wwPDB EM Validation Summary Report (i)

Sep 22, 2026 – 01:16 AM EDT

PDB ID	:	7UMH / pdb_00007umh
EMDB ID	:	EMD-26601
Title	:	Energetic robustness to large scale structural dynamics in a photosynthetic supercomplex
Authors	:	Harris, D.; Toporik, H.; Schlau-Cohen, G.S.; Mazor, Y.
Deposited on	:	2022-04-07
Resolution	:	2.60 Å(reported)
Based on initial model	:	6NWA

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

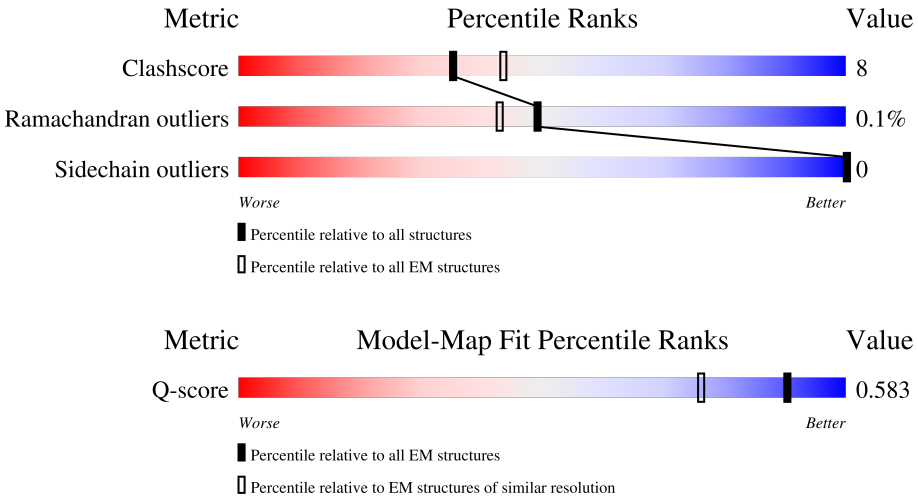
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	83% 15%
1	H	751	82% 17%
1	a	751	83% 15%
2	B	731	85% 15%

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Mol	Chain	Length	Quality of chain
2	G	731	85% 15%
2	b	731	84% 15%
3	C	81	80% 19%
3	N	81	85% 14%
3	c	81	90% 9%
4	D	141	10% 82% 16%
4	P	141	10% 86% 12%
4	d	141	14% 84% 14%
5	E	74	9% 80% 12% 8%
5	O	74	16% 78% 14% 8%
5	e	74	19% 84% 8% 8%
6	F	165	14% 75% 10% 15%
6	Q	165	12% 76% 10% 15%
6	f	165	11% 75% 11% 15%
7	I	40	5% 65% 28% 8%
7	R	40	5% 70% 22% 8%
7	i	40	78% 15% 8%
8	J	40	5% 80% 18%
8	S	40	8% 72% 25%
8	j	40	8% 82% 15%
9	K	86	15% 80% 9% 10%
9	T	86	17% 83% 7% 10%
9	k	86	14% 81% 8% 10%
10	L	157	7% 85% 12%
10	U	157	6% 82% 15%

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Mol	Chain	Length	Quality of chain
10	l	157	8% 85% 12%
11	M	31	6% 94% 6%
11	V	31	6% 97%
11	m	31	6% 97%
12	W	342	15% 82% 16%
12	X	342	6% 82% 17%
12	Y	342	6% 82% 17%
12	Z	342	84% 15%
12	g	342	8% 82% 15%
12	h	342	29% 85% 11%
12	n	342	12% 82% 17%
12	o	342	7% 89% 11%
12	p	342	7% 86% 14%
12	q	342	5% 82% 16%
12	r	342	9% 82% 15%
12	s	342	6% 83% 15%
12	t	342	15% 85% 14%
12	u	342	7% 85% 14%
12	v	342	26% 84% 13%
12	w	342	85% 13%
12	x	342	9% 85% 12%
12	y	342	29% 82% 15%

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 140516 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	H	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	G	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	b	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	N	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			537	337	95	105		
5	O	68	Total	C	N	O	0	0
			537	337	95	105		
5	e	68	Total	C	N	O	0	0
			537	337	95	105		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	R	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	52	3		
8	S	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	T	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	k	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	U	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	l	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	V	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

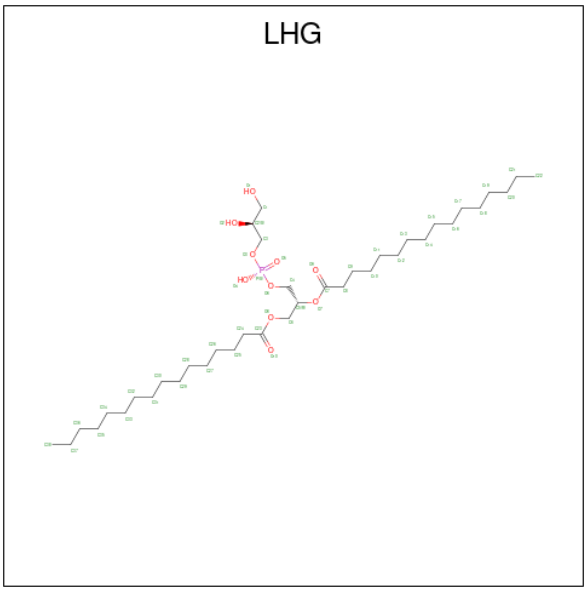
Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	X	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	Y	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	g	333	Total	C	N	O	S	0	0
			2573	1714	420	434	5		
12	h	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	n	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	o	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	p	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		
12	q	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	r	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	s	339	Total	C	N	O	S	0	0
			2617	1741	427	444	5		
12	t	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	u	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	v	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	w	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	x	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	y	330	Total	C	N	O	S	0	0
			2532	1689	409	429	5		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



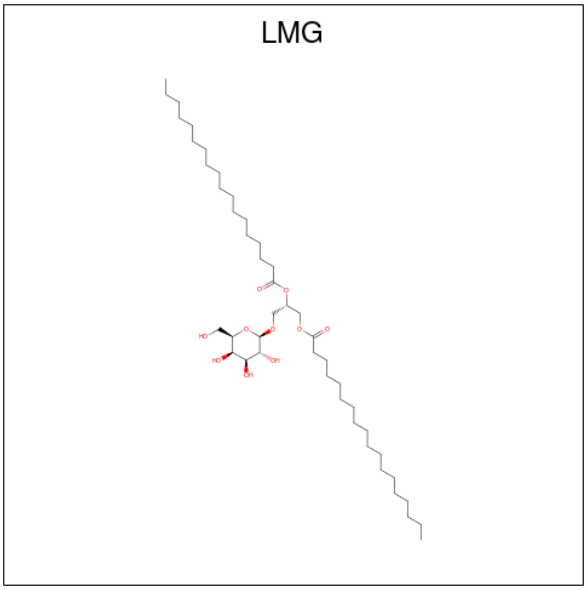
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			43	32	10	1	
13	A	1	Total	C	O	P	0
			26	15	10	1	
13	B	1	Total	C	O	P	0
			38	27	10	1	
13	G	1	Total	C	O	P	0
			38	27	10	1	
13	H	1	Total	C	O	P	0
			43	32	10	1	
13	H	1	Total	C	O	P	0
			26	15	10	1	
13	I	1	Total	C	O	P	0
			40	29	10	1	
13	R	1	Total	C	O	P	0
			40	29	10	1	
13	X	1	Total	C	O	P	0
			27	16	10	1	
13	Y	1	Total	C	O	P	0
			32	21	10	1	
13	a	1	Total	C	O	P	0
			43	32	10	1	
13	a	1	Total	C	O	P	0
			26	15	10	1	
13	b	1	Total	C	O	P	0
			38	27	10	1	
13	g	1	Total	C	O	P	0
			31	20	10	1	

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Mol	Chain	Residues	Atoms				AltConf
13	i	1	Total	C	O	P	0
			40	29	10	1	
13	o	1	Total	C	O	P	0
			27	16	10	1	
13	p	1	Total	C	O	P	0
			32	21	10	1	
13	r	1	Total	C	O	P	0
			31	20	10	1	
13	s	1	Total	C	O	P	0
			32	21	10	1	
13	u	1	Total	C	O	P	0
			27	16	10	1	
13	x	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



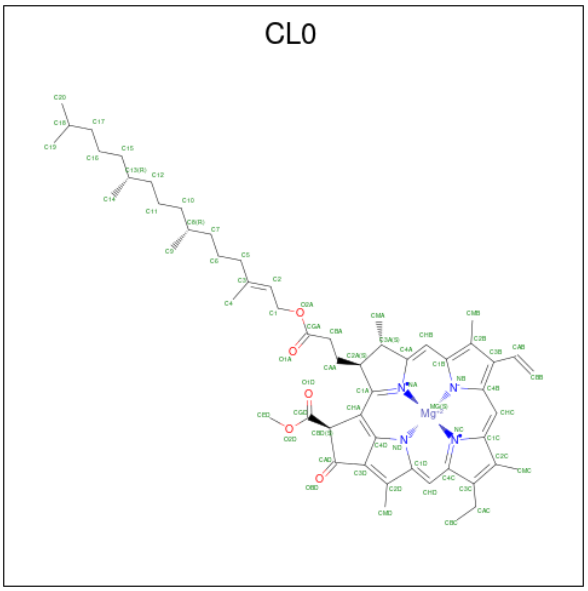
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			38	28	10	
14	A	1	Total	C	O	0
			46	36	10	
14	A	1	Total	C	O	0
			32	22	10	
14	B	1	Total	C	O	0
			43	33	10	

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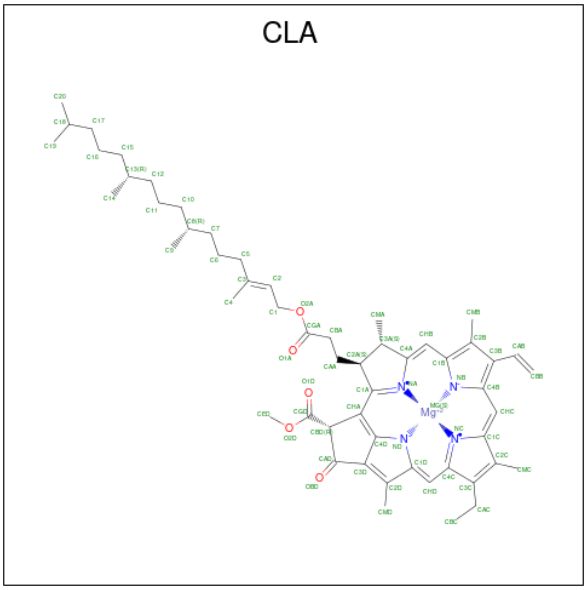
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total C O 27 17 10	0
14	G	1	Total C O 43 33 10	0
14	H	1	Total C O 38 28 10	0
14	H	1	Total C O 46 36 10	0
14	H	1	Total C O 32 22 10	0
14	Q	1	Total C O 27 17 10	0
14	a	1	Total C O 38 28 10	0
14	a	1	Total C O 46 36 10	0
14	a	1	Total C O 32 22 10	0
14	b	1	Total C O 43 33 10	0
14	f	1	Total C O 27 17 10	0

- Molecule 15 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	S	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	t	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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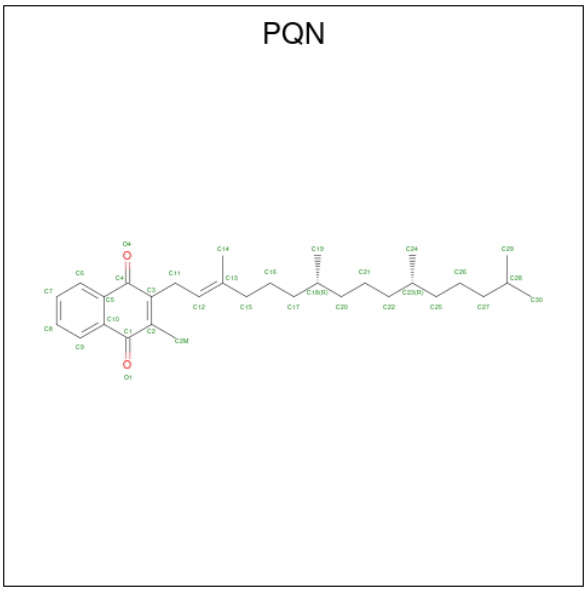
Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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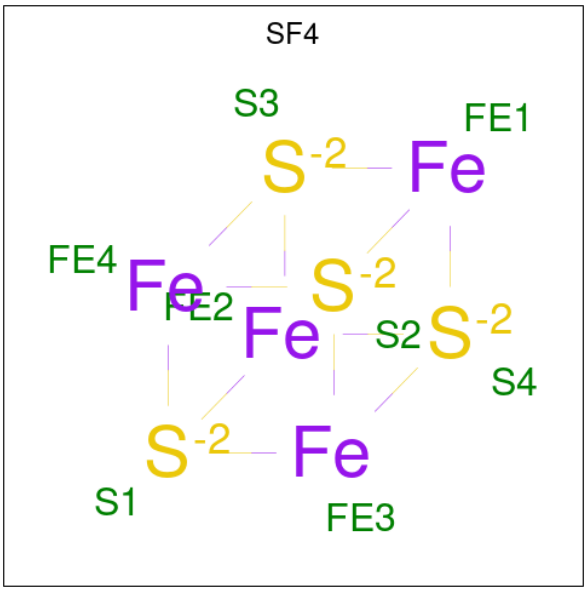
Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	y	1	Total 55	C 45	Mg 1	N 4	O 5	0

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



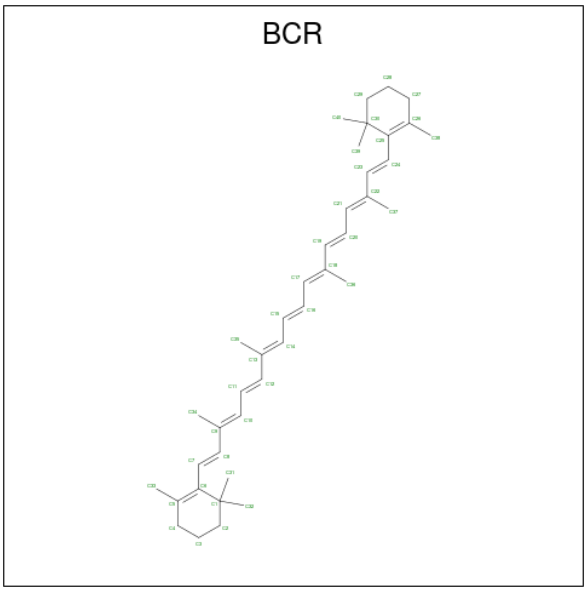
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C O 33 31 2	0
17	B	1	Total C O 33 31 2	0
17	G	1	Total C O 33 31 2	0
17	H	1	Total C O 33 31 2	0
17	a	1	Total C O 33 31 2	0
17	b	1	Total C O 33 31 2	0

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total Fe S 8 4 4	0
18	C	1	Total Fe S 8 4 4	0
18	C	1	Total Fe S 8 4 4	0
18	H	1	Total Fe S 8 4 4	0
18	N	1	Total Fe S 8 4 4	0
18	N	1	Total Fe S 8 4 4	0
18	a	1	Total Fe S 8 4 4	0
18	c	1	Total Fe S 8 4 4	0
18	c	1	Total Fe S 8 4 4	0

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 30 30	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C 30 30	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	Q	1	Total C 40 40	0
19	R	1	Total C 40 40	0
19	S	1	Total C 40 40	0
19	S	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	S	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 30 30	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	f	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	i	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	k	1	Total C 40 40	0
19	k	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0

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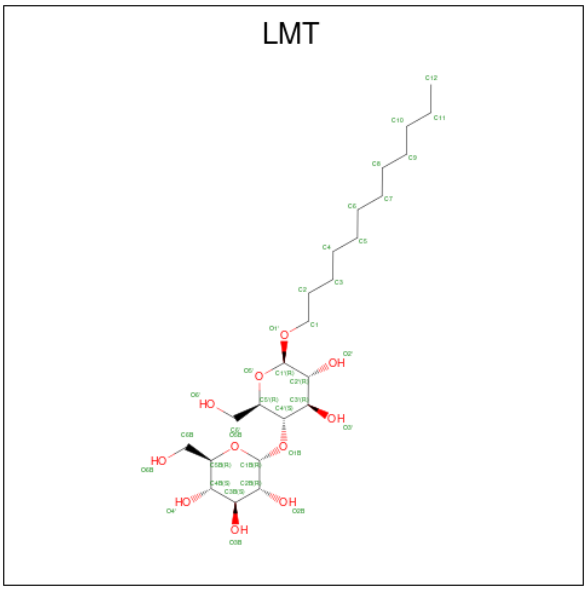
Mol	Chain	Residues	Atoms	AltConf
19	r	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0

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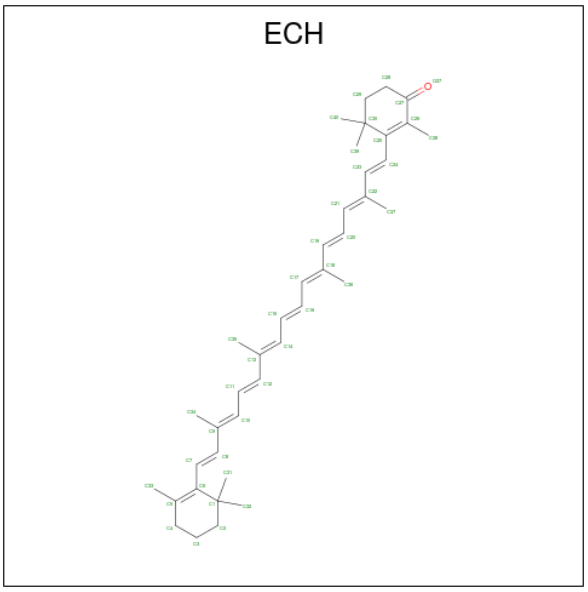
Mol	Chain	Residues	Atoms	AltConf
19	x	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0

- Molecule 20 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C O 35 24 11	0
20	H	1	Total C O 35 24 11	0
20	L	1	Total C O 35 24 11	0
20	U	1	Total C O 35 24 11	0
20	a	1	Total C O 35 24 11	0
20	l	1	Total C O 35 24 11	0

- Molecule 21 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).

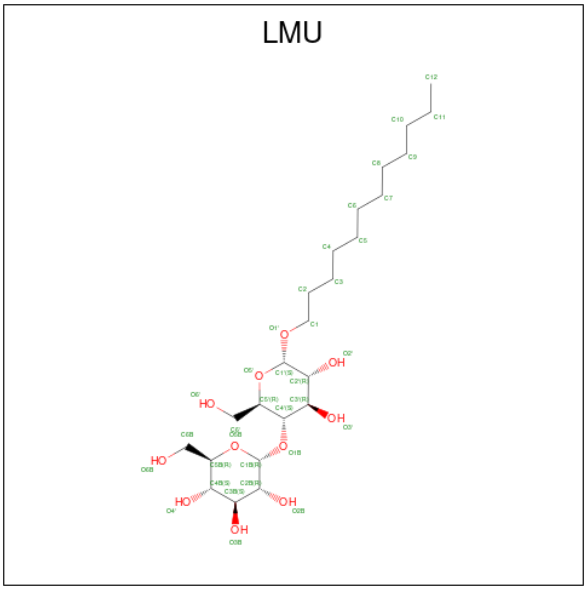


Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C O 41 40 1	0
21	G	1	Total C O 41 40 1	0
21	I	1	Total C O 41 40 1	0
21	M	1	Total C O 41 40 1	0
21	R	1	Total C O 41 40 1	0
21	V	1	Total C O 41 40 1	0
21	b	1	Total C O 41 40 1	0
21	i	1	Total C O 41 40 1	0
21	m	1	Total C O 41 40 1	0

- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

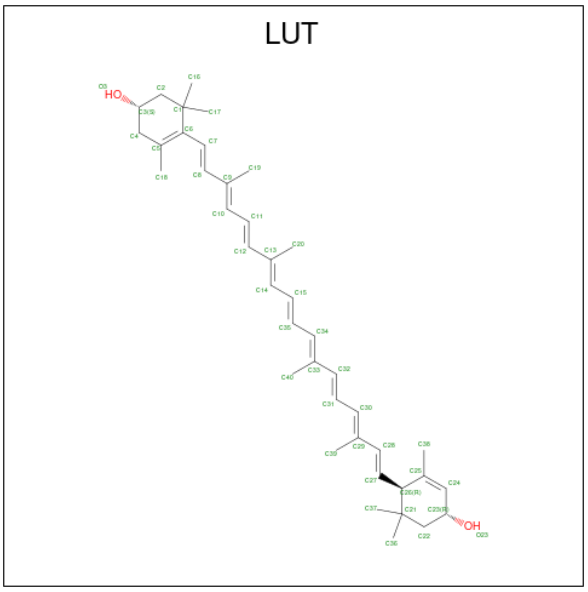
Mol	Chain	Residues	Atoms	AltConf
22	L	1	Total Ca 1 1	0
22	U	1	Total Ca 1 1	0
22	l	1	Total Ca 1 1	0

- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
23	Y	1	Total	C	O	0
			35	24	11	
23	Z	1	Total	C	O	0
			35	24	11	
23	g	1	Total	C	O	0
			35	24	11	
23	p	1	Total	C	O	0
			35	24	11	
23	q	1	Total	C	O	0
			35	24	11	
23	r	1	Total	C	O	0
			35	24	11	
23	s	1	Total	C	O	0
			35	24	11	
23	w	1	Total	C	O	0
			35	24	11	
23	x	1	Total	C	O	0
			35	24	11	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
24	Z	1	Total C O 42 40 2	0
24	q	1	Total C O 42 40 2	0
24	w	1	Total C O 42 40 2	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	A	56	Total O 56 56	0
25	B	52	Total O 52 52	0
25	C	7	Total O 7 7	0
25	D	3	Total O 3 3	0
25	E	4	Total O 4 4	0
25	F	3	Total O 3 3	0
25	G	55	Total O 55 55	0
25	H	52	Total O 52 52	0
25	I	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
25	J	1	Total O 1 1	0
25	L	5	Total O 5 5	0
25	N	13	Total O 13 13	0
25	O	11	Total O 11 11	0
25	P	6	Total O 6 6	0
25	Q	4	Total O 4 4	0
25	R	1	Total O 1 1	0
25	S	3	Total O 3 3	0
25	U	3	Total O 3 3	0
25	a	57	Total O 57 57	0
25	b	74	Total O 74 74	0
25	c	17	Total O 17 17	0
25	d	7	Total O 7 7	0
25	e	10	Total O 10 10	0
25	f	7	Total O 7 7	0
25	i	1	Total O 1 1	0
25	j	1	Total O 1 1	0
25	k	1	Total O 1 1	0
25	l	6	Total O 6 6	0

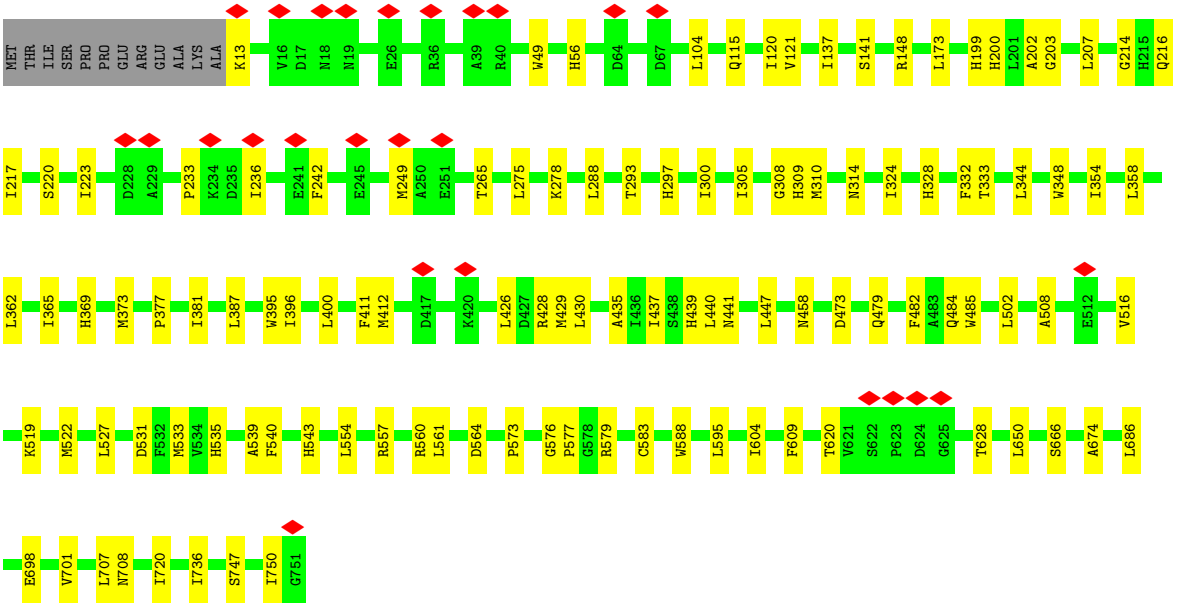
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

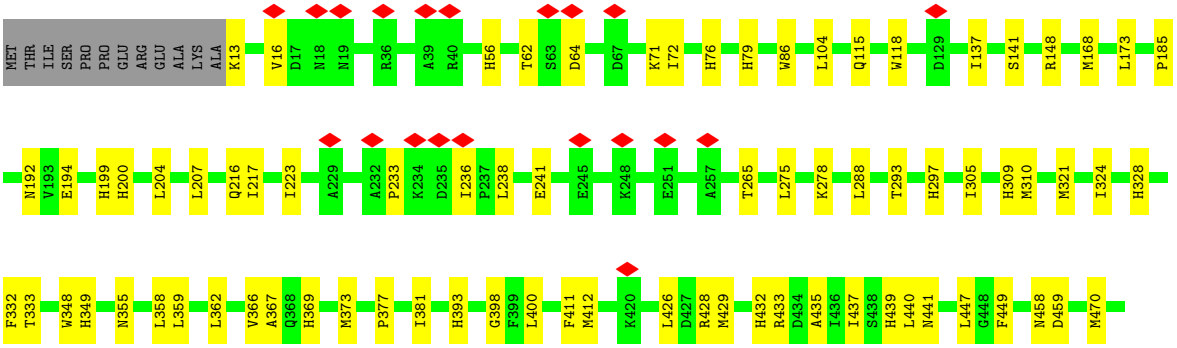


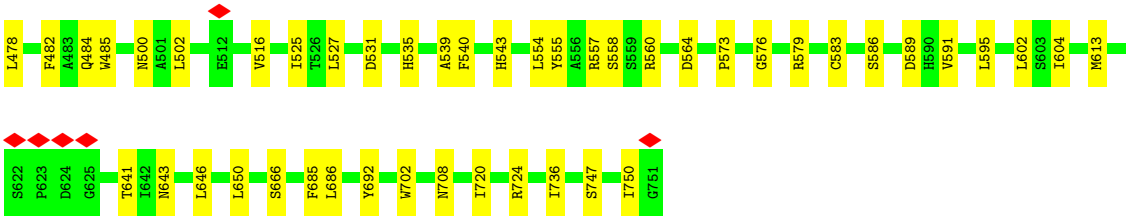


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

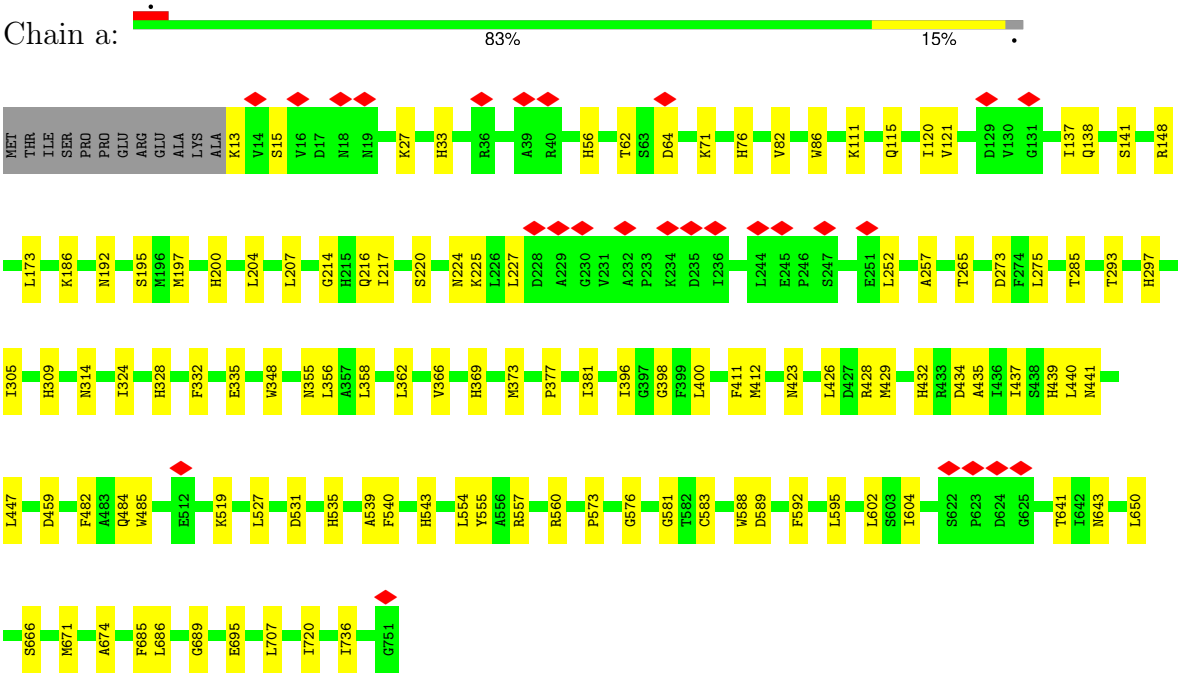
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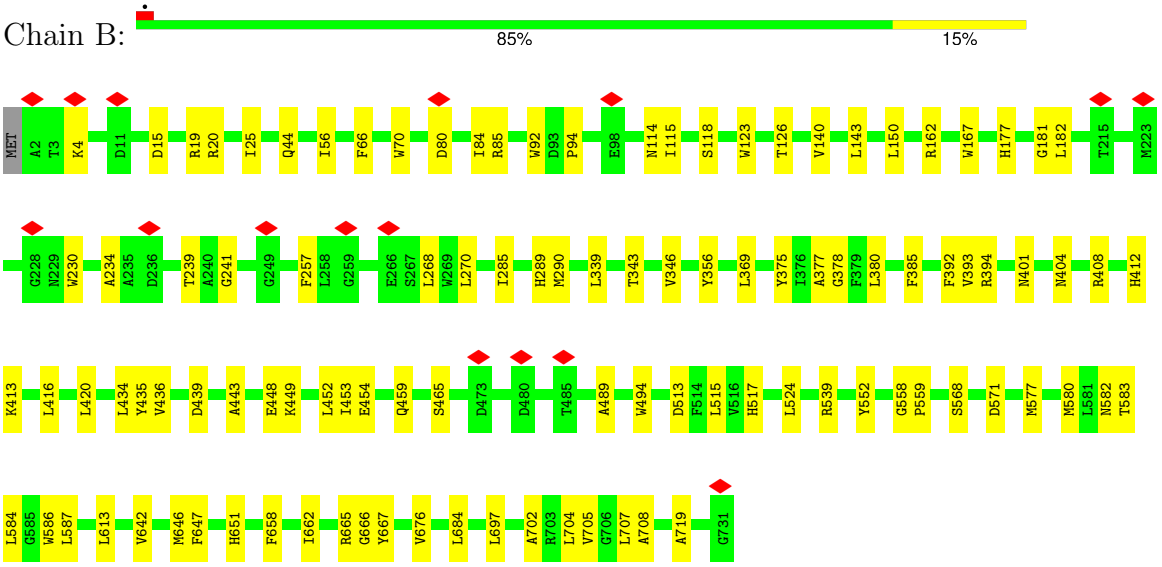




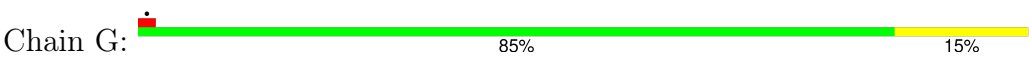
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

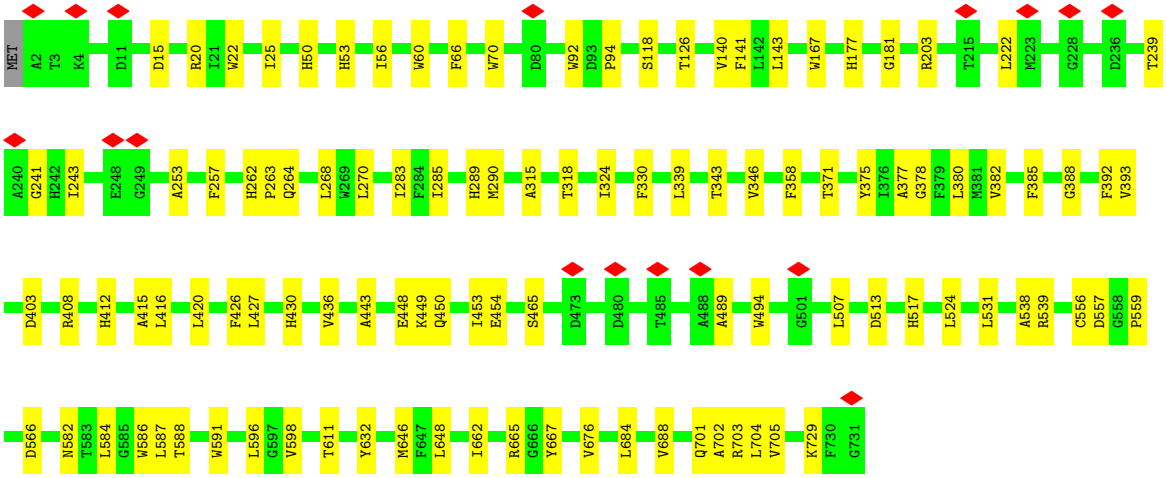


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

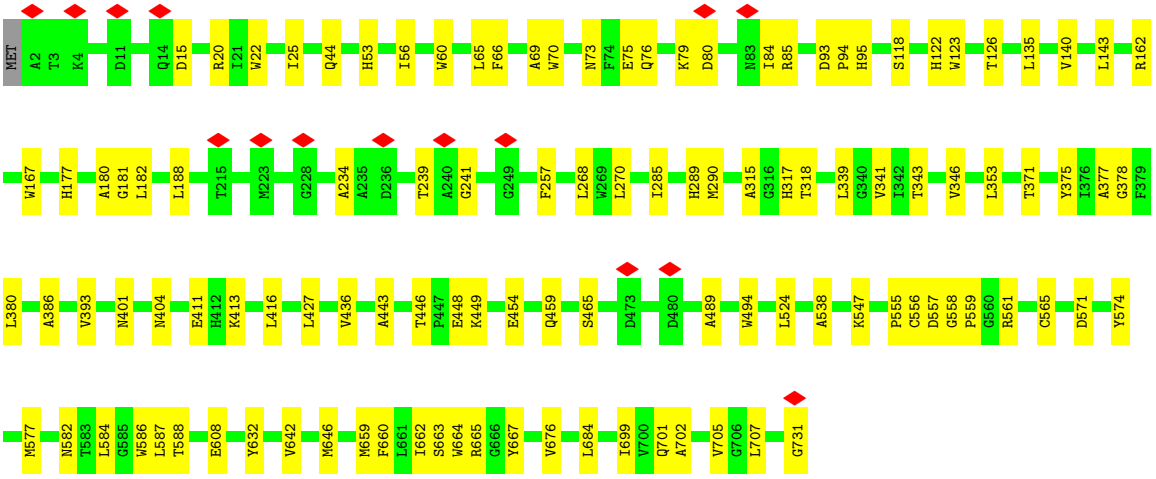




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:

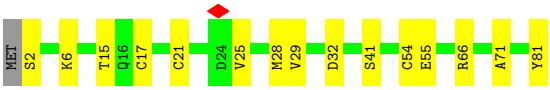




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

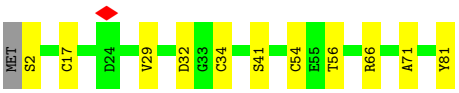




• Molecule 3: Photosystem I iron-sulfur center

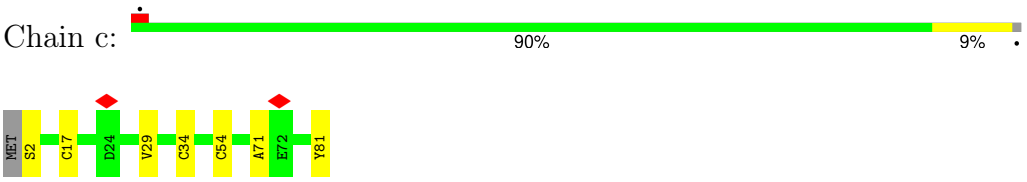
Chain N:





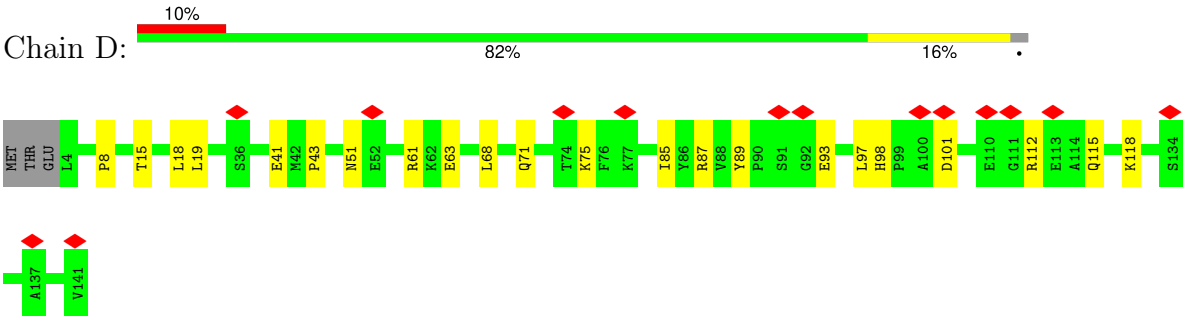
• Molecule 3: Photosystem I iron-sulfur center

Chain c:



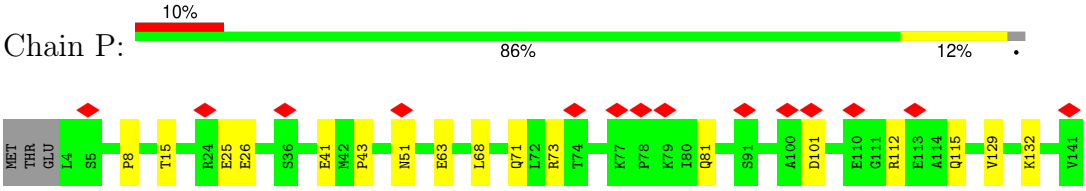
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



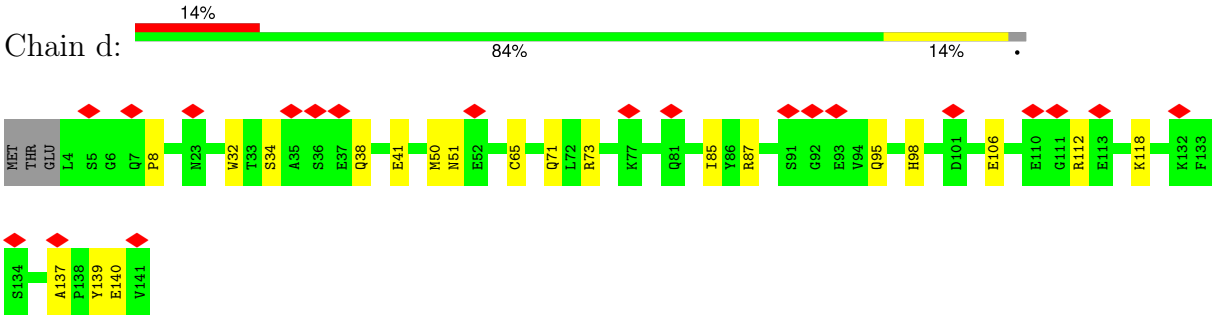
• Molecule 4: Photosystem I reaction center subunit II

Chain P:



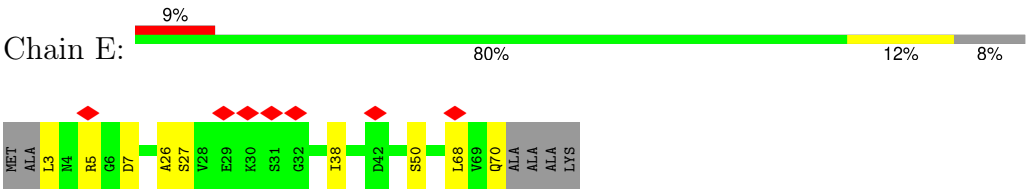
• Molecule 4: Photosystem I reaction center subunit II

Chain d:



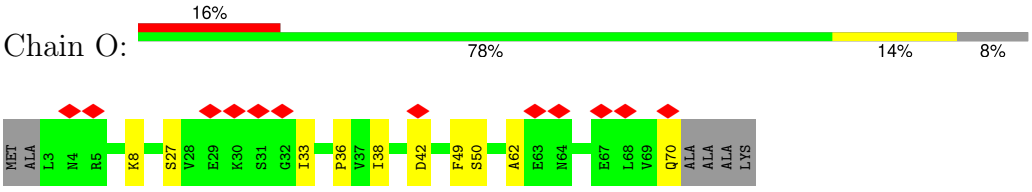
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



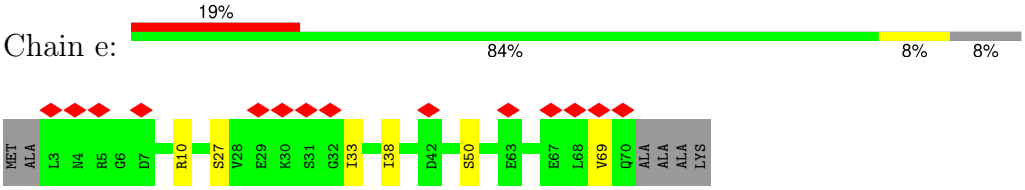
• Molecule 5: Photosystem I reaction center subunit IV

Chain O:



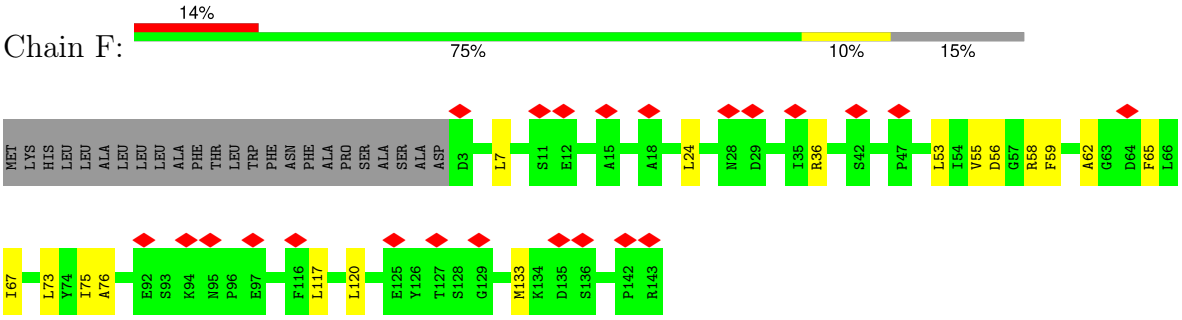
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:



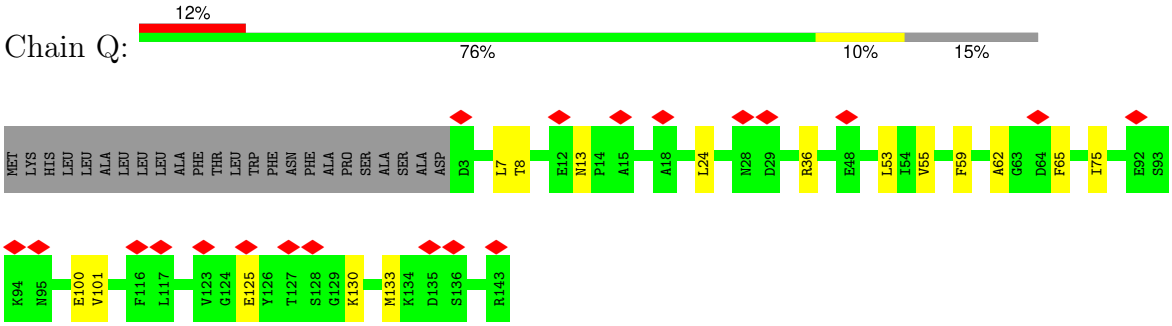
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



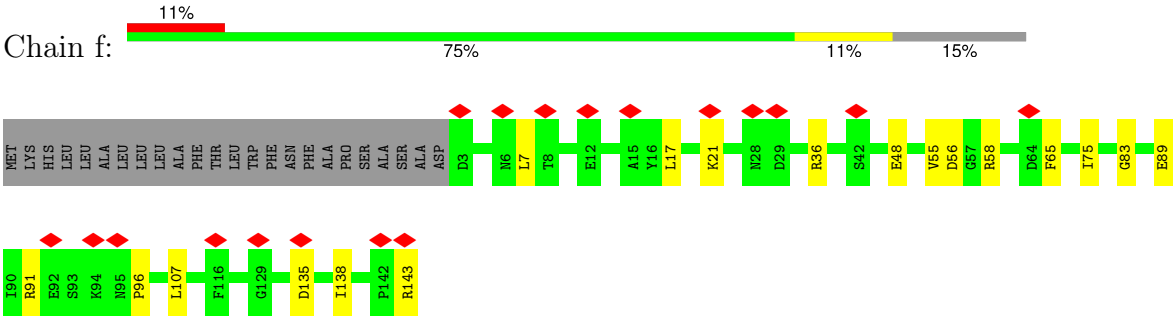
• Molecule 6: Photosystem I reaction center subunit III

Chain Q:



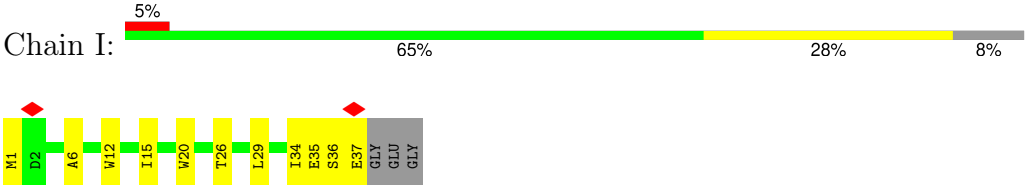
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



• Molecule 7: Photosystem I reaction center subunit VIII

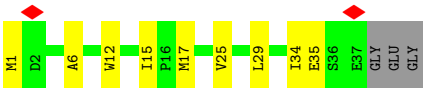
Chain I:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain R:

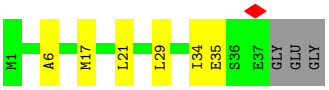




• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

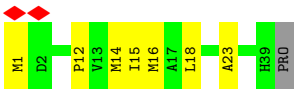




• Molecule 8: Photosystem I reaction center subunit IX

Chain J:





• Molecule 8: Photosystem I reaction center subunit IX

Chain S:

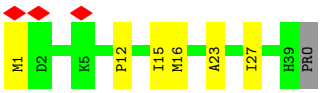




• Molecule 8: Photosystem I reaction center subunit IX

Chain j:

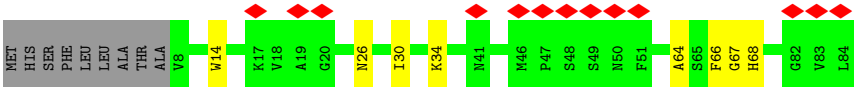




• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:

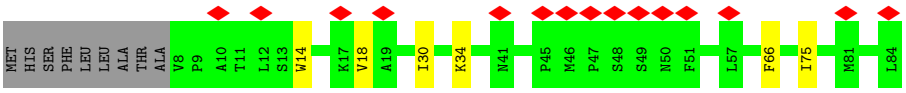




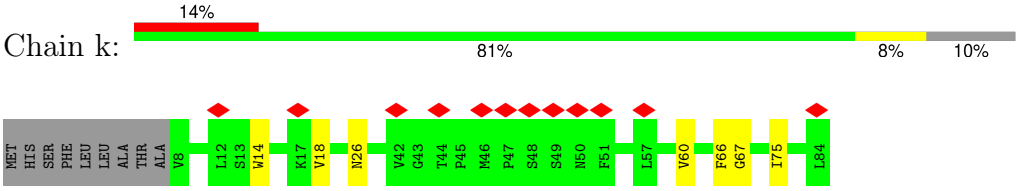
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain T:

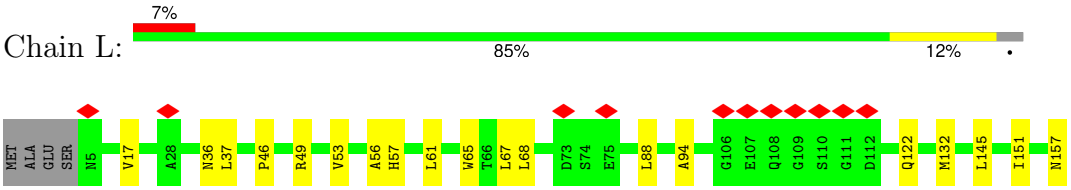




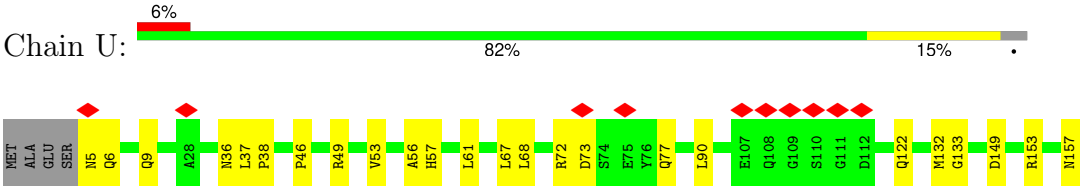
• Molecule 9: Photosystem I reaction center subunit PsaK 1



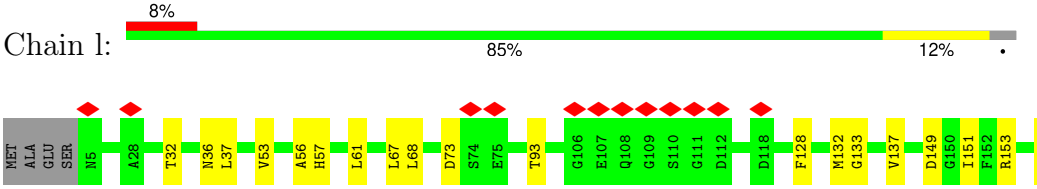
• Molecule 10: Photosystem I reaction center subunit XI



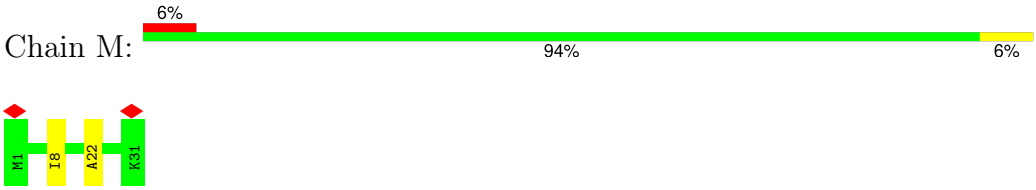
• Molecule 10: Photosystem I reaction center subunit XI



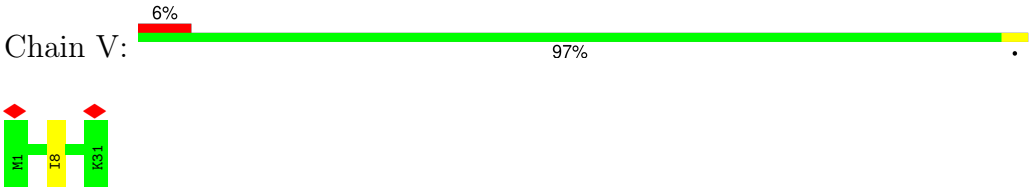
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Photosystem I reaction center subunit XII

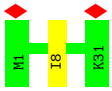


• Molecule 11: Photosystem I reaction center subunit XII



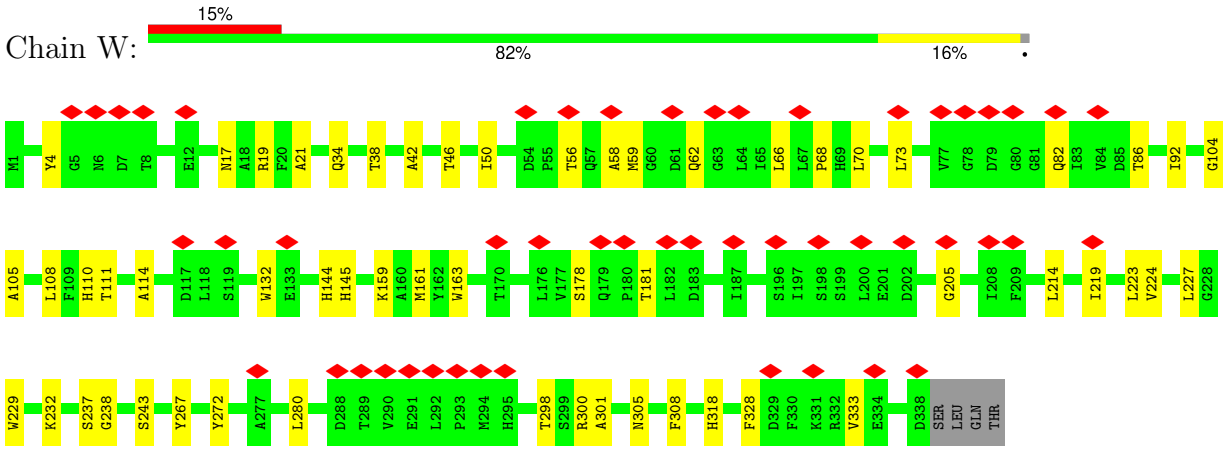
• Molecule 11: Photosystem I reaction center subunit XII





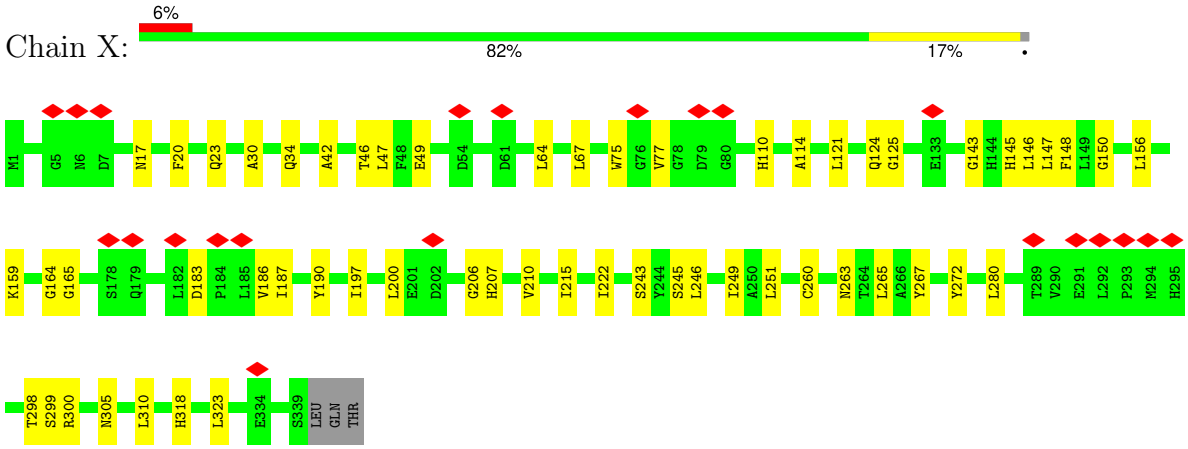
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain W:



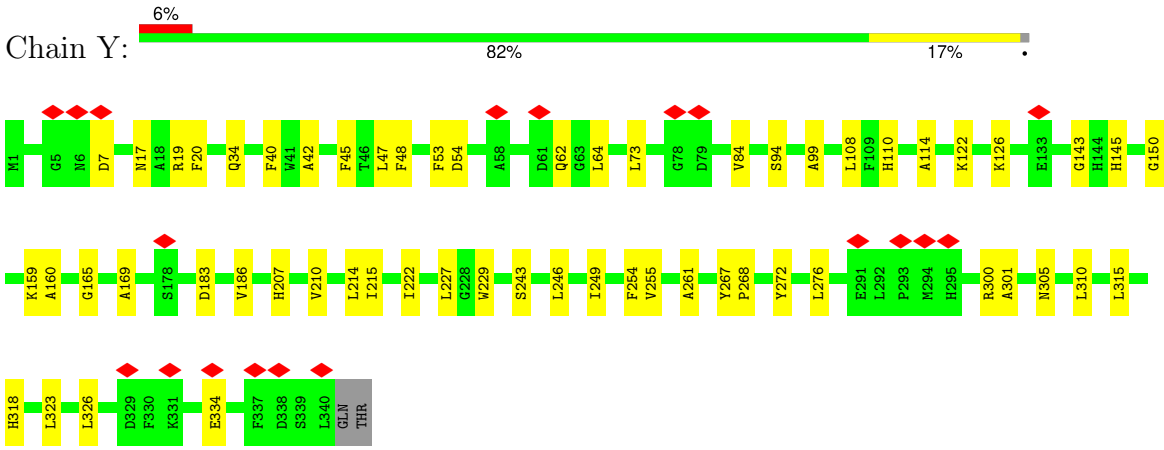
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain X:



• Molecule 12: Iron stress-induced chlorophyll-binding protein

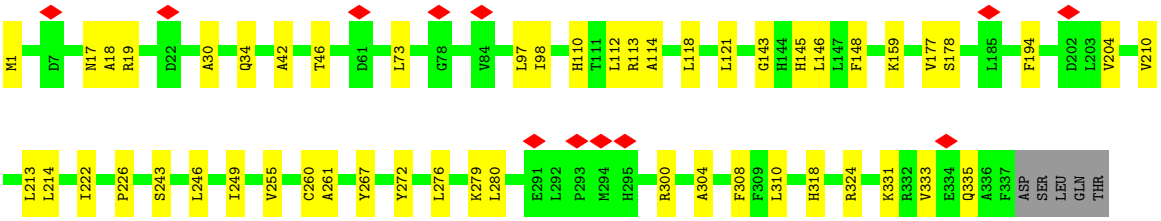
Chain Y:



• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Z:

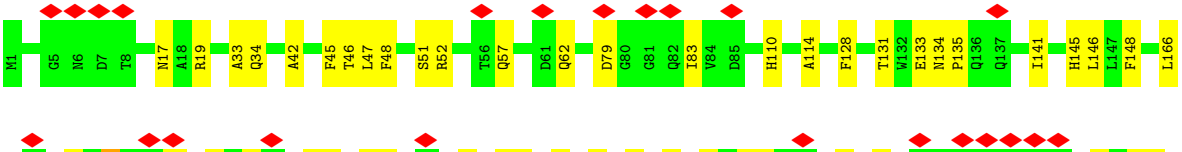


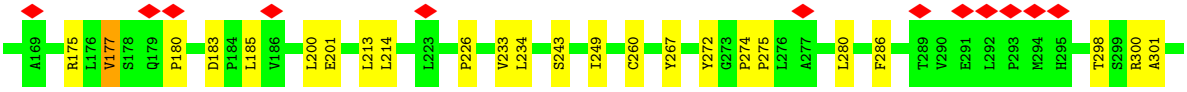


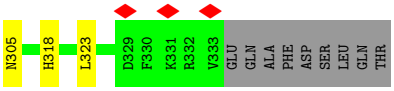
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain g:





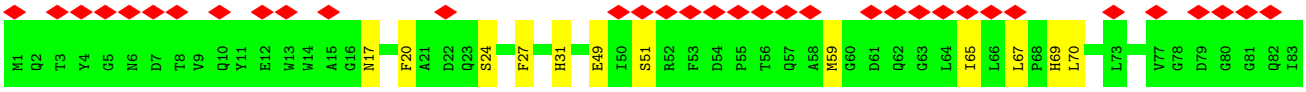


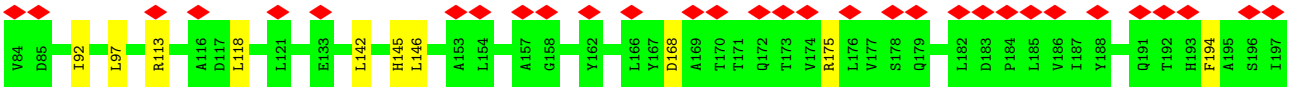


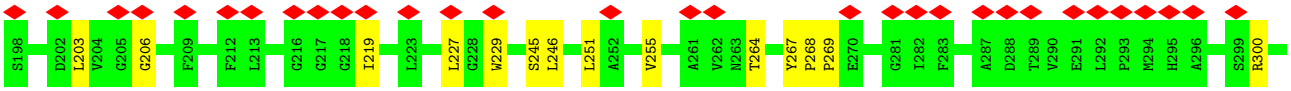
• Molecule 12: Iron stress-induced chlorophyll-binding protein

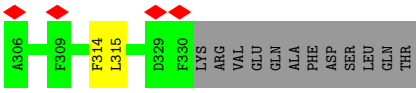
Chain h:







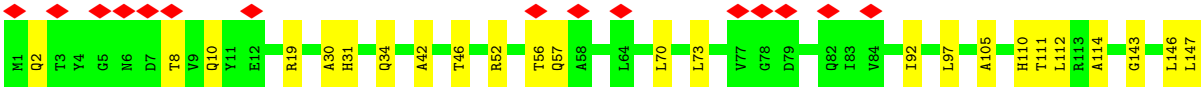


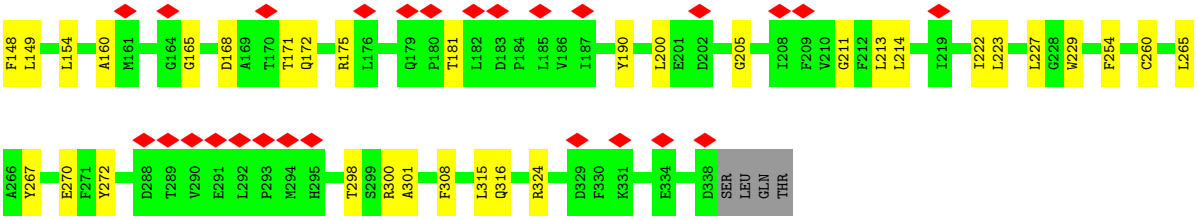


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain n:



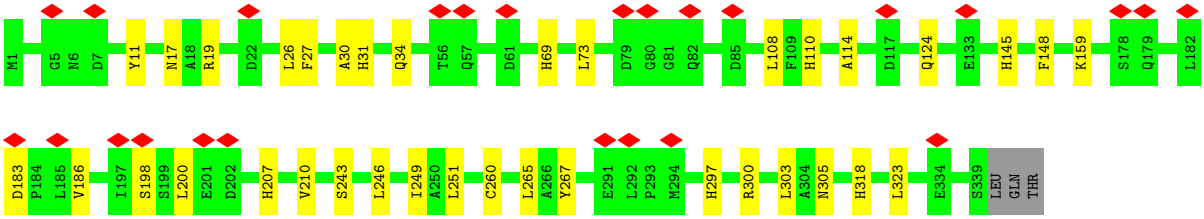




• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain o:

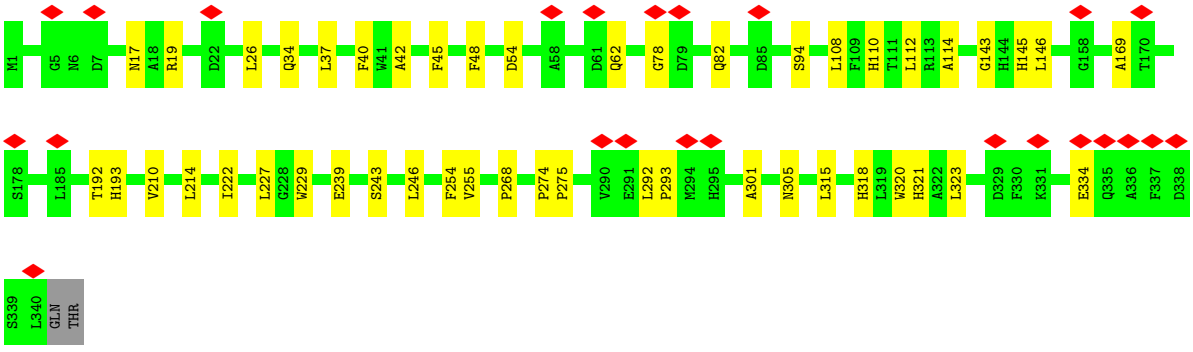




• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain p:

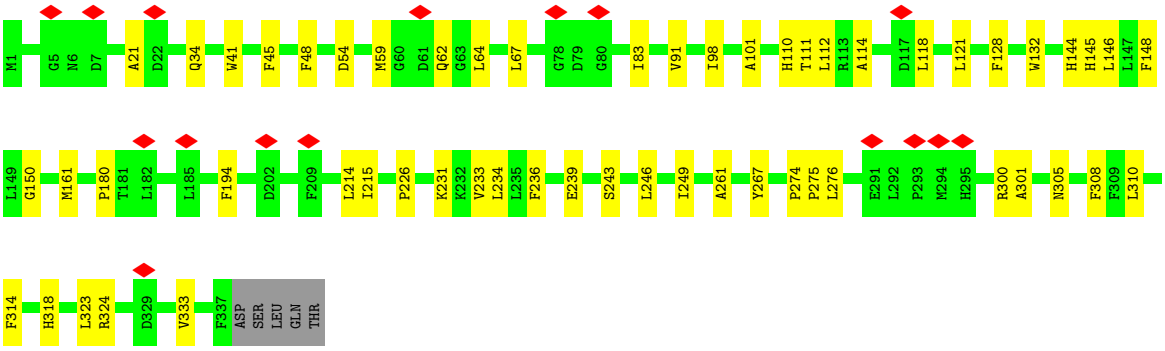




• Molecule 12: Iron stress-induced chlorophyll-binding protein

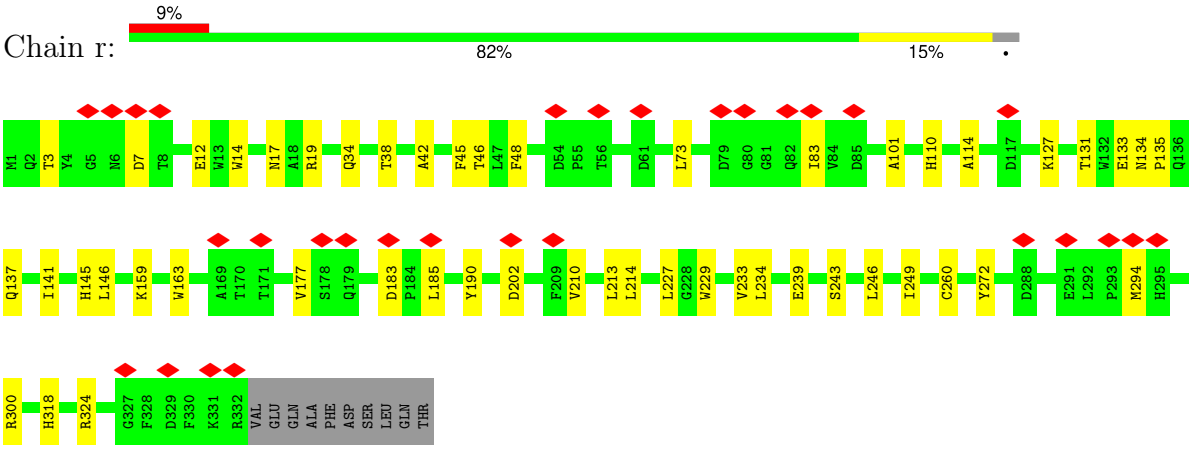
Chain q:





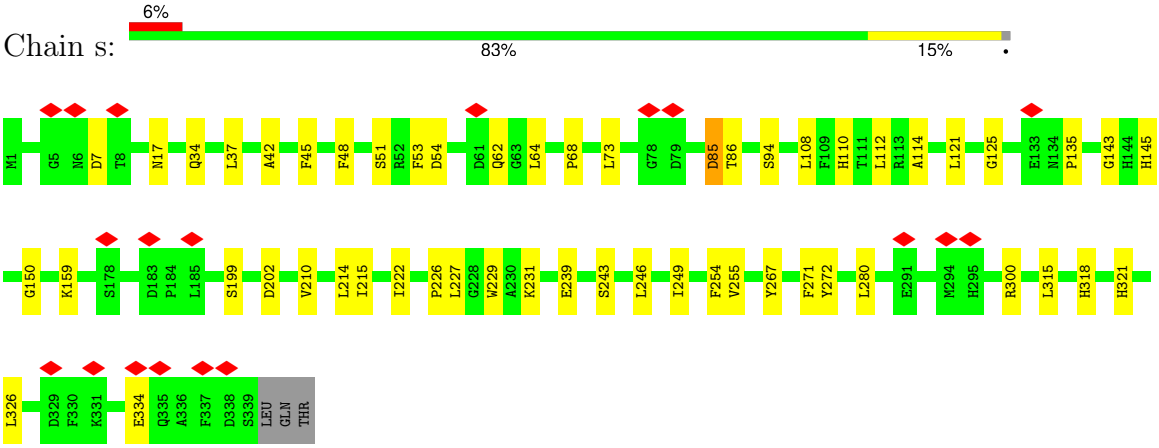
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain r:



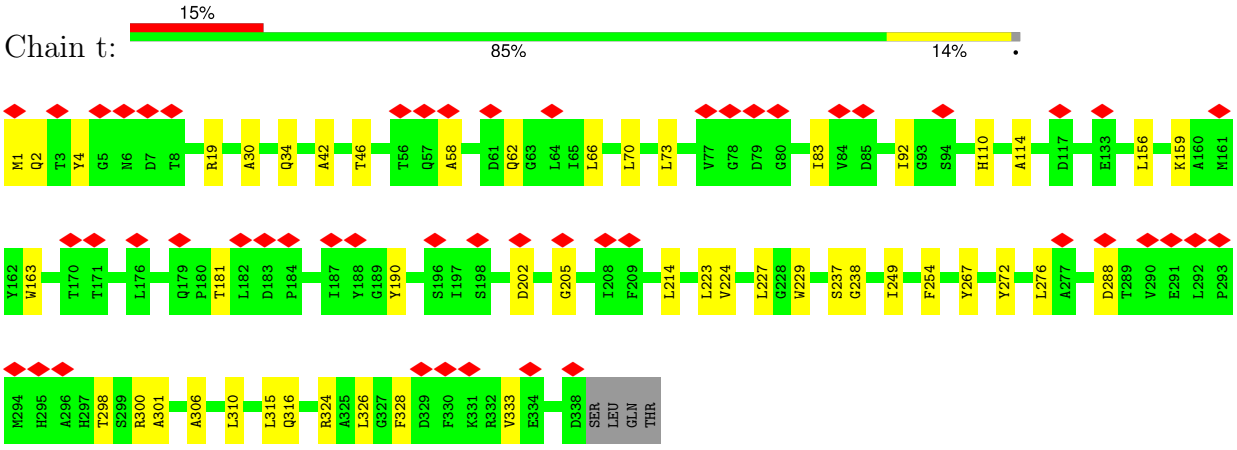
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain s:



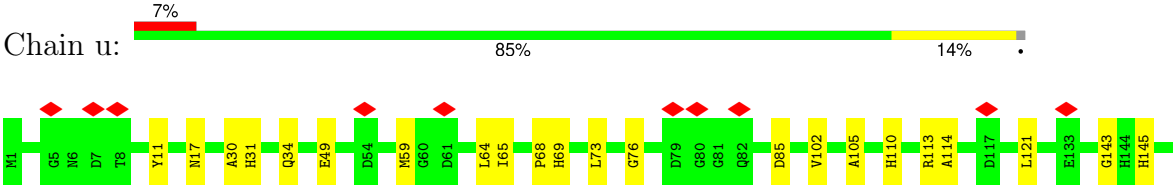
• Molecule 12: Iron stress-induced chlorophyll-binding protein

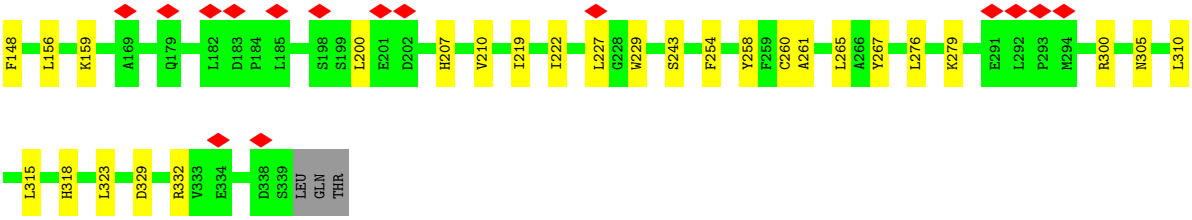
Chain t:



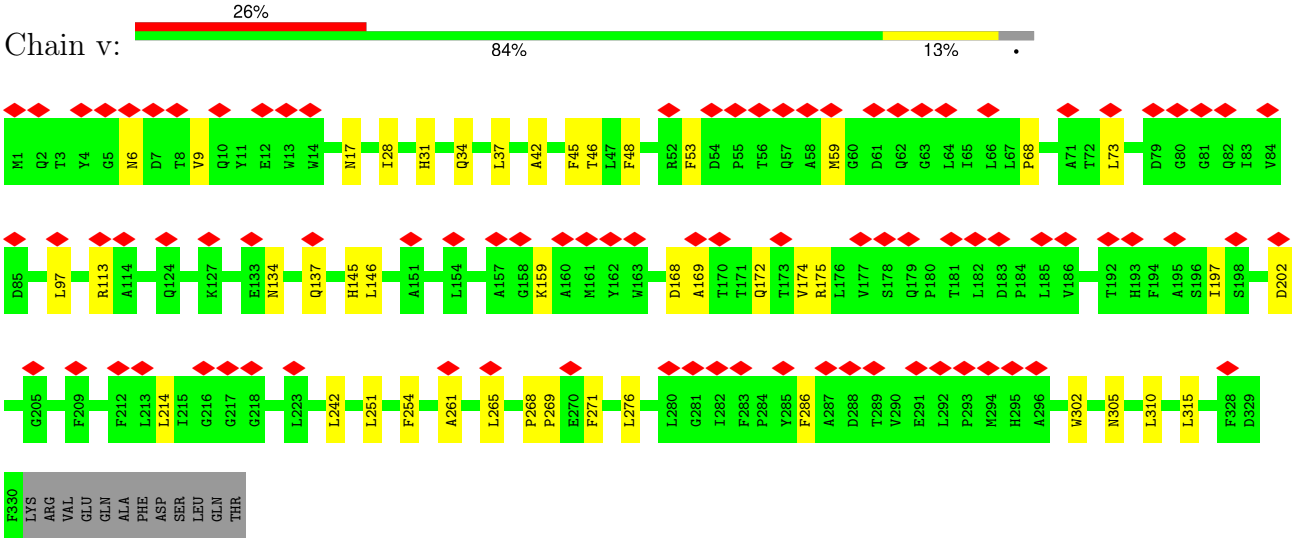
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain u:

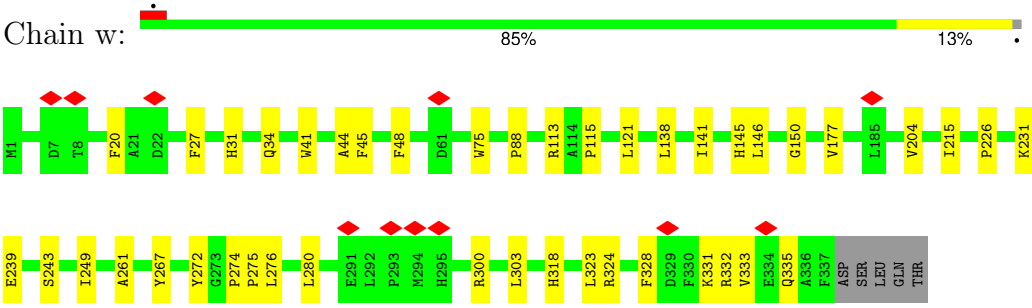




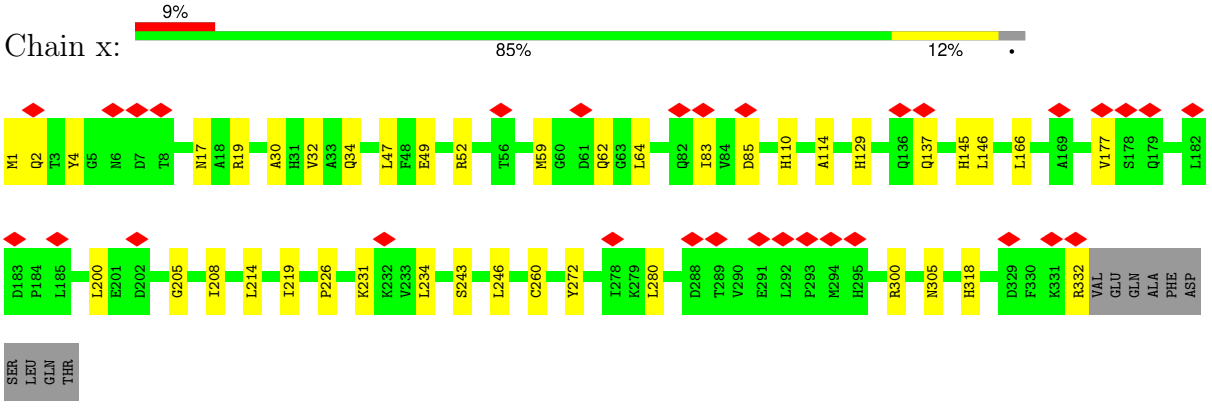
• Molecule 12: Iron stress-induced chlorophyll-binding protein



• Molecule 12: Iron stress-induced chlorophyll-binding protein

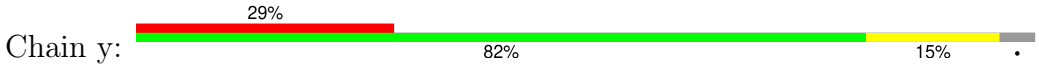


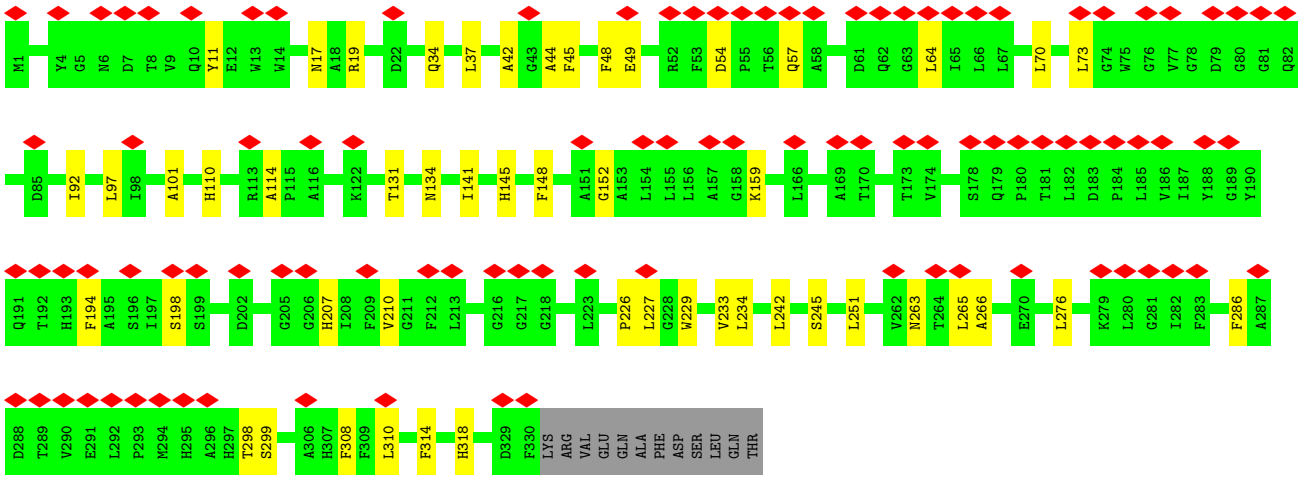
• Molecule 12: Iron stress-induced chlorophyll-binding protein



• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain y:


29%
82%
15%


M1 Y4 G5 N6 D7 T8 V9 Q10 Y11 E12 W13 W14 N17 A18 R19 D22 Q34 L37 A42 G43 A44 F45 F48 E49 R52 F53 D54 P55 T56 Q57 A58 D61 Q62 G63 L64 I65 L66 L67 L70 L73 G74 W75 G76 V77 G78 D79 G80 G81 Q82
D85 I92 L97 I98 A101 H110 R113 A114 P115 A116 K122 T131 N134 I141 H145 F148 A151 G152 A153 L154 L155 L156 A157 G158 K159 L166 A169 T170 T173 V174 S178 Q179 P180 T181 L182 D183 P184 L185 V186 I187 Y188 G189 Y190
Q191 T192 H193 F194 A195 S196 I197 S198 S199 D202 G205 G206 H207 I208 F209 V210 G211 F212 L213 G216 G217 G218 L223 P226 L227 G228 W229 V233 L234 L242 S245 L251 V262 N263 T264 L265 A266 E270 L276 K279 L280 G281 I282 F283 F286 A287
D288 T289 V290 E291 L292 P293 M294 H295 A296 H297 T298 S299 A306 H307 F308 F309 L310 F314 H318 D329 F330 LYS ARG VAL GLU GLN ALA PHE ASP SER LEU GLN THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.466	Depositor
Minimum map value	-42.667	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	2.305	Depositor
Recommended contour level	9.2	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LUT, SF4, LHG, LMG, CL0, CA, LMT, CLA, LMU, ECH, PQN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.23	0/5985	0.43	0/8158
1	H	0.23	0/5985	0.44	0/8158
1	a	0.23	0/5985	0.45	0/8158
2	B	0.22	0/5986	0.44	0/8185
2	G	0.23	0/5986	0.45	0/8185
2	b	0.23	0/5986	0.45	0/8185
3	C	0.20	0/610	0.48	0/826
3	N	0.21	0/610	0.48	0/826
3	c	0.22	0/610	0.51	0/826
4	D	0.19	0/1102	0.44	0/1485
4	P	0.18	0/1102	0.38	0/1485
4	d	0.18	0/1102	0.40	0/1485
5	E	0.13	0/546	0.31	0/738
5	O	0.13	0/546	0.32	0/738
5	e	0.14	0/546	0.33	0/738
6	F	0.20	0/1130	0.43	0/1535
6	Q	0.22	0/1130	0.46	0/1535
6	f	0.21	0/1130	0.44	0/1535
7	I	0.27	0/304	0.55	0/416
7	R	0.30	0/304	0.57	0/416
7	i	0.31	0/304	0.61	0/416
8	J	0.20	0/319	0.45	0/431
8	S	0.22	0/319	0.47	0/431
8	j	0.30	0/319	0.48	0/431
9	K	0.15	0/549	0.36	0/745
9	T	0.16	0/549	0.43	0/745
9	k	0.16	0/549	0.44	0/745
10	L	0.20	0/1180	0.47	0/1603
10	U	0.21	0/1180	0.49	0/1603
10	l	0.21	0/1180	0.46	0/1603
11	M	0.19	0/241	0.38	0/326
11	V	0.22	0/241	0.45	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	m	0.24	0/241	0.50	0/326
12	W	0.18	0/2691	0.44	1/3678 (0.0%)
12	X	0.20	0/2712	0.47	0/3703
12	Y	0.21	0/2712	0.45	0/3704
12	Z	0.20	0/2693	0.44	1/3678 (0.0%)
12	g	0.19	0/2662	0.45	0/3636
12	h	0.17	0/2627	0.42	0/3592
12	n	0.16	0/2691	0.37	0/3678
12	o	0.20	0/2712	0.47	0/3703
12	p	0.20	0/2712	0.43	0/3704
12	q	0.18	0/2693	0.39	0/3678
12	r	0.20	0/2655	0.49	0/3626
12	s	0.20	0/2707	0.42	0/3697
12	t	0.17	0/2691	0.41	0/3678
12	u	0.20	0/2712	0.45	0/3703
12	v	0.16	0/2627	0.40	0/3592
12	w	0.19	0/2693	0.43	0/3678
12	x	0.18	0/2655	0.45	2/3626 (0.1%)
12	y	0.16	0/2621	0.40	0/3585
All	All	0.21	0/102122	0.44	4/139283 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
12	Y	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	x	85	ASP	CA-C-N	5.76	131.60	122.61
12	x	85	ASP	C-N-CA	5.76	131.60	122.61
12	W	308	PHE	N-CA-C	-5.49	106.25	113.12
12	Z	333	VAL	N-CA-C	-5.27	108.36	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Y	84	VAL	Peptide
2	b	664	TRP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5648	95	0
1	H	5787	0	5648	100	0
1	a	5787	0	5648	90	0
2	B	5775	0	5554	86	0
2	G	5775	0	5554	86	0
2	b	5775	0	5554	85	0
3	C	600	0	589	12	0
3	N	600	0	589	9	0
3	c	600	0	589	5	0
4	D	1078	0	1076	17	0
4	P	1078	0	1076	11	0
4	d	1078	0	1076	12	0
5	E	537	0	520	5	0
5	O	537	0	520	7	0
5	e	537	0	520	4	0
6	F	1100	0	1096	14	0
6	Q	1100	0	1096	12	0
6	f	1100	0	1096	13	0
7	I	293	0	292	10	0
7	R	293	0	292	8	0
7	i	293	0	292	4	0
8	J	311	0	321	7	0
8	S	311	0	321	10	0
8	j	311	0	321	6	0
9	K	538	0	565	6	0
9	T	538	0	565	5	0
9	k	538	0	565	5	0
10	L	1150	0	1122	19	0
10	U	1150	0	1122	23	0
10	l	1150	0	1122	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	238	0	260	2	0
11	V	238	0	260	1	0
11	m	238	0	260	1	0
12	W	2601	0	2532	39	0
12	X	2622	0	2567	47	0
12	Y	2622	0	2561	43	0
12	Z	2603	0	2550	38	0
12	g	2573	0	2526	39	0
12	h	2538	0	2476	32	0
12	n	2601	0	2532	47	0
12	o	2622	0	2567	32	0
12	p	2622	0	2561	34	0
12	q	2603	0	2550	44	0
12	r	2566	0	2517	36	0
12	s	2617	0	2559	38	0
12	t	2601	0	2532	34	0
12	u	2622	0	2567	38	0
12	v	2538	0	2476	33	0
12	w	2603	0	2550	37	0
12	x	2566	0	2517	29	0
12	y	2532	0	2465	35	0
13	A	69	0	78	2	0
13	B	38	0	49	1	0
13	G	38	0	49	1	0
13	H	69	0	78	2	0
13	I	40	0	50	2	0
13	R	40	0	50	2	0
13	X	27	0	24	1	0
13	Y	32	0	34	0	0
13	a	69	0	78	0	0
13	b	38	0	49	3	0
13	g	31	0	32	0	0
13	i	40	0	50	2	0
13	o	27	0	24	1	0
13	p	32	0	34	1	0
13	r	31	0	32	2	0
13	s	32	0	34	1	0
13	u	27	0	24	1	0
13	x	31	0	32	0	0
14	A	116	0	142	6	0
14	B	43	0	56	2	0
14	F	27	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	43	0	56	2	0
14	H	116	0	142	8	0
14	Q	27	0	24	1	0
14	a	116	0	142	3	0
14	b	43	0	56	0	0
14	f	27	0	24	1	0
15	A	65	0	72	3	0
15	H	65	0	72	4	0
15	a	65	0	72	4	0
16	A	2545	0	2497	100	0
16	B	2309	0	2201	99	0
16	F	91	0	66	1	0
16	G	2310	0	2204	89	0
16	H	2545	0	2497	105	0
16	J	82	0	58	1	0
16	K	145	0	115	3	0
16	L	185	0	190	11	0
16	Q	91	0	66	3	0
16	S	82	0	58	0	0
16	T	145	0	115	3	0
16	U	185	0	190	11	0
16	W	963	0	910	26	0
16	X	959	0	904	40	0
16	Y	973	0	936	33	0
16	Z	977	0	942	37	0
16	a	2540	0	2487	97	0
16	b	2310	0	2204	84	0
16	f	91	0	66	2	0
16	g	978	0	949	31	0
16	h	969	0	930	32	0
16	j	82	0	58	0	0
16	k	145	0	115	2	0
16	l	185	0	190	15	0
16	n	968	0	923	41	0
16	o	959	0	904	34	0
16	p	973	0	936	36	0
16	q	977	0	942	43	0
16	r	978	0	949	38	0
16	s	973	0	936	34	0
16	t	968	0	923	24	0
16	u	959	0	904	32	0
16	v	969	0	930	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	w	977	0	942	35	0
16	x	978	0	949	35	0
16	y	969	0	930	38	0
17	A	33	0	46	4	0
17	B	33	0	46	5	0
17	G	33	0	46	5	0
17	H	33	0	46	4	0
17	a	33	0	46	4	0
17	b	33	0	46	2	0
18	A	8	0	0	0	0
18	C	16	0	0	0	0
18	H	8	0	0	0	0
18	N	16	0	0	0	0
18	a	8	0	0	0	0
18	c	16	0	0	0	0
19	A	200	0	280	12	0
19	B	230	0	319	15	0
19	F	40	0	56	4	0
19	G	230	0	319	16	0
19	H	200	0	280	13	0
19	I	40	0	56	3	0
19	J	120	0	168	8	0
19	K	80	0	112	5	0
19	L	80	0	112	9	0
19	Q	40	0	56	2	0
19	R	40	0	56	0	0
19	S	120	0	168	9	0
19	T	80	0	112	3	0
19	U	80	0	112	13	0
19	W	120	0	168	6	0
19	X	160	0	224	11	0
19	Y	160	0	224	6	0
19	Z	120	0	168	4	0
19	a	200	0	280	15	0
19	b	230	0	319	15	0
19	f	40	0	56	4	0
19	g	160	0	224	12	0
19	h	120	0	168	9	0
19	i	40	0	56	5	0
19	j	120	0	168	7	0
19	k	80	0	112	4	0
19	l	80	0	112	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	n	120	0	168	9	0
19	o	160	0	224	5	0
19	p	160	0	224	10	0
19	q	120	0	168	13	0
19	r	160	0	224	7	0
19	s	160	0	224	11	0
19	t	120	0	168	5	0
19	u	160	0	224	8	0
19	v	120	0	168	7	0
19	w	120	0	168	8	0
19	x	160	0	224	9	0
19	y	120	0	168	11	0
20	A	35	0	46	1	0
20	H	35	0	46	1	0
20	L	35	0	46	3	0
20	U	35	0	46	2	0
20	a	35	0	45	1	0
20	l	35	0	46	3	0
21	B	41	0	54	3	0
21	G	41	0	54	2	0
21	I	41	0	54	2	0
21	M	41	0	54	2	0
21	R	41	0	54	2	0
21	V	41	0	54	4	0
21	b	41	0	54	2	0
21	i	41	0	54	1	0
21	m	41	0	54	2	0
22	L	1	0	0	0	0
22	U	1	0	0	0	0
22	l	1	0	0	0	0
23	Y	35	0	46	1	0
23	Z	35	0	46	0	0
23	g	35	0	46	1	0
23	p	35	0	46	1	0
23	q	35	0	46	2	0
23	r	35	0	46	3	0
23	s	35	0	46	0	0
23	w	35	0	46	0	0
23	x	35	0	46	2	0
24	Z	42	0	55	0	0
24	q	42	0	55	1	0
24	w	42	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	56	0	0	1	0
25	B	52	0	0	1	0
25	C	7	0	0	0	0
25	D	3	0	0	0	0
25	E	4	0	0	0	0
25	F	3	0	0	0	0
25	G	55	0	0	1	0
25	H	52	0	0	0	0
25	I	1	0	0	0	0
25	J	1	0	0	0	0
25	L	5	0	0	0	0
25	N	13	0	0	0	0
25	O	11	0	0	0	0
25	P	6	0	0	0	0
25	Q	4	0	0	0	0
25	R	1	0	0	0	0
25	S	3	0	0	0	0
25	U	3	0	0	0	0
25	a	57	0	0	0	0
25	b	74	0	0	1	0
25	c	17	0	0	0	0
25	d	7	0	0	0	0
25	e	10	0	0	0	0
25	f	7	0	0	0	0
25	i	1	0	0	0	0
25	j	1	0	0	0	0
25	k	1	0	0	0	0
25	l	6	0	0	0	0
All	All	140516	0	138986	2192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2192 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HB2	16:A:1137:CLA:HBB1	1.61	0.81
16:b:1206:CLA:H3A	16:b:1207:CLA:HBB1	1.64	0.78
16:H:1107:CLA:HBB1	19:S:4012:BCR:HC7	1.67	0.77
16:B:1206:CLA:H3A	16:B:1207:CLA:HBB1	1.66	0.77
1:a:440:LEU:HB2	16:a:1137:CLA:HBB1	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	H	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
1	a	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
2	B	728/731 (100%)	713 (98%)	15 (2%)	0	100	100
2	G	728/731 (100%)	712 (98%)	16 (2%)	0	100	100
2	b	728/731 (100%)	711 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	P	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	d	136/141 (96%)	130 (96%)	6 (4%)	0	100	100
5	E	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
5	O	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
5	e	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
6	Q	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
6	f	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	R	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	i	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
8	J	37/40 (92%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	37/40 (92%)	37 (100%)	0	0	100	100
8	j	37/40 (92%)	37 (100%)	0	0	100	100
9	K	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	T	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	k	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
10	L	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	U	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	l	151/157 (96%)	147 (97%)	4 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	336/342 (98%)	317 (94%)	18 (5%)	1 (0%)	36	58
12	X	337/342 (98%)	318 (94%)	19 (6%)	0	100	100
12	Y	338/342 (99%)	320 (95%)	17 (5%)	1 (0%)	36	58
12	Z	335/342 (98%)	326 (97%)	8 (2%)	1 (0%)	36	58
12	g	331/342 (97%)	304 (92%)	25 (8%)	2 (1%)	21	42
12	h	328/342 (96%)	308 (94%)	20 (6%)	0	100	100
12	n	336/342 (98%)	322 (96%)	14 (4%)	0	100	100
12	o	337/342 (98%)	318 (94%)	17 (5%)	2 (1%)	21	42
12	p	338/342 (99%)	317 (94%)	21 (6%)	0	100	100
12	q	335/342 (98%)	326 (97%)	9 (3%)	0	100	100
12	r	330/342 (96%)	316 (96%)	12 (4%)	2 (1%)	21	42
12	s	337/342 (98%)	321 (95%)	14 (4%)	2 (1%)	21	42
12	t	336/342 (98%)	319 (95%)	16 (5%)	1 (0%)	36	58
12	u	337/342 (98%)	322 (96%)	14 (4%)	1 (0%)	36	58
12	v	328/342 (96%)	312 (95%)	15 (5%)	1 (0%)	36	58
12	w	335/342 (98%)	322 (96%)	13 (4%)	0	100	100
12	x	330/342 (96%)	311 (94%)	17 (5%)	2 (1%)	21	42
12	y	328/342 (96%)	307 (94%)	21 (6%)	0	100	100
All	All	12645/13047 (97%)	12150 (96%)	479 (4%)	16 (0%)	49	70

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	W	59	MET
12	v	174	VAL
12	s	85	ASP
12	o	11	TYR
12	s	7	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	593 (100%)	0	100	100
1	H	593/603 (98%)	593 (100%)	0	100	100
1	a	593/603 (98%)	593 (100%)	0	100	100
2	B	582/583 (100%)	582 (100%)	0	100	100
2	G	582/583 (100%)	582 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	113/116 (97%)	113 (100%)	0	100	100
4	P	113/116 (97%)	113 (100%)	0	100	100
4	d	113/116 (97%)	113 (100%)	0	100	100
5	E	58/60 (97%)	58 (100%)	0	100	100
5	O	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	118/137 (86%)	118 (100%)	0	100	100
6	Q	118/137 (86%)	118 (100%)	0	100	100
6	f	118/137 (86%)	118 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	R	31/32 (97%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	i	31/32 (97%)	31 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
8	S	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
9	T	55/62 (89%)	55 (100%)	0	100	100
9	k	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100
10	U	115/118 (98%)	115 (100%)	0	100	100
10	l	115/118 (98%)	115 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
11	V	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	W	252/260 (97%)	252 (100%)	0	100	100
12	X	256/260 (98%)	256 (100%)	0	100	100
12	Y	255/260 (98%)	255 (100%)	0	100	100
12	Z	253/260 (97%)	253 (100%)	0	100	100
12	g	251/260 (96%)	251 (100%)	0	100	100
12	h	246/260 (95%)	246 (100%)	0	100	100
12	n	252/260 (97%)	252 (100%)	0	100	100
12	o	256/260 (98%)	256 (100%)	0	100	100
12	p	255/260 (98%)	255 (100%)	0	100	100
12	q	253/260 (97%)	253 (100%)	0	100	100
12	r	250/260 (96%)	250 (100%)	0	100	100
12	s	255/260 (98%)	255 (100%)	0	100	100
12	t	252/260 (97%)	252 (100%)	0	100	100
12	u	256/260 (98%)	256 (100%)	0	100	100
12	v	246/260 (95%)	246 (100%)	0	100	100
12	w	253/260 (97%)	253 (100%)	0	100	100
12	x	250/260 (96%)	250 (100%)	0	100	100
12	y	245/260 (94%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9912/10200 (97%)	9912 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
12	r	124	GLN
12	x	6	ASN
12	s	129	HIS
12	u	179	GLN
12	y	17	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 798 ligands modelled in this entry, 3 are monoatomic - leaving 795 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	CLA	H	1132	1	69,73,73	0.99	6 (8%)	82,113,113	1.11	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	b	1207	2	69,73,73	0.99	4 (5%)	82,113,113	1.17	4 (4%)
16	CLA	p	502	12	54,58,73	1.10	5 (9%)	64,95,113	1.07	4 (6%)
16	CLA	y	511	12	69,73,73	1.00	4 (5%)	82,113,113	1.12	5 (6%)
16	CLA	w	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.17	5 (7%)
16	CLA	Y	513	-	50,54,73	1.16	4 (8%)	59,90,113	1.08	5 (8%)
16	CLA	g	501	12	54,58,73	1.11	4 (7%)	64,95,113	1.08	5 (7%)
16	CLA	h	512	12	69,73,73	1.03	6 (8%)	82,113,113	1.06	7 (8%)
16	CLA	r	505	12	69,73,73	0.99	5 (7%)	82,113,113	1.17	4 (4%)
16	CLA	u	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.20	6 (9%)
16	CLA	Z	516	-	50,54,73	1.13	4 (8%)	59,90,113	1.07	4 (6%)
16	CLA	H	1103	-	69,73,73	0.99	4 (5%)	82,113,113	1.01	4 (4%)
19	BCR	w	602	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	u	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
13	LHG	s	605	-	31,31,48	0.79	1 (3%)	34,37,54	1.28	4 (11%)
19	BCR	B	4014	-	41,41,41	0.88	0	56,56,56	1.25	7 (12%)
16	CLA	g	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.01	6 (7%)
16	CLA	b	1226	2	64,68,73	1.04	6 (9%)	76,107,113	1.08	4 (5%)
16	CLA	H	1022	25	69,73,73	1.00	5 (7%)	82,113,113	1.15	8 (9%)
23	LMU	p	606	-	36,36,36	0.83	0	47,47,47	1.33	5 (10%)
16	CLA	B	1226	2	64,68,73	1.05	6 (9%)	76,107,113	1.05	3 (3%)
16	CLA	G	1220	2	58,62,73	1.10	4 (6%)	68,99,113	1.09	5 (7%)
16	CLA	A	1108	1	49,53,73	1.18	5 (10%)	58,89,113	1.10	2 (3%)
16	CLA	Y	503	-	50,54,73	1.14	4 (8%)	59,90,113	1.19	5 (8%)
16	CLA	a	1126	1	69,73,73	0.99	5 (7%)	82,113,113	1.08	3 (3%)
16	CLA	q	502	12	54,58,73	1.13	6 (11%)	64,95,113	1.04	3 (4%)
16	CLA	t	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.22	5 (7%)
16	CLA	g	509	12	69,73,73	1.01	6 (8%)	82,113,113	1.09	5 (6%)
16	CLA	s	506	12	64,68,73	1.02	6 (9%)	76,107,113	1.12	8 (10%)
19	BCR	r	603	-	41,41,41	0.83	0	56,56,56	1.20	6 (10%)
16	CLA	A	1116	1	58,62,73	1.04	5 (8%)	68,99,113	1.20	7 (10%)
16	CLA	a	1136	1	69,73,73	0.99	5 (7%)	82,113,113	1.00	3 (3%)
16	CLA	b	1216	25	51,55,73	1.16	5 (9%)	60,91,113	1.46	8 (13%)
16	CLA	F	1302	6	50,54,73	1.17	5 (10%)	59,90,113	1.05	3 (5%)
19	BCR	K	4005	-	41,41,41	0.86	0	56,56,56	1.28	6 (10%)
16	CLA	p	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.02	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	a	1113	1	49,53,73	1.21	7 (14%)	58,89,113	1.15	2 (3%)
16	CLA	G	1211	2	69,73,73	0.98	4 (5%)	82,113,113	1.01	2 (2%)
16	CLA	w	506	-	64,68,73	1.03	5 (7%)	76,107,113	1.09	4 (5%)
16	CLA	a	1121	1	55,59,73	1.12	5 (9%)	64,96,113	1.11	5 (7%)
16	CLA	A	1124	25	64,68,73	1.03	4 (6%)	76,107,113	1.05	4 (5%)
14	LMG	B	848	-	43,43,55	0.87	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	v	514	-	54,58,73	1.13	4 (7%)	64,95,113	1.05	2 (3%)
19	BCR	F	4016	-	41,41,41	0.86	0	56,56,56	1.31	8 (14%)
16	CLA	A	1102	16,1	60,64,73	1.06	4 (6%)	71,102,113	0.95	3 (4%)
16	CLA	y	504	12	64,68,73	1.05	6 (9%)	76,107,113	1.19	8 (10%)
16	CLA	X	510	-	64,68,73	1.03	4 (6%)	76,107,113	0.97	4 (5%)
19	BCR	T	4005	-	41,41,41	0.85	0	56,56,56	1.26	7 (12%)
18	SF4	N	101	-	0,12,12	-	-	-		
16	CLA	H	1801	13	50,54,73	1.13	4 (8%)	59,90,113	1.15	5 (8%)
14	LMG	Q	4017	-	27,27,55	1.07	1 (3%)	35,35,63	1.18	3 (8%)
16	CLA	f	1302	6	50,54,73	1.17	5 (10%)	59,90,113	1.07	4 (6%)
19	BCR	X	603	-	41,41,41	0.85	0	56,56,56	1.15	4 (7%)
19	BCR	r	602	-	41,41,41	0.86	0	56,56,56	1.24	4 (7%)
16	CLA	w	516	12	50,54,73	1.14	4 (8%)	59,90,113	1.01	4 (6%)
16	CLA	G	1236	2	54,58,73	1.10	4 (7%)	64,95,113	1.14	3 (4%)
19	BCR	W	601	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	a	1127	1	69,73,73	1.00	6 (8%)	82,113,113	1.08	4 (4%)
16	CLA	A	1127	1	69,73,73	0.99	6 (8%)	82,113,113	1.07	4 (4%)
16	CLA	G	1213	2	59,63,73	1.08	5 (8%)	70,101,113	1.10	4 (5%)
19	BCR	f	4016	-	41,41,41	0.87	0	56,56,56	1.29	5 (8%)
16	CLA	a	1131	1	69,73,73	1.01	6 (8%)	82,113,113	1.13	3 (3%)
16	CLA	g	505	12	69,73,73	0.99	5 (7%)	82,113,113	1.19	7 (8%)
16	CLA	w	509	12	69,73,73	1.00	5 (7%)	82,113,113	1.02	5 (6%)
14	LMG	b	848	-	43,43,55	0.86	1 (2%)	51,51,63	1.28	6 (11%)
19	BCR	B	4004	-	41,41,41	0.83	0	56,56,56	1.26	5 (8%)
20	LMT	L	4101	-	36,36,36	1.17	6 (16%)	47,47,47	1.15	3 (6%)
16	CLA	a	1101	1	69,73,73	0.98	4 (5%)	82,113,113	1.06	4 (4%)
16	CLA	b	1227	2	53,57,73	1.11	6 (11%)	61,93,113	1.15	6 (9%)
16	CLA	u	501	12	50,54,73	1.14	4 (8%)	59,90,113	0.99	3 (5%)
19	BCR	u	601	-	41,41,41	0.91	1 (2%)	56,56,56	1.38	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	s	604	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
16	CLA	B	1239	2	69,73,73	0.95	3 (4%)	82,113,113	1.11	6 (7%)
19	BCR	X	602	-	41,41,41	0.88	0	56,56,56	1.36	7 (12%)
16	CLA	B	1209	2	49,53,73	1.17	4 (8%)	58,89,113	1.10	3 (5%)
16	CLA	h	509	12	69,73,73	1.02	6 (8%)	82,113,113	1.07	6 (7%)
16	CLA	L	1502	10	64,68,73	1.00	5 (7%)	76,107,113	1.12	4 (5%)
16	CLA	p	517	12	59,63,73	1.07	4 (6%)	70,101,113	1.02	4 (5%)
16	CLA	b	1212	2	49,53,73	1.19	5 (10%)	58,89,113	1.19	4 (6%)
21	ECH	M	4021	-	42,42,42	0.86	0	55,58,58	1.53	9 (16%)
16	CLA	k	4004	-	59,63,73	1.07	4 (6%)	70,101,113	0.98	5 (7%)
16	CLA	g	516	-	50,54,73	1.15	4 (8%)	59,90,113	1.19	3 (5%)
19	BCR	G	4005	-	41,41,41	0.85	0	56,56,56	1.14	4 (7%)
16	CLA	x	513	-	50,54,73	1.18	5 (10%)	59,90,113	1.03	2 (3%)
16	CLA	a	1137	1	51,55,73	1.13	4 (7%)	60,91,113	1.14	5 (8%)
16	CLA	X	517	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	5 (7%)
16	CLA	n	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.07	5 (6%)
16	CLA	A	1112	1	49,53,73	1.19	4 (8%)	58,89,113	1.07	4 (6%)
19	BCR	L	4022	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
16	CLA	b	1202	-	69,73,73	0.97	4 (5%)	82,113,113	0.97	3 (3%)
13	LHG	A	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.23	5 (11%)
16	CLA	a	1801	13	50,54,73	1.16	4 (8%)	59,90,113	1.20	4 (6%)
16	CLA	A	1801	13	50,54,73	1.14	4 (8%)	59,90,113	1.22	5 (8%)
16	CLA	o	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.03	5 (6%)
16	CLA	w	503	12	50,54,73	1.16	6 (12%)	59,90,113	1.18	5 (8%)
16	CLA	b	1221	25	69,73,73	1.00	5 (7%)	82,113,113	1.10	5 (6%)
16	CLA	A	1126	1	69,73,73	0.98	5 (7%)	82,113,113	1.13	2 (2%)
16	CLA	a	1105	-	62,66,73	1.07	5 (8%)	73,104,113	1.03	5 (6%)
16	CLA	o	513	-	50,54,73	1.16	4 (8%)	59,90,113	0.98	1 (1%)
21	ECH	i	4020	-	42,42,42	0.84	1 (2%)	55,58,58	1.84	10 (18%)
16	CLA	o	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	G	1206	2	69,73,73	0.98	5 (7%)	82,113,113	0.95	3 (3%)
16	CLA	J	1302	8	49,53,73	1.19	5 (10%)	58,89,113	1.26	6 (10%)
16	CLA	Y	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.12	5 (7%)
19	BCR	B	4010	-	41,41,41	0.91	0	56,56,56	1.35	8 (14%)
19	BCR	v	601	-	41,41,41	0.83	0	56,56,56	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	w	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.11	5 (6%)
16	CLA	G	1224	2	64,68,73	1.05	5 (7%)	76,107,113	1.12	4 (5%)
17	PQN	b	2002	-	34,34,34	0.36	0	43,45,45	1.06	2 (4%)
24	LUT	w	601	-	42,43,43	0.74	0	51,60,60	1.46	7 (13%)
16	CLA	G	1012	25	59,63,73	1.13	6 (10%)	70,101,113	1.19	7 (10%)
19	BCR	S	4012	-	41,41,41	0.88	0	56,56,56	1.28	7 (12%)
16	CLA	W	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
19	BCR	k	4005	-	41,41,41	0.85	0	56,56,56	1.26	5 (8%)
16	CLA	a	1130	1	64,68,73	1.04	5 (7%)	76,107,113	1.01	6 (7%)
16	CLA	H	1104	1	69,73,73	1.00	6 (8%)	82,113,113	1.07	6 (7%)
16	CLA	n	511	12	69,73,73	1.00	5 (7%)	82,113,113	1.05	5 (6%)
16	CLA	a	1237	25	69,73,73	0.99	4 (5%)	82,113,113	1.12	6 (7%)
19	BCR	Z	603	-	41,41,41	0.84	0	56,56,56	1.17	4 (7%)
20	LMT	A	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	0
16	CLA	b	1201	2	58,62,73	1.07	4 (6%)	68,99,113	1.15	5 (7%)
16	CLA	t	517	12	59,63,73	1.09	5 (8%)	70,101,113	1.00	3 (4%)
19	BCR	H	4002	-	41,41,41	0.85	0	56,56,56	1.19	5 (8%)
16	CLA	G	1208	2	49,53,73	1.16	4 (8%)	58,89,113	1.22	6 (10%)
16	CLA	B	1235	2	66,70,73	1.03	5 (7%)	78,109,113	1.19	9 (11%)
18	SF4	c	101	-	0,12,12	-	-	-		
16	CLA	b	1211	2	69,73,73	0.98	5 (7%)	82,113,113	0.98	4 (4%)
16	CLA	B	1206	2	69,73,73	0.98	5 (7%)	82,113,113	0.94	4 (4%)
16	CLA	b	1234	2	54,58,73	1.14	5 (9%)	64,95,113	1.13	8 (12%)
16	CLA	B	1234	2	54,58,73	1.13	6 (11%)	64,95,113	1.13	5 (7%)
23	LMU	x	606	-	36,36,36	0.88	0	47,47,47	1.26	6 (12%)
16	CLA	a	1118	1	59,63,73	1.06	4 (6%)	70,101,113	0.96	2 (2%)
16	CLA	w	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.05	5 (6%)
19	BCR	t	604	-	41,41,41	0.83	0	56,56,56	1.23	4 (7%)
19	BCR	X	601	-	41,41,41	0.87	1 (2%)	56,56,56	1.33	6 (10%)
16	CLA	a	1128	1	69,73,73	0.97	6 (8%)	82,113,113	1.10	6 (7%)
16	CLA	B	1221	25	69,73,73	0.99	4 (5%)	82,113,113	1.02	3 (3%)
16	CLA	B	1203	2	69,73,73	0.99	5 (7%)	82,113,113	1.14	5 (6%)
16	CLA	x	511	12	69,73,73	1.00	6 (8%)	82,113,113	0.94	2 (2%)
16	CLA	x	517	12	59,63,73	1.09	4 (6%)	70,101,113	0.96	2 (2%)
16	CLA	W	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.12	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	y	501	12	50,54,73	1.15	4 (8%)	59,90,113	1.27	7 (11%)
19	BCR	G	4017	-	41,41,41	0.87	0	56,56,56	1.18	6 (10%)
16	CLA	b	1224	2	64,68,73	1.05	6 (9%)	76,107,113	1.20	4 (5%)
19	BCR	y	601	-	41,41,41	0.83	0	56,56,56	1.24	6 (10%)
17	PQN	B	2002	-	34,34,34	0.36	0	43,45,45	1.04	2 (4%)
16	CLA	o	501	12	50,54,73	1.14	4 (8%)	59,90,113	1.13	4 (6%)
16	CLA	u	506	-	64,68,73	1.08	6 (9%)	76,107,113	1.64	12 (15%)
23	LMU	Z	605	-	36,36,36	0.87	0	47,47,47	1.20	4 (8%)
16	CLA	U	1501	10	64,68,73	1.03	5 (7%)	76,107,113	1.01	4 (5%)
16	CLA	F	1301	25	49,53,73	1.18	4 (8%)	58,89,113	1.13	3 (5%)
16	CLA	r	510	-	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
14	LMG	A	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	h	514	-	54,58,73	1.13	4 (7%)	64,95,113	1.14	7 (10%)
16	CLA	b	1203	2	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
18	SF4	A	3001	-	0,12,12	-	-	-		
19	BCR	Y	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	x	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.11	6 (7%)
16	CLA	h	501	12	50,54,73	1.17	5 (10%)	59,90,113	1.26	6 (10%)
23	LMU	Y	606	-	36,36,36	0.84	0	47,47,47	1.36	6 (12%)
16	CLA	t	507	12	69,73,73	1.01	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	A	1136	1	69,73,73	0.98	4 (5%)	82,113,113	1.00	3 (3%)
16	CLA	T	4002	9	49,53,73	1.17	4 (8%)	58,89,113	1.03	3 (5%)
16	CLA	h	504	-	64,68,73	1.05	5 (7%)	76,107,113	1.24	7 (9%)
16	CLA	a	1102	16,1	60,64,73	1.06	5 (8%)	71,102,113	1.05	3 (4%)
14	LMG	H	4101	-	46,46,55	0.91	1 (2%)	54,54,63	1.23	4 (7%)
16	CLA	G	1205	2	69,73,73	0.99	5 (7%)	82,113,113	1.09	4 (4%)
19	BCR	b	4009	-	30,30,41	0.85	0	39,39,56	1.35	6 (15%)
16	CLA	A	1104	1	69,73,73	0.99	5 (7%)	82,113,113	0.98	6 (7%)
16	CLA	B	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.01	4 (4%)
16	CLA	Z	513	-	54,58,73	1.12	4 (7%)	64,95,113	1.07	5 (7%)
16	CLA	A	1121	1	55,59,73	1.11	5 (9%)	64,96,113	1.11	4 (6%)
16	CLA	q	513	-	54,58,73	1.12	4 (7%)	64,95,113	1.08	4 (6%)
16	CLA	Z	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.12	5 (7%)
16	CLA	x	501	-	54,58,73	1.12	5 (9%)	64,95,113	1.34	7 (10%)
19	BCR	x	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	o	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.16	5 (6%)
16	CLA	t	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.12	5 (7%)
16	CLA	b	1238	25	69,73,73	0.98	4 (5%)	82,113,113	1.06	8 (9%)
16	CLA	G	1218	-	59,63,73	1.08	4 (6%)	70,101,113	1.10	4 (5%)
19	BCR	g	603	-	41,41,41	0.84	0	56,56,56	1.21	6 (10%)
14	LMG	f	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	B	1228	2	59,63,73	1.08	4 (6%)	70,101,113	1.09	4 (5%)
16	CLA	H	1115	1	58,62,73	1.06	4 (6%)	68,99,113	1.16	2 (2%)
16	CLA	b	1206	2	69,73,73	0.99	5 (7%)	82,113,113	0.94	2 (2%)
16	CLA	s	513	-	50,54,73	1.15	4 (8%)	59,90,113	1.16	5 (8%)
16	CLA	w	517	12	59,63,73	1.09	6 (10%)	70,101,113	1.07	3 (4%)
16	CLA	Z	507	12	69,73,73	1.00	3 (4%)	82,113,113	1.08	5 (6%)
16	CLA	Z	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.12	4 (4%)
16	CLA	U	1502	10	64,68,73	1.01	5 (7%)	76,107,113	1.14	5 (6%)
16	CLA	A	1131	1	69,73,73	1.02	5 (7%)	82,113,113	1.16	5 (6%)
19	BCR	o	601	-	41,41,41	0.88	1 (2%)	56,56,56	1.37	8 (14%)
19	BCR	J	4012	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	b	1205	2	69,73,73	0.98	4 (5%)	82,113,113	1.08	4 (4%)
16	CLA	g	511	12	69,73,73	0.99	5 (7%)	82,113,113	0.98	3 (3%)
16	CLA	y	507	12	69,73,73	1.02	5 (7%)	82,113,113	0.96	4 (4%)
16	CLA	W	506	12	64,68,73	1.03	3 (4%)	76,107,113	1.09	5 (6%)
16	CLA	s	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	5 (6%)
16	CLA	v	507	12	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	H	1107	1	54,58,73	1.11	4 (7%)	64,95,113	1.07	6 (9%)
19	BCR	a	4003	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
14	LMG	H	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	Z	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.13	5 (7%)
19	BCR	a	4011	-	41,41,41	0.89	0	56,56,56	1.26	5 (8%)
19	BCR	h	601	-	41,41,41	0.84	0	56,56,56	1.28	7 (12%)
21	ECH	m	4021	-	42,42,42	0.84	0	55,58,58	1.55	9 (16%)
16	CLA	H	1129	1	50,54,73	1.13	5 (10%)	59,90,113	1.16	6 (10%)
16	CLA	A	1117	1	69,73,73	0.99	5 (7%)	82,113,113	1.14	4 (4%)
16	CLA	A	1119	25	69,73,73	1.00	4 (5%)	82,113,113	0.99	4 (4%)
16	CLA	g	517	12	59,63,73	1.09	4 (6%)	70,101,113	0.99	3 (4%)
16	CLA	v	509	12	69,73,73	1.02	6 (8%)	82,113,113	1.06	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	t	603	-	41,41,41	0.84	0	56,56,56	1.18	4 (7%)
16	CLA	b	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.02	5 (6%)
16	CLA	p	511	12	69,73,73	0.98	4 (5%)	82,113,113	1.05	5 (6%)
16	CLA	Z	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.18	7 (10%)
16	CLA	s	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	W	505	12	69,73,73	1.00	4 (5%)	82,113,113	1.15	6 (7%)
16	CLA	X	516	12	50,54,73	1.13	5 (10%)	59,90,113	1.09	3 (5%)
16	CLA	s	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.22	5 (7%)
16	CLA	G	1222	25	54,58,73	1.13	6 (11%)	64,95,113	1.15	8 (12%)
16	CLA	B	1224	2	64,68,73	1.05	6 (9%)	76,107,113	1.07	4 (5%)
16	CLA	G	1209	2	49,53,73	1.18	4 (8%)	58,89,113	1.17	4 (6%)
16	CLA	p	509	12	64,68,73	1.05	4 (6%)	76,107,113	0.98	3 (3%)
19	BCR	b	4017	-	41,41,41	0.87	0	56,56,56	1.16	4 (7%)
16	CLA	X	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.10	6 (7%)
16	CLA	a	1124	25	64,68,73	1.03	4 (6%)	76,107,113	0.99	2 (2%)
16	CLA	X	509	12	64,68,73	1.05	5 (7%)	76,107,113	1.00	6 (7%)
16	CLA	b	1217	2	49,53,73	1.16	4 (8%)	58,89,113	1.20	5 (8%)
16	CLA	G	1214	2	59,63,73	1.06	6 (10%)	70,101,113	1.11	5 (7%)
16	CLA	o	516	12	50,54,73	1.14	5 (10%)	59,90,113	1.05	2 (3%)
19	BCR	H	4008	-	41,41,41	0.90	1 (2%)	56,56,56	1.37	4 (7%)
16	CLA	g	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.16	6 (7%)
16	CLA	s	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.19	6 (9%)
16	CLA	L	1503	25	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	G	1215	2	64,68,73	1.00	4 (6%)	76,107,113	1.09	2 (2%)
16	CLA	W	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.08	5 (6%)
16	CLA	X	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.97	4 (5%)
16	CLA	p	514	-	54,58,73	1.13	5 (9%)	64,95,113	1.10	4 (6%)
16	CLA	w	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.07	5 (7%)
16	CLA	a	1135	1	55,59,73	1.14	7 (12%)	64,96,113	1.08	5 (7%)
16	CLA	y	509	12	69,73,73	1.00	4 (5%)	82,113,113	0.97	5 (6%)
16	CLA	p	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	t	505	12	69,73,73	1.00	5 (7%)	82,113,113	1.19	6 (7%)
16	CLA	G	1210	2	69,73,73	1.00	5 (7%)	82,113,113	1.05	5 (6%)
16	CLA	B	1212	2	49,53,73	1.19	5 (10%)	58,89,113	1.14	4 (6%)
19	BCR	W	603	-	41,41,41	0.85	0	56,56,56	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	A	1130	1	64,68,73	1.03	5 (7%)	76,107,113	0.94	4 (5%)
16	CLA	B	1215	2	64,68,73	1.00	5 (7%)	76,107,113	1.11	3 (3%)
16	CLA	j	1302	8	49,53,73	1.19	5 (10%)	58,89,113	1.18	6 (10%)
19	BCR	y	603	-	41,41,41	0.83	0	56,56,56	1.17	5 (8%)
16	CLA	b	1222	25	54,58,73	1.14	5 (9%)	64,95,113	1.08	4 (6%)
16	CLA	u	513	-	50,54,73	1.15	5 (10%)	59,90,113	1.03	3 (5%)
19	BCR	o	604	-	41,41,41	0.88	0	56,56,56	1.31	10 (17%)
16	CLA	v	506	-	64,68,73	1.05	5 (7%)	76,107,113	1.33	7 (9%)
16	CLA	g	503	-	50,54,73	1.15	4 (8%)	59,90,113	1.13	4 (6%)
16	CLA	h	506	12	64,68,73	1.05	6 (9%)	76,107,113	1.38	10 (13%)
16	CLA	n	514	-	54,58,73	1.11	6 (11%)	64,95,113	1.10	5 (7%)
19	BCR	p	601	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
19	BCR	G	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	v	510	-	69,73,73	1.02	4 (5%)	82,113,113	1.01	7 (8%)
16	CLA	p	504	12	69,73,73	1.00	4 (5%)	82,113,113	1.00	3 (3%)
19	BCR	Z	602	-	41,41,41	0.87	0	56,56,56	1.36	8 (14%)
19	BCR	a	4007	-	41,41,41	0.89	1 (2%)	56,56,56	1.30	5 (8%)
16	CLA	K	4002	9	49,53,73	1.17	4 (8%)	58,89,113	1.02	2 (3%)
16	CLA	u	511	-	69,73,73	0.97	4 (5%)	82,113,113	1.10	4 (4%)
16	CLA	Z	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.03	6 (7%)
16	CLA	X	501	12	50,54,73	1.14	4 (8%)	59,90,113	1.11	5 (8%)
16	CLA	b	1218	-	59,63,73	1.07	4 (6%)	70,101,113	1.10	7 (10%)
16	CLA	a	1107	1	54,58,73	1.11	4 (7%)	64,95,113	1.14	3 (4%)
16	CLA	j	1303	8	41,45,73	1.24	5 (12%)	50,78,113	1.10	3 (6%)
16	CLA	s	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.15	6 (7%)
19	BCR	X	604	-	41,41,41	0.88	0	56,56,56	1.31	5 (8%)
16	CLA	y	505	12	69,73,73	1.02	5 (7%)	82,113,113	1.21	5 (6%)
16	CLA	S	1302	8	49,53,73	1.18	5 (10%)	58,89,113	1.11	5 (8%)
16	CLA	G	1235	2	66,70,73	1.02	5 (7%)	78,109,113	1.19	10 (12%)
16	CLA	q	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.15	5 (7%)
19	BCR	Q	4016	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
14	LMG	A	4101	-	46,46,55	0.92	2 (4%)	54,54,63	1.23	4 (7%)
20	LMT	H	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	0
16	CLA	W	517	12	59,63,73	1.09	5 (8%)	70,101,113	0.98	4 (5%)
19	BCR	q	603	-	41,41,41	0.84	0	56,56,56	1.16	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	y	512	12	69,73,73	1.00	5 (7%)	82,113,113	1.01	6 (7%)
16	CLA	G	1240	13	50,54,73	1.18	5 (10%)	59,90,113	1.30	6 (10%)
16	CLA	y	517	-	59,63,73	1.11	5 (8%)	70,101,113	1.26	6 (8%)
19	BCR	s	601	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	b	1232	25	49,53,73	1.19	5 (10%)	58,89,113	1.35	4 (6%)
16	CLA	Z	506	-	64,68,73	1.02	3 (4%)	76,107,113	1.03	2 (2%)
13	LHG	i	103	-	39,39,48	0.69	2 (5%)	42,45,54	1.24	5 (11%)
16	CLA	B	1219	-	49,53,73	1.21	6 (12%)	58,89,113	1.15	4 (6%)
16	CLA	a	1114	-	50,54,73	1.15	5 (10%)	59,90,113	1.31	5 (8%)
17	PQN	a	2001	-	34,34,34	0.39	0	43,45,45	1.06	2 (4%)
16	CLA	v	515	12	69,73,73	1.02	4 (5%)	82,113,113	1.18	7 (8%)
16	CLA	y	516	12	50,54,73	1.17	5 (10%)	59,90,113	1.18	5 (8%)
16	CLA	a	1120	1	53,57,73	1.08	4 (7%)	61,93,113	1.21	5 (8%)
21	ECH	G	4006	-	42,42,42	0.79	0	55,58,58	1.50	8 (14%)
16	CLA	y	506	12	64,68,73	1.04	4 (6%)	76,107,113	1.40	9 (11%)
19	BCR	A	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.40	9 (16%)
19	BCR	A	4008	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
16	CLA	v	517	-	59,63,73	1.11	5 (8%)	70,101,113	1.03	6 (8%)
19	BCR	t	601	-	41,41,41	0.83	0	56,56,56	1.18	6 (10%)
16	CLA	h	516	12	50,54,73	1.16	4 (8%)	59,90,113	1.12	4 (6%)
19	BCR	q	602	-	41,41,41	0.85	0	56,56,56	1.24	6 (10%)
16	CLA	X	505	12	69,73,73	1.00	5 (7%)	82,113,113	1.12	6 (7%)
16	CLA	o	510	-	64,68,73	1.04	4 (6%)	76,107,113	0.98	5 (6%)
21	ECH	V	4021	-	42,42,42	0.84	1 (2%)	55,58,58	1.55	7 (12%)
16	CLA	h	507	12	69,73,73	0.99	4 (5%)	82,113,113	1.11	5 (6%)
16	CLA	Y	511	12	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	B	1021	2	69,73,73	1.00	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	H	1127	1	69,73,73	1.00	6 (8%)	82,113,113	1.11	5 (6%)
19	BCR	v	603	-	41,41,41	0.85	0	56,56,56	1.27	8 (14%)
21	ECH	R	4020	-	42,42,42	0.99	3 (7%)	55,58,58	1.93	14 (25%)
16	CLA	H	1135	1	55,59,73	1.12	4 (7%)	64,96,113	1.26	6 (9%)
19	BCR	w	604	-	41,41,41	0.87	0	56,56,56	1.27	6 (10%)
16	CLA	q	517	12	59,63,73	1.08	5 (8%)	70,101,113	1.13	6 (8%)
16	CLA	A	1107	1	54,58,73	1.12	4 (7%)	64,95,113	1.15	5 (7%)
13	LHG	G	4018	16	37,37,48	0.73	1 (2%)	40,43,54	1.32	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	u	512	12	69,73,73	0.98	6 (8%)	82,113,113	1.02	2 (2%)
16	CLA	b	1214	2	59,63,73	1.06	5 (8%)	70,101,113	1.03	4 (5%)
16	CLA	t	504	12	64,68,73	1.04	4 (6%)	76,107,113	1.02	3 (3%)
16	CLA	r	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.13	4 (6%)
16	CLA	H	1111	1	59,63,73	1.09	4 (6%)	70,101,113	1.03	2 (2%)
19	BCR	l	4022	-	41,41,41	0.89	1 (2%)	56,56,56	1.41	8 (14%)
19	BCR	K	4001	-	41,41,41	0.86	0	56,56,56	1.31	7 (12%)
19	BCR	Z	604	-	41,41,41	0.87	0	56,56,56	1.24	6 (10%)
16	CLA	G	1023	-	69,73,73	1.02	8 (11%)	82,113,113	1.13	8 (9%)
16	CLA	v	516	12	50,54,73	1.14	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	H	1112	1	49,53,73	1.19	4 (8%)	58,89,113	0.99	3 (5%)
19	BCR	g	602	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
19	BCR	q	604	-	41,41,41	0.87	0	56,56,56	1.26	6 (10%)
23	LMU	g	606	-	36,36,36	0.86	0	47,47,47	1.32	5 (10%)
16	CLA	q	509	12	69,73,73	1.01	5 (7%)	82,113,113	0.98	6 (7%)
19	BCR	o	603	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	A	1113	1	49,53,73	1.19	4 (8%)	58,89,113	1.06	2 (3%)
16	CLA	H	1136	1	69,73,73	0.98	5 (7%)	82,113,113	0.99	3 (3%)
16	CLA	H	1138	1	69,73,73	0.99	5 (7%)	82,113,113	1.07	4 (4%)
13	LHG	b	4018	16	37,37,48	0.71	0	40,43,54	1.31	5 (12%)
16	CLA	l	1502	10	64,68,73	1.00	5 (7%)	76,107,113	1.16	5 (6%)
16	CLA	W	514	-	54,58,73	1.11	5 (9%)	64,95,113	1.11	4 (6%)
16	CLA	B	1223	2	69,73,73	0.98	4 (5%)	82,113,113	1.07	3 (3%)
19	BCR	v	604	-	41,41,41	0.86	0	56,56,56	1.28	8 (14%)
16	CLA	A	1110	1	58,62,73	1.05	4 (6%)	68,99,113	1.01	3 (4%)
16	CLA	a	1103	1	69,73,73	0.97	4 (5%)	82,113,113	0.98	2 (2%)
19	BCR	G	4004	-	41,41,41	0.83	0	56,56,56	1.25	6 (10%)
16	CLA	n	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.00	6 (7%)
16	CLA	K	4003	9	49,53,73	1.20	4 (8%)	58,89,113	1.14	4 (6%)
16	CLA	h	505	12	69,73,73	1.02	5 (7%)	82,113,113	1.15	6 (7%)
16	CLA	y	503	-	50,54,73	1.18	6 (12%)	59,90,113	1.21	6 (10%)
19	BCR	H	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.30	7 (12%)
19	BCR	s	602	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
19	BCR	n	603	-	41,41,41	0.83	0	56,56,56	1.20	5 (8%)
19	BCR	h	603	-	41,41,41	0.83	0	56,56,56	1.19	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	u	517	12	59,63,73	1.09	4 (6%)	70,101,113	1.04	5 (7%)
16	CLA	t	502	12	54,58,73	1.14	6 (11%)	64,95,113	1.13	4 (6%)
16	CLA	Q	1301	25	49,53,73	1.17	4 (8%)	58,89,113	1.13	4 (6%)
17	PQN	H	2001	-	34,34,34	0.38	0	43,45,45	1.06	2 (4%)
16	CLA	b	1219	-	49,53,73	1.21	5 (10%)	58,89,113	1.21	5 (8%)
16	CLA	b	1213	2	59,63,73	1.08	6 (10%)	70,101,113	1.09	6 (8%)
16	CLA	W	502	12	54,58,73	1.14	6 (11%)	64,95,113	1.16	5 (7%)
16	CLA	h	510	-	69,73,73	1.01	5 (7%)	82,113,113	1.00	6 (7%)
16	CLA	r	513	-	50,54,73	1.18	4 (8%)	59,90,113	1.10	5 (8%)
16	CLA	o	517	12	59,63,73	1.08	4 (6%)	70,101,113	0.98	4 (5%)
16	CLA	A	1135	1	55,59,73	1.13	7 (12%)	64,96,113	1.12	5 (7%)
16	CLA	y	502	12	54,58,73	1.13	5 (9%)	64,95,113	1.01	4 (6%)
16	CLA	L	1501	10	64,68,73	1.02	5 (7%)	76,107,113	0.98	5 (6%)
16	CLA	a	1106	1	69,73,73	0.97	4 (5%)	82,113,113	1.10	3 (3%)
20	LMT	l	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
16	CLA	a	1139	25	59,63,73	1.07	5 (8%)	70,101,113	1.00	5 (7%)
16	CLA	q	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.17	5 (7%)
16	CLA	X	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	Z	510	-	64,68,73	1.04	4 (6%)	76,107,113	1.04	3 (3%)
16	CLA	b	1209	2	49,53,73	1.17	4 (8%)	58,89,113	1.10	3 (5%)
18	SF4	N	102	-	0,12,12	-	-	-		
19	BCR	i	4018	-	41,41,41	0.87	0	56,56,56	1.23	8 (14%)
18	SF4	H	3001	-	0,12,12	-	-	-		
16	CLA	t	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.10	4 (6%)
16	CLA	A	1111	1	59,63,73	1.08	6 (10%)	70,101,113	1.20	5 (7%)
16	CLA	X	513	-	50,54,73	1.14	4 (8%)	59,90,113	1.09	3 (5%)
16	CLA	t	506	12	64,68,73	1.04	5 (7%)	76,107,113	1.07	5 (6%)
16	CLA	h	517	-	59,63,73	1.10	4 (6%)	70,101,113	0.99	5 (7%)
19	BCR	J	4015	-	41,41,41	0.87	0	56,56,56	1.26	9 (16%)
16	CLA	x	509	12	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	U	1503	-	69,73,73	1.00	4 (5%)	82,113,113	0.87	3 (3%)
16	CLA	s	510	-	69,73,73	1.01	4 (5%)	82,113,113	0.97	4 (4%)
16	CLA	Y	504	12	69,73,73	1.01	5 (7%)	82,113,113	0.99	3 (3%)
16	CLA	v	502	12	54,58,73	1.12	5 (9%)	64,95,113	1.06	5 (7%)
16	CLA	s	502	12	54,58,73	1.10	5 (9%)	64,95,113	1.09	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	t	510	-	69,73,73	1.00	4 (5%)	82,113,113	0.99	5 (6%)
16	CLA	t	509	12	64,68,73	1.06	5 (7%)	76,107,113	1.15	6 (7%)
16	CLA	G	1212	2	49,53,73	1.19	5 (10%)	58,89,113	1.20	4 (6%)
16	CLA	G	1231	25	49,53,73	1.19	4 (8%)	58,89,113	1.13	4 (6%)
16	CLA	o	506	-	64,68,73	1.04	5 (7%)	76,107,113	1.06	4 (5%)
13	LHG	Y	605	-	31,31,48	0.78	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	p	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.07	3 (5%)
16	CLA	W	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	4 (4%)
16	CLA	A	1237	25	69,73,73	0.99	4 (5%)	82,113,113	1.10	6 (7%)
18	SF4	c	102	-	0,12,12	-	-	-		
16	CLA	r	501	12	54,58,73	1.10	4 (7%)	64,95,113	1.21	6 (9%)
16	CLA	v	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.24	7 (11%)
16	CLA	X	514	-	54,58,73	1.12	6 (11%)	64,95,113	1.30	6 (9%)
16	CLA	a	1112	1	49,53,73	1.19	5 (10%)	58,89,113	1.00	3 (5%)
16	CLA	A	1114	-	50,54,73	1.12	4 (8%)	59,90,113	1.23	4 (6%)
16	CLA	H	1131	1	69,73,73	1.01	4 (5%)	82,113,113	1.11	4 (4%)
19	BCR	a	4008	-	41,41,41	0.91	1 (2%)	56,56,56	1.35	6 (10%)
17	PQN	A	2001	-	34,34,34	0.37	0	43,45,45	1.08	2 (4%)
19	BCR	B	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	H	1137	1	51,55,73	1.12	5 (9%)	60,91,113	1.11	5 (8%)
19	BCR	x	603	-	41,41,41	0.85	0	56,56,56	1.26	6 (10%)
16	CLA	w	513	-	54,58,73	1.13	4 (7%)	64,95,113	1.15	6 (9%)
16	CLA	Y	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	5 (6%)
19	BCR	b	4004	-	41,41,41	0.84	0	56,56,56	1.26	6 (10%)
16	CLA	B	1204	2	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
19	BCR	I	4018	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	o	504	12	64,68,73	1.05	5 (7%)	76,107,113	1.05	4 (5%)
16	CLA	t	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.13	5 (6%)
19	BCR	b	4005	-	41,41,41	0.85	0	56,56,56	1.15	5 (8%)
16	CLA	w	511	12	69,73,73	0.99	5 (7%)	82,113,113	1.04	5 (6%)
16	CLA	A	1022	25	69,73,73	1.01	5 (7%)	82,113,113	1.08	9 (10%)
16	CLA	u	503	-	50,54,73	1.15	4 (8%)	59,90,113	1.06	3 (5%)
16	CLA	Z	517	12	59,63,73	1.09	5 (8%)	70,101,113	1.03	3 (4%)
16	CLA	b	1223	2	69,73,73	0.99	4 (5%)	82,113,113	1.09	1 (1%)
16	CLA	B	1227	2	53,57,73	1.13	6 (11%)	61,93,113	1.13	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	T	4001	-	41,41,41	0.86	1 (2%)	56,56,56	1.26	6 (10%)
19	BCR	a	4002	-	41,41,41	0.85	0	56,56,56	1.18	5 (8%)
16	CLA	Y	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.04	5 (6%)
16	CLA	Z	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.16	5 (6%)
19	BCR	l	4019	-	41,41,41	0.88	0	56,56,56	1.44	8 (14%)
16	CLA	A	1103	-	69,73,73	0.97	4 (5%)	82,113,113	1.00	1 (1%)
16	CLA	g	513	-	50,54,73	1.18	4 (8%)	59,90,113	1.00	5 (8%)
16	CLA	q	511	12	69,73,73	1.00	4 (5%)	82,113,113	1.05	3 (3%)
16	CLA	W	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.24	5 (7%)
19	BCR	k	4001	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
23	LMU	w	605	-	36,36,36	0.84	0	47,47,47	1.10	4 (8%)
16	CLA	x	504	12	69,73,73	1.01	4 (5%)	82,113,113	1.04	6 (7%)
16	CLA	s	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.02	6 (7%)
16	CLA	n	510	-	69,73,73	1.01	3 (4%)	82,113,113	1.04	4 (4%)
16	CLA	A	1133	1	58,62,73	1.08	6 (10%)	68,99,113	1.22	7 (10%)
16	CLA	a	1115	1	58,62,73	1.07	5 (8%)	68,99,113	1.14	3 (4%)
16	CLA	o	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.06	4 (4%)
16	CLA	G	1203	2	69,73,73	0.99	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	o	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.03	4 (6%)
16	CLA	s	517	12	59,63,73	1.10	5 (8%)	70,101,113	1.09	5 (7%)
16	CLA	w	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.14	6 (9%)
16	CLA	B	1232	-	49,53,73	1.18	5 (10%)	58,89,113	1.30	5 (8%)
16	CLA	q	515	12	69,73,73	0.99	5 (7%)	82,113,113	1.20	7 (8%)
16	CLA	b	1208	2	49,53,73	1.16	5 (10%)	58,89,113	1.19	6 (10%)
16	CLA	r	506	12	64,68,73	1.01	3 (4%)	76,107,113	1.07	7 (9%)
23	LMU	q	605	-	36,36,36	0.83	0	47,47,47	1.13	4 (8%)
16	CLA	a	1132	1	69,73,73	0.99	6 (8%)	82,113,113	1.20	5 (6%)
16	CLA	B	1220	2	57,61,73	1.11	4 (7%)	67,98,113	1.11	6 (8%)
16	CLA	p	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.11	6 (7%)
16	CLA	r	508	12	59,63,73	1.08	4 (6%)	70,101,113	1.01	3 (4%)
16	CLA	A	1137	1	51,55,73	1.14	4 (7%)	60,91,113	1.09	6 (10%)
16	CLA	B	1229	2	62,66,73	1.06	4 (6%)	73,104,113	1.05	5 (6%)
16	CLA	H	1130	1	64,68,73	1.03	5 (7%)	76,107,113	1.01	7 (9%)
16	CLA	s	511	12	69,73,73	0.98	5 (7%)	82,113,113	1.01	4 (4%)
16	CLA	v	511	12	69,73,73	0.99	4 (5%)	82,113,113	1.08	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	y	514	-	54,58,73	1.13	6 (11%)	64,95,113	1.13	6 (9%)
16	CLA	t	513	-	50,54,73	1.17	5 (10%)	59,90,113	1.15	6 (10%)
16	CLA	g	514	-	54,58,73	1.13	6 (11%)	64,95,113	1.08	5 (7%)
16	CLA	H	1126	1	69,73,73	0.99	4 (5%)	82,113,113	1.12	5 (6%)
16	CLA	G	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.14	4 (4%)
16	CLA	v	508	12	59,63,73	1.07	5 (8%)	70,101,113	1.31	7 (10%)
16	CLA	q	501	12	54,58,73	1.13	5 (9%)	64,95,113	1.19	6 (9%)
16	CLA	w	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.06	5 (7%)
13	LHG	o	605	-	26,26,48	0.85	0	29,32,54	1.27	2 (6%)
16	CLA	B	1207	2	69,73,73	0.99	5 (7%)	82,113,113	1.18	6 (7%)
16	CLA	X	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.04	3 (4%)
16	CLA	h	502	12	54,58,73	1.13	5 (9%)	64,95,113	1.05	5 (7%)
16	CLA	u	510	-	64,68,73	1.04	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	G	1238	25	69,73,73	0.98	4 (5%)	82,113,113	1.04	6 (7%)
16	CLA	a	1104	1	69,73,73	1.00	6 (8%)	82,113,113	1.03	4 (4%)
16	CLA	t	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.28	5 (8%)
16	CLA	A	1106	1	69,73,73	0.98	4 (5%)	82,113,113	1.12	4 (4%)
16	CLA	x	507	12	69,73,73	1.00	5 (7%)	82,113,113	1.07	6 (7%)
19	BCR	p	603	-	41,41,41	0.86	0	56,56,56	1.21	5 (8%)
19	BCR	L	4019	-	41,41,41	0.90	0	56,56,56	1.41	6 (10%)
16	CLA	Z	504	12	69,73,73	1.01	6 (8%)	82,113,113	1.09	6 (7%)
16	CLA	q	504	12	69,73,73	1.02	5 (7%)	82,113,113	1.11	4 (4%)
16	CLA	o	509	12	64,68,73	1.03	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	a	1134	1	49,53,73	1.16	4 (8%)	58,89,113	1.16	4 (6%)
16	CLA	W	513	-	50,54,73	1.16	5 (10%)	59,90,113	1.14	6 (10%)
16	CLA	G	1226	2	64,68,73	1.04	6 (9%)	76,107,113	1.10	5 (6%)
16	CLA	x	502	12	54,58,73	1.13	6 (11%)	64,95,113	1.12	3 (4%)
16	CLA	y	513	-	50,54,73	1.16	4 (8%)	59,90,113	1.01	3 (5%)
16	CLA	H	1110	1	58,62,73	1.05	4 (6%)	68,99,113	1.03	4 (5%)
19	BCR	A	4002	-	41,41,41	0.84	0	56,56,56	1.15	3 (5%)
19	BCR	r	604	-	41,41,41	0.89	0	56,56,56	1.27	6 (10%)
16	CLA	n	506	12	64,68,73	1.03	4 (6%)	76,107,113	1.08	5 (6%)
16	CLA	s	504	12	69,73,73	0.99	4 (5%)	82,113,113	0.95	3 (3%)
19	BCR	o	602	-	41,41,41	0.88	0	56,56,56	1.37	7 (12%)
16	CLA	a	1013	-	69,73,73	0.99	6 (8%)	82,113,113	1.17	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	Y	510	-	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	H	1116	1	58,62,73	1.05	5 (8%)	68,99,113	1.08	5 (7%)
16	CLA	Y	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.04	5 (7%)
16	CLA	Z	503	12	50,54,73	1.15	6 (12%)	59,90,113	1.19	6 (10%)
16	CLA	H	1118	1	59,63,73	1.07	4 (6%)	70,101,113	1.07	7 (10%)
16	CLA	g	512	12	69,73,73	1.00	5 (7%)	82,113,113	1.17	4 (4%)
16	CLA	A	1128	1	69,73,73	0.98	5 (7%)	82,113,113	1.08	4 (4%)
16	CLA	b	1023	-	69,73,73	1.01	7 (10%)	82,113,113	1.12	5 (6%)
16	CLA	G	1216	25	51,55,73	1.13	5 (9%)	60,91,113	1.33	4 (6%)
13	LHG	x	605	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
16	CLA	p	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.18	5 (6%)
16	CLA	o	505	12	69,73,73	0.99	4 (5%)	82,113,113	1.09	4 (4%)
16	CLA	B	1216	25	51,55,73	1.17	6 (11%)	60,91,113	1.15	4 (6%)
16	CLA	s	503	-	50,54,73	1.16	6 (12%)	59,90,113	1.25	5 (8%)
19	BCR	g	601	-	41,41,41	0.88	0	56,56,56	1.44	9 (16%)
16	CLA	q	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.13	6 (7%)
19	BCR	u	603	-	41,41,41	0.88	0	56,56,56	1.35	8 (14%)
16	CLA	Z	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.11	5 (7%)
16	CLA	b	1239	2	69,73,73	0.97	3 (4%)	82,113,113	1.07	7 (8%)
19	BCR	A	4003	-	41,41,41	0.85	0	56,56,56	1.29	7 (12%)
16	CLA	a	1109	16,1	69,73,73	0.98	4 (5%)	82,113,113	1.16	6 (7%)
16	CLA	G	1234	2	54,58,73	1.13	6 (11%)	64,95,113	1.16	4 (6%)
21	ECH	I	4020	-	42,42,42	0.88	1 (2%)	55,58,58	1.90	14 (25%)
19	BCR	U	4022	-	41,41,41	0.88	0	56,56,56	1.32	6 (10%)
19	BCR	A	4011	-	41,41,41	0.88	0	56,56,56	1.29	4 (7%)
16	CLA	Q	1302	6	50,54,73	1.16	5 (10%)	59,90,113	1.07	4 (6%)
16	CLA	n	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.08	4 (4%)
16	CLA	B	1238	25	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
19	BCR	G	4010	-	41,41,41	0.94	0	56,56,56	1.39	9 (16%)
16	CLA	n	508	12	59,63,73	1.07	5 (8%)	70,101,113	0.99	2 (2%)
14	LMG	a	4101	-	46,46,55	0.90	2 (4%)	54,54,63	1.22	4 (7%)
16	CLA	g	502	12	54,58,73	1.10	5 (9%)	64,95,113	1.07	2 (3%)
16	CLA	S	1303	8	41,45,73	1.25	5 (12%)	50,78,113	1.03	2 (4%)
16	CLA	x	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.18	5 (8%)
16	CLA	h	515	12	69,73,73	1.01	4 (5%)	82,113,113	1.24	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	n	516	-	50,54,73	1.17	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	B	1230	2	49,53,73	1.18	4 (8%)	58,89,113	1.11	4 (6%)
15	CL0	A	1011	1	69,73,73	1.01	6 (8%)	82,113,113	1.03	5 (6%)
16	CLA	u	504	12	64,68,73	1.06	6 (9%)	76,107,113	1.05	4 (5%)
19	BCR	x	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	a	1125	1	69,73,73	0.97	5 (7%)	82,113,113	1.06	3 (3%)
16	CLA	n	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.03	4 (4%)
16	CLA	b	1240	13	50,54,73	1.15	4 (8%)	59,90,113	1.16	2 (3%)
24	LUT	q	601	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
16	CLA	v	505	12	69,73,73	1.02	5 (7%)	82,113,113	1.24	5 (6%)
14	LMG	a	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	B	1202	-	69,73,73	0.99	4 (5%)	82,113,113	0.92	2 (2%)
16	CLA	J	1303	8	41,45,73	1.24	5 (12%)	50,78,113	1.07	3 (6%)
16	CLA	q	510	-	64,68,73	1.03	4 (6%)	76,107,113	0.96	3 (3%)
16	CLA	b	1215	2	64,68,73	1.00	4 (6%)	76,107,113	1.15	3 (3%)
19	BCR	Y	603	-	41,41,41	0.85	0	56,56,56	1.16	4 (7%)
19	BCR	j	4015	-	41,41,41	0.88	0	56,56,56	1.22	7 (12%)
16	CLA	A	1118	1	59,63,73	1.06	4 (6%)	70,101,113	1.00	3 (4%)
16	CLA	W	512	12	64,68,73	1.04	6 (9%)	76,107,113	1.08	4 (5%)
16	CLA	B	1231	25	49,53,73	1.19	4 (8%)	58,89,113	1.16	4 (6%)
16	CLA	n	517	12	59,63,73	1.08	5 (8%)	70,101,113	1.02	3 (4%)
16	CLA	H	1013	-	69,73,73	1.01	7 (10%)	82,113,113	1.20	9 (10%)
16	CLA	G	1021	2	69,73,73	0.99	5 (7%)	82,113,113	1.16	5 (6%)
21	ECH	b	4006	-	42,42,42	0.85	2 (4%)	55,58,58	1.52	8 (14%)
16	CLA	u	509	12	64,68,73	1.03	5 (7%)	76,107,113	1.07	6 (7%)
21	ECH	B	4006	-	42,42,42	0.74	0	55,58,58	1.53	11 (20%)
16	CLA	A	1115	1	58,62,73	1.06	6 (10%)	68,99,113	1.17	3 (4%)
16	CLA	r	511	12	69,73,73	1.01	5 (7%)	82,113,113	0.89	2 (2%)
19	BCR	H	4003	-	41,41,41	0.86	0	56,56,56	1.22	4 (7%)
13	LHG	p	605	-	31,31,48	0.77	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	B	1217	2	49,53,73	1.18	4 (8%)	58,89,113	1.11	3 (5%)
16	CLA	p	503	-	50,54,73	1.14	6 (12%)	59,90,113	1.17	6 (10%)
19	BCR	g	604	-	41,41,41	0.88	0	56,56,56	1.28	6 (10%)
16	CLA	u	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.05	6 (7%)
19	BCR	j	4013	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	a	1110	1	58,62,73	1.04	4 (6%)	68,99,113	1.01	2 (2%)
16	CLA	k	4003	9	49,53,73	1.20	4 (8%)	58,89,113	1.14	3 (5%)
16	CLA	b	1231	25	49,53,73	1.18	4 (8%)	58,89,113	1.21	4 (6%)
19	BCR	n	604	-	41,41,41	0.86	0	56,56,56	1.33	7 (12%)
19	BCR	Y	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	A	1132	1	69,73,73	0.99	6 (8%)	82,113,113	1.14	6 (7%)
13	LHG	H	851	16	25,25,48	0.88	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	G	1227	2	53,57,73	1.12	6 (11%)	61,93,113	1.15	5 (8%)
16	CLA	B	1211	2	69,73,73	0.98	6 (8%)	82,113,113	1.02	5 (6%)
16	CLA	p	506	12	64,68,73	1.01	4 (6%)	76,107,113	1.12	5 (6%)
16	CLA	s	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.04	4 (5%)
16	CLA	G	1219	-	49,53,73	1.21	5 (10%)	58,89,113	1.14	5 (8%)
16	CLA	H	1105	-	62,66,73	1.05	5 (8%)	73,104,113	1.08	5 (6%)
16	CLA	b	1021	2	69,73,73	1.00	5 (7%)	82,113,113	1.12	6 (7%)
16	CLA	r	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	n	513	-	50,54,73	1.16	5 (10%)	59,90,113	1.05	4 (6%)
16	CLA	B	1222	25	54,58,73	1.13	5 (9%)	64,95,113	1.10	5 (7%)
16	CLA	Y	517	12	59,63,73	1.08	4 (6%)	70,101,113	1.05	3 (4%)
16	CLA	x	510	-	69,73,73	0.99	5 (7%)	82,113,113	1.05	4 (4%)
16	CLA	w	510	-	64,68,73	1.04	3 (4%)	76,107,113	0.98	2 (2%)
15	CL0	a	1011	1	69,73,73	1.00	6 (8%)	82,113,113	0.98	5 (6%)
16	CLA	H	1139	25	64,68,73	1.03	5 (7%)	76,107,113	1.01	4 (5%)
16	CLA	l	1501	10	64,68,73	1.03	5 (7%)	76,107,113	0.99	4 (5%)
19	BCR	R	4018	-	41,41,41	0.85	0	56,56,56	1.20	7 (12%)
19	BCR	S	4013	-	41,41,41	0.87	0	56,56,56	1.32	7 (12%)
16	CLA	H	1237	25	69,73,73	0.99	5 (7%)	82,113,113	1.08	6 (7%)
20	LMT	U	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
19	BCR	x	604	-	41,41,41	0.88	0	56,56,56	1.29	6 (10%)
16	CLA	q	516	-	50,54,73	1.14	5 (10%)	59,90,113	0.99	2 (3%)
16	CLA	v	513	-	50,54,73	1.17	4 (8%)	59,90,113	1.01	3 (5%)
16	CLA	q	506	-	64,68,73	1.03	4 (6%)	76,107,113	1.05	4 (5%)
16	CLA	r	504	12	69,73,73	1.01	4 (5%)	82,113,113	0.99	3 (3%)
14	LMG	a	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.24	4 (8%)
16	CLA	H	1125	1	69,73,73	0.98	4 (5%)	82,113,113	0.99	2 (2%)
16	CLA	A	1134	1	49,53,73	1.19	5 (10%)	58,89,113	1.09	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	G	1207	2	69,73,73	1.00	4 (5%)	82,113,113	1.15	5 (6%)
16	CLA	n	505	12	69,73,73	1.00	6 (8%)	82,113,113	1.22	6 (7%)
13	LHG	R	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.24	4 (9%)
16	CLA	B	1205	2	69,73,73	0.99	4 (5%)	82,113,113	1.06	3 (3%)
16	CLA	s	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.15	7 (8%)
14	LMG	A	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.18	3 (7%)
16	CLA	A	1101	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	7 (8%)
16	CLA	B	1201	2	58,62,73	1.07	4 (6%)	68,99,113	1.04	4 (5%)
16	CLA	A	1013	-	69,73,73	0.99	6 (8%)	82,113,113	1.20	10 (12%)
16	CLA	v	512	12	69,73,73	1.02	4 (5%)	82,113,113	1.08	7 (8%)
19	BCR	p	604	-	41,41,41	0.87	0	56,56,56	1.23	6 (10%)
16	CLA	W	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.22	5 (8%)
16	CLA	a	1138	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	7 (8%)
16	CLA	A	1140	1	69,73,73	0.98	5 (7%)	82,113,113	1.12	5 (6%)
16	CLA	t	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	K	4004	-	59,63,73	1.07	4 (6%)	70,101,113	1.10	4 (5%)
16	CLA	H	1119	25	69,73,73	0.98	5 (7%)	82,113,113	1.02	4 (4%)
16	CLA	p	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	s	516	-	50,54,73	1.15	4 (8%)	59,90,113	1.06	3 (5%)
19	BCR	h	604	-	41,41,41	0.86	0	56,56,56	1.25	6 (10%)
16	CLA	u	502	12	54,58,73	1.12	6 (11%)	64,95,113	1.12	3 (4%)
16	CLA	Y	501	12	54,58,73	1.10	4 (7%)	64,95,113	1.20	7 (10%)
13	LHG	X	605	-	26,26,48	0.82	0	29,32,54	1.27	2 (6%)
13	LHG	a	851	16	25,25,48	0.88	2 (8%)	28,31,54	1.26	2 (7%)
13	LHG	A	851	16	25,25,48	0.87	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	H	1121	1	55,59,73	1.12	5 (9%)	64,96,113	1.14	4 (6%)
16	CLA	X	512	12	69,73,73	0.99	5 (7%)	82,113,113	1.00	5 (6%)
16	CLA	G	1239	2	69,73,73	0.96	3 (4%)	82,113,113	1.14	6 (7%)
16	CLA	a	1140	1	69,73,73	0.97	5 (7%)	82,113,113	1.11	5 (6%)
19	BCR	U	4019	-	41,41,41	0.86	0	56,56,56	1.49	8 (14%)
16	CLA	Z	511	12	69,73,73	0.99	5 (7%)	82,113,113	1.08	4 (4%)
16	CLA	A	1105	-	62,66,73	1.06	5 (8%)	73,104,113	1.00	4 (5%)
16	CLA	A	1109	16,1	69,73,73	0.98	5 (7%)	82,113,113	1.13	5 (6%)
16	CLA	x	506	12	64,68,73	1.02	6 (9%)	76,107,113	1.12	4 (5%)
16	CLA	b	1204	2	69,73,73	0.97	4 (5%)	82,113,113	0.98	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	n	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.24	5 (8%)
16	CLA	X	506	-	64,68,73	1.02	4 (6%)	76,107,113	1.24	4 (5%)
16	CLA	a	1123	-	69,73,73	1.00	4 (5%)	82,113,113	1.01	4 (4%)
13	LHG	u	605	-	26,26,48	0.83	0	29,32,54	1.27	2 (6%)
16	CLA	x	505	12	69,73,73	0.99	5 (7%)	82,113,113	1.23	6 (7%)
16	CLA	b	1012	25	59,63,73	1.13	4 (6%)	70,101,113	1.20	8 (11%)
16	CLA	B	1012	25	59,63,73	1.12	4 (6%)	70,101,113	1.11	6 (8%)
16	CLA	W	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.96	3 (4%)
16	CLA	H	1102	16,1	60,64,73	1.05	4 (6%)	71,102,113	0.94	2 (2%)
16	CLA	a	1129	1	50,54,73	1.11	5 (10%)	59,90,113	1.13	5 (8%)
16	CLA	q	503	12	50,54,73	1.15	6 (12%)	59,90,113	1.26	5 (8%)
16	CLA	B	1208	2	49,53,73	1.16	4 (8%)	58,89,113	1.16	6 (10%)
16	CLA	h	511	12	69,73,73	1.00	6 (8%)	82,113,113	1.08	8 (9%)
16	CLA	o	514	-	54,58,73	1.12	6 (11%)	64,95,113	1.35	4 (6%)
19	BCR	r	601	-	41,41,41	0.86	1 (2%)	56,56,56	1.28	7 (12%)
16	CLA	A	1120	1	53,57,73	1.10	4 (7%)	61,93,113	1.12	5 (8%)
19	BCR	G	4014	-	41,41,41	0.90	1 (2%)	56,56,56	1.29	8 (14%)
16	CLA	g	510	-	69,73,73	0.99	5 (7%)	82,113,113	1.11	5 (6%)
16	CLA	h	513	-	50,54,73	1.17	4 (8%)	59,90,113	0.99	4 (6%)
16	CLA	A	1125	1	69,73,73	0.98	4 (5%)	82,113,113	0.97	3 (3%)
16	CLA	H	1114	-	50,54,73	1.13	5 (10%)	59,90,113	1.27	7 (11%)
16	CLA	b	1235	2	66,70,73	1.04	6 (9%)	78,109,113	1.15	8 (10%)
16	CLA	l	1503	-	69,73,73	1.00	4 (5%)	82,113,113	0.91	4 (4%)
16	CLA	X	504	12	64,68,73	1.06	6 (9%)	76,107,113	1.16	3 (3%)
16	CLA	G	1204	2	69,73,73	0.98	4 (5%)	82,113,113	0.98	3 (3%)
14	LMG	H	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	r	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.11	5 (7%)
16	CLA	Y	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.06	6 (7%)
16	CLA	u	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.03	4 (5%)
16	CLA	f	1301	25	49,53,73	1.17	4 (8%)	58,89,113	1.06	4 (6%)
24	LUT	Z	601	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	6 (11%)
14	LMG	G	848	-	43,43,55	0.86	0	51,51,63	1.27	7 (13%)
16	CLA	H	1117	1	69,73,73	0.99	5 (7%)	82,113,113	1.15	6 (7%)
16	CLA	G	1223	2	69,73,73	0.98	4 (5%)	82,113,113	1.09	4 (4%)
16	CLA	a	1111	1	59,63,73	1.09	5 (8%)	70,101,113	1.03	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	u	516	12	50,54,73	1.14	5 (10%)	59,90,113	1.15	4 (6%)
16	CLA	W	510	-	69,73,73	1.01	3 (4%)	82,113,113	1.01	5 (6%)
16	CLA	x	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.14	6 (7%)
16	CLA	B	1210	2	69,73,73	1.01	5 (7%)	82,113,113	1.09	6 (7%)
16	CLA	T	4003	9	49,53,73	1.18	4 (8%)	58,89,113	1.05	3 (5%)
16	CLA	G	1230	2	49,53,73	1.17	4 (8%)	58,89,113	1.03	2 (3%)
19	BCR	w	603	-	41,41,41	0.85	0	56,56,56	1.17	6 (10%)
16	CLA	G	1201	2	58,62,73	1.08	4 (6%)	68,99,113	1.05	4 (5%)
16	CLA	r	507	12	69,73,73	1.00	5 (7%)	82,113,113	0.95	3 (3%)
19	BCR	b	4014	-	41,41,41	0.91	0	56,56,56	1.45	8 (14%)
16	CLA	a	1119	-	69,73,73	1.00	5 (7%)	82,113,113	0.98	4 (4%)
16	CLA	B	1023	-	69,73,73	1.01	7 (10%)	82,113,113	1.12	5 (6%)
16	CLA	G	1228	2	59,63,73	1.07	4 (6%)	70,101,113	1.09	5 (7%)
16	CLA	G	1217	2	49,53,73	1.17	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	H	1106	1	69,73,73	0.96	4 (5%)	82,113,113	1.11	4 (4%)
16	CLA	n	504	12	64,68,73	1.04	4 (6%)	76,107,113	1.10	4 (5%)
16	CLA	o	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.07	6 (7%)
16	CLA	G	1202	2	69,73,73	0.96	4 (5%)	82,113,113	0.99	5 (6%)
23	LMU	r	606	-	36,36,36	0.87	0	47,47,47	1.10	2 (4%)
19	BCR	H	4011	-	41,41,41	0.88	0	56,56,56	1.26	6 (10%)
19	BCR	J	4013	-	41,41,41	0.86	0	56,56,56	1.23	8 (14%)
16	CLA	H	1109	16,1	69,73,73	0.98	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	b	1210	2	69,73,73	1.02	5 (7%)	82,113,113	1.05	6 (7%)
16	CLA	Y	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.06	7 (8%)
16	CLA	X	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.16	4 (6%)
16	CLA	r	502	12	54,58,73	1.11	5 (9%)	64,95,113	1.07	3 (4%)
16	CLA	G	1221	25	69,73,73	1.00	4 (5%)	82,113,113	1.07	3 (3%)
16	CLA	X	507	12	69,73,73	1.00	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	y	508	12	59,63,73	1.08	4 (6%)	70,101,113	1.20	6 (8%)
16	CLA	w	515	12	69,73,73	0.99	5 (7%)	82,113,113	1.12	4 (4%)
16	CLA	b	1230	2	49,53,73	1.18	5 (10%)	58,89,113	1.15	4 (6%)
16	CLA	a	1108	1	49,53,73	1.17	5 (10%)	58,89,113	1.25	5 (8%)
16	CLA	x	514	-	54,58,73	1.11	5 (9%)	64,95,113	1.10	5 (7%)
18	SF4	C	101	-	0,12,12	-	-	-		
23	LMU	s	606	-	36,36,36	0.83	0	47,47,47	1.27	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	Y	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.18	8 (9%)
17	PQN	G	2002	-	34,34,34	0.38	0	43,45,45	1.04	2 (4%)
16	CLA	v	504	12	64,68,73	1.04	5 (7%)	76,107,113	1.09	6 (7%)
14	LMG	F	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	o	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.10	4 (6%)
19	BCR	p	602	-	41,41,41	0.87	0	56,56,56	1.31	7 (12%)
16	CLA	H	1133	1	58,62,73	1.08	6 (10%)	68,99,113	1.28	6 (8%)
16	CLA	H	1120	1	53,57,73	1.09	4 (7%)	61,93,113	1.18	5 (8%)
16	CLA	B	1236	2	54,58,73	1.11	6 (11%)	64,95,113	1.14	4 (6%)
16	CLA	g	506	12	64,68,73	1.01	4 (6%)	76,107,113	1.01	5 (6%)
16	CLA	a	1116	1	58,62,73	1.07	5 (8%)	68,99,113	1.02	4 (5%)
16	CLA	B	1213	2	59,63,73	1.07	6 (10%)	70,101,113	1.08	4 (5%)
13	LHG	r	605	-	30,30,48	0.81	2 (6%)	33,36,54	1.28	3 (9%)
16	CLA	H	1123	-	69,73,73	1.00	4 (5%)	82,113,113	0.96	3 (3%)
16	CLA	Y	516	-	50,54,73	1.13	4 (8%)	59,90,113	1.11	4 (6%)
16	CLA	n	502	12	54,58,73	1.12	6 (11%)	64,95,113	1.13	3 (4%)
19	BCR	u	604	-	41,41,41	0.89	0	56,56,56	1.35	10 (17%)
16	CLA	Y	506	12	64,68,73	1.01	4 (6%)	76,107,113	1.12	5 (6%)
16	CLA	w	504	12	69,73,73	1.01	5 (7%)	82,113,113	1.02	5 (6%)
16	CLA	q	505	-	69,73,73	0.99	6 (8%)	82,113,113	1.16	8 (9%)
13	LHG	a	849	-	42,42,48	0.71	1 (2%)	45,48,54	1.22	4 (8%)
19	BCR	B	4017	-	41,41,41	0.88	0	56,56,56	1.22	6 (10%)
16	CLA	k	4002	9	49,53,73	1.17	4 (8%)	58,89,113	1.12	4 (6%)
16	CLA	H	1140	1	69,73,73	0.97	5 (7%)	82,113,113	1.07	3 (3%)
16	CLA	y	510	-	69,73,73	1.01	4 (5%)	82,113,113	0.95	5 (6%)
19	BCR	s	603	-	41,41,41	0.86	0	56,56,56	1.18	6 (10%)
16	CLA	h	503	-	50,54,73	1.18	5 (10%)	59,90,113	1.26	6 (10%)
16	CLA	a	1022	-	69,73,73	1.01	5 (7%)	82,113,113	1.04	6 (7%)
16	CLA	T	4004	-	59,63,73	1.07	4 (6%)	70,101,113	1.13	4 (5%)
16	CLA	a	1117	1	69,73,73	0.98	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	H	1113	1	49,53,73	1.20	6 (12%)	58,89,113	1.18	3 (5%)
16	CLA	H	1128	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	5 (6%)
16	CLA	n	501	12	54,58,73	1.12	4 (7%)	64,95,113	1.21	7 (10%)
16	CLA	b	1229	2	62,66,73	1.06	4 (6%)	73,104,113	1.04	5 (6%)
18	SF4	a	3001	-	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	n	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	p	513	-	50,54,73	1.14	5 (10%)	59,90,113	1.04	4 (6%)
19	BCR	B	4005	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
19	BCR	W	604	-	41,41,41	0.86	0	56,56,56	1.37	9 (16%)
16	CLA	t	511	12	69,73,73	1.00	4 (5%)	82,113,113	1.04	5 (6%)
16	CLA	r	516	-	50,54,73	1.15	5 (10%)	59,90,113	1.13	4 (6%)
19	BCR	j	4012	-	41,41,41	0.88	0	56,56,56	1.29	7 (12%)
16	CLA	q	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.03	3 (3%)
13	LHG	B	4018	16	37,37,48	0.72	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	v	501	12	50,54,73	1.17	5 (10%)	59,90,113	1.26	7 (11%)
16	CLA	a	1122	1	63,67,73	1.04	5 (7%)	74,105,113	1.10	4 (5%)
16	CLA	A	1122	1	63,67,73	1.05	5 (7%)	74,105,113	1.09	6 (8%)
16	CLA	u	505	12	69,73,73	0.99	4 (5%)	82,113,113	1.08	5 (6%)
16	CLA	r	509	12	69,73,73	1.01	5 (7%)	82,113,113	1.03	5 (6%)
18	SF4	C	102	-	0,12,12	-	-	-		
16	CLA	B	1240	13	50,54,73	1.18	5 (10%)	59,90,113	1.21	4 (6%)
13	LHG	I	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.23	4 (9%)
16	CLA	a	1133	1	58,62,73	1.09	5 (8%)	68,99,113	1.10	5 (7%)
16	CLA	B	1214	2	59,63,73	1.06	4 (6%)	70,101,113	1.19	4 (5%)
16	CLA	w	507	12	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	A	1139	25	64,68,73	1.03	5 (7%)	76,107,113	1.03	4 (5%)
16	CLA	b	1236	2	54,58,73	1.12	5 (9%)	64,95,113	1.14	6 (9%)
16	CLA	B	1218	-	59,63,73	1.07	4 (6%)	70,101,113	1.15	5 (7%)
19	BCR	Y	604	-	41,41,41	0.86	0	56,56,56	1.16	6 (10%)
16	CLA	t	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.15	5 (6%)
15	CL0	H	1011	1	69,73,73	1.01	6 (8%)	82,113,113	1.04	5 (6%)
16	CLA	W	511	12	69,73,73	1.01	5 (7%)	82,113,113	1.09	6 (7%)
16	CLA	b	1228	2	59,63,73	1.07	4 (6%)	70,101,113	1.07	5 (7%)
16	CLA	G	1232	25	49,53,73	1.19	5 (10%)	58,89,113	1.29	6 (10%)
16	CLA	H	1134	1	49,53,73	1.18	4 (8%)	58,89,113	1.09	2 (3%)
16	CLA	Z	509	12	69,73,73	1.00	5 (7%)	82,113,113	1.01	4 (4%)
16	CLA	x	508	12	59,63,73	1.08	4 (6%)	70,101,113	0.99	3 (4%)
16	CLA	r	517	12	59,63,73	1.09	4 (6%)	70,101,113	1.01	3 (4%)
16	CLA	H	1108	1	49,53,73	1.17	5 (10%)	58,89,113	1.24	4 (6%)
16	CLA	A	1123	25	69,73,73	0.99	4 (5%)	82,113,113	1.07	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	G	1229	2	62,66,73	1.05	4 (6%)	73,104,113	1.03	4 (5%)
16	CLA	p	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.16	6 (9%)
16	CLA	A	1129	1	50,54,73	1.12	4 (8%)	59,90,113	1.15	5 (8%)
16	CLA	g	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.98	3 (4%)
16	CLA	H	1101	1	69,73,73	0.98	4 (5%)	82,113,113	1.04	3 (3%)
19	BCR	y	604	-	41,41,41	0.87	0	56,56,56	1.29	7 (12%)
20	LMT	a	4202	-	36,36,36	1.17	5 (13%)	47,47,47	0.93	0
16	CLA	g	504	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	6 (7%)
16	CLA	y	515	12	69,73,73	1.01	4 (5%)	82,113,113	1.14	8 (9%)
16	CLA	A	1138	1	69,73,73	0.99	4 (5%)	82,113,113	0.98	4 (4%)
13	LHG	H	849	-	42,42,48	0.68	0	45,48,54	1.21	4 (8%)
16	CLA	r	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.20	4 (4%)
16	CLA	H	1124	-	64,68,73	1.02	5 (7%)	76,107,113	0.98	3 (3%)
19	BCR	u	602	-	41,41,41	0.88	0	56,56,56	1.36	6 (10%)
16	CLA	Y	502	12	54,58,73	1.11	4 (7%)	64,95,113	1.03	4 (6%)
19	BCR	S	4015	-	41,41,41	0.87	0	56,56,56	1.20	8 (14%)
16	CLA	x	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.16	4 (6%)
13	LHG	g	605	-	30,30,48	0.80	2 (6%)	33,36,54	1.26	3 (9%)
16	CLA	p	510	-	69,73,73	1.01	4 (5%)	82,113,113	1.01	3 (3%)
16	CLA	h	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.15	6 (8%)
16	CLA	H	1122	1	63,67,73	1.06	5 (7%)	74,105,113	1.09	6 (8%)
19	BCR	b	4010	-	41,41,41	0.91	0	56,56,56	1.33	7 (12%)
16	CLA	W	504	12	64,68,73	1.05	5 (7%)	76,107,113	1.01	3 (3%)
16	CLA	b	1220	2	58,62,73	1.10	6 (10%)	68,99,113	1.11	5 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1132	1	-	16/39/115/115	-
16	CLA	b	1207	2	-	14/39/115/115	-
16	CLA	p	502	12	-	5/21/97/115	-
16	CLA	y	511	12	-	11/39/115/115	-
16	CLA	w	502	12	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Y	513	-	-	10/17/93/115	-
16	CLA	g	501	12	-	8/21/97/115	-
16	CLA	h	512	12	-	16/39/115/115	-
16	CLA	r	505	12	-	13/39/115/115	-
16	CLA	u	514	-	-	6/21/97/115	-
16	CLA	Z	516	-	-	11/17/93/115	-
16	CLA	H	1103	-	-	12/39/115/115	-
19	BCR	w	602	-	-	11/29/63/63	0/2/2/2
16	CLA	u	515	12	-	17/39/115/115	-
13	LHG	s	605	-	-	12/36/36/53	-
19	BCR	B	4014	-	-	16/29/63/63	0/2/2/2
16	CLA	g	507	12	-	9/39/115/115	-
16	CLA	b	1226	2	-	16/33/109/115	-
16	CLA	H	1022	25	-	10/39/115/115	-
23	LMU	p	606	-	-	9/21/61/61	0/2/2/2
16	CLA	B	1226	2	-	13/33/109/115	-
16	CLA	G	1220	2	-	15/26/102/115	-
16	CLA	A	1108	1	-	3/15/91/115	-
16	CLA	Y	503	-	-	7/17/93/115	-
16	CLA	a	1126	1	-	11/39/115/115	-
16	CLA	q	502	12	-	7/21/97/115	-
16	CLA	t	501	12	-	7/21/97/115	-
16	CLA	g	509	12	-	8/39/115/115	-
16	CLA	s	506	12	-	11/33/109/115	-
19	BCR	r	603	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1116	1	-	12/26/102/115	-
16	CLA	a	1136	1	-	11/39/115/115	-
16	CLA	b	1216	25	-	2/18/94/115	-
16	CLA	F	1302	6	-	8/17/93/115	-
19	BCR	K	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	p	508	12	-	10/27/103/115	-
16	CLA	a	1113	1	-	3/15/91/115	-
16	CLA	G	1211	2	-	22/39/115/115	-
16	CLA	w	506	-	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	a	1121	1	-	6/23/99/115	-
16	CLA	A	1124	25	-	7/33/109/115	-
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	v	514	-	-	7/21/97/115	-
19	BCR	F	4016	-	-	9/29/63/63	0/2/2/2
16	CLA	A	1102	16,1	-	6/29/105/115	-
16	CLA	y	504	12	-	12/33/109/115	-
16	CLA	X	510	-	-	8/33/109/115	-
19	BCR	T	4005	-	-	9/29/63/63	0/2/2/2
18	SF4	N	101	-	-	-	0/6/5/5
16	CLA	H	1801	13	-	5/17/93/115	-
14	LMG	Q	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	f	1302	6	-	8/17/93/115	-
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2
19	BCR	r	602	-	-	16/29/63/63	0/2/2/2
16	CLA	w	516	12	-	10/17/93/115	-
16	CLA	G	1236	2	-	7/21/97/115	-
19	BCR	W	601	-	-	16/29/63/63	0/2/2/2
16	CLA	a	1127	1	-	4/39/115/115	-
16	CLA	A	1127	1	-	5/39/115/115	-
16	CLA	G	1213	2	-	8/27/103/115	-
19	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1131	1	-	13/39/115/115	-
16	CLA	g	505	12	-	11/39/115/115	-
16	CLA	w	509	12	-	12/39/115/115	-
14	LMG	b	848	-	-	19/38/58/70	0/1/1/1
19	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
20	LMT	L	4101	-	-	9/21/61/61	0/2/2/2
16	CLA	a	1101	1	-	19/39/115/115	-
16	CLA	b	1227	2	-	6/20/96/115	-
16	CLA	u	501	12	-	6/17/93/115	-
19	BCR	u	601	-	-	8/29/63/63	0/2/2/2
19	BCR	s	604	-	-	16/29/63/63	0/2/2/2
16	CLA	B	1239	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	X	602	-	-	17/29/63/63	0/2/2/2
16	CLA	B	1209	2	-	7/15/91/115	-
16	CLA	h	509	12	-	18/39/115/115	-
16	CLA	L	1502	10	-	9/33/109/115	-
16	CLA	p	517	12	-	10/27/103/115	-
16	CLA	b	1212	2	-	4/15/91/115	-
21	ECH	M	4021	-	-	15/29/66/66	0/2/2/2
16	CLA	k	4004	-	-	6/27/103/115	-
16	CLA	g	516	-	-	5/17/93/115	-
19	BCR	G	4005	-	-	11/29/63/63	0/2/2/2
16	CLA	x	513	-	-	10/17/93/115	-
16	CLA	a	1137	1	-	6/18/94/115	-
16	CLA	X	517	12	-	7/27/103/115	-
16	CLA	n	515	12	-	15/39/115/115	-
16	CLA	A	1112	1	-	4/15/91/115	-
19	BCR	L	4022	-	-	14/29/63/63	0/2/2/2
16	CLA	b	1202	-	-	16/39/115/115	-
13	LHG	A	849	-	-	19/47/47/53	-
16	CLA	a	1801	13	-	7/17/93/115	-
16	CLA	A	1801	13	-	9/17/93/115	-
16	CLA	o	511	-	-	10/39/115/115	-
16	CLA	w	503	12	-	8/17/93/115	-
16	CLA	b	1221	25	-	19/39/115/115	-
16	CLA	A	1126	1	-	11/39/115/115	-
16	CLA	a	1105	-	-	7/31/107/115	-
16	CLA	o	513	-	-	5/17/93/115	-
21	ECH	i	4020	-	-	12/29/66/66	0/2/2/2
16	CLA	o	508	12	-	14/27/103/115	-
16	CLA	G	1206	2	-	12/39/115/115	-
16	CLA	J	1302	8	-	6/15/91/115	-
16	CLA	Y	514	-	-	7/21/97/115	-
19	BCR	B	4010	-	-	16/29/63/63	0/2/2/2
19	BCR	v	601	-	-	11/29/63/63	0/2/2/2
16	CLA	w	512	12	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1224	2	-	12/33/109/115	-
17	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
24	LUT	w	601	-	-	7/29/67/67	0/2/2/2
16	CLA	G	1012	25	-	7/27/103/115	-
19	BCR	S	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	W	515	12	-	16/39/115/115	-
19	BCR	k	4005	-	-	7/29/63/63	0/2/2/2
16	CLA	a	1130	1	-	10/33/109/115	-
16	CLA	H	1104	1	-	17/39/115/115	-
16	CLA	n	511	12	-	7/39/115/115	-
16	CLA	a	1237	25	-	13/39/115/115	-
19	BCR	Z	603	-	-	8/29/63/63	0/2/2/2
20	LMT	A	4202	-	-	7/21/61/61	0/2/2/2
16	CLA	b	1201	2	-	4/26/102/115	-
16	CLA	t	517	12	-	8/27/103/115	-
19	BCR	H	4002	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1208	2	-	8/15/91/115	-
16	CLA	B	1235	2	-	11/36/112/115	-
18	SF4	c	101	-	-	-	0/6/5/5
16	CLA	b	1211	2	-	13/39/115/115	-
16	CLA	B	1206	2	-	17/39/115/115	-
16	CLA	b	1234	2	-	4/21/97/115	-
16	CLA	B	1234	2	-	5/21/97/115	-
23	LMU	x	606	-	-	14/21/61/61	0/2/2/2
16	CLA	a	1118	1	-	11/27/103/115	-
16	CLA	w	505	-	-	9/39/115/115	-
19	BCR	t	604	-	-	14/29/63/63	0/2/2/2
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
16	CLA	a	1128	1	-	18/39/115/115	-
16	CLA	B	1221	25	-	15/39/115/115	-
16	CLA	B	1203	2	-	15/39/115/115	-
16	CLA	x	511	12	-	7/39/115/115	-
16	CLA	x	517	12	-	9/27/103/115	-
16	CLA	W	516	-	-	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	y	501	12	-	8/17/93/115	-
19	BCR	G	4017	-	-	13/29/63/63	0/2/2/2
16	CLA	b	1224	2	-	9/33/109/115	-
19	BCR	y	601	-	-	15/29/63/63	0/2/2/2
17	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
16	CLA	o	501	12	-	9/17/93/115	-
16	CLA	u	506	-	-	11/33/109/115	-
23	LMU	Z	605	-	-	5/21/61/61	0/2/2/2
16	CLA	U	1501	10	-	13/33/109/115	-
16	CLA	F	1301	25	-	3/15/91/115	-
16	CLA	r	510	-	-	12/39/115/115	-
14	LMG	A	852	-	-	10/33/53/70	0/1/1/1
16	CLA	h	514	-	-	6/21/97/115	-
16	CLA	b	1203	2	-	16/39/115/115	-
18	SF4	A	3001	-	-	-	0/6/5/5
19	BCR	Y	601	-	-	12/29/63/63	0/2/2/2
16	CLA	x	512	12	-	9/39/115/115	-
16	CLA	h	501	12	-	9/17/93/115	-
23	LMU	Y	606	-	-	6/21/61/61	0/2/2/2
16	CLA	t	507	12	-	11/39/115/115	-
16	CLA	A	1136	1	-	7/39/115/115	-
16	CLA	T	4002	9	-	7/15/91/115	-
16	CLA	h	504	-	-	14/33/109/115	-
16	CLA	a	1102	16,1	-	7/29/105/115	-
14	LMG	H	4101	-	-	23/41/61/70	0/1/1/1
16	CLA	G	1205	2	-	10/39/115/115	-
19	BCR	b	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	A	1104	1	-	19/39/115/115	-
16	CLA	B	1225	-	-	11/39/115/115	-
16	CLA	Z	513	-	-	8/21/97/115	-
16	CLA	A	1121	1	-	8/23/99/115	-
16	CLA	q	513	-	-	8/21/97/115	-
16	CLA	Z	508	12	-	9/27/103/115	-
16	CLA	x	501	-	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	x	601	-	-	11/29/63/63	0/2/2/2
16	CLA	o	512	12	-	8/39/115/115	-
16	CLA	t	514	-	-	8/21/97/115	-
16	CLA	b	1238	25	-	18/39/115/115	-
16	CLA	G	1218	-	-	14/27/103/115	-
19	BCR	g	603	-	-	15/29/63/63	0/2/2/2
14	LMG	f	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	B	1228	2	-	14/27/103/115	-
16	CLA	H	1115	1	-	10/26/102/115	-
16	CLA	b	1206	2	-	15/39/115/115	-
16	CLA	s	513	-	-	9/17/93/115	-
16	CLA	w	517	12	-	8/27/103/115	-
16	CLA	Z	507	12	-	15/39/115/115	-
16	CLA	Z	512	12	-	14/39/115/115	-
16	CLA	U	1502	10	-	9/33/109/115	-
16	CLA	A	1131	1	-	14/39/115/115	-
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
19	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
16	CLA	b	1205	2	-	12/39/115/115	-
16	CLA	g	511	12	-	9/39/115/115	-
16	CLA	y	507	12	-	13/39/115/115	-
16	CLA	W	506	12	-	11/33/109/115	-
16	CLA	s	507	12	-	11/39/115/115	-
16	CLA	v	507	12	-	9/39/115/115	-
16	CLA	H	1107	1	-	5/21/97/115	-
19	BCR	a	4003	-	-	12/29/63/63	0/2/2/2
14	LMG	H	852	-	-	6/33/53/70	0/1/1/1
16	CLA	Z	514	-	-	9/21/97/115	-
19	BCR	a	4011	-	-	16/29/63/63	0/2/2/2
19	BCR	h	601	-	-	14/29/63/63	0/2/2/2
21	ECH	m	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	H	1129	1	-	6/17/93/115	-
16	CLA	A	1117	1	-	7/39/115/115	-
16	CLA	A	1119	25	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	g	517	12	-	10/27/103/115	-
16	CLA	v	509	12	-	16/39/115/115	-
19	BCR	t	603	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1225	-	-	12/39/115/115	-
16	CLA	p	511	12	-	15/39/115/115	-
16	CLA	Z	501	12	-	7/21/97/115	-
16	CLA	s	508	12	-	10/27/103/115	-
16	CLA	W	505	12	-	20/39/115/115	-
16	CLA	X	516	12	-	8/17/93/115	-
16	CLA	s	514	-	-	7/21/97/115	-
16	CLA	G	1222	25	-	8/21/97/115	-
16	CLA	B	1224	2	-	10/33/109/115	-
16	CLA	G	1209	2	-	5/15/91/115	-
16	CLA	p	509	12	-	20/33/109/115	-
19	BCR	b	4017	-	-	12/29/63/63	0/2/2/2
16	CLA	X	511	-	-	10/39/115/115	-
16	CLA	a	1124	25	-	7/33/109/115	-
16	CLA	X	509	12	-	13/33/109/115	-
16	CLA	b	1217	2	-	3/15/91/115	-
16	CLA	G	1214	2	-	13/27/103/115	-
16	CLA	o	516	12	-	11/17/93/115	-
19	BCR	H	4008	-	-	13/29/63/63	0/2/2/2
16	CLA	g	515	12	-	9/39/115/115	-
16	CLA	s	501	12	-	9/21/97/115	-
16	CLA	L	1503	25	-	11/39/115/115	-
16	CLA	G	1215	2	-	8/33/109/115	-
16	CLA	W	509	12	-	5/33/109/115	-
16	CLA	X	508	12	-	15/27/103/115	-
16	CLA	p	514	-	-	8/21/97/115	-
16	CLA	w	514	-	-	8/21/97/115	-
16	CLA	a	1135	1	-	3/23/99/115	-
16	CLA	y	509	12	-	19/39/115/115	-
16	CLA	p	515	12	-	14/39/115/115	-
16	CLA	t	505	12	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1210	2	-	16/39/115/115	-
16	CLA	B	1212	2	-	6/15/91/115	-
19	BCR	W	603	-	-	13/29/63/63	0/2/2/2
16	CLA	A	1130	1	-	10/33/109/115	-
16	CLA	B	1215	2	-	7/33/109/115	-
16	CLA	j	1302	8	-	7/15/91/115	-
19	BCR	y	603	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1222	25	-	8/21/97/115	-
16	CLA	u	513	-	-	7/17/93/115	-
19	BCR	o	604	-	-	18/29/63/63	0/2/2/2
16	CLA	v	506	-	-	5/33/109/115	-
16	CLA	g	503	-	-	9/17/93/115	-
16	CLA	h	506	12	-	11/33/109/115	-
16	CLA	n	514	-	-	7/21/97/115	-
19	BCR	p	601	-	-	9/29/63/63	0/2/2/2
19	BCR	G	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	v	510	-	-	6/39/115/115	-
16	CLA	p	504	12	-	16/39/115/115	-
19	BCR	Z	602	-	-	11/29/63/63	0/2/2/2
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	K	4002	9	-	4/15/91/115	-
16	CLA	u	511	-	-	8/39/115/115	-
16	CLA	Z	505	-	-	14/39/115/115	-
16	CLA	X	501	12	-	9/17/93/115	-
16	CLA	b	1218	-	-	9/27/103/115	-
16	CLA	a	1107	1	-	8/21/97/115	-
16	CLA	j	1303	8	-	2/4/76/115	-
16	CLA	s	512	12	-	8/39/115/115	-
19	BCR	X	604	-	-	19/29/63/63	0/2/2/2
16	CLA	y	505	12	-	9/39/115/115	-
16	CLA	S	1302	8	-	7/15/91/115	-
16	CLA	G	1235	2	-	11/36/112/115	-
16	CLA	q	508	12	-	10/27/103/115	-
19	BCR	Q	4016	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMG	A	4101	-	-	24/41/61/70	0/1/1/1
20	LMT	H	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	W	517	12	-	10/27/103/115	-
19	BCR	q	603	-	-	6/29/63/63	0/2/2/2
16	CLA	y	512	12	-	12/39/115/115	-
16	CLA	G	1240	13	-	5/17/93/115	-
16	CLA	y	517	-	-	15/27/103/115	-
19	BCR	s	601	-	-	12/29/63/63	0/2/2/2
16	CLA	b	1232	25	-	8/15/91/115	-
16	CLA	Z	506	-	-	8/33/109/115	-
13	LHG	i	103	-	-	22/44/44/53	-
16	CLA	B	1219	-	-	4/15/91/115	-
16	CLA	a	1114	-	-	10/17/93/115	-
17	PQN	a	2001	-	-	5/23/43/43	0/2/2/2
16	CLA	v	515	12	-	17/39/115/115	-
16	CLA	y	516	12	-	7/17/93/115	-
16	CLA	a	1120	1	-	8/20/96/115	-
21	ECH	G	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	y	506	12	-	9/33/109/115	-
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	v	517	-	-	15/27/103/115	-
19	BCR	t	601	-	-	14/29/63/63	0/2/2/2
16	CLA	h	516	12	-	8/17/93/115	-
19	BCR	q	602	-	-	12/29/63/63	0/2/2/2
16	CLA	X	505	12	-	12/39/115/115	-
16	CLA	o	510	-	-	5/33/109/115	-
21	ECH	V	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	h	507	12	-	15/39/115/115	-
16	CLA	Y	511	12	-	14/39/115/115	-
16	CLA	B	1021	2	-	13/39/115/115	-
16	CLA	H	1127	1	-	7/39/115/115	-
19	BCR	v	603	-	-	12/29/63/63	0/2/2/2
21	ECH	R	4020	-	-	11/29/66/66	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1135	1	-	4/23/99/115	-
19	BCR	w	604	-	-	17/29/63/63	0/2/2/2
16	CLA	q	517	12	-	11/27/103/115	-
16	CLA	A	1107	1	-	6/21/97/115	-
13	LHG	G	4018	16	-	12/42/42/53	-
16	CLA	u	512	12	-	11/39/115/115	-
16	CLA	b	1214	2	-	7/27/103/115	-
16	CLA	t	504	12	-	6/33/109/115	-
16	CLA	r	503	-	-	9/17/93/115	-
16	CLA	H	1111	1	-	8/27/103/115	-
19	BCR	l	4022	-	-	18/29/63/63	0/2/2/2
19	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
19	BCR	Z	604	-	-	19/29/63/63	0/2/2/2
16	CLA	G	1023	-	-	8/39/115/115	-
16	CLA	v	516	12	-	6/17/93/115	-
16	CLA	H	1112	1	-	2/15/91/115	-
19	BCR	g	602	-	-	14/29/63/63	0/2/2/2
19	BCR	q	604	-	-	16/29/63/63	0/2/2/2
23	LMU	g	606	-	-	5/21/61/61	0/2/2/2
16	CLA	q	509	12	-	12/39/115/115	-
19	BCR	o	603	-	-	9/29/63/63	0/2/2/2
16	CLA	A	1113	1	-	7/15/91/115	-
16	CLA	H	1136	1	-	10/39/115/115	-
16	CLA	H	1138	1	-	11/39/115/115	-
13	LHG	b	4018	16	-	16/42/42/53	-
16	CLA	l	1502	10	-	9/33/109/115	-
16	CLA	W	514	-	-	8/21/97/115	-
16	CLA	B	1223	2	-	11/39/115/115	-
19	BCR	v	604	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1110	1	-	10/26/102/115	-
16	CLA	a	1103	1	-	12/39/115/115	-
19	BCR	G	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	n	509	12	-	9/33/109/115	-
16	CLA	K	4003	9	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	h	505	12	-	6/39/115/115	-
16	CLA	y	503	-	-	4/17/93/115	-
19	BCR	H	4007	-	-	8/29/63/63	0/2/2/2
19	BCR	s	602	-	-	11/29/63/63	0/2/2/2
19	BCR	n	603	-	-	12/29/63/63	0/2/2/2
19	BCR	h	603	-	-	11/29/63/63	0/2/2/2
16	CLA	u	517	12	-	8/27/103/115	-
16	CLA	t	502	12	-	10/21/97/115	-
16	CLA	Q	1301	25	-	2/15/91/115	-
17	PQN	H	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	b	1219	-	-	6/15/91/115	-
16	CLA	b	1213	2	-	6/27/103/115	-
16	CLA	W	502	12	-	10/21/97/115	-
16	CLA	h	510	-	-	9/39/115/115	-
16	CLA	r	513	-	-	13/17/93/115	-
16	CLA	o	517	12	-	11/27/103/115	-
16	CLA	A	1135	1	-	3/23/99/115	-
16	CLA	y	502	12	-	5/21/97/115	-
16	CLA	L	1501	10	-	13/33/109/115	-
16	CLA	a	1106	1	-	17/39/115/115	-
20	LMT	l	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	a	1139	25	-	6/27/103/115	-
16	CLA	q	514	-	-	10/21/97/115	-
16	CLA	X	515	12	-	16/39/115/115	-
16	CLA	Z	510	-	-	11/33/109/115	-
16	CLA	b	1209	2	-	5/15/91/115	-
18	SF4	N	102	-	-	-	0/6/5/5
19	BCR	i	4018	-	-	13/29/63/63	0/2/2/2
18	SF4	H	3001	-	-	-	0/6/5/5
16	CLA	t	516	-	-	9/17/93/115	-
16	CLA	A	1111	1	-	7/27/103/115	-
16	CLA	X	513	-	-	9/17/93/115	-
16	CLA	t	506	12	-	13/33/109/115	-
16	CLA	h	517	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	J	4015	-	-	7/29/63/63	0/2/2/2
16	CLA	x	509	12	-	14/39/115/115	-
16	CLA	U	1503	-	-	9/39/115/115	-
16	CLA	s	510	-	-	9/39/115/115	-
16	CLA	Y	504	12	-	16/39/115/115	-
16	CLA	v	502	12	-	6/21/97/115	-
16	CLA	s	502	12	-	6/21/97/115	-
16	CLA	t	510	-	-	9/39/115/115	-
16	CLA	t	509	12	-	6/33/109/115	-
16	CLA	G	1212	2	-	8/15/91/115	-
16	CLA	G	1231	25	-	5/15/91/115	-
16	CLA	o	506	-	-	16/33/109/115	-
13	LHG	Y	605	-	-	16/36/36/53	-
16	CLA	p	516	-	-	9/17/93/115	-
16	CLA	W	507	12	-	12/39/115/115	-
16	CLA	A	1237	25	-	11/39/115/115	-
18	SF4	c	102	-	-	-	0/6/5/5
16	CLA	r	501	12	-	6/21/97/115	-
16	CLA	v	503	-	-	7/17/93/115	-
16	CLA	X	514	-	-	4/21/97/115	-
16	CLA	a	1112	1	-	6/15/91/115	-
16	CLA	A	1114	-	-	9/17/93/115	-
16	CLA	H	1131	1	-	10/39/115/115	-
19	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
17	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
19	BCR	B	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	H	1137	1	-	6/18/94/115	-
19	BCR	x	603	-	-	14/29/63/63	0/2/2/2
16	CLA	w	513	-	-	8/21/97/115	-
16	CLA	Y	507	12	-	10/39/115/115	-
19	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1204	2	-	9/39/115/115	-
19	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
16	CLA	o	504	12	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	t	512	12	-	11/39/115/115	-
19	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
16	CLA	w	511	12	-	9/39/115/115	-
16	CLA	A	1022	25	-	10/39/115/115	-
16	CLA	u	503	-	-	9/17/93/115	-
16	CLA	Z	517	12	-	6/27/103/115	-
16	CLA	b	1223	2	-	11/39/115/115	-
16	CLA	B	1227	2	-	11/20/96/115	-
19	BCR	T	4001	-	-	12/29/63/63	0/2/2/2
19	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	Y	515	12	-	8/39/115/115	-
16	CLA	Z	515	12	-	11/39/115/115	-
19	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1103	-	-	10/39/115/115	-
16	CLA	g	513	-	-	11/17/93/115	-
16	CLA	q	511	12	-	5/39/115/115	-
16	CLA	W	501	12	-	8/21/97/115	-
19	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
23	LMU	w	605	-	-	5/21/61/61	0/2/2/2
16	CLA	x	504	12	-	21/39/115/115	-
16	CLA	s	515	12	-	12/39/115/115	-
16	CLA	n	510	-	-	14/39/115/115	-
16	CLA	A	1133	1	-	11/26/102/115	-
16	CLA	a	1115	1	-	8/26/102/115	-
16	CLA	o	507	12	-	13/39/115/115	-
16	CLA	G	1203	2	-	16/39/115/115	-
16	CLA	o	502	12	-	8/21/97/115	-
16	CLA	s	517	12	-	9/27/103/115	-
16	CLA	w	501	12	-	10/21/97/115	-
16	CLA	B	1232	-	-	8/15/91/115	-
16	CLA	q	515	12	-	12/39/115/115	-
16	CLA	b	1208	2	-	8/15/91/115	-
16	CLA	r	506	12	-	12/33/109/115	-
23	LMU	q	605	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	a	1132	1	-	14/39/115/115	-
16	CLA	B	1220	2	-	12/25/101/115	-
16	CLA	p	505	-	-	14/39/115/115	-
16	CLA	r	508	12	-	9/27/103/115	-
16	CLA	A	1137	1	-	7/18/94/115	-
16	CLA	B	1229	2	-	9/31/107/115	-
16	CLA	H	1130	1	-	10/33/109/115	-
16	CLA	s	511	12	-	14/39/115/115	-
16	CLA	v	511	12	-	11/39/115/115	-
16	CLA	y	514	-	-	8/21/97/115	-
16	CLA	t	513	-	-	8/17/93/115	-
16	CLA	g	514	-	-	7/21/97/115	-
16	CLA	H	1126	1	-	12/39/115/115	-
16	CLA	G	1225	-	-	11/39/115/115	-
16	CLA	v	508	12	-	13/27/103/115	-
16	CLA	q	501	12	-	7/21/97/115	-
16	CLA	w	508	12	-	8/27/103/115	-
13	LHG	o	605	-	-	12/31/31/53	-
16	CLA	B	1207	2	-	18/39/115/115	-
16	CLA	X	502	12	-	6/21/97/115	-
16	CLA	h	502	12	-	7/21/97/115	-
16	CLA	u	510	-	-	9/33/109/115	-
16	CLA	G	1238	25	-	11/39/115/115	-
16	CLA	a	1104	1	-	18/39/115/115	-
16	CLA	t	503	-	-	7/17/93/115	-
16	CLA	A	1106	1	-	15/39/115/115	-
16	CLA	x	507	12	-	10/39/115/115	-
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
19	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
16	CLA	Z	504	12	-	14/39/115/115	-
16	CLA	q	504	12	-	14/39/115/115	-
16	CLA	o	509	12	-	11/33/109/115	-
16	CLA	a	1134	1	-	6/15/91/115	-
16	CLA	W	513	-	-	10/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1226	2	-	17/33/109/115	-
16	CLA	x	502	12	-	5/21/97/115	-
16	CLA	y	513	-	-	7/17/93/115	-
16	CLA	H	1110	1	-	9/26/102/115	-
19	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
19	BCR	r	604	-	-	15/29/63/63	0/2/2/2
16	CLA	n	506	12	-	8/33/109/115	-
16	CLA	s	504	12	-	16/39/115/115	-
19	BCR	o	602	-	-	14/29/63/63	0/2/2/2
16	CLA	a	1013	-	-	12/39/115/115	-
16	CLA	Y	510	-	-	11/39/115/115	-
16	CLA	H	1116	1	-	10/26/102/115	-
16	CLA	Y	508	12	-	13/27/103/115	-
16	CLA	Z	503	12	-	9/17/93/115	-
16	CLA	H	1118	1	-	13/27/103/115	-
16	CLA	g	512	12	-	10/39/115/115	-
16	CLA	A	1128	1	-	20/39/115/115	-
16	CLA	b	1023	-	-	12/39/115/115	-
16	CLA	G	1216	25	-	4/18/94/115	-
13	LHG	x	605	-	-	20/35/35/53	-
16	CLA	p	512	12	-	10/39/115/115	-
16	CLA	o	505	12	-	16/39/115/115	-
16	CLA	B	1216	25	-	5/18/94/115	-
16	CLA	s	503	-	-	10/17/93/115	-
19	BCR	g	601	-	-	17/29/63/63	0/2/2/2
16	CLA	q	507	12	-	12/39/115/115	-
19	BCR	u	603	-	-	9/29/63/63	0/2/2/2
16	CLA	Z	502	12	-	7/21/97/115	-
16	CLA	b	1239	2	-	14/39/115/115	-
19	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1109	16,1	-	9/39/115/115	-
16	CLA	G	1234	2	-	3/21/97/115	-
21	ECH	I	4020	-	-	11/29/66/66	0/2/2/2
19	BCR	U	4022	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
16	CLA	Q	1302	6	-	6/17/93/115	-
16	CLA	n	512	12	-	19/39/115/115	-
16	CLA	B	1238	25	-	9/39/115/115	-
19	BCR	G	4010	-	-	17/29/63/63	0/2/2/2
16	CLA	n	508	12	-	9/27/103/115	-
14	LMG	a	4101	-	-	21/41/61/70	0/1/1/1
16	CLA	g	502	12	-	6/21/97/115	-
16	CLA	S	1303	8	-	2/4/76/115	-
16	CLA	x	516	-	-	5/17/93/115	-
16	CLA	h	515	12	-	17/39/115/115	-
16	CLA	n	516	-	-	8/17/93/115	-
16	CLA	B	1230	2	-	7/15/91/115	-
15	CL0	A	1011	1	-	8/39/115/115	-
16	CLA	u	504	12	-	18/33/109/115	-
19	BCR	x	602	-	-	17/29/63/63	0/2/2/2
16	CLA	a	1125	1	-	10/39/115/115	-
16	CLA	n	507	12	-	11/39/115/115	-
16	CLA	b	1240	13	-	5/17/93/115	-
24	LUT	q	601	-	-	7/29/67/67	0/2/2/2
16	CLA	v	505	12	-	13/39/115/115	-
14	LMG	a	4201	-	-	11/27/47/70	0/1/1/1
16	CLA	B	1202	-	-	16/39/115/115	-
16	CLA	J	1303	8	-	2/4/76/115	-
16	CLA	q	510	-	-	10/33/109/115	-
16	CLA	b	1215	2	-	6/33/109/115	-
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
19	BCR	j	4015	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1118	1	-	11/27/103/115	-
16	CLA	W	512	12	-	18/33/109/115	-
16	CLA	B	1231	25	-	9/15/91/115	-
16	CLA	n	517	12	-	11/27/103/115	-
16	CLA	H	1013	-	-	13/39/115/115	-
16	CLA	G	1021	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	ECH	b	4006	-	-	9/29/66/66	0/2/2/2
16	CLA	u	509	12	-	8/33/109/115	-
21	ECH	B	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	A	1115	1	-	8/26/102/115	-
16	CLA	r	511	12	-	6/39/115/115	-
19	BCR	H	4003	-	-	10/29/63/63	0/2/2/2
13	LHG	p	605	-	-	13/36/36/53	-
16	CLA	B	1217	2	-	7/15/91/115	-
16	CLA	p	503	-	-	6/17/93/115	-
19	BCR	g	604	-	-	16/29/63/63	0/2/2/2
16	CLA	u	507	12	-	12/39/115/115	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1110	1	-	9/26/102/115	-
16	CLA	k	4003	9	-	5/15/91/115	-
16	CLA	b	1231	25	-	8/15/91/115	-
19	BCR	n	604	-	-	13/29/63/63	0/2/2/2
19	BCR	Y	602	-	-	10/29/63/63	0/2/2/2
16	CLA	A	1132	1	-	15/39/115/115	-
13	LHG	H	851	16	-	7/30/30/53	-
16	CLA	G	1227	2	-	9/20/96/115	-
16	CLA	B	1211	2	-	17/39/115/115	-
16	CLA	p	506	12	-	15/33/109/115	-
16	CLA	s	509	12	-	15/33/109/115	-
16	CLA	G	1219	-	-	6/15/91/115	-
16	CLA	H	1105	-	-	9/31/107/115	-
16	CLA	b	1021	2	-	17/39/115/115	-
16	CLA	r	515	12	-	12/39/115/115	-
16	CLA	n	513	-	-	9/17/93/115	-
16	CLA	B	1222	25	-	8/21/97/115	-
16	CLA	Y	517	12	-	10/27/103/115	-
16	CLA	x	510	-	-	13/39/115/115	-
16	CLA	w	510	-	-	10/33/109/115	-
15	CL0	a	1011	1	-	7/39/115/115	-
16	CLA	H	1139	25	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	l	1501	10	-	15/33/109/115	-
19	BCR	R	4018	-	-	13/29/63/63	0/2/2/2
19	BCR	S	4013	-	-	10/29/63/63	0/2/2/2
16	CLA	H	1237	25	-	11/39/115/115	-
20	LMT	U	4101	-	-	8/21/61/61	0/2/2/2
19	BCR	x	604	-	-	12/29/63/63	0/2/2/2
16	CLA	q	516	-	-	11/17/93/115	-
16	CLA	v	513	-	-	4/17/93/115	-
16	CLA	q	506	-	-	12/33/109/115	-
16	CLA	r	504	12	-	17/39/115/115	-
14	LMG	a	852	-	-	10/33/53/70	0/1/1/1
16	CLA	H	1125	1	-	11/39/115/115	-
16	CLA	A	1134	1	-	6/15/91/115	-
16	CLA	G	1207	2	-	14/39/115/115	-
16	CLA	n	505	12	-	22/39/115/115	-
13	LHG	R	103	-	-	23/44/44/53	-
16	CLA	B	1205	2	-	10/39/115/115	-
16	CLA	s	505	-	-	13/39/115/115	-
14	LMG	A	4201	-	-	13/27/47/70	0/1/1/1
16	CLA	A	1101	1	-	15/39/115/115	-
16	CLA	B	1201	2	-	4/26/102/115	-
16	CLA	A	1013	-	-	14/39/115/115	-
16	CLA	v	512	12	-	12/39/115/115	-
19	BCR	p	604	-	-	15/29/63/63	0/2/2/2
16	CLA	W	503	-	-	10/17/93/115	-
16	CLA	a	1138	1	-	15/39/115/115	-
16	CLA	A	1140	1	-	12/39/115/115	-
16	CLA	t	508	12	-	9/27/103/115	-
16	CLA	K	4004	-	-	5/27/103/115	-
16	CLA	H	1119	25	-	12/39/115/115	-
16	CLA	p	507	12	-	9/39/115/115	-
16	CLA	s	516	-	-	10/17/93/115	-
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
16	CLA	u	502	12	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Y	501	12	-	6/21/97/115	-
13	LHG	X	605	-	-	12/31/31/53	-
13	LHG	a	851	16	-	9/30/30/53	-
13	LHG	A	851	16	-	7/30/30/53	-
16	CLA	H	1121	1	-	8/23/99/115	-
16	CLA	X	512	12	-	11/39/115/115	-
16	CLA	G	1239	2	-	15/39/115/115	-
16	CLA	a	1140	1	-	13/39/115/115	-
19	BCR	U	4019	-	-	10/29/63/63	0/2/2/2
16	CLA	Z	511	12	-	4/39/115/115	-
16	CLA	A	1105	-	-	9/31/107/115	-
16	CLA	A	1109	16,1	-	9/39/115/115	-
16	CLA	x	506	12	-	14/33/109/115	-
16	CLA	b	1204	2	-	13/39/115/115	-
16	CLA	n	503	-	-	8/17/93/115	-
16	CLA	X	506	-	-	13/33/109/115	-
16	CLA	a	1123	-	-	13/39/115/115	-
13	LHG	u	605	-	-	12/31/31/53	-
16	CLA	x	505	12	-	10/39/115/115	-
16	CLA	b	1012	25	-	10/27/103/115	-
16	CLA	B	1012	25	-	11/27/103/115	-
16	CLA	W	508	12	-	9/27/103/115	-
16	CLA	H	1102	16,1	-	5/29/105/115	-
16	CLA	a	1129	1	-	3/17/93/115	-
16	CLA	q	503	12	-	9/17/93/115	-
16	CLA	B	1208	2	-	6/15/91/115	-
16	CLA	h	511	12	-	15/39/115/115	-
16	CLA	o	514	-	-	8/21/97/115	-
19	BCR	r	601	-	-	15/29/63/63	0/2/2/2
16	CLA	A	1120	1	-	7/20/96/115	-
19	BCR	G	4014	-	-	16/29/63/63	0/2/2/2
16	CLA	g	510	-	-	12/39/115/115	-
16	CLA	h	513	-	-	6/17/93/115	-
16	CLA	A	1125	1	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1114	-	-	9/17/93/115	-
16	CLA	b	1235	2	-	14/36/112/115	-
16	CLA	l	1503	-	-	12/39/115/115	-
16	CLA	X	504	12	-	16/33/109/115	-
16	CLA	G	1204	2	-	9/39/115/115	-
14	LMG	H	4201	-	-	10/27/47/70	0/1/1/1
16	CLA	r	514	-	-	10/21/97/115	-
16	CLA	Y	509	12	-	15/33/109/115	-
16	CLA	u	508	12	-	12/27/103/115	-
16	CLA	f	1301	25	-	4/15/91/115	-
24	LUT	Z	601	-	-	7/29/67/67	0/2/2/2
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	H	1117	1	-	9/39/115/115	-
16	CLA	G	1223	2	-	6/39/115/115	-
16	CLA	a	1111	1	-	8/27/103/115	-
16	CLA	u	516	12	-	9/17/93/115	-
16	CLA	W	510	-	-	14/39/115/115	-
16	CLA	x	515	12	-	10/39/115/115	-
16	CLA	B	1210	2	-	14/39/115/115	-
16	CLA	T	4003	9	-	9/15/91/115	-
16	CLA	G	1230	2	-	8/15/91/115	-
19	BCR	w	603	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1201	2	-	4/26/102/115	-
16	CLA	r	507	12	-	11/39/115/115	-
19	BCR	b	4014	-	-	15/29/63/63	0/2/2/2
16	CLA	a	1119	-	-	8/39/115/115	-
16	CLA	B	1023	-	-	9/39/115/115	-
16	CLA	G	1228	2	-	15/27/103/115	-
16	CLA	G	1217	2	-	9/15/91/115	-
16	CLA	H	1106	1	-	16/39/115/115	-
16	CLA	n	504	12	-	5/33/109/115	-
16	CLA	o	515	12	-	16/39/115/115	-
16	CLA	G	1202	2	-	18/39/115/115	-
23	LMU	r	606	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	H	4011	-	-	16/29/63/63	0/2/2/2
19	BCR	J	4013	-	-	9/29/63/63	0/2/2/2
16	CLA	H	1109	16,1	-	11/39/115/115	-
16	CLA	b	1210	2	-	12/39/115/115	-
16	CLA	Y	505	-	-	15/39/115/115	-
16	CLA	X	503	-	-	11/17/93/115	-
16	CLA	r	502	12	-	6/21/97/115	-
16	CLA	G	1221	25	-	18/39/115/115	-
16	CLA	X	507	12	-	10/39/115/115	-
16	CLA	y	508	12	-	10/27/103/115	-
16	CLA	w	515	12	-	13/39/115/115	-
16	CLA	b	1230	2	-	7/15/91/115	-
16	CLA	a	1108	1	-	7/15/91/115	-
16	CLA	x	514	-	-	7/21/97/115	-
23	LMU	s	606	-	-	6/21/61/61	0/2/2/2
18	SF4	C	101	-	-	-	0/6/5/5
16	CLA	Y	512	12	-	9/39/115/115	-
17	PQN	G	2002	-	-	10/23/43/43	0/2/2/2
16	CLA	v	504	12	-	13/33/109/115	-
14	LMG	F	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	o	503	-	-	5/17/93/115	-
19	BCR	p	602	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1133	1	-	10/26/102/115	-
16	CLA	H	1120	1	-	9/20/96/115	-
16	CLA	B	1236	2	-	11/21/97/115	-
16	CLA	g	506	12	-	11/33/109/115	-
16	CLA	a	1116	1	-	9/26/102/115	-
16	CLA	B	1213	2	-	8/27/103/115	-
13	LHG	r	605	-	-	17/35/35/53	-
16	CLA	H	1123	-	-	10/39/115/115	-
16	CLA	Y	516	-	-	11/17/93/115	-
16	CLA	n	502	12	-	7/21/97/115	-
19	BCR	u	604	-	-	17/29/63/63	0/2/2/2
16	CLA	Y	506	12	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	504	12	-	12/39/115/115	-
16	CLA	q	505	-	-	13/39/115/115	-
13	LHG	a	849	-	-	17/47/47/53	-
19	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
16	CLA	k	4002	9	-	7/15/91/115	-
16	CLA	H	1140	1	-	15/39/115/115	-
16	CLA	y	510	-	-	6/39/115/115	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
16	CLA	h	503	-	-	5/17/93/115	-
16	CLA	a	1022	-	-	8/39/115/115	-
16	CLA	T	4004	-	-	4/27/103/115	-
16	CLA	a	1117	1	-	10/39/115/115	-
16	CLA	H	1113	1	-	1/15/91/115	-
16	CLA	H	1128	1	-	17/39/115/115	-
16	CLA	n	501	12	-	10/21/97/115	-
16	CLA	b	1229	2	-	9/31/107/115	-
19	BCR	n	601	-	-	12/29/63/63	0/2/2/2
18	SF4	a	3001	-	-	-	0/6/5/5
16	CLA	p	513	-	-	8/17/93/115	-
19	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
19	BCR	W	604	-	-	10/29/63/63	0/2/2/2
16	CLA	t	511	12	-	9/39/115/115	-
16	CLA	r	516	-	-	5/17/93/115	-
19	BCR	j	4012	-	-	9/29/63/63	0/2/2/2
16	CLA	q	512	12	-	15/39/115/115	-
13	LHG	B	4018	16	-	17/42/42/53	-
16	CLA	v	501	12	-	6/17/93/115	-
16	CLA	a	1122	1	-	10/32/108/115	-
16	CLA	A	1122	1	-	9/32/108/115	-
16	CLA	u	505	12	-	14/39/115/115	-
16	CLA	r	509	12	-	10/39/115/115	-
18	SF4	C	102	-	-	-	0/6/5/5
16	CLA	B	1240	13	-	6/17/93/115	-
13	LHG	I	103	-	-	20/44/44/53	-
16	CLA	a	1133	1	-	8/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1214	2	-	10/27/103/115	-
16	CLA	w	507	12	-	10/39/115/115	-
16	CLA	A	1139	25	-	15/33/109/115	-
16	CLA	b	1236	2	-	7/21/97/115	-
16	CLA	B	1218	-	-	9/27/103/115	-
19	BCR	Y	604	-	-	14/29/63/63	0/2/2/2
16	CLA	t	515	12	-	15/39/115/115	-
15	CL0	H	1011	1	-	6/39/115/115	-
16	CLA	W	511	12	-	9/39/115/115	-
16	CLA	b	1228	2	-	12/27/103/115	-
16	CLA	G	1232	25	-	6/15/91/115	-
16	CLA	H	1134	1	-	4/15/91/115	-
16	CLA	Z	509	12	-	16/39/115/115	-
16	CLA	x	508	12	-	12/27/103/115	-
16	CLA	r	517	12	-	12/27/103/115	-
16	CLA	H	1108	1	-	5/15/91/115	-
16	CLA	A	1123	25	-	8/39/115/115	-
16	CLA	G	1229	2	-	10/31/107/115	-
16	CLA	p	501	12	-	7/21/97/115	-
16	CLA	A	1129	1	-	6/17/93/115	-
16	CLA	g	508	12	-	7/27/103/115	-
16	CLA	H	1101	1	-	17/39/115/115	-
19	BCR	y	604	-	-	11/29/63/63	0/2/2/2
20	LMT	a	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	g	504	12	-	22/39/115/115	-
16	CLA	y	515	12	-	15/39/115/115	-
16	CLA	A	1138	1	-	12/39/115/115	-
13	LHG	H	849	-	-	17/47/47/53	-
16	CLA	r	512	12	-	11/39/115/115	-
16	CLA	H	1124	-	-	6/33/109/115	-
19	BCR	u	602	-	-	13/29/63/63	0/2/2/2
16	CLA	Y	502	12	-	6/21/97/115	-
19	BCR	S	4015	-	-	10/29/63/63	0/2/2/2
16	CLA	x	503	-	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LHG	g	605	-	-	16/35/35/53	-
16	CLA	p	510	-	-	11/39/115/115	-
16	CLA	h	508	12	-	12/27/103/115	-
16	CLA	H	1122	1	-	9/32/108/115	-
19	BCR	b	4010	-	-	15/29/63/63	0/2/2/2
16	CLA	W	504	12	-	6/33/109/115	-
16	CLA	b	1220	2	-	13/26/102/115	-

The worst 5 of 2891 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1012	CLA	C1D-ND	3.66	1.42	1.37
16	G	1218	CLA	C1D-ND	3.63	1.42	1.37
16	n	510	CLA	C1D-ND	3.61	1.42	1.37
16	g	504	CLA	C1D-ND	3.56	1.42	1.37
16	p	510	CLA	C1D-ND	3.56	1.42	1.37

The worst 5 of 3850 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	506	CLA	C4A-NA-C1A	8.41	110.52	106.68
21	i	4020	ECH	C8-C9-C10	6.94	129.93	119.01
16	x	505	CLA	C4A-NA-C1A	6.63	109.70	106.68
16	v	505	CLA	C4A-NA-C1A	6.59	109.69	106.68
16	b	1216	CLA	C4A-NA-C1A	6.57	109.68	106.68

There are no chirality outliers.

5 of 8156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	849	LHG	O1-C1-C2-O2
13	A	849	LHG	O1-C1-C2-C3
13	A	849	LHG	C3-O3-P-O5
13	A	851	LHG	C3-O3-P-O5
13	B	4018	LHG	O1-C1-C2-O2

There are no ring outliers.

673 monomers are involved in 1441 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	H	1132	CLA	1	0
16	b	1207	CLA	6	0
16	p	502	CLA	1	0
16	y	511	CLA	6	0
16	w	502	CLA	1	0
16	h	512	CLA	3	0
16	r	505	CLA	7	0
16	u	514	CLA	1	0
16	Z	516	CLA	4	0
16	H	1103	CLA	8	0
19	w	602	BCR	3	0
16	u	515	CLA	2	0
13	s	605	LHG	1	0
19	B	4014	BCR	6	0
16	g	507	CLA	4	0
16	b	1226	CLA	5	0
16	H	1022	CLA	2	0
23	p	606	LMU	1	0
16	B	1226	CLA	2	0
16	G	1220	CLA	3	0
16	A	1108	CLA	1	0
16	a	1126	CLA	4	0
16	q	502	CLA	4	0
16	g	509	CLA	3	0
16	s	506	CLA	4	0
19	r	603	BCR	3	0
16	A	1116	CLA	4	0
16	a	1136	CLA	2	0
16	b	1216	CLA	2	0
19	K	4005	BCR	2	0
16	p	508	CLA	2	0
16	a	1113	CLA	1	0
16	G	1211	CLA	3	0
16	w	506	CLA	3	0
16	A	1124	CLA	6	0
14	B	848	LMG	2	0
16	v	514	CLA	2	0
19	F	4016	BCR	4	0
16	A	1102	CLA	2	0
16	y	504	CLA	2	0
16	X	510	CLA	6	0
16	H	1801	CLA	3	0
14	Q	4017	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	X	603	BCR	2	0
19	r	602	BCR	2	0
16	w	516	CLA	1	0
16	G	1236	CLA	5	0
19	W	601	BCR	5	0
16	a	1127	CLA	1	0
16	A	1127	CLA	4	0
16	G	1213	CLA	2	0
19	f	4016	BCR	4	0
16	a	1131	CLA	3	0
16	g	505	CLA	6	0
16	w	509	CLA	6	0
20	L	4101	LMT	3	0
16	a	1101	CLA	5	0
16	b	1227	CLA	1	0
16	u	501	CLA	1	0
19	u	601	BCR	4	0
19	s	604	BCR	3	0
16	B	1239	CLA	3	0
19	X	602	BCR	3	0
16	h	509	CLA	4	0
16	L	1502	CLA	3	0
16	p	517	CLA	2	0
21	M	4021	ECH	2	0
16	g	516	CLA	2	0
19	G	4005	BCR	2	0
16	a	1137	CLA	4	0
16	X	517	CLA	1	0
16	n	515	CLA	2	0
16	A	1112	CLA	1	0
19	L	4022	BCR	6	0
16	b	1202	CLA	2	0
16	a	1801	CLA	1	0
16	A	1801	CLA	2	0
16	o	511	CLA	1	0
16	w	503	CLA	3	0
16	b	1221	CLA	6	0
16	A	1126	CLA	8	0
16	a	1105	CLA	4	0
16	o	513	CLA	1	0
21	i	4020	ECH	1	0
16	o	508	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1206	CLA	3	0
19	B	4010	BCR	2	0
19	v	601	BCR	1	0
16	w	512	CLA	1	0
16	G	1224	CLA	2	0
17	b	2002	PQN	2	0
16	G	1012	CLA	2	0
19	S	4012	BCR	4	0
16	W	515	CLA	1	0
16	a	1130	CLA	2	0
16	H	1104	CLA	5	0
16	n	511	CLA	5	0
16	a	1237	CLA	2	0
19	Z	603	BCR	1	0
20	A	4202	LMT	1	0
16	b	1201	CLA	2	0
19	H	4002	BCR	3	0
16	G	1208	CLA	1	0
16	B	1235	CLA	3	0
16	b	1211	CLA	2	0
16	B	1206	CLA	7	0
16	b	1234	CLA	1	0
16	B	1234	CLA	1	0
23	x	606	LMU	2	0
16	a	1118	CLA	1	0
16	w	505	CLA	3	0
19	X	601	BCR	3	0
16	a	1128	CLA	5	0
16	B	1221	CLA	2	0
16	B	1203	CLA	7	0
16	x	511	CLA	6	0
16	x	517	CLA	1	0
19	G	4017	BCR	3	0
16	b	1224	CLA	2	0
19	y	601	BCR	1	0
17	B	2002	PQN	5	0
16	o	501	CLA	1	0
16	u	506	CLA	5	0
16	U	1501	CLA	4	0
16	F	1301	CLA	1	0
16	r	510	CLA	6	0
14	A	852	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	1203	CLA	7	0
19	Y	601	BCR	2	0
16	x	512	CLA	3	0
16	h	501	CLA	1	0
23	Y	606	LMU	1	0
16	t	507	CLA	1	0
16	A	1136	CLA	3	0
16	T	4002	CLA	1	0
16	h	504	CLA	2	0
16	a	1102	CLA	5	0
14	H	4101	LMG	6	0
16	G	1205	CLA	5	0
16	A	1104	CLA	4	0
16	B	1225	CLA	8	0
16	A	1121	CLA	1	0
16	q	513	CLA	2	0
16	Z	508	CLA	1	0
16	x	501	CLA	1	0
19	x	601	BCR	5	0
16	o	512	CLA	3	0
16	b	1238	CLA	2	0
16	G	1218	CLA	2	0
19	g	603	BCR	3	0
14	f	4017	LMG	1	0
16	B	1228	CLA	1	0
16	b	1206	CLA	4	0
16	s	513	CLA	1	0
16	w	517	CLA	1	0
16	Z	507	CLA	6	0
16	Z	512	CLA	2	0
16	U	1502	CLA	3	0
16	A	1131	CLA	2	0
19	o	601	BCR	1	0
19	J	4012	BCR	5	0
16	b	1205	CLA	3	0
16	g	511	CLA	1	0
16	y	507	CLA	2	0
16	W	506	CLA	3	0
16	s	507	CLA	5	0
16	v	507	CLA	5	0
16	H	1107	CLA	3	0
19	a	4003	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	852	LMG	2	0
19	a	4011	BCR	4	0
19	h	601	BCR	1	0
21	m	4021	ECH	2	0
16	H	1129	CLA	3	0
16	A	1117	CLA	7	0
16	A	1119	CLA	5	0
16	g	517	CLA	1	0
16	v	509	CLA	7	0
19	t	603	BCR	2	0
16	b	1225	CLA	5	0
16	p	511	CLA	1	0
16	s	508	CLA	2	0
16	W	505	CLA	2	0
16	G	1222	CLA	3	0
16	B	1224	CLA	2	0
16	p	509	CLA	3	0
19	b	4017	BCR	1	0
16	X	511	CLA	1	0
16	a	1124	CLA	7	0
16	X	509	CLA	6	0
16	G	1214	CLA	2	0
19	H	4008	BCR	4	0
16	g	515	CLA	3	0
16	L	1503	CLA	5	0
16	G	1215	CLA	2	0
16	W	509	CLA	2	0
16	X	508	CLA	2	0
16	a	1135	CLA	3	0
16	y	509	CLA	8	0
16	p	515	CLA	6	0
16	t	505	CLA	3	0
16	G	1210	CLA	6	0
16	A	1130	CLA	4	0
16	B	1215	CLA	3	0
19	y	603	BCR	5	0
16	b	1222	CLA	2	0
19	o	604	BCR	1	0
16	v	506	CLA	3	0
16	g	503	CLA	1	0
16	h	506	CLA	1	0
16	n	514	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	p	601	BCR	2	0
19	G	4009	BCR	1	0
16	v	510	CLA	5	0
16	p	504	CLA	7	0
19	Z	602	BCR	2	0
19	a	4007	BCR	1	0
16	u	511	CLA	3	0
16	Z	505	CLA	7	0
16	X	501	CLA	2	0
16	b	1218	CLA	1	0
16	a	1107	CLA	2	0
16	s	512	CLA	3	0
19	X	604	BCR	4	0
16	y	505	CLA	3	0
16	G	1235	CLA	2	0
16	q	508	CLA	3	0
19	Q	4016	BCR	2	0
14	A	4101	LMG	5	0
20	H	4202	LMT	1	0
16	W	517	CLA	1	0
19	q	603	BCR	4	0
16	y	512	CLA	4	0
16	G	1240	CLA	2	0
16	y	517	CLA	3	0
19	s	601	BCR	2	0
16	Z	506	CLA	3	0
13	i	103	LHG	2	0
16	B	1219	CLA	1	0
16	a	1114	CLA	1	0
17	a	2001	PQN	4	0
16	v	515	CLA	1	0
16	y	516	CLA	1	0
16	a	1120	CLA	2	0
21	G	4006	ECH	2	0
16	y	506	CLA	2	0
19	A	4007	BCR	1	0
19	A	4008	BCR	3	0
19	t	601	BCR	3	0
16	h	516	CLA	2	0
19	q	602	BCR	4	0
16	X	505	CLA	4	0
16	o	510	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	V	4021	ECH	4	0
16	h	507	CLA	4	0
16	Y	511	CLA	3	0
16	B	1021	CLA	4	0
16	H	1127	CLA	1	0
19	v	603	BCR	3	0
21	R	4020	ECH	2	0
16	H	1135	CLA	1	0
19	w	604	BCR	2	0
16	q	517	CLA	3	0
16	A	1107	CLA	4	0
13	G	4018	LHG	1	0
16	u	512	CLA	2	0
16	b	1214	CLA	2	0
16	t	504	CLA	2	0
16	H	1111	CLA	3	0
19	l	4022	BCR	6	0
19	K	4001	BCR	3	0
19	Z	604	BCR	1	0
16	G	1023	CLA	3	0
16	v	516	CLA	3	0
16	H	1112	CLA	1	0
19	g	602	BCR	4	0
19	q	604	BCR	5	0
23	g	606	LMU	1	0
16	q	509	CLA	4	0
19	o	603	BCR	2	0
16	A	1113	CLA	1	0
16	H	1136	CLA	2	0
16	H	1138	CLA	4	0
13	b	4018	LHG	3	0
16	l	1502	CLA	2	0
16	B	1223	CLA	2	0
19	v	604	BCR	3	0
16	A	1110	CLA	1	0
16	a	1103	CLA	5	0
19	G	4004	BCR	2	0
16	n	509	CLA	5	0
16	K	4003	CLA	2	0
16	h	505	CLA	2	0
19	H	4007	BCR	1	0
19	s	602	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	n	603	BCR	1	0
19	h	603	BCR	5	0
16	u	517	CLA	1	0
16	t	502	CLA	1	0
16	Q	1301	CLA	2	0
17	H	2001	PQN	4	0
16	b	1219	CLA	1	0
16	b	1213	CLA	1	0
16	W	502	CLA	4	0
16	h	510	CLA	6	0
16	r	513	CLA	1	0
16	o	517	CLA	3	0
16	A	1135	CLA	2	0
16	y	502	CLA	2	0
16	L	1501	CLA	3	0
16	a	1106	CLA	2	0
20	l	4101	LMT	3	0
16	X	515	CLA	3	0
16	Z	510	CLA	6	0
16	b	1209	CLA	1	0
19	i	4018	BCR	5	0
16	A	1111	CLA	3	0
16	X	513	CLA	2	0
16	t	506	CLA	3	0
19	J	4015	BCR	2	0
16	x	509	CLA	3	0
16	U	1503	CLA	4	0
16	s	510	CLA	5	0
16	Y	504	CLA	4	0
16	v	502	CLA	3	0
16	s	502	CLA	2	0
16	t	510	CLA	3	0
16	t	509	CLA	3	0
16	G	1231	CLA	1	0
16	o	506	CLA	3	0
16	p	516	CLA	1	0
16	W	507	CLA	5	0
16	A	1237	CLA	3	0
16	X	514	CLA	1	0
16	a	1112	CLA	1	0
16	H	1131	CLA	5	0
19	a	4008	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	2001	PQN	4	0
19	B	4009	BCR	2	0
16	H	1137	CLA	5	0
19	x	603	BCR	2	0
16	w	513	CLA	1	0
16	Y	507	CLA	5	0
19	b	4004	BCR	1	0
16	B	1204	CLA	5	0
19	I	4018	BCR	3	0
16	o	504	CLA	2	0
16	t	512	CLA	3	0
19	b	4005	BCR	4	0
16	w	511	CLA	1	0
16	A	1022	CLA	4	0
16	u	503	CLA	2	0
16	Z	517	CLA	1	0
16	b	1223	CLA	1	0
16	B	1227	CLA	1	0
19	T	4001	BCR	3	0
19	a	4002	BCR	4	0
16	Y	515	CLA	3	0
16	Z	515	CLA	3	0
19	l	4019	BCR	4	0
16	A	1103	CLA	3	0
16	g	513	CLA	1	0
16	q	511	CLA	3	0
16	W	501	CLA	2	0
19	k	4001	BCR	4	0
16	x	504	CLA	2	0
16	s	515	CLA	2	0
16	n	510	CLA	6	0
16	a	1115	CLA	1	0
16	G	1203	CLA	4	0
16	o	502	CLA	3	0
16	s	517	CLA	2	0
16	q	515	CLA	4	0
16	b	1208	CLA	2	0
16	r	506	CLA	2	0
23	q	605	LMU	2	0
16	a	1132	CLA	2	0
16	B	1220	CLA	3	0
16	p	505	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	r	508	CLA	2	0
16	A	1137	CLA	3	0
16	B	1229	CLA	2	0
16	H	1130	CLA	1	0
16	v	511	CLA	5	0
16	H	1126	CLA	5	0
16	G	1225	CLA	4	0
16	w	508	CLA	2	0
13	o	605	LHG	1	0
16	B	1207	CLA	6	0
16	X	502	CLA	3	0
16	u	510	CLA	3	0
16	G	1238	CLA	2	0
16	a	1104	CLA	4	0
16	A	1106	CLA	2	0
16	x	507	CLA	6	0
19	p	603	BCR	4	0
19	L	4019	BCR	3	0
16	Z	504	CLA	2	0
16	q	504	CLA	3	0
16	o	509	CLA	5	0
16	G	1226	CLA	4	0
16	y	513	CLA	1	0
16	H	1110	CLA	2	0
19	A	4002	BCR	3	0
16	n	506	CLA	4	0
16	s	504	CLA	6	0
19	o	602	BCR	1	0
16	a	1013	CLA	2	0
16	Y	510	CLA	5	0
16	H	1116	CLA	3	0
16	Y	508	CLA	1	0
16	Z	503	CLA	2	0
16	H	1118	CLA	2	0
16	g	512	CLA	2	0
16	A	1128	CLA	5	0
16	b	1023	CLA	3	0
16	G	1216	CLA	2	0
16	p	512	CLA	2	0
16	o	505	CLA	7	0
19	g	601	BCR	2	0
16	q	507	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	u	603	BCR	2	0
16	Z	502	CLA	2	0
16	b	1239	CLA	5	0
19	A	4003	BCR	2	0
16	a	1109	CLA	2	0
16	G	1234	CLA	2	0
21	I	4020	ECH	2	0
19	U	4022	BCR	12	0
19	A	4011	BCR	4	0
16	Q	1302	CLA	1	0
16	n	512	CLA	1	0
16	B	1238	CLA	3	0
19	G	4010	BCR	3	0
16	n	508	CLA	4	0
14	a	4101	LMG	1	0
16	g	502	CLA	2	0
16	x	516	CLA	2	0
16	h	515	CLA	4	0
16	n	516	CLA	2	0
16	B	1230	CLA	3	0
15	A	1011	CL0	3	0
16	u	504	CLA	3	0
19	x	602	BCR	1	0
16	a	1125	CLA	1	0
16	n	507	CLA	6	0
16	b	1240	CLA	2	0
24	q	601	LUT	1	0
16	v	505	CLA	5	0
16	B	1202	CLA	4	0
16	J	1303	CLA	1	0
16	q	510	CLA	7	0
16	b	1215	CLA	3	0
19	Y	603	BCR	2	0
19	j	4015	BCR	2	0
16	A	1118	CLA	1	0
16	W	512	CLA	2	0
16	B	1231	CLA	2	0
16	n	517	CLA	1	0
16	H	1013	CLA	3	0
16	G	1021	CLA	2	0
21	b	4006	ECH	2	0
16	u	509	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	4006	ECH	3	0
16	r	511	CLA	3	0
19	H	4003	BCR	2	0
13	p	605	LHG	1	0
16	p	503	CLA	1	0
19	g	604	BCR	4	0
16	u	507	CLA	1	0
19	j	4013	BCR	2	0
16	a	1110	CLA	3	0
16	k	4003	CLA	1	0
16	b	1231	CLA	1	0
19	n	604	BCR	4	0
19	Y	602	BCR	2	0
16	A	1132	CLA	3	0
13	H	851	LHG	2	0
16	G	1227	CLA	2	0
16	B	1211	CLA	3	0
16	p	506	CLA	2	0
16	s	509	CLA	4	0
16	G	1219	CLA	1	0
16	H	1105	CLA	3	0
16	b	1021	CLA	2	0
16	r	515	CLA	4	0
16	B	1222	CLA	3	0
16	Y	517	CLA	2	0
16	x	510	CLA	8	0
16	w	510	CLA	5	0
15	a	1011	CL0	4	0
16	H	1139	CLA	7	0
16	l	1501	CLA	7	0
19	S	4013	BCR	3	0
16	H	1237	CLA	3	0
20	U	4101	LMT	2	0
19	x	604	BCR	1	0
16	q	516	CLA	2	0
16	q	506	CLA	4	0
16	r	504	CLA	2	0
14	a	852	LMG	2	0
16	H	1125	CLA	2	0
16	A	1134	CLA	1	0
16	G	1207	CLA	5	0
16	n	505	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	R	103	LHG	2	0
16	B	1205	CLA	4	0
16	s	505	CLA	6	0
14	A	4201	LMG	1	0
16	A	1101	CLA	5	0
16	B	1201	CLA	3	0
16	A	1013	CLA	1	0
16	v	512	CLA	4	0
19	p	604	BCR	1	0
16	a	1138	CLA	1	0
16	A	1140	CLA	2	0
16	t	508	CLA	2	0
16	K	4004	CLA	1	0
16	H	1119	CLA	9	0
16	p	507	CLA	2	0
16	s	516	CLA	1	0
19	h	604	BCR	3	0
16	u	502	CLA	2	0
13	X	605	LHG	1	0
13	A	851	LHG	2	0
16	H	1121	CLA	1	0
16	X	512	CLA	3	0
16	G	1239	CLA	5	0
16	a	1140	CLA	3	0
19	U	4019	BCR	1	0
16	Z	511	CLA	2	0
16	A	1105	CLA	1	0
16	A	1109	CLA	1	0
16	x	506	CLA	2	0
16	b	1204	CLA	4	0
16	n	503	CLA	1	0
16	X	506	CLA	2	0
16	a	1123	CLA	6	0
13	u	605	LHG	1	0
16	x	505	CLA	3	0
16	b	1012	CLA	3	0
16	B	1012	CLA	4	0
16	a	1129	CLA	2	0
16	q	503	CLA	2	0
16	B	1208	CLA	2	0
16	h	511	CLA	6	0
16	o	514	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	r	601	BCR	2	0
16	A	1120	CLA	2	0
19	G	4014	BCR	5	0
16	g	510	CLA	4	0
16	A	1125	CLA	1	0
16	b	1235	CLA	3	0
16	l	1503	CLA	6	0
16	X	504	CLA	4	0
16	G	1204	CLA	5	0
14	H	4201	LMG	1	0
16	Y	509	CLA	5	0
16	u	508	CLA	2	0
16	f	1301	CLA	2	0
14	G	848	LMG	2	0
16	H	1117	CLA	4	0
16	G	1223	CLA	2	0
16	a	1111	CLA	4	0
16	W	510	CLA	4	0
16	x	515	CLA	4	0
16	B	1210	CLA	7	0
16	T	4003	CLA	2	0
16	G	1230	CLA	2	0
19	w	603	BCR	3	0
16	G	1201	CLA	2	0
16	r	507	CLA	6	0
19	b	4014	BCR	7	0
16	a	1119	CLA	6	0
16	B	1023	CLA	5	0
16	G	1228	CLA	2	0
16	H	1106	CLA	2	0
16	n	504	CLA	5	0
16	o	515	CLA	1	0
16	G	1202	CLA	6	0
23	r	606	LMU	3	0
19	H	4011	BCR	3	0
19	J	4013	BCR	1	0
16	H	1109	CLA	2	0
16	b	1210	CLA	5	0
16	Y	505	CLA	4	0
16	X	503	CLA	2	0
16	r	502	CLA	1	0
16	G	1221	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	X	507	CLA	1	0
16	y	508	CLA	5	0
16	w	515	CLA	4	0
16	b	1230	CLA	1	0
16	a	1108	CLA	1	0
16	x	514	CLA	1	0
16	Y	512	CLA	3	0
17	G	2002	PQN	5	0
16	v	504	CLA	4	0
16	o	503	CLA	1	0
19	p	602	BCR	3	0
16	H	1133	CLA	1	0
16	H	1120	CLA	2	0
16	B	1236	CLA	3	0
16	g	506	CLA	2	0
16	a	1116	CLA	4	0
16	B	1213	CLA	3	0
13	r	605	LHG	2	0
16	H	1123	CLA	2	0
16	Y	516	CLA	1	0
16	n	502	CLA	3	0
16	Y	506	CLA	5	0
16	w	504	CLA	3	0
16	q	505	CLA	4	0
19	B	4017	BCR	2	0
16	k	4002	CLA	1	0
16	H	1140	CLA	4	0
16	y	510	CLA	5	0
19	s	603	BCR	5	0
16	a	1022	CLA	3	0
16	a	1117	CLA	4	0
16	H	1128	CLA	5	0
16	n	501	CLA	3	0
16	b	1229	CLA	4	0
19	n	601	BCR	4	0
16	p	513	CLA	1	0
19	B	4005	BCR	3	0
19	W	604	BCR	1	0
16	t	511	CLA	2	0
16	r	516	CLA	3	0
19	j	4012	BCR	3	0
16	q	512	CLA	3	0

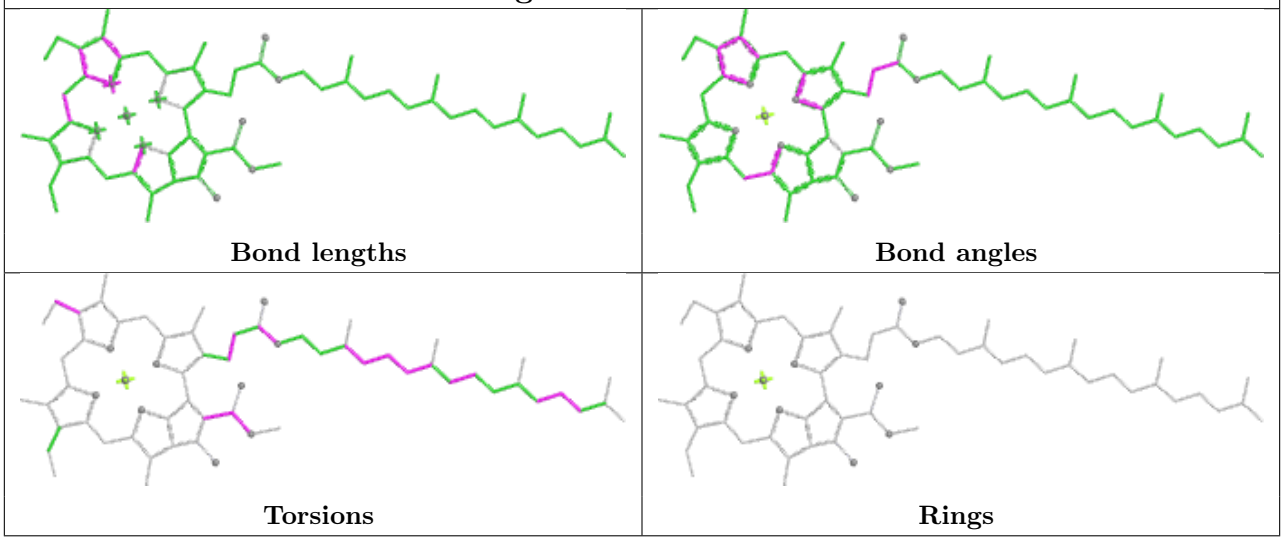
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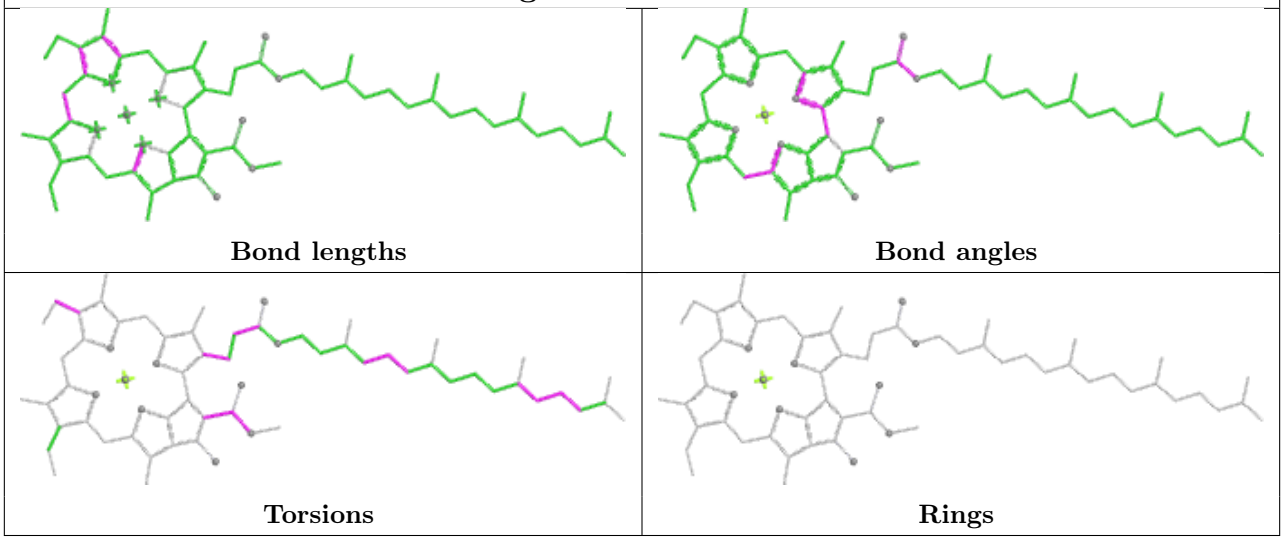
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	4018	LHG	1	0
16	a	1122	CLA	5	0
16	A	1122	CLA	3	0
16	u	505	CLA	3	0
16	r	509	CLA	6	0
16	B	1240	CLA	4	0
13	I	103	LHG	2	0
16	a	1133	CLA	2	0
16	B	1214	CLA	4	0
16	w	507	CLA	6	0
16	A	1139	CLA	5	0
16	b	1236	CLA	1	0
16	B	1218	CLA	1	0
16	t	515	CLA	4	0
15	H	1011	CL0	4	0
16	W	511	CLA	2	0
16	b	1228	CLA	1	0
16	G	1232	CLA	1	0
16	H	1134	CLA	3	0
16	Z	509	CLA	5	0
16	x	508	CLA	1	0
16	H	1108	CLA	1	0
16	A	1123	CLA	4	0
16	A	1129	CLA	1	0
16	g	508	CLA	3	0
16	H	1101	CLA	5	0
19	y	604	BCR	5	0
20	a	4202	LMT	1	0
16	g	504	CLA	2	0
16	y	515	CLA	5	0
16	A	1138	CLA	3	0
16	r	512	CLA	3	0
16	H	1124	CLA	4	0
19	u	602	BCR	2	0
19	S	4015	BCR	2	0
16	x	503	CLA	2	0
16	p	510	CLA	7	0
16	h	508	CLA	2	0
16	H	1122	CLA	3	0
19	b	4010	BCR	2	0
16	W	504	CLA	5	0
16	b	1220	CLA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

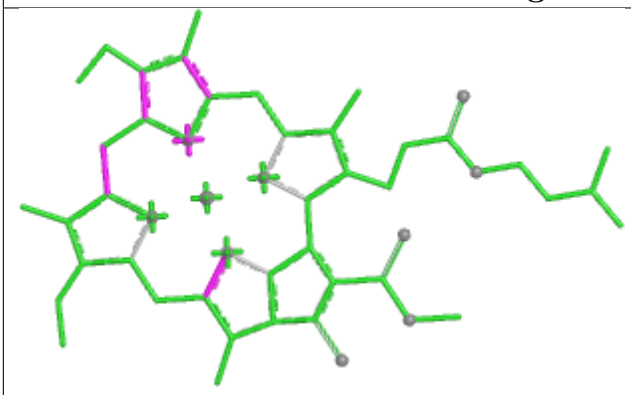
Ligand CLA H 1132



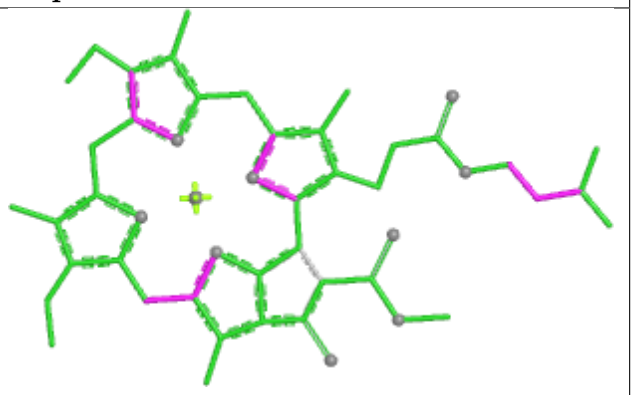
Ligand CLA b 1207



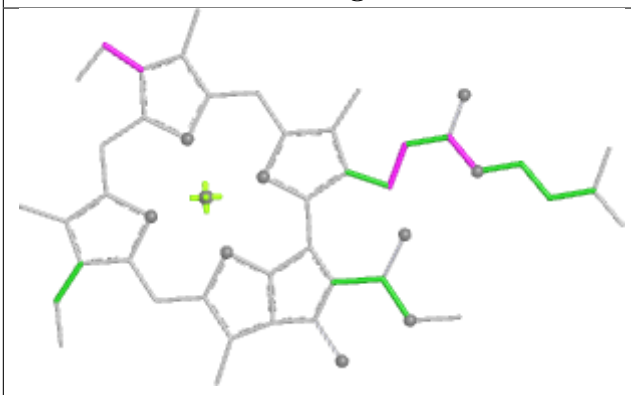
Ligand CLA p 502



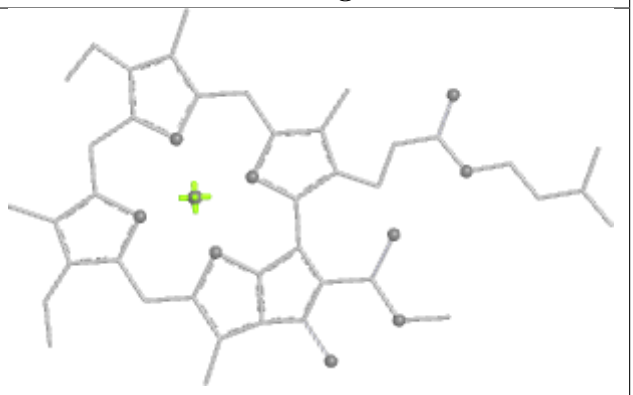
Bond lengths



Bond angles

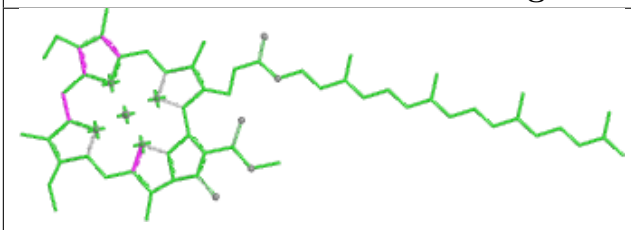


Torsions

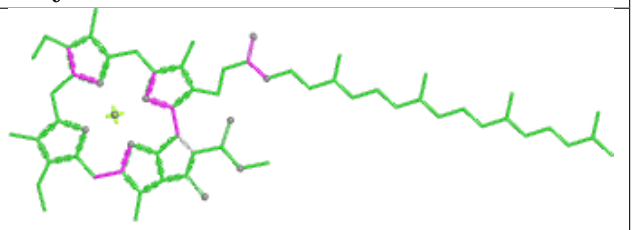


Rings

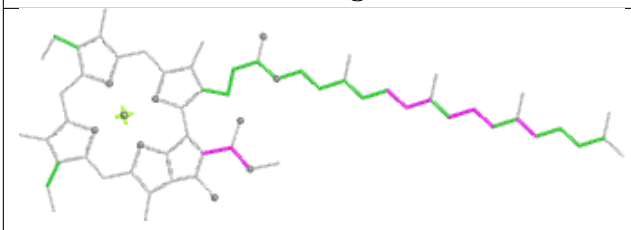
Ligand CLA y 511



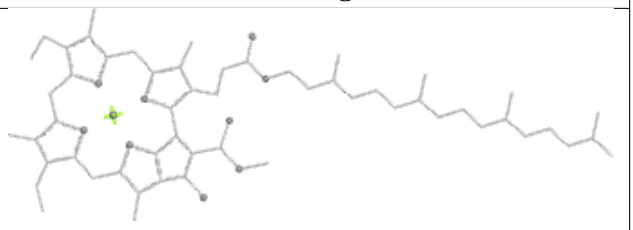
Bond lengths



Bond angles

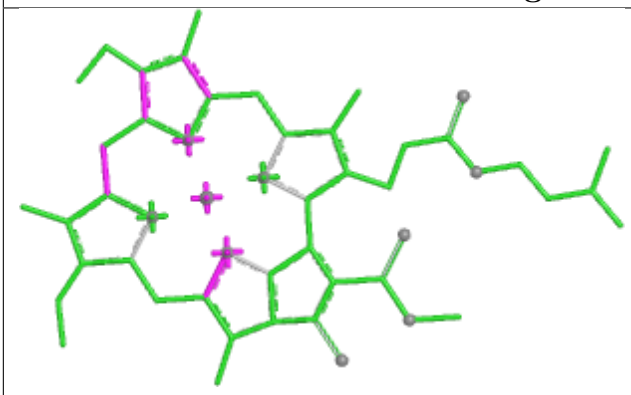


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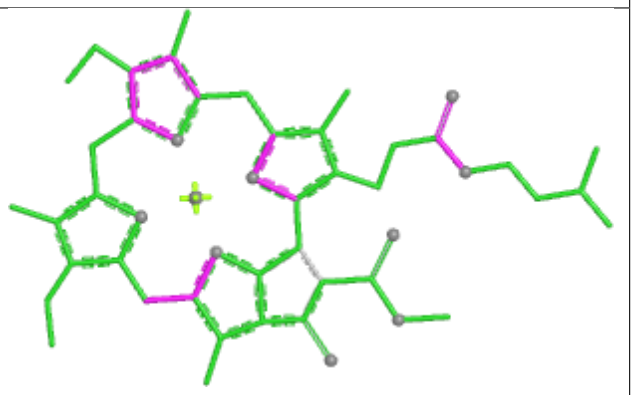


Rings

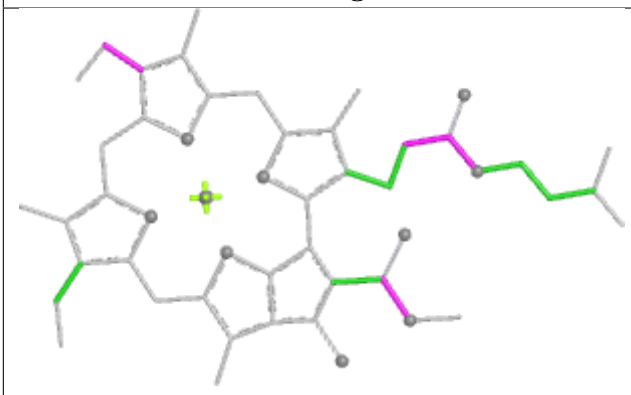
Ligand CLA w 502



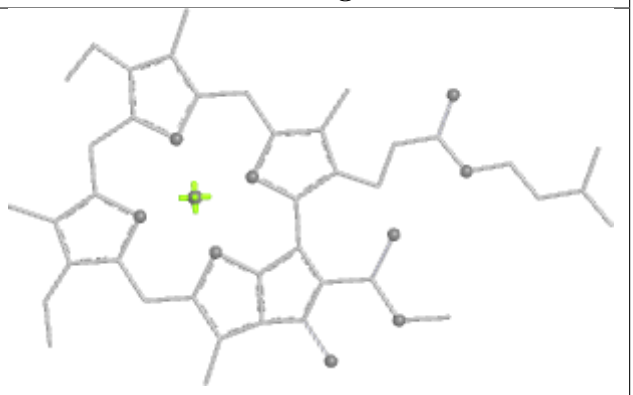
Bond lengths



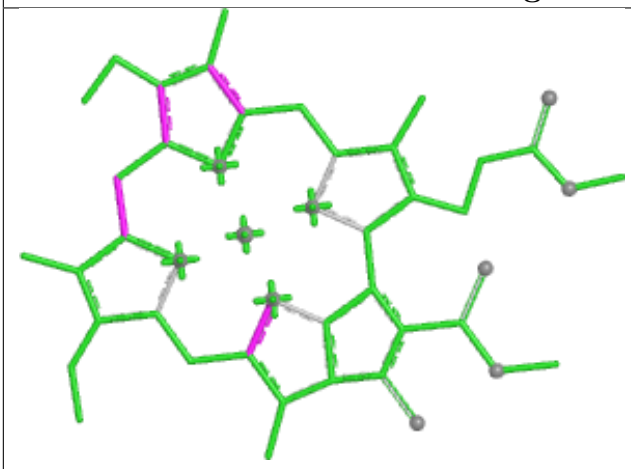
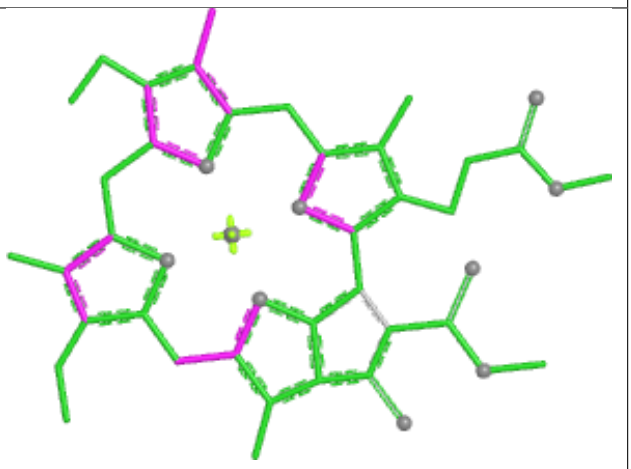
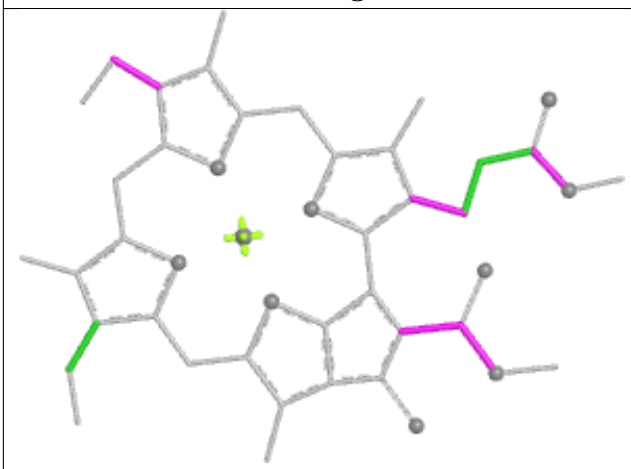
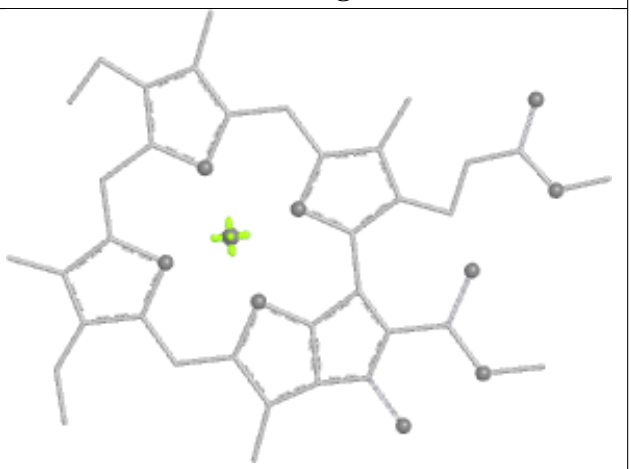
Bond angles



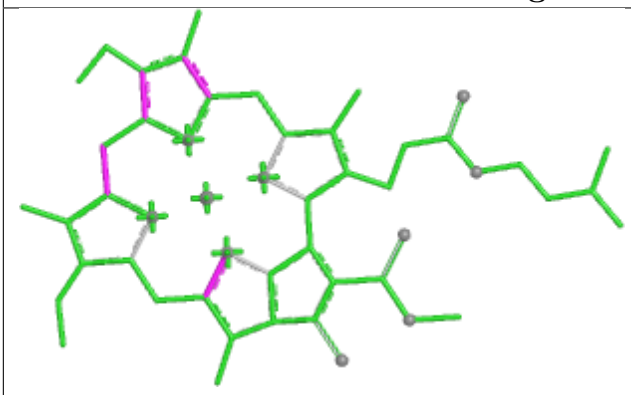
Torsions



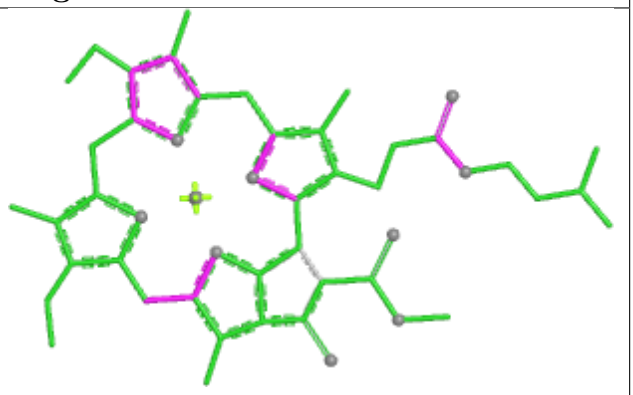
Rings

Ligand CLA Y 513	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

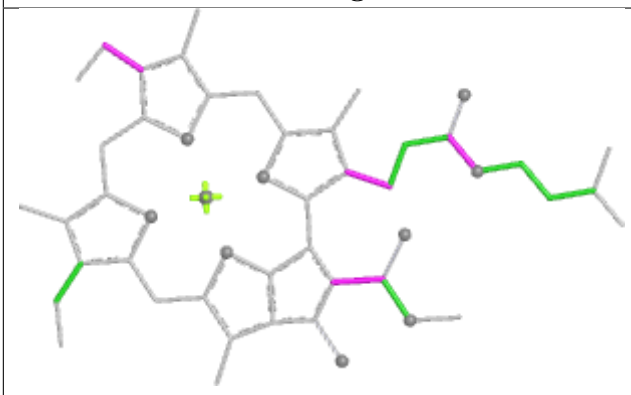
Ligand CLA g 501



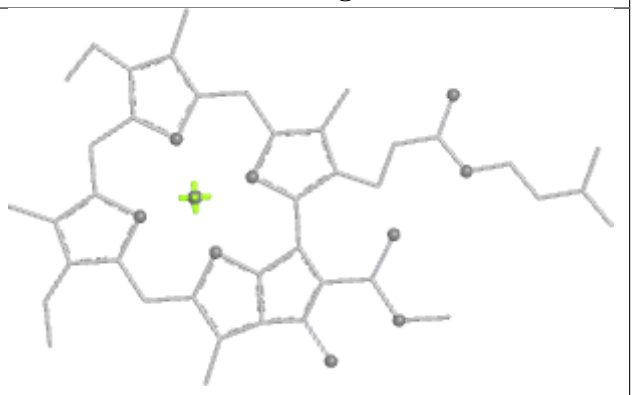
Bond lengths



Bond angles

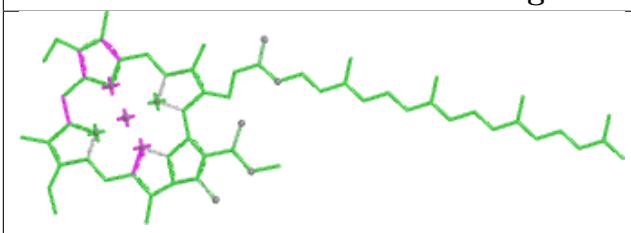


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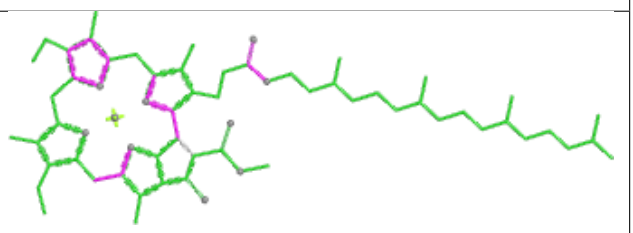


Rings

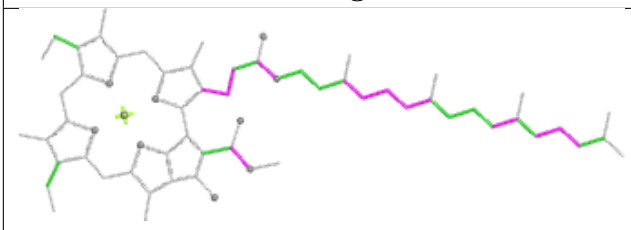
Ligand CLA h 512



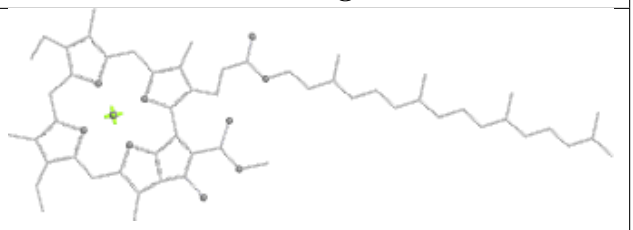
Bond lengths



Bond angles

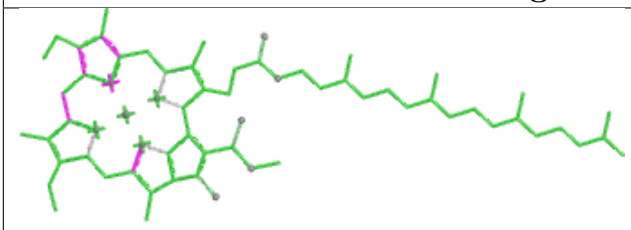


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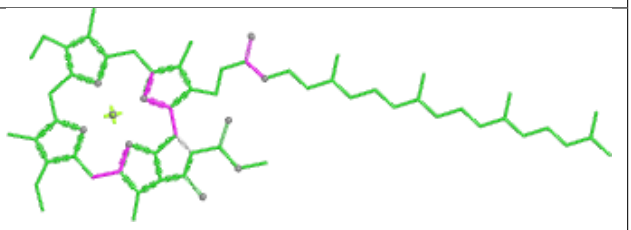


Rings

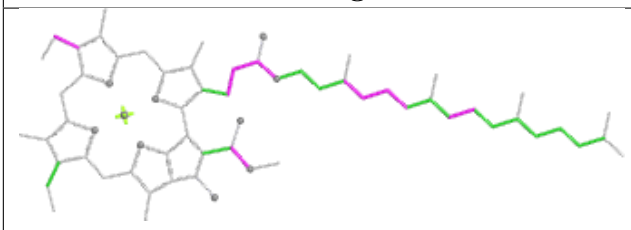
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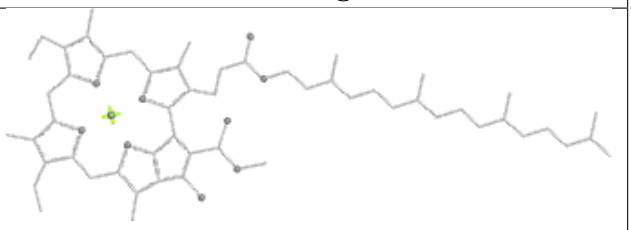
Bond lengths



Bond angles

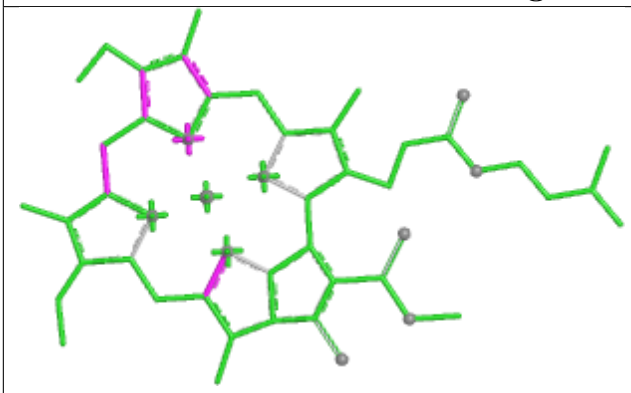


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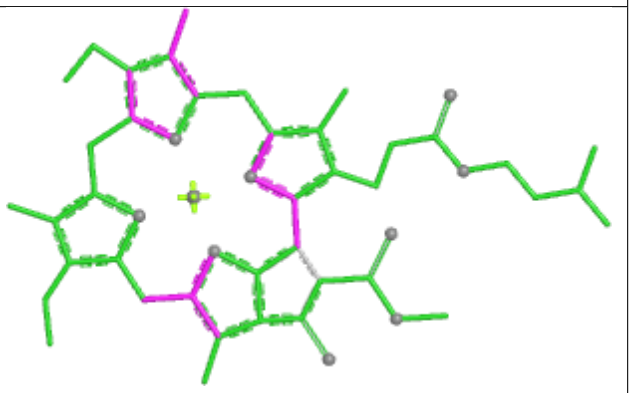


Rings

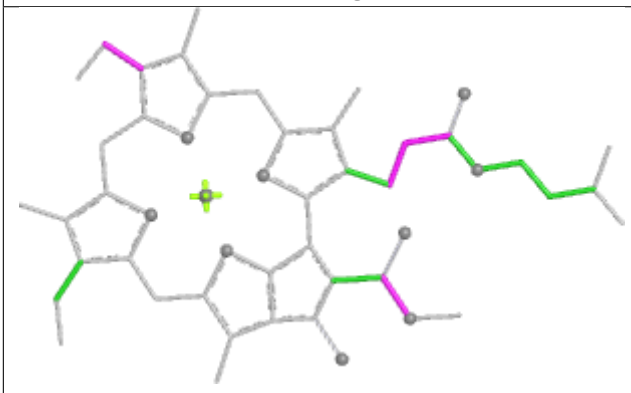
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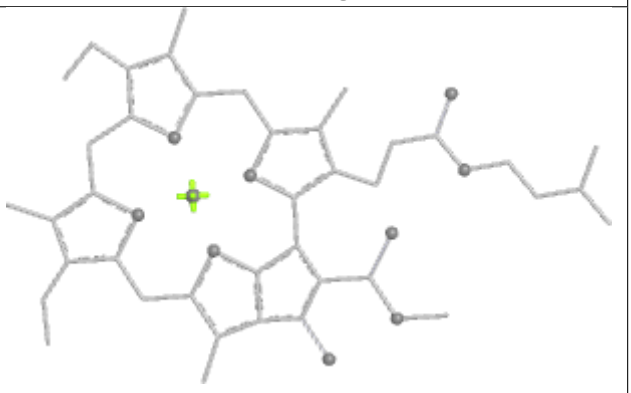
Bond lengths



Bond angles

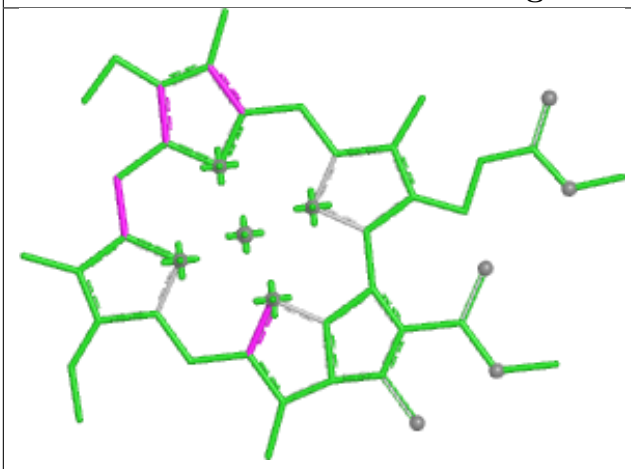


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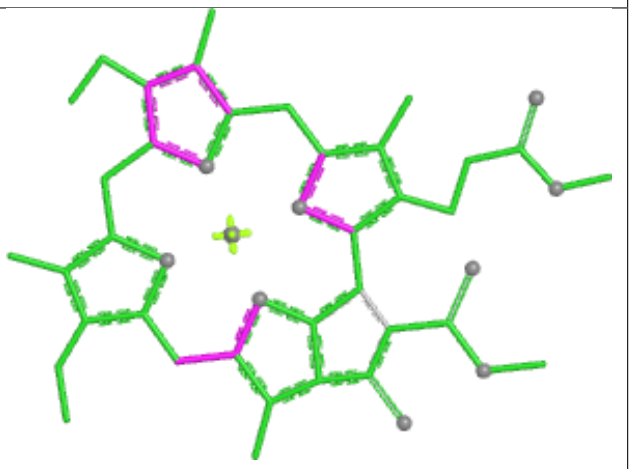


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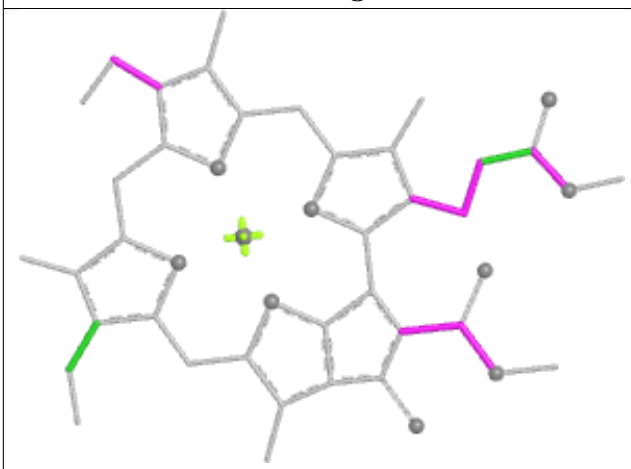
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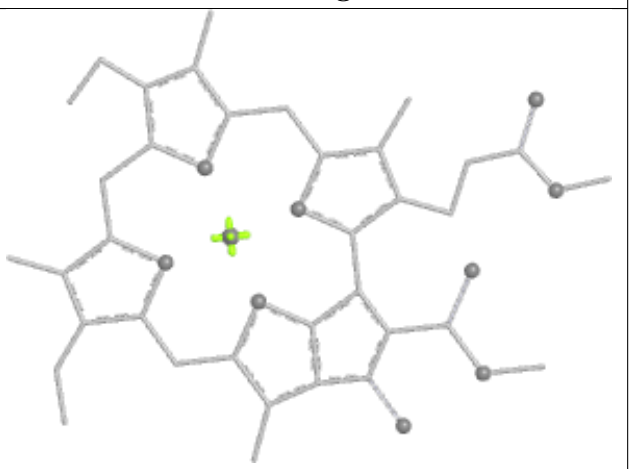
Bond lengths



Bond angles

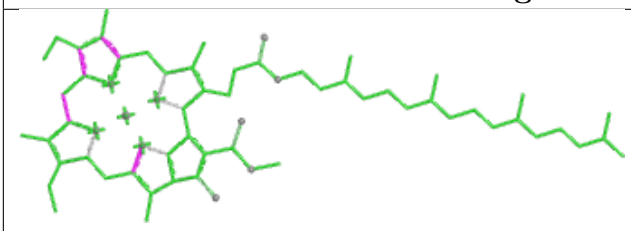


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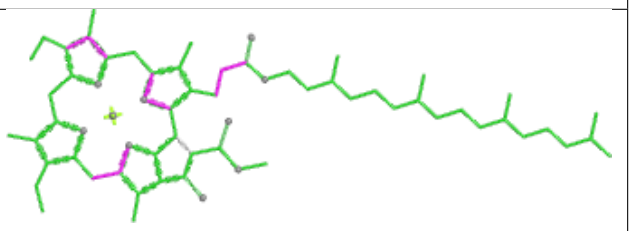


Rings

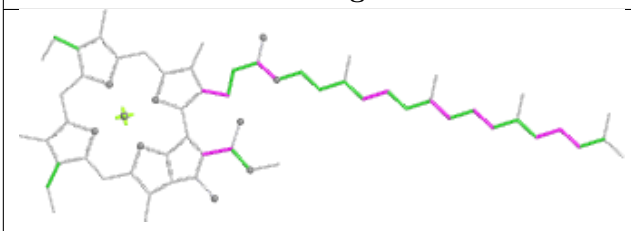
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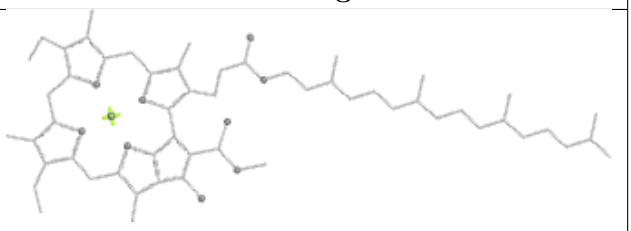
Bond lengths



Bond angles

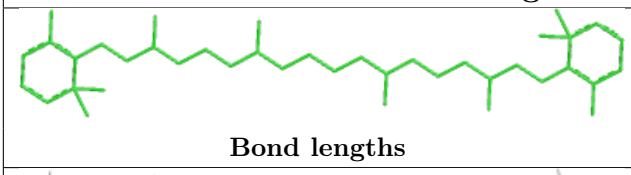


Torsions

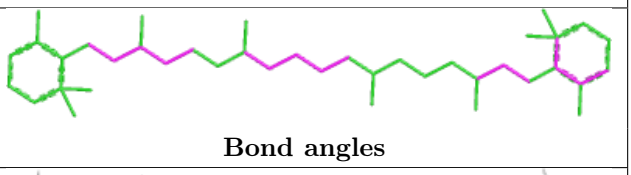


Rings

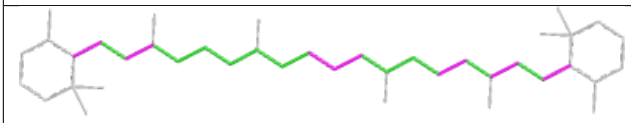
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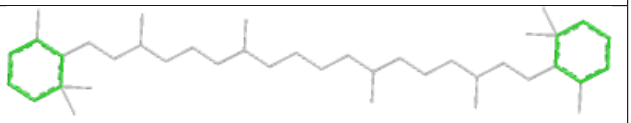
Bond lengths



Bond angles

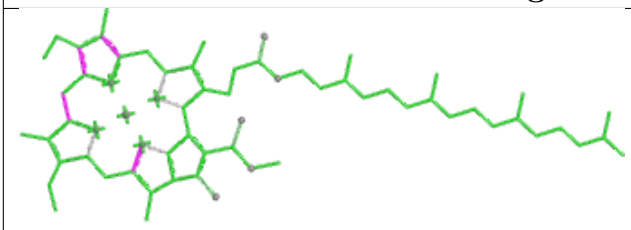


Torsions

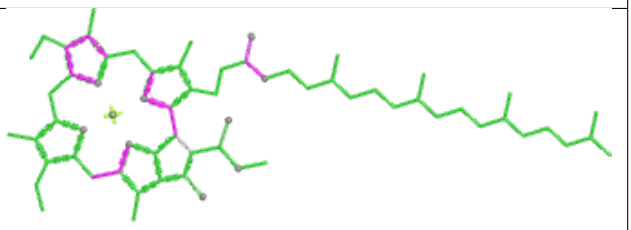


Rings

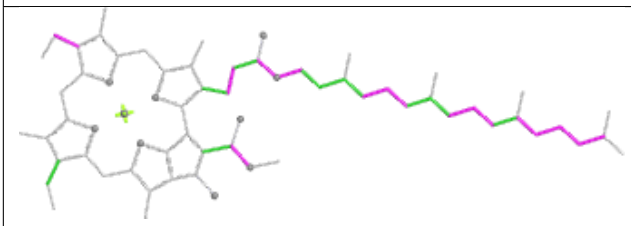
Ligand CLA u 515



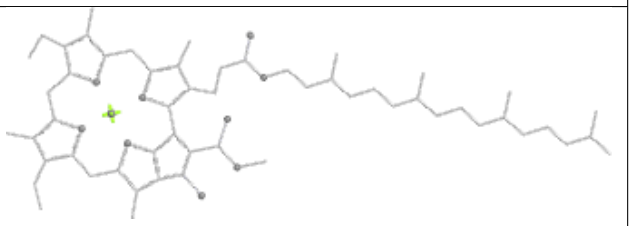
Bond lengths



Bond angles

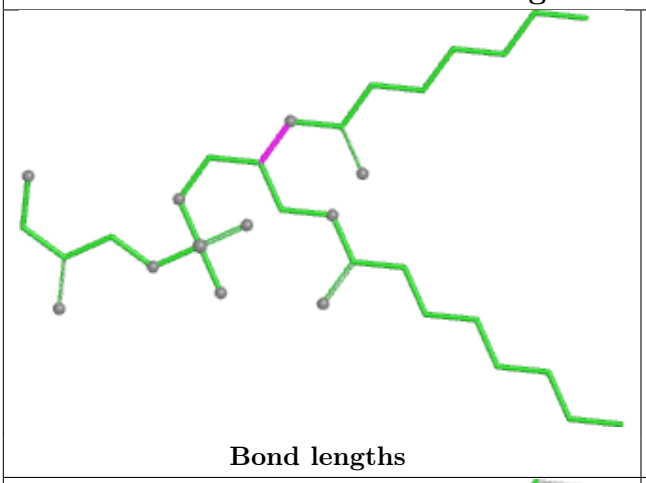


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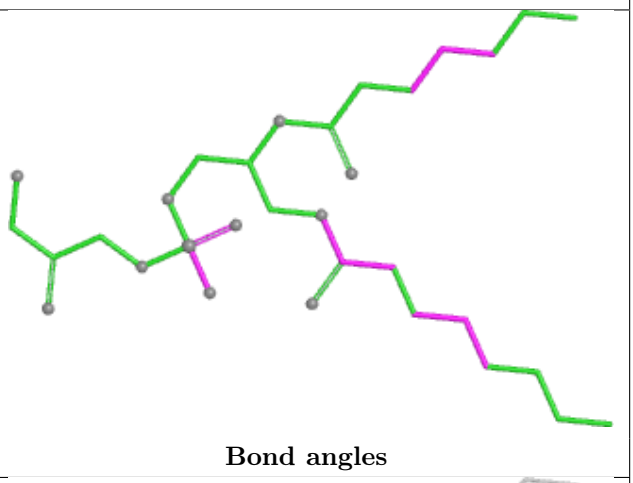


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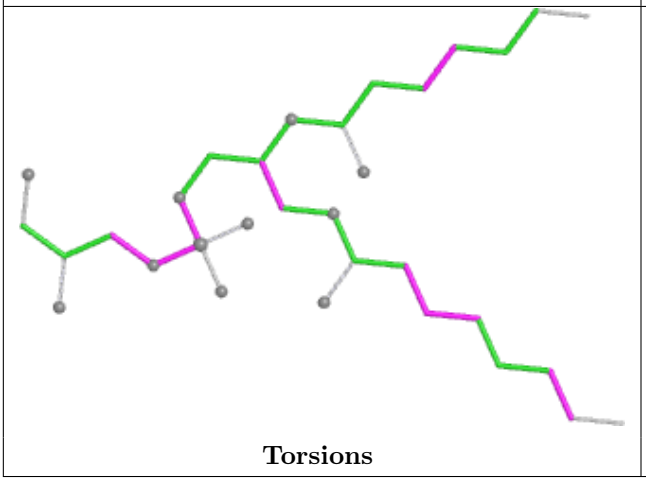
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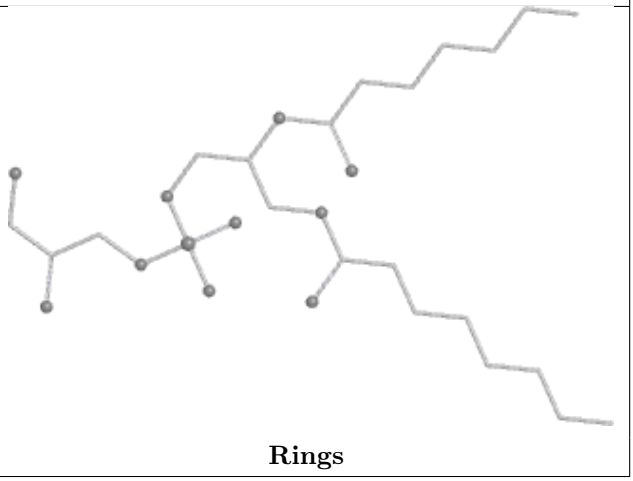
Bond lengths



Bond angles

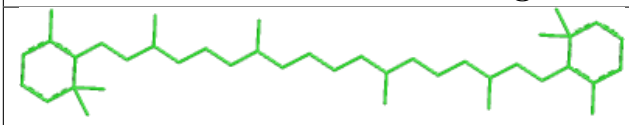


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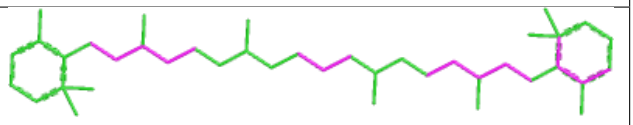


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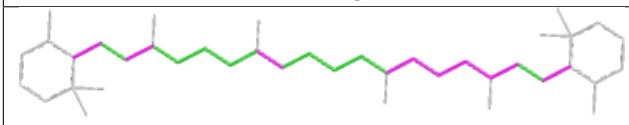
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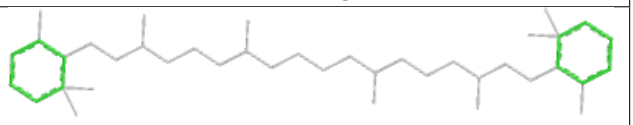
Bond lengths



Bond angles

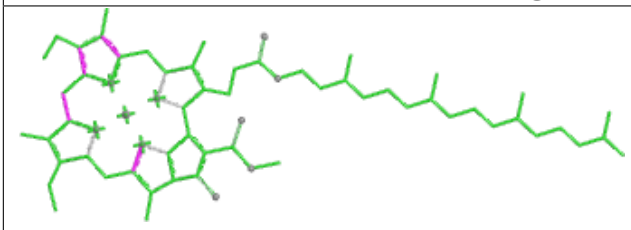


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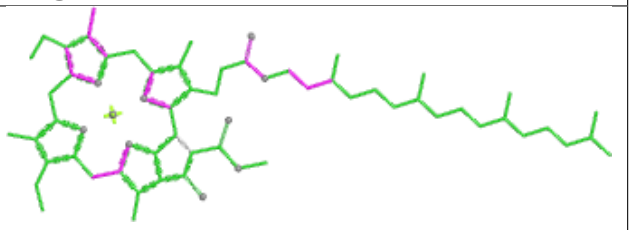


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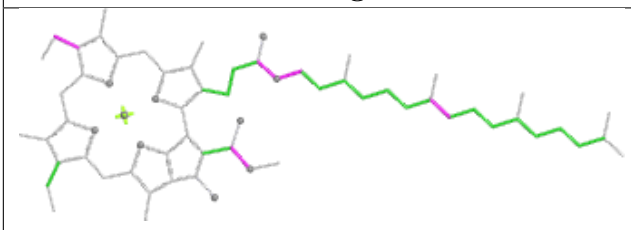
Ligand CLA g 507



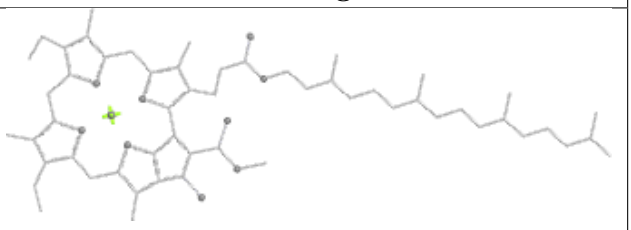
Bond lengths



Bond angles

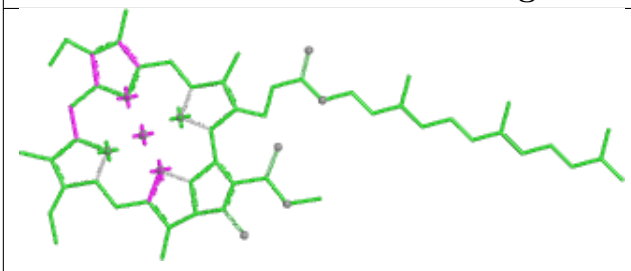


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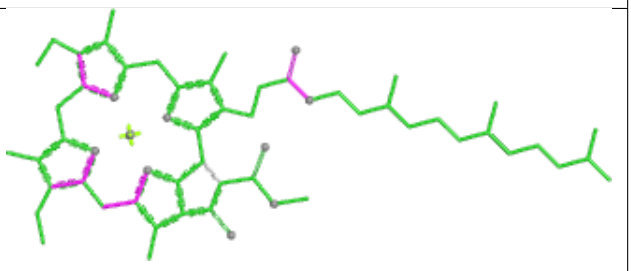


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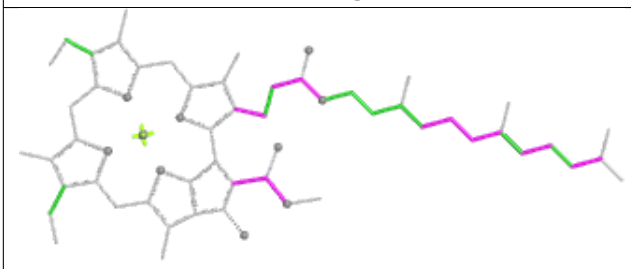
Ligand CLA b 1226



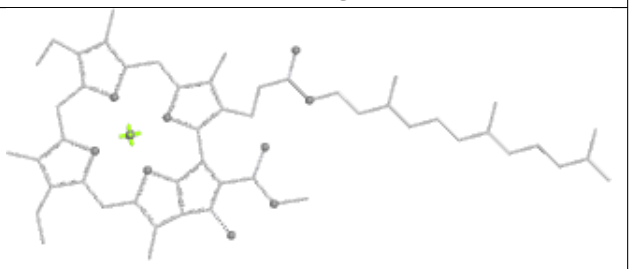
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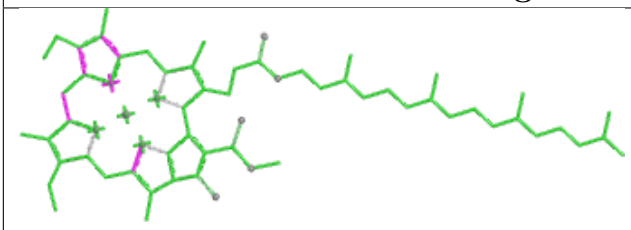


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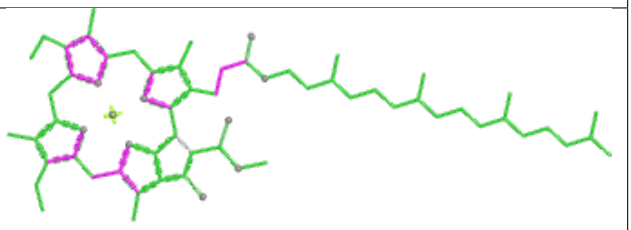


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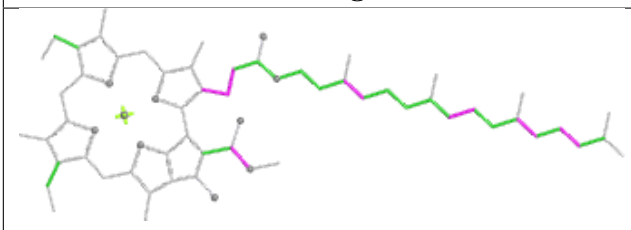
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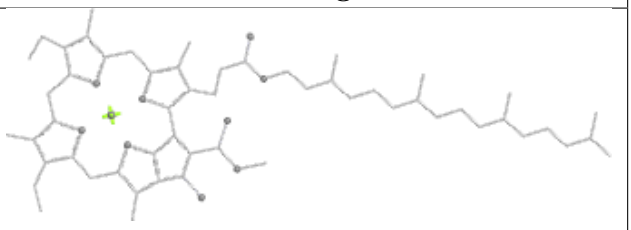
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Bond angles

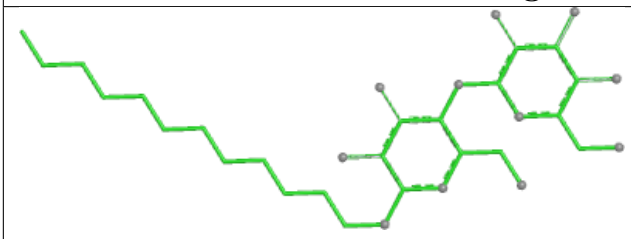


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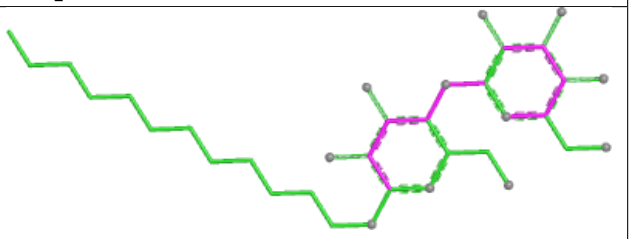


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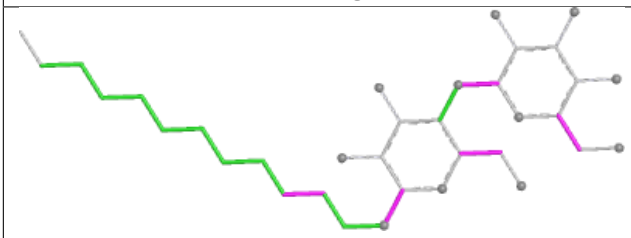
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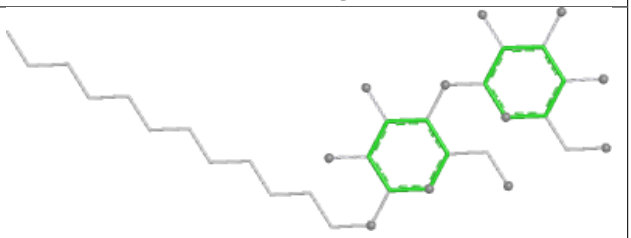
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Bond angles

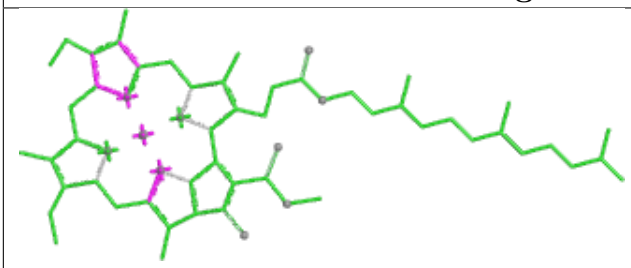


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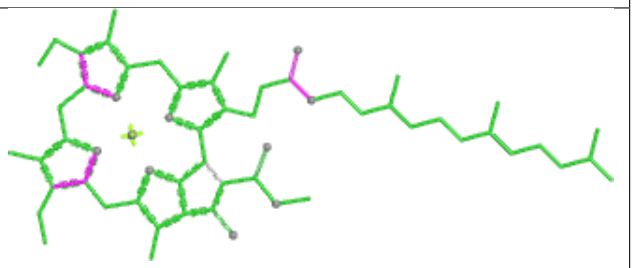


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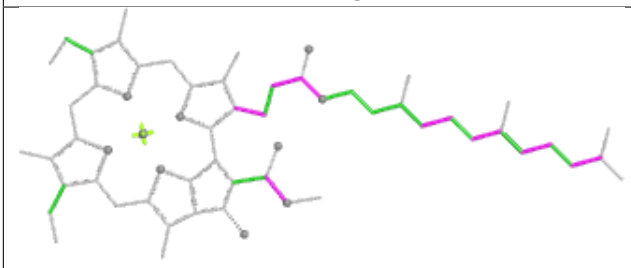
Ligand CLA B 1226



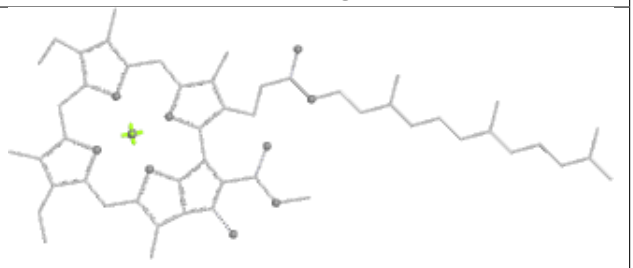
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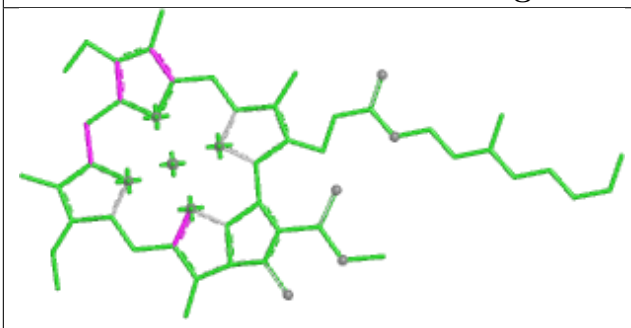


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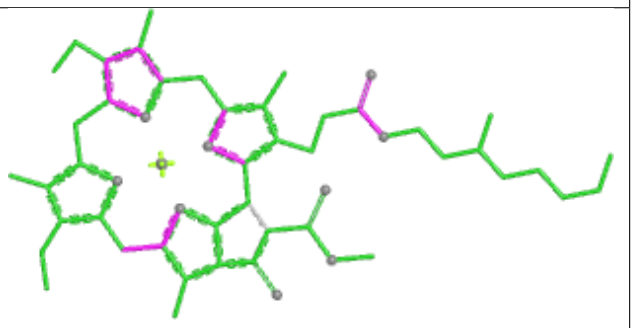


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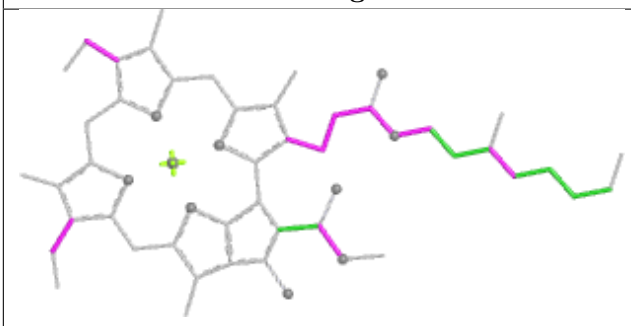
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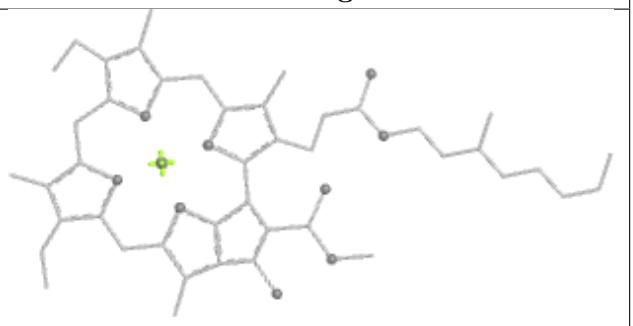
Bond lengths



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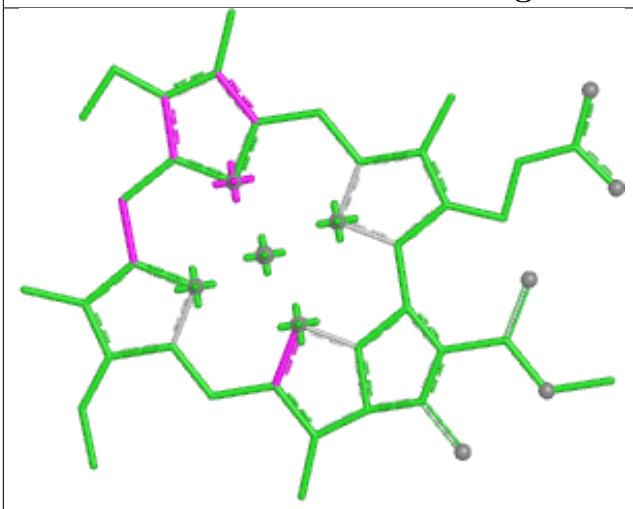


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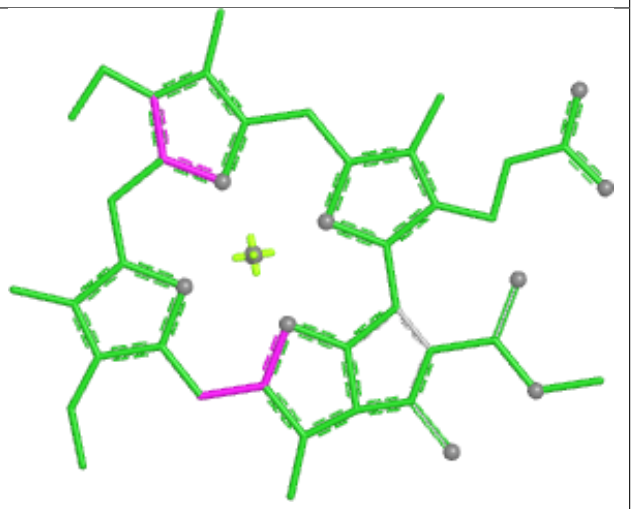


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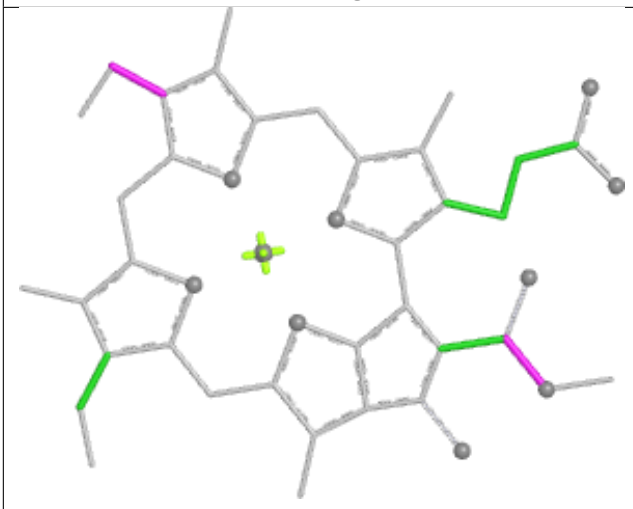
Ligand CLA A 1108



Bond lengths



Bond angles

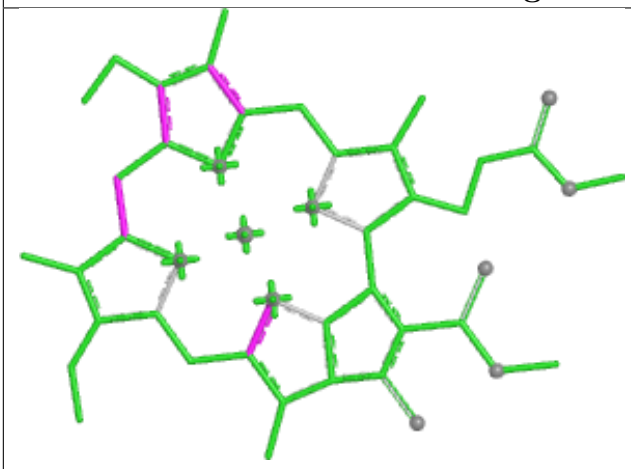


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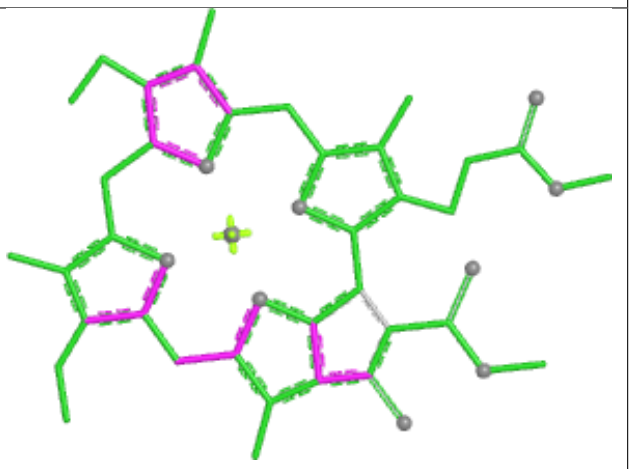


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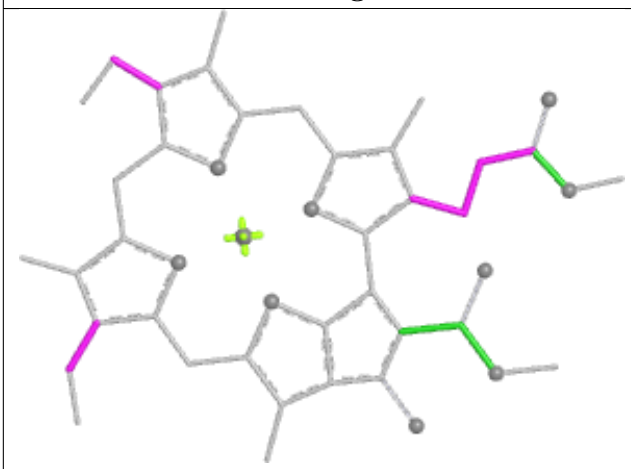
Ligand CLA Y 503



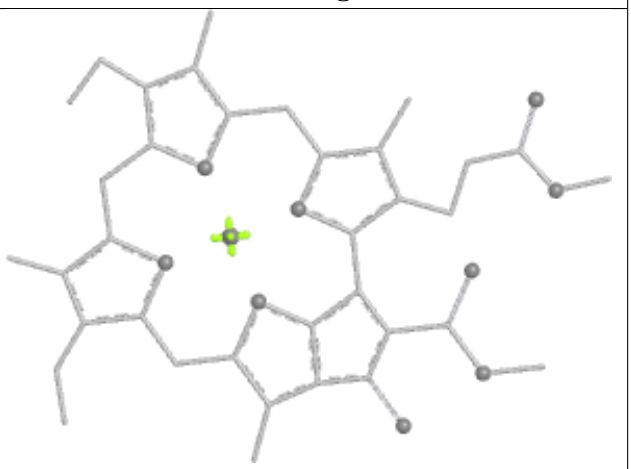
Bond lengths



Bond angles

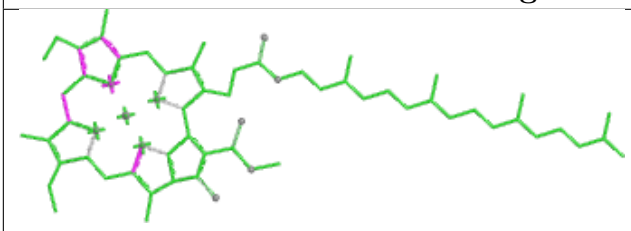


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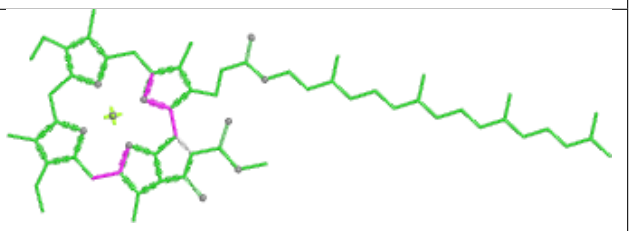


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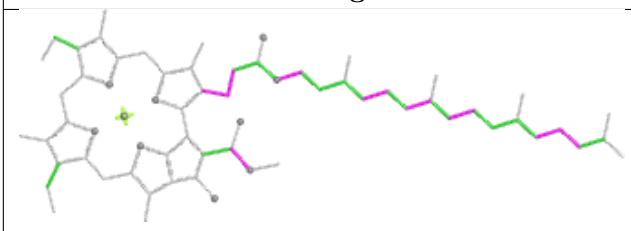
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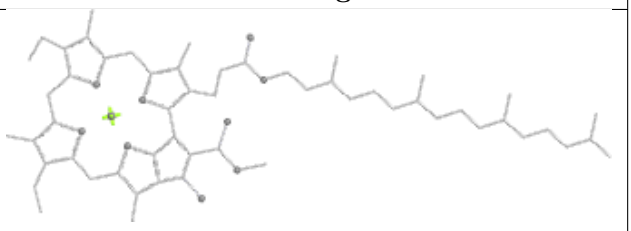
Bond lengths



Bond angles

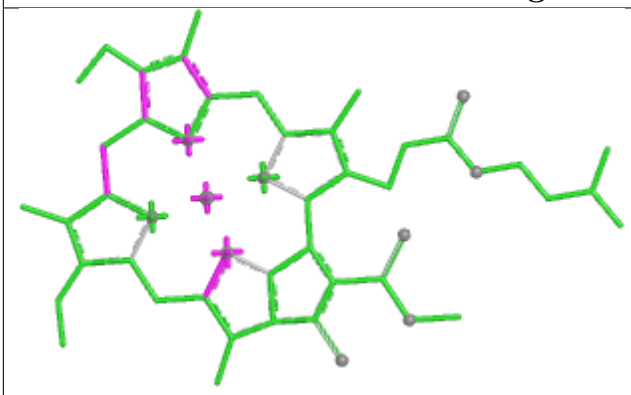


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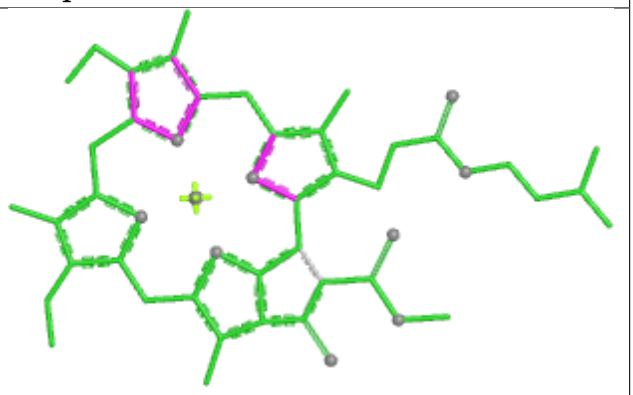


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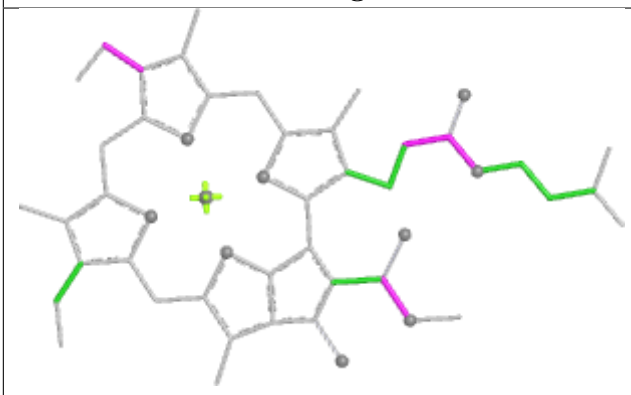
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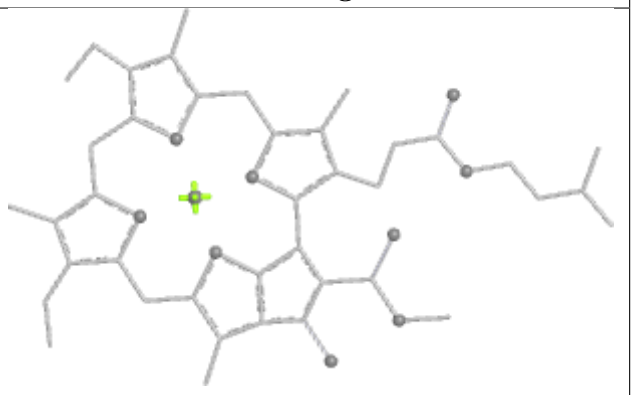
Bond lengths



Bond angles

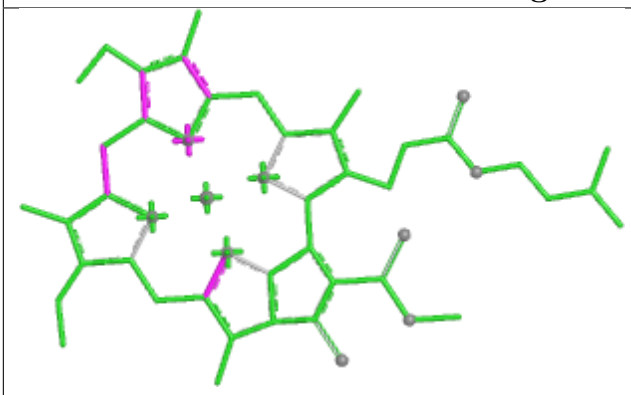


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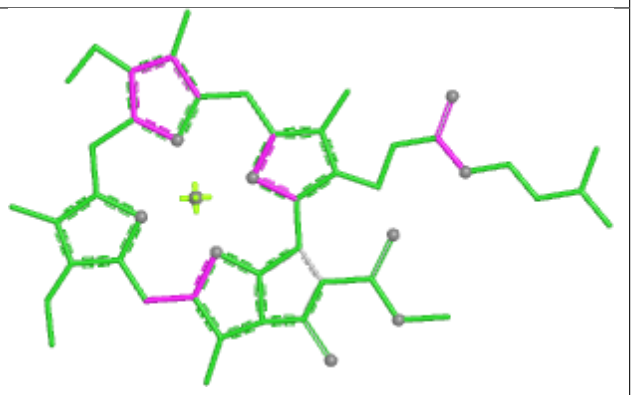


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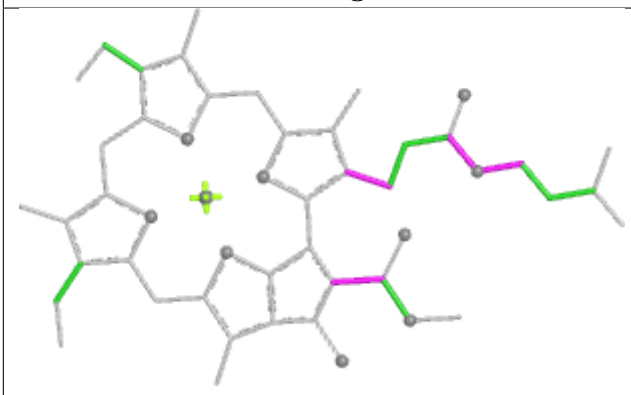
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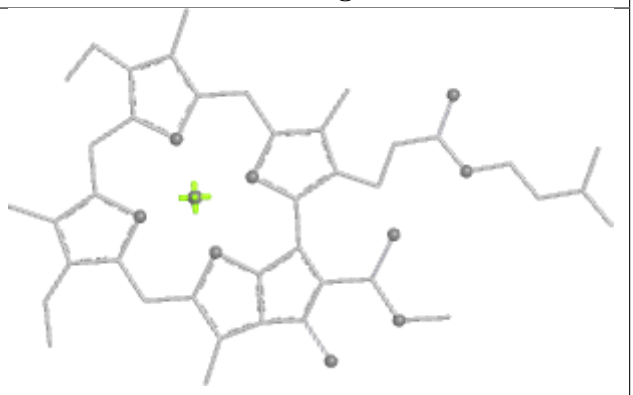
Bond lengths



Bond angles

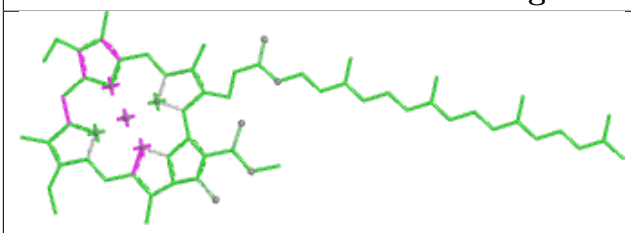


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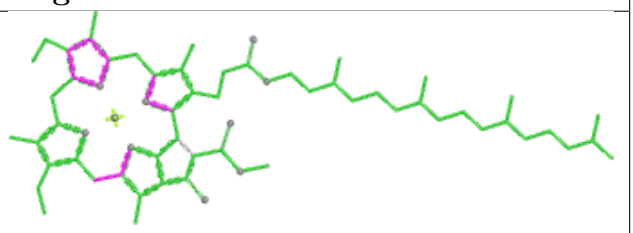


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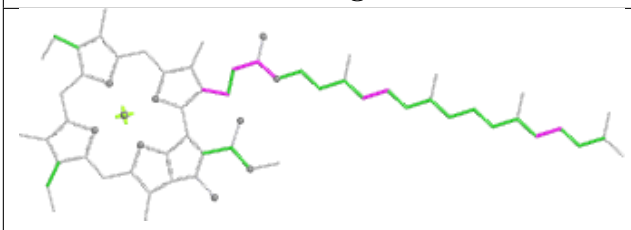
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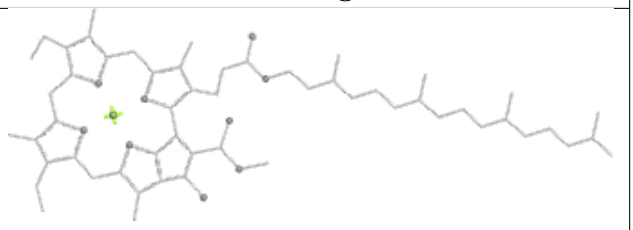
Bond lengths



Bond angles

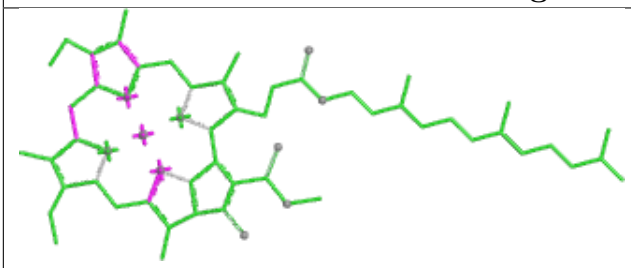


Torsions

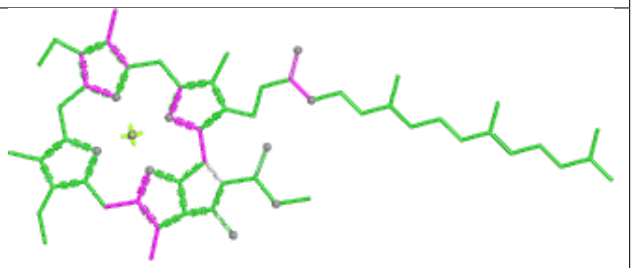


Rings

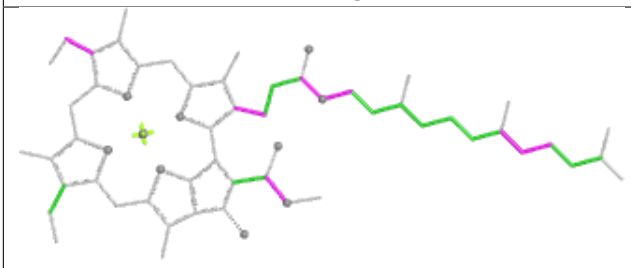
Ligand CLA s 506



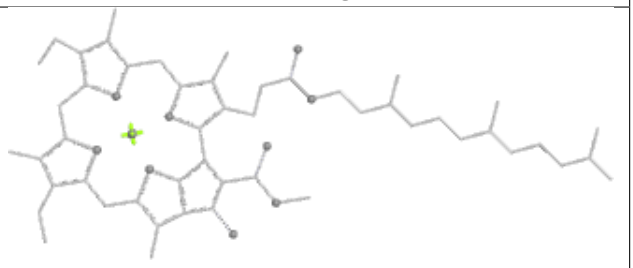
Bond lengths



Bond angles

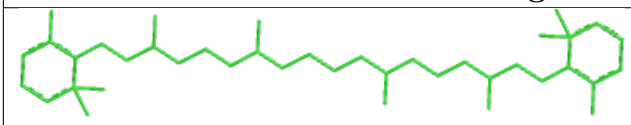


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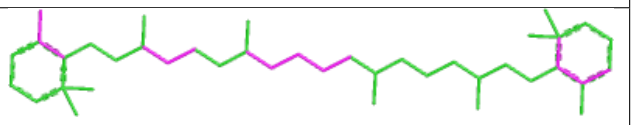


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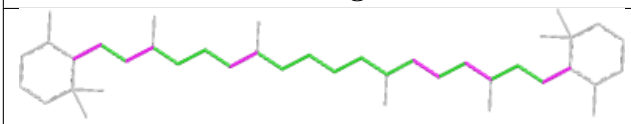
Ligand BCR r 603



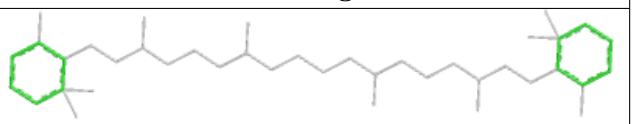
Bond lengths



Bond angles

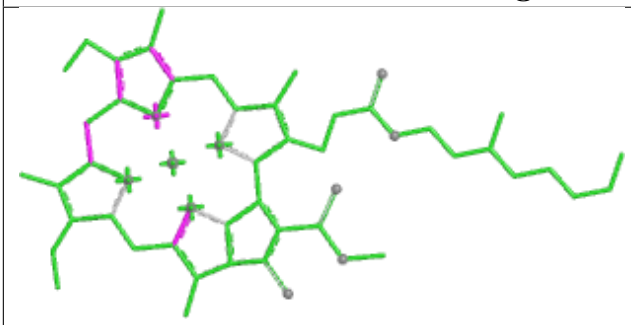


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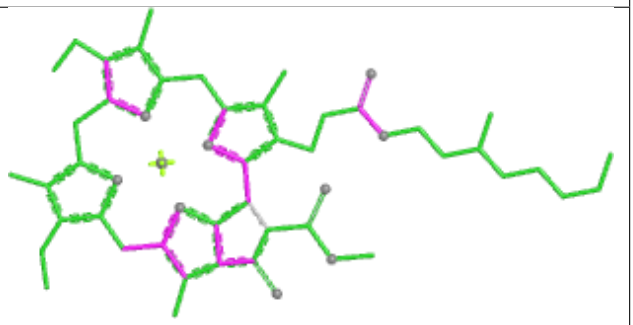


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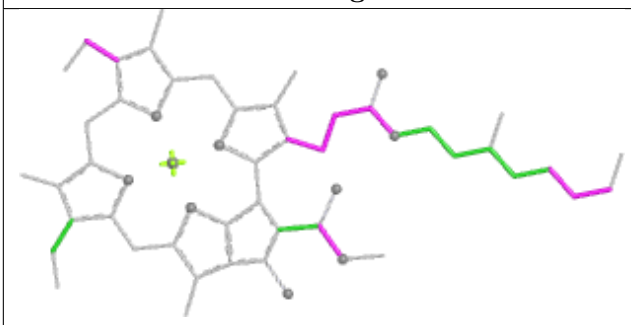
Ligand CLA A 1116



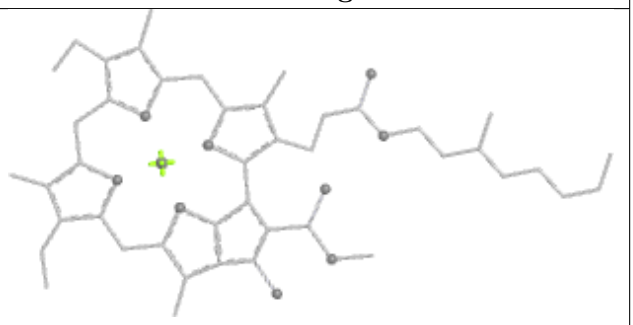
Bond lengths



Bond angles

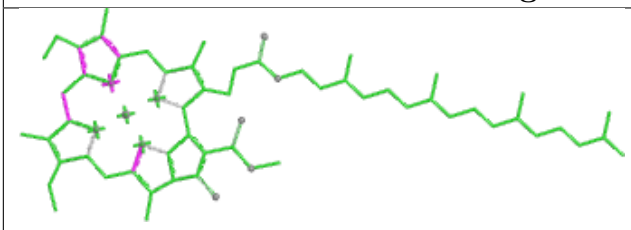


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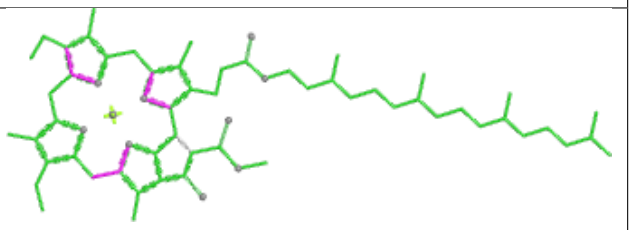


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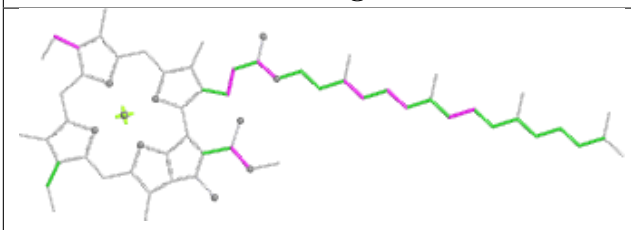
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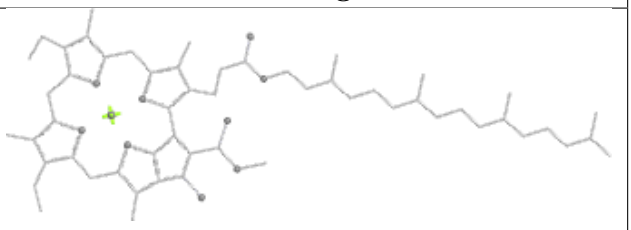
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Bond angles

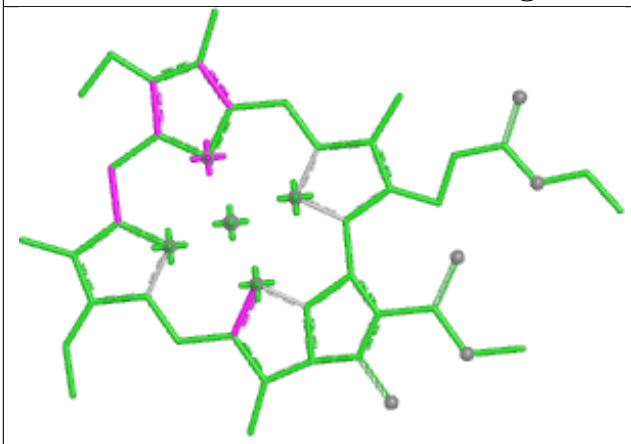


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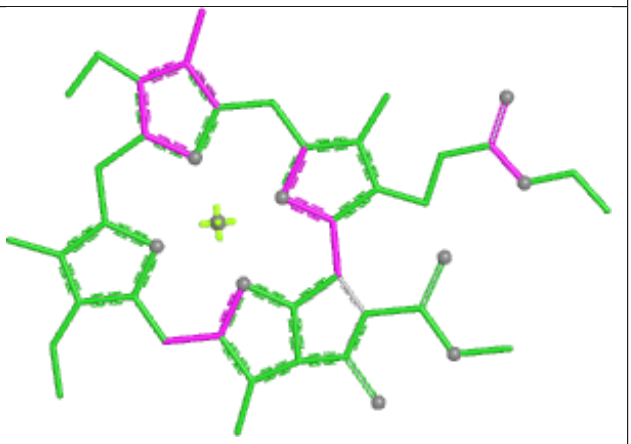


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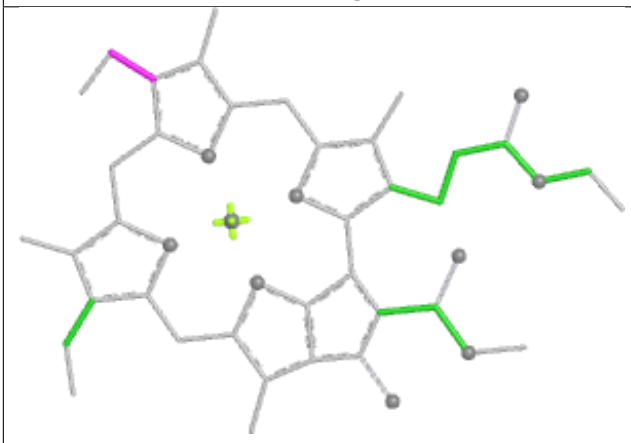
Ligand CLA b 1216



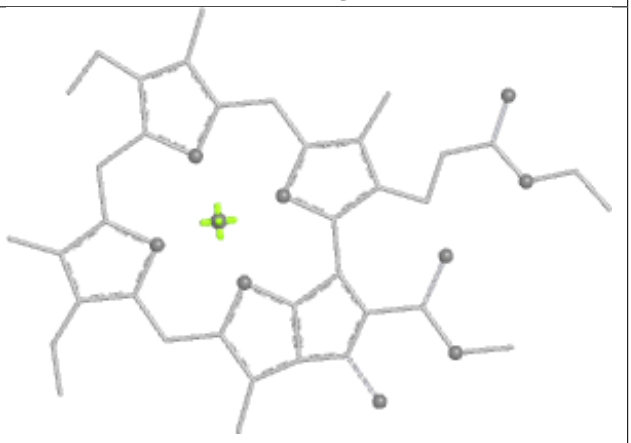
Bond lengths



Bond angles

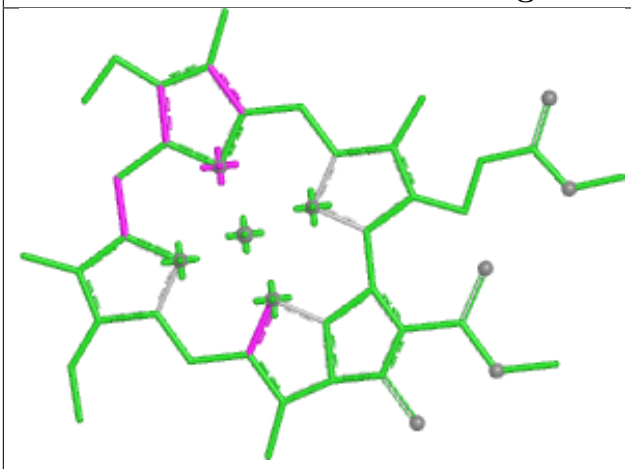


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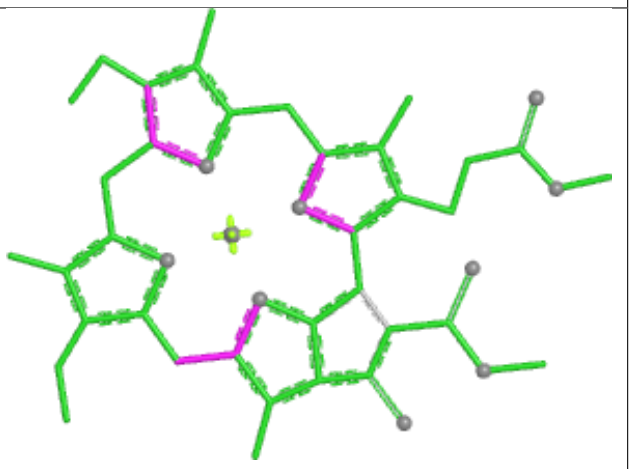


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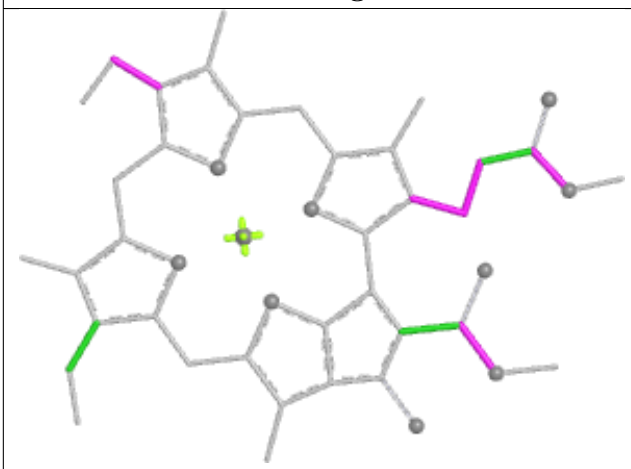
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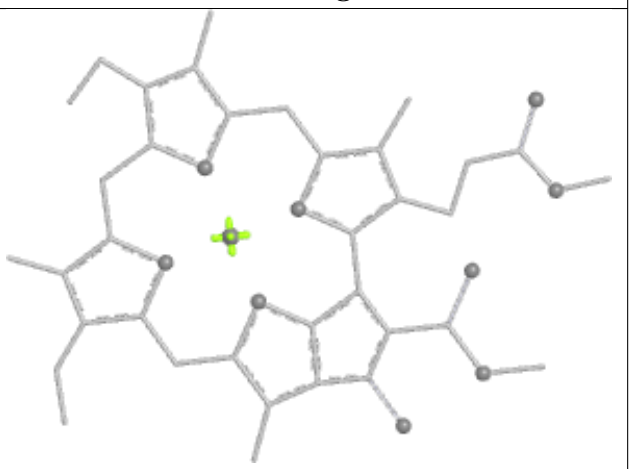
Bond lengths



Bond angles



Torsions

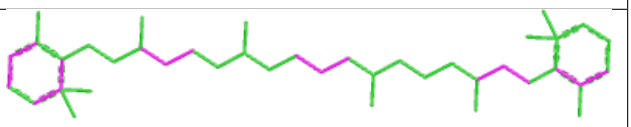


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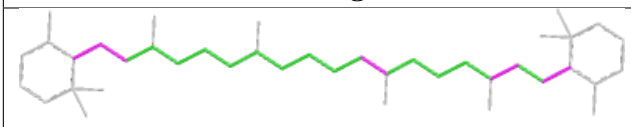
Ligand BCR K 4005



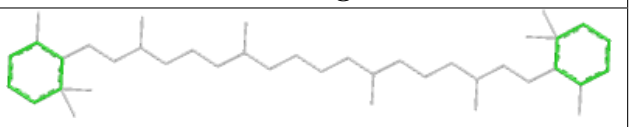
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Bond angles

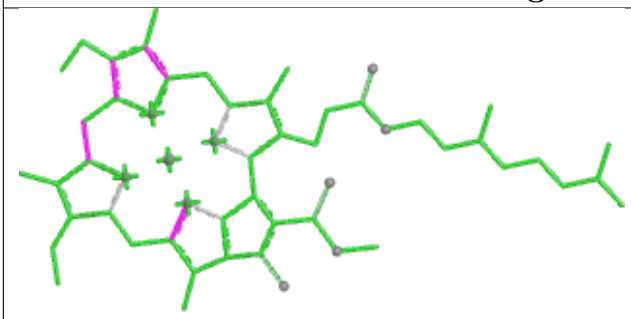


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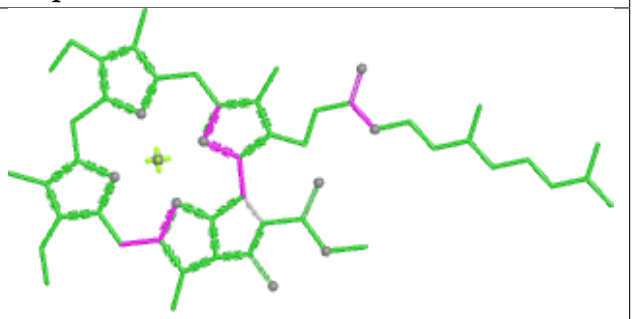


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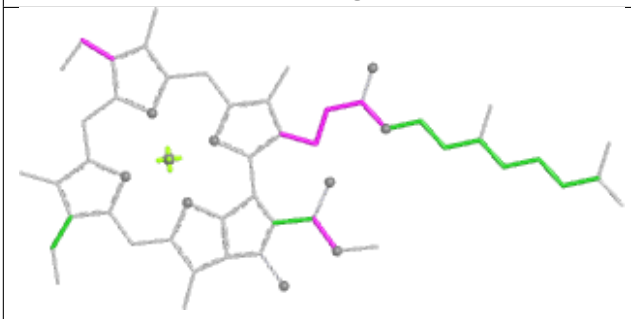
Ligand CLA p 508



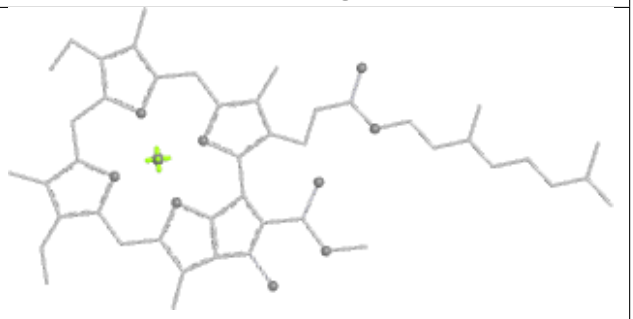
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Bond angles

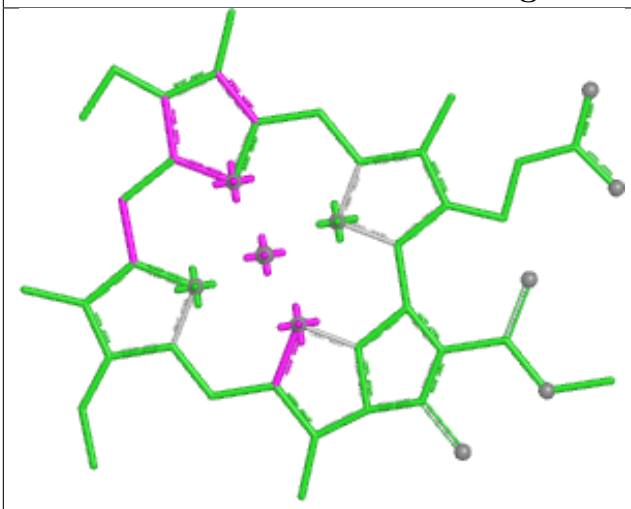


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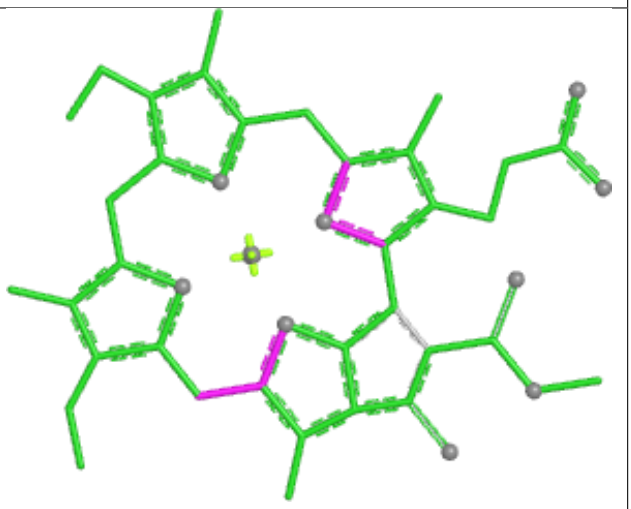


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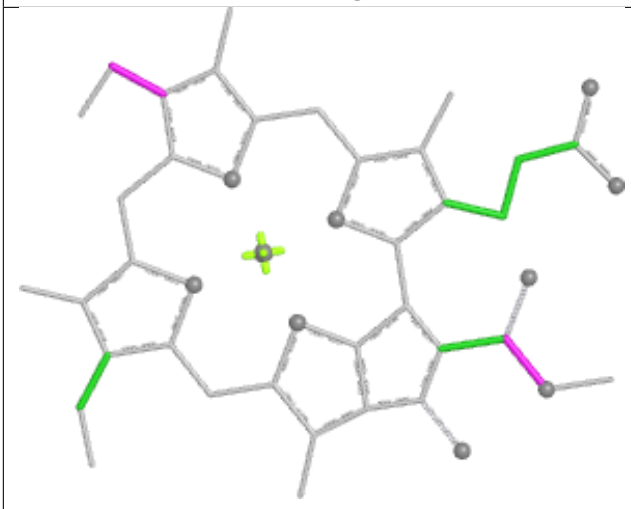
Ligand CLA a 1113



Bond lengths



Bond angles

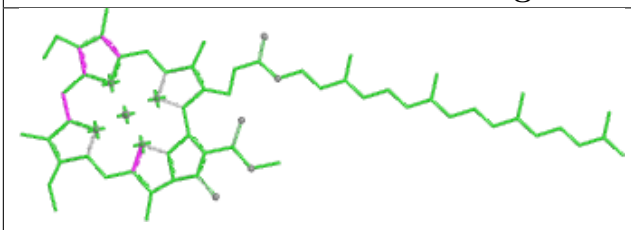


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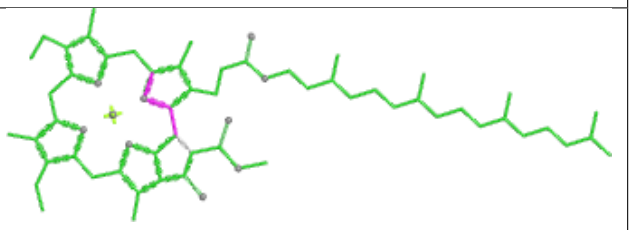


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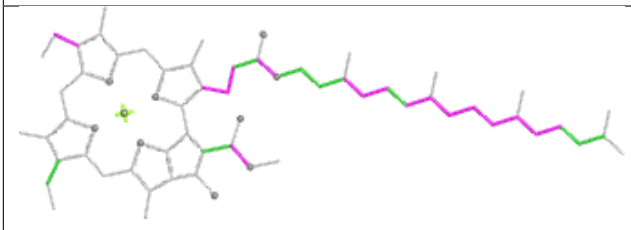
Ligand CLA G 1211



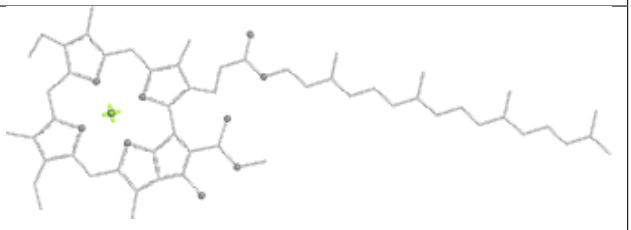
Bond lengths



Bond angles

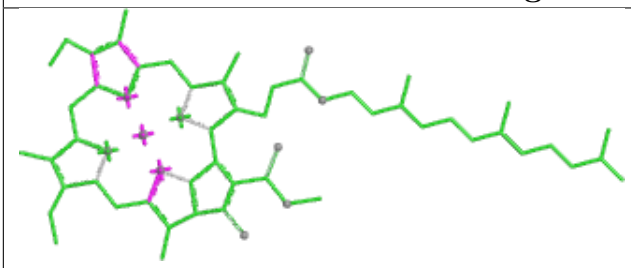


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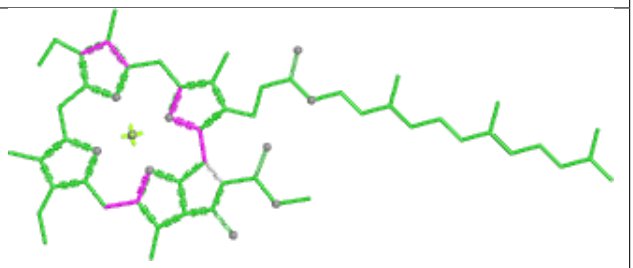


Rings

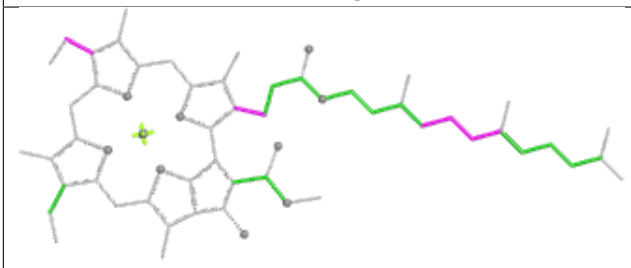
Ligand CLA w 506



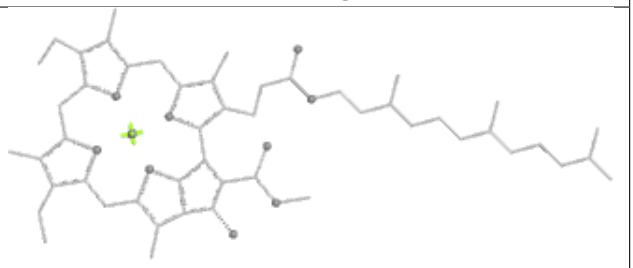
Bond lengths



Bond angles

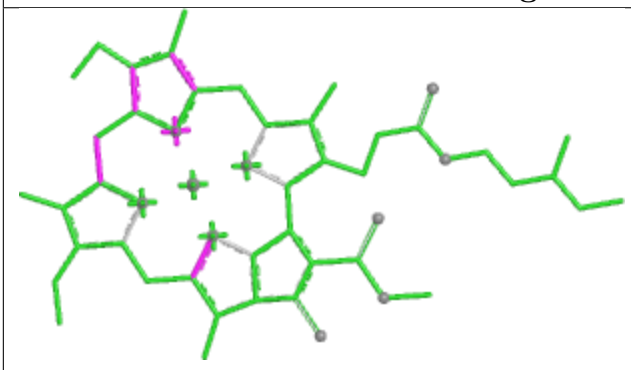


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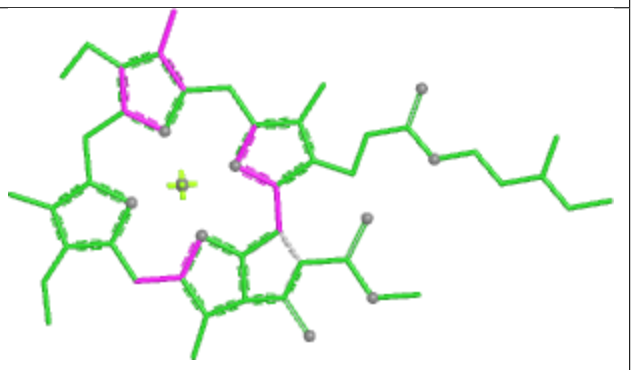


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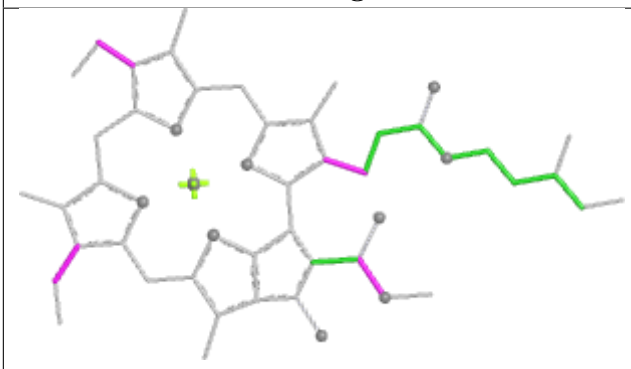
Ligand CLA a 1121



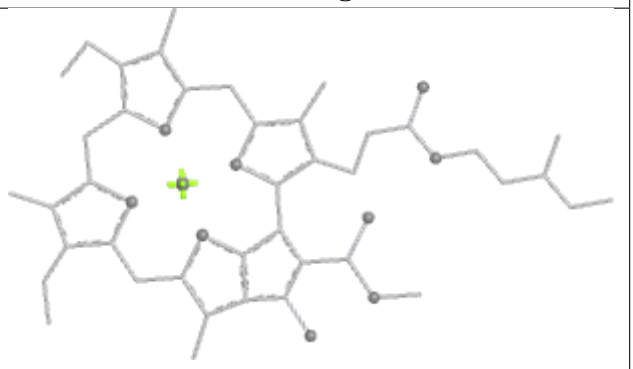
Bond lengths



Bond angles

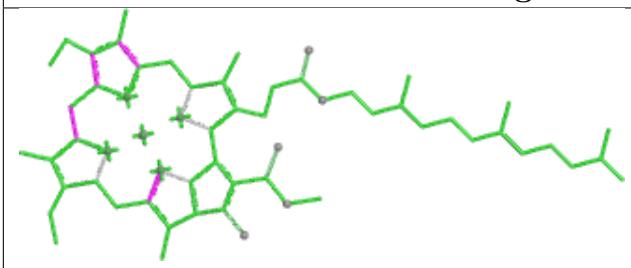


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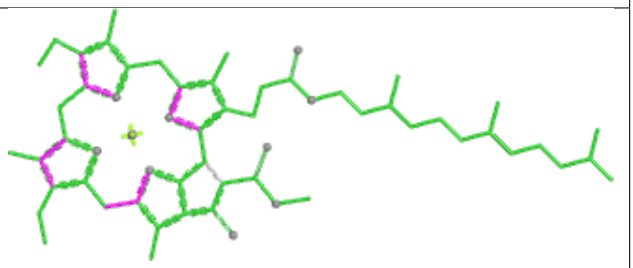


Rings

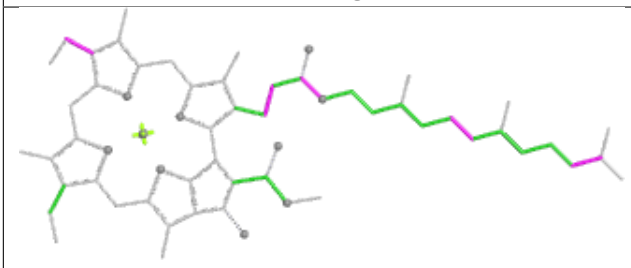
Ligand CLA A 1124



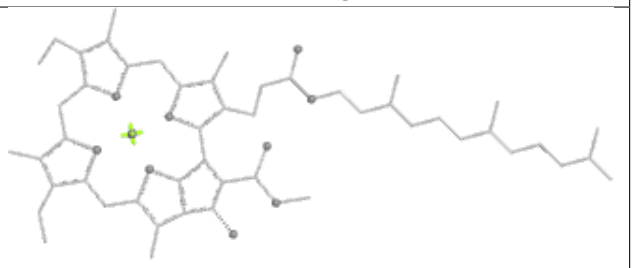
Bond lengths



Bond angles

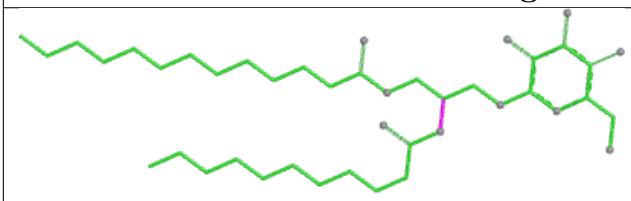


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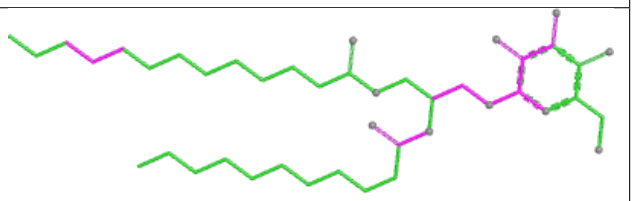


Rings

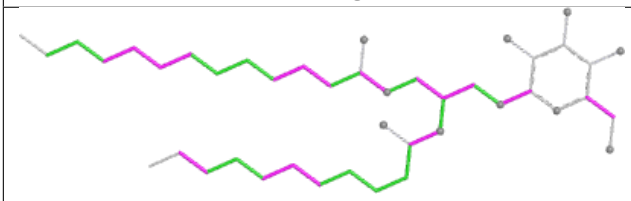
Ligand LMG B 848



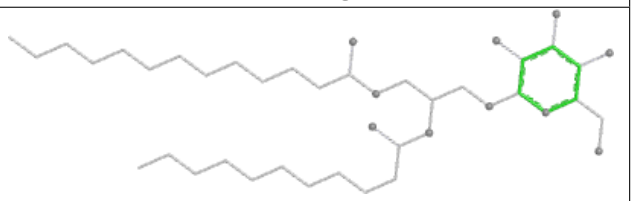
Bond lengths



Bond angles

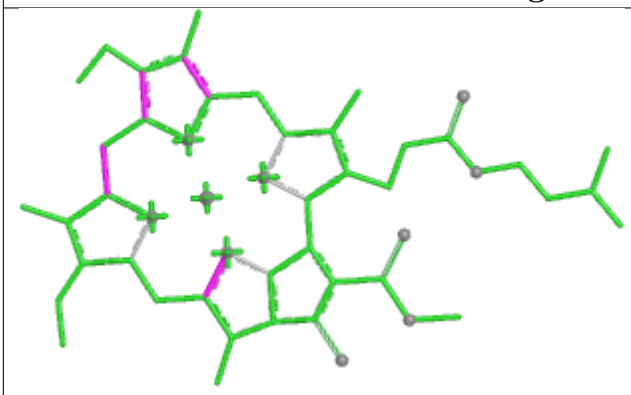


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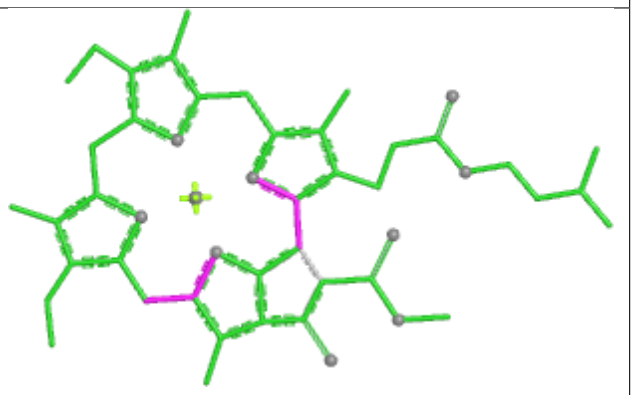


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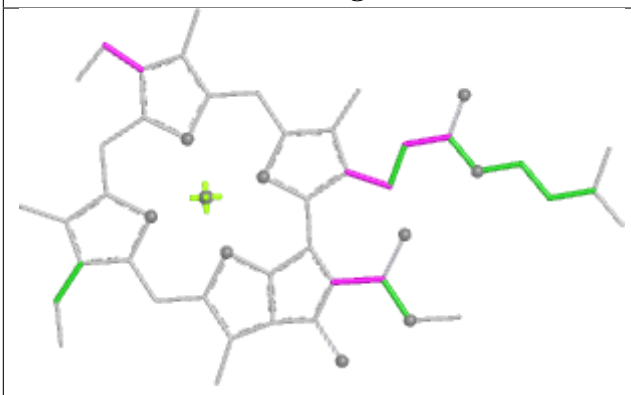
Ligand CLA v 514



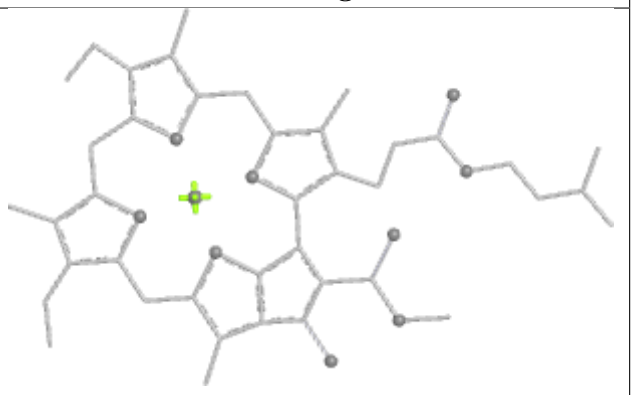
Bond lengths



Bond angles



Torsions

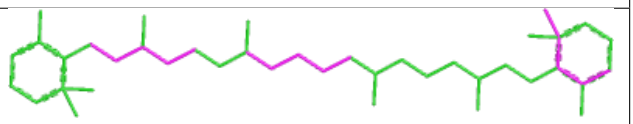


Rings

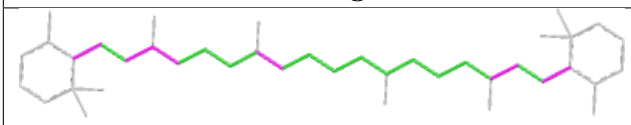
Ligand BCR F 4016



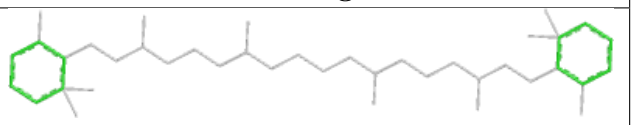
Bond lengths



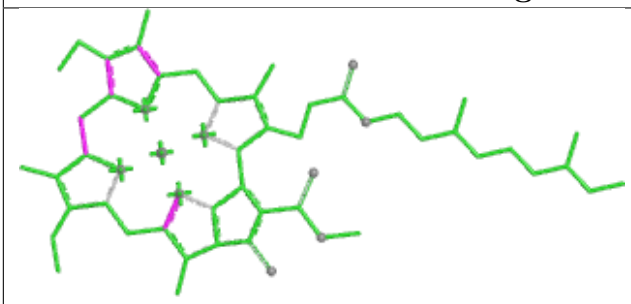
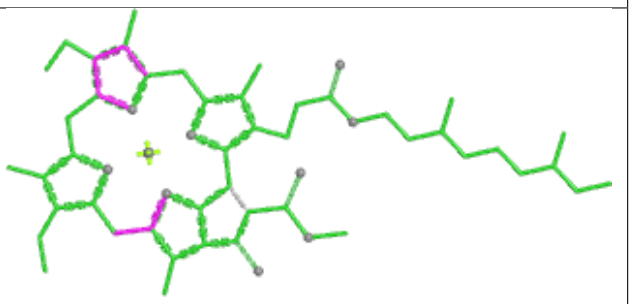
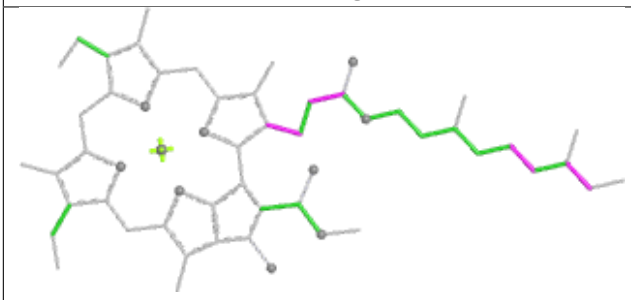
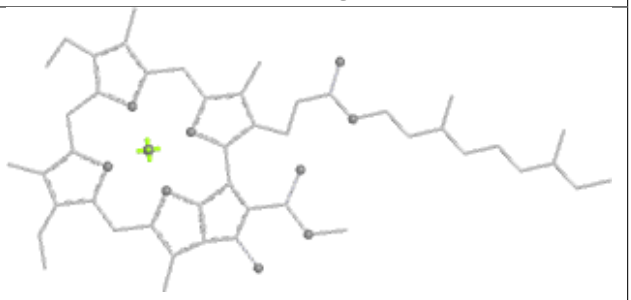
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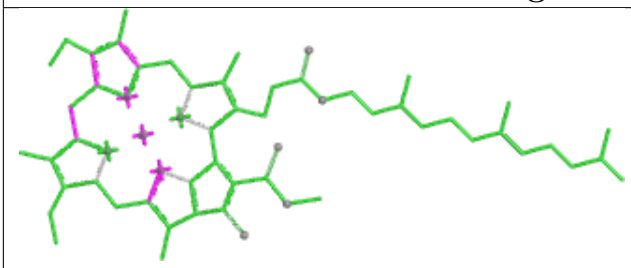
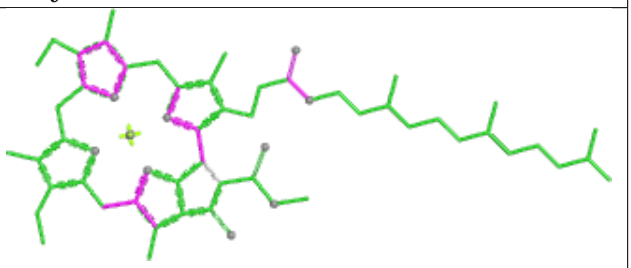
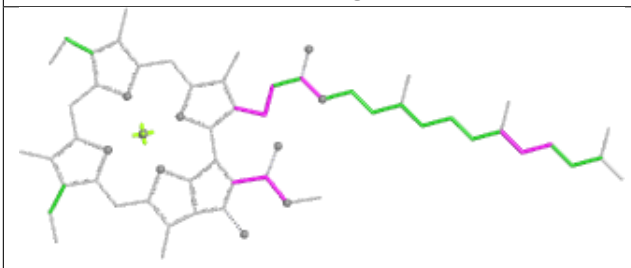
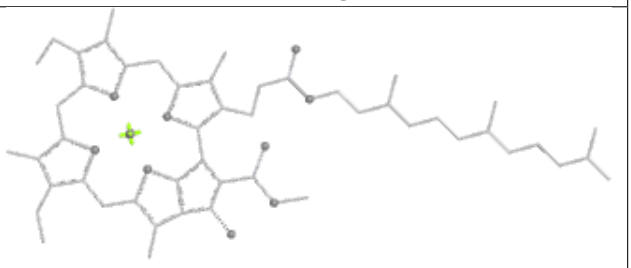


Torsions

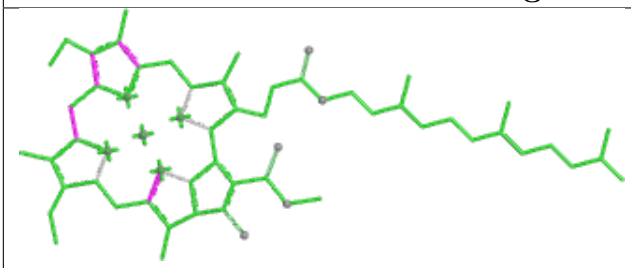


Rings

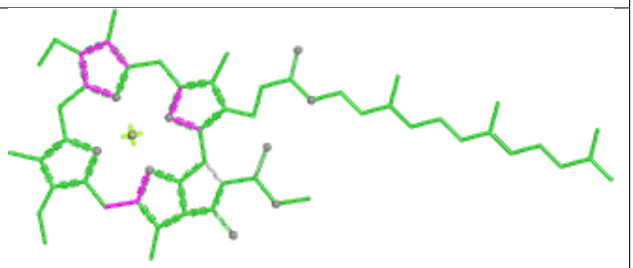
Ligand CLA A 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA y 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

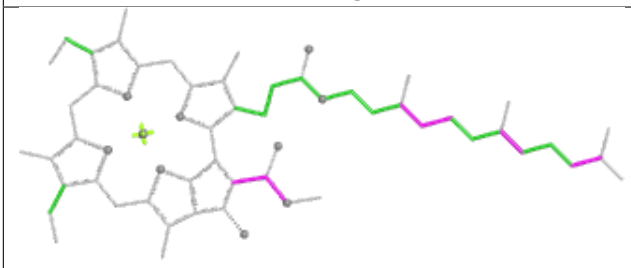
Ligand CLA X 510



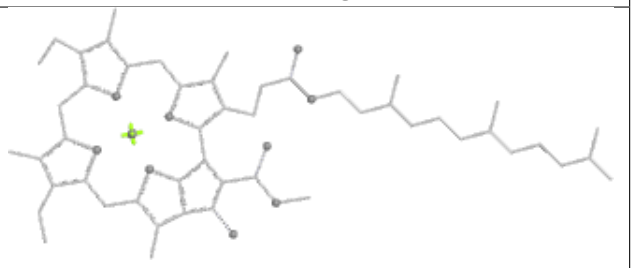
Bond lengths



Bond angles

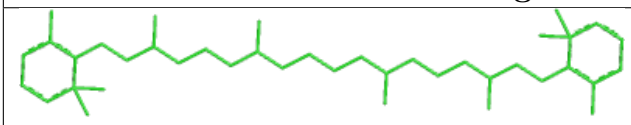


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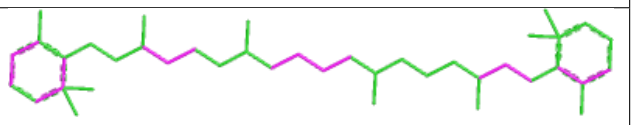


Rings

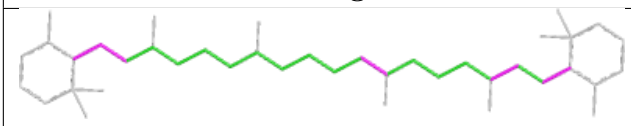
Ligand BCR T 4005



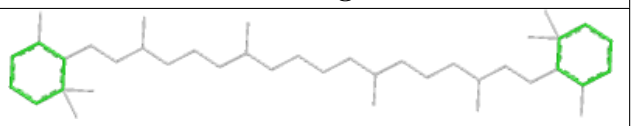
Bond lengths



Bond angles

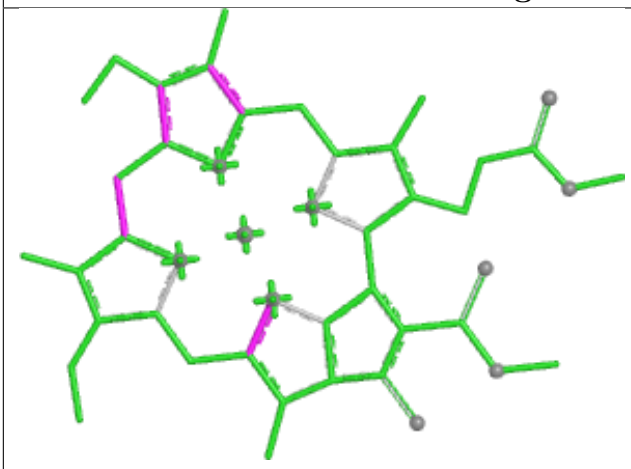


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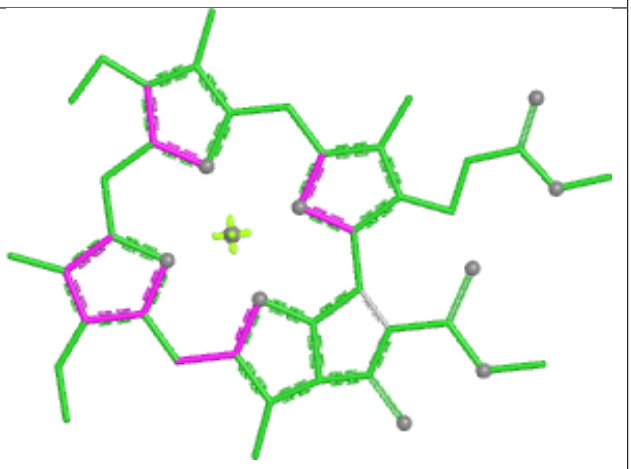


Rings

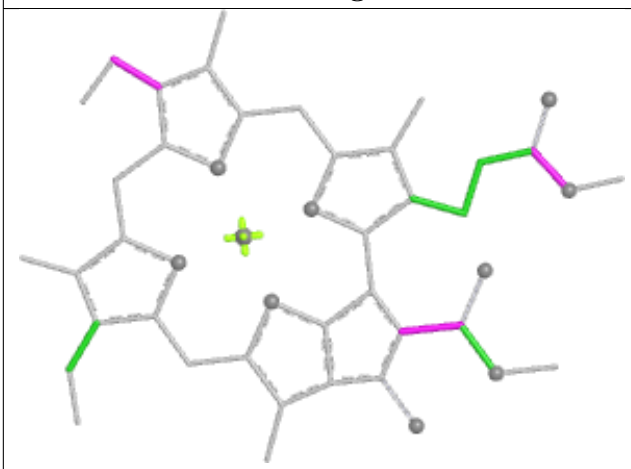
Ligand CLA H 1801



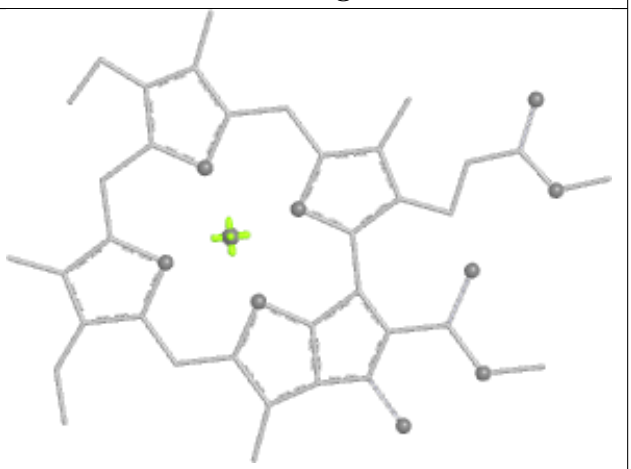
Bond lengths



Bond angles

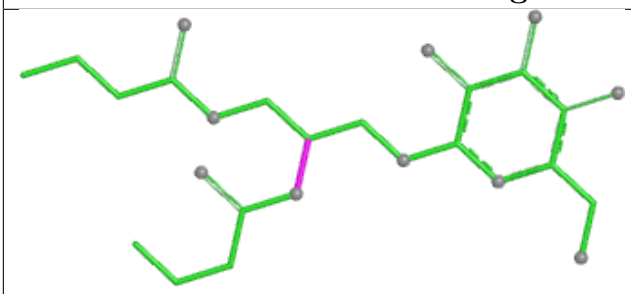


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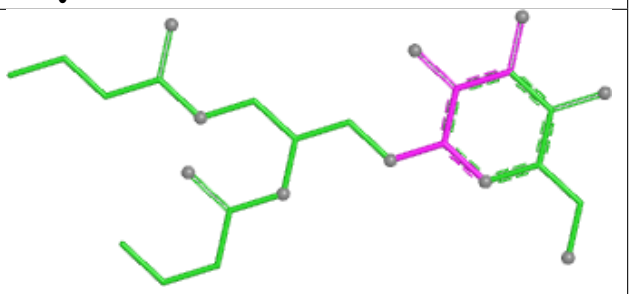


Rings

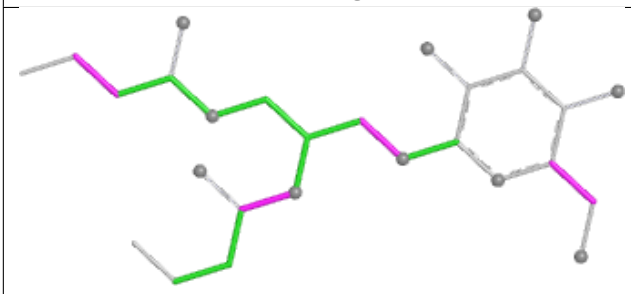
Ligand LMG Q 4017



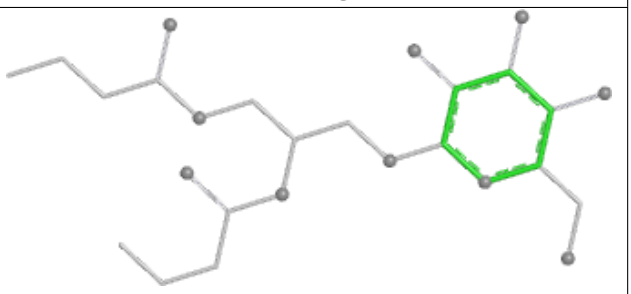
Bond lengths



Bond angles

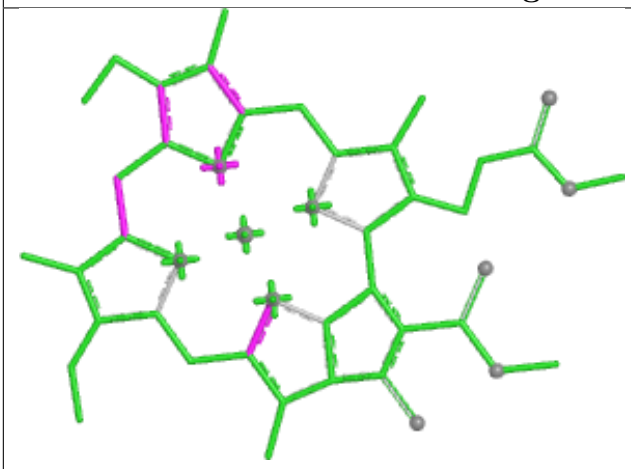


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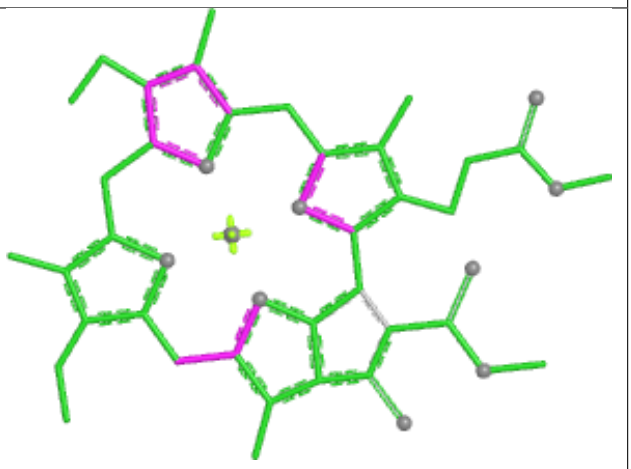


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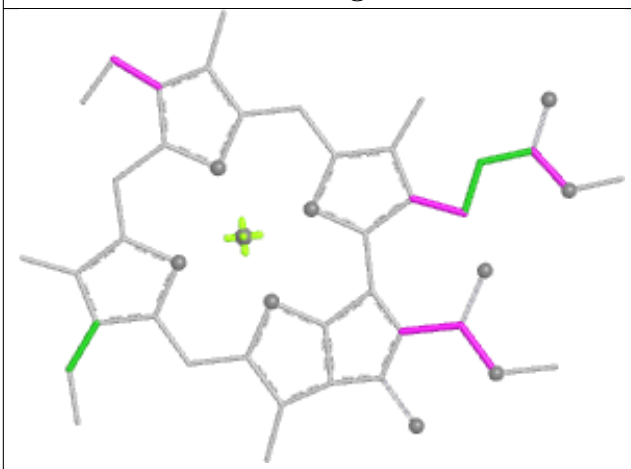
Ligand CLA f 1302



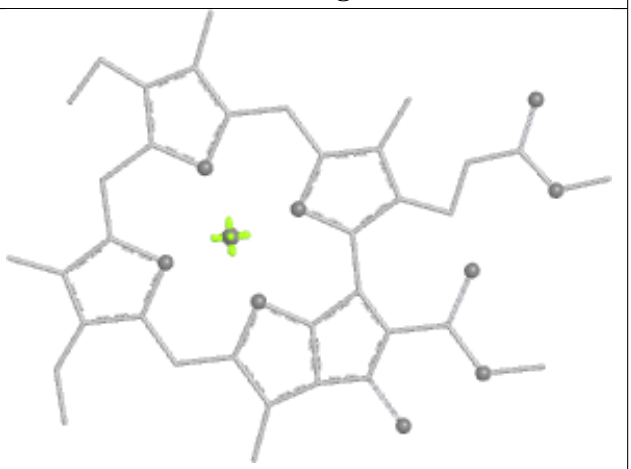
Bond lengths



Bond angles



Torsions

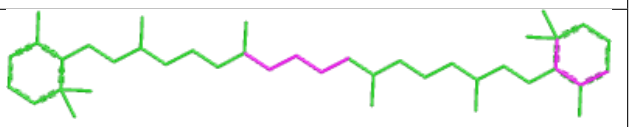


Rings

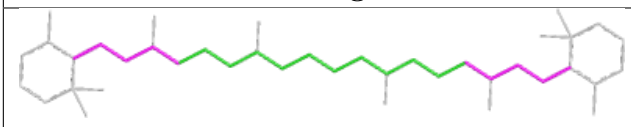
Ligand BCR X 603



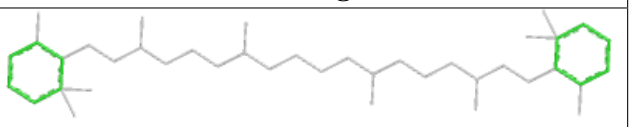
Bond lengths



Bond angles

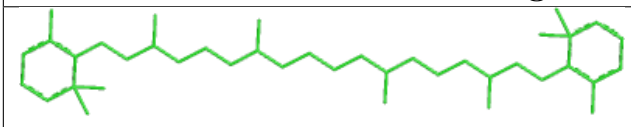


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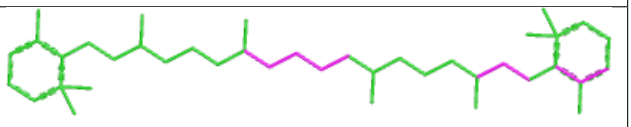


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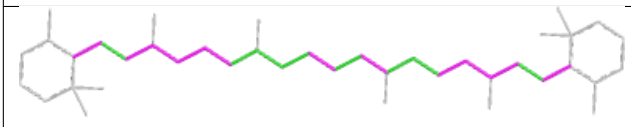
Ligand BCR r 602



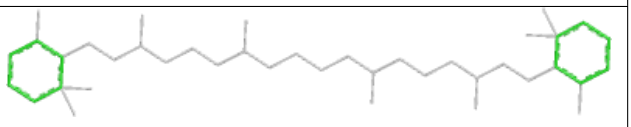
Bond lengths



Bond angles

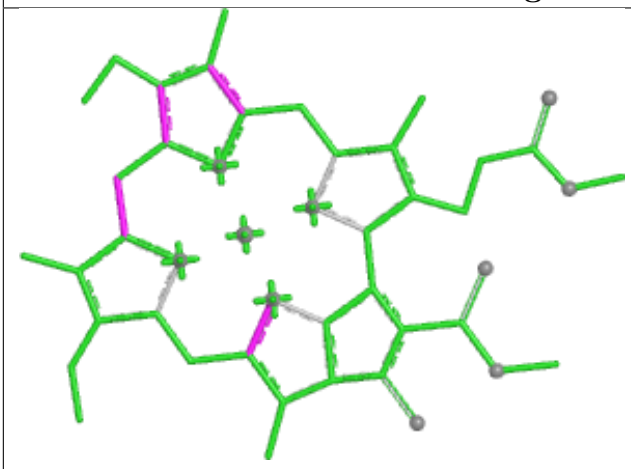


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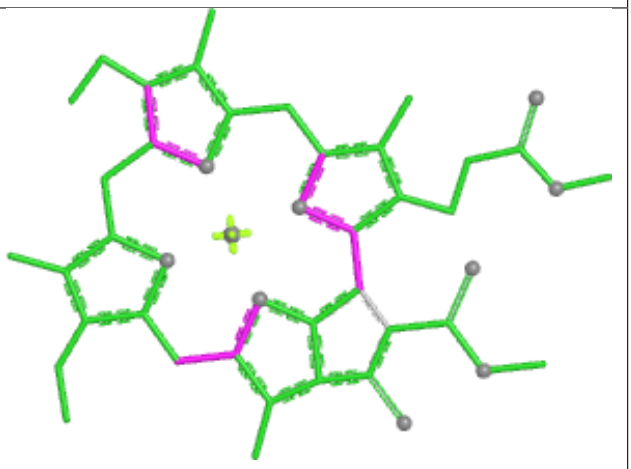


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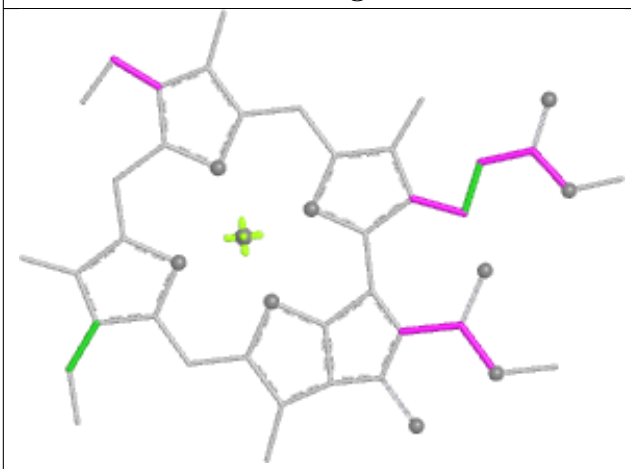
Ligand CLA w 516



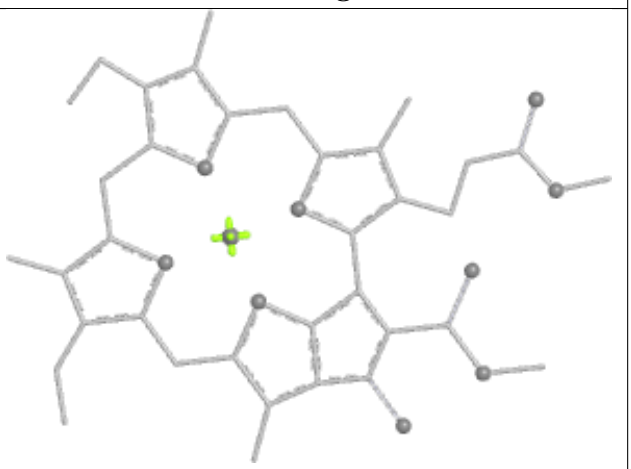
Bond lengths



Bond angles

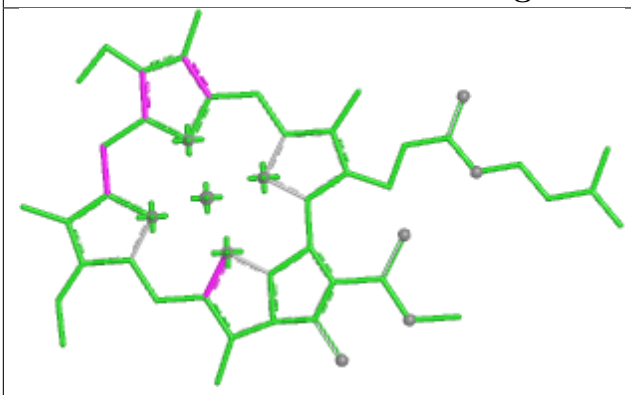


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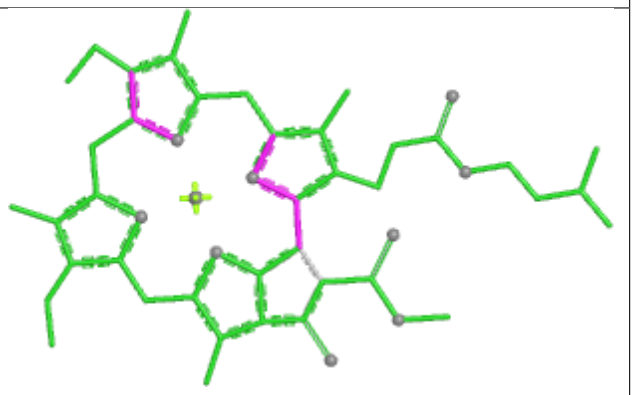


Rings

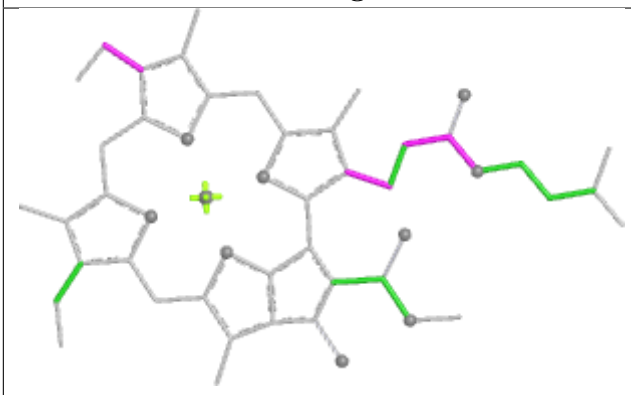
Ligand CLA G 1236



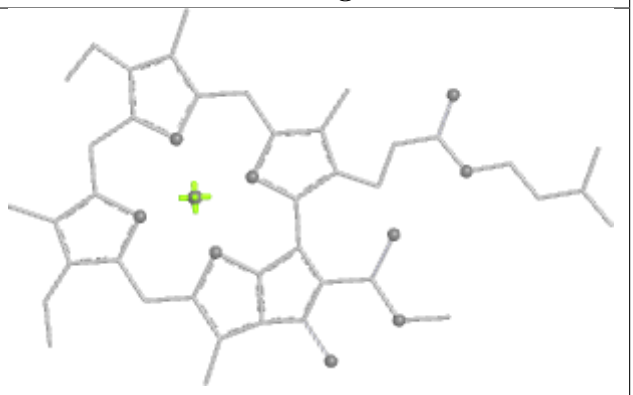
Bond lengths



Bond angles



Torsions

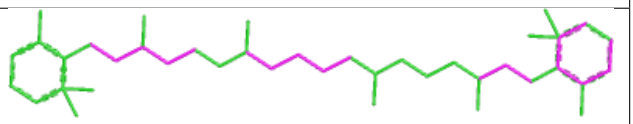


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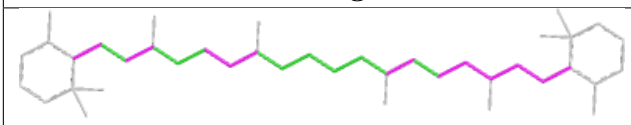
Ligand BCR W 601



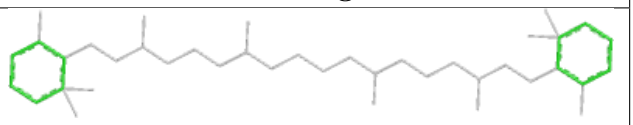
Bond lengths



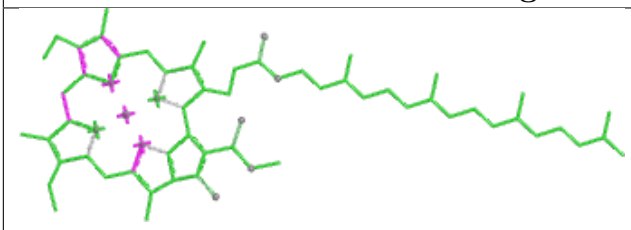
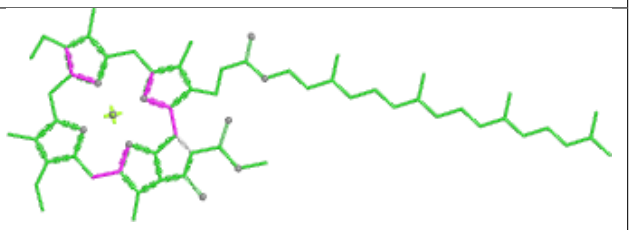
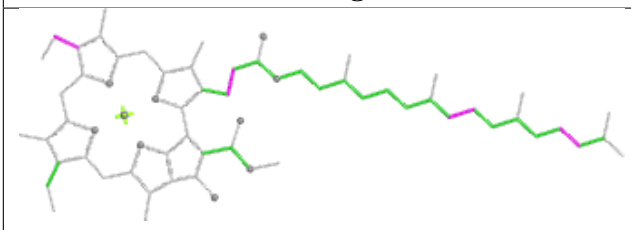
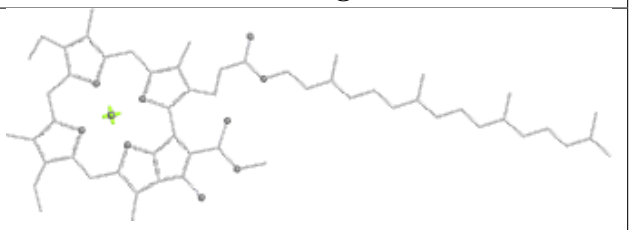
Bond angles

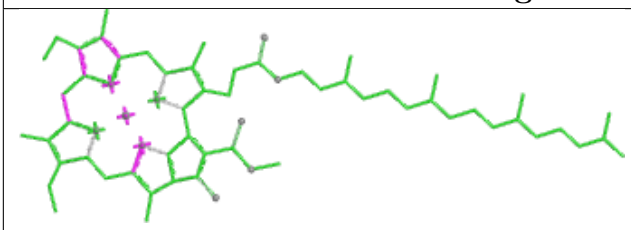
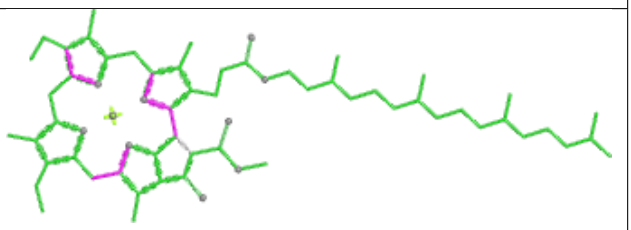
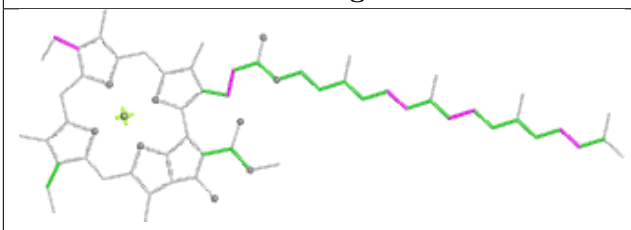
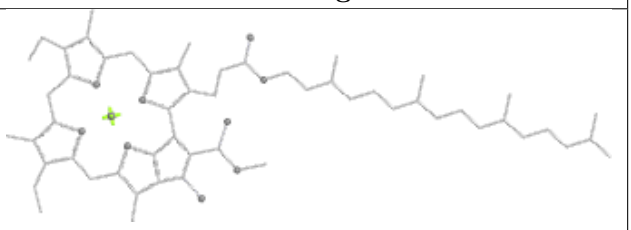


Torsions

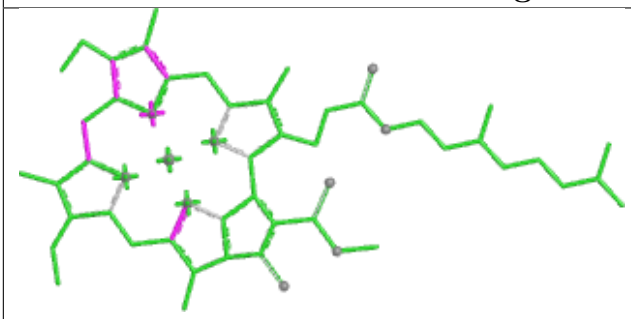


Rings

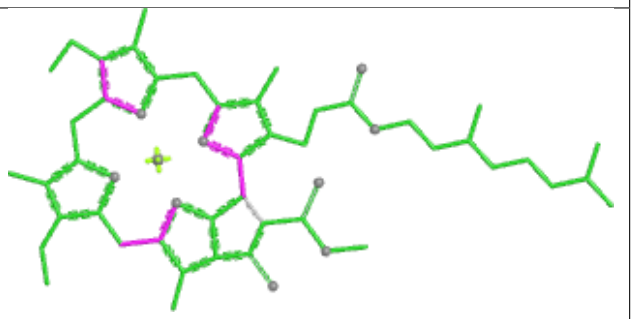
Ligand CLA a 1127	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 1127	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

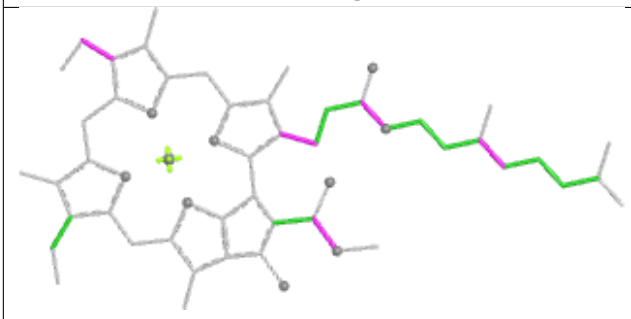
Ligand CLA G 1213



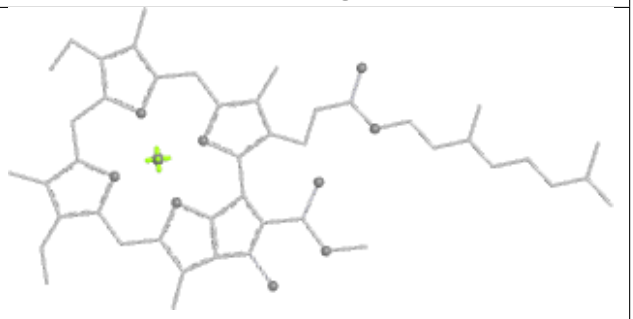
Bond lengths



Bond angles

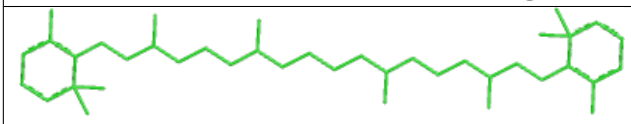


Torsions

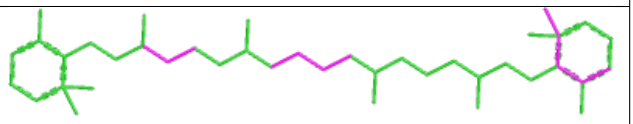


Rings

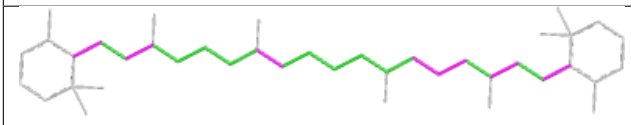
Ligand BCR f 4016



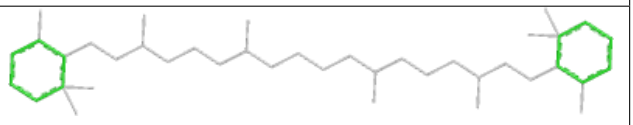
Bond lengths



Bond angles

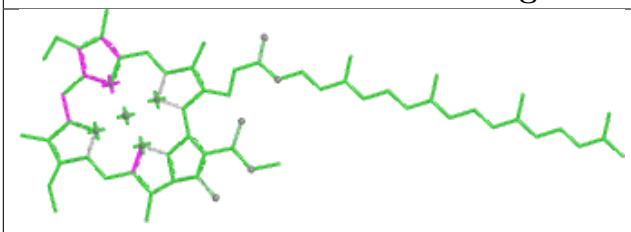


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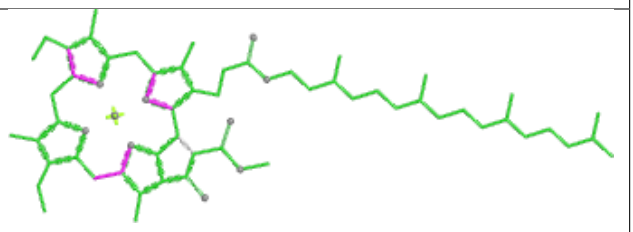


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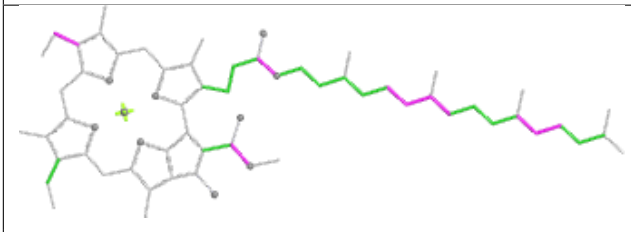
Ligand CLA a 1131



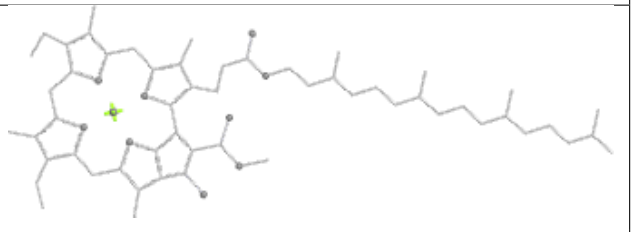
Bond lengths



Bond angles

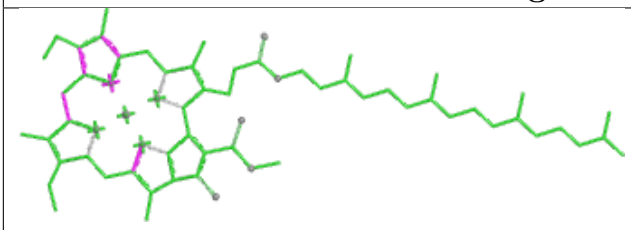


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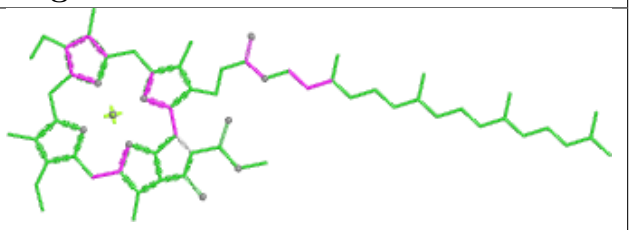


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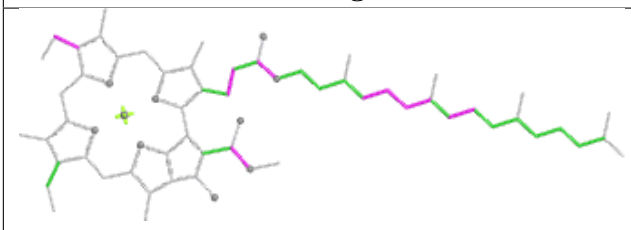
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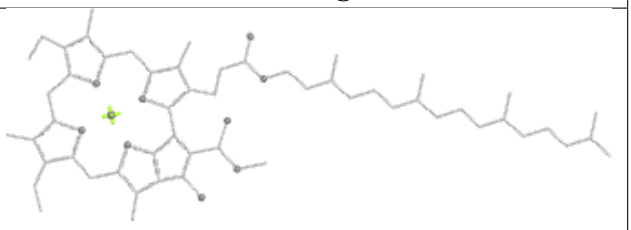
Bond lengths



Bond angles

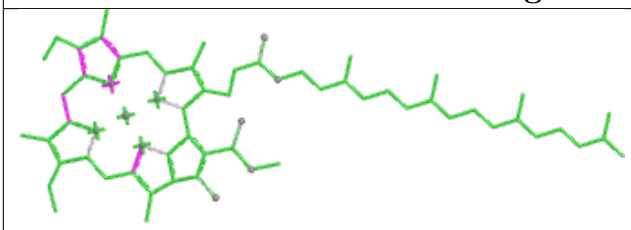


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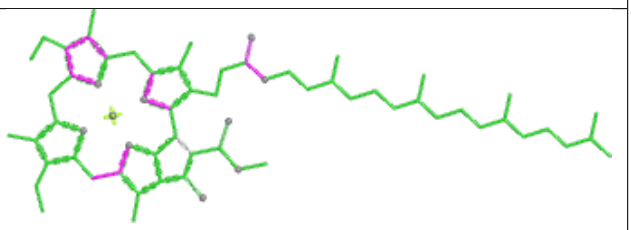


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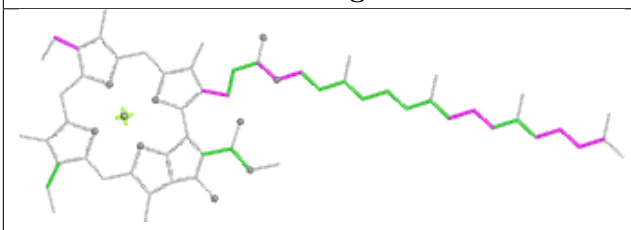
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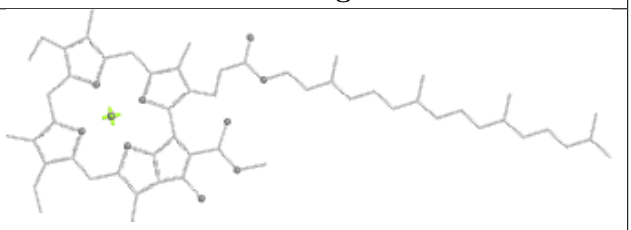
Bond lengths



Bond angles

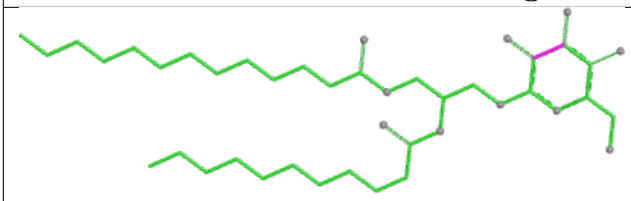


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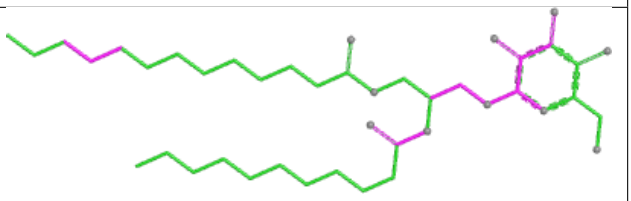


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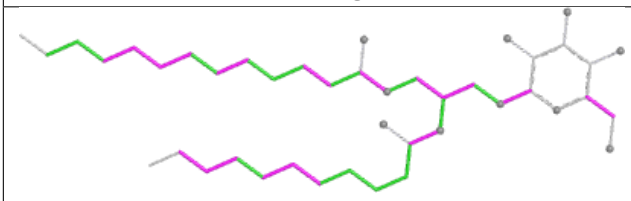
Ligand LMG b 848



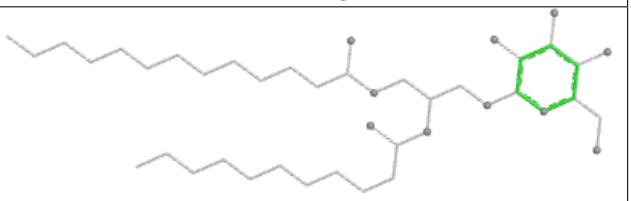
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Bond angles

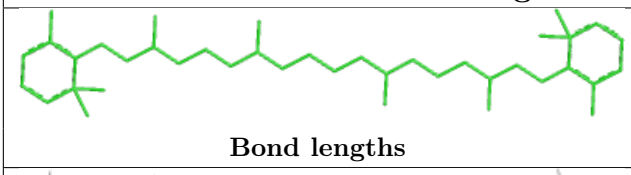


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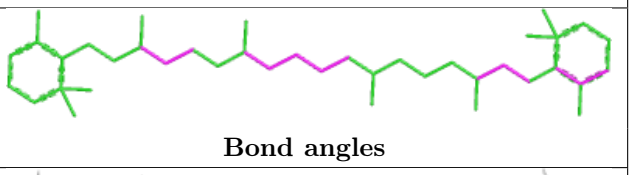


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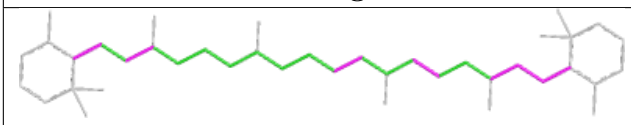
Ligand BCR B 4004



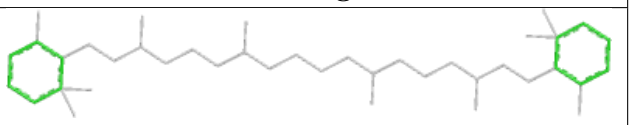
Bond lengths



Bond angles

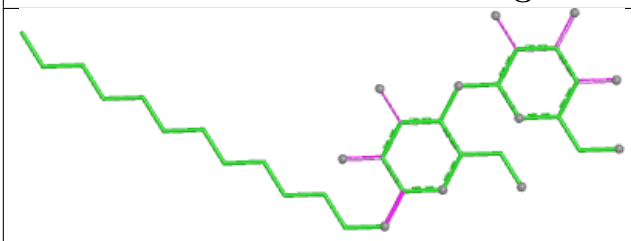


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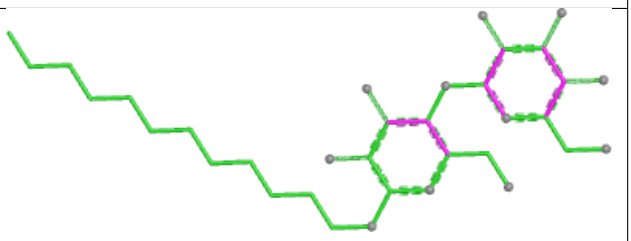


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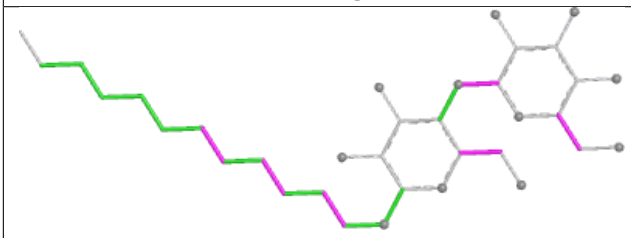
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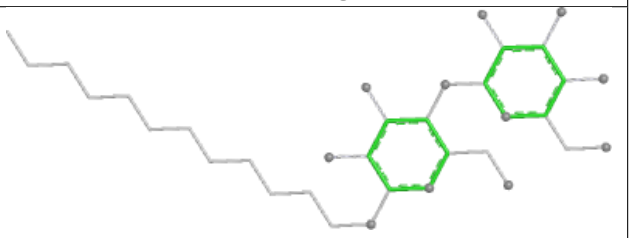
Bond lengths



Bond angles

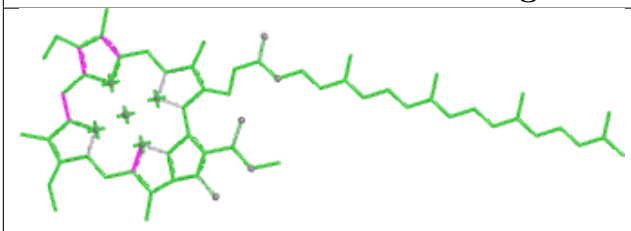


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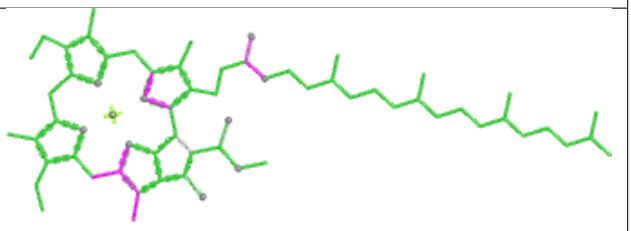


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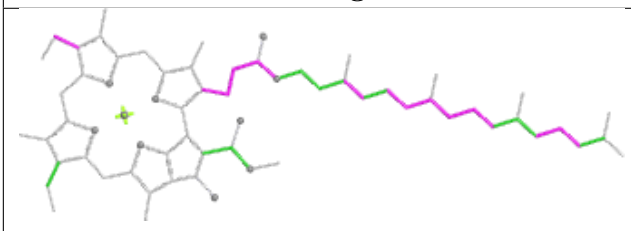
Ligand CLA a 1101



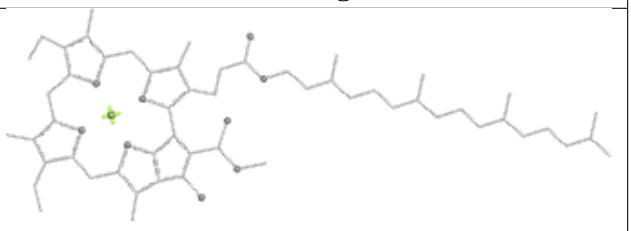
Bond lengths



Bond angles

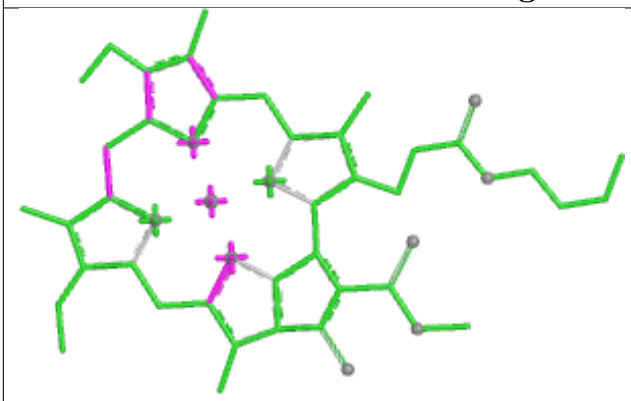


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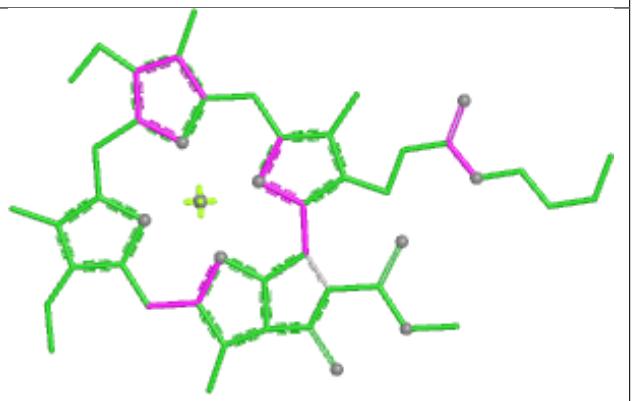


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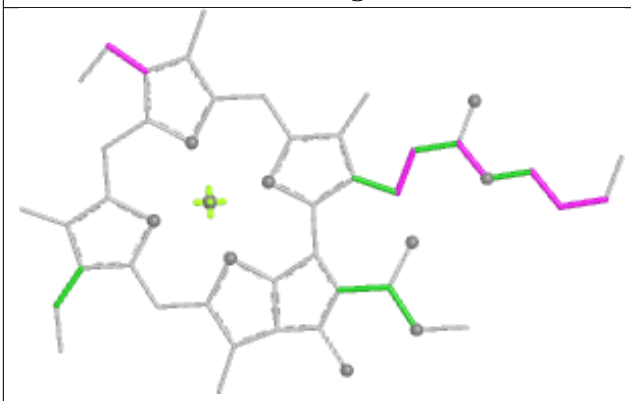
Ligand CLA b 1227



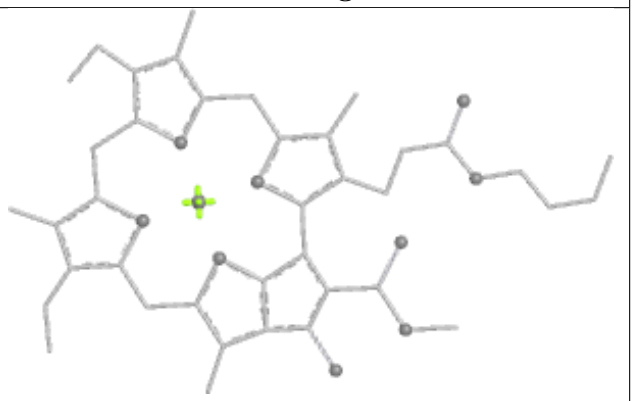
Bond lengths



Bond angles

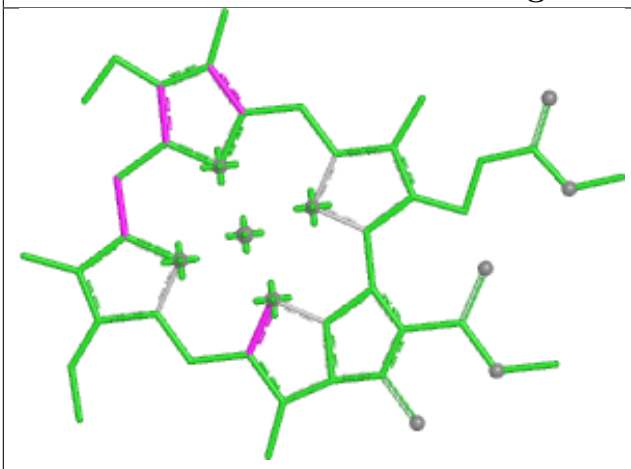


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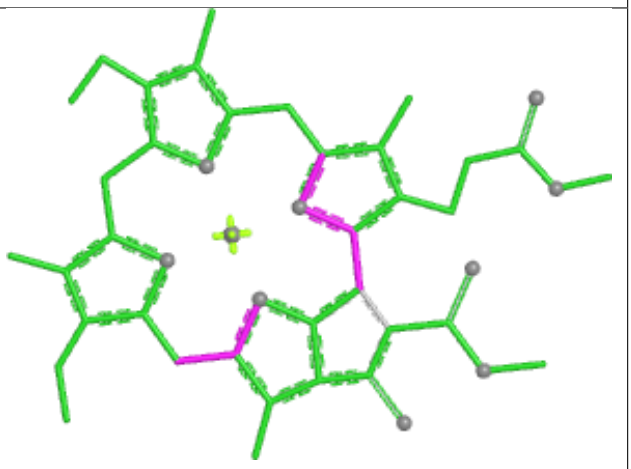


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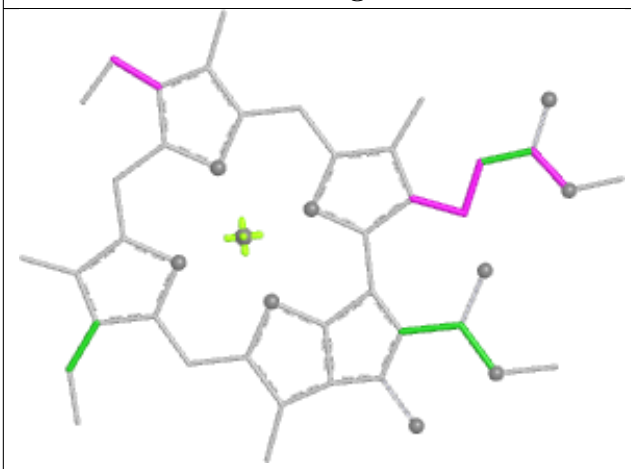
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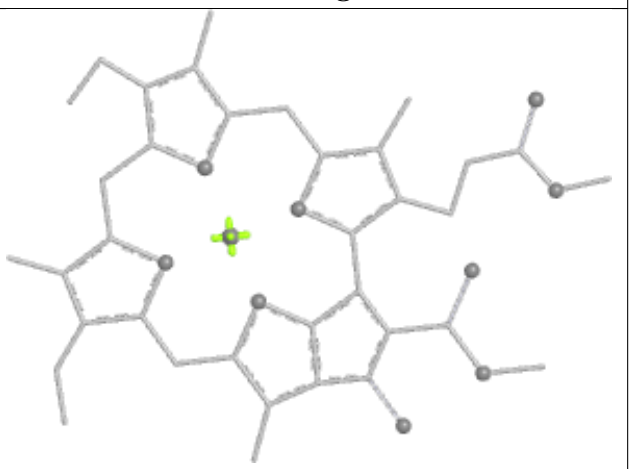
Bond lengths



Bond angles



Torsions

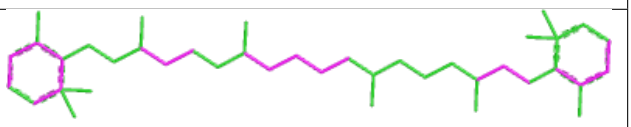


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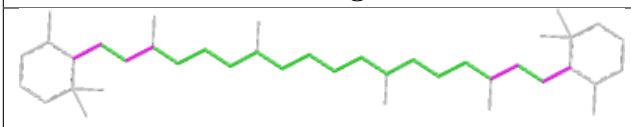
Ligand BCR u 601



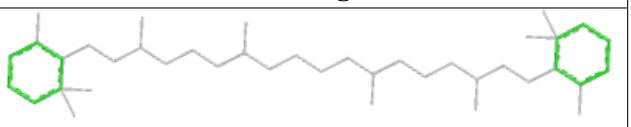
Bond lengths



Bond angles

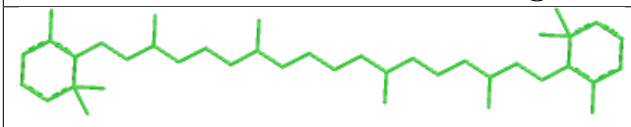


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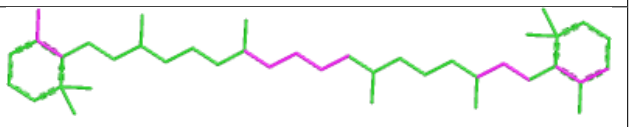


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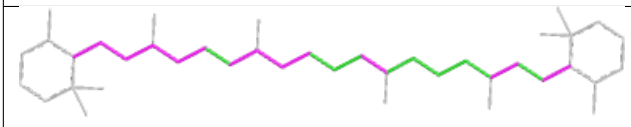
Ligand BCR s 604



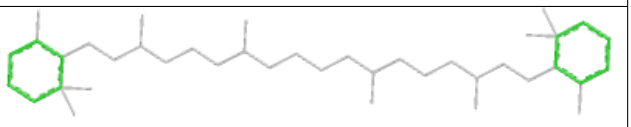
Bond lengths



Bond angles

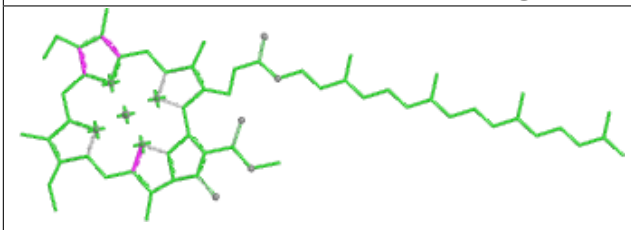


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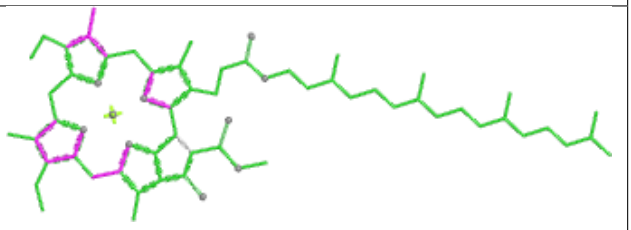


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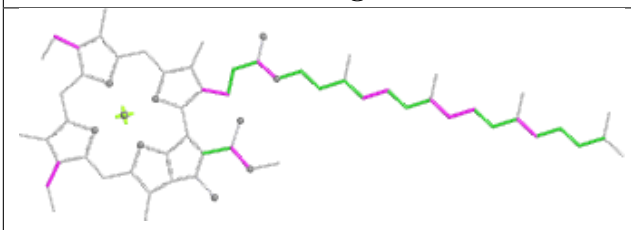
Ligand CLA B 1239



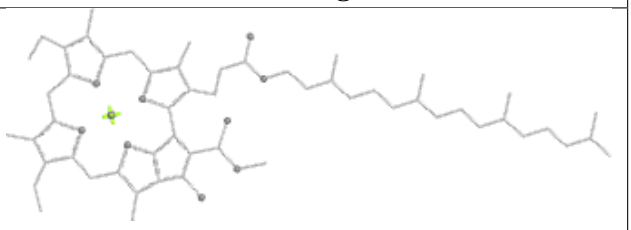
Bond lengths



Bond angles



Torsions

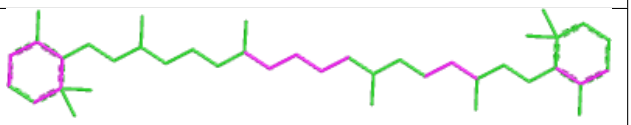


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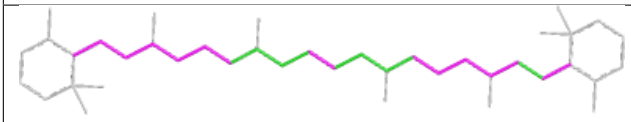
Ligand BCR X 602



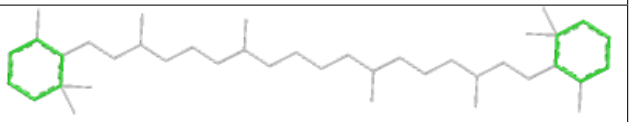
Bond lengths



Bond angles

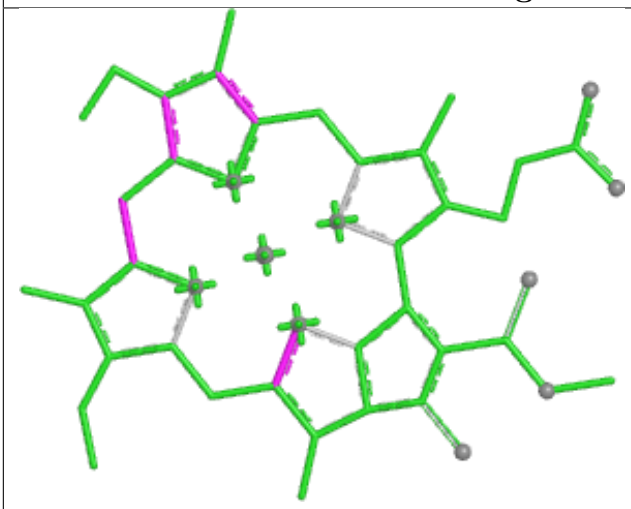


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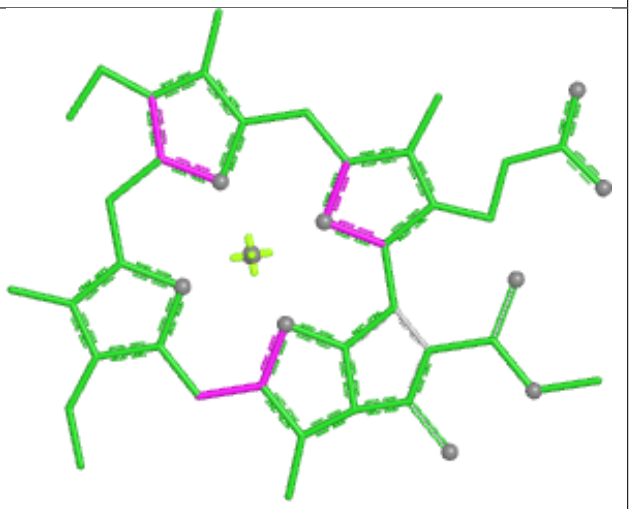


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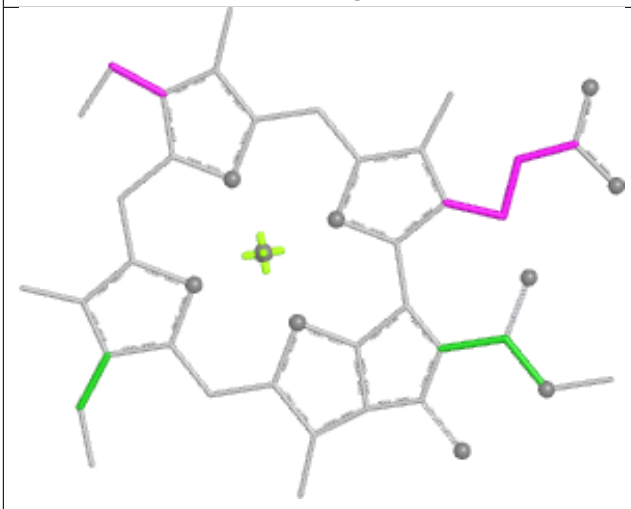
Ligand CLA B 1209



Bond lengths



Bond angles

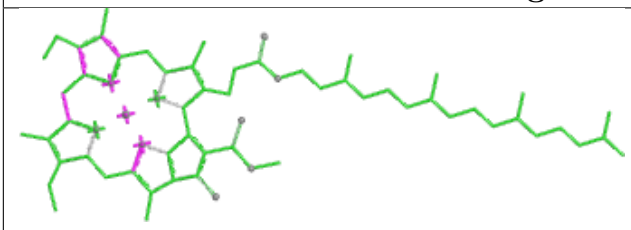


Torsions

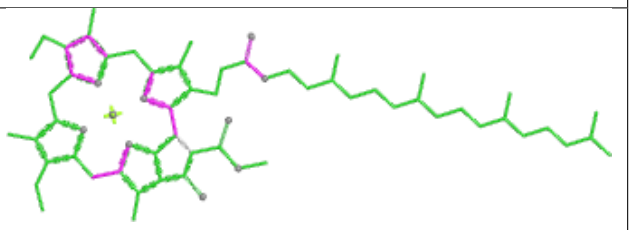


Rings

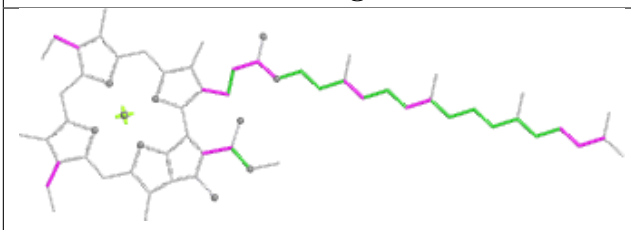
Ligand CLA h 509



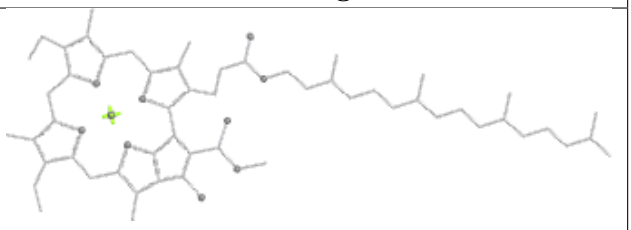
Bond lengths



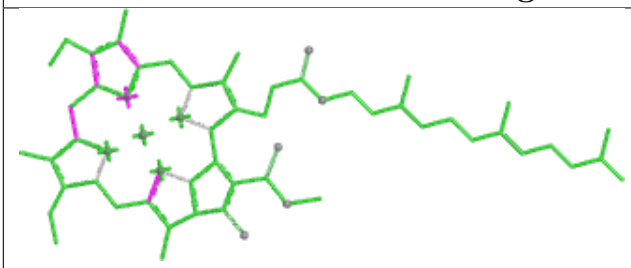
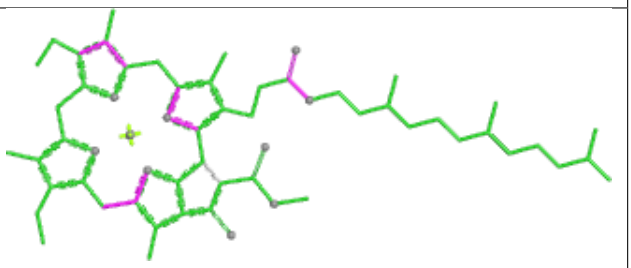
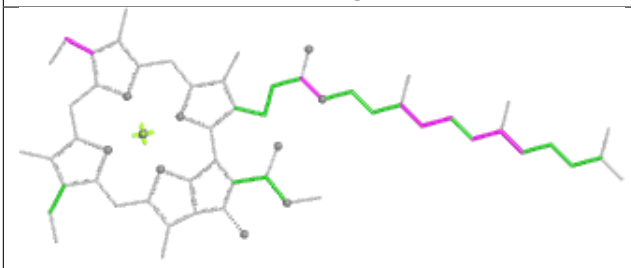
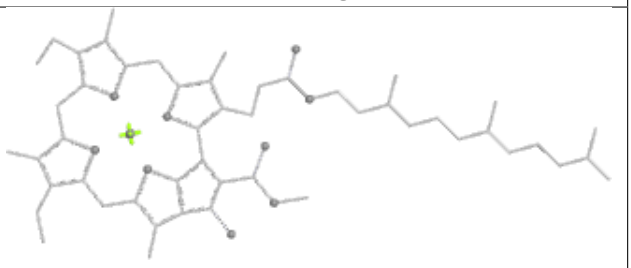
Bond angles

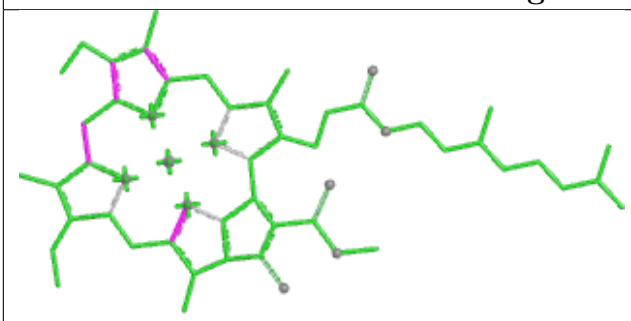
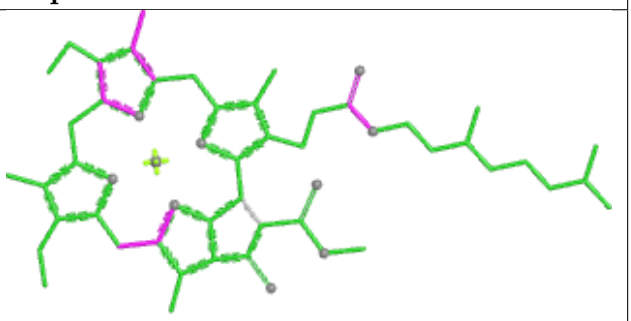
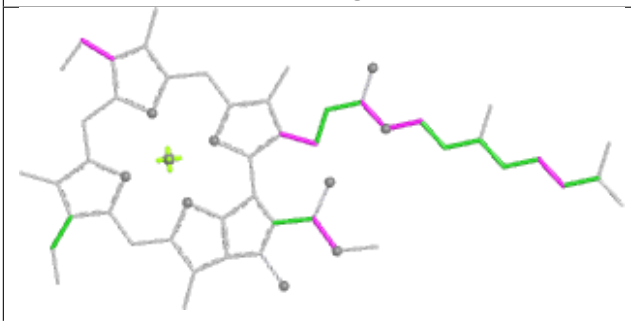
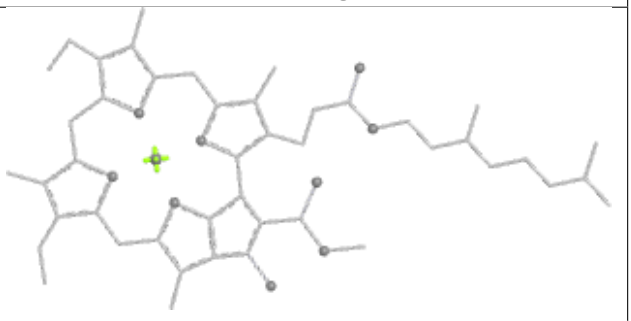


Torsions

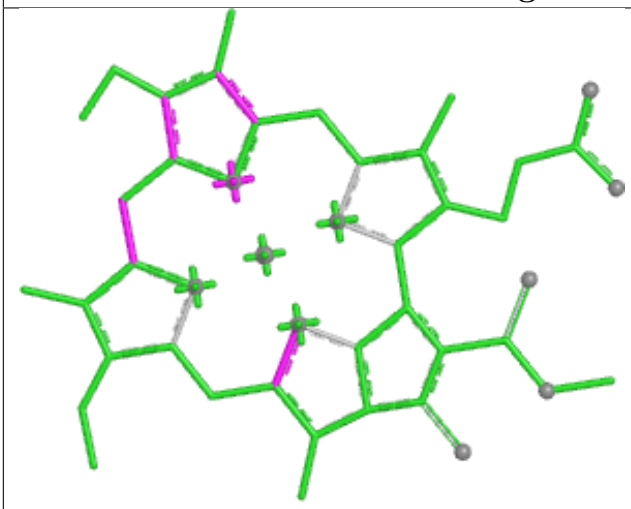


Rings

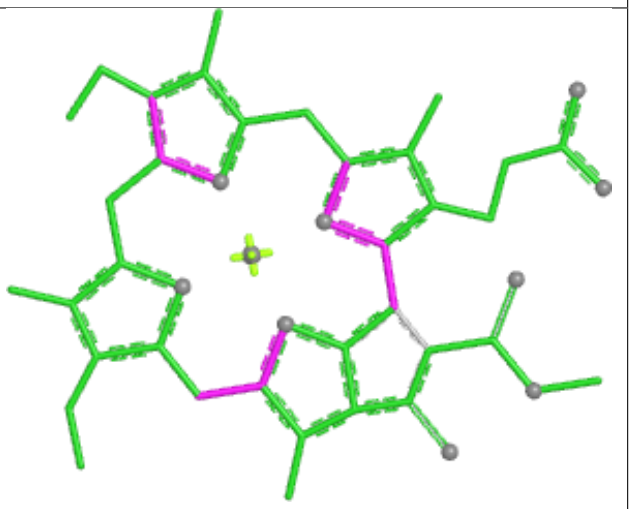
Ligand CLA L 1502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

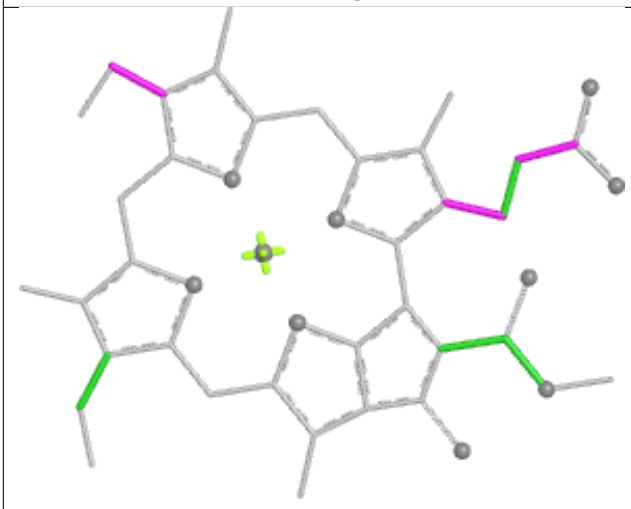
Ligand CLA b 1212



Bond lengths



Bond angles

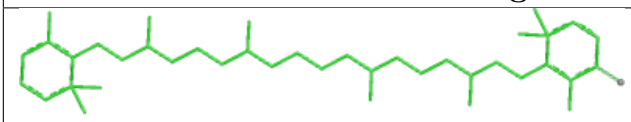


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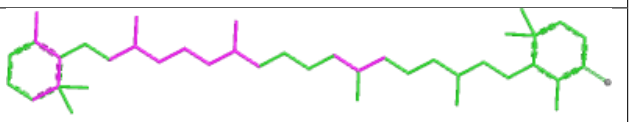


Rings

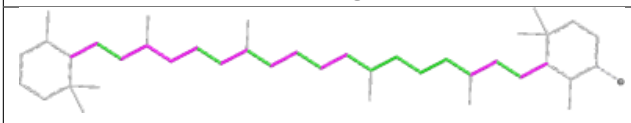
Ligand ECH M 4021



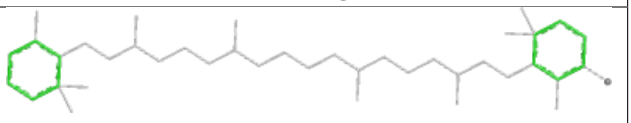
Bond lengths



Bond angles

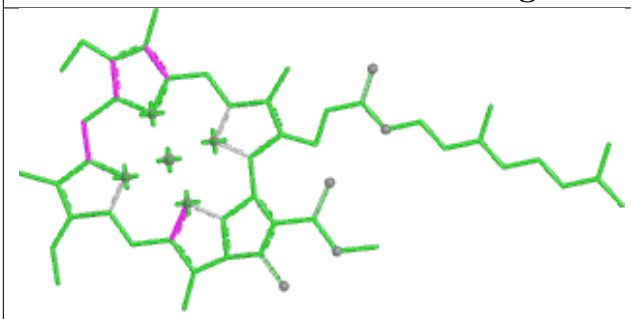


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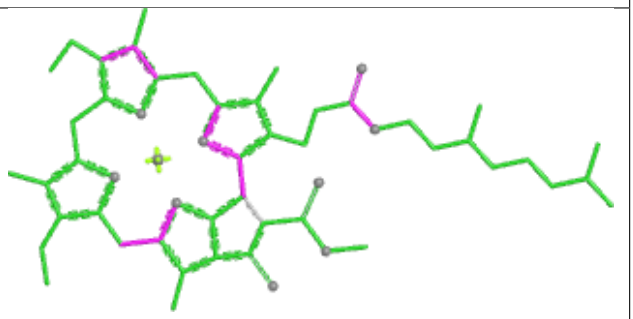


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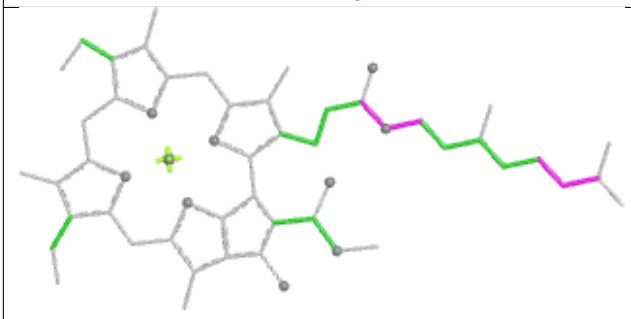
Ligand CLA k 4004



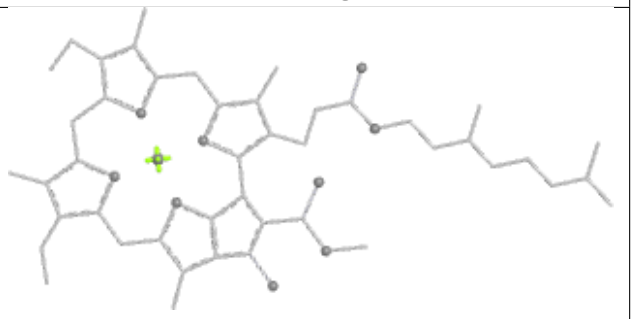
Bond lengths



Bond angles

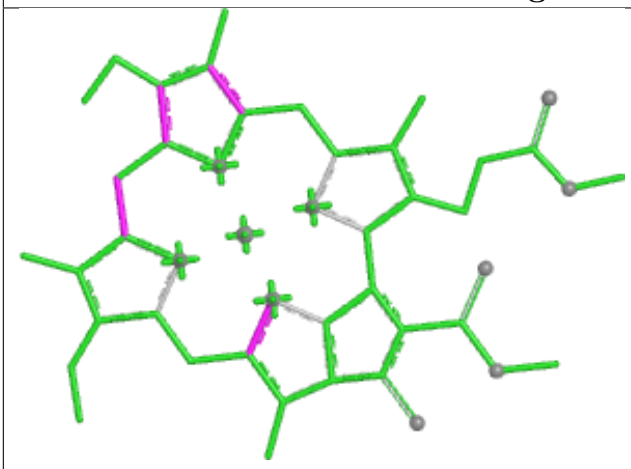


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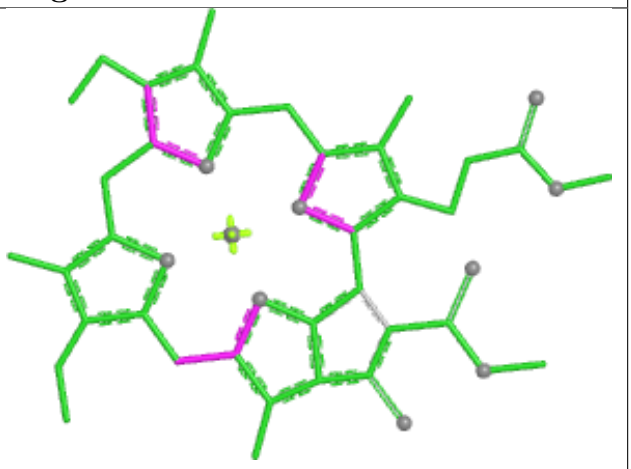


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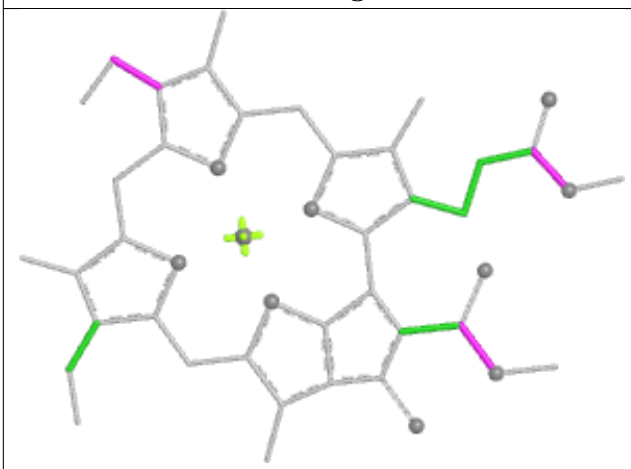
Ligand CLA g 516



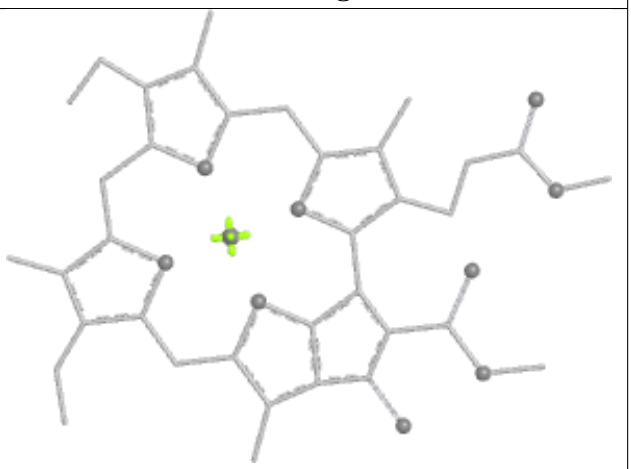
Bond lengths



Bond angles



Torsions

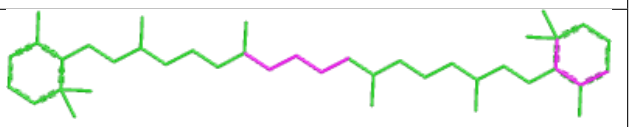


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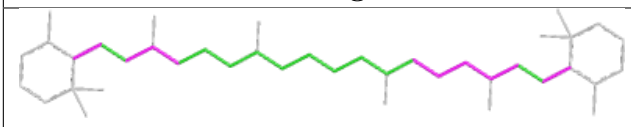
Ligand BCR G 4005



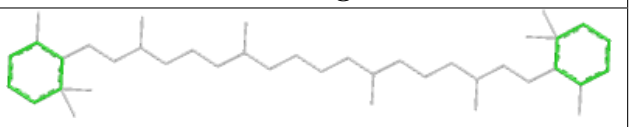
Bond lengths



Bond angles

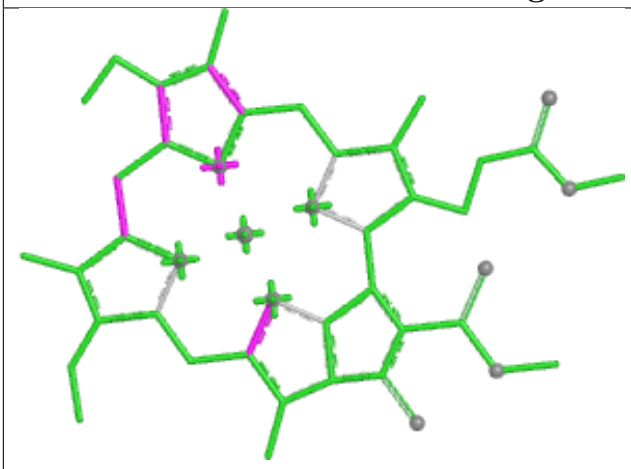


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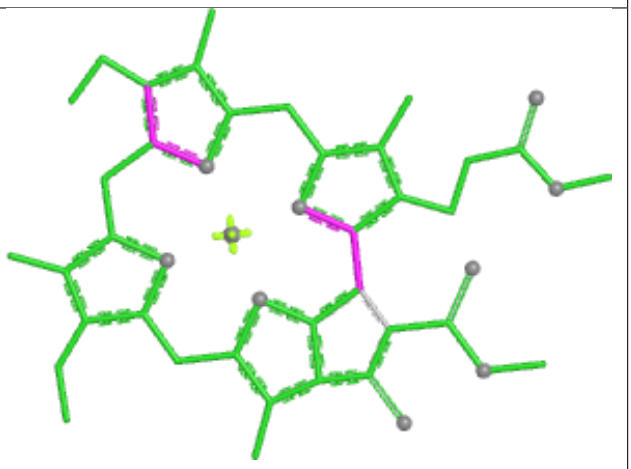


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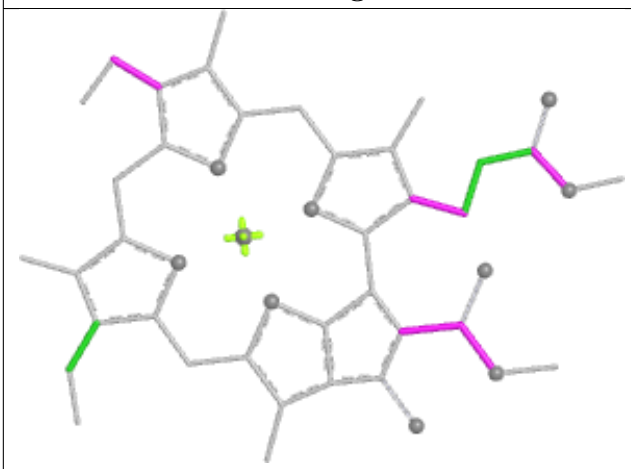
Ligand CLA x 513



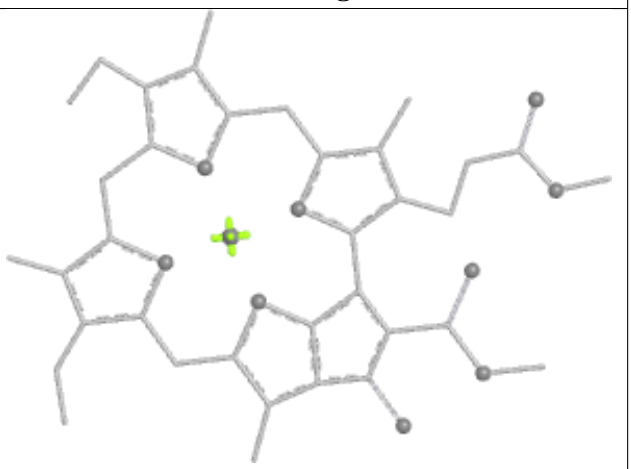
Bond lengths



Bond angles

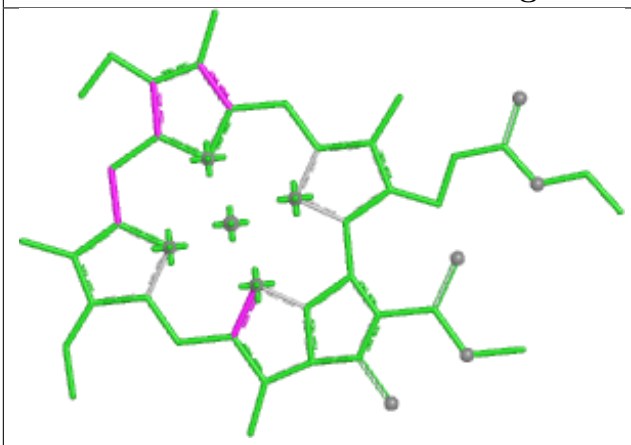


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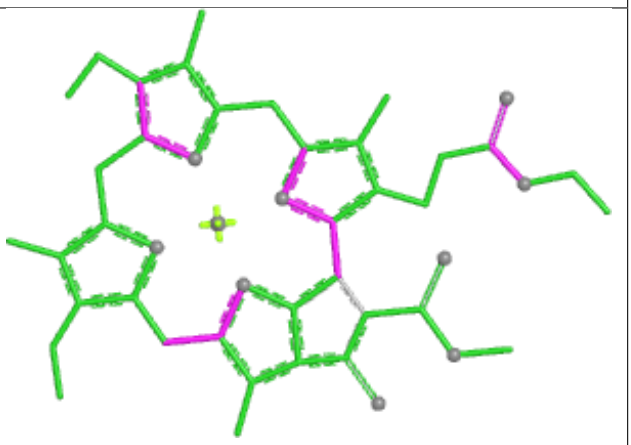


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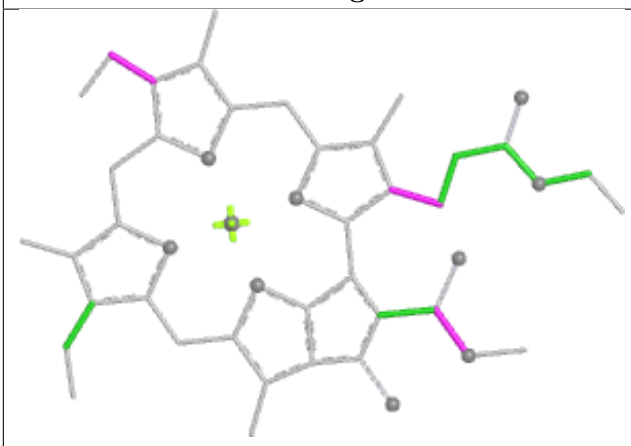
Ligand CLA a 1137



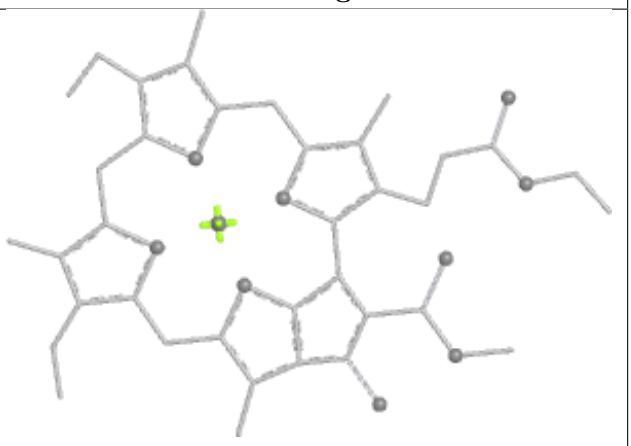
Bond lengths



Bond angles

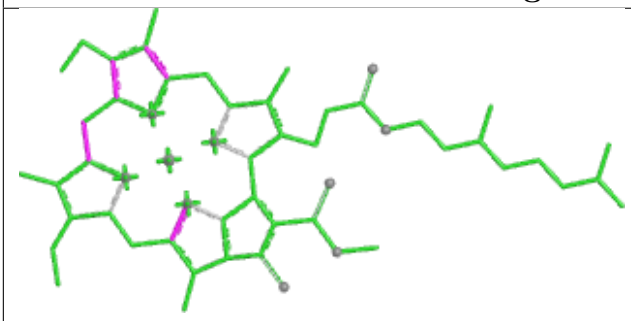


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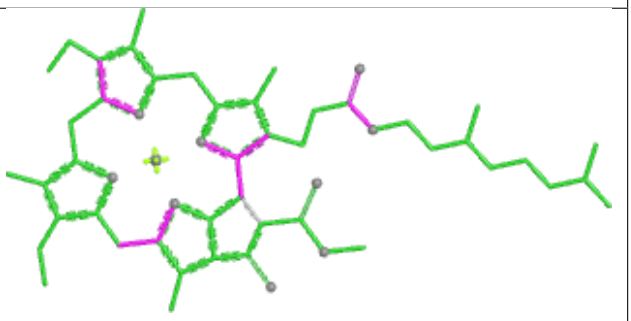


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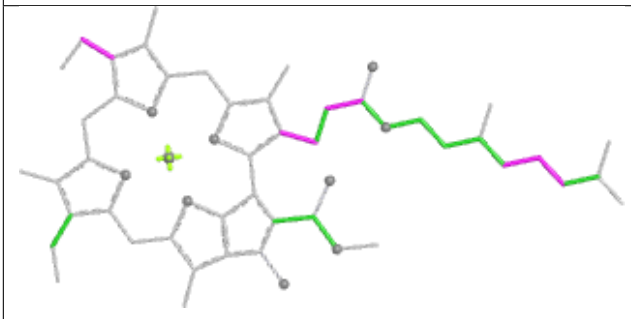
Ligand CLA X 517



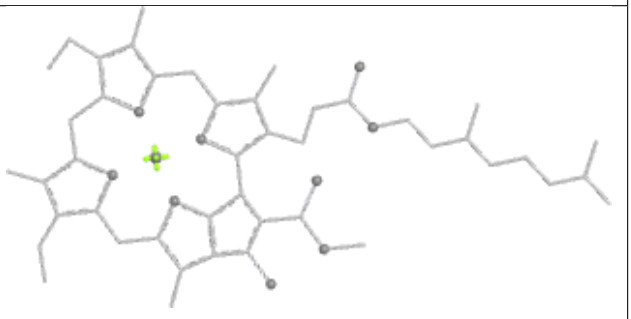
Bond lengths



Bond angles

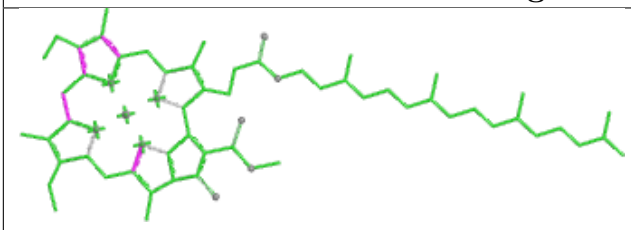


Torsions

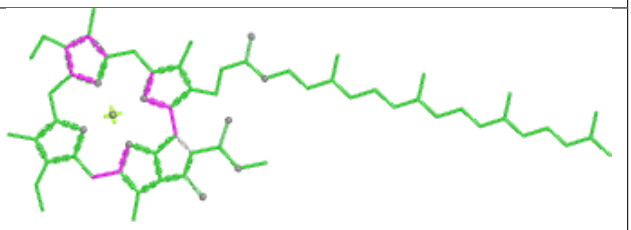


Rings

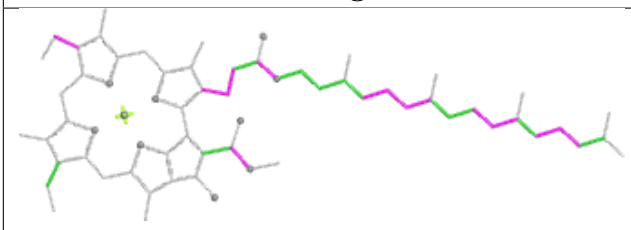
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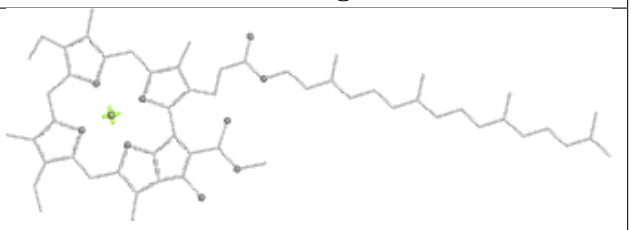
Bond lengths



Bond angles

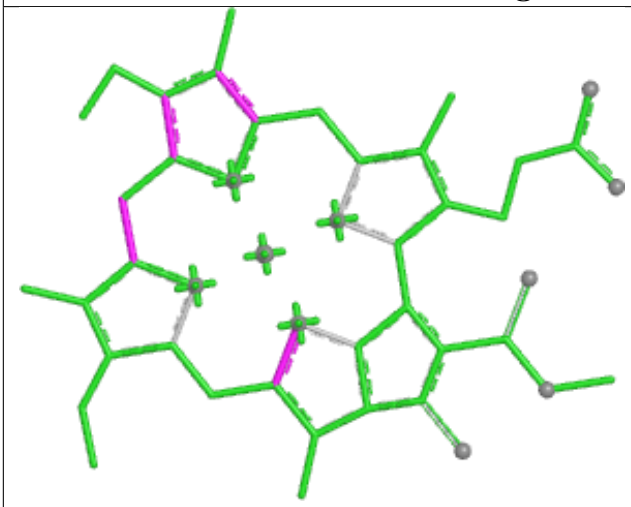


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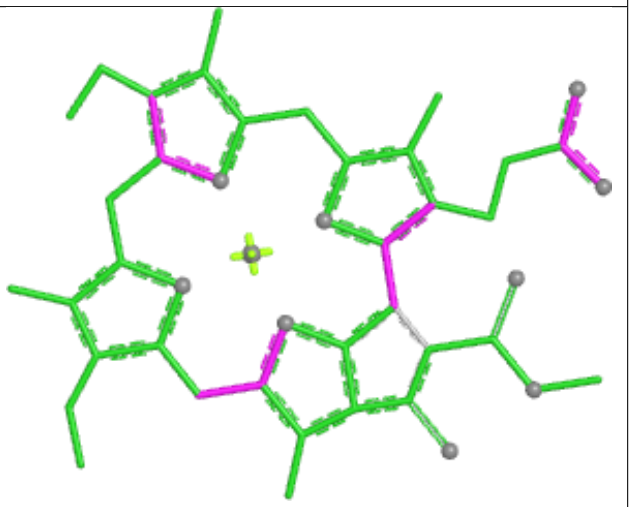


Rings

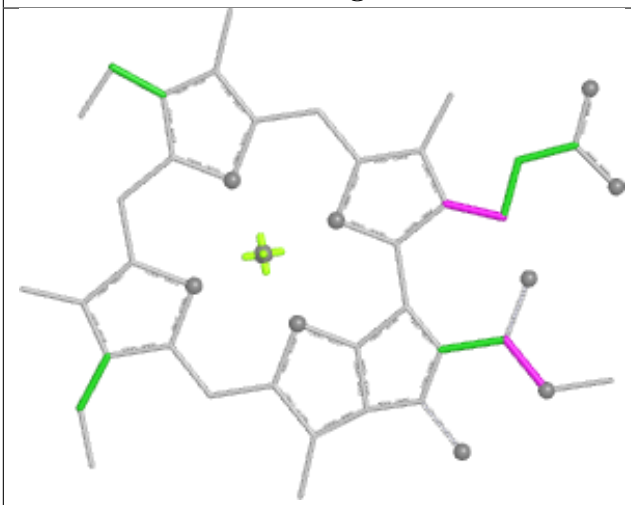
Ligand CLA A 1112



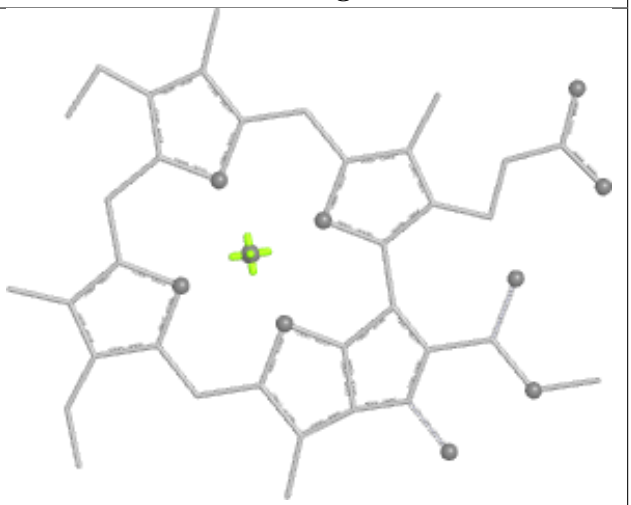
Bond lengths



Bond angles

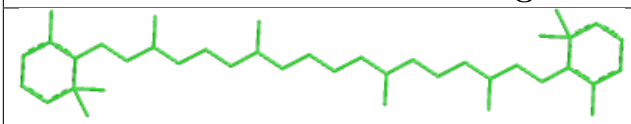


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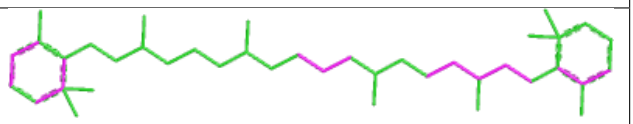


Rings

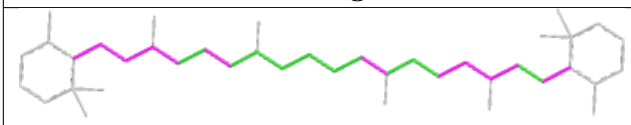
Ligand BCR L 4022



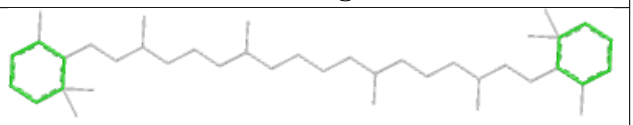
Bond lengths



Bond angles

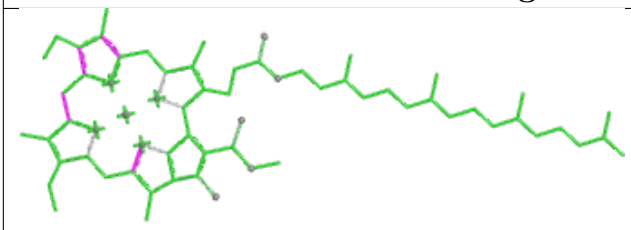


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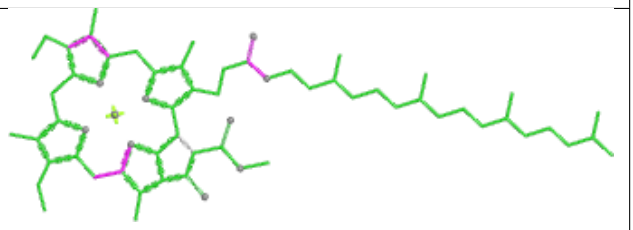


Rings

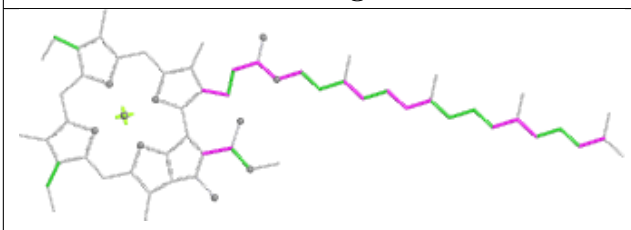
Ligand CLA b 1202



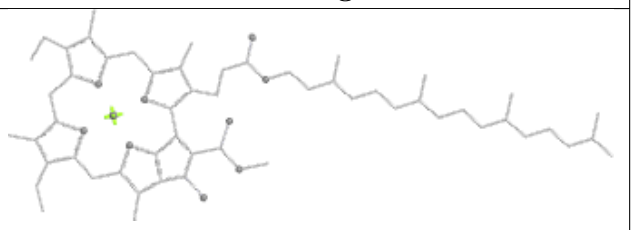
Bond lengths



Bond angles

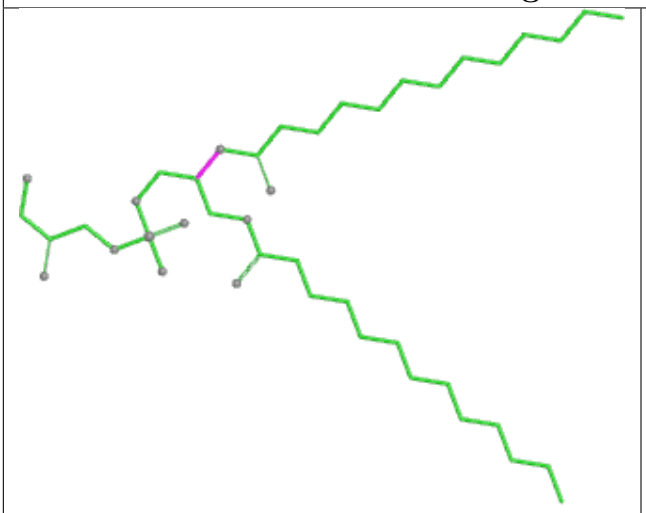


Torsions

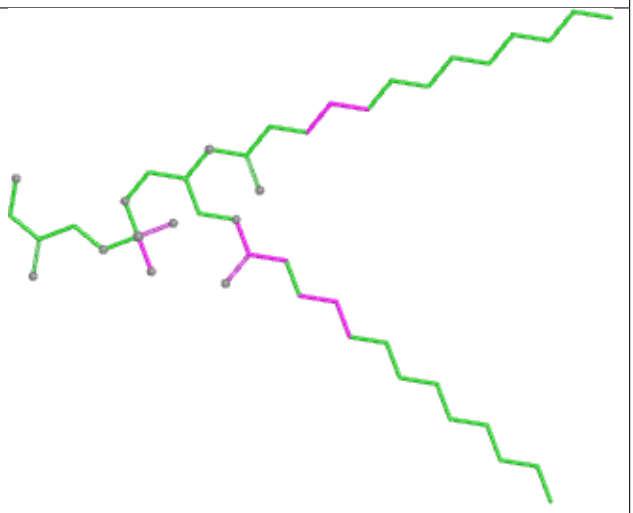


Rings

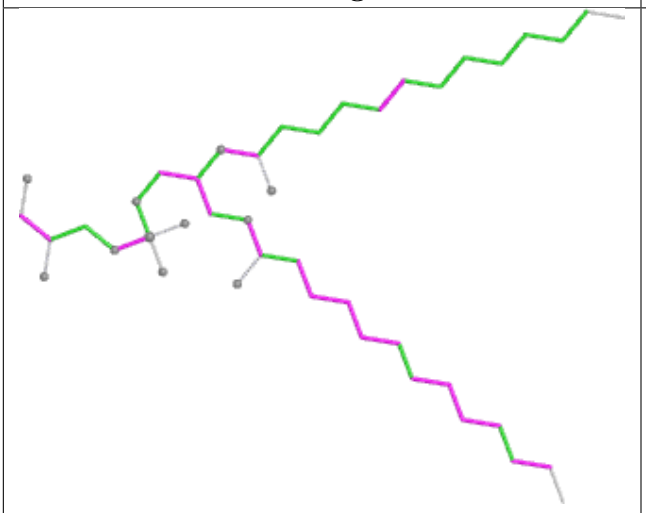
Ligand LHG A 849



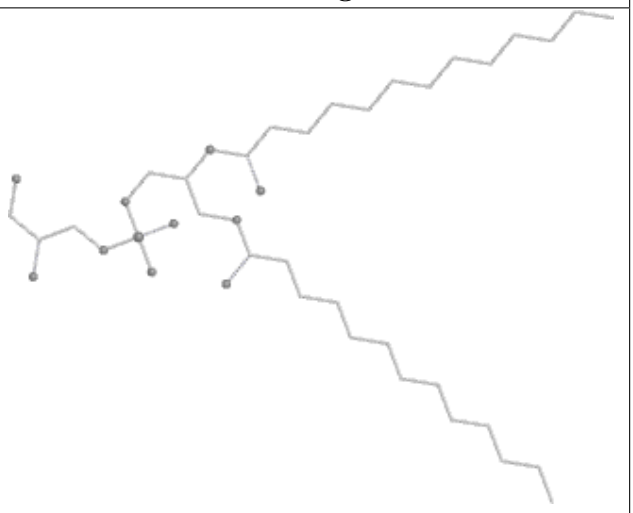
Bond lengths



Bond angles

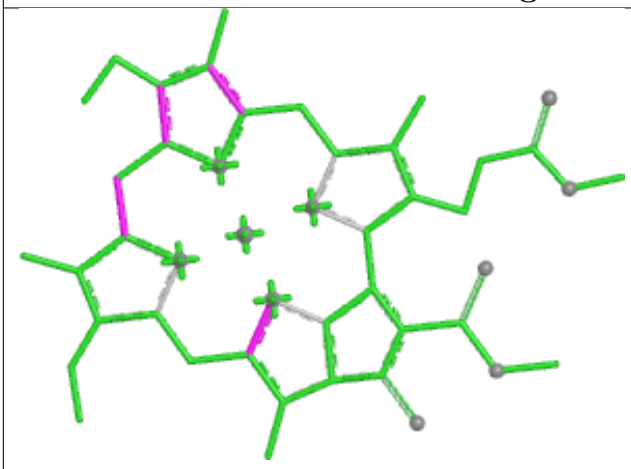


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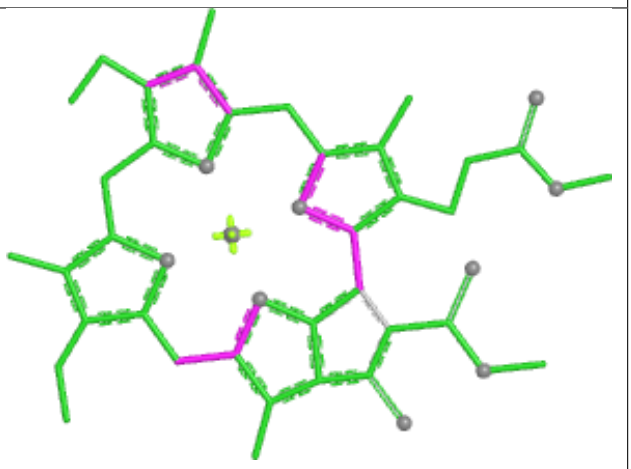


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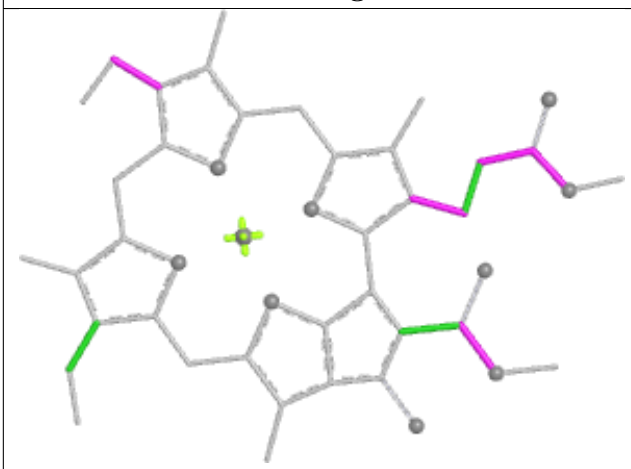
Ligand CLA a 1801



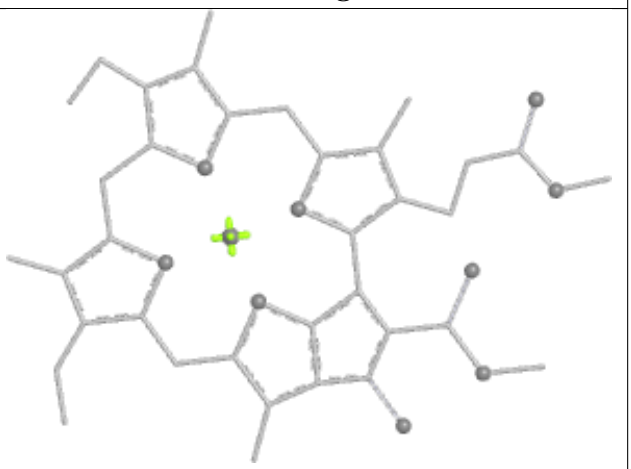
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Bond angles

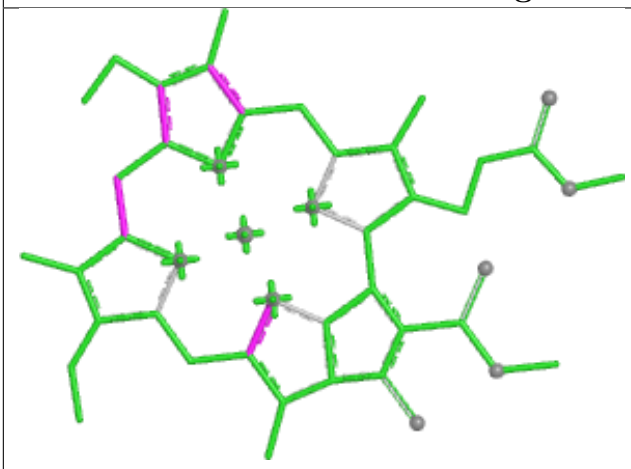


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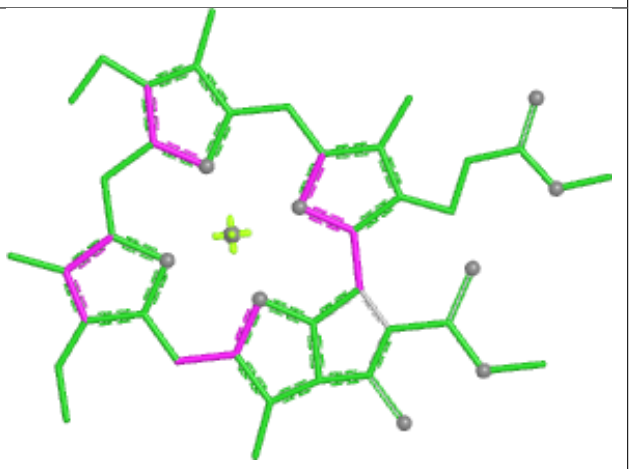


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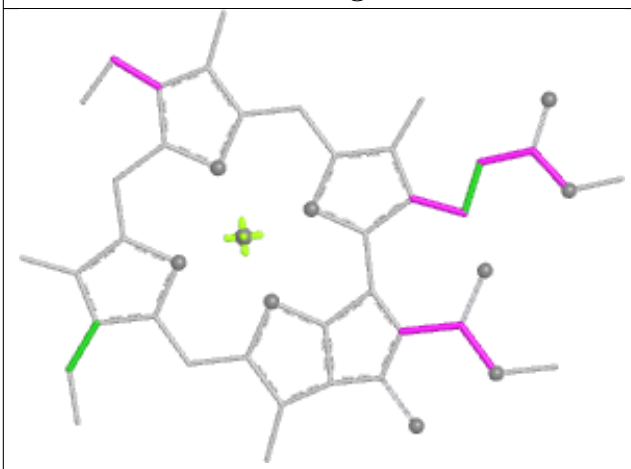
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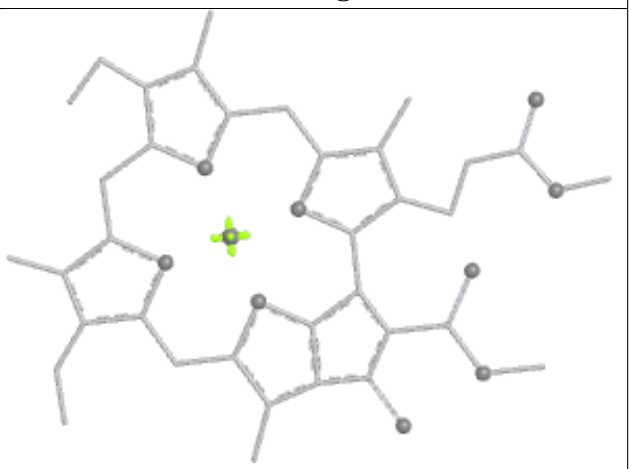
Bond lengths



Bond angles

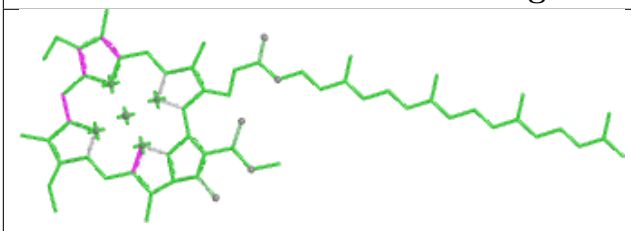


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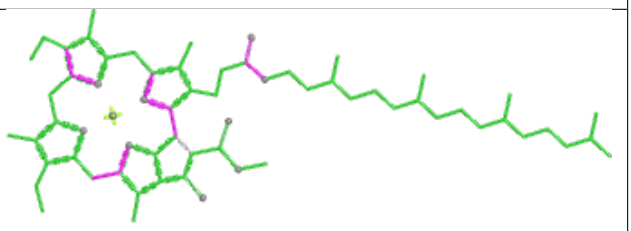


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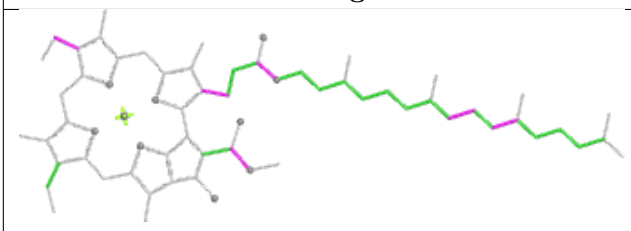
Ligand CLA o 511



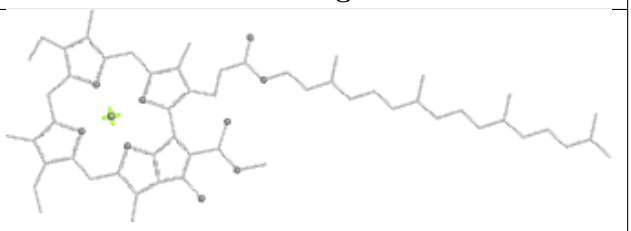
Bond lengths



Bond angles

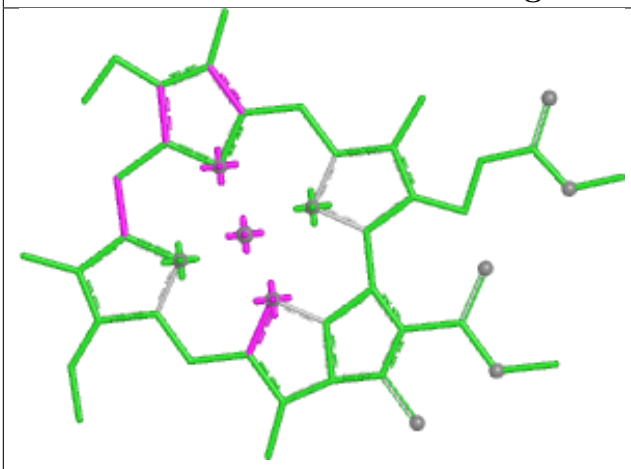


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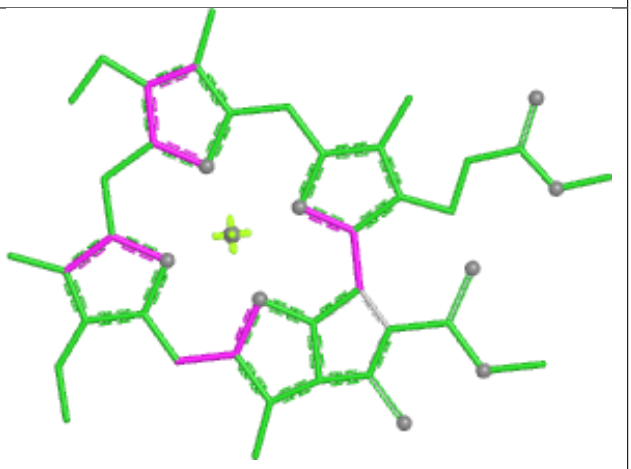


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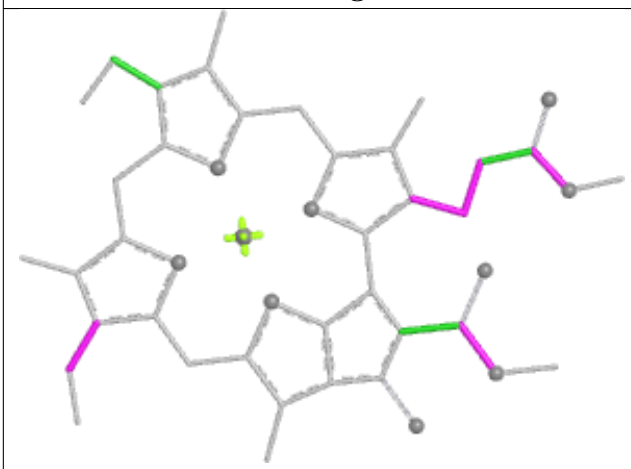
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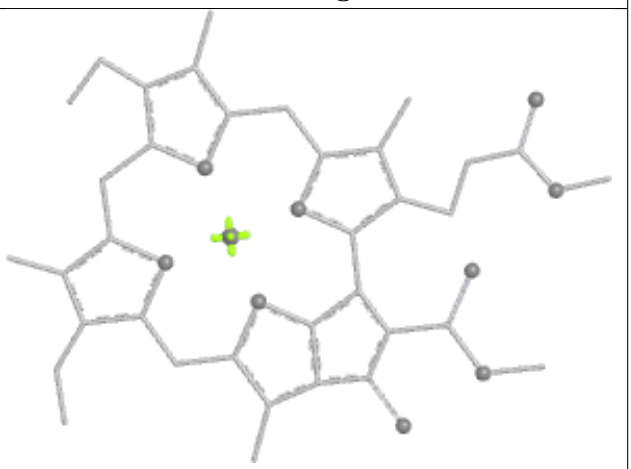
Bond lengths



Bond angles

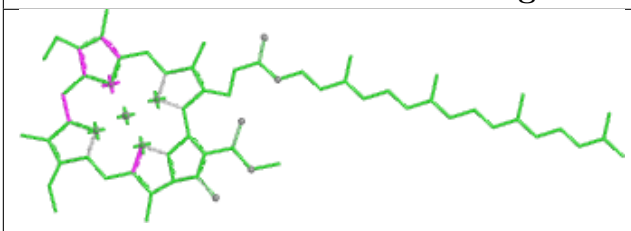


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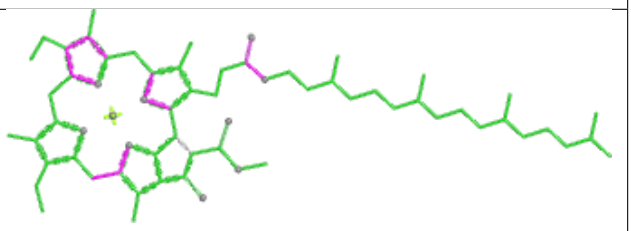


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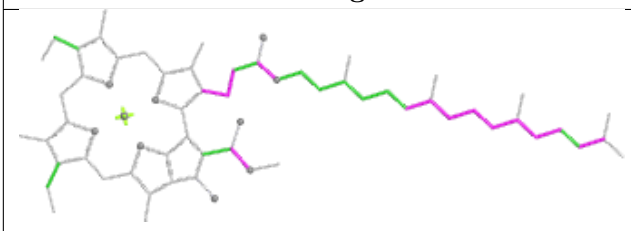
Ligand CLA b 1221



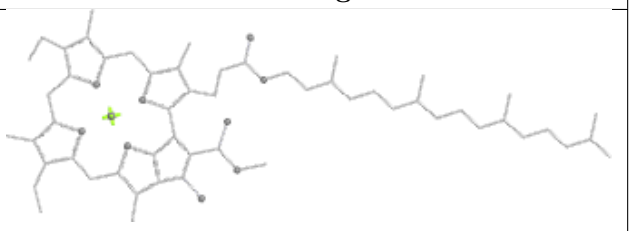
Bond lengths



Bond angles

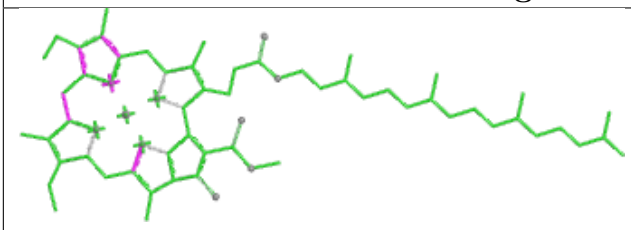


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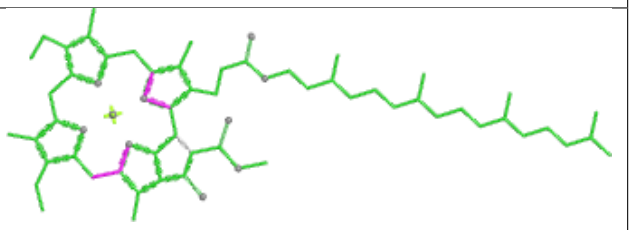


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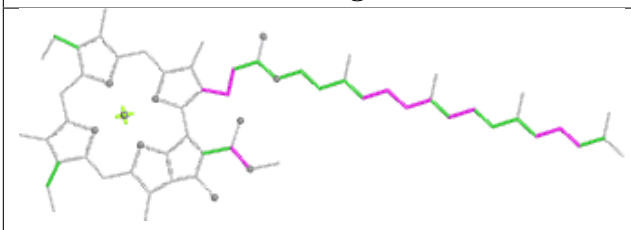
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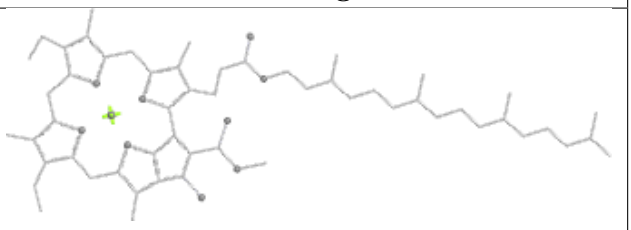
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Bond angles

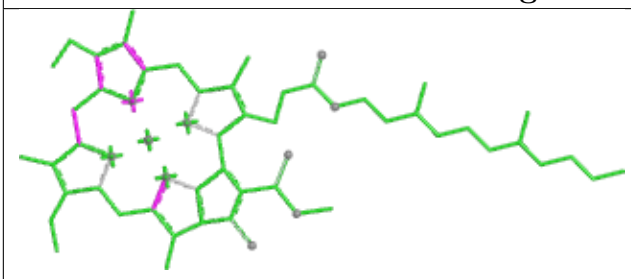


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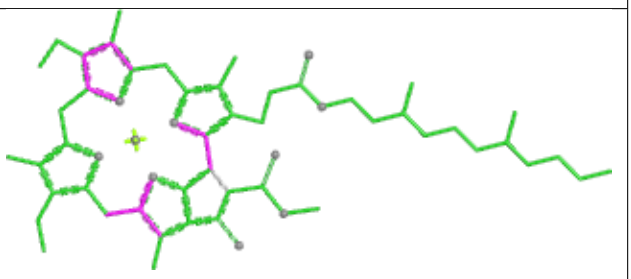


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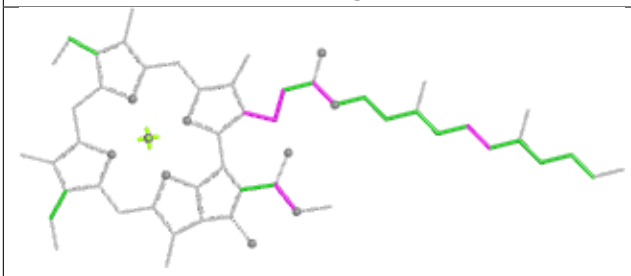
Ligand CLA a 1105



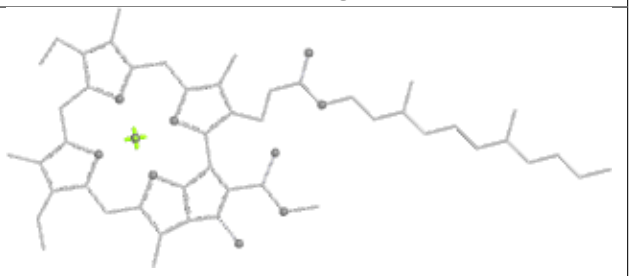
Bond lengths



Bond angles

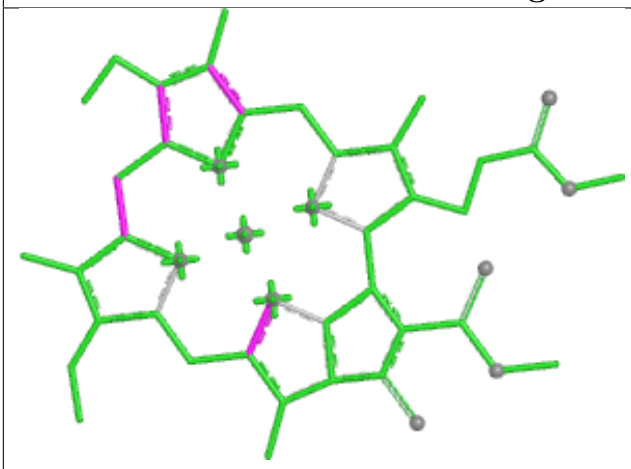


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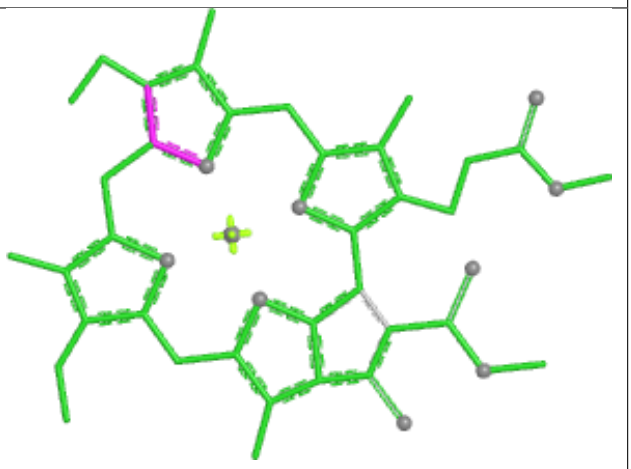


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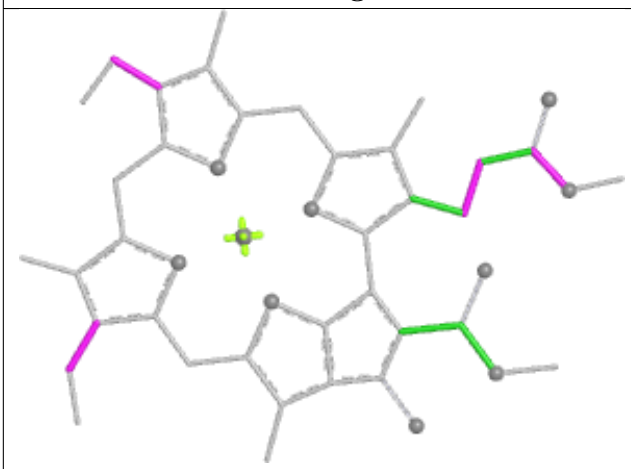
Ligand CLA o 513



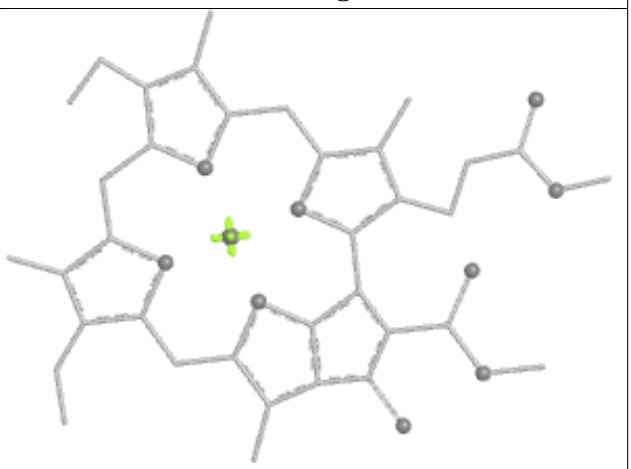
Bond lengths



Bond angles



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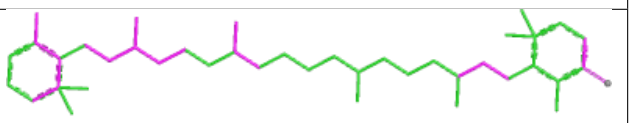


Rings

Ligand ECH i 4020



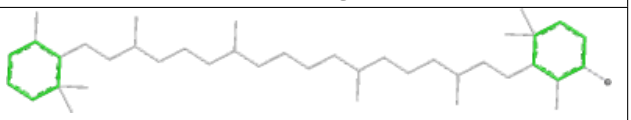
Bond lengths



Bond angles

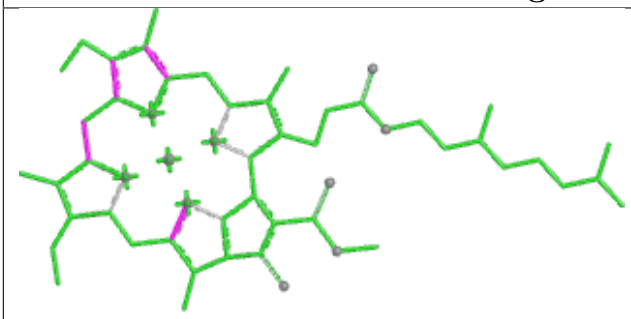


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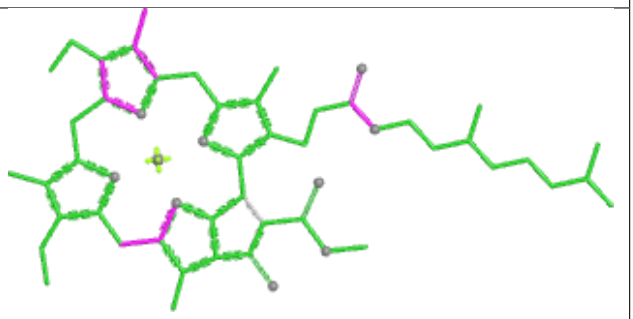


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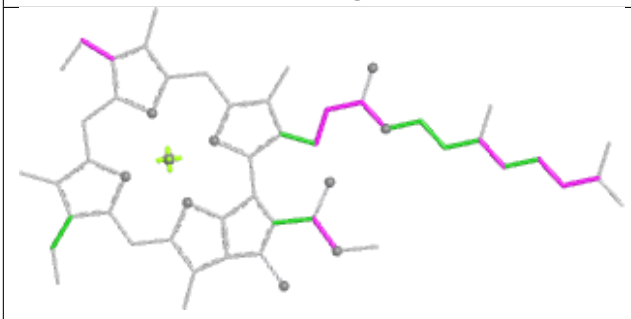
Ligand CLA o 508



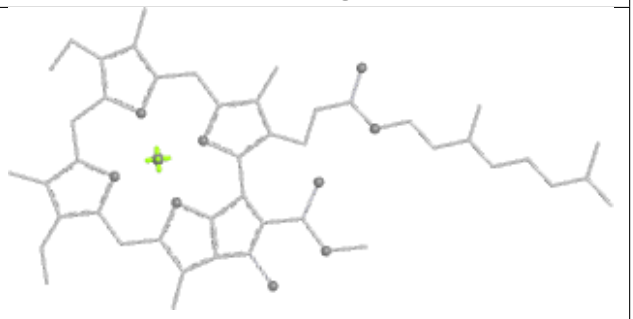
Bond lengths



Bond angles

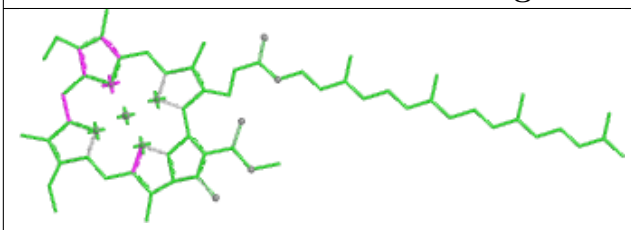


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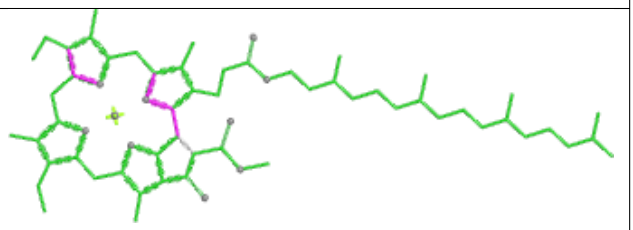


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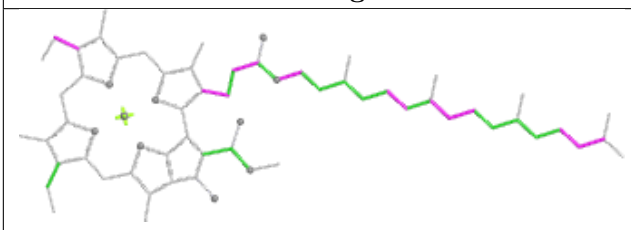
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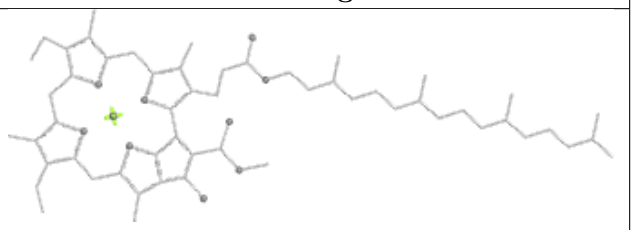
Bond lengths



Bond angles

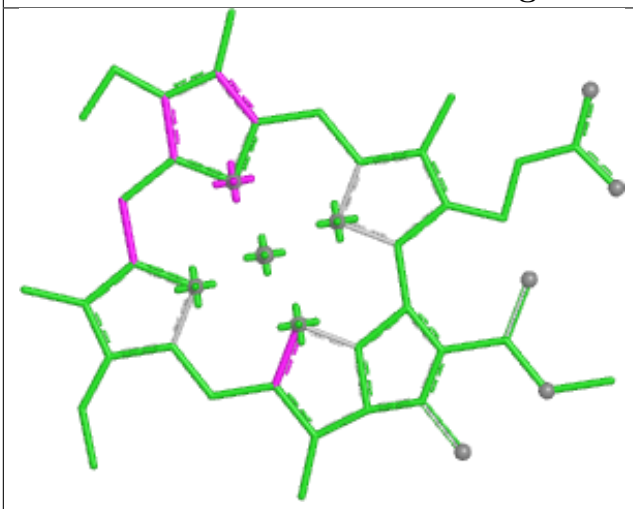


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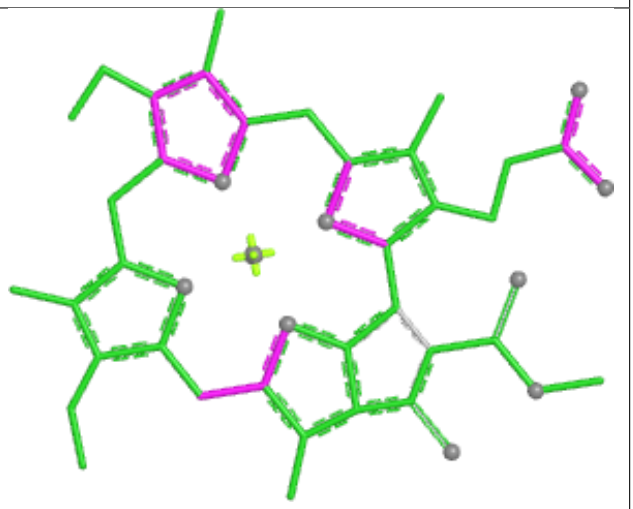


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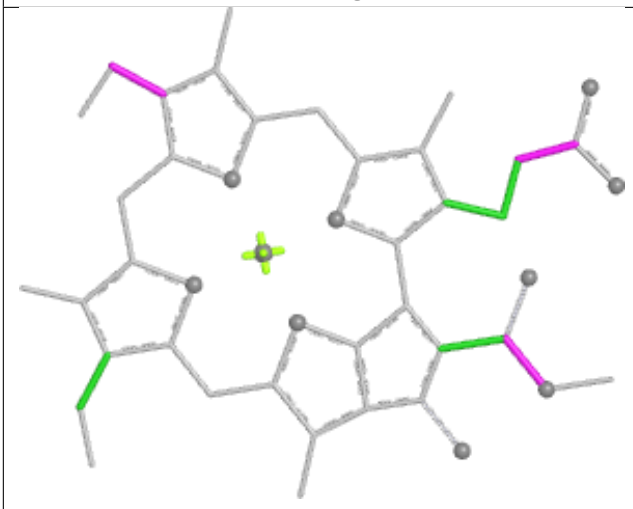
Ligand CLA J 1302



Bond lengths



Bond angles

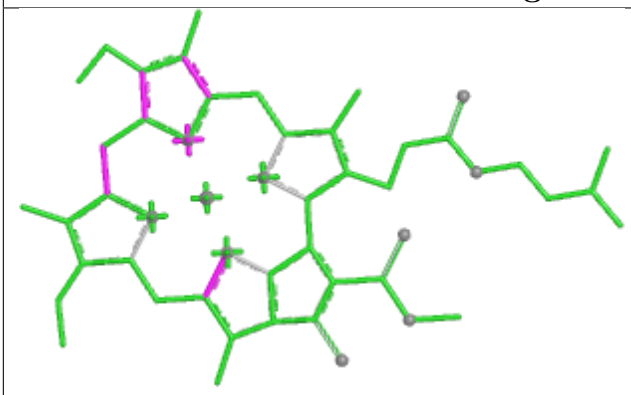


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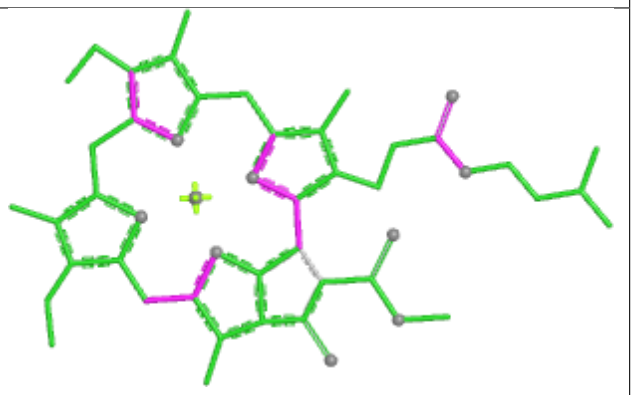


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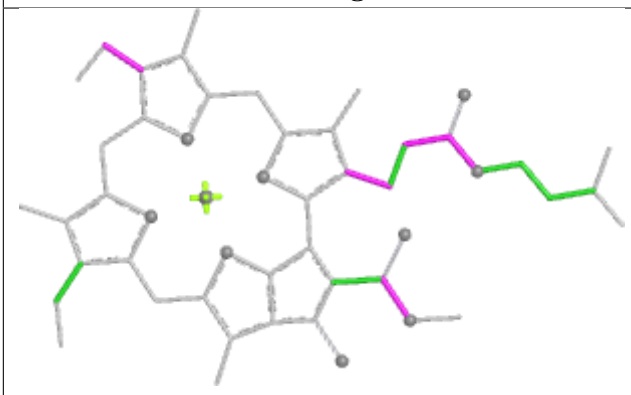
Ligand CLA Y 514



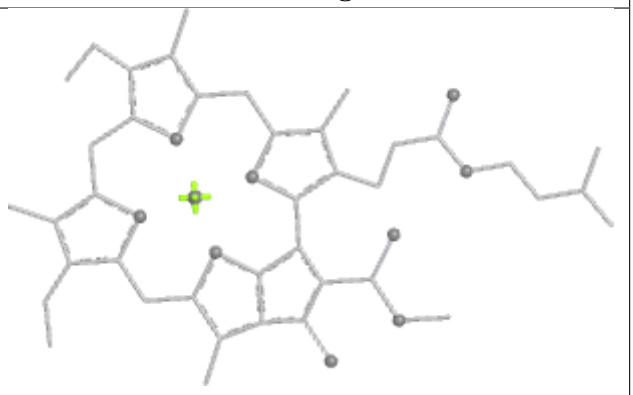
Bond lengths



Bond angles



Torsions

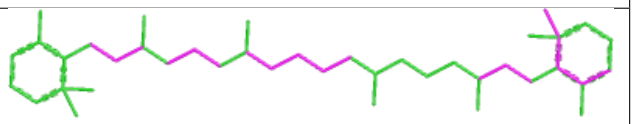


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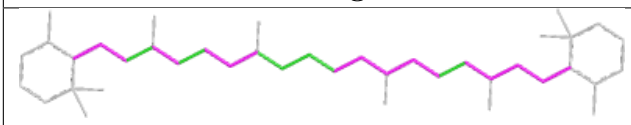
Ligand BCR B 4010



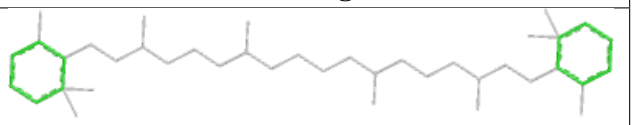
Bond lengths



Bond angles

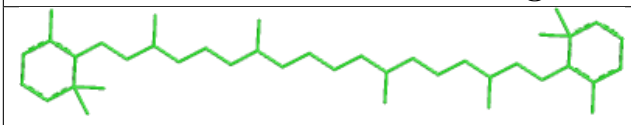


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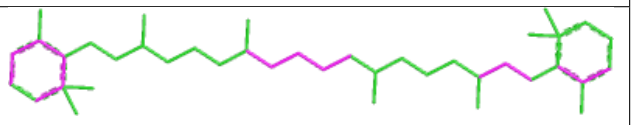


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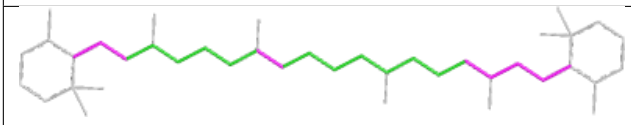
Ligand BCR v 601



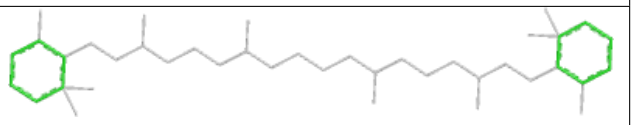
Bond lengths



Bond angles

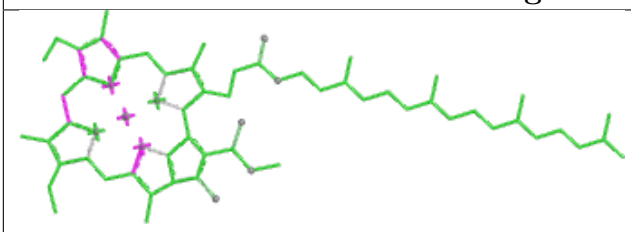


Torsions

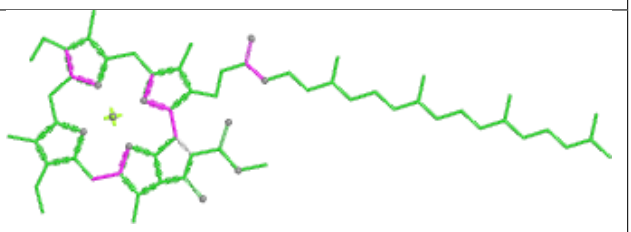


Rings

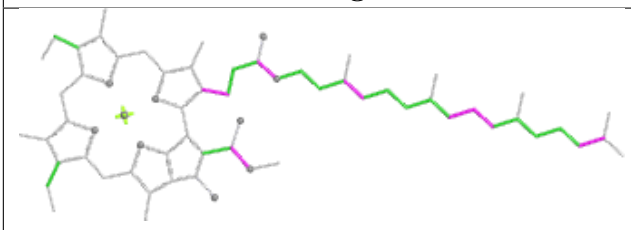
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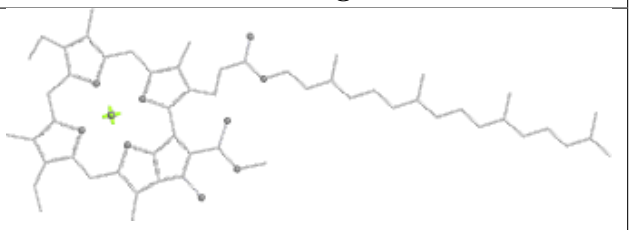
Bond lengths



Bond angles

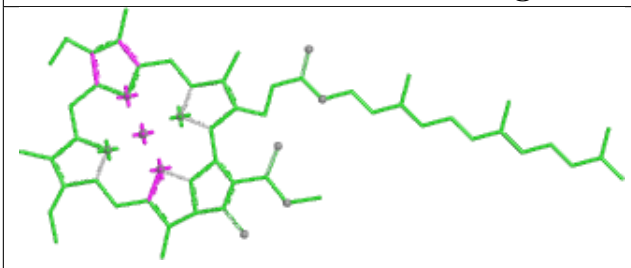


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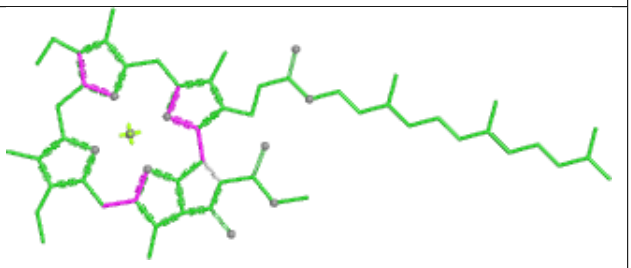


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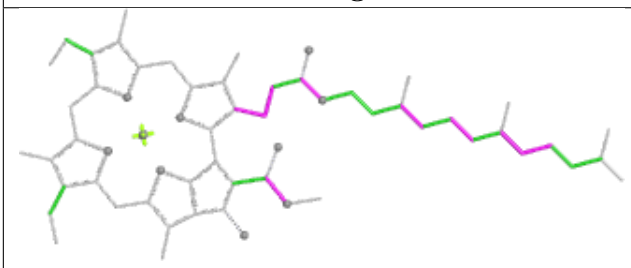
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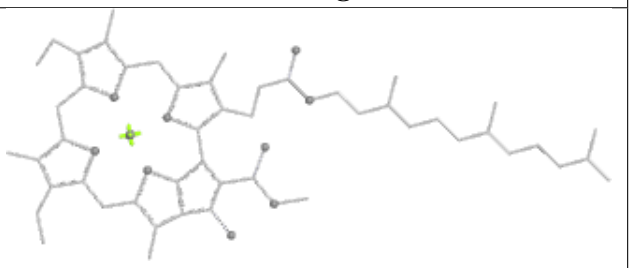
Bond lengths



Bond angles

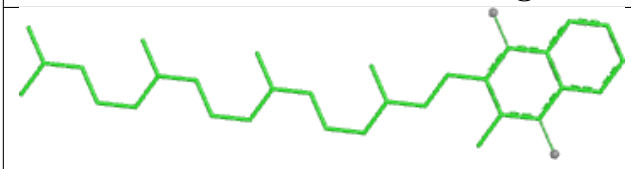


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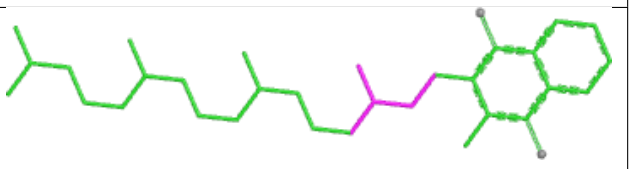


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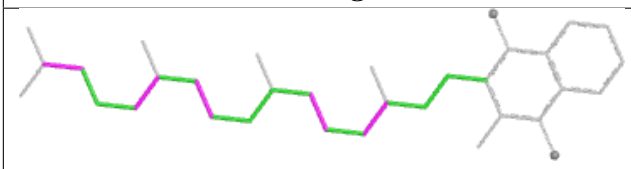
Ligand PQN b 2002



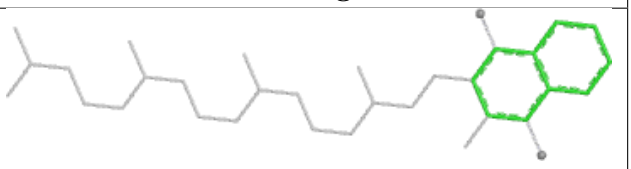
Bond lengths



Bond angles

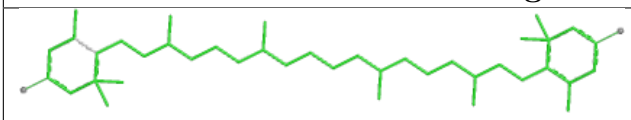


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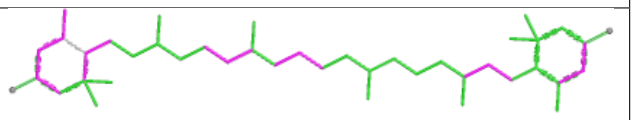


Rings

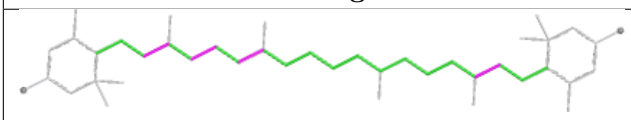
Ligand LUT w 601



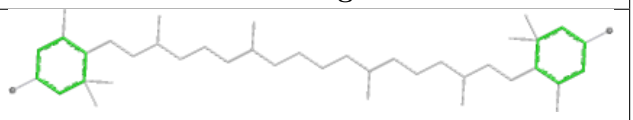
Bond lengths



Bond angles

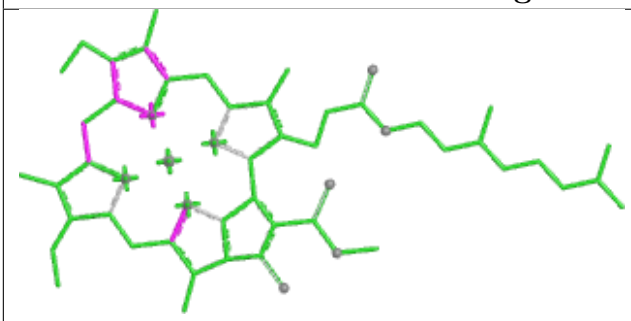


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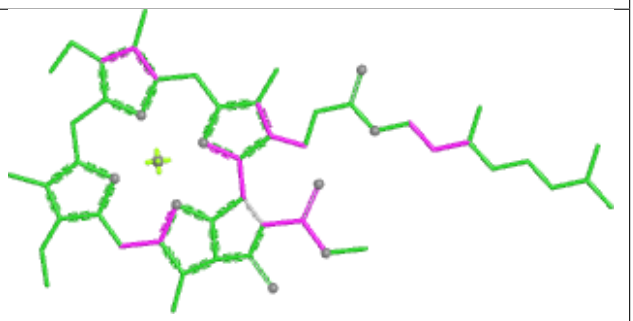


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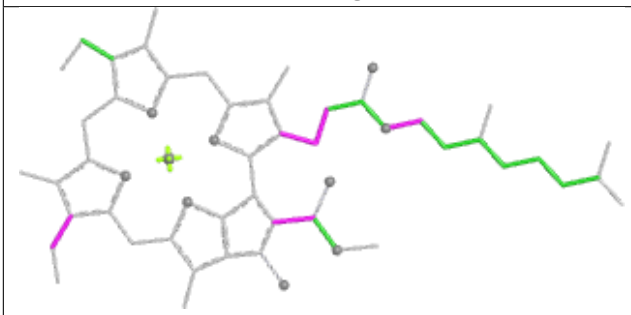
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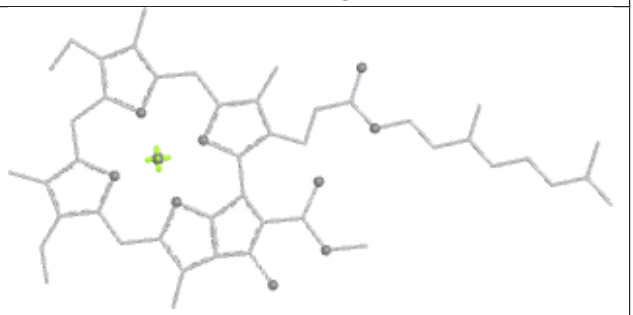
Bond lengths



Bond angles

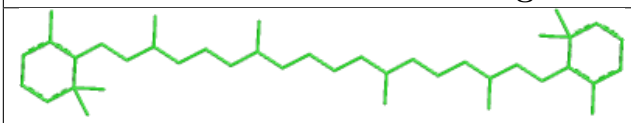


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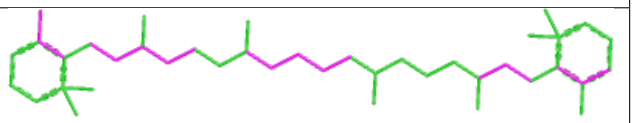


Rings

Ligand BCR S 4012



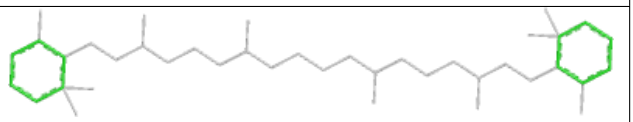
Bond lengths



Bond angles

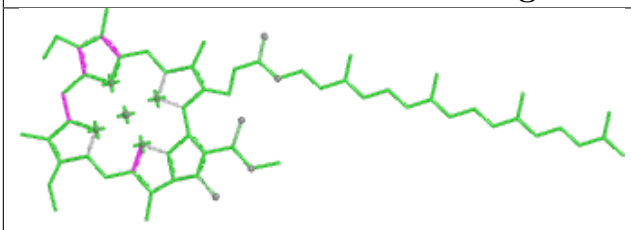


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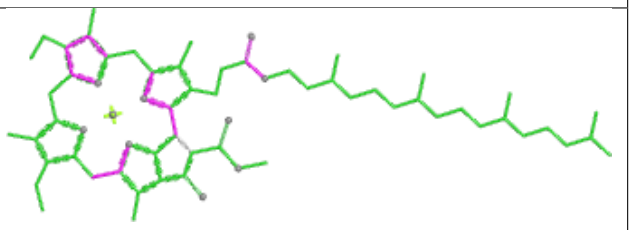


Rings

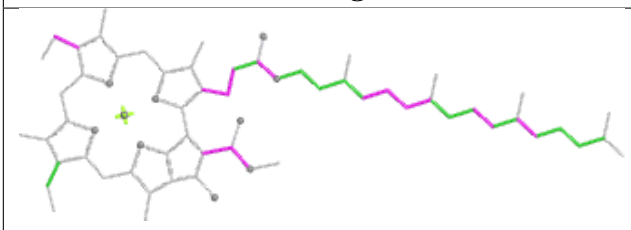
Ligand CLA W 515



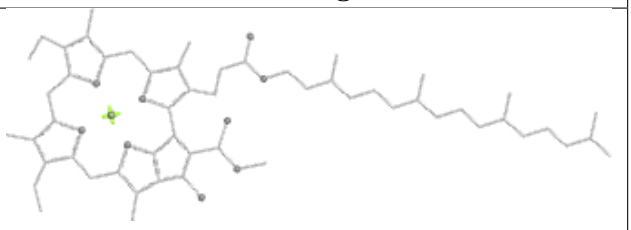
Bond lengths



Bond angles

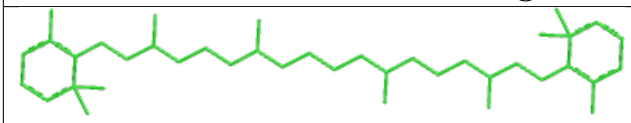


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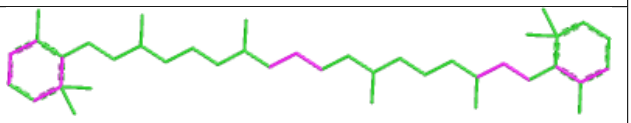


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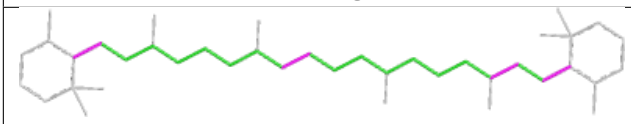
Ligand BCR k 4005



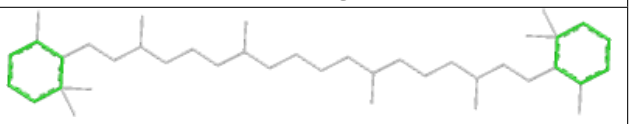
Bond lengths



Bond angles

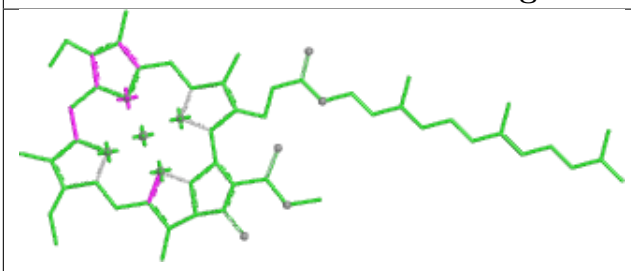


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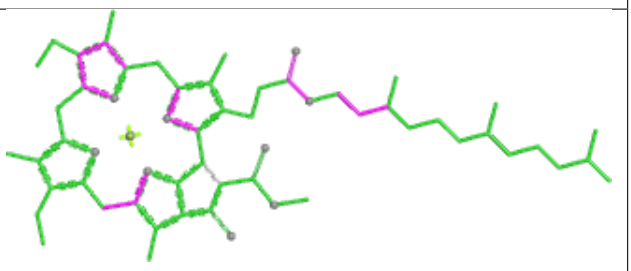


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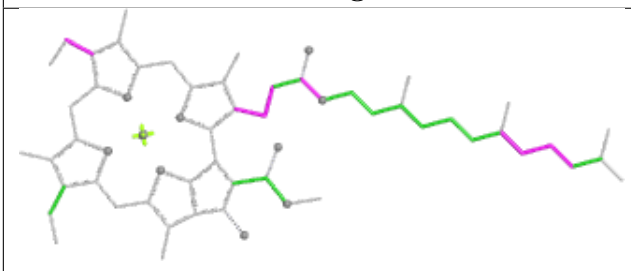
Ligand CLA a 1130



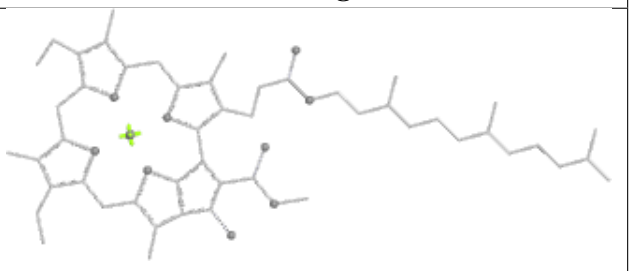
Bond lengths



Bond angles

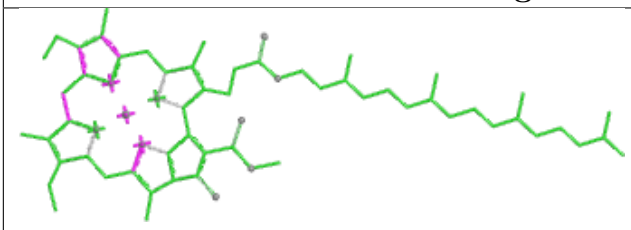


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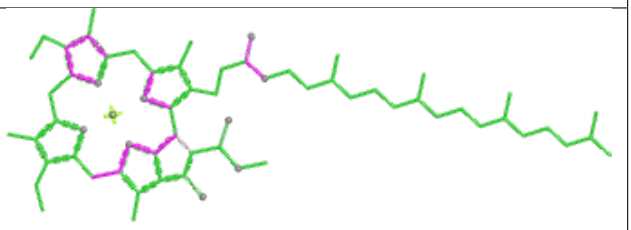


Rings

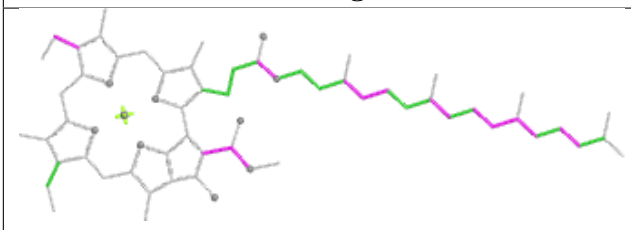
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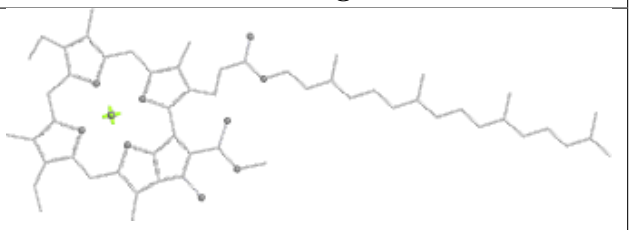
Bond lengths



Bond angles

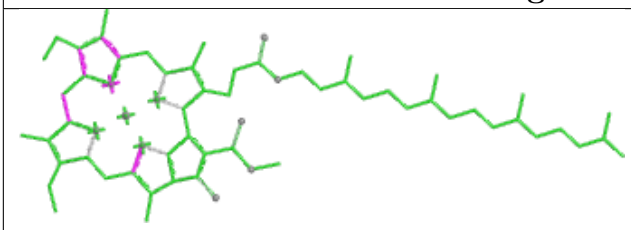


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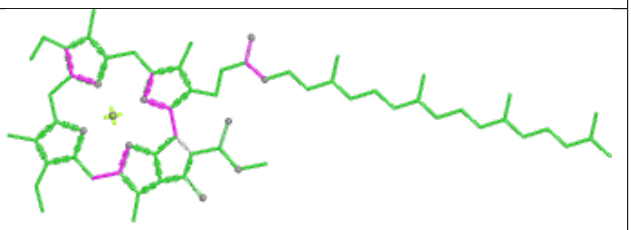


Rings

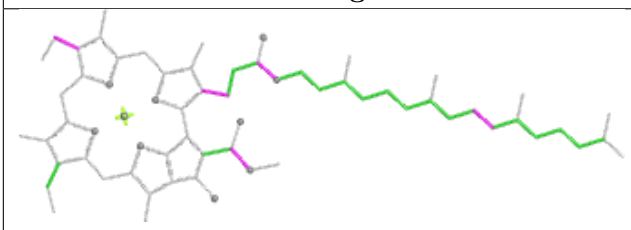
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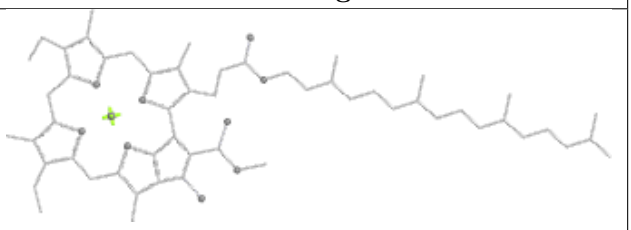
Bond lengths



Bond angles

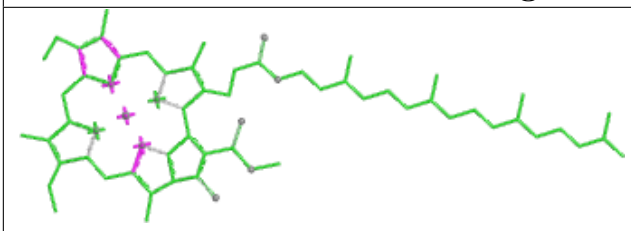


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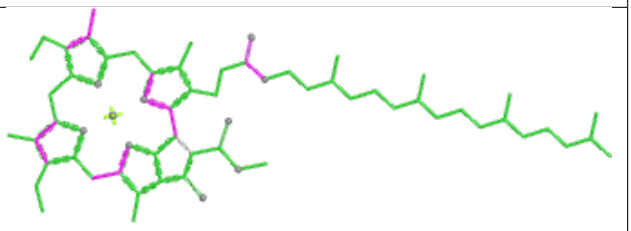


Rings

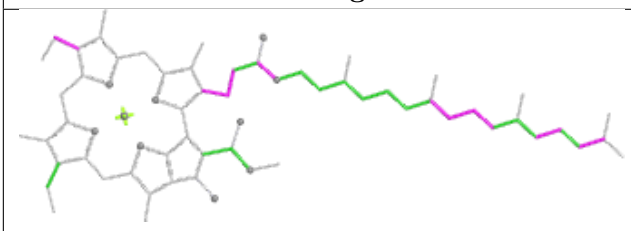
Ligand CLA a 1237



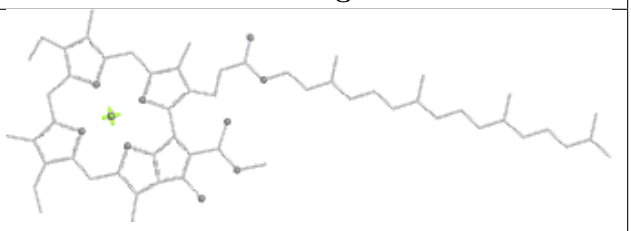
Bond lengths



Bond angles

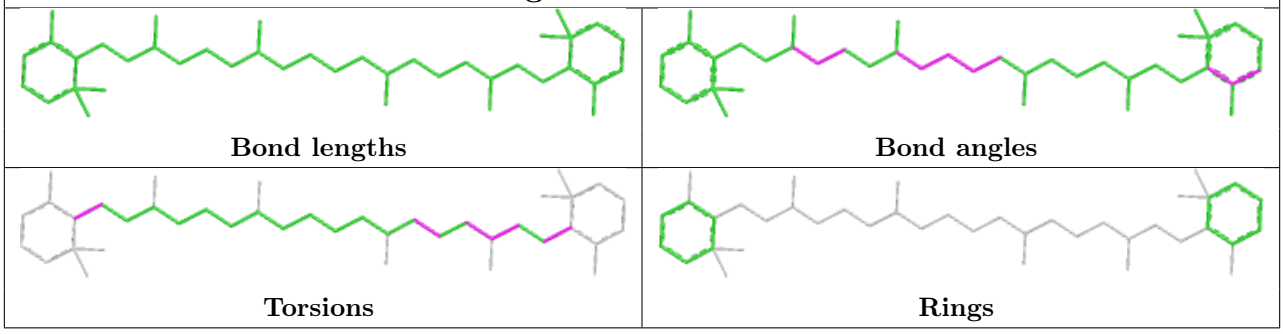


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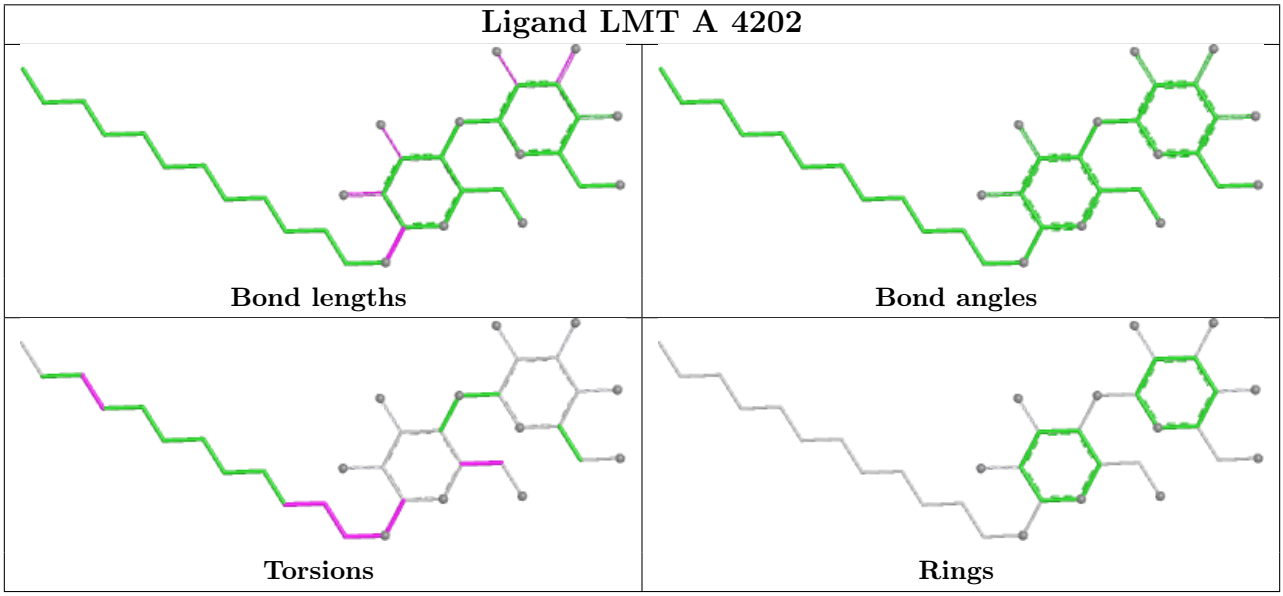


Rings

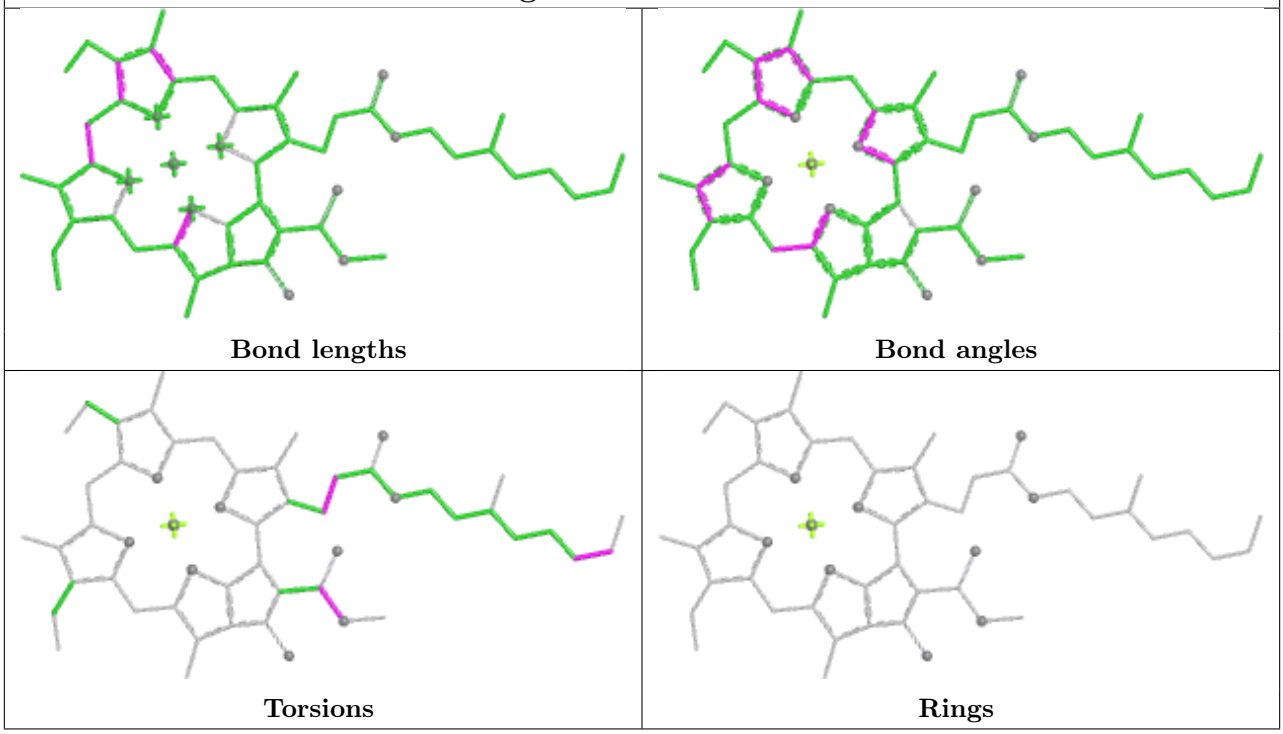
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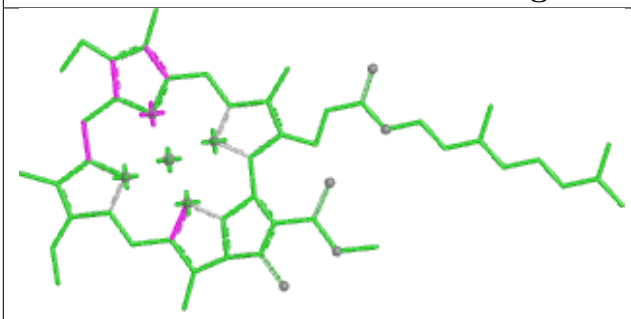
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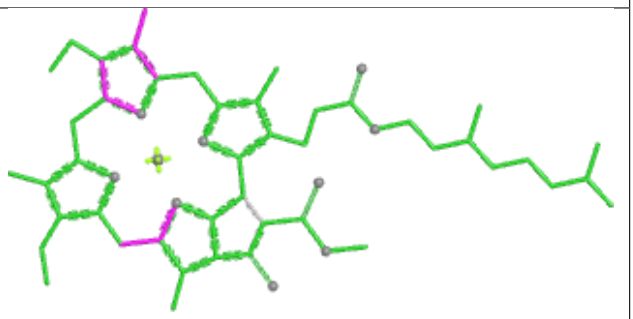
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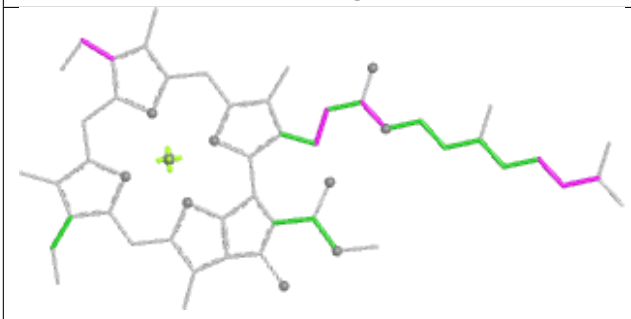
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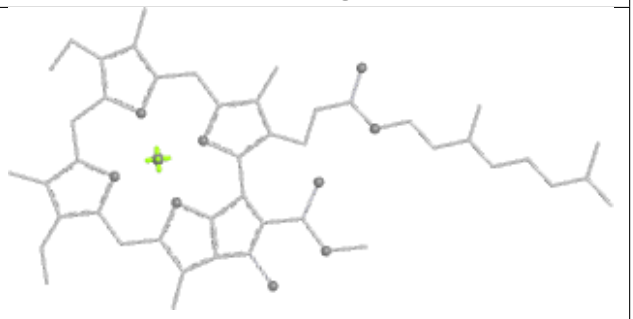
Bond lengths



Bond angles

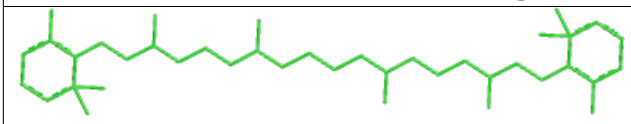


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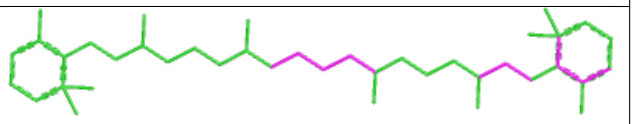


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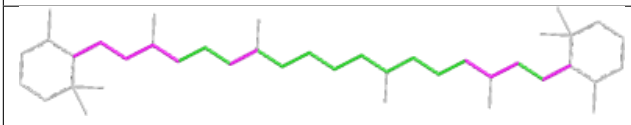
Ligand BCR H 4002



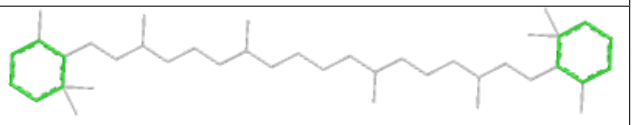
Bond lengths



Bond angles

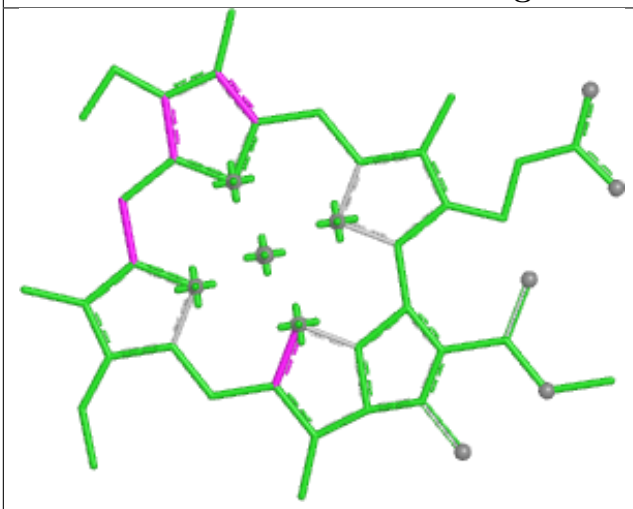


Torsions

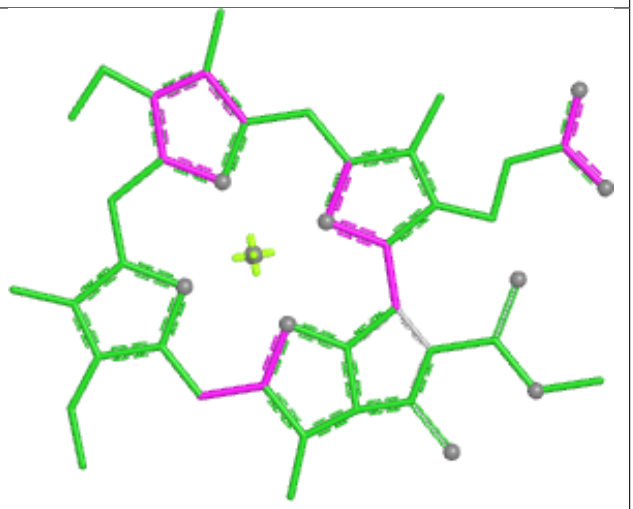


Rings

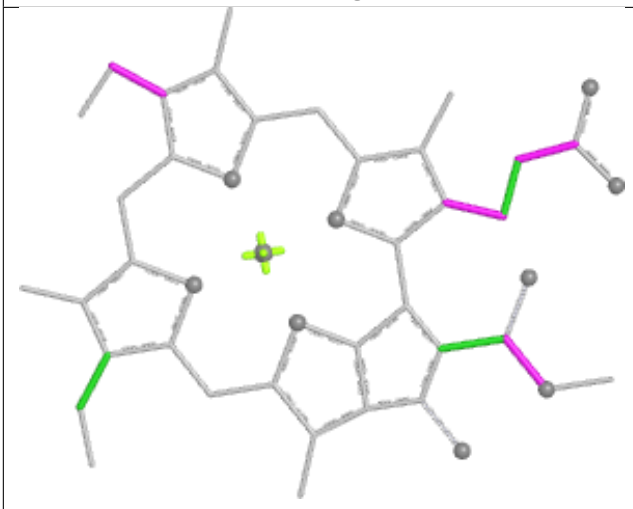
Ligand CLA G 1208



Bond lengths



Bond angles

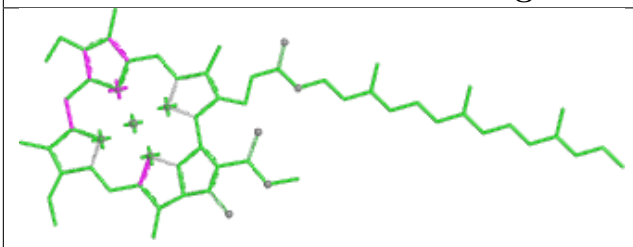


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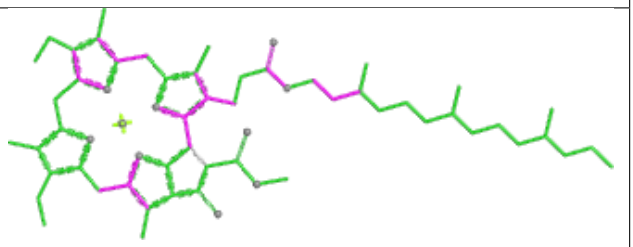


Rings

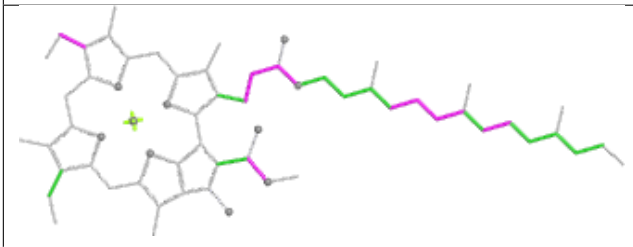
Ligand CLA B 1235



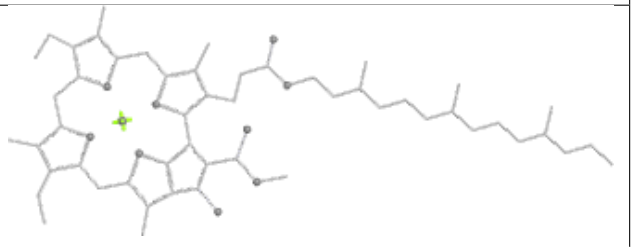
Bond lengths



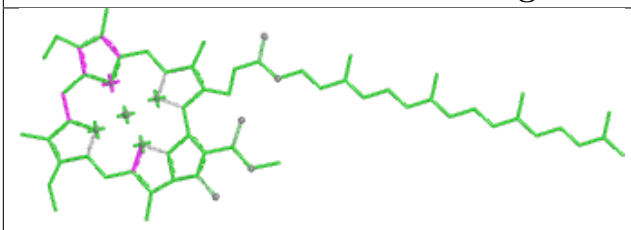
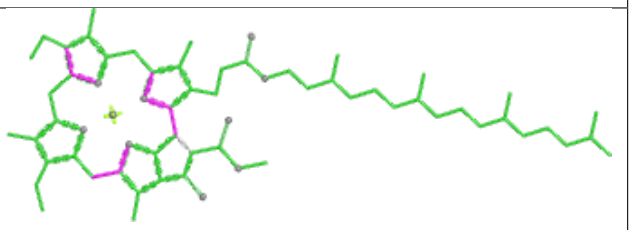
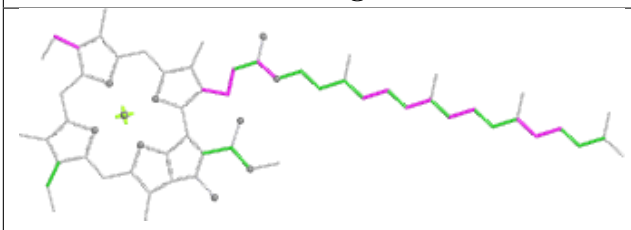
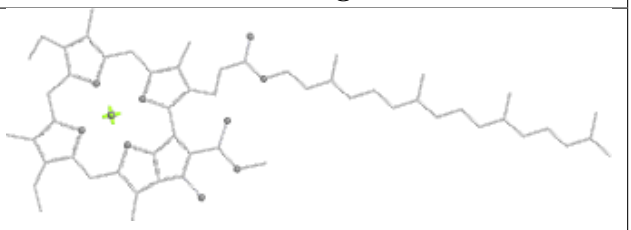
Bond angles

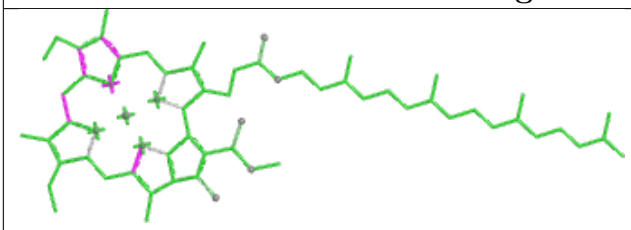
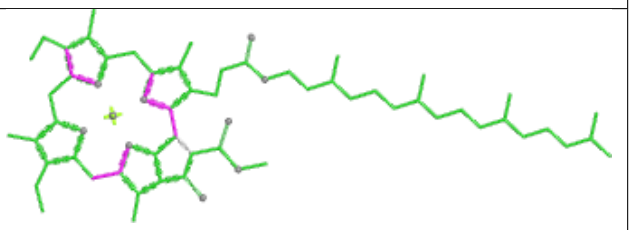
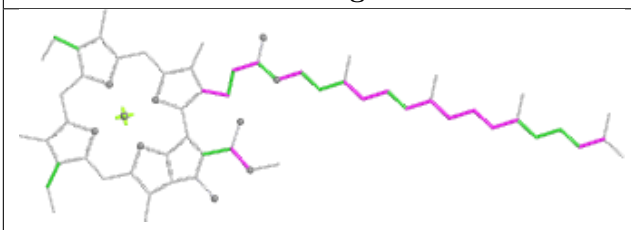
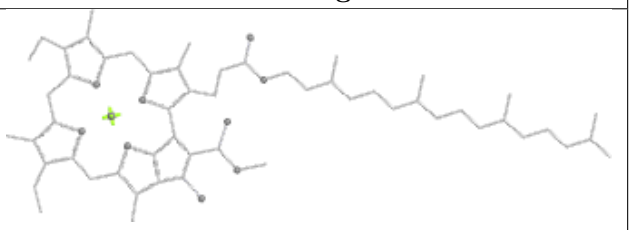


Torsions

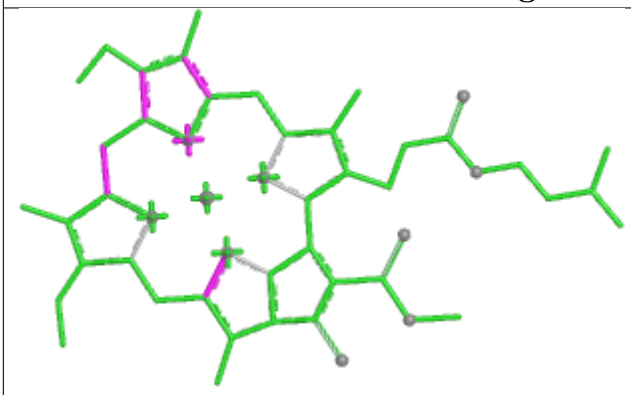


Rings

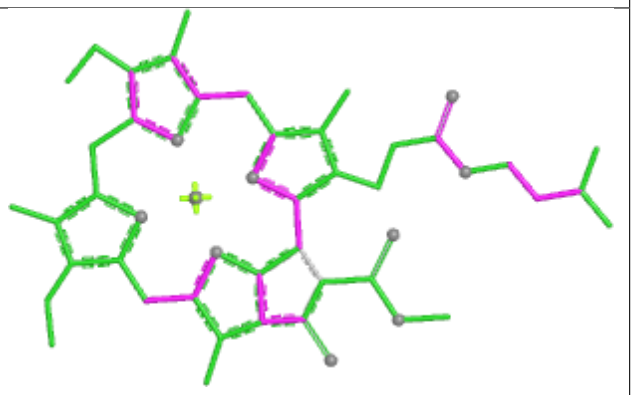
Ligand CLA b 1211	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 1206	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

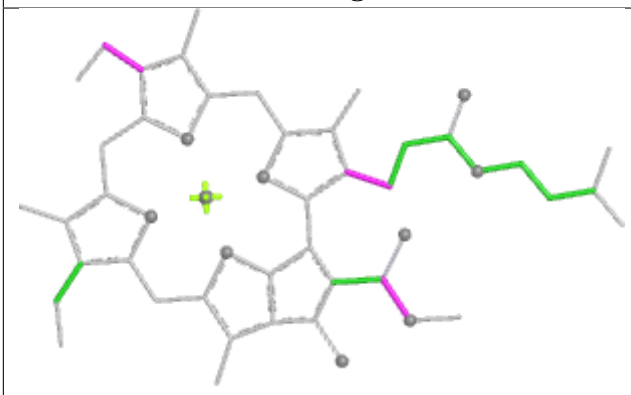
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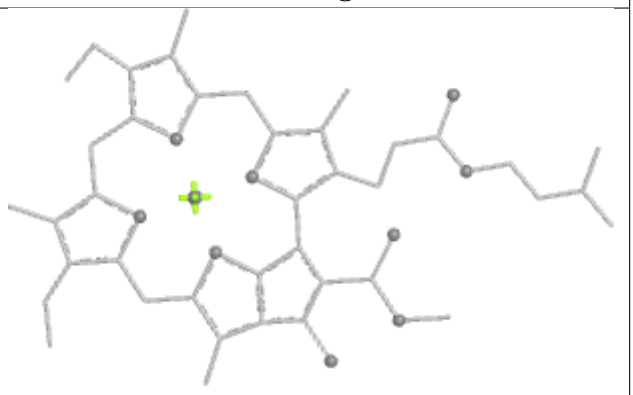
Bond lengths



Bond angles

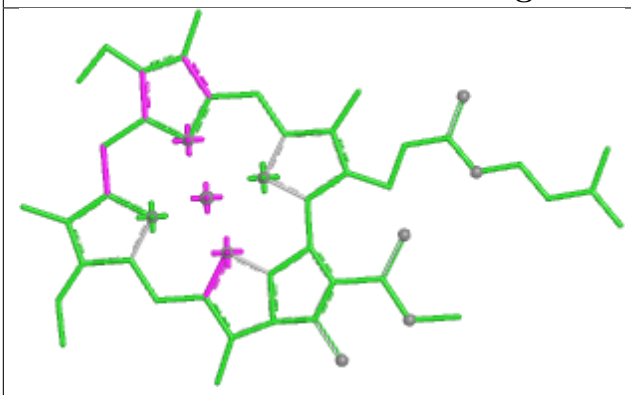


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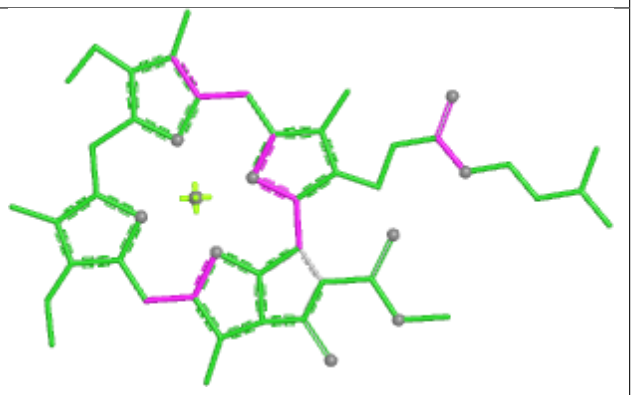


Rings

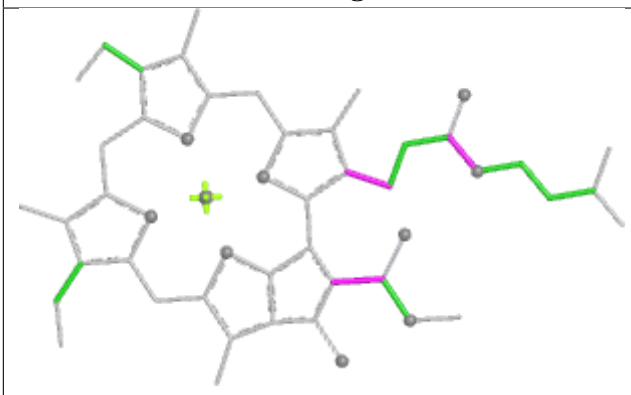
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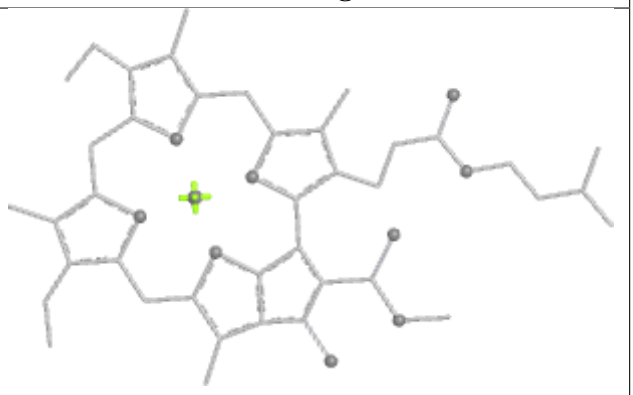
Bond lengths



Bond angles

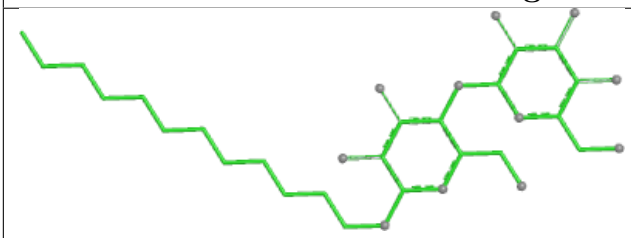


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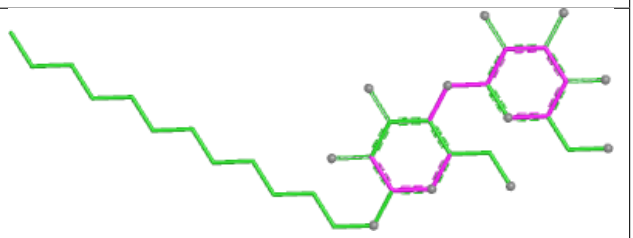


Rings

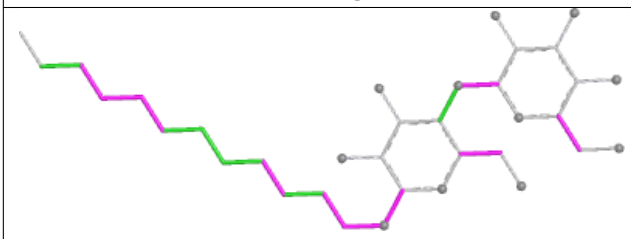
Ligand LMU x 606



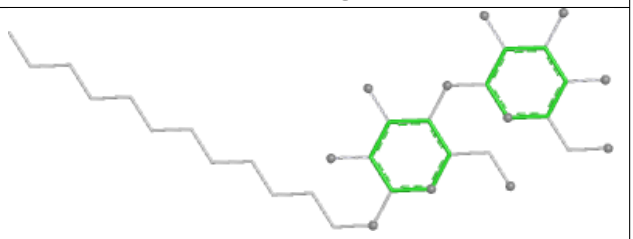
Bond lengths



Bond angles

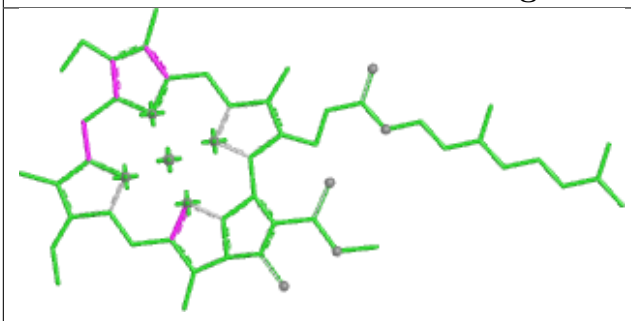


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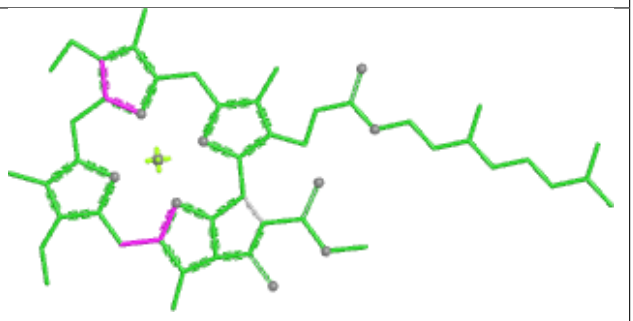


Rings

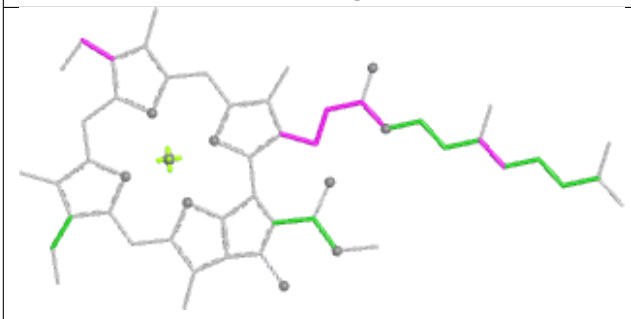
Ligand CLA a 1118



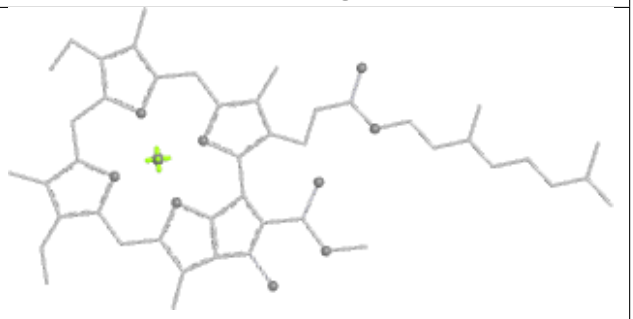
Bond lengths



Bond angles

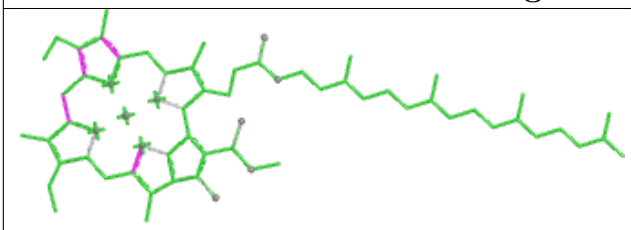


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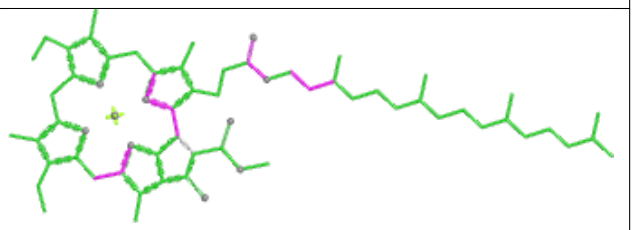


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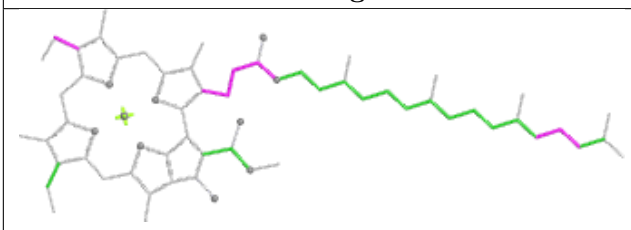
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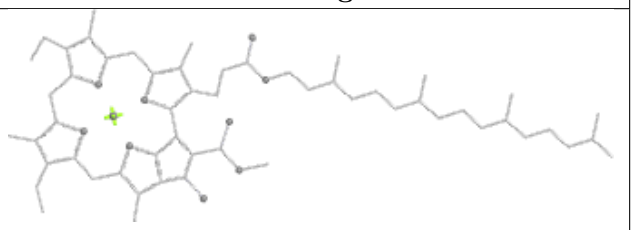
Bond lengths



Bond angles



Torsions

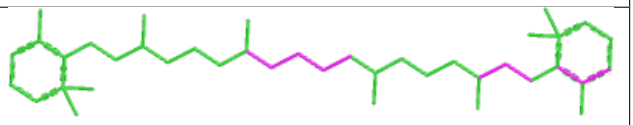


Rings

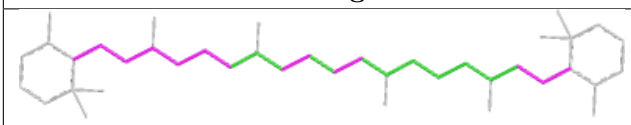
Ligand BCR t 604



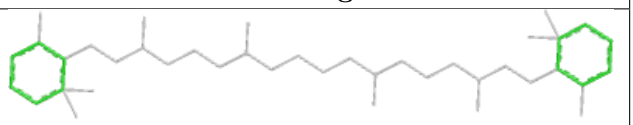
Bond lengths



Bond angles

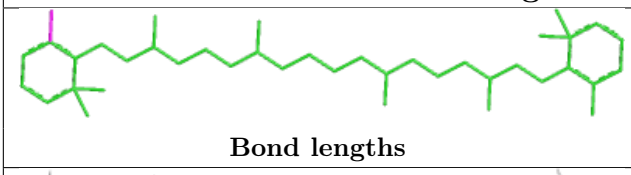


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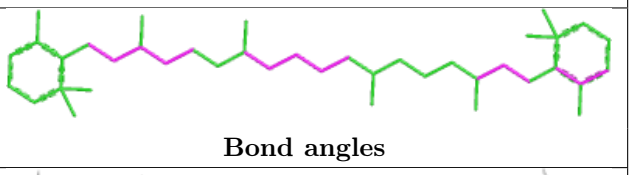


Rings

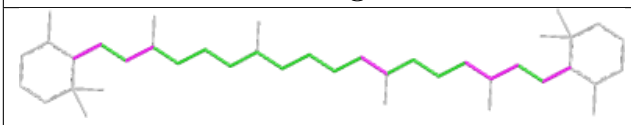
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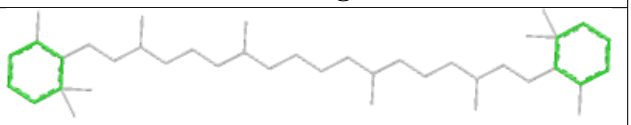
Bond lengths



Bond angles

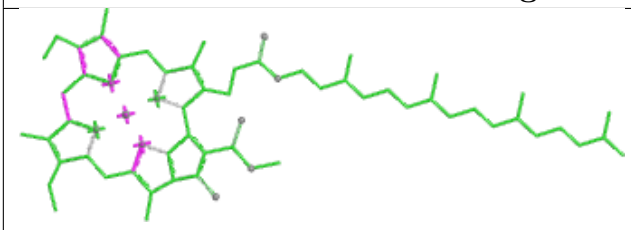


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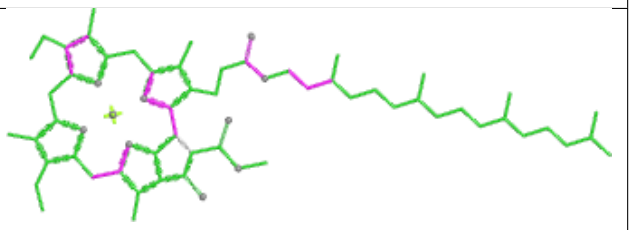


Rings

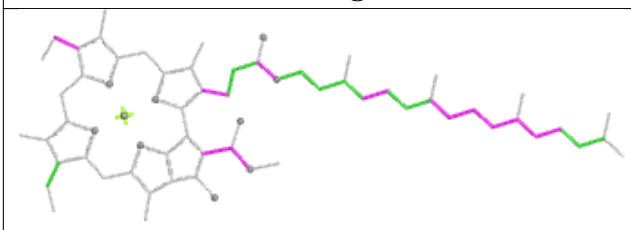
Ligand CLA a 1128



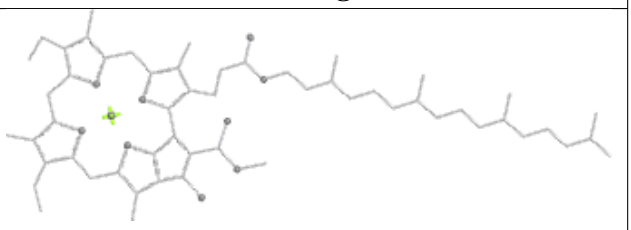
Bond lengths



Bond angles

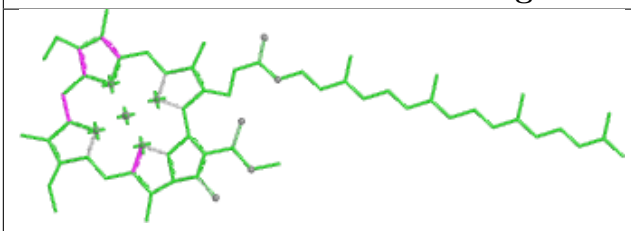


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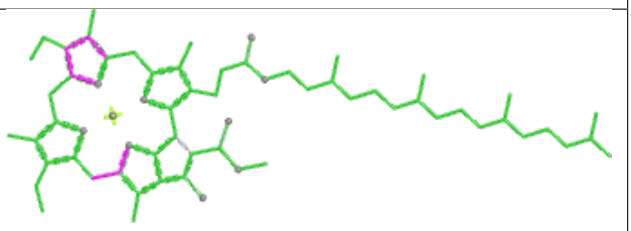


Rings

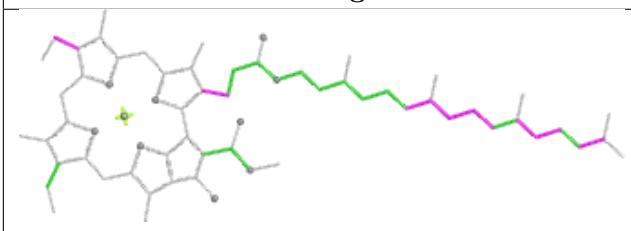
Ligand CLA B 1221



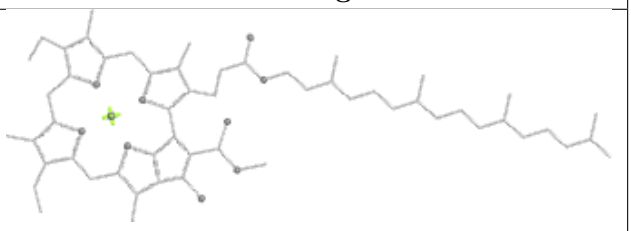
Bond lengths



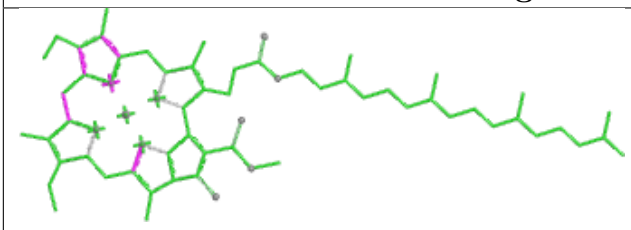
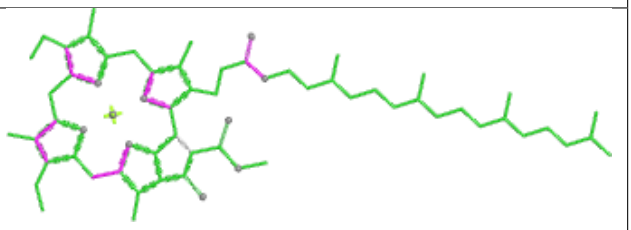
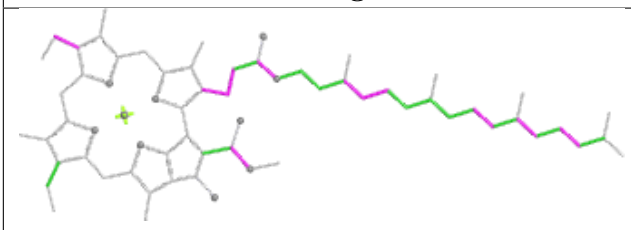
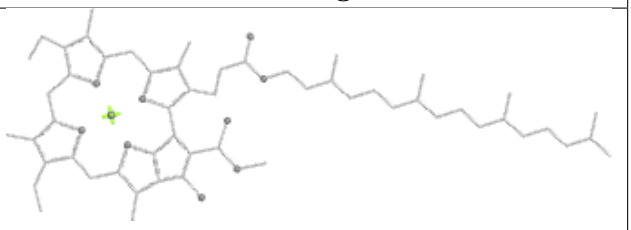
Bond angles

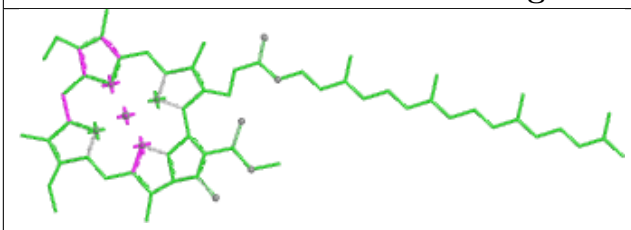
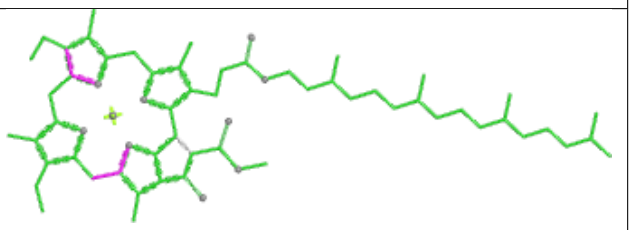
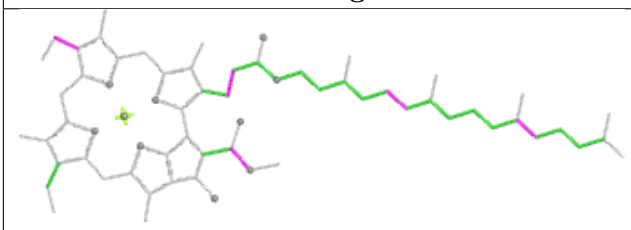
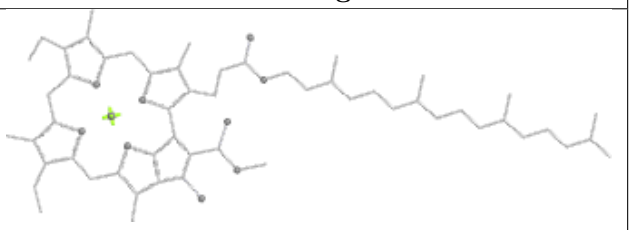


Torsions

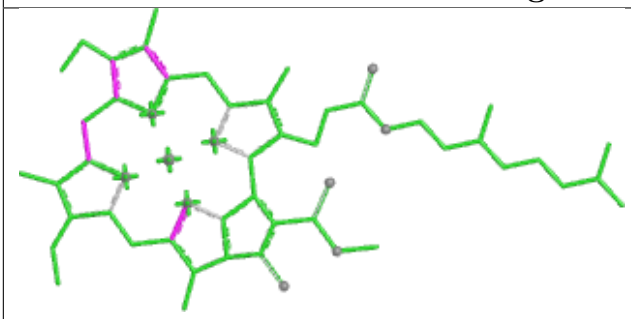


Rings

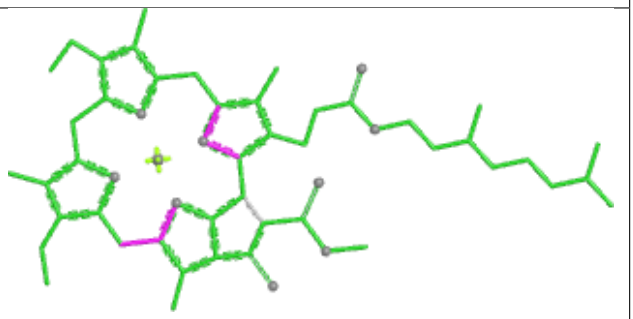
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA x 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

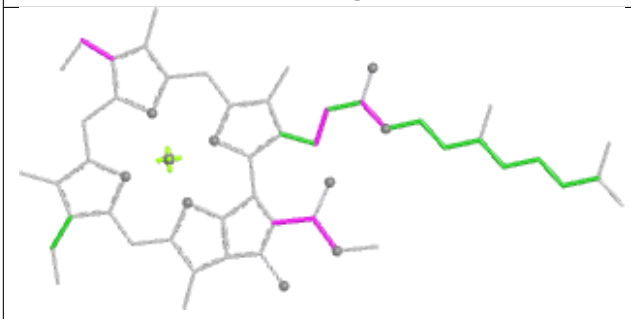
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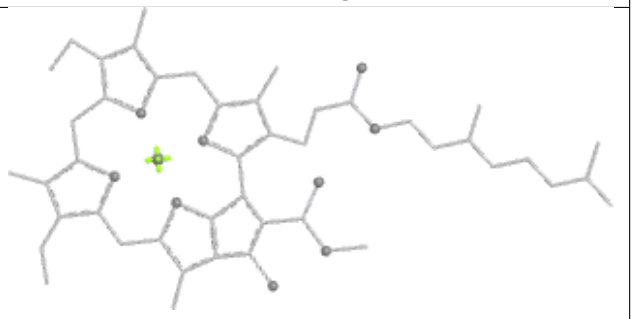
Bond lengths



Bond angles

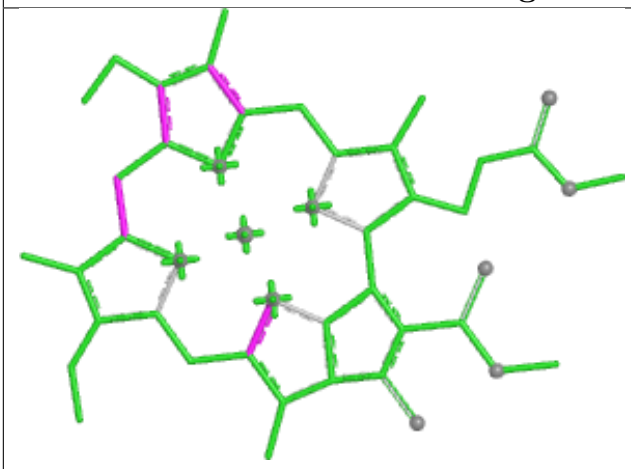


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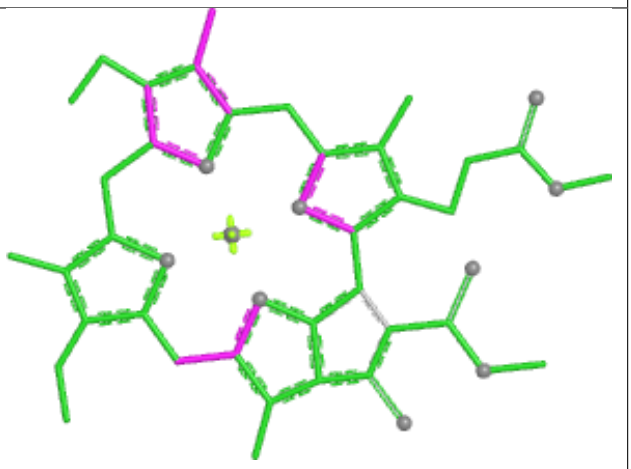


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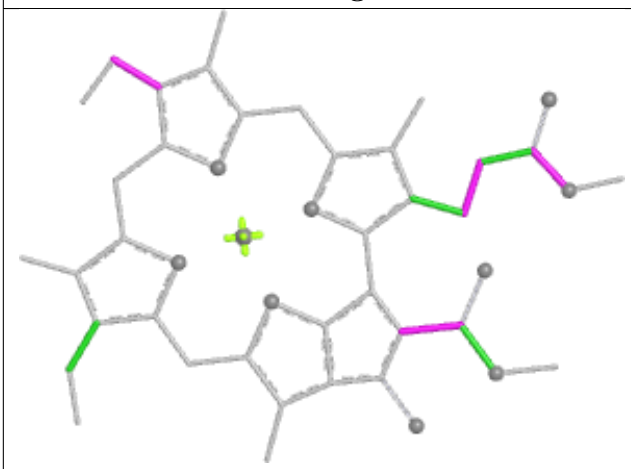
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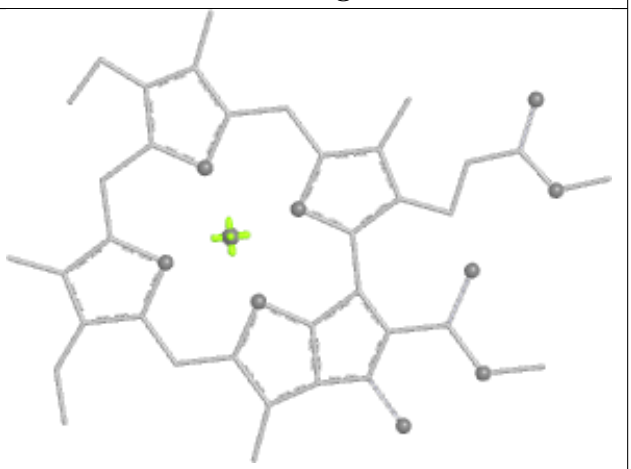
Bond lengths



Bond angles

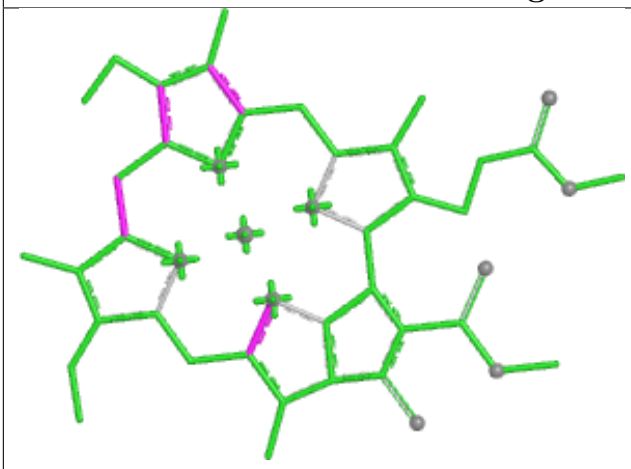


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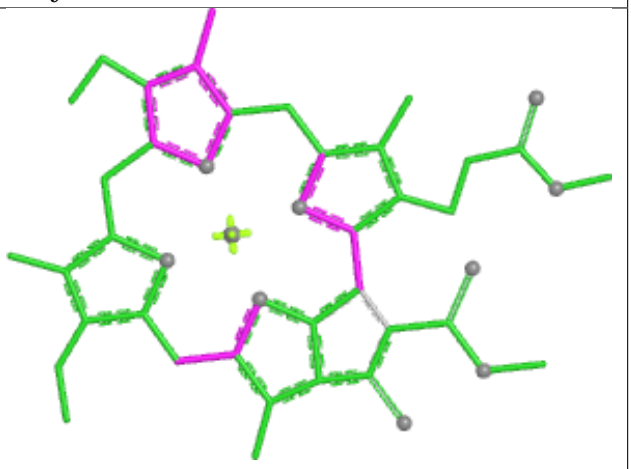


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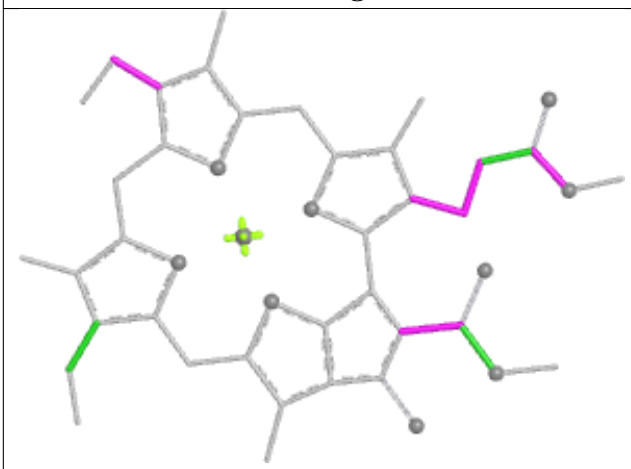
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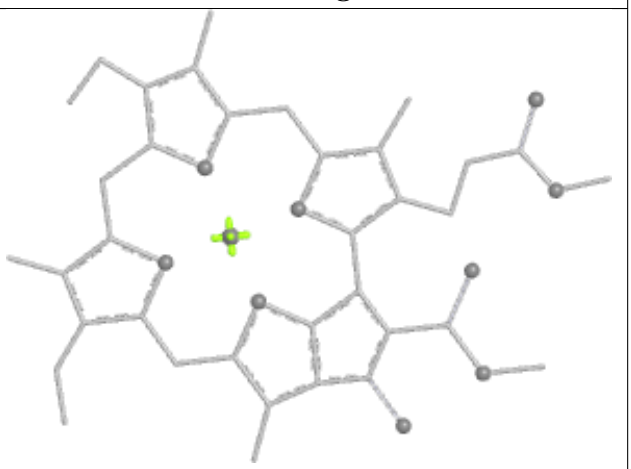
Bond lengths



Bond angles



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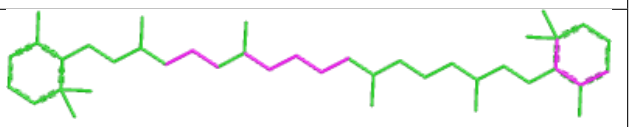


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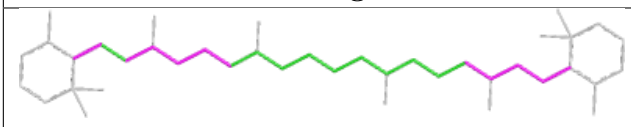
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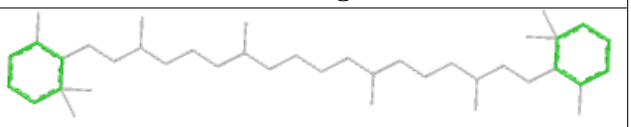
Bond lengths



Bond angles

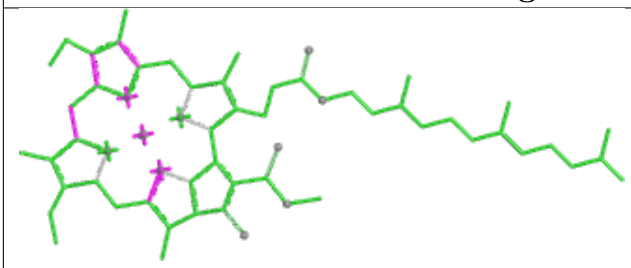


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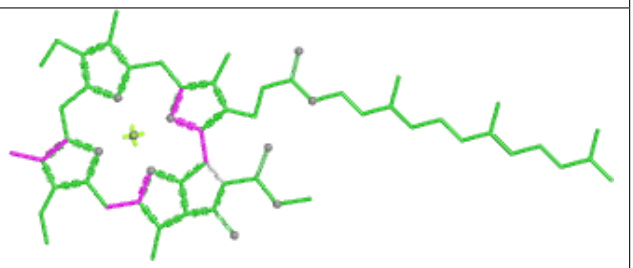


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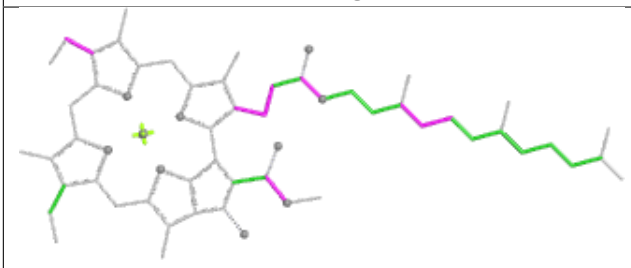
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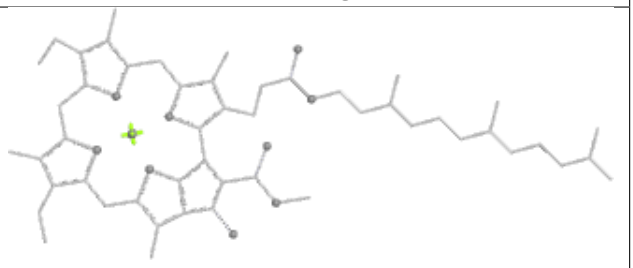
Bond lengths



Bond angles

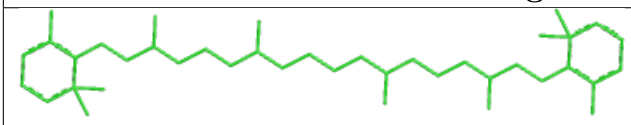


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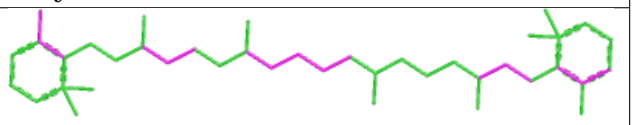


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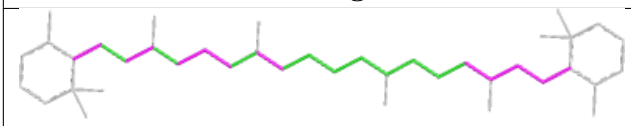
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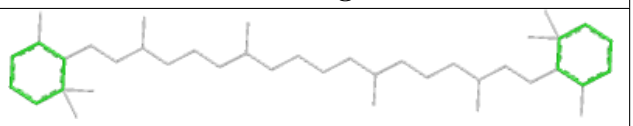
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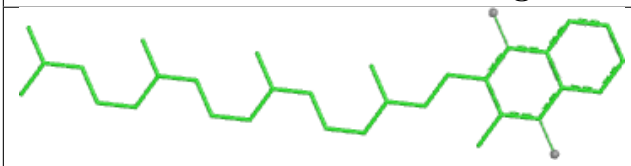


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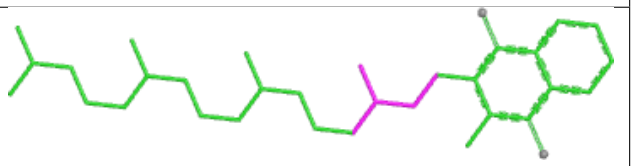


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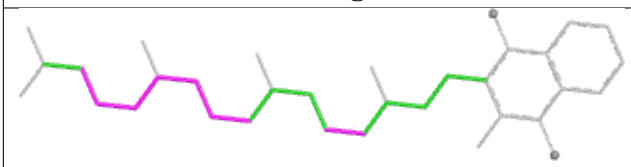
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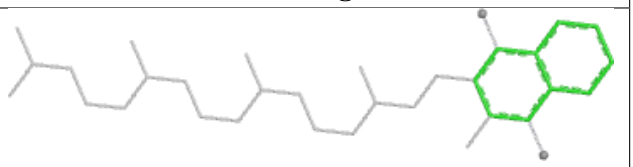
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Bond angles

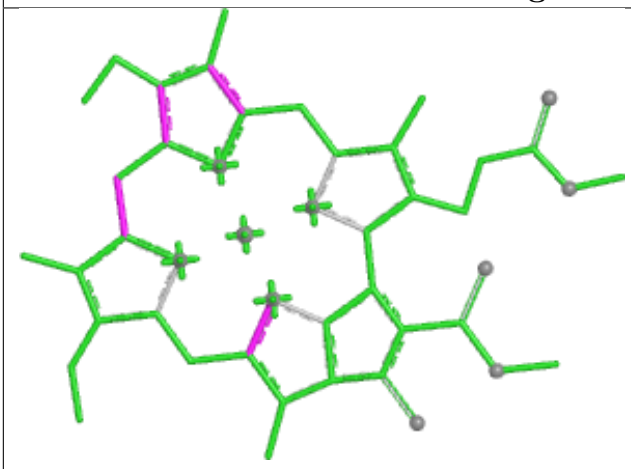


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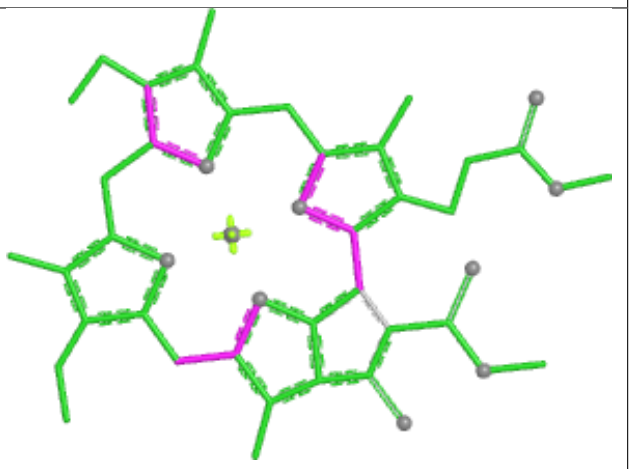


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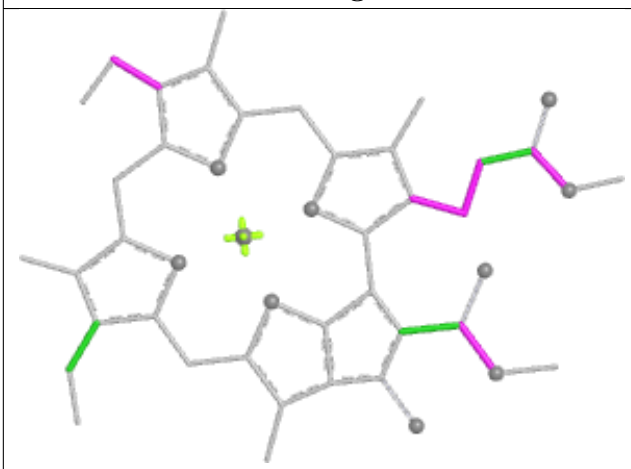
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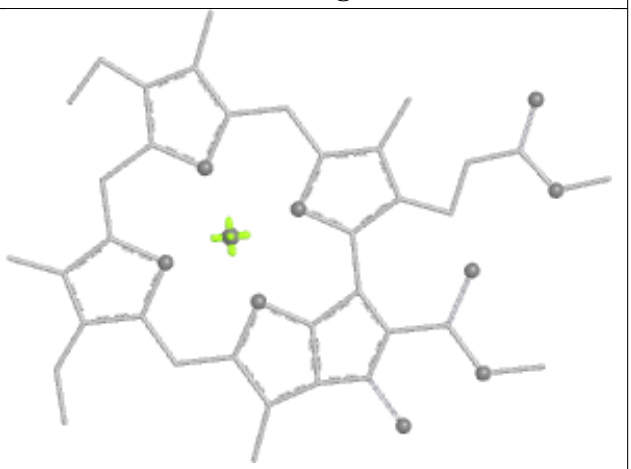
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Bond angles

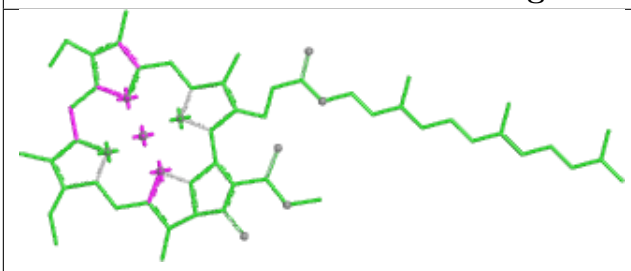


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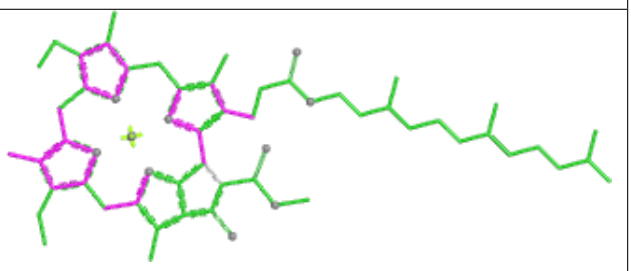


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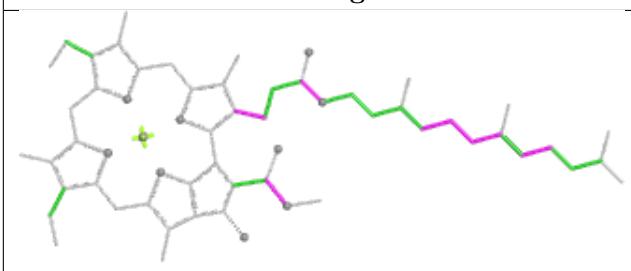
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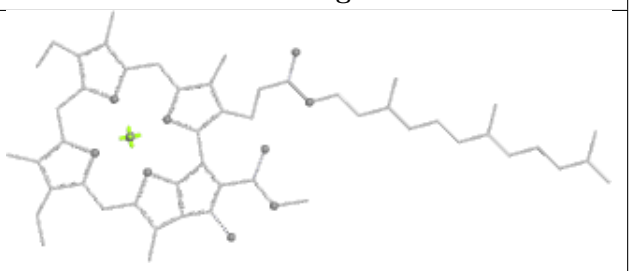
Bond lengths



Bond angles

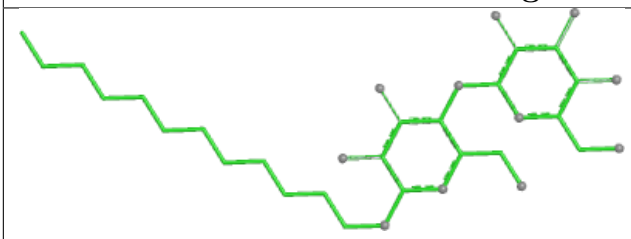


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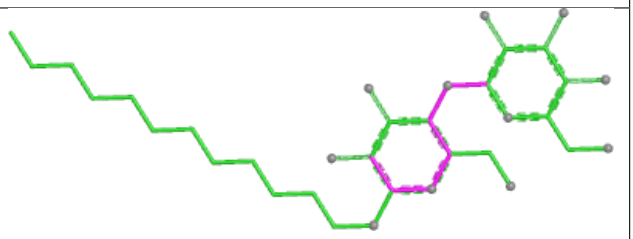


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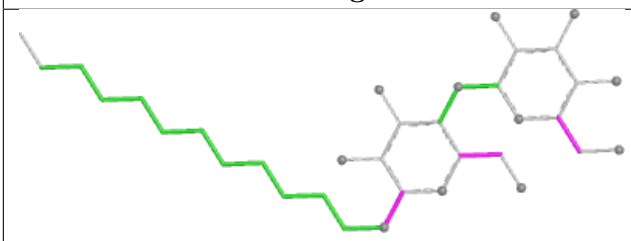
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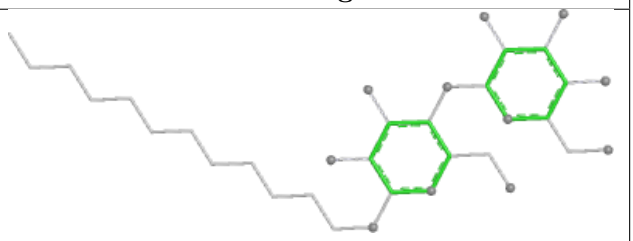
Bond lengths



Bond angles

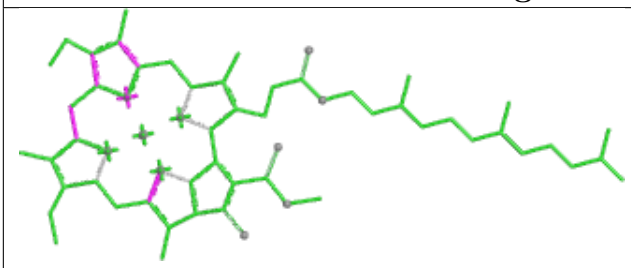


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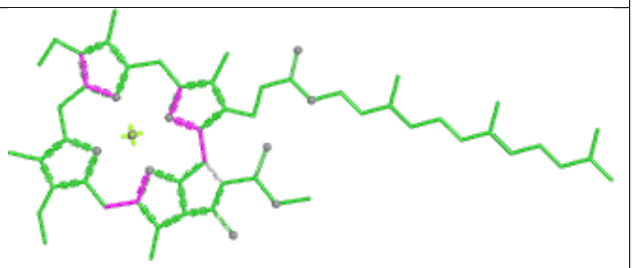


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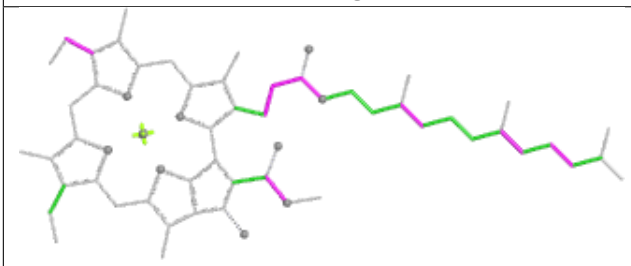
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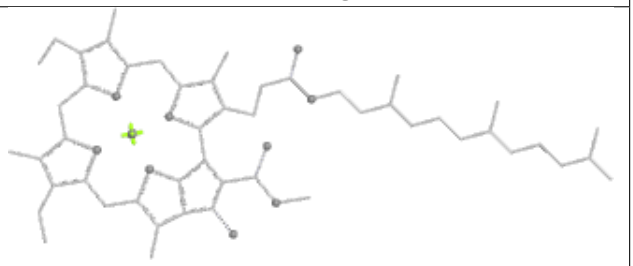
Bond lengths



Bond angles

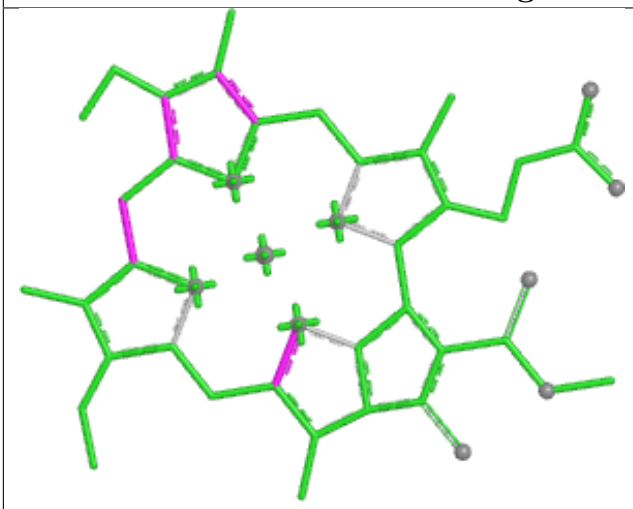


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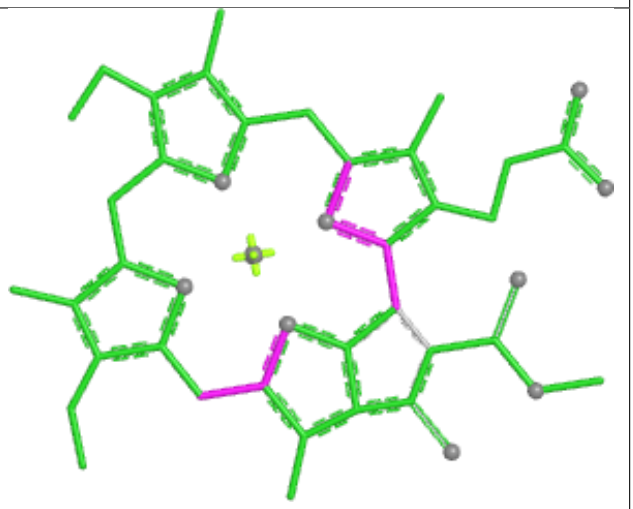


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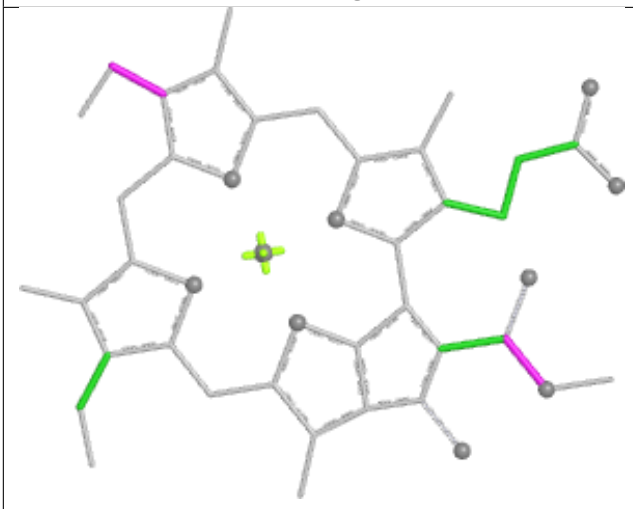
Ligand CLA F 1301



Bond lengths



Bond angles

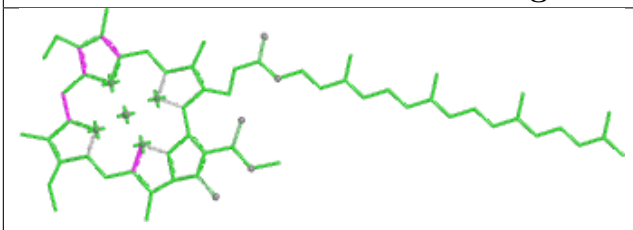


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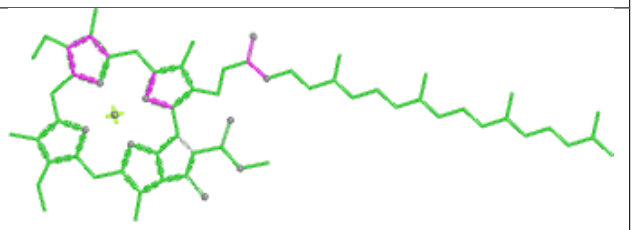


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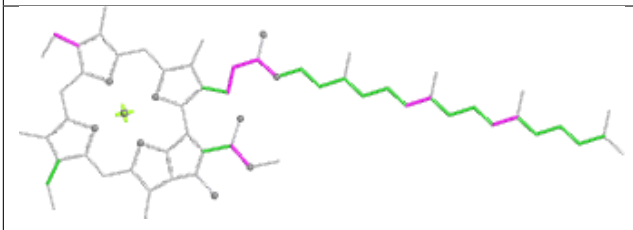
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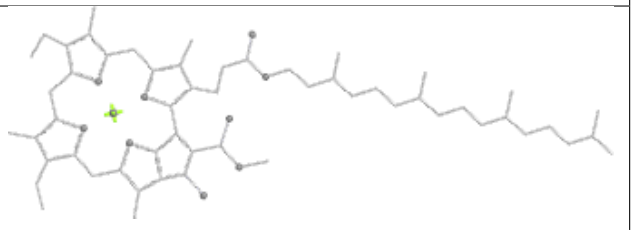
Bond lengths



Bond angles

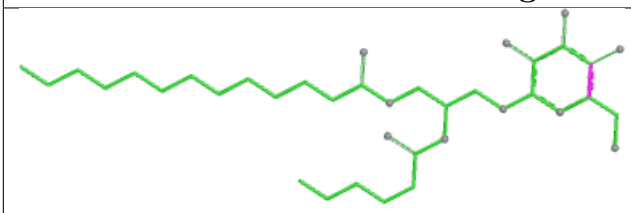


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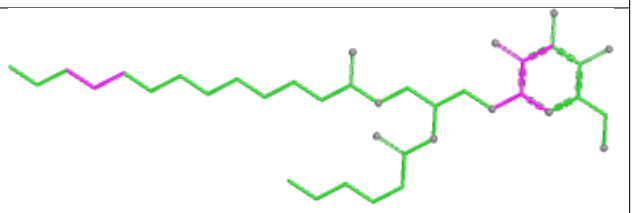


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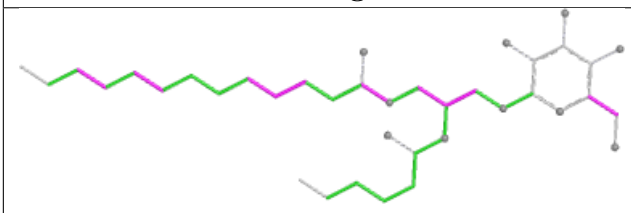
Ligand LMG A 852



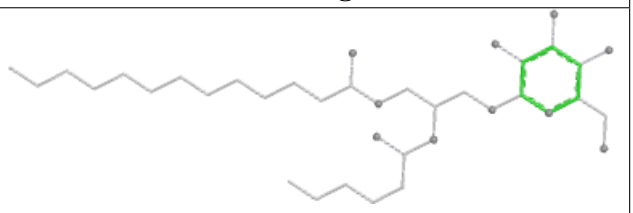
Bond lengths



Bond angles

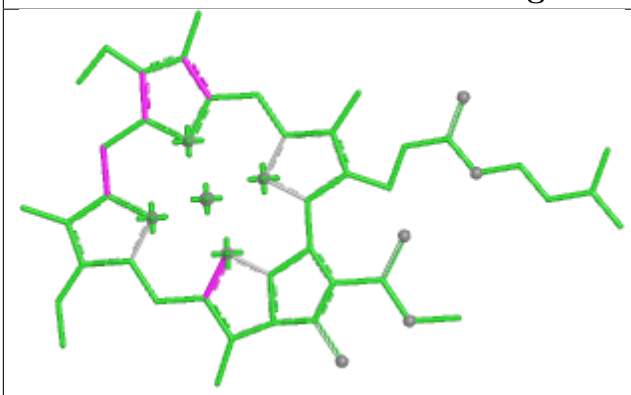


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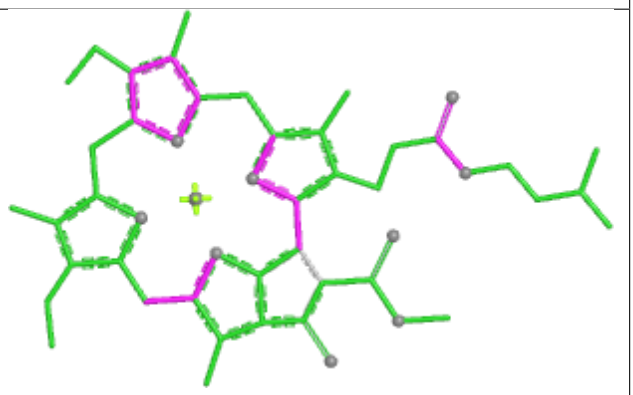


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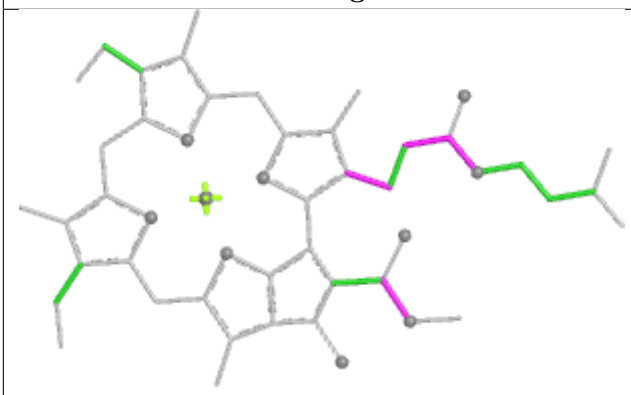
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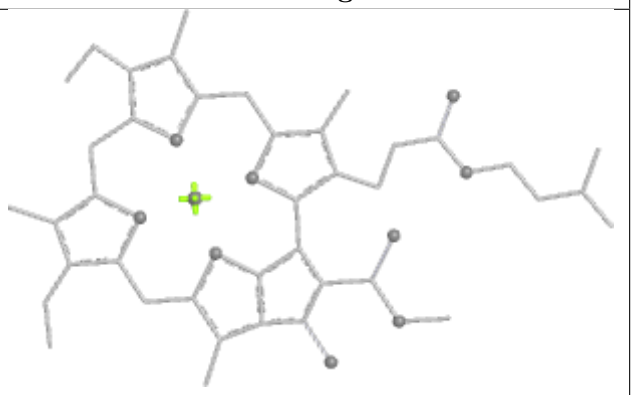
Bond lengths



Bond angles

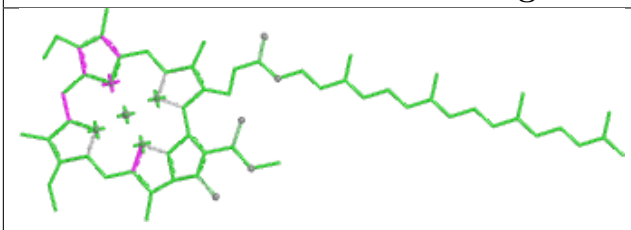


Torsions

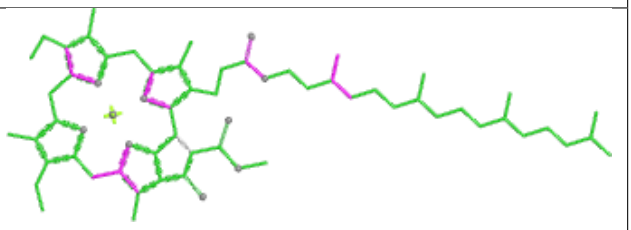


Rings

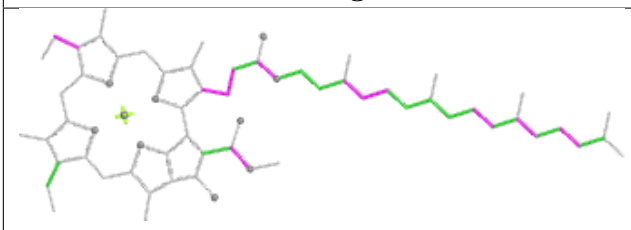
Ligand CLA b 1203



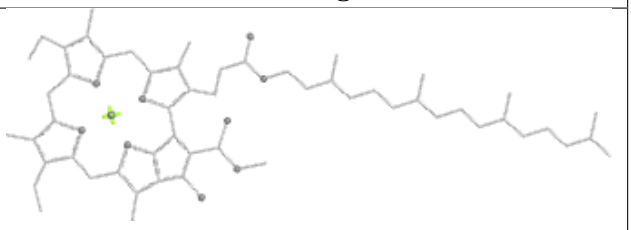
Bond lengths



Bond angles

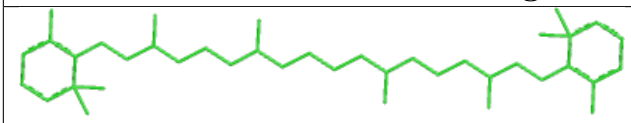


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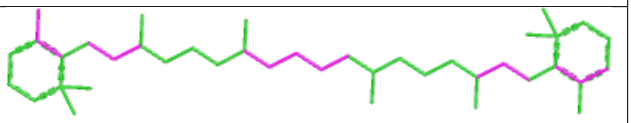


Rings

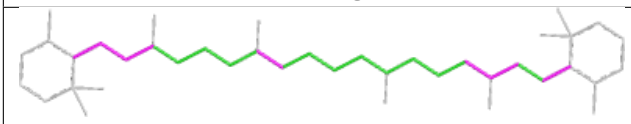
Ligand BCR Y 601



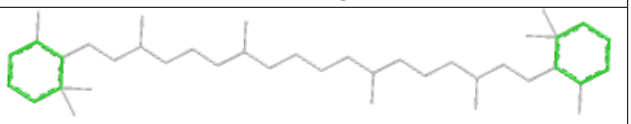
Bond lengths



Bond angles

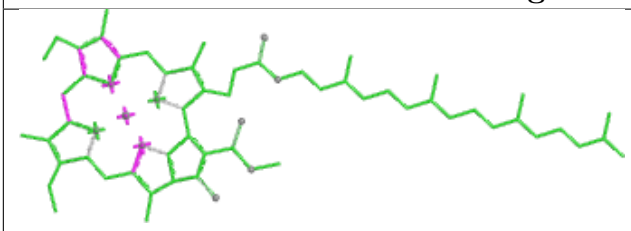


Torsions

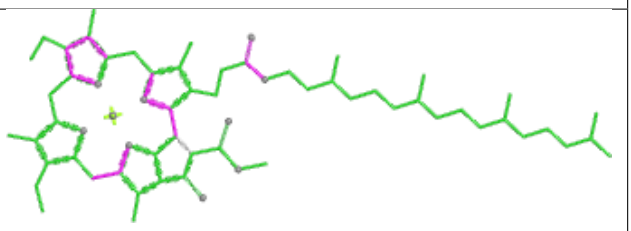


Rings

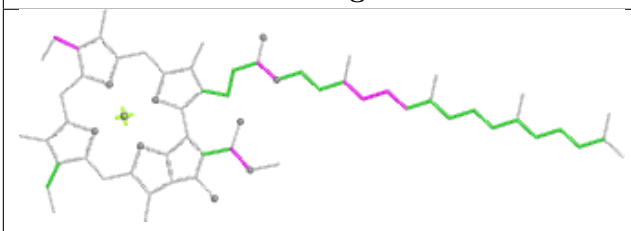
Ligand CLA x 512



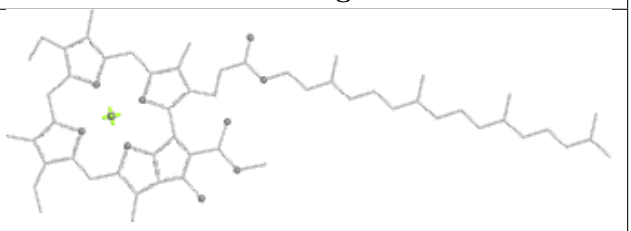
Bond lengths



Bond angles

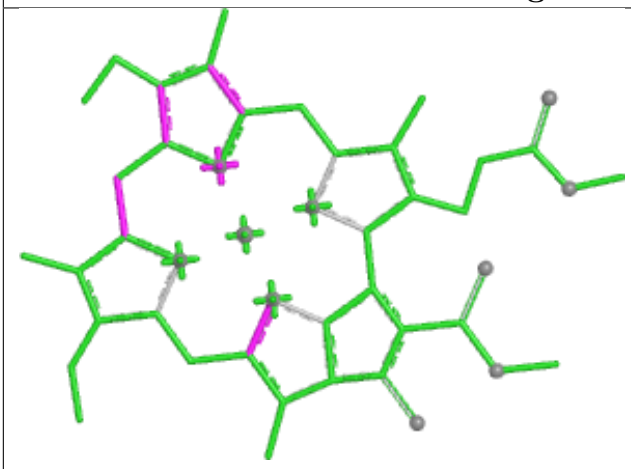


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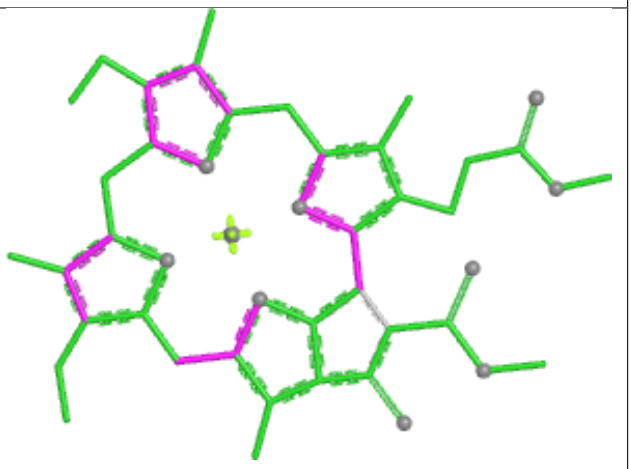


Rings

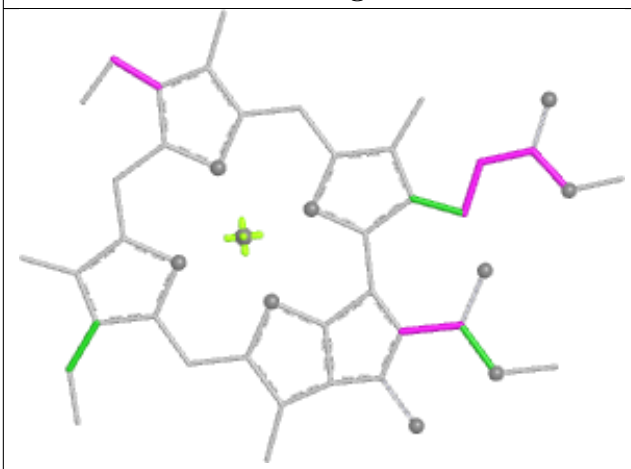
Ligand CLA h 501



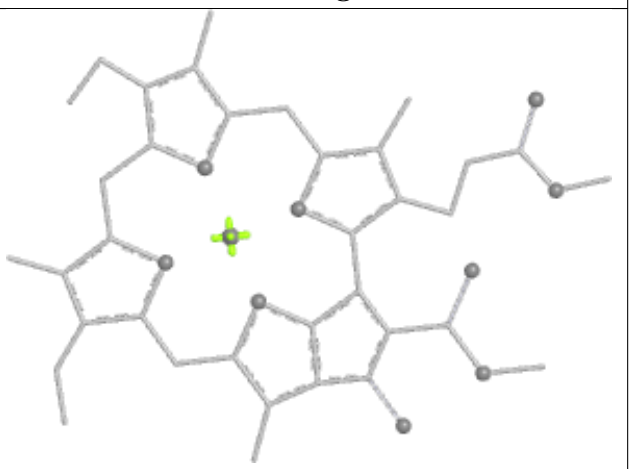
Bond lengths



Bond angles

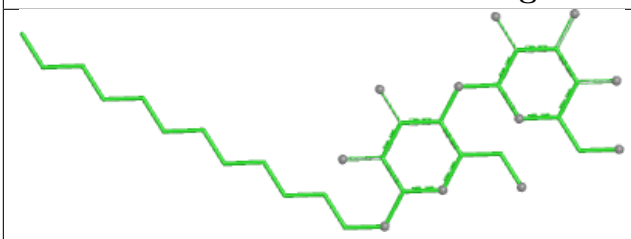


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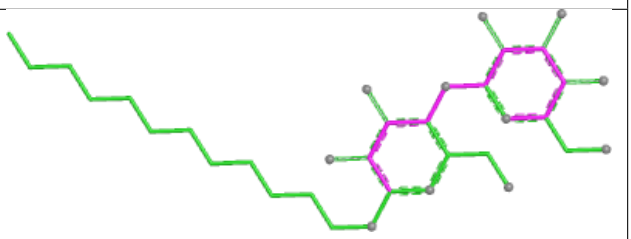


Rings

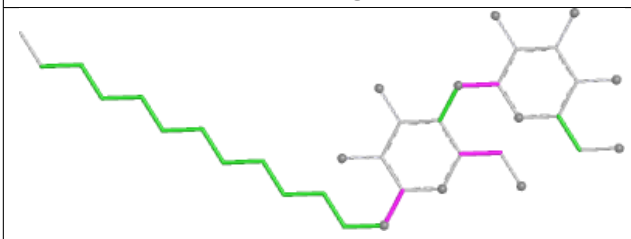
Ligand LMU Y 606



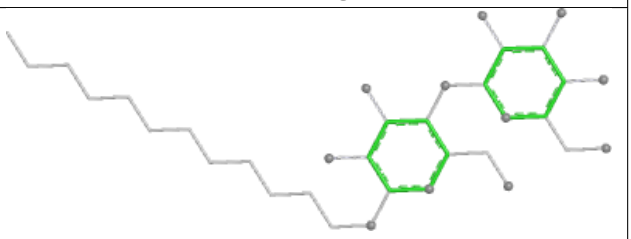
Bond lengths



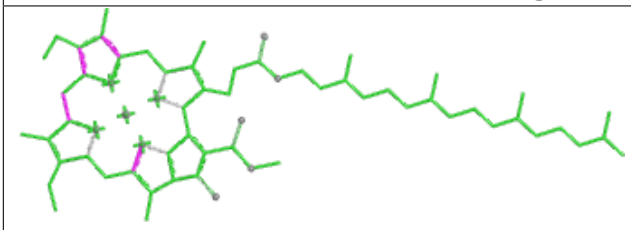
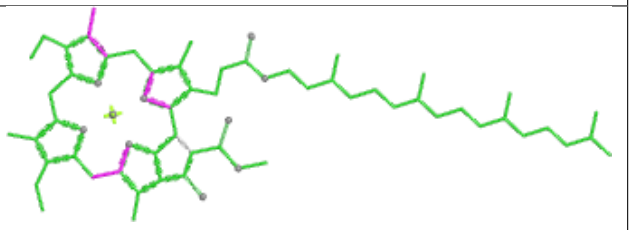
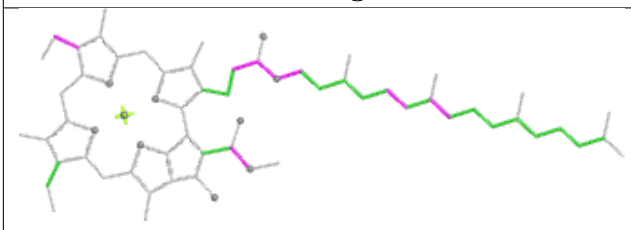
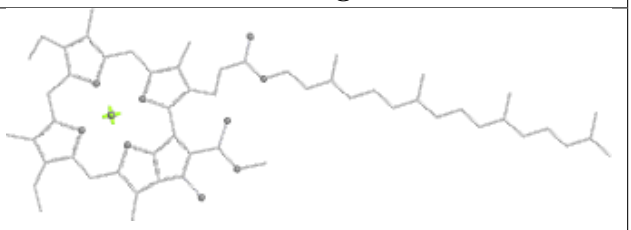
Bond angles

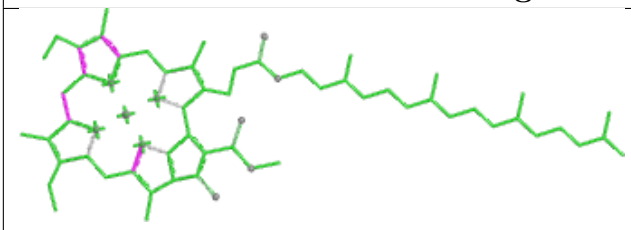
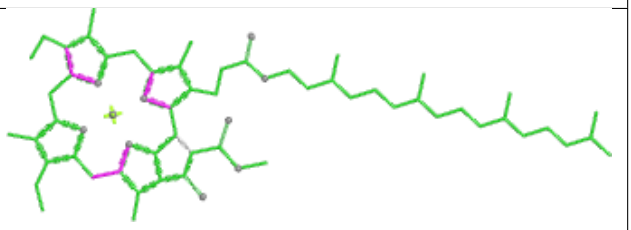
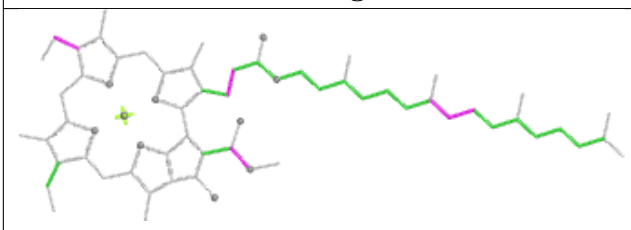
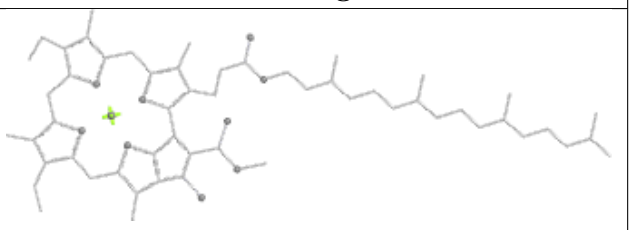


Torsions

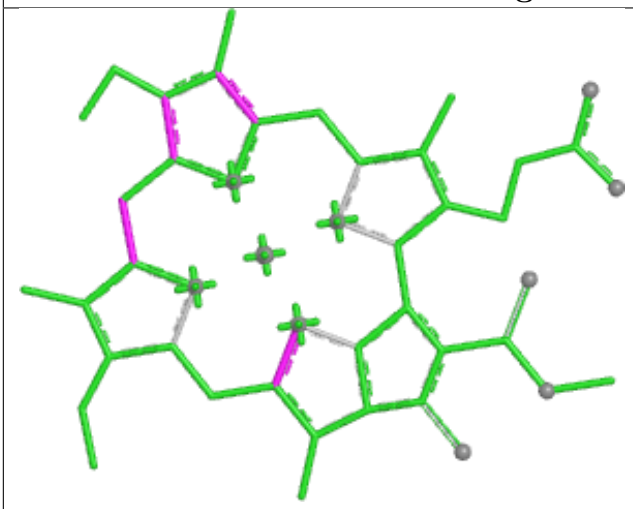


Rings

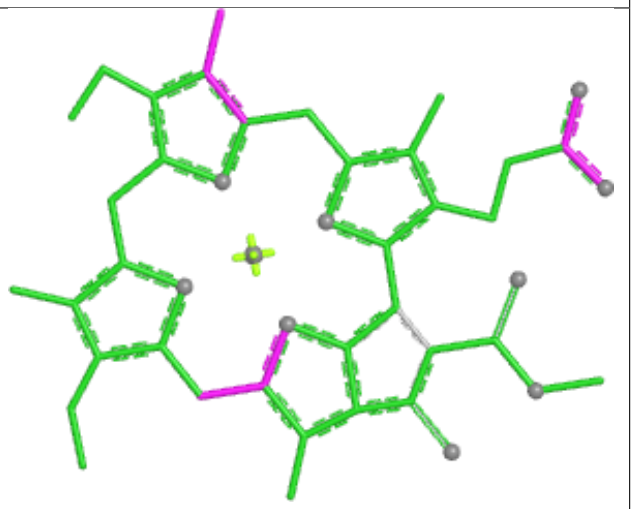
Ligand CLA t 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

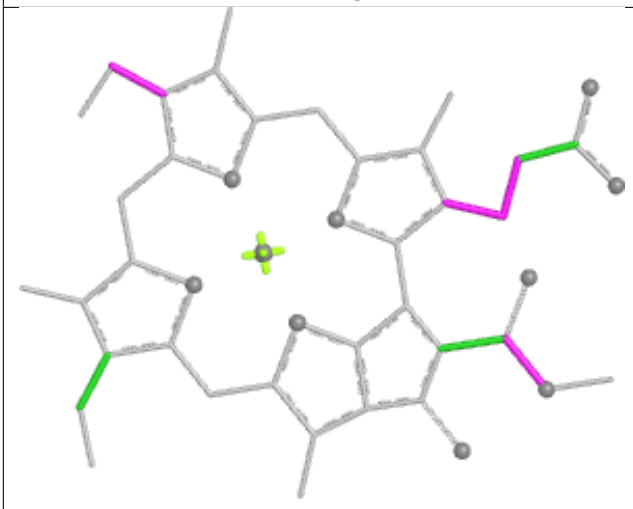
Ligand CLA T 4002



Bond lengths



Bond angles

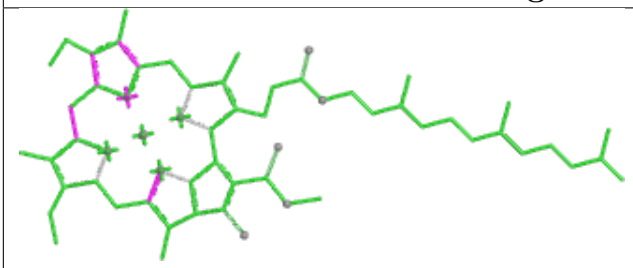


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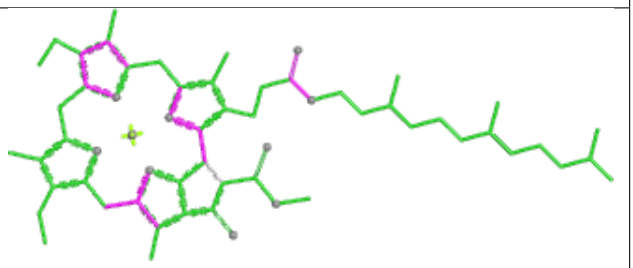


Rings

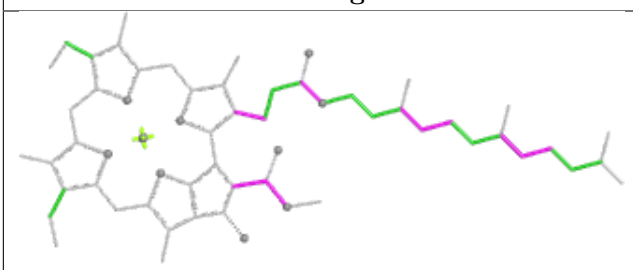
Ligand CLA h 504



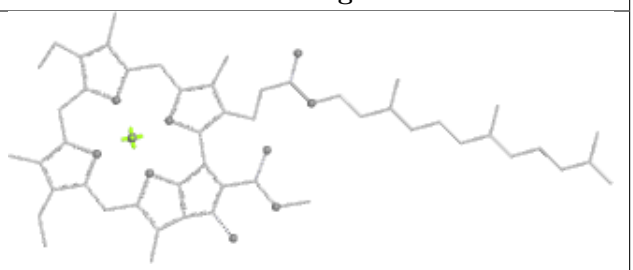
Bond lengths



Bond angles

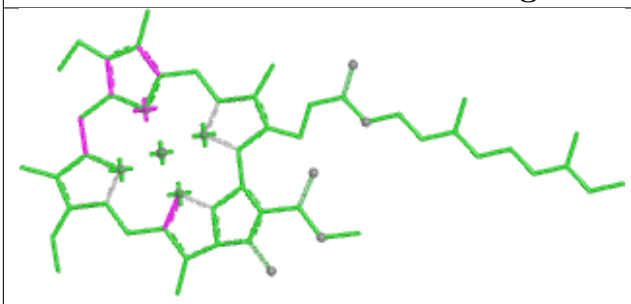


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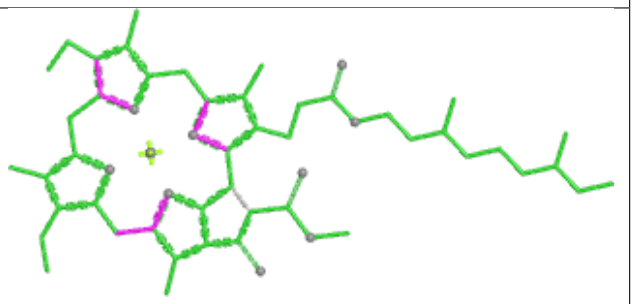


Rings

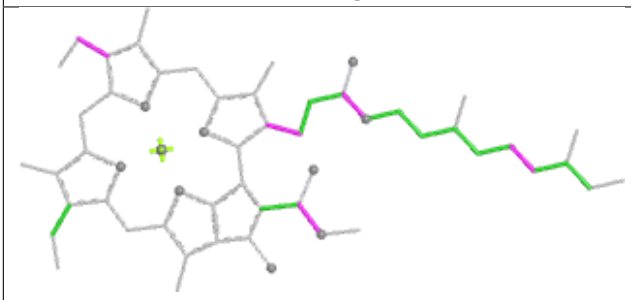
Ligand CLA a 1102



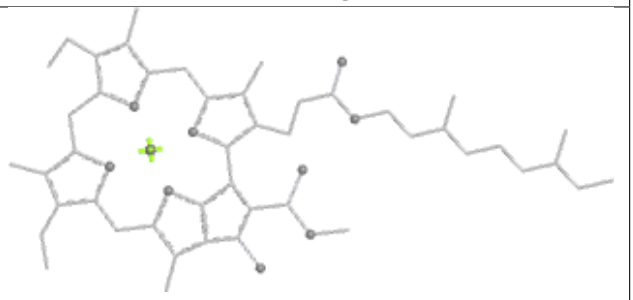
Bond lengths



Bond angles

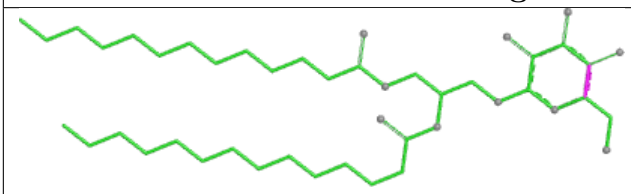


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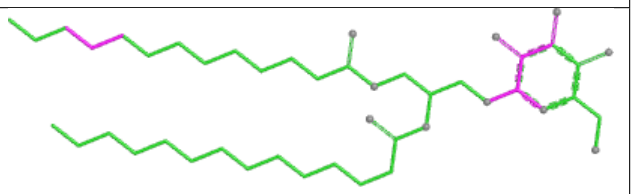


Rings

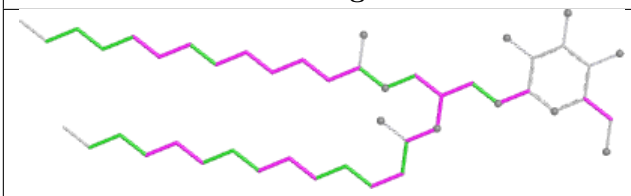
Ligand LMG H 4101



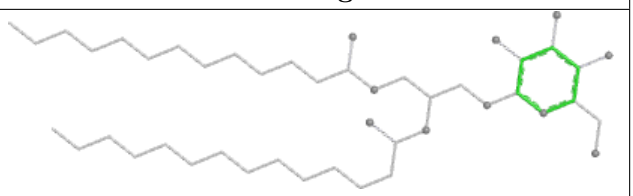
Bond lengths



Bond angles

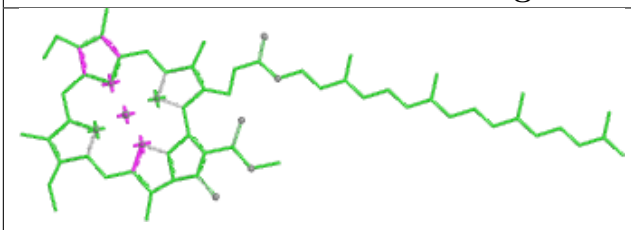


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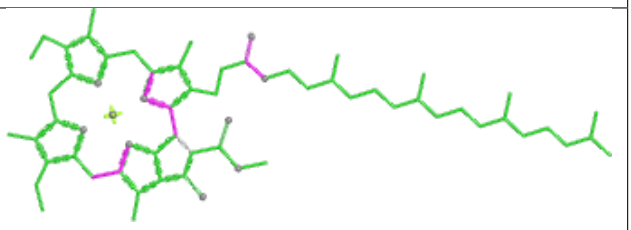


Rings

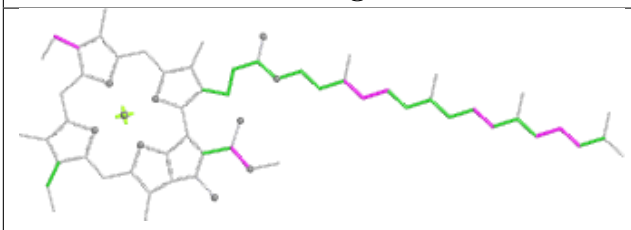
Ligand CLA G 1205



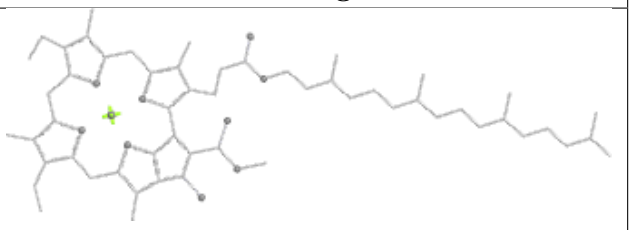
Bond lengths



Bond angles

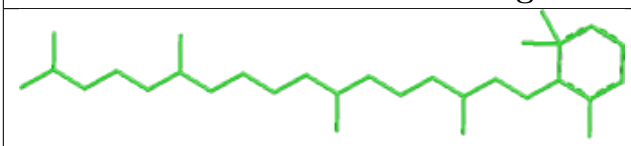


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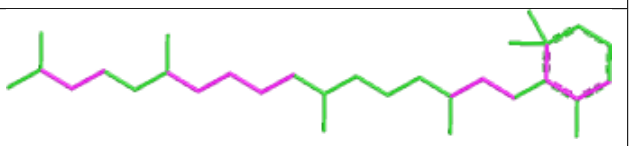


Rings

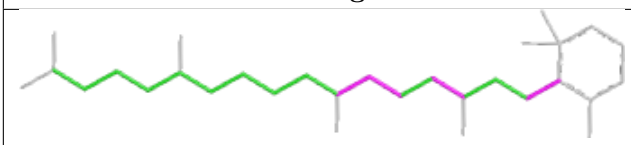
Ligand BCR b 4009



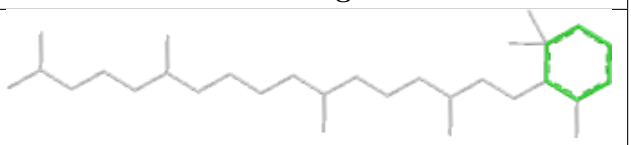
Bond lengths



Bond angles

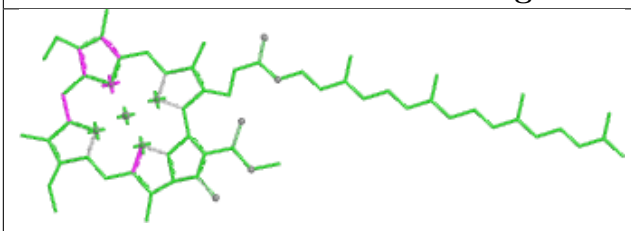


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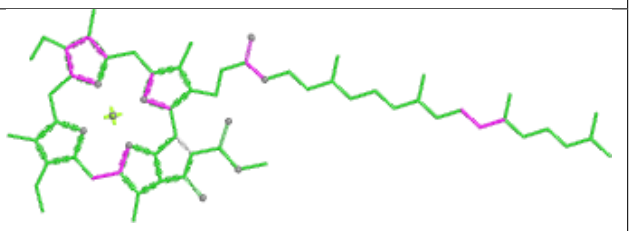


Rings

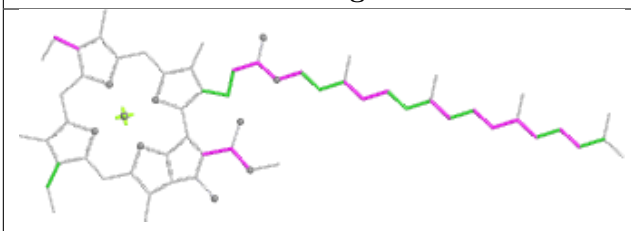
Ligand CLA A 1104



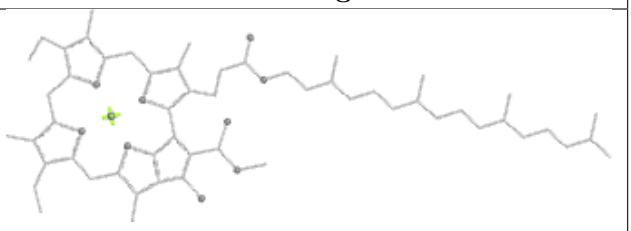
Bond lengths



Bond angles

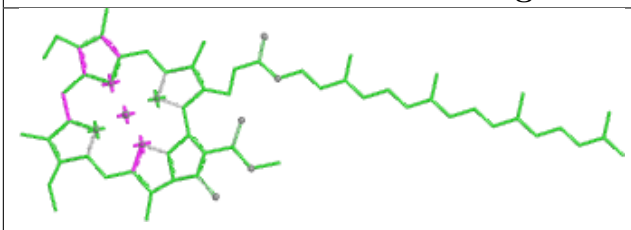


Torsions

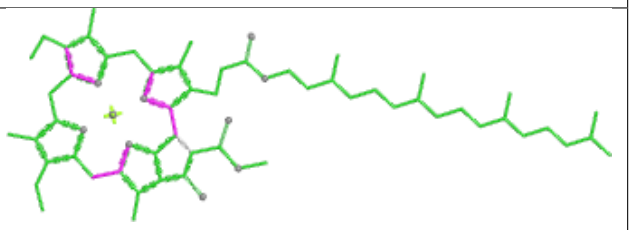


Rings

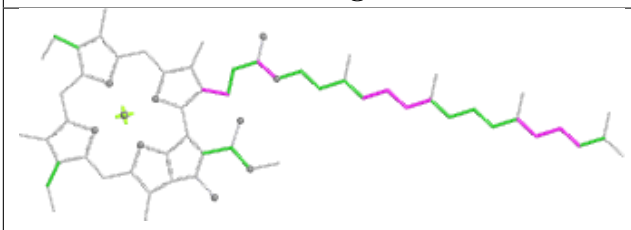
Ligand CLA B 1225



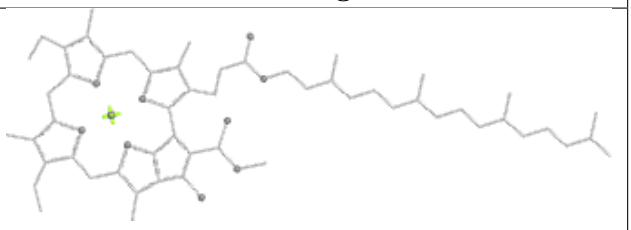
Bond lengths



Bond angles

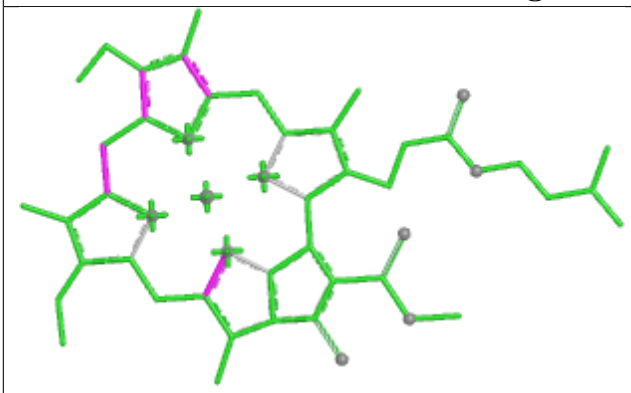


Torsions

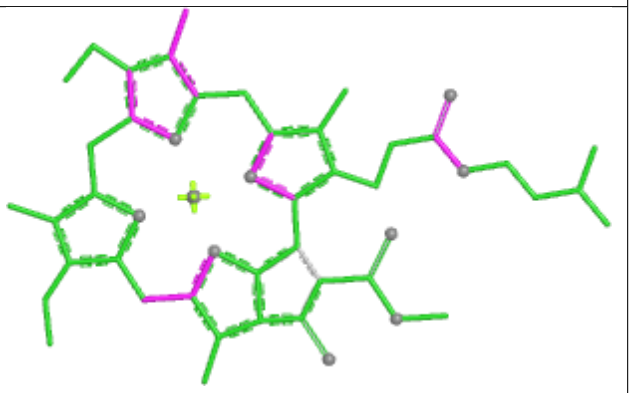


Rings

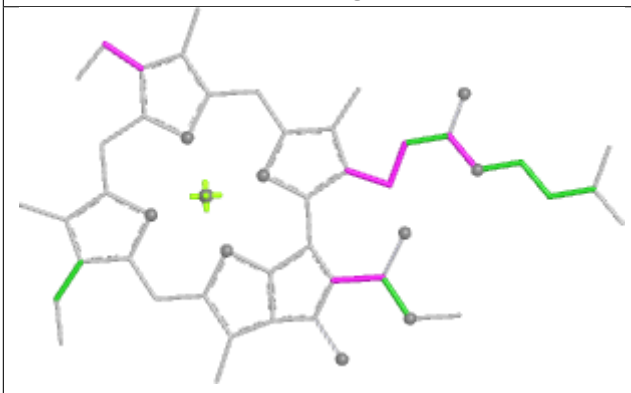
Ligand CLA Z 513



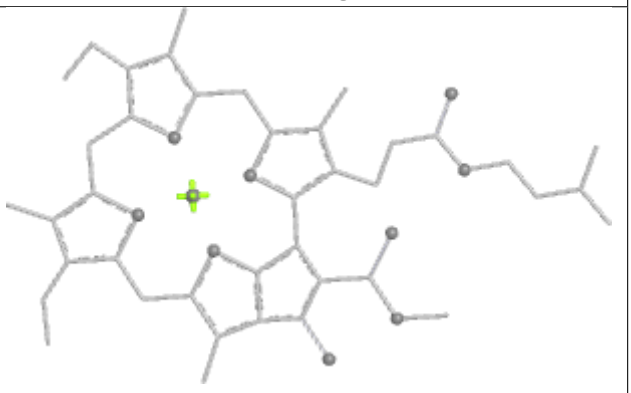
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Bond angles

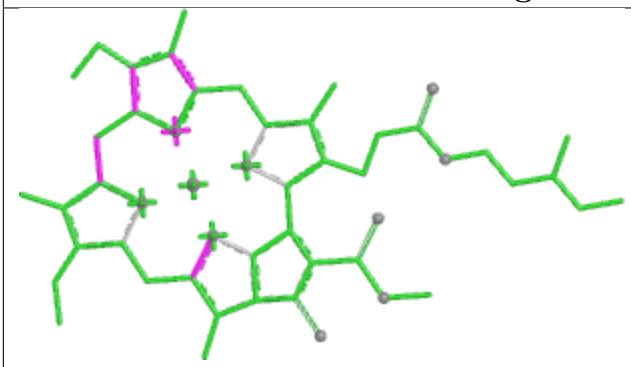


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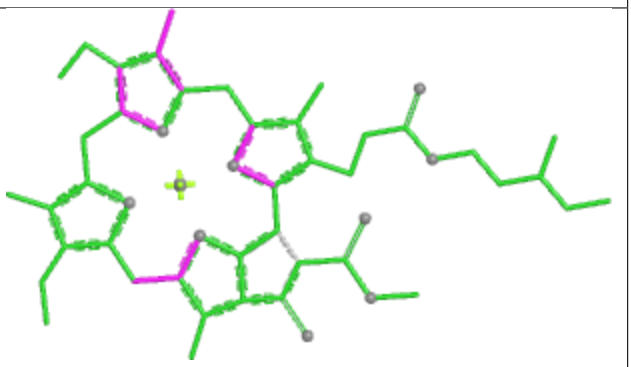


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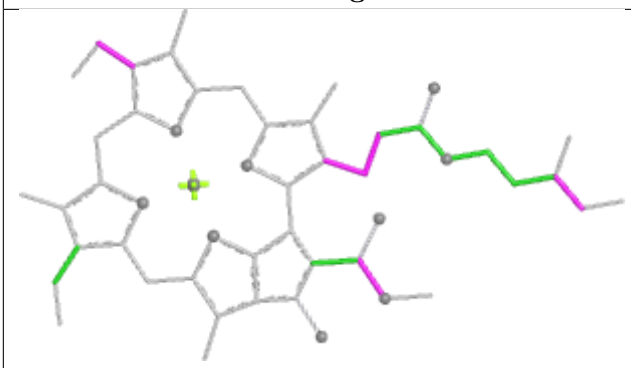
Ligand CLA A 1121



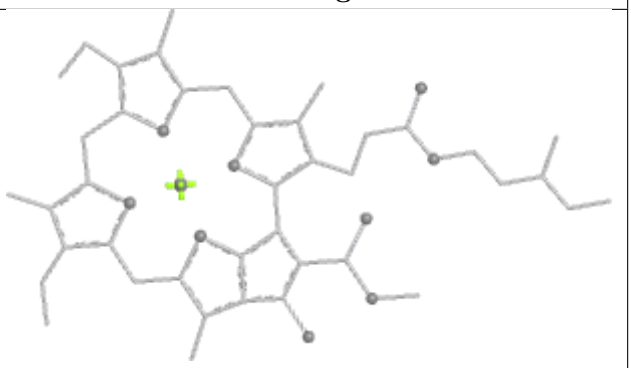
Bond lengths



Bond angles

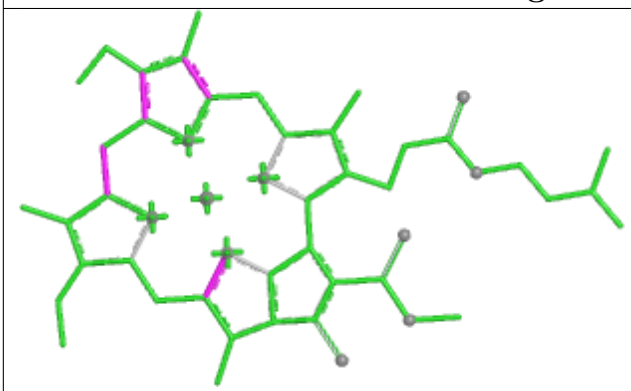


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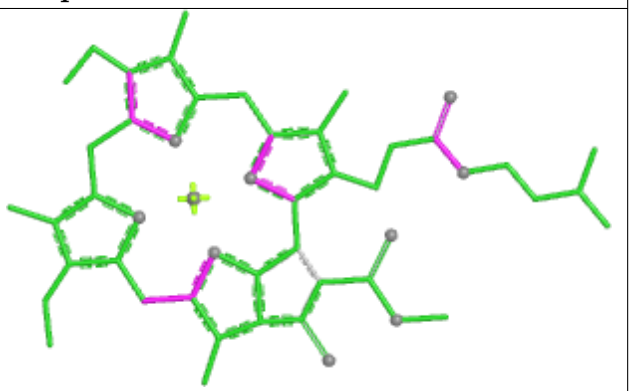


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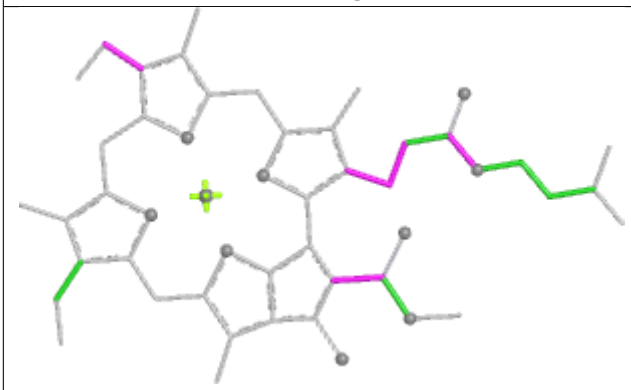
Ligand CLA q 513



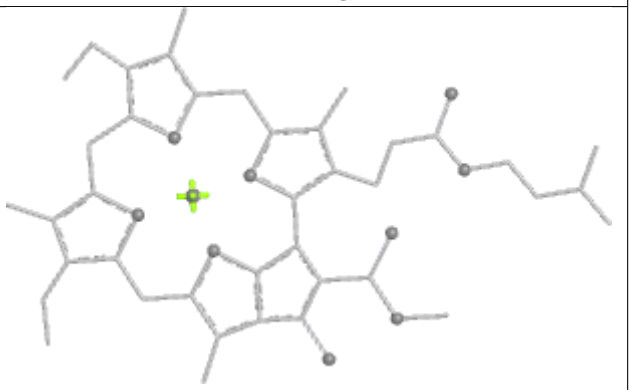
Bond lengths



Bond angles

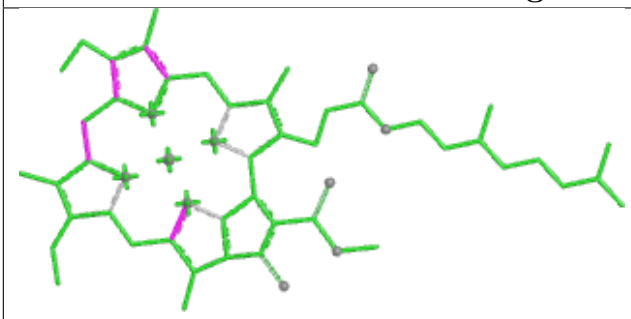


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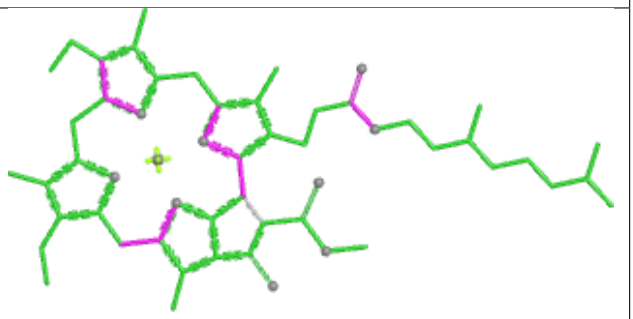


Rings

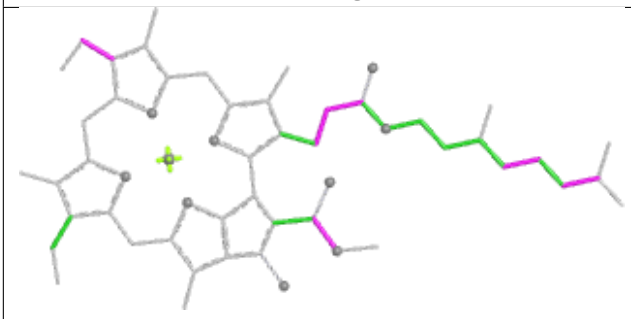
Ligand CLA Z 508



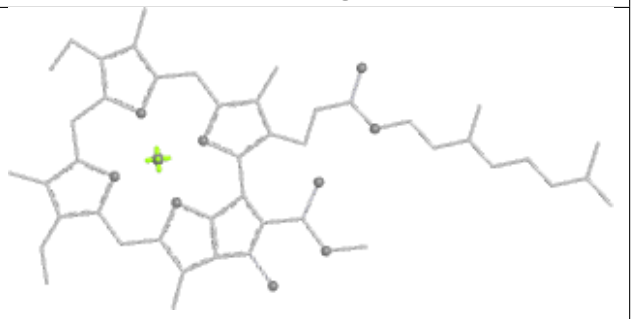
Bond lengths



Bond angles

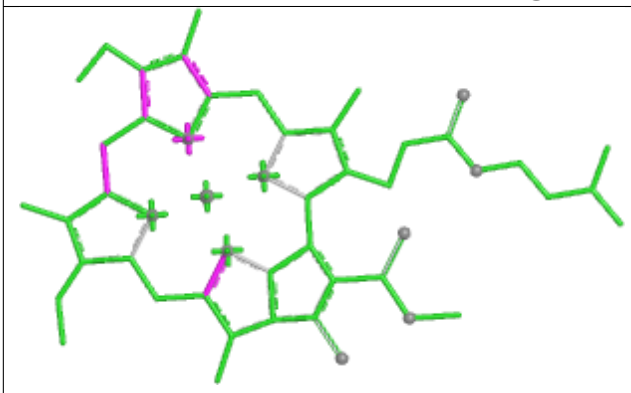


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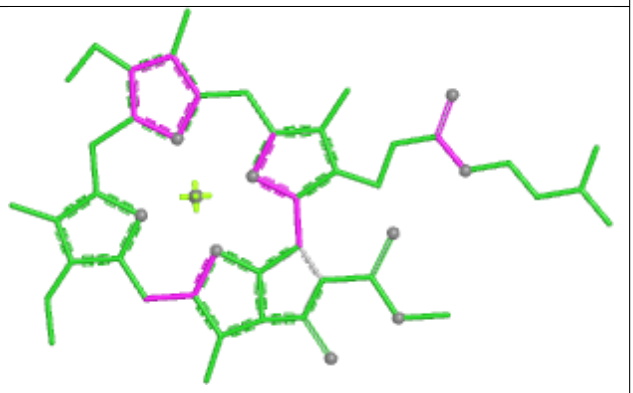


Rings

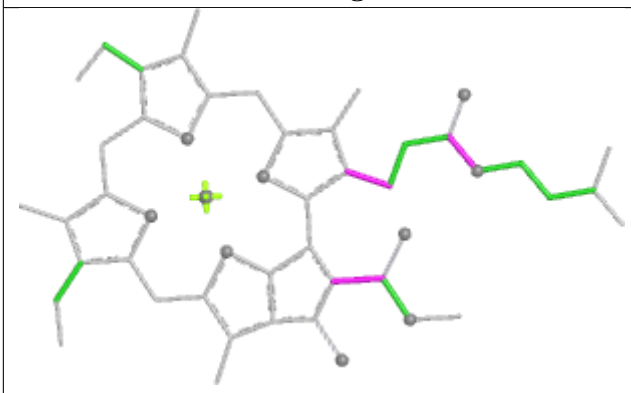
Ligand CLA x 501



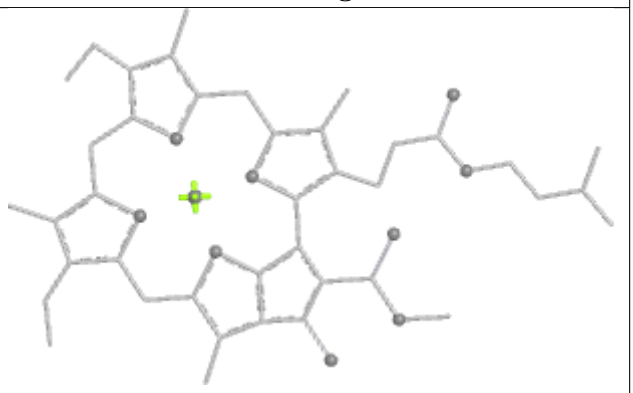
Bond lengths



Bond angles

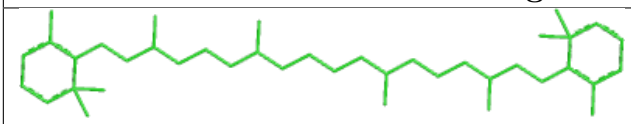


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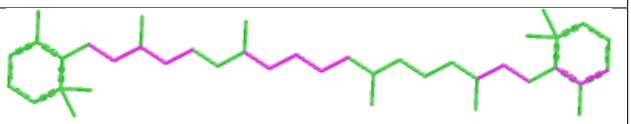


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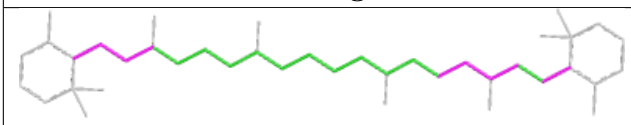
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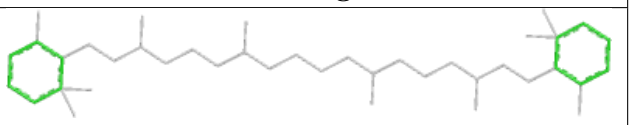
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Bond angles

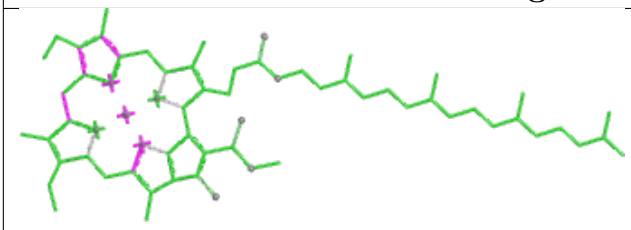


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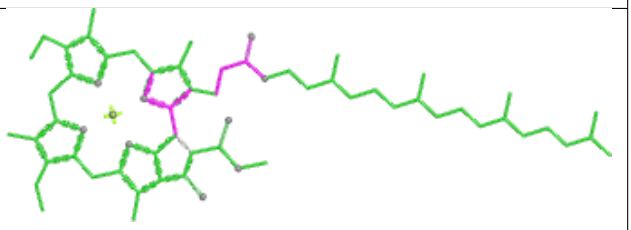


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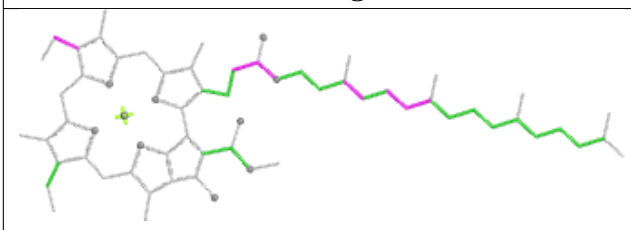
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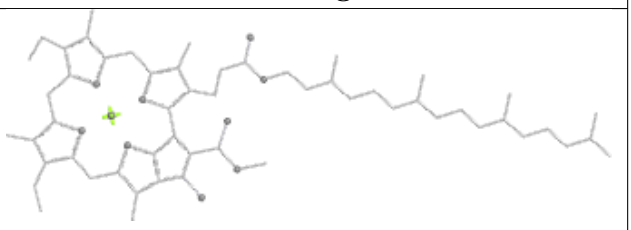
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Bond angles

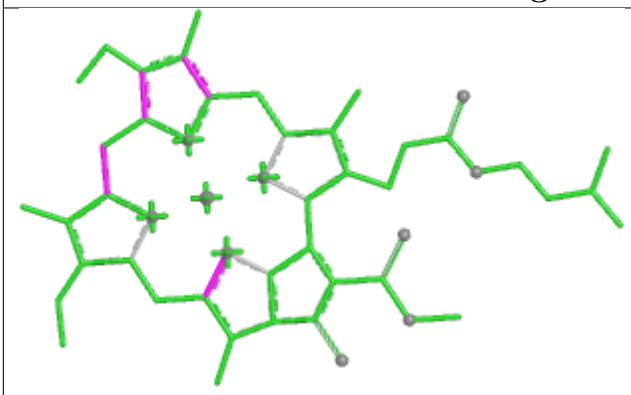


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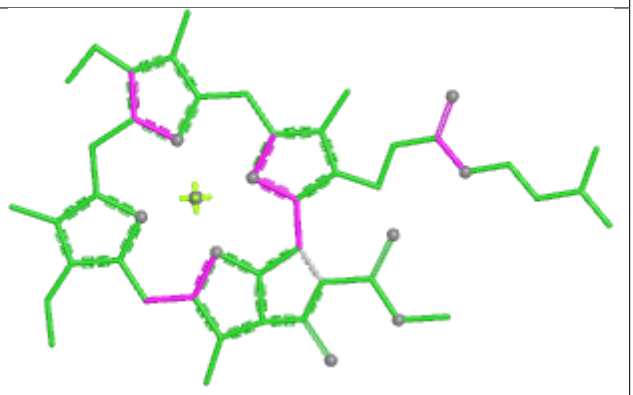


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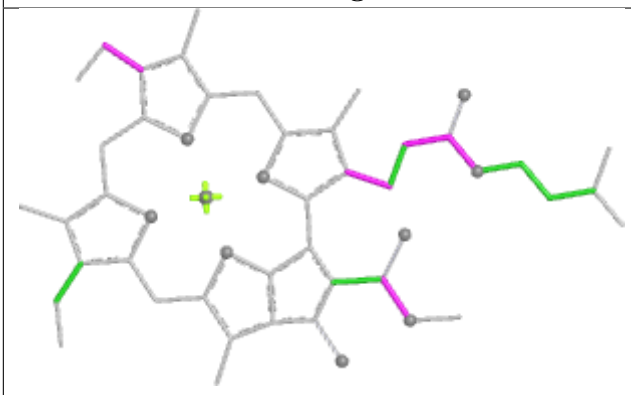
Ligand CLA t 514



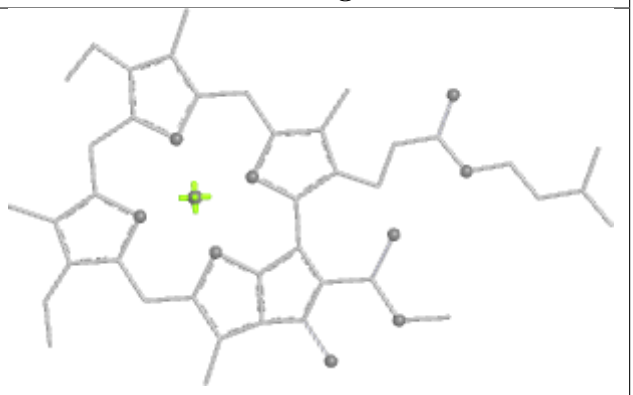
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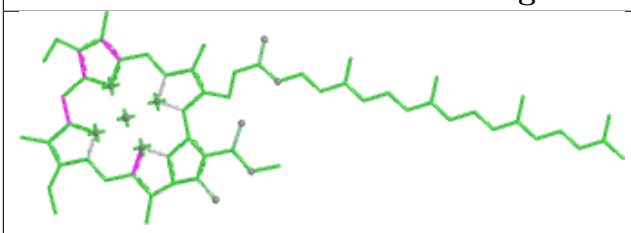


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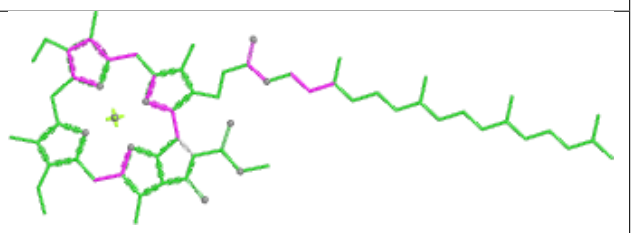


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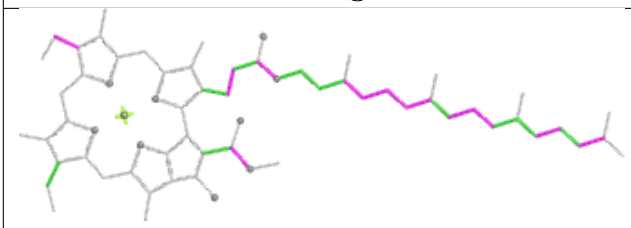
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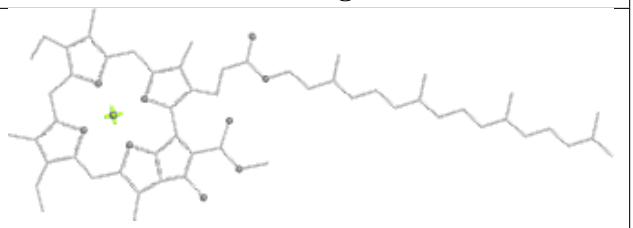
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Bond angles

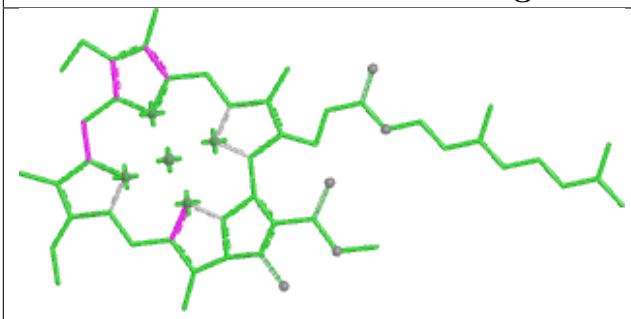


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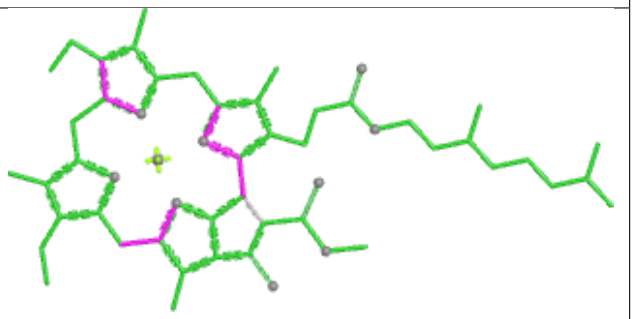


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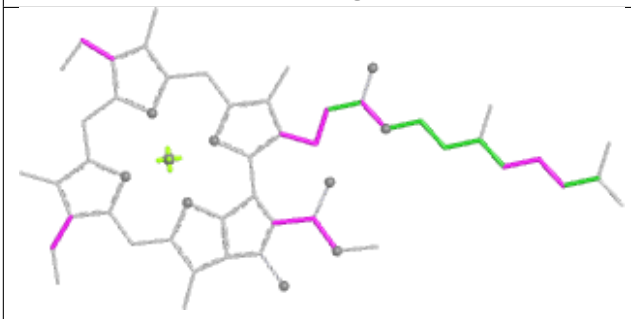
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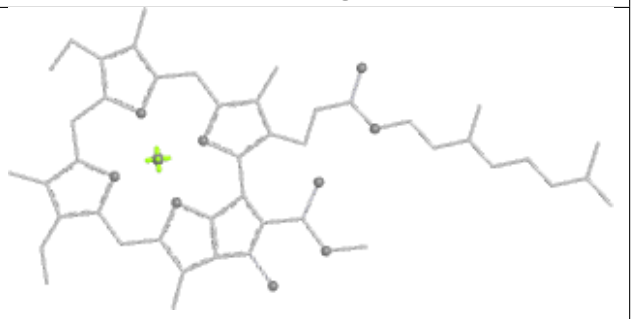
Bond lengths



Bond angles

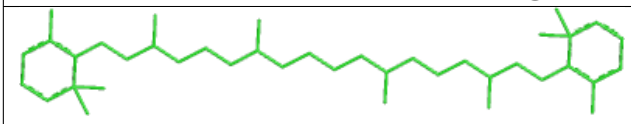


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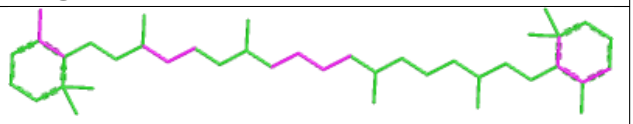


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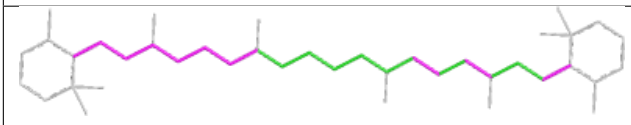
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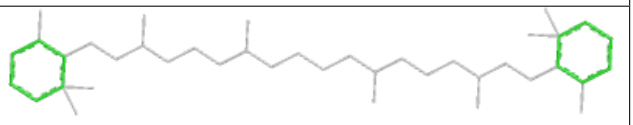
Bond lengths



Bond angles

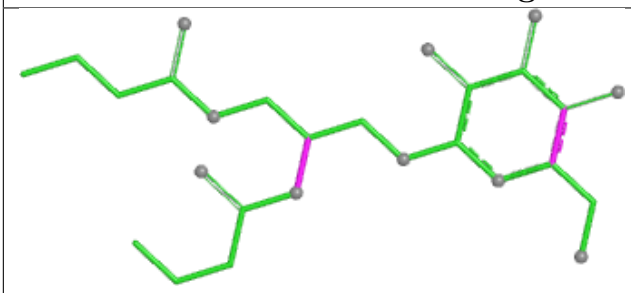


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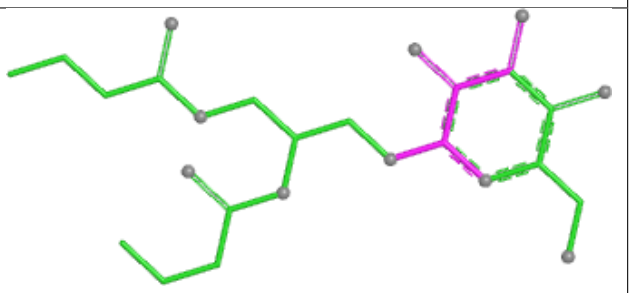


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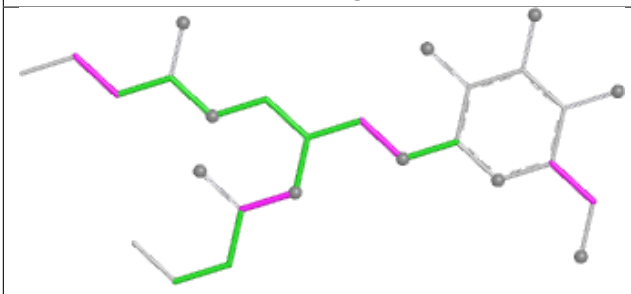
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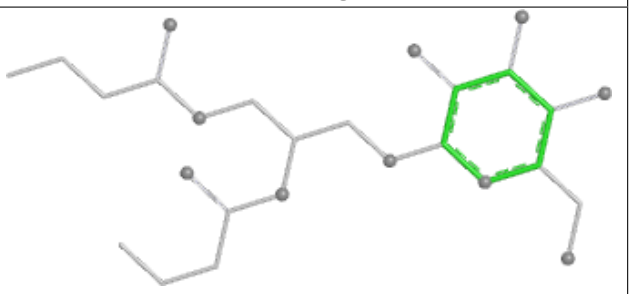
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Bond angles

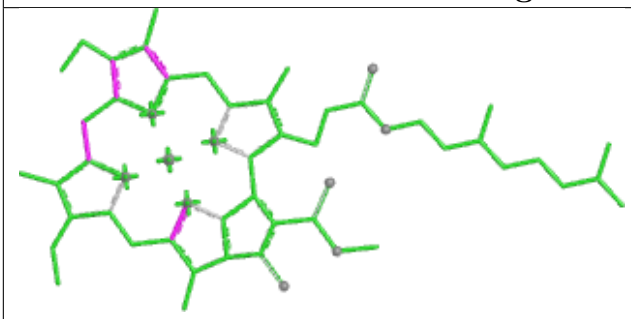


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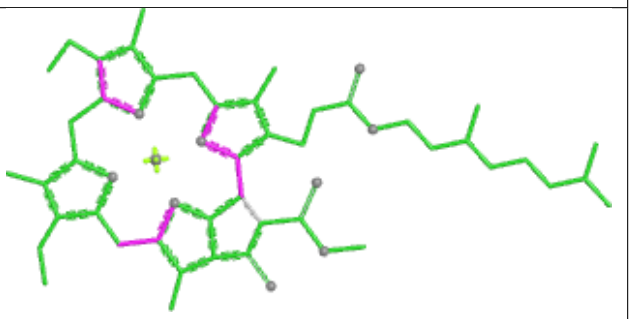


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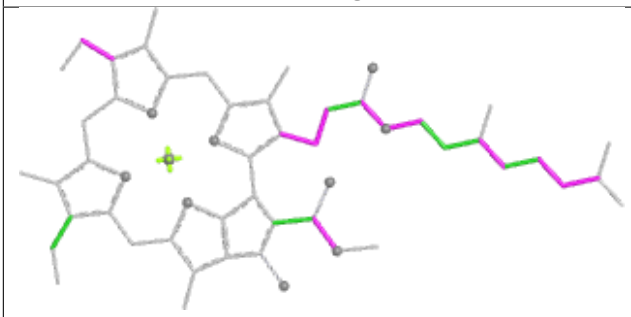
Ligand CLA B 1228



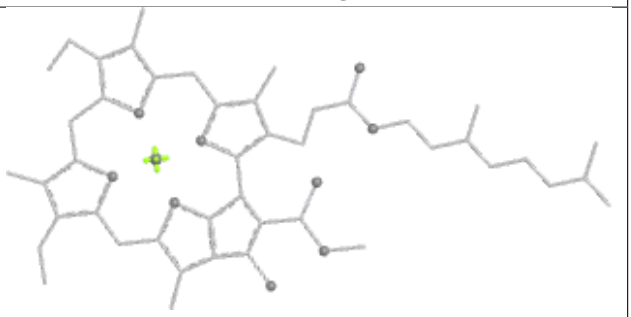
Bond lengths



Bond angles

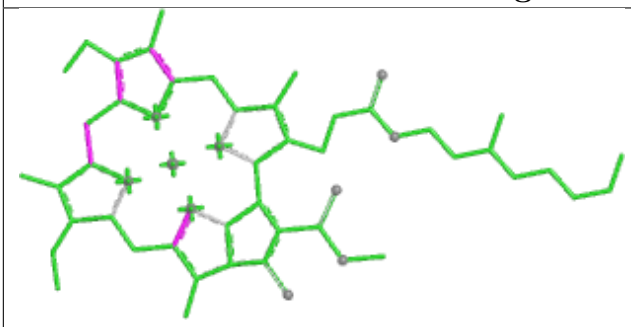


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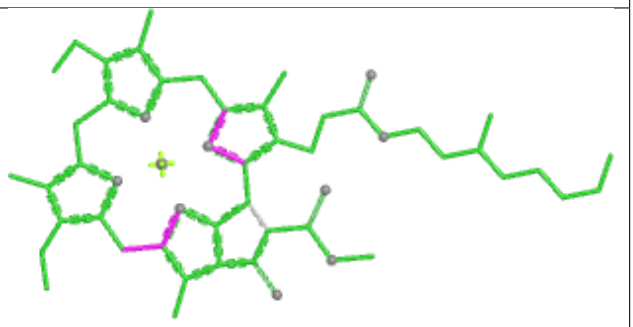


Rings

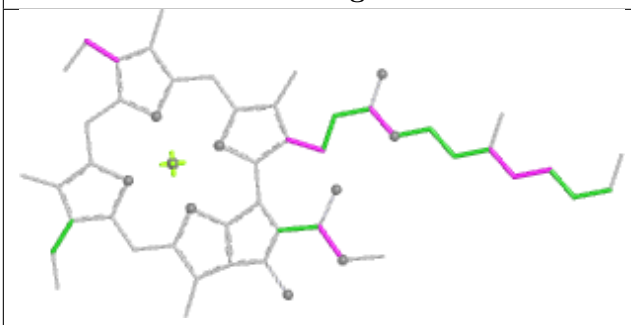
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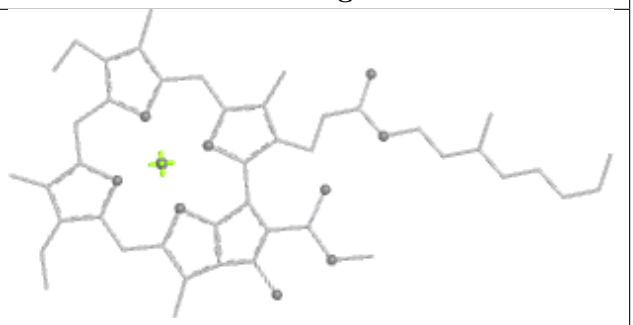
Bond lengths



Bond angles

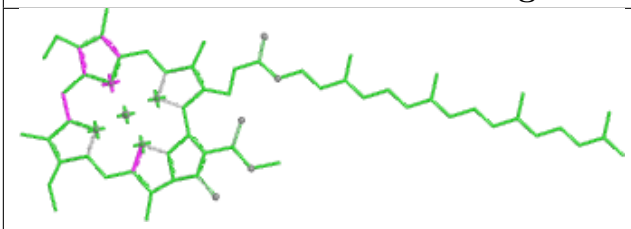


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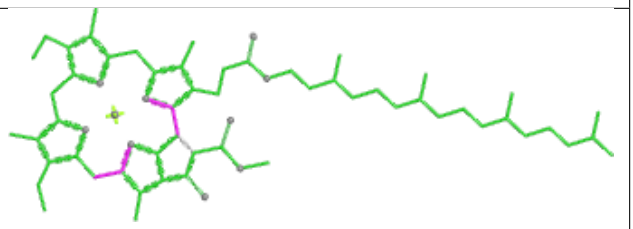


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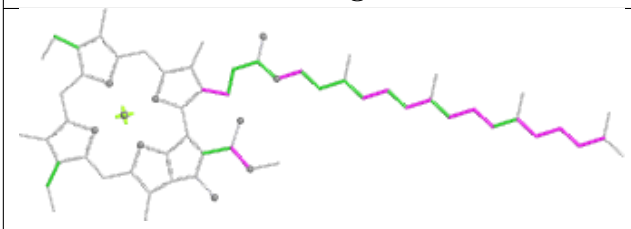
Ligand CLA b 1206



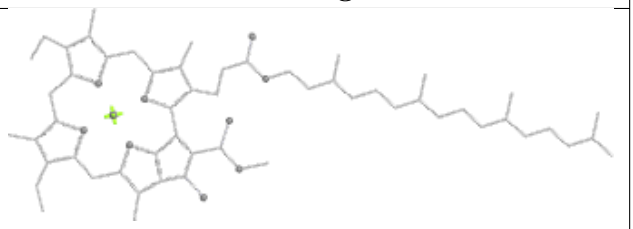
Bond lengths



Bond angles

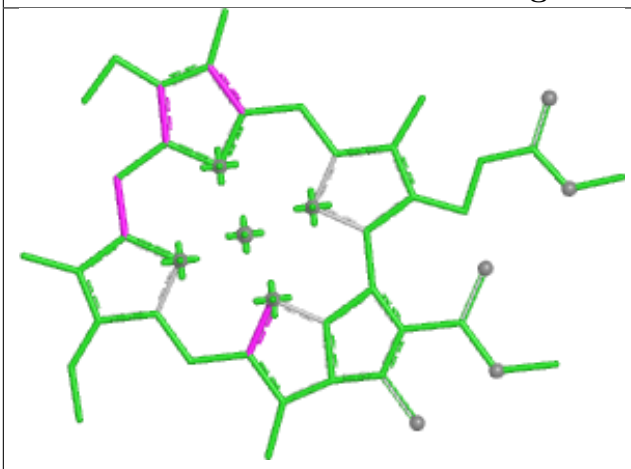


Torsions

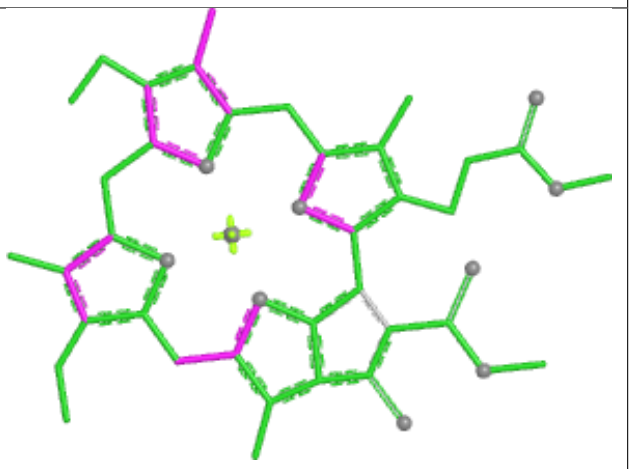


Rings

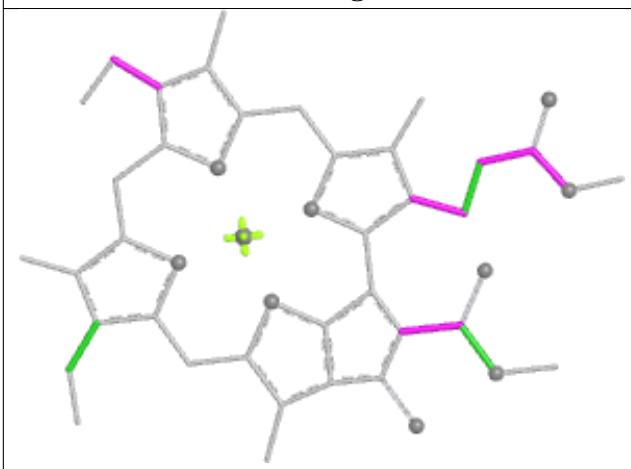
Ligand CLA s 513



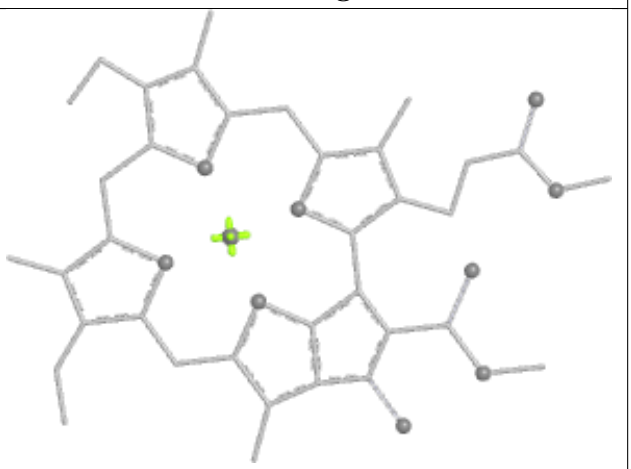
Bond lengths



Bond angles

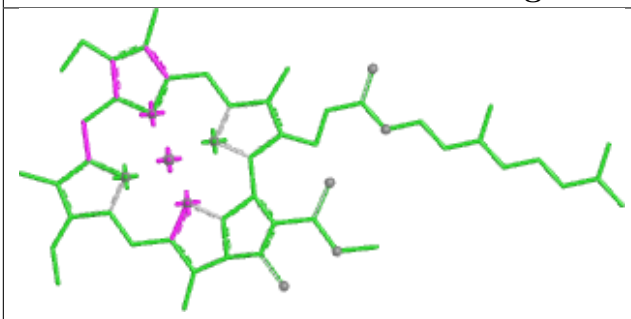


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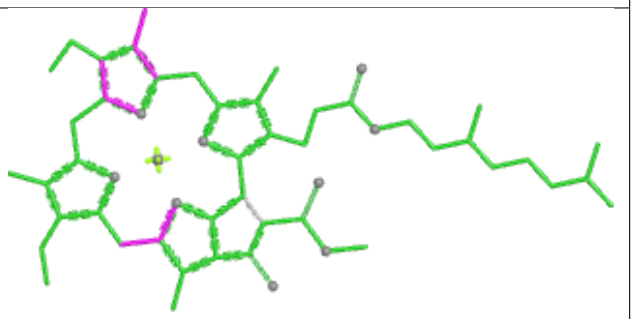


Rings

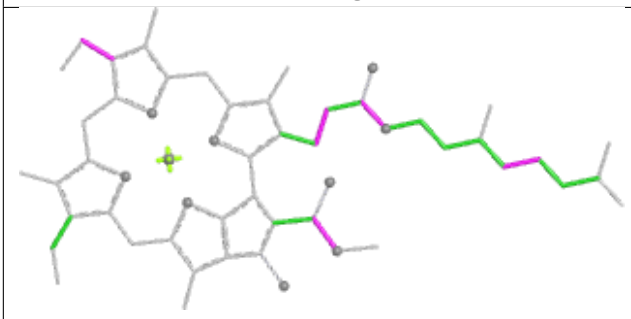
Ligand CLA w 517



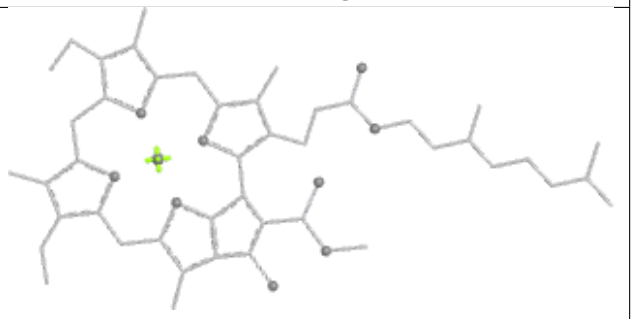
Bond lengths



Bond angles

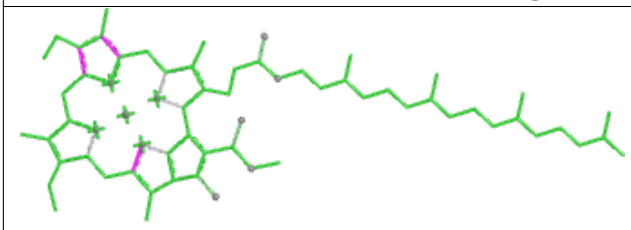


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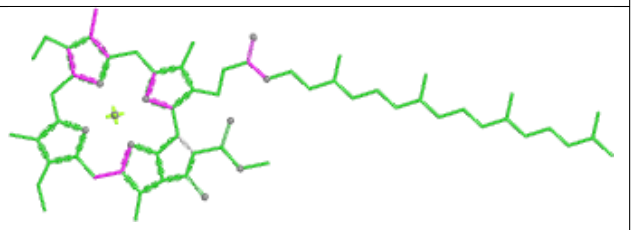


Rings

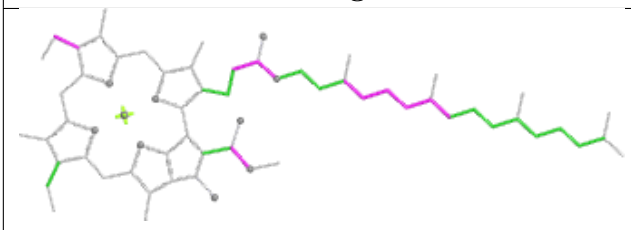
Ligand CLA Z 507



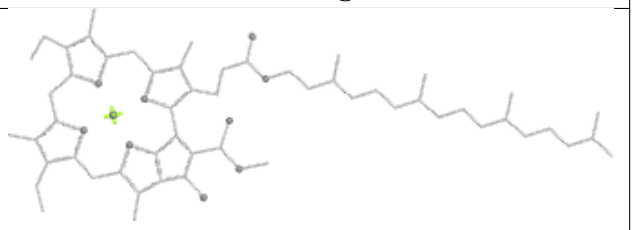
Bond lengths



Bond angles

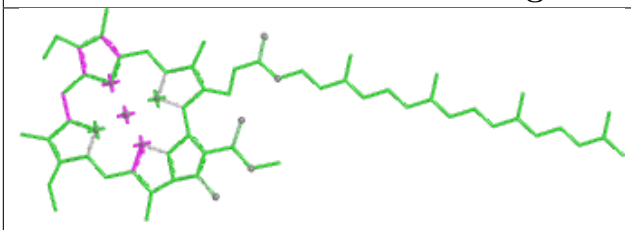


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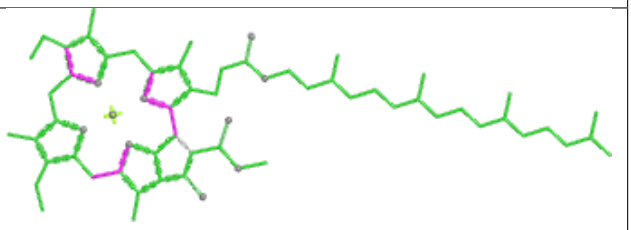


Rings

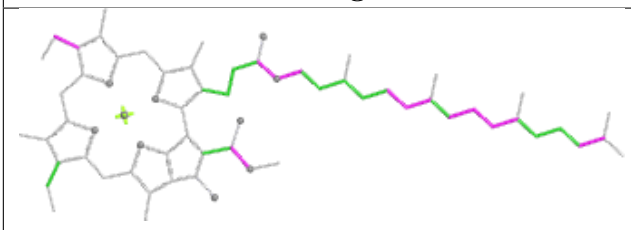
Ligand CLA Z 512



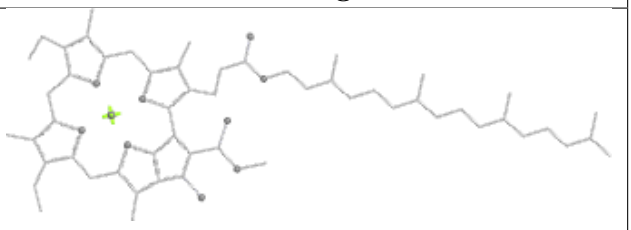
Bond lengths



Bond angles

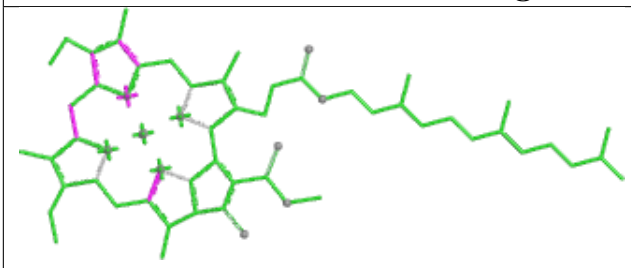


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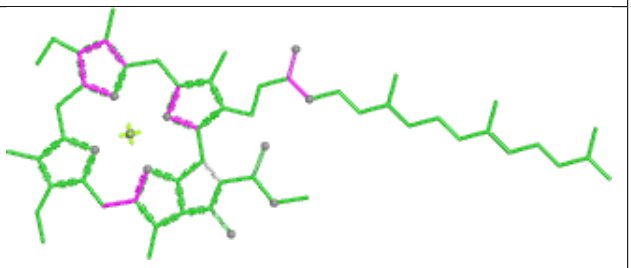


Rings

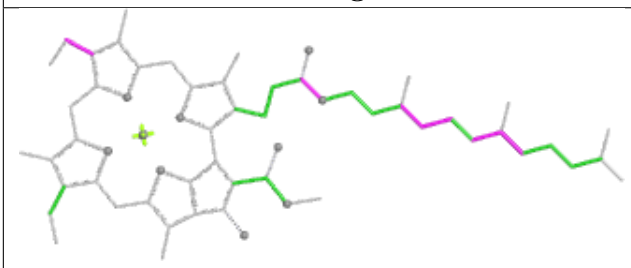
Ligand CLA U 1502



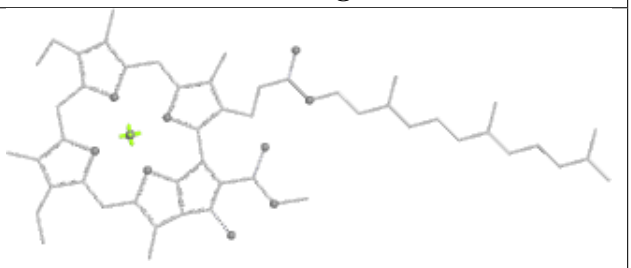
Bond lengths



Bond angles

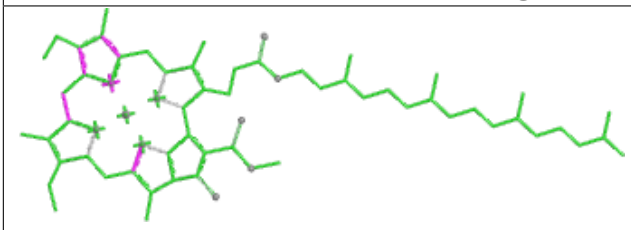


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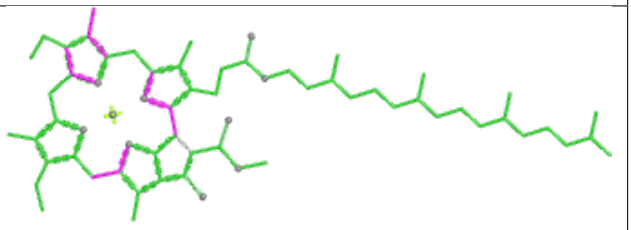


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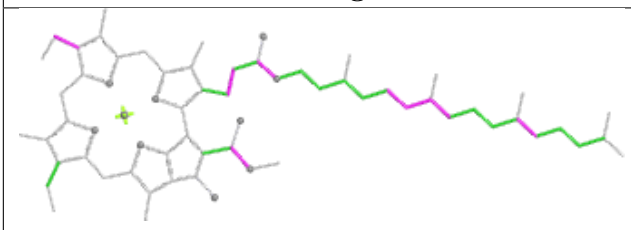
Ligand CLA A 1131



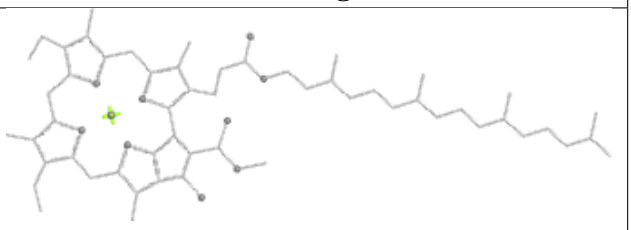
Bond lengths



Bond angles



Torsions

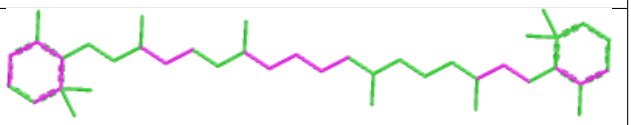


Rings

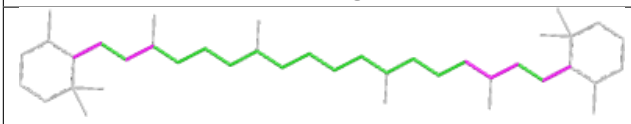
Ligand BCR o 601



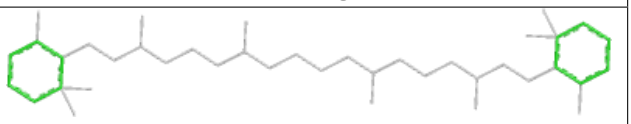
Bond lengths



Bond angles

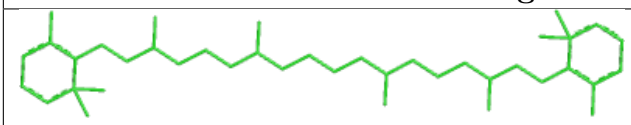


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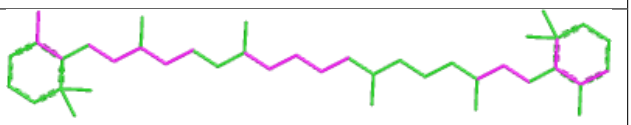


Rings

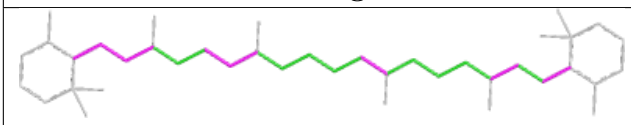
Ligand BCR J 4012



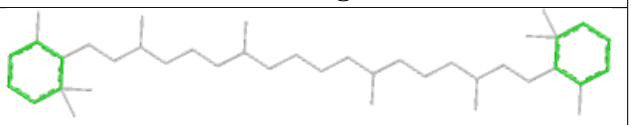
Bond lengths



Bond angles

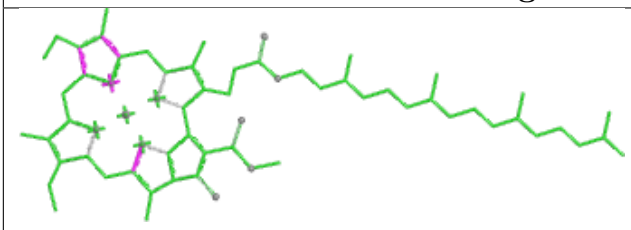


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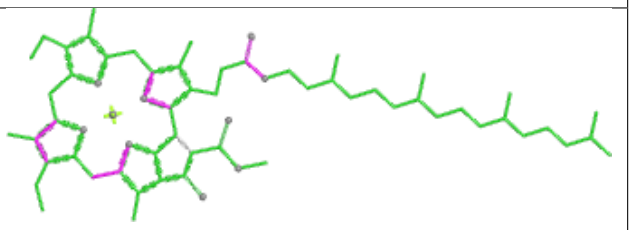


Rings

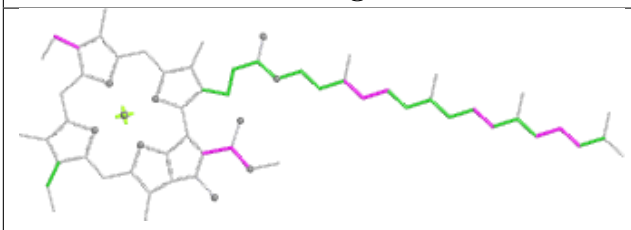
Ligand CLA b 1205



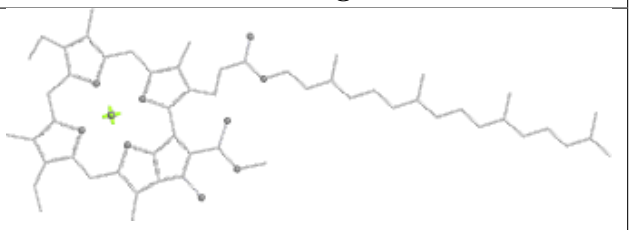
Bond lengths



Bond angles

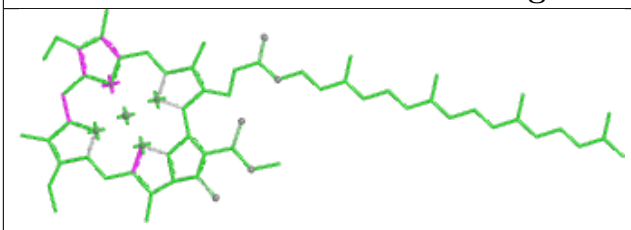


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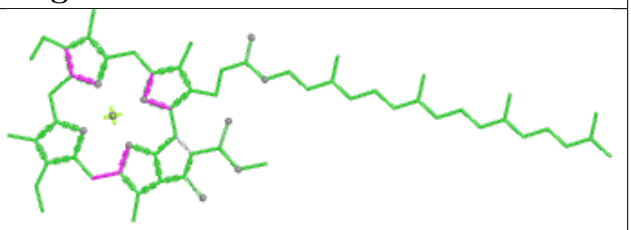


Rings

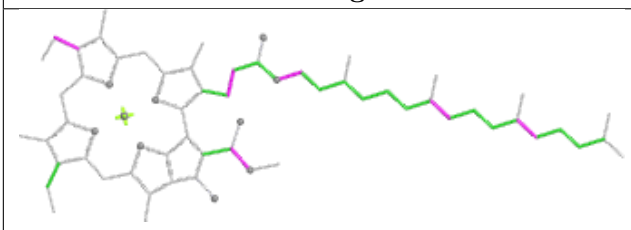
Ligand CLA g 511



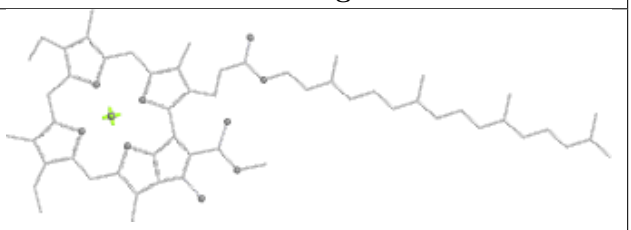
Bond lengths



Bond angles

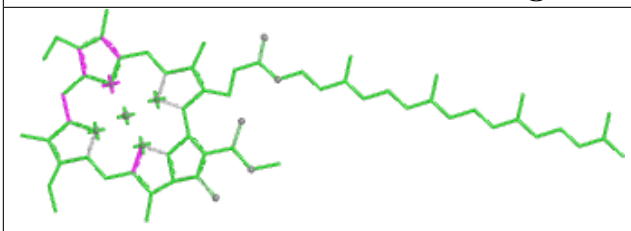


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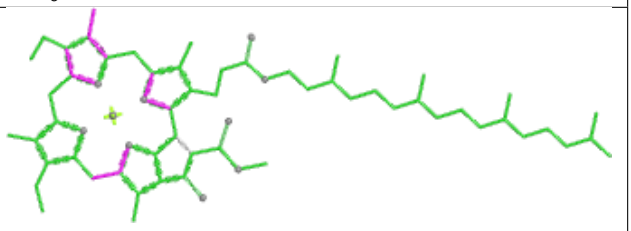


Rings

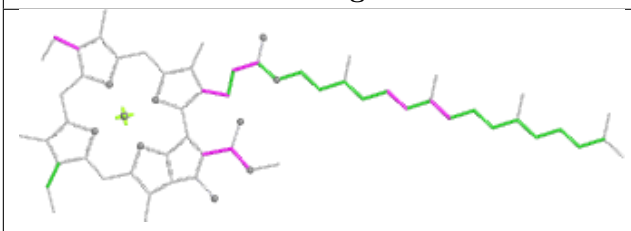
Ligand CLA y 507



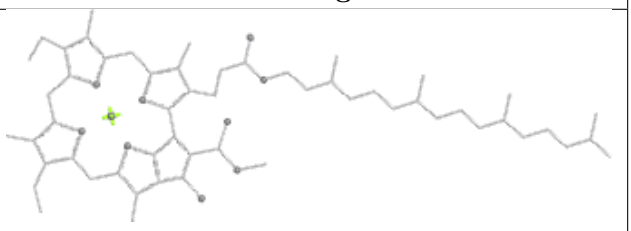
Bond lengths



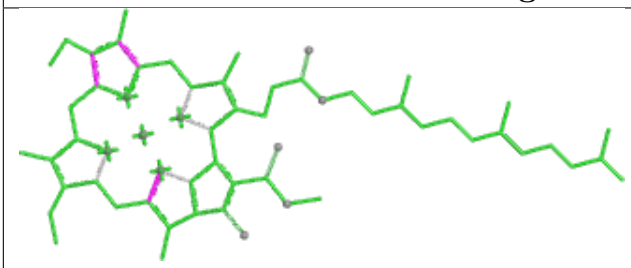
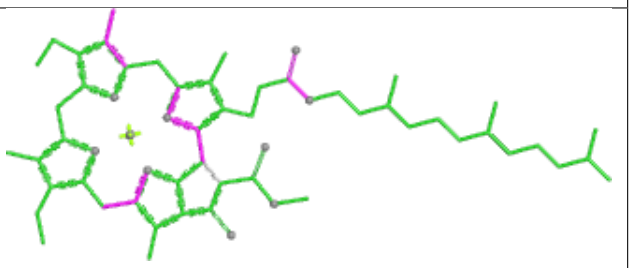
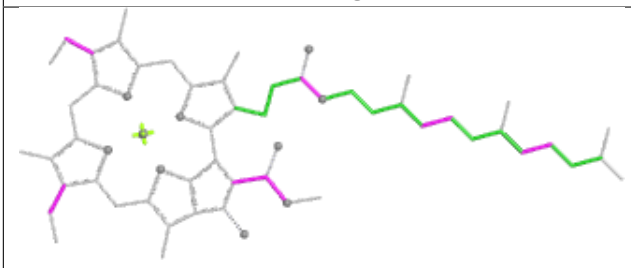
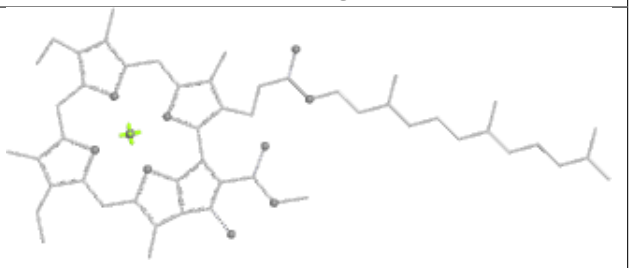
Bond angles

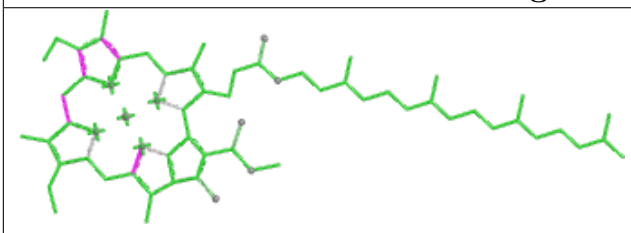
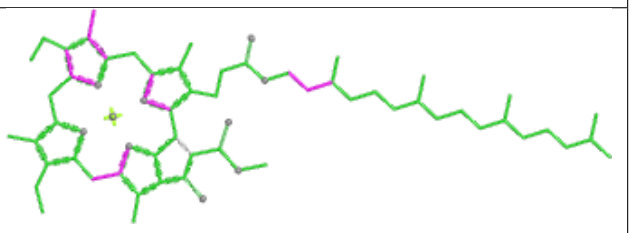
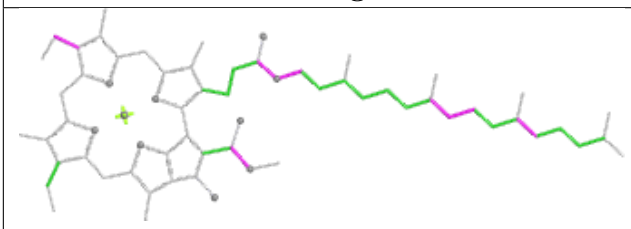
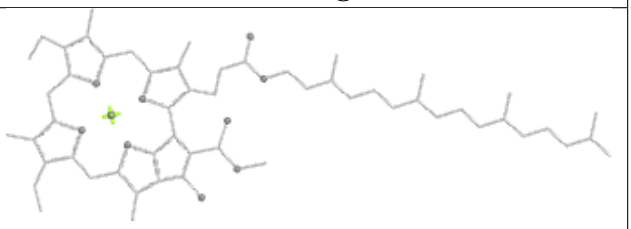


Torsions

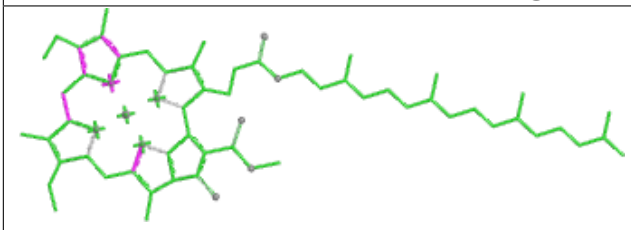


Rings

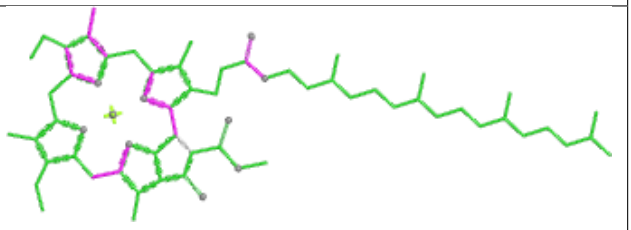
Ligand CLA W 506	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA s 507	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

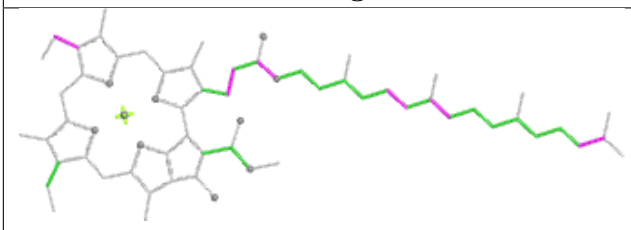
Ligand CLA v 507



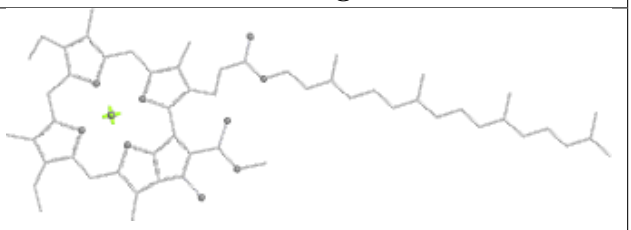
Bond lengths



Bond angles

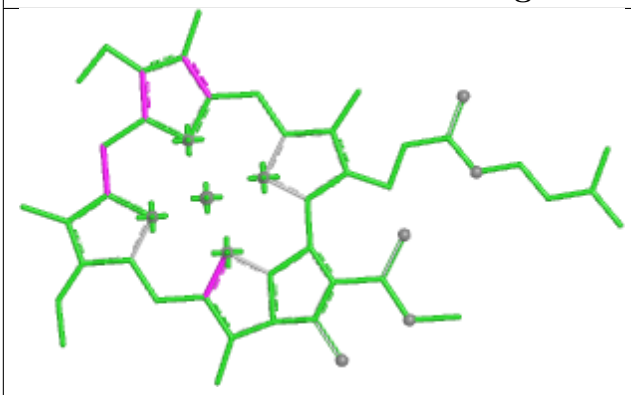


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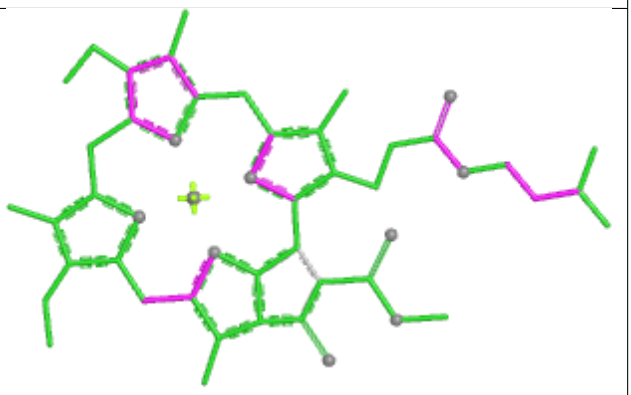


Rings

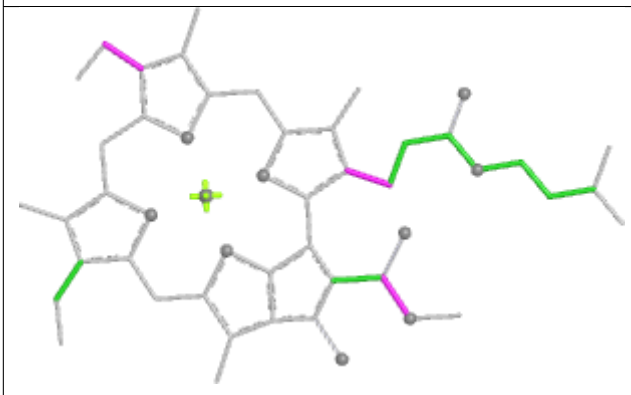
Ligand CLA H 1107



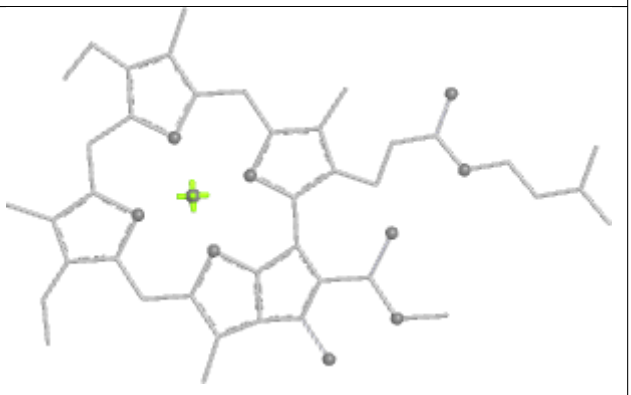
Bond lengths



Bond angles

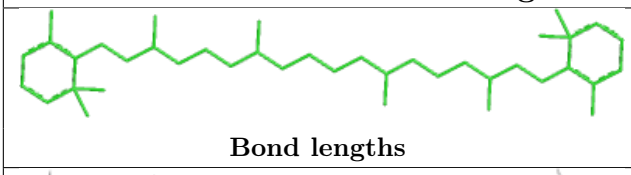


Torsions

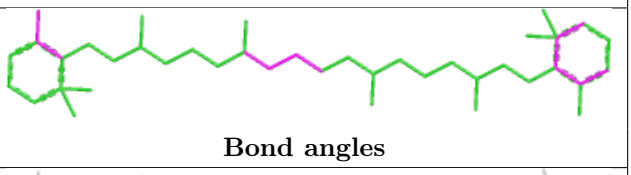


Rings

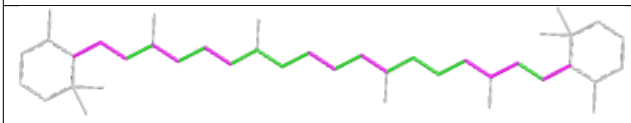
Ligand BCR a 4003



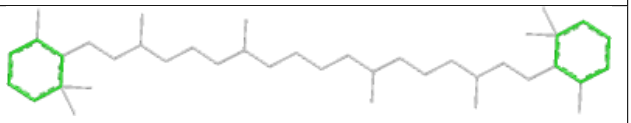
Bond lengths



Bond angles

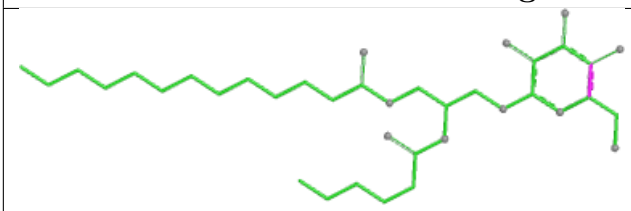


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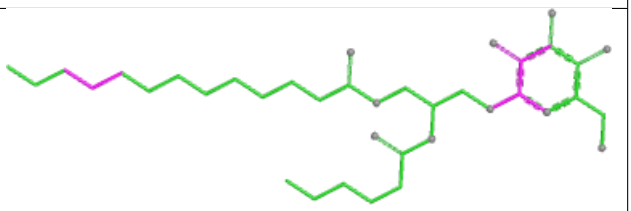


Rings

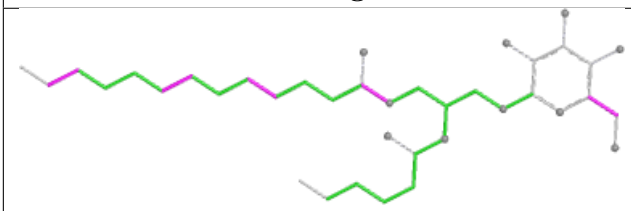
Ligand LMG H 852



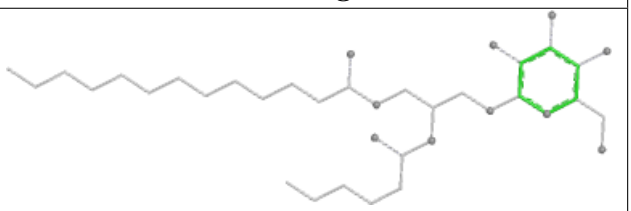
Bond lengths



Bond angles

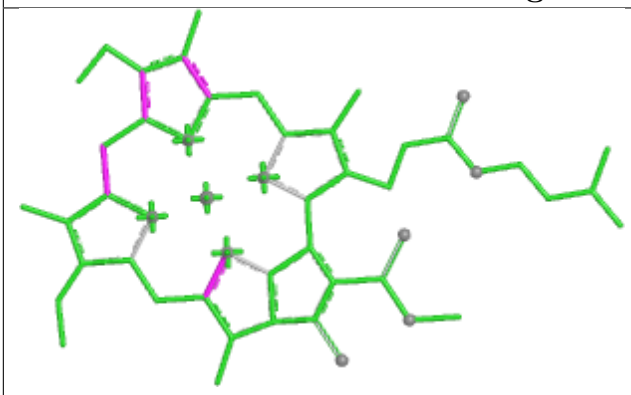


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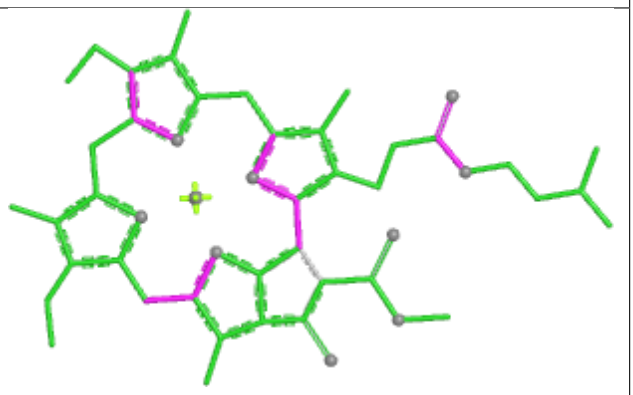


Rings

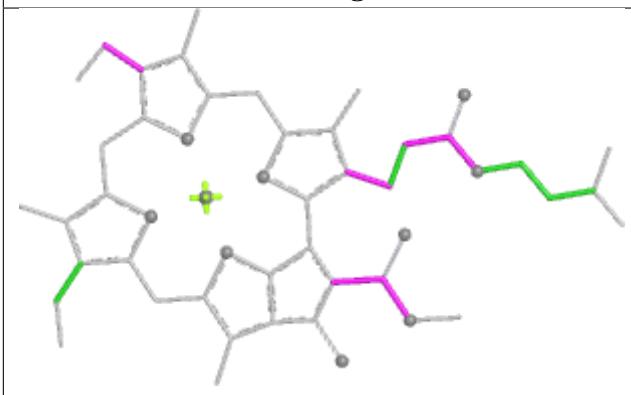
Ligand CLA Z 514



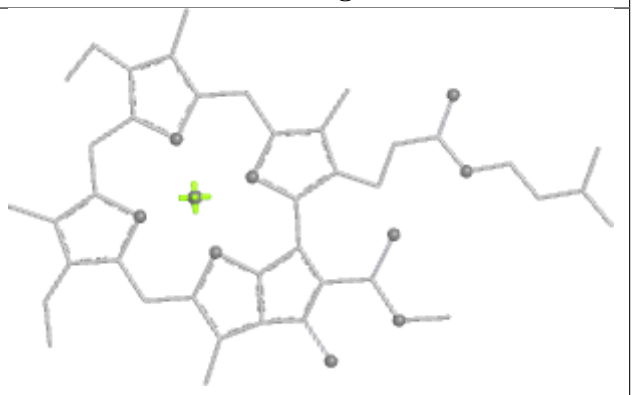
Bond lengths



Bond angles



Torsions

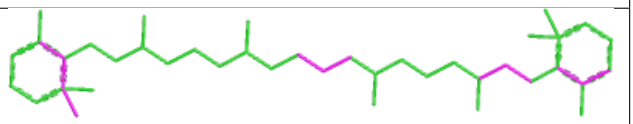


Rings

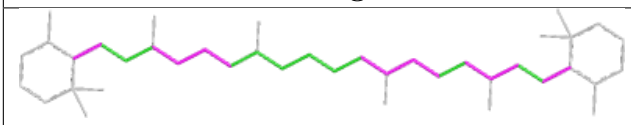
Ligand BCR a 4011



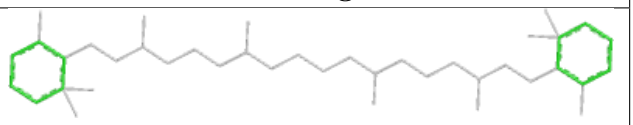
Bond lengths



Bond angles

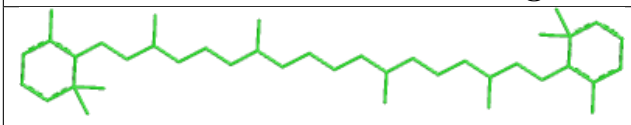


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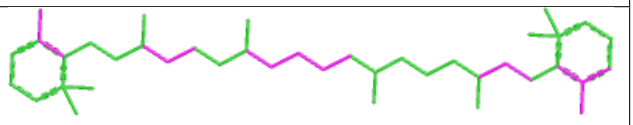


Rings

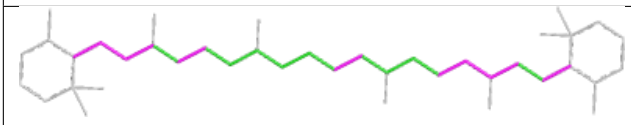
Ligand BCR h 601



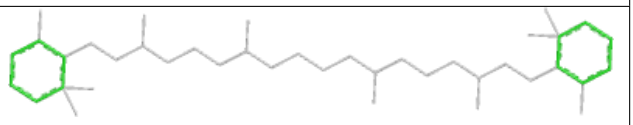
Bond lengths



Bond angles

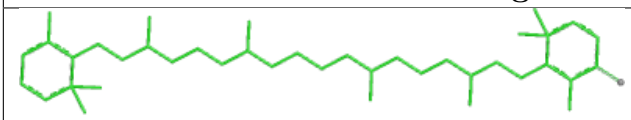


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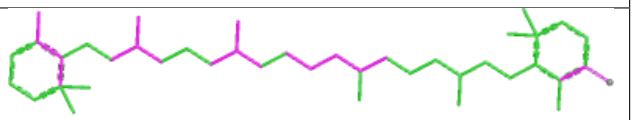


Rings

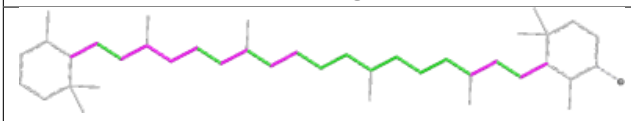
Ligand ECH m 4021



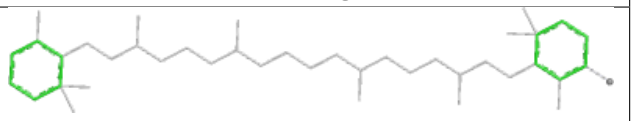
Bond lengths



Bond angles

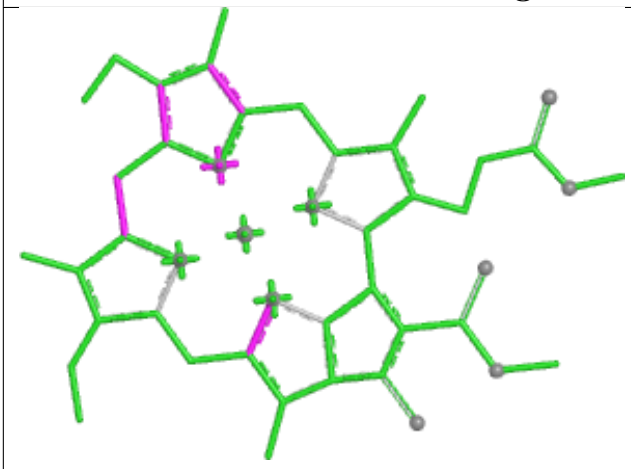


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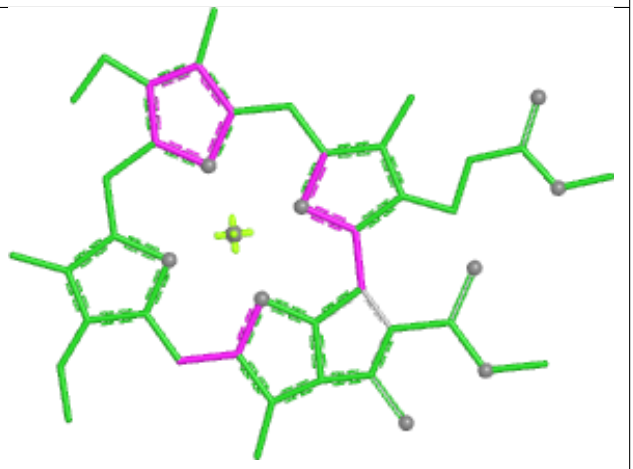


Rings

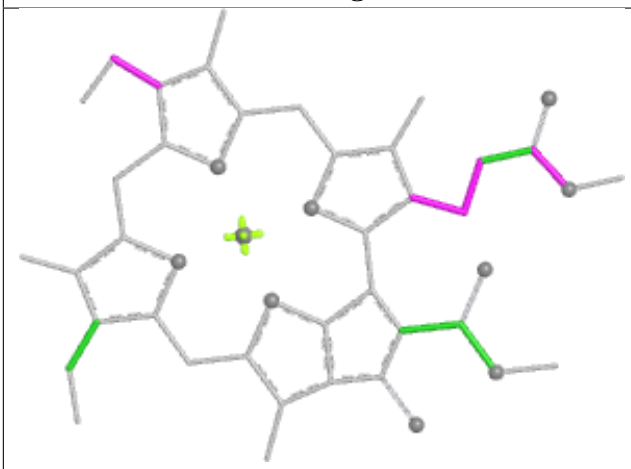
Ligand CLA H 1129



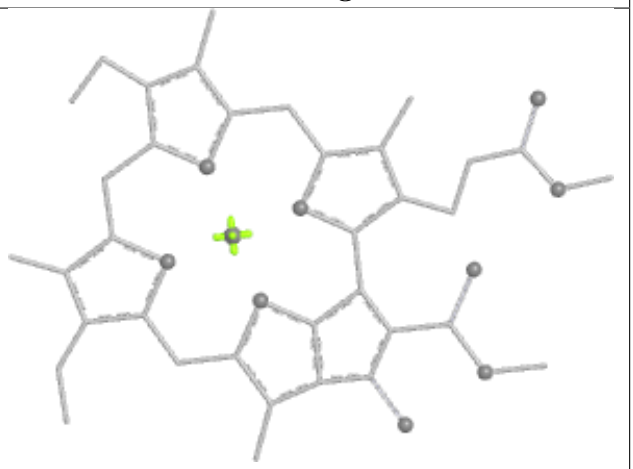
Bond lengths



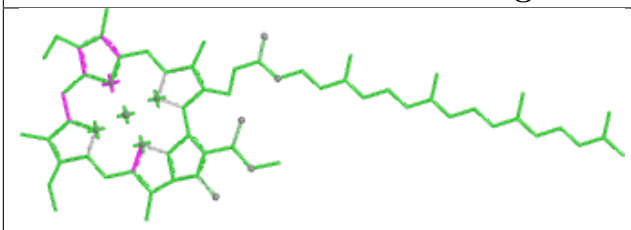
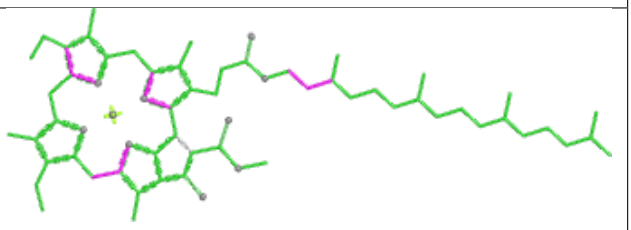
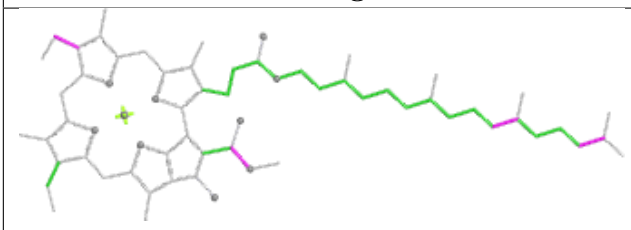
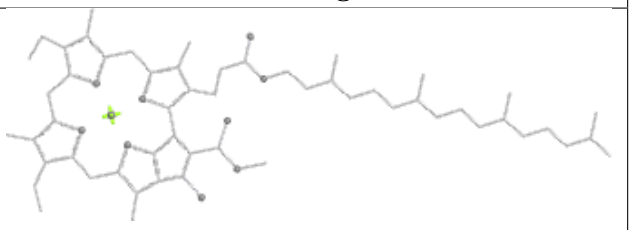
Bond angles

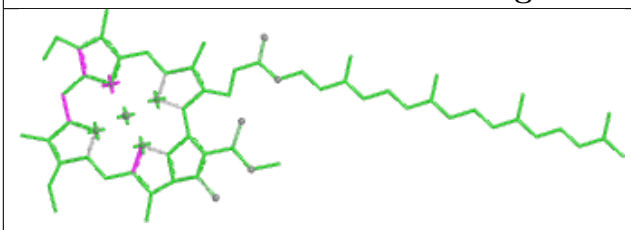
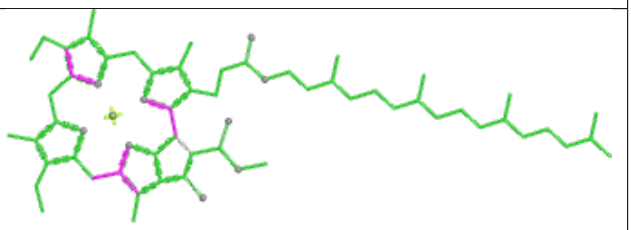
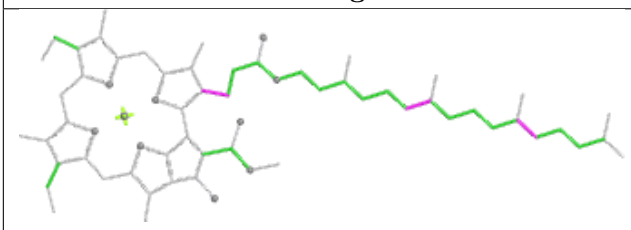
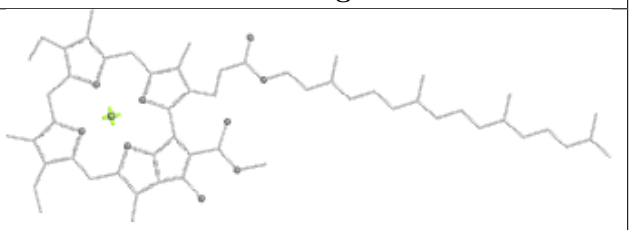


Torsions

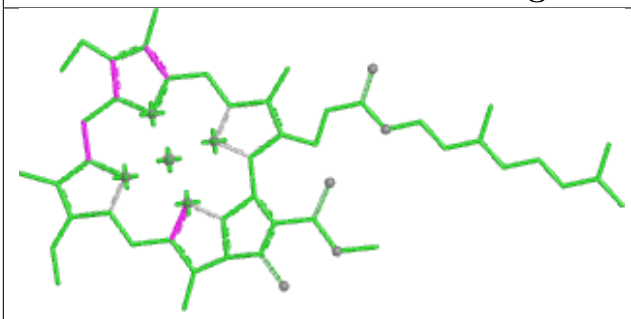


Rings

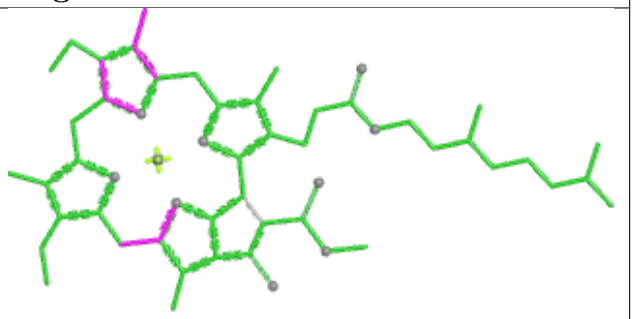
Ligand CLA A 1117	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1119	
	
Bond lengths	Bond angles
	
Torsions	Rings

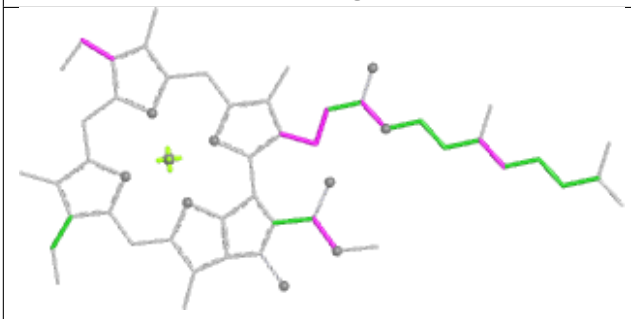
Ligand CLA g 517



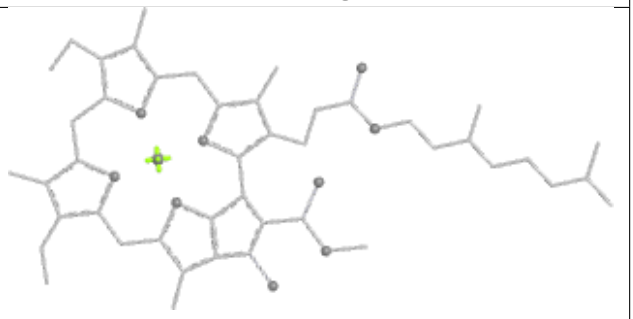
Bond lengths



Bond angles

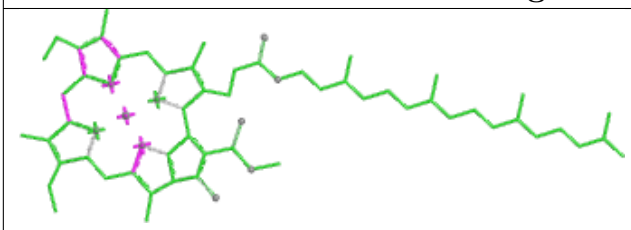


Torsions

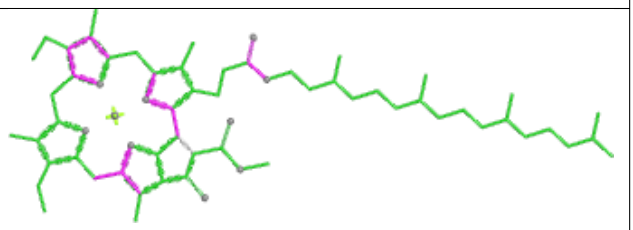


Rings

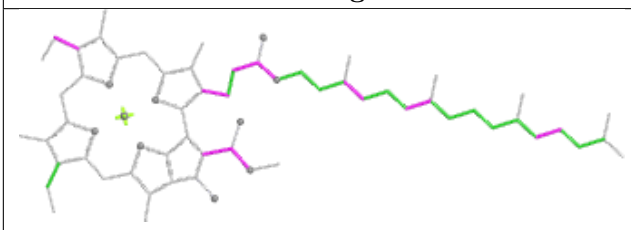
Ligand CLA v 509



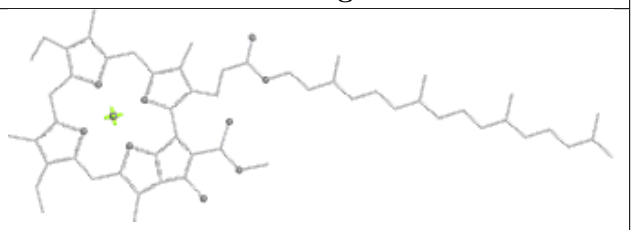
Bond lengths



Bond angles



Torsions

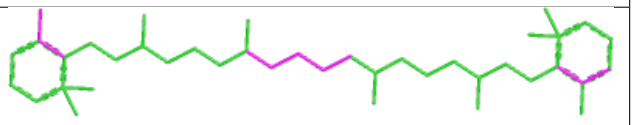


Rings

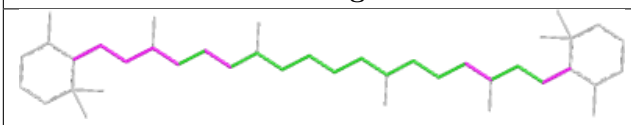
Ligand BCR t 603



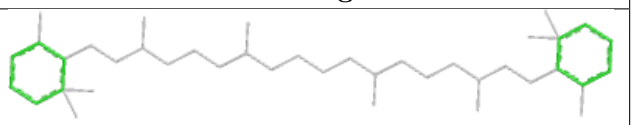
Bond lengths



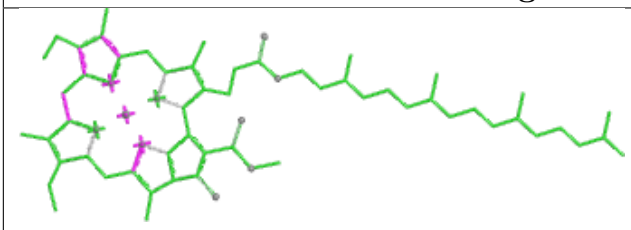
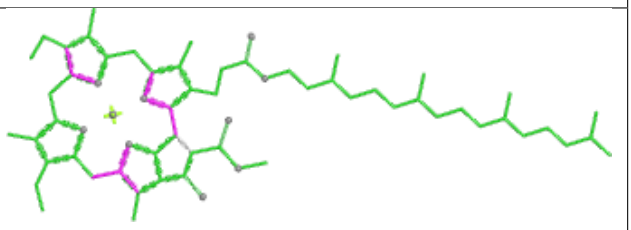
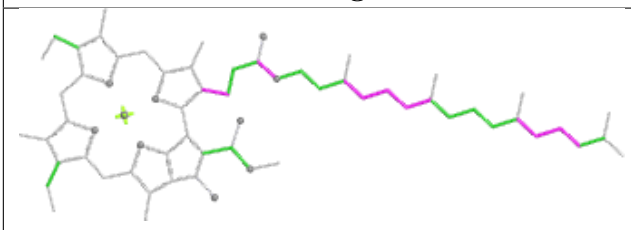
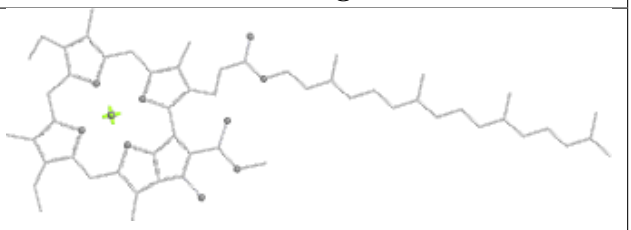
Bond angles

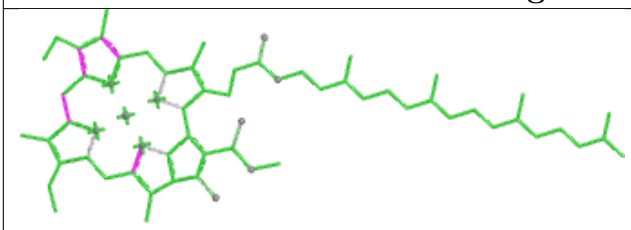
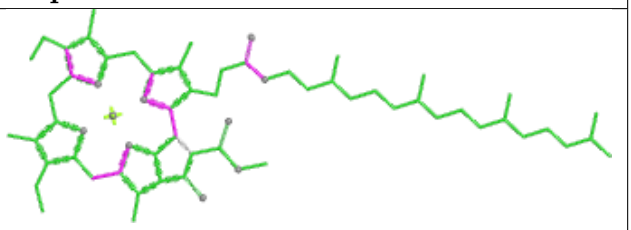
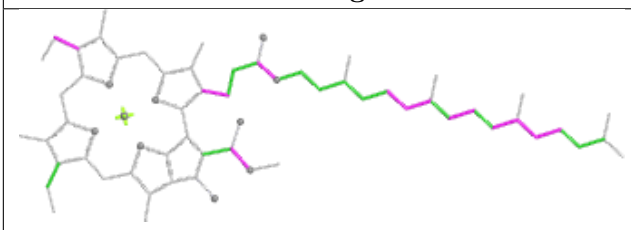
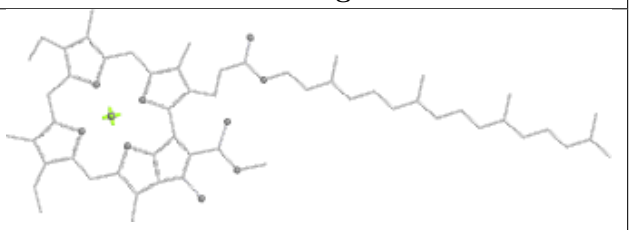


Torsions

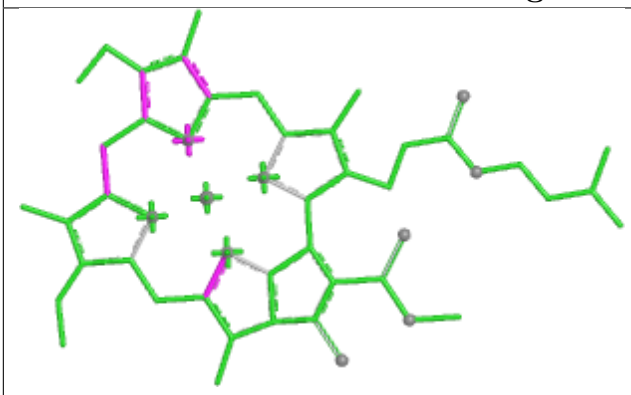


Rings

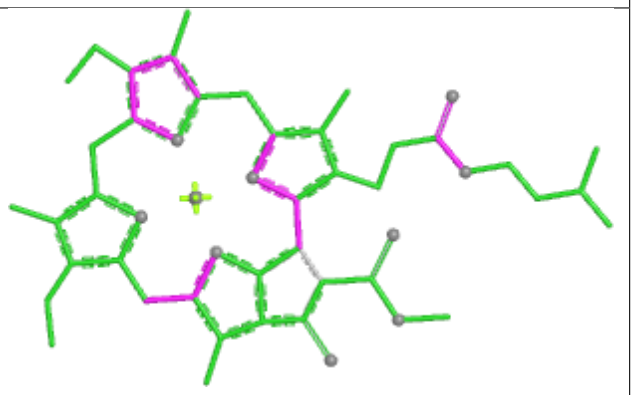
Ligand CLA b 1225	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

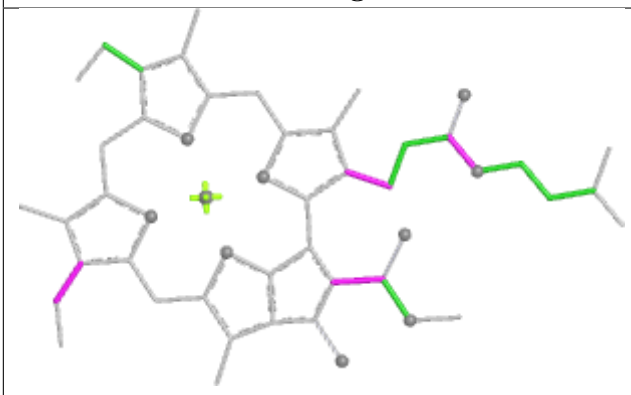
Ligand CLA Z 501



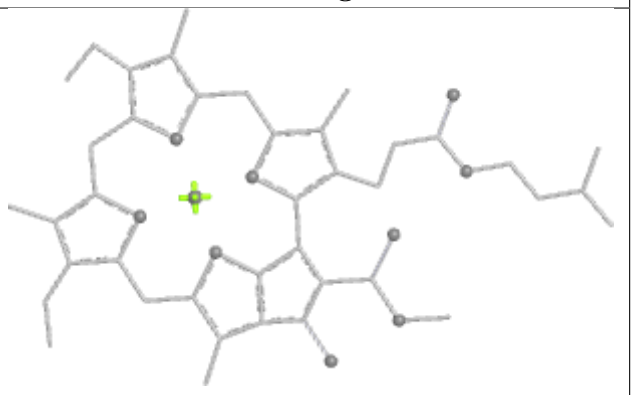
Bond lengths



Bond angles

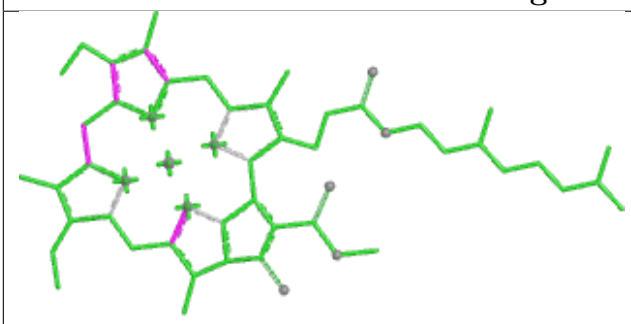


Torsions

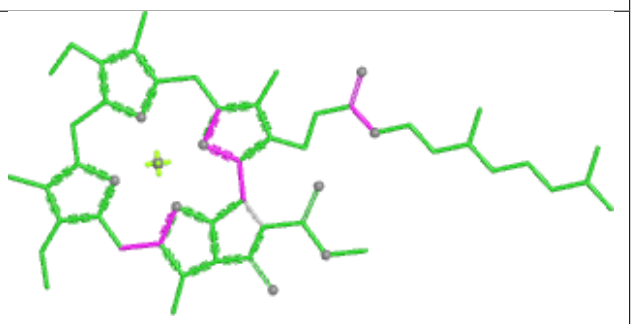


Rings

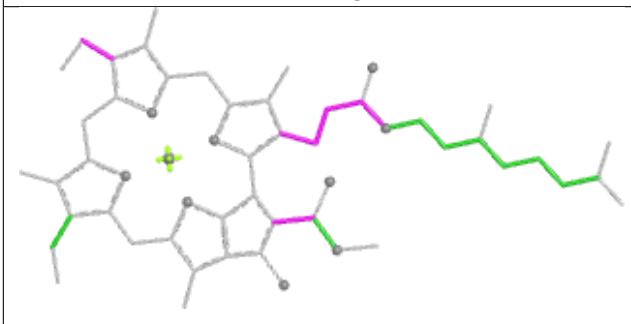
Ligand CLA s 508



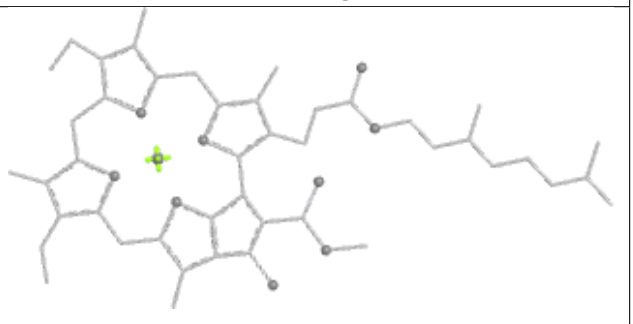
Bond lengths



Bond angles

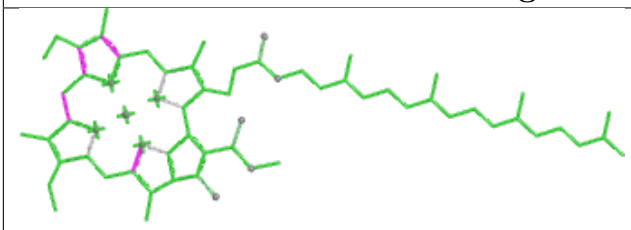


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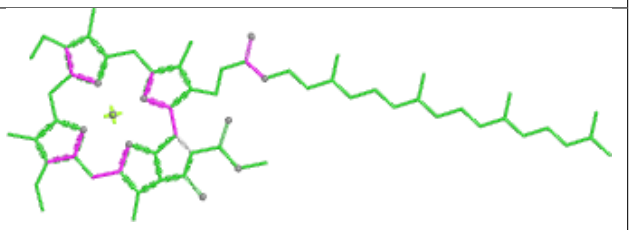


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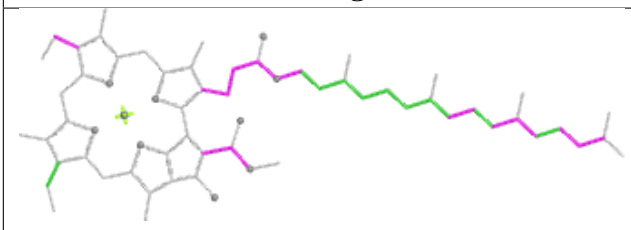
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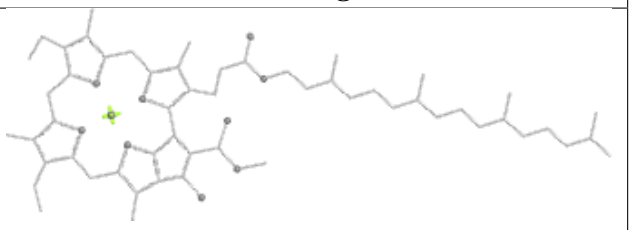
Bond lengths



Bond angles

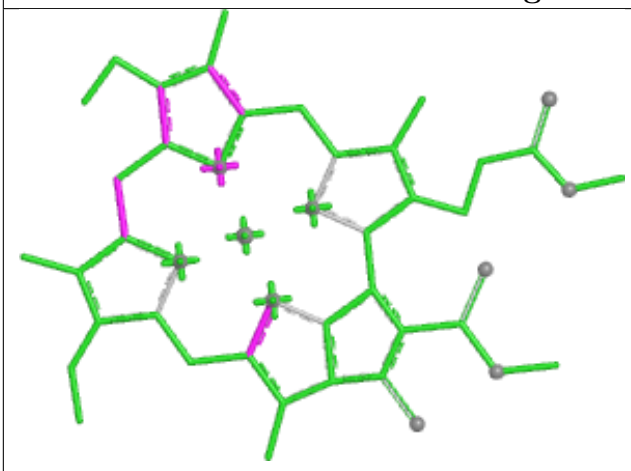


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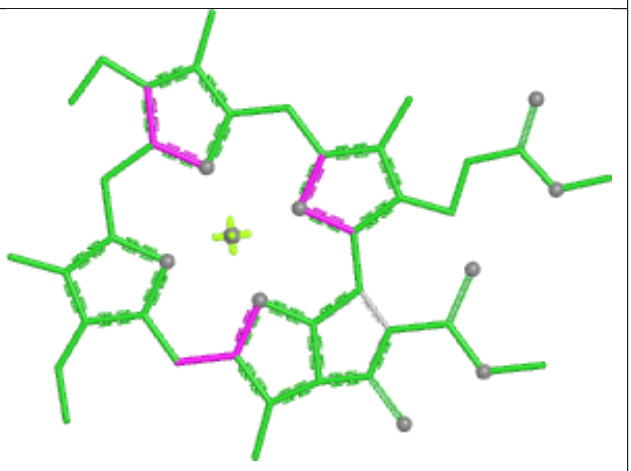


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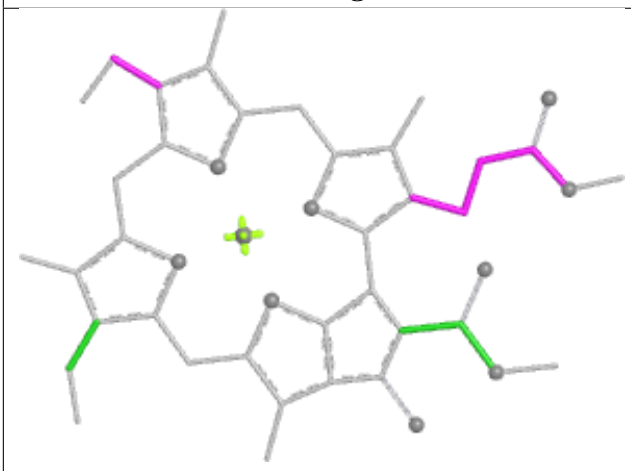
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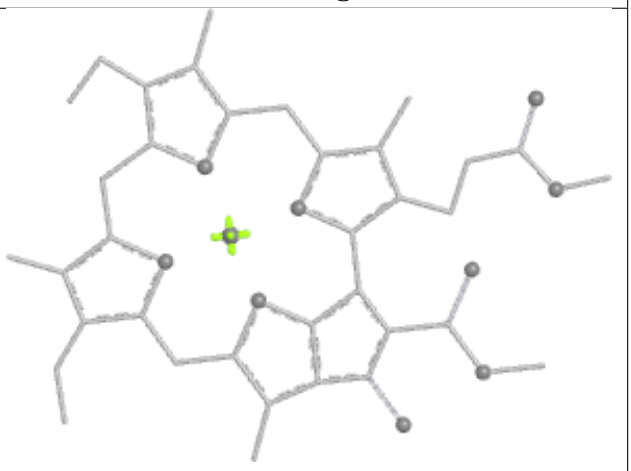
Bond lengths



Bond angles

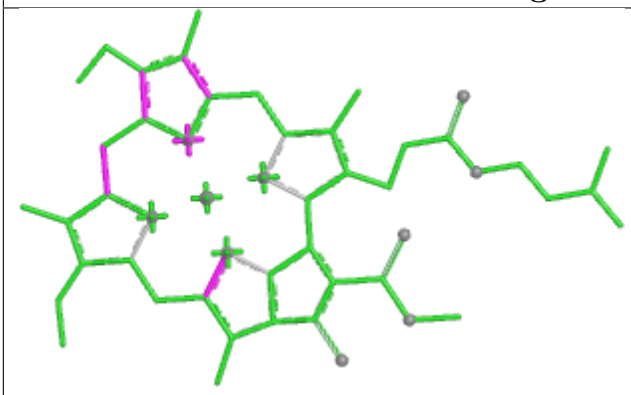


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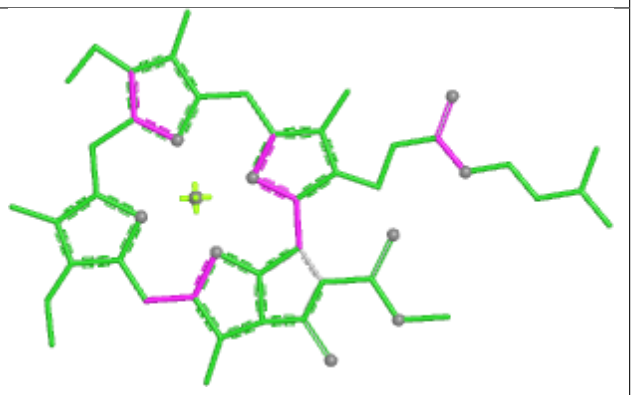


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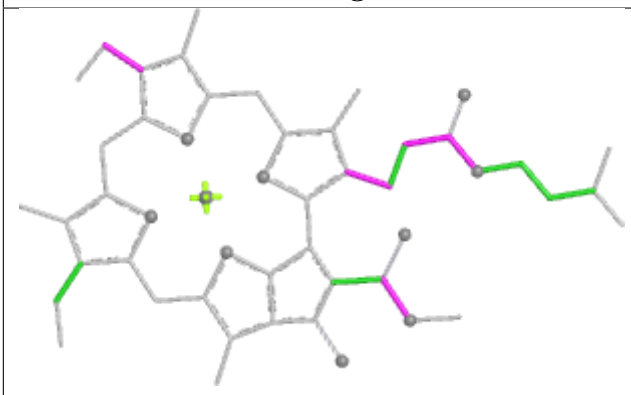
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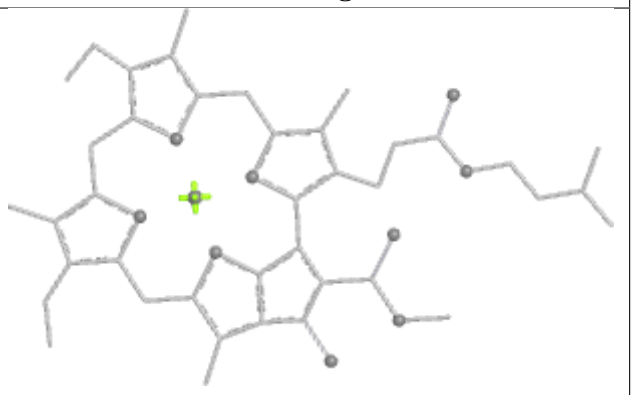
Bond lengths



Bond angles

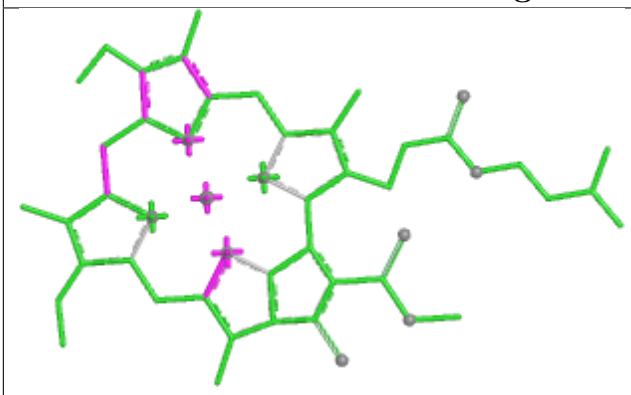


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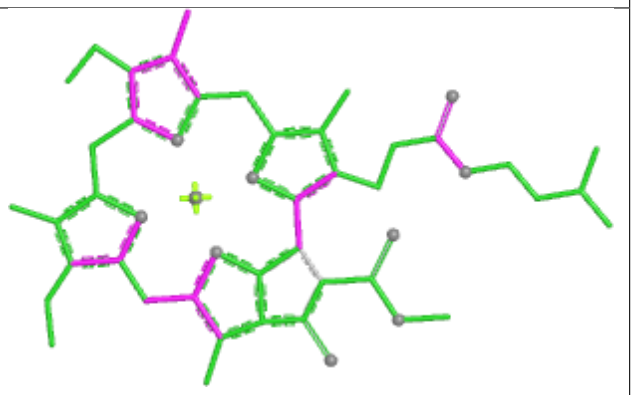


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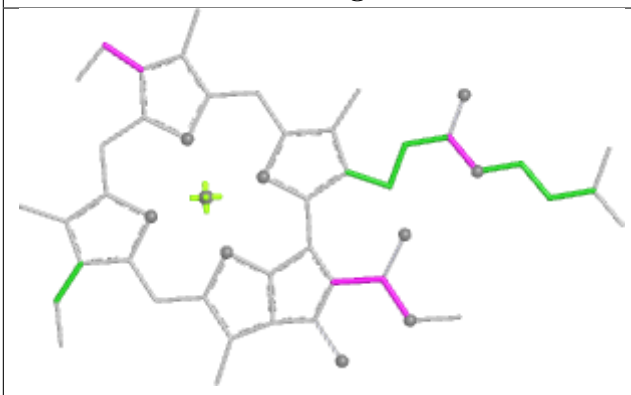
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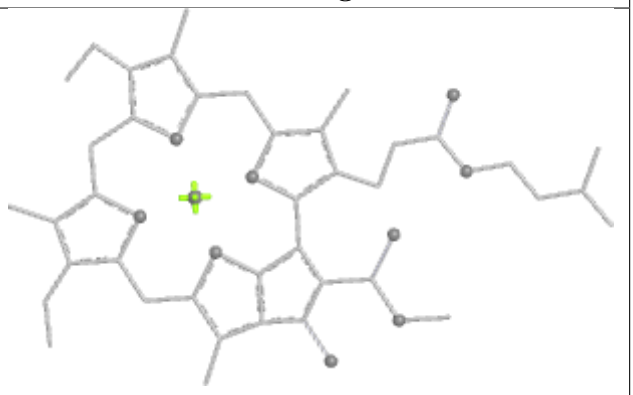
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Bond angles

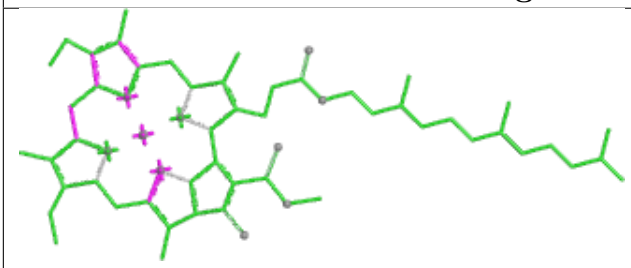


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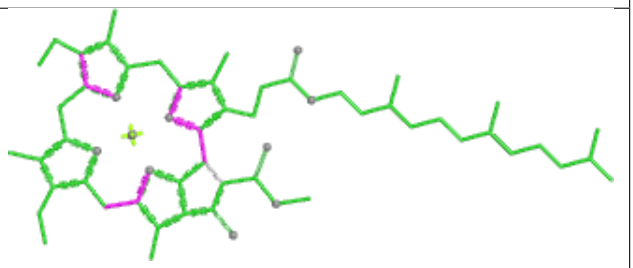


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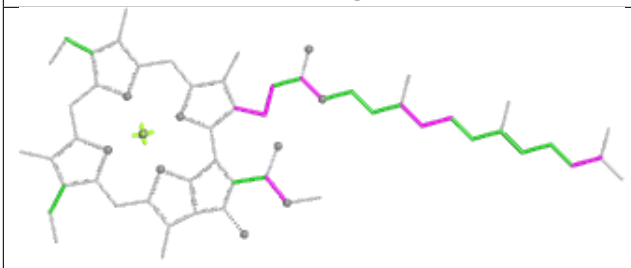
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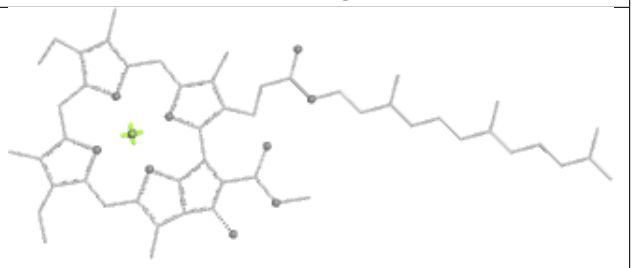
Bond lengths



Bond angles

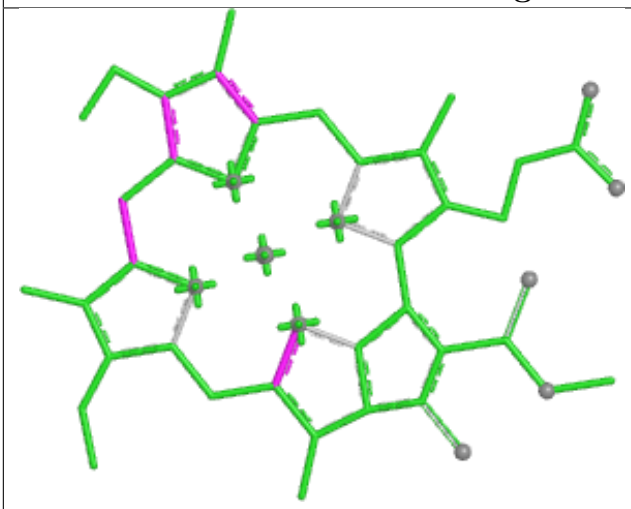


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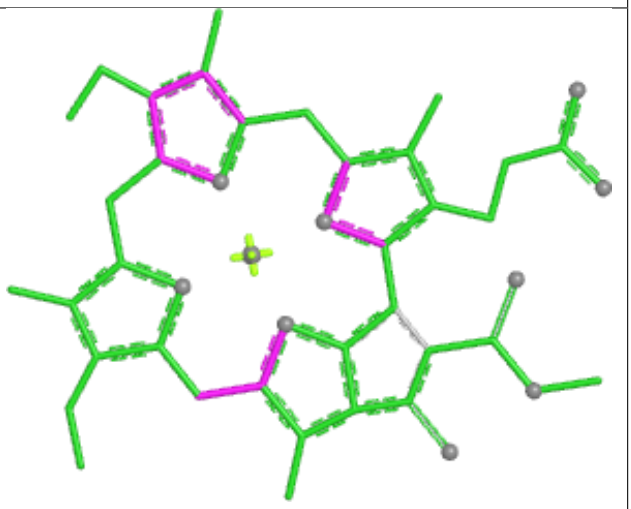


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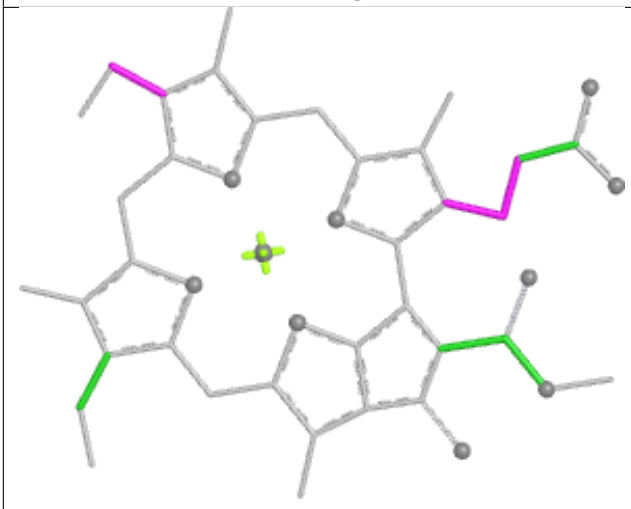
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Bond lengths



Bond angles

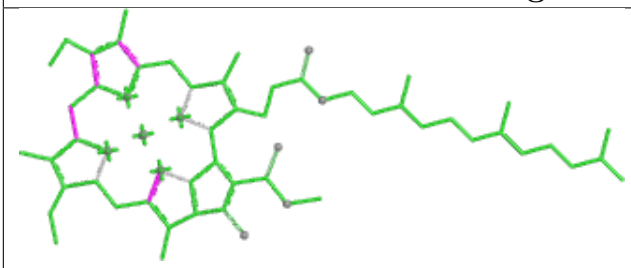


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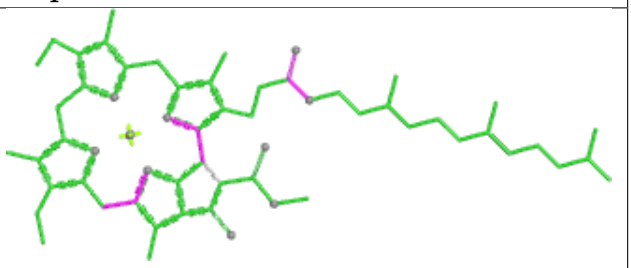


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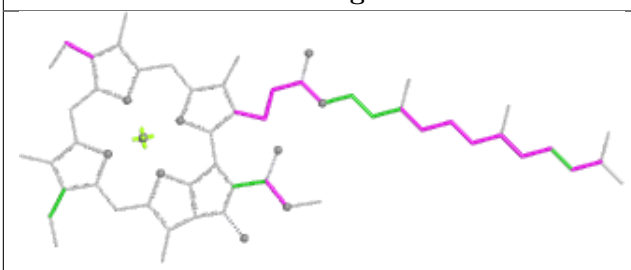
Ligand CLA p 509



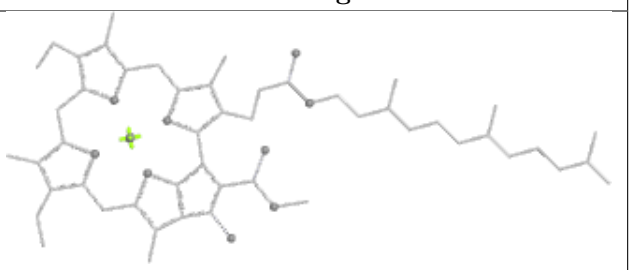
Bond lengths



Bond angles

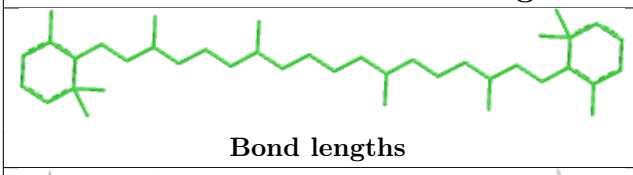


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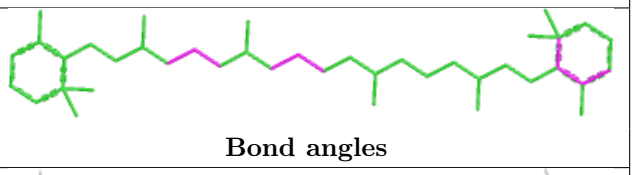


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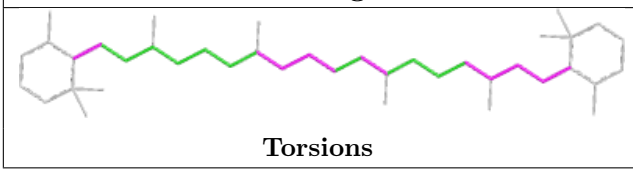
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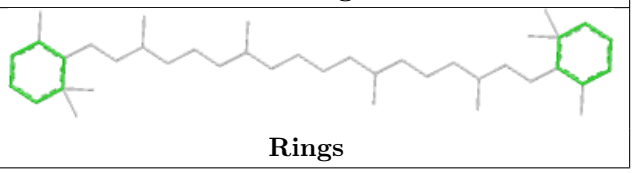
Bond lengths



Bond angles

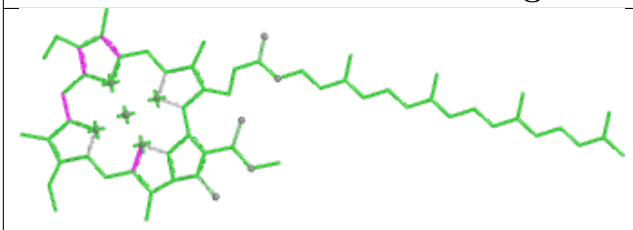


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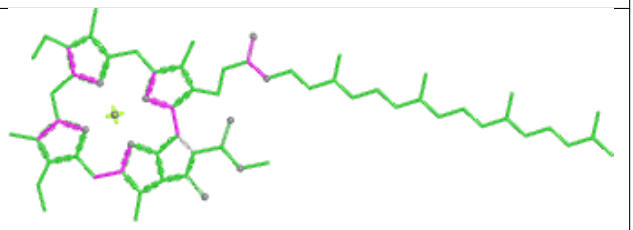


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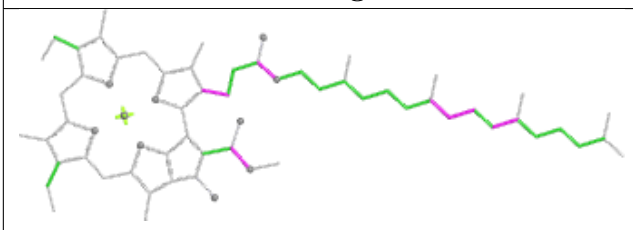
Ligand CLA X 511



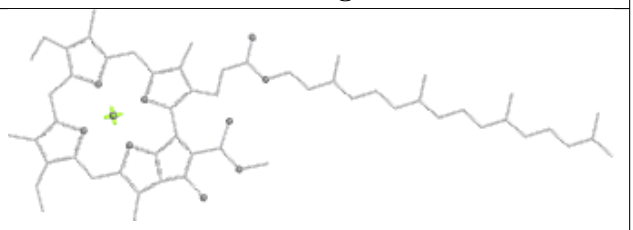
Bond lengths



Bond angles

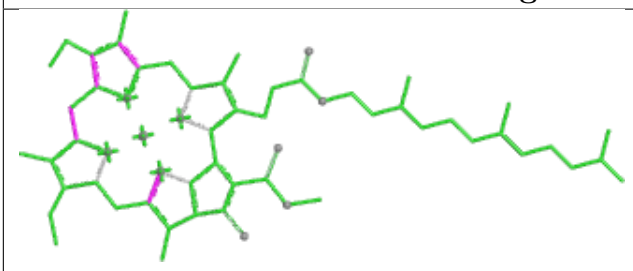


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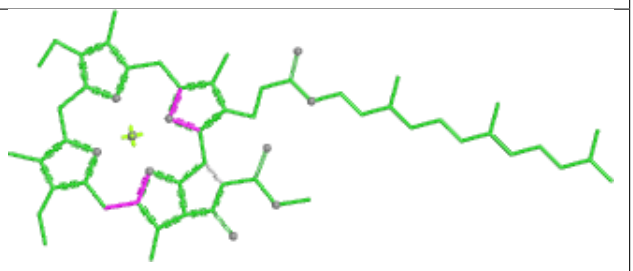


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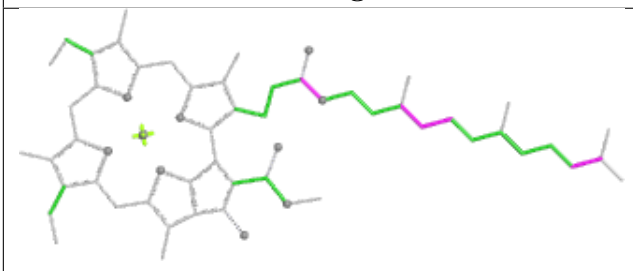
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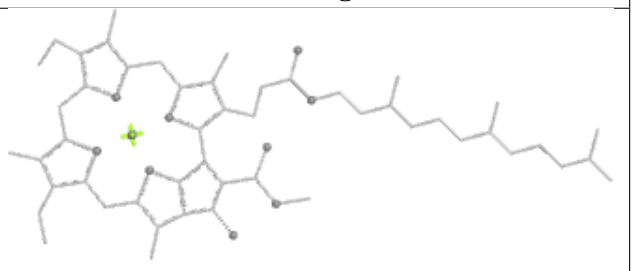
Bond lengths



Bond angles

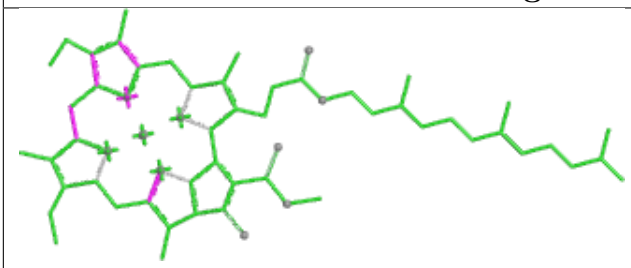


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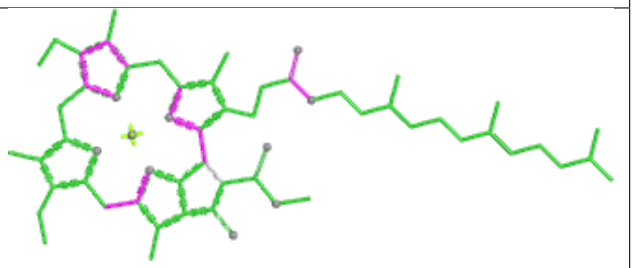


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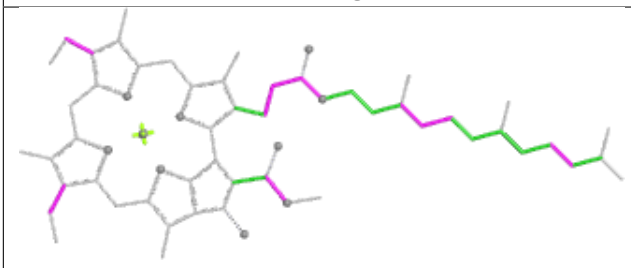
Ligand CLA X 509



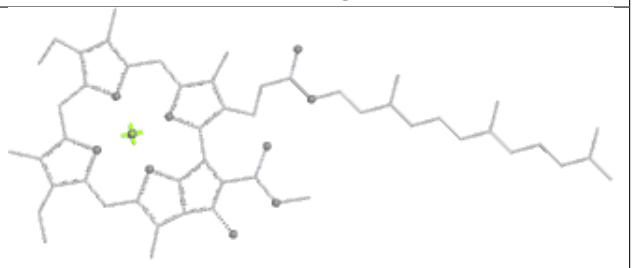
Bond lengths



Bond angles

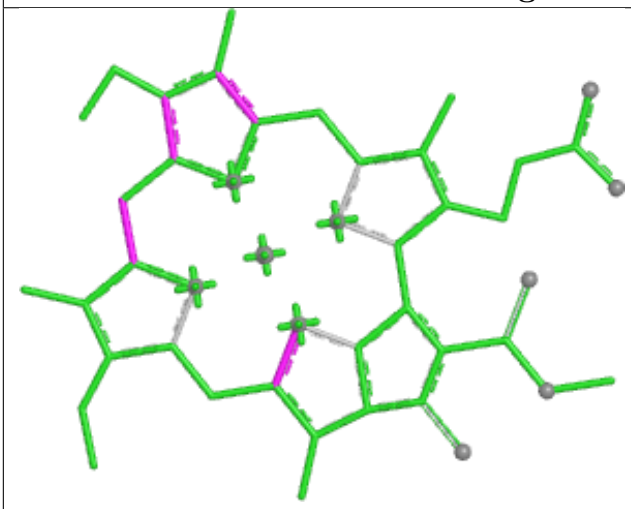


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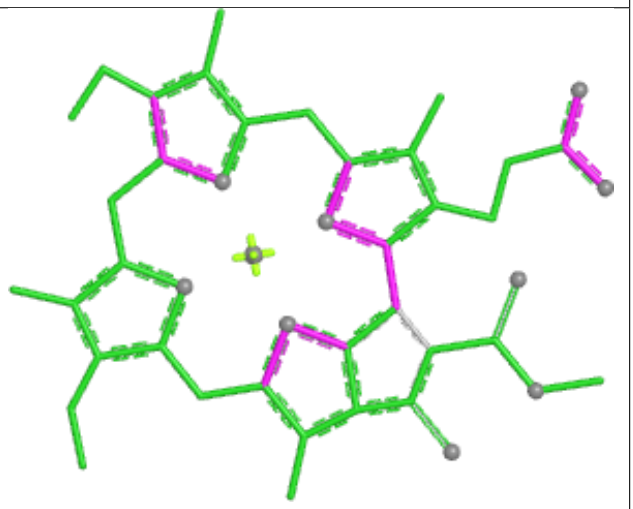


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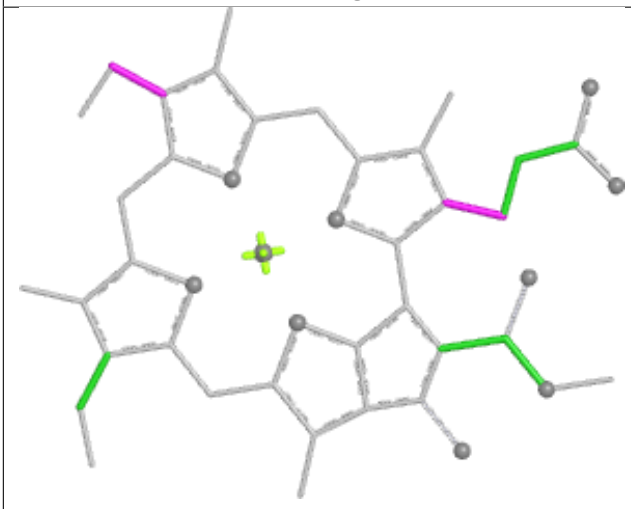
Ligand CLA b 1217



Bond lengths



Bond angles

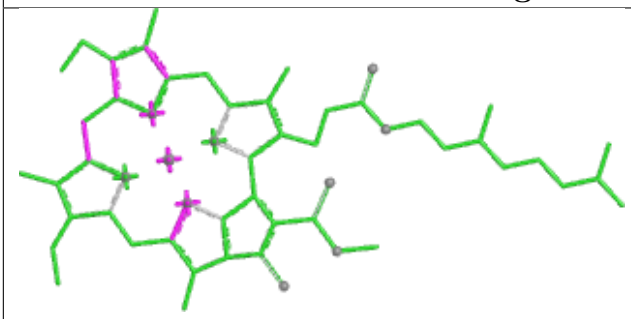


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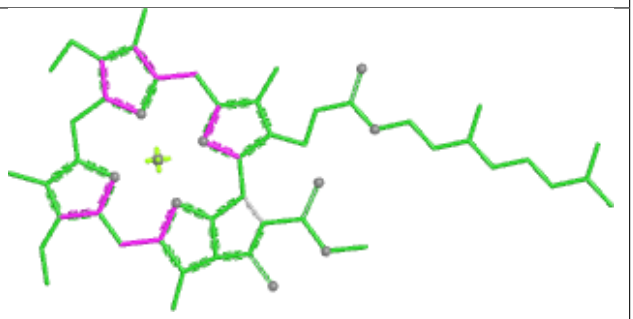


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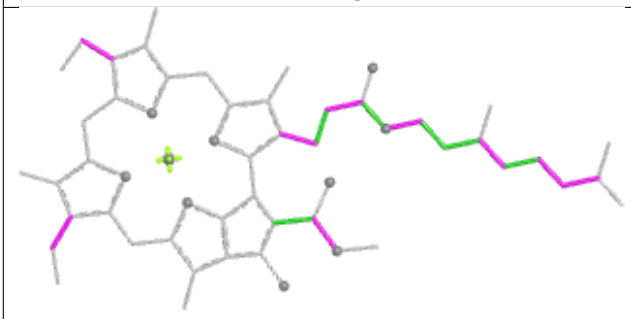
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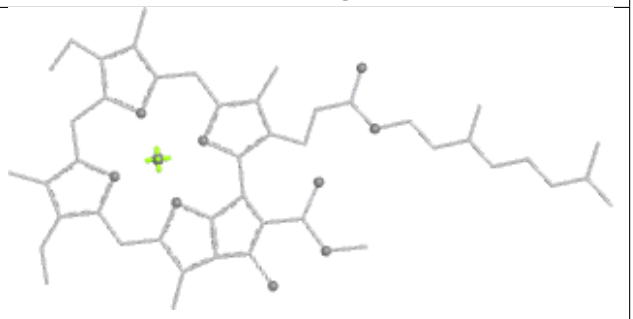
Bond lengths



Bond angles

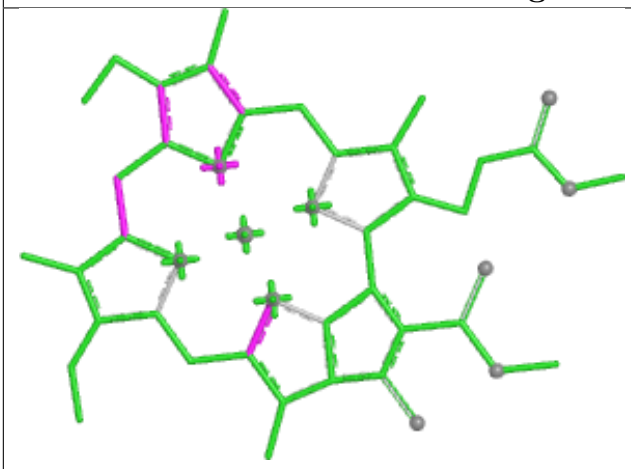


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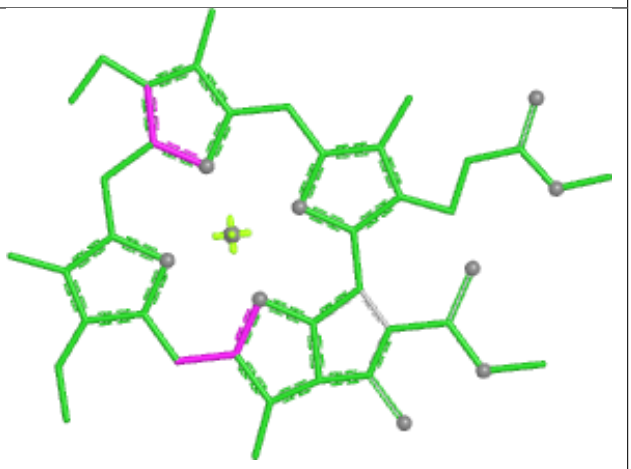


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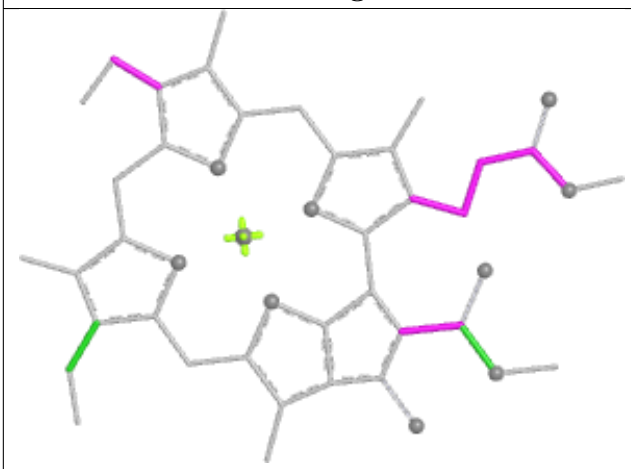
Ligand CLA o 516



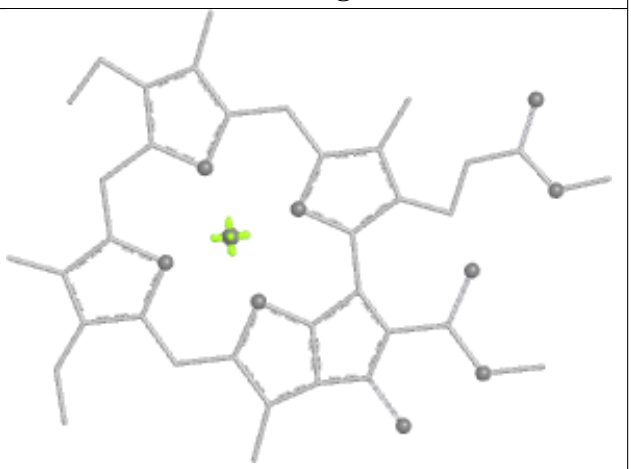
Bond lengths



Bond angles



Torsions

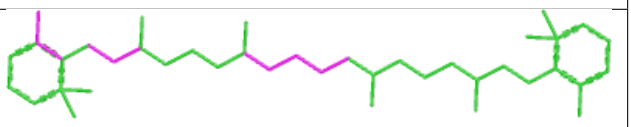


Rings

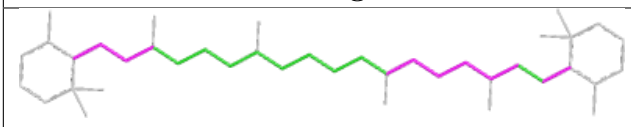
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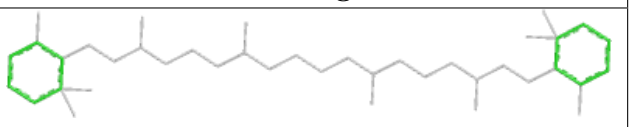
Bond lengths



Bond angles

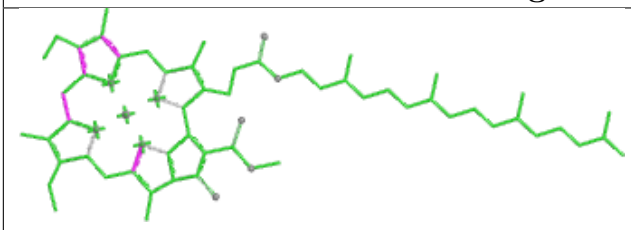


Torsions

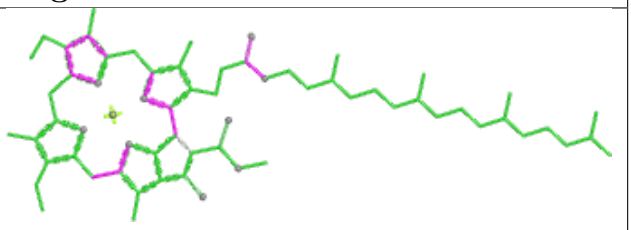


Rings

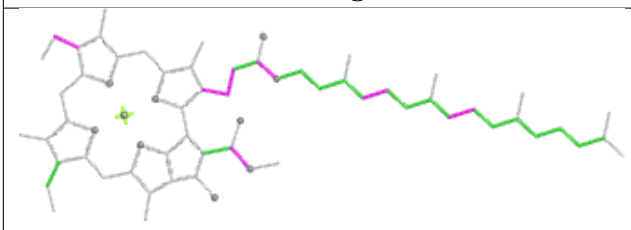
Ligand CLA g 515



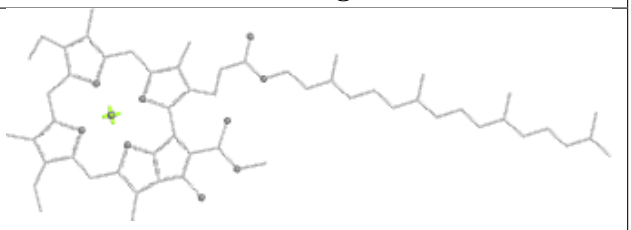
Bond lengths



Bond angles

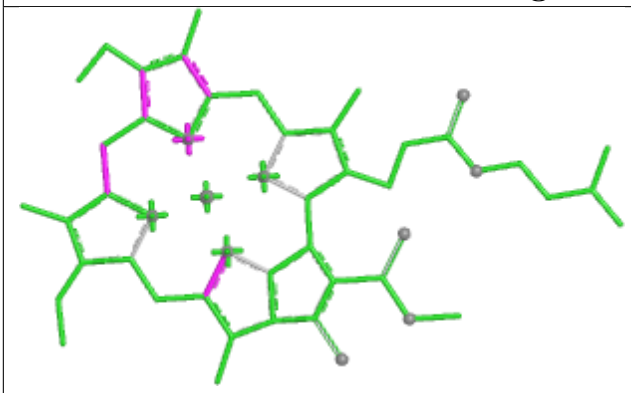


Torsions

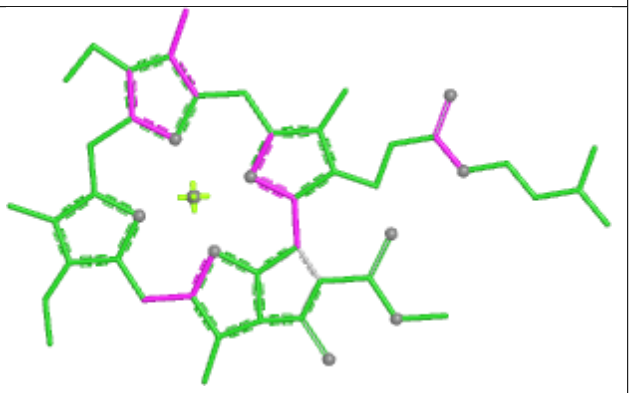


Rings

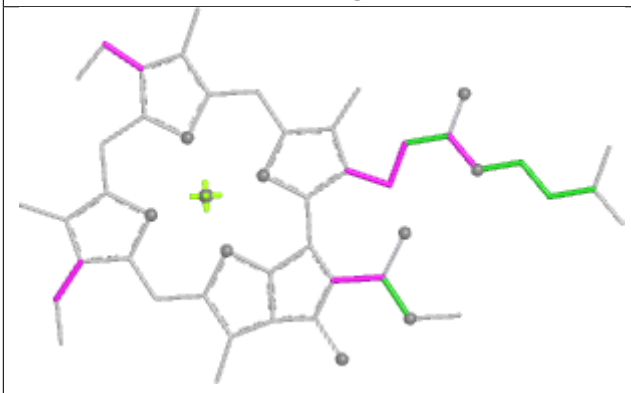
Ligand CLA s 501



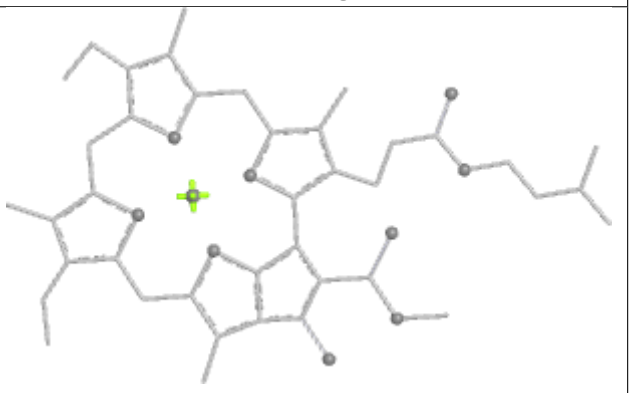
Bond lengths



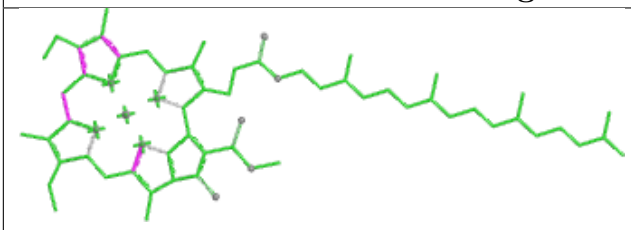
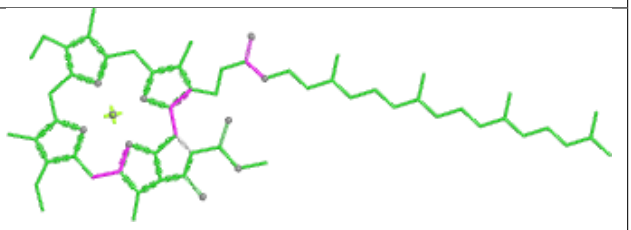
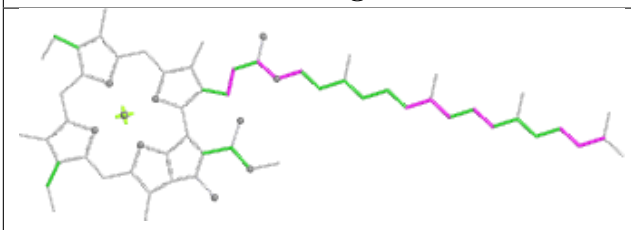
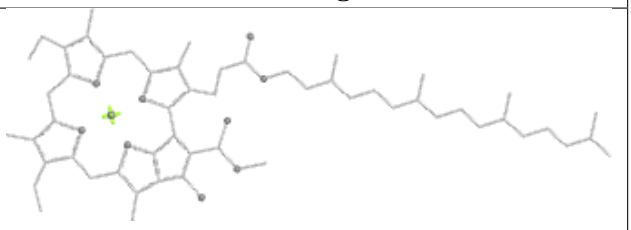
Bond angles

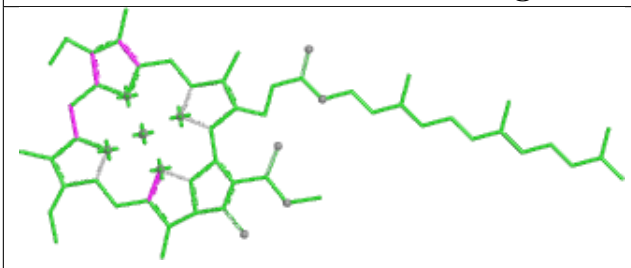
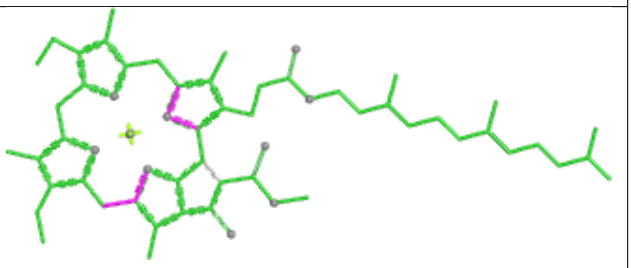
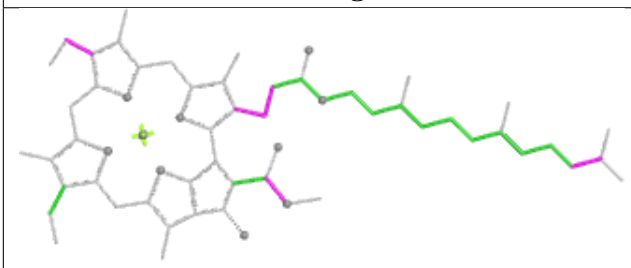
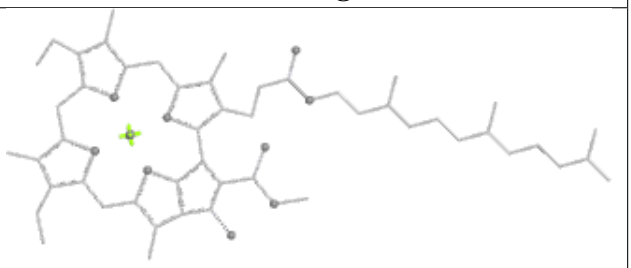


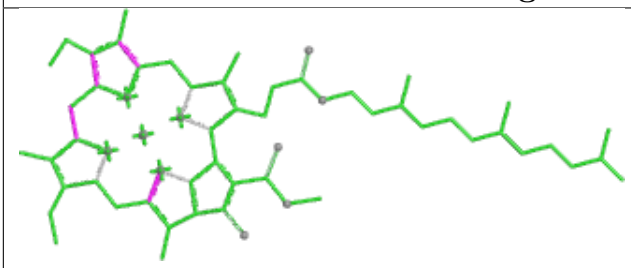
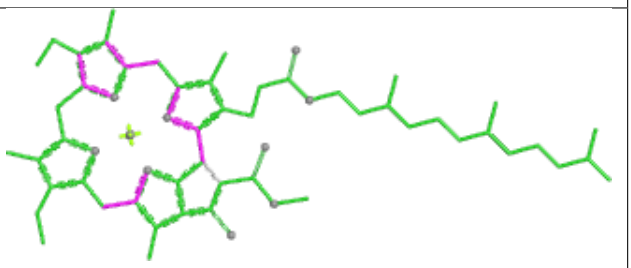
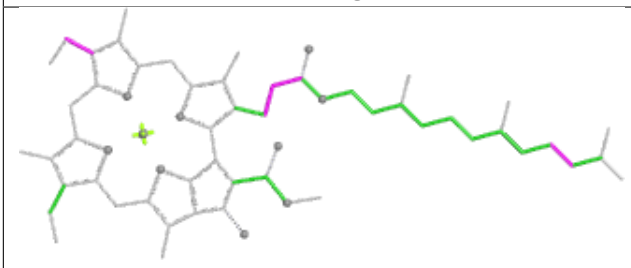
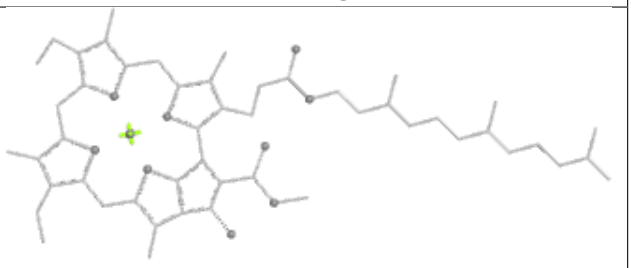
Torsions

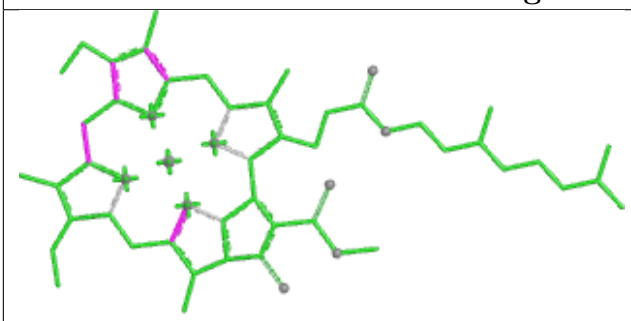
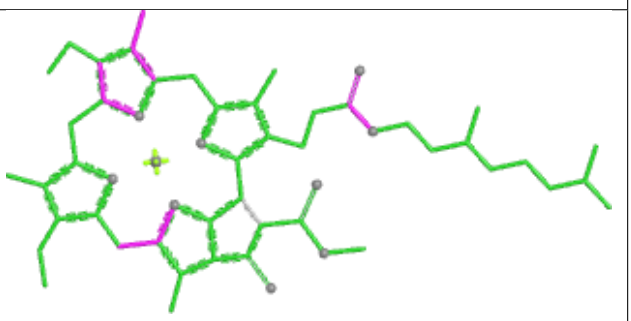
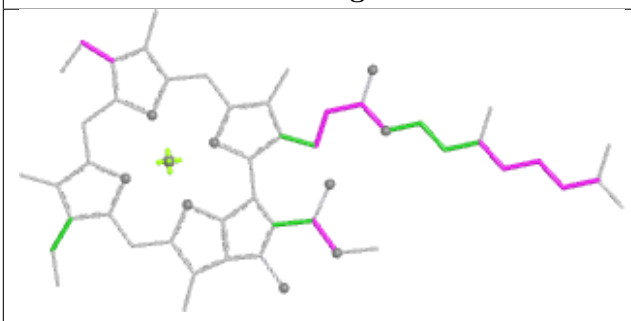
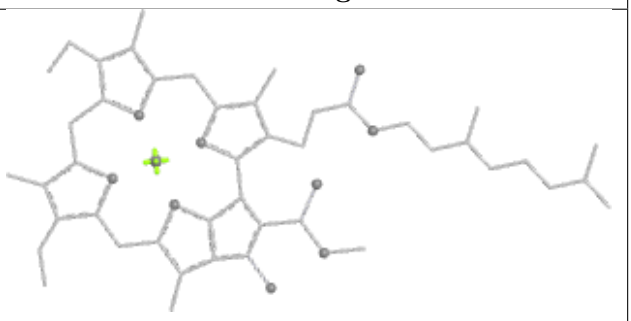


Rings

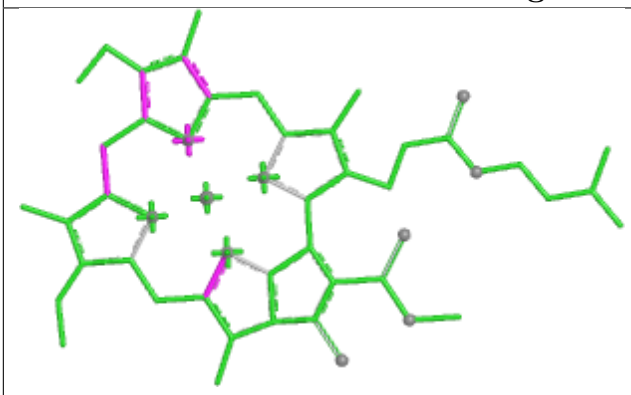
Ligand CLA L 1503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1215	
	
Bond lengths	Bond angles
	
Torsions	Rings

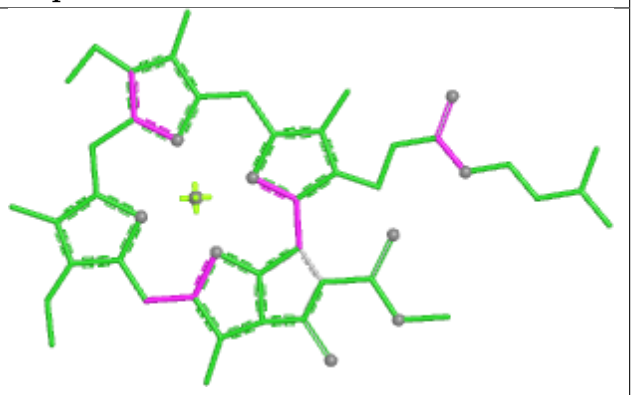
Ligand CLA W 509	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA X 508	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

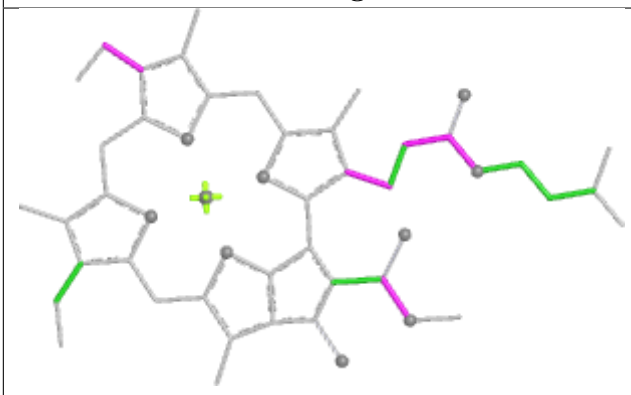
Ligand CLA p 514



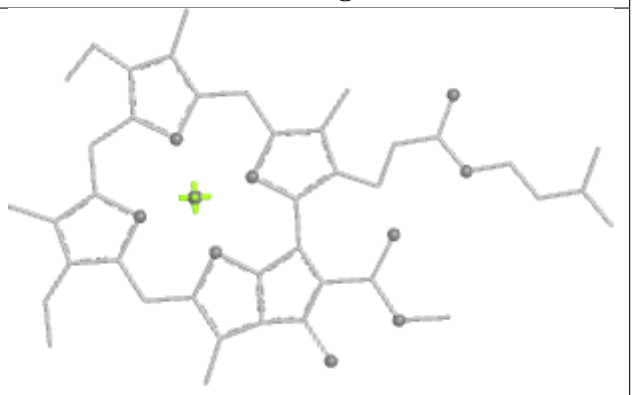
Bond lengths



Bond angles

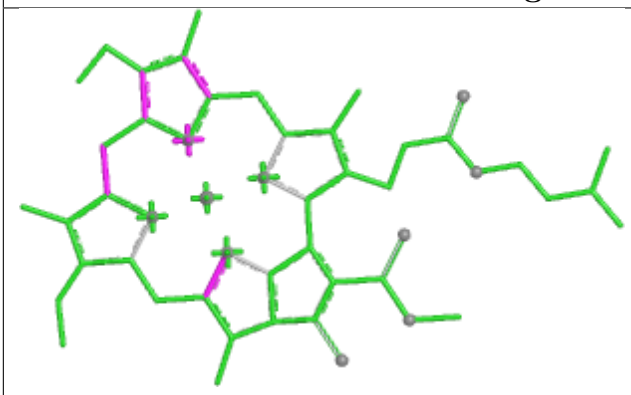


Torsions

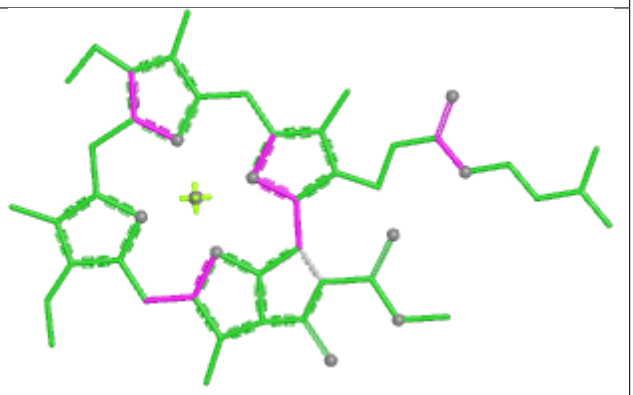


Rings

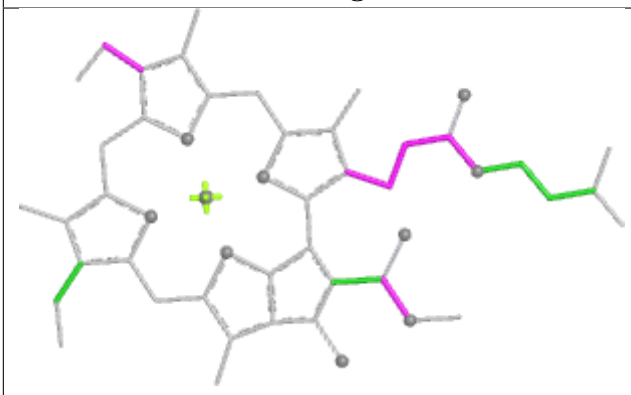
Ligand CLA w 514



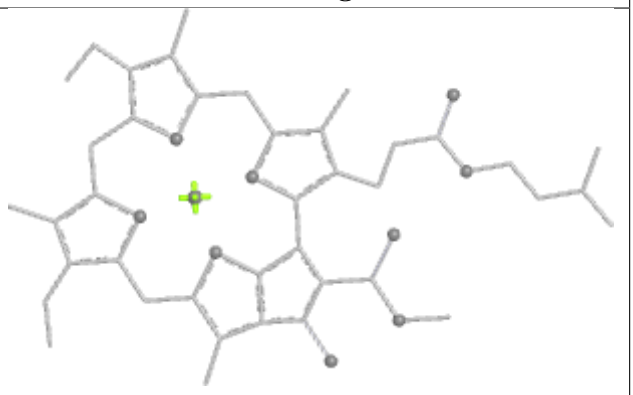
Bond lengths



Bond angles

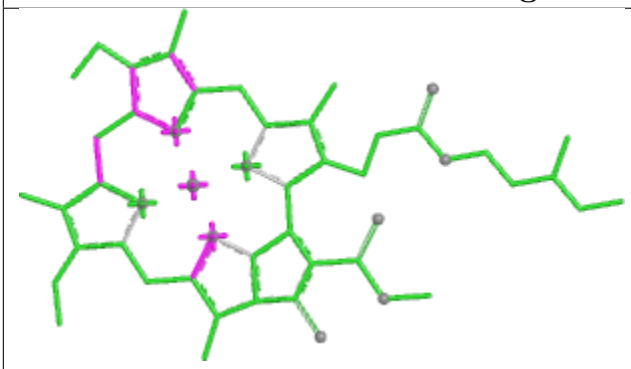


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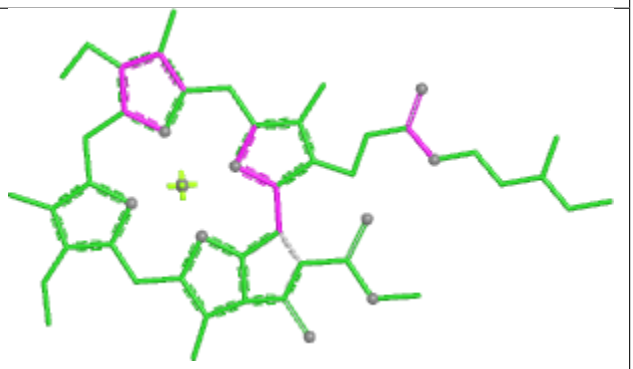


Rings

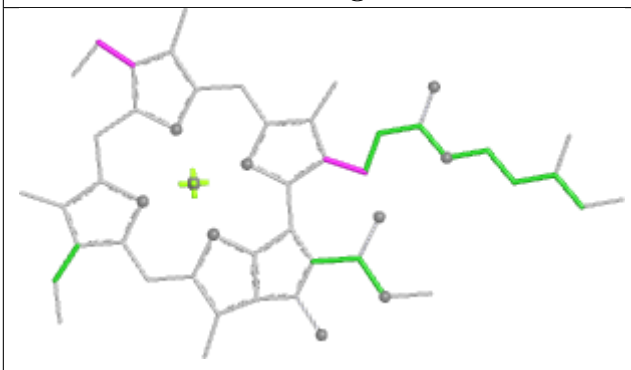
Ligand CLA a 1135



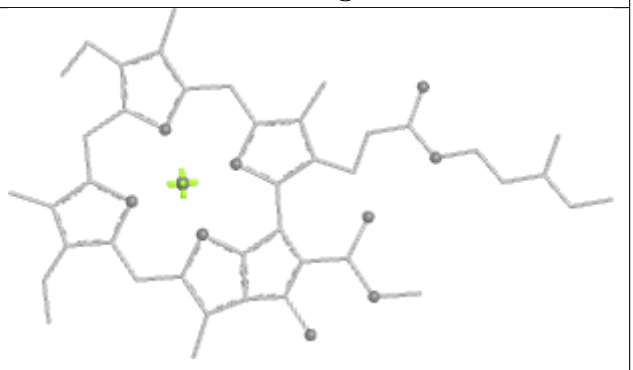
Bond lengths



Bond angles

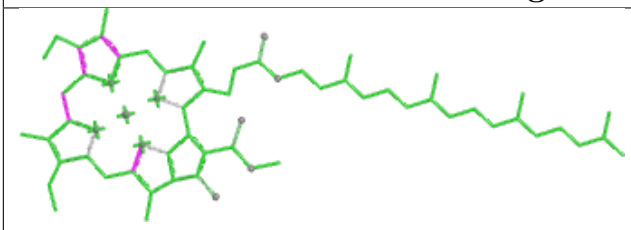


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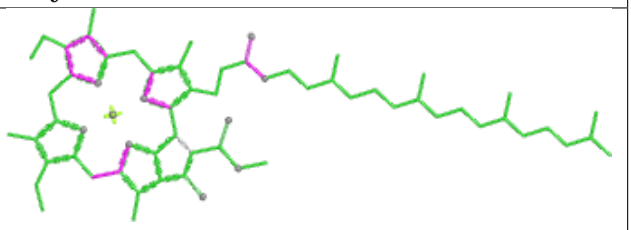


Rings

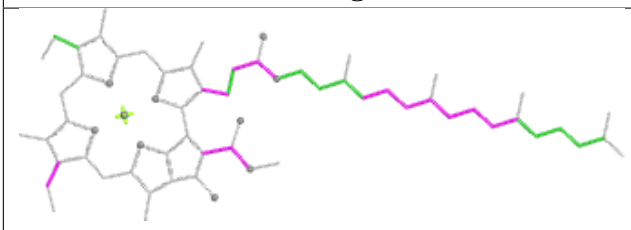
Ligand CLA y 509



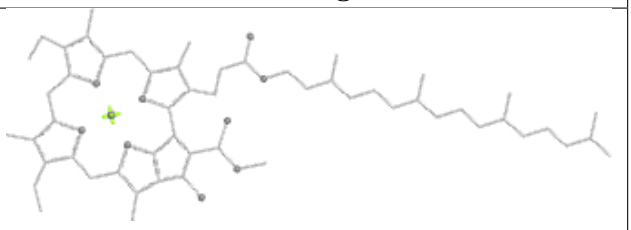
Bond lengths



Bond angles

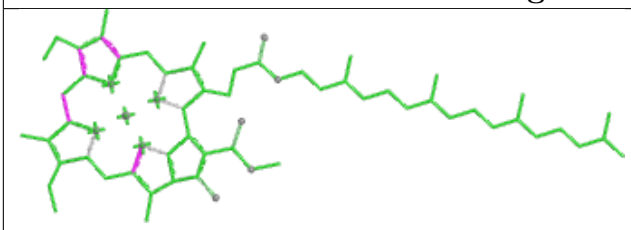


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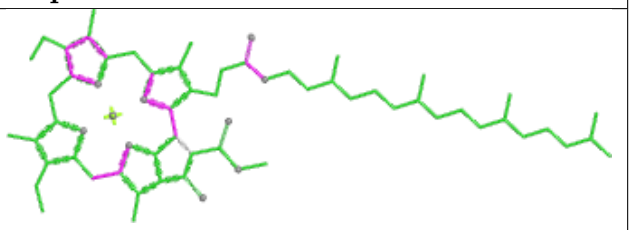


Rings

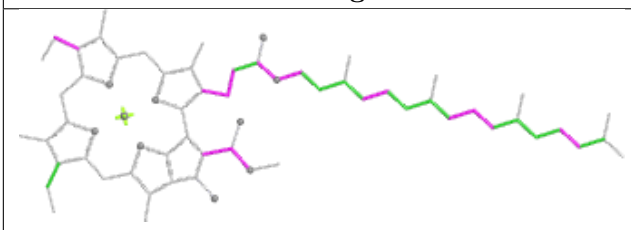
Ligand CLA p 515



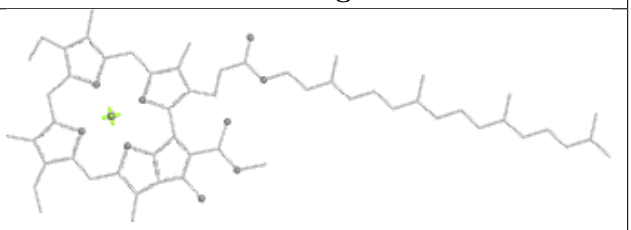
Bond lengths



Bond angles

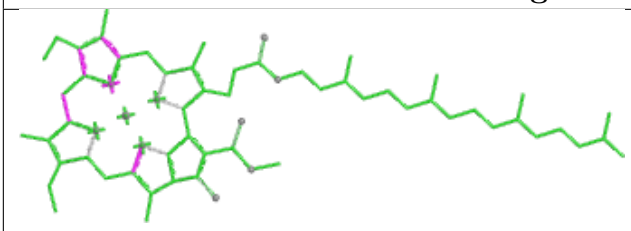


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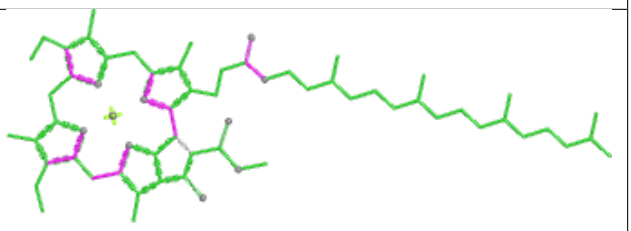


Rings

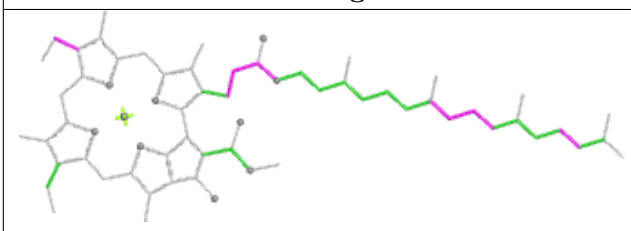
Ligand CLA t 505



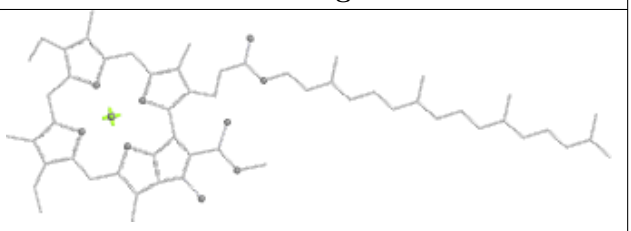
Bond lengths



Bond angles

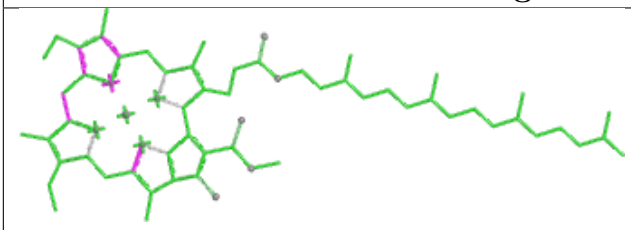


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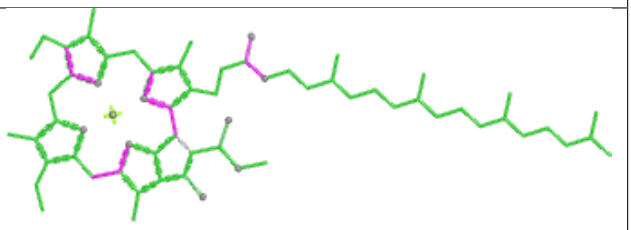


Rings

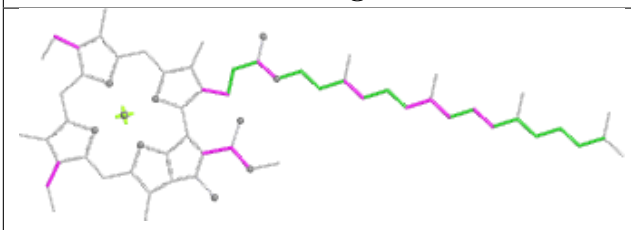
Ligand CLA G 1210



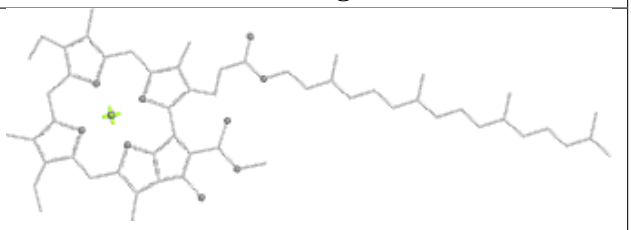
Bond lengths



Bond angles

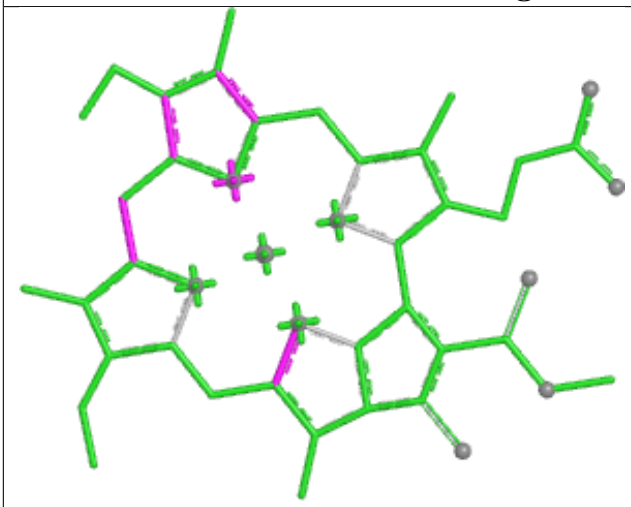


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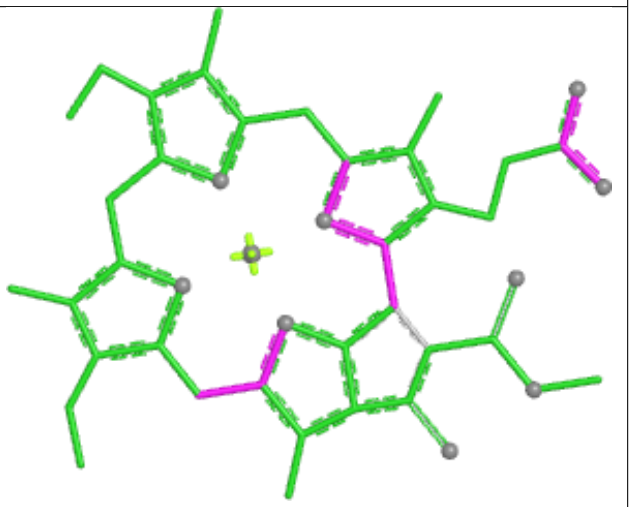


Rings

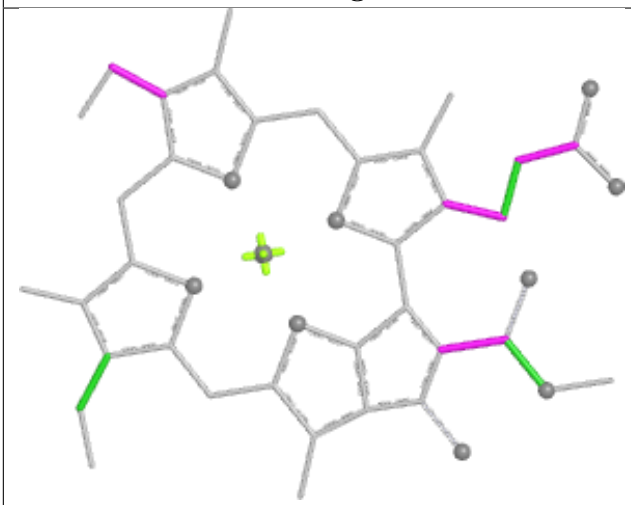
Ligand CLA B 1212



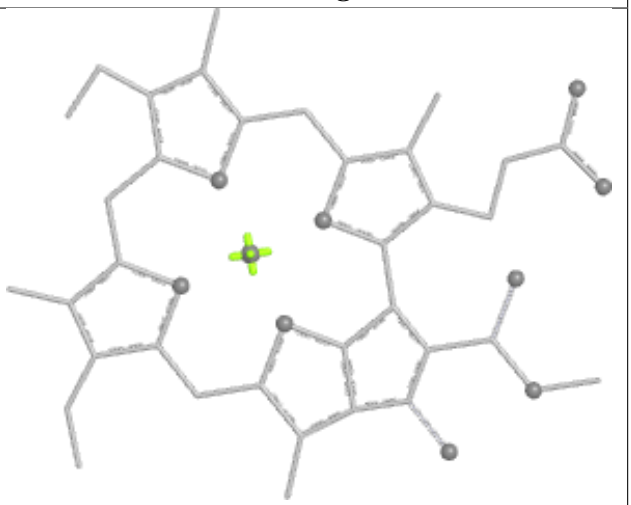
Bond lengths



Bond angles

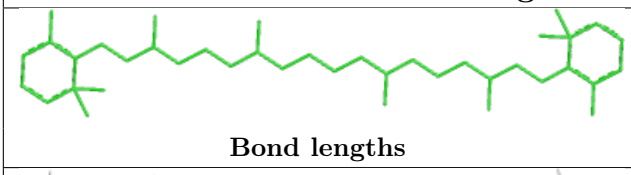


Torsions

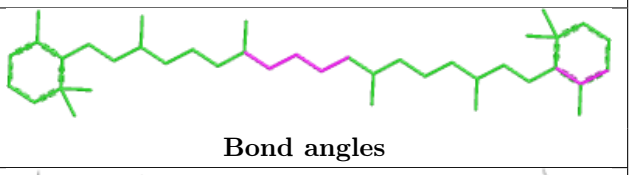


Rings

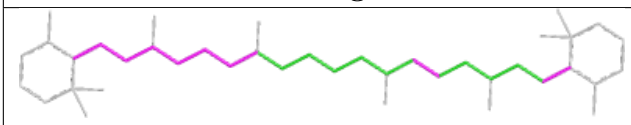
Ligand BCR W 603



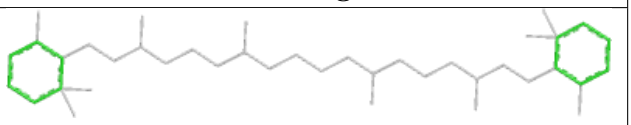
Bond lengths



Bond angles

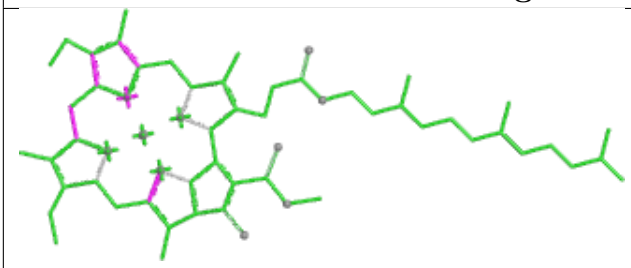


Torsions

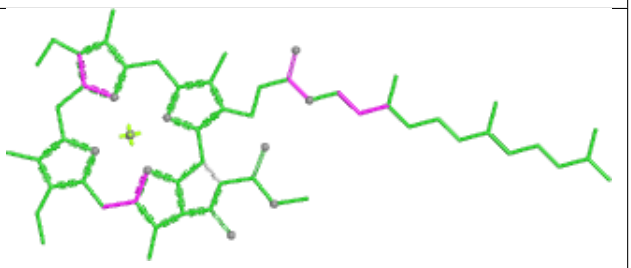


Rings

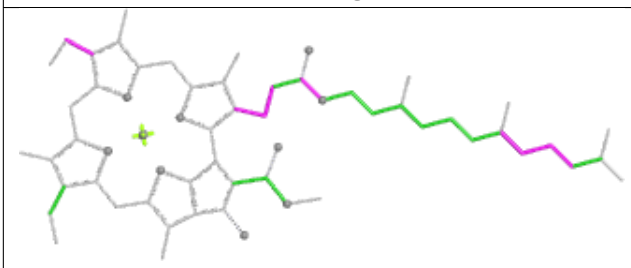
Ligand CLA A 1130



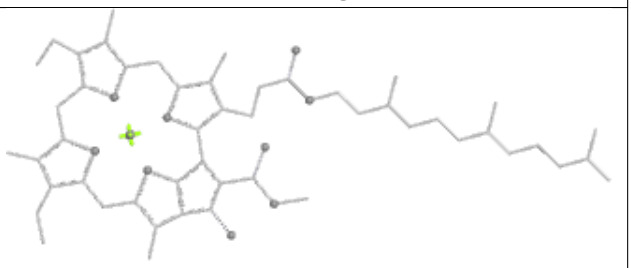
Bond lengths



Bond angles

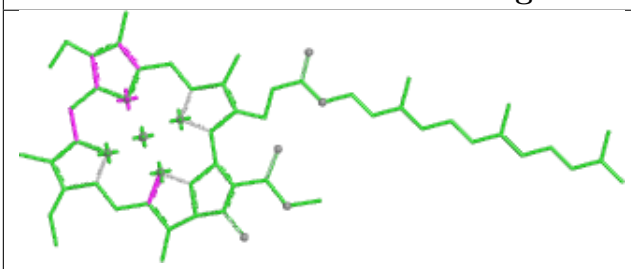


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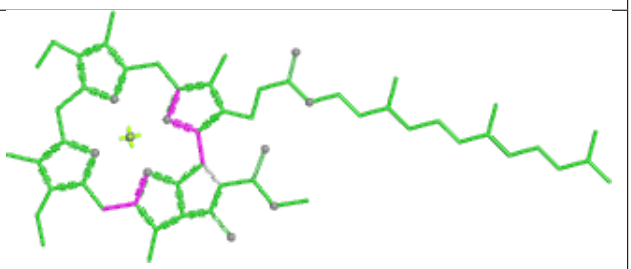


Rings

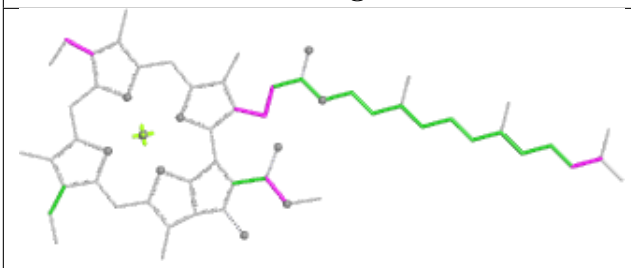
Ligand CLA B 1215



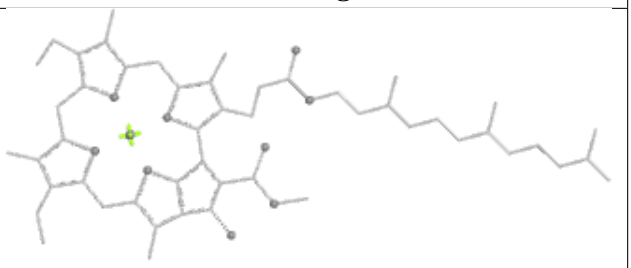
Bond lengths



Bond angles

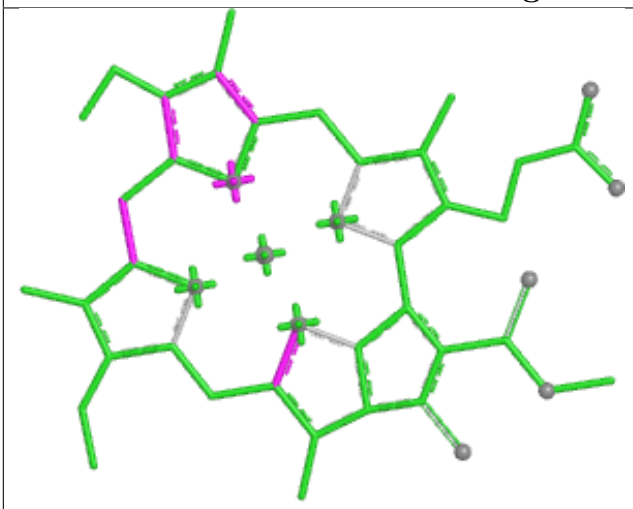


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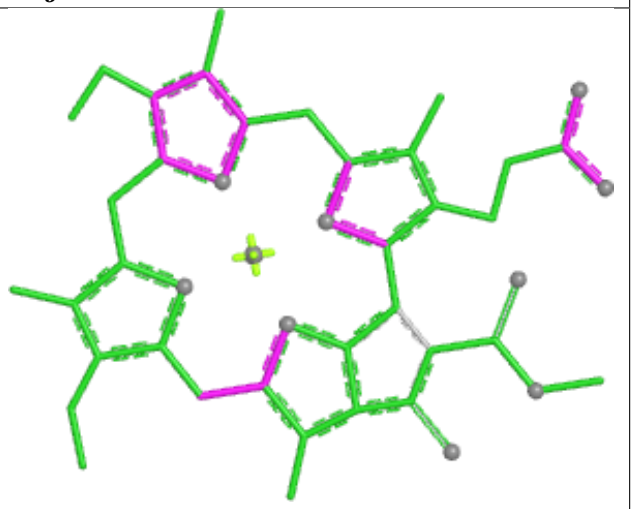


Rings

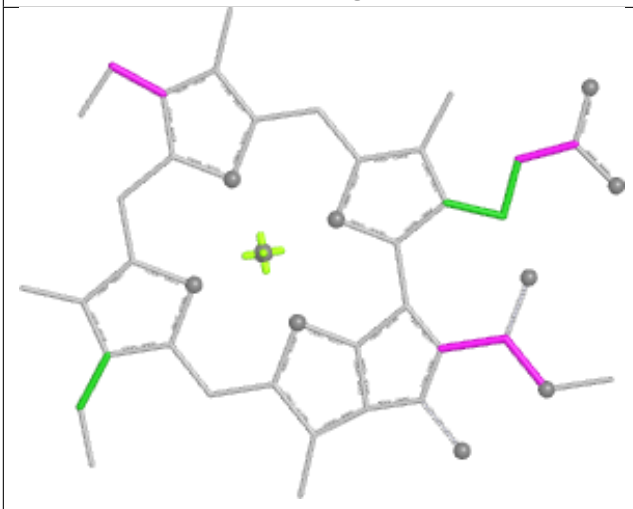
Ligand CLA j 1302



Bond lengths



Bond angles

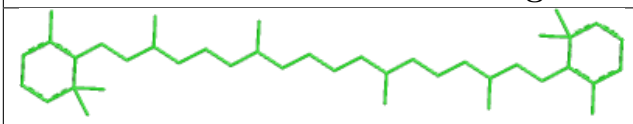


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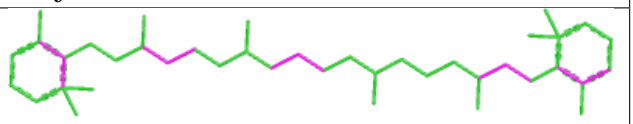


Rings

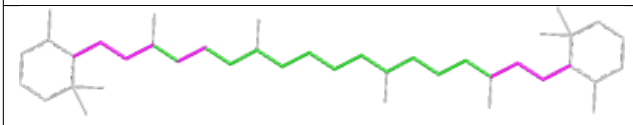
Ligand BCR y 603



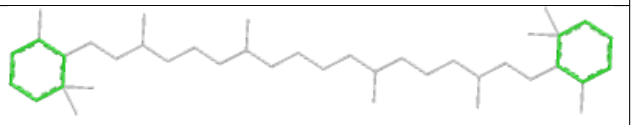
Bond lengths



Bond angles

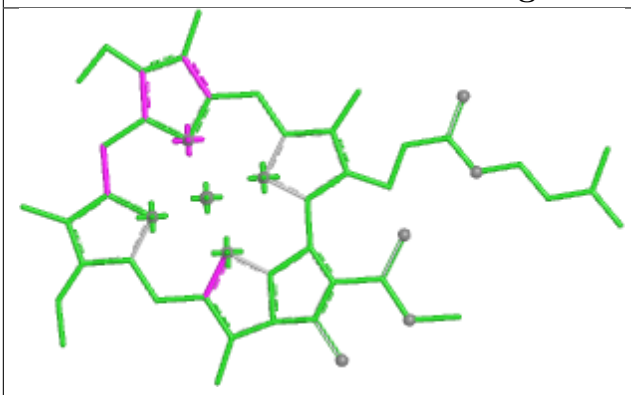


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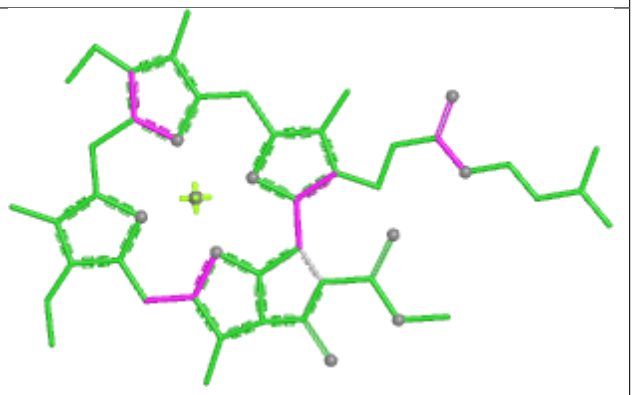


Rings

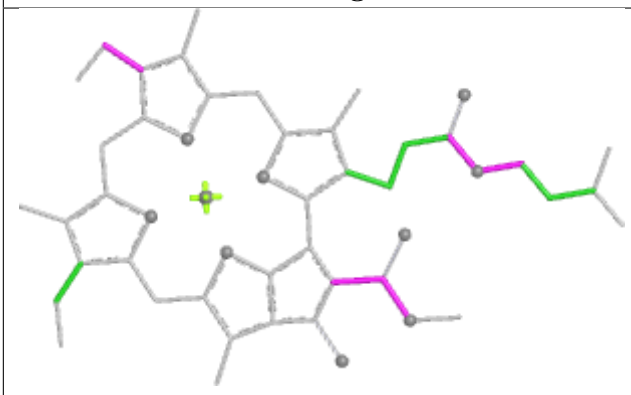
Ligand CLA b 1222



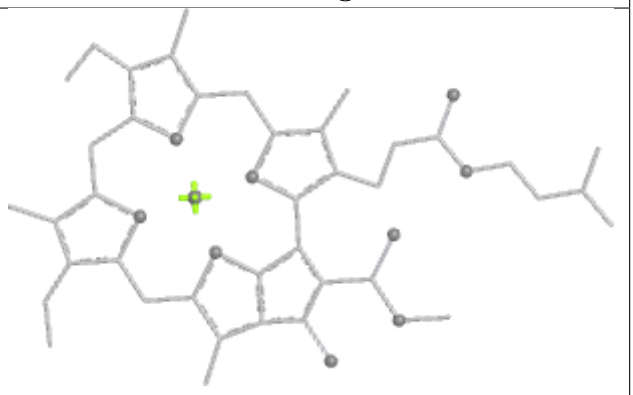
Bond lengths



Bond angles

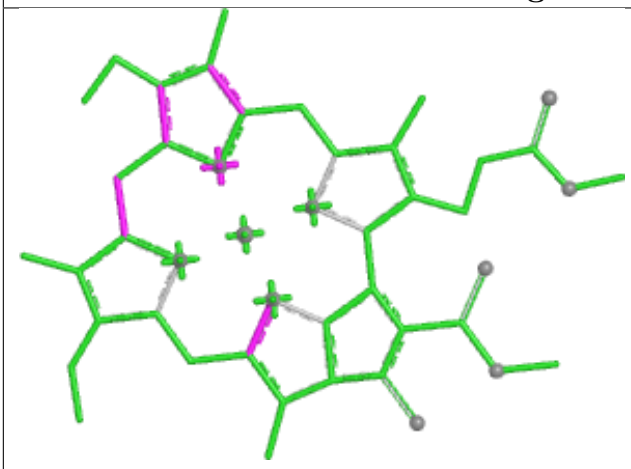


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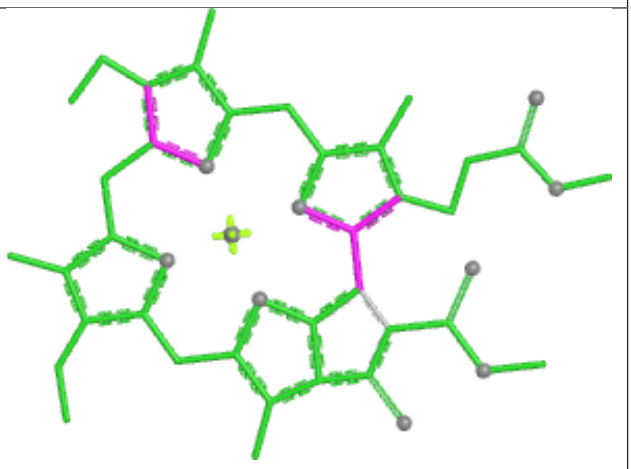


Rings

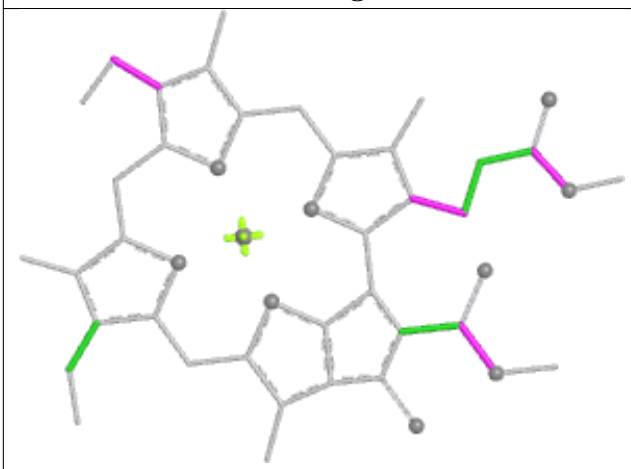
Ligand CLA u 513



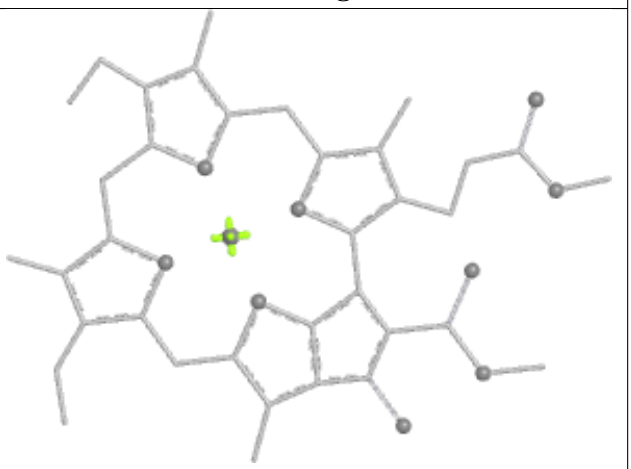
Bond lengths



Bond angles



Torsions

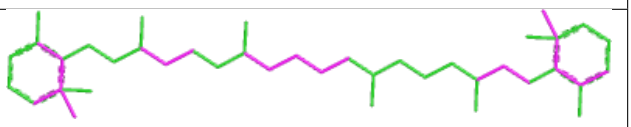


Rings

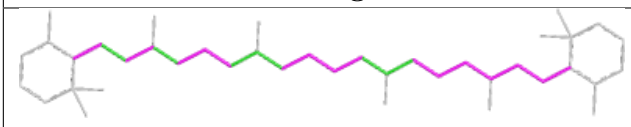
Ligand BCR o 604



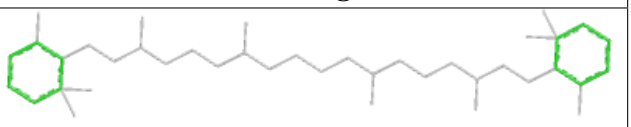
Bond lengths



Bond angles

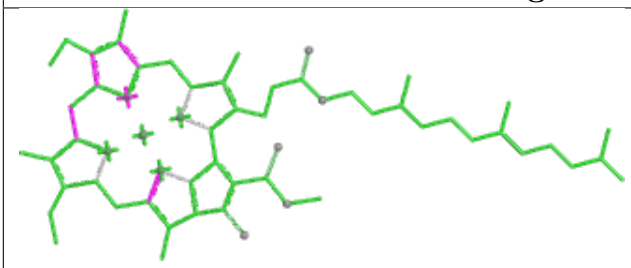


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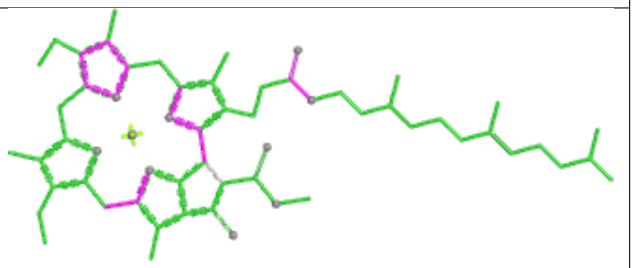


Rings

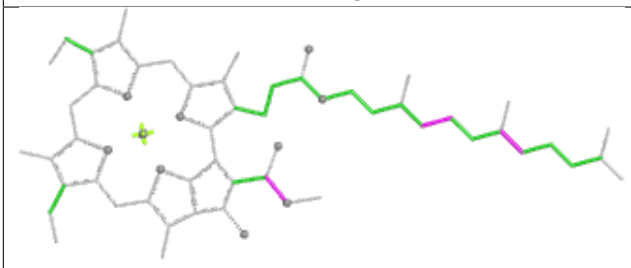
Ligand CLA v 506



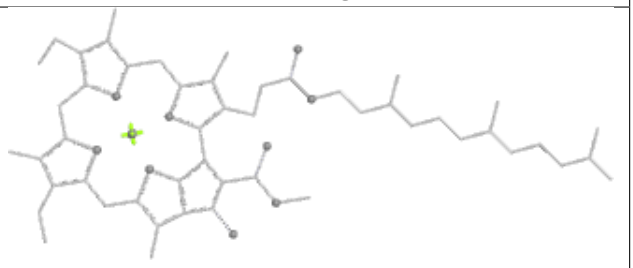
Bond lengths



Bond angles

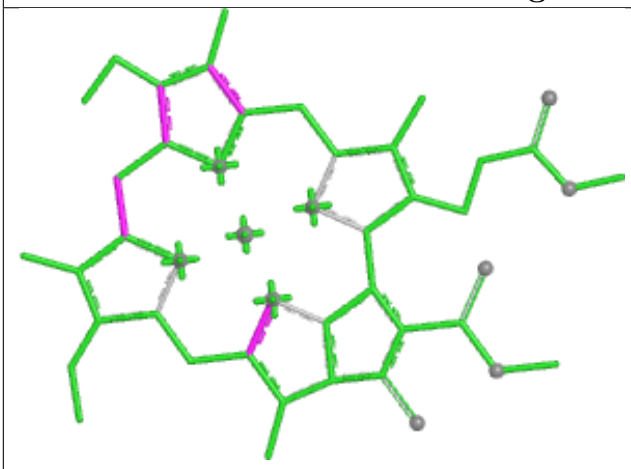


Torsions

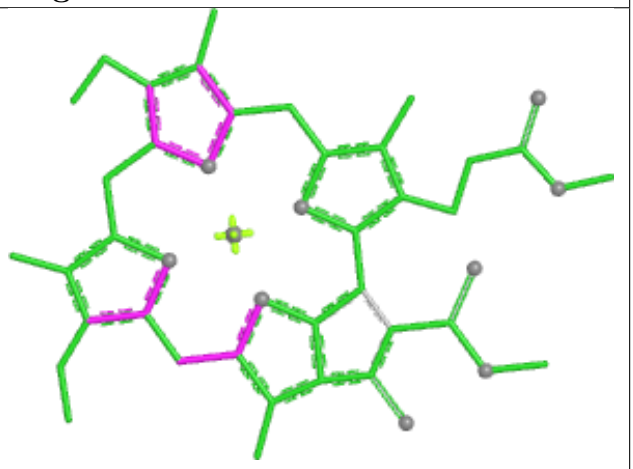


Rings

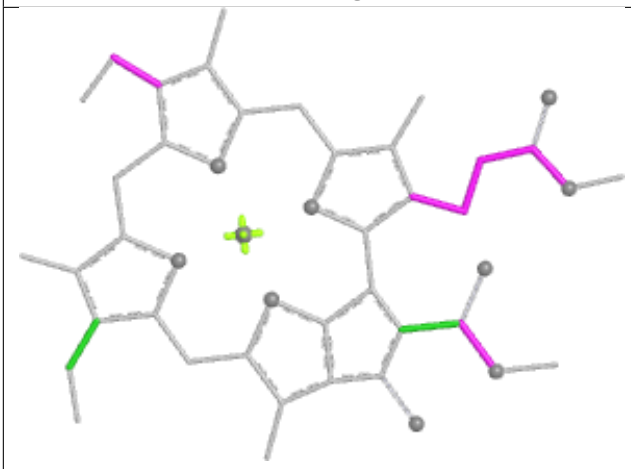
Ligand CLA g 503



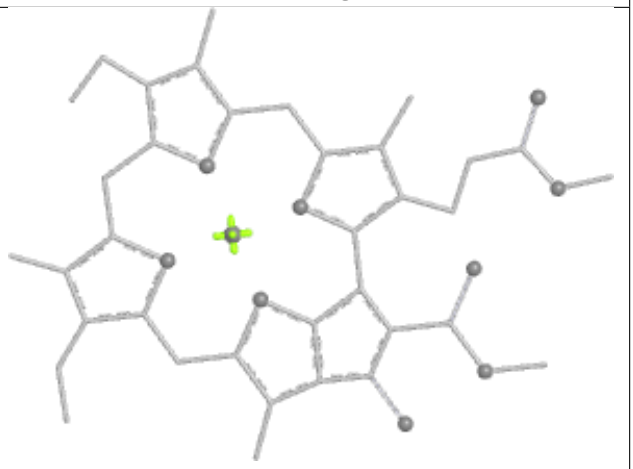
Bond lengths



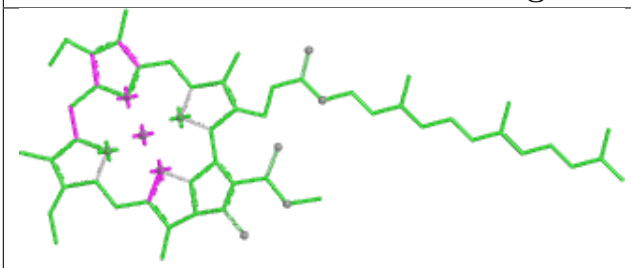
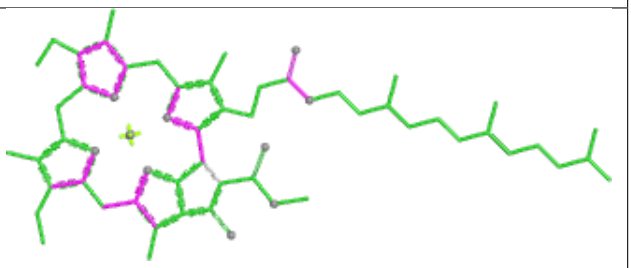
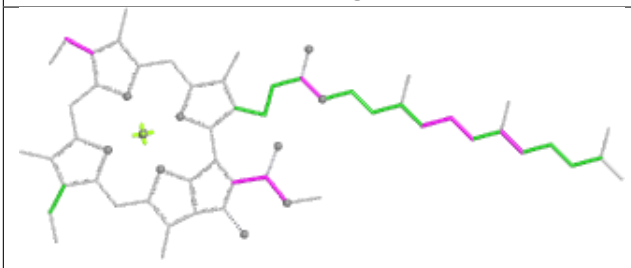
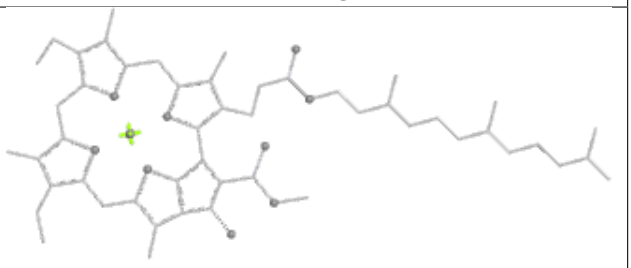
Bond angles

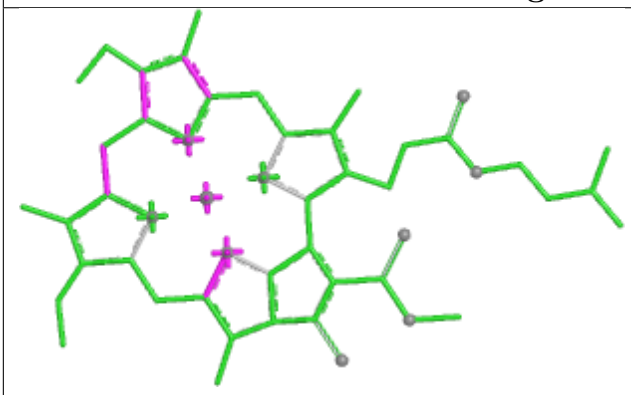
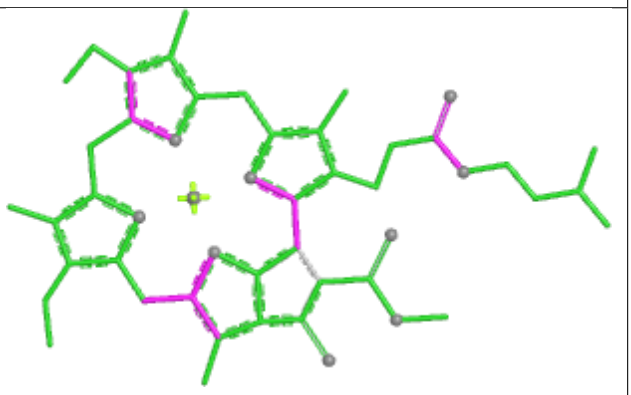
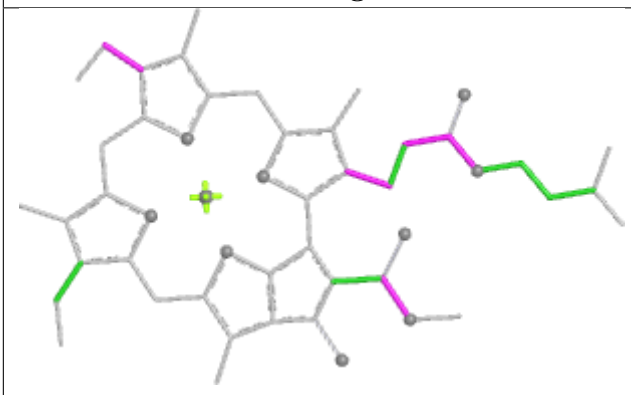
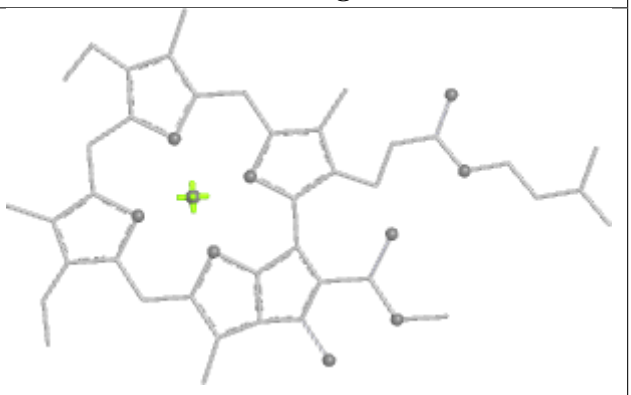


Torsions

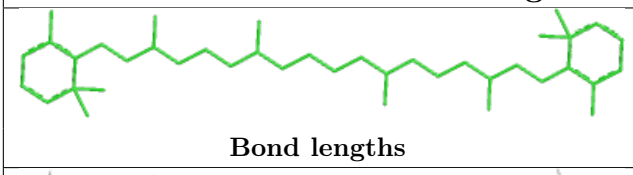


Rings

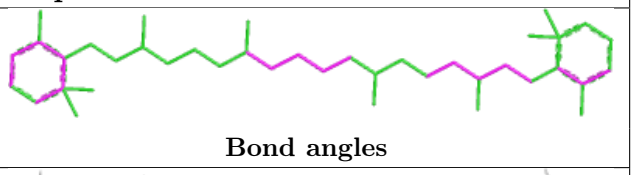
Ligand CLA h 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

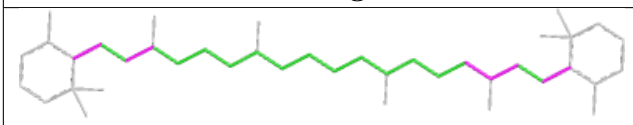
Ligand BCR p 601



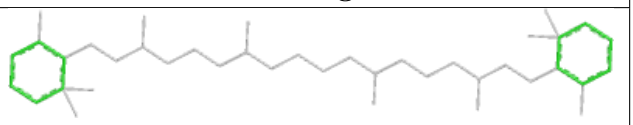
Bond lengths



Bond angles



Torsions

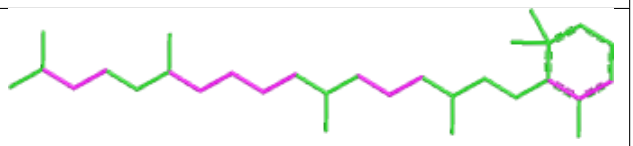


Rings

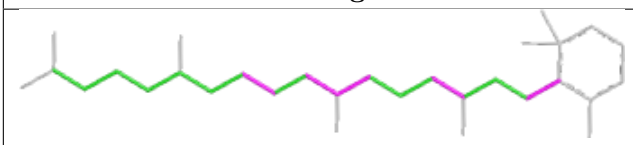
Ligand BCR G 4009



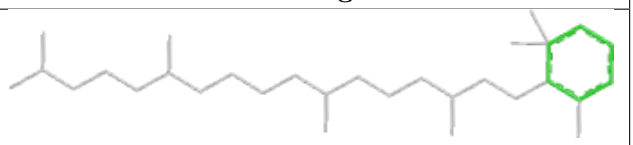
Bond lengths



Bond angles

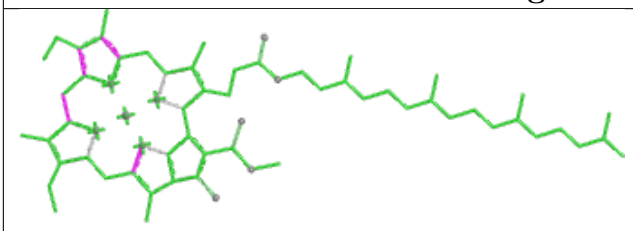


Torsions

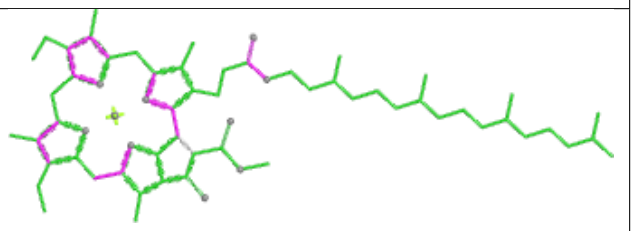


Rings

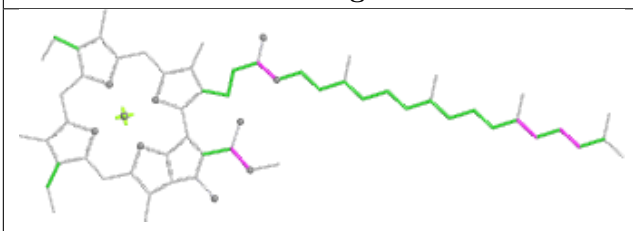
Ligand CLA v 510



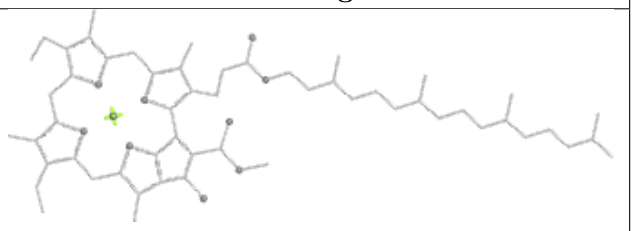
Bond lengths



Bond angles

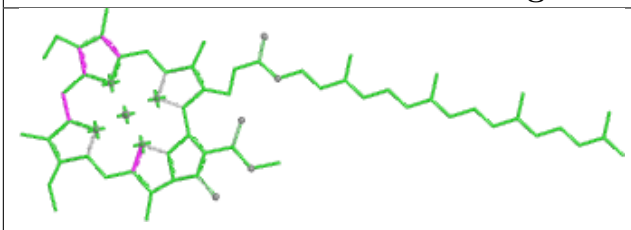


Torsions

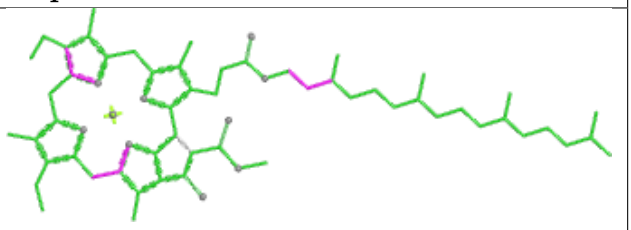


Rings

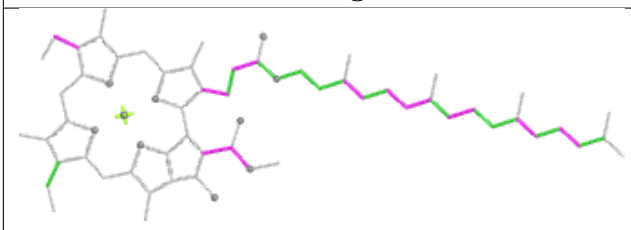
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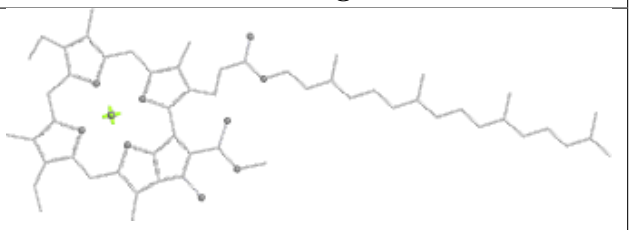
Bond lengths



Bond angles

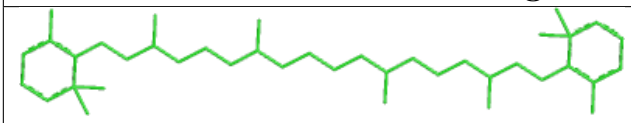


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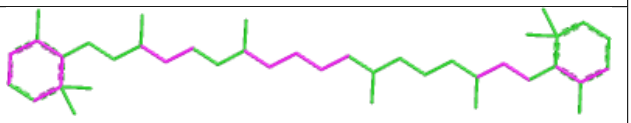


Rings

Ligand BCR Z 602



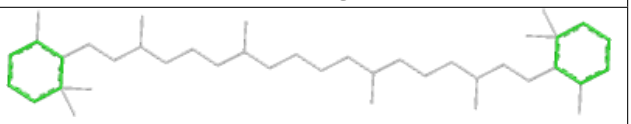
Bond lengths



Bond angles

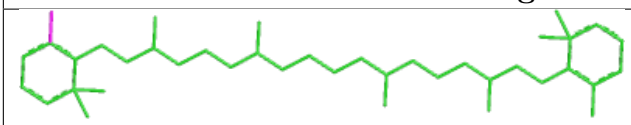


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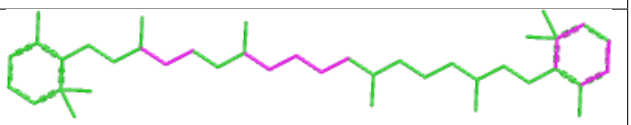


Rings

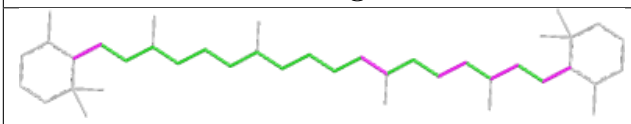
Ligand BCR a 4007



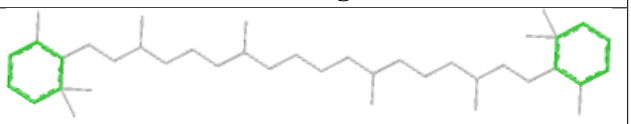
Bond lengths



Bond angles

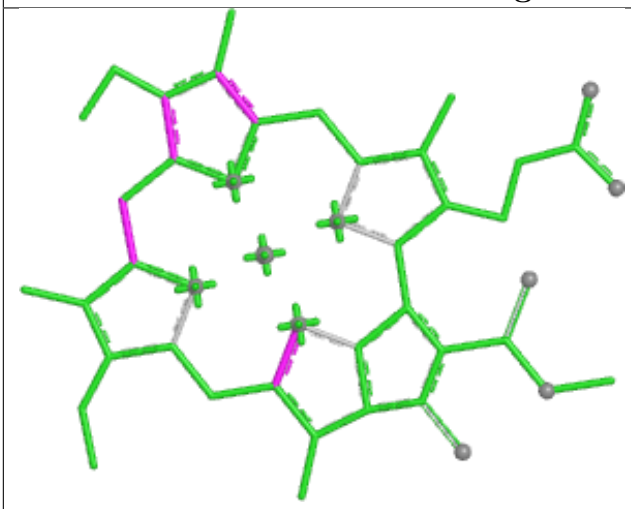


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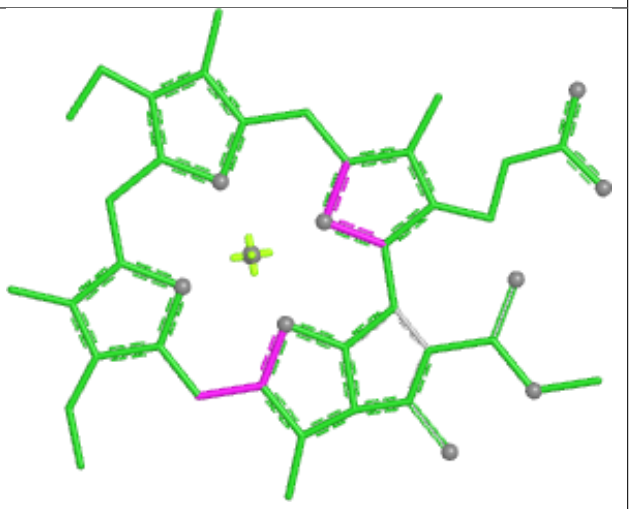


Rings

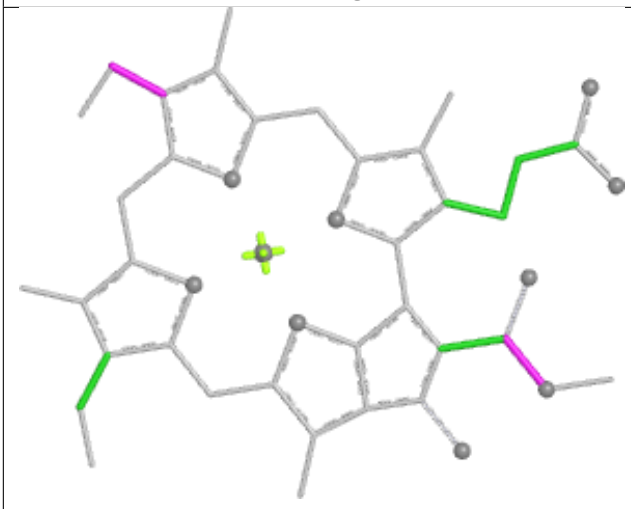
Ligand CLA K 4002



Bond lengths



Bond angles

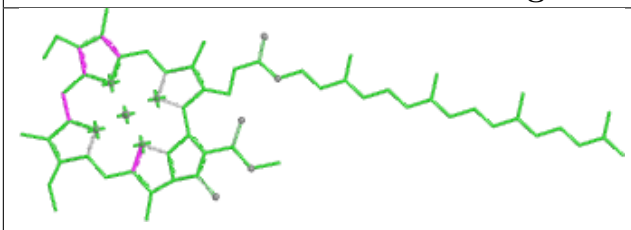


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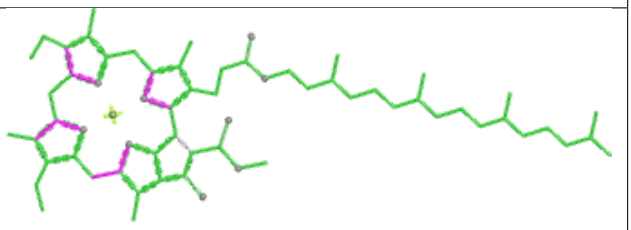


Rings

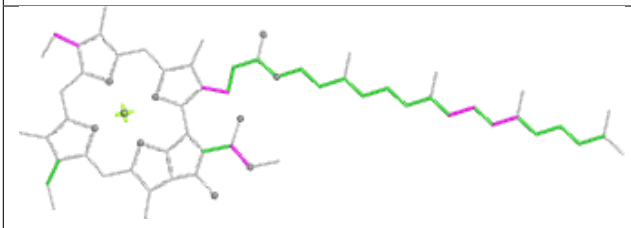
Ligand CLA u 511



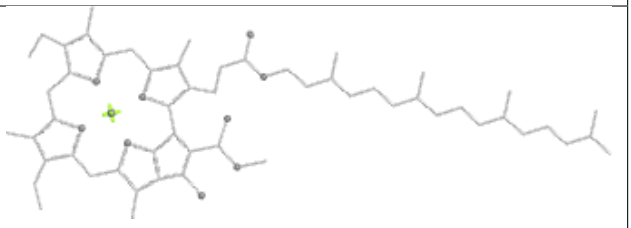
Bond lengths



Bond angles

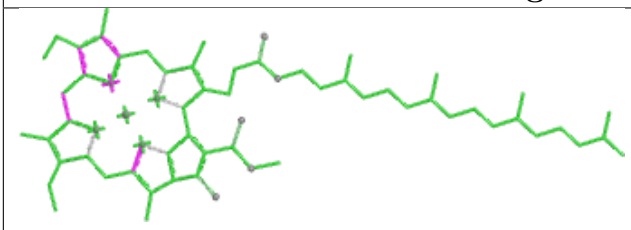


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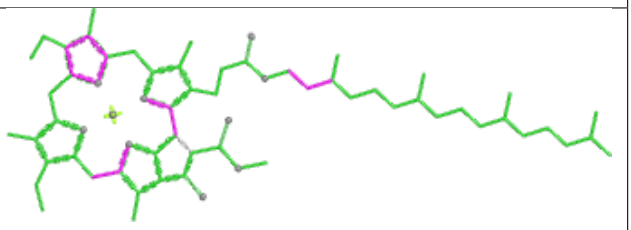


Rings

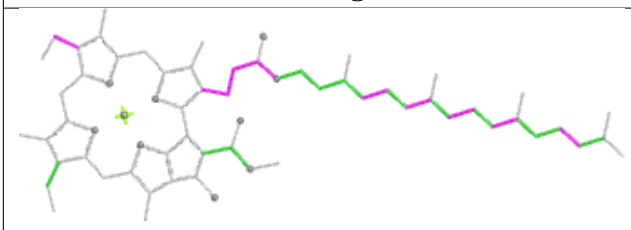
Ligand CLA Z 505



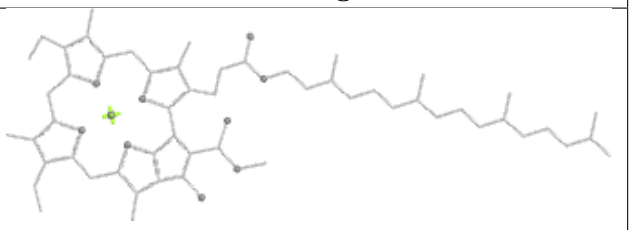
Bond lengths



Bond angles

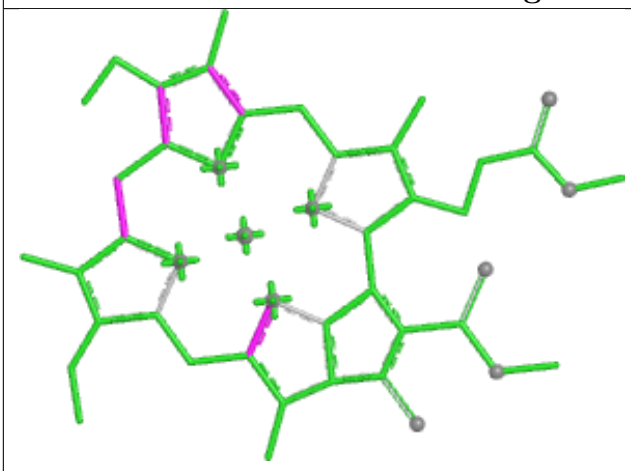


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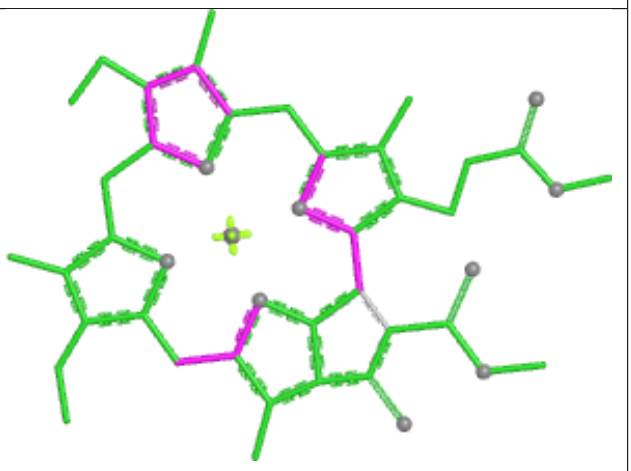


Rings

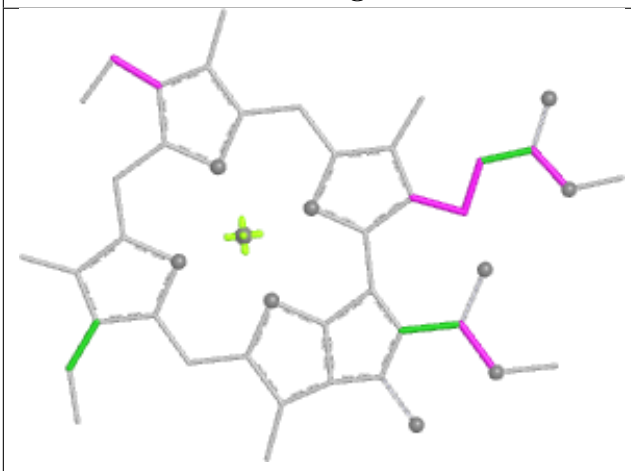
Ligand CLA X 501



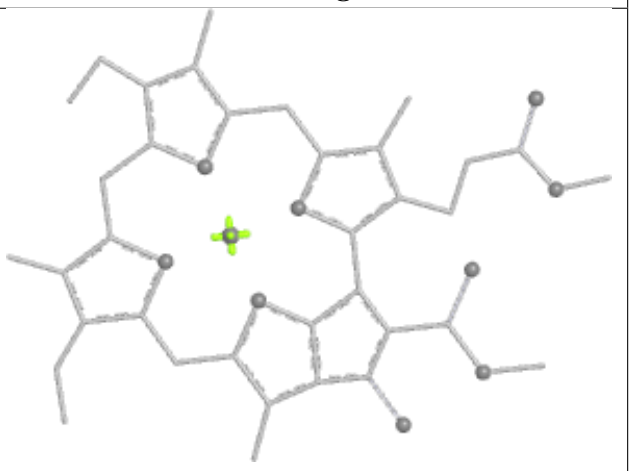
Bond lengths



Bond angles

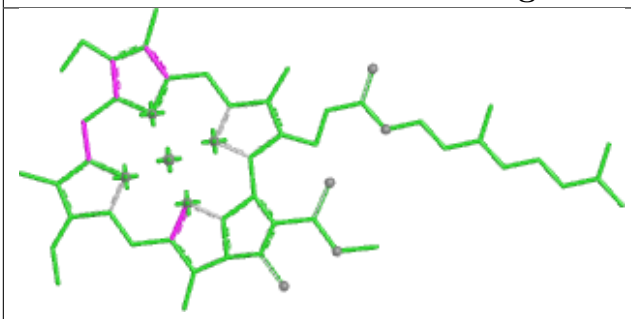


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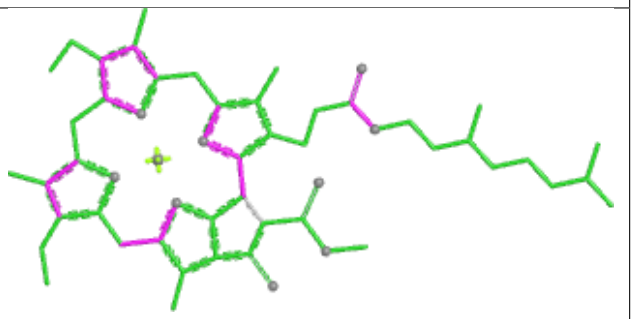


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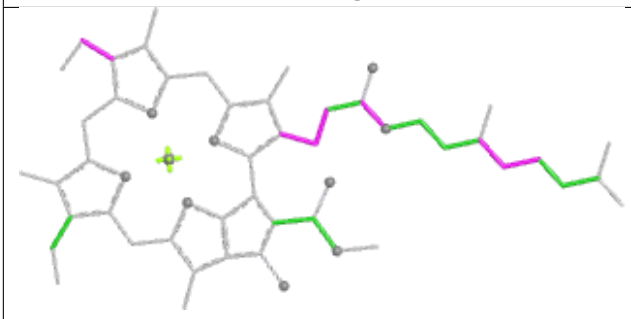
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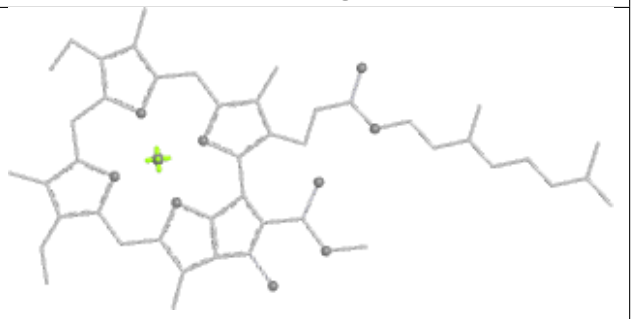
Bond lengths



Bond angles

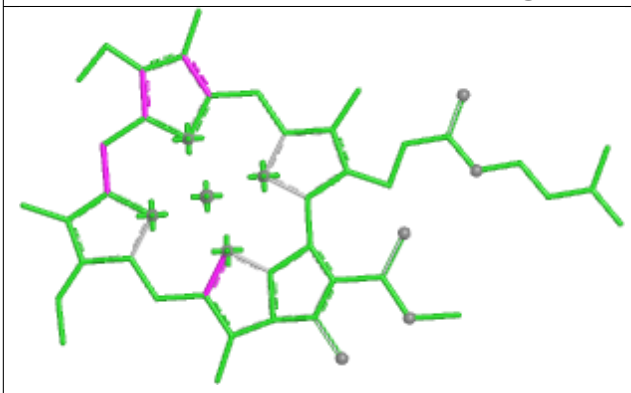


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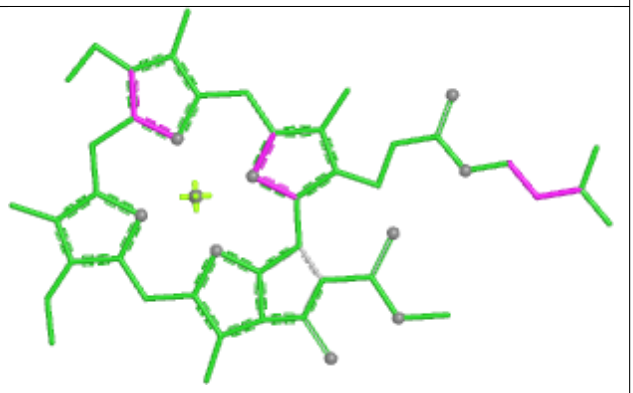


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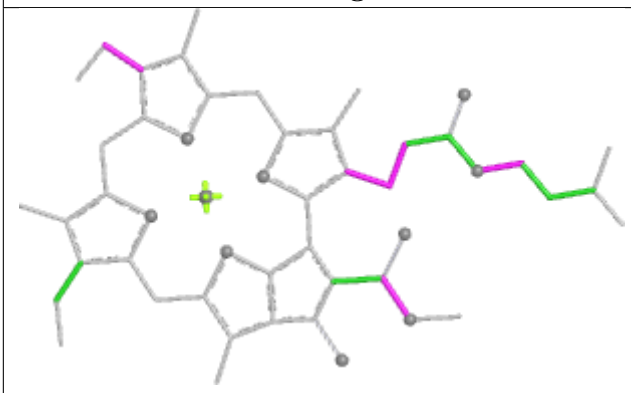
Ligand CLA a 1107



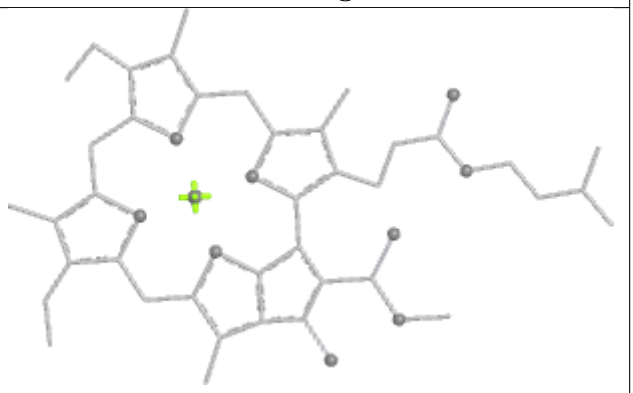
Bond lengths



Bond angles

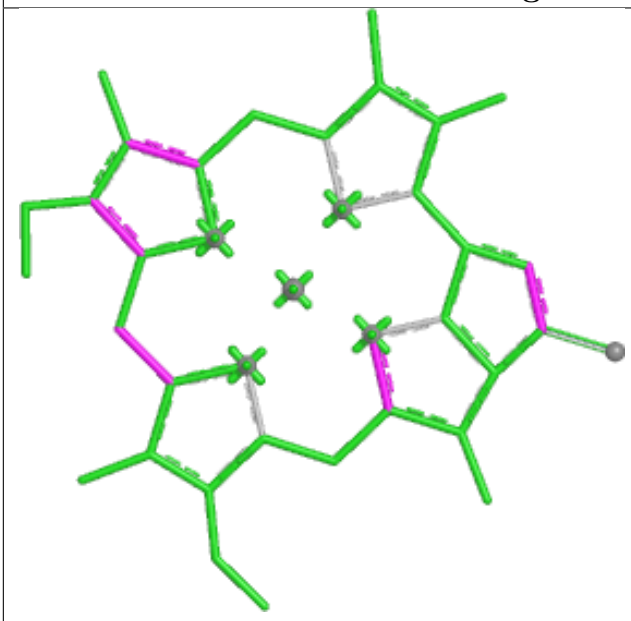


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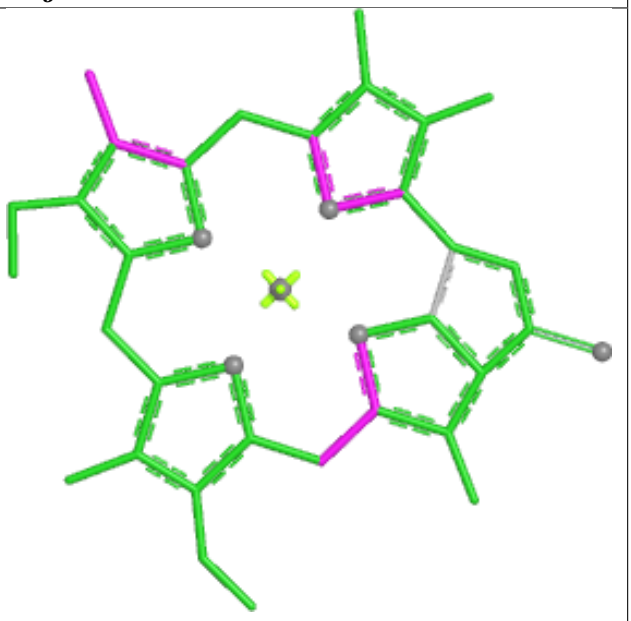


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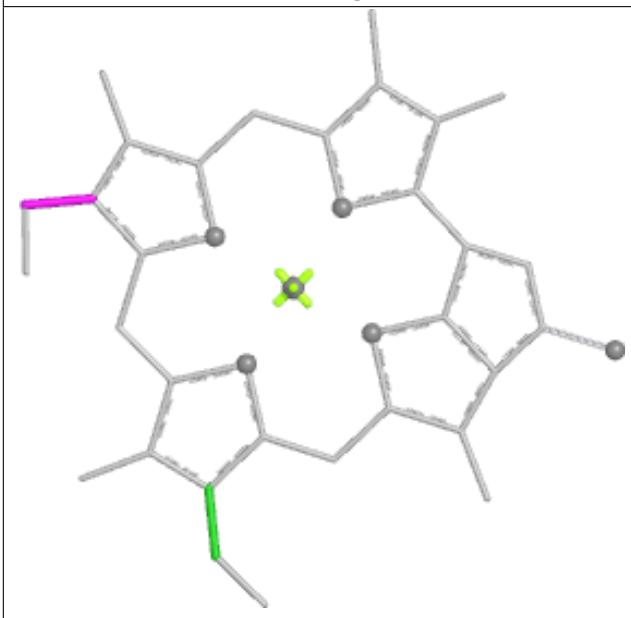
Ligand CLA j 1303



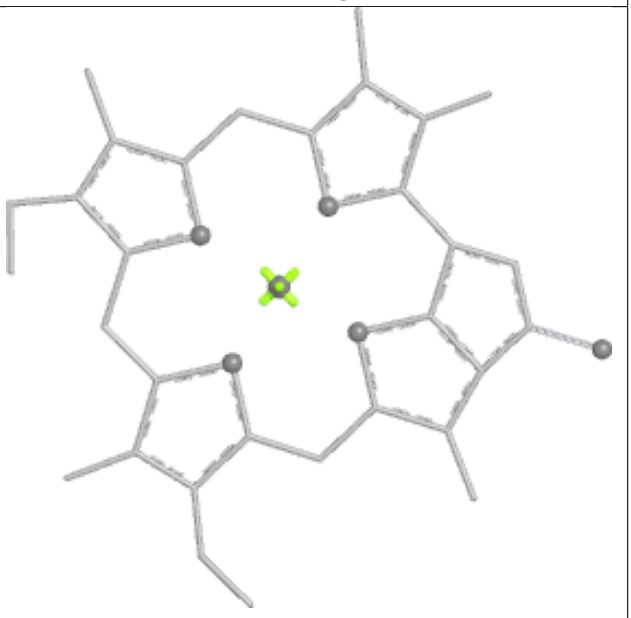
Bond lengths



Bond angles

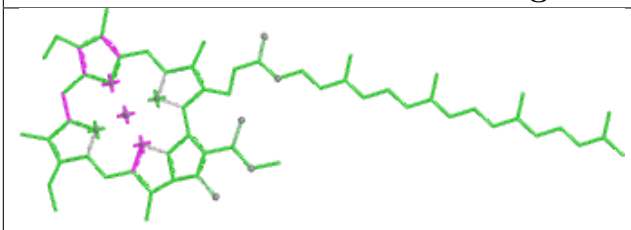


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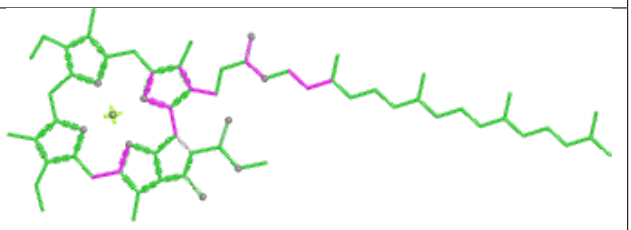


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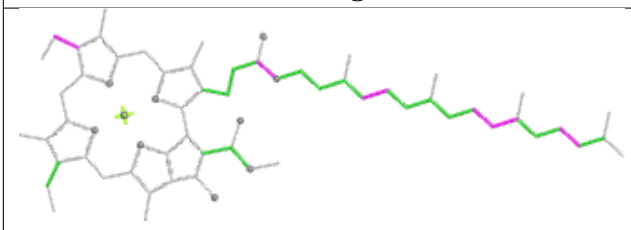
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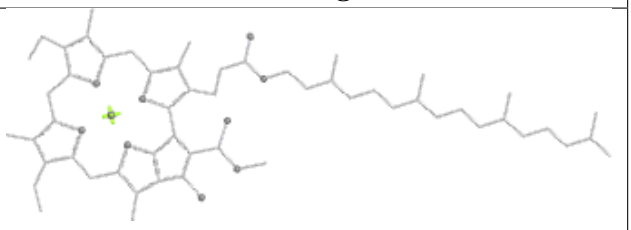
Bond lengths



Bond angles

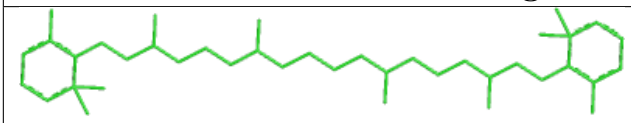


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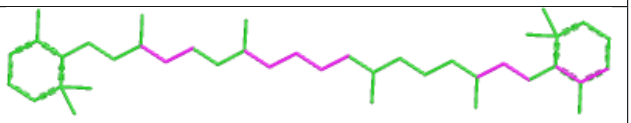


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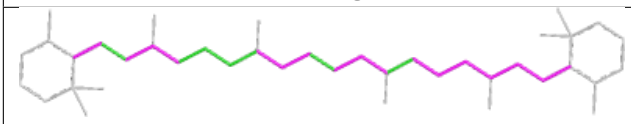
Ligand BCR X 604



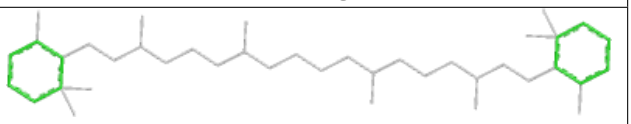
Bond lengths



Bond angles

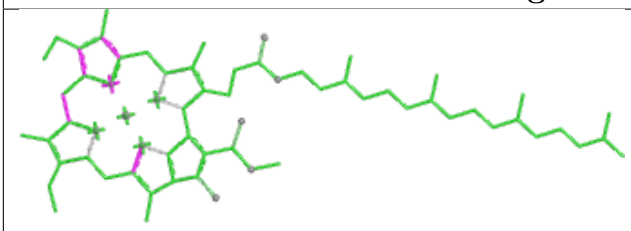


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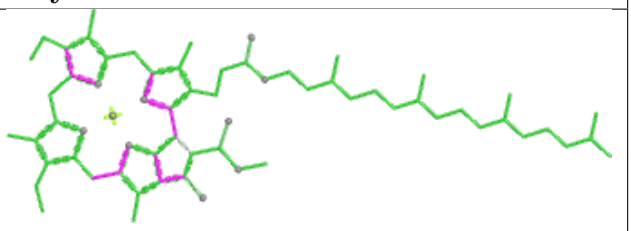


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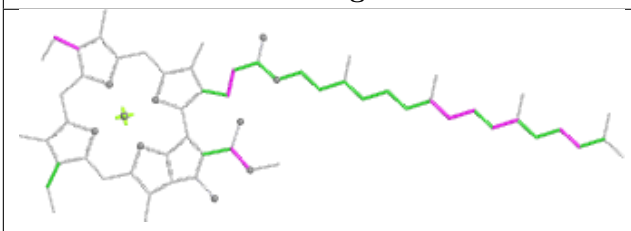
Ligand CLA y 505



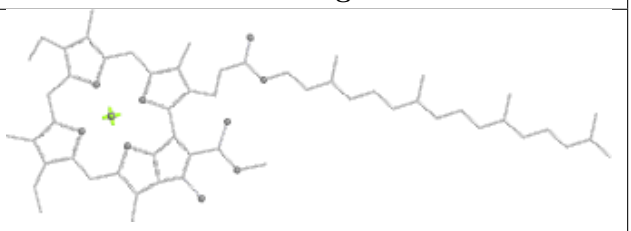
Bond lengths



Bond angles

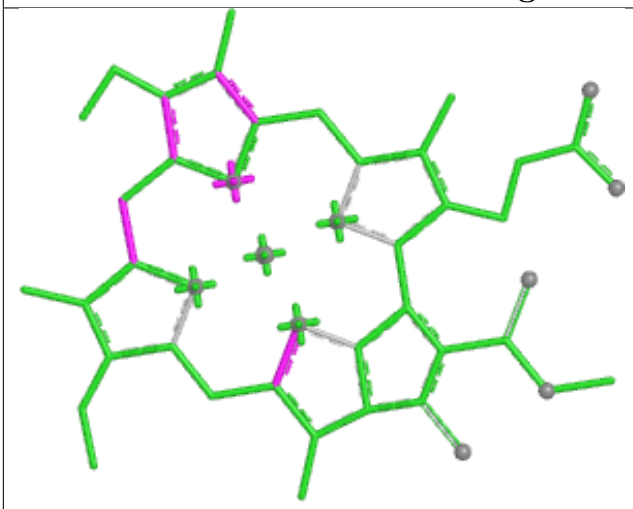


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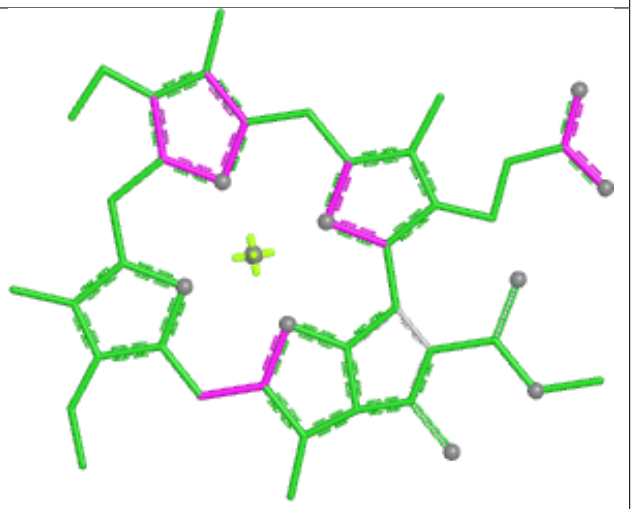


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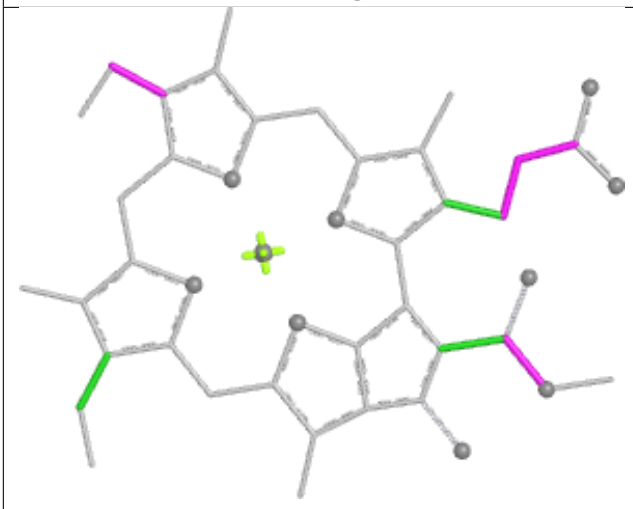
Ligand CLA S 1302



Bond lengths



Bond angles

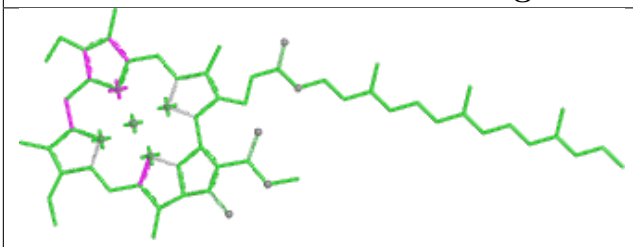


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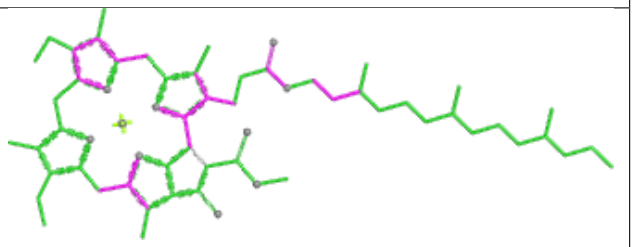


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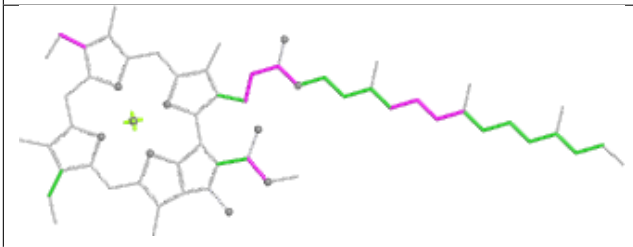
Ligand CLA G 1235



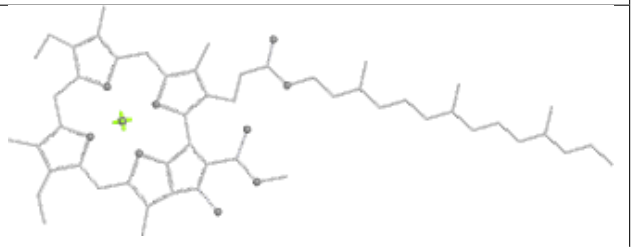
Bond lengths



Bond angles

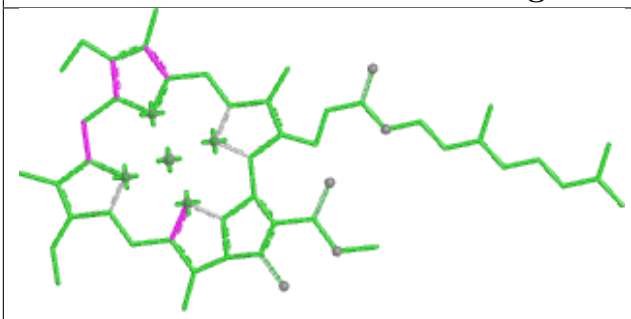


Torsions

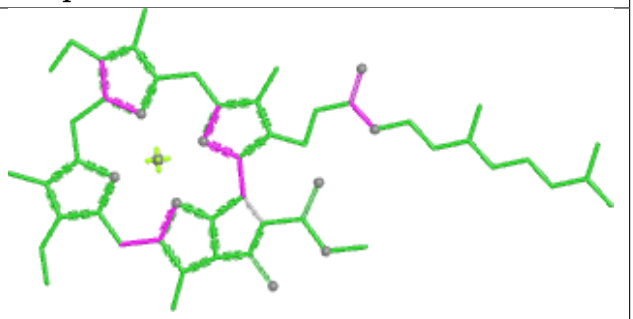


Rings

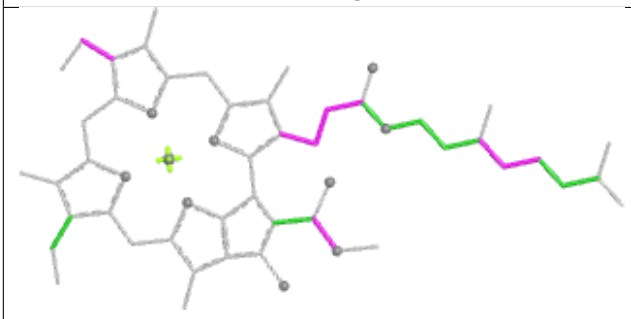
Ligand CLA q 508



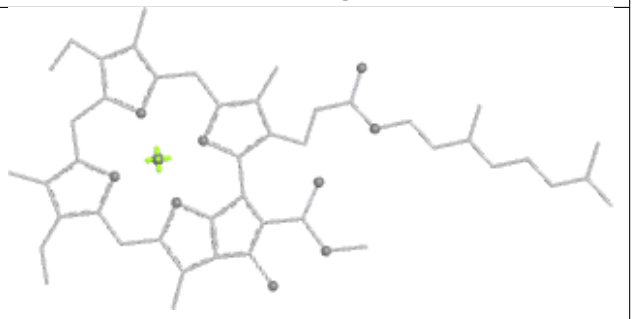
Bond lengths



Bond angles

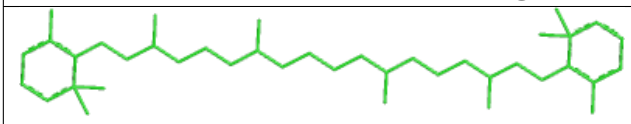


Torsions

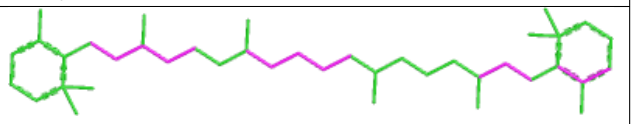


Rings

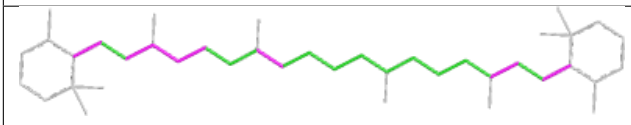
Ligand BCR Q 4016



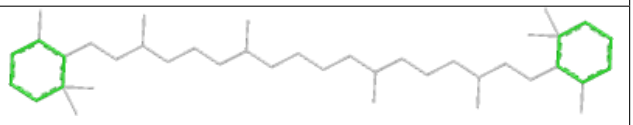
Bond lengths



Bond angles

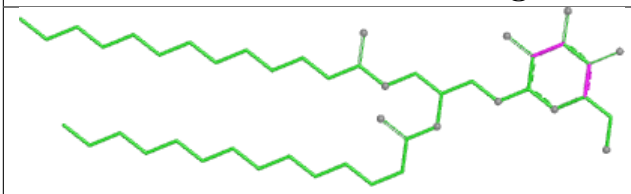


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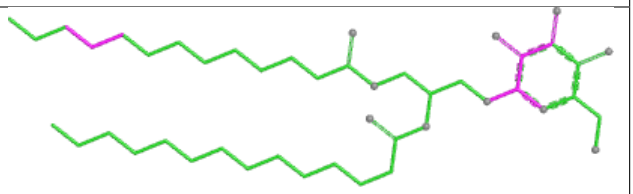


Rings

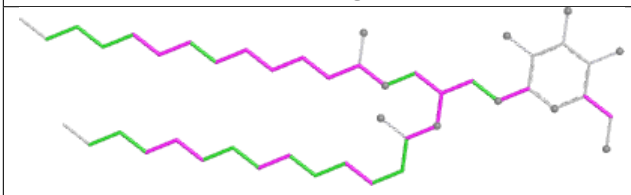
Ligand LMG A 4101



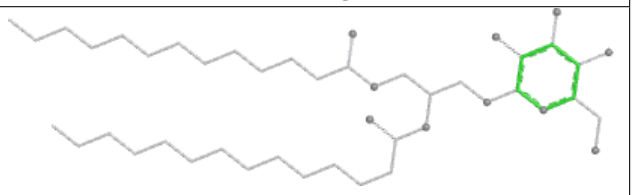
Bond lengths



Bond angles

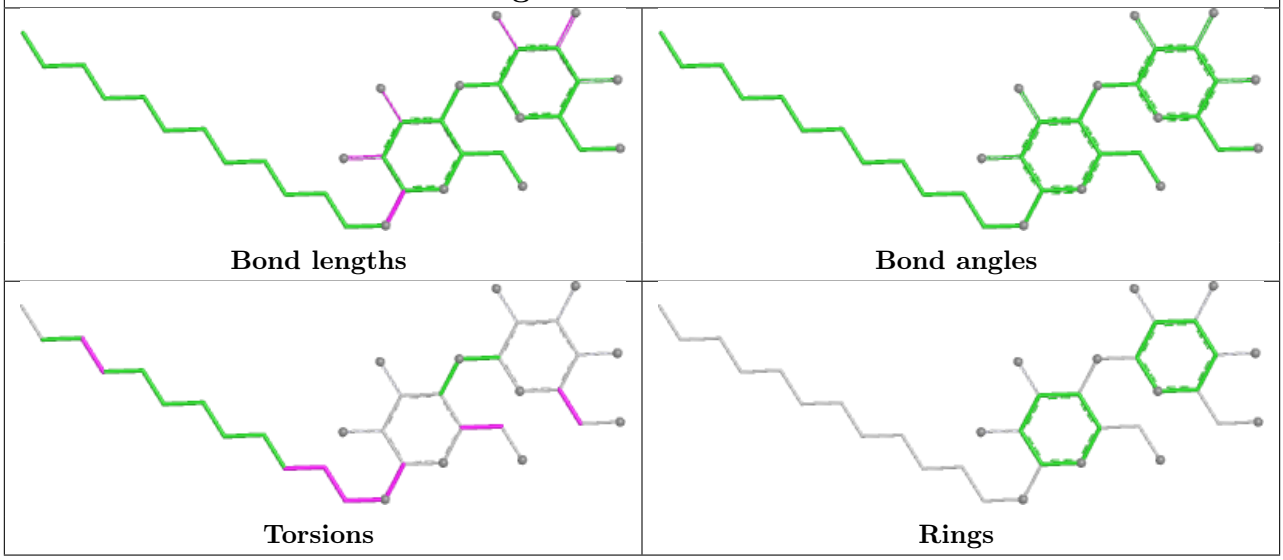


Torsions

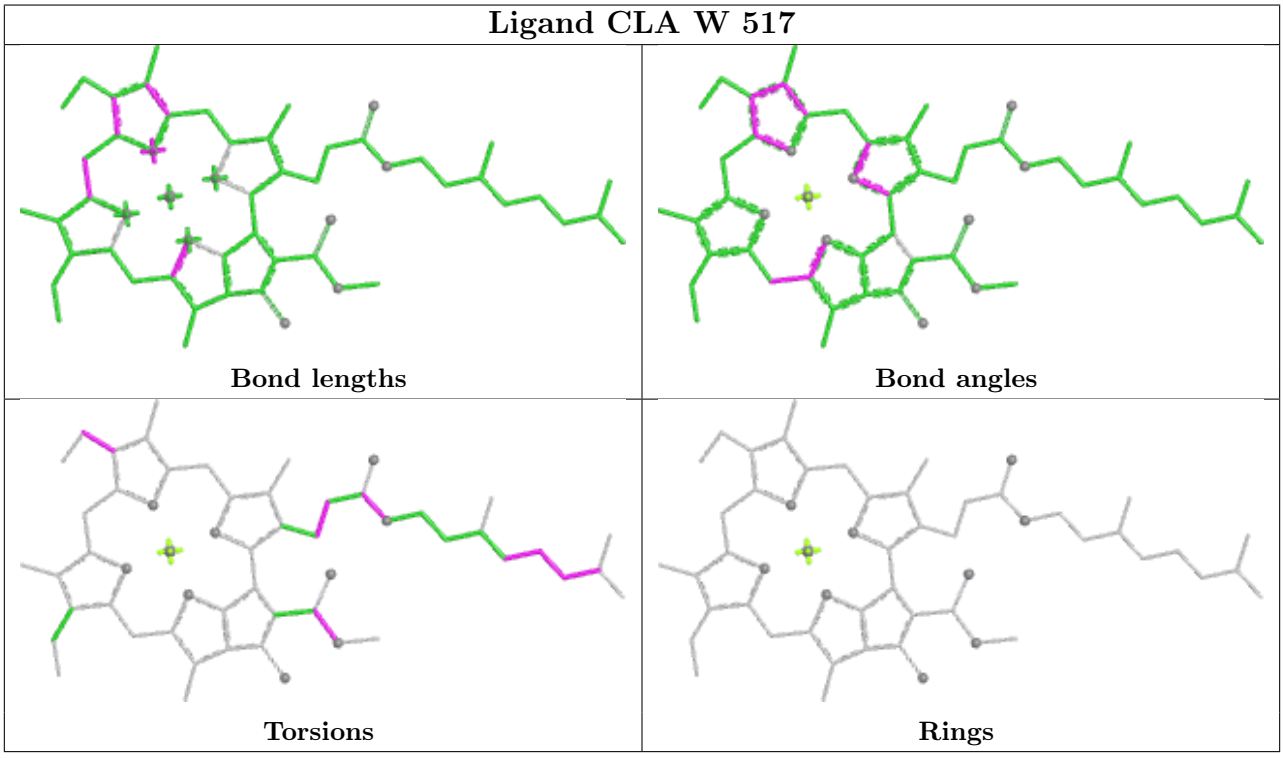


Rings

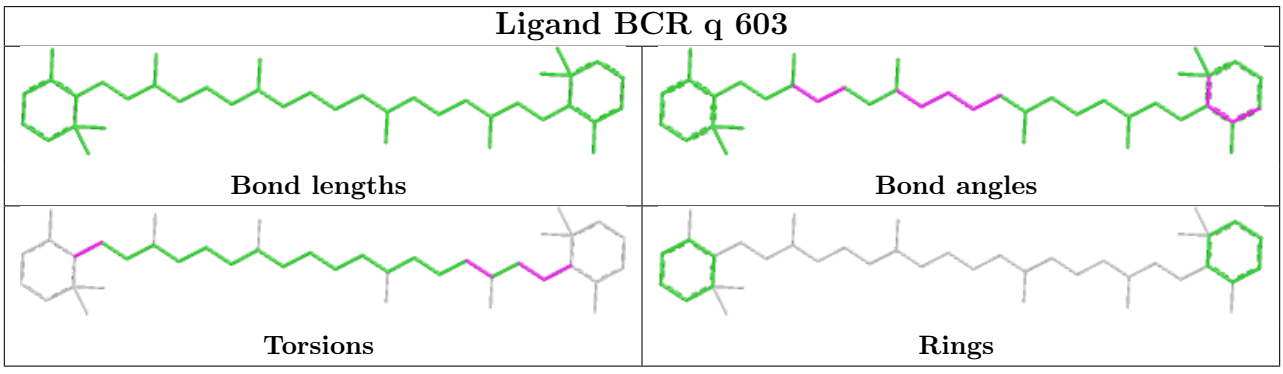
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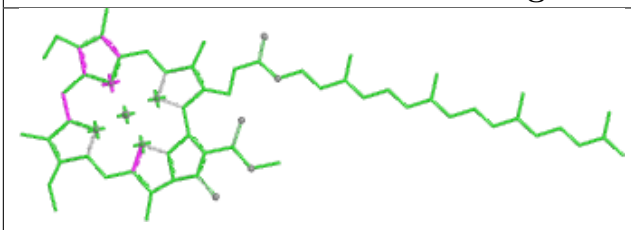
Ligand CLA W 517



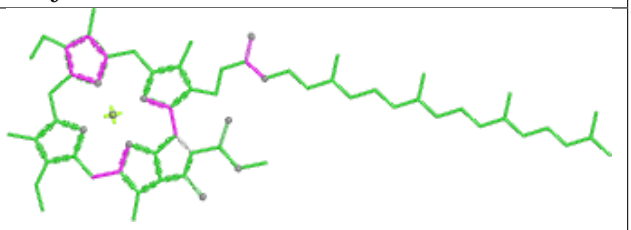
Ligand BCR q 603



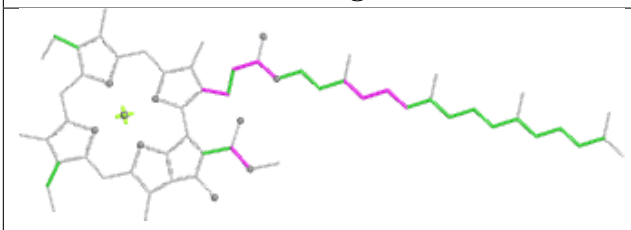
Ligand CLA y 512



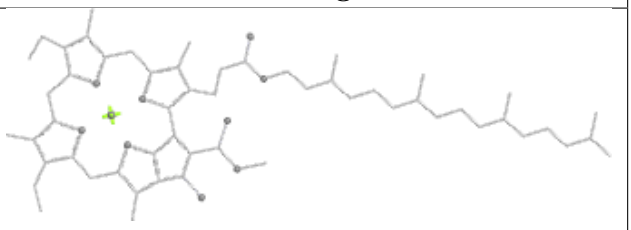
Bond lengths



Bond angles

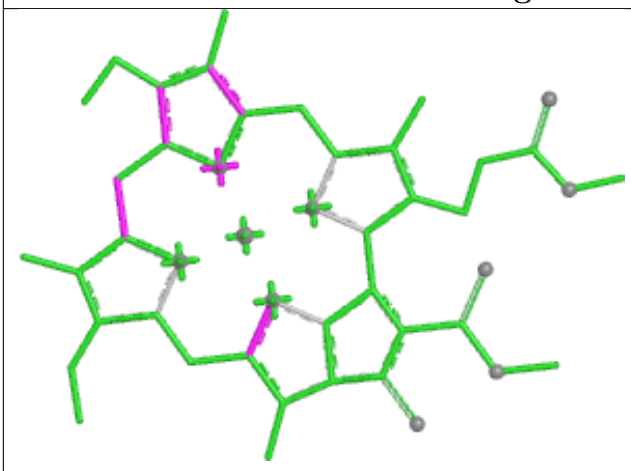


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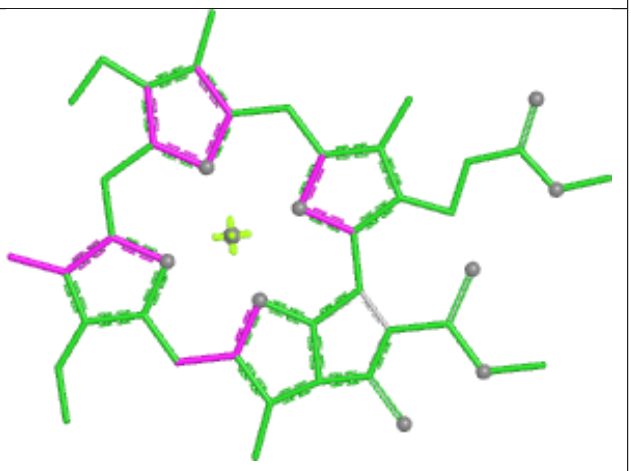


Rings

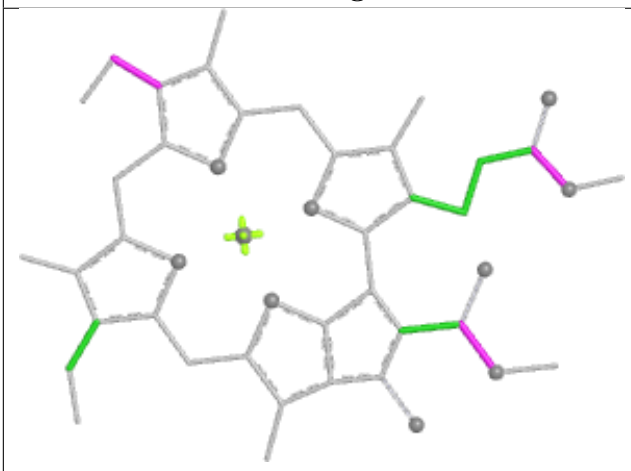
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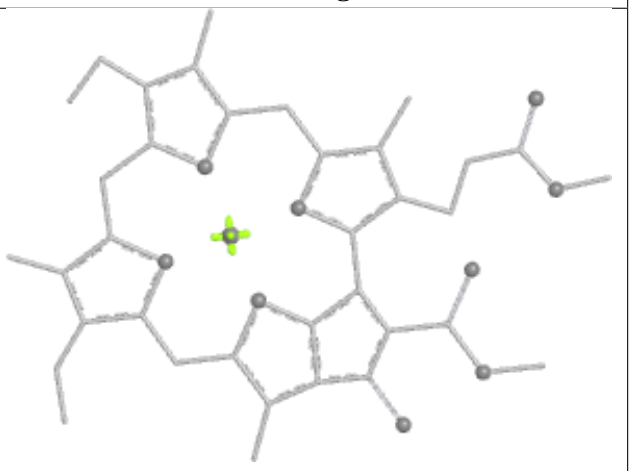
Bond lengths



Bond angles

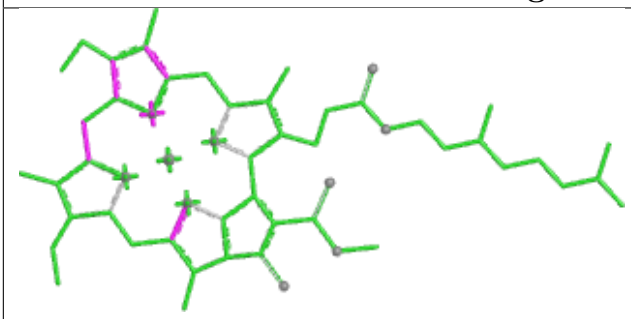


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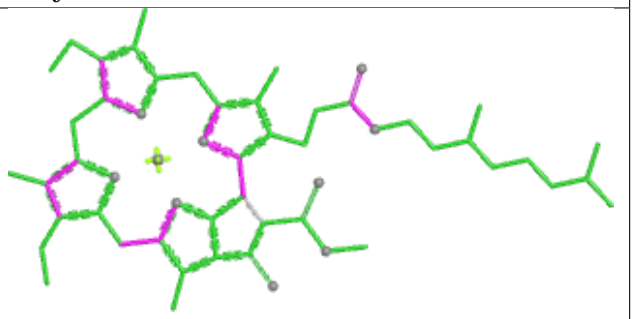


Rings

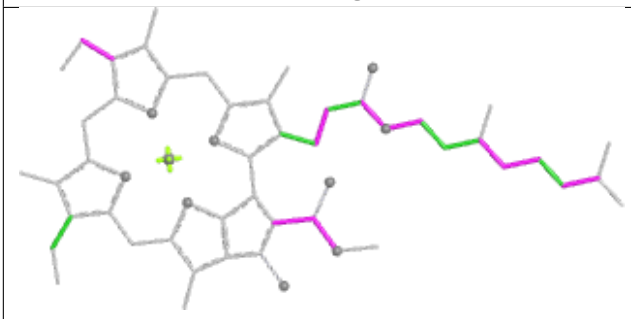
Ligand CLA y 517



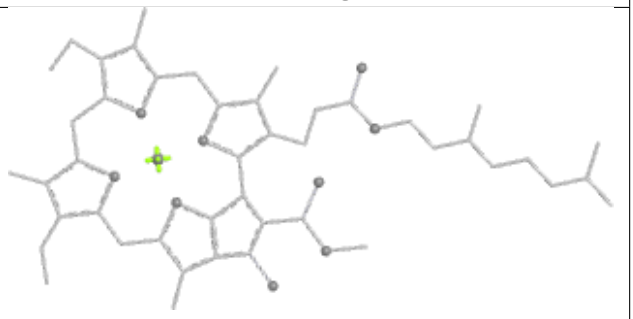
Bond lengths



Bond angles

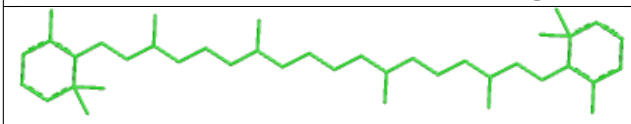


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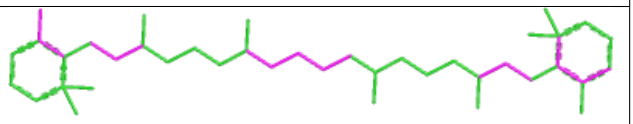


Rings

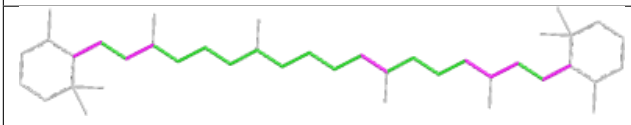
Ligand BCR s 601



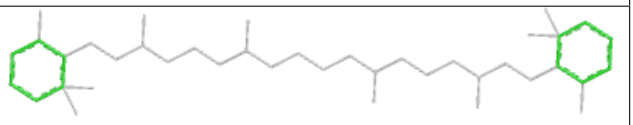
Bond lengths



Bond angles

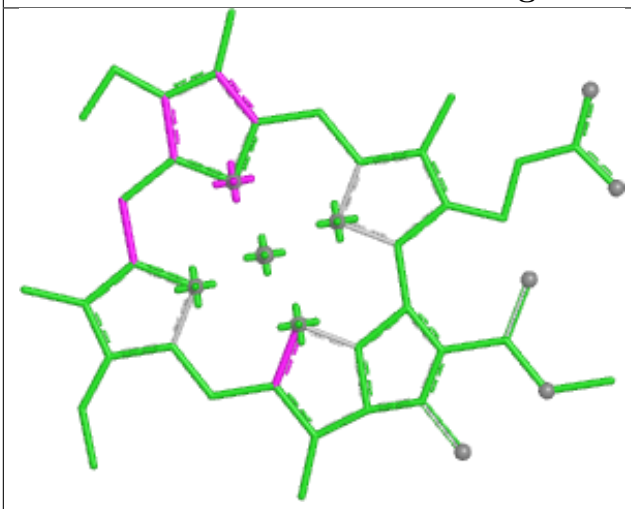


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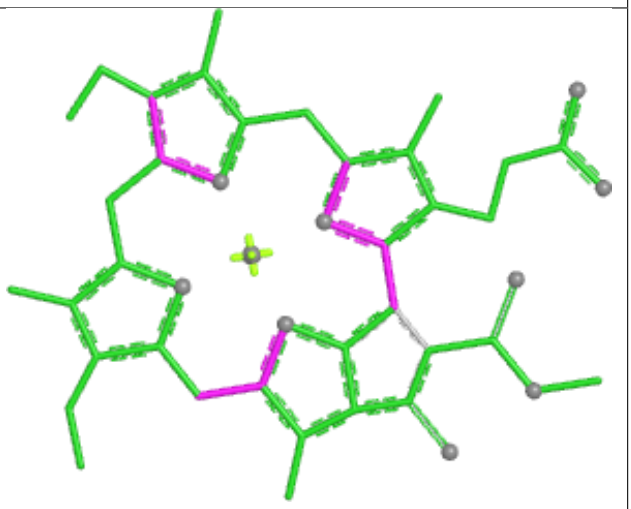


Rings

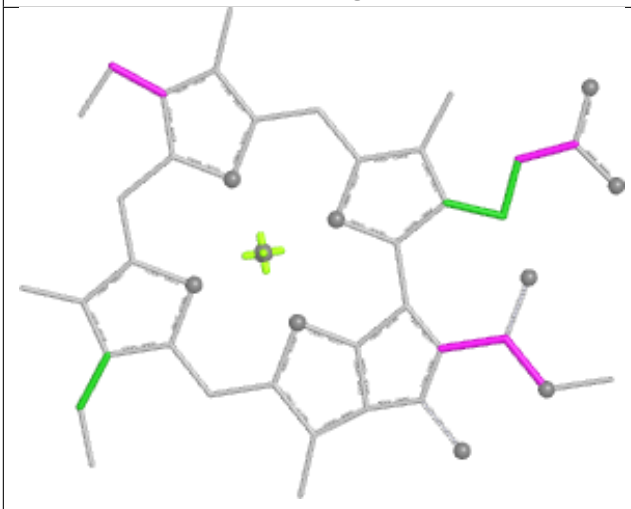
Ligand CLA b 1232



Bond lengths



Bond angles

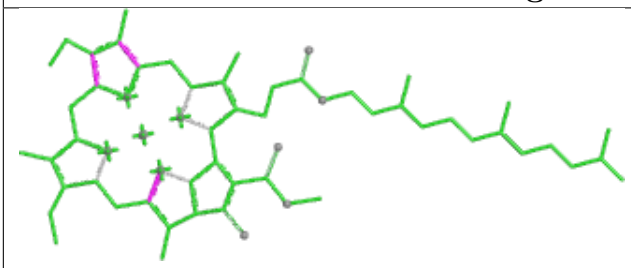


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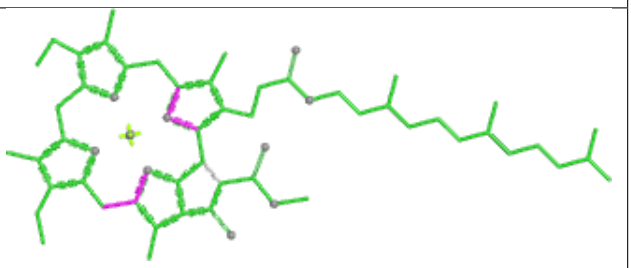


Rings

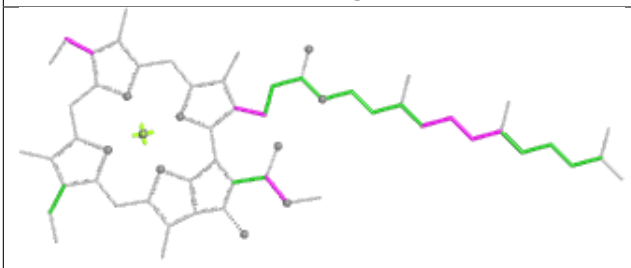
Ligand CLA Z 506



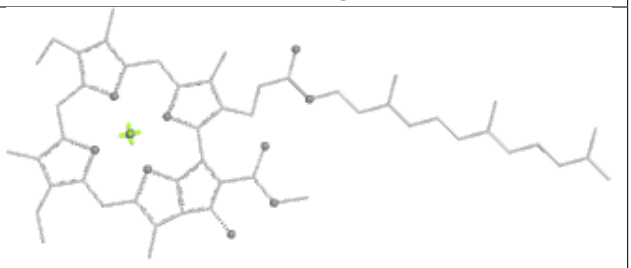
Bond lengths



Bond angles

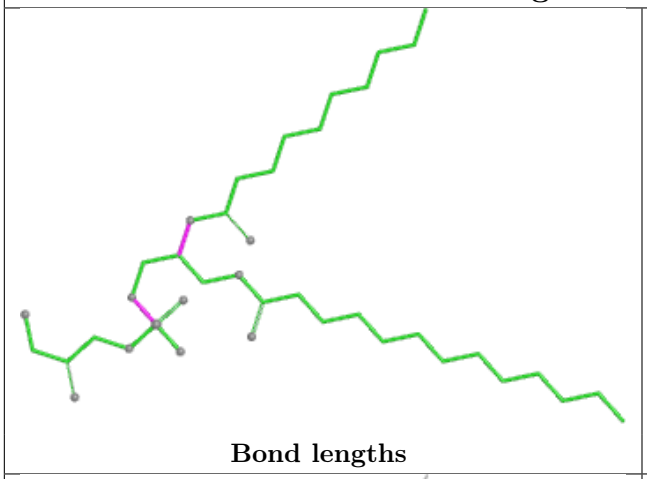


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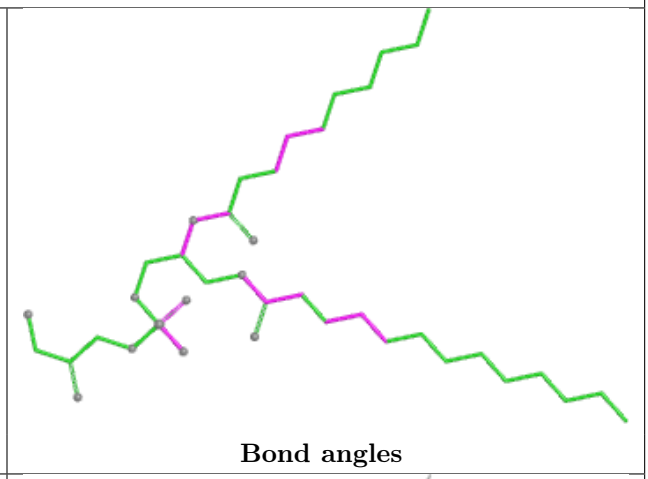


Rings

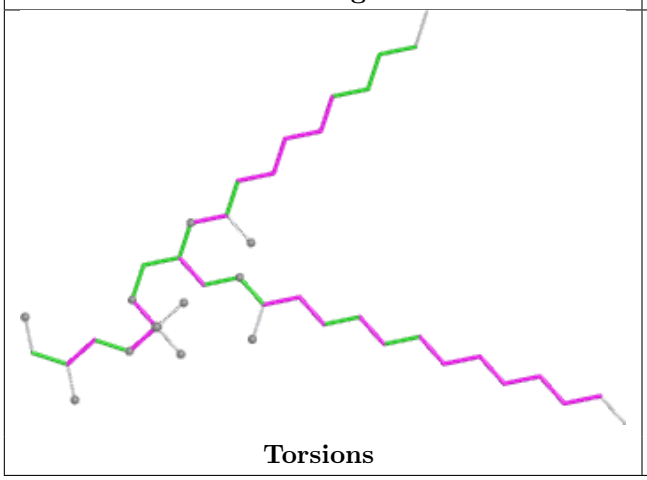
Ligand LHG i 103



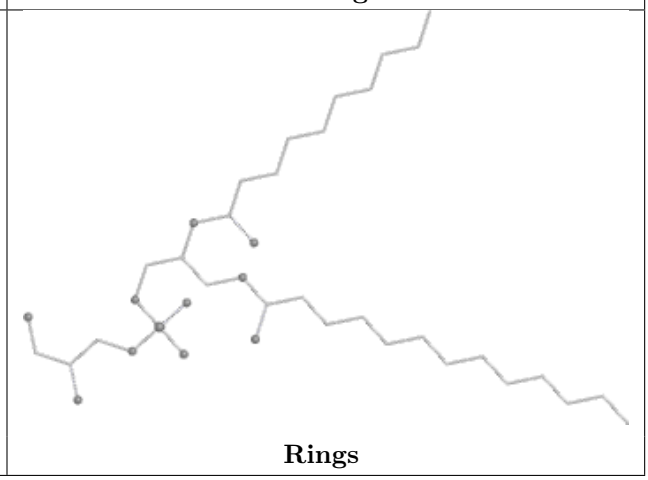
Bond lengths



Bond angles

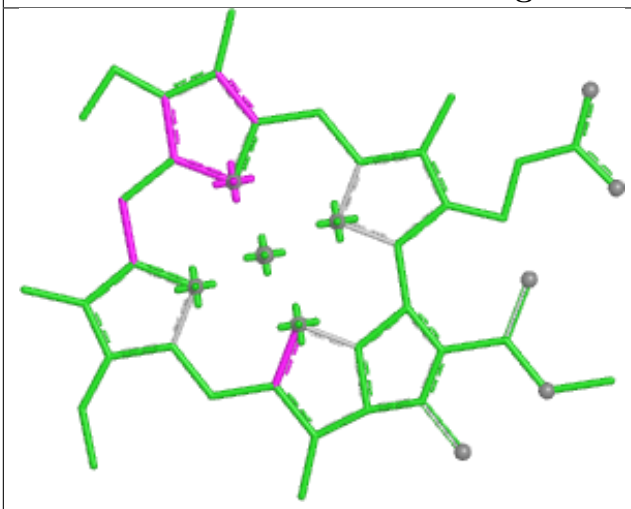


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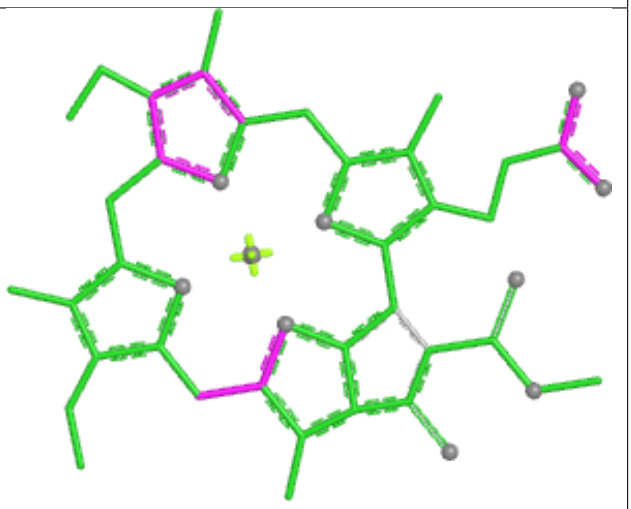


Rings

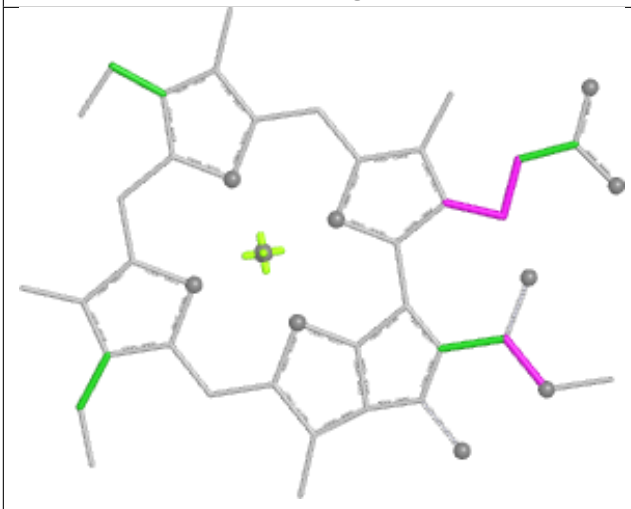
Ligand CLA B 1219



Bond lengths



Bond angles

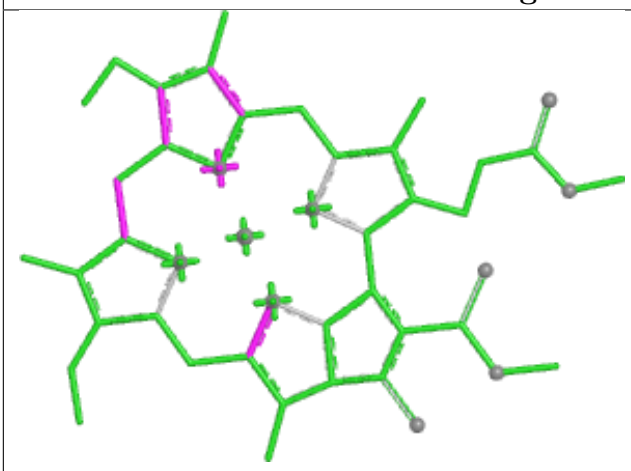


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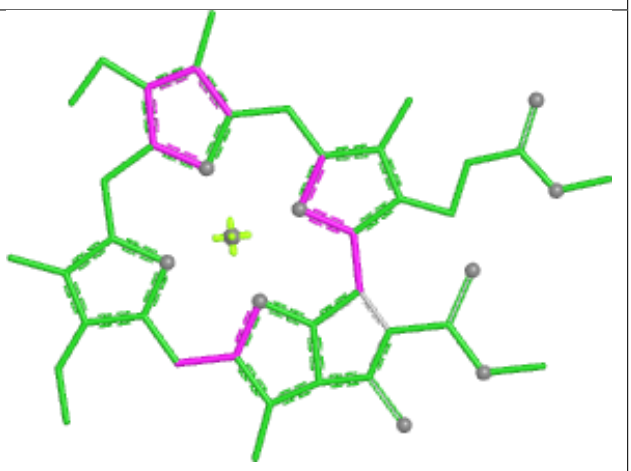


Rings

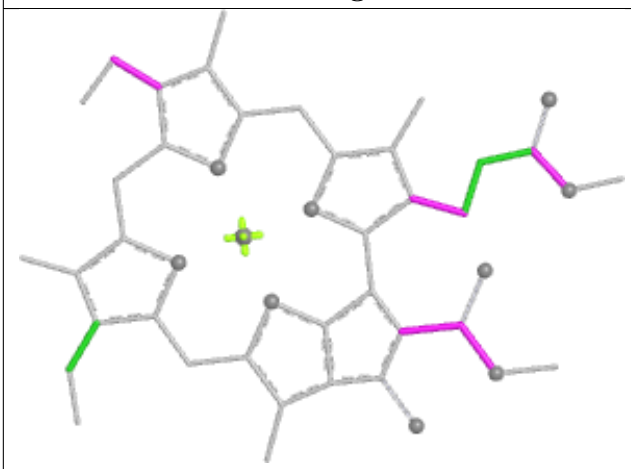
Ligand CLA a 1114



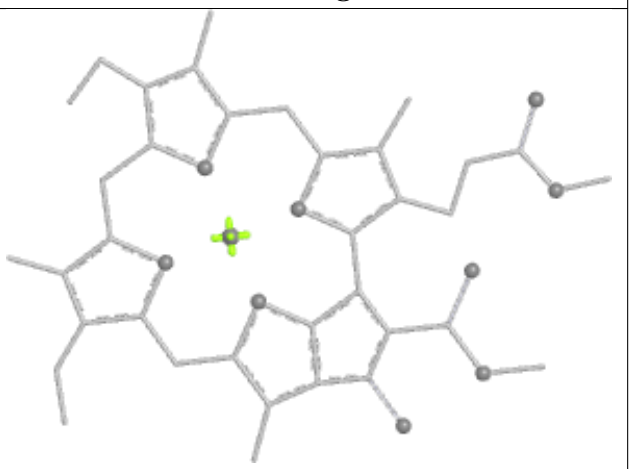
Bond lengths



Bond angles

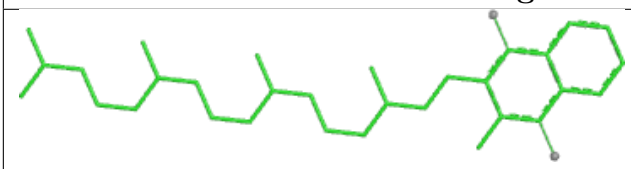


Torsions

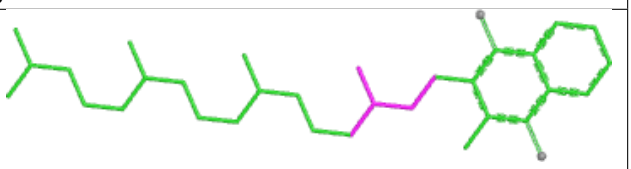


Rings

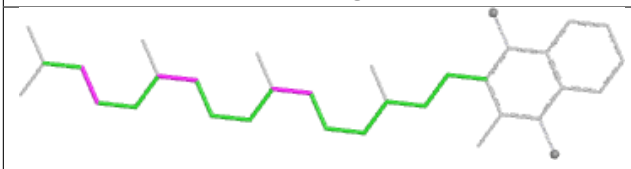
Ligand PQN a 2001



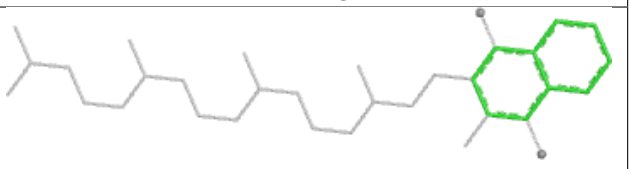
Bond lengths



Bond angles

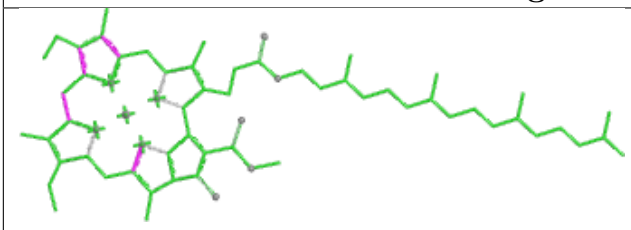


Torsions

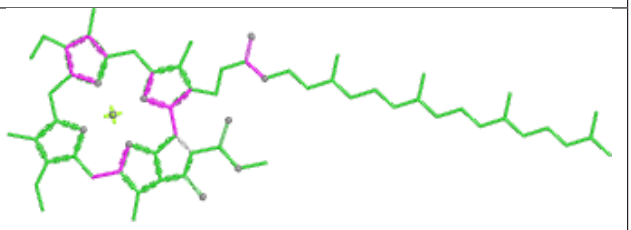


Rings

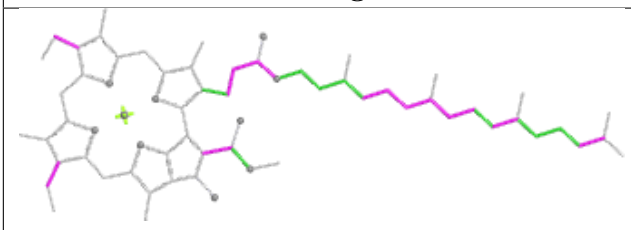
Ligand CLA v 515



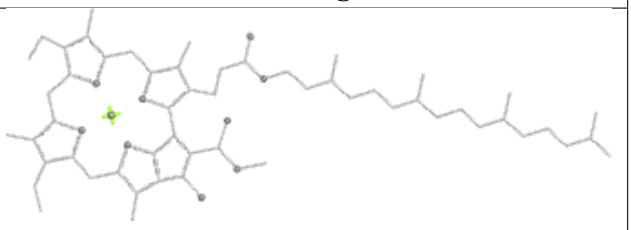
Bond lengths



Bond angles

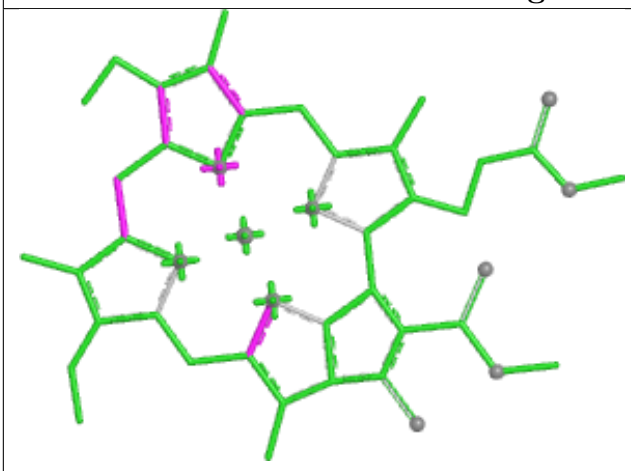


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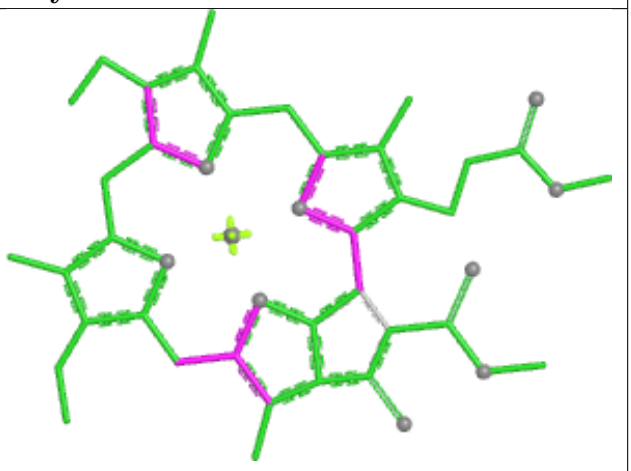


Rings

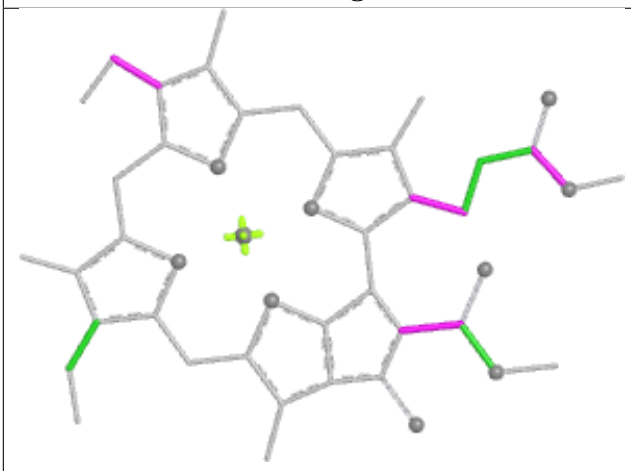
Ligand CLA y 516



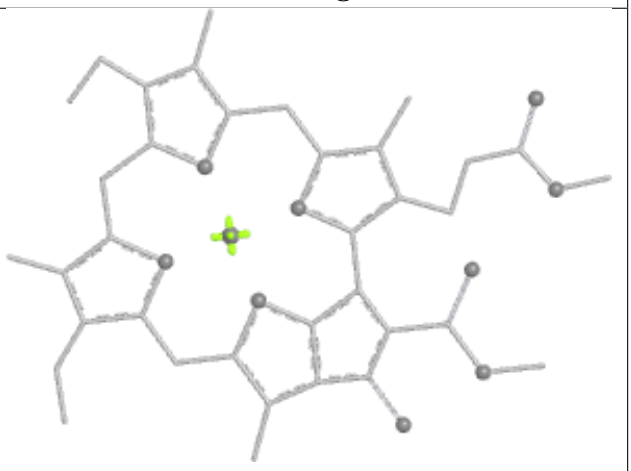
Bond lengths



Bond angles

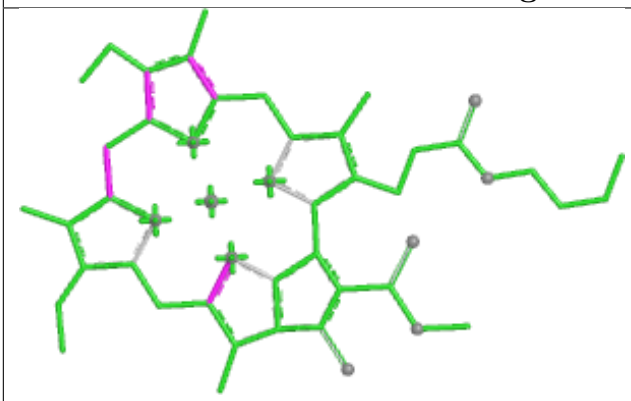


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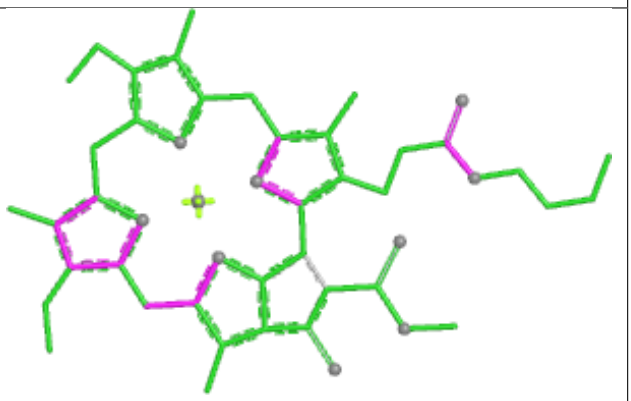


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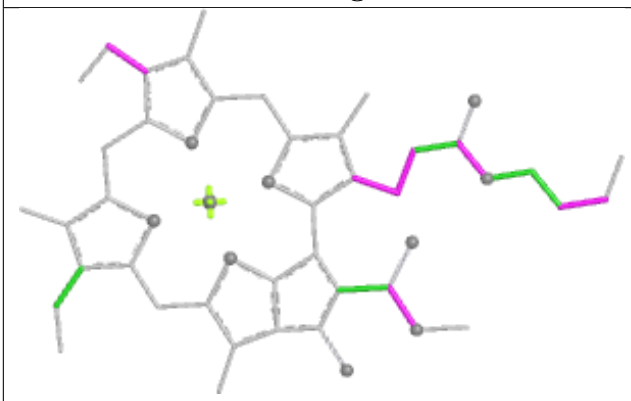
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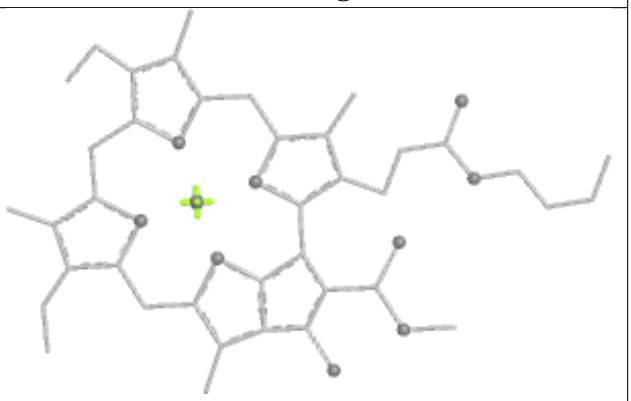
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Bond angles

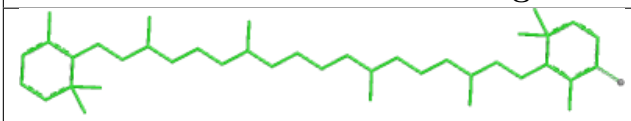


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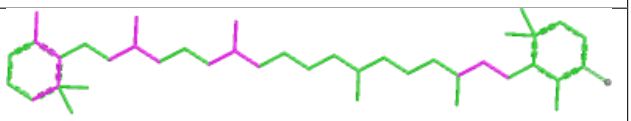


Rings

Ligand ECH G 4006



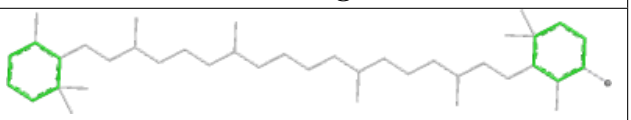
Bond lengths



Bond angles

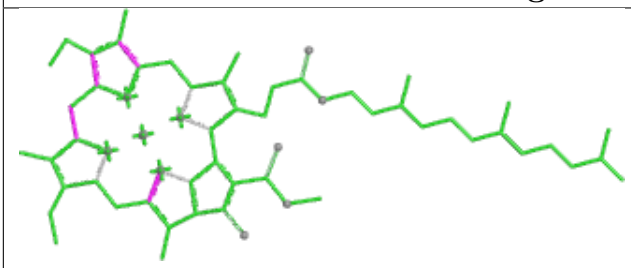


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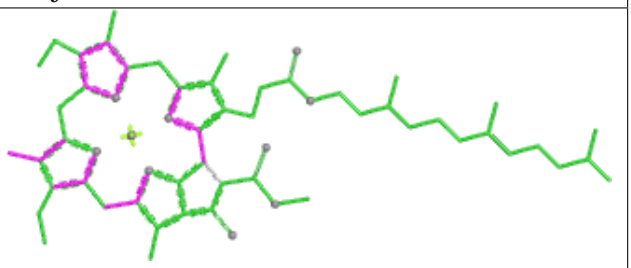


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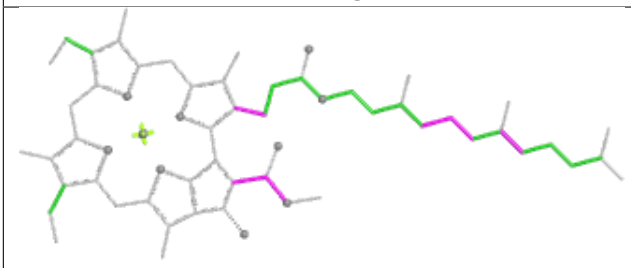
Ligand CLA y 506



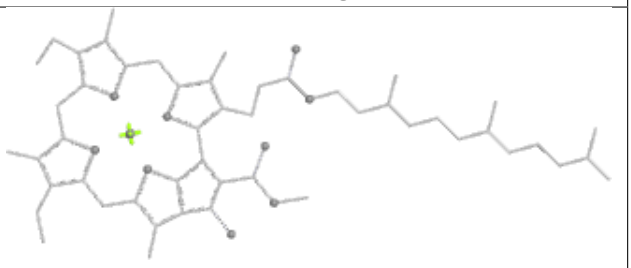
Bond lengths



Bond angles

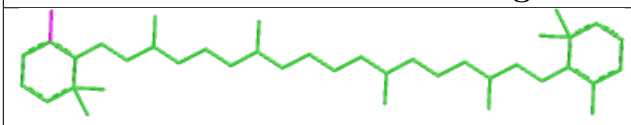


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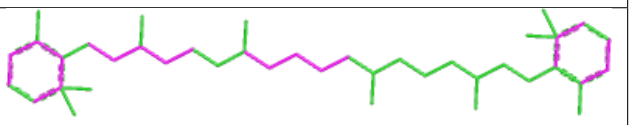


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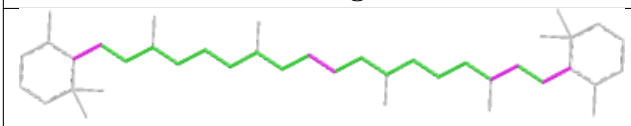
Ligand BCR A 4007



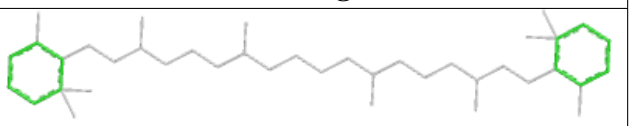
Bond lengths



Bond angles



Torsions

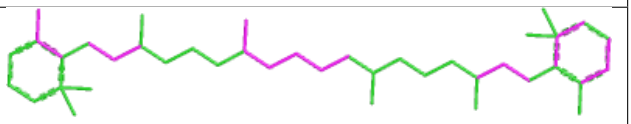


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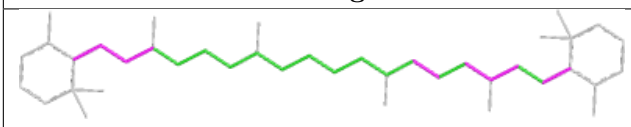
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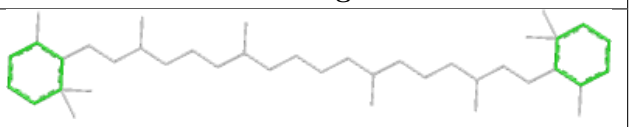
Bond lengths



Bond angles

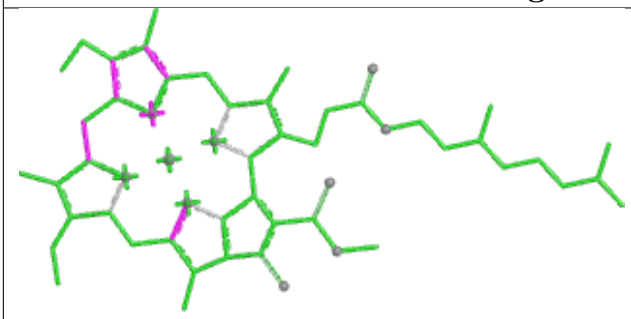


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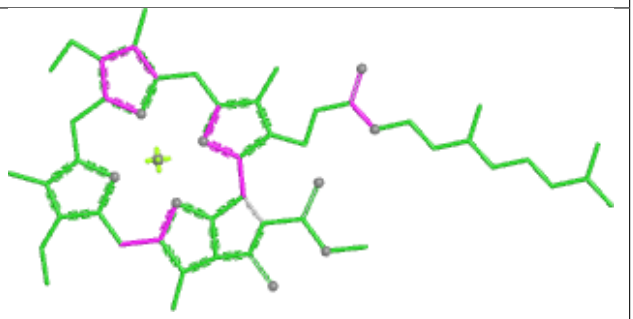


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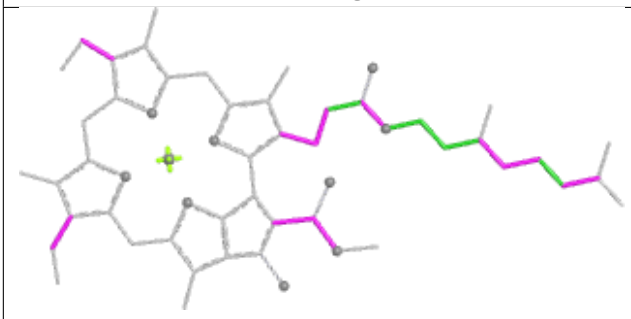
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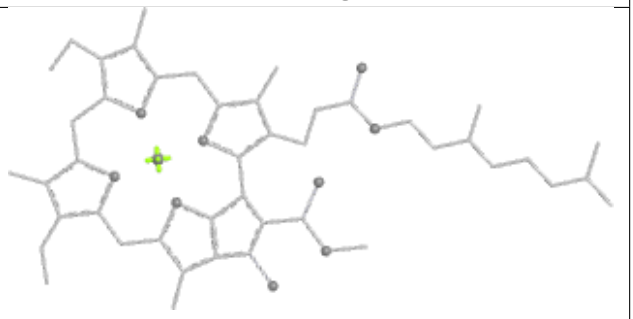
Bond lengths



Bond angles

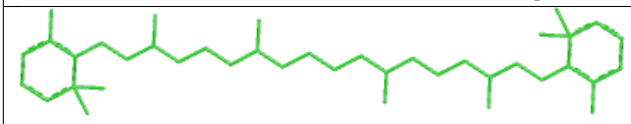


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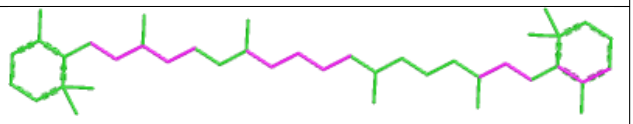


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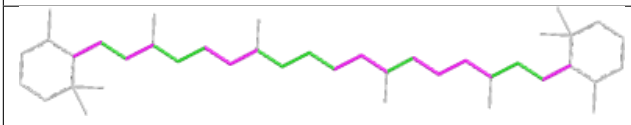
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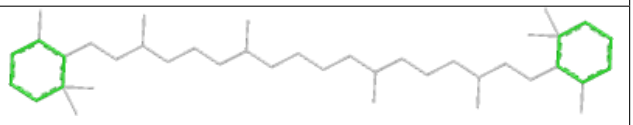
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Bond angles

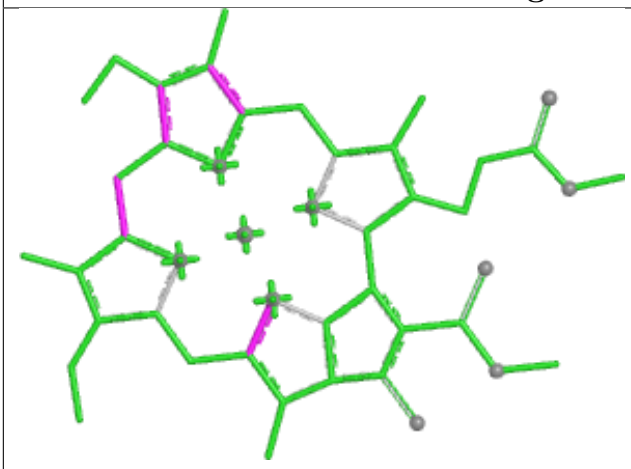


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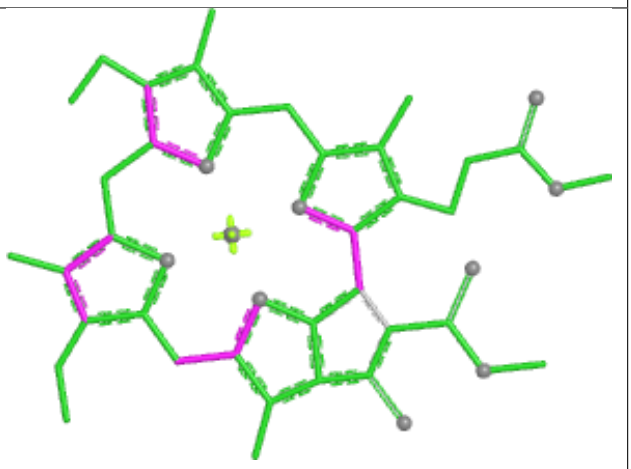


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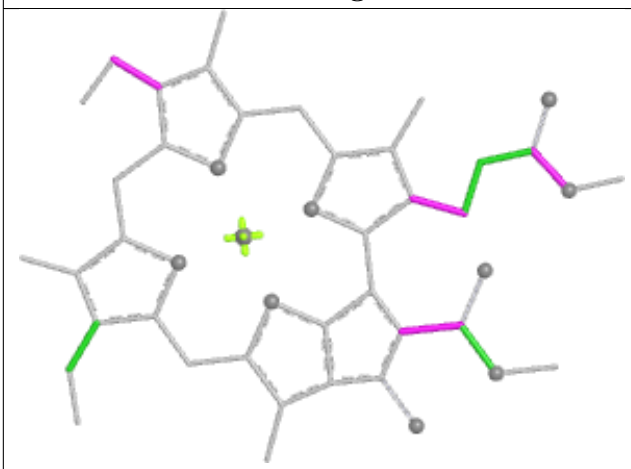
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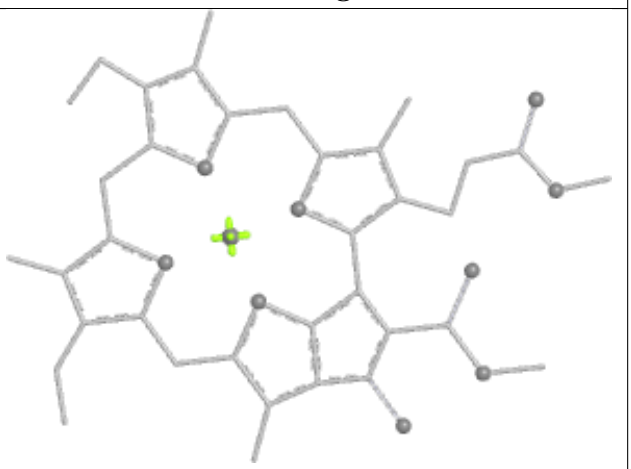
Bond lengths



Bond angles



Torsions

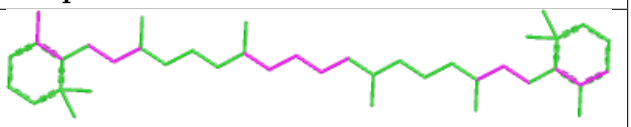


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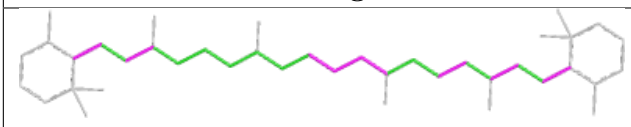
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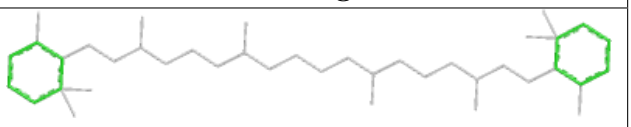
Bond lengths



Bond angles

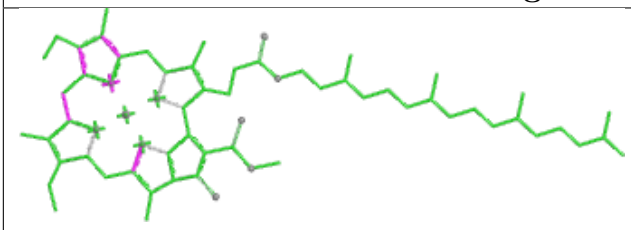


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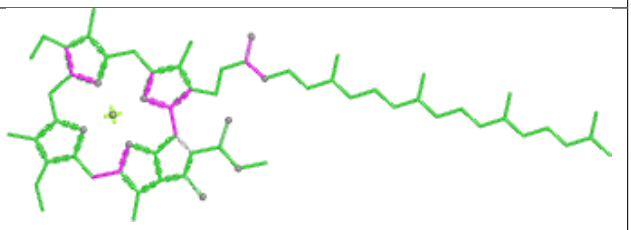


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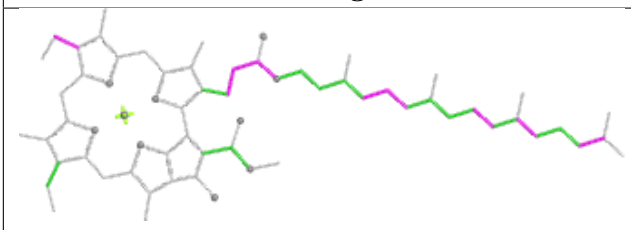
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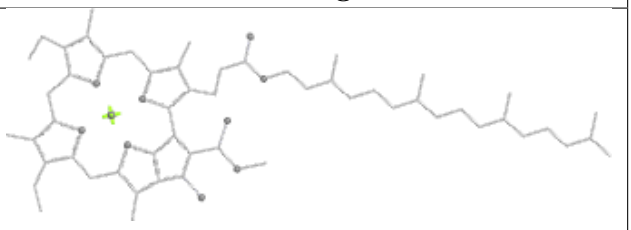
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Bond angles

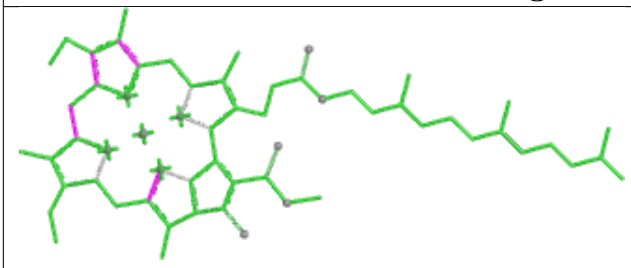


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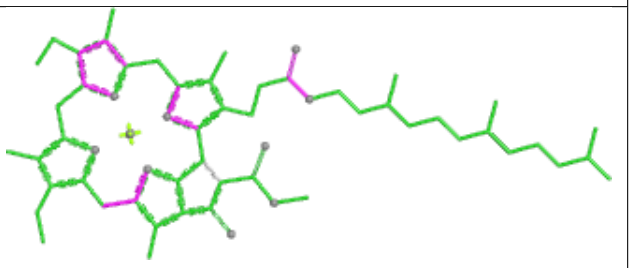


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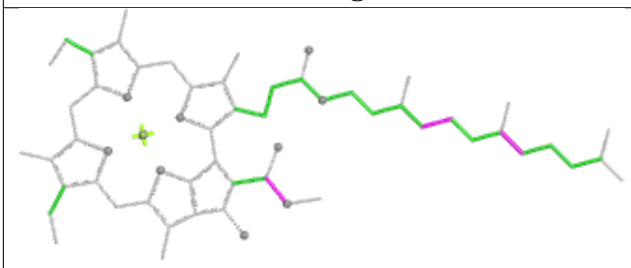
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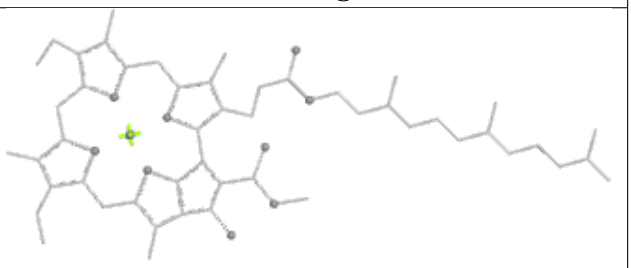
Bond lengths



Bond angles



Torsions



Rings

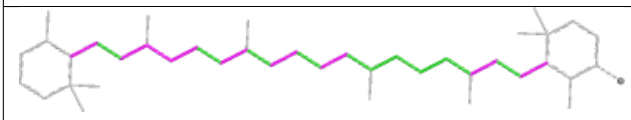
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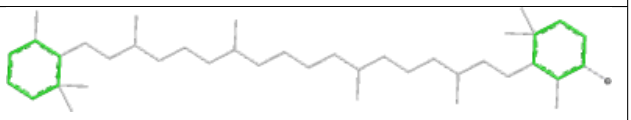
Bond lengths



Bond angles

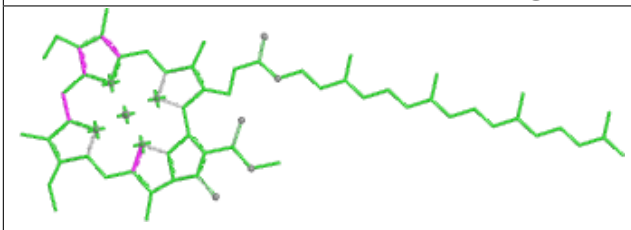


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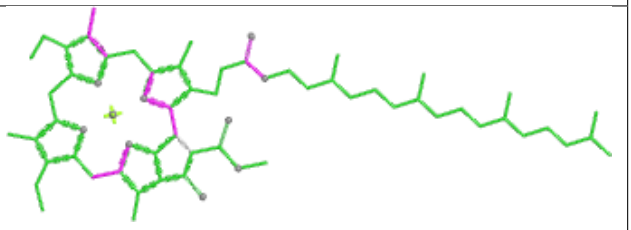


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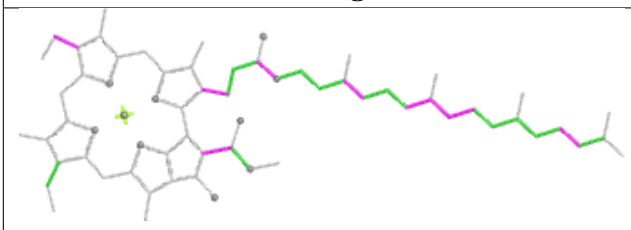
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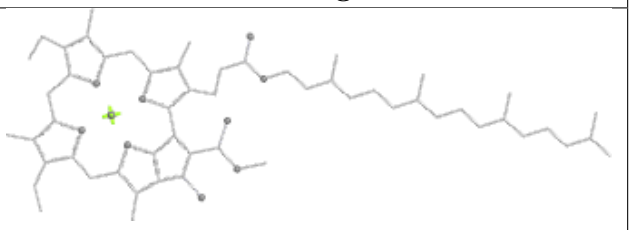
Bond lengths



Bond angles

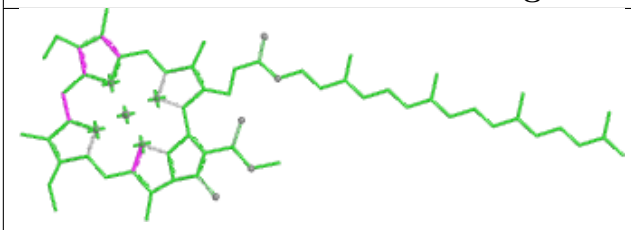


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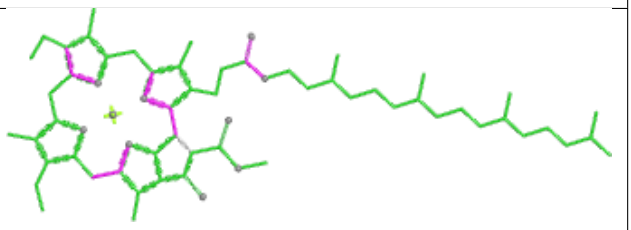


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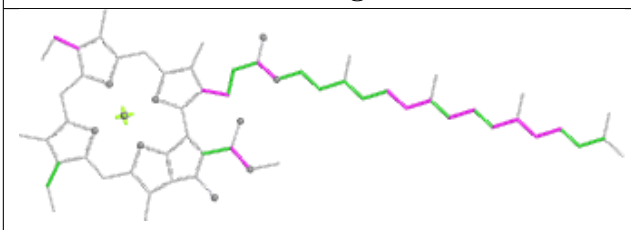
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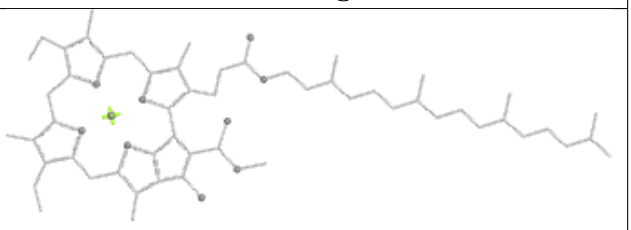
Bond lengths



Bond angles

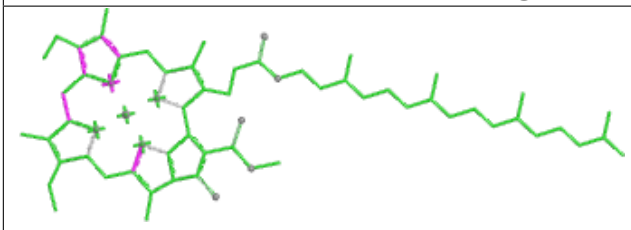


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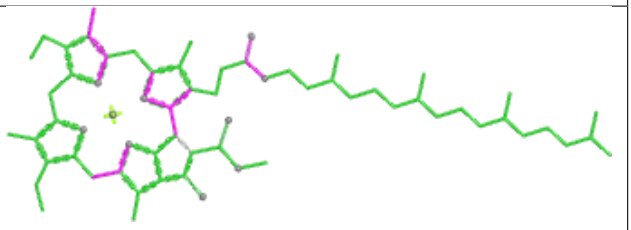


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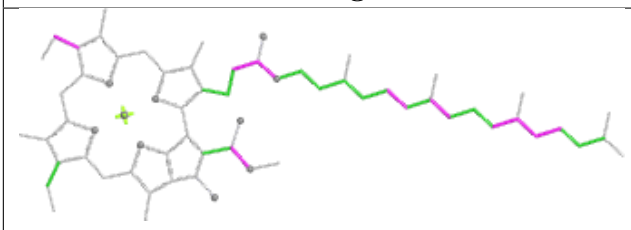
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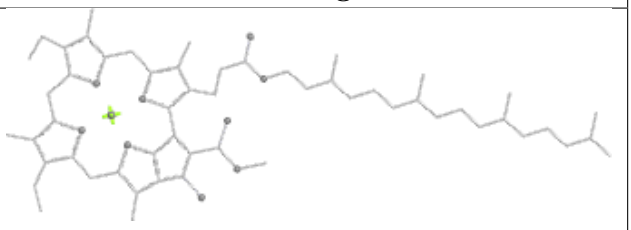
Bond lengths



Bond angles

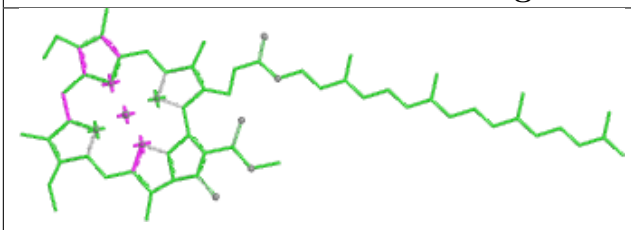


Torsions

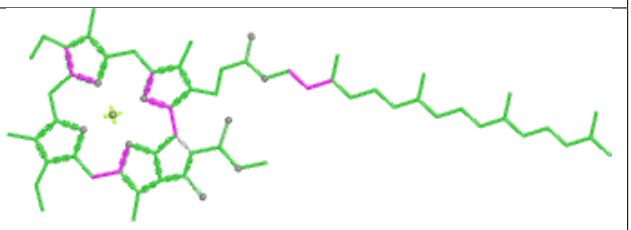


Rings

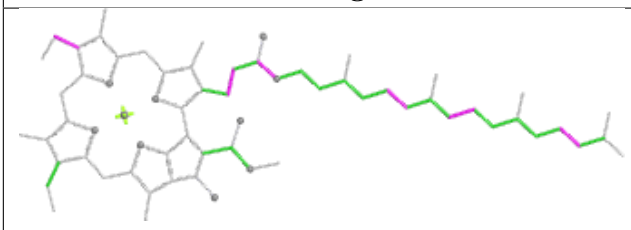
Ligand CLA H 1127



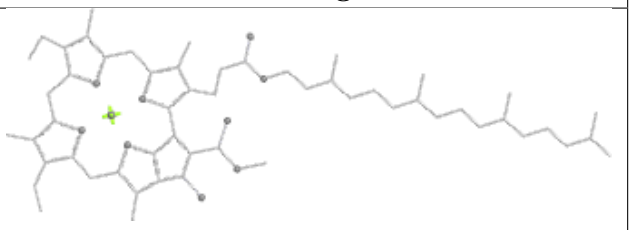
Bond lengths



Bond angles

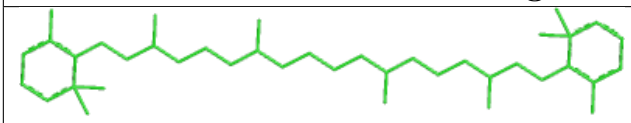


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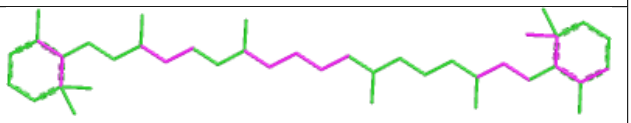


Rings

Ligand BCR v 603



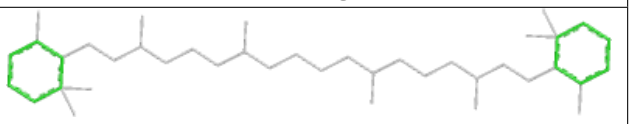
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Bond angles

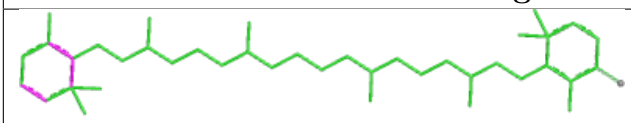


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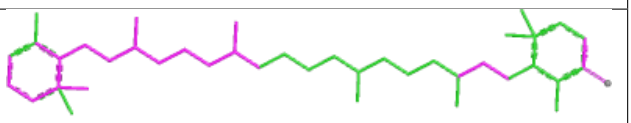


Rings

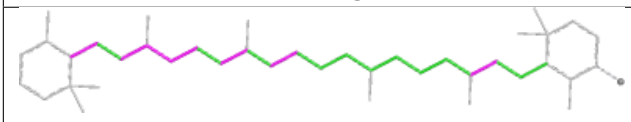
Ligand ECH R 4020



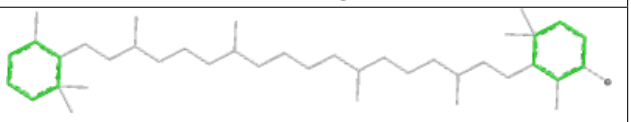
Bond lengths



Bond angles

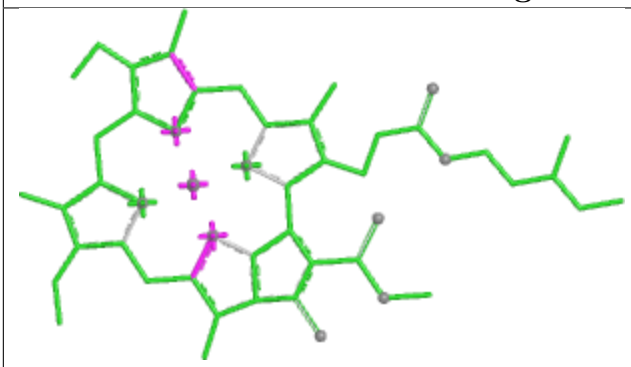


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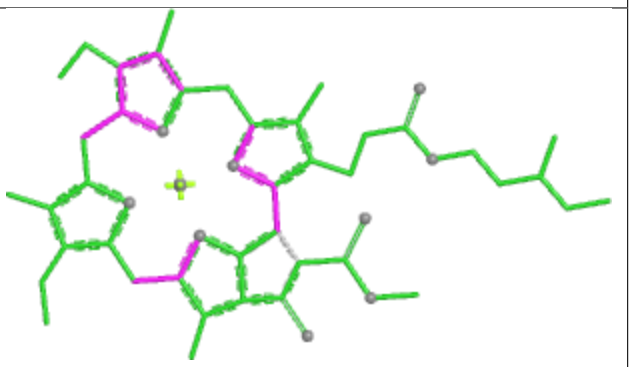


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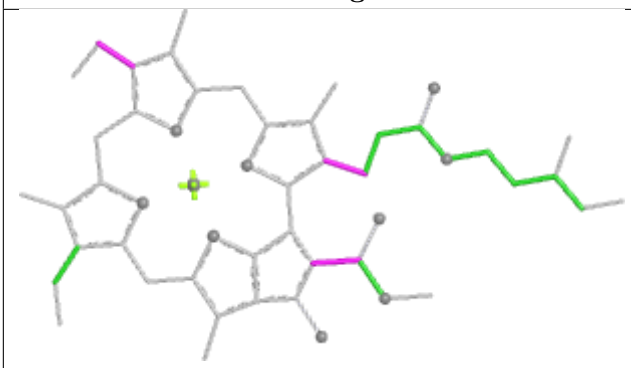
Ligand CLA H 1135



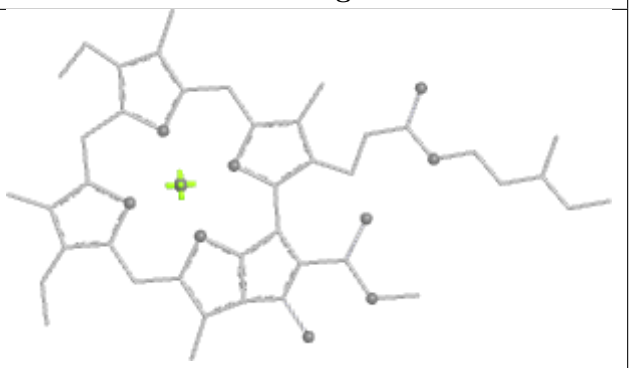
Bond lengths



Bond angles

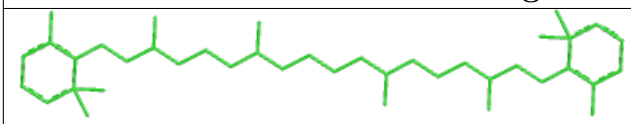


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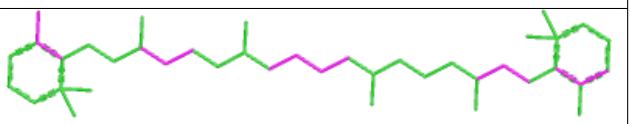


Rings

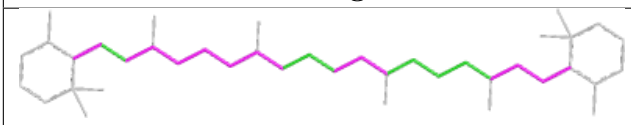
Ligand BCR w 604



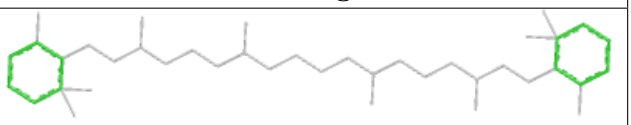
Bond lengths



Bond angles

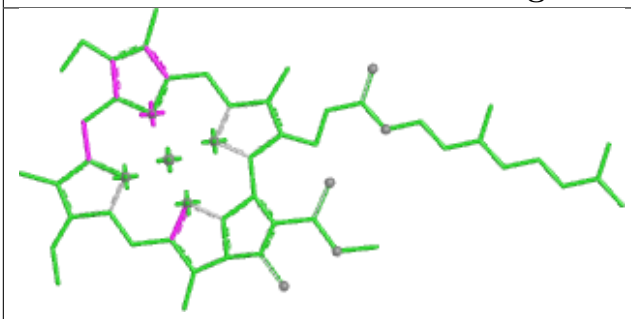


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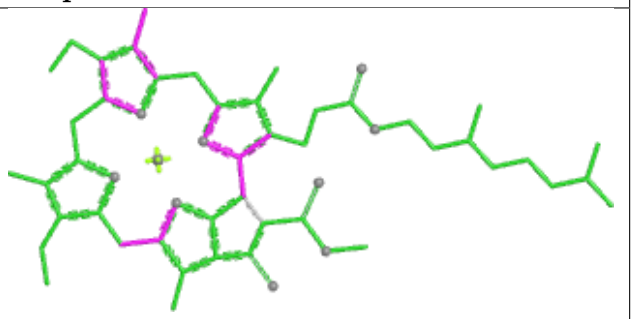


Rings

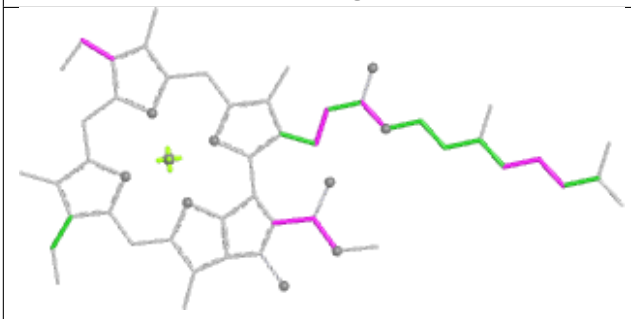
Ligand CLA q 517



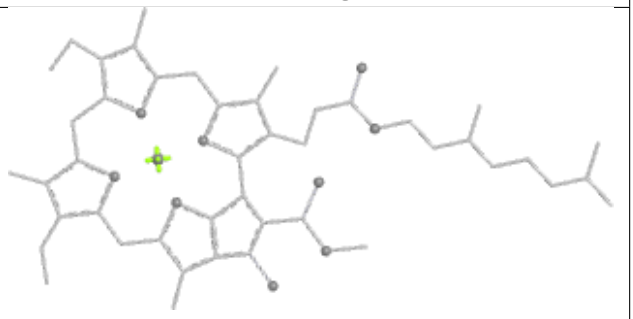
Bond lengths



Bond angles

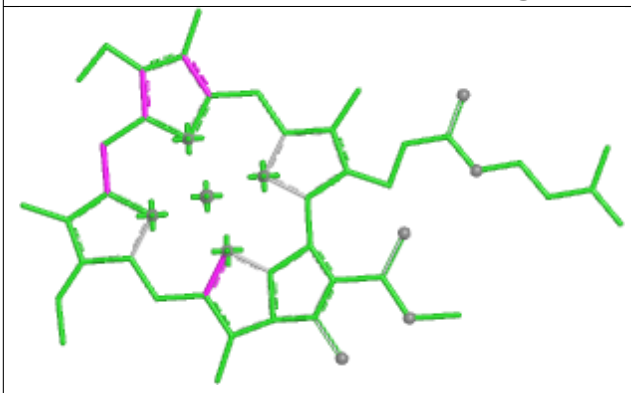


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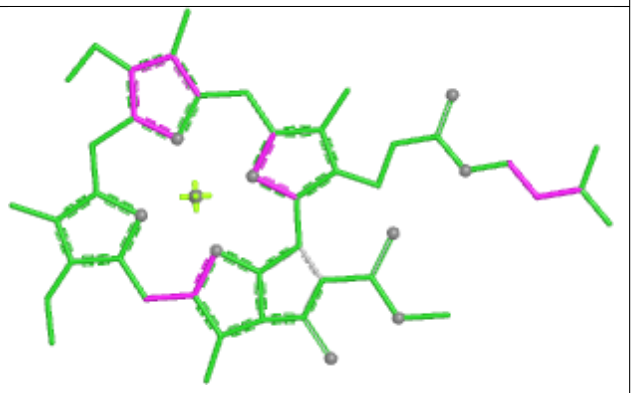


Rings

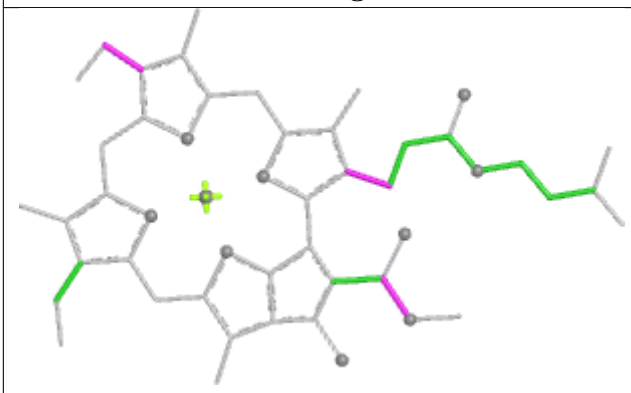
Ligand CLA A 1107



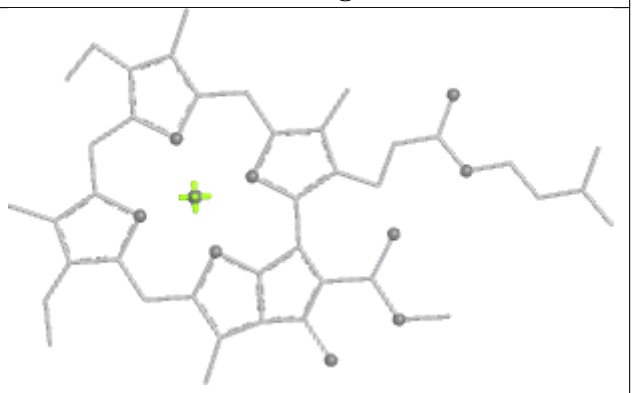
Bond lengths



Bond angles

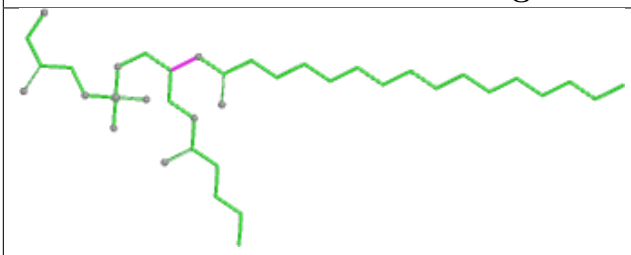


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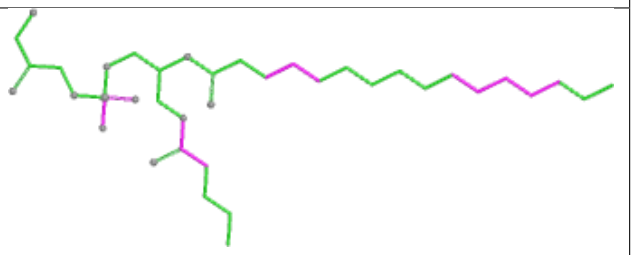


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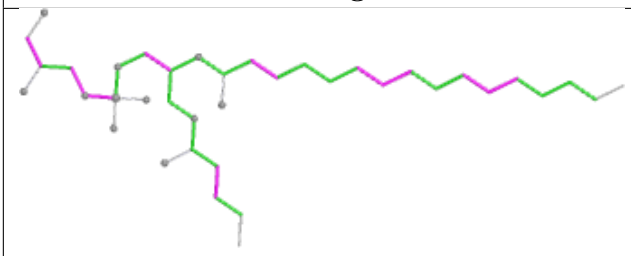
Ligand LHG G 4018



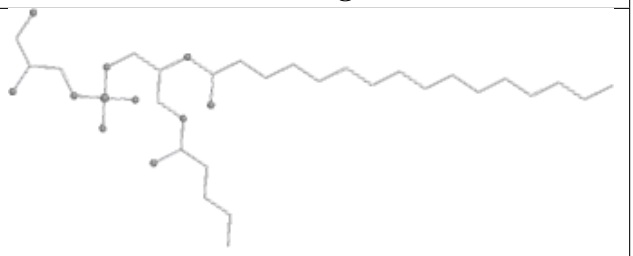
Bond lengths



Bond angles

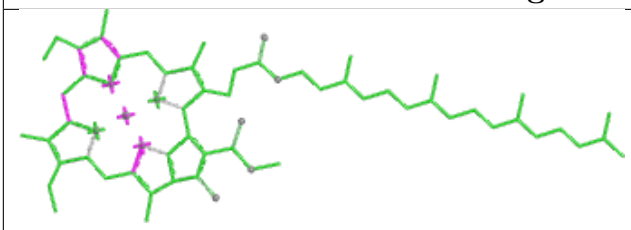


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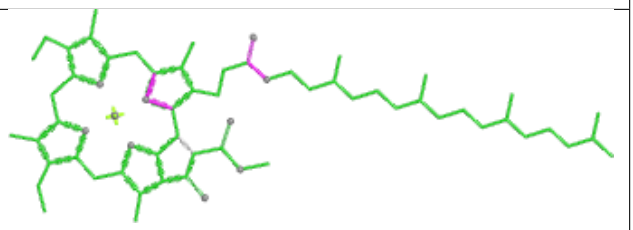


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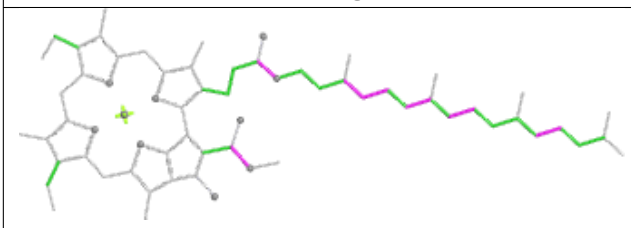
Ligand CLA u 512



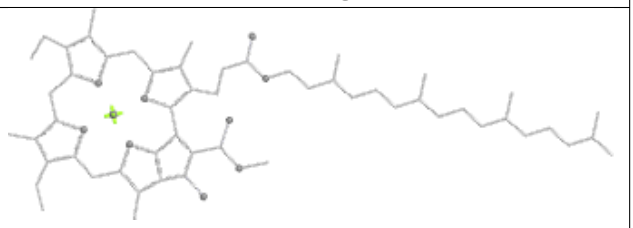
Bond lengths



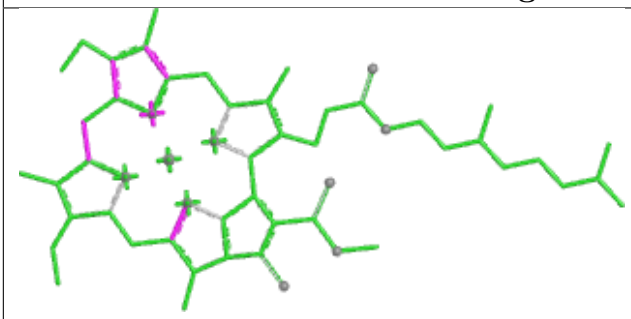
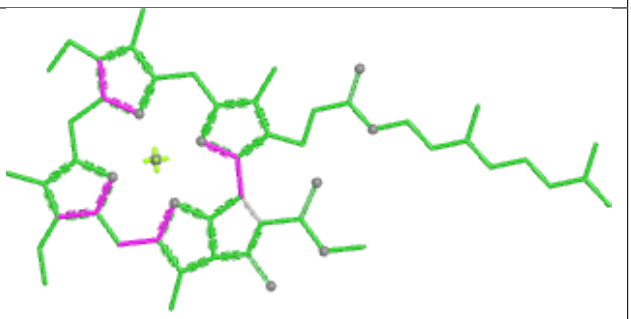
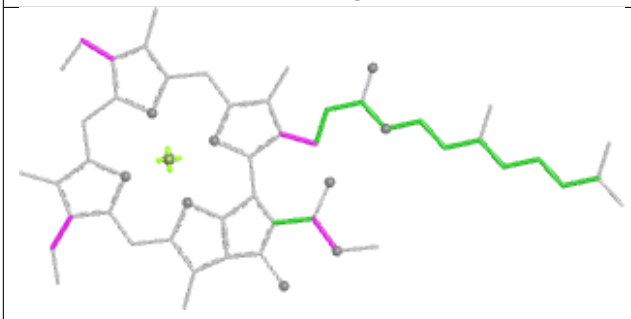
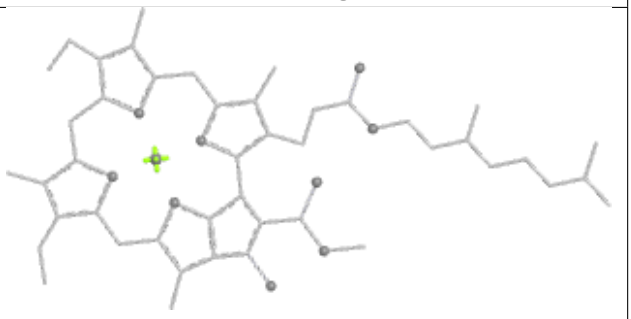
Bond angles

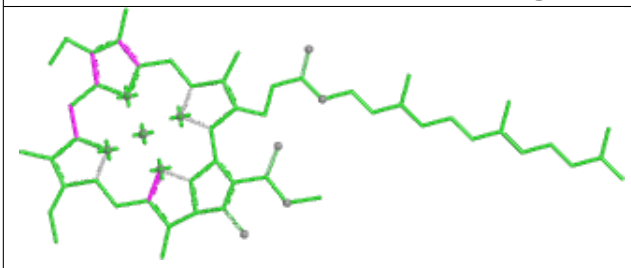
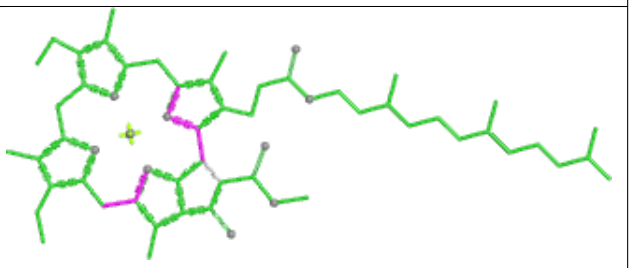
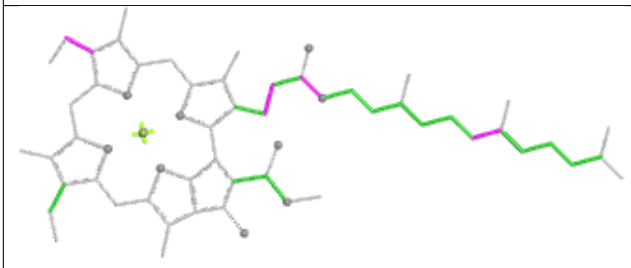
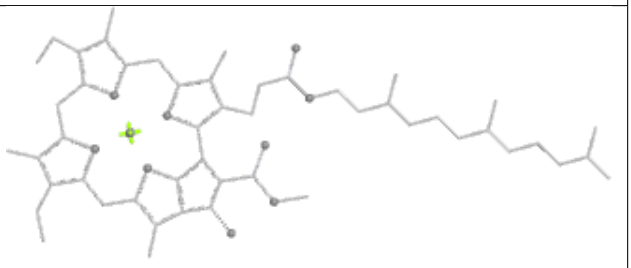


Torsions

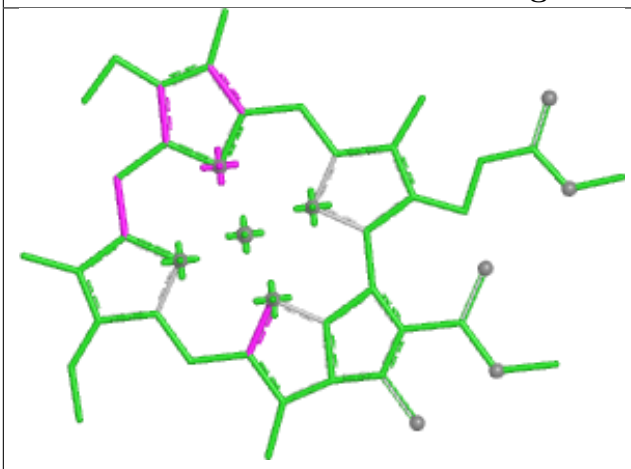


Rings

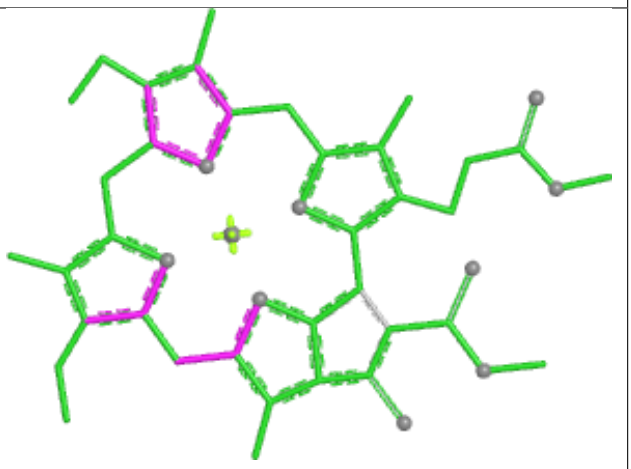
Ligand CLA b 1214	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA t 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

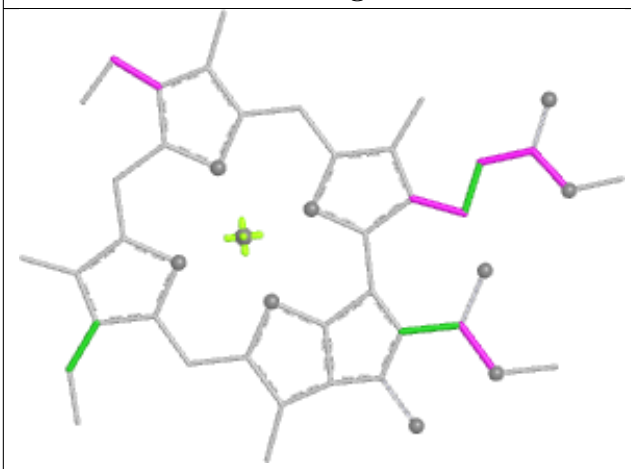
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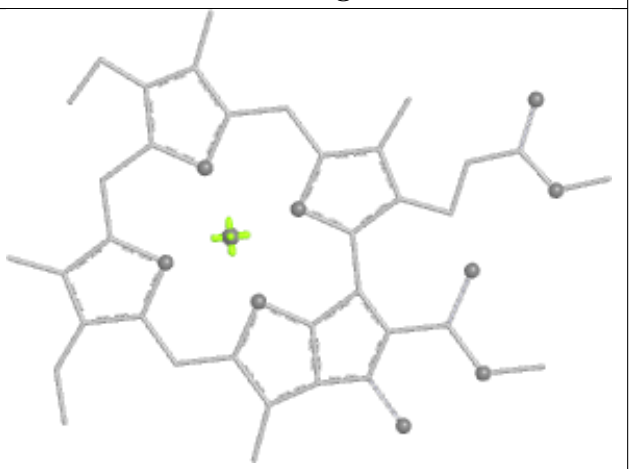
Bond lengths



Bond angles

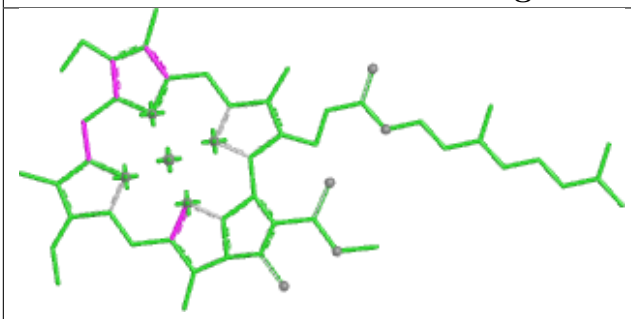


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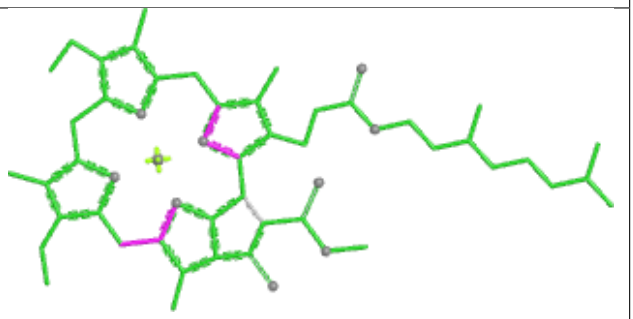


Rings

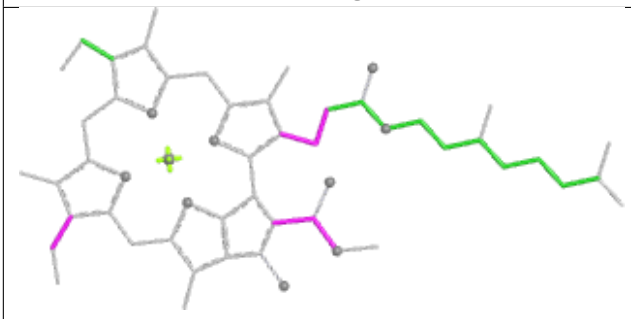
Ligand CLA H 1111



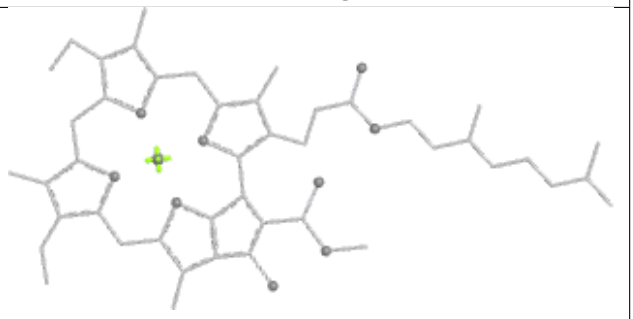
Bond lengths



Bond angles

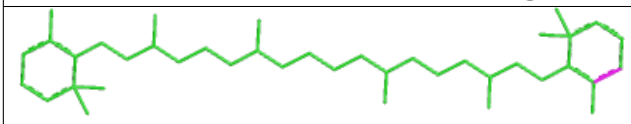


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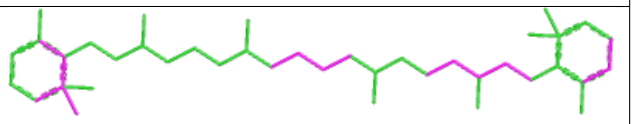


Rings

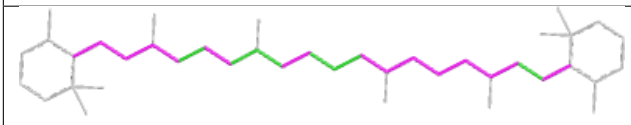
Ligand BCR l 4022



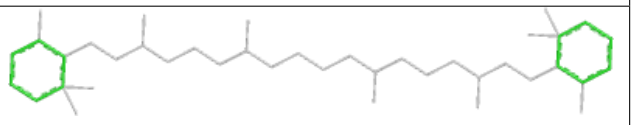
Bond lengths



Bond angles

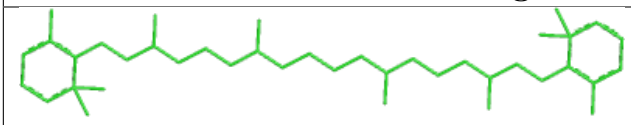


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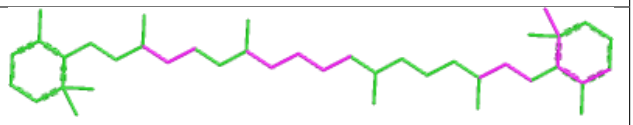


Rings

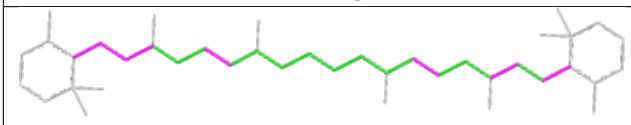
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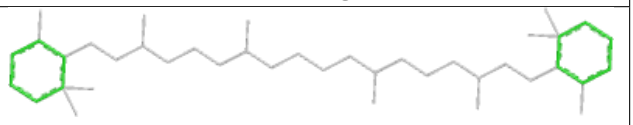
Bond lengths



Bond angles

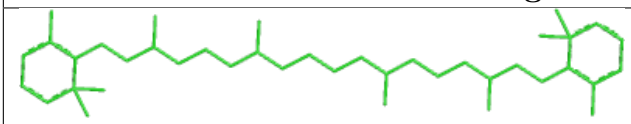


Torsions

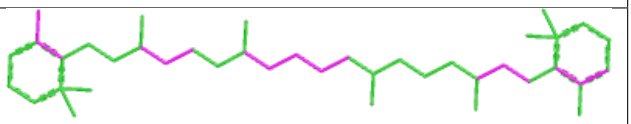


Rings

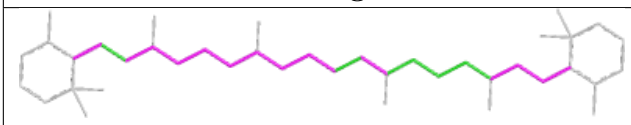
Ligand BCR Z 604



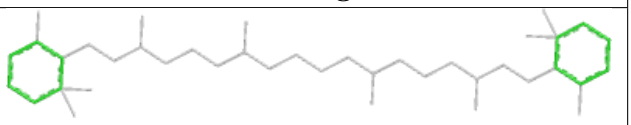
Bond lengths



Bond angles

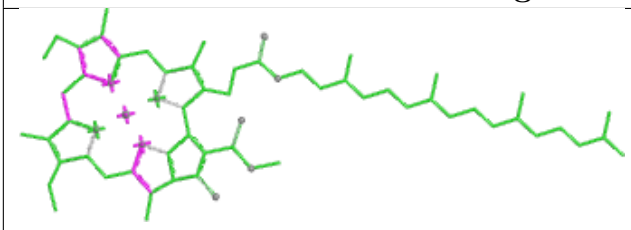


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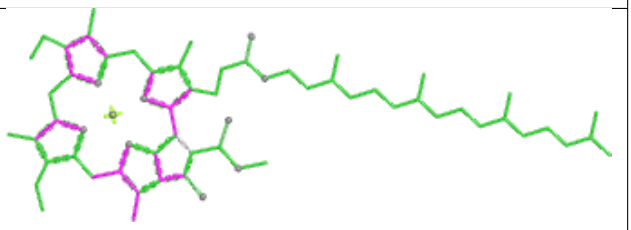


Rings

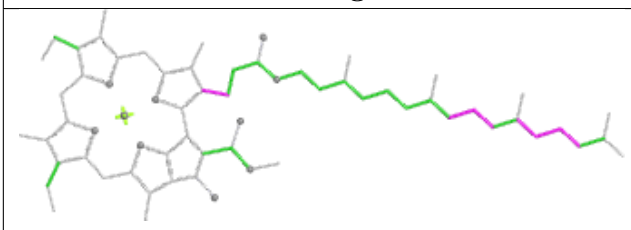
Ligand CLA G 1023



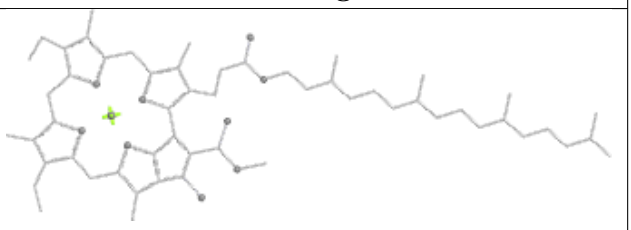
Bond lengths



Bond angles

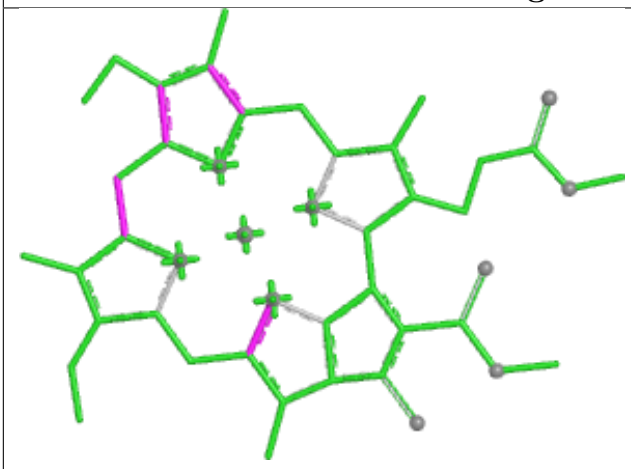


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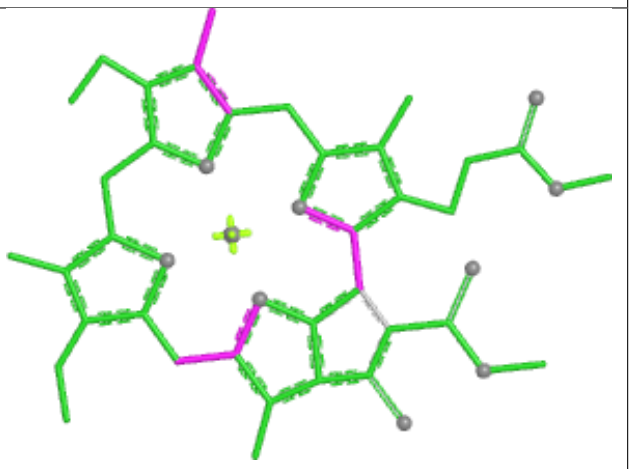


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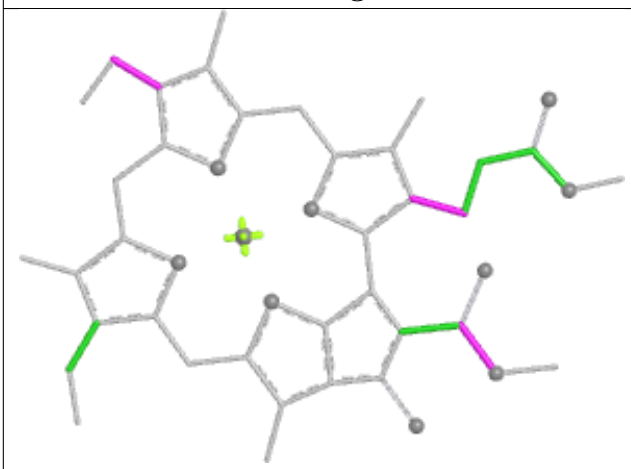
Ligand CLA v 516



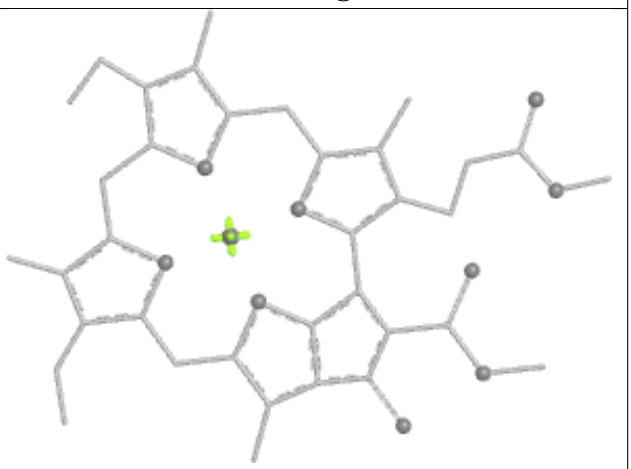
Bond lengths



Bond angles

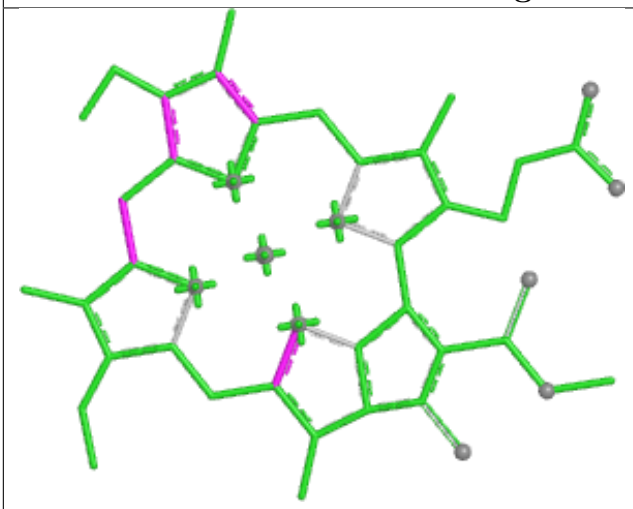


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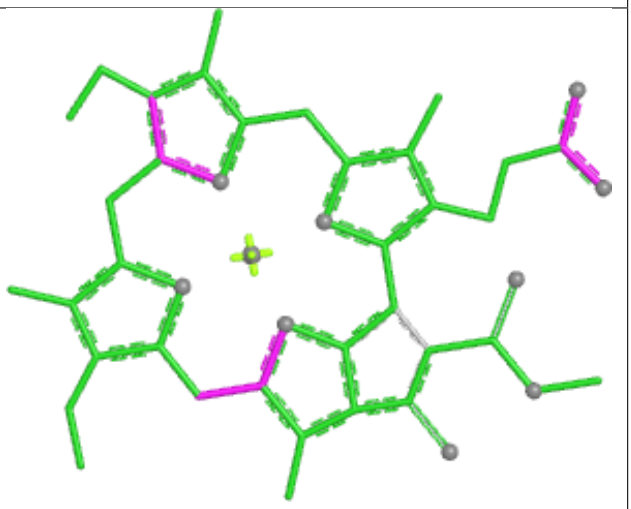


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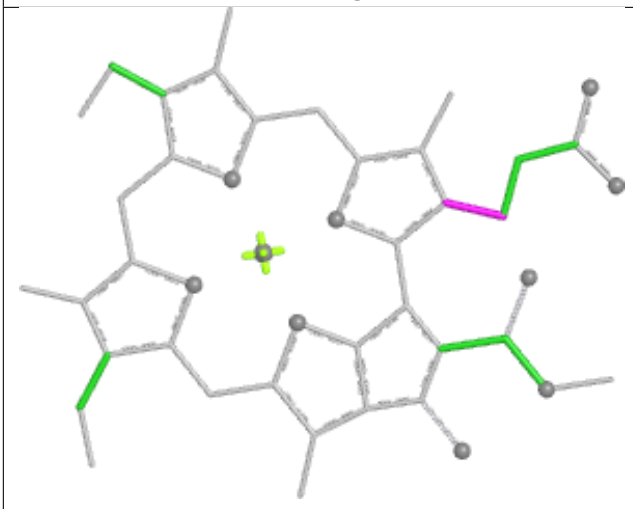
Ligand CLA H 1112



Bond lengths



Bond angles

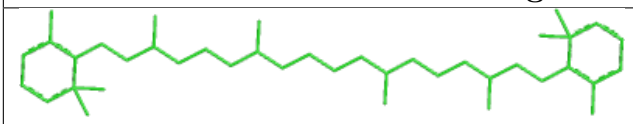


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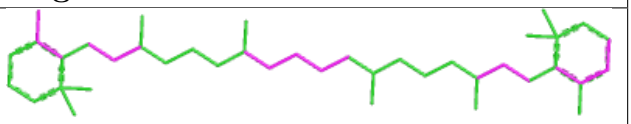


Rings

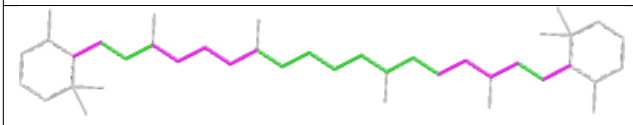
Ligand BCR g 602



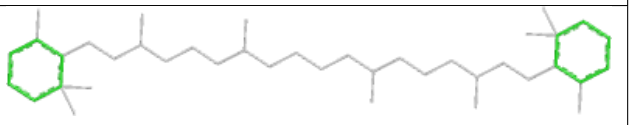
Bond lengths



Bond angles

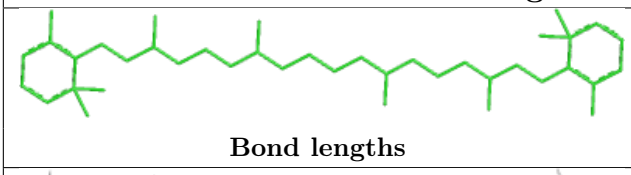


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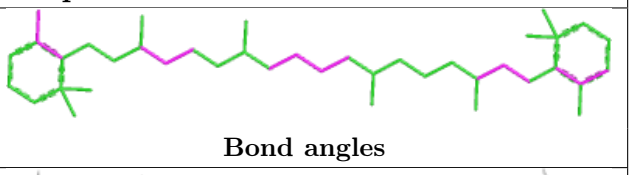


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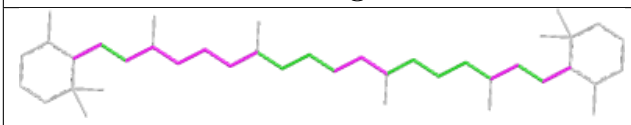
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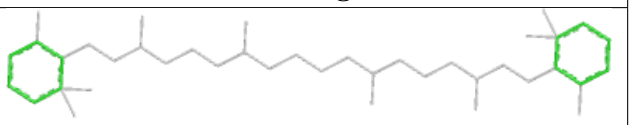
Bond lengths



Bond angles

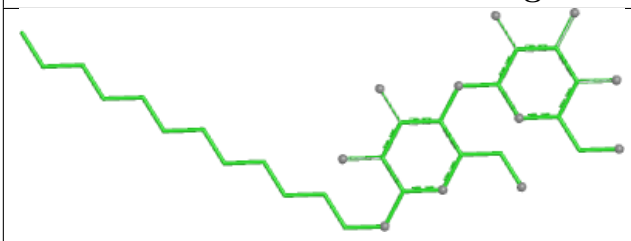


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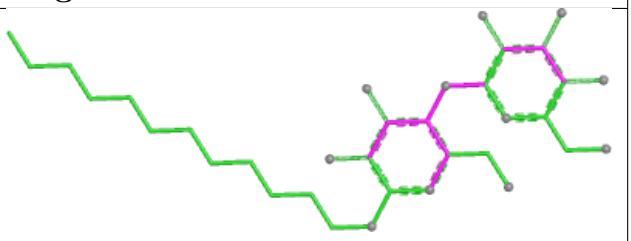


Rings

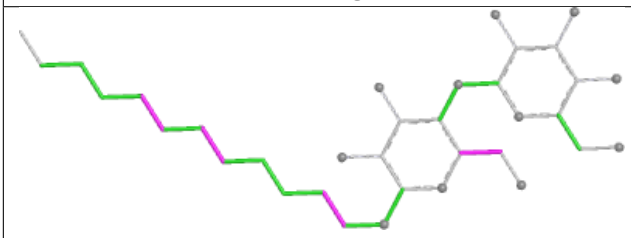
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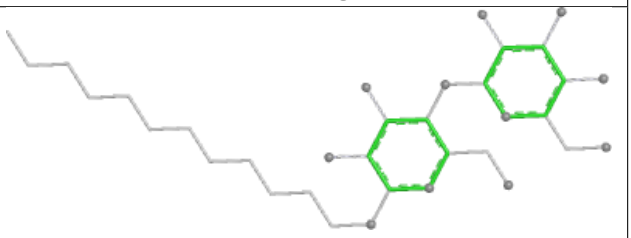
Bond lengths



Bond angles

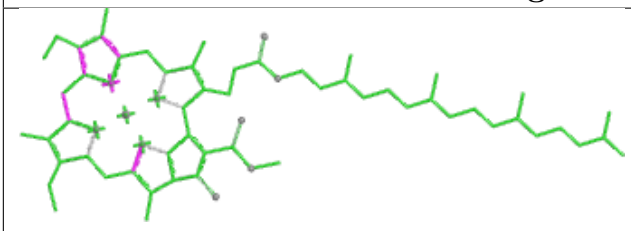


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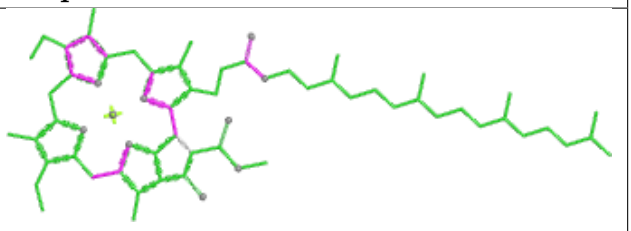


Rings

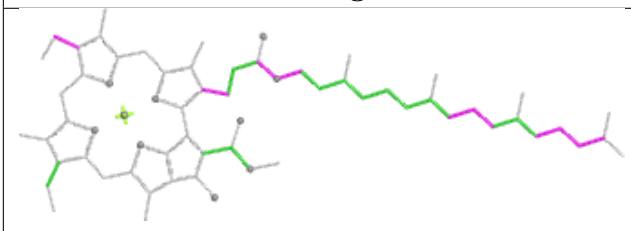
Ligand CLA q 509



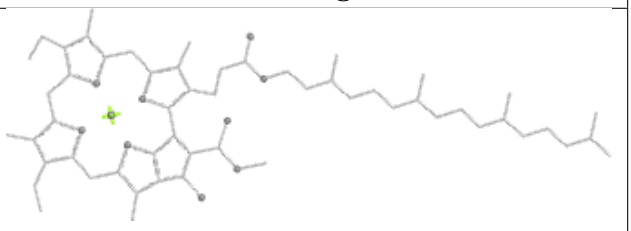
Bond lengths



Bond angles

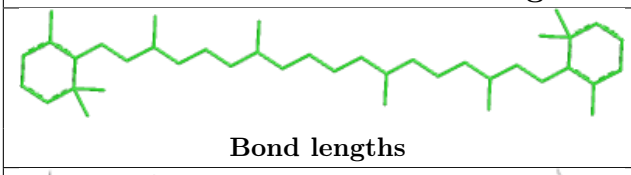


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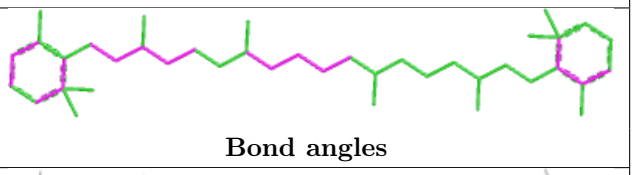


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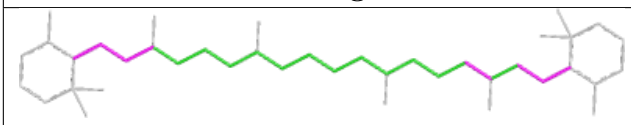
Ligand BCR o 603



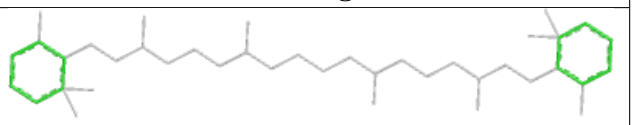
Bond lengths



Bond angles

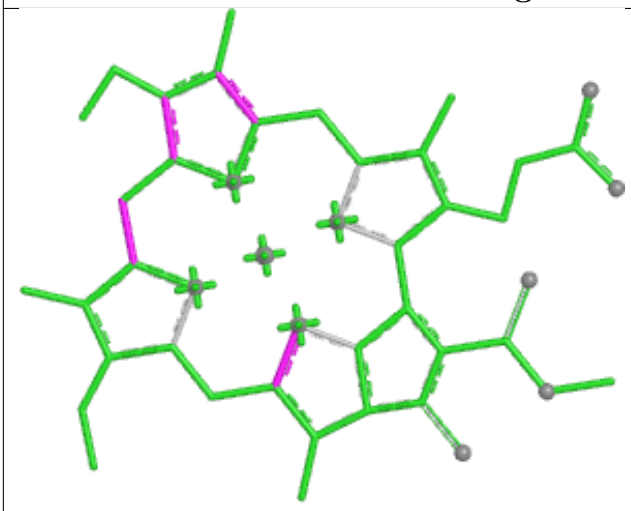


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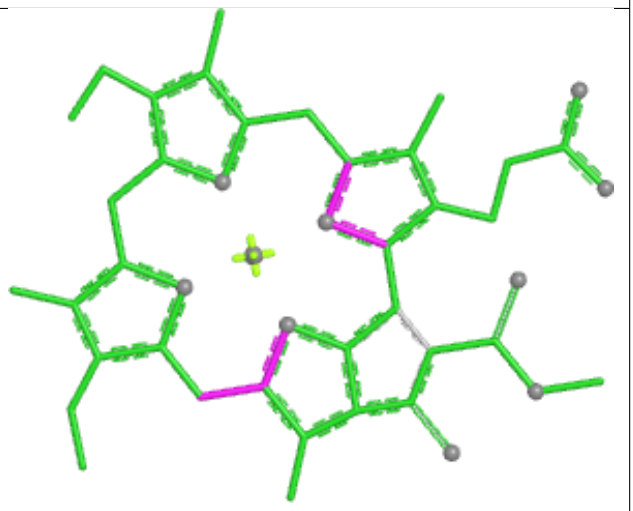


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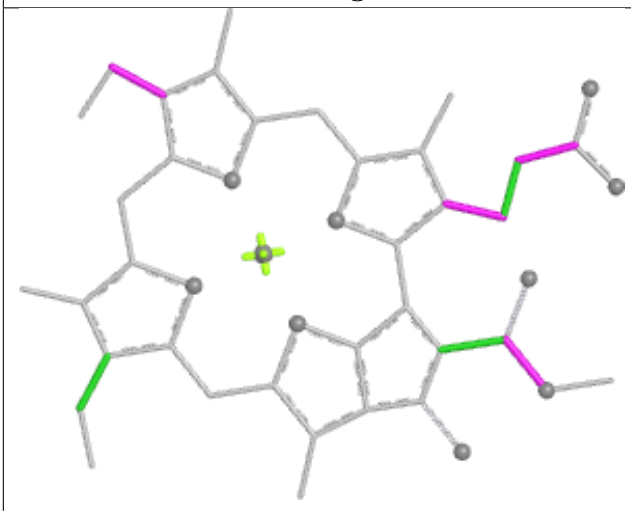
Ligand CLA A 1113



Bond lengths



Bond angles

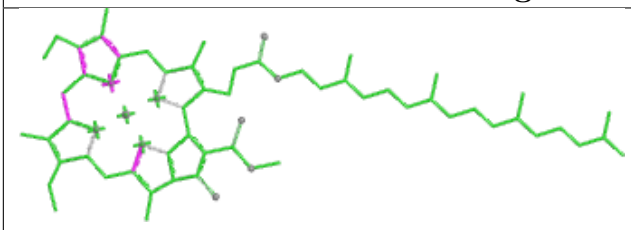


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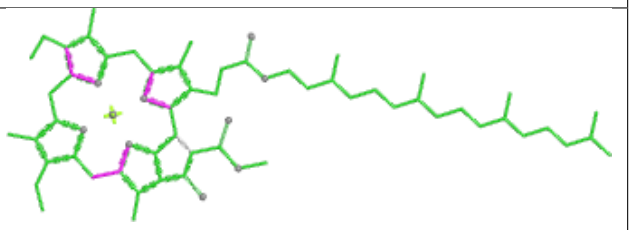


Rings

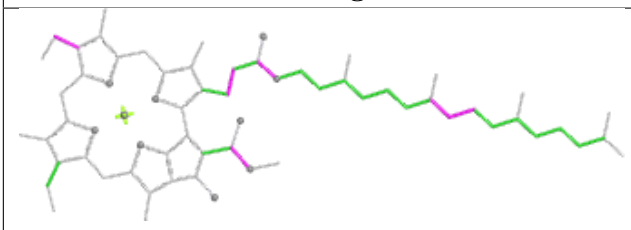
Ligand CLA H 1136



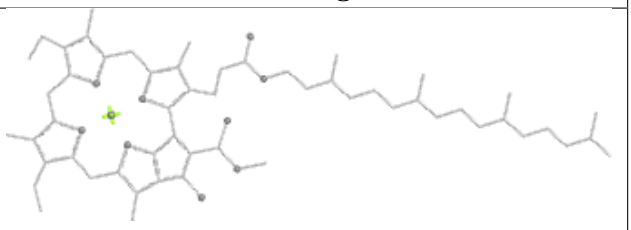
Bond lengths



Bond angles

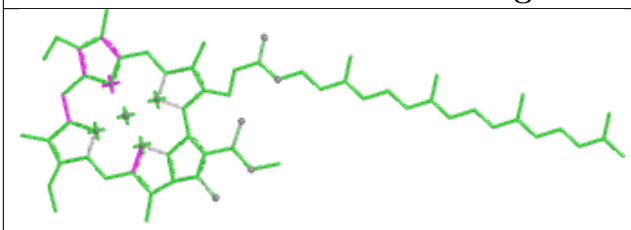


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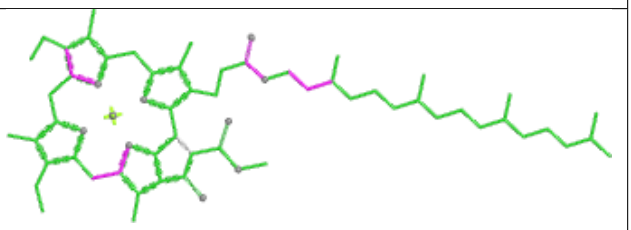


Rings

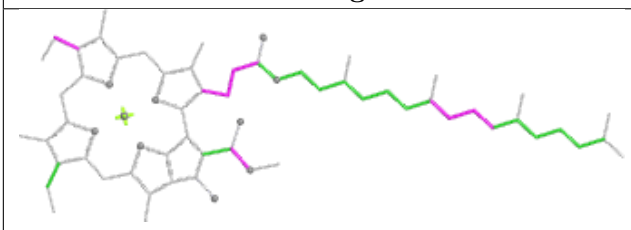
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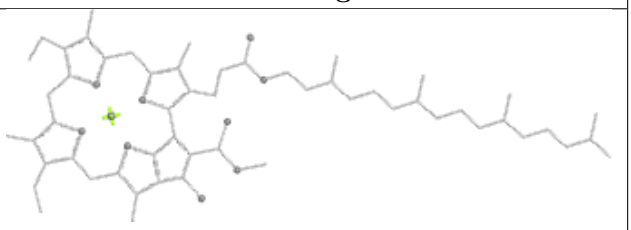
Bond lengths



Bond angles

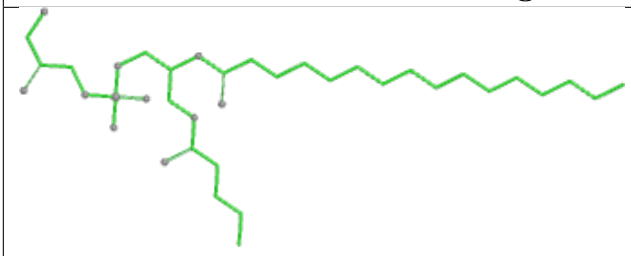


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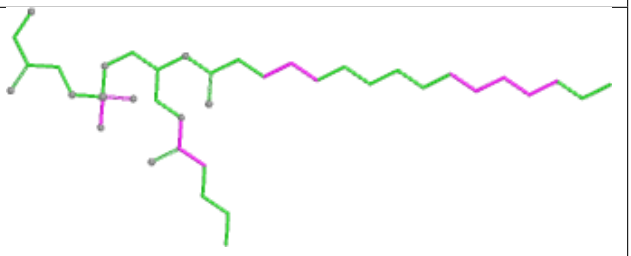


Rings

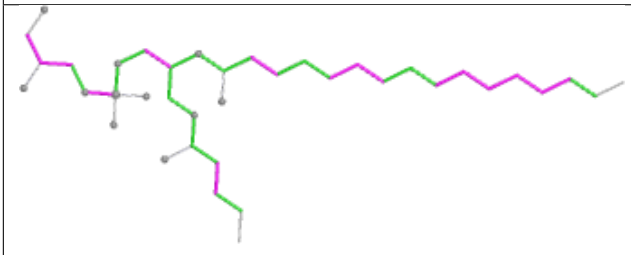
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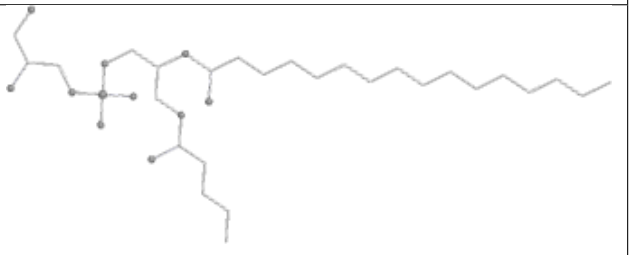
Bond lengths



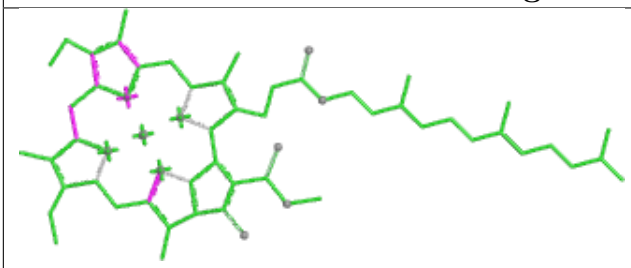
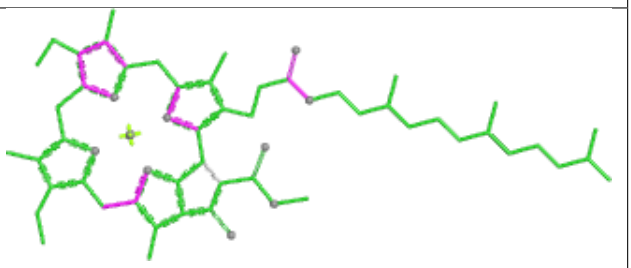
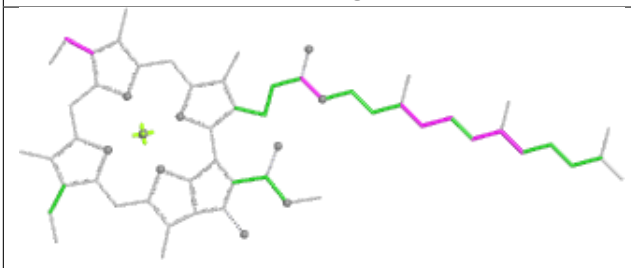
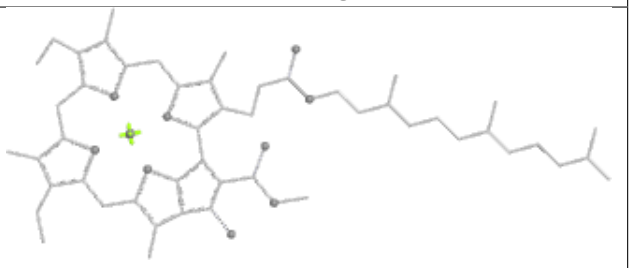
Bond angles

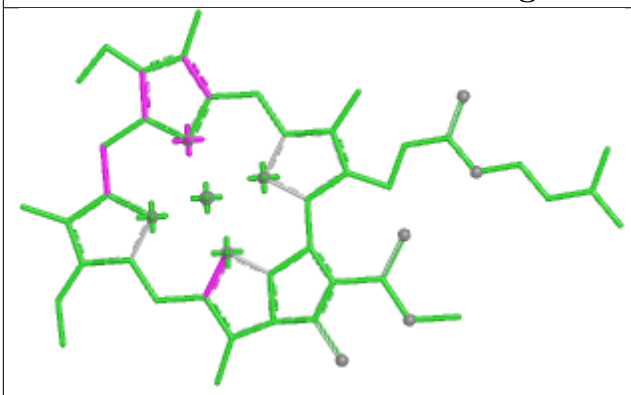
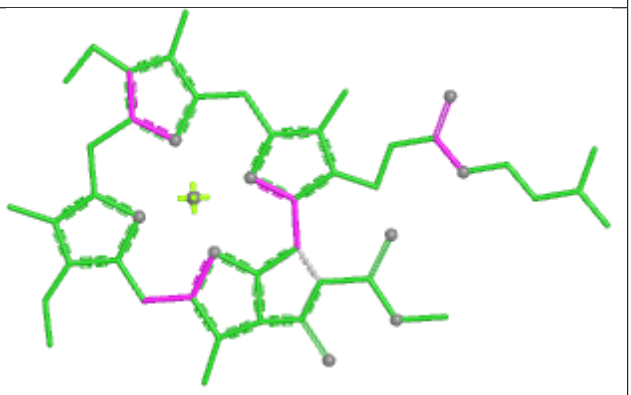
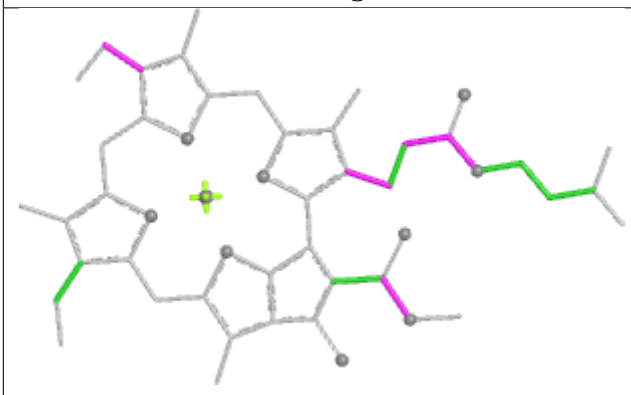
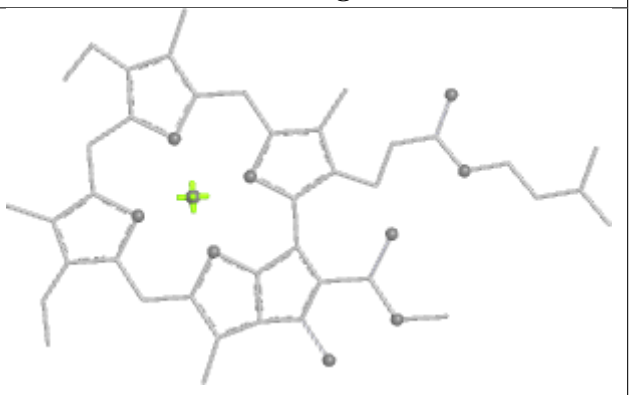


Torsions

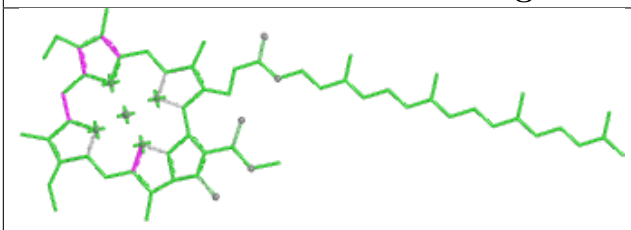


Rings

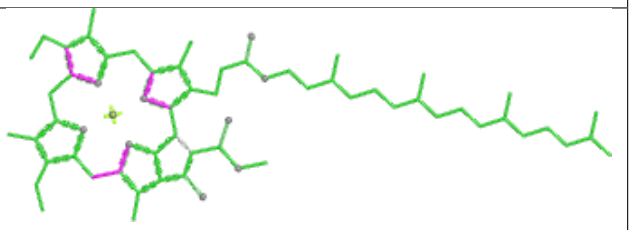
Ligand CLA l 1502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA W 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

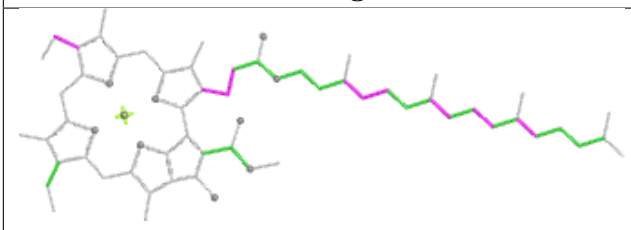
Ligand CLA B 1223



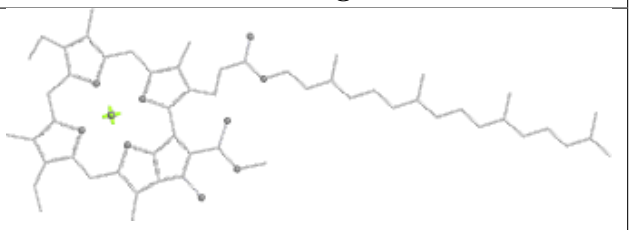
Bond lengths



Bond angles

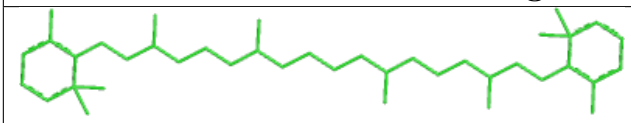


Torsions

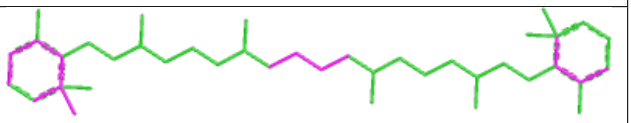


Rings

Ligand BCR v 604



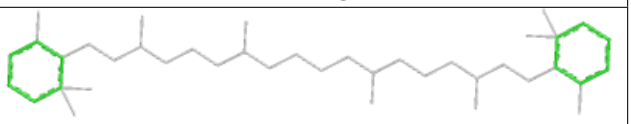
Bond lengths



Bond angles

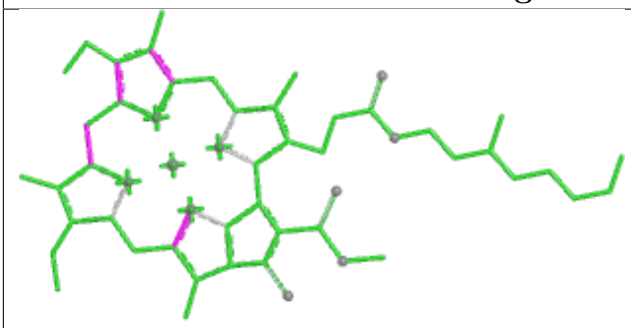


Torsions

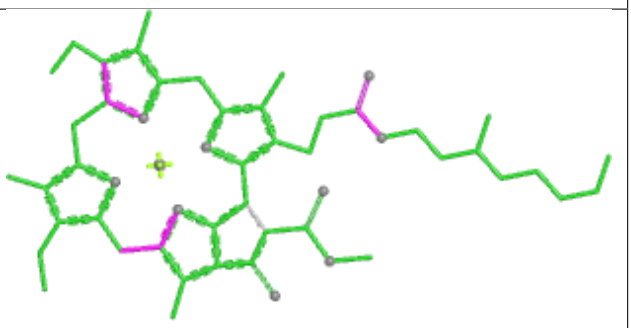


Rings

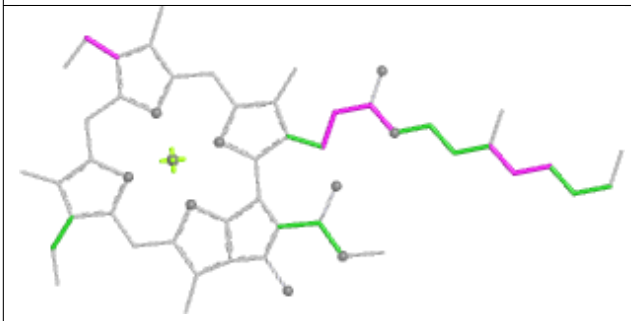
Ligand CLA A 1110



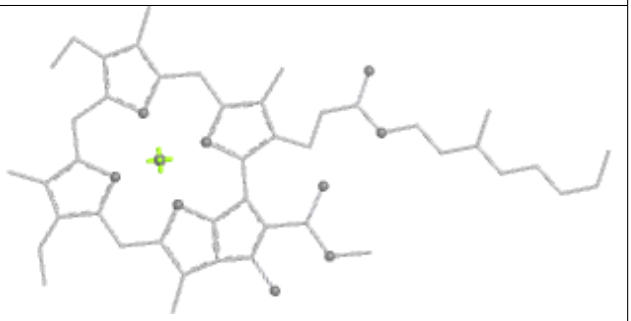
Bond lengths



Bond angles

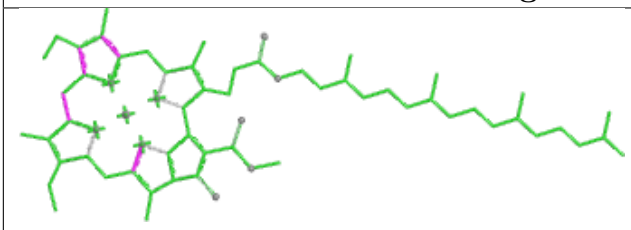


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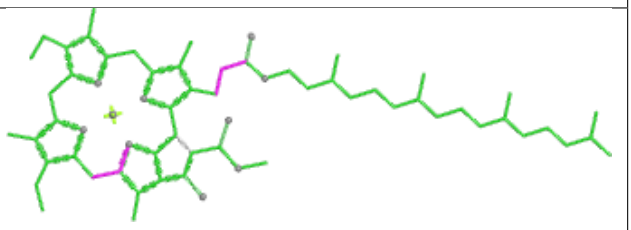


Rings

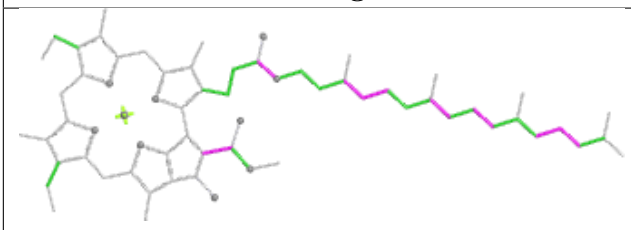
Ligand CLA a 1103



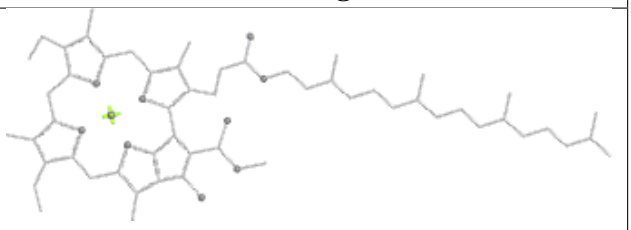
Bond lengths



Bond angles

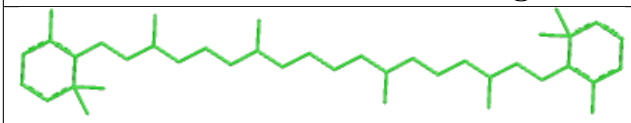


Torsions

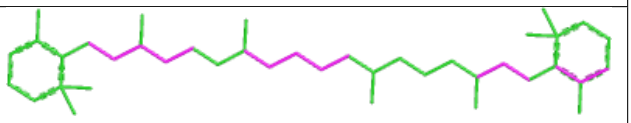


Rings

Ligand BCR G 4004



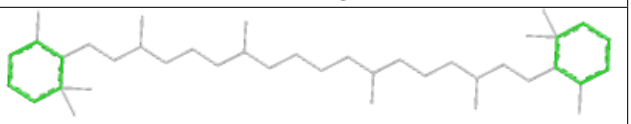
Bond lengths



Bond angles

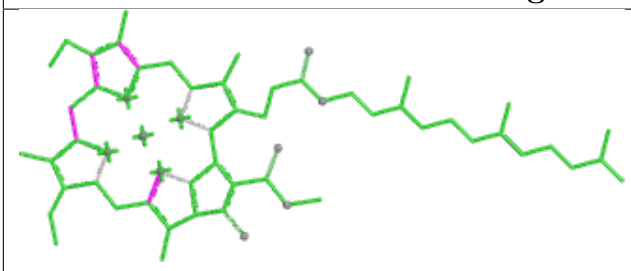


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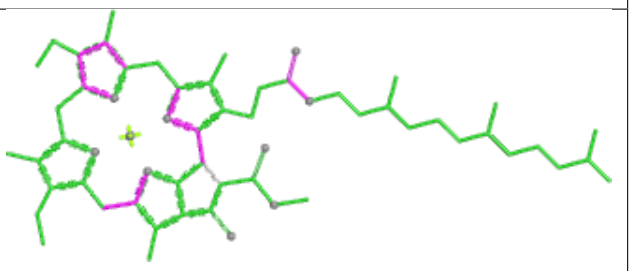


Rings

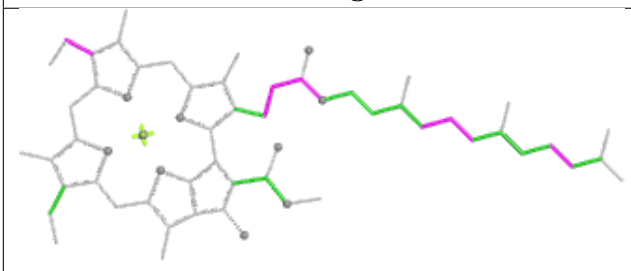
Ligand CLA n 509



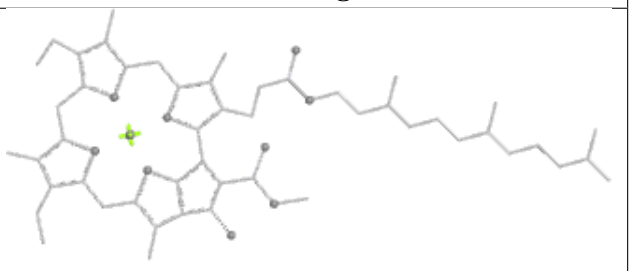
Bond lengths



Bond angles

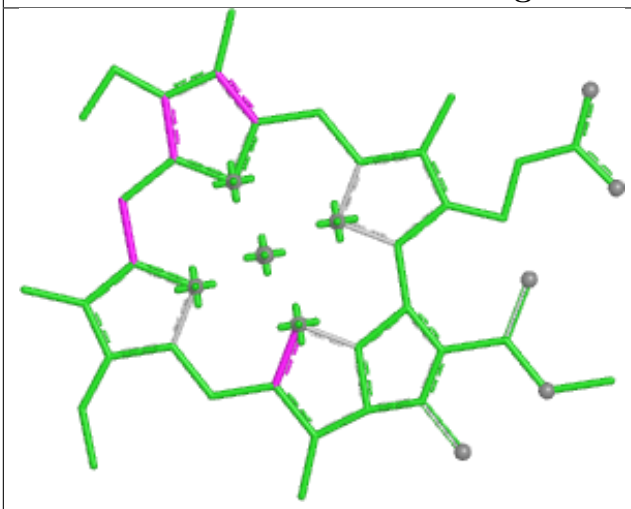


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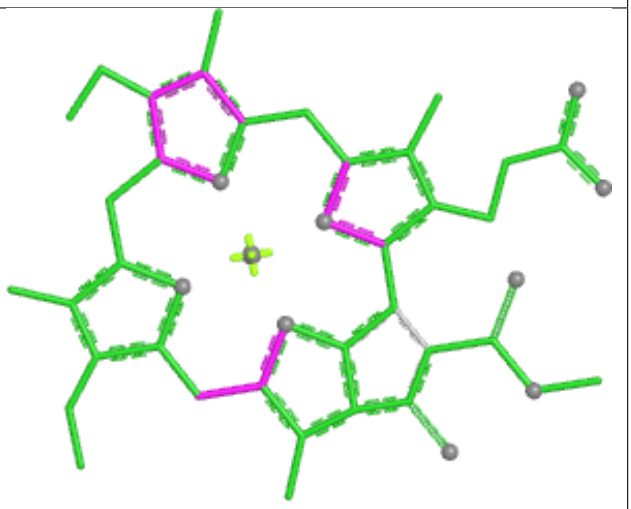


Rings

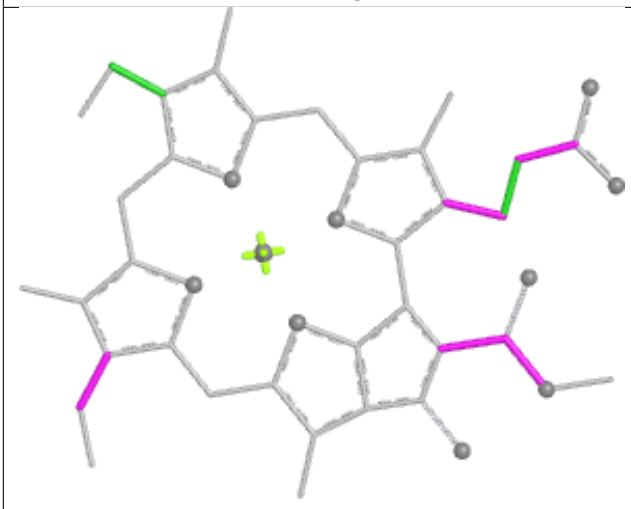
Ligand CLA K 4003



Bond lengths



Bond angles

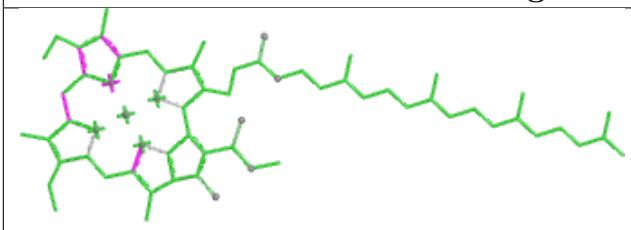


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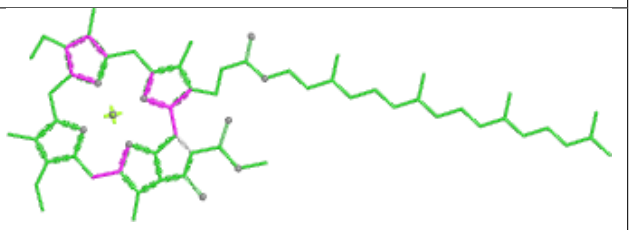


Rings

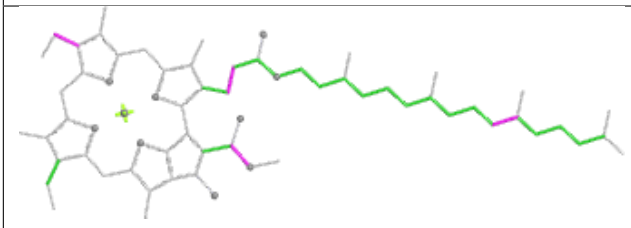
Ligand CLA h 505



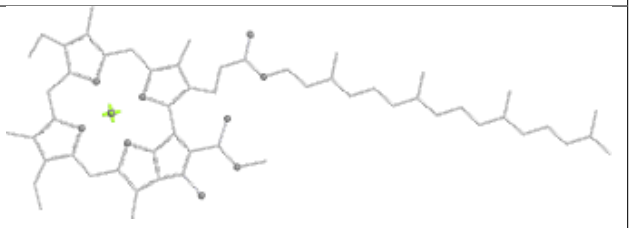
Bond lengths



Bond angles

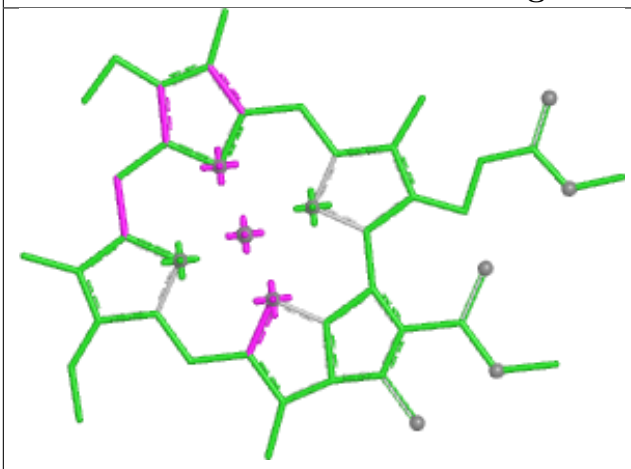


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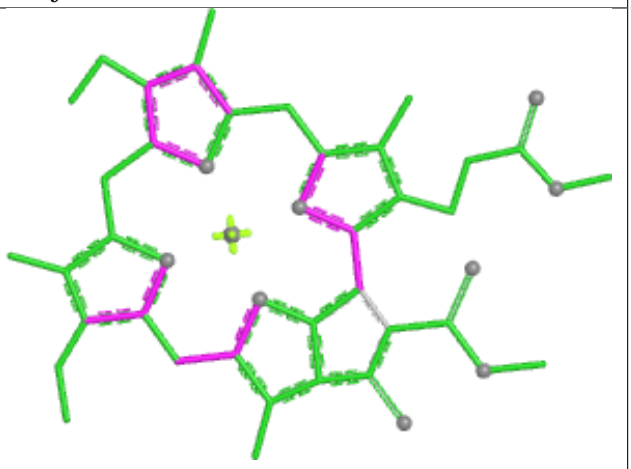


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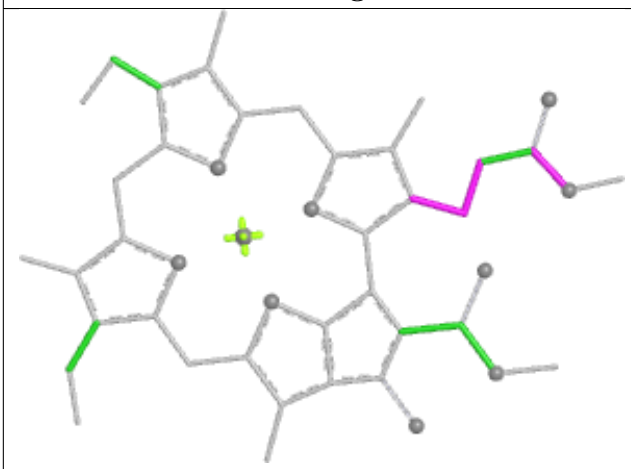
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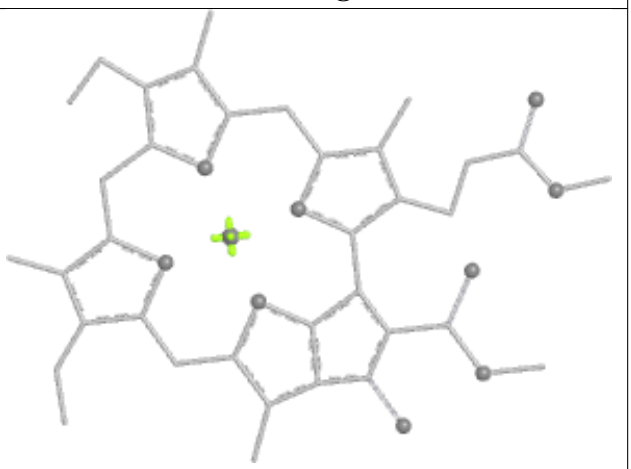
Bond lengths



Bond angles



Torsions

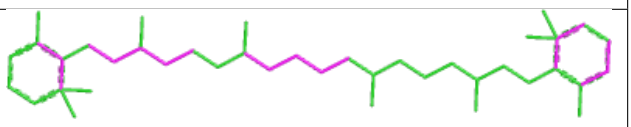


Rings

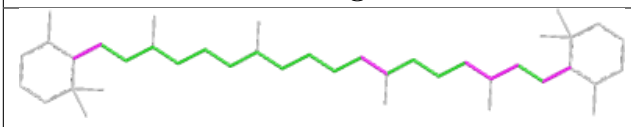
Ligand BCR H 4007



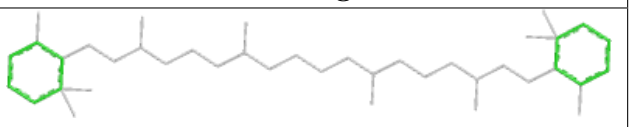
Bond lengths



Bond angles

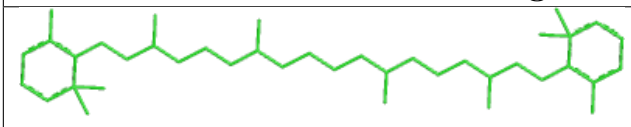


Torsions

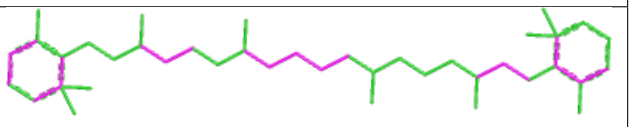


Rings

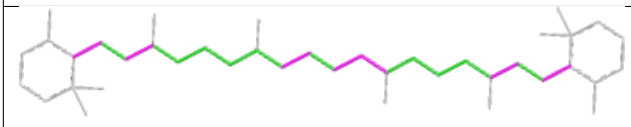
Ligand BCR s 602



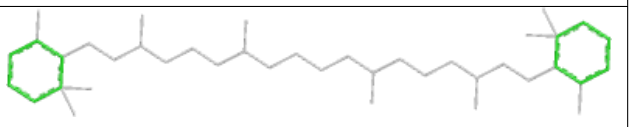
Bond lengths



Bond angles

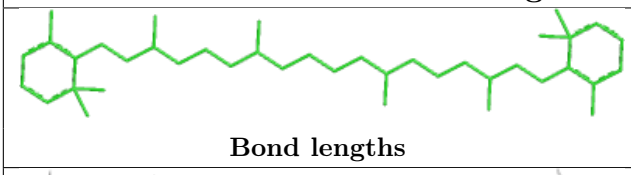


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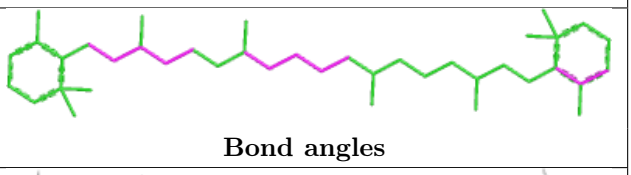


Rings

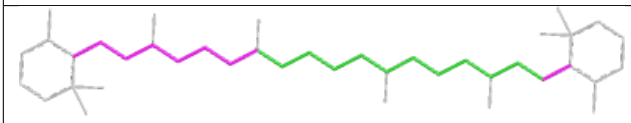
Ligand BCR n 603



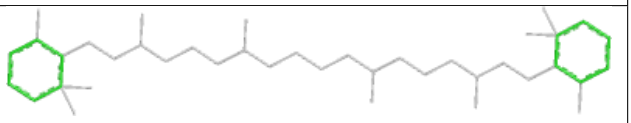
Bond lengths



Bond angles



Torsions

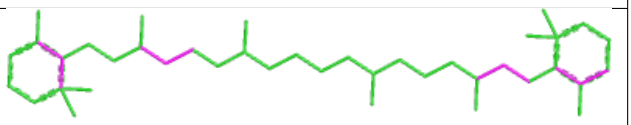


Rings

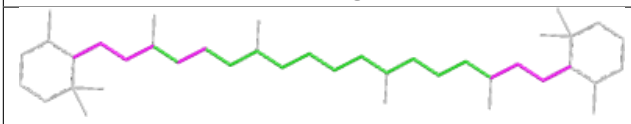
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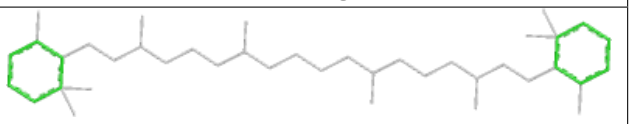
Bond lengths



Bond angles

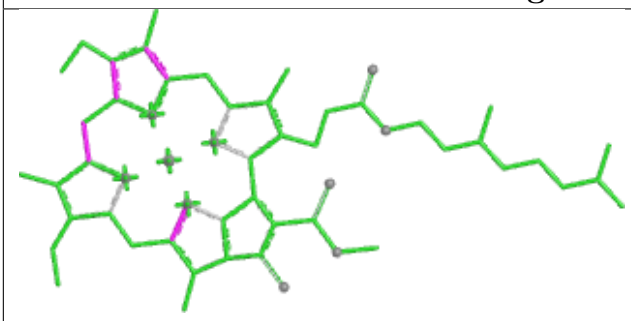


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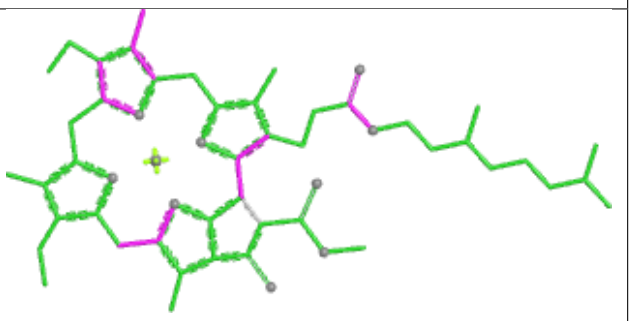


Rings

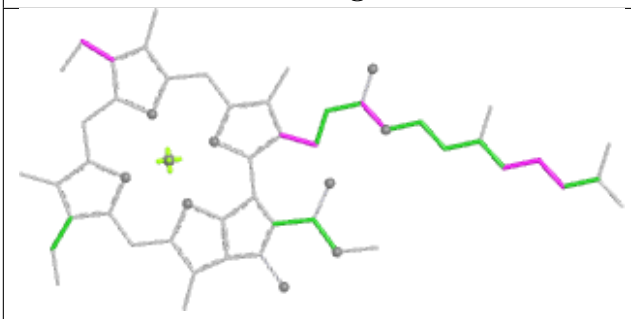
Ligand CLA u 517



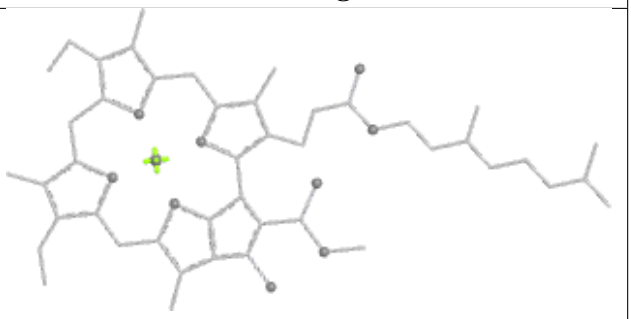
Bond lengths



Bond angles

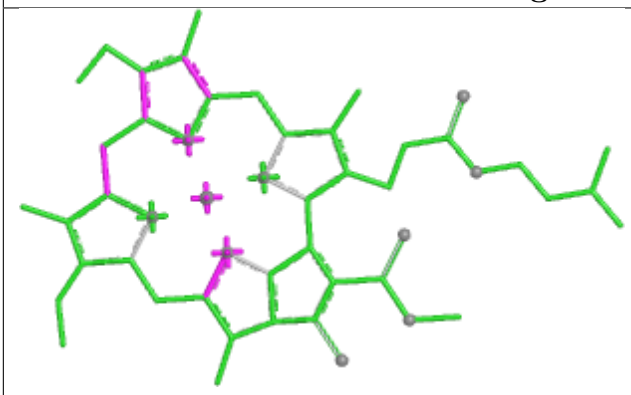


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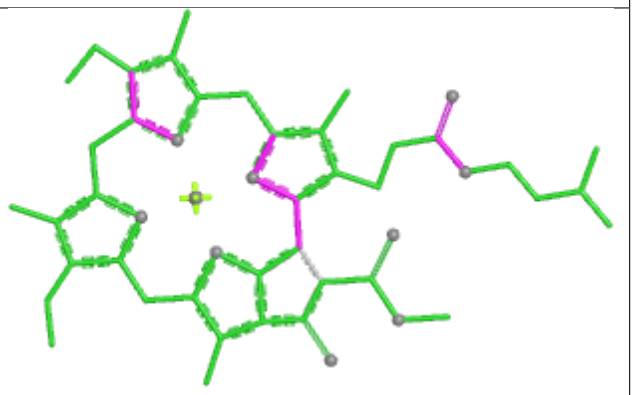


Rings

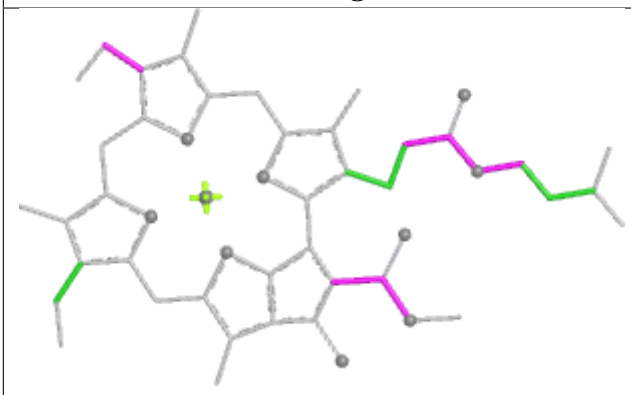
Ligand CLA t 502



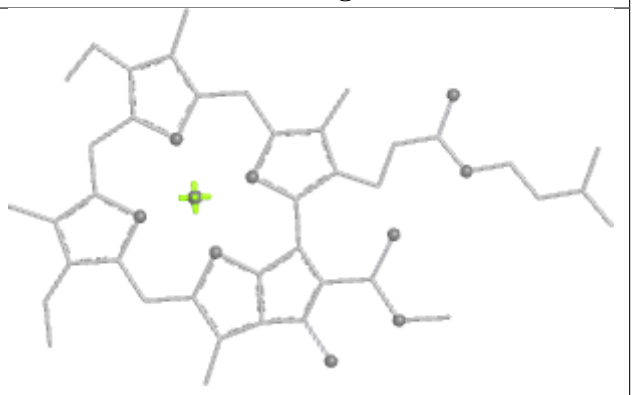
Bond lengths



Bond angles

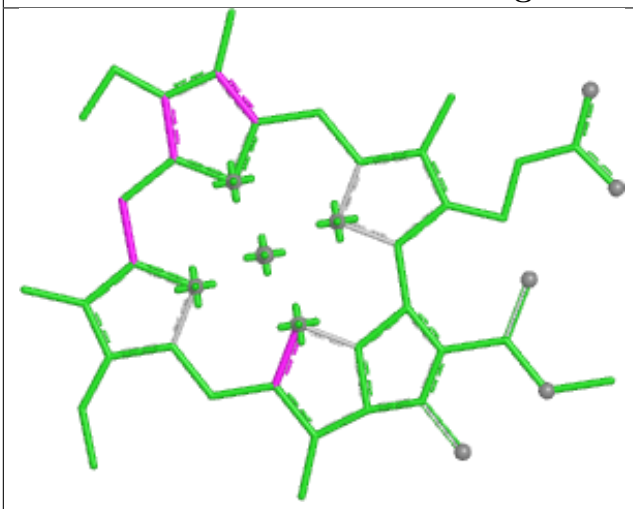


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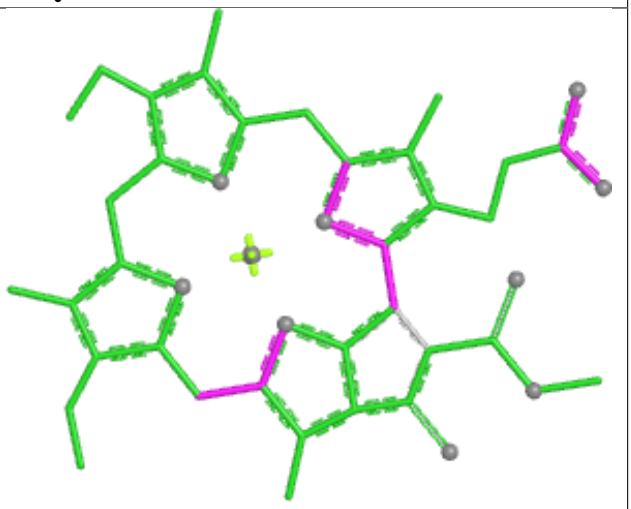


Rings

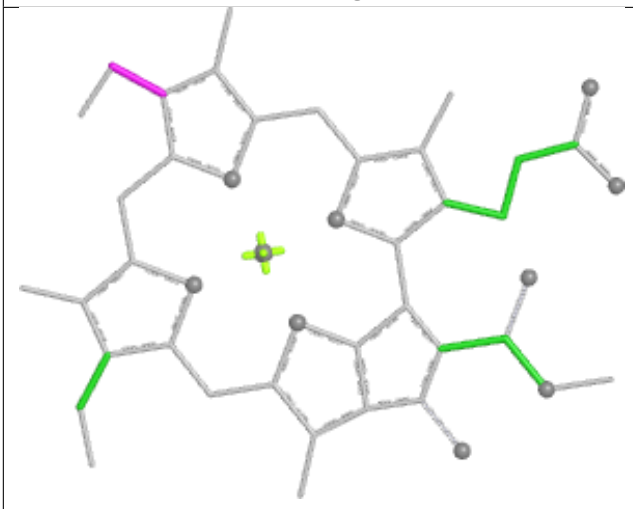
Ligand CLA Q 1301



Bond lengths



Bond angles

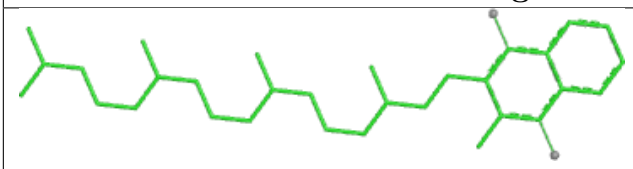


Torsions

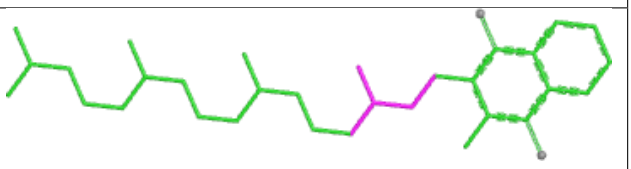


Rings

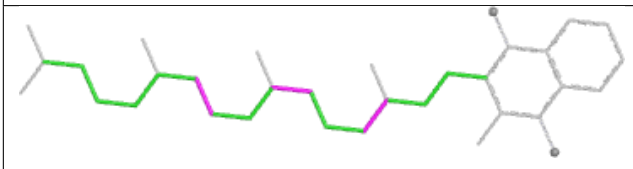
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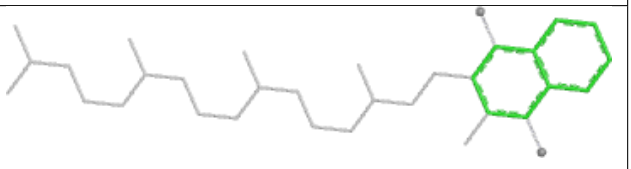
Bond lengths



Bond angles

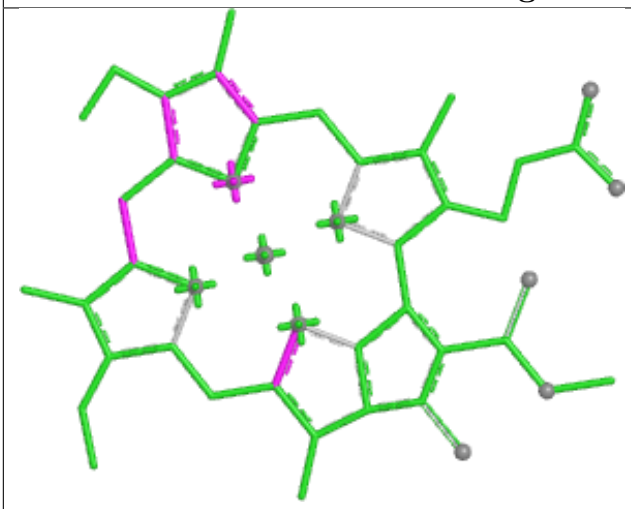


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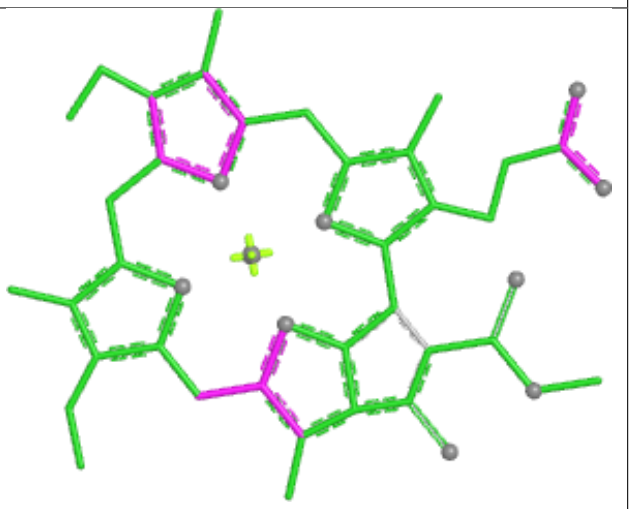


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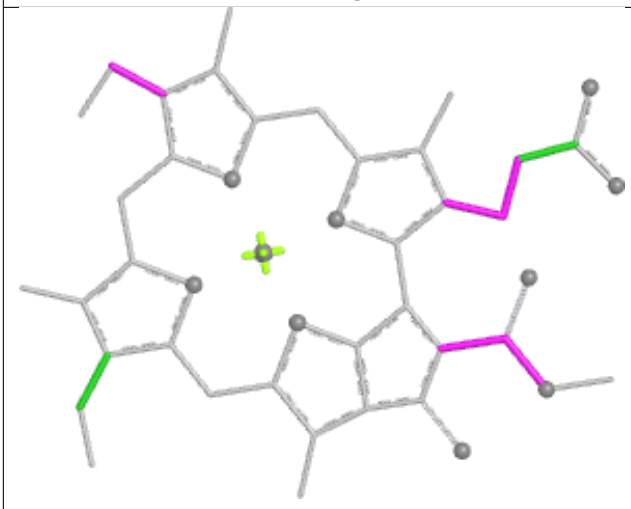
Ligand CLA b 1219



Bond lengths



Bond angles

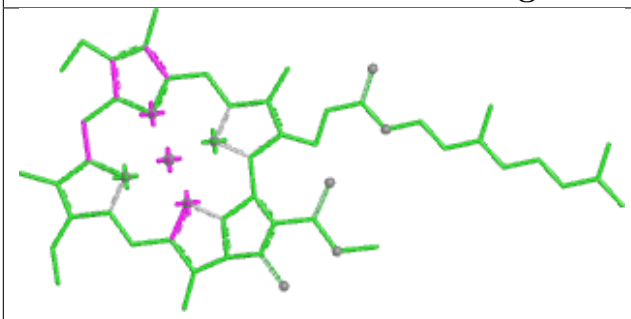


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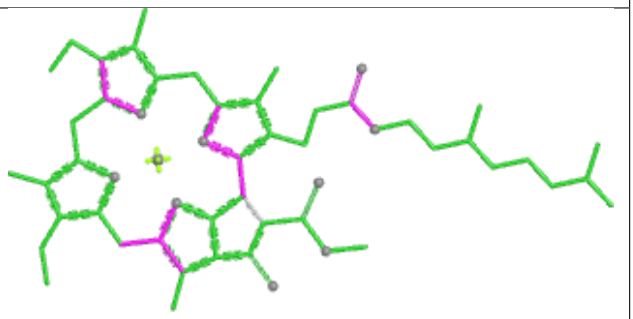


Rings

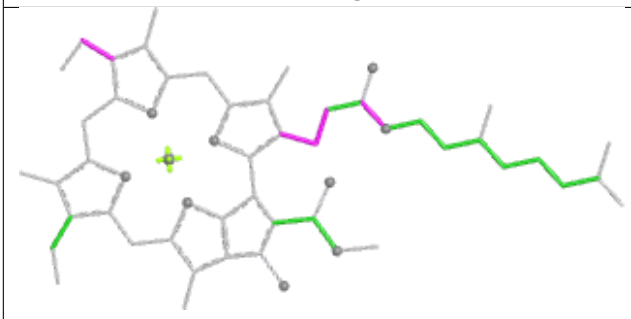
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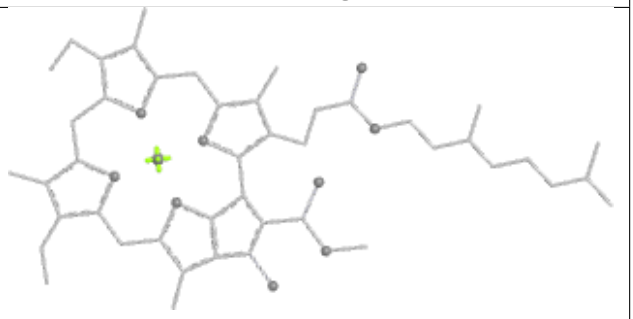
Bond lengths



Bond angles

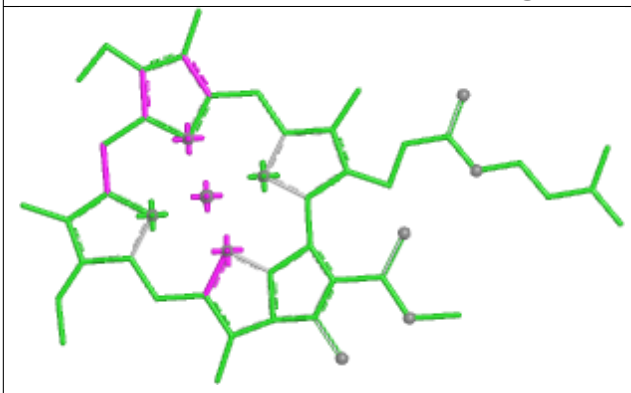


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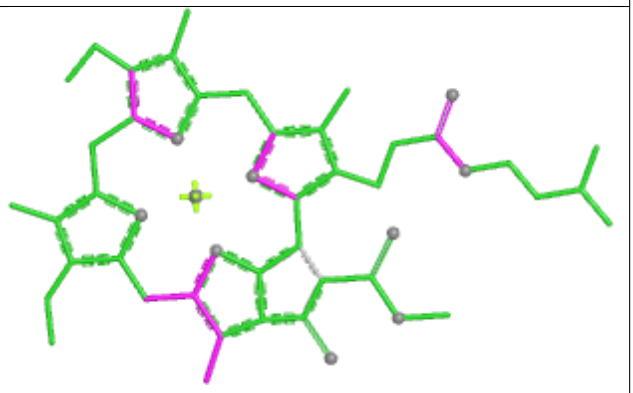


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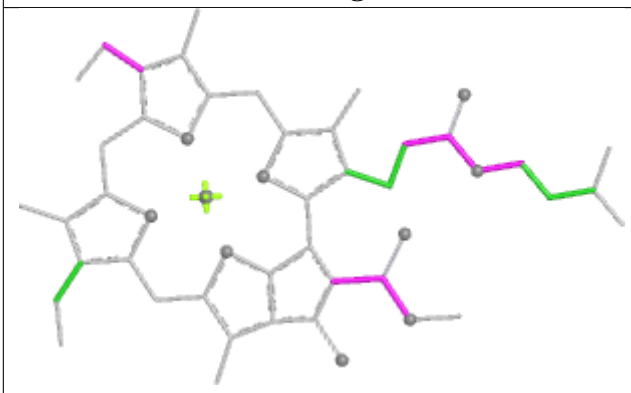
Ligand CLA W 502



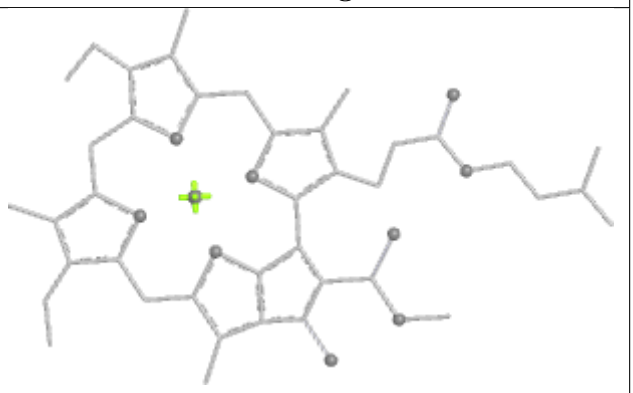
Bond lengths



Bond angles

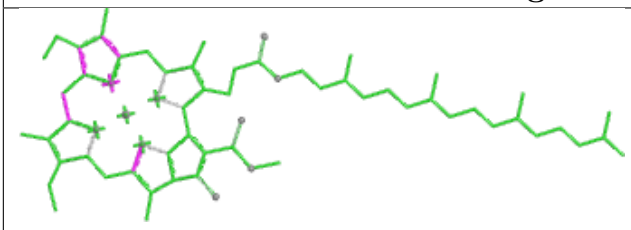


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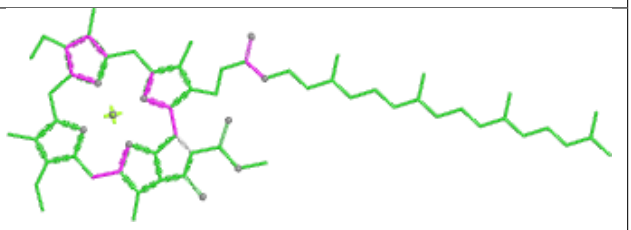


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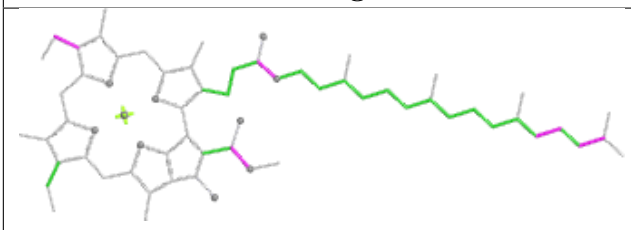
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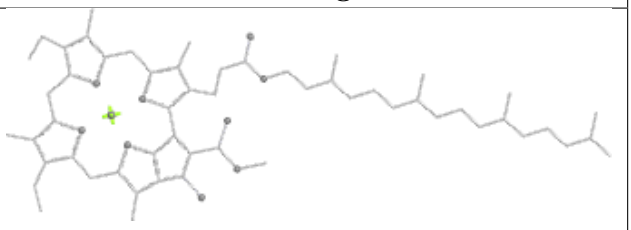
Bond lengths



Bond angles

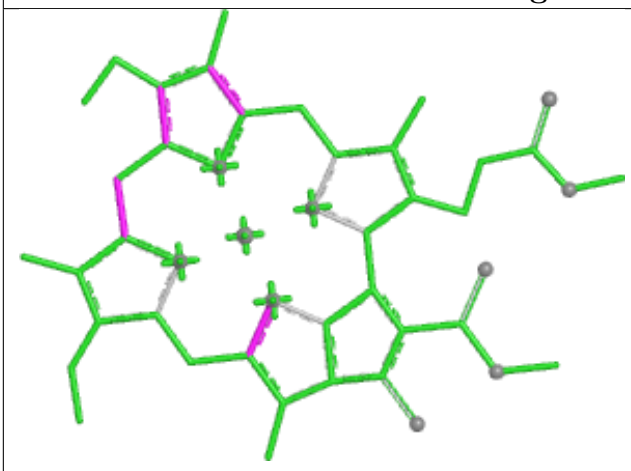


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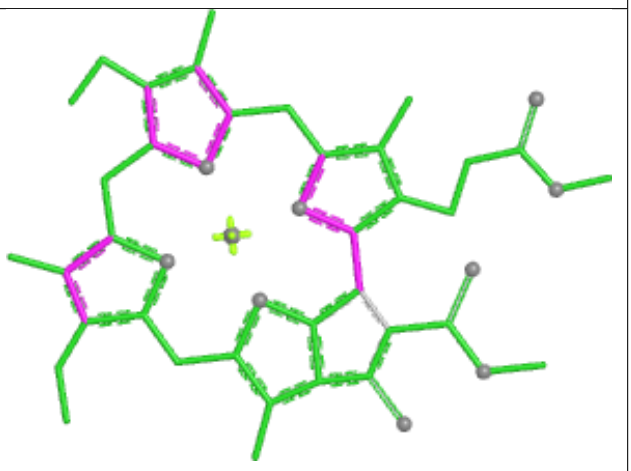


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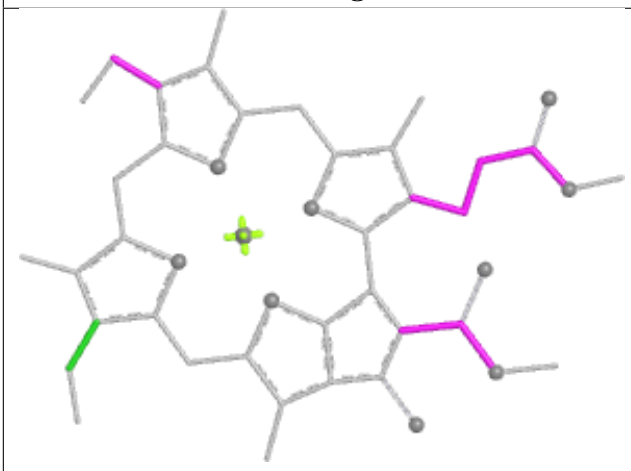
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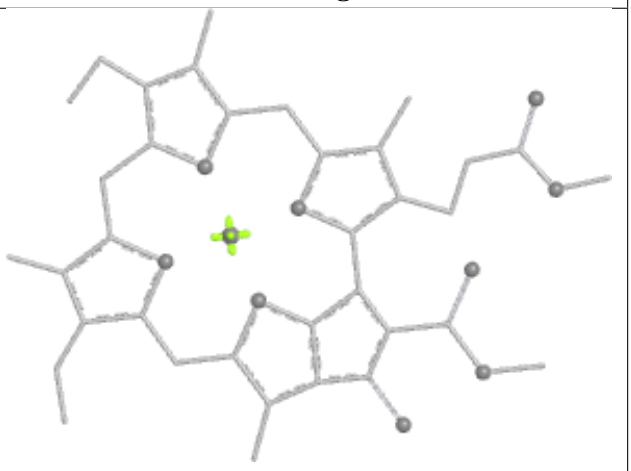
Bond lengths



Bond angles

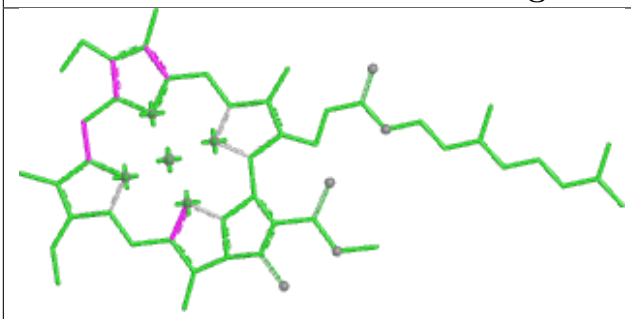


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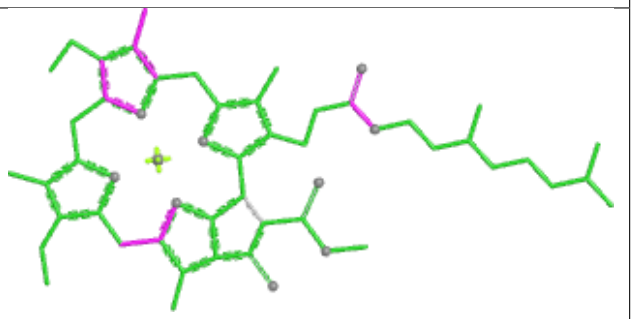


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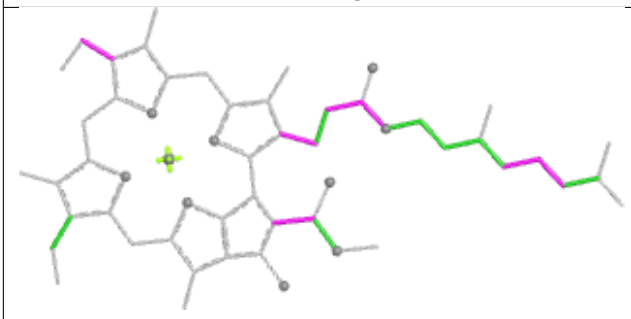
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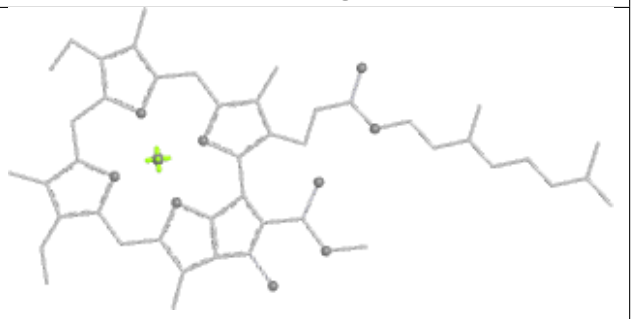
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Bond angles

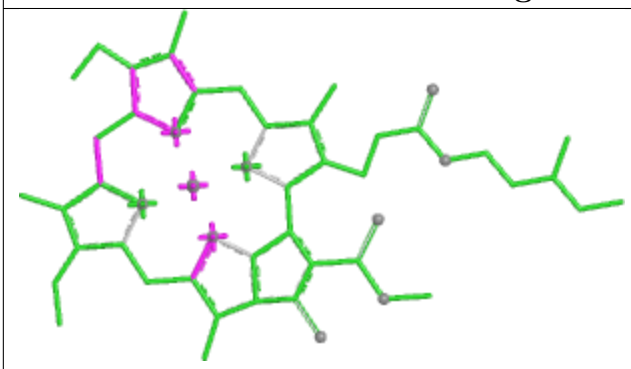


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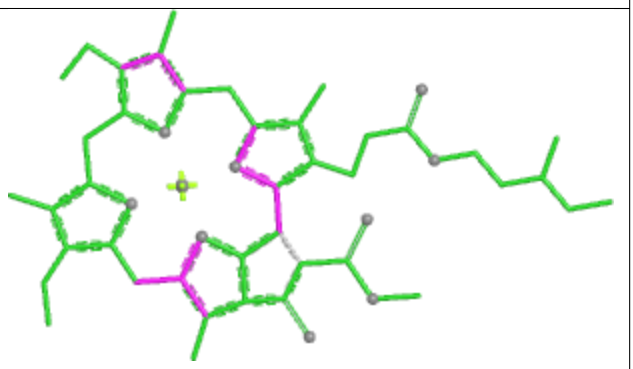


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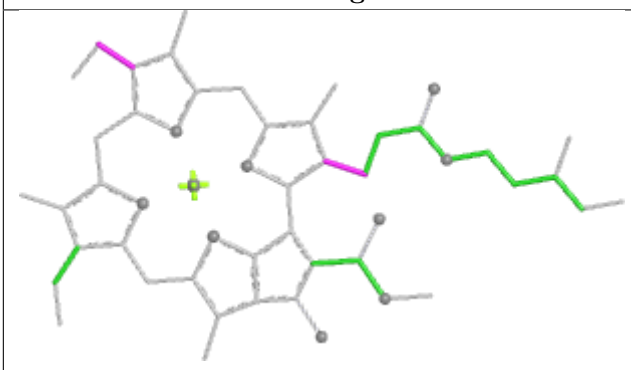
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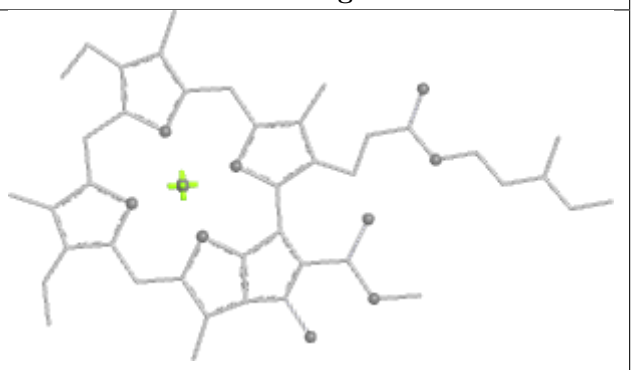
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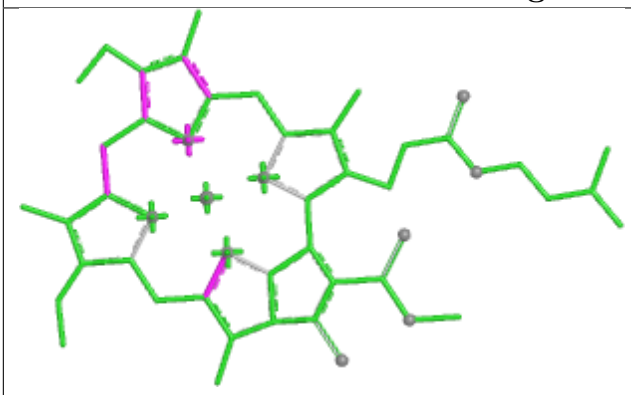


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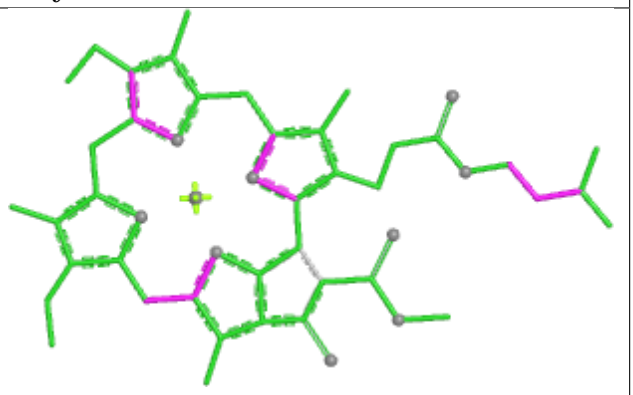


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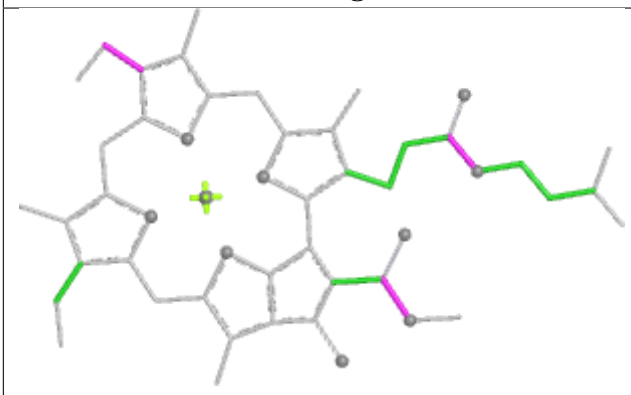
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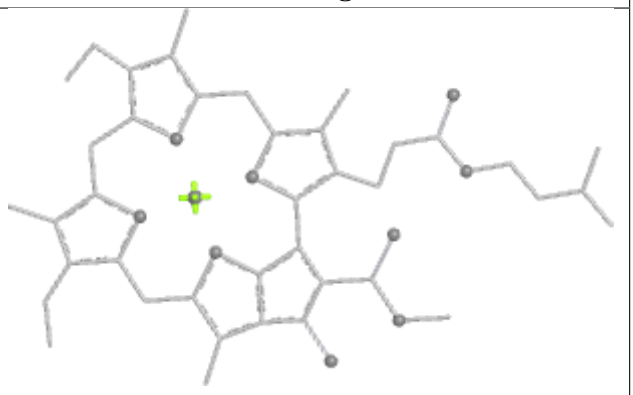
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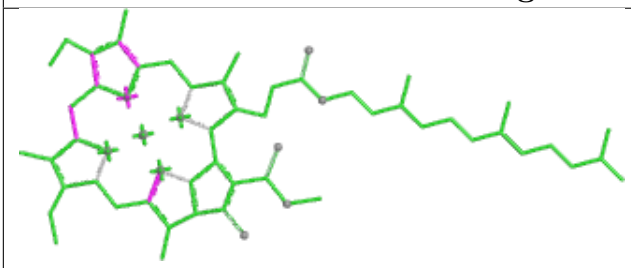


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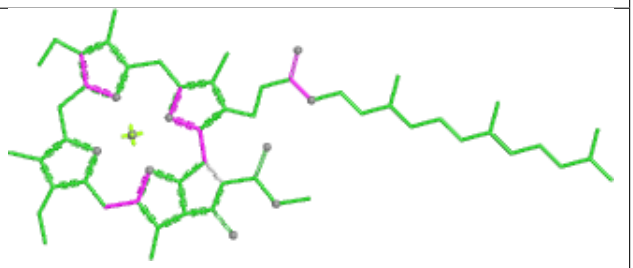


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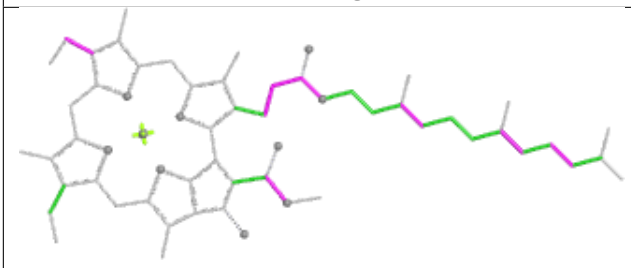
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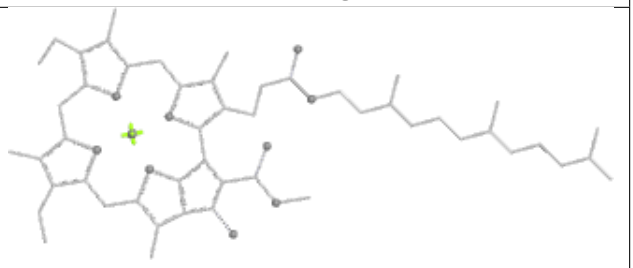
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Bond angles

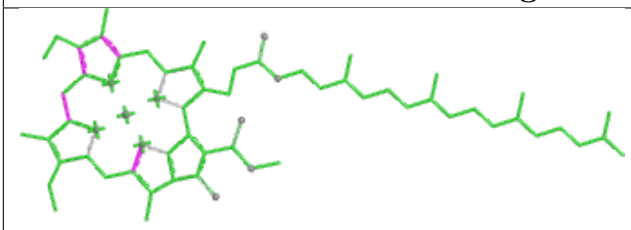


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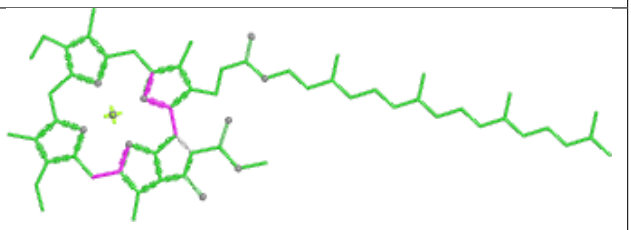


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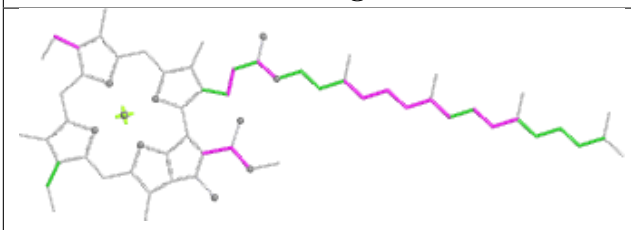
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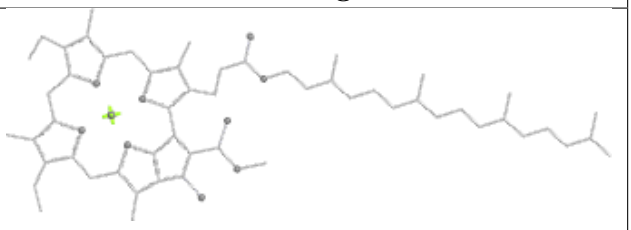
Bond lengths



Bond angles

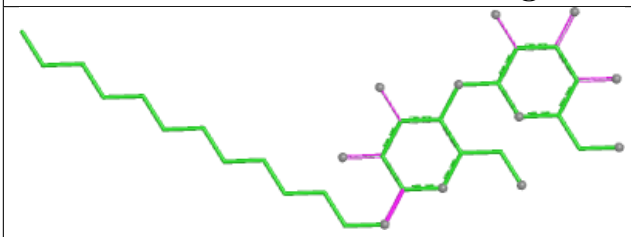


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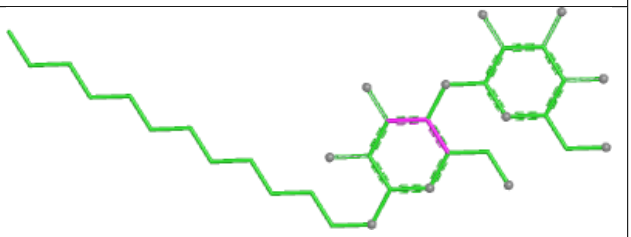


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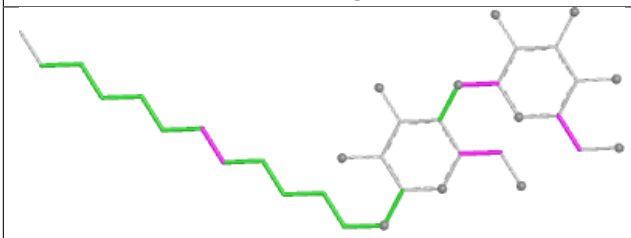
Ligand LMT l 4101



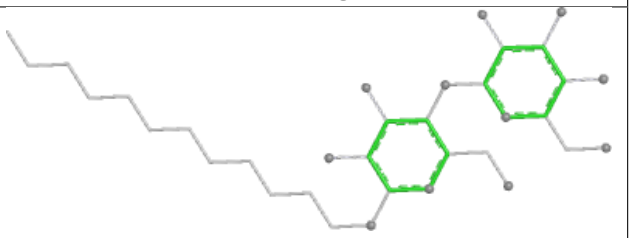
Bond lengths



Bond angles

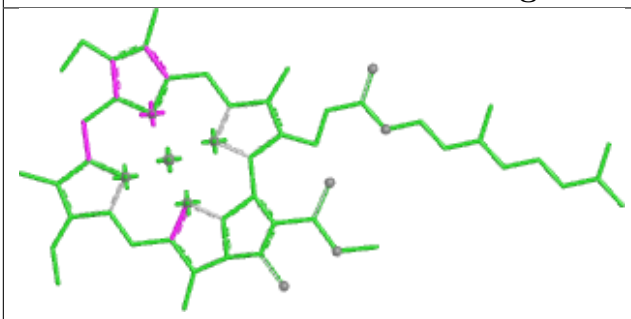


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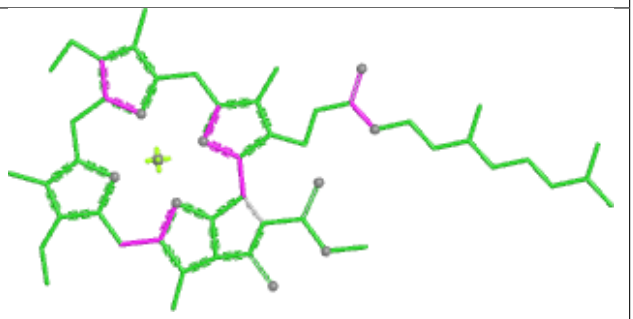


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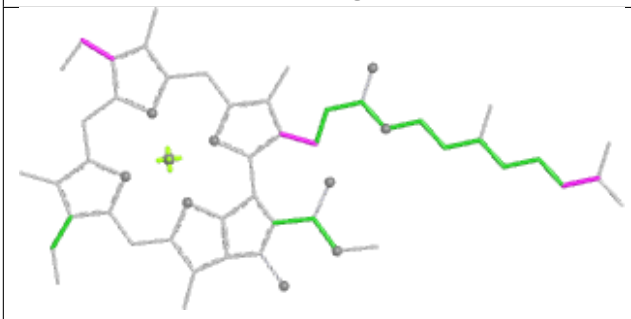
Ligand CLA a 1139



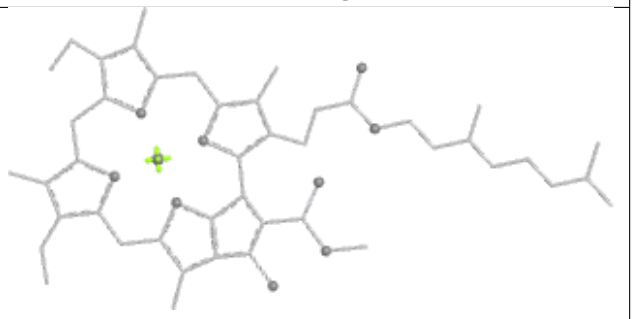
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Bond angles

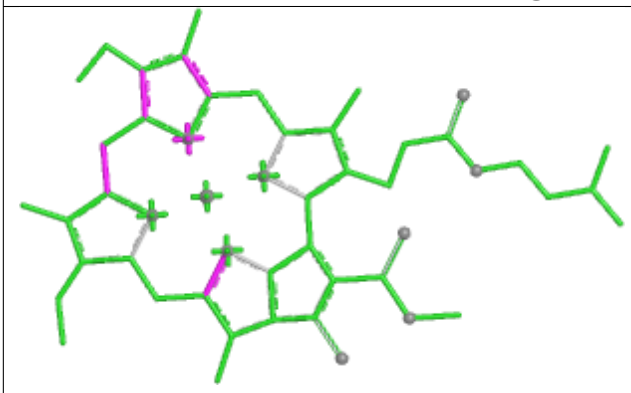


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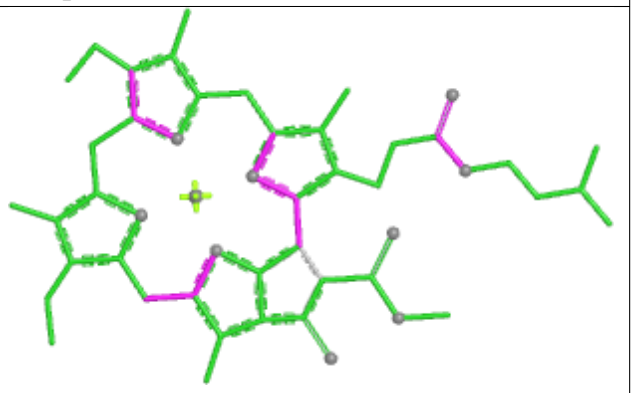


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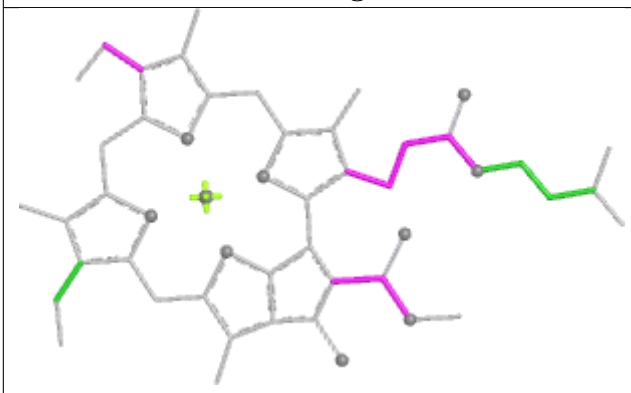
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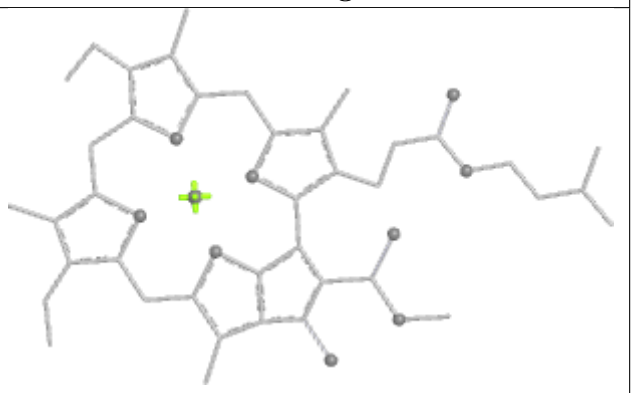
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Bond angles

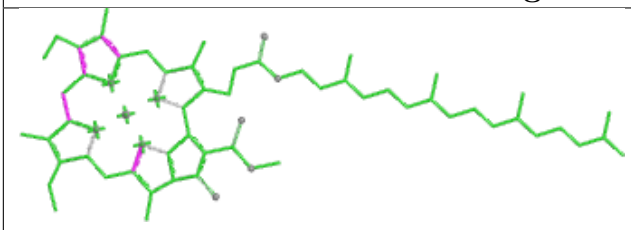


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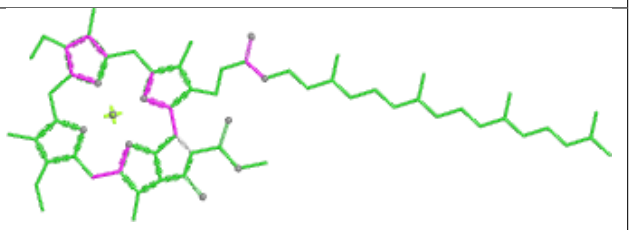


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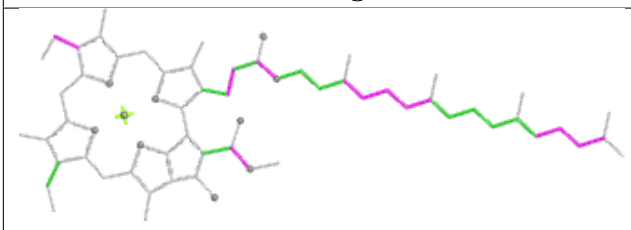
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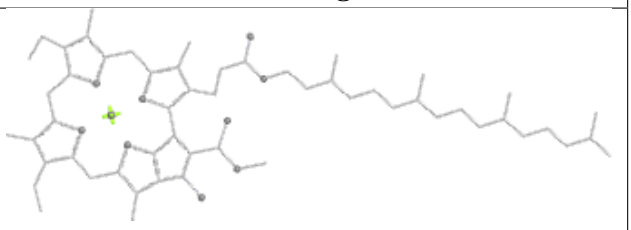
Bond lengths



Bond angles

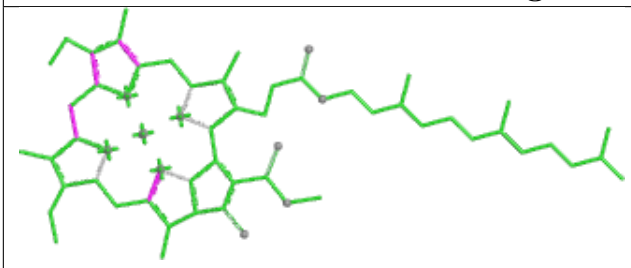


Torsions

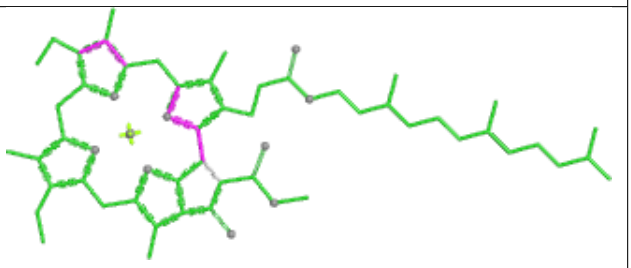


Rings

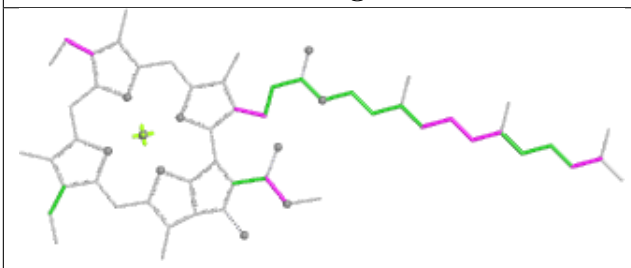
Ligand CLA Z 510



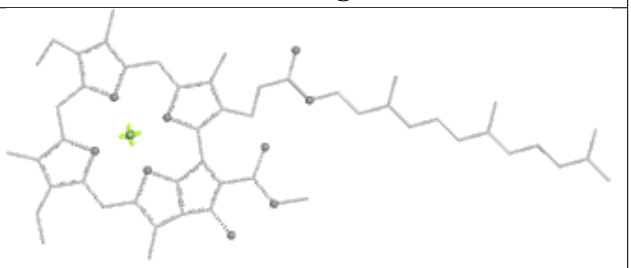
Bond lengths



Bond angles

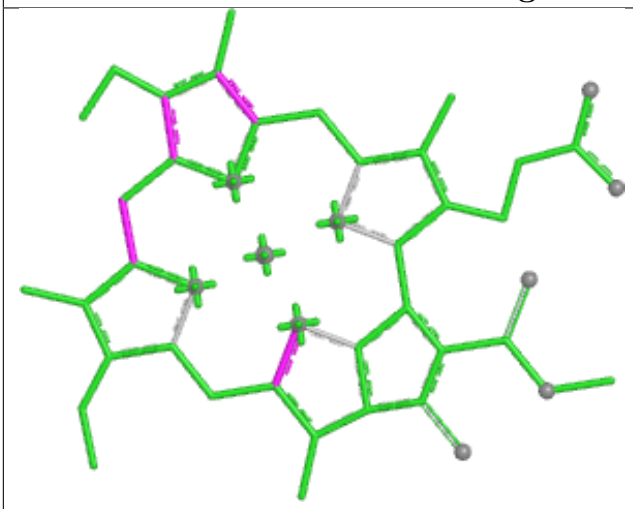


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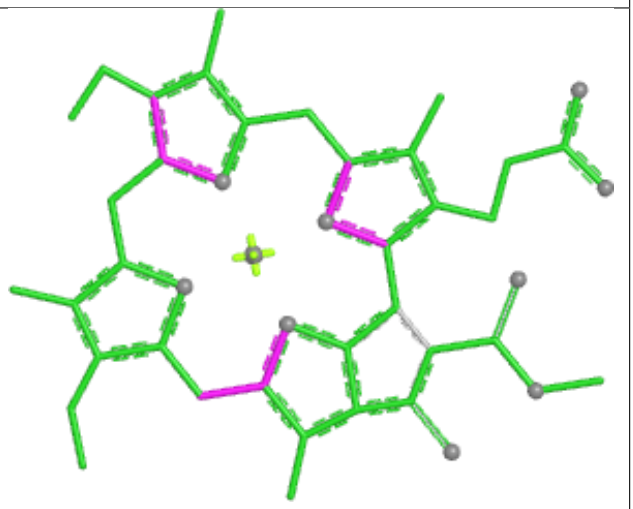


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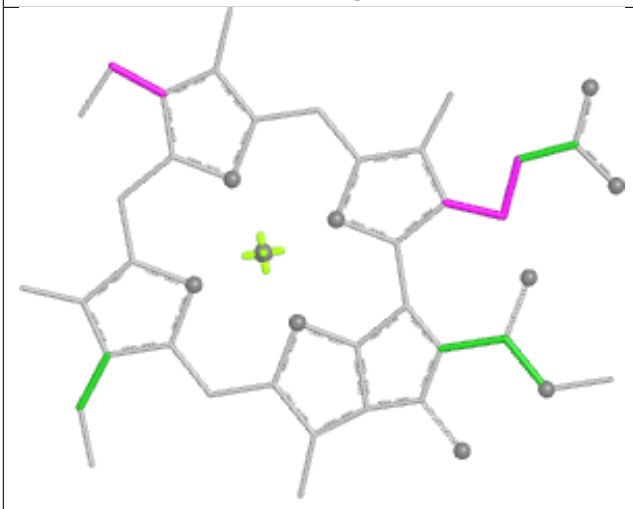
Ligand CLA b 1209



Bond lengths



Bond angles

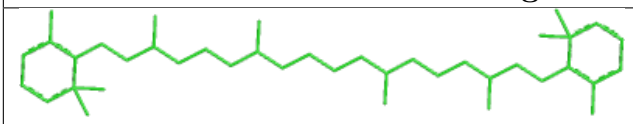


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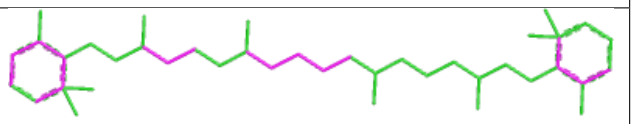


Rings

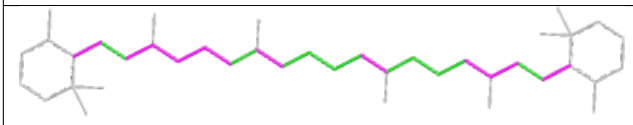
Ligand BCR i 4018



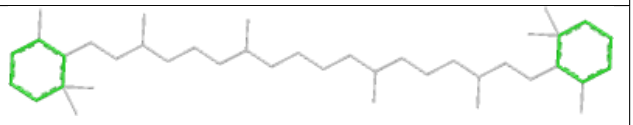
Bond lengths



Bond angles

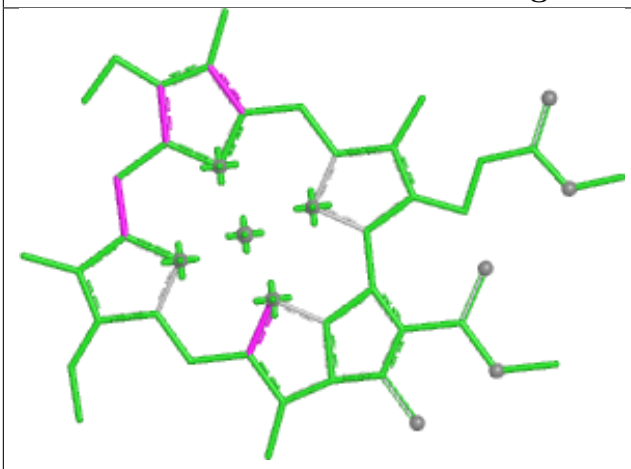


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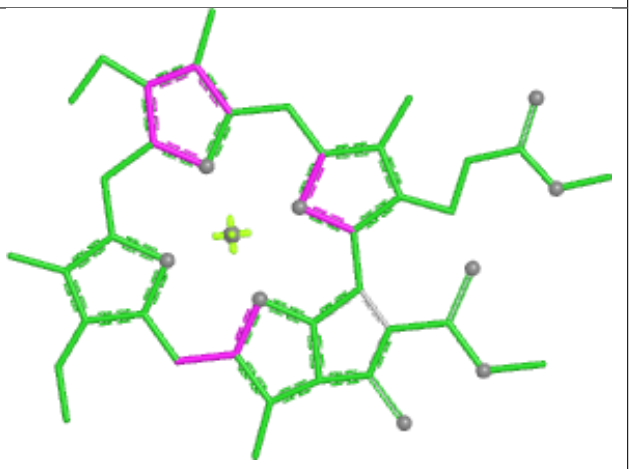


Rings

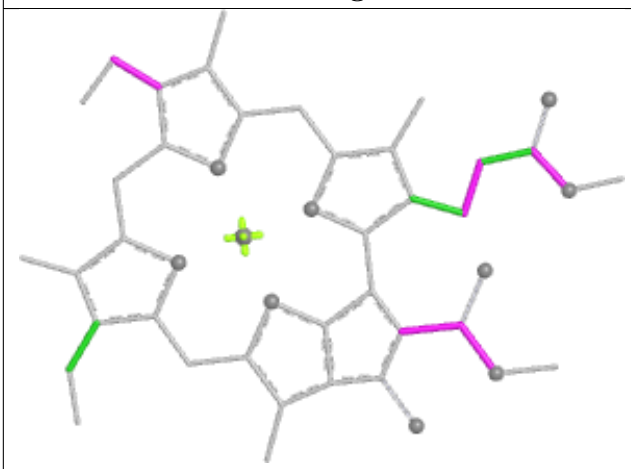
Ligand CLA t 516



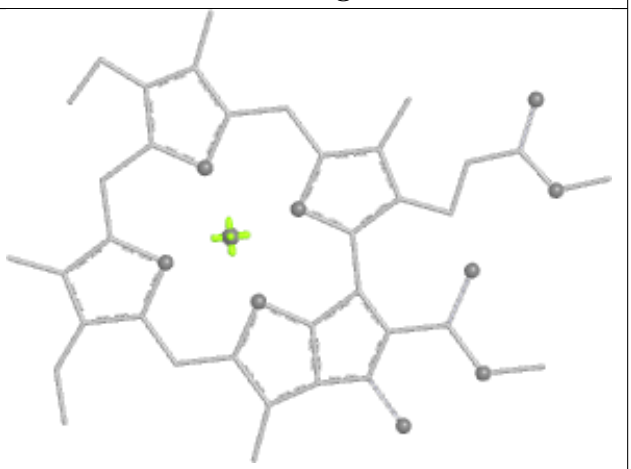
Bond lengths



Bond angles

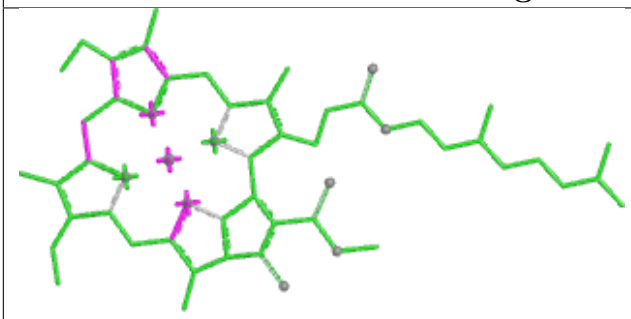


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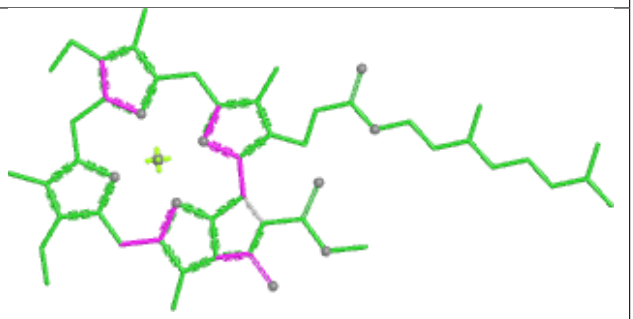


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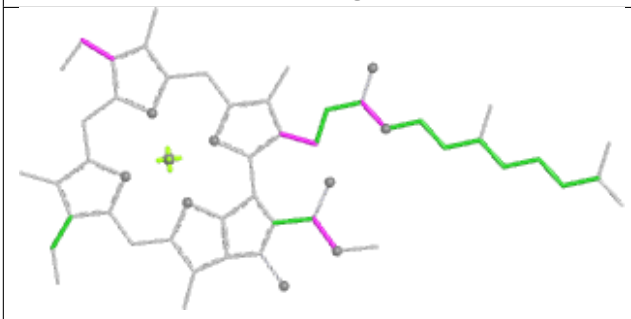
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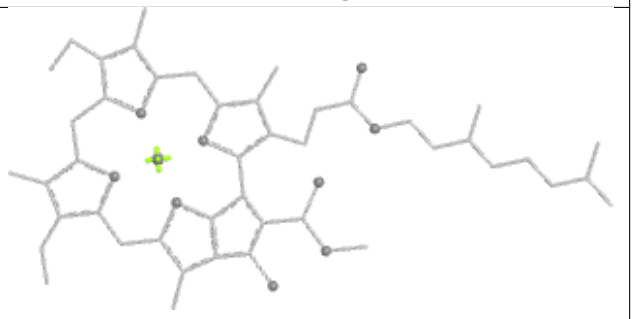
Bond lengths



Bond angles

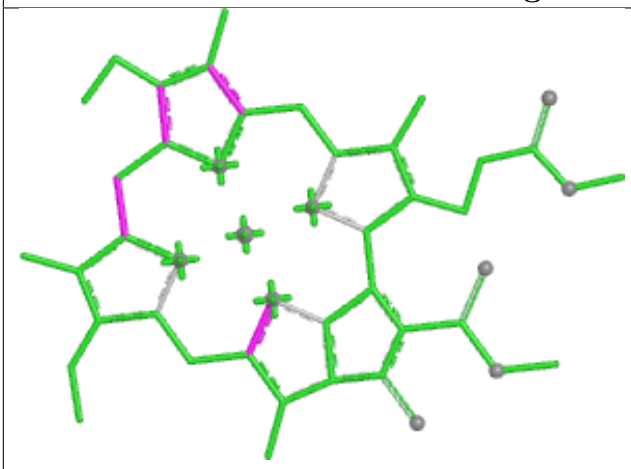


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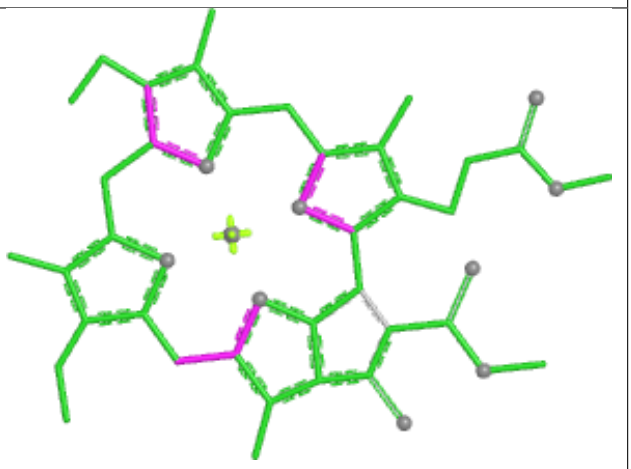


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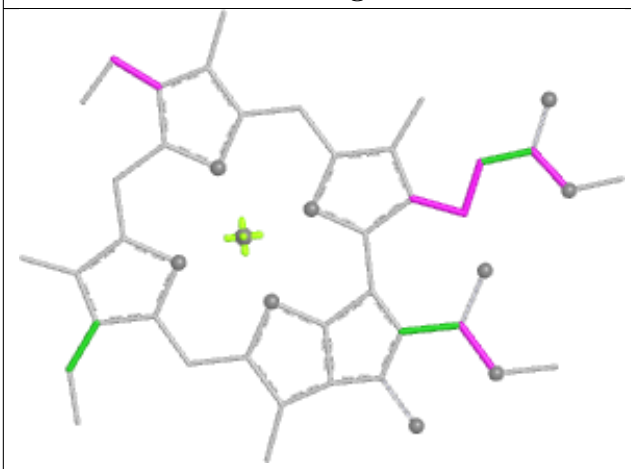
Ligand CLA X 513



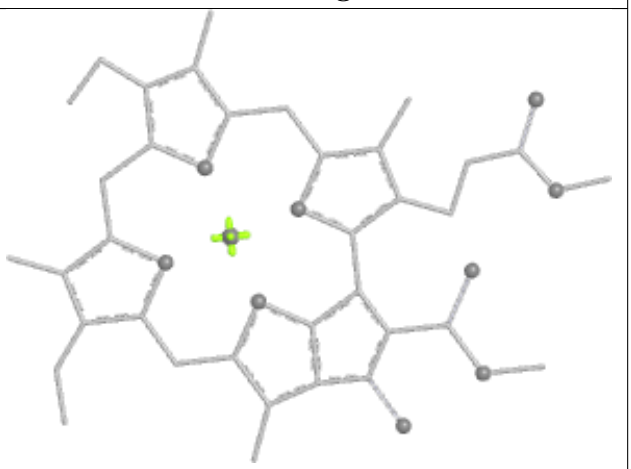
Bond lengths



Bond angles

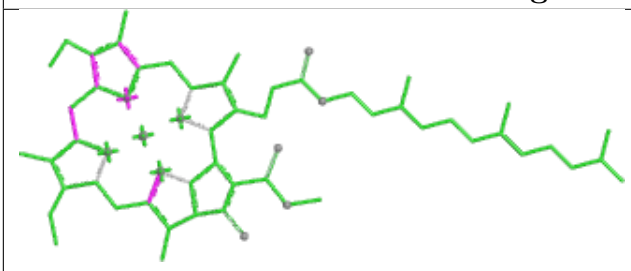


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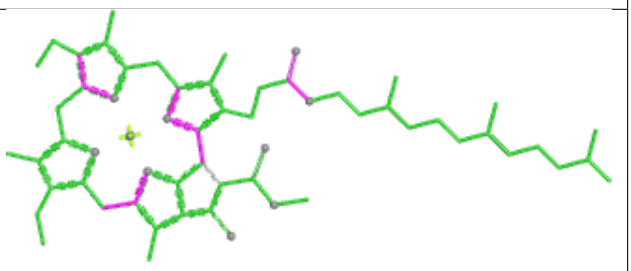


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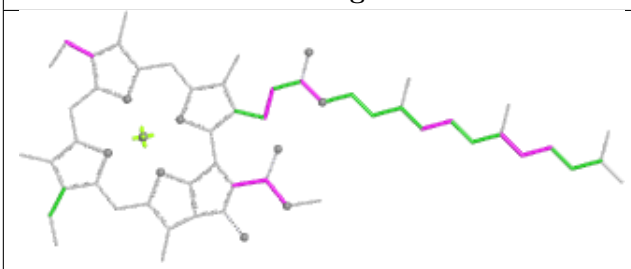
Ligand CLA t 506



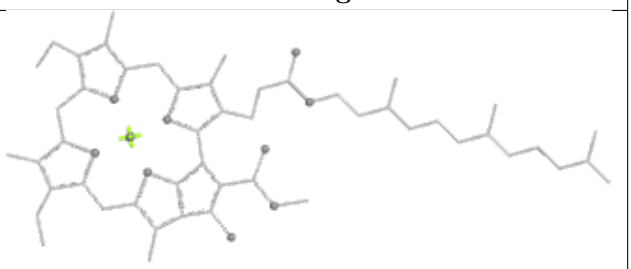
Bond lengths



Bond angles

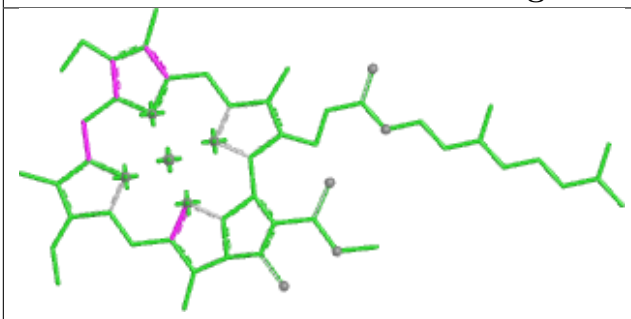


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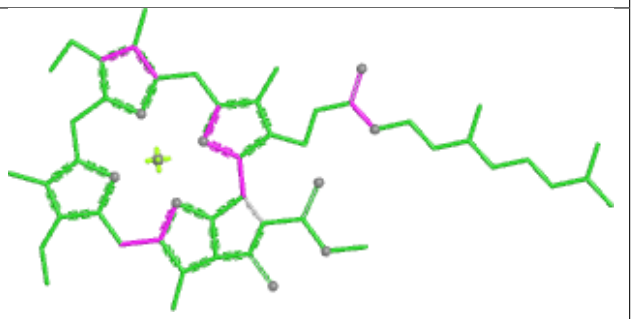


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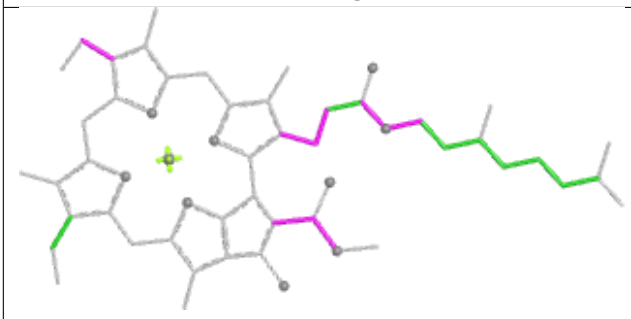
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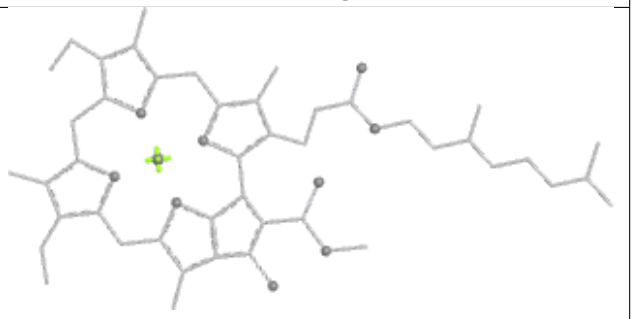
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Bond angles

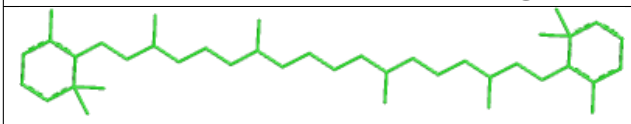


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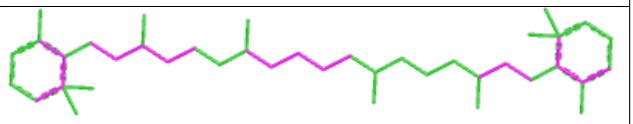


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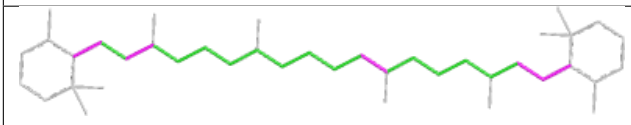
Ligand BCR J 4015



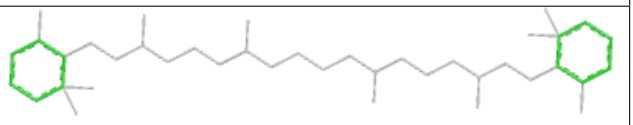
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Bond angles

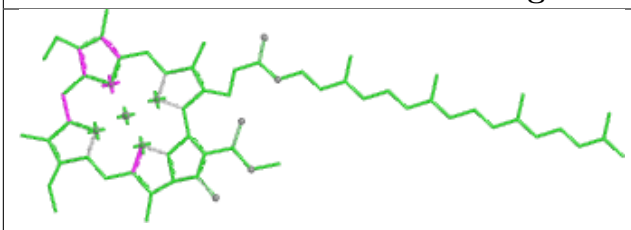


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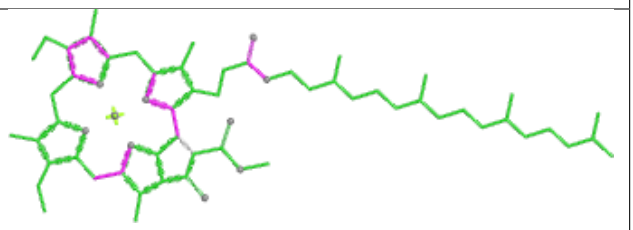


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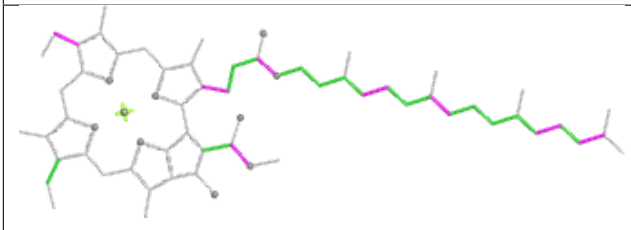
Ligand CLA x 509



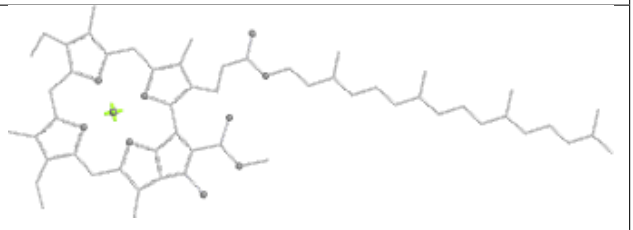
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Bond angles

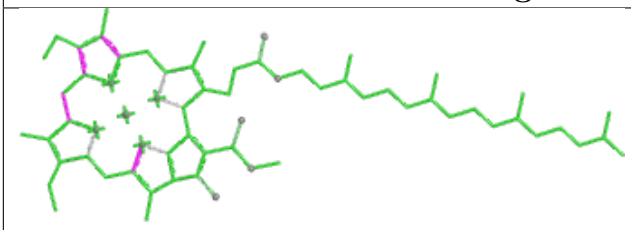


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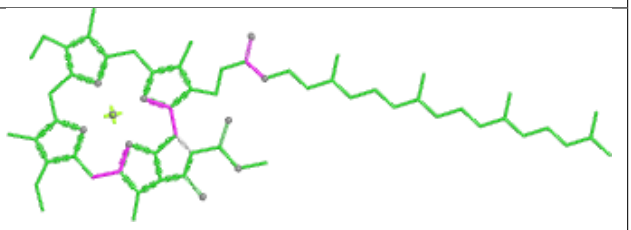


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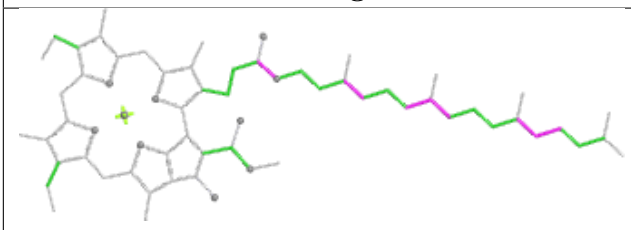
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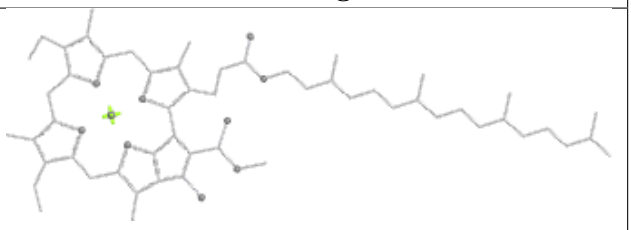
Bond lengths



Bond angles

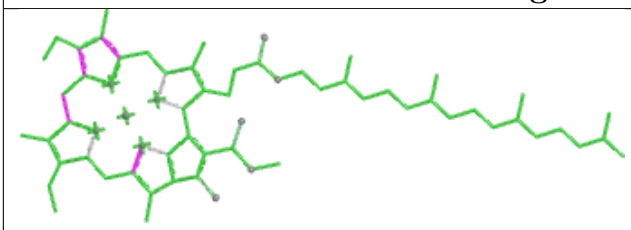


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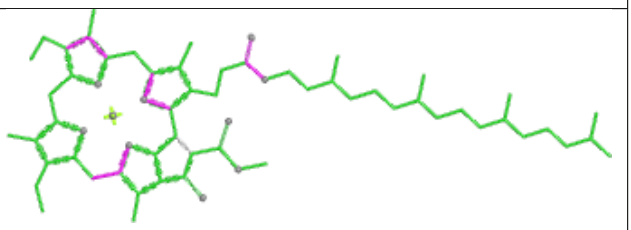


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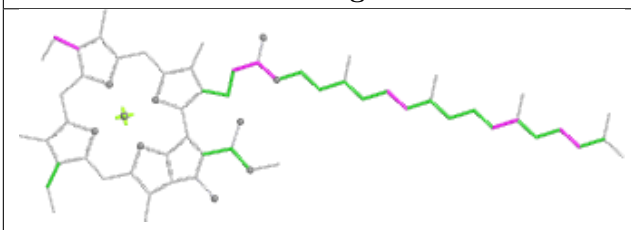
Ligand CLA s 510



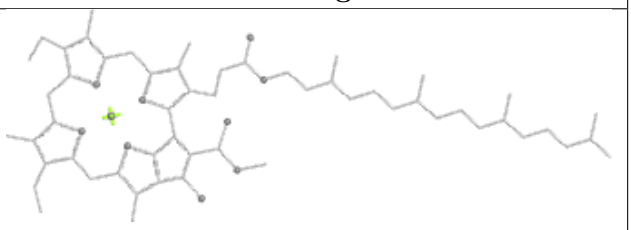
Bond lengths



Bond angles

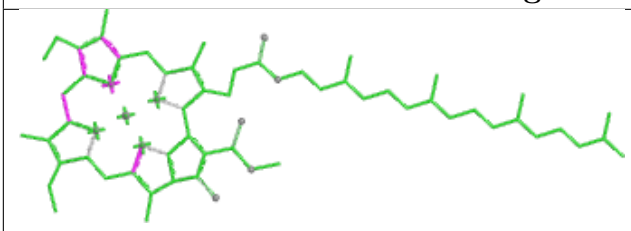


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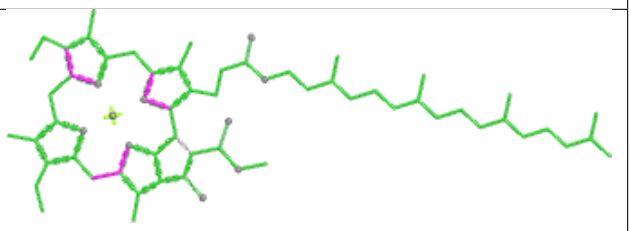


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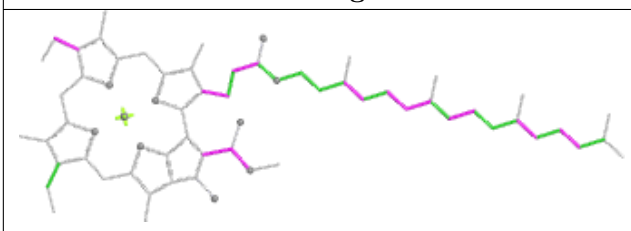
Ligand CLA Y 504



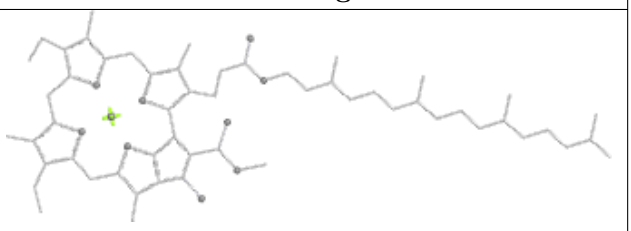
Bond lengths



Bond angles

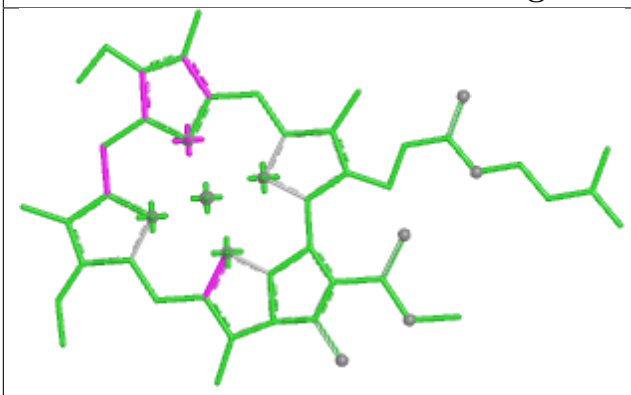


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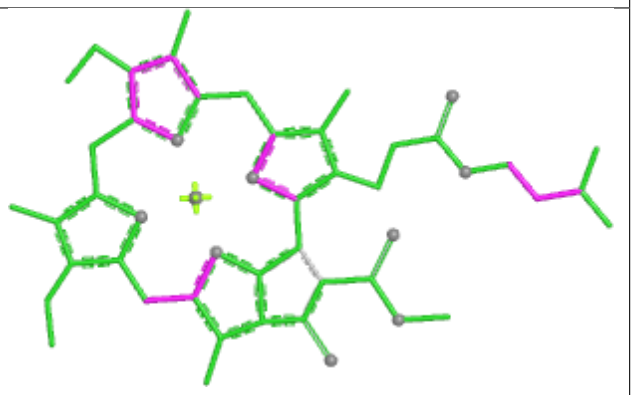


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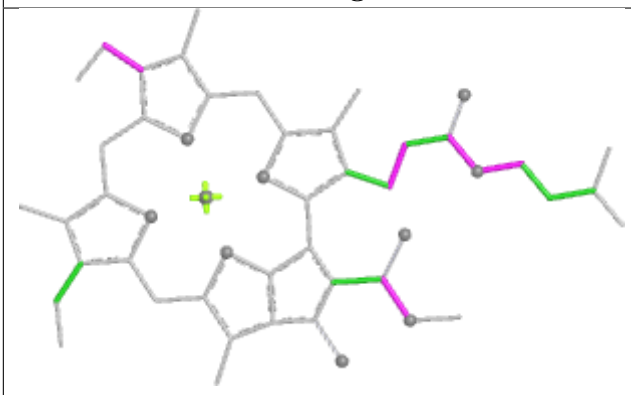
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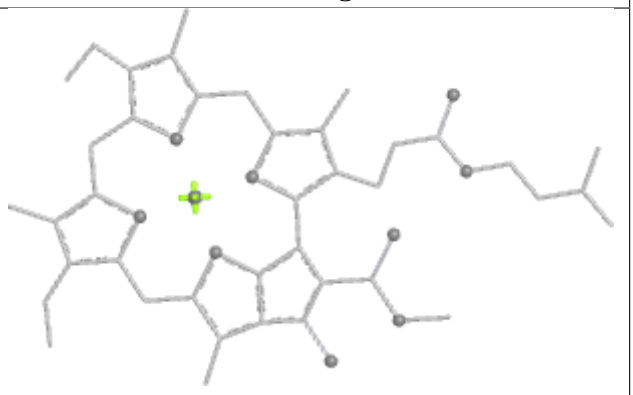
Bond lengths



Bond angles

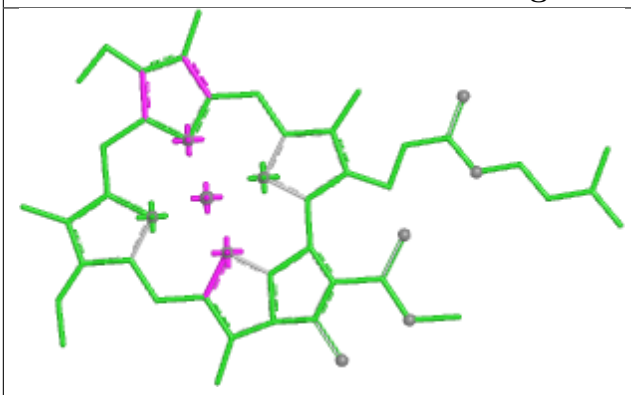


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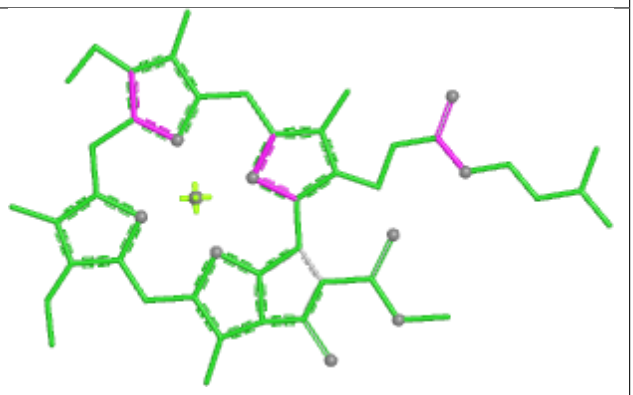


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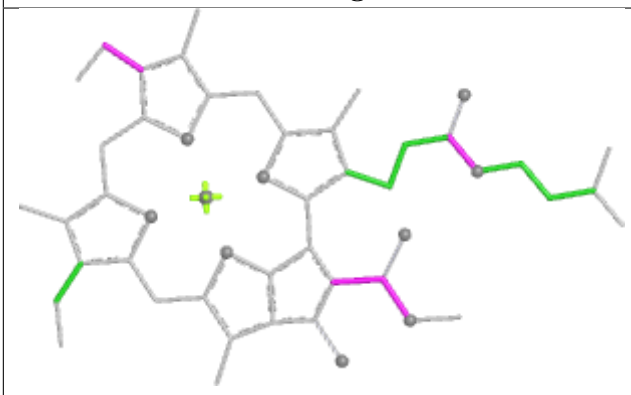
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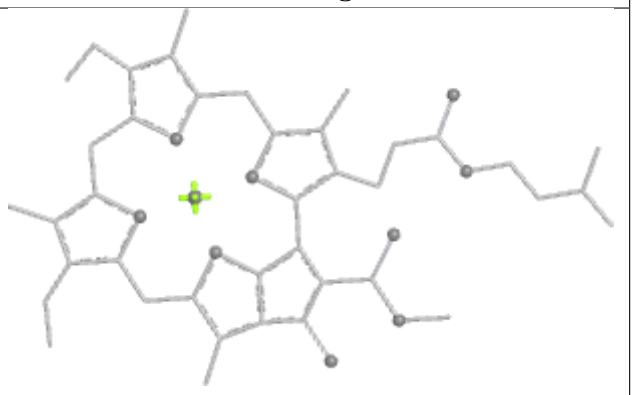
Bond lengths



Bond angles

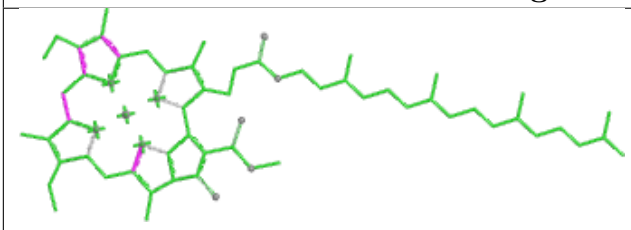


Torsions

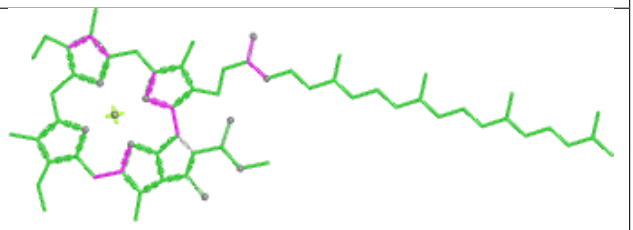


Rings

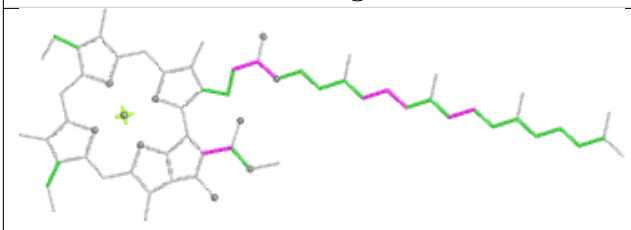
Ligand CLA t 510



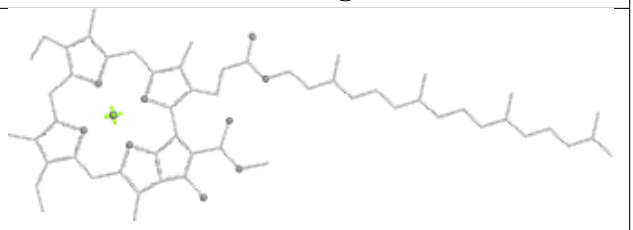
Bond lengths



Bond angles

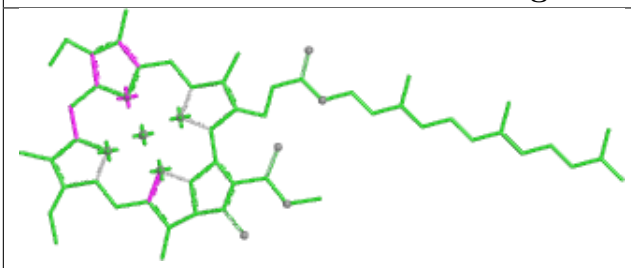


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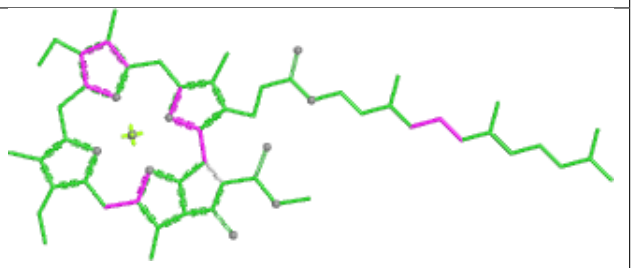


Rings

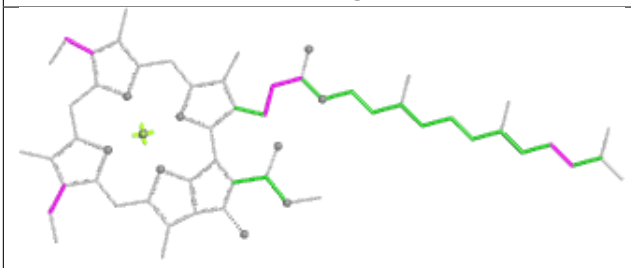
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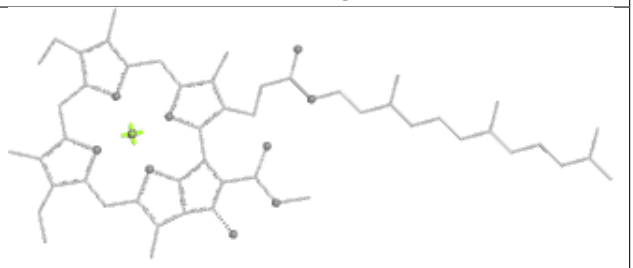
Bond lengths



Bond angles

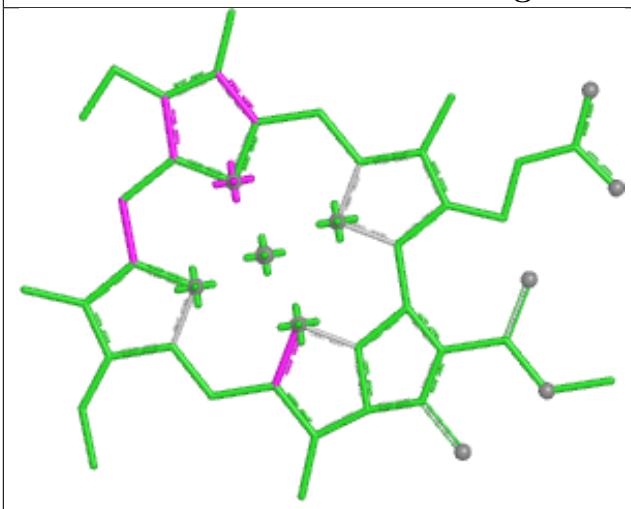


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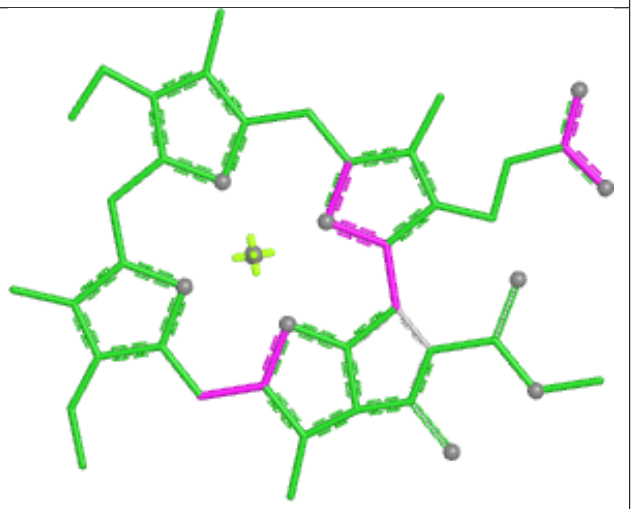


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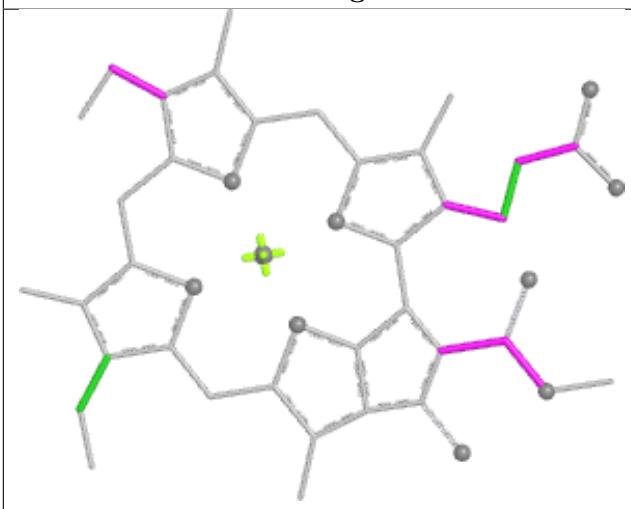
Ligand CLA G 1212



Bond lengths



Bond angles

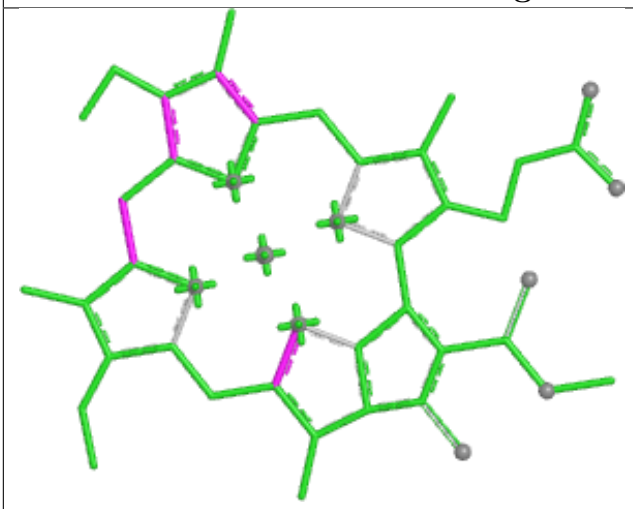


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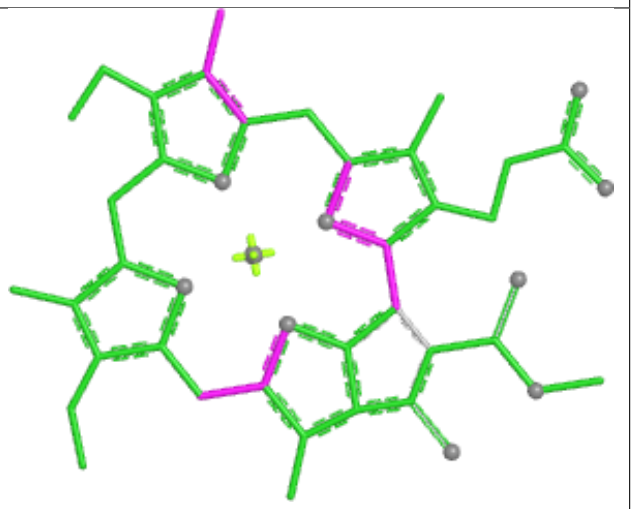


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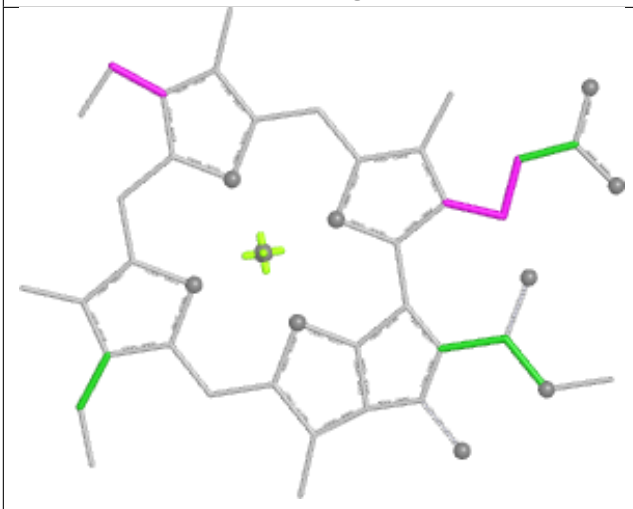
Ligand CLA G 1231



Bond lengths



Bond angles

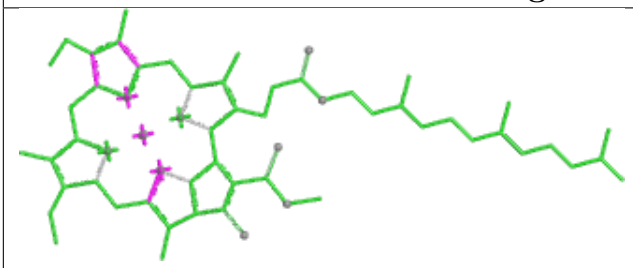


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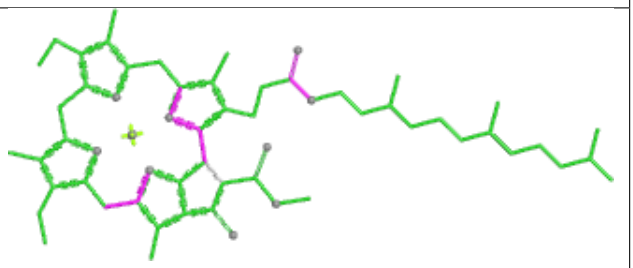


Rings

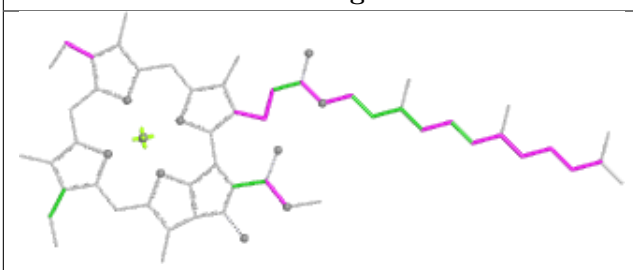
Ligand CLA o 506



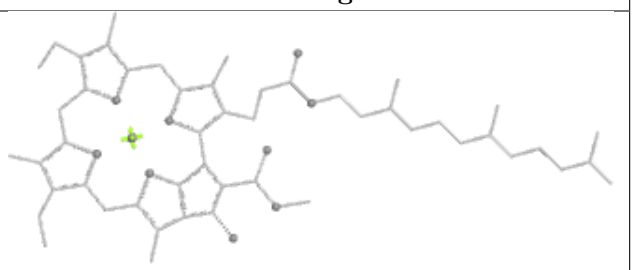
Bond lengths



Bond angles

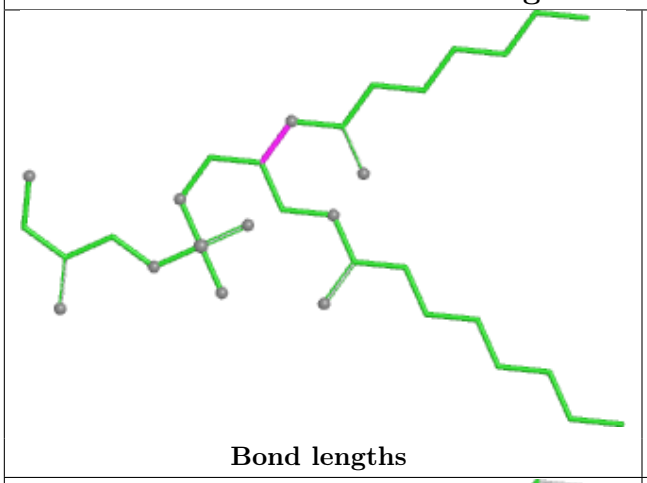


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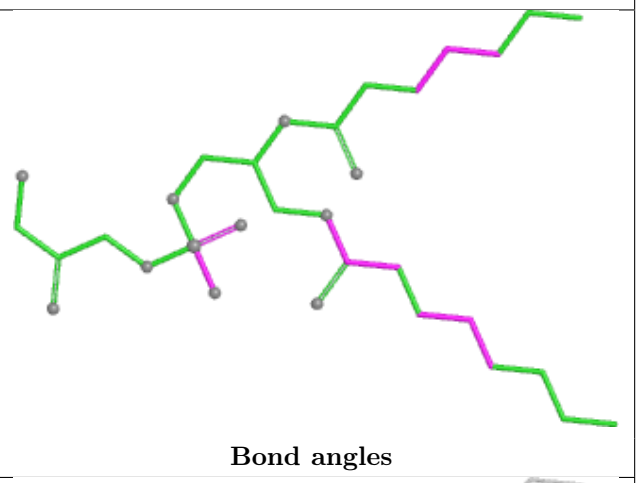


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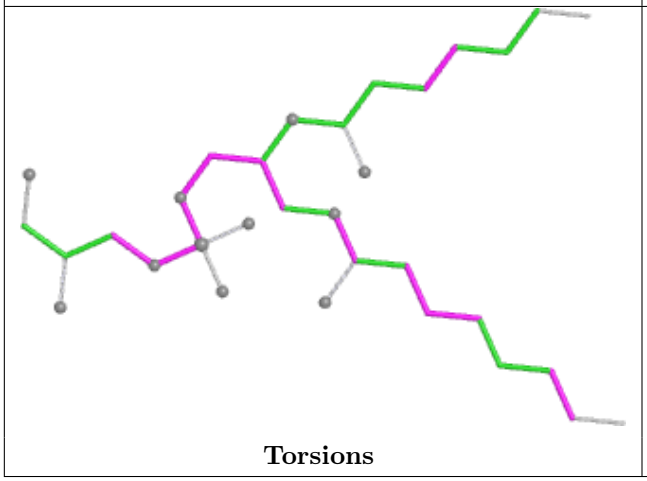
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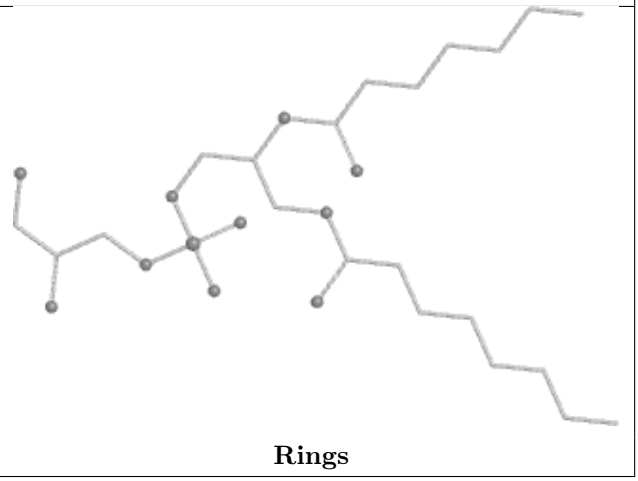
Bond lengths



Bond angles

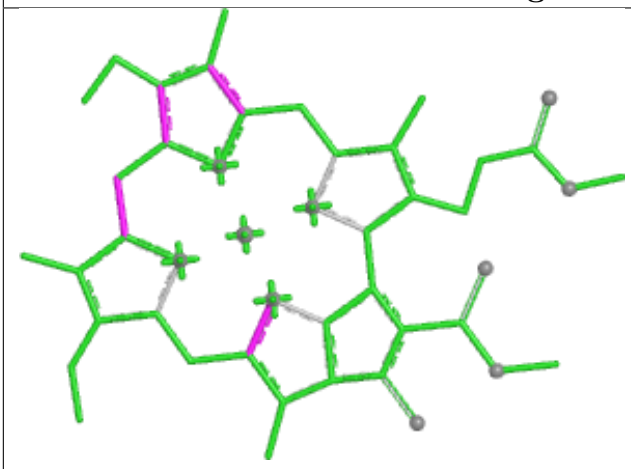


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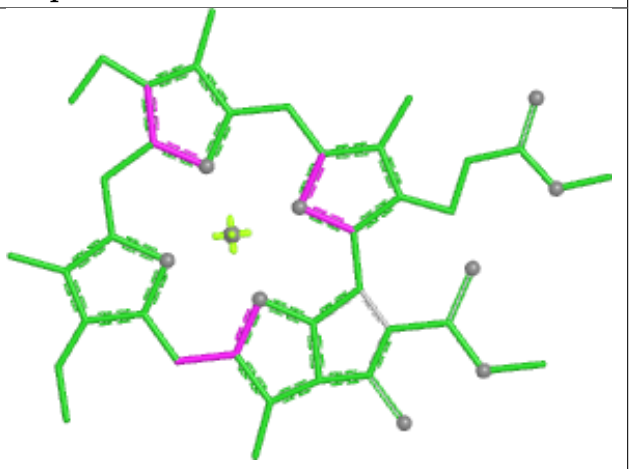


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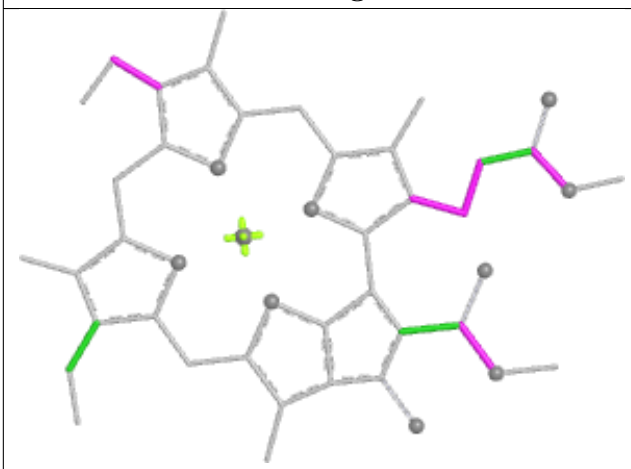
Ligand CLA p 516



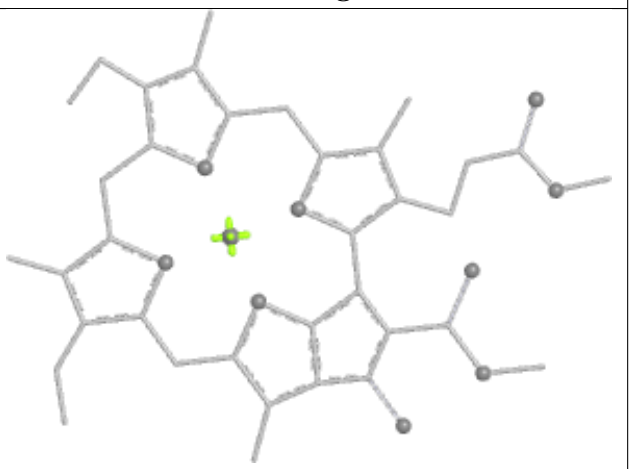
Bond lengths



Bond angles

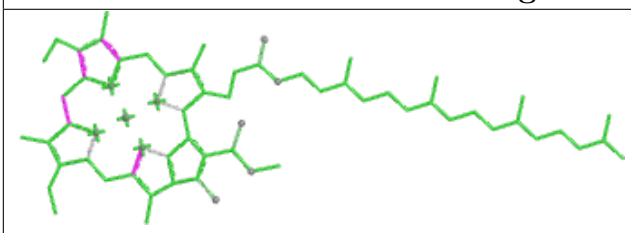


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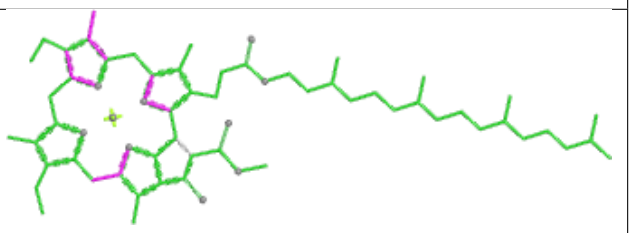


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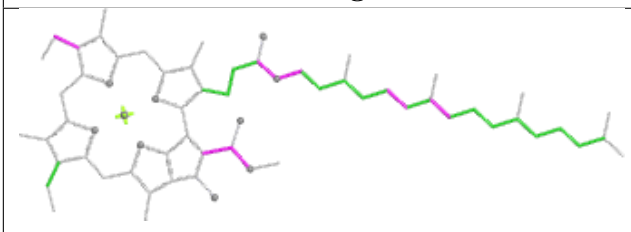
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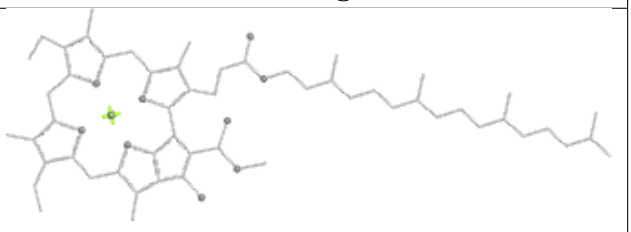
Bond lengths



Bond angles

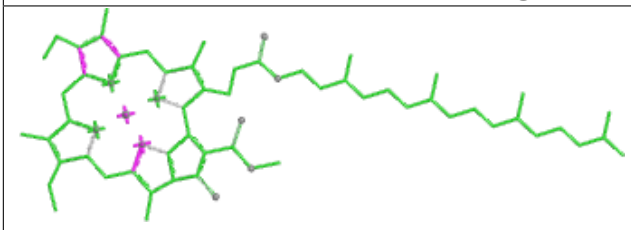


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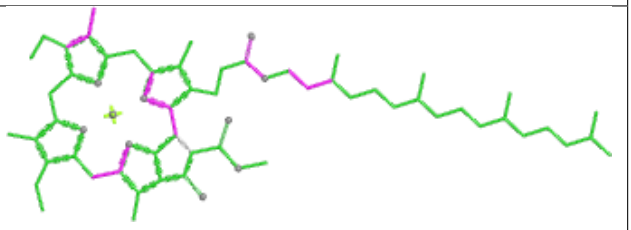


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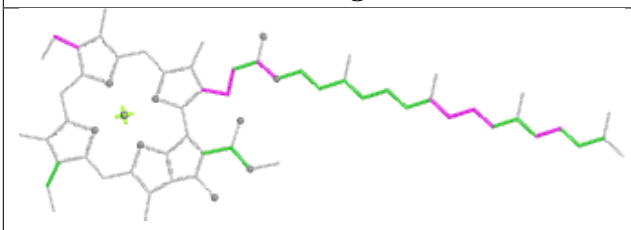
Ligand CLA A 1237



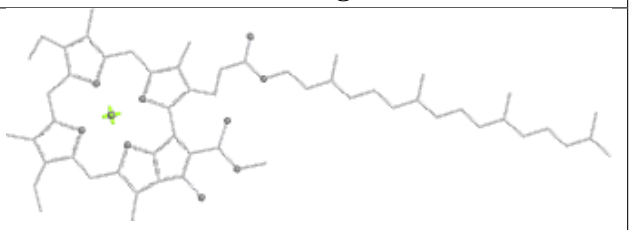
Bond lengths



Bond angles

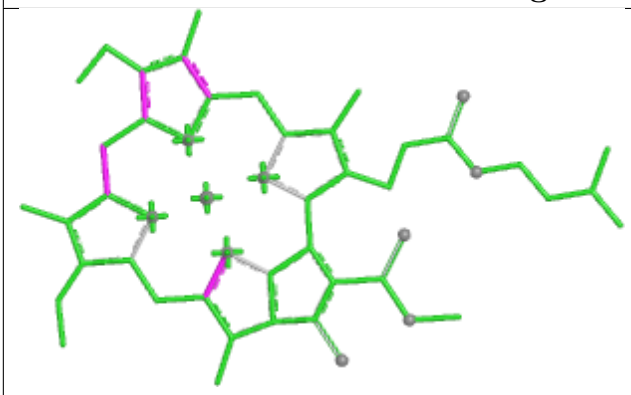


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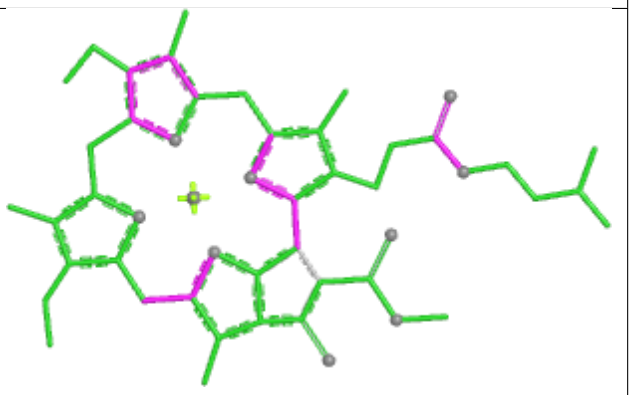


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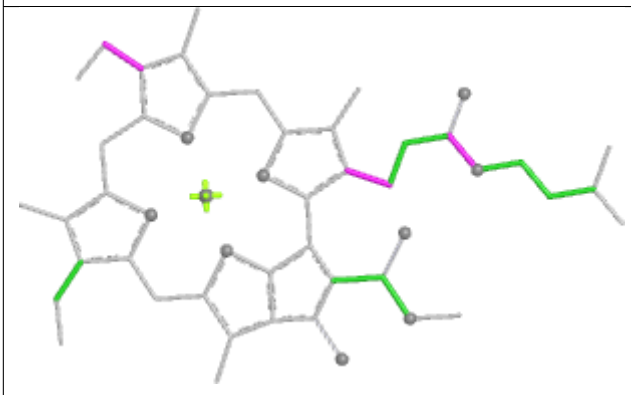
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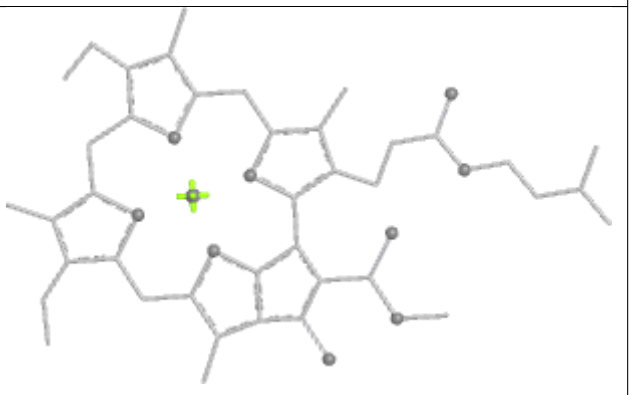
Bond lengths



Bond angles

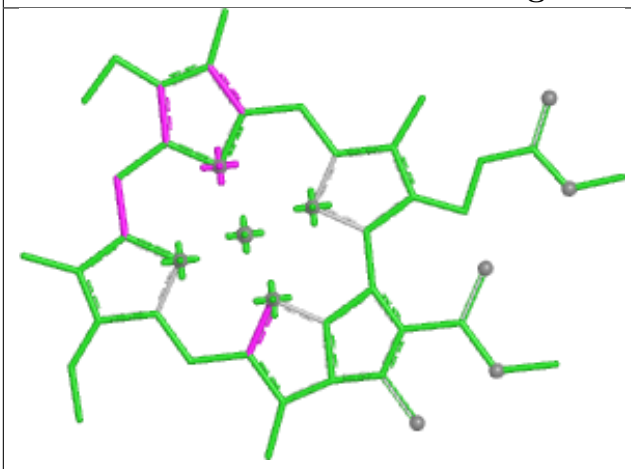


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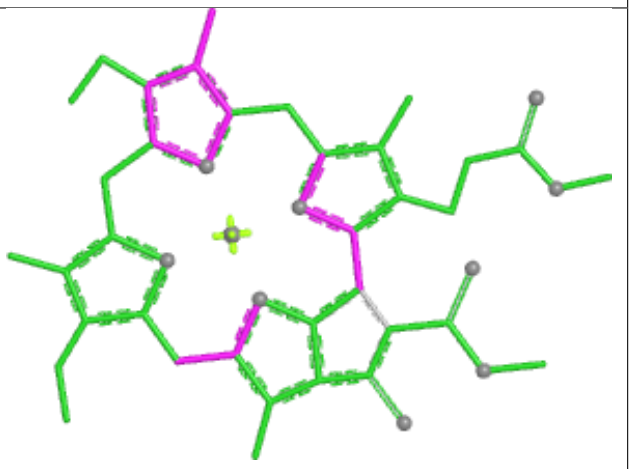


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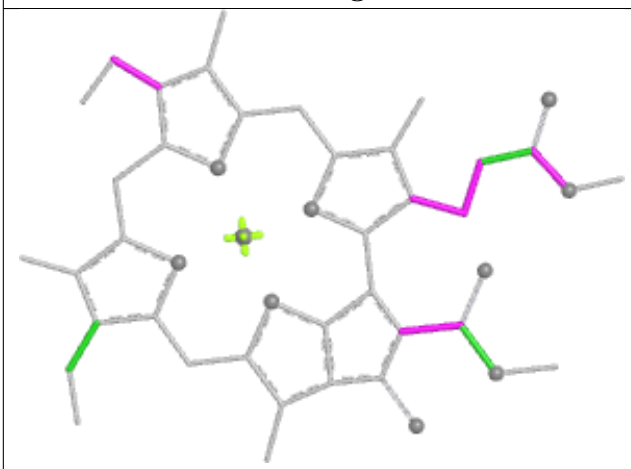
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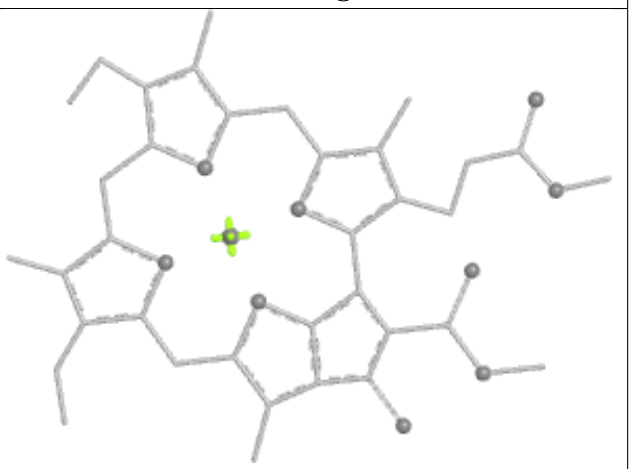
Bond lengths



Bond angles

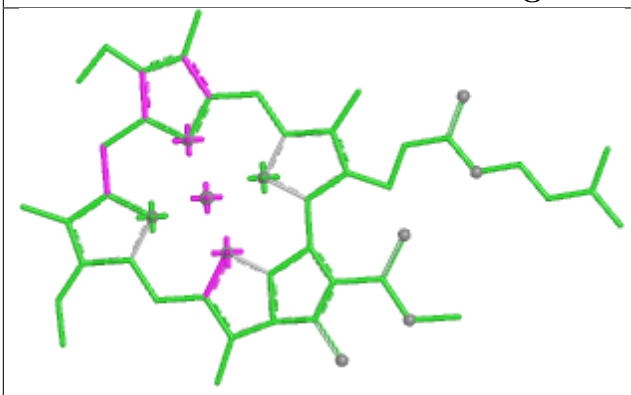


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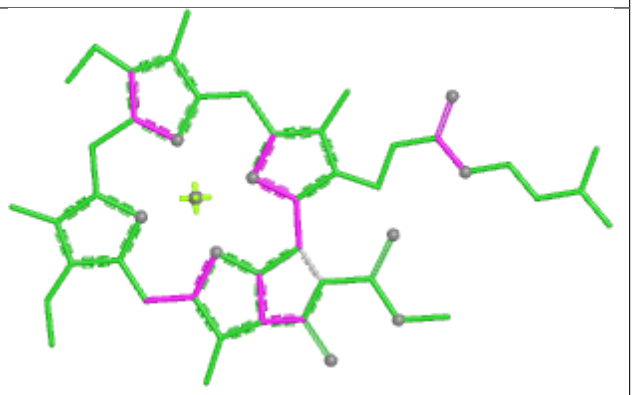


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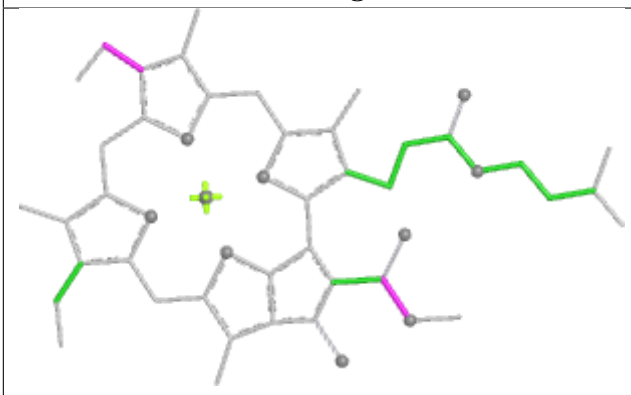
Ligand CLA X 514



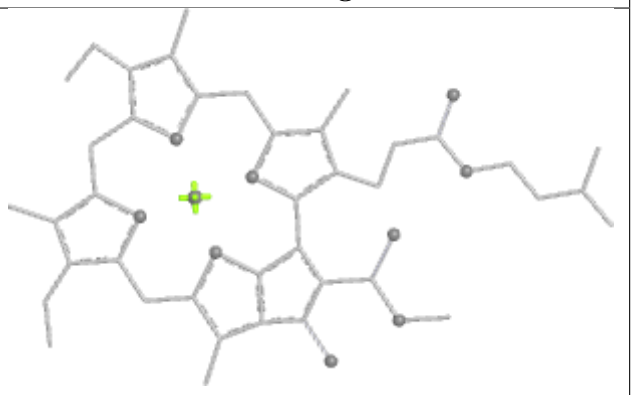
Bond lengths



Bond angles

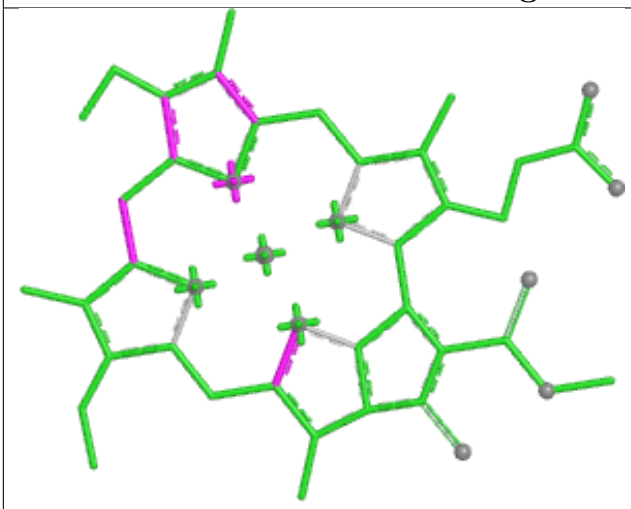


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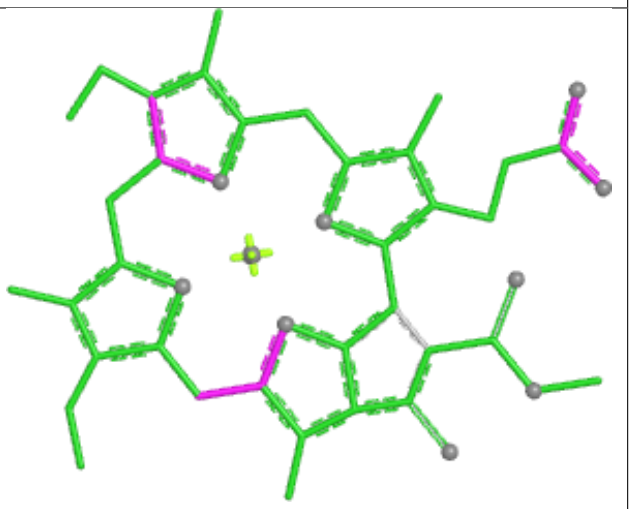


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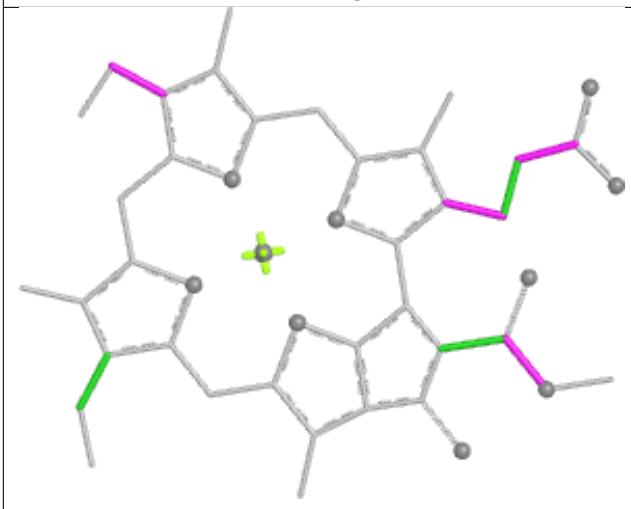
Ligand CLA a 1112



Bond lengths



Bond angles

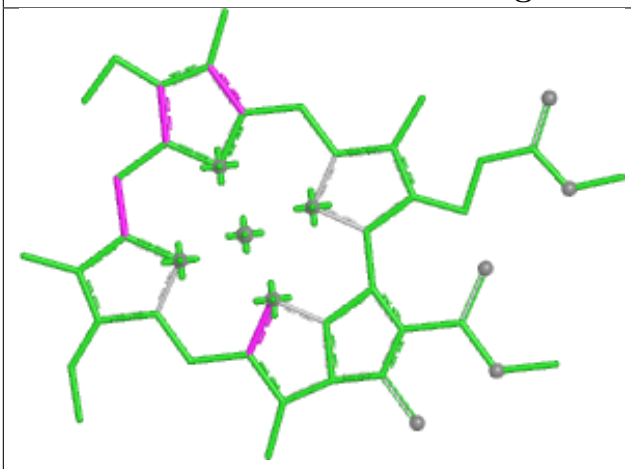


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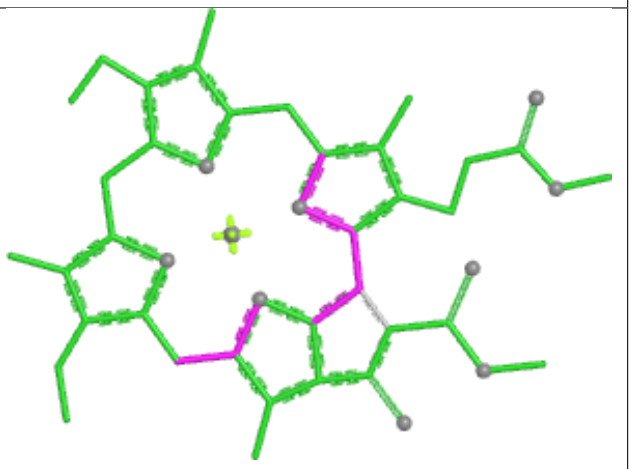


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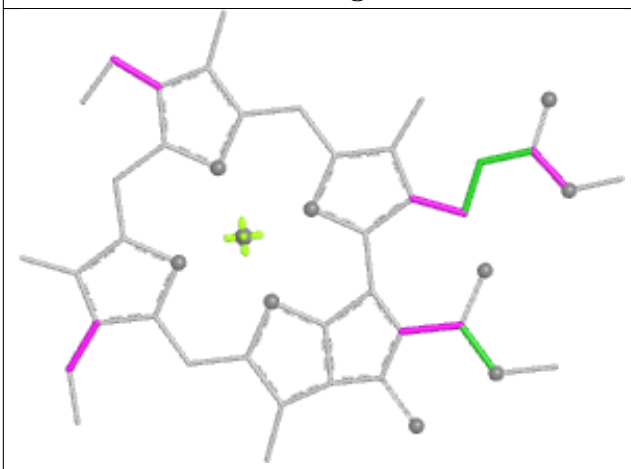
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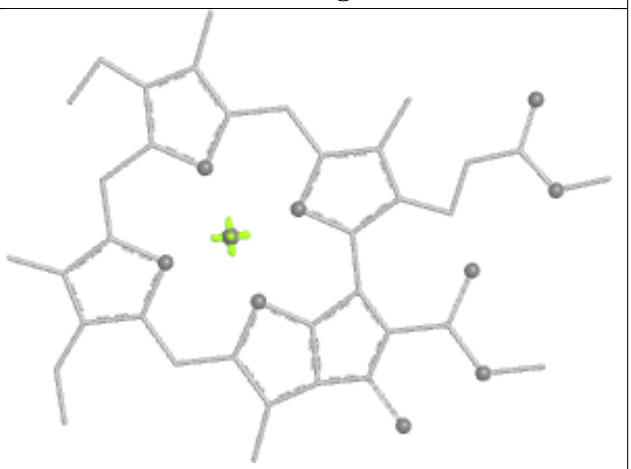
Bond lengths



Bond angles

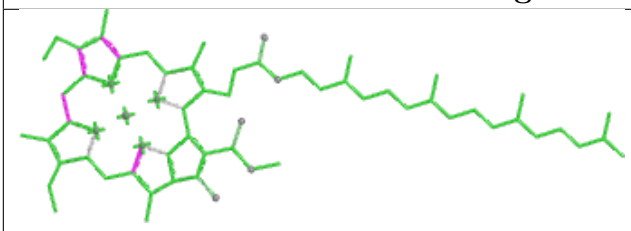


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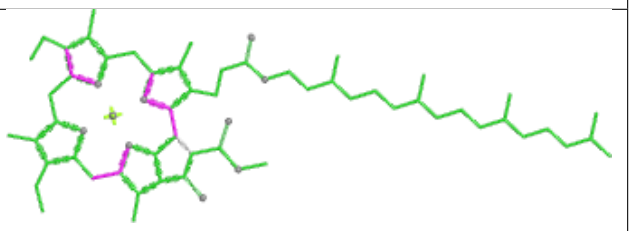


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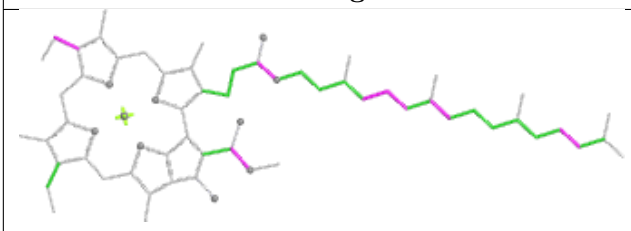
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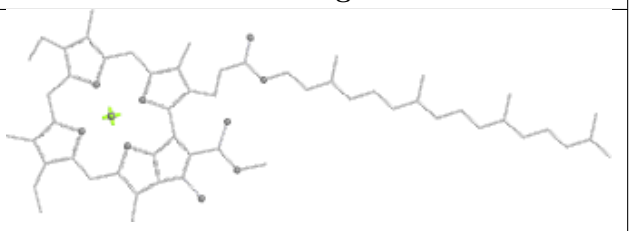
Bond lengths



Bond angles

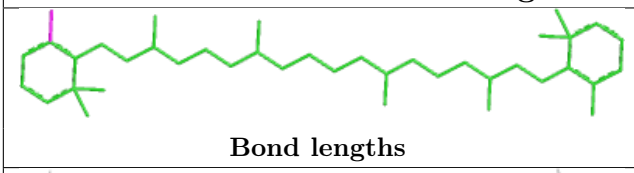


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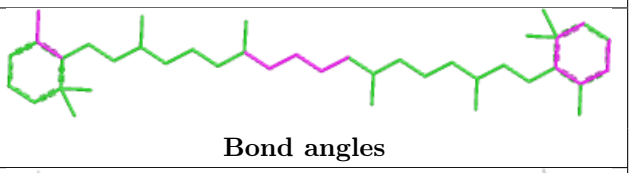


Rings

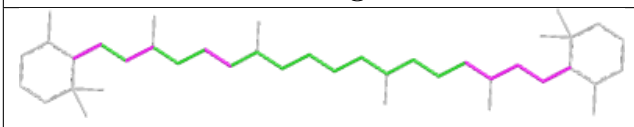
Ligand BCR a 4008



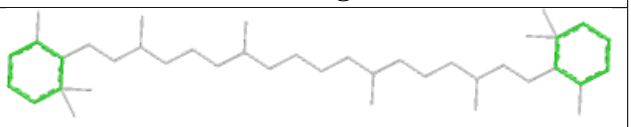
Bond lengths



Bond angles

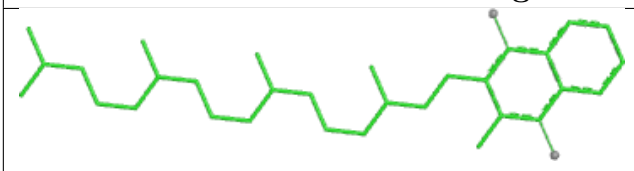


Torsions

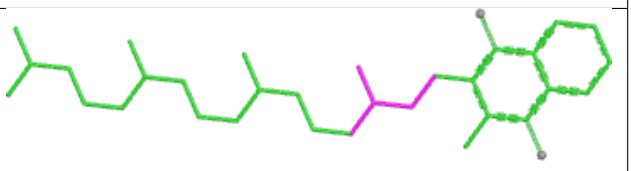


Rings

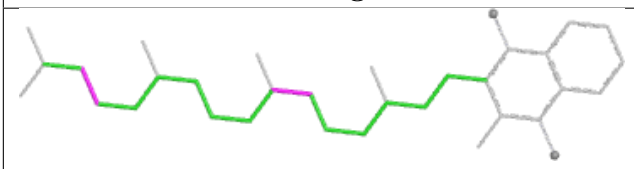
Ligand PQN A 2001



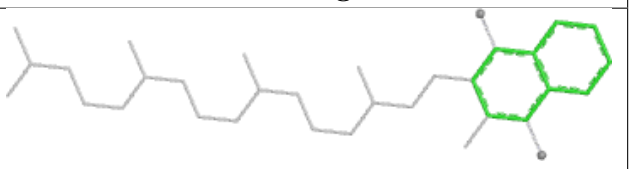
Bond lengths



Bond angles

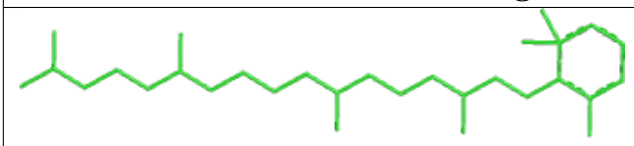


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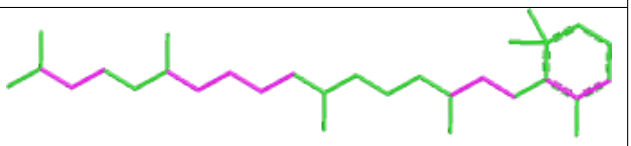


Rings

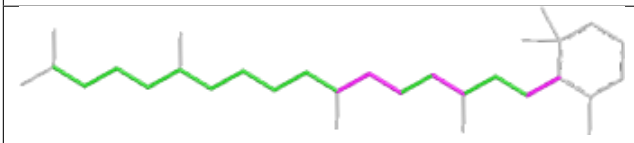
Ligand BCR B 4009



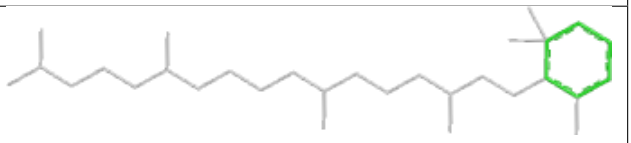
Bond lengths



Bond angles

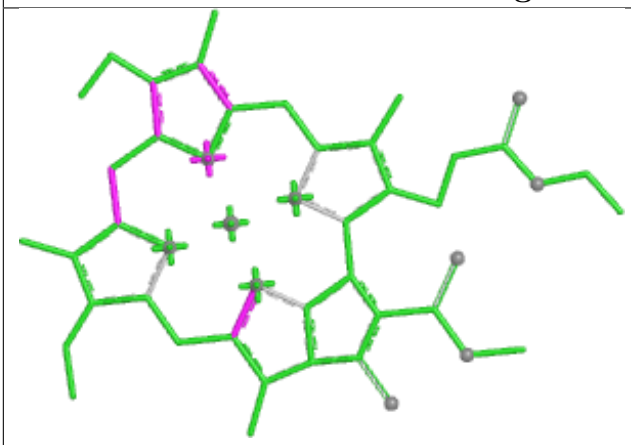


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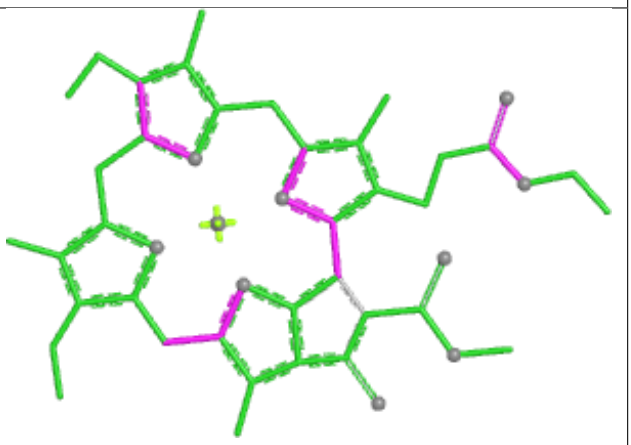


Rings

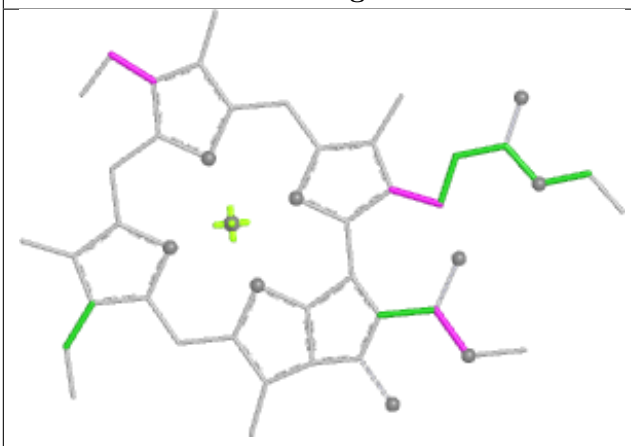
Ligand CLA H 1137



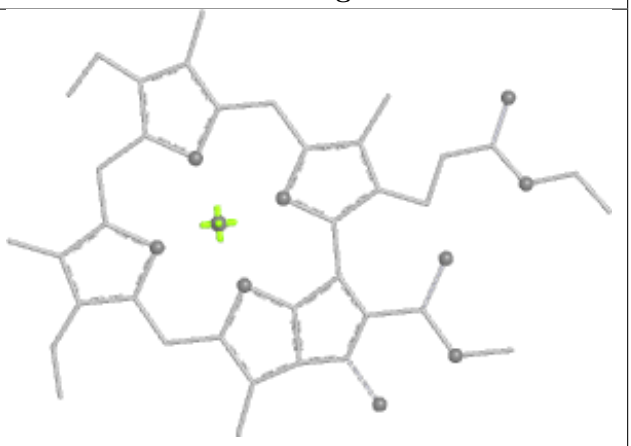
Bond lengths



Bond angles



Torsions

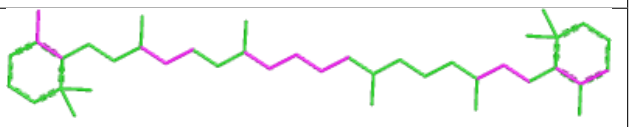


Rings

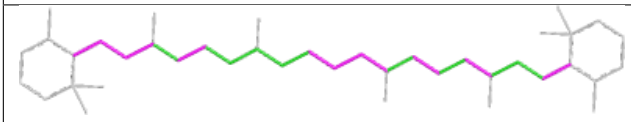
Ligand BCR x 603



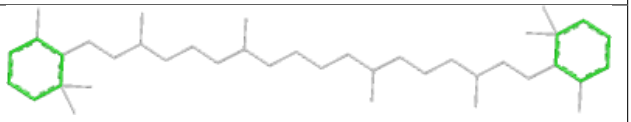
Bond lengths



Bond angles

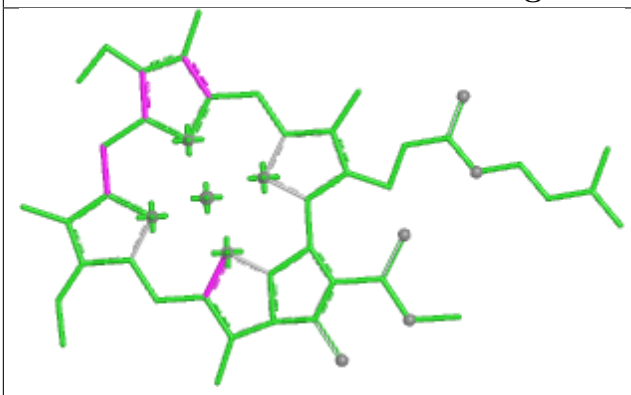


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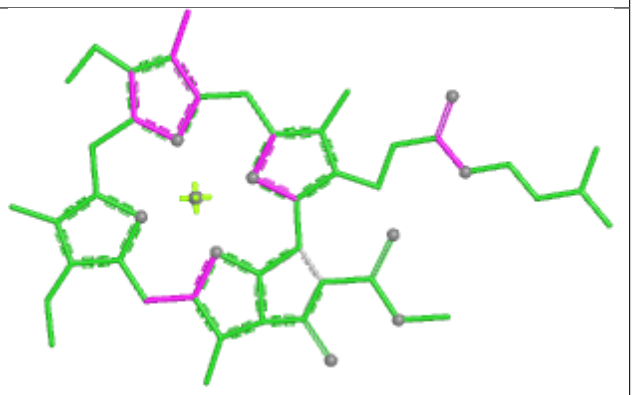


Rings

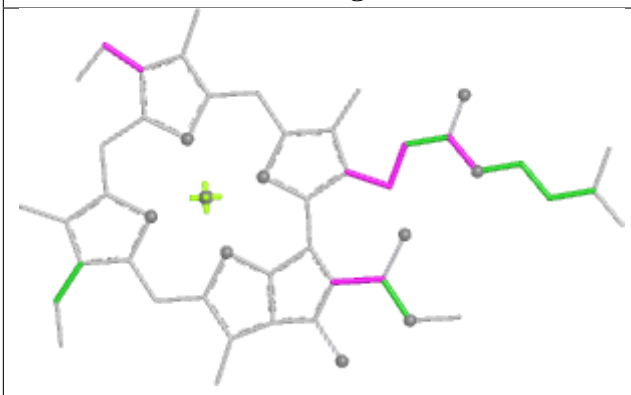
Ligand CLA w 513



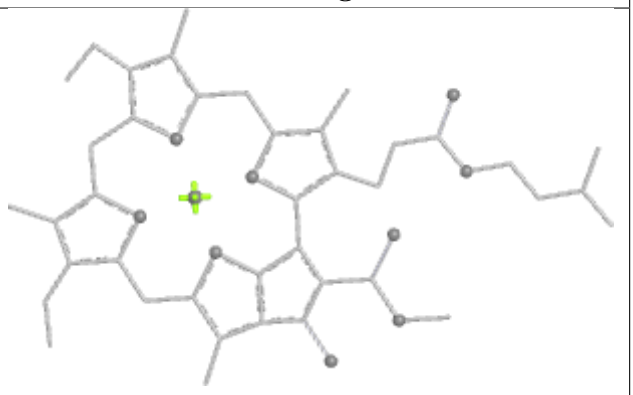
Bond lengths



Bond angles

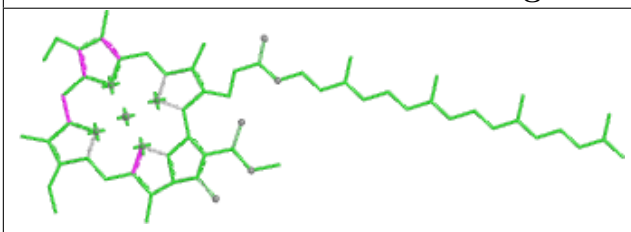


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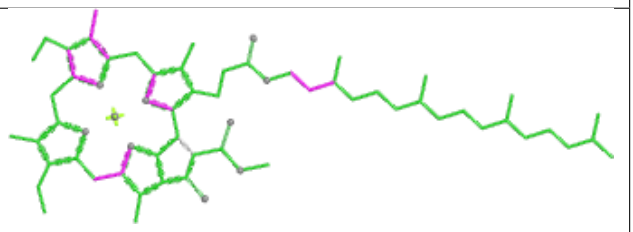


Rings

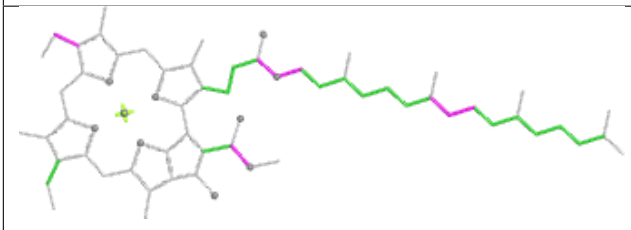
Ligand CLA Y 507



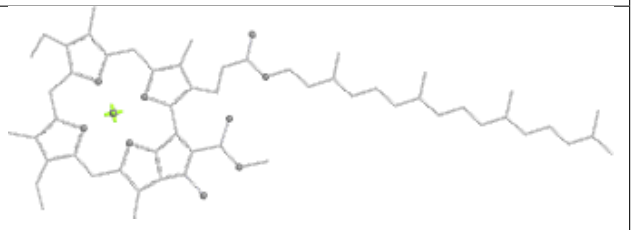
Bond lengths



Bond angles

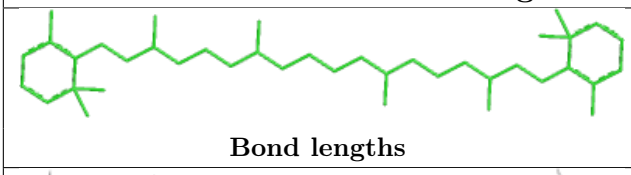


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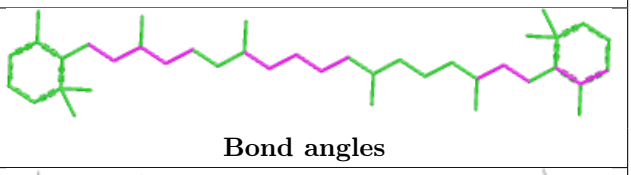


Rings

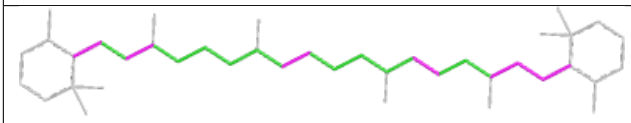
Ligand BCR b 4004



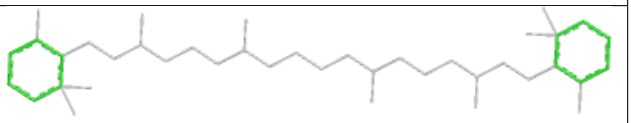
Bond lengths



Bond angles

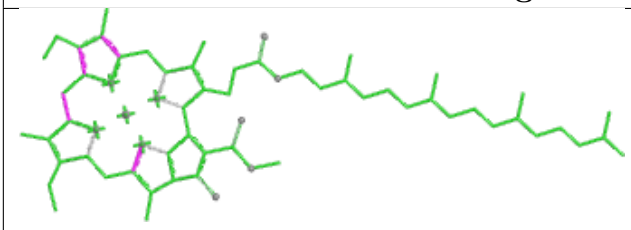


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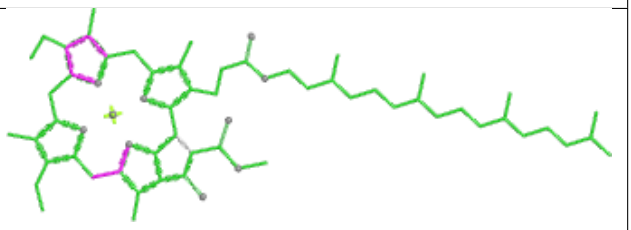


Rings

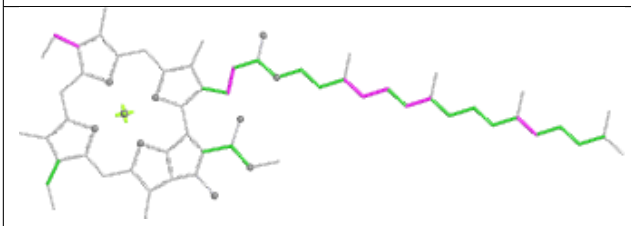
Ligand CLA B 1204



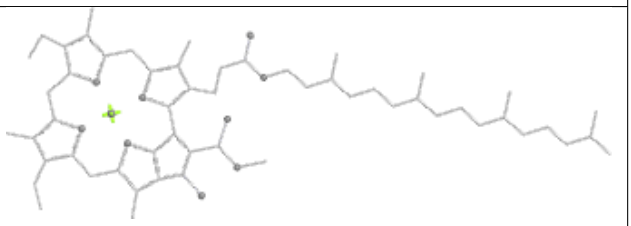
Bond lengths



Bond angles



Torsions

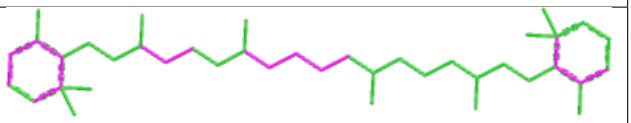


Rings

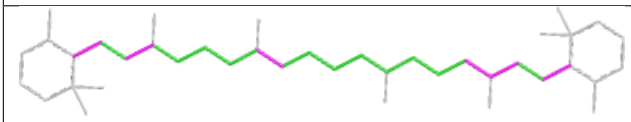
Ligand BCR I 4018



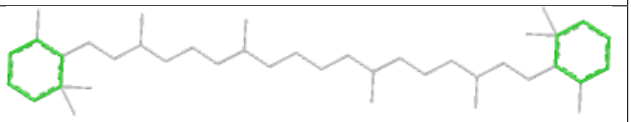
Bond lengths



Bond angles

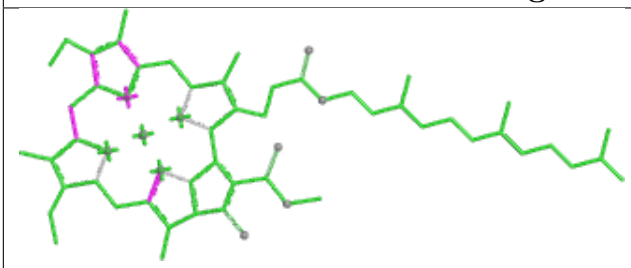


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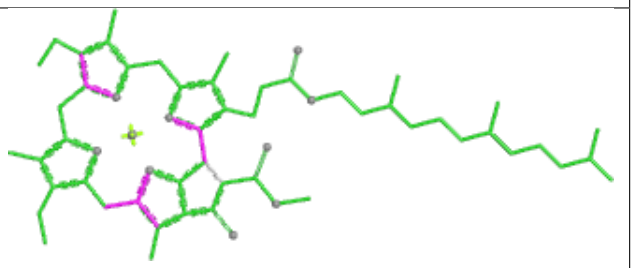


Rings

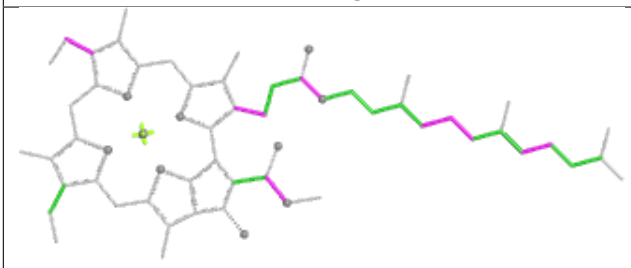
Ligand CLA o 504



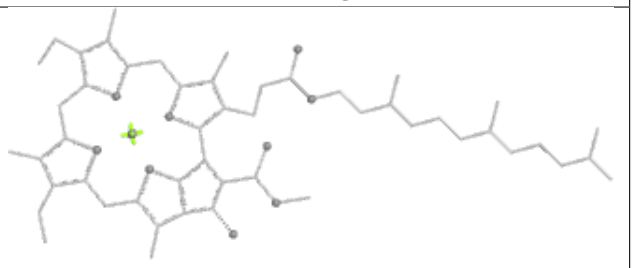
Bond lengths



Bond angles

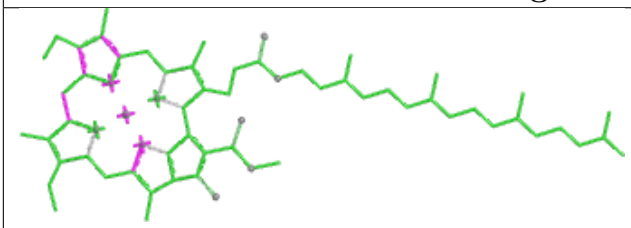


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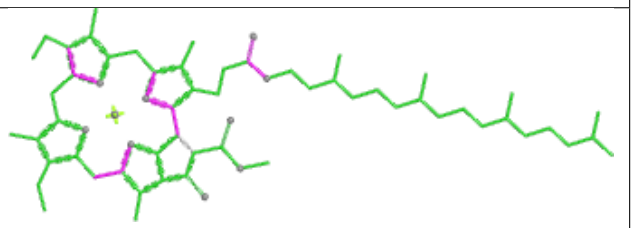


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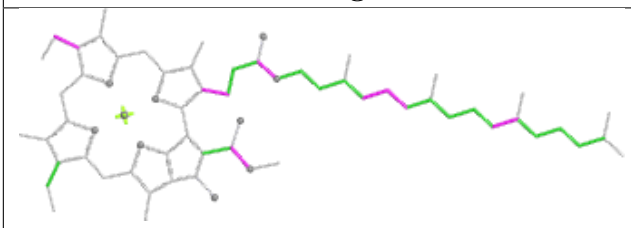
Ligand CLA t 512



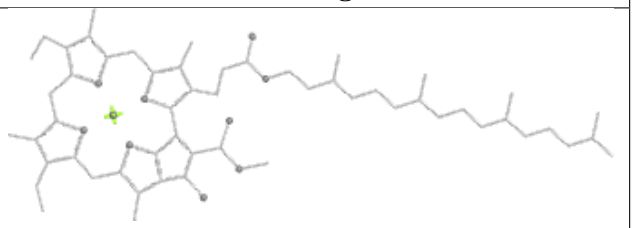
Bond lengths



Bond angles



Torsions

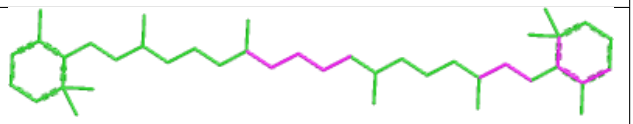


Rings

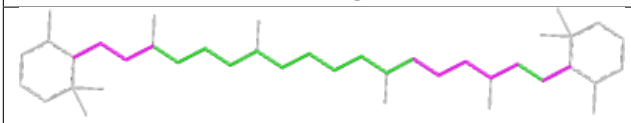
Ligand BCR b 4005



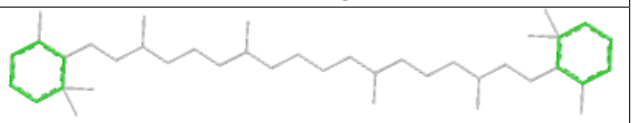
Bond lengths



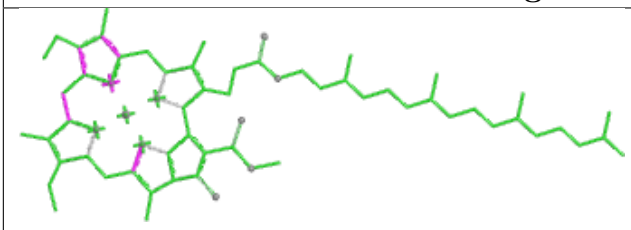
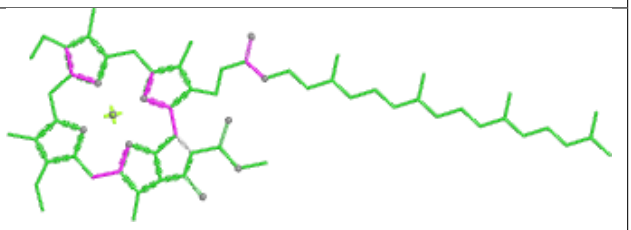
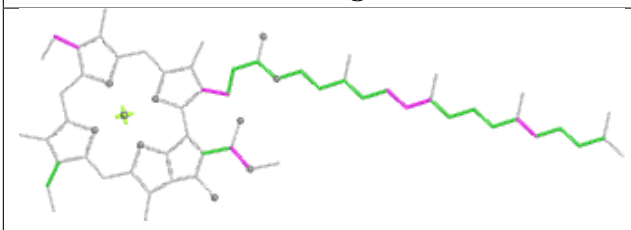
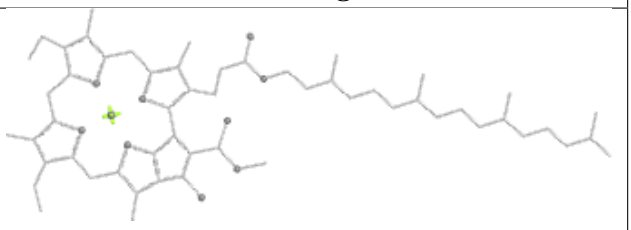
Bond angles

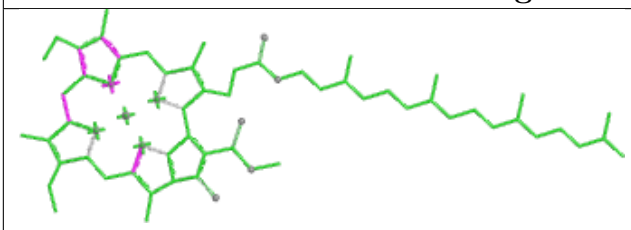
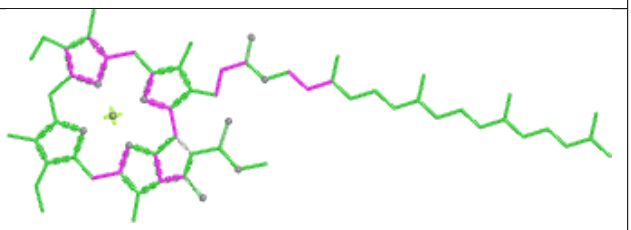
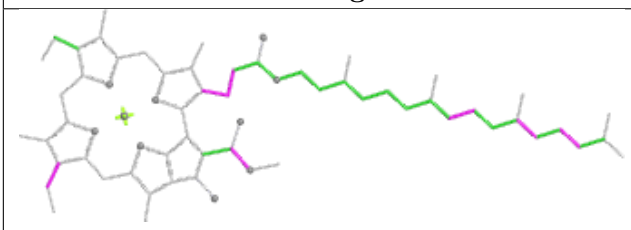
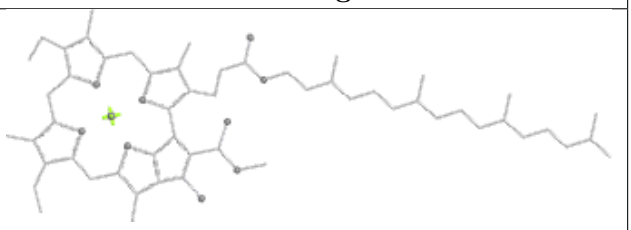


Torsions

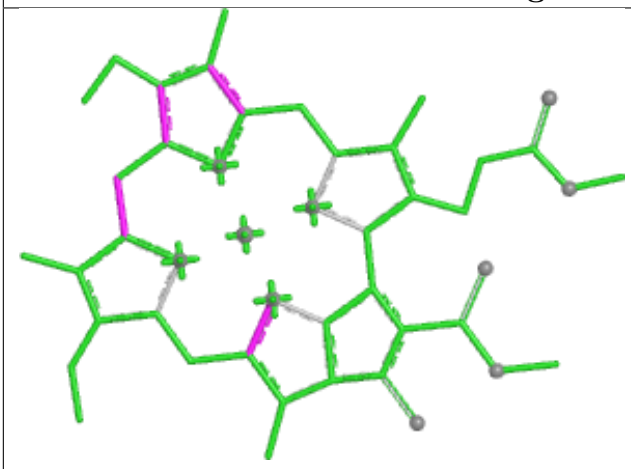


Rings

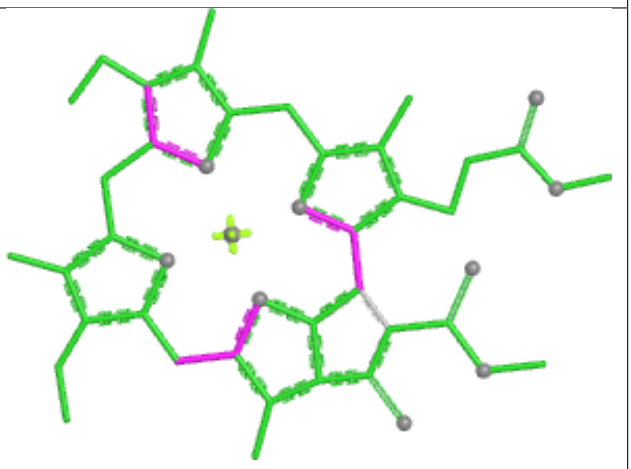
Ligand CLA w 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1022	
	
Bond lengths	Bond angles
	
Torsions	Rings

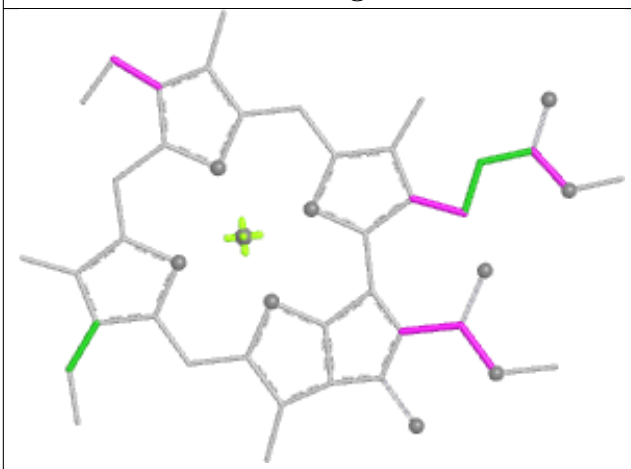
Ligand CLA u 503



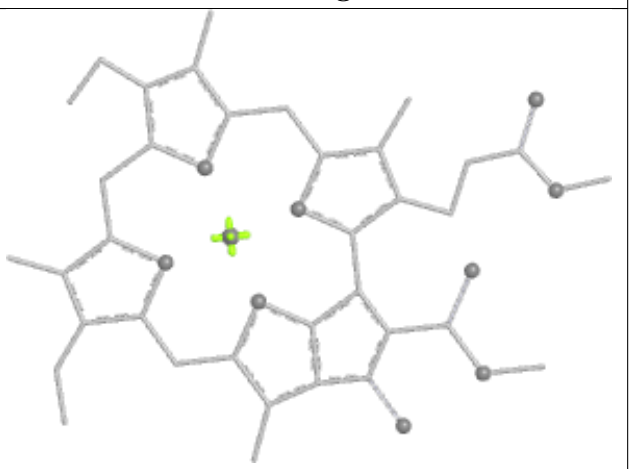
Bond lengths



Bond angles

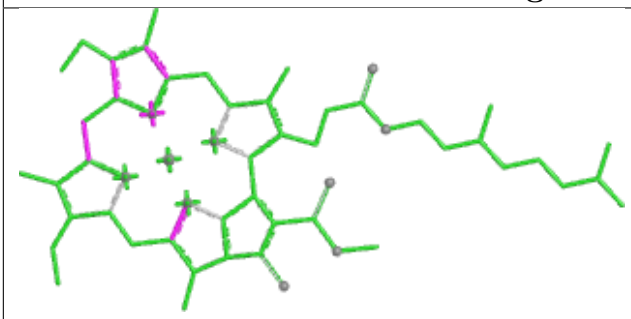


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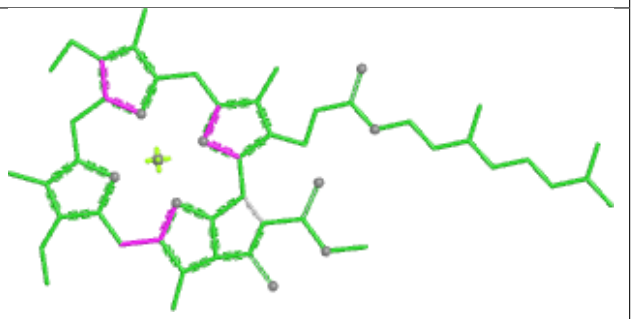


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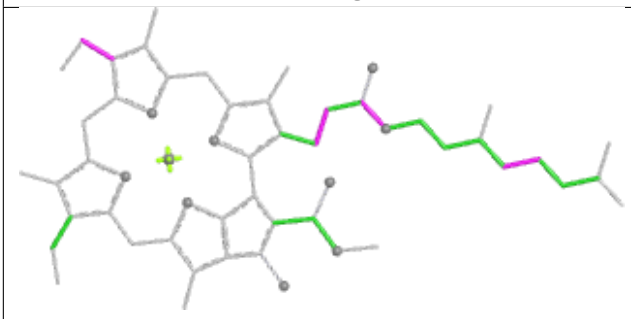
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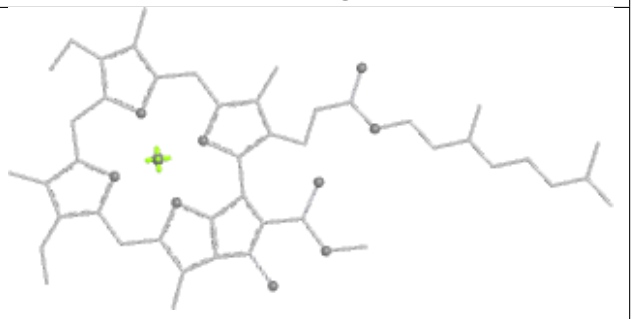
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Bond angles

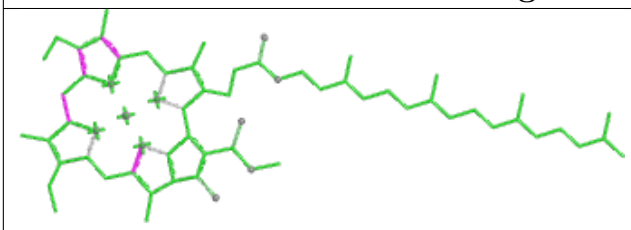


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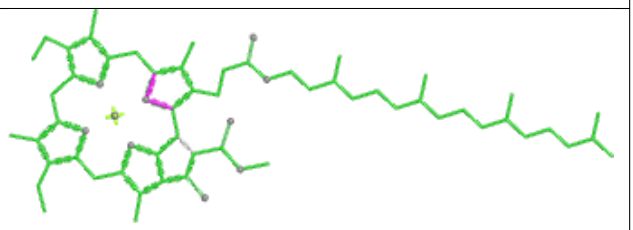


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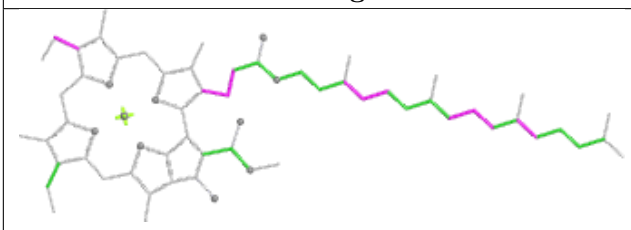
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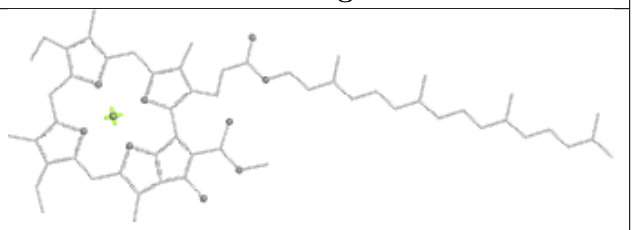
Bond lengths



Bond angles

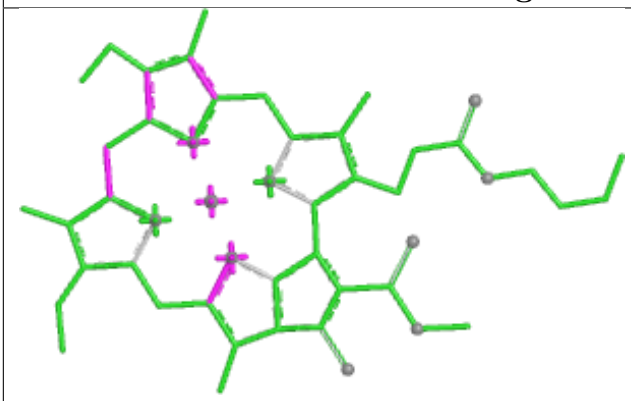


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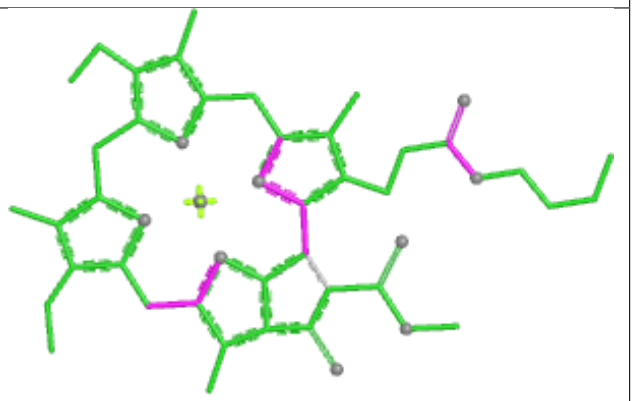


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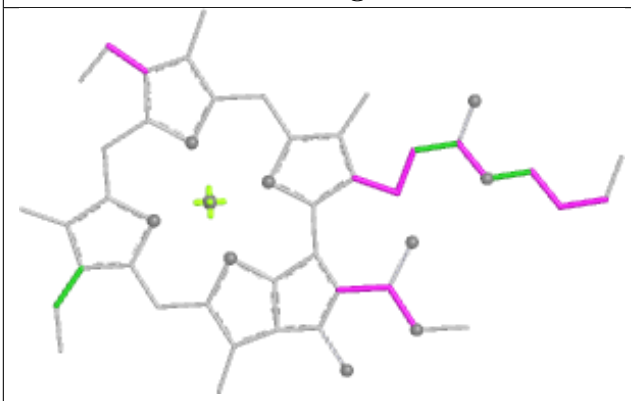
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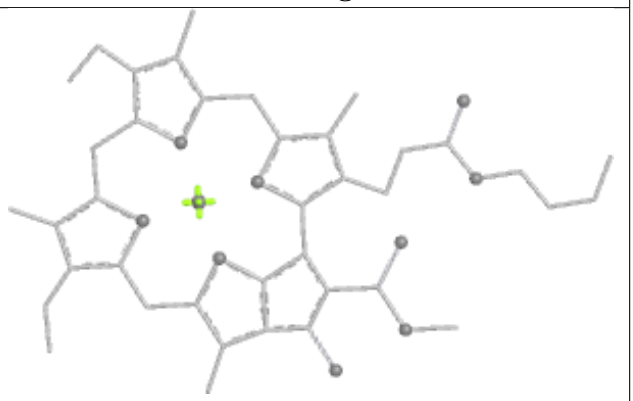
Bond lengths



Bond angles



Torsions

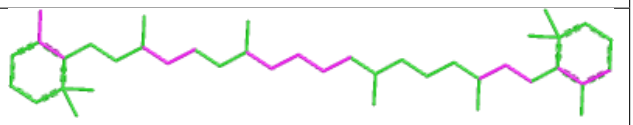


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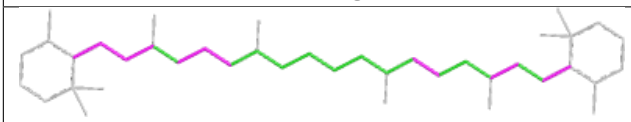
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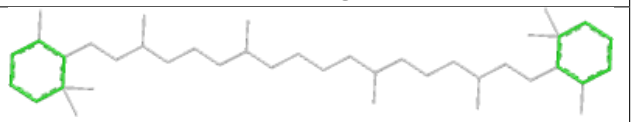
Bond lengths



Bond angles

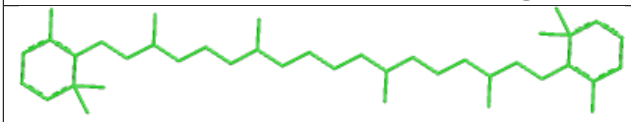


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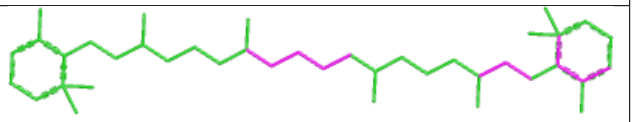


Rings

Ligand BCR a 4002



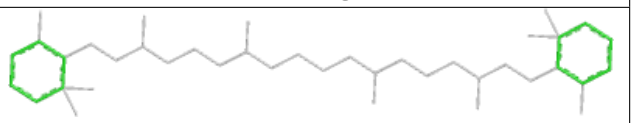
Bond lengths



Bond angles

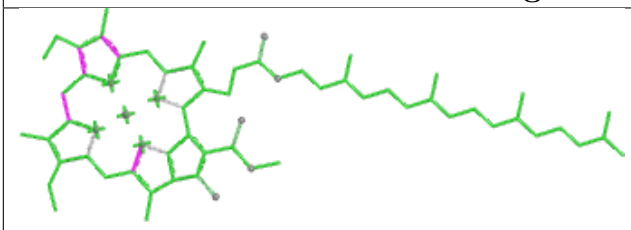


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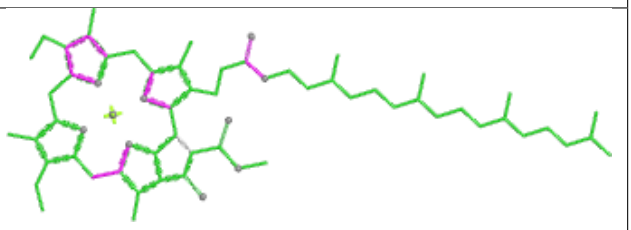


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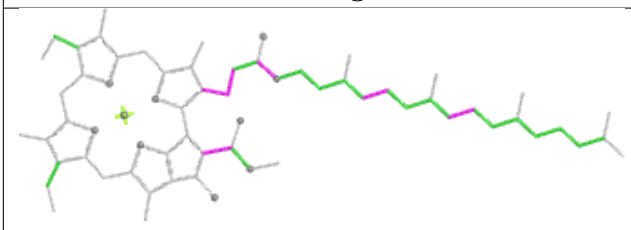
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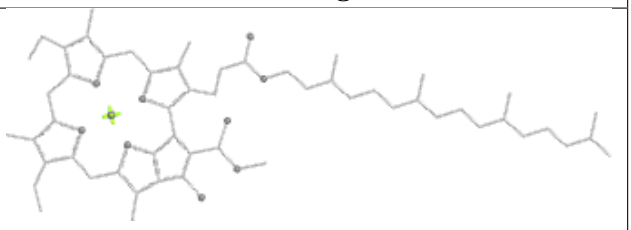
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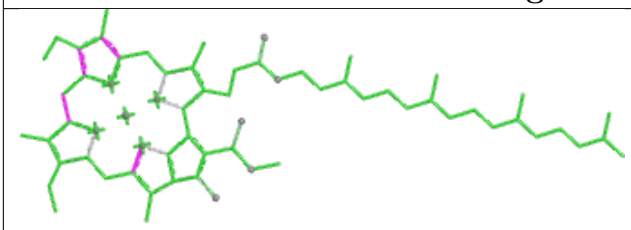


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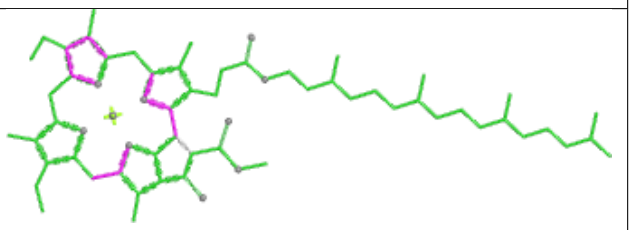


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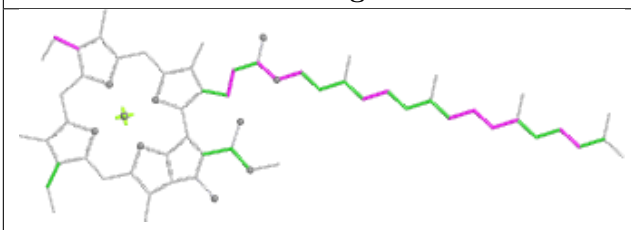
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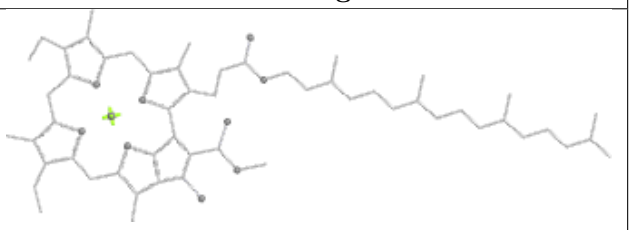
Bond lengths



Bond angles



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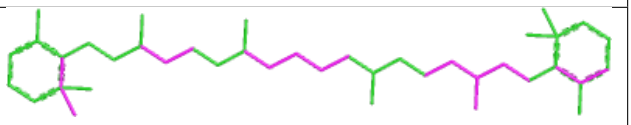


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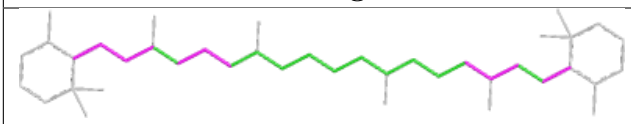
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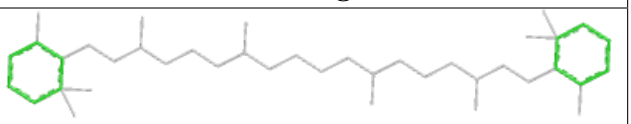
Bond lengths



Bond angles

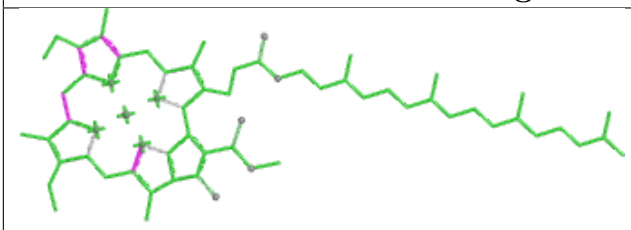


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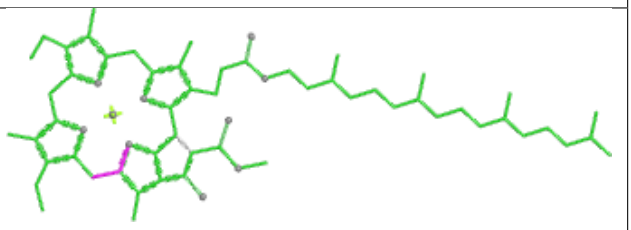


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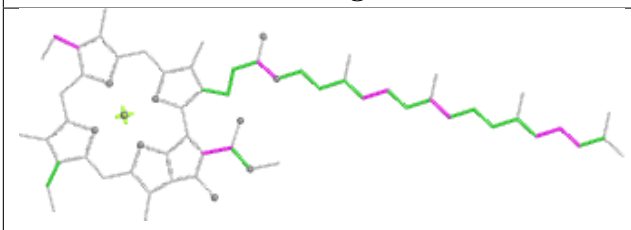
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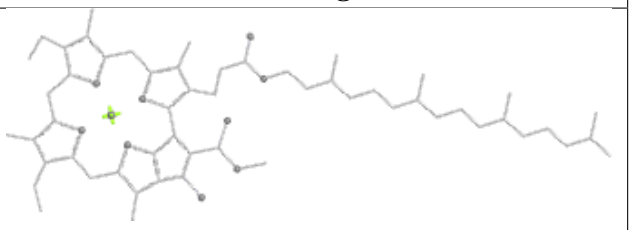
Bond lengths



Bond angles

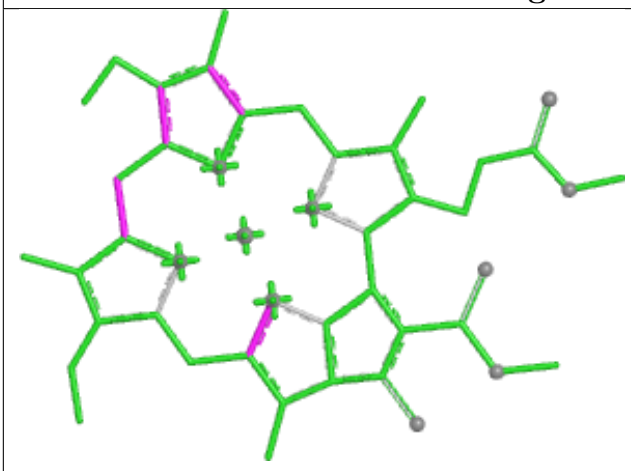


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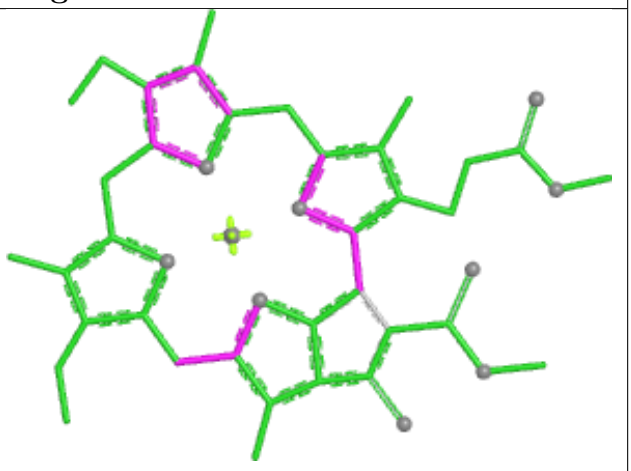


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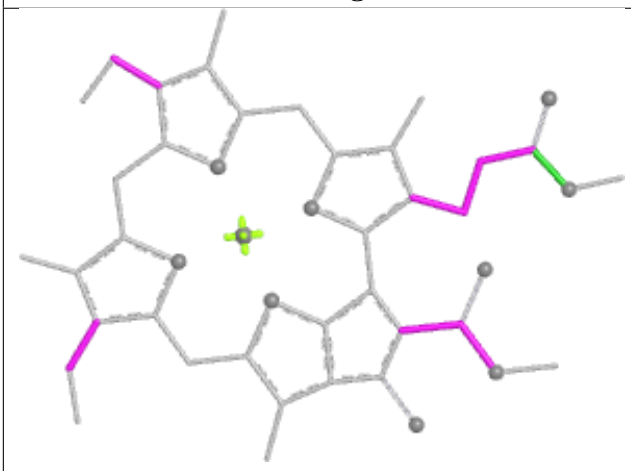
Ligand CLA g 513



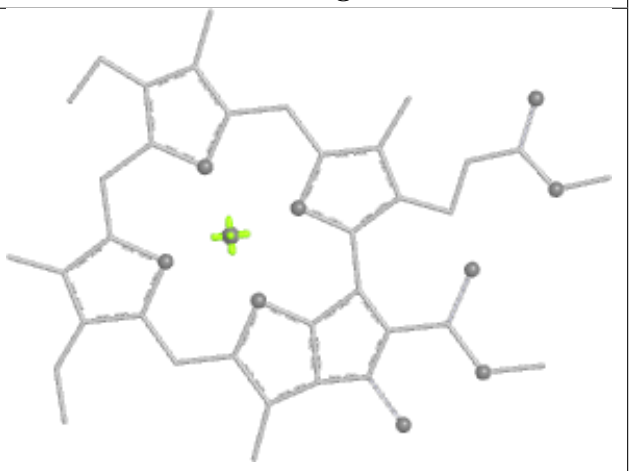
Bond lengths



Bond angles

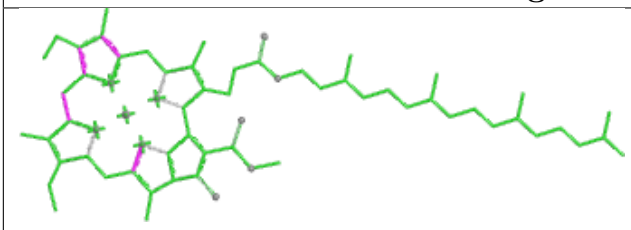


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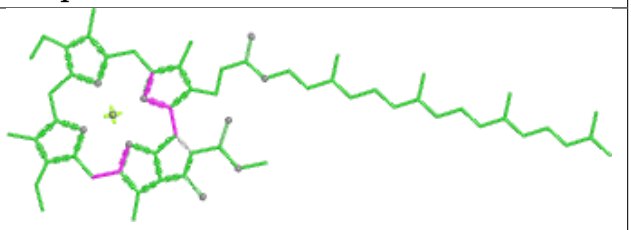


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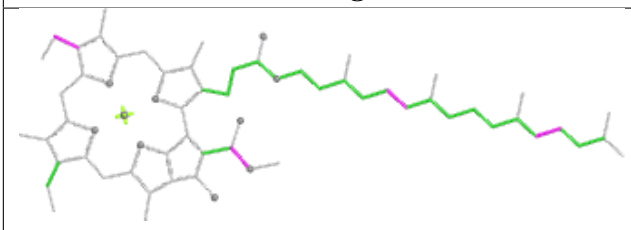
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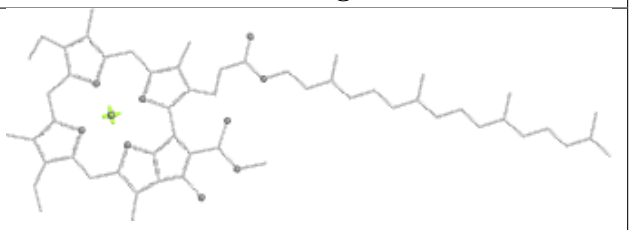
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Bond angles

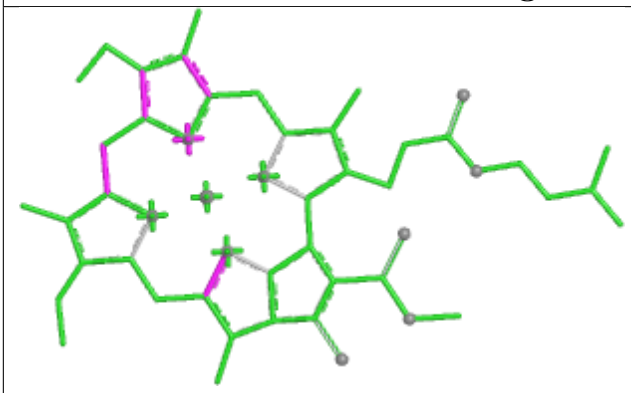


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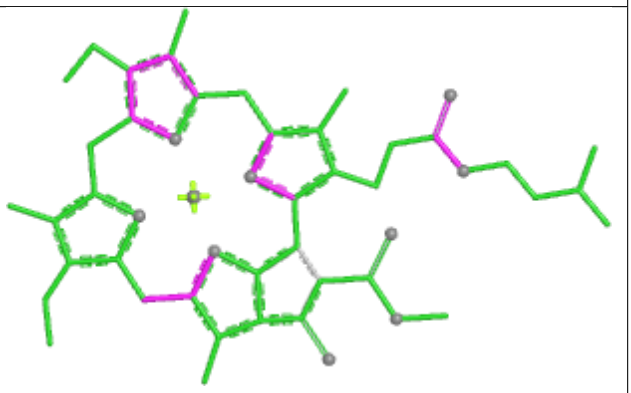


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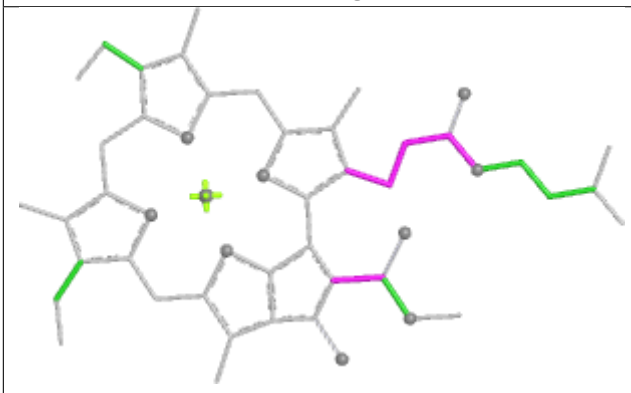
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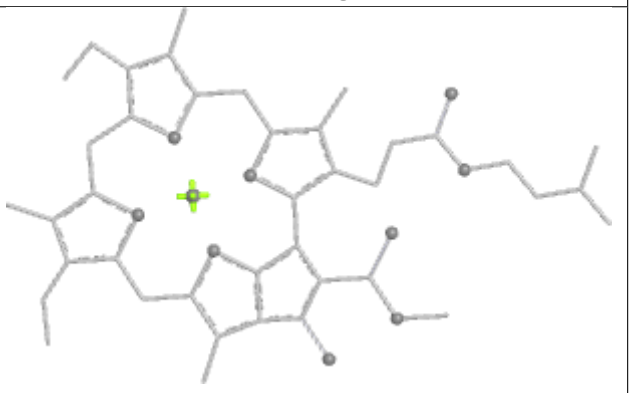
Bond lengths



Bond angles

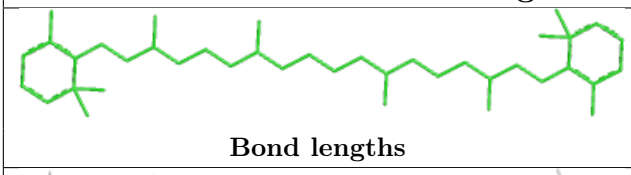


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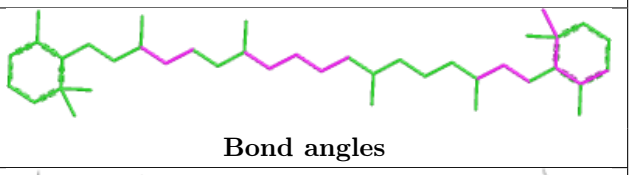


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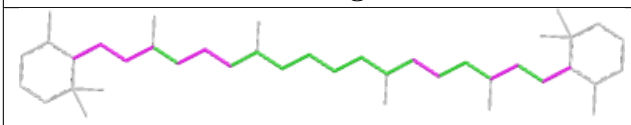
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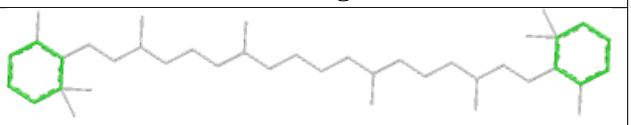
Bond lengths



Bond angles

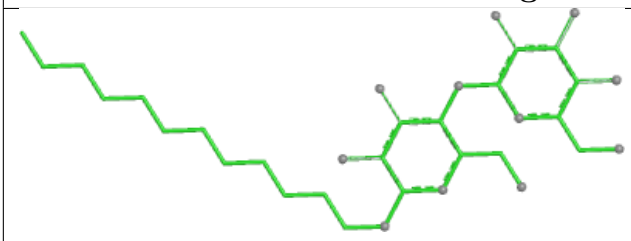


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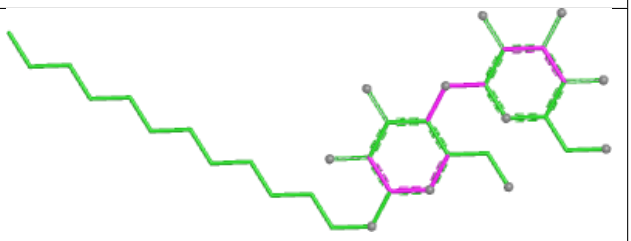


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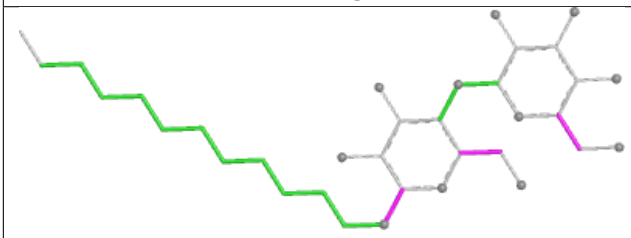
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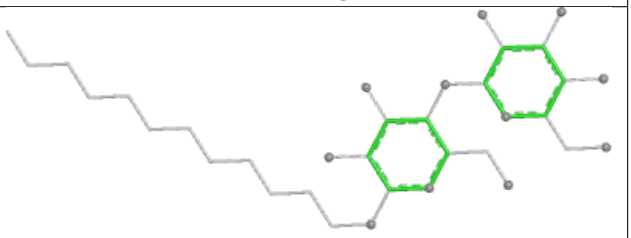
Bond lengths



Bond angles

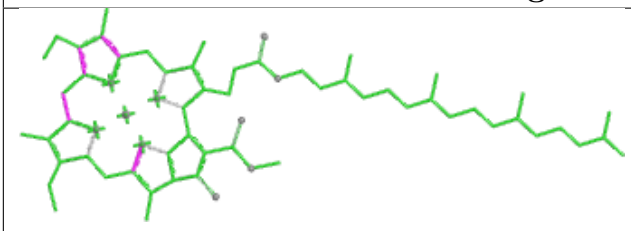


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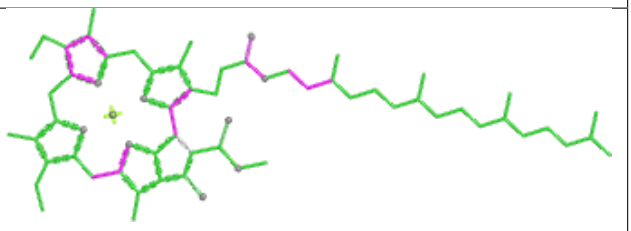


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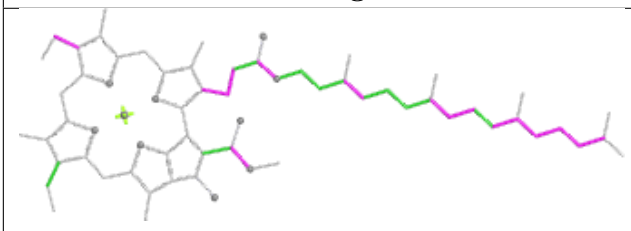
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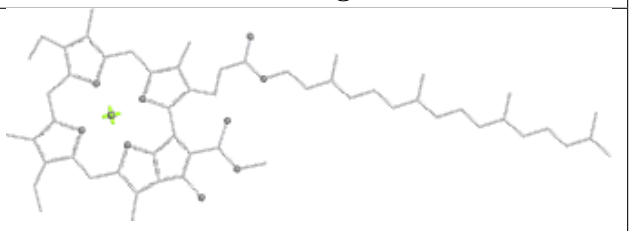
Bond lengths



Bond angles

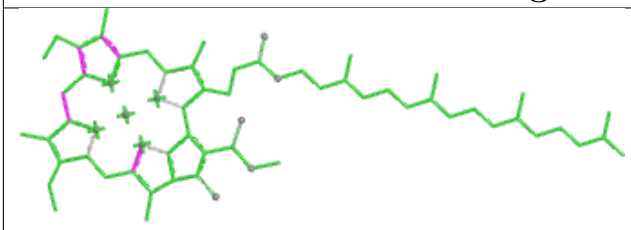


Torsions

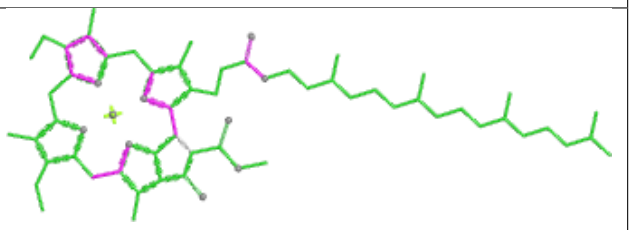


Rings

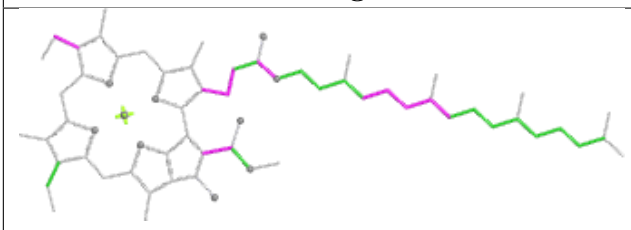
Ligand CLA s 515



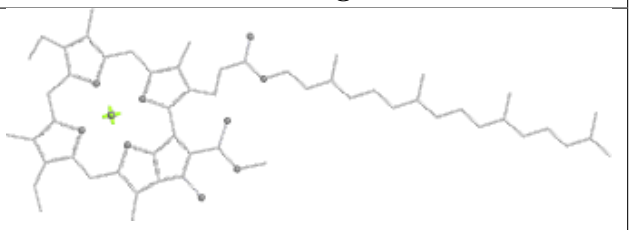
Bond lengths



Bond angles

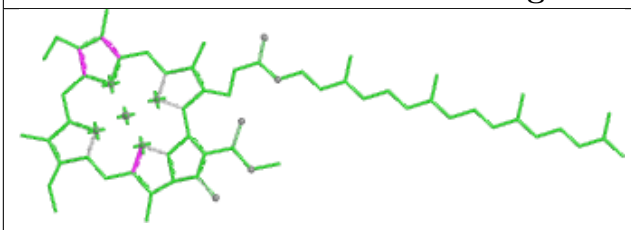


Torsions

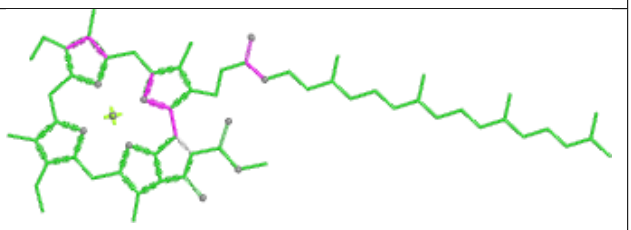


Rings

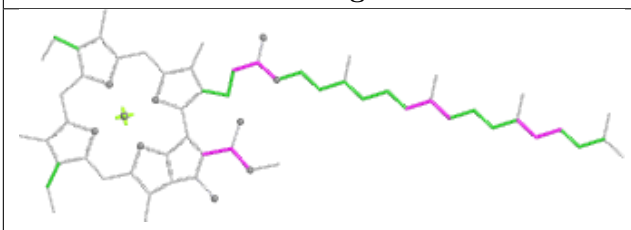
Ligand CLA n 510



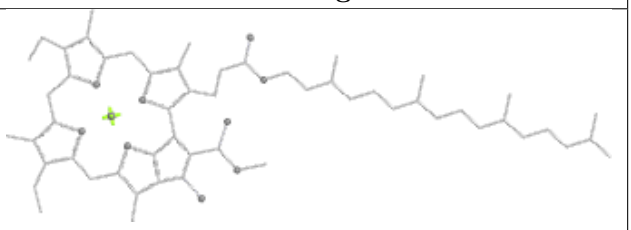
Bond lengths



Bond angles

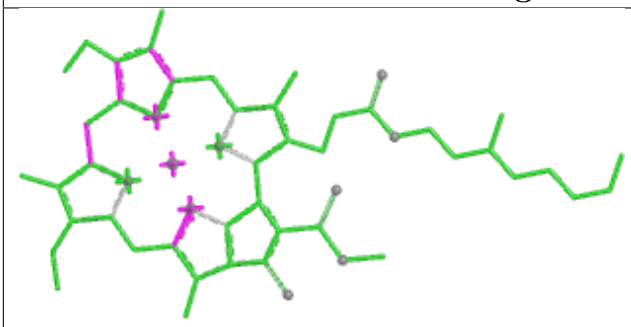


Torsions

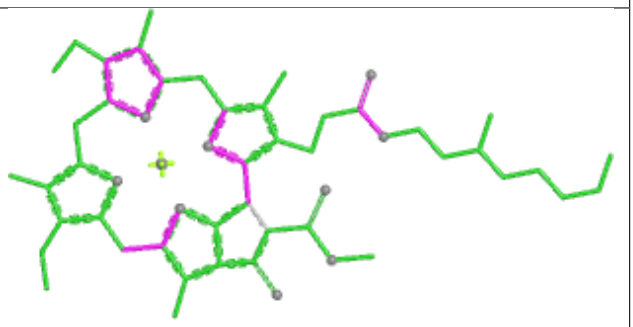


Rings

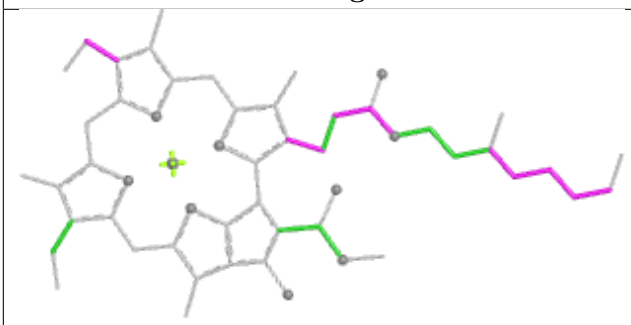
Ligand CLA A 1133



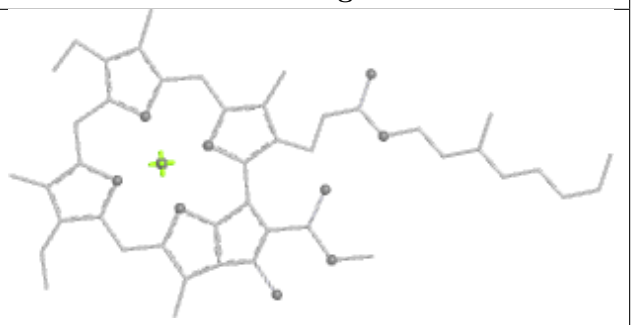
Bond lengths



Bond angles

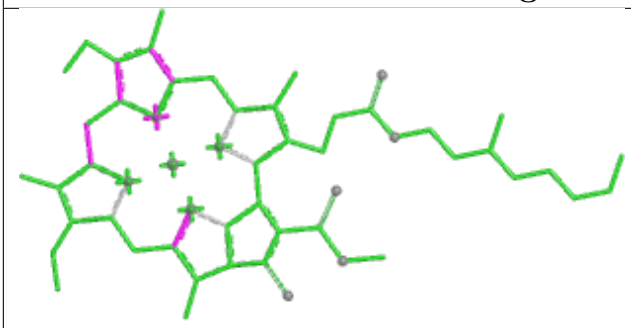


Torsions

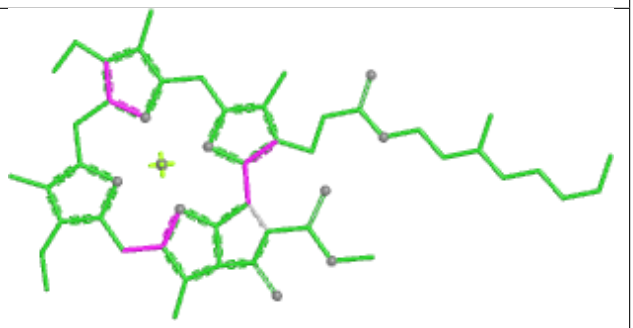


Rings

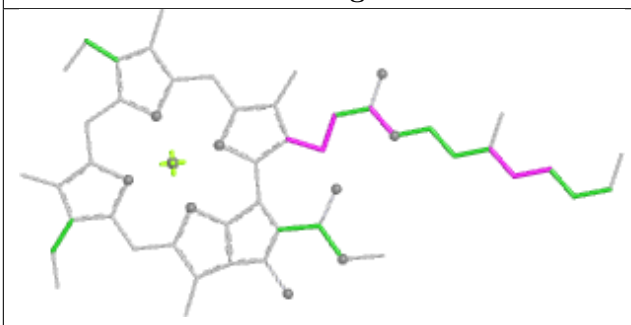
Ligand CLA a 1115



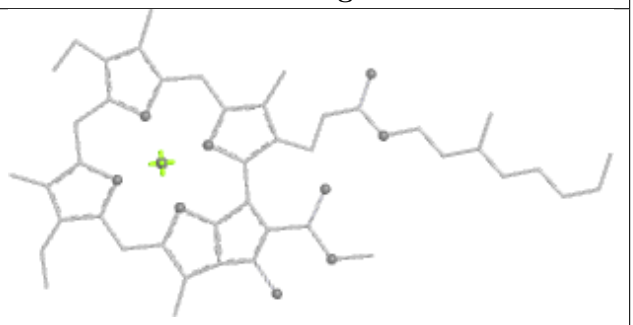
Bond lengths



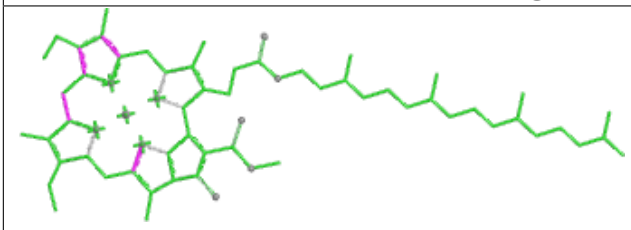
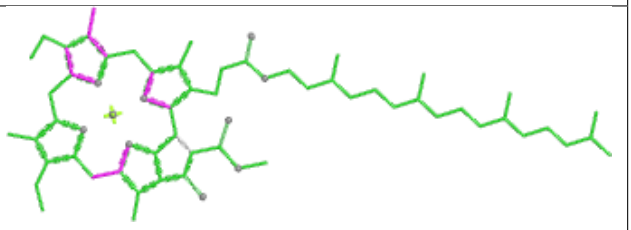
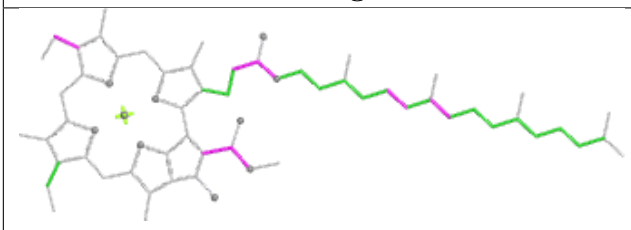
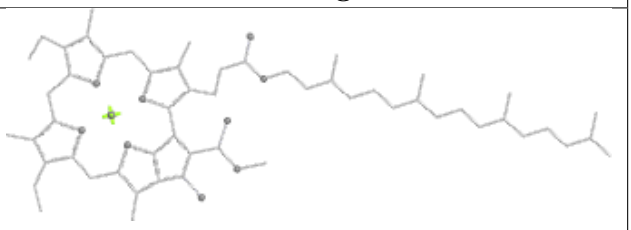
Bond angles

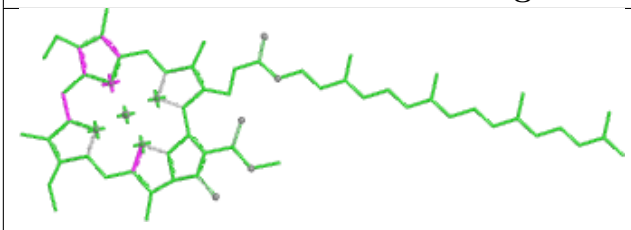
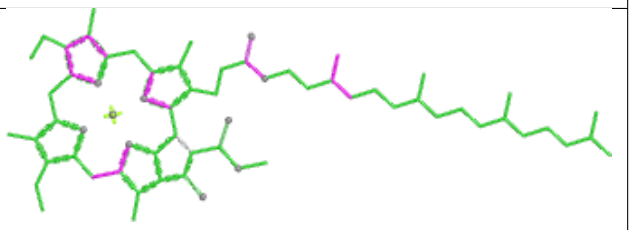
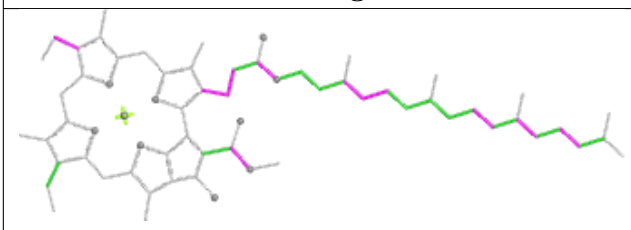
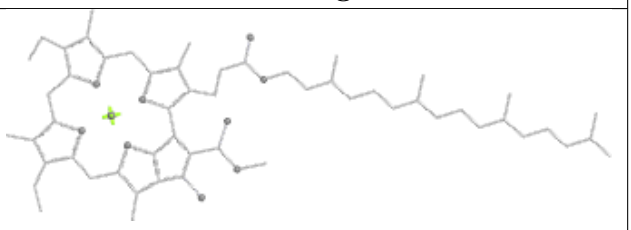


Torsions

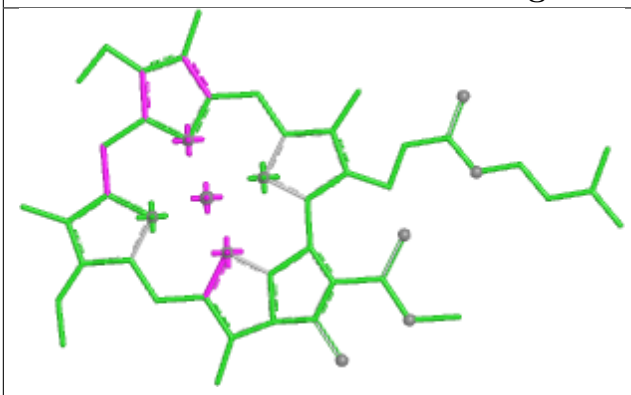


Rings

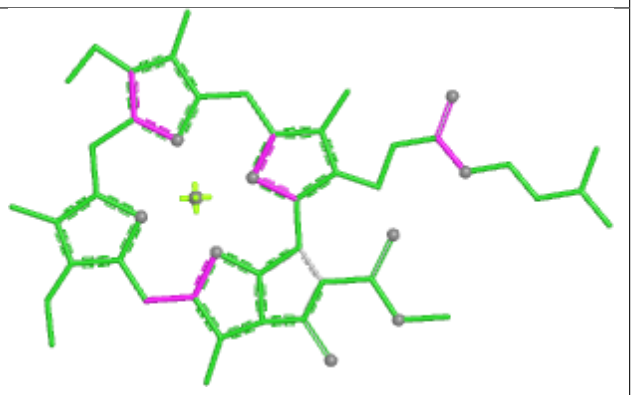
Ligand CLA o 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

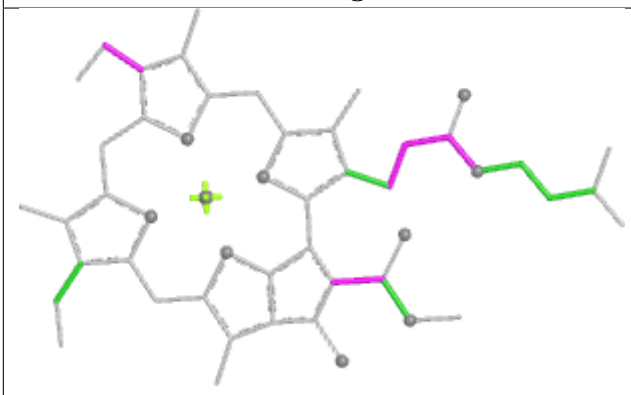
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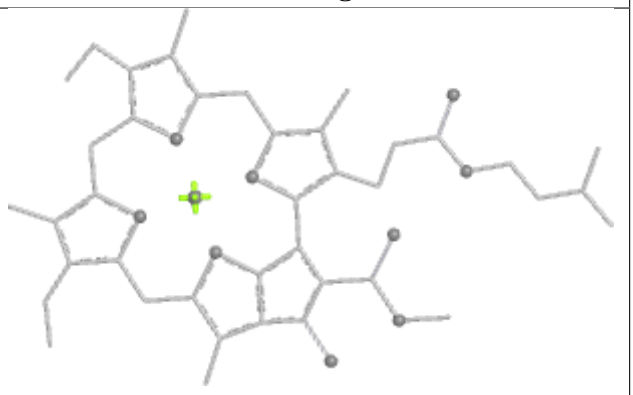
Bond lengths



Bond angles

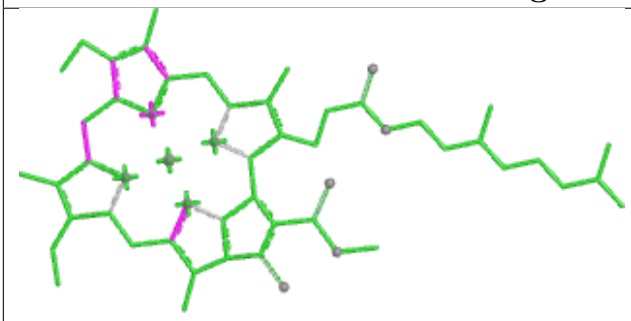


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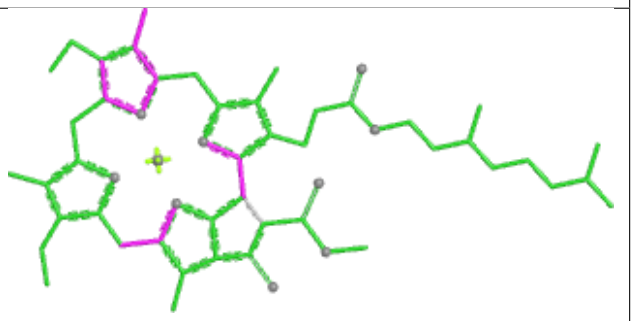


Rings

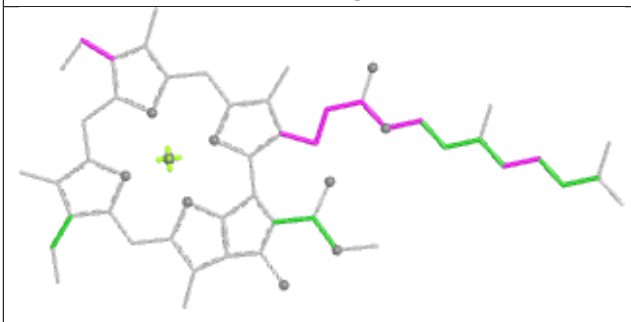
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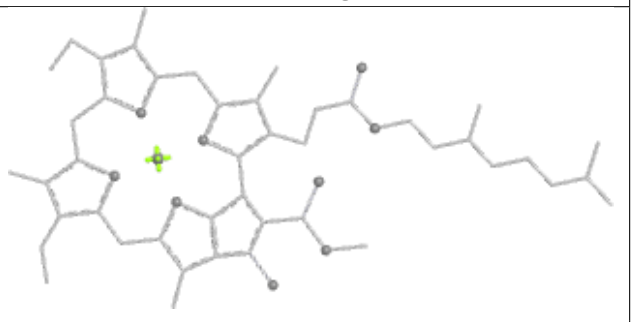
Bond lengths



Bond angles

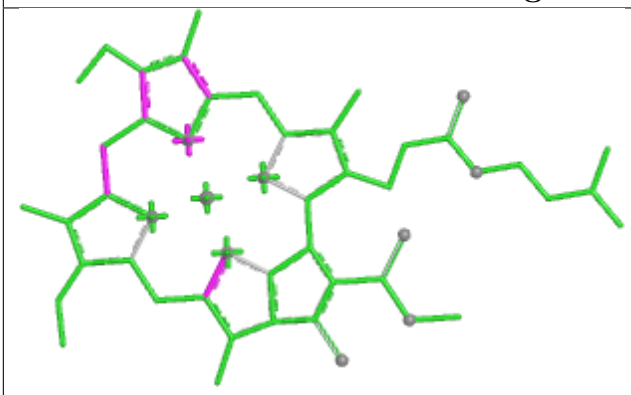


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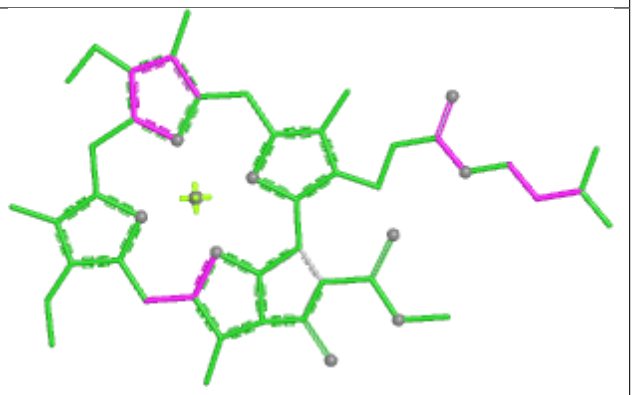


Rings

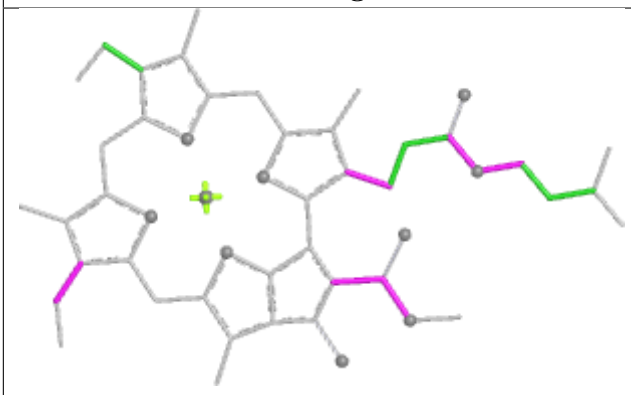
Ligand CLA w 501



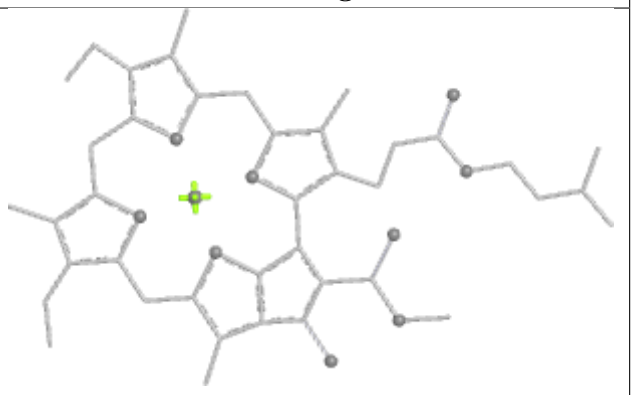
Bond lengths



Bond angles

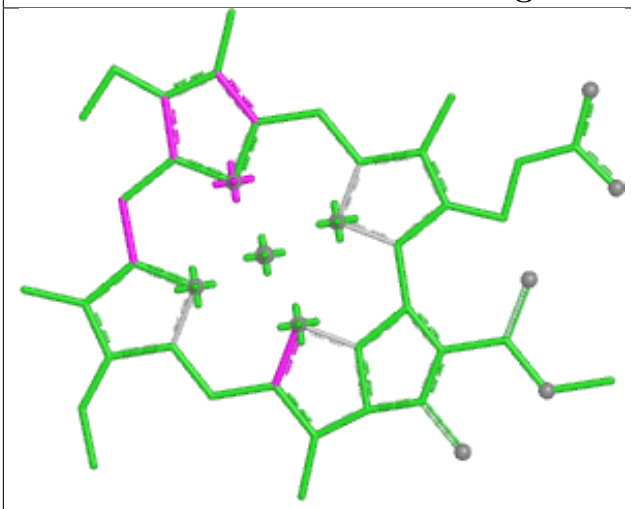


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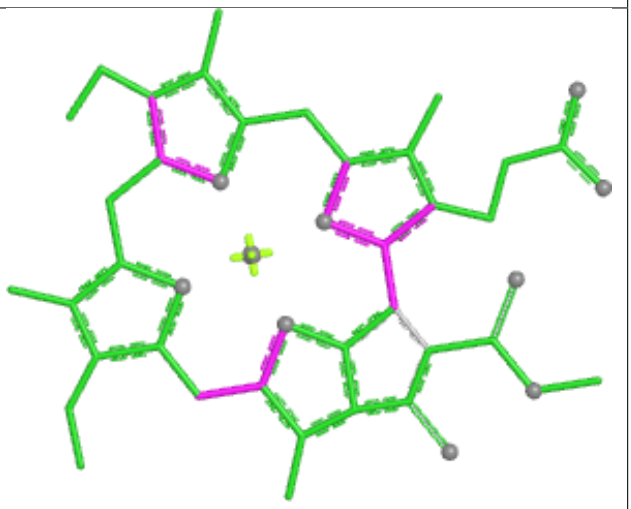


Rings

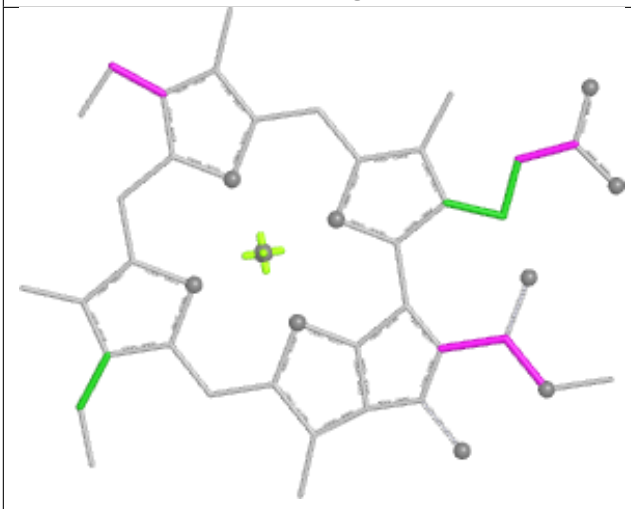
Ligand CLA B 1232



Bond lengths



Bond angles

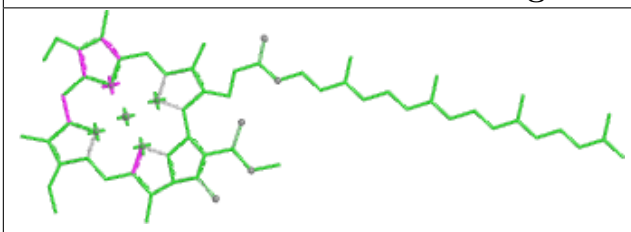


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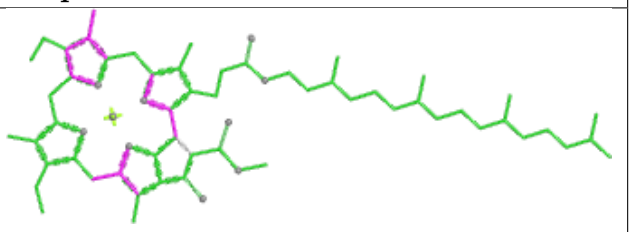


Rings

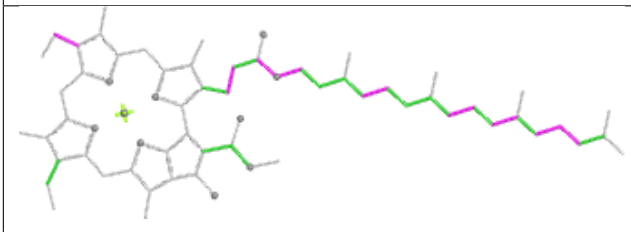
Ligand CLA q 515



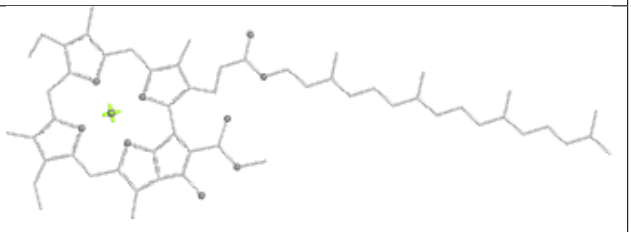
Bond lengths



Bond angles

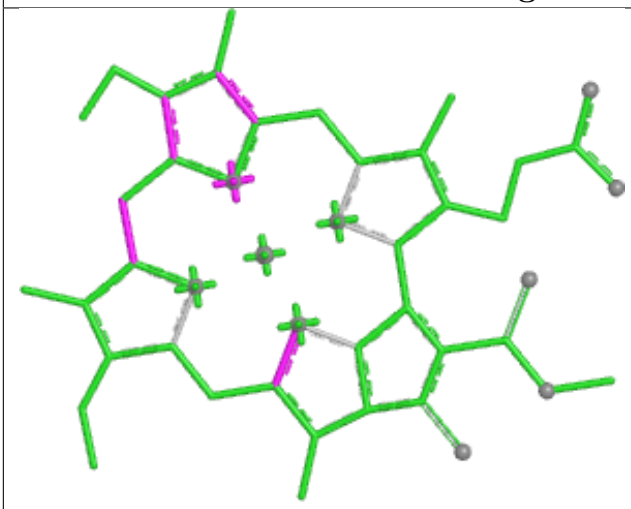


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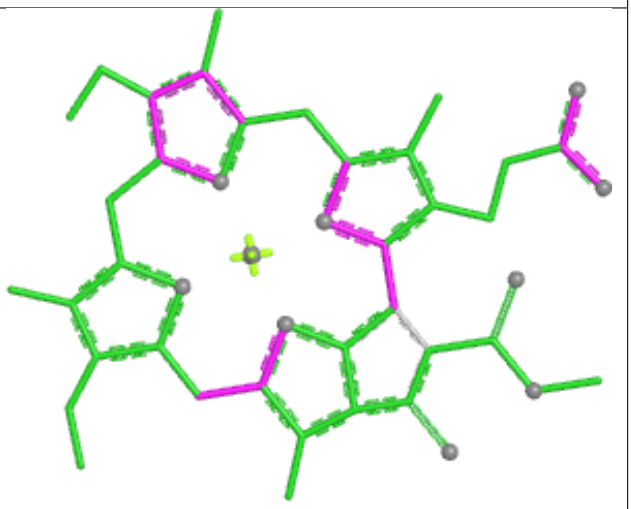


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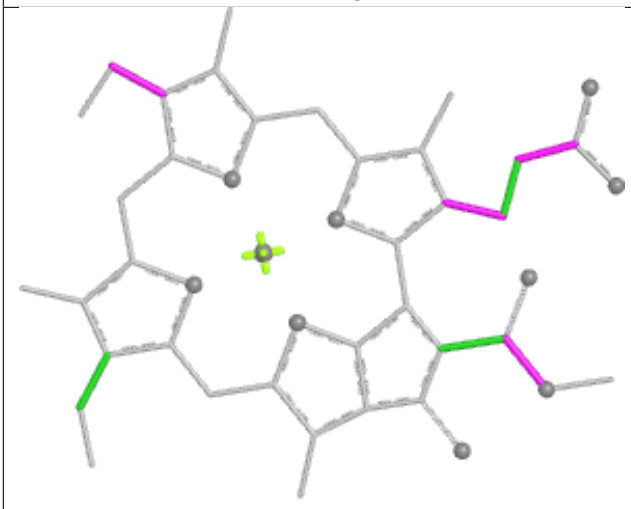
Ligand CLA b 1208



Bond lengths



Bond angles

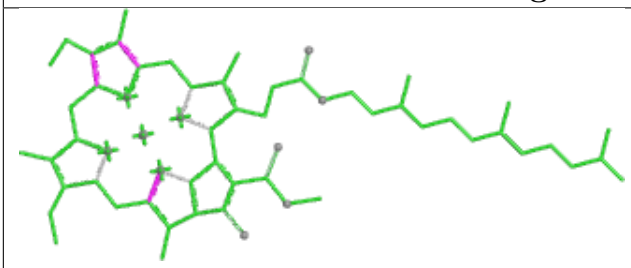


Torsions

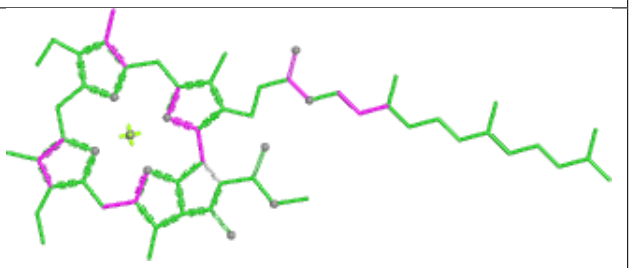


Rings

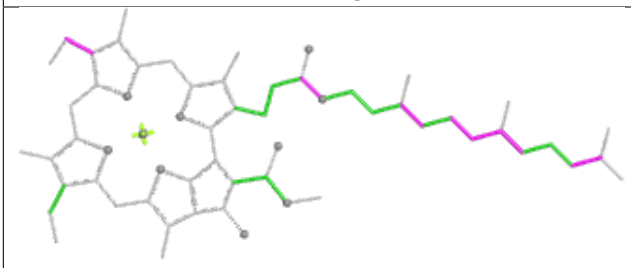
Ligand CLA r 506



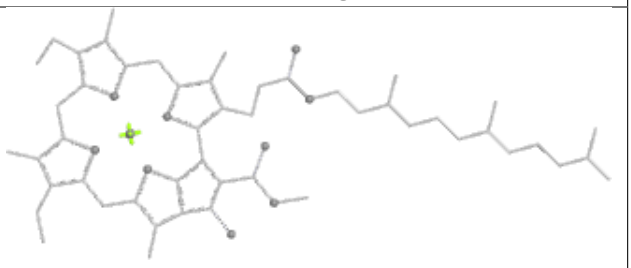
Bond lengths



Bond angles

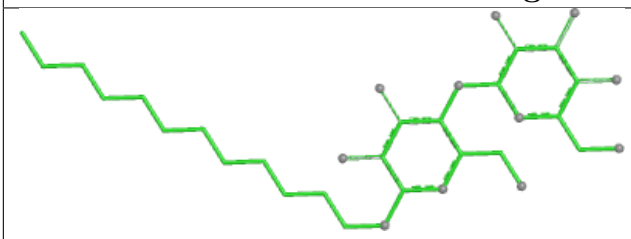


Torsions

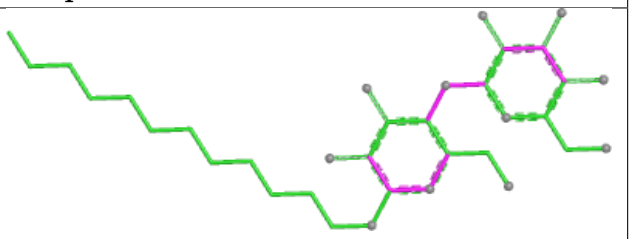


Rings

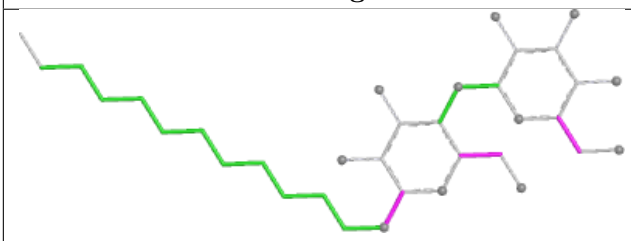
Ligand LMU q 605



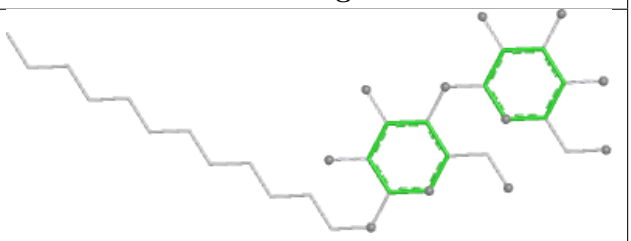
Bond lengths



Bond angles

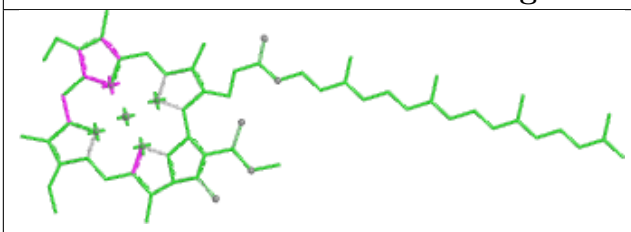


Torsions

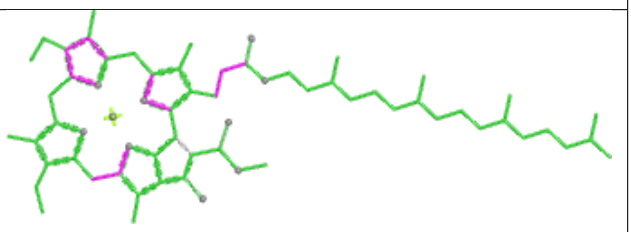


Rings

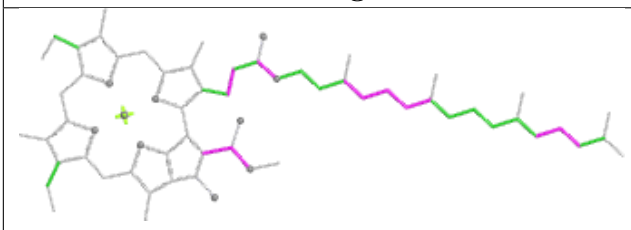
Ligand CLA a 1132



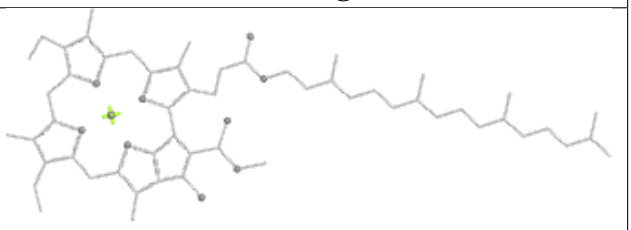
Bond lengths



Bond angles

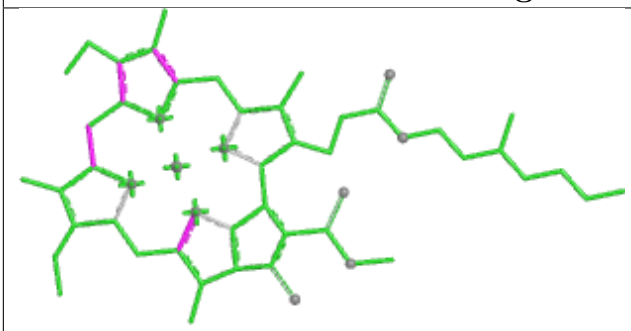


Torsions

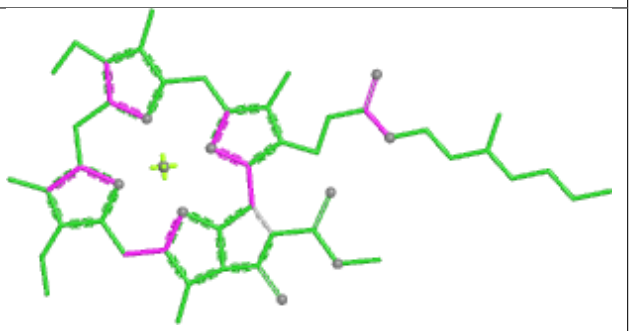


Rings

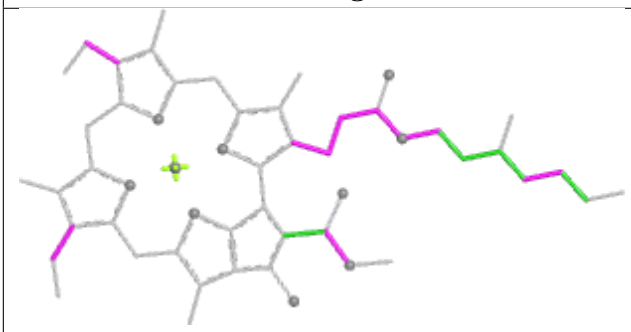
Ligand CLA B 1220



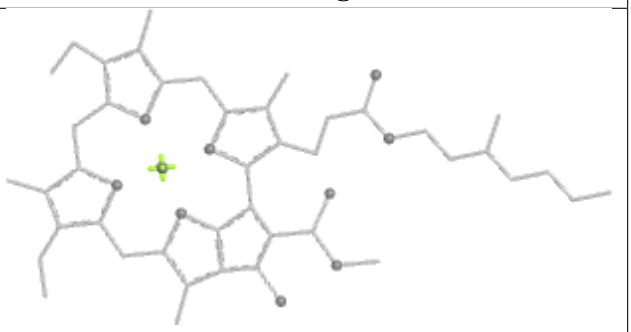
Bond lengths



Bond angles

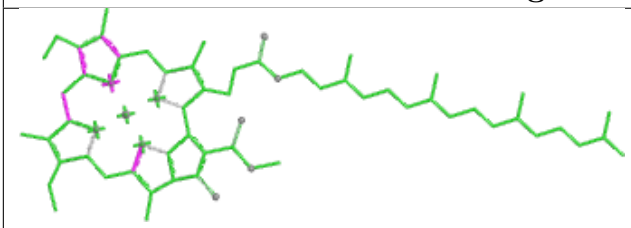


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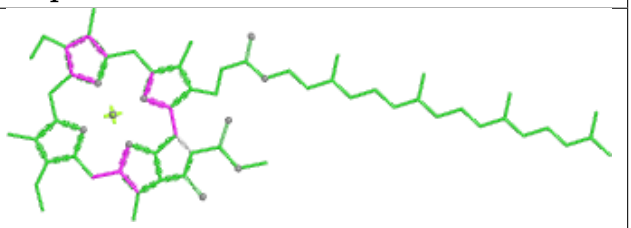


Rings

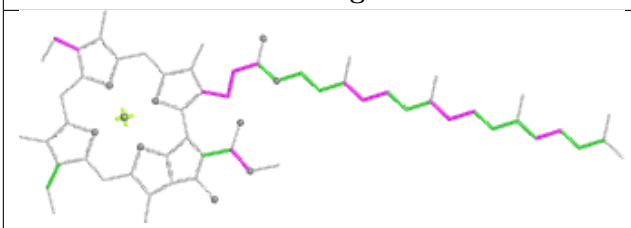
Ligand CLA p 505



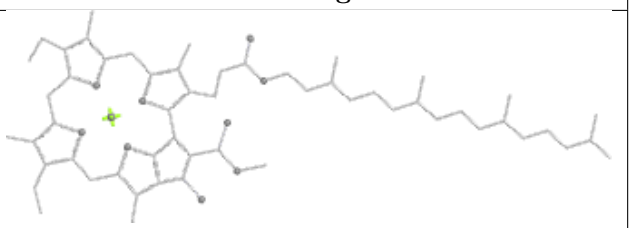
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Bond angles

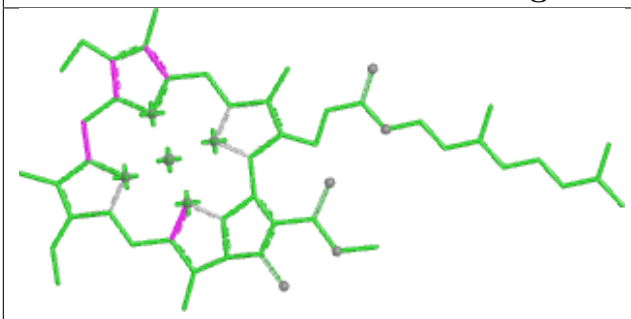


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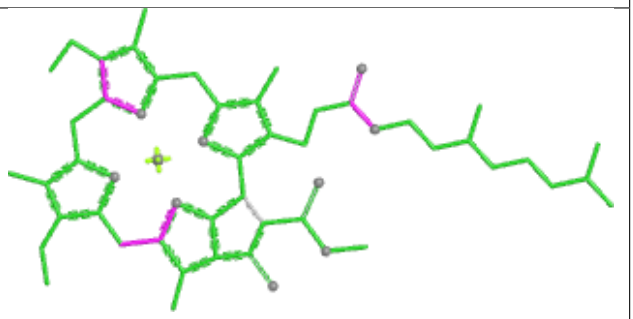


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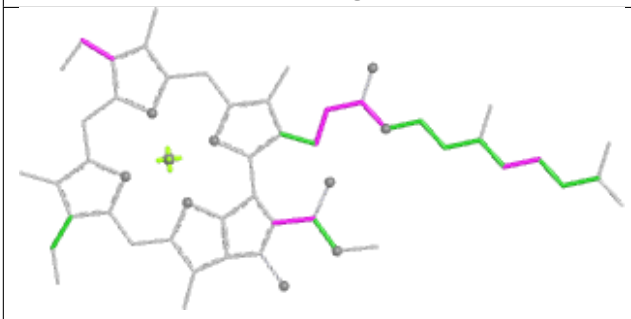
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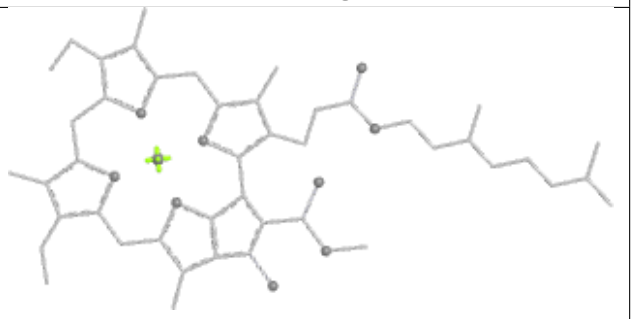
Bond lengths



Bond angles

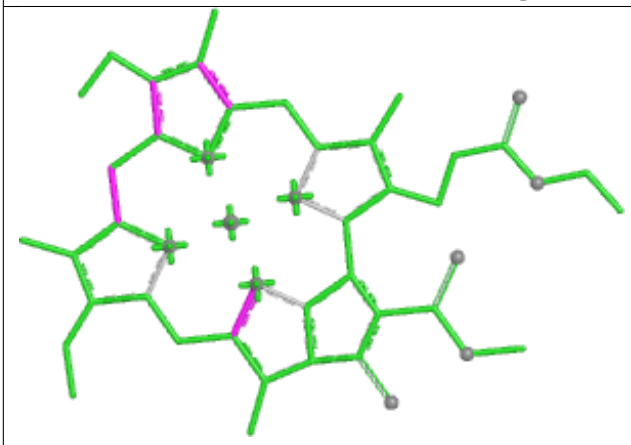


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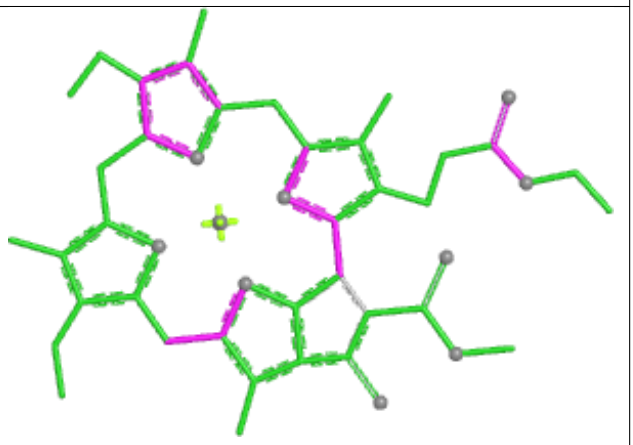


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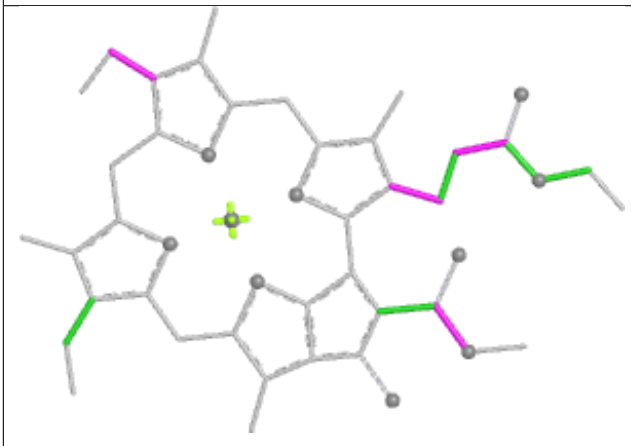
Ligand CLA A 1137



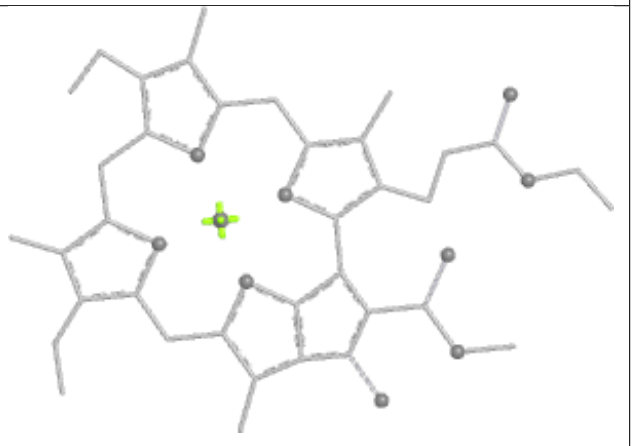
Bond lengths



Bond angles

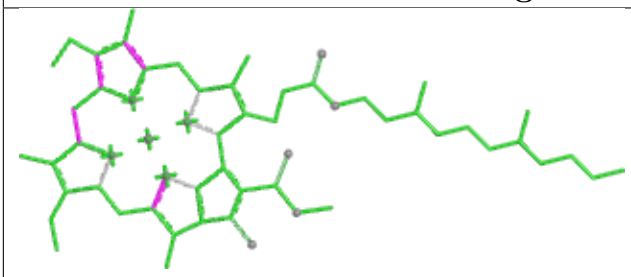


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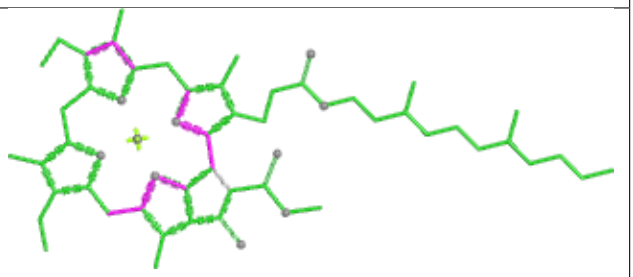


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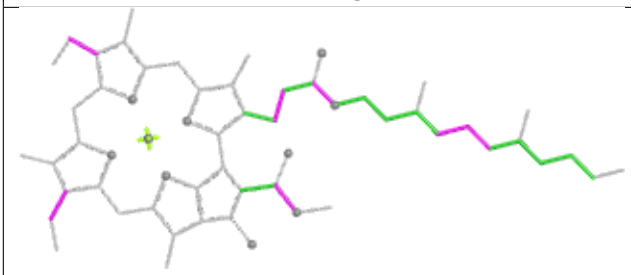
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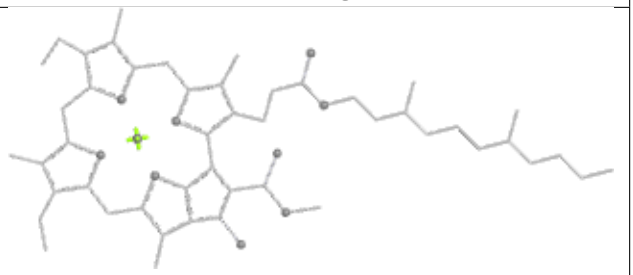
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Bond angles

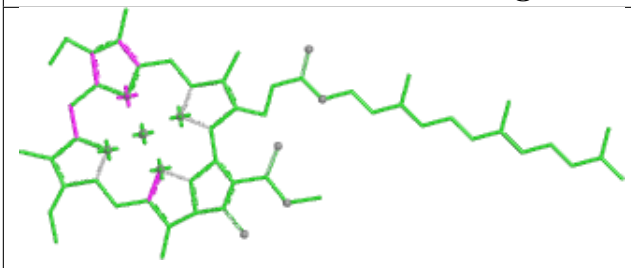


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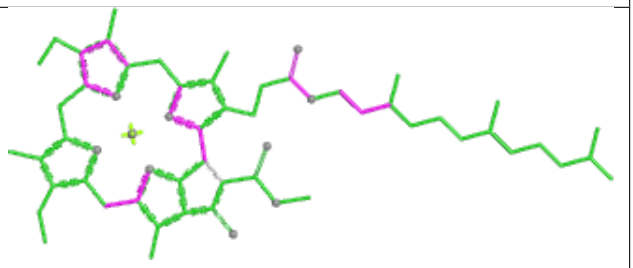


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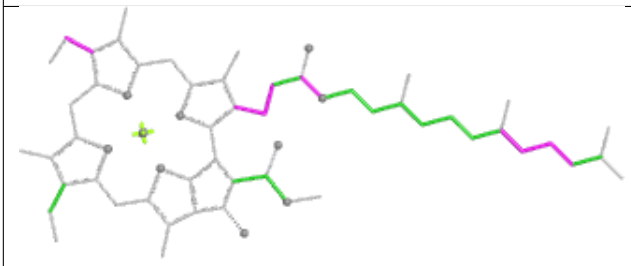
Ligand CLA H 1130



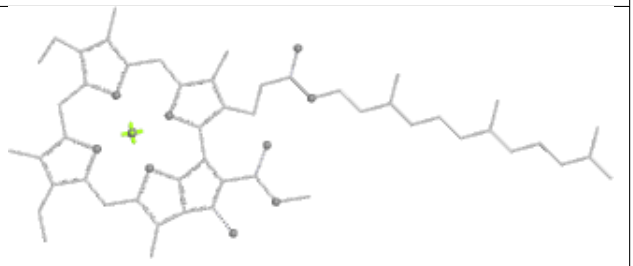
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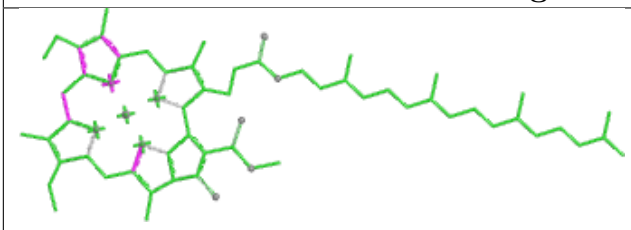


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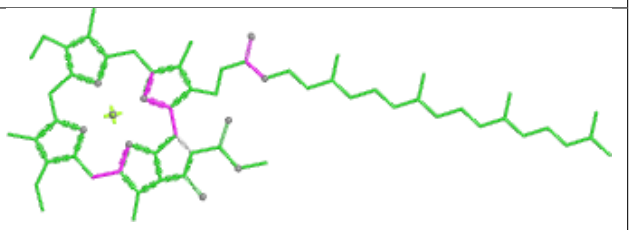


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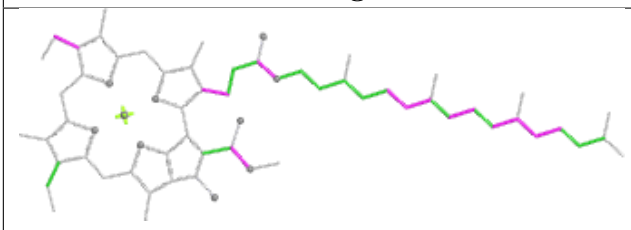
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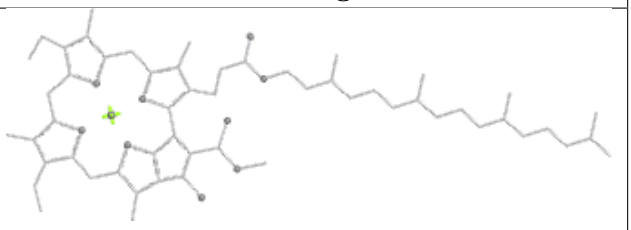
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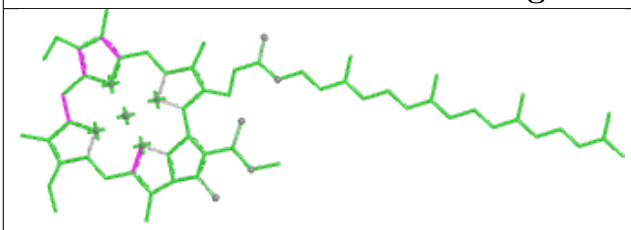


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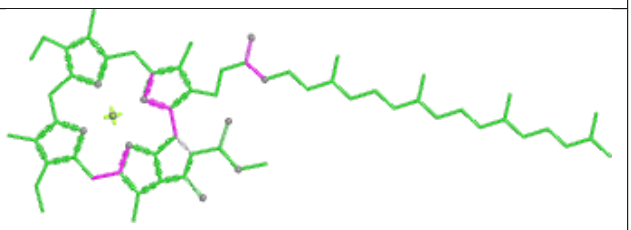


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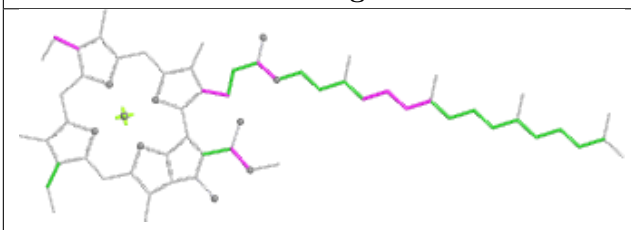
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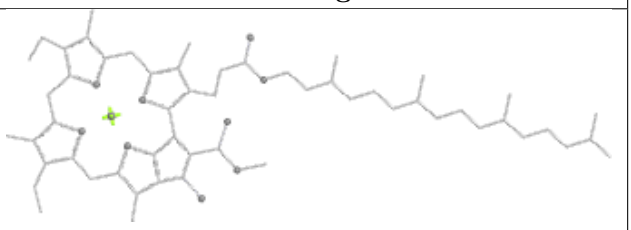
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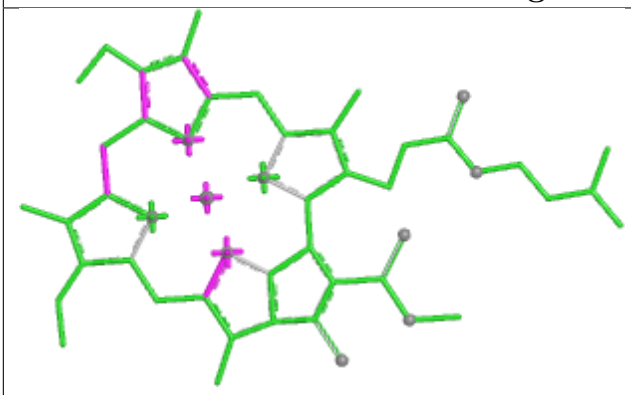


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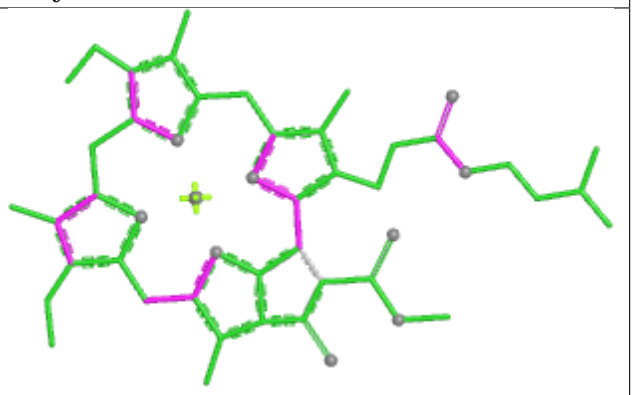


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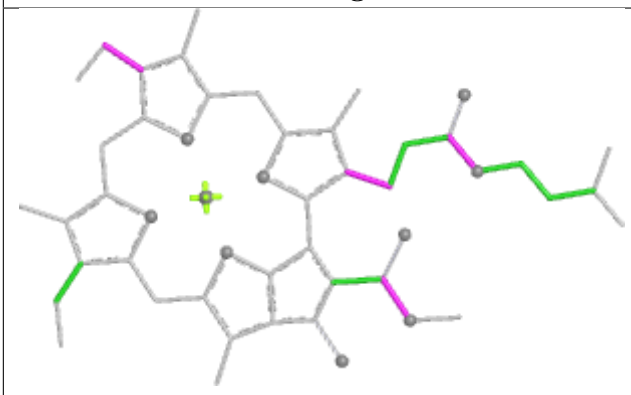
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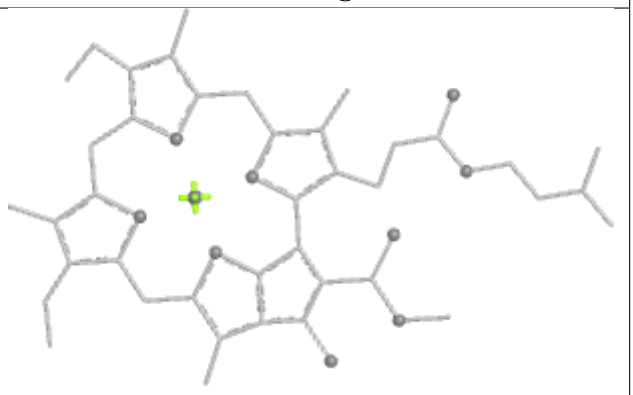
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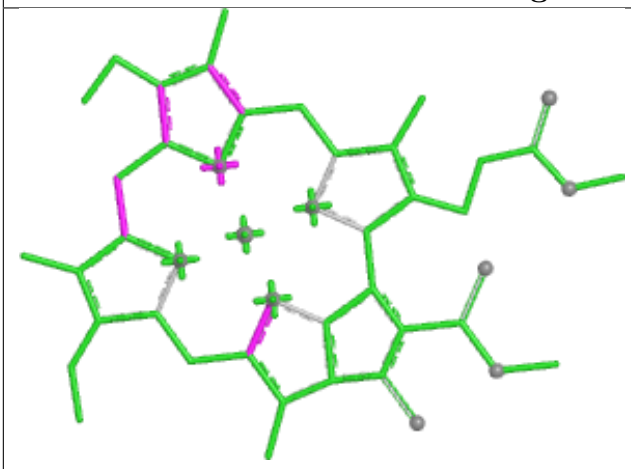


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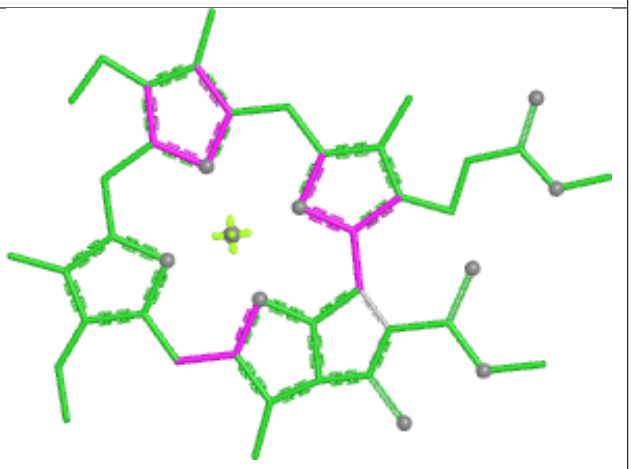


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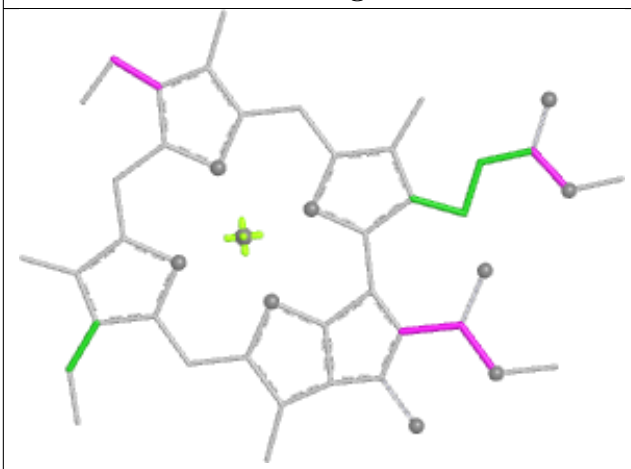
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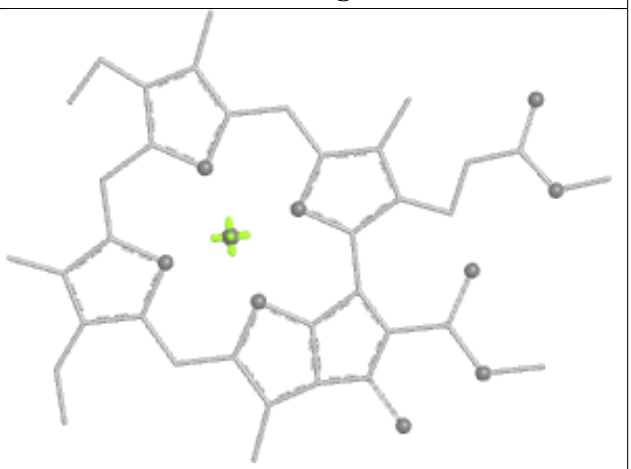
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Bond angles

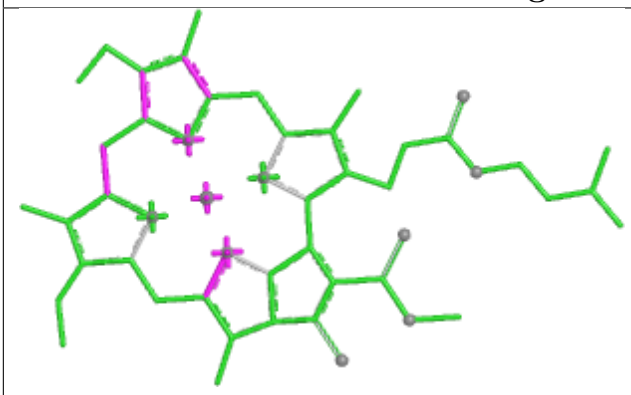


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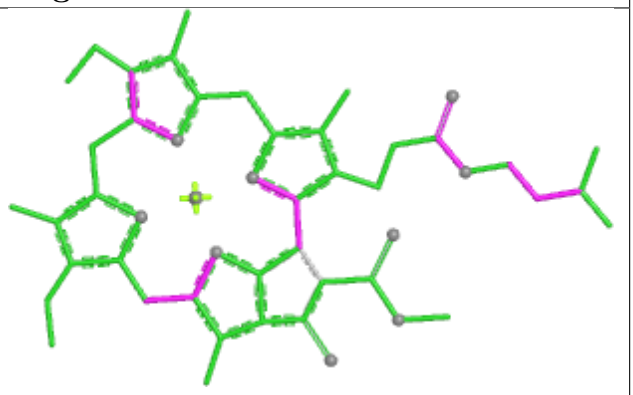


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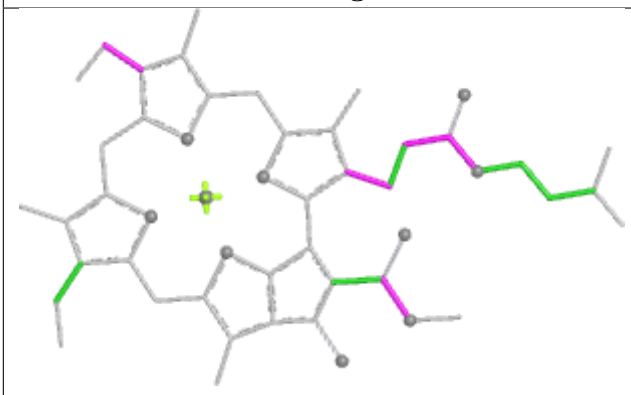
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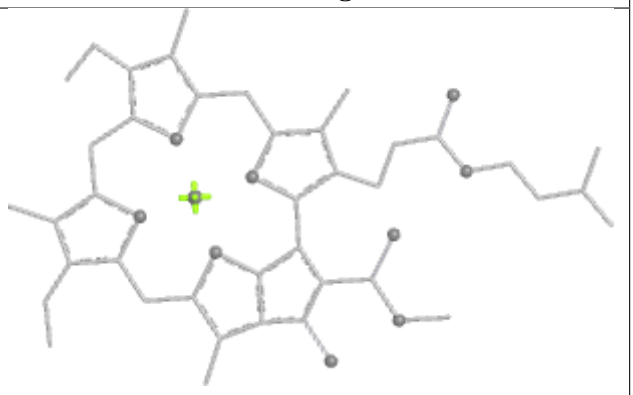
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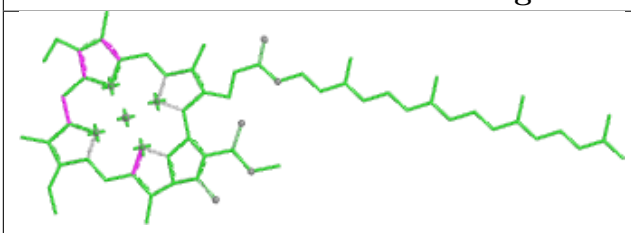


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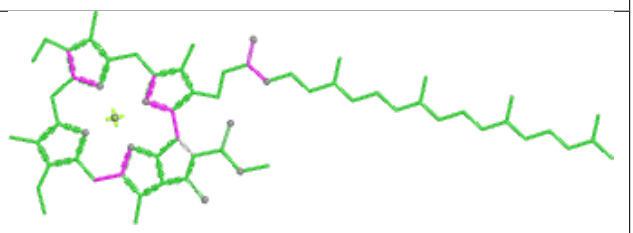


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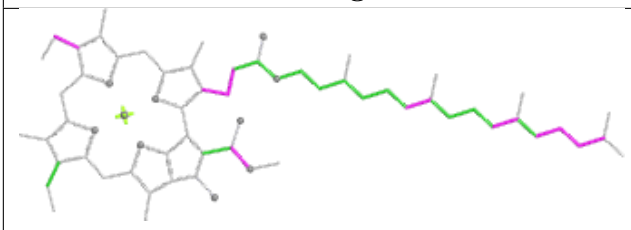
Ligand CLA H 1126



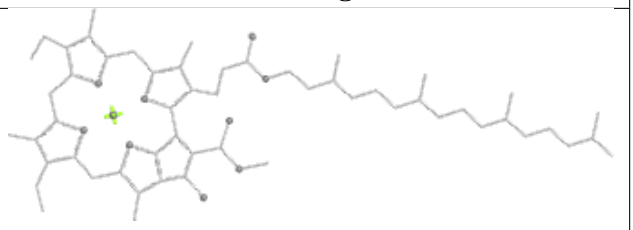
Bond lengths



Bond angles

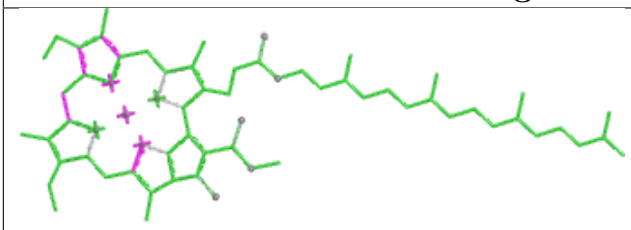


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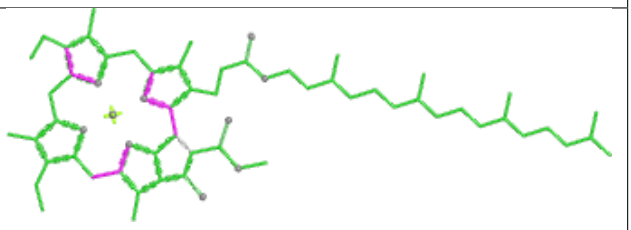


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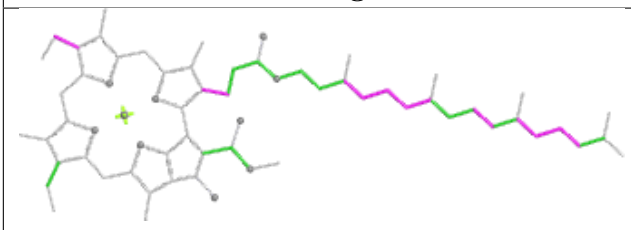
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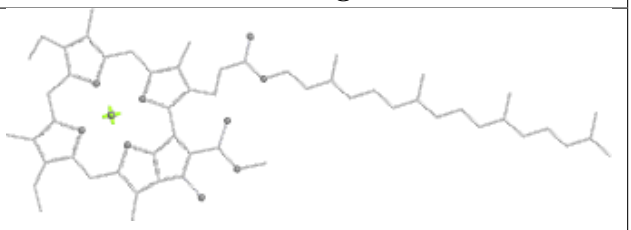
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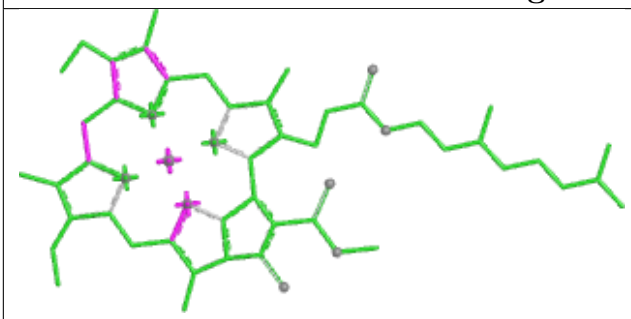


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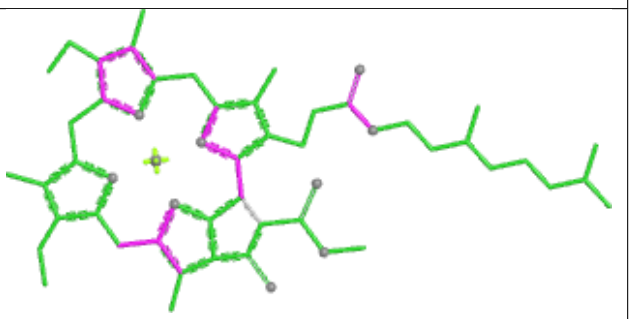


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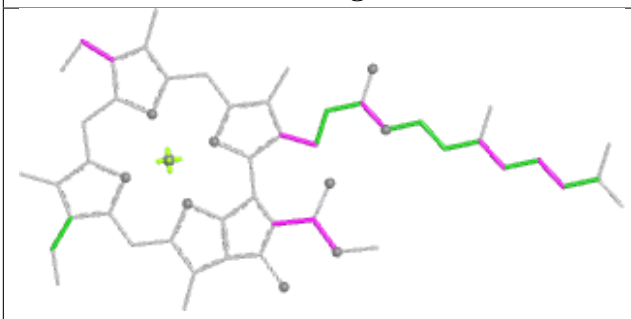
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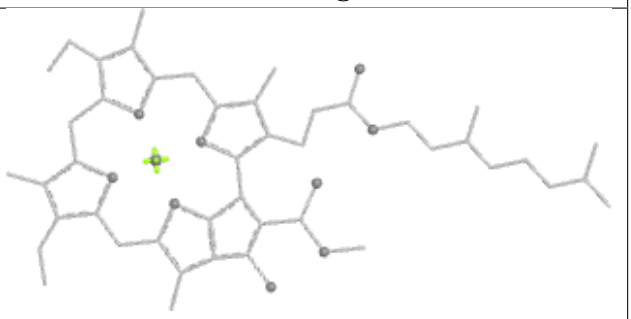
Bond lengths



Bond angles

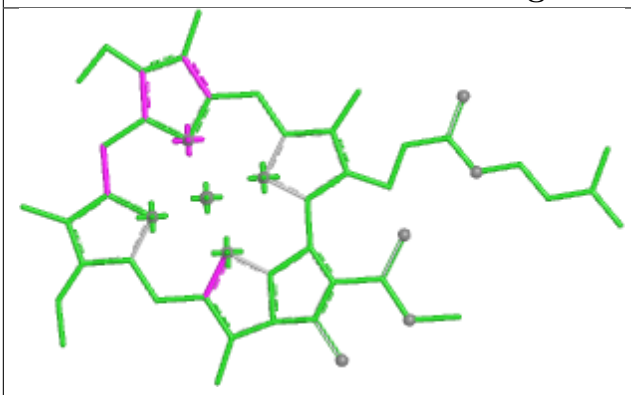


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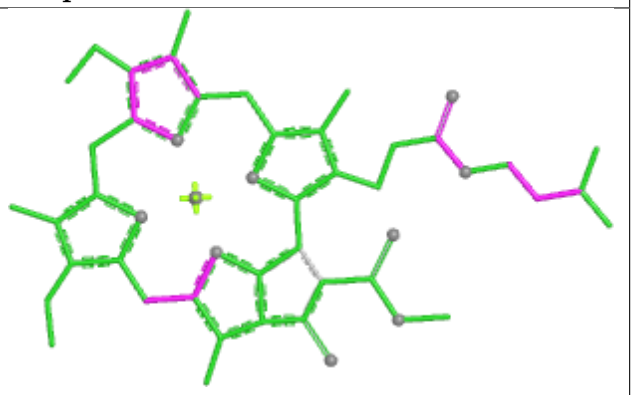


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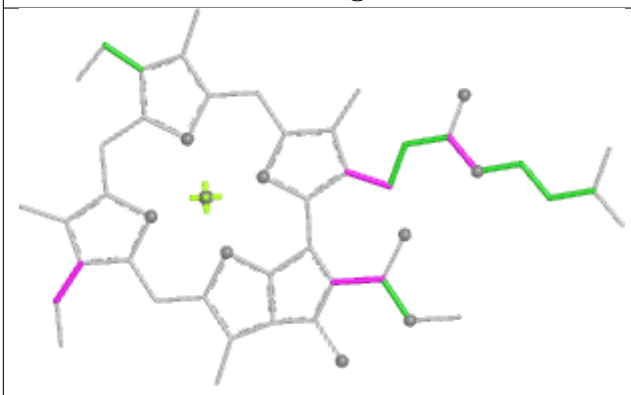
Ligand CLA q 501



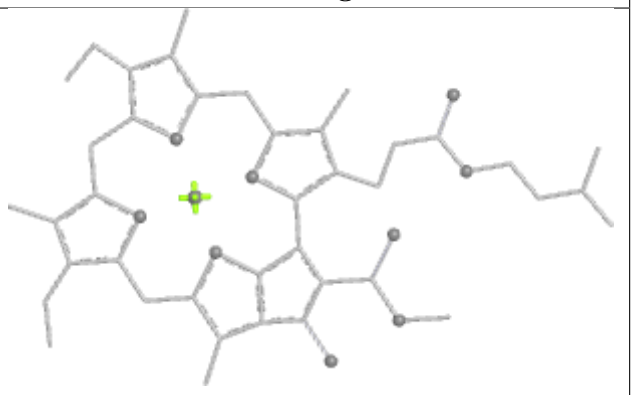
Bond lengths



Bond angles

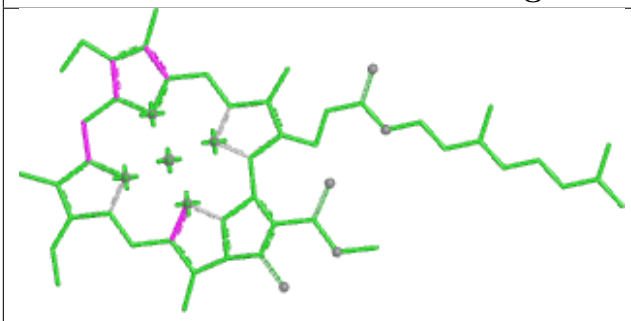


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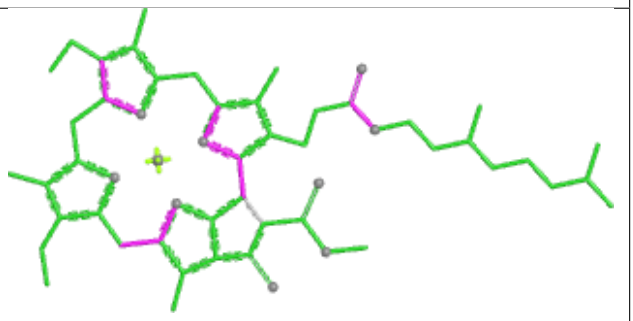


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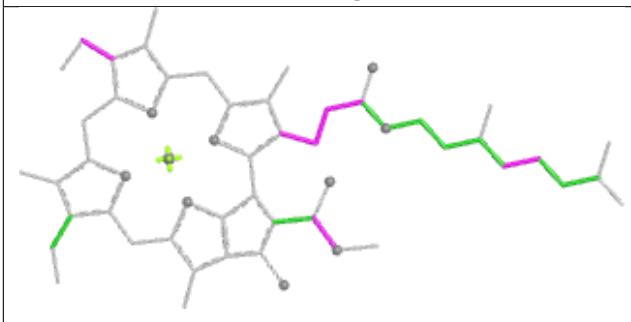
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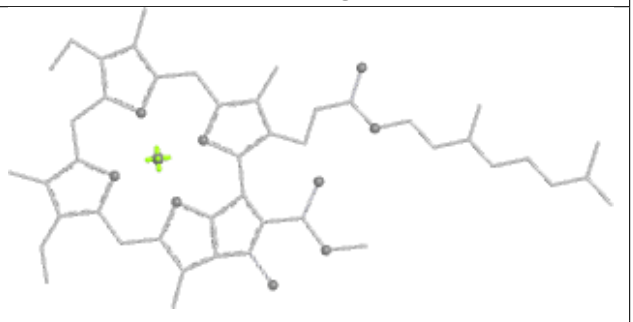
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Bond angles

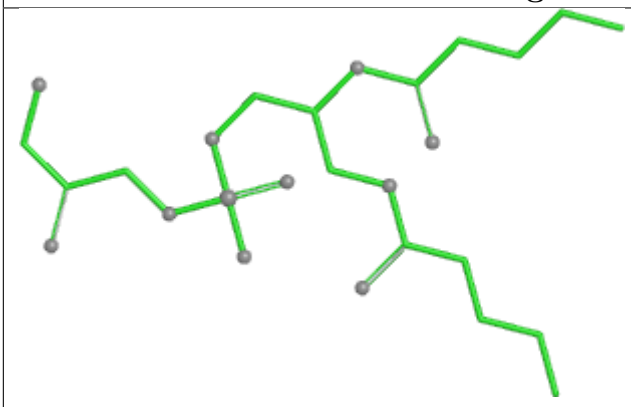


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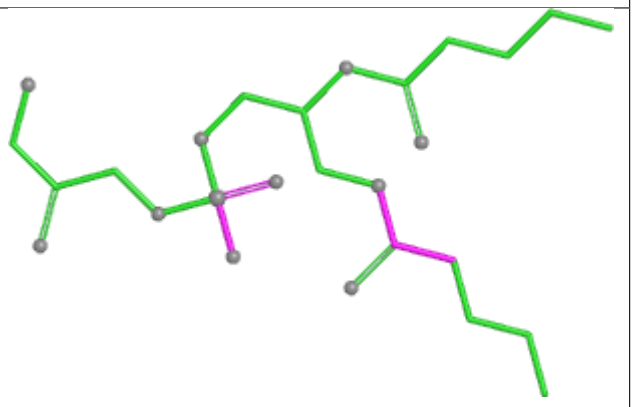


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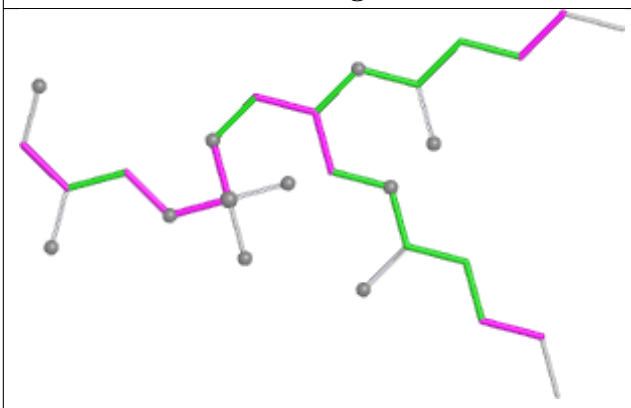
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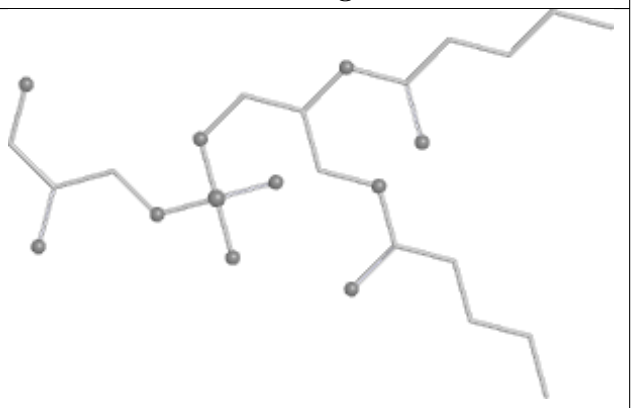
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Bond angles

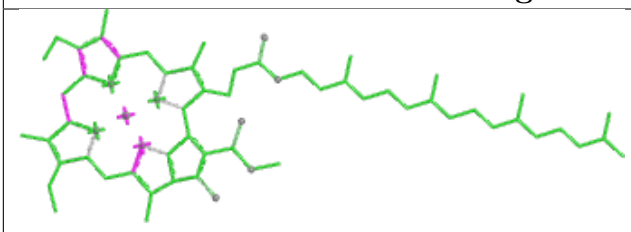


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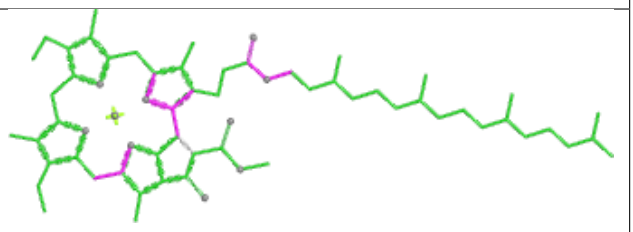


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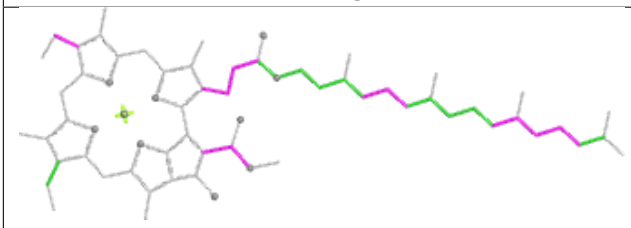
Ligand CLA B 1207



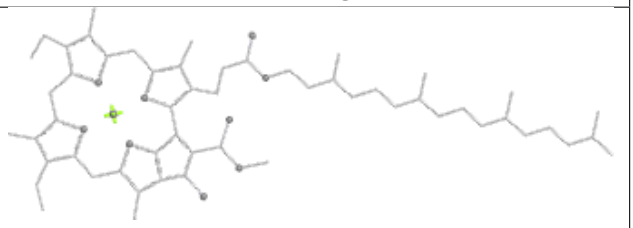
Bond lengths



Bond angles

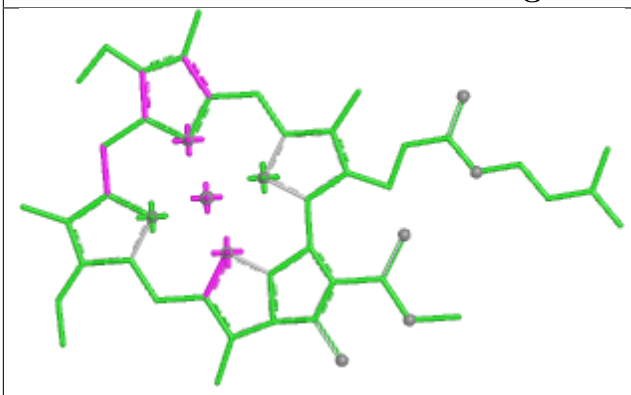


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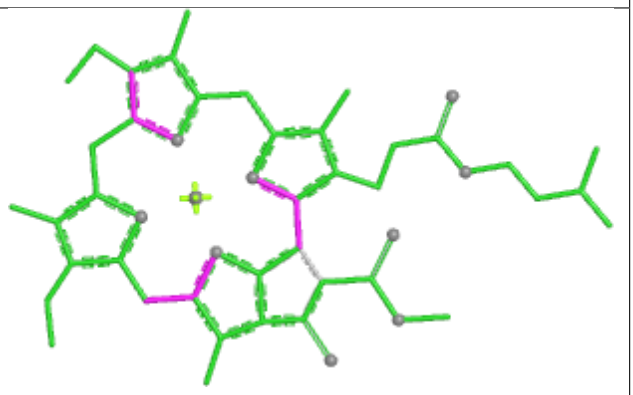


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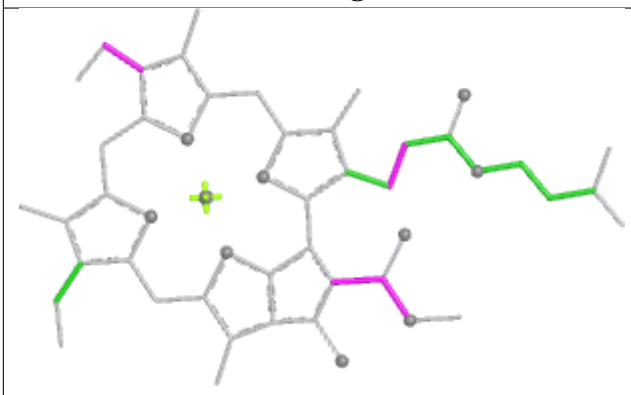
Ligand CLA X 502



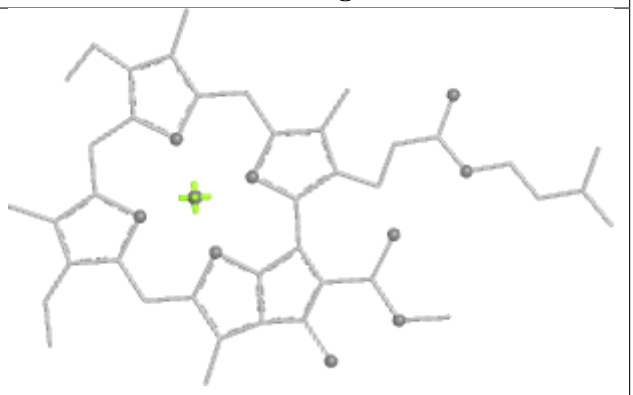
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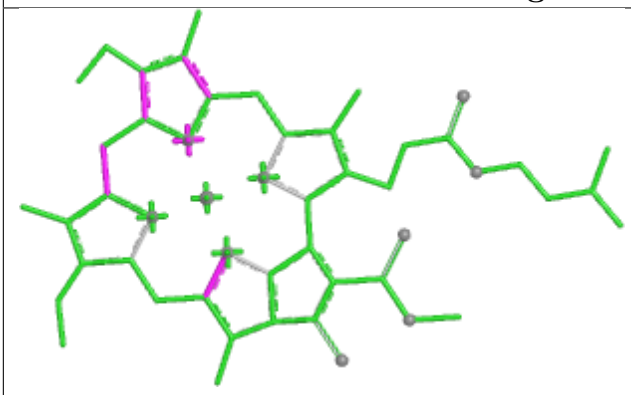


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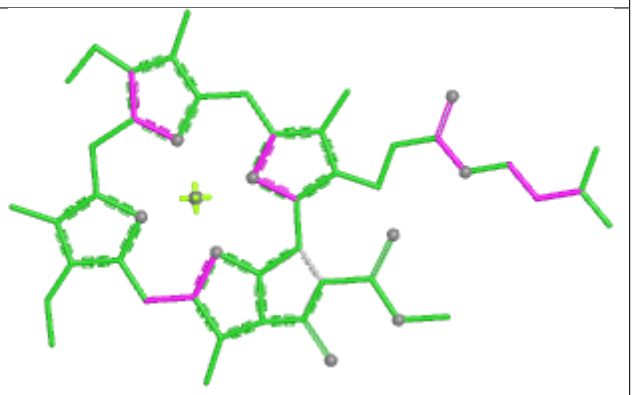


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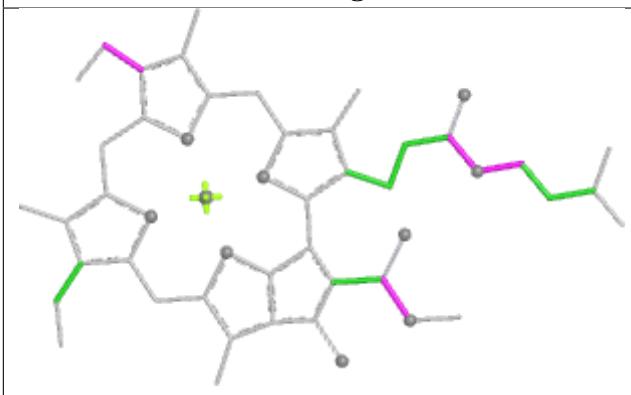
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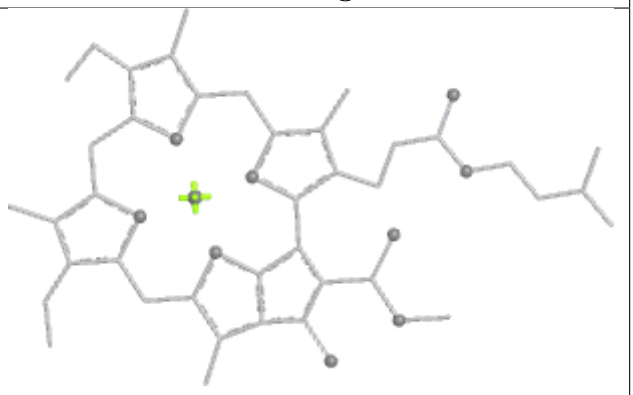
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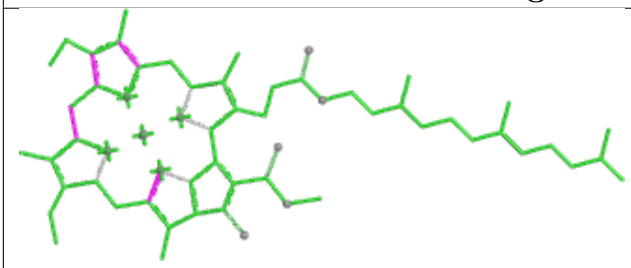


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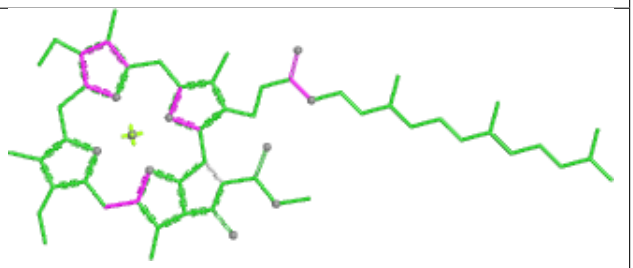


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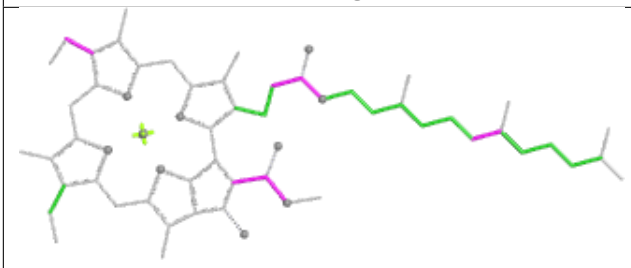
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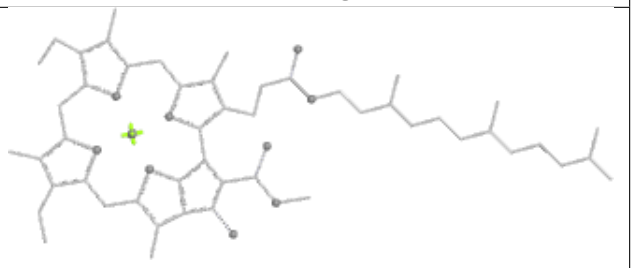
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Bond angles

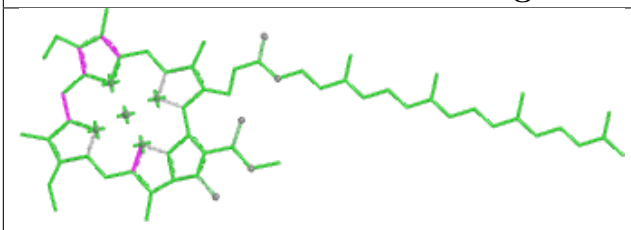


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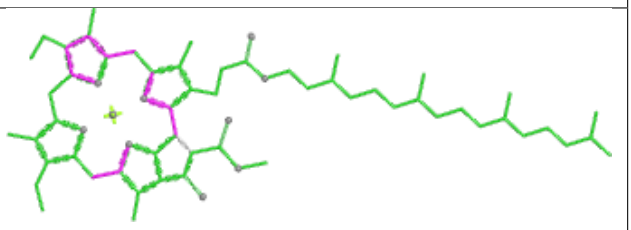


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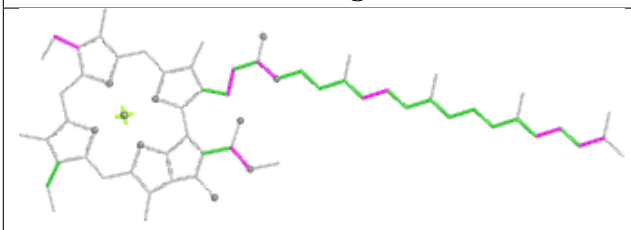
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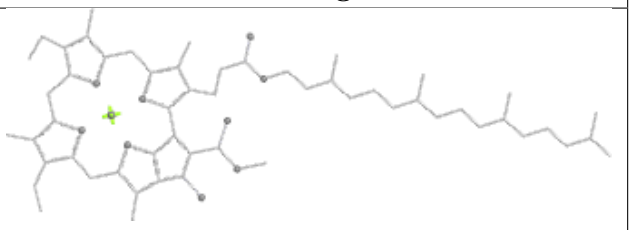
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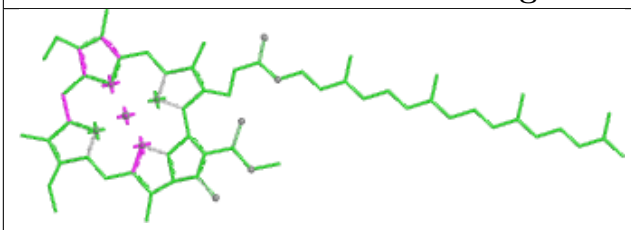


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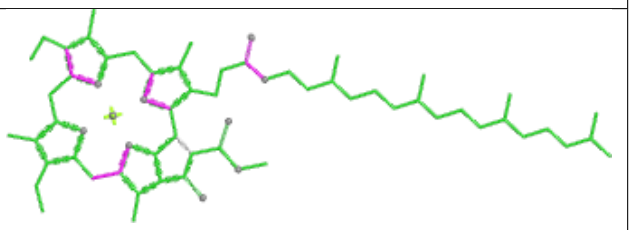


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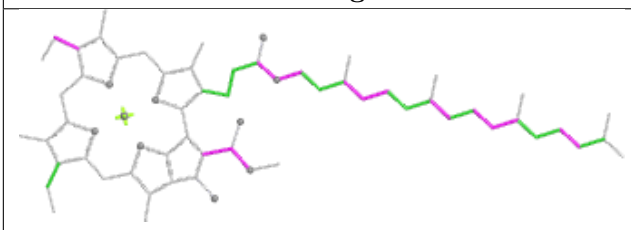
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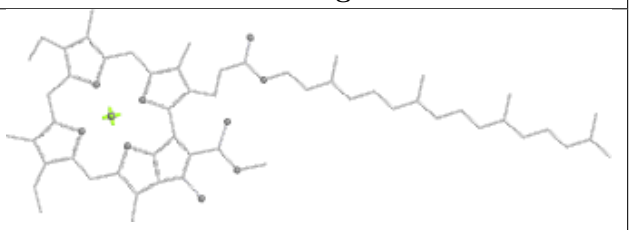
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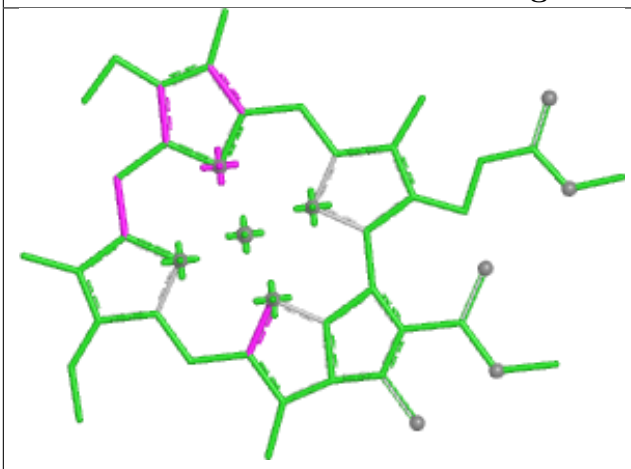


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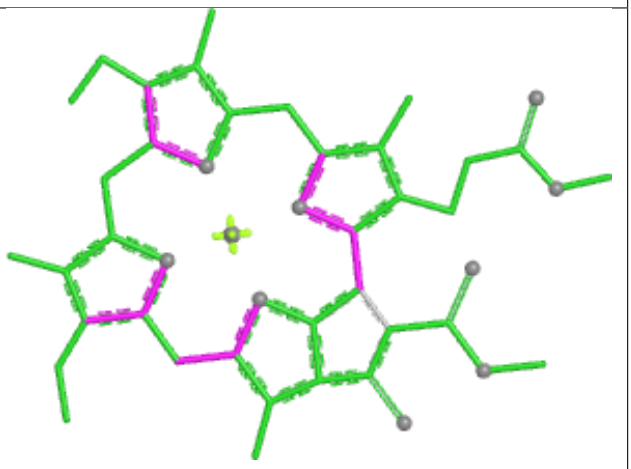


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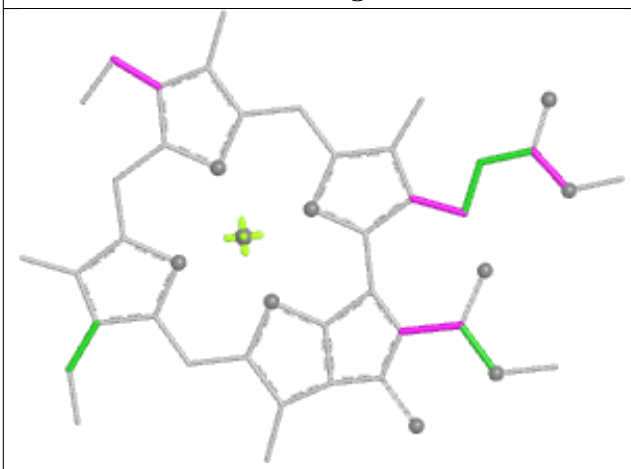
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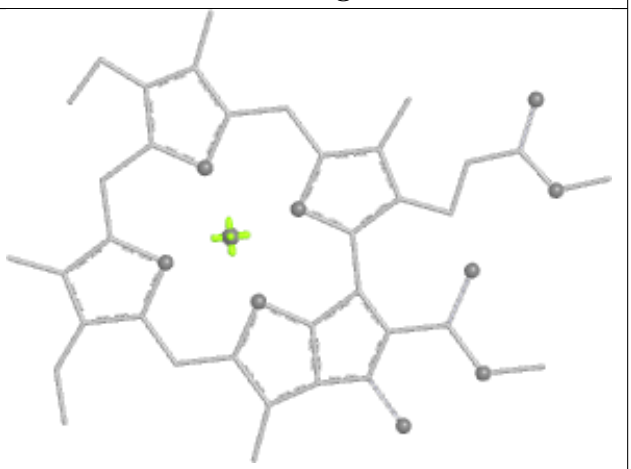
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Bond angles

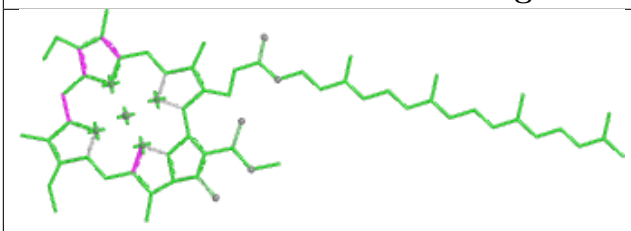


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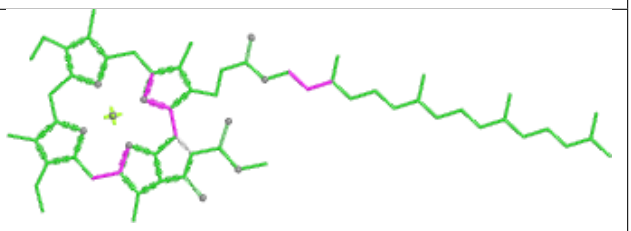


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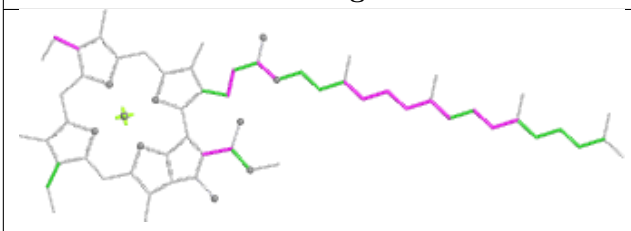
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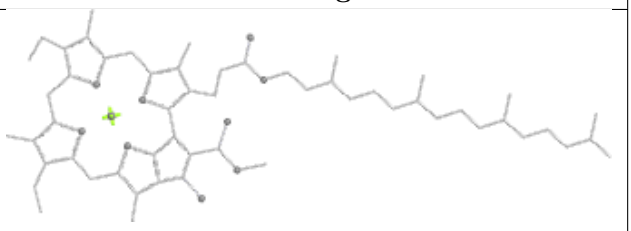
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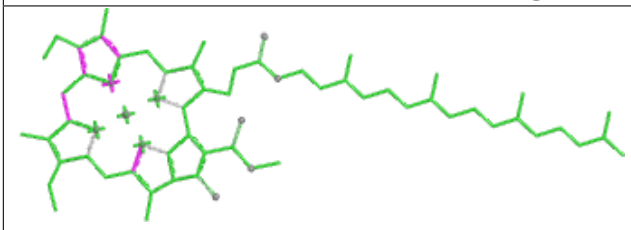


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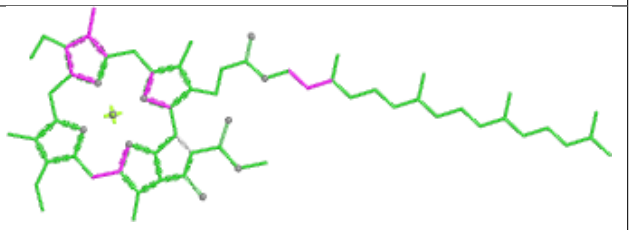


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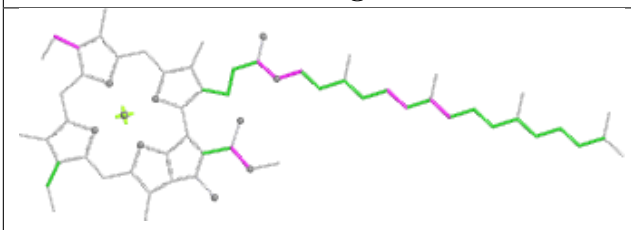
Ligand CLA x 507



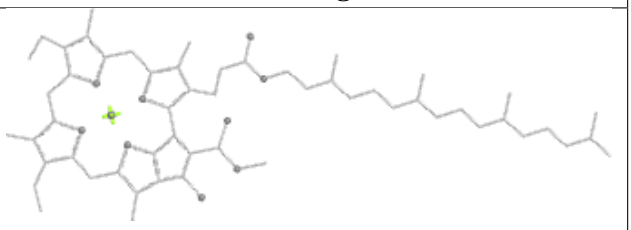
Bond lengths



Bond angles



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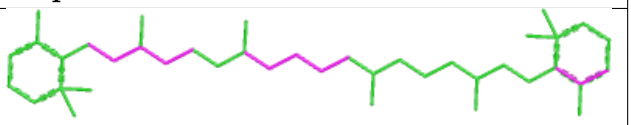


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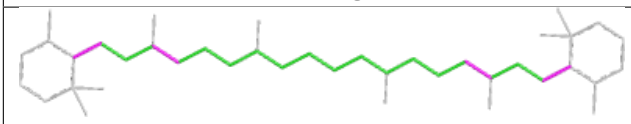
Ligand BCR p 603



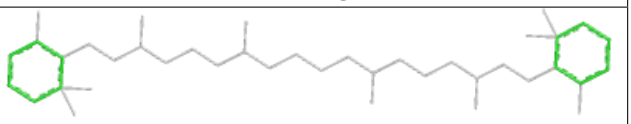
Bond lengths



Bond angles

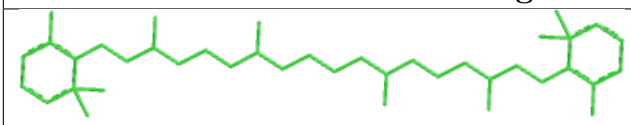


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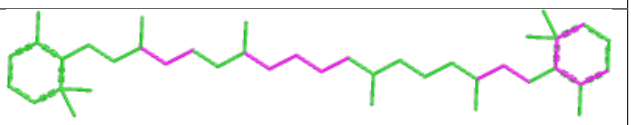


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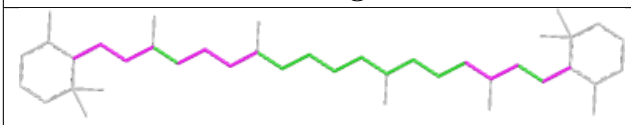
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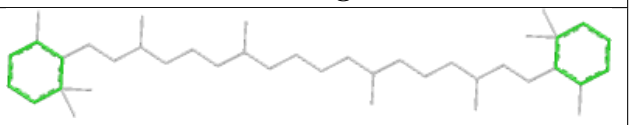
Bond lengths



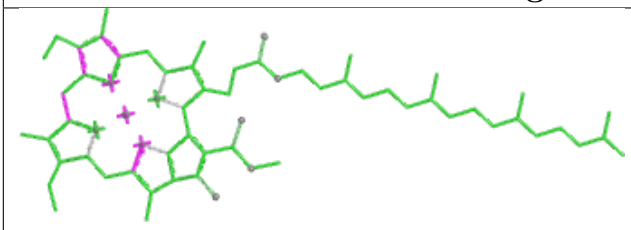
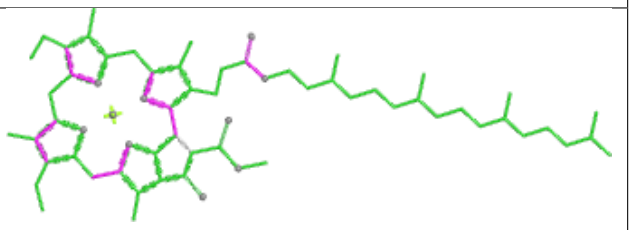
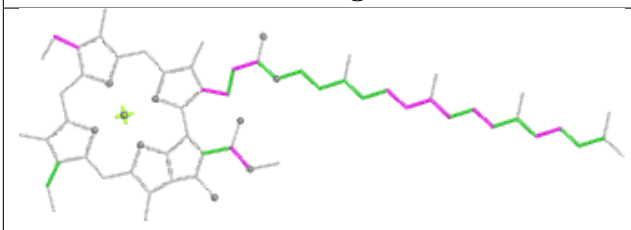
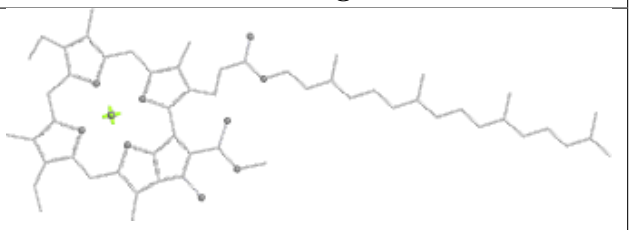
Bond angles

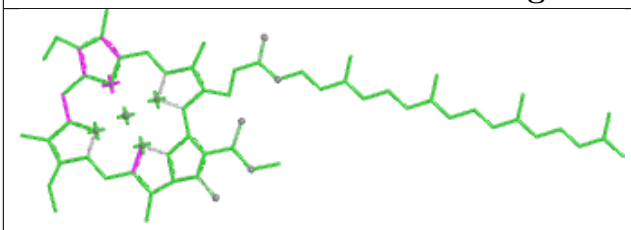
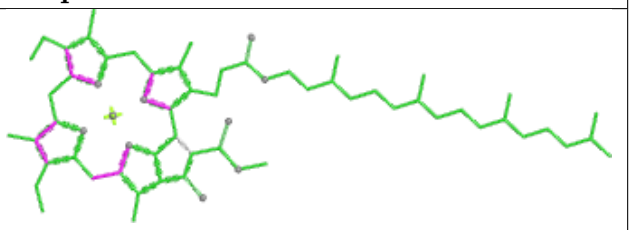
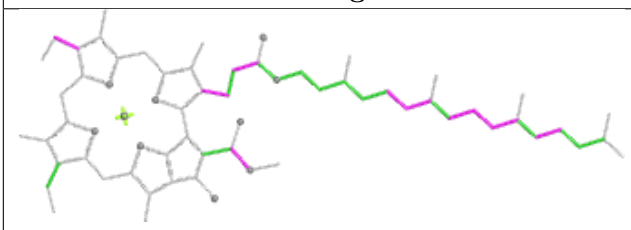
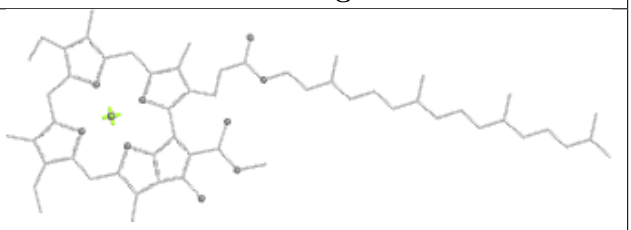


Torsions

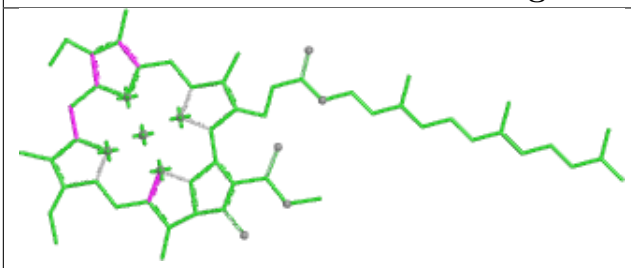


Rings

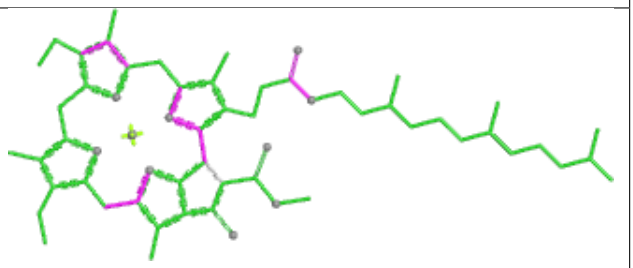
Ligand CLA Z 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

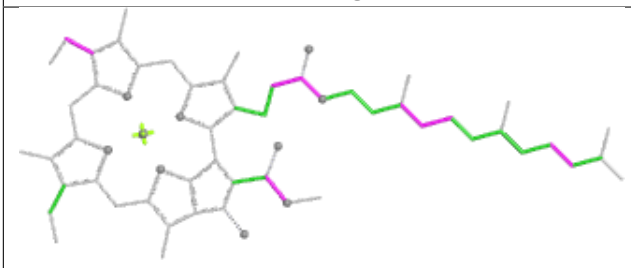
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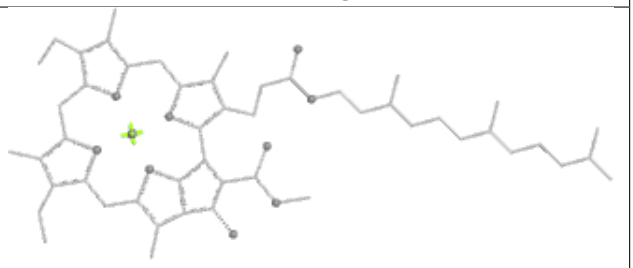
Bond lengths



Bond angles

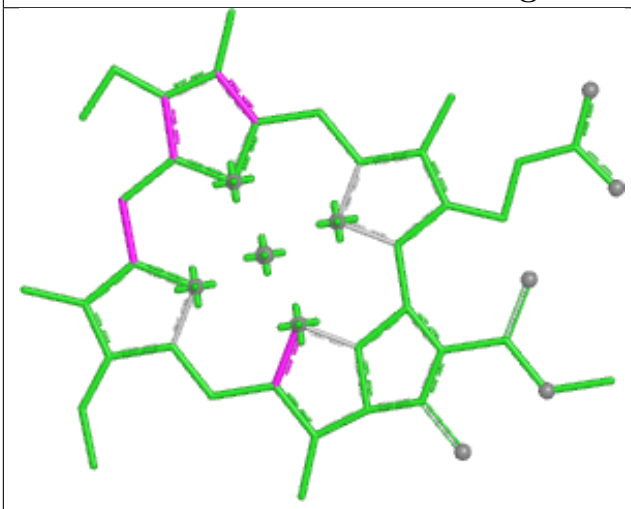


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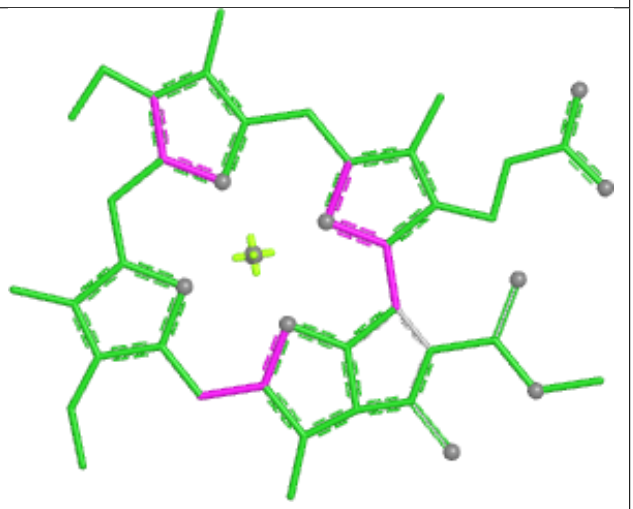


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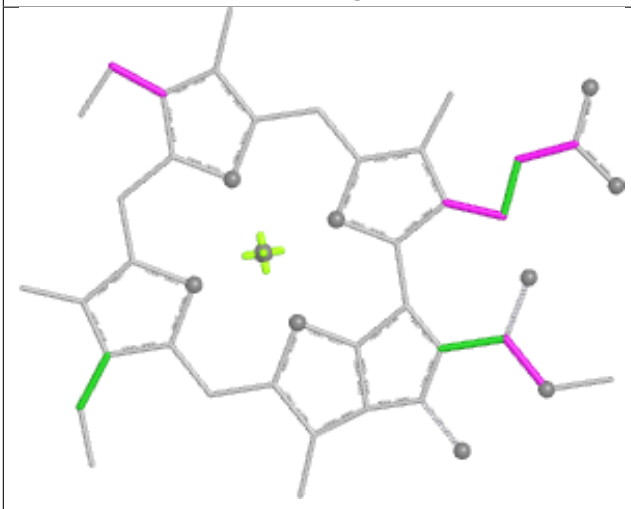
Ligand CLA a 1134



Bond lengths



Bond angles

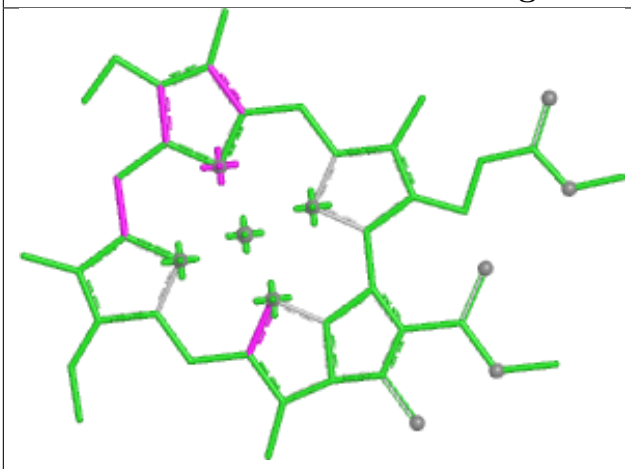


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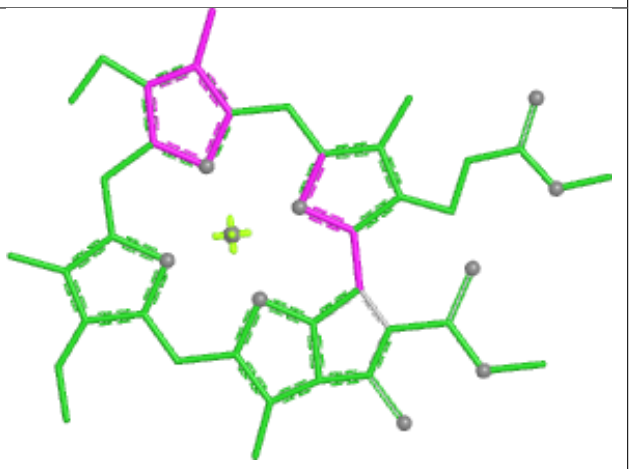


Rings

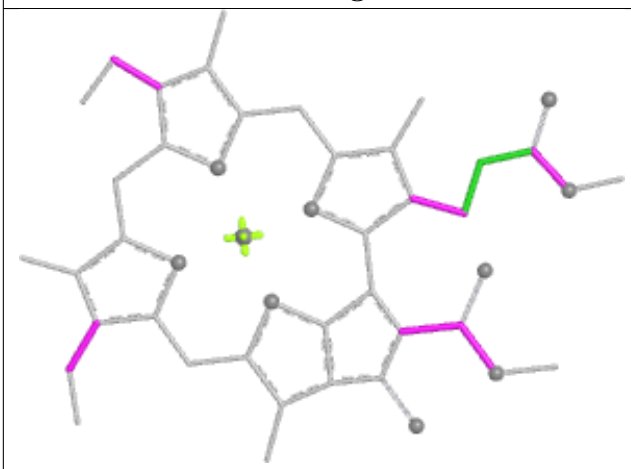
Ligand CLA W 513



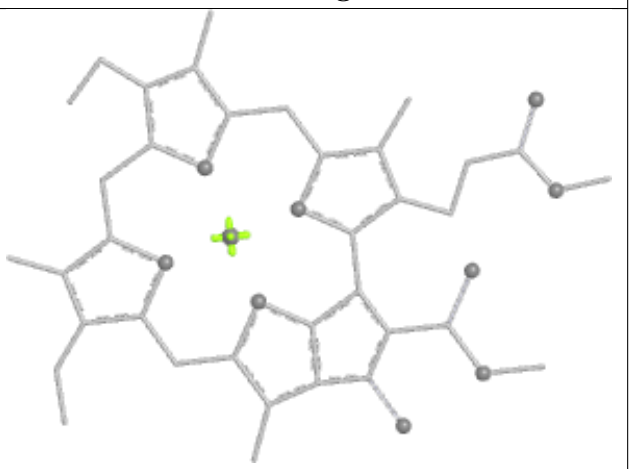
Bond lengths



Bond angles

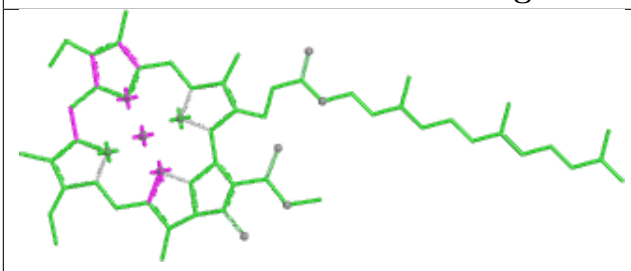


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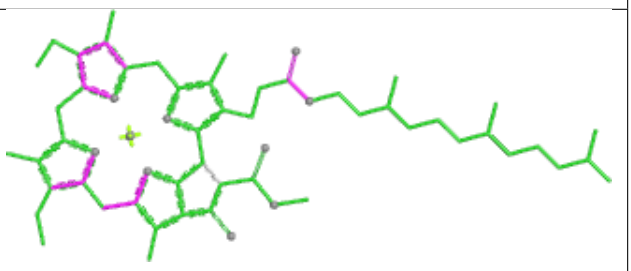


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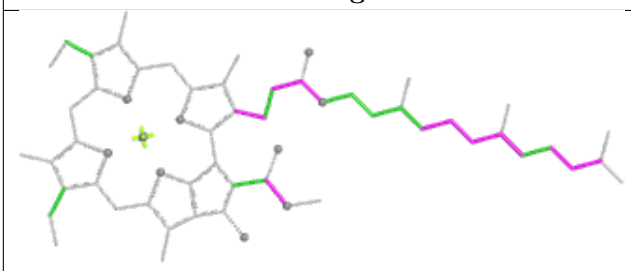
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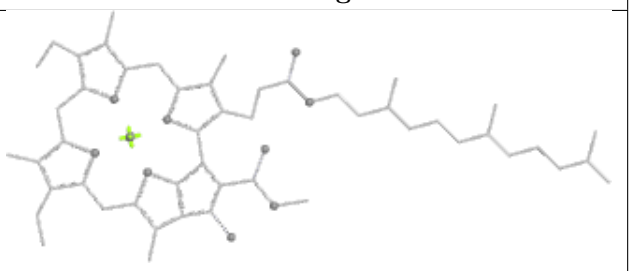
Bond lengths



Bond angles

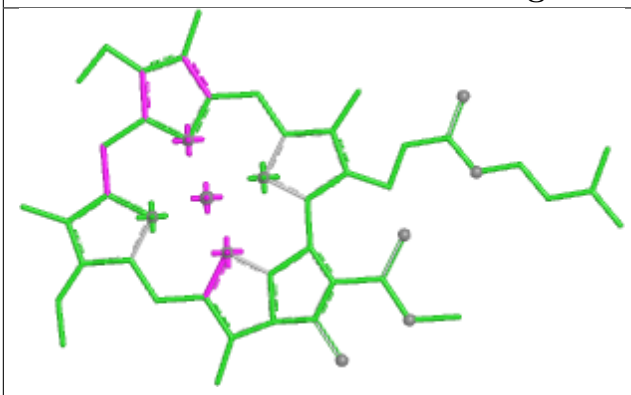


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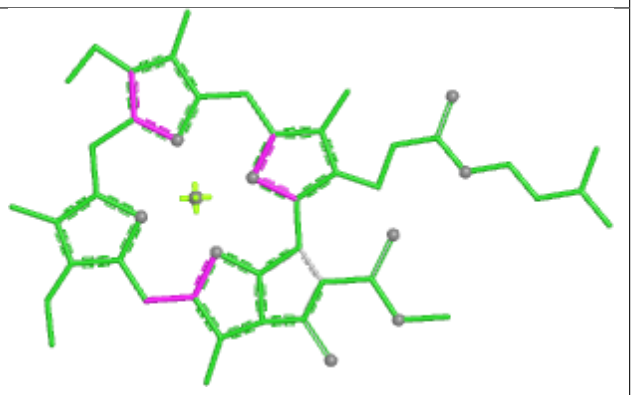


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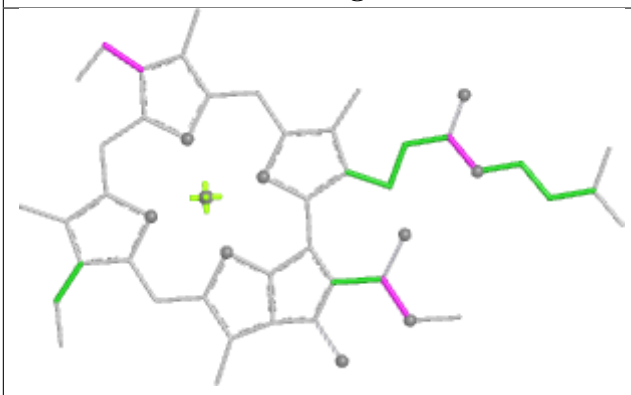
Ligand CLA x 502



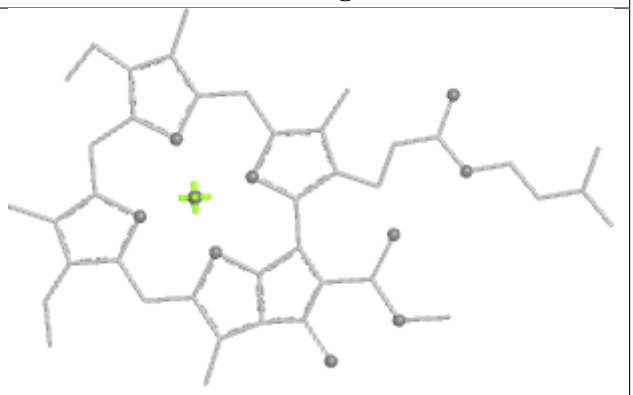
Bond lengths



Bond angles

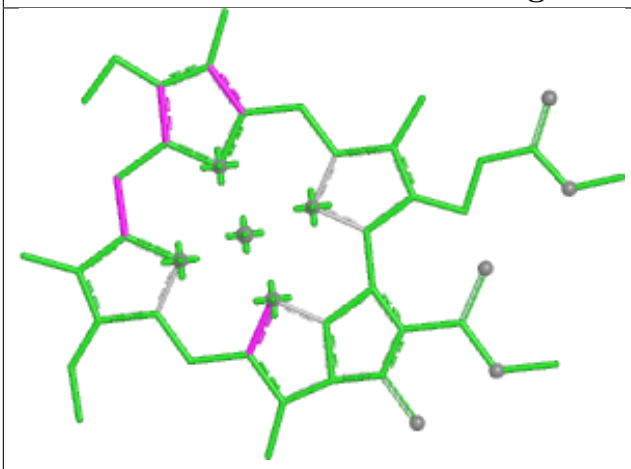


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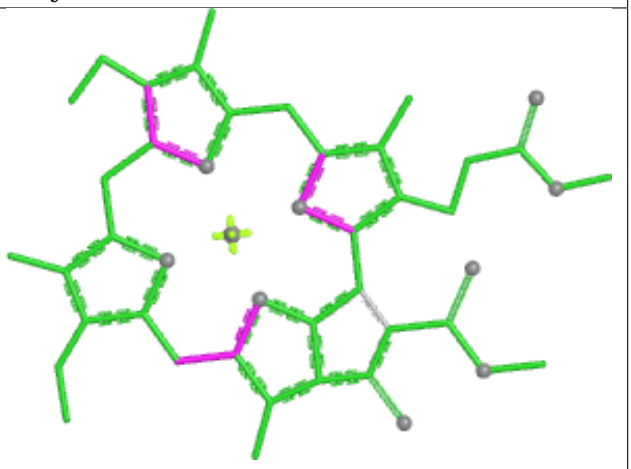


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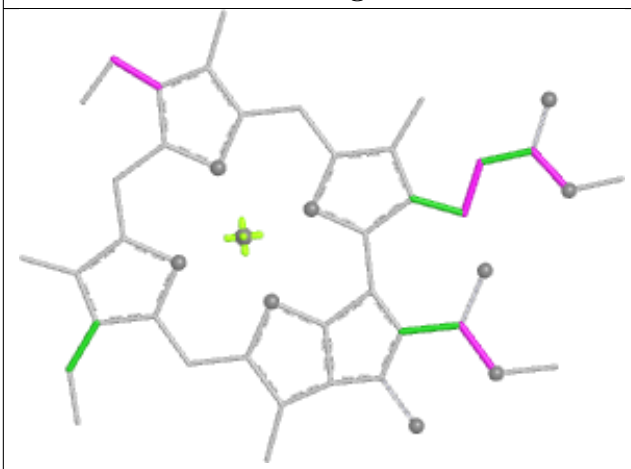
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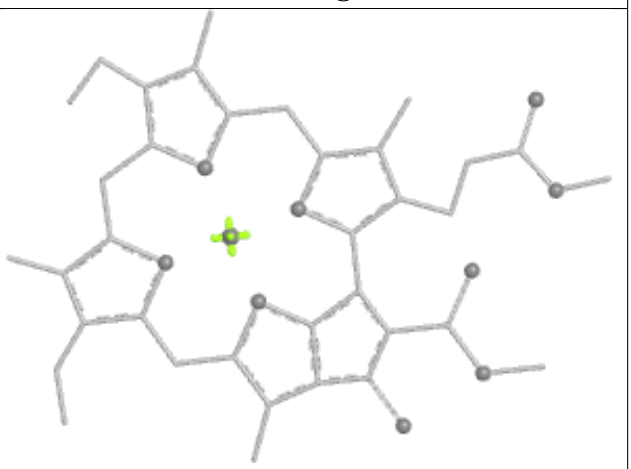
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Bond angles

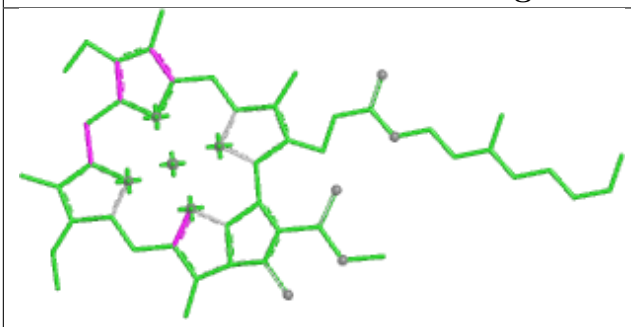


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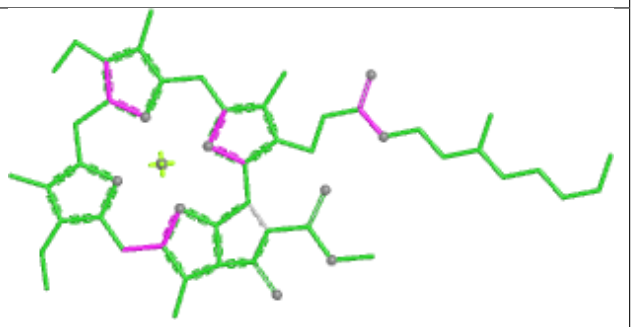


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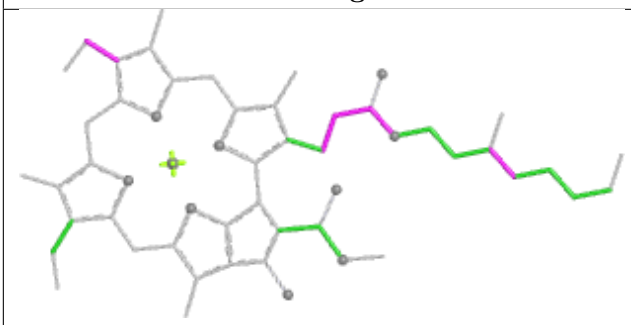
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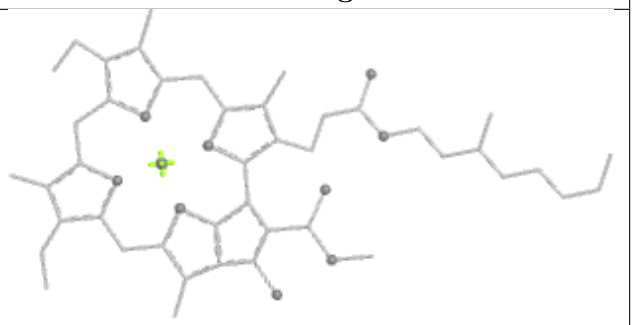
Bond lengths



Bond angles



Torsions

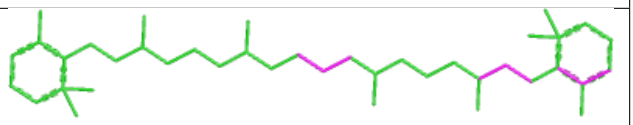


Rings

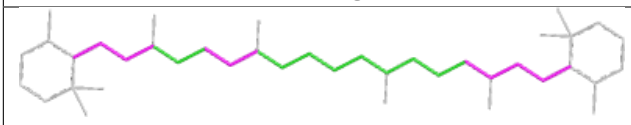
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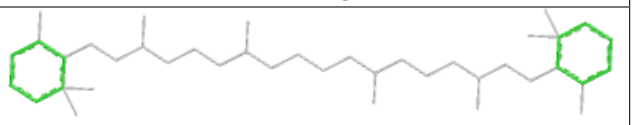
Bond lengths



Bond angles

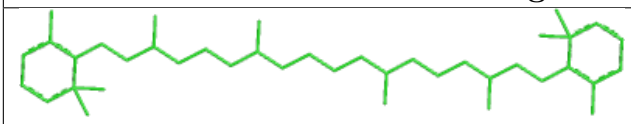


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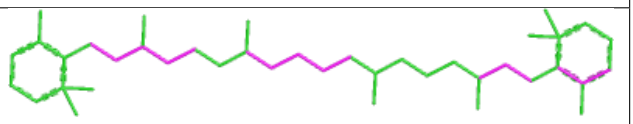


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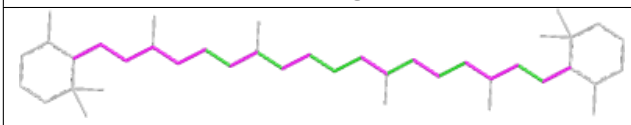
Ligand BCR r 604



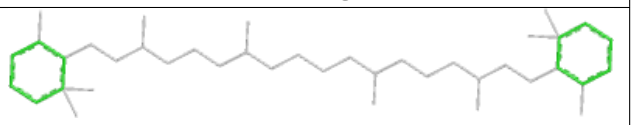
Bond lengths



Bond angles

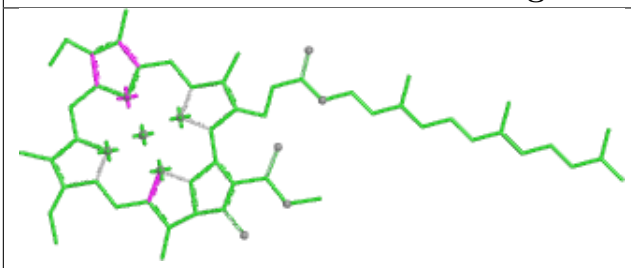


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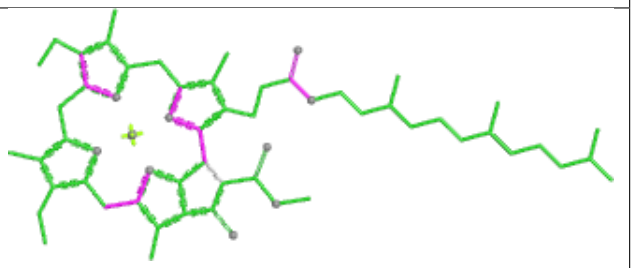


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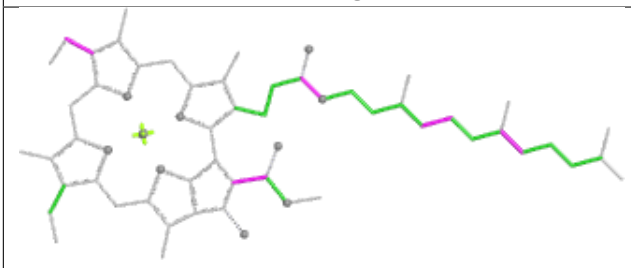
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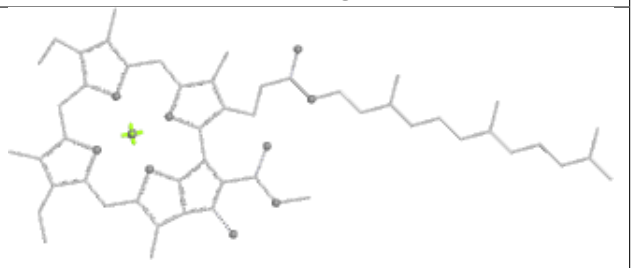
Bond lengths



Bond angles

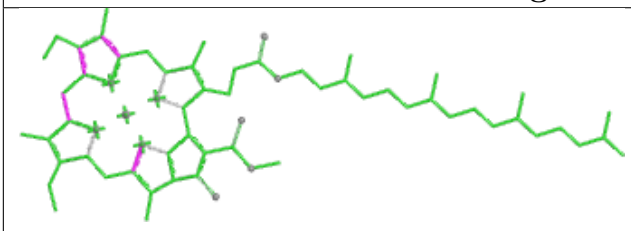


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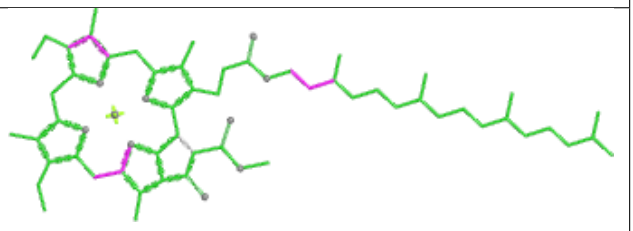


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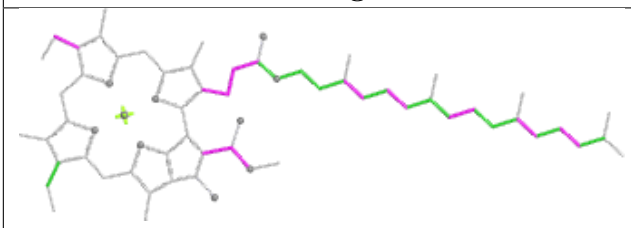
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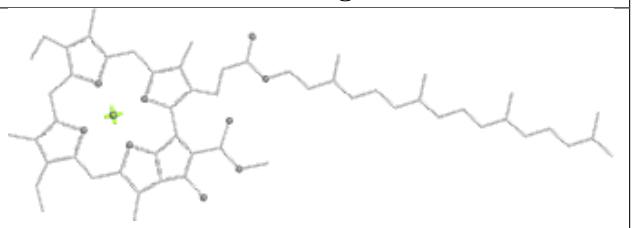
Bond lengths



Bond angles



Torsions

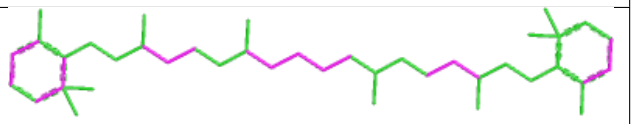


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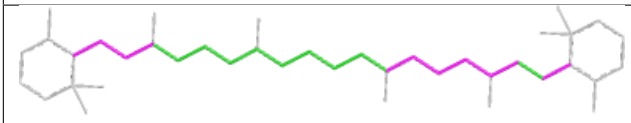
Ligand BCR o 602



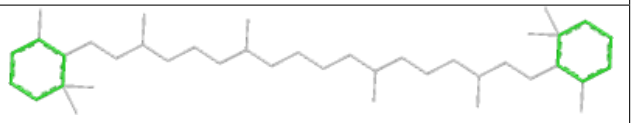
Bond lengths



Bond angles

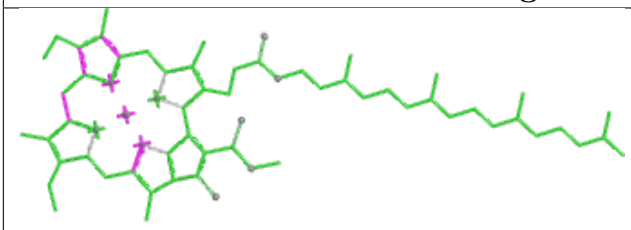


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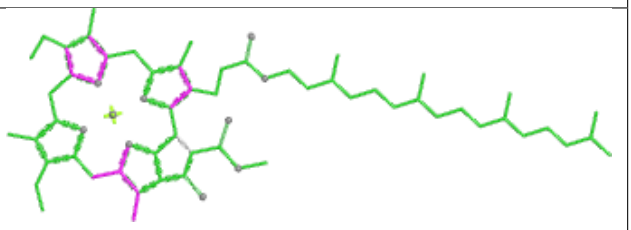


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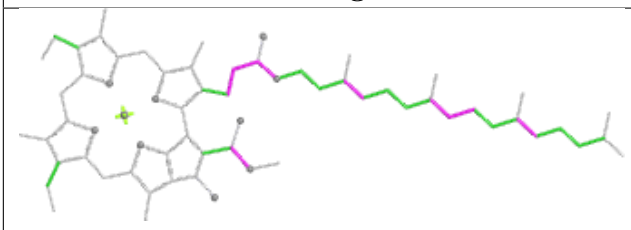
Ligand CLA a 1013



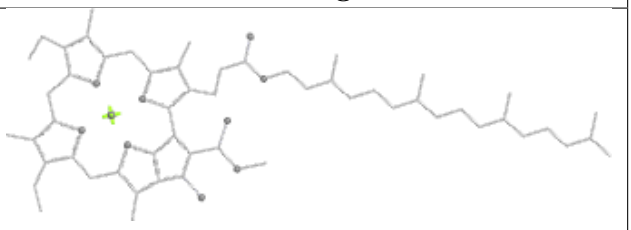
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Bond angles

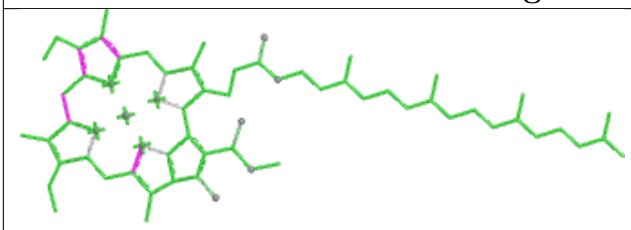


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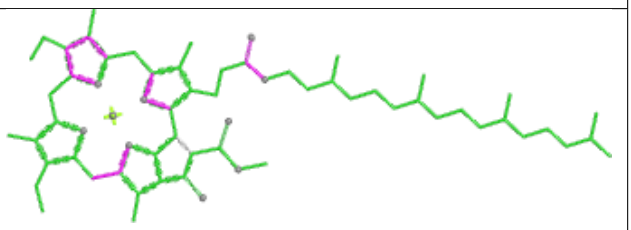


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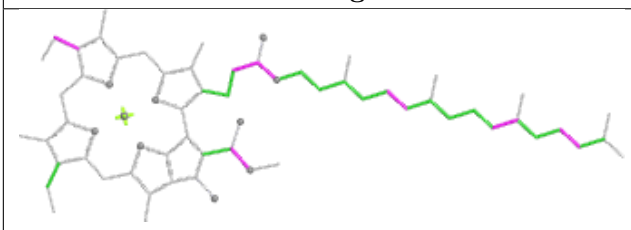
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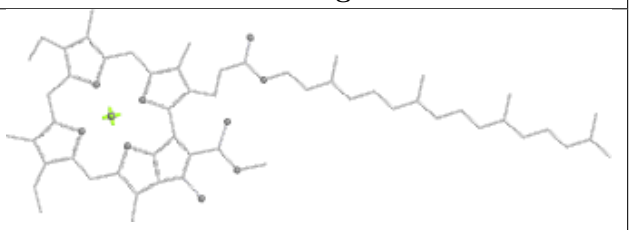
Bond lengths



Bond angles

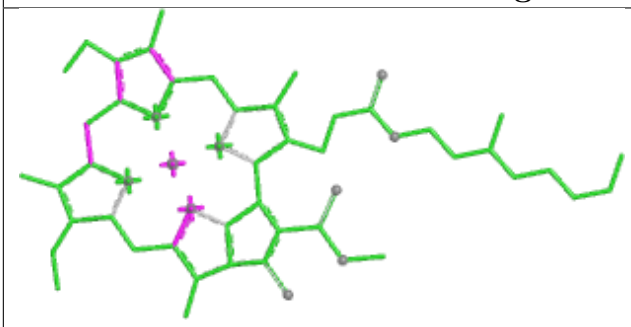


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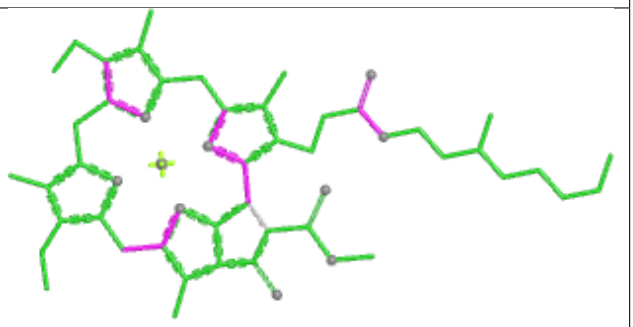


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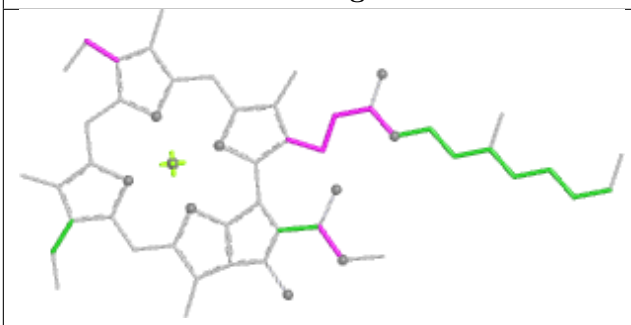
Ligand CLA H 1116



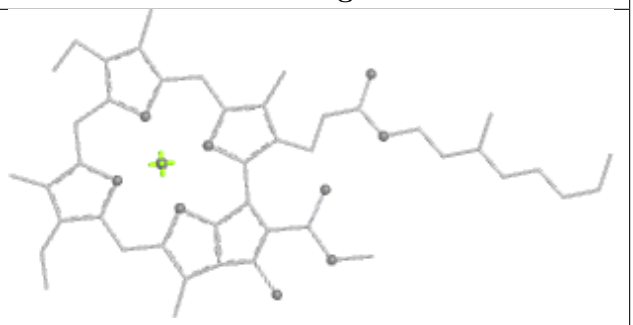
Bond lengths



Bond angles

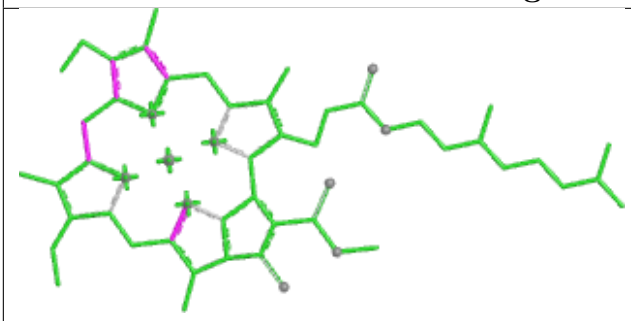


Torsions

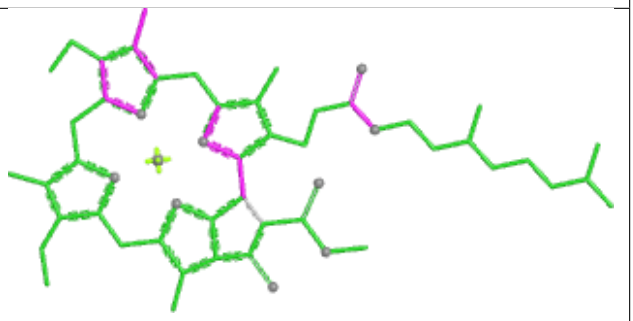


Rings

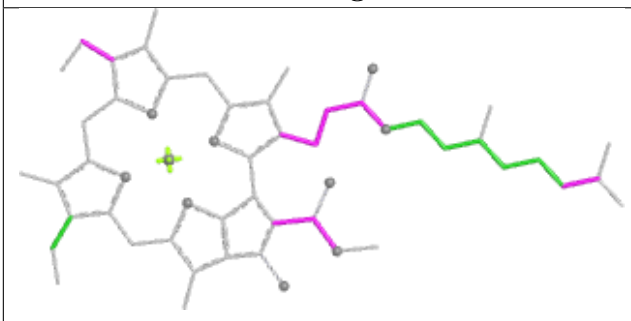
Ligand CLA Y 508



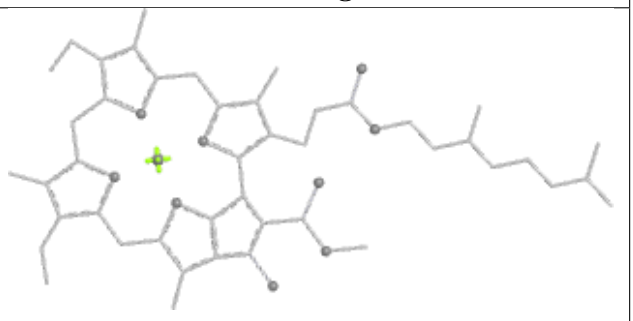
Bond lengths



Bond angles

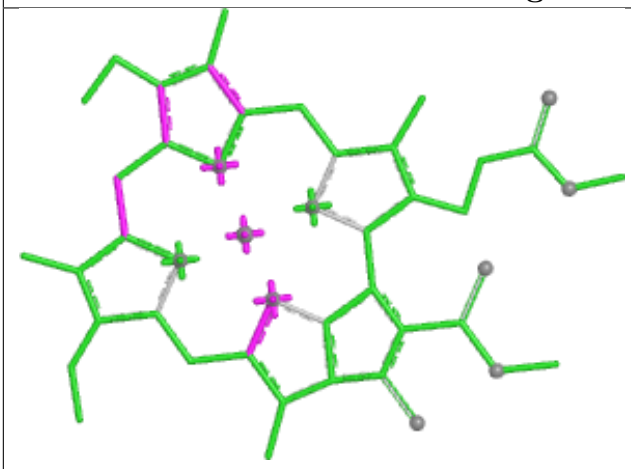


Torsions

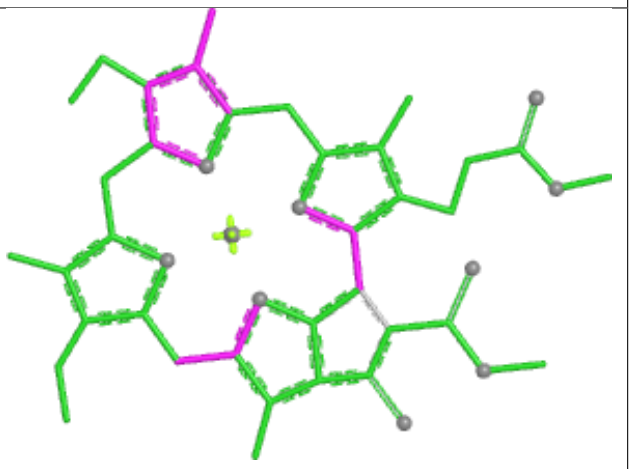


Rings

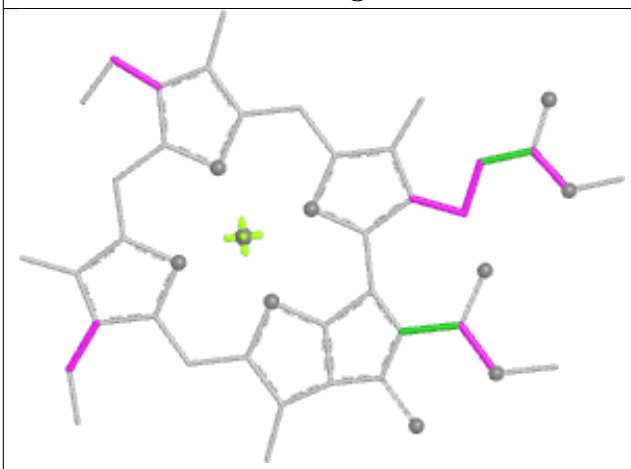
Ligand CLA Z 503



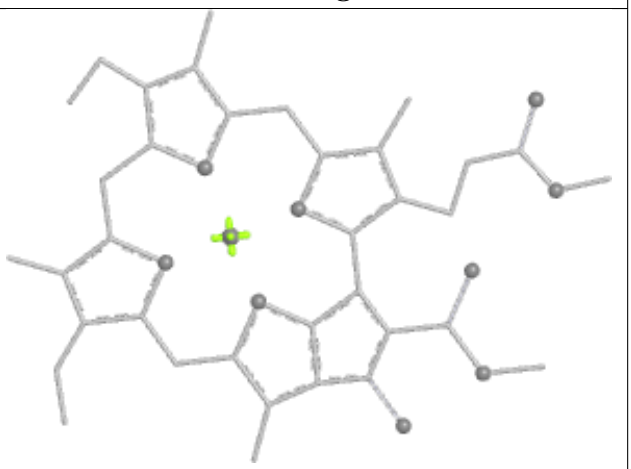
Bond lengths



Bond angles

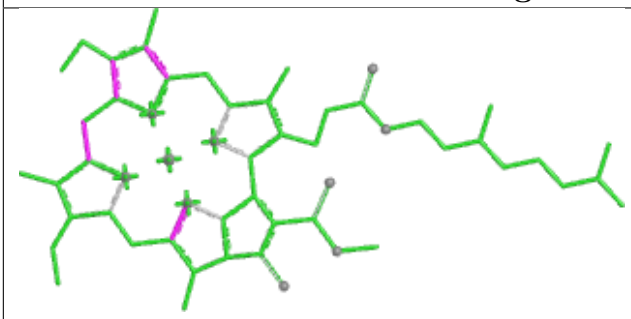


Torsions

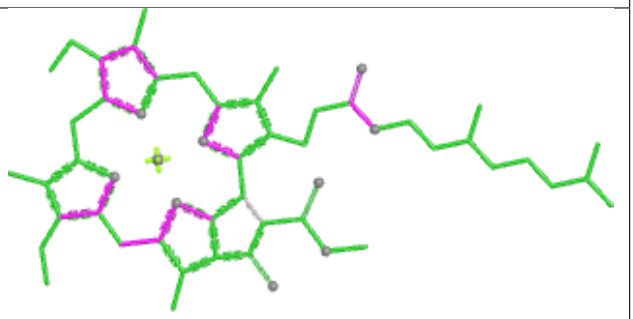


Rings

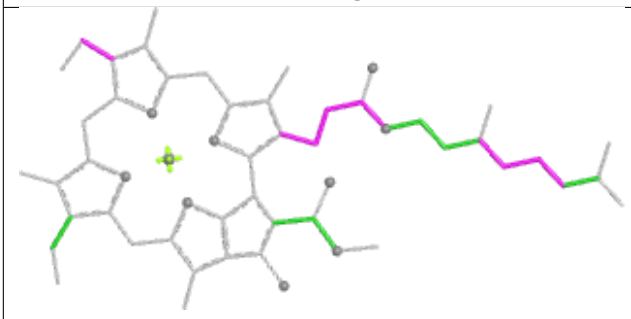
Ligand CLA H 1118



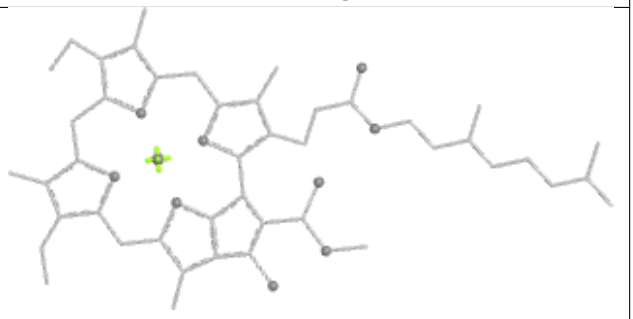
Bond lengths



Bond angles

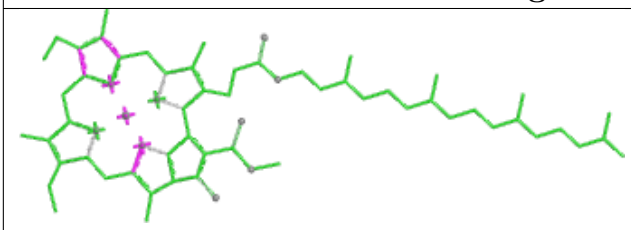


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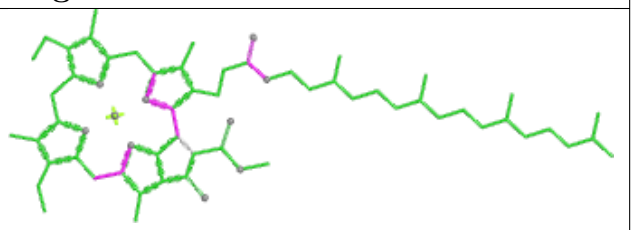


Rings

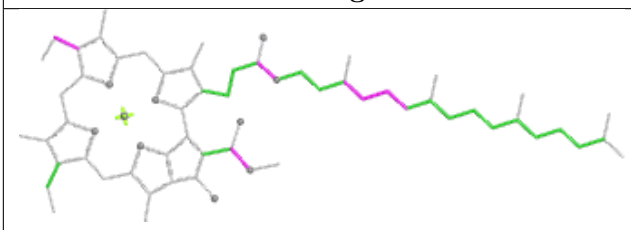
Ligand CLA g 512



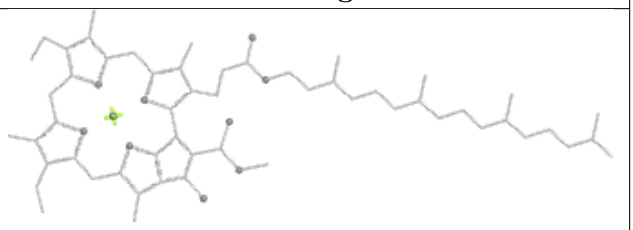
Bond lengths



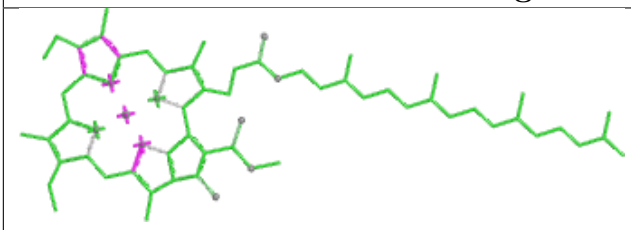
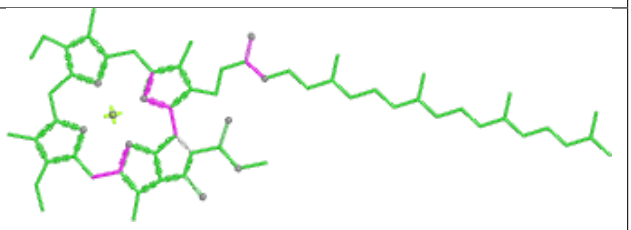
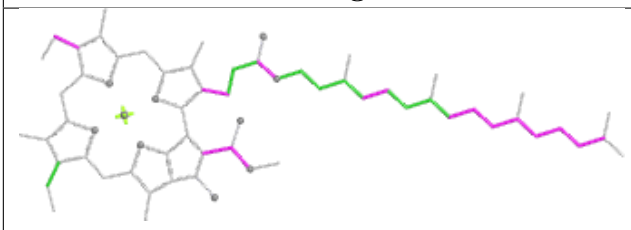
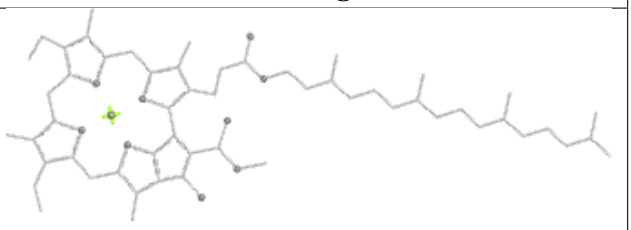
Bond angles

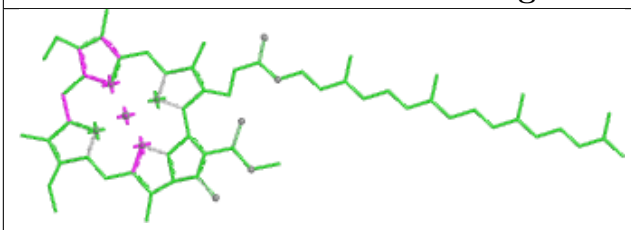
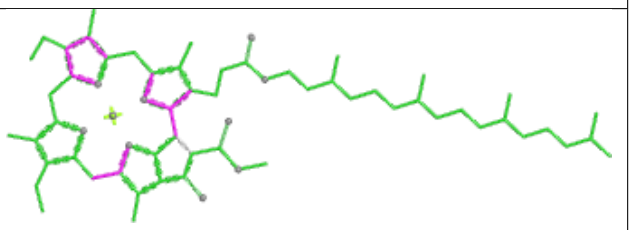
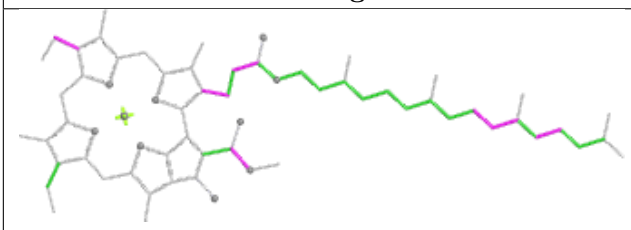
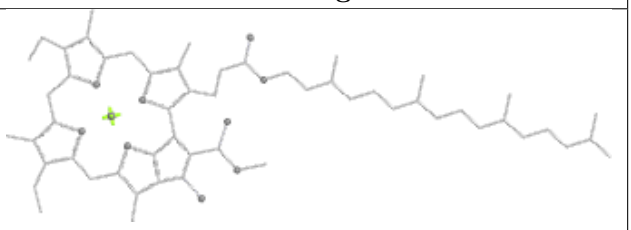


Torsions

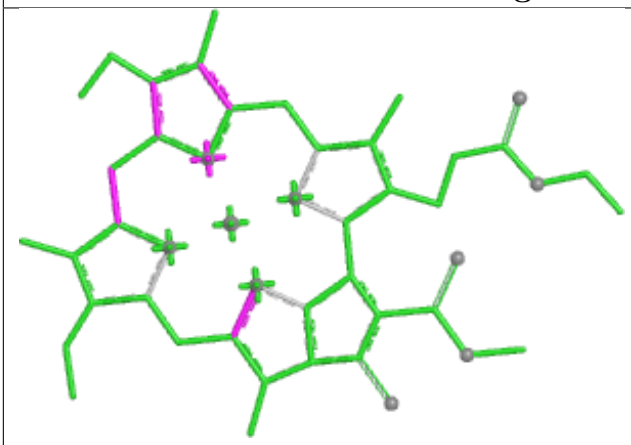


Rings

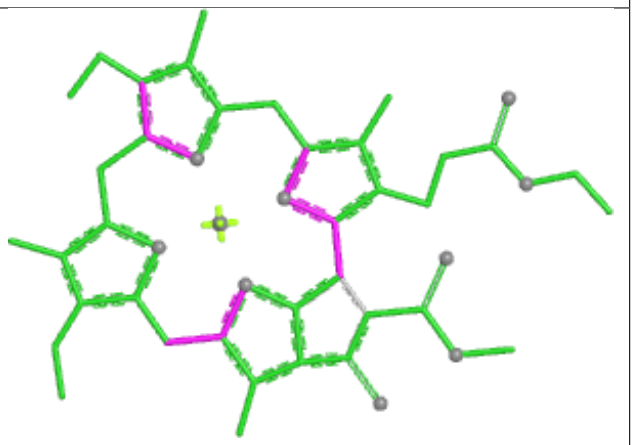
Ligand CLA A 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1023	
	
Bond lengths	Bond angles
	
Torsions	Rings

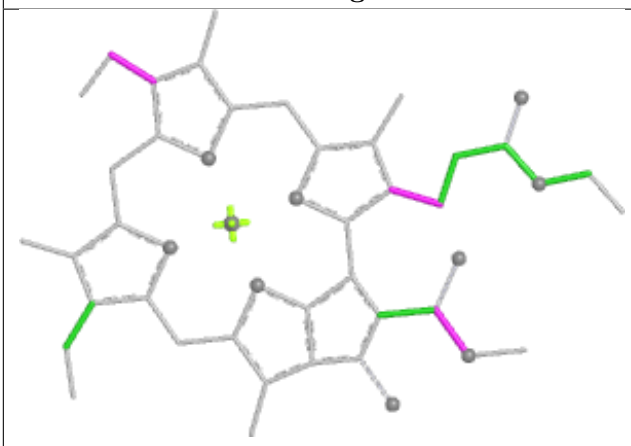
Ligand CLA G 1216



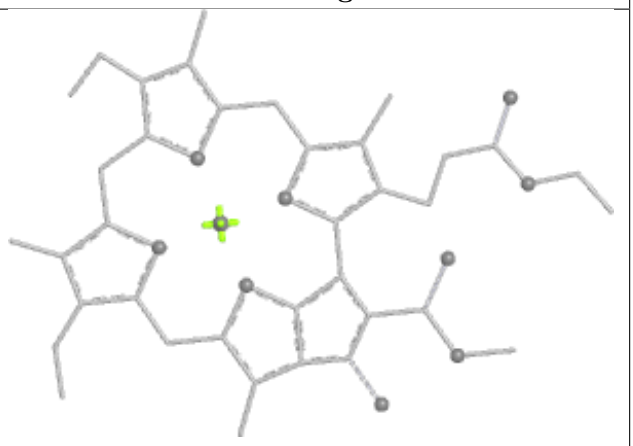
Bond lengths



Bond angles

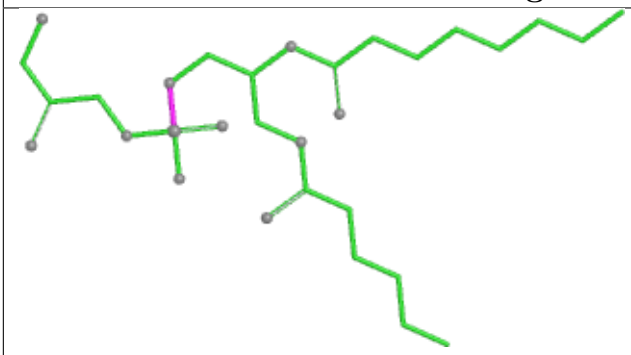


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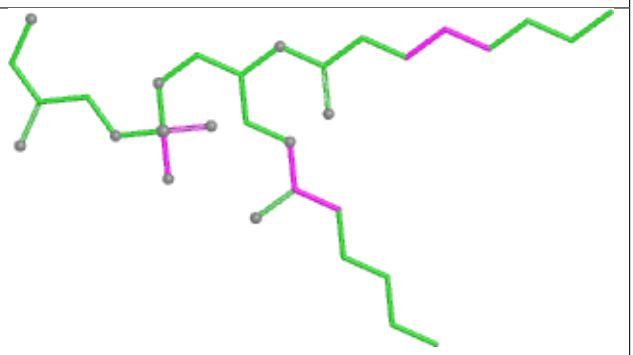


Rings

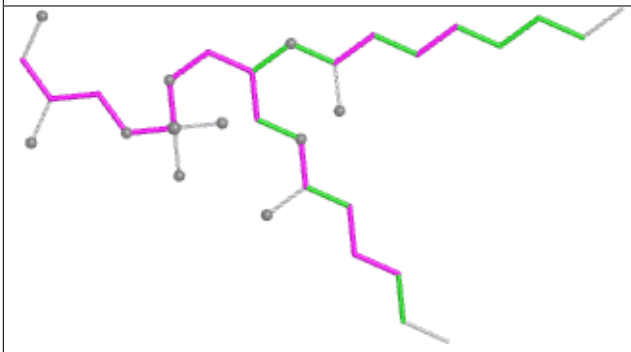
Ligand LHG x 605



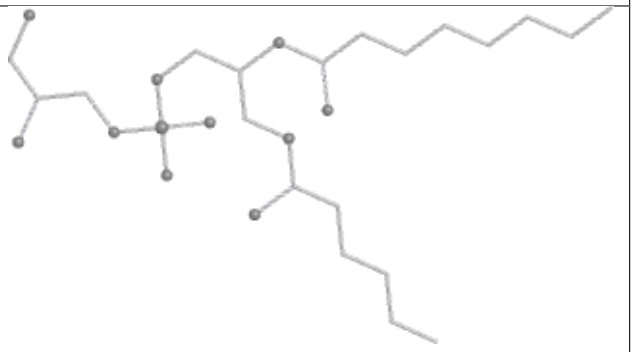
Bond lengths



Bond angles

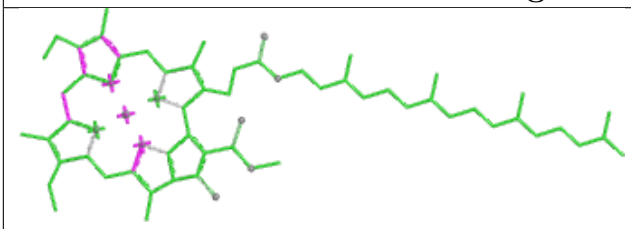


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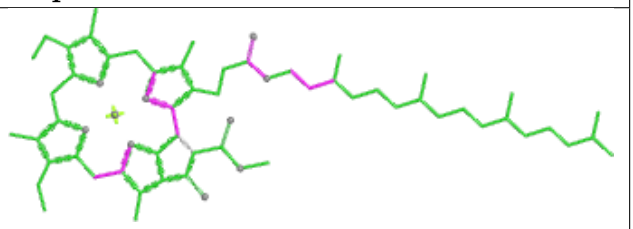


Rings

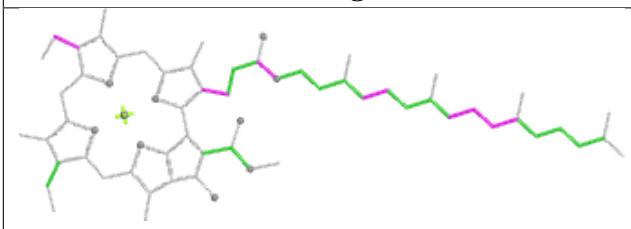
Ligand CLA p 512



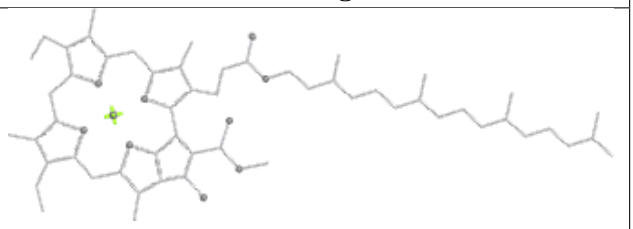
Bond lengths



Bond angles

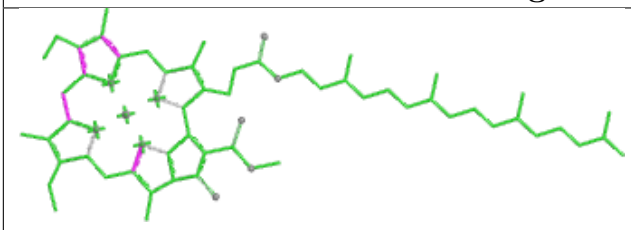


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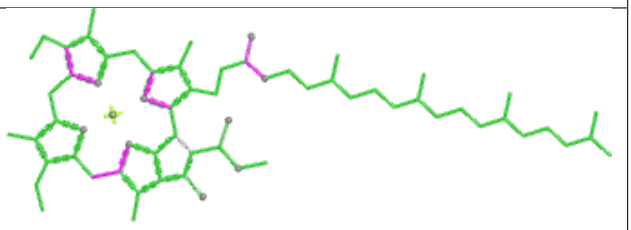


Rings

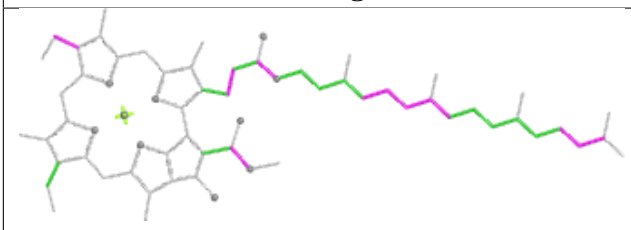
Ligand CLA o 505



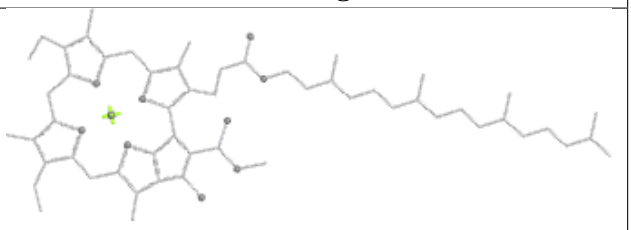
Bond lengths



Bond angles

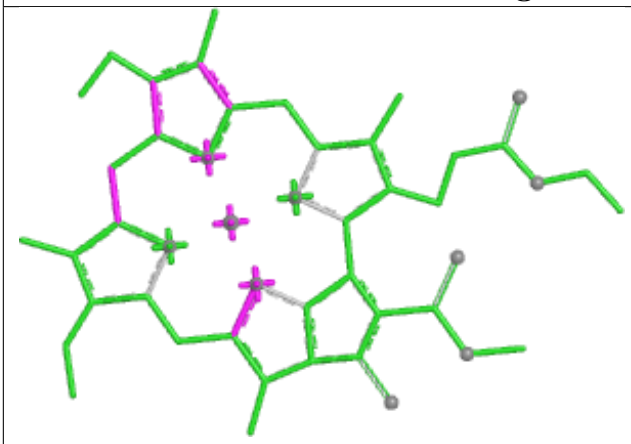


Torsions

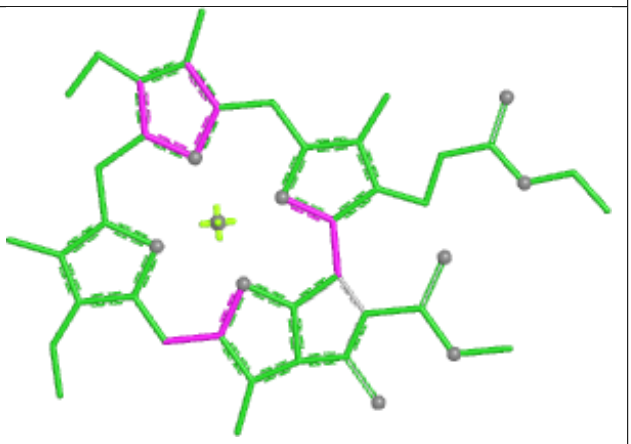


Rings

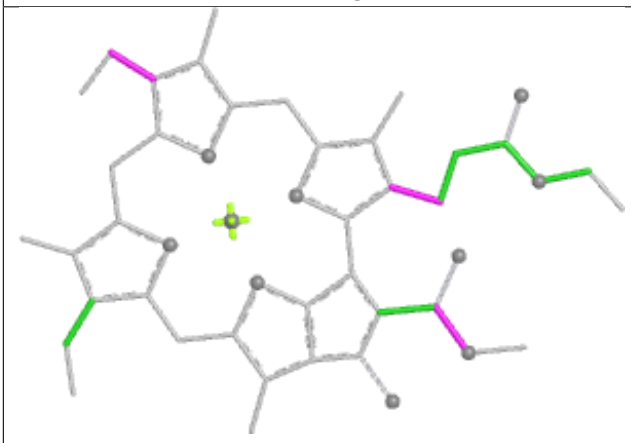
Ligand CLA B 1216



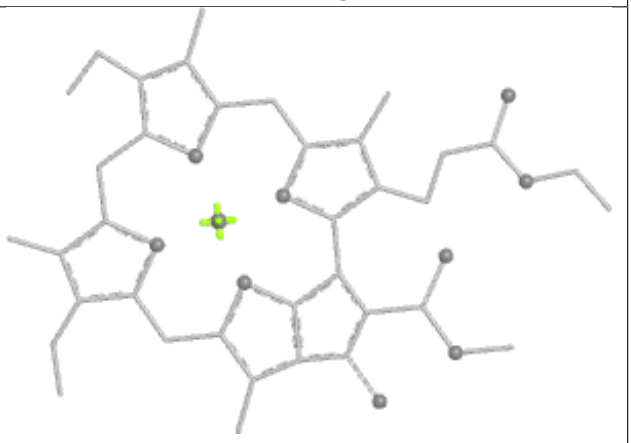
Bond lengths



Bond angles

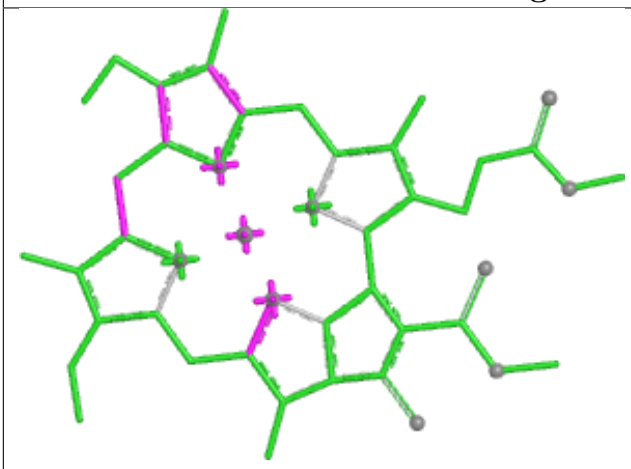


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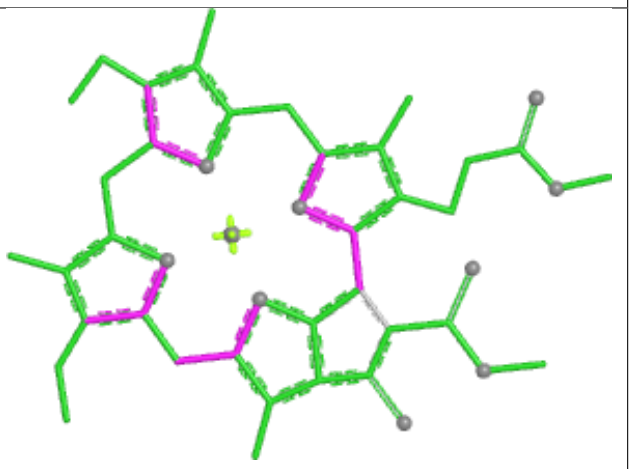


Rings

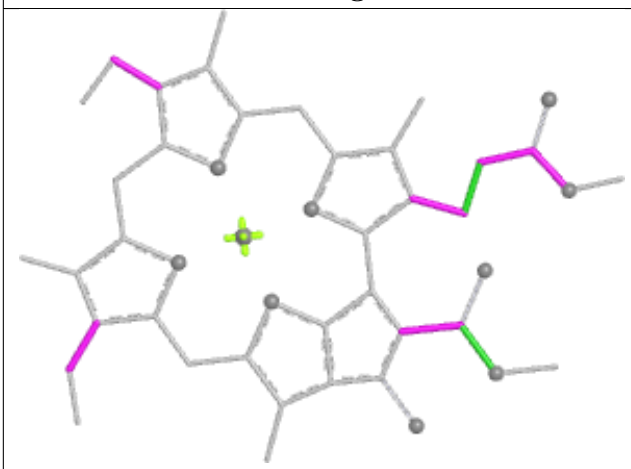
Ligand CLA s 503



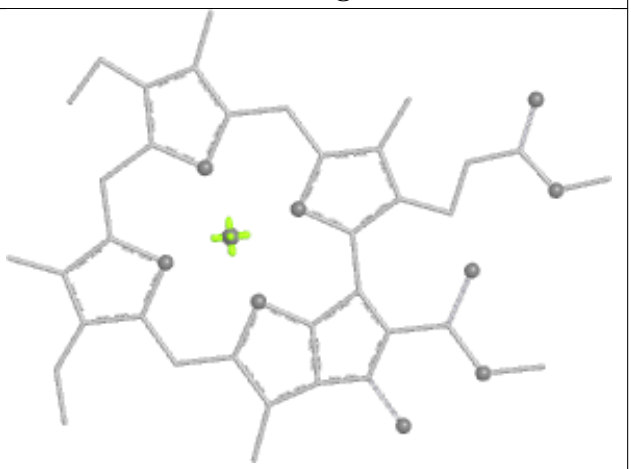
Bond lengths



Bond angles



Torsions

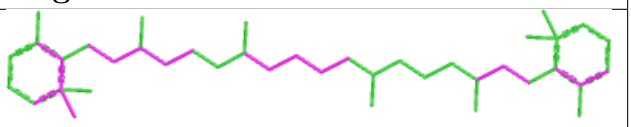


Rings

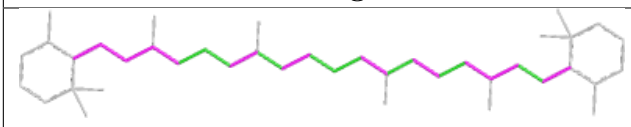
Ligand BCR g 601



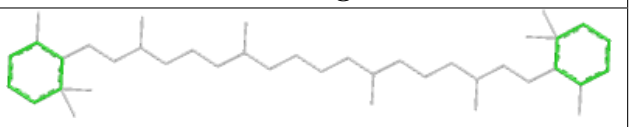
Bond lengths



Bond angles

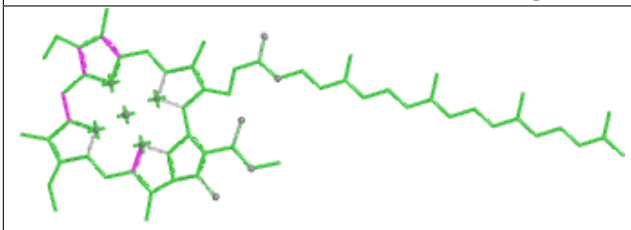


Torsions

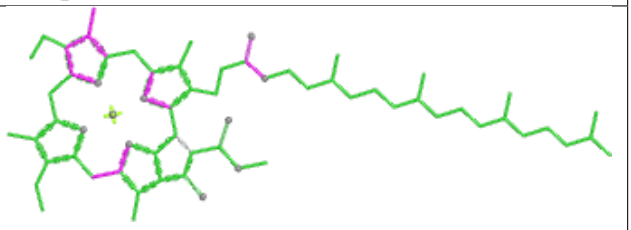


Rings

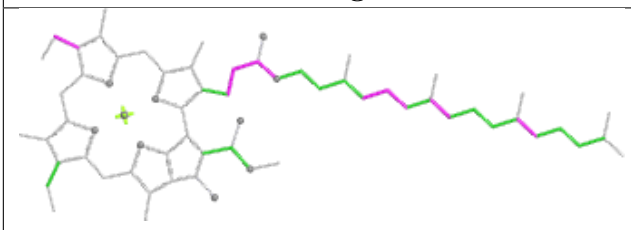
Ligand CLA q 507



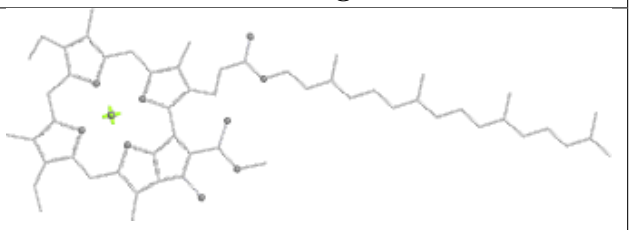
Bond lengths



Bond angles



Torsions

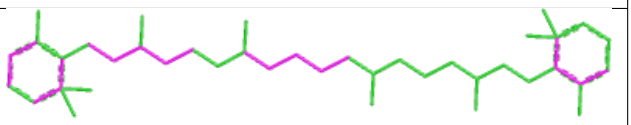


Rings

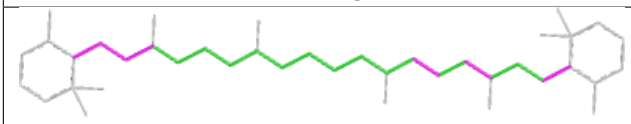
Ligand BCR u 603



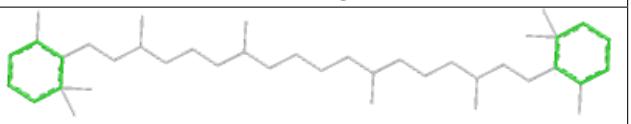
Bond lengths



Bond angles

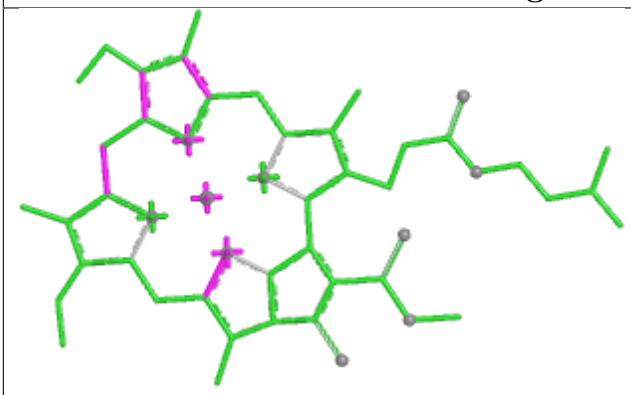


Torsions

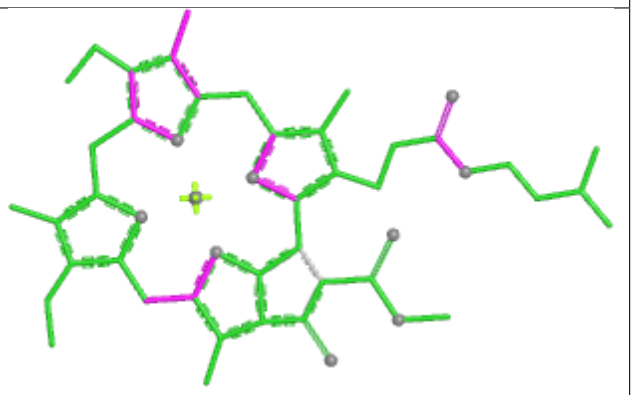


Rings

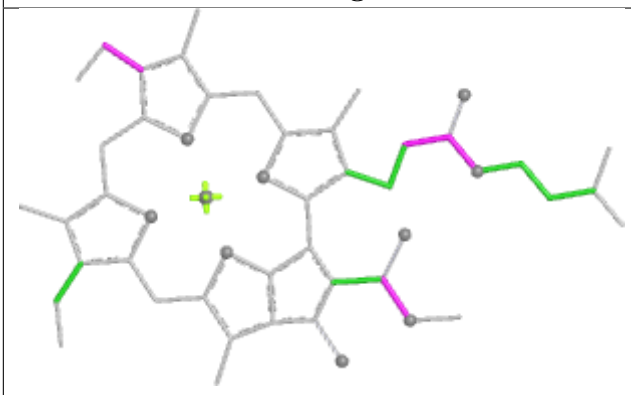
Ligand CLA Z 502



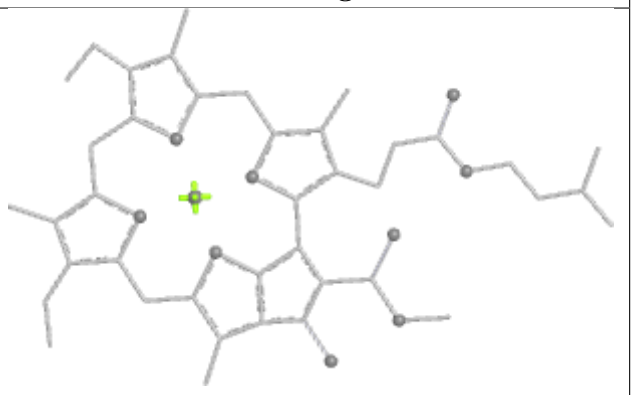
Bond lengths



Bond angles

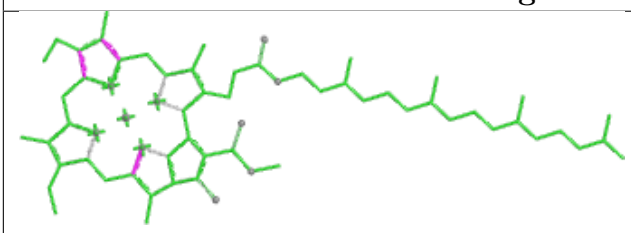


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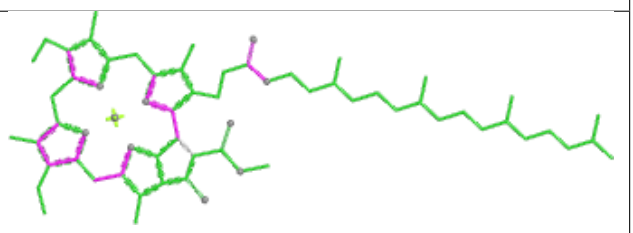


Rings

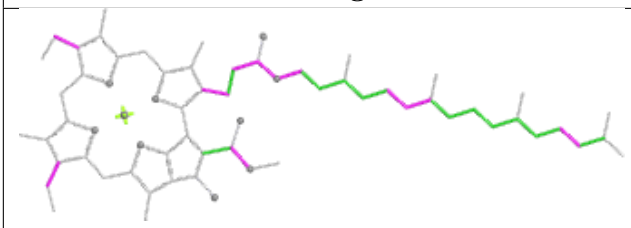
Ligand CLA b 1239



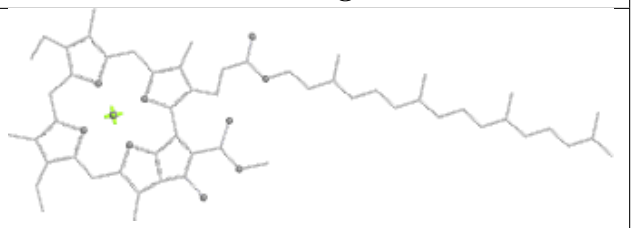
Bond lengths



Bond angles

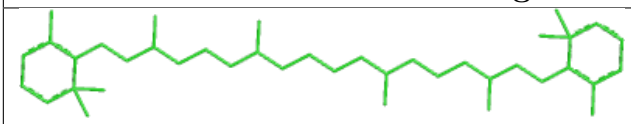


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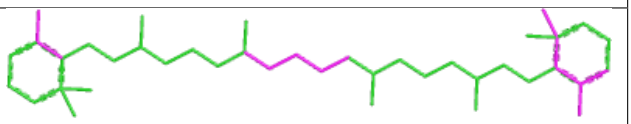


Rings

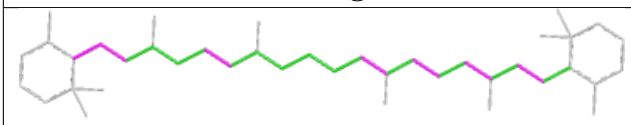
Ligand BCR A 4003



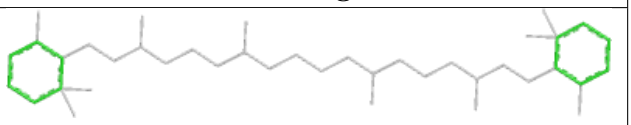
Bond lengths



Bond angles

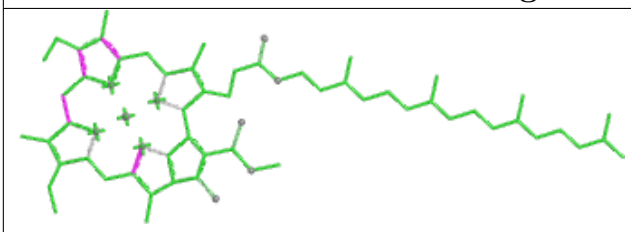


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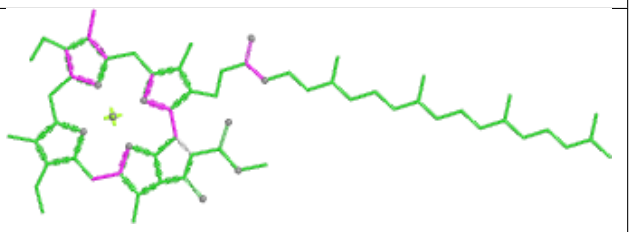


Rings

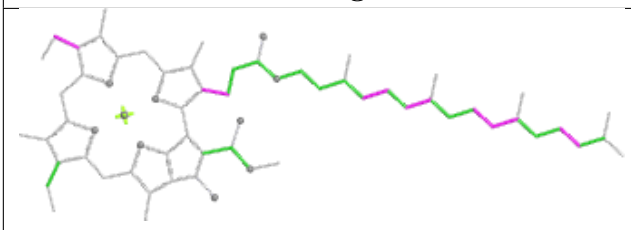
Ligand CLA a 1109



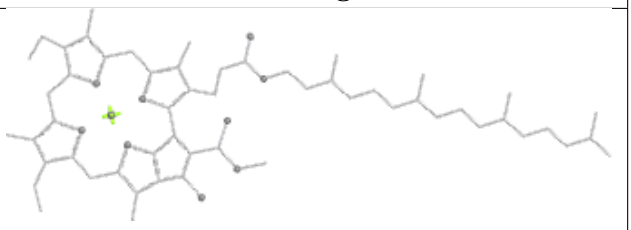
Bond lengths



Bond angles

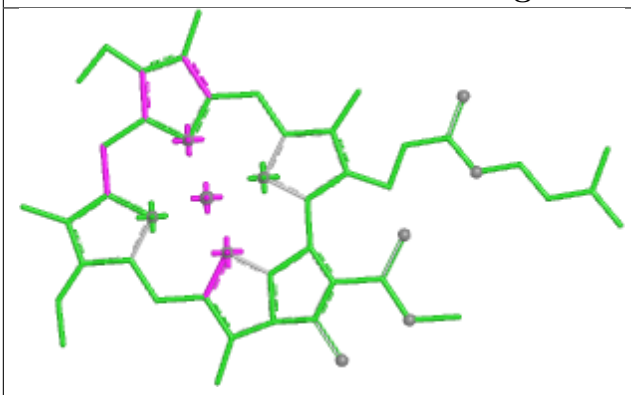


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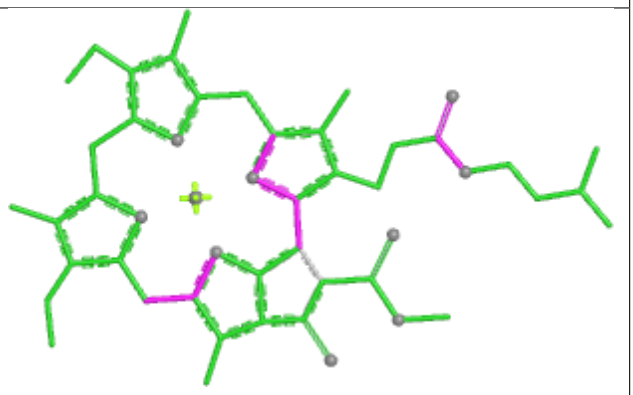


Rings

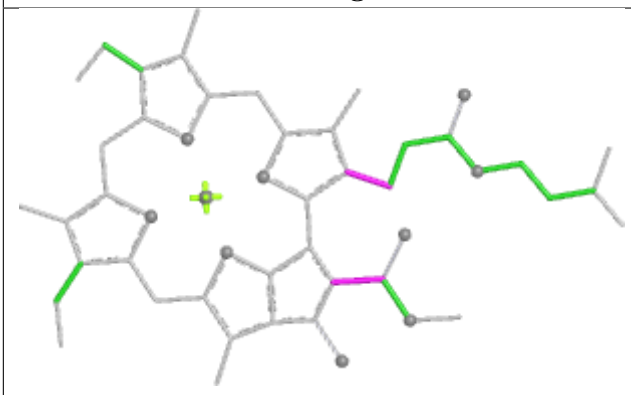
Ligand CLA G 1234



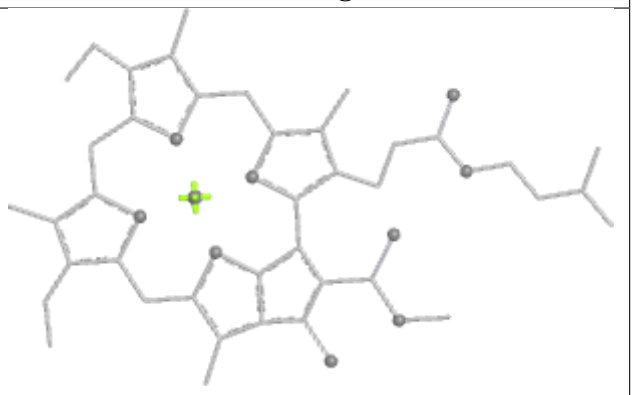
Bond lengths



Bond angles



Torsions

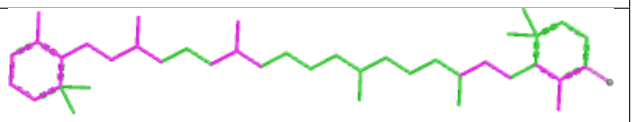


Rings

Ligand ECH I 4020



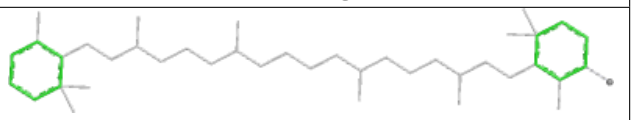
Bond lengths



Bond angles

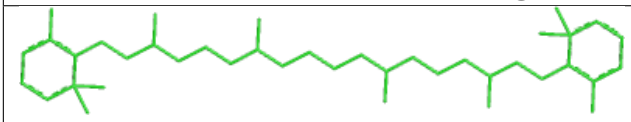


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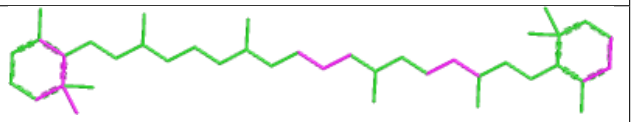


Rings

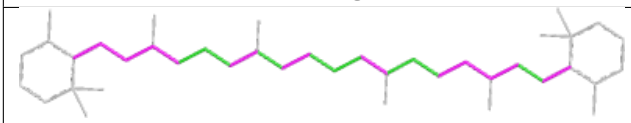
Ligand BCR U 4022



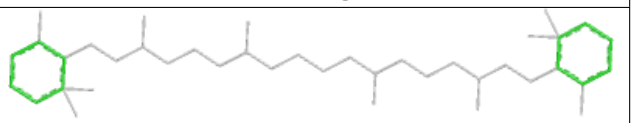
Bond lengths



Bond angles

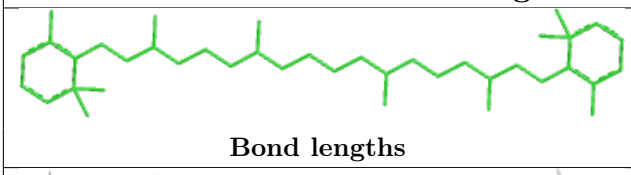


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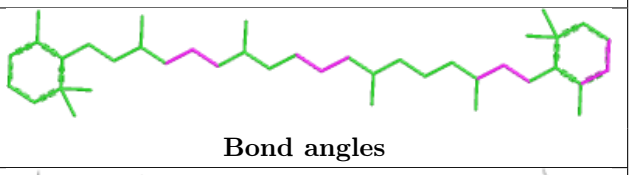


Rings

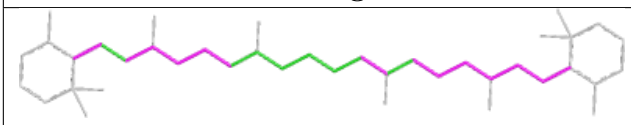
Ligand BCR A 4011



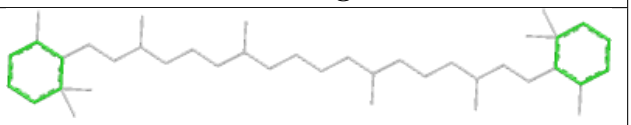
Bond lengths



Bond angles

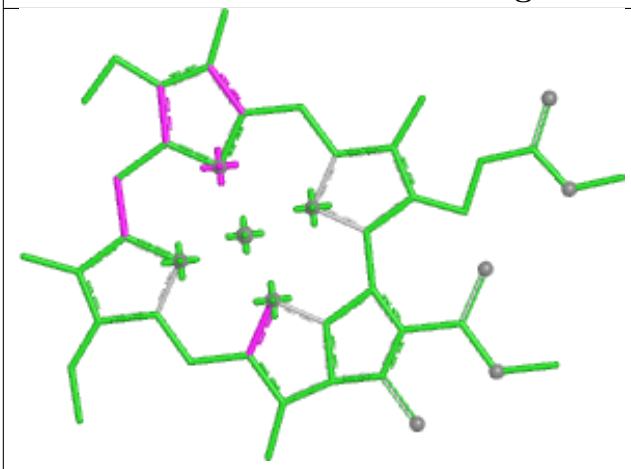


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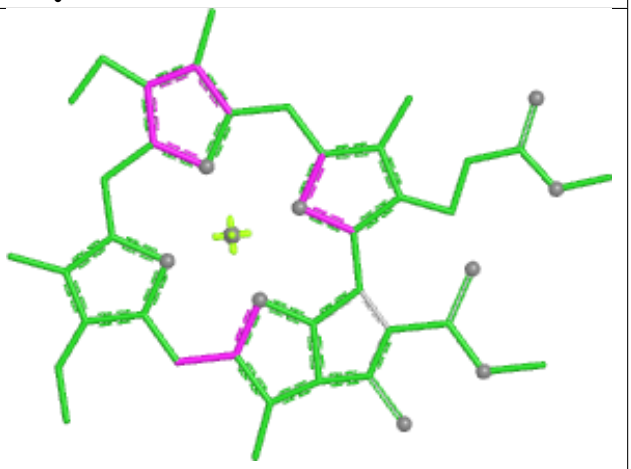


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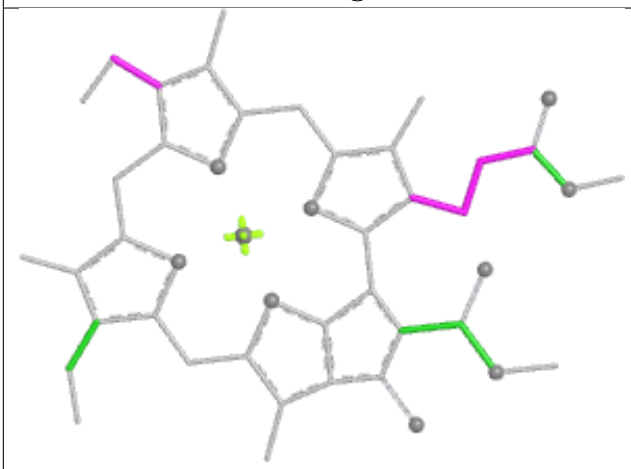
Ligand CLA Q 1302



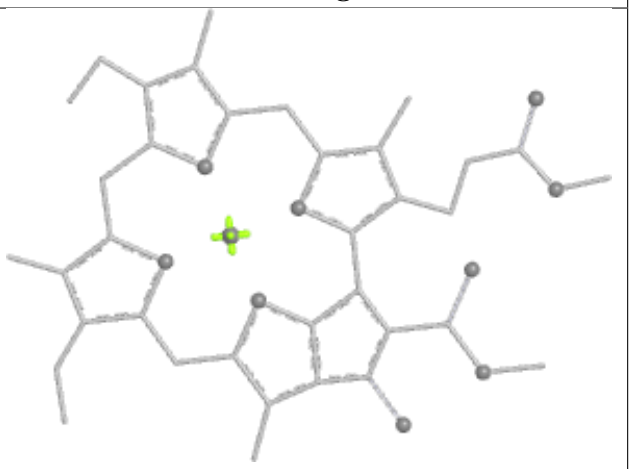
Bond lengths



Bond angles

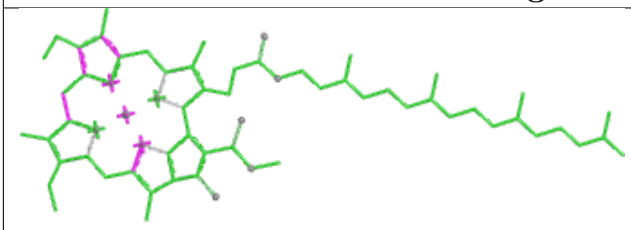


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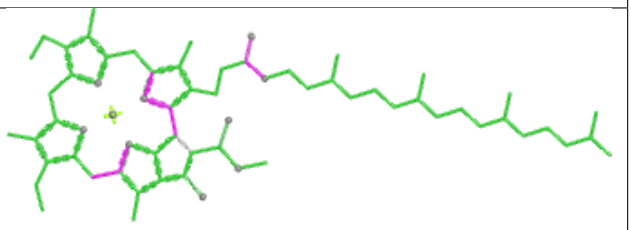


Rings

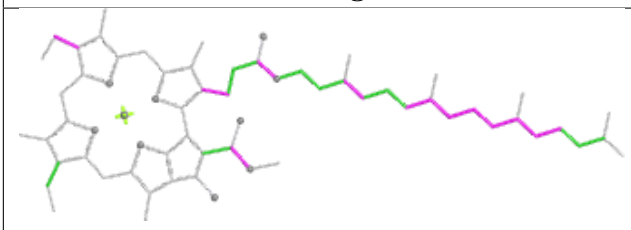
Ligand CLA n 512



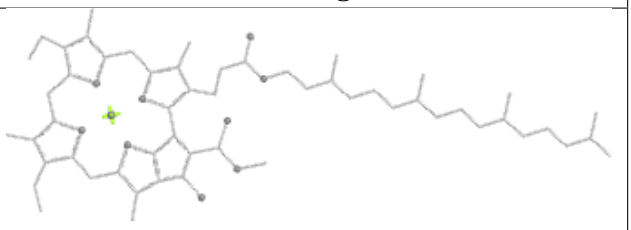
Bond lengths



Bond angles

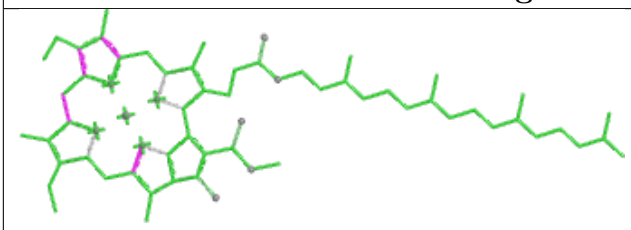


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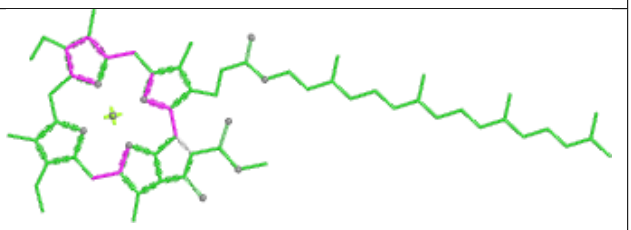


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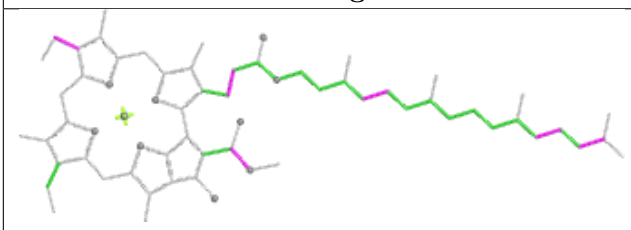
Ligand CLA B 1238



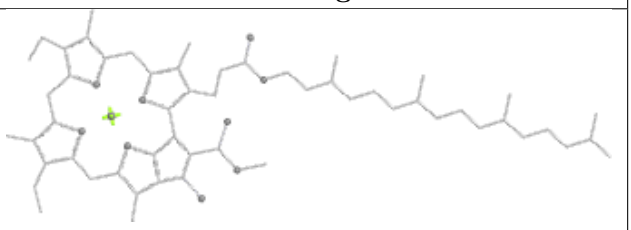
Bond lengths



Bond angles



Torsions

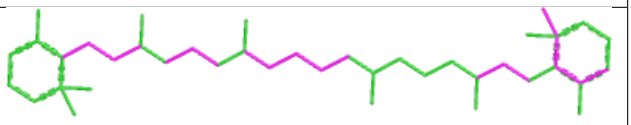


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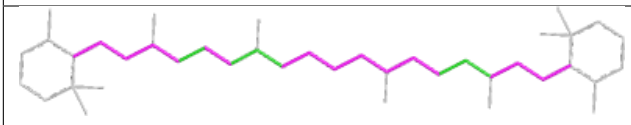
Ligand BCR G 4010



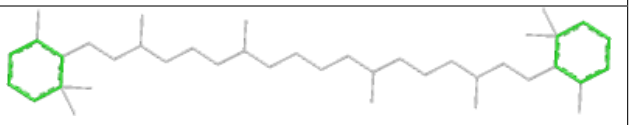
Bond lengths



Bond angles

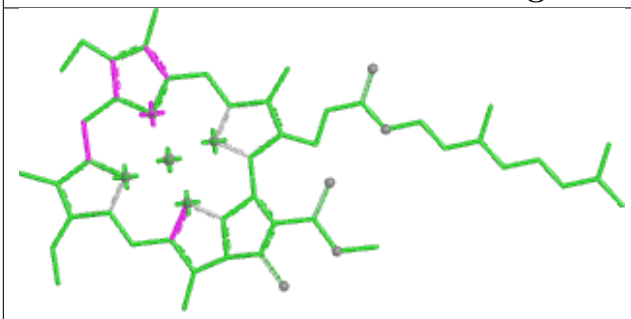


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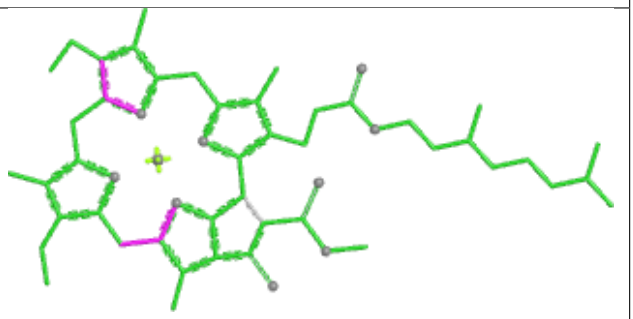


Rings

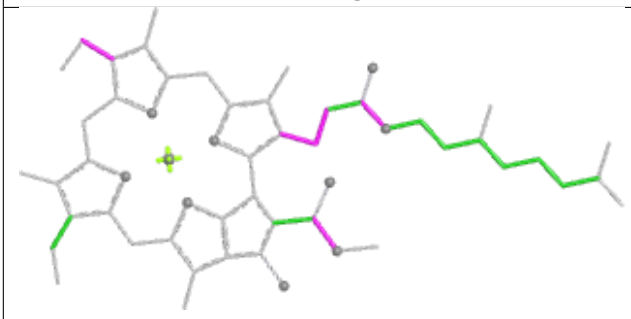
Ligand CLA n 508



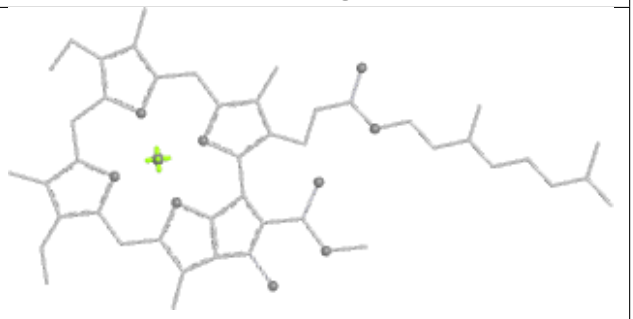
Bond lengths



Bond angles

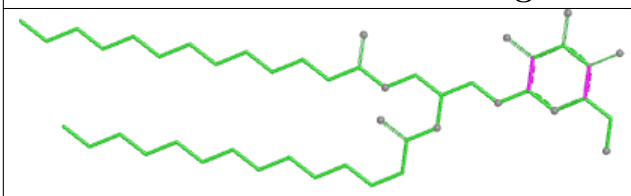


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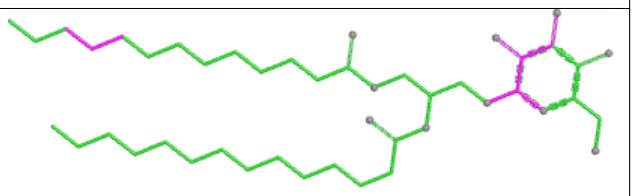


Rings

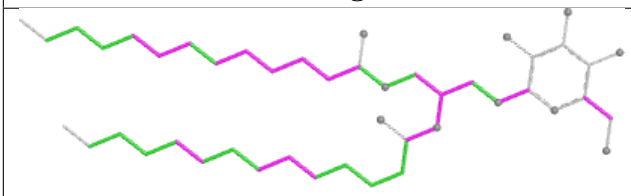
Ligand LMG a 4101



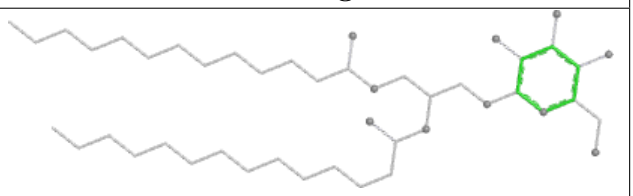
Bond lengths



Bond angles

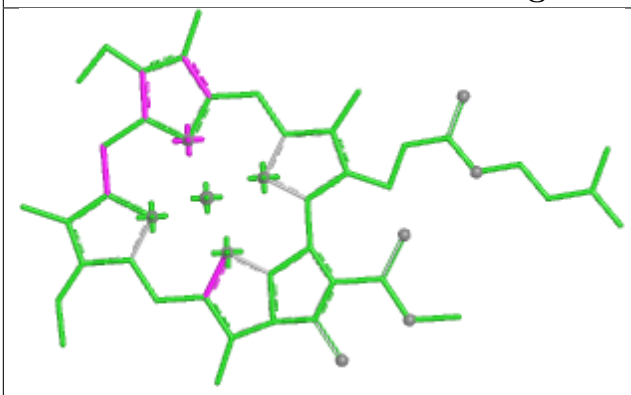


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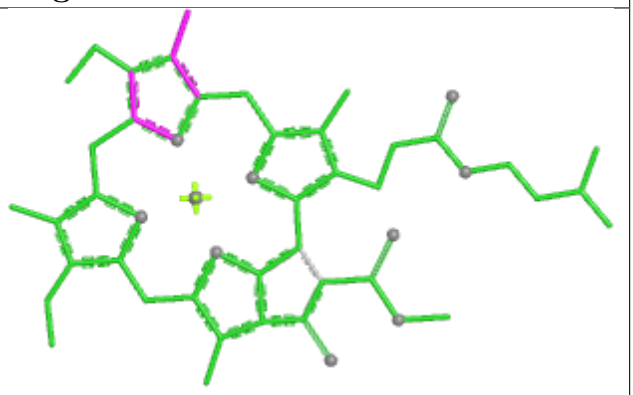


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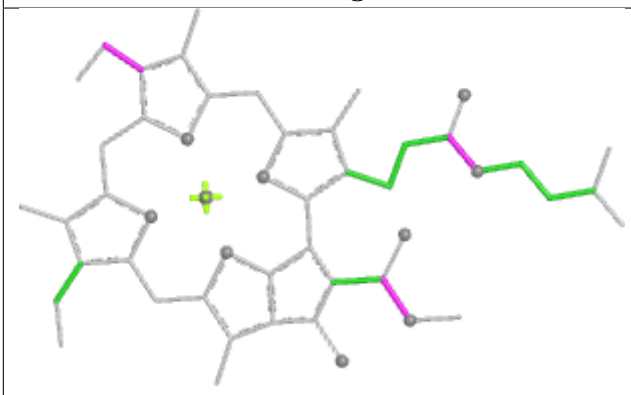
Ligand CLA g 502



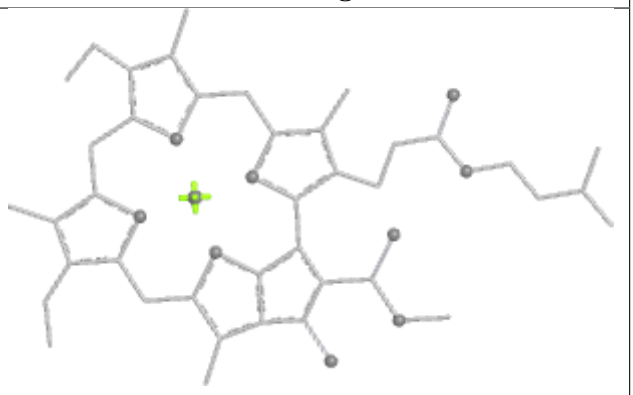
Bond lengths



Bond angles

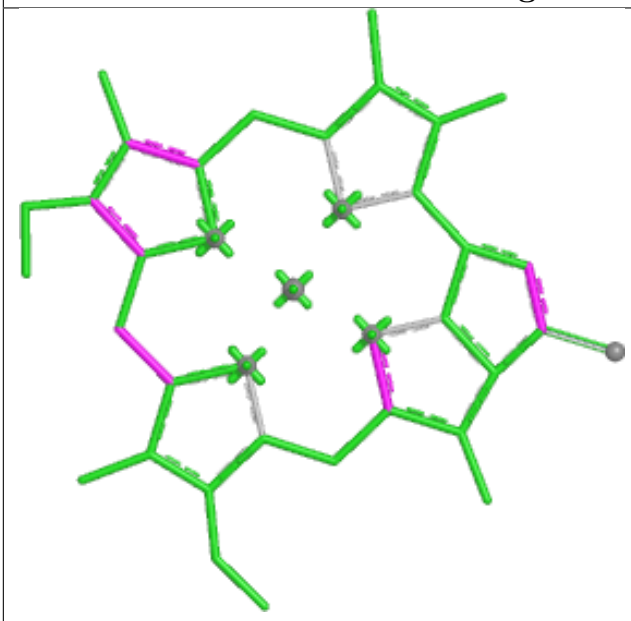


Torsions

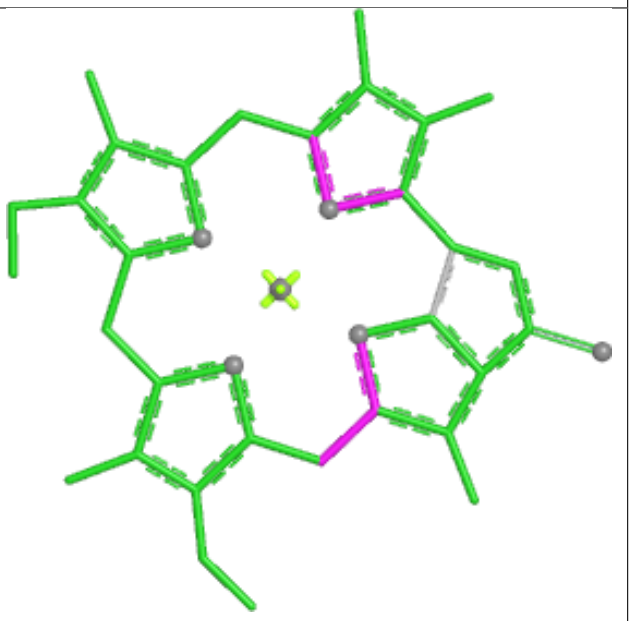


Rings

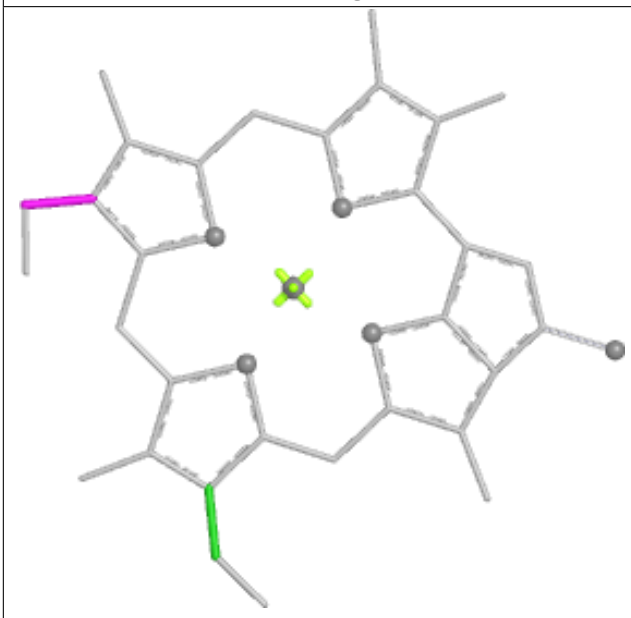
Ligand CLA S 1303



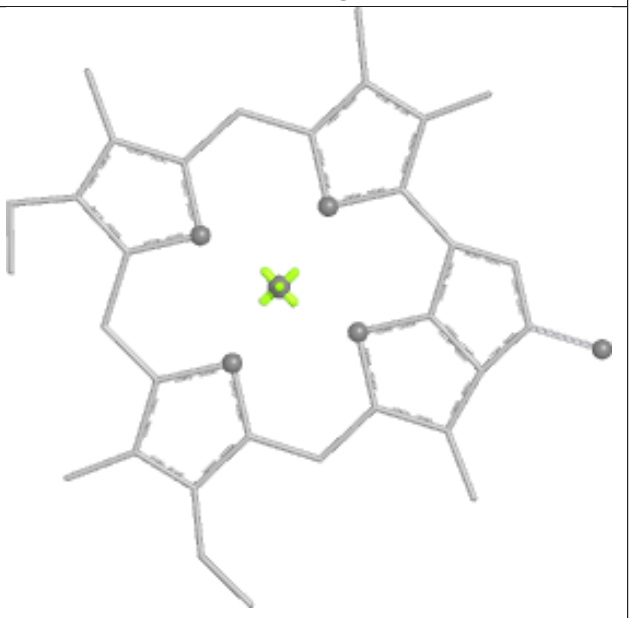
Bond lengths



Bond angles

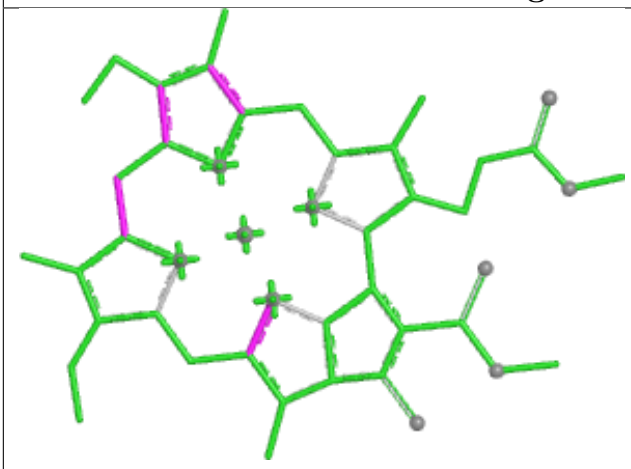


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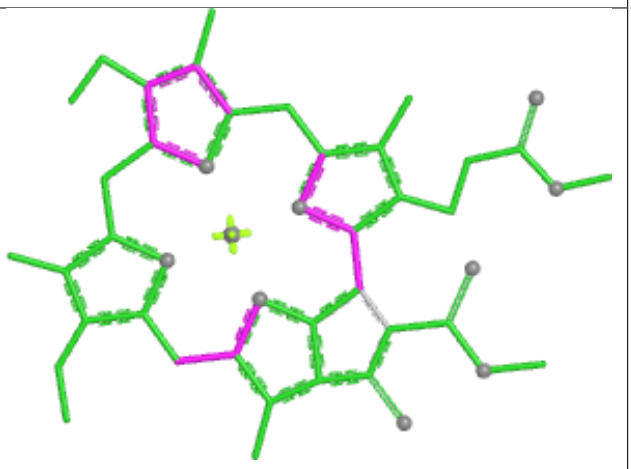


Rings

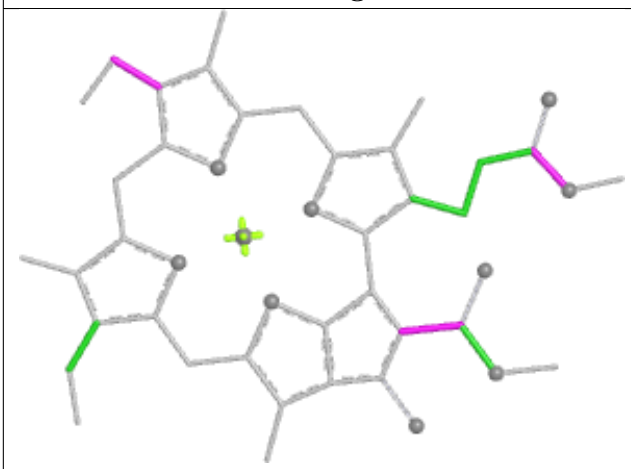
Ligand CLA x 516



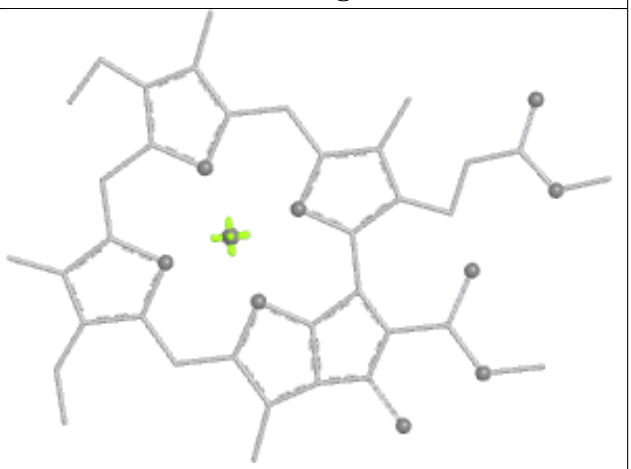
Bond lengths



Bond angles

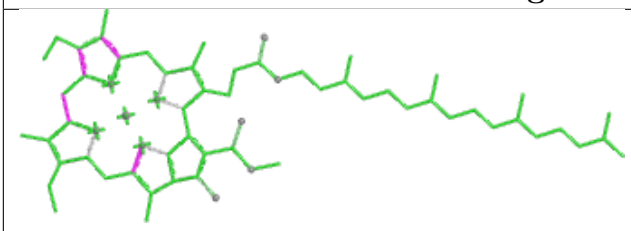


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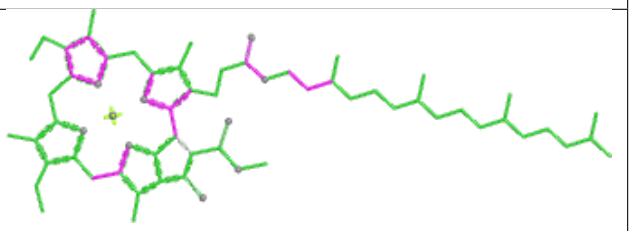


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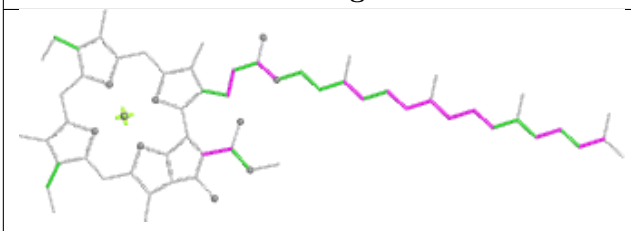
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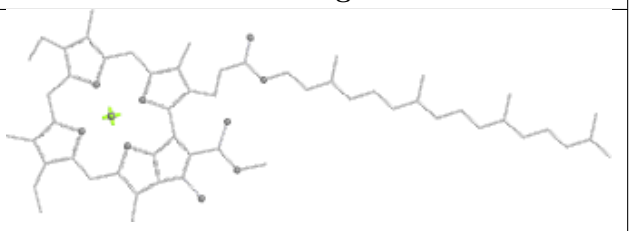
Bond lengths



Bond angles

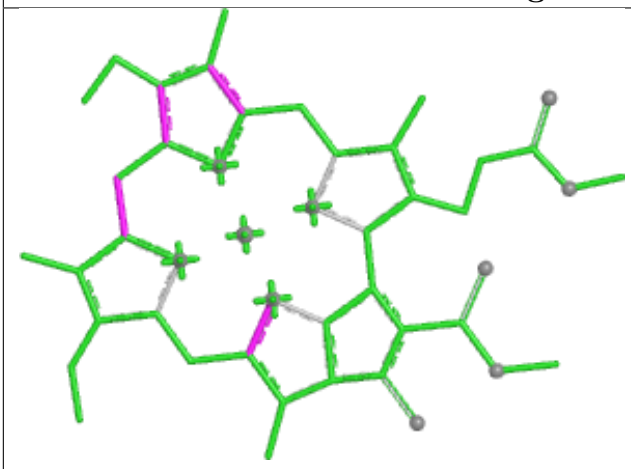


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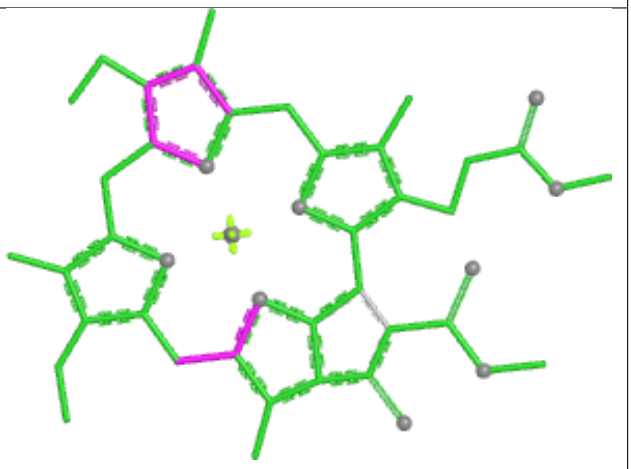


Rings

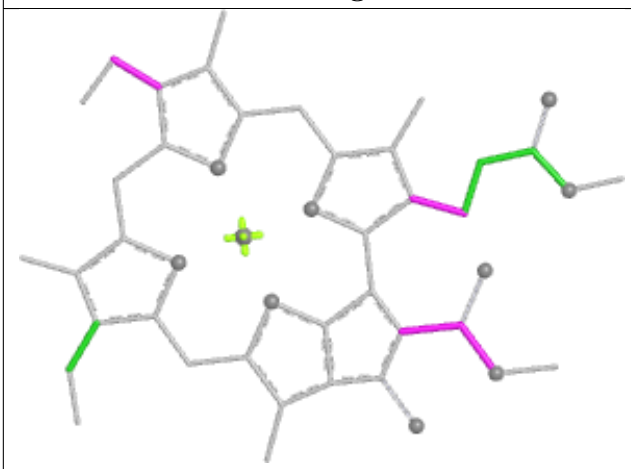
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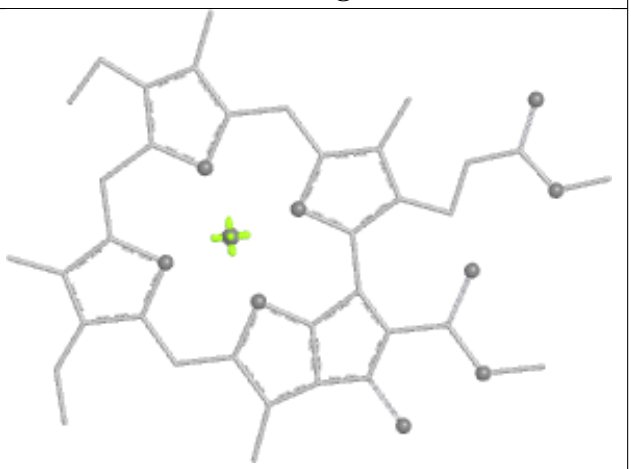
Bond lengths



Bond angles

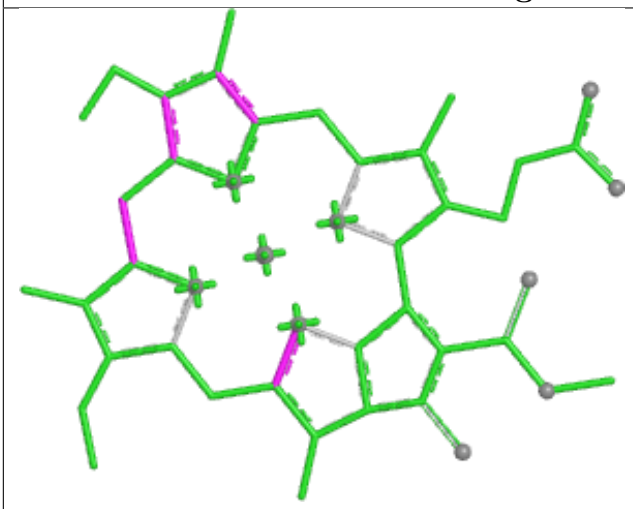


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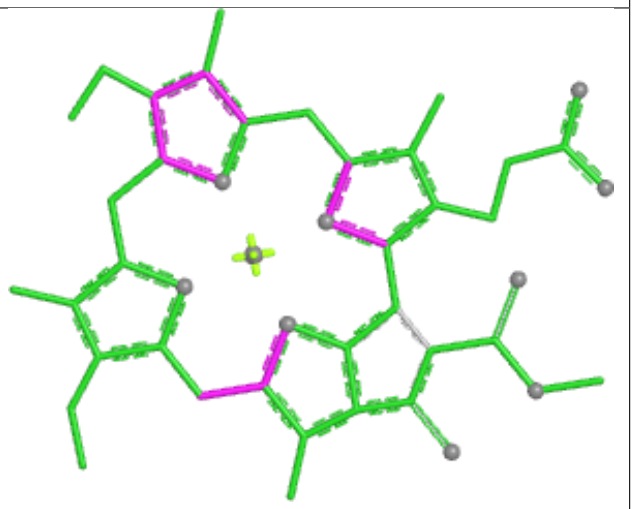


Rings

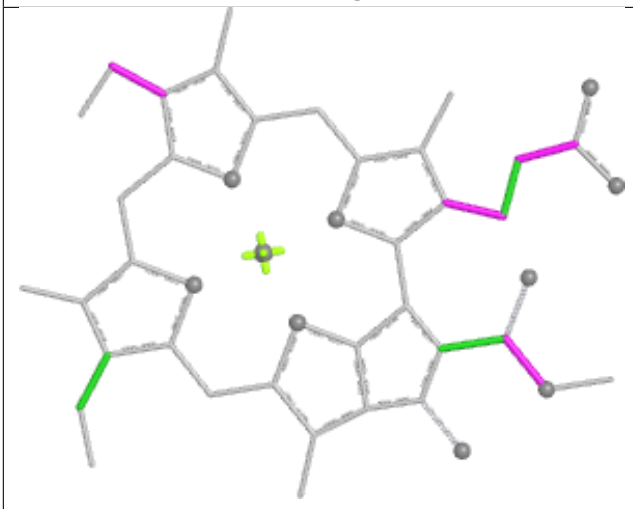
Ligand CLA B 1230



Bond lengths



Bond angles

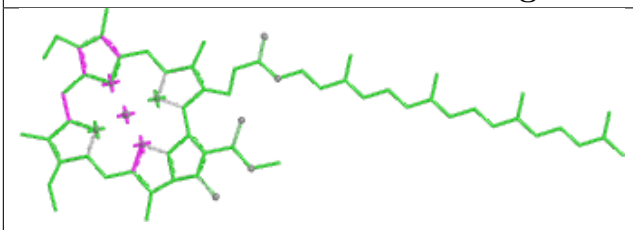


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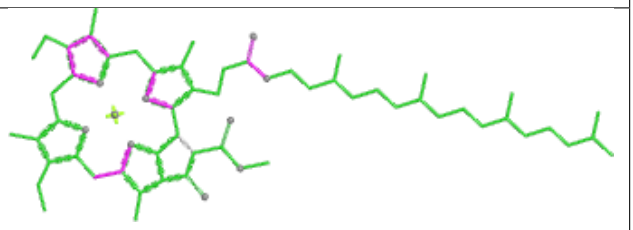


Rings

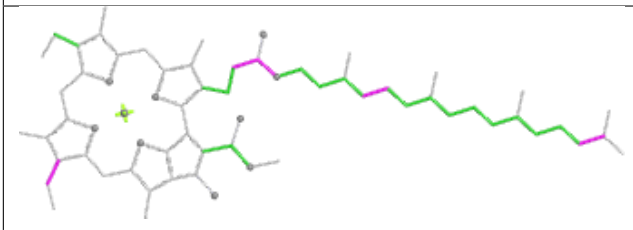
Ligand CL0 A 1011



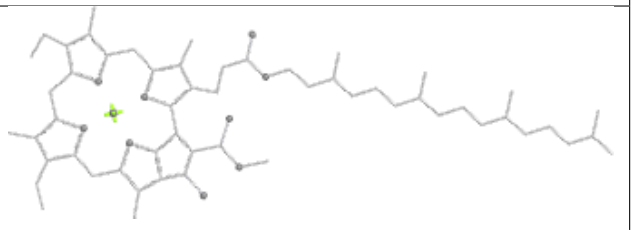
Bond lengths



Bond angles

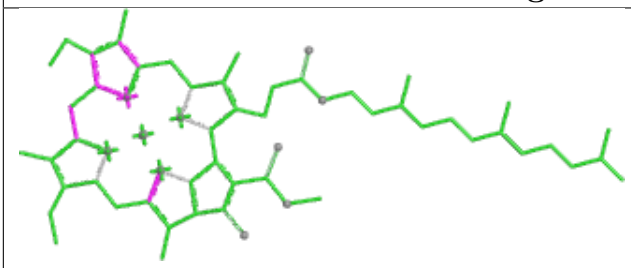


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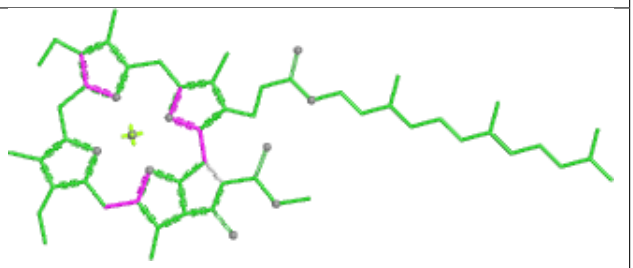


Rings

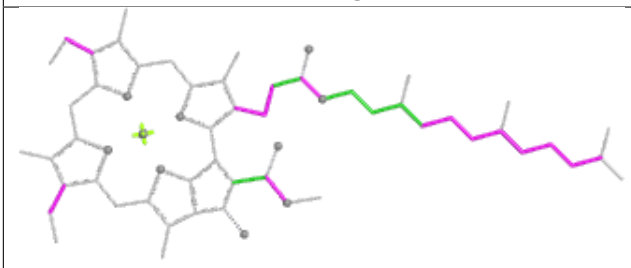
Ligand CLA u 504



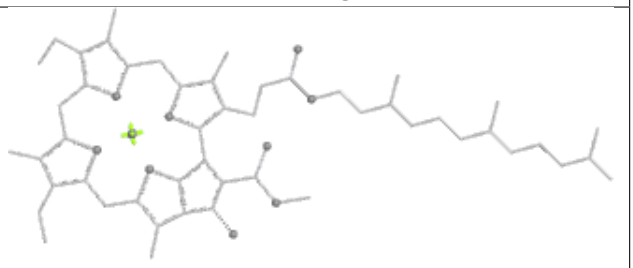
Bond lengths



Bond angles

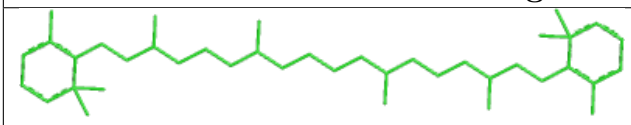


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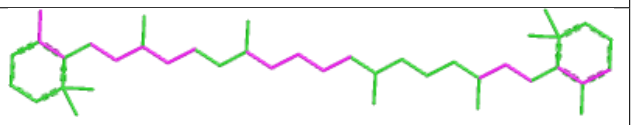


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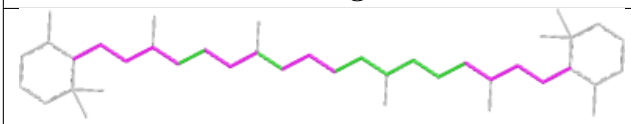
Ligand BCR x 602



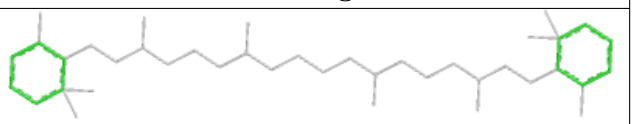
Bond lengths



Bond angles

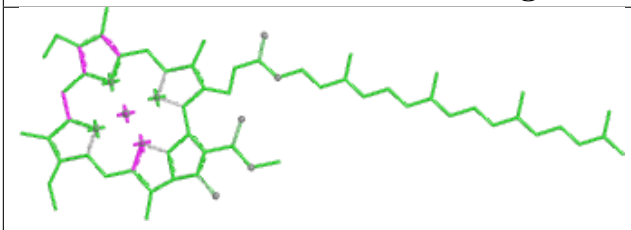


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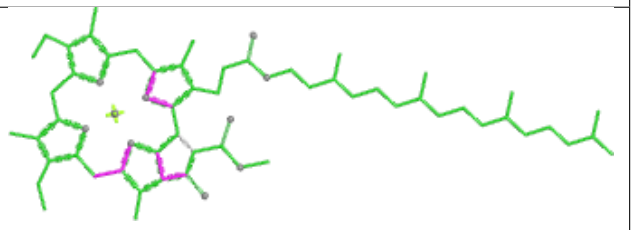


Rings

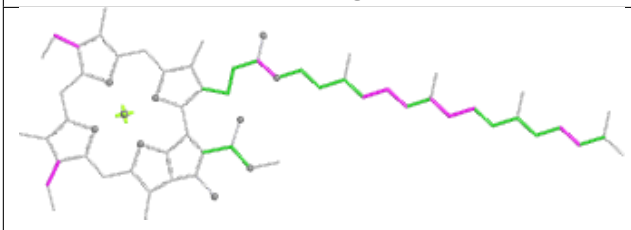
Ligand CLA a 1125



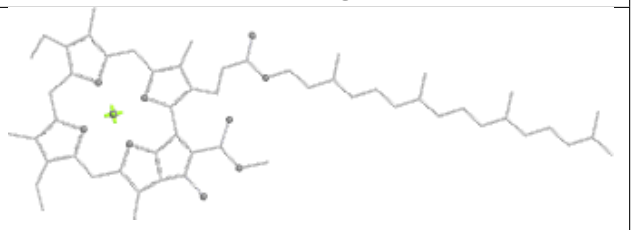
Bond lengths



Bond angles

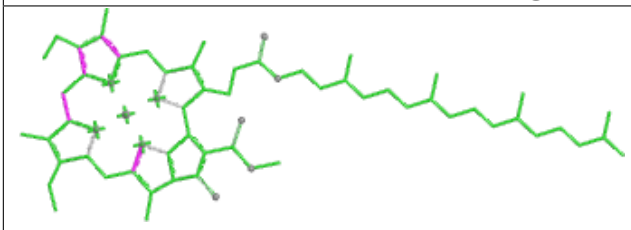


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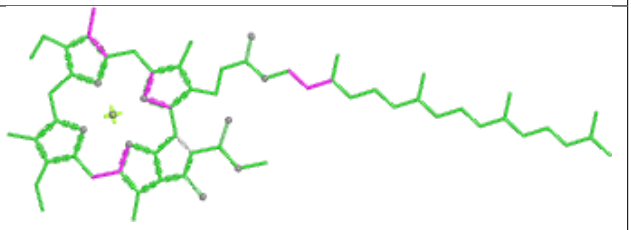


Rings

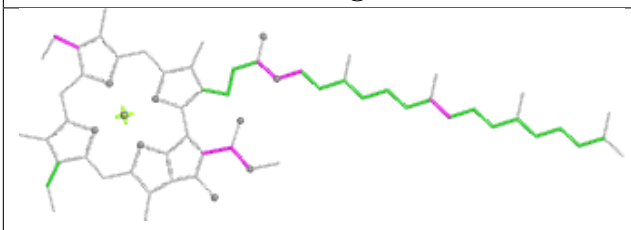
Ligand CLA n 507



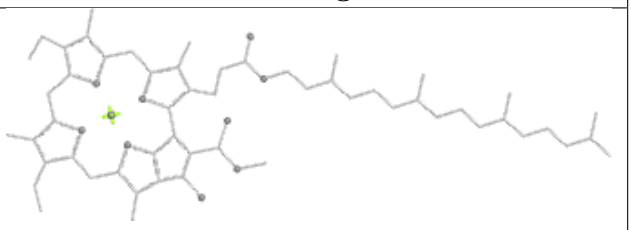
Bond lengths



Bond angles

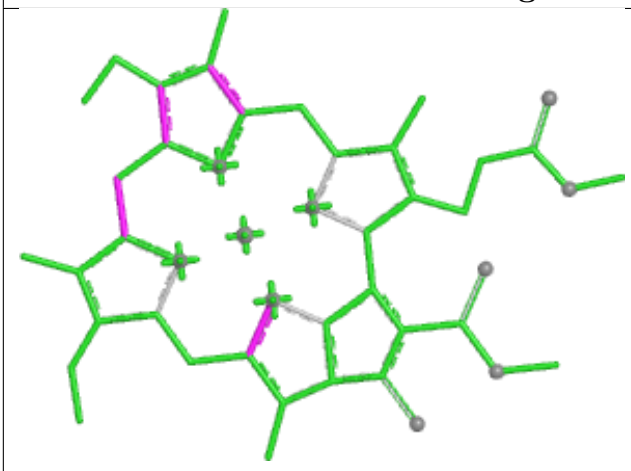


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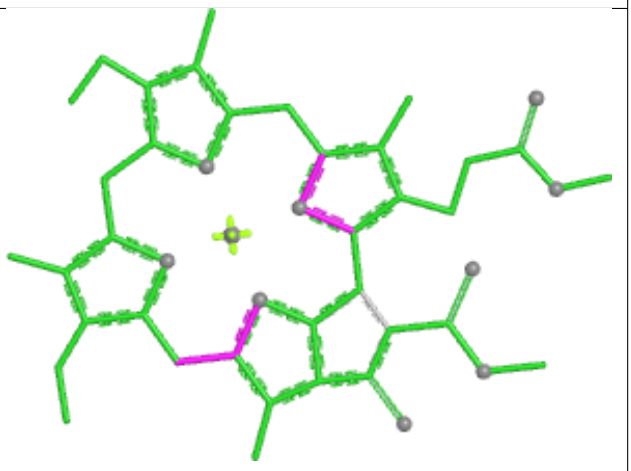


Rings

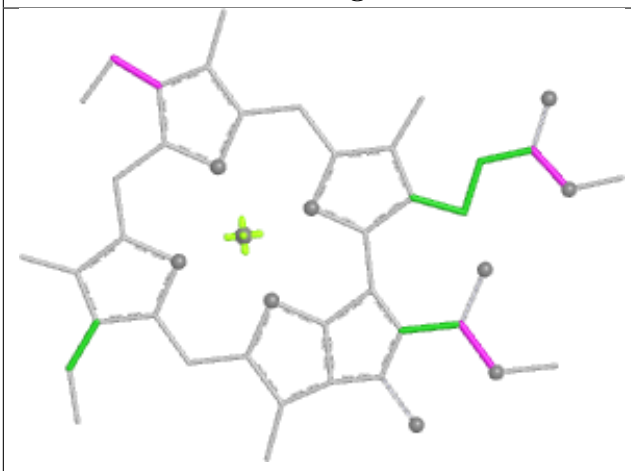
Ligand CLA b 1240



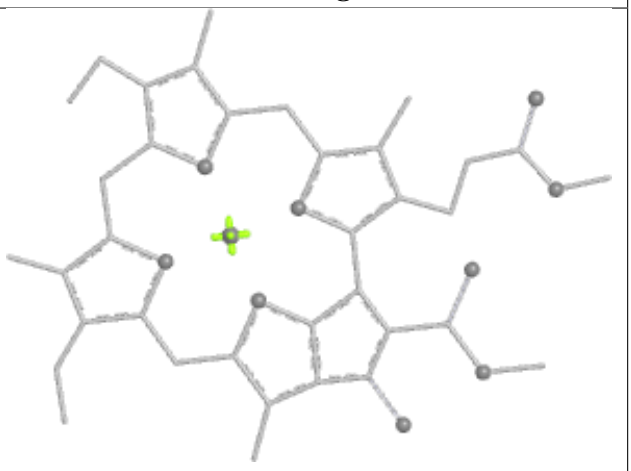
Bond lengths



Bond angles

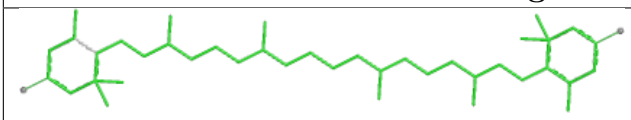


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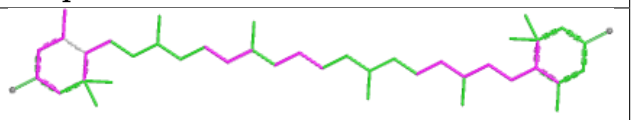


Rings

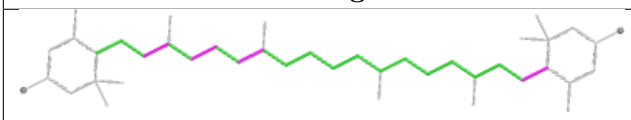
Ligand LUT q 601



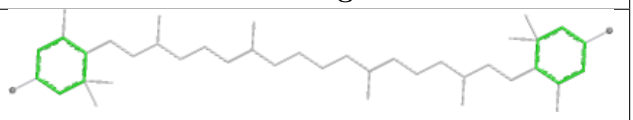
Bond lengths



Bond angles

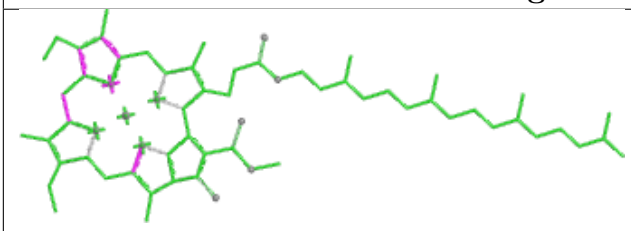


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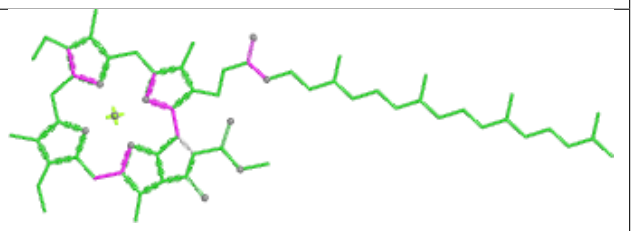


Rings

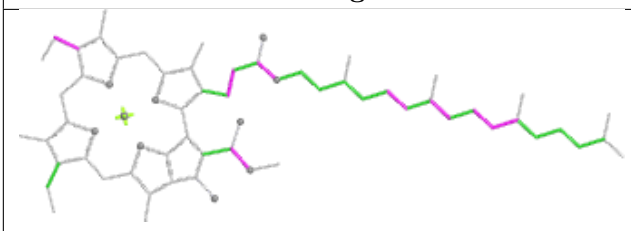
Ligand CLA v 505



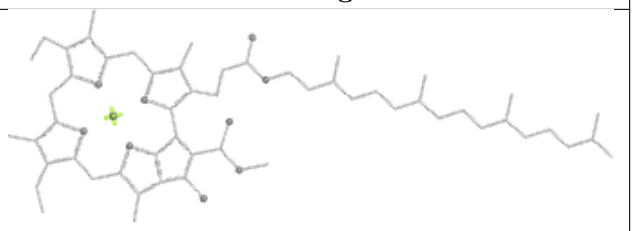
Bond lengths



Bond angles

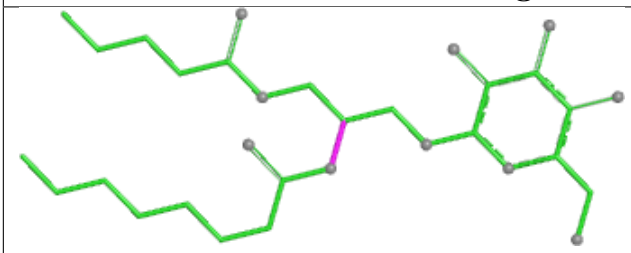


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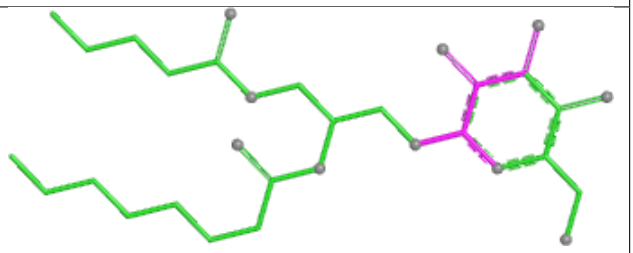


Rings

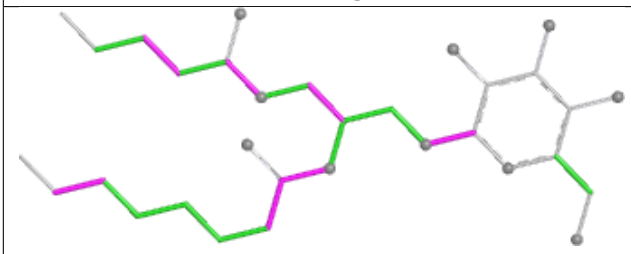
Ligand LMG a 4201



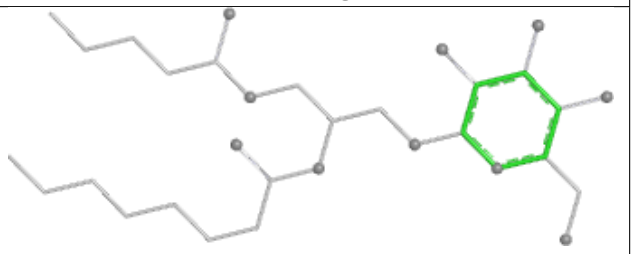
Bond lengths



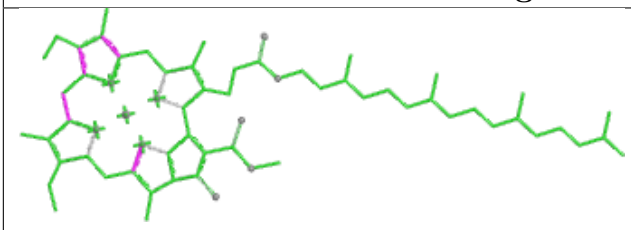
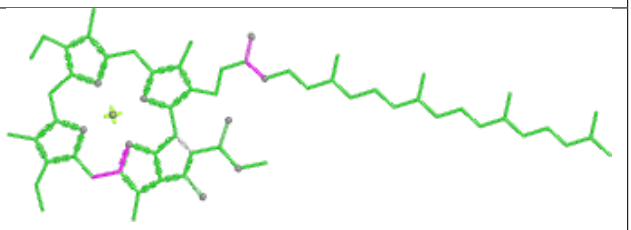
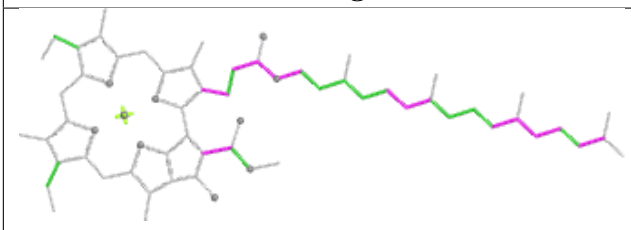
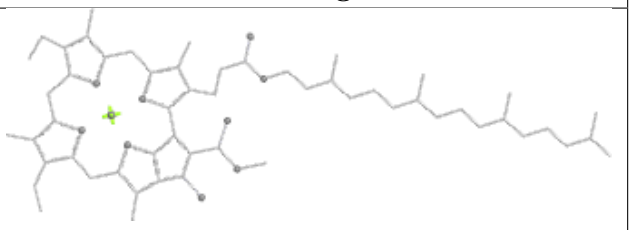
Bond angles



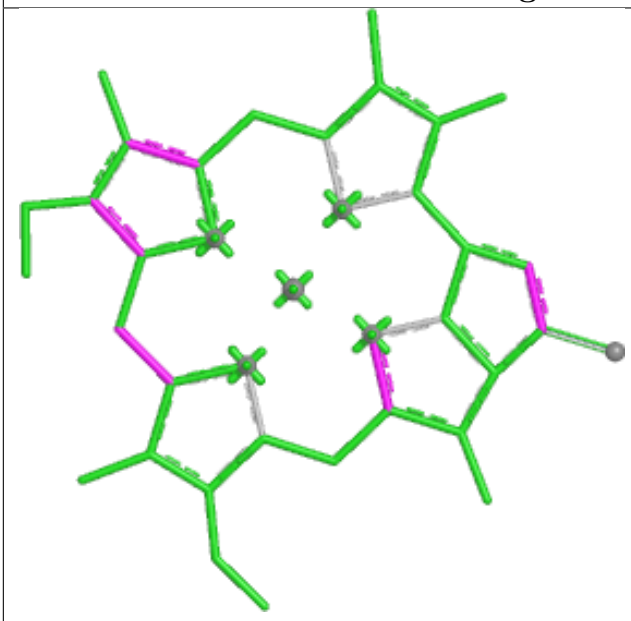
Torsions



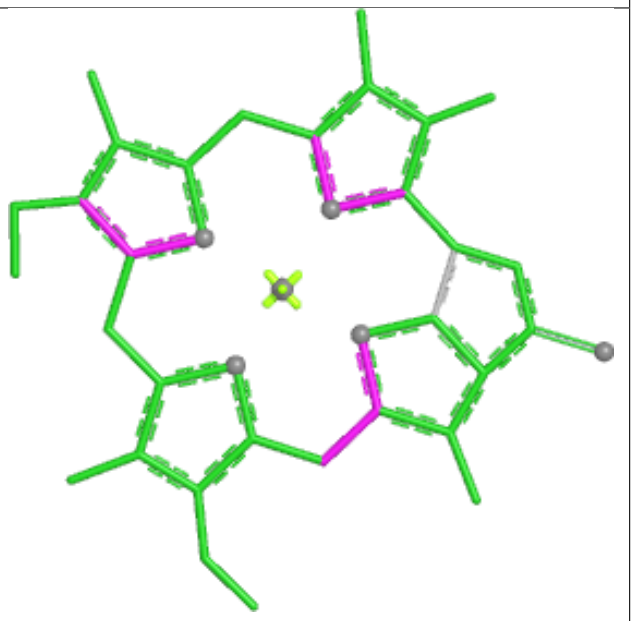
Rings

Ligand CLA B 1202	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

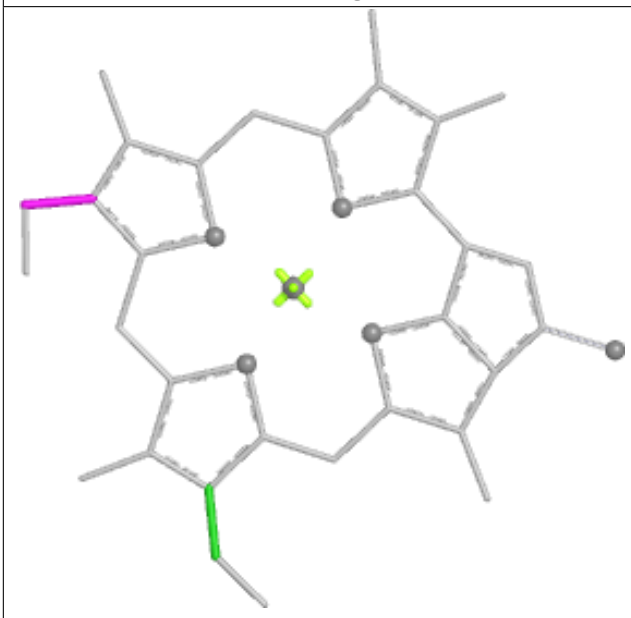
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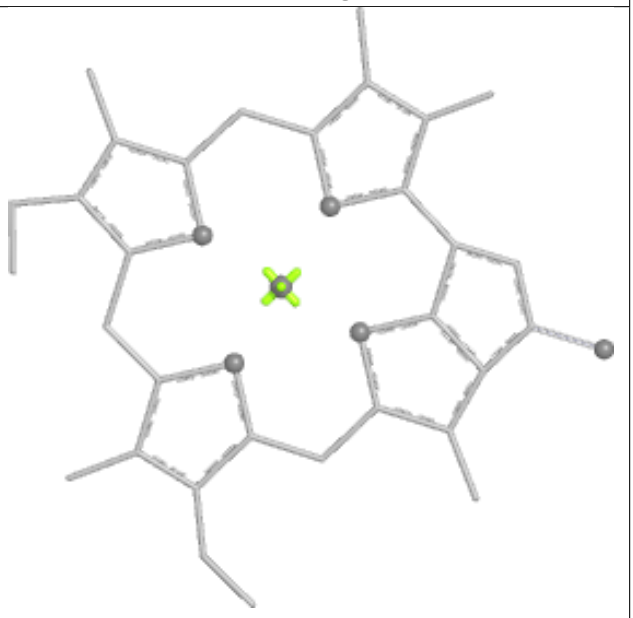
Bond lengths



Bond angles

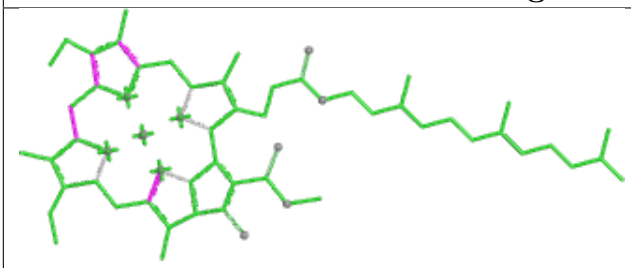


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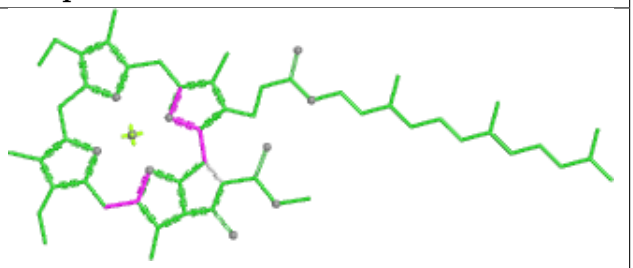


Rings

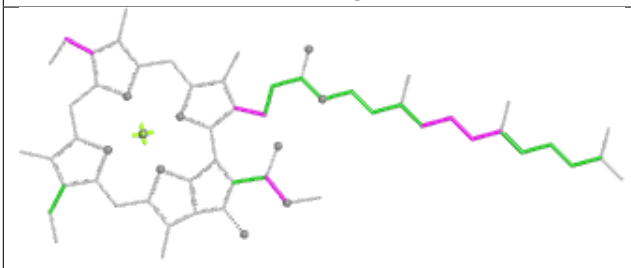
Ligand CLA q 510



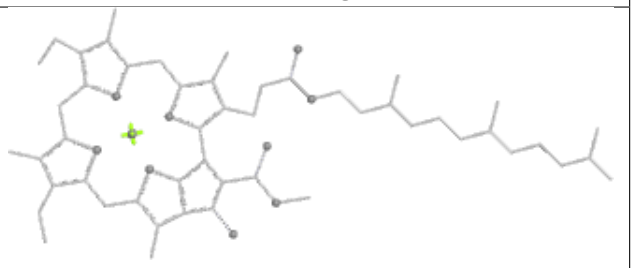
Bond lengths



Bond angles

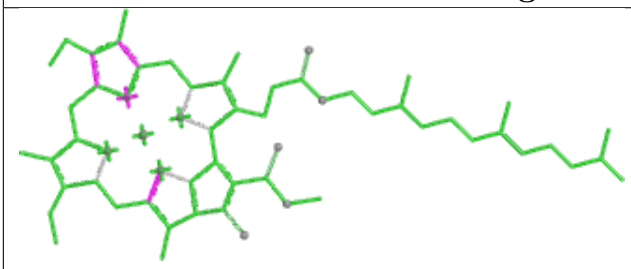


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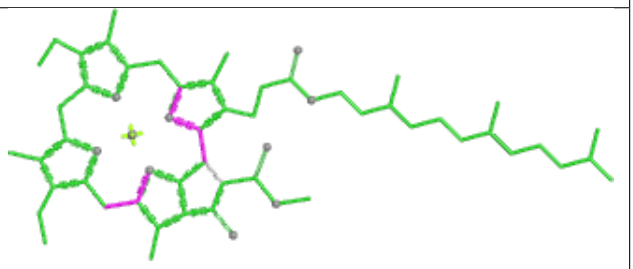


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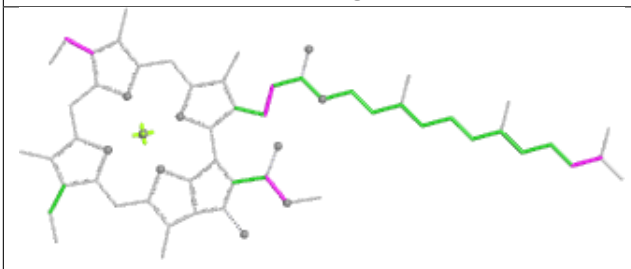
Ligand CLA b 1215



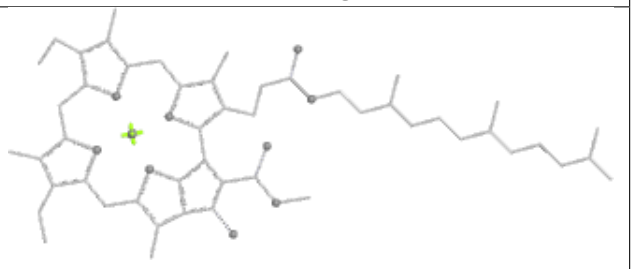
Bond lengths



Bond angles

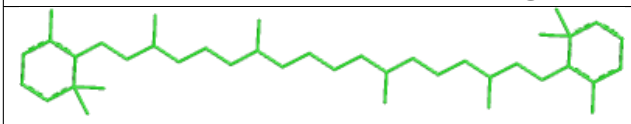


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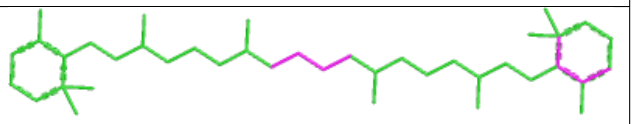


Rings

Ligand BCR Y 603



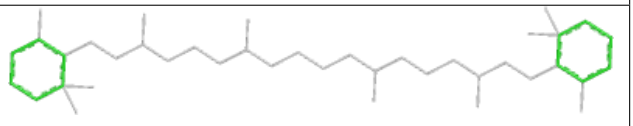
Bond lengths



Bond angles

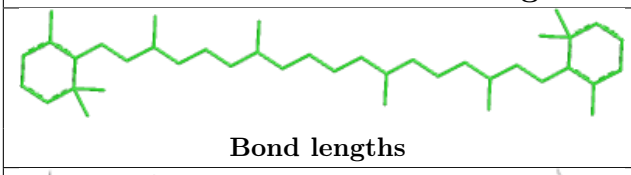


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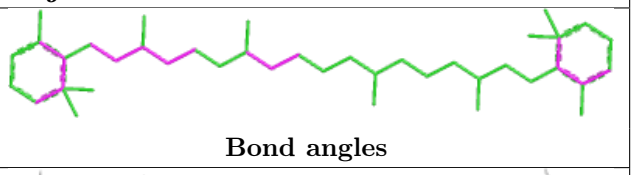


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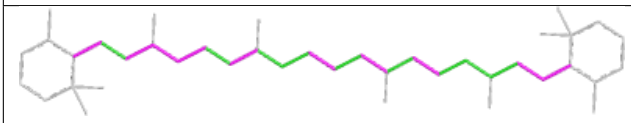
Ligand BCR j 4015



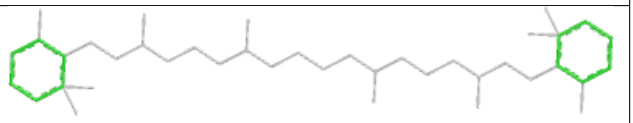
Bond lengths



Bond angles

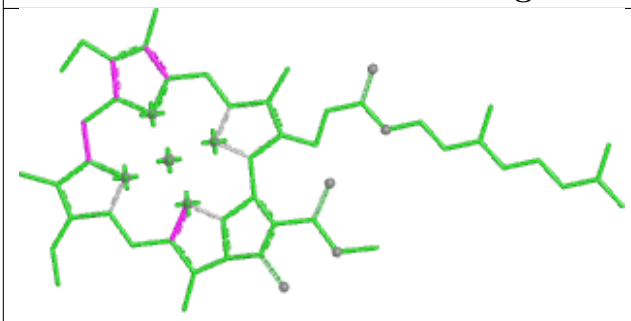


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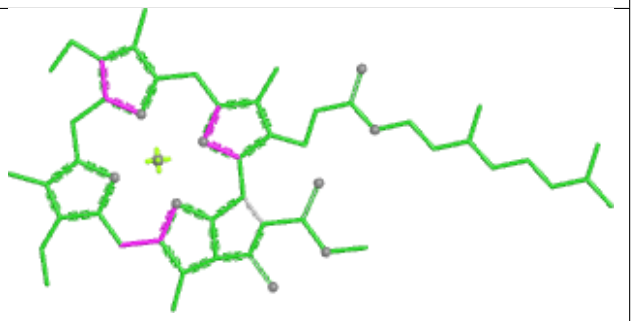


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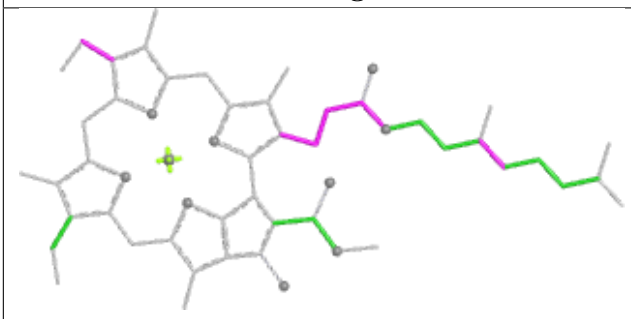
Ligand CLA A 1118



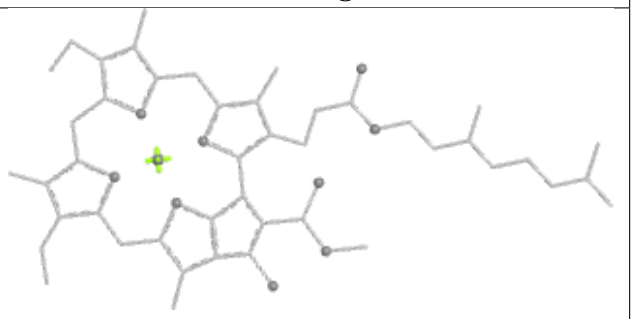
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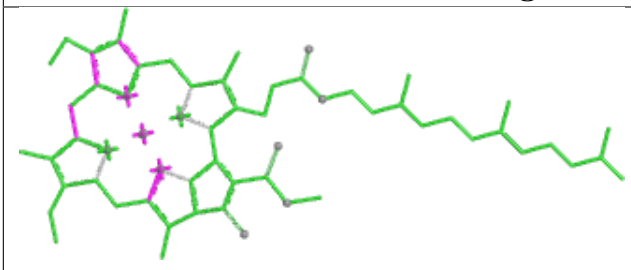


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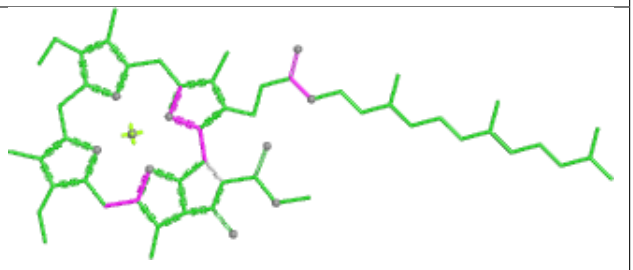


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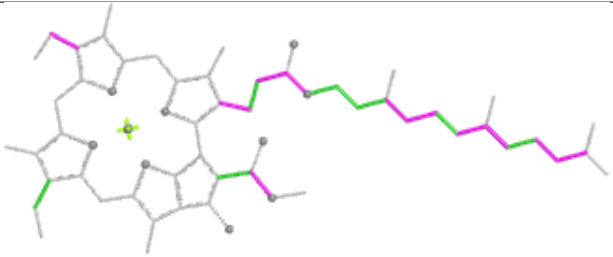
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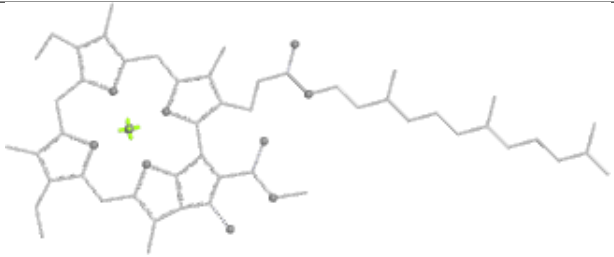
Bond lengths



Bond angles

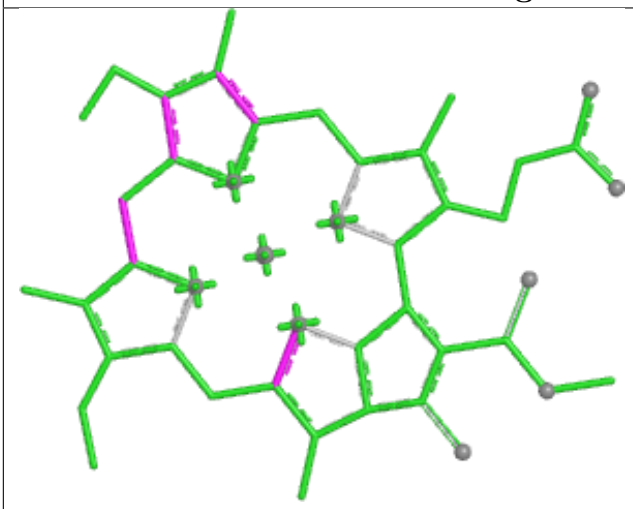


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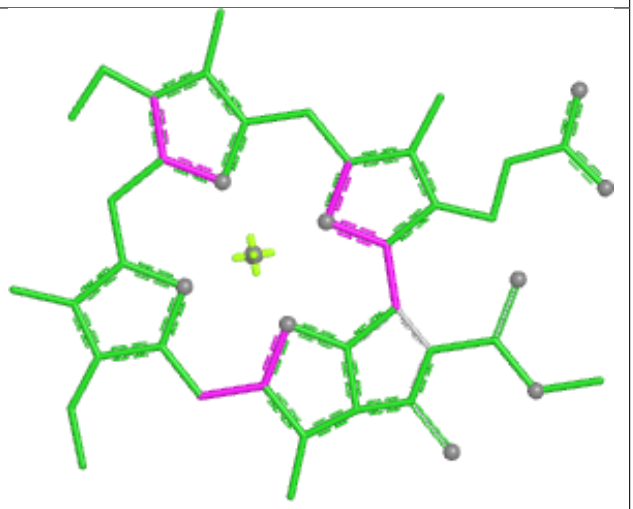


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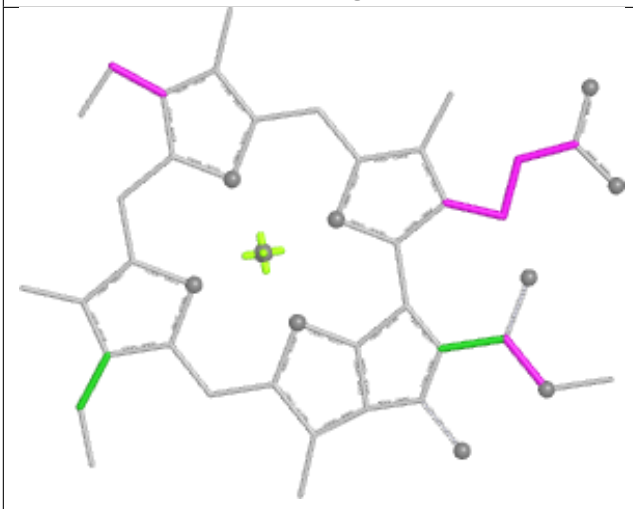
Ligand CLA B 1231



Bond lengths



Bond angles

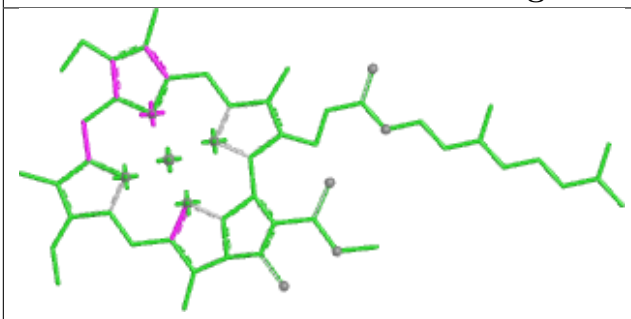


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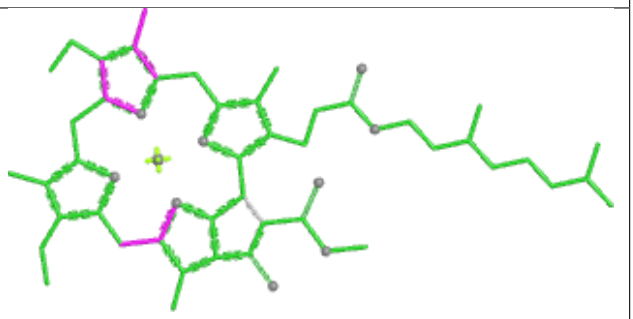


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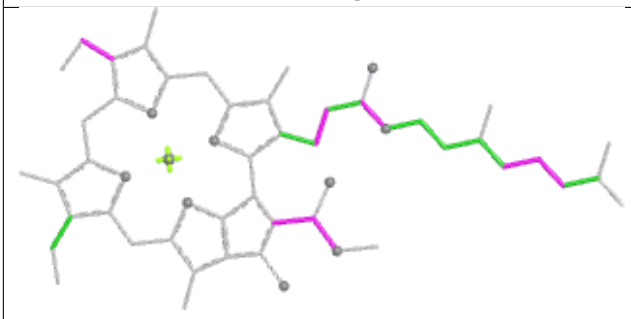
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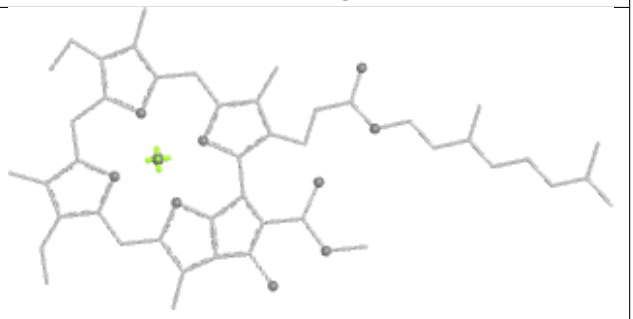
Bond lengths



Bond angles

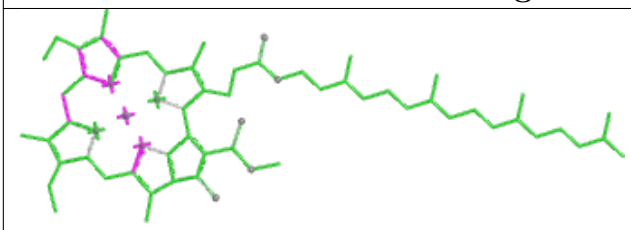


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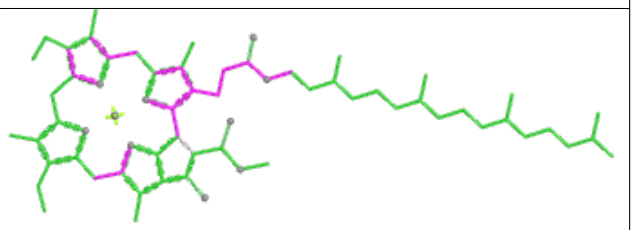


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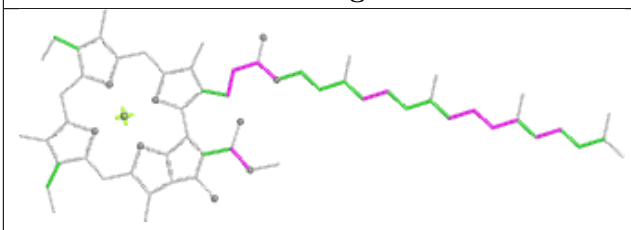
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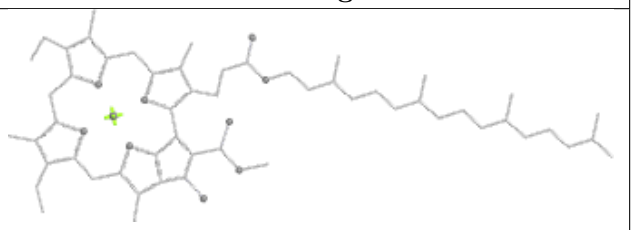
Bond lengths



Bond angles

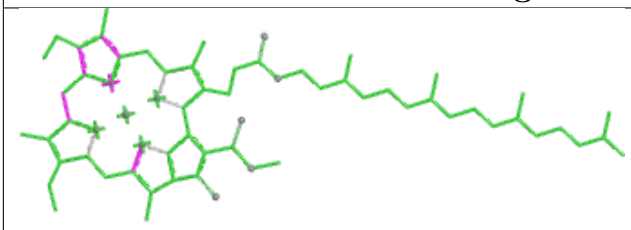


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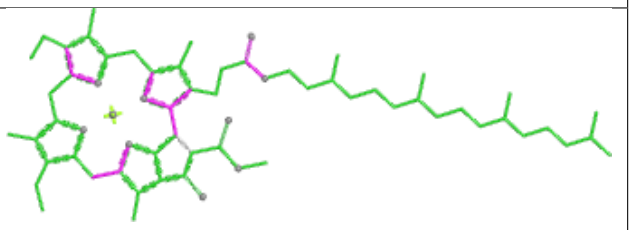


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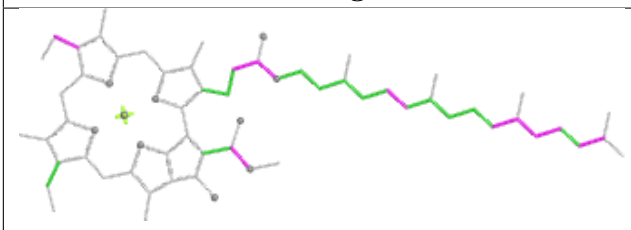
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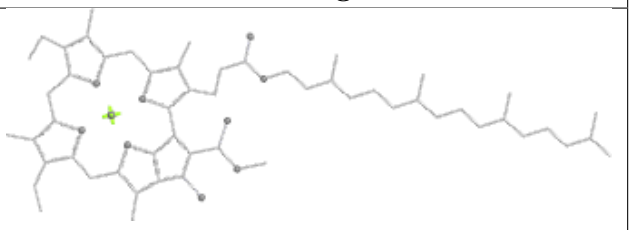
Bond lengths



Bond angles

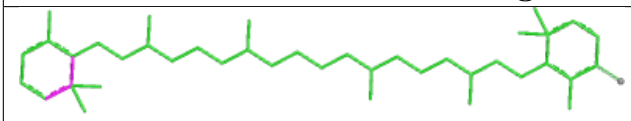


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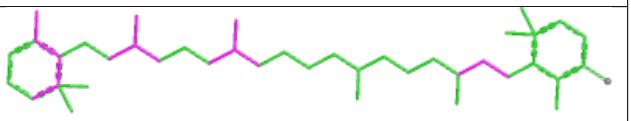


Rings

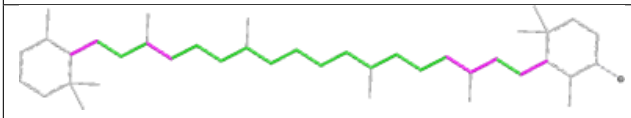
Ligand ECH b 4006



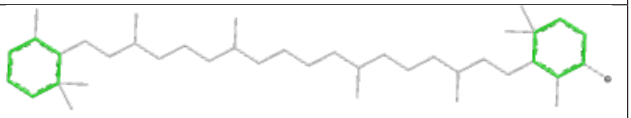
Bond lengths



Bond angles

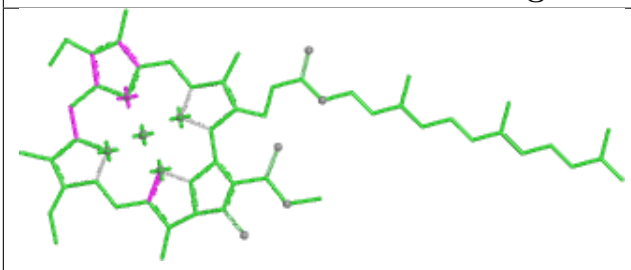


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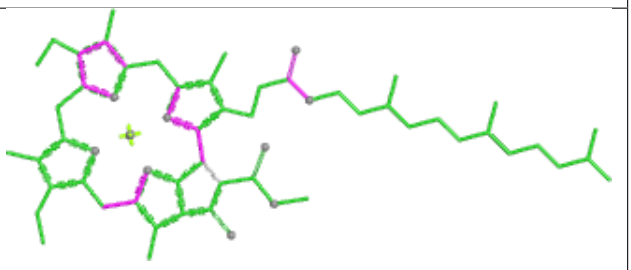


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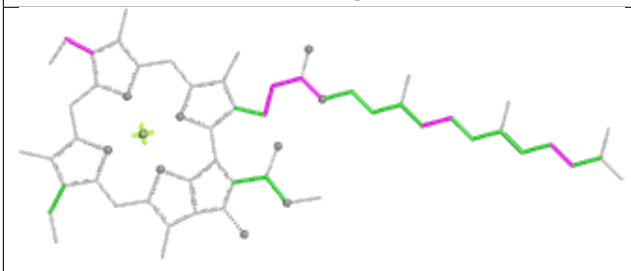
Ligand CLA u 509



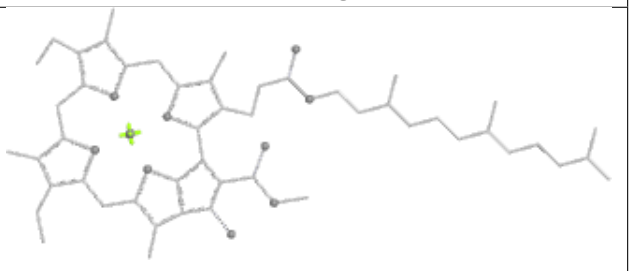
Bond lengths



Bond angles

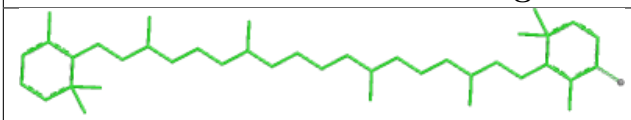


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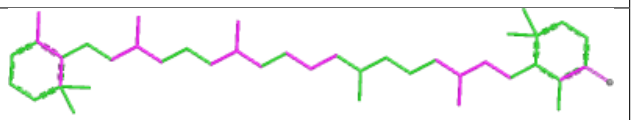


Rings

Ligand ECH B 4006



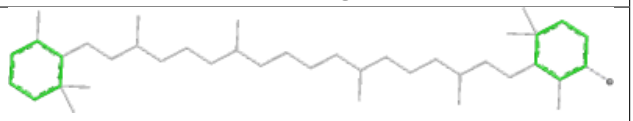
Bond lengths



Bond angles

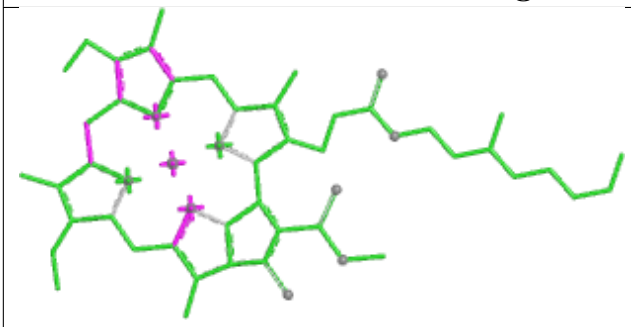


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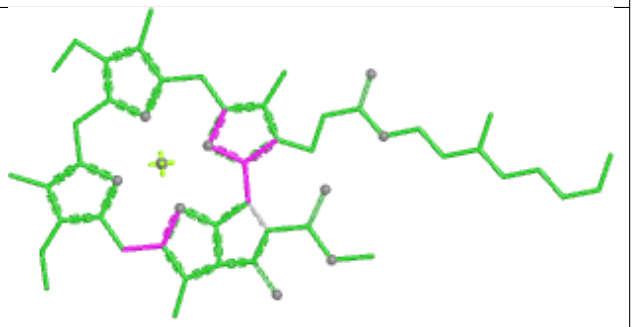


Rings

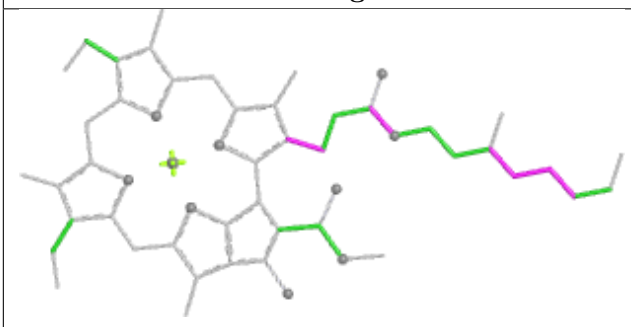
Ligand CLA A 1115



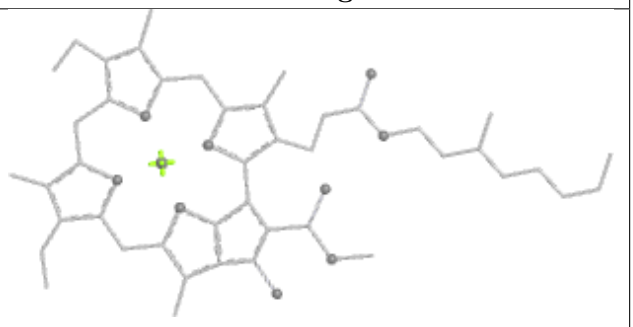
Bond lengths



Bond angles

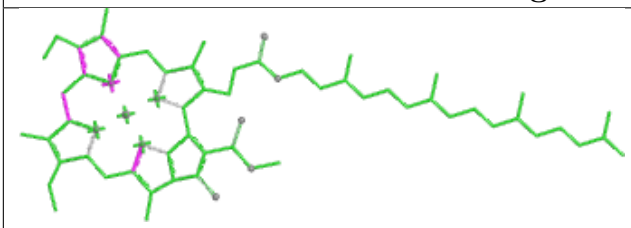


Torsions

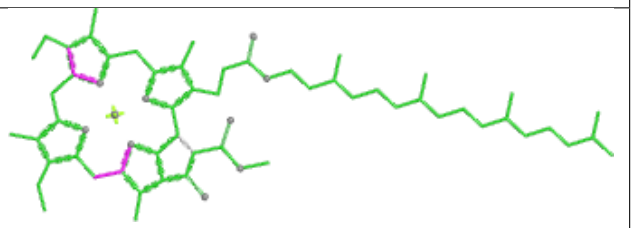


Rings

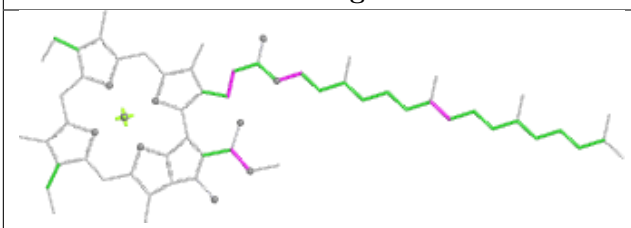
Ligand CLA r 511



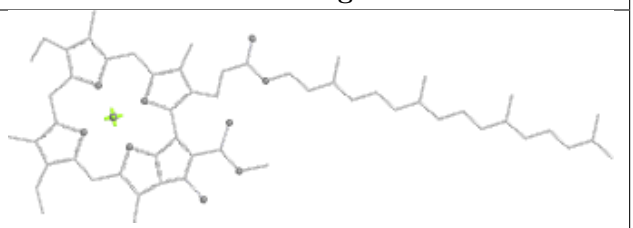
Bond lengths



Bond angles

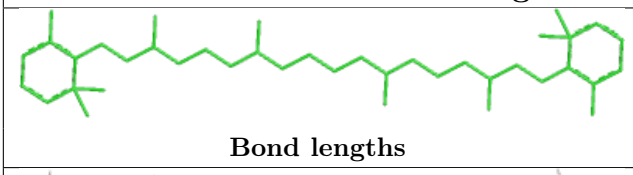


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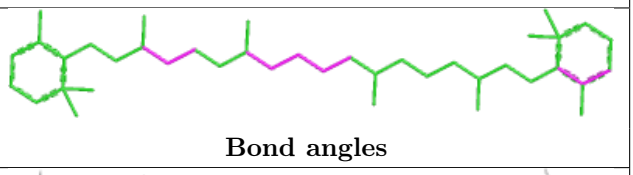


Rings

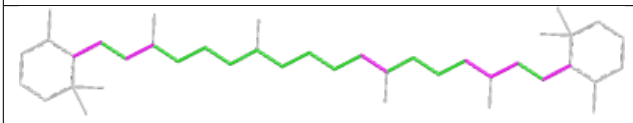
Ligand BCR H 4003



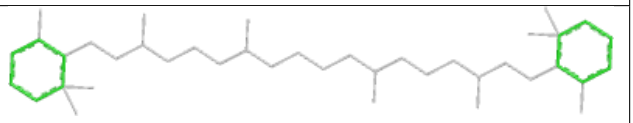
Bond lengths



Bond angles

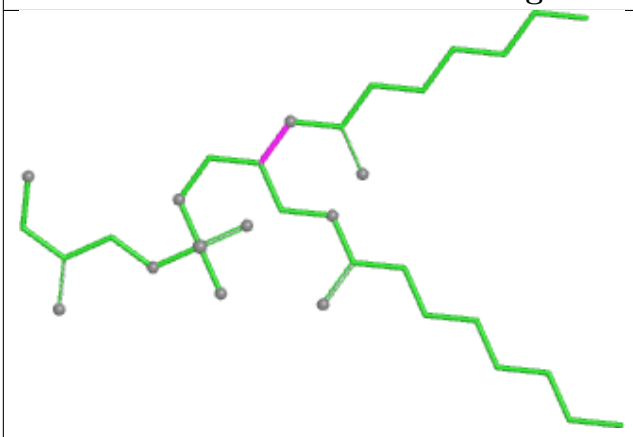


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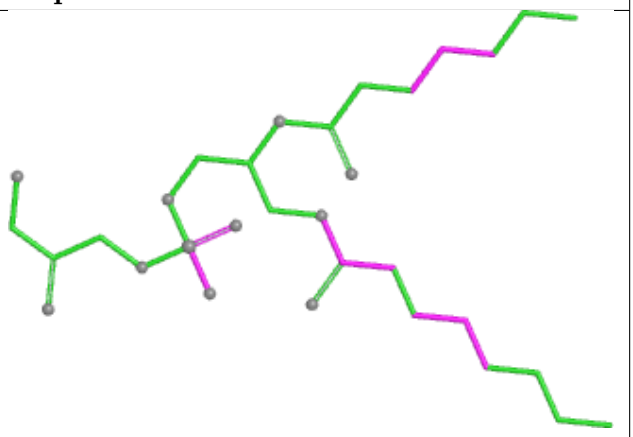


Rings

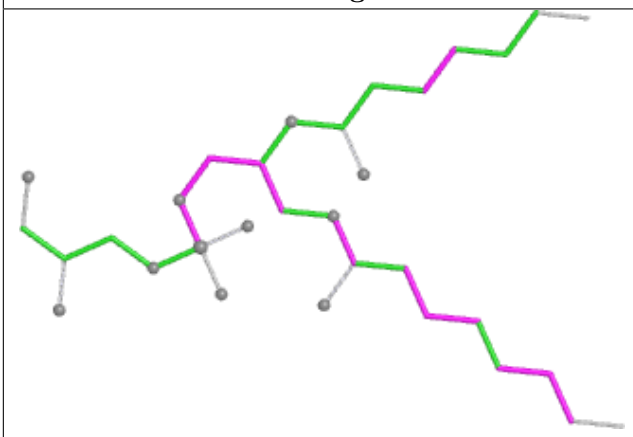
Ligand LHG p 605



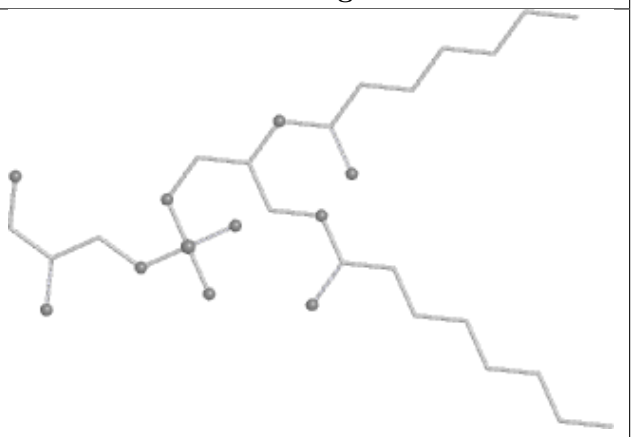
Bond lengths



Bond angles

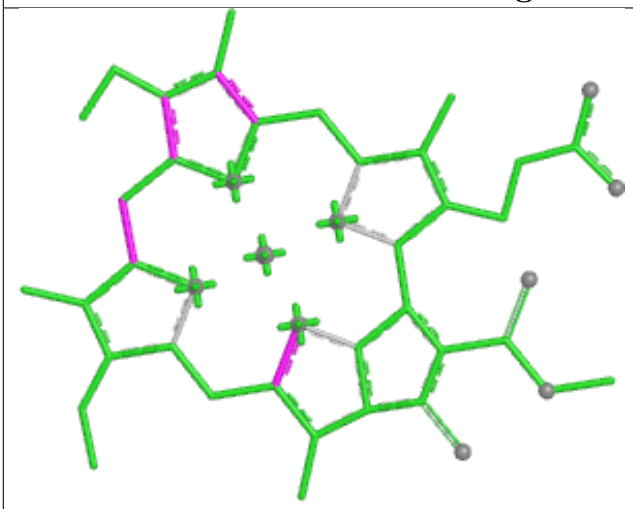


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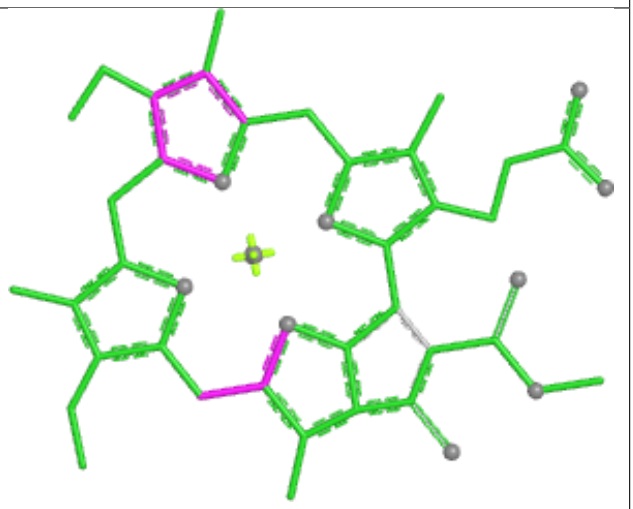


Rings

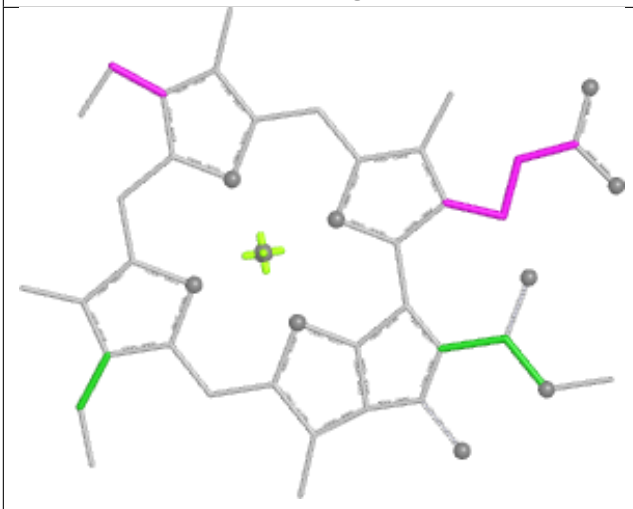
Ligand CLA B 1217



Bond lengths



Bond angles

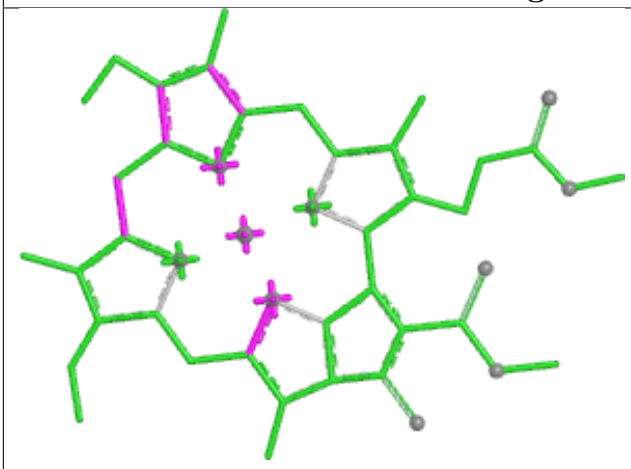


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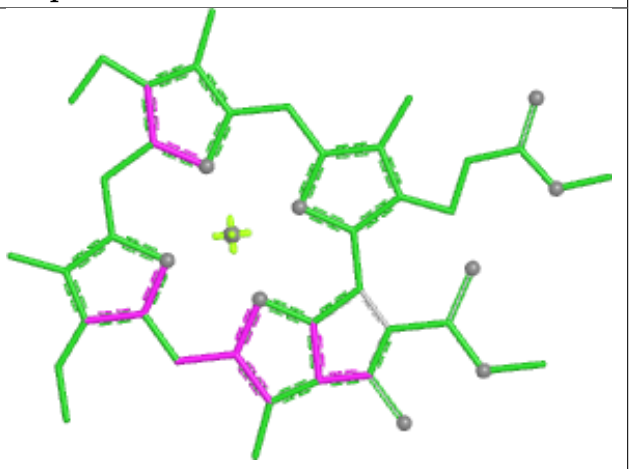


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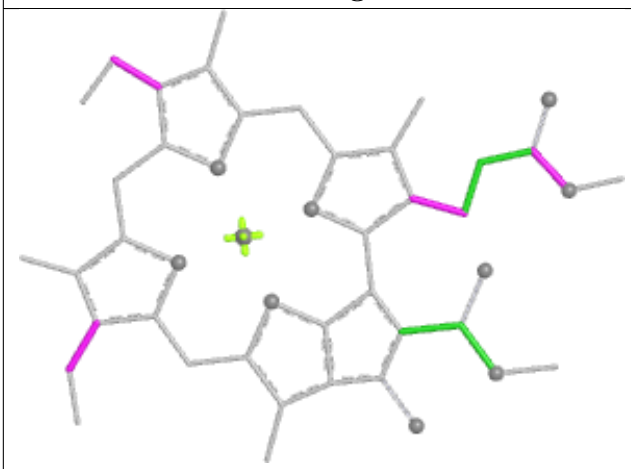
Ligand CLA p 503



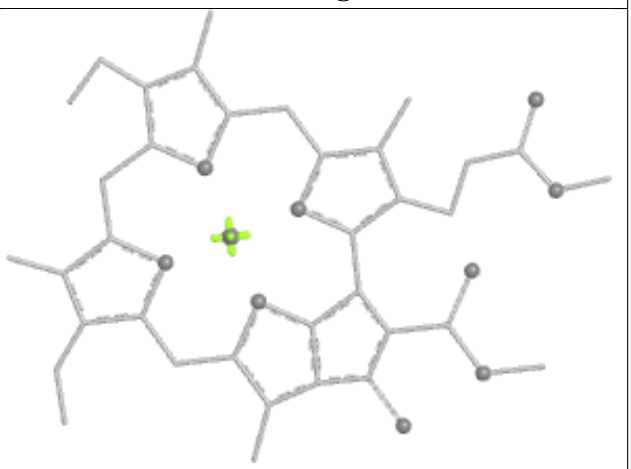
Bond lengths



Bond angles



Torsions

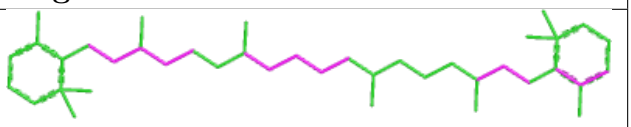


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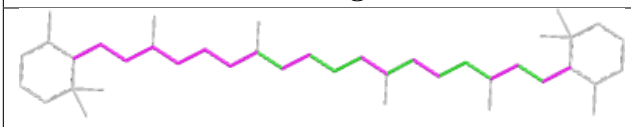
Ligand BCR g 604



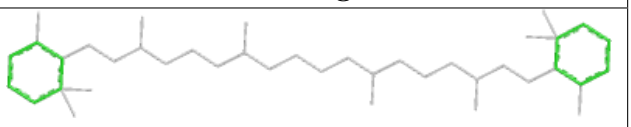
Bond lengths



Bond angles

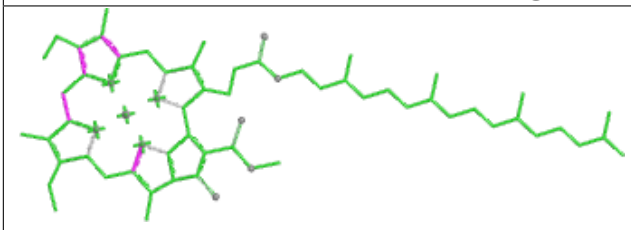


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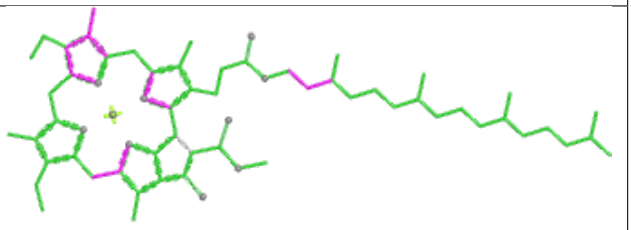


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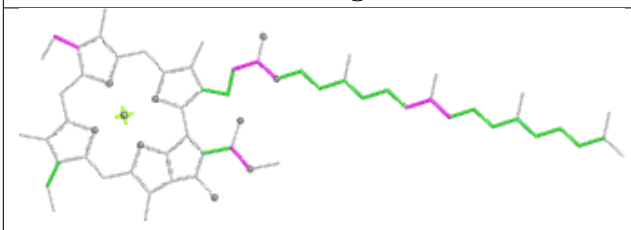
Ligand CLA u 507



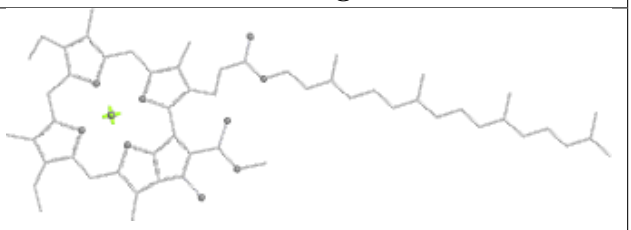
Bond lengths



Bond angles



Torsions

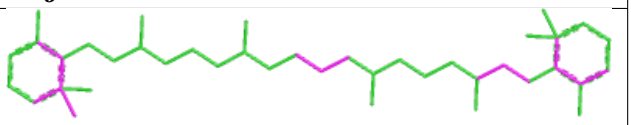


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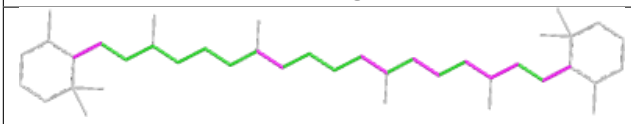
Ligand BCR j 4013



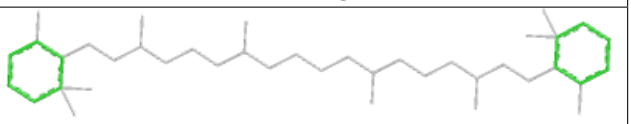
Bond lengths



Bond angles

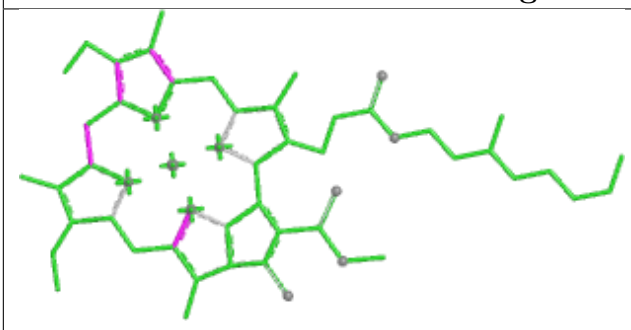


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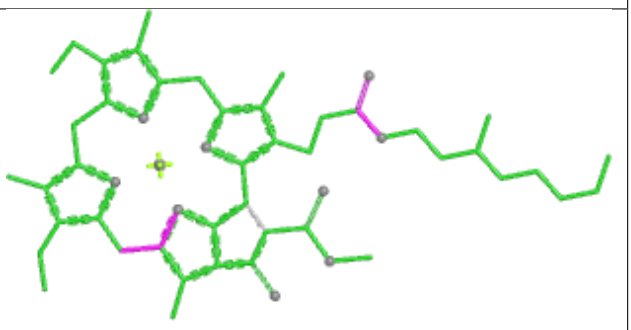


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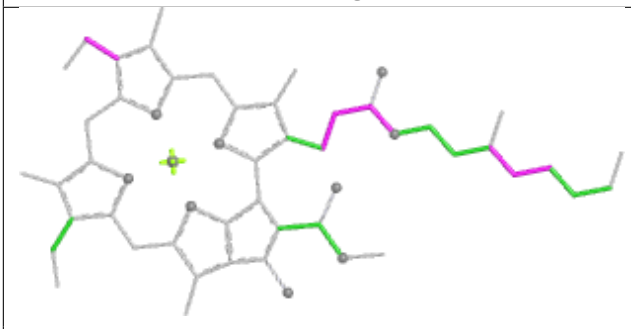
Ligand CLA a 1110



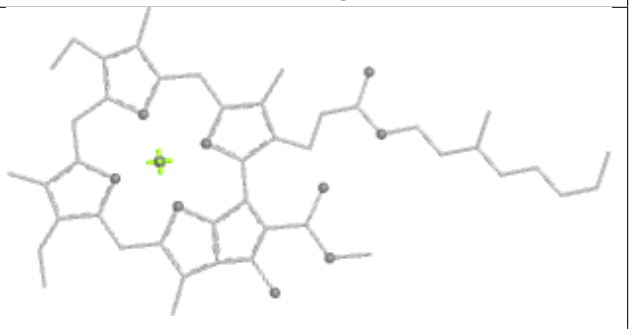
Bond lengths



Bond angles

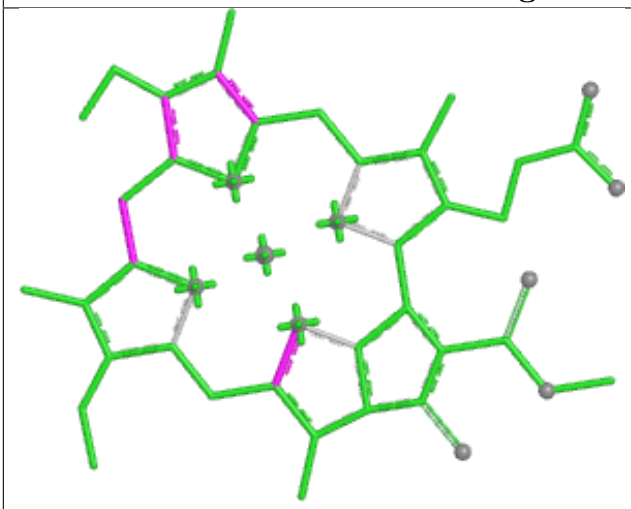


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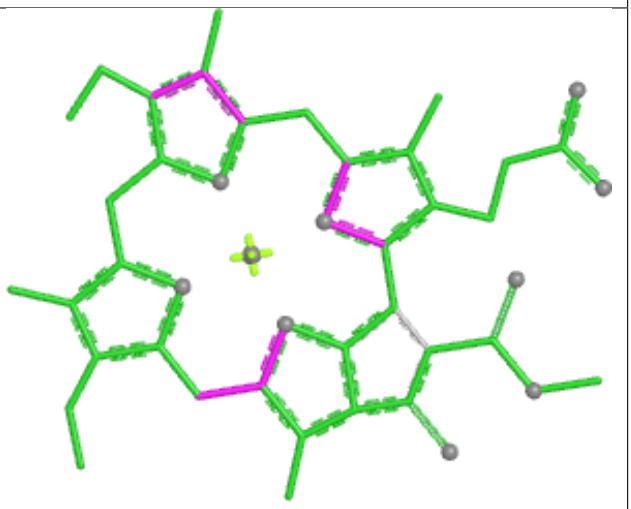


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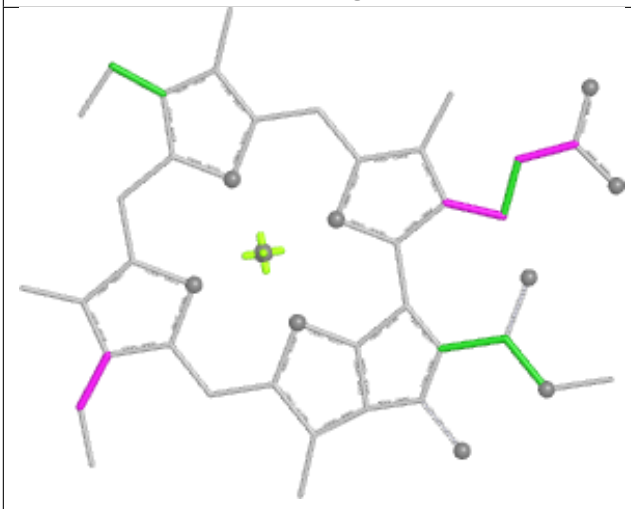
Ligand CLA k 4003



Bond lengths



Bond angles

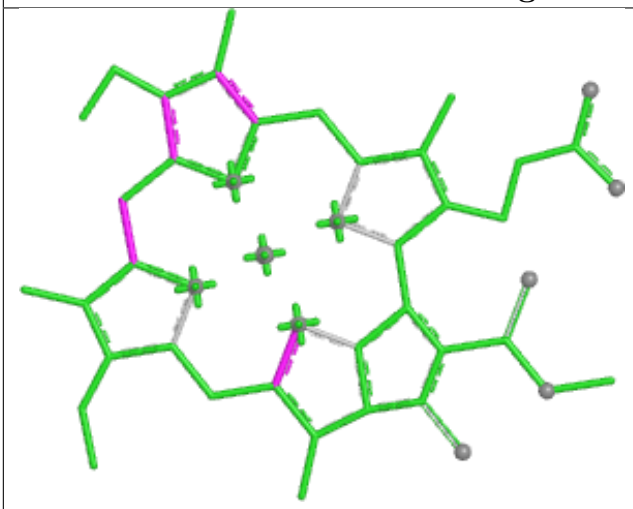


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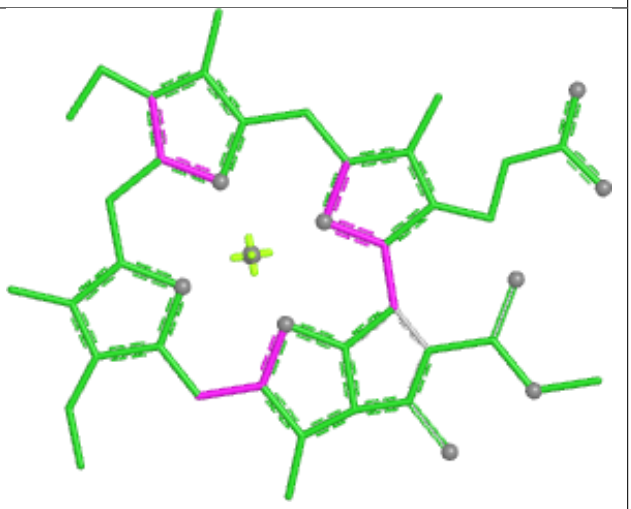


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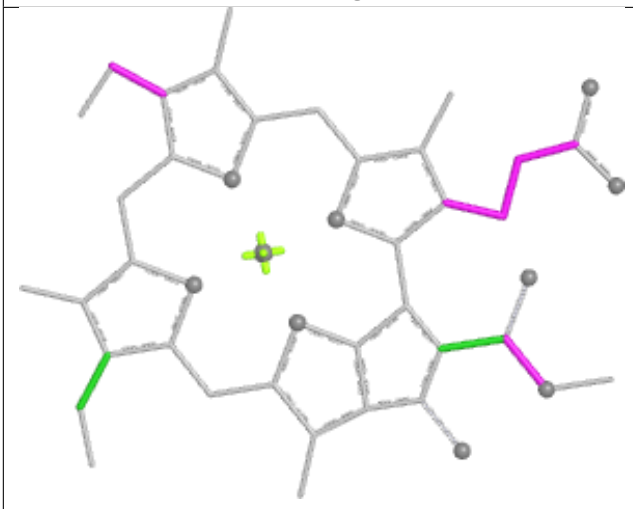
Ligand CLA b 1231



Bond lengths



Bond angles

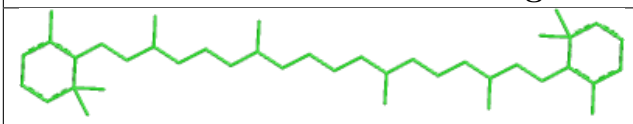


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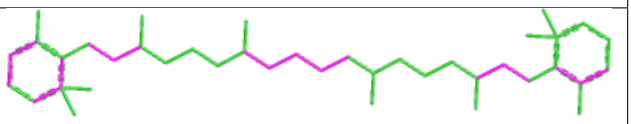


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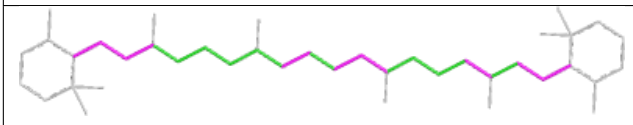
Ligand BCR n 604



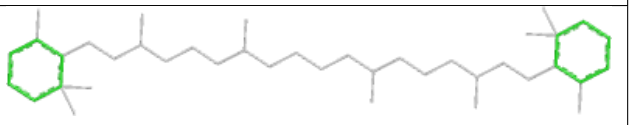
Bond lengths



Bond angles

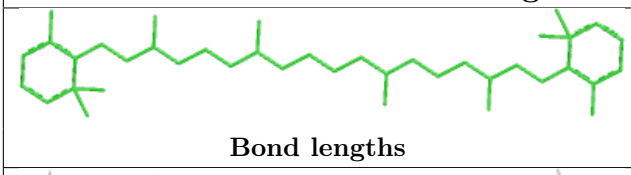


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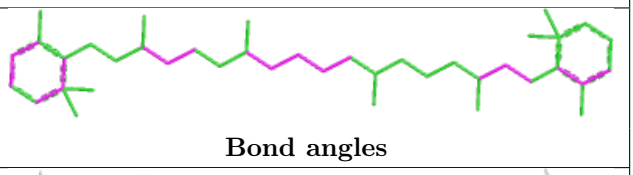


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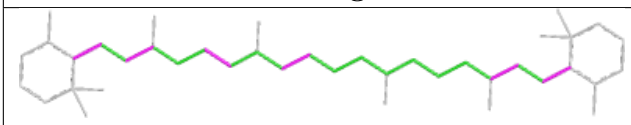
Ligand BCR Y 602



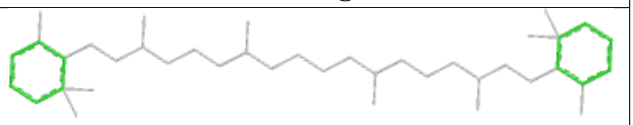
Bond lengths



Bond angles

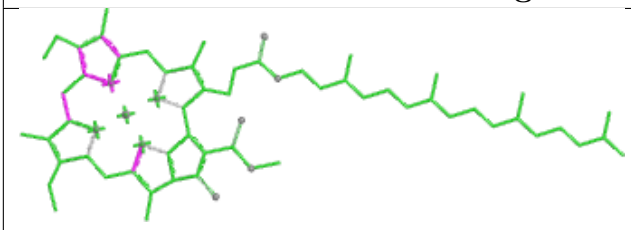


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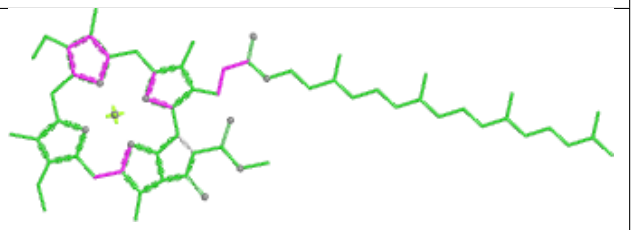


Rings

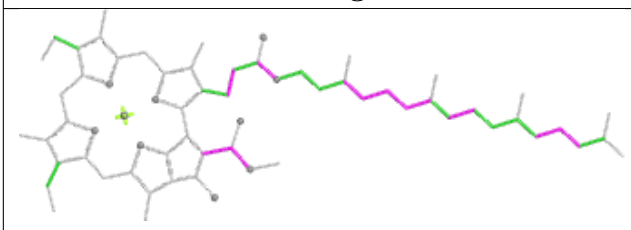
Ligand CLA A 1132



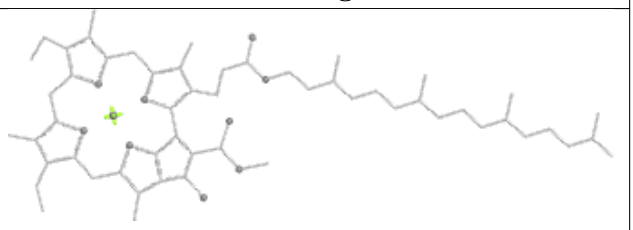
Bond lengths



Bond angles

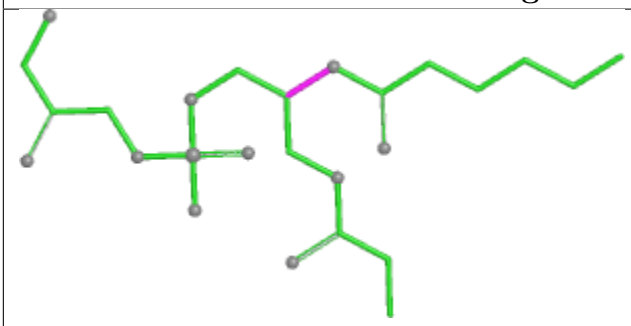


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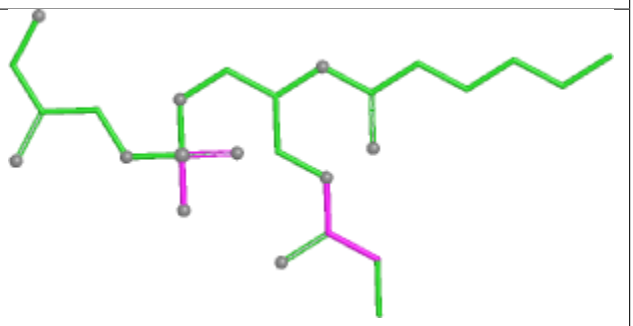


Rings

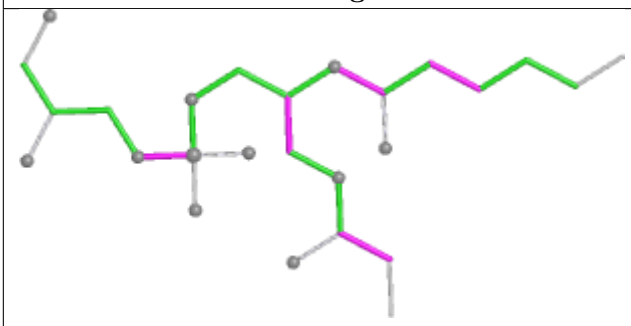
Ligand LHG H 851



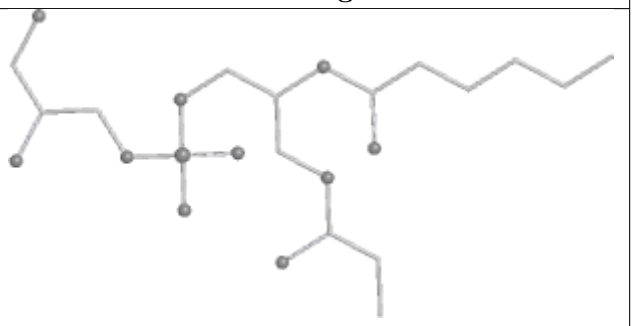
Bond lengths



Bond angles

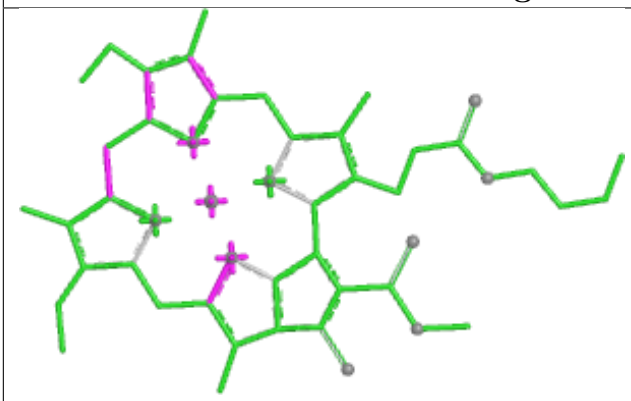


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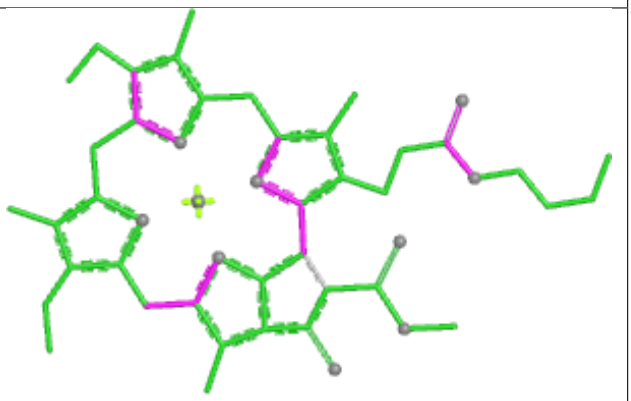


Rings

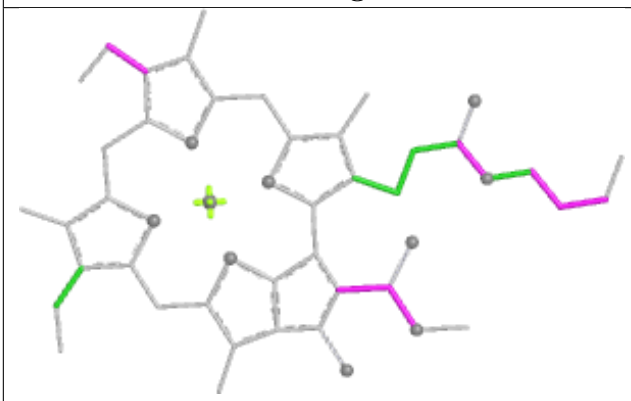
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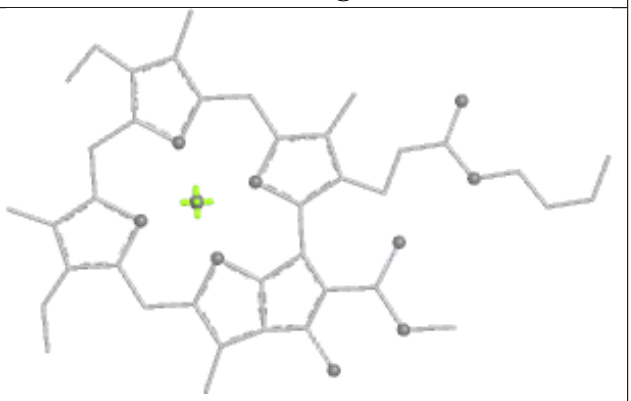
Bond lengths



Bond angles

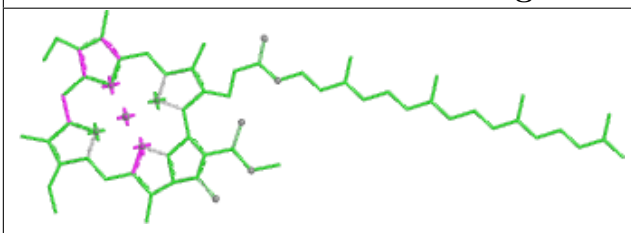


Torsions

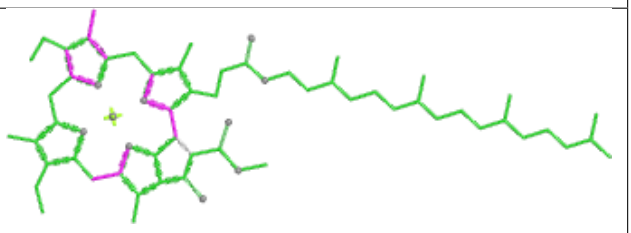


Rings

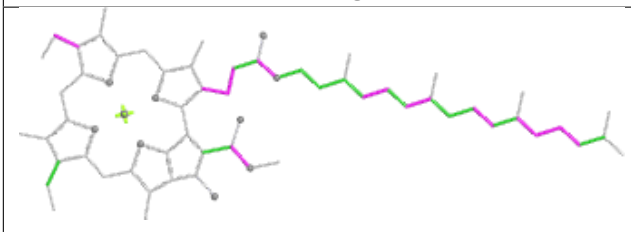
Ligand CLA B 1211



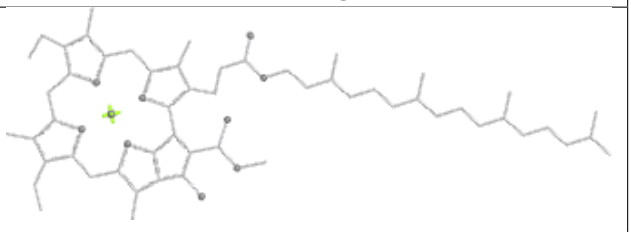
Bond lengths



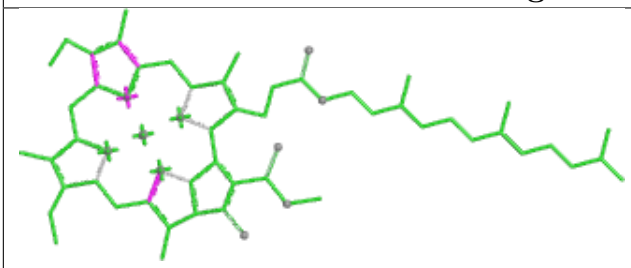
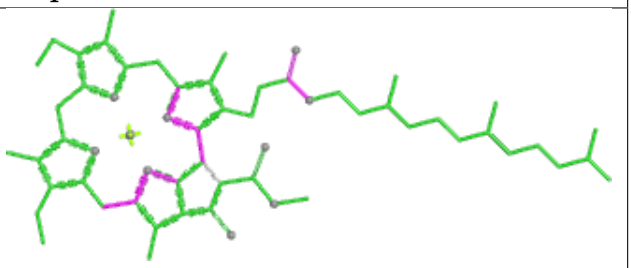
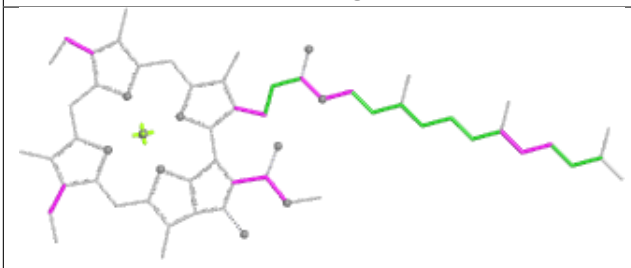
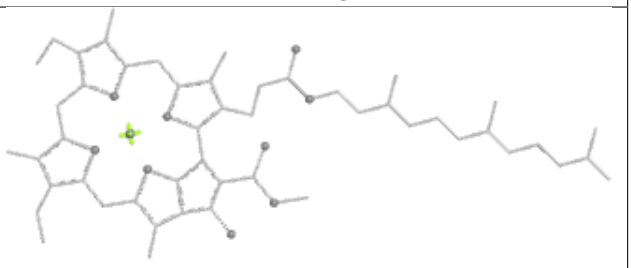
Bond angles

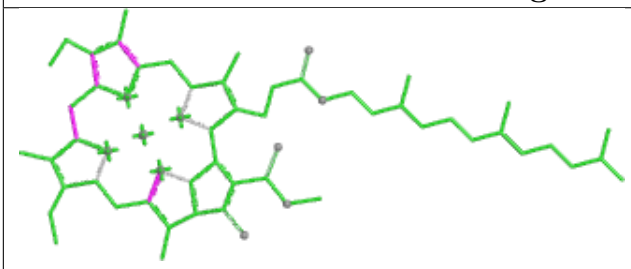
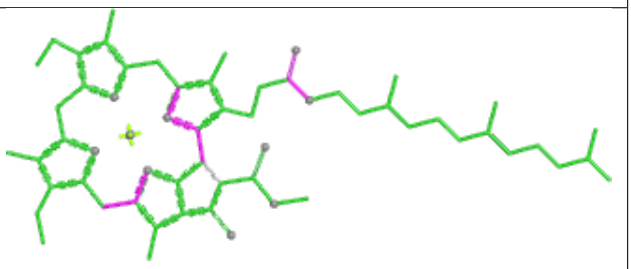
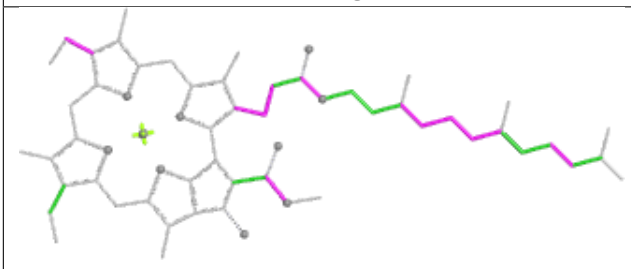
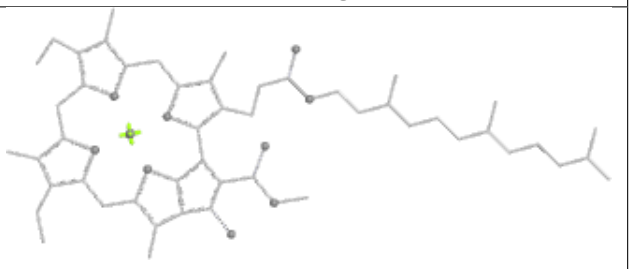


Torsions

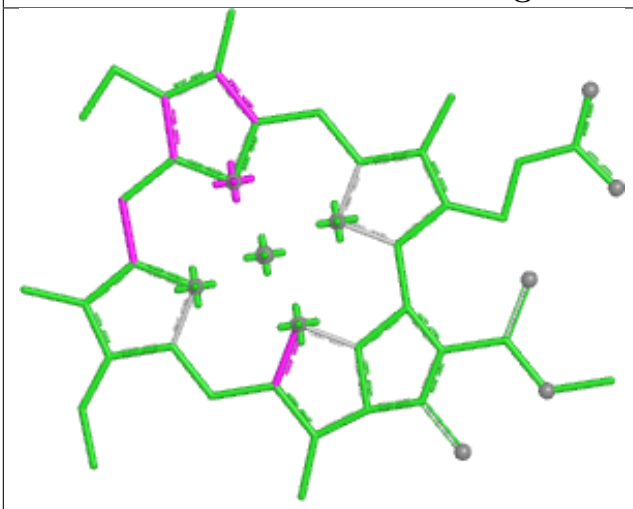


Rings

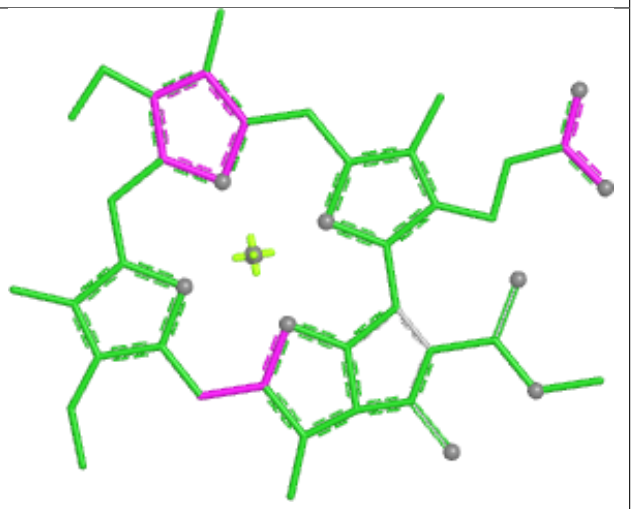
Ligand CLA p 506	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA s 509	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

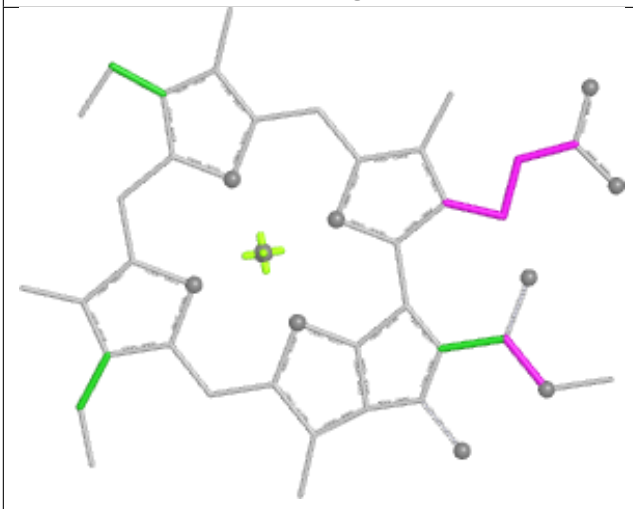
Ligand CLA G 1219



Bond lengths



Bond angles

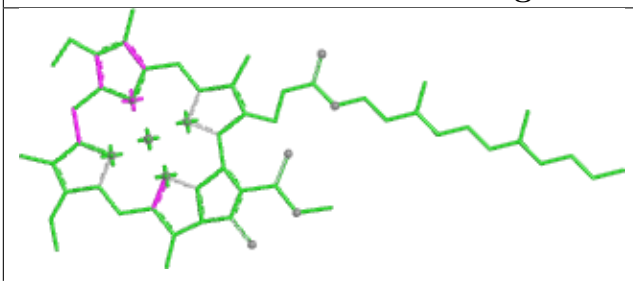


Torsions

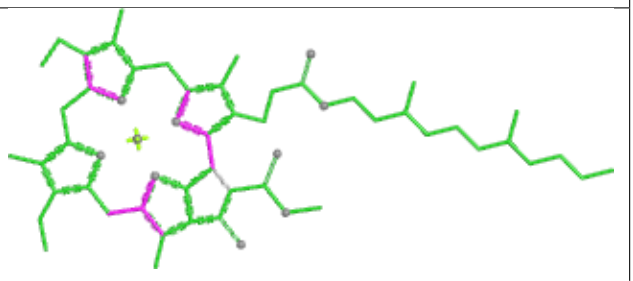


Rings

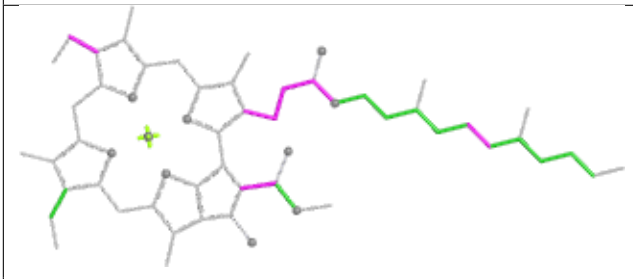
Ligand CLA H 1105



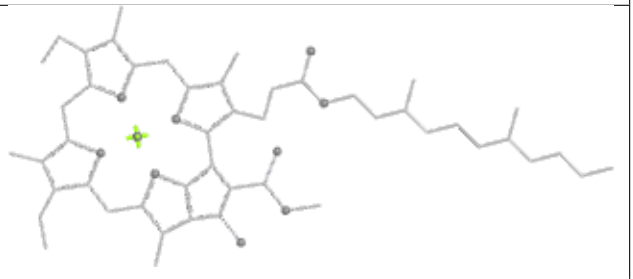
Bond lengths



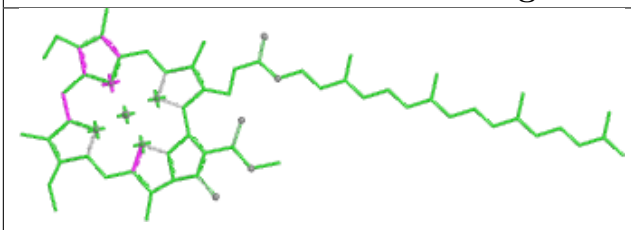
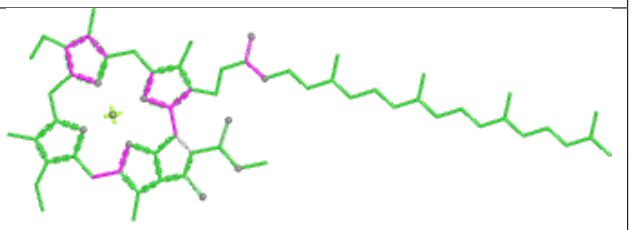
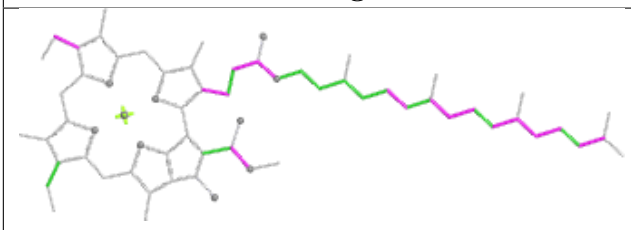
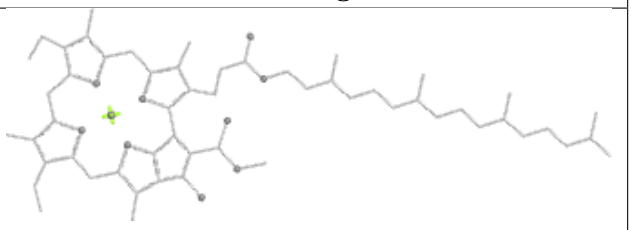
Bond angles

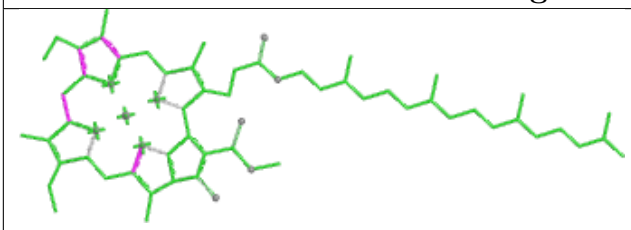
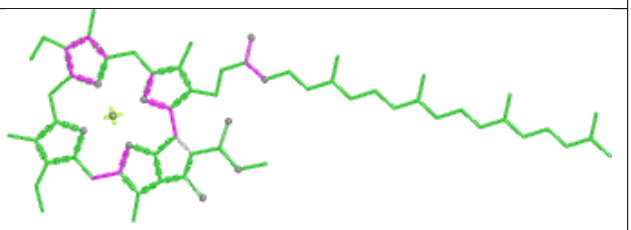
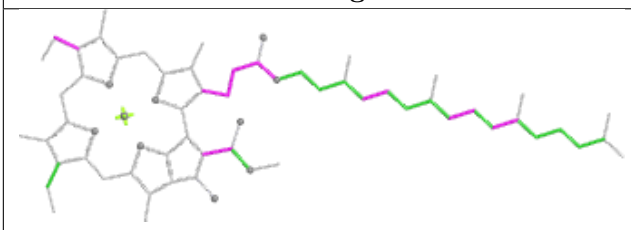
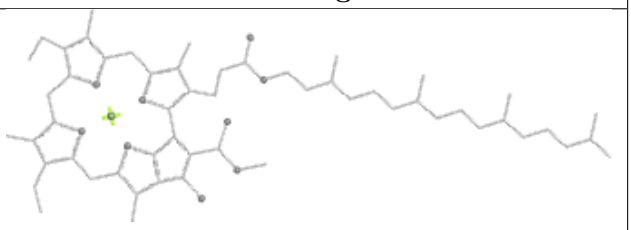


Torsions

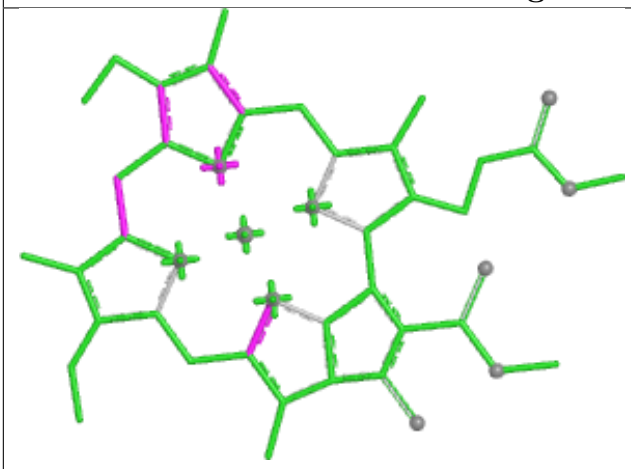


Rings

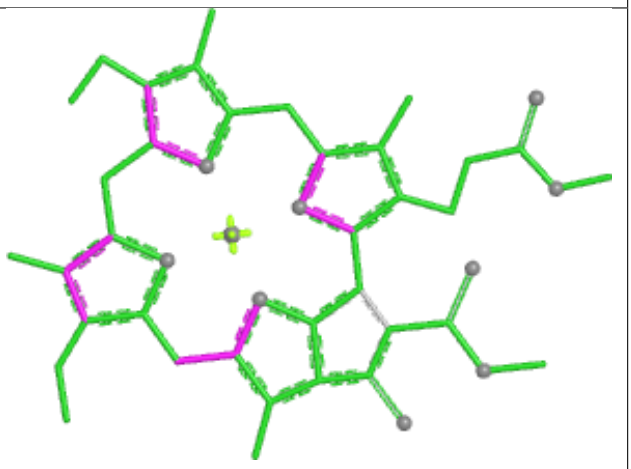
Ligand CLA b 1021	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

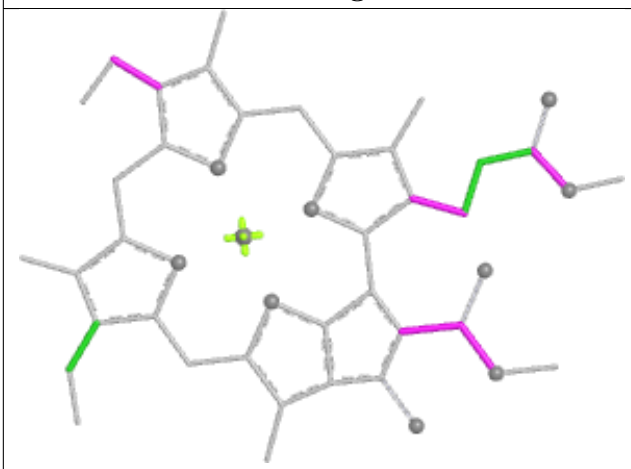
Ligand CLA n 513



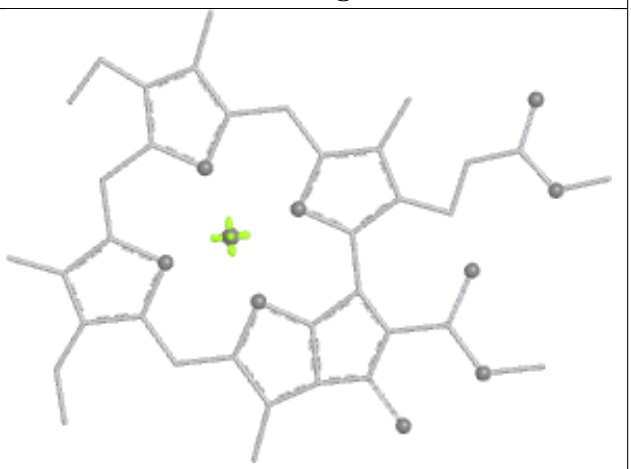
Bond lengths



Bond angles

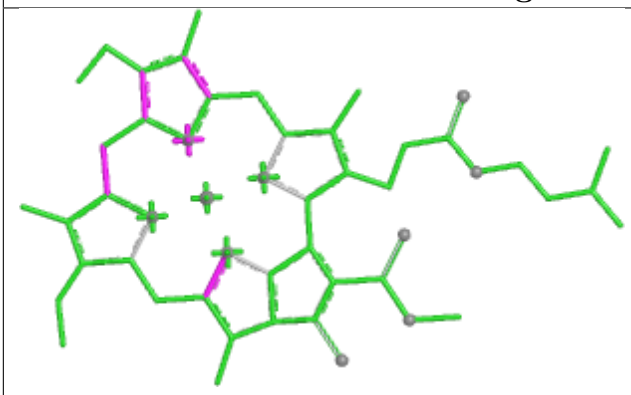


Torsions

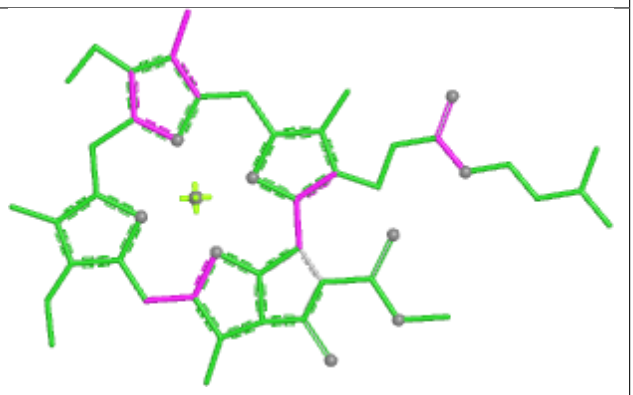


Rings

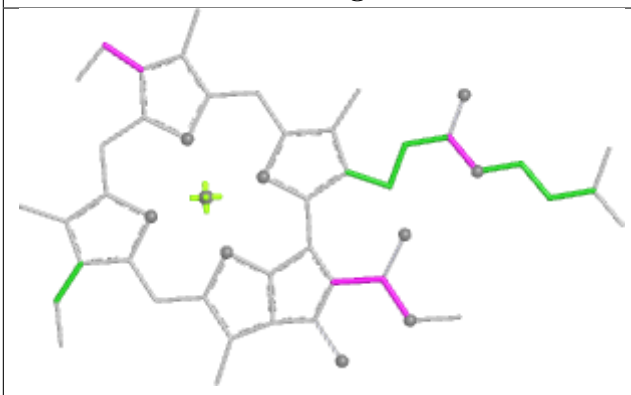
Ligand CLA B 1222



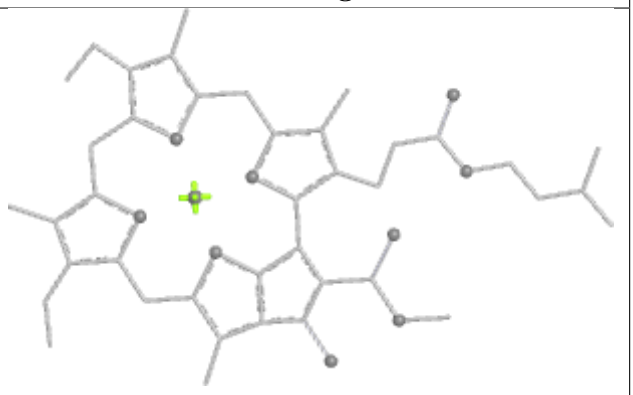
Bond lengths



Bond angles

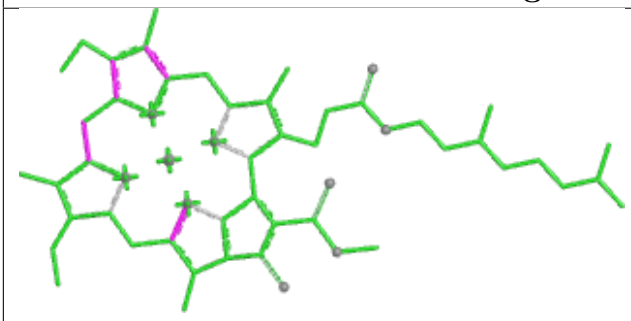


Torsions

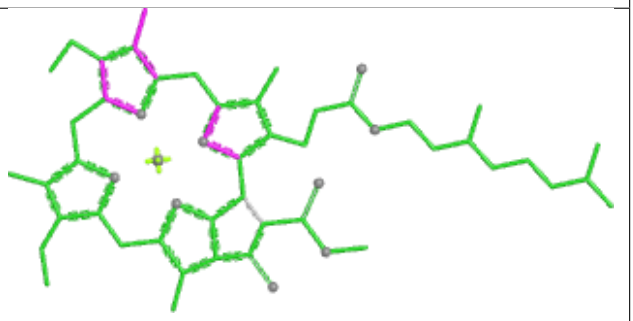


Rings

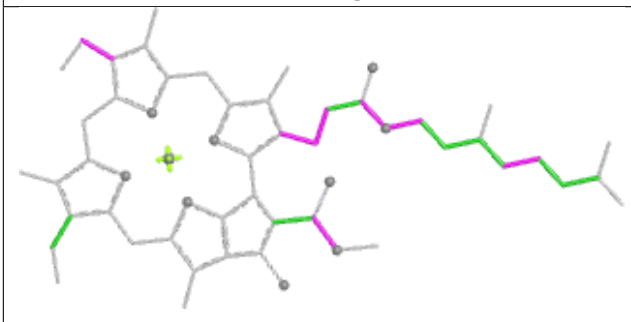
Ligand CLA Y 517



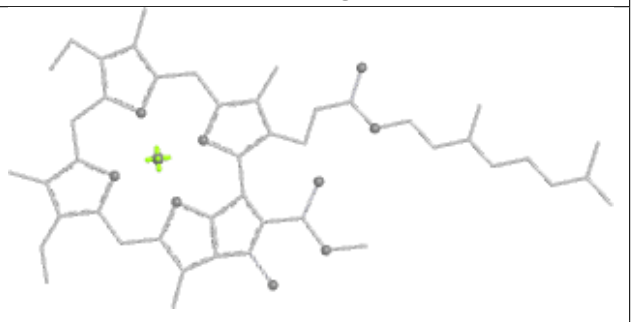
Bond lengths



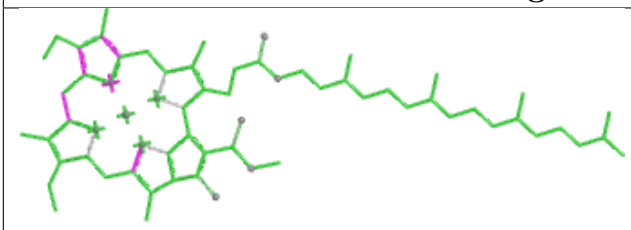
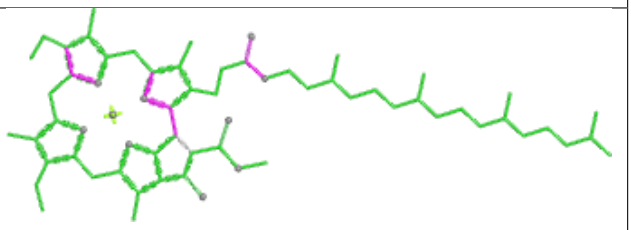
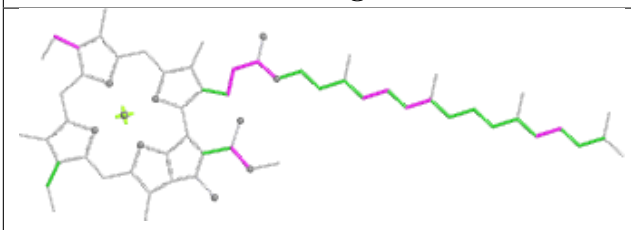
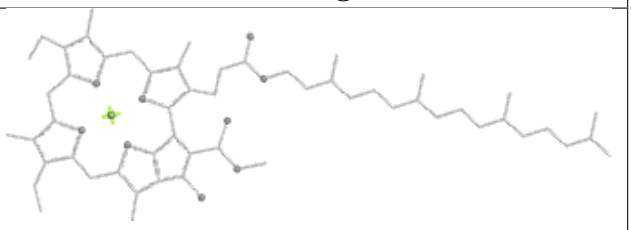
Bond angles

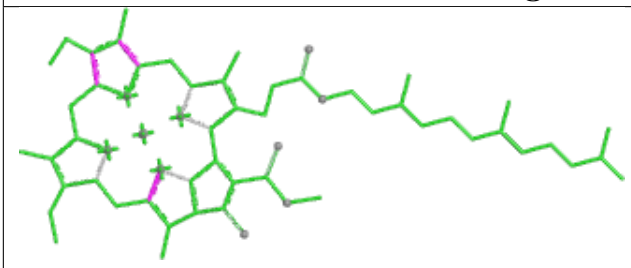
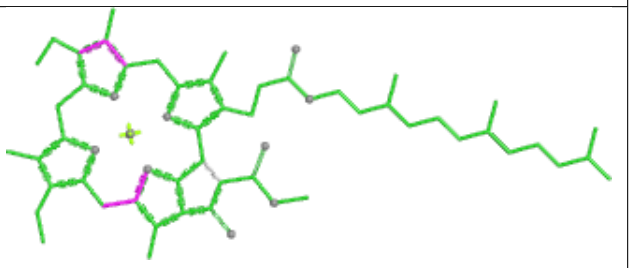
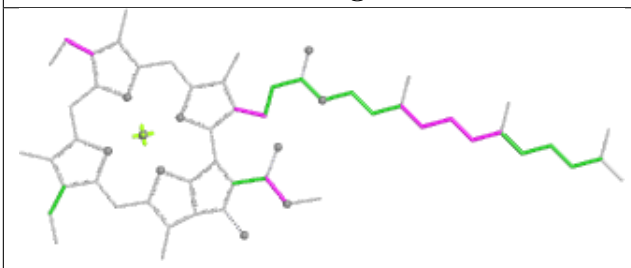
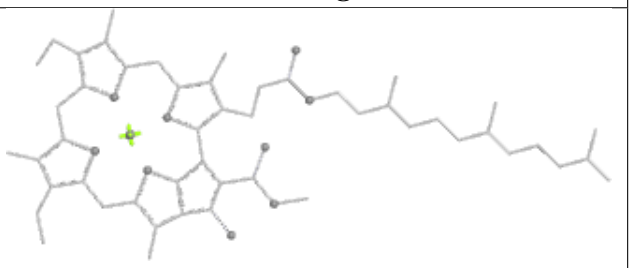


Torsions

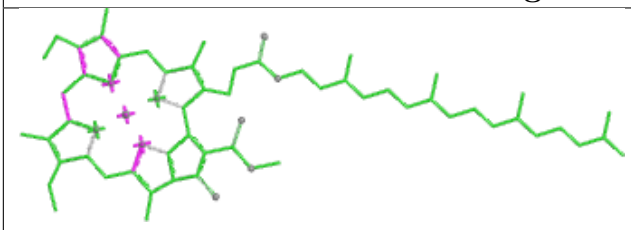


Rings

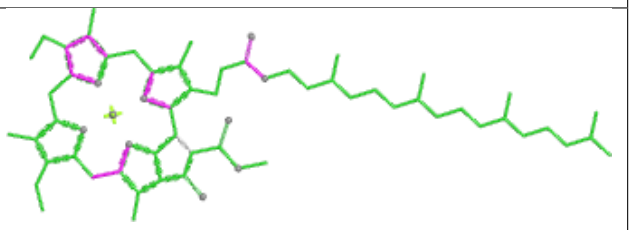
Ligand CLA x 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA w 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

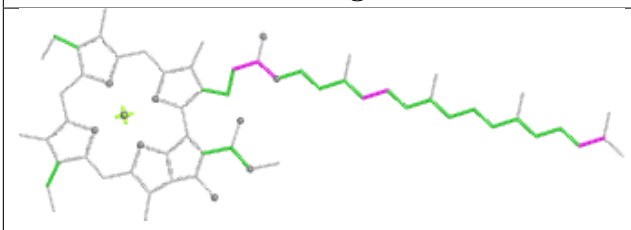
Ligand CL0 a 1011



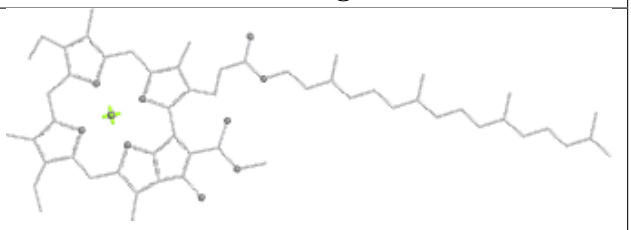
Bond lengths



Bond angles

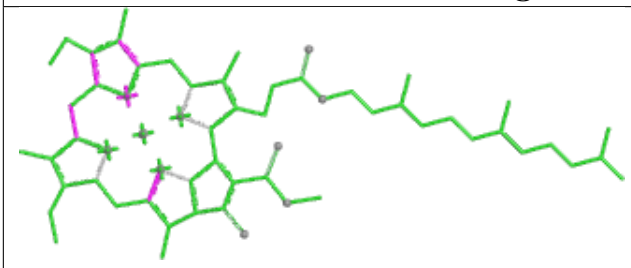


Torsions

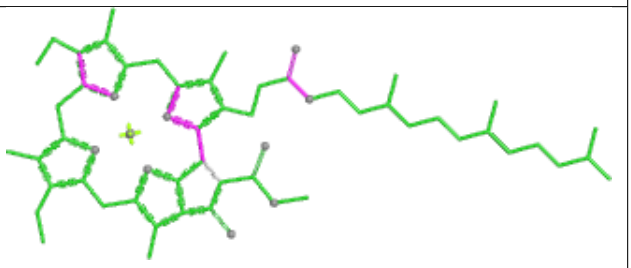


Rings

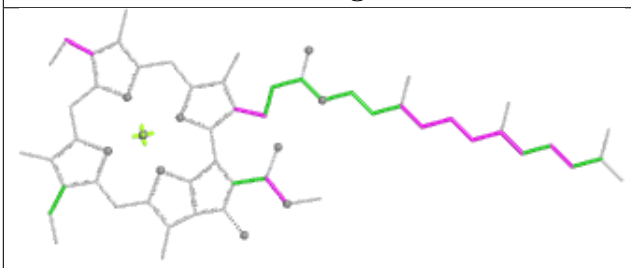
Ligand CLA H 1139



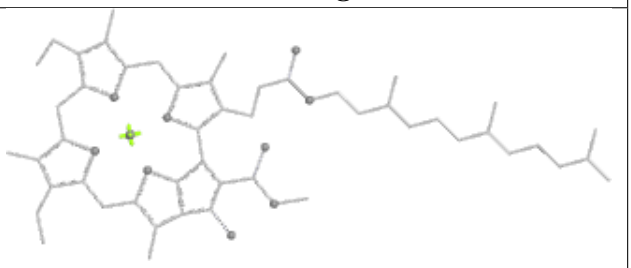
Bond lengths



Bond angles

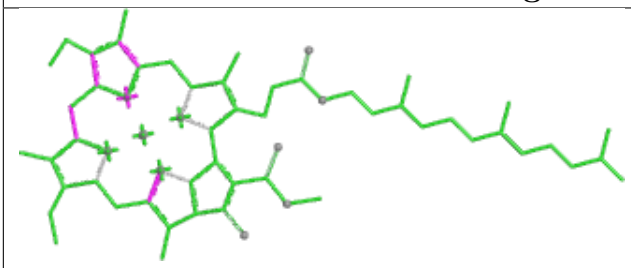


Torsions

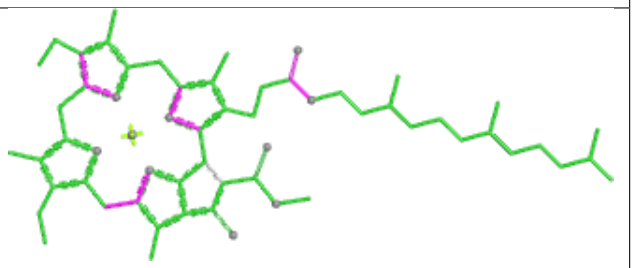


Rings

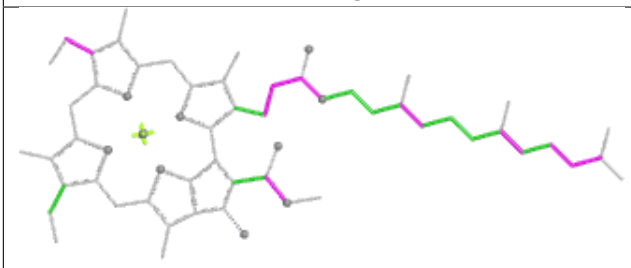
Ligand CLA l 1501



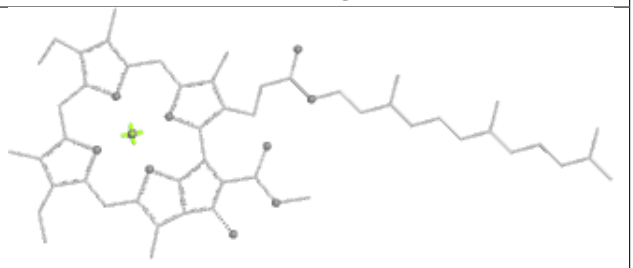
Bond lengths



Bond angles

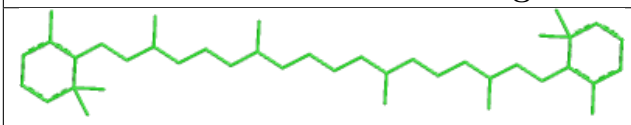


Torsions

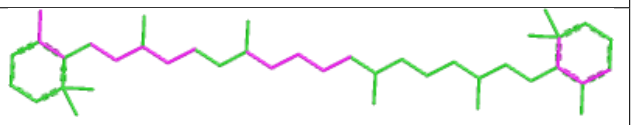


Rings

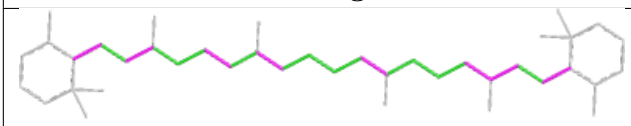
Ligand BCR R 4018



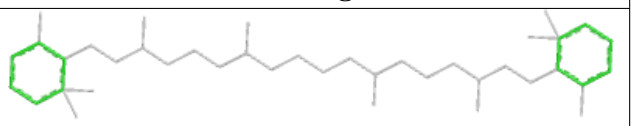
Bond lengths



Bond angles



Torsions

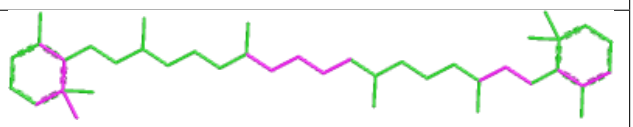


Rings

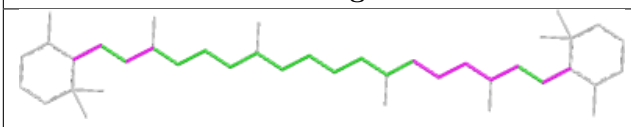
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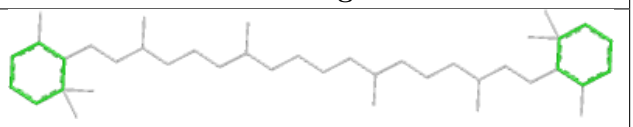
Bond lengths



Bond angles

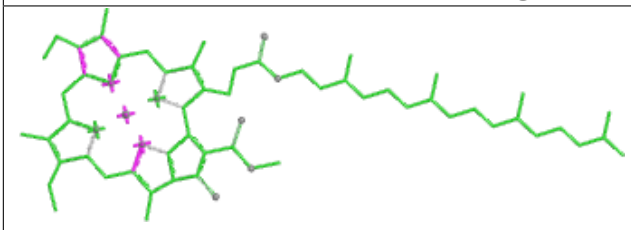


Torsions

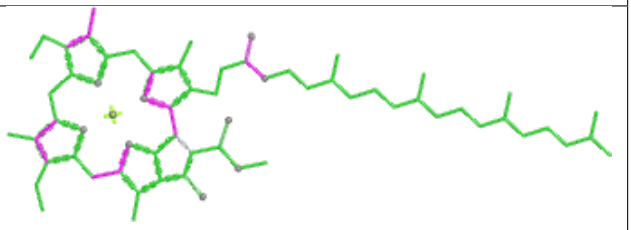


Rings

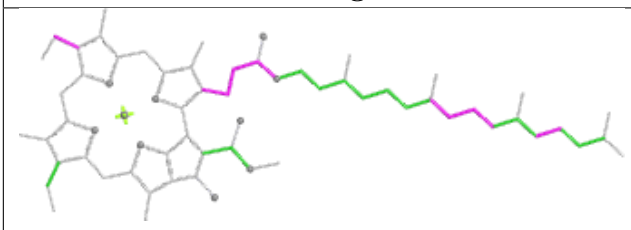
Ligand CLA H 1237



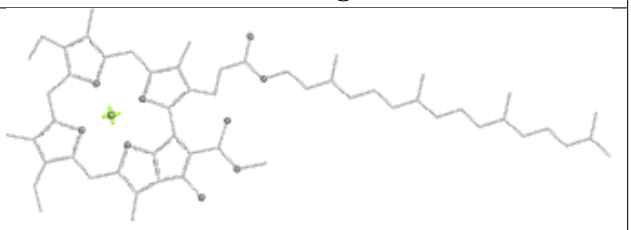
Bond lengths



Bond angles

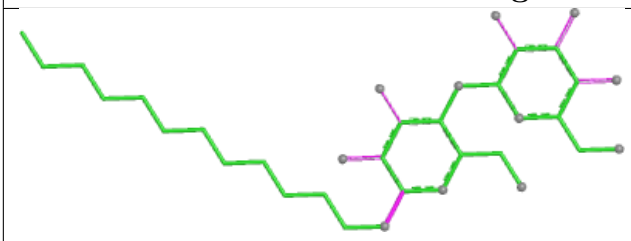


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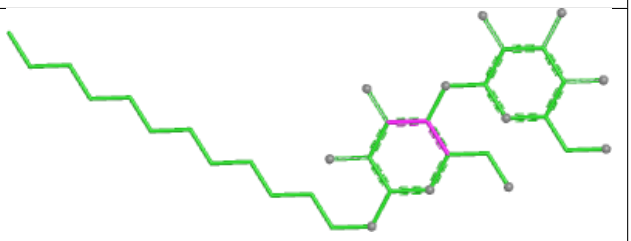


Rings

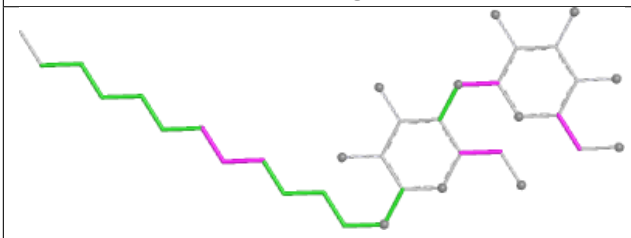
Ligand LMT U 4101



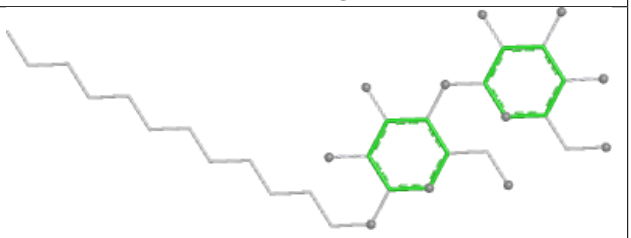
Bond lengths



Bond angles



Torsions

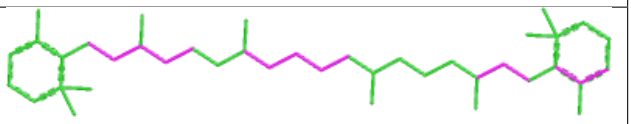


Rings

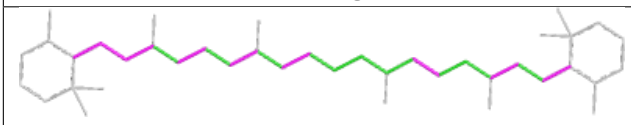
Ligand BCR x 604



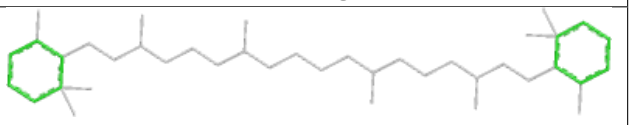
Bond lengths



Bond angles

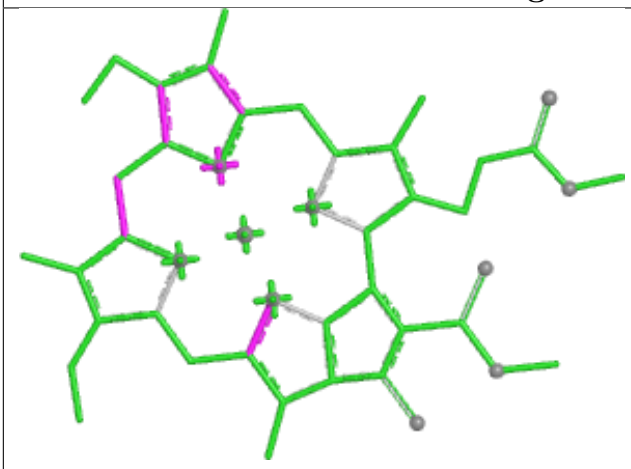


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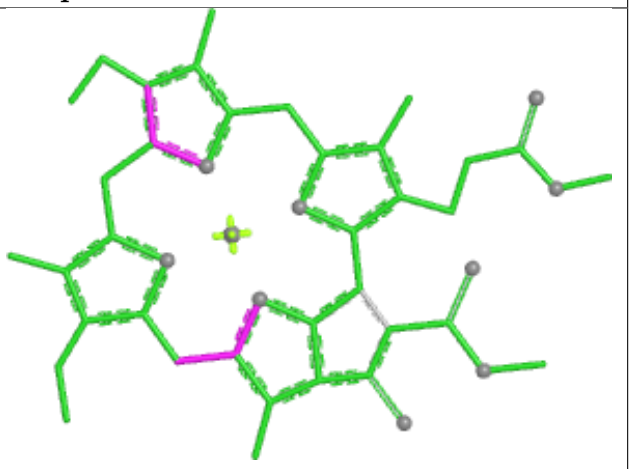


Rings

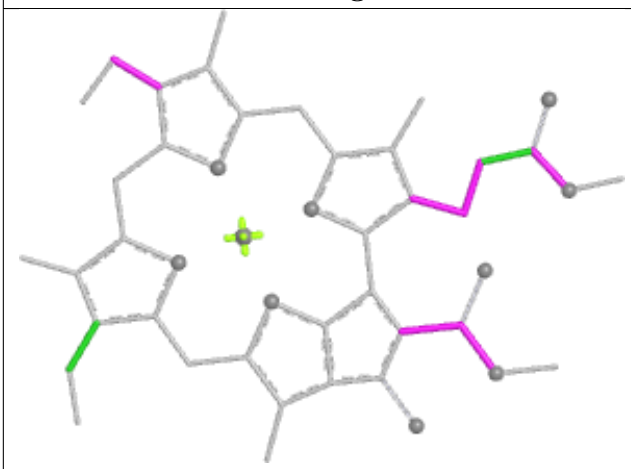
Ligand CLA q 516



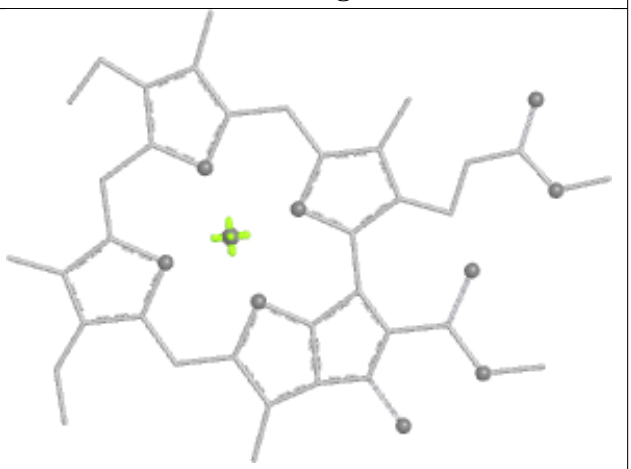
Bond lengths



Bond angles

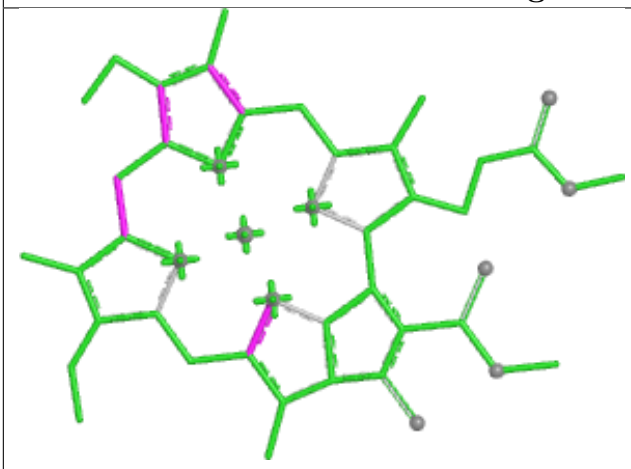


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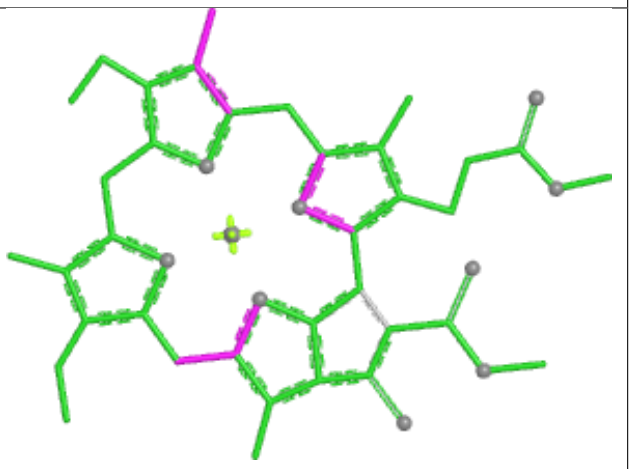


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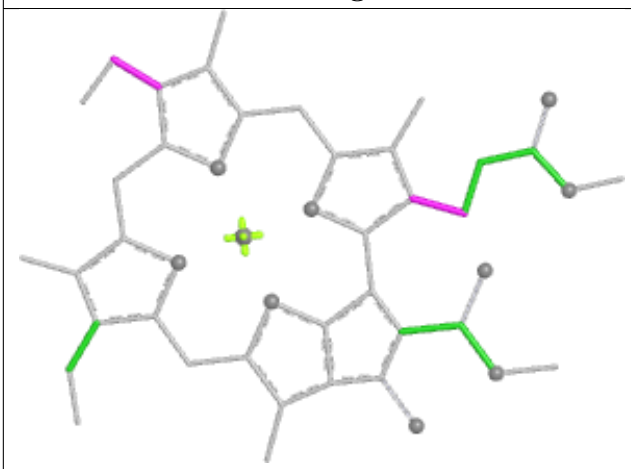
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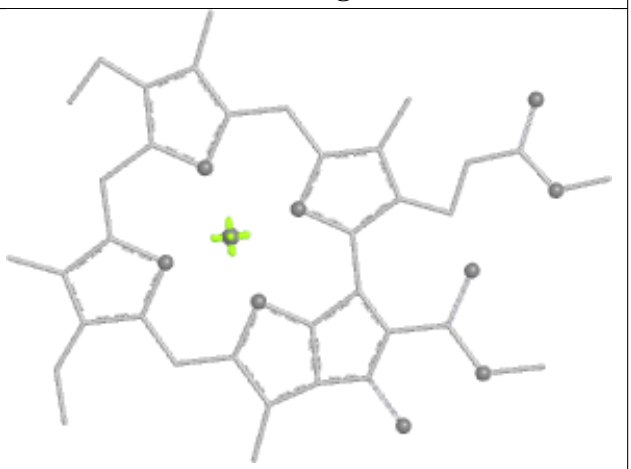
Bond lengths



Bond angles

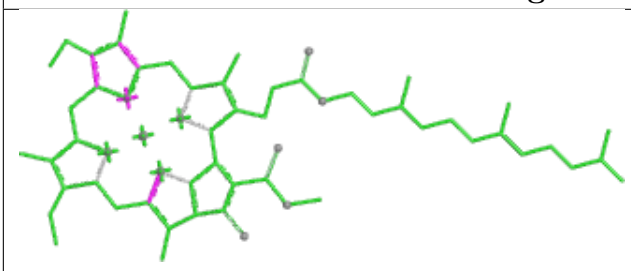


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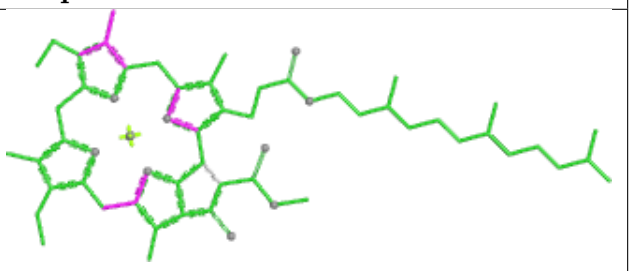


Rings

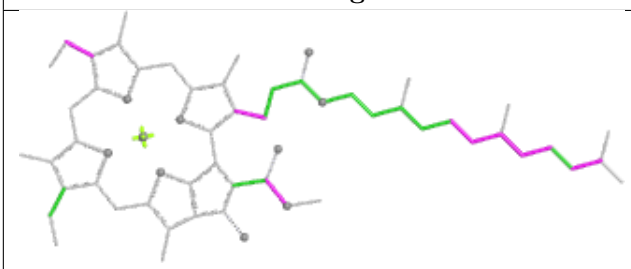
Ligand CLA q 506



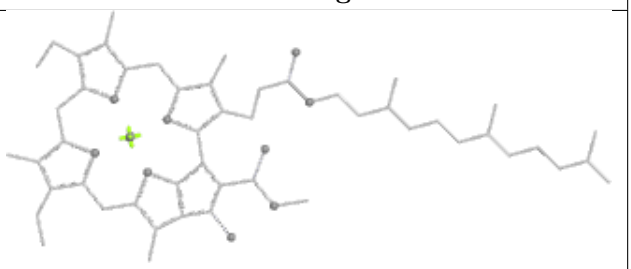
Bond lengths



Bond angles

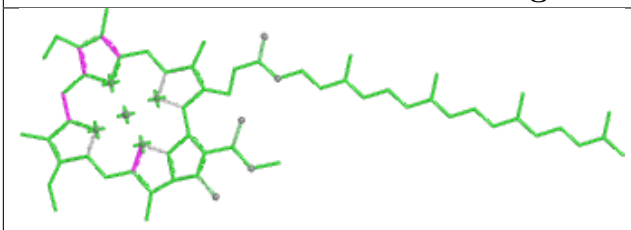


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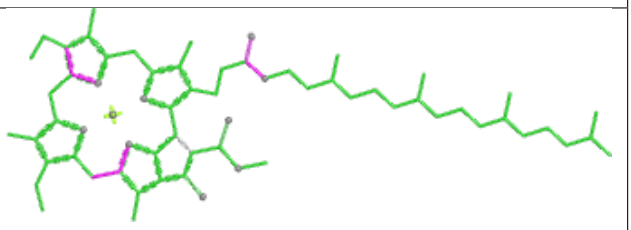


Rings

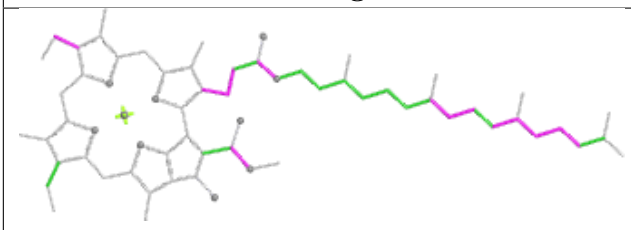
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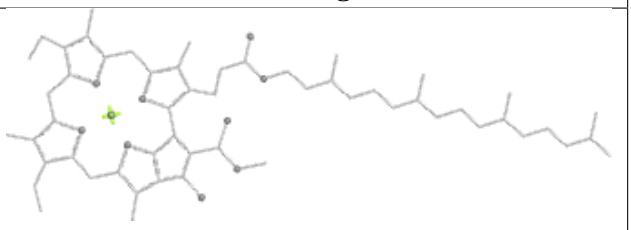
Bond lengths



Bond angles

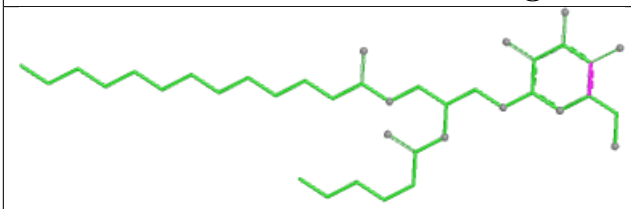


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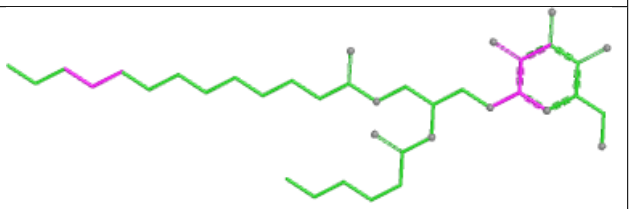


Rings

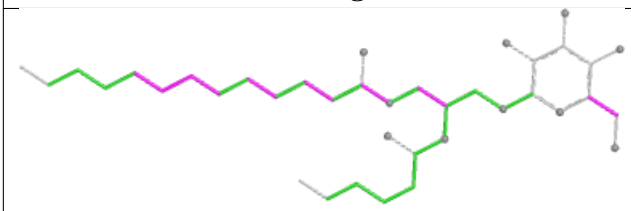
Ligand LMG a 852



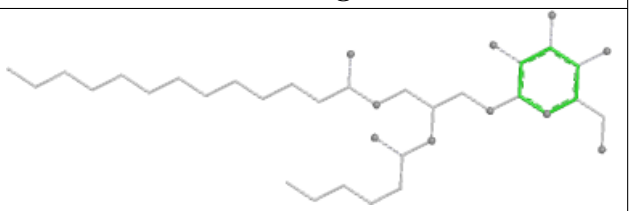
Bond lengths



Bond angles

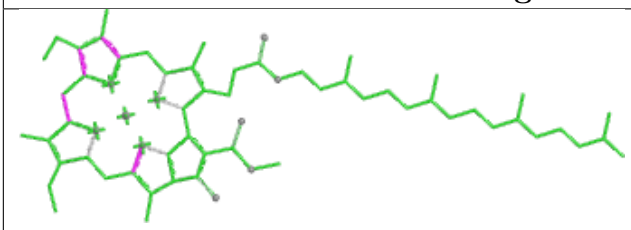


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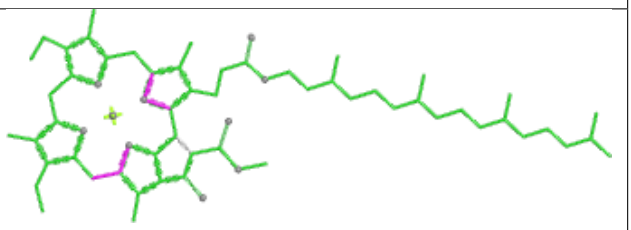


Rings

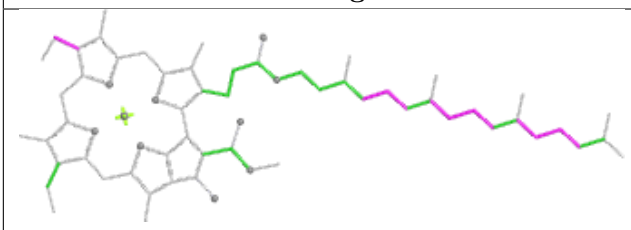
Ligand CLA H 1125



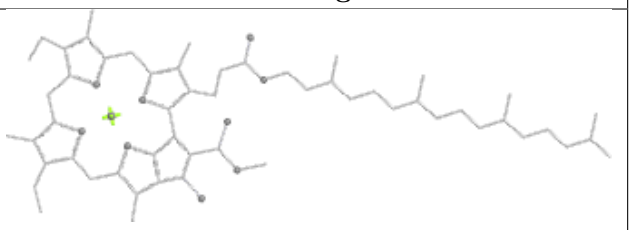
Bond lengths



Bond angles

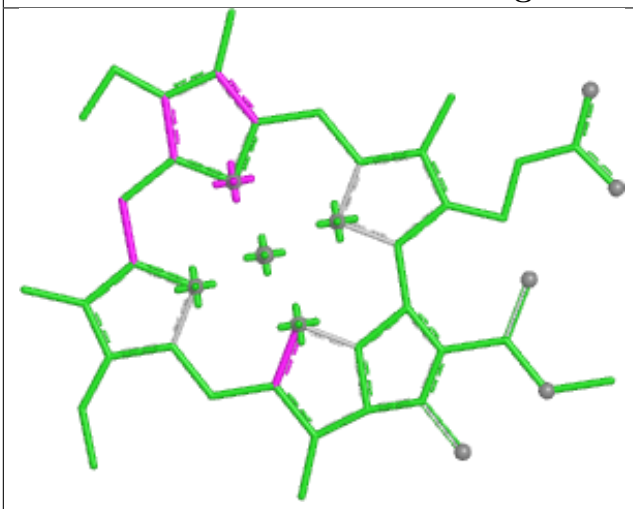


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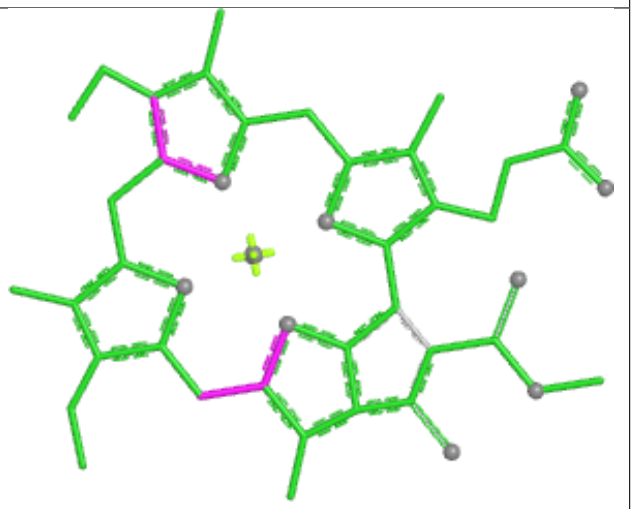


Rings

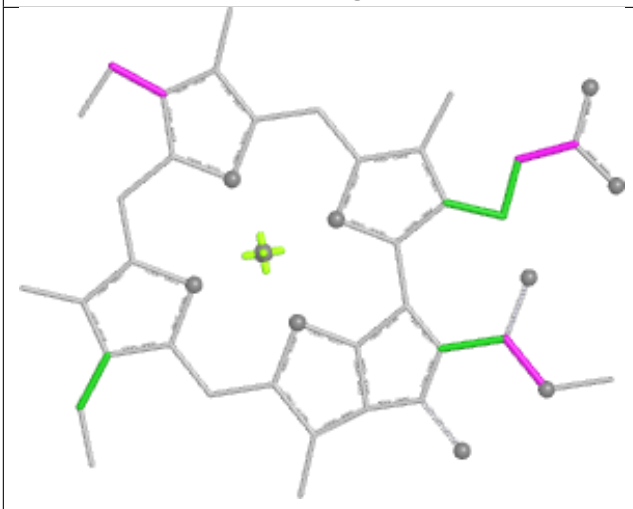
Ligand CLA A 1134



Bond lengths



Bond angles

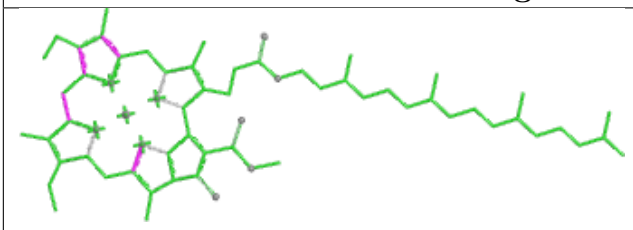


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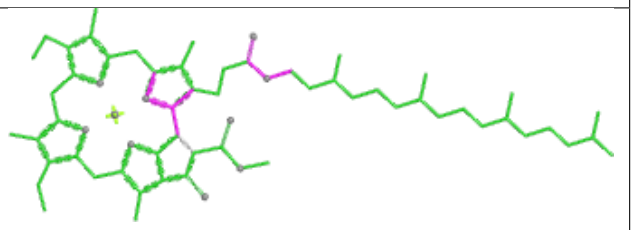


Rings

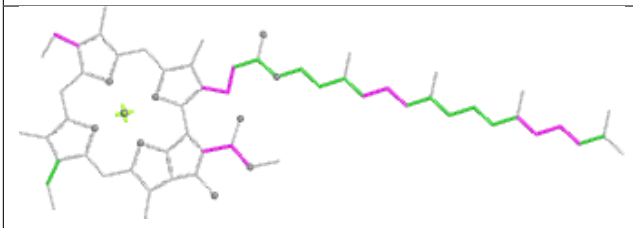
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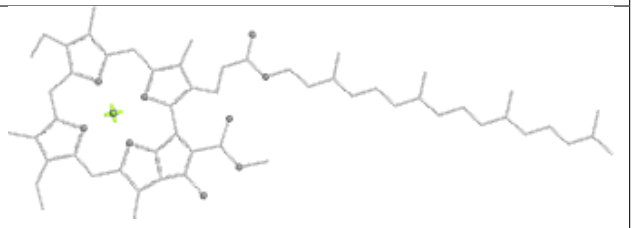
Bond lengths



Bond angles

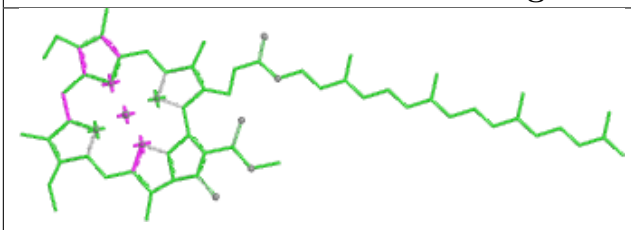


Torsions

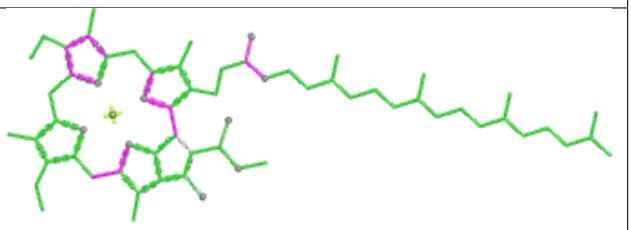


Rings

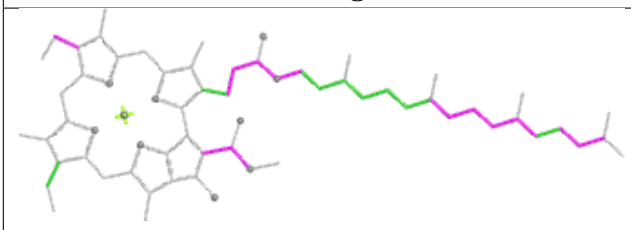
Ligand CLA n 505



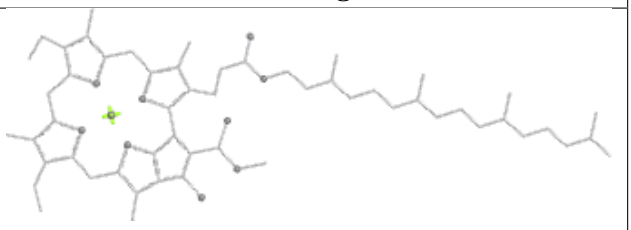
Bond lengths



Bond angles

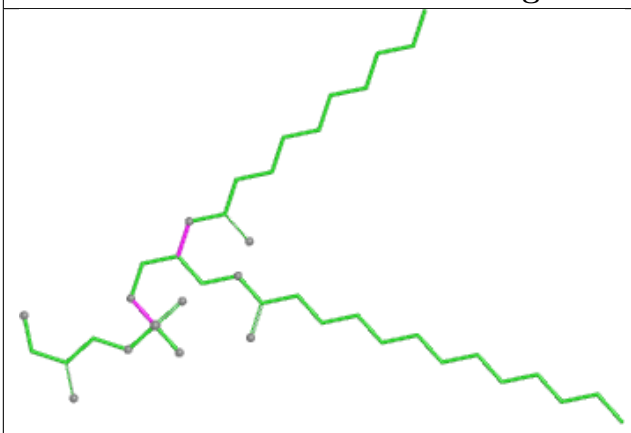


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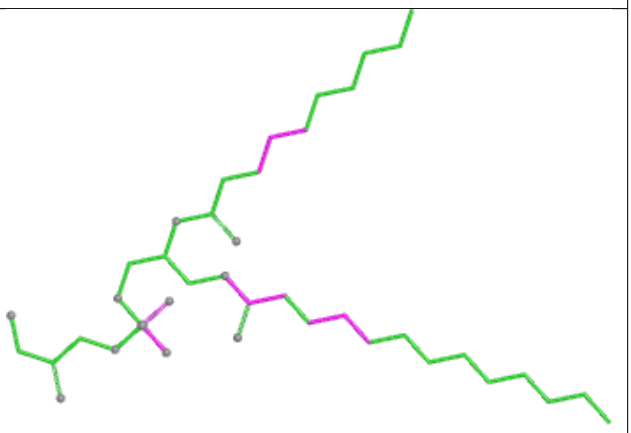


Rings

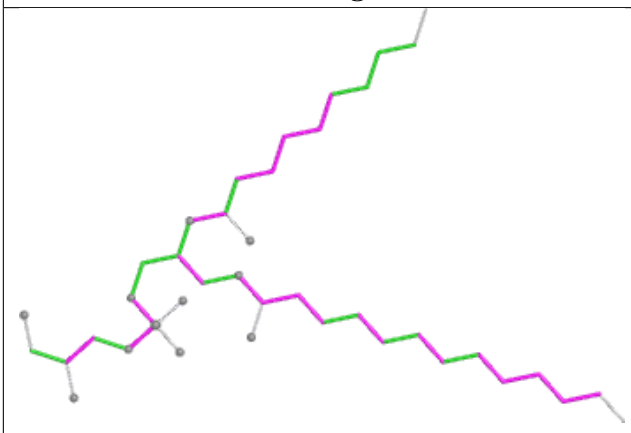
Ligand LHG R 103



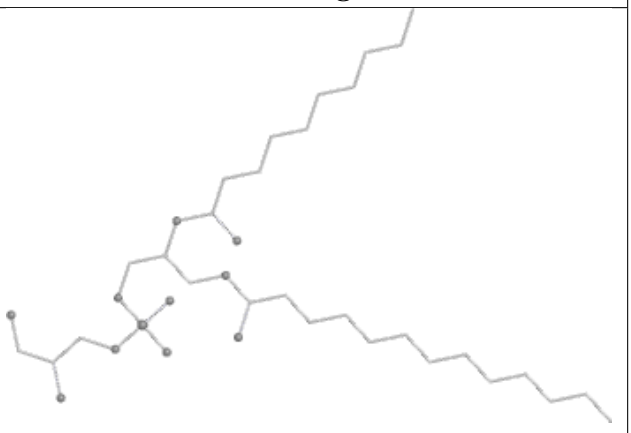
Bond lengths



Bond angles

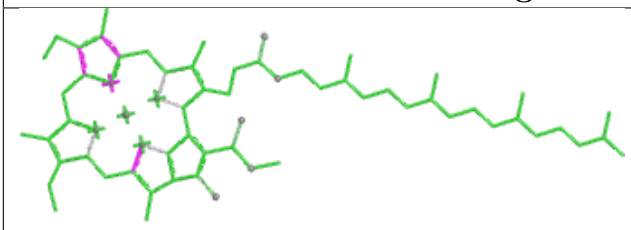


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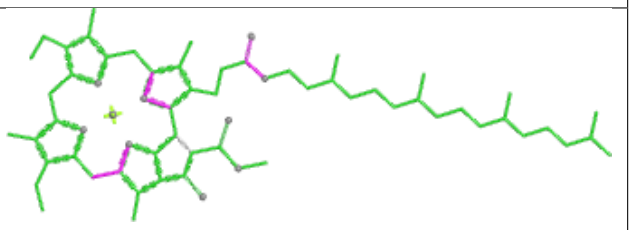


Rings

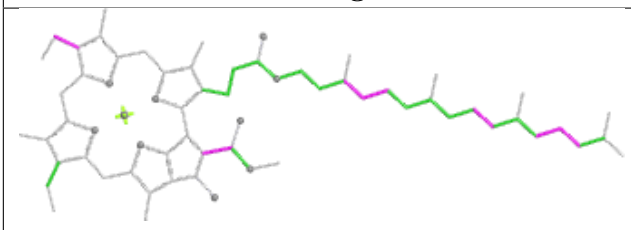
Ligand CLA B 1205



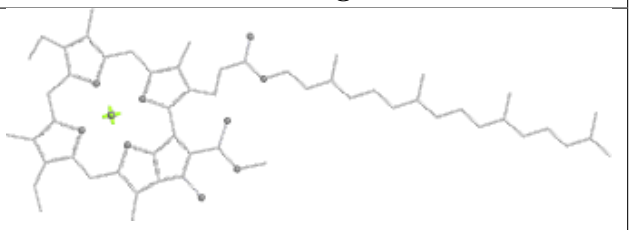
Bond lengths



Bond angles

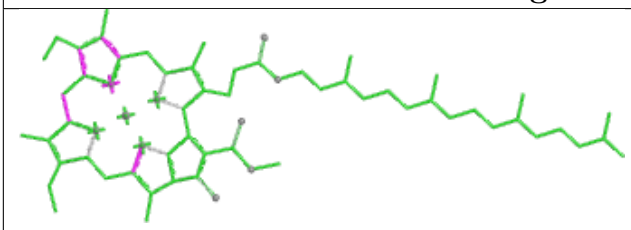


Torsions

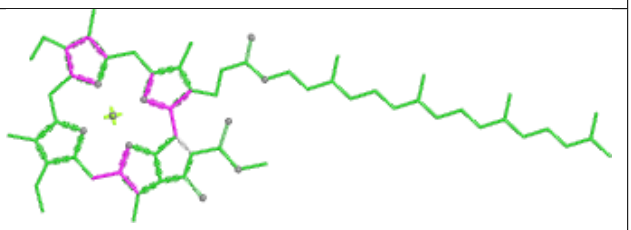


Rings

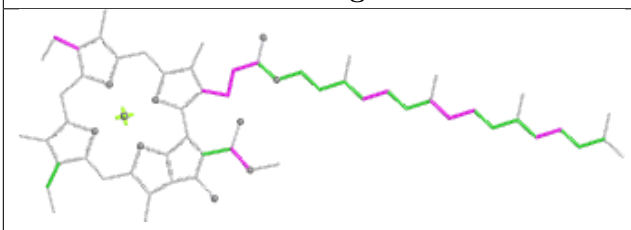
Ligand CLA s 505



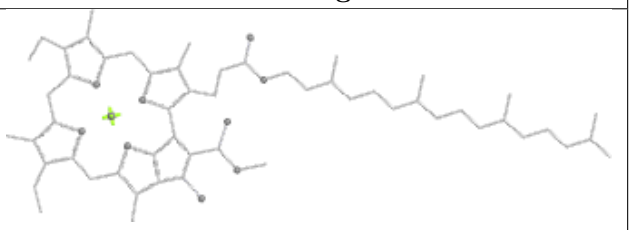
Bond lengths



Bond angles

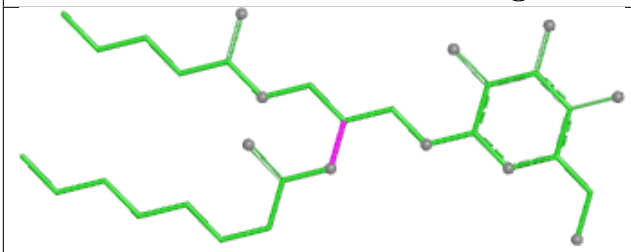


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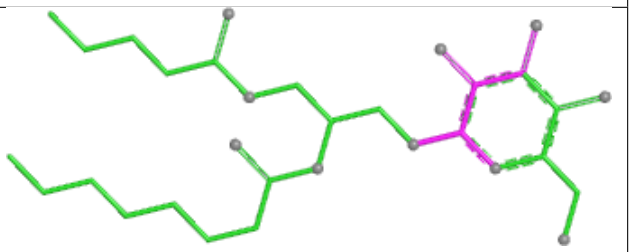


Rings

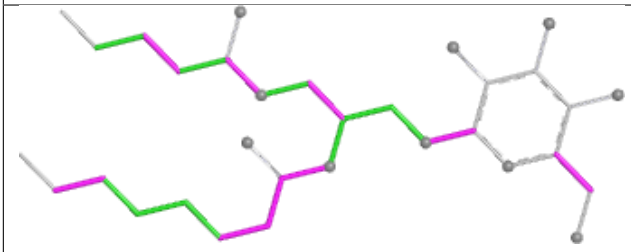
Ligand LMG A 4201



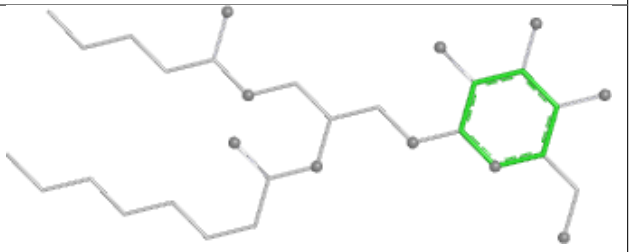
Bond lengths



Bond angles

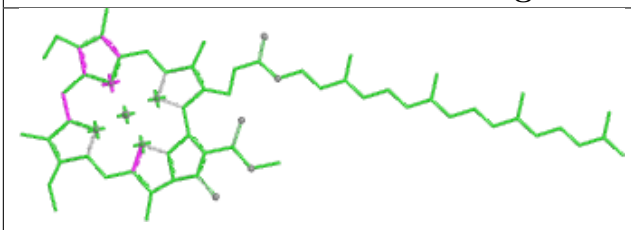


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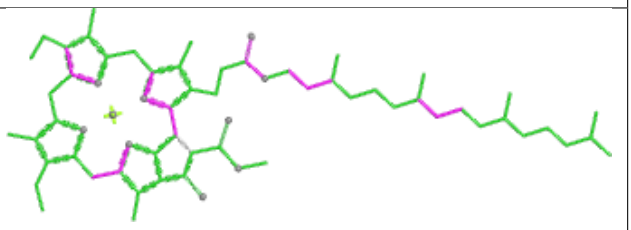


Rings

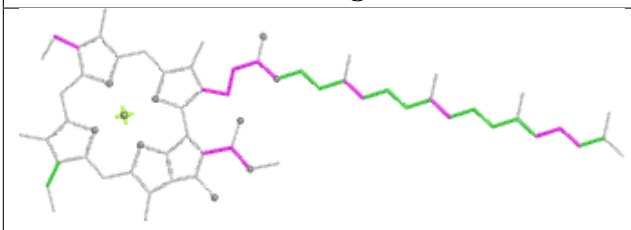
Ligand CLA A 1101



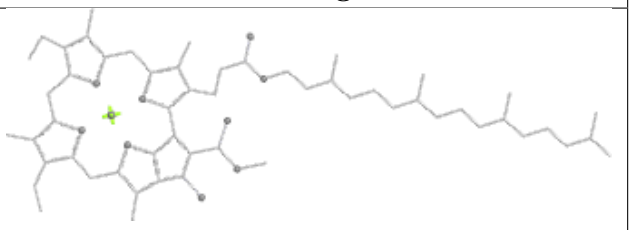
Bond lengths



Bond angles

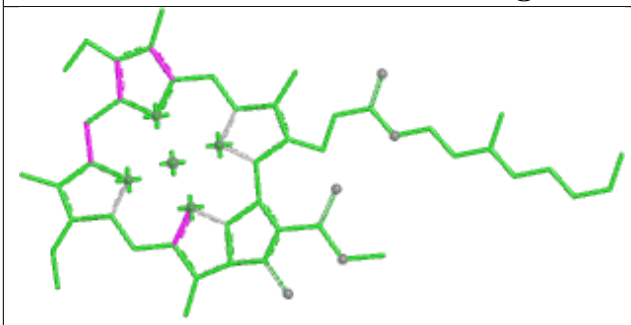


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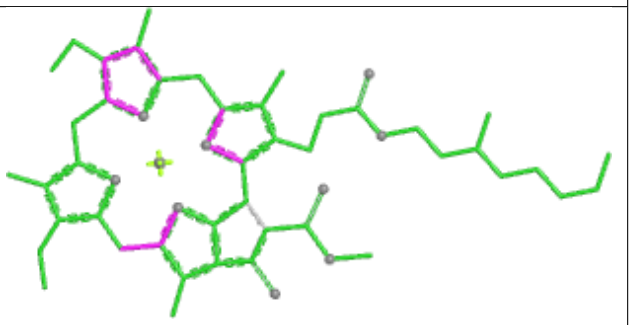


Rings

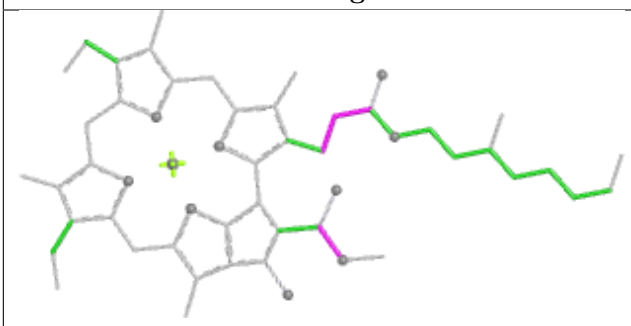
Ligand CLA B 1201



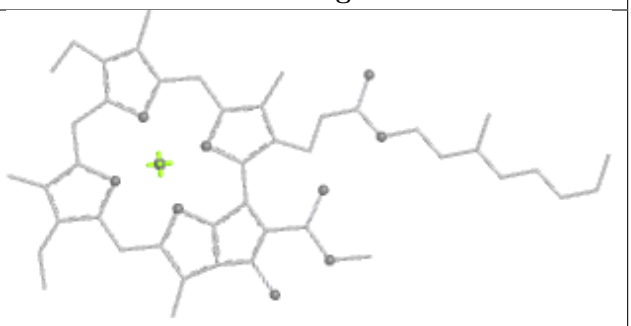
Bond lengths



Bond angles

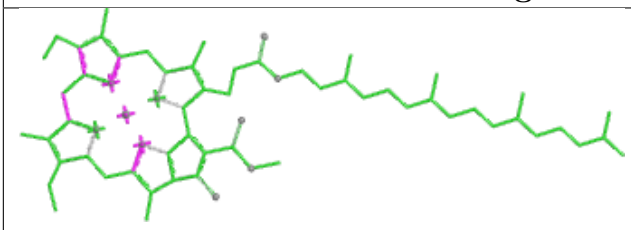


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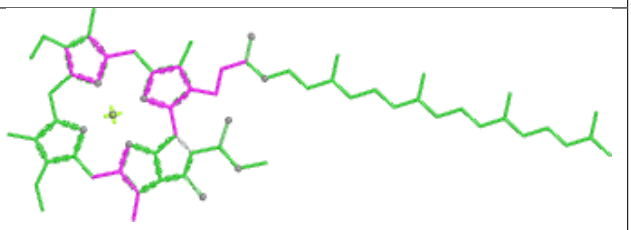


Rings

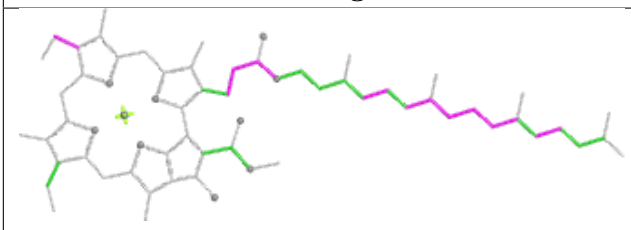
Ligand CLA A 1013



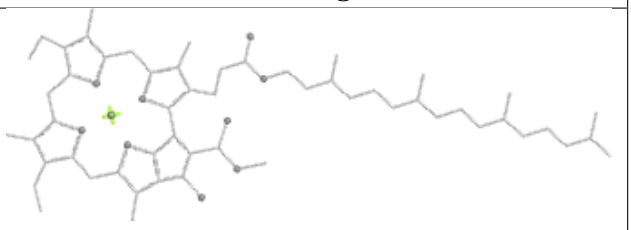
Bond lengths



Bond angles

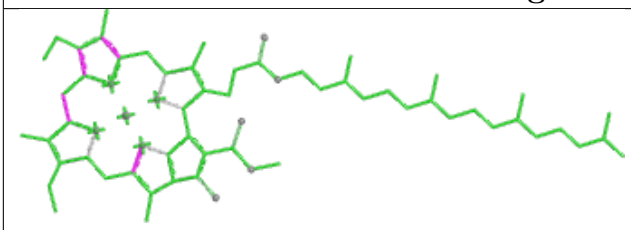


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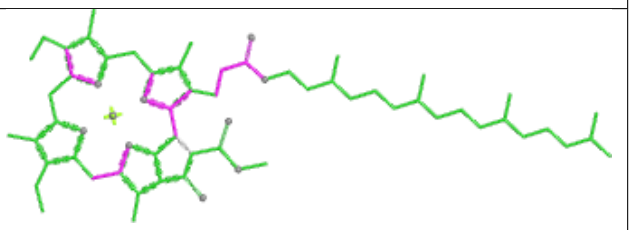


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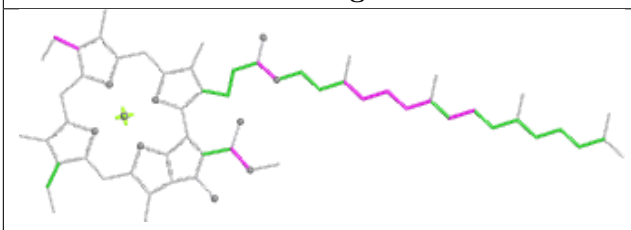
Ligand CLA v 512



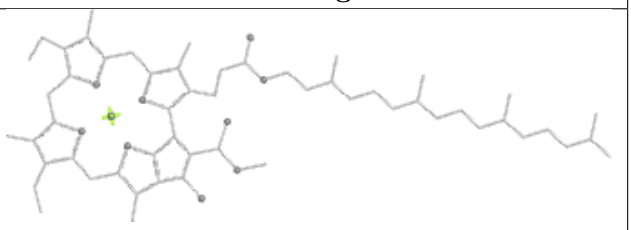
Bond lengths



Bond angles



Torsions

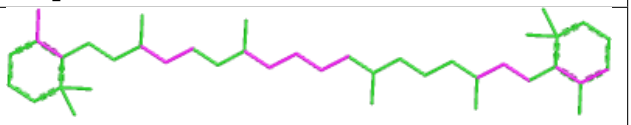


Rings

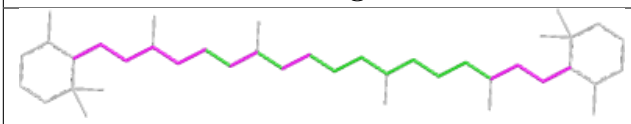
Ligand BCR p 604



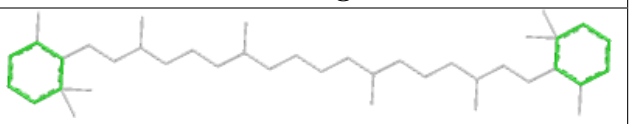
Bond lengths



Bond angles

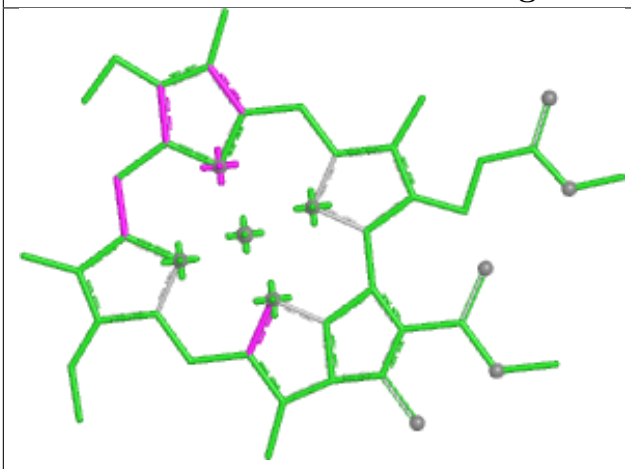


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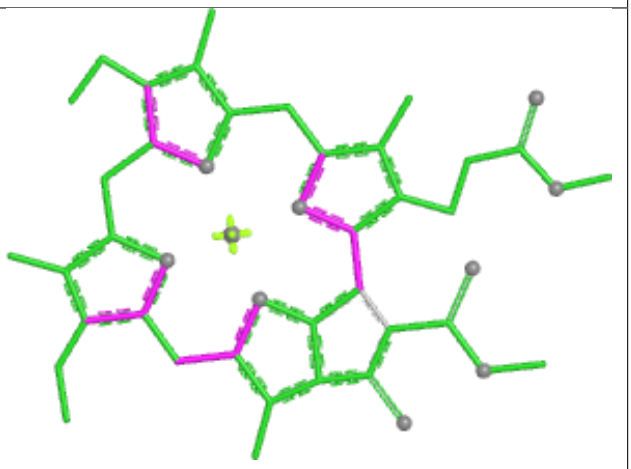


Rings

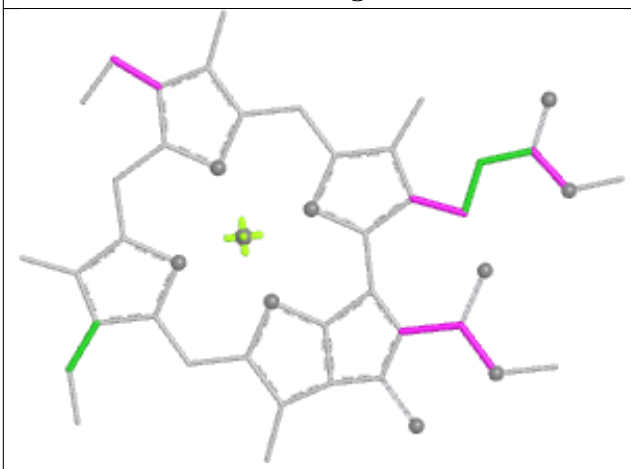
Ligand CLA W 503



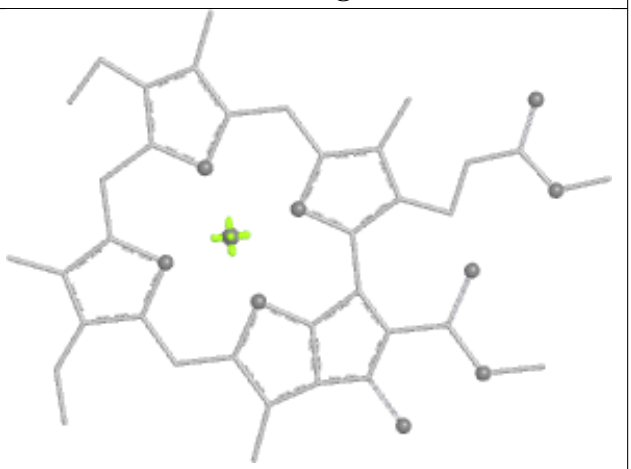
Bond lengths



Bond angles

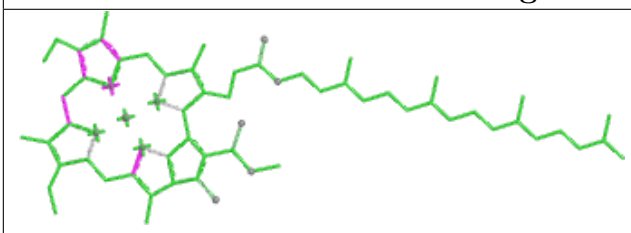


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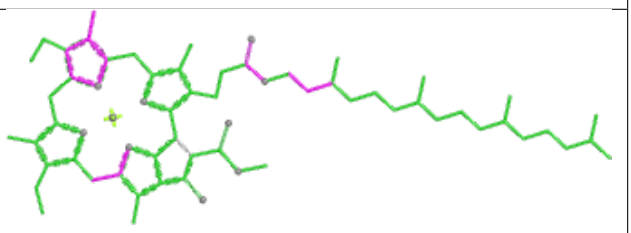


Rings

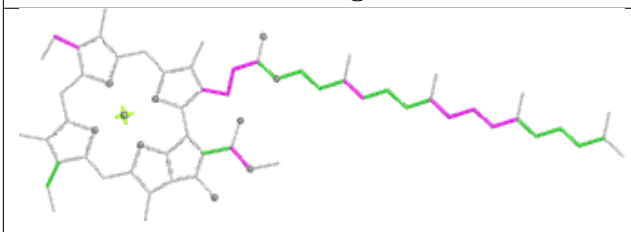
Ligand CLA a 1138



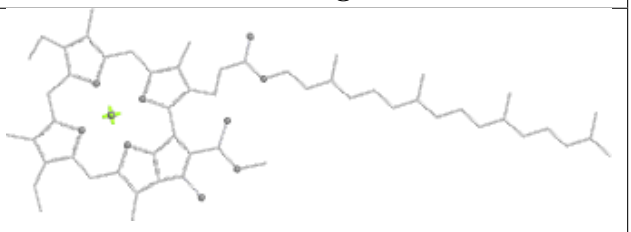
Bond lengths



Bond angles

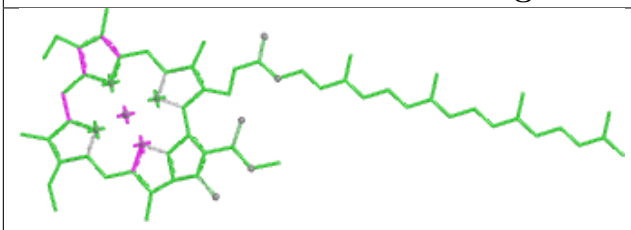


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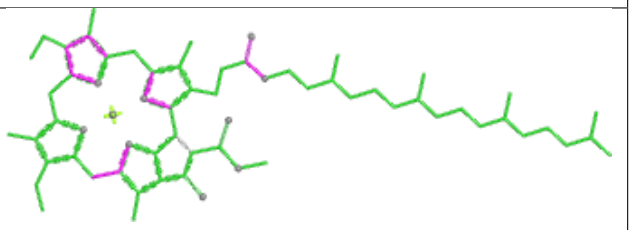


Rings

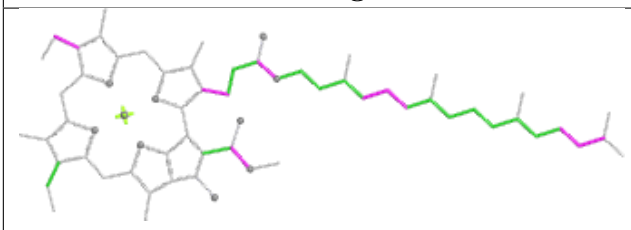
Ligand CLA A 1140



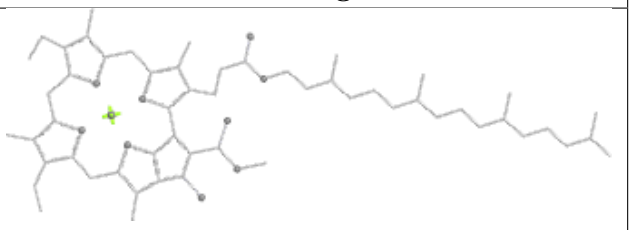
Bond lengths



Bond angles

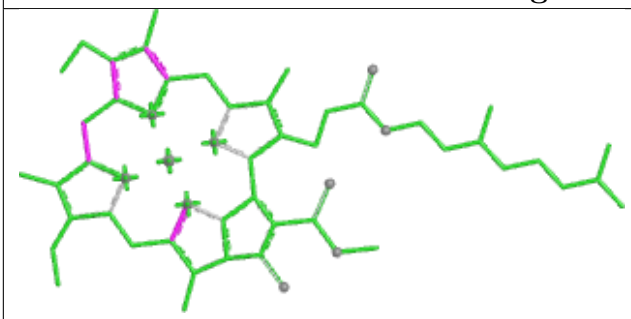


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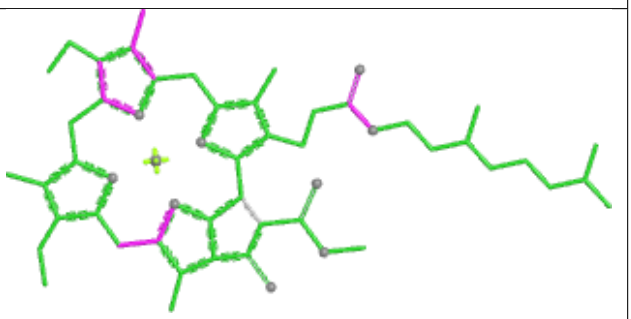


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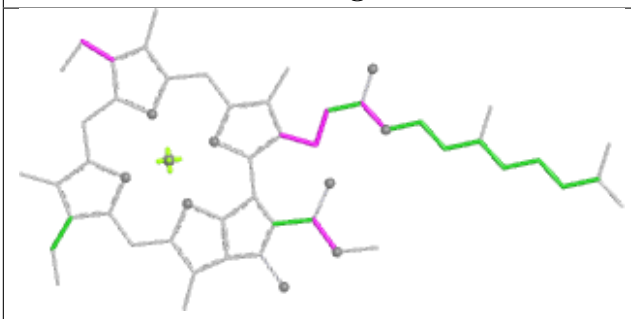
Ligand CLA t 508



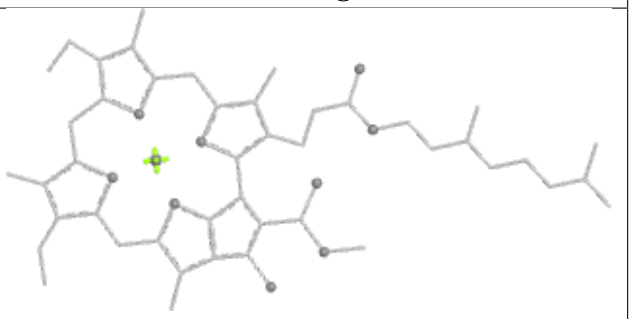
Bond lengths



Bond angles

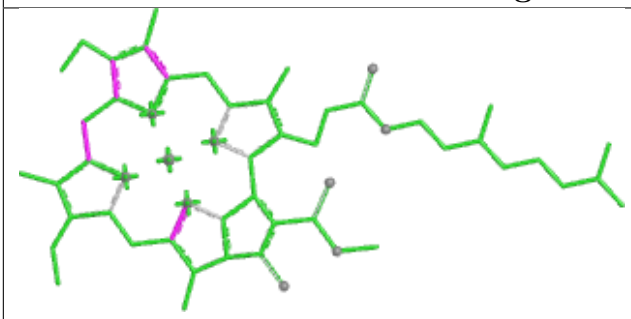


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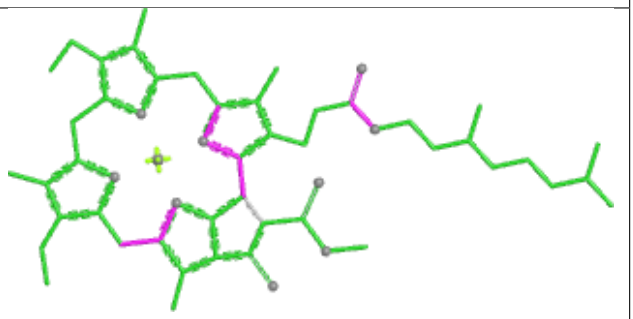


Rings

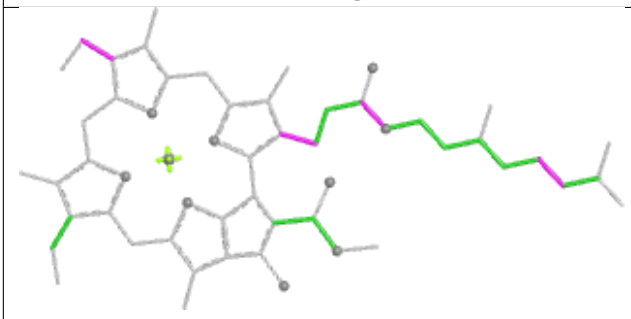
Ligand CLA K 4004



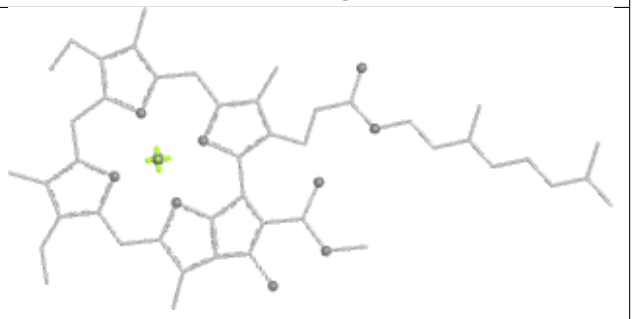
Bond lengths



Bond angles

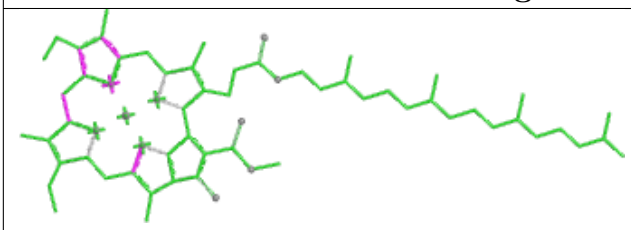


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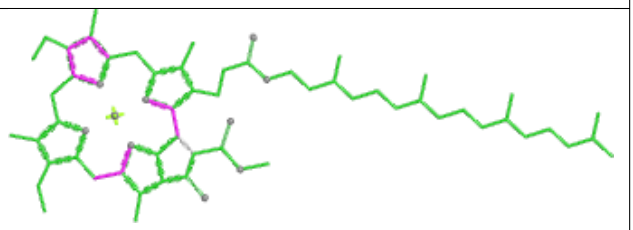


Rings

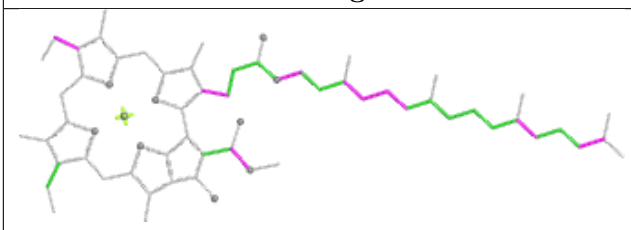
Ligand CLA H 1119



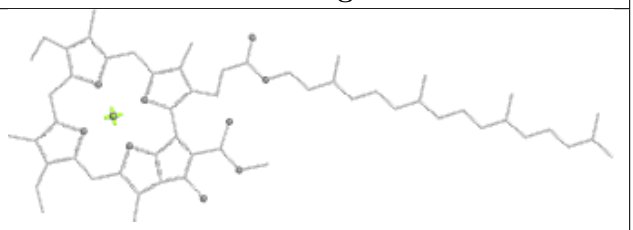
Bond lengths



Bond angles

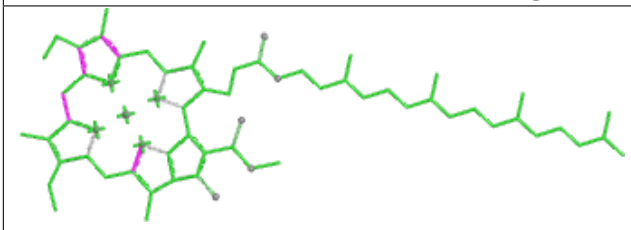


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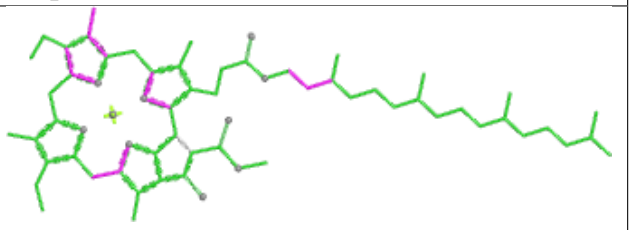


Rings

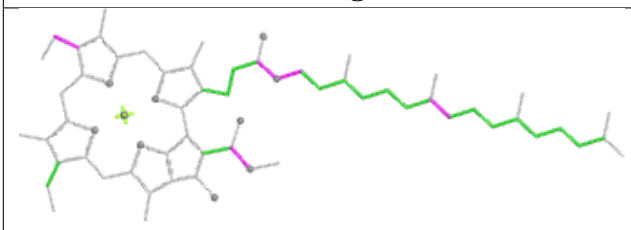
Ligand CLA p 507



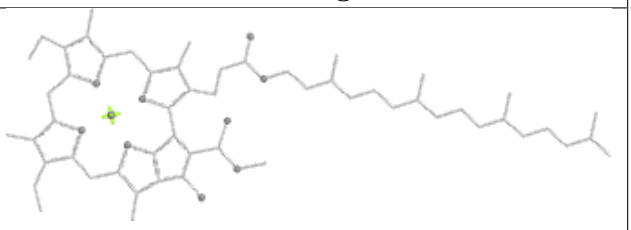
Bond lengths



Bond angles

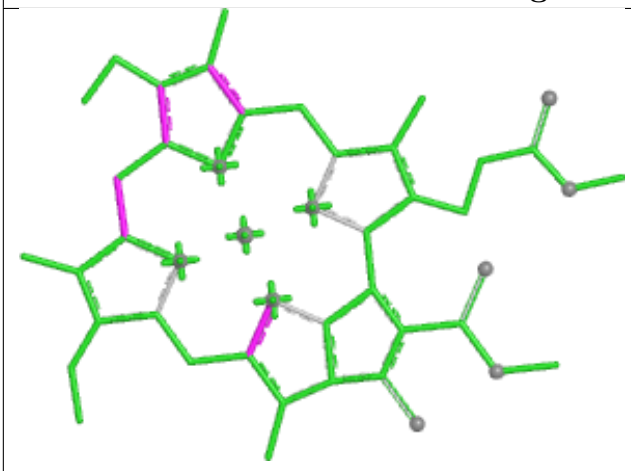


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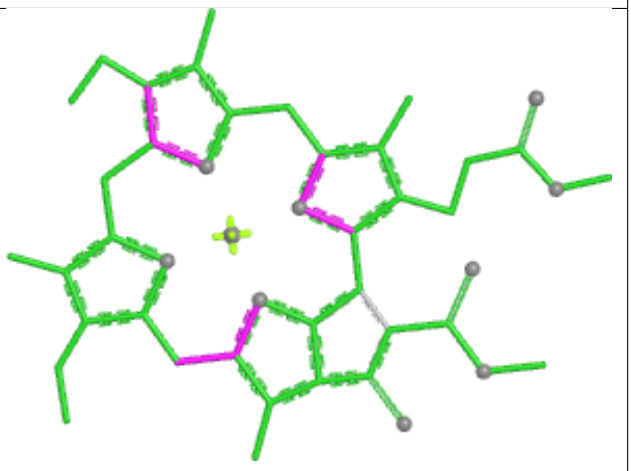


Rings

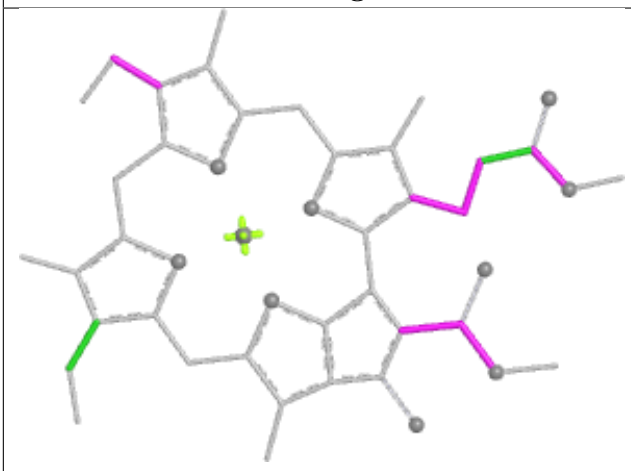
Ligand CLA s 516



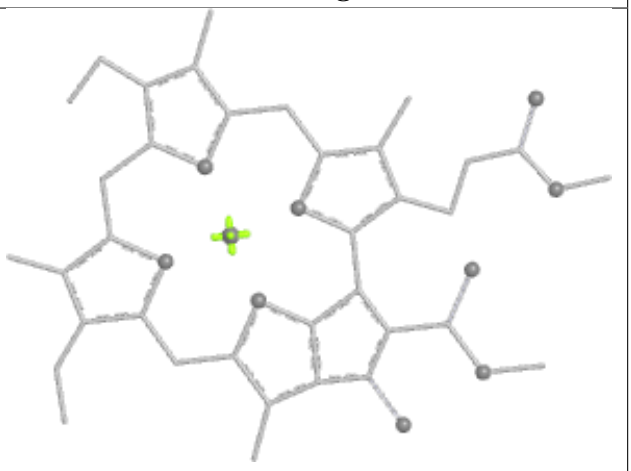
Bond lengths



Bond angles

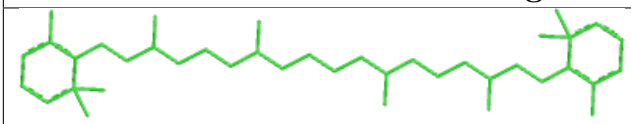


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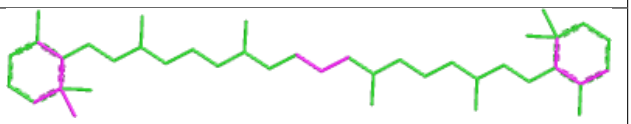


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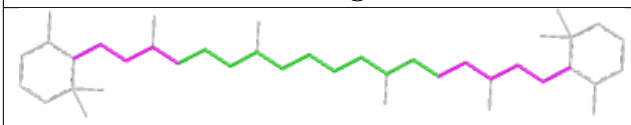
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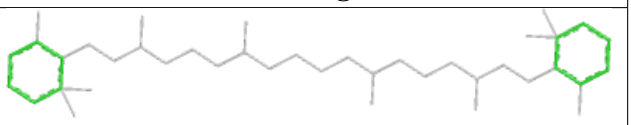
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Bond angles

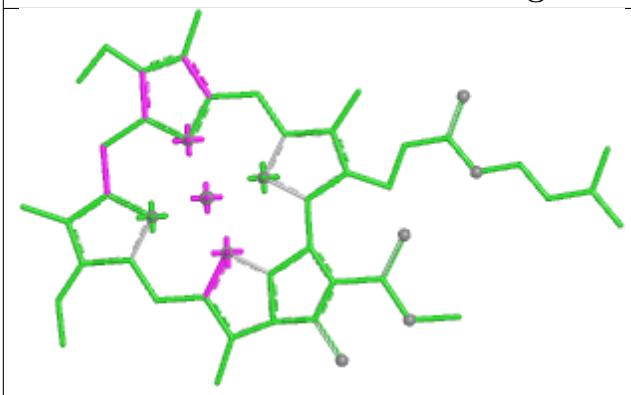


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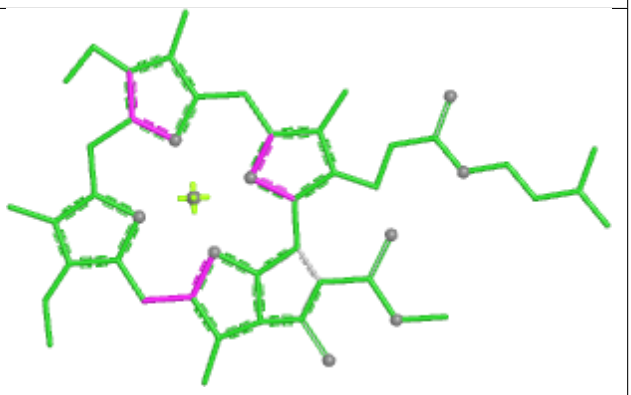


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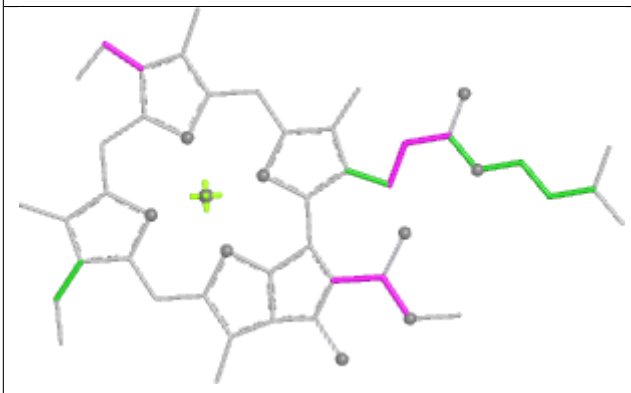
Ligand CLA u 502



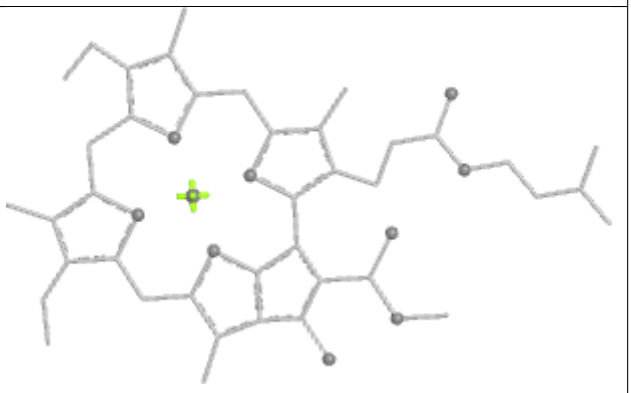
Bond lengths



Bond angles

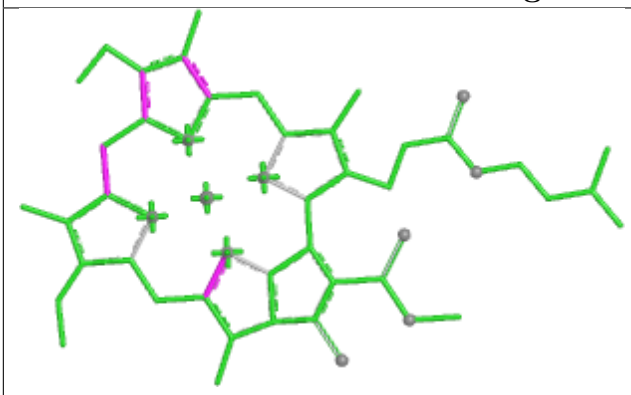


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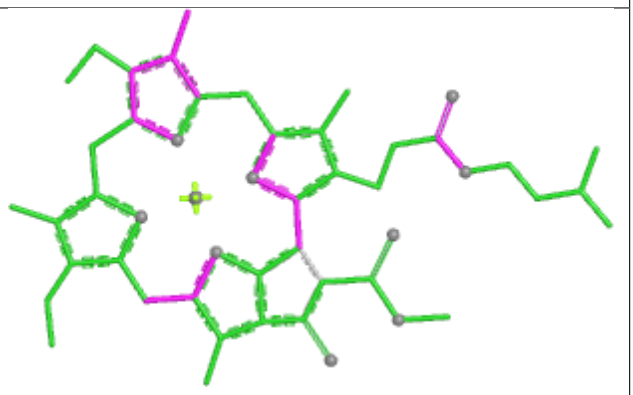


Rings

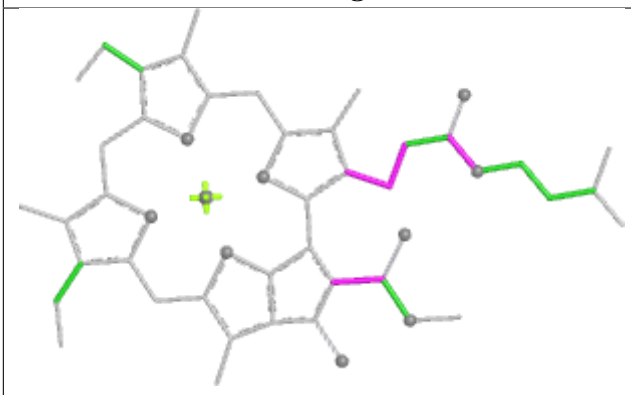
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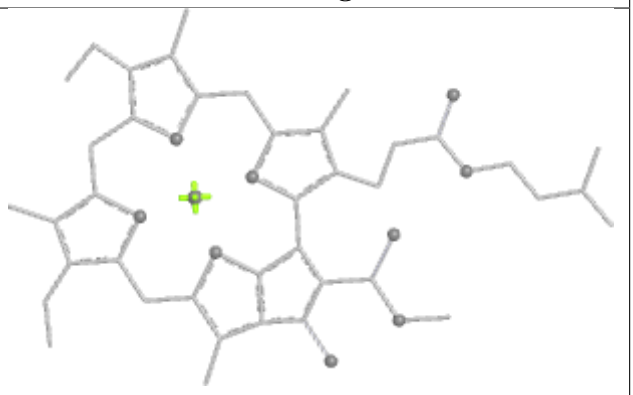
Bond lengths



Bond angles

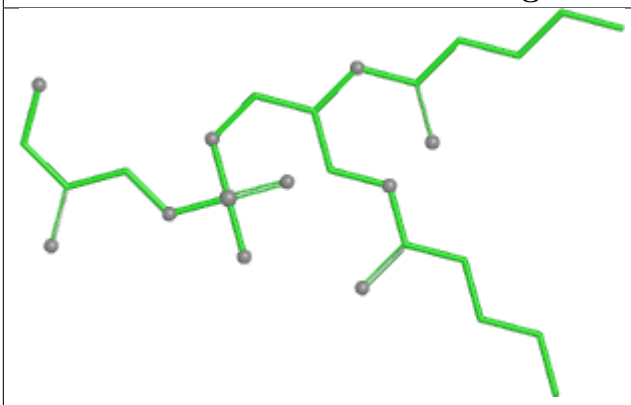


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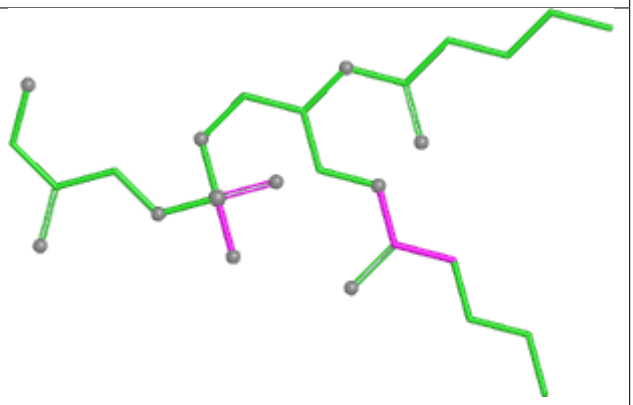


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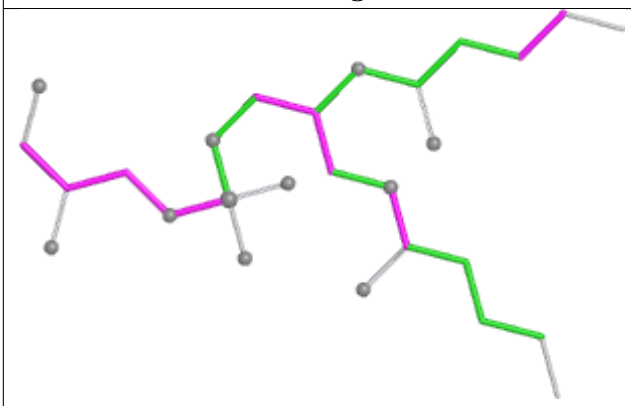
Ligand LHG X 605



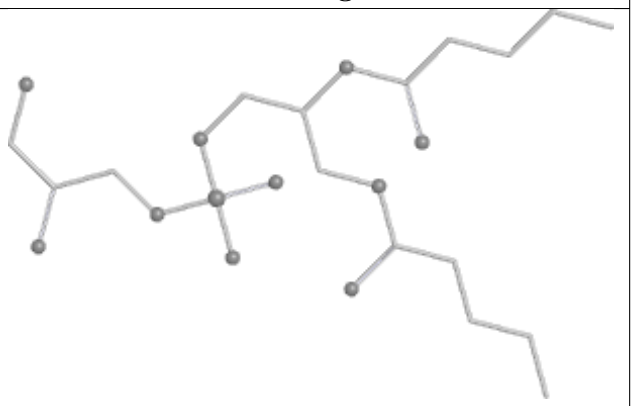
Bond lengths



Bond angles

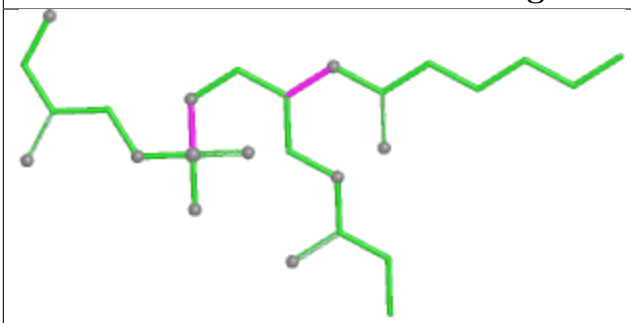


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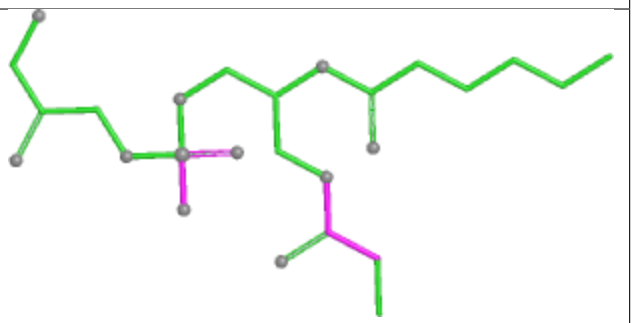


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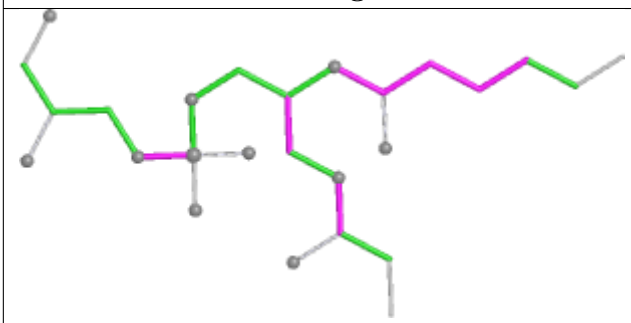
Ligand LHG a 851



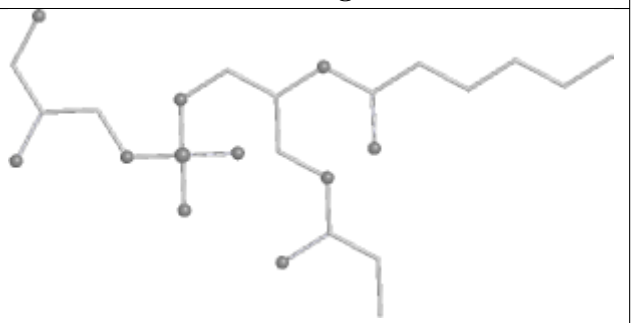
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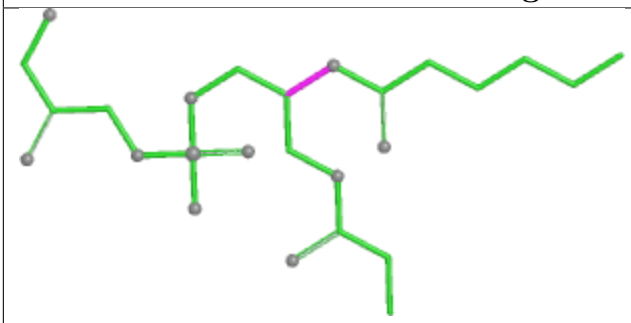


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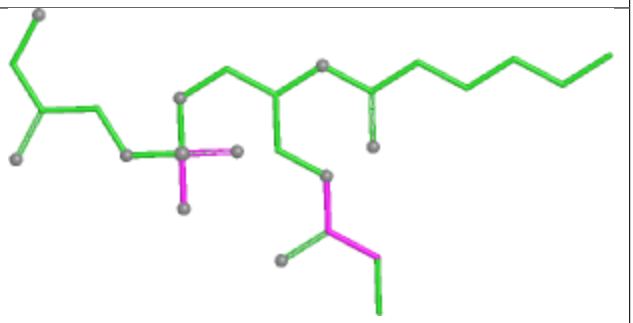


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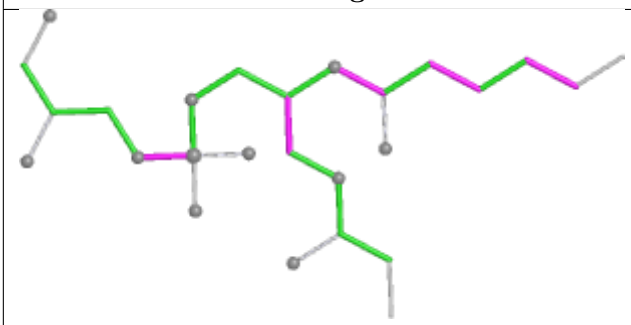
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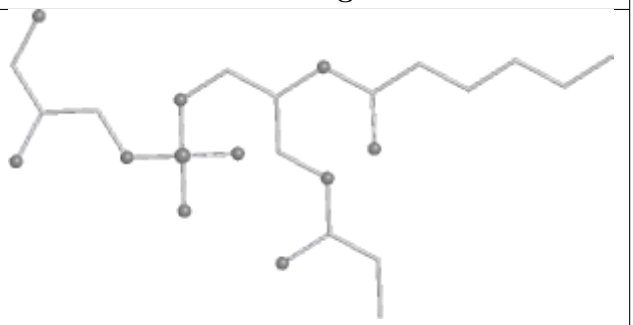
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Bond angles

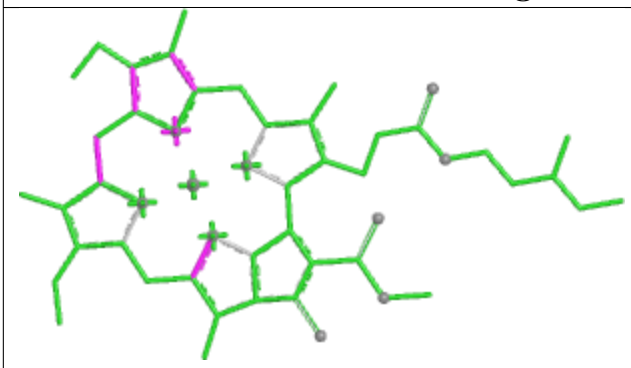


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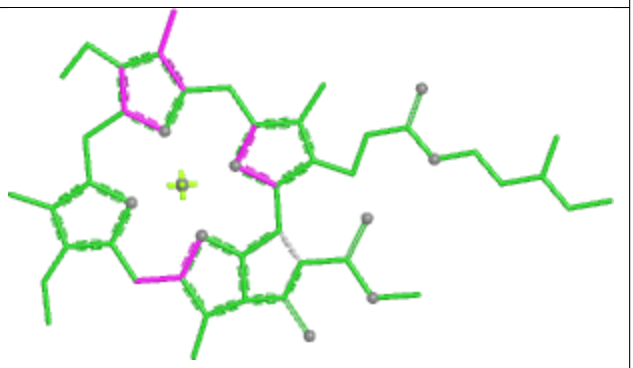


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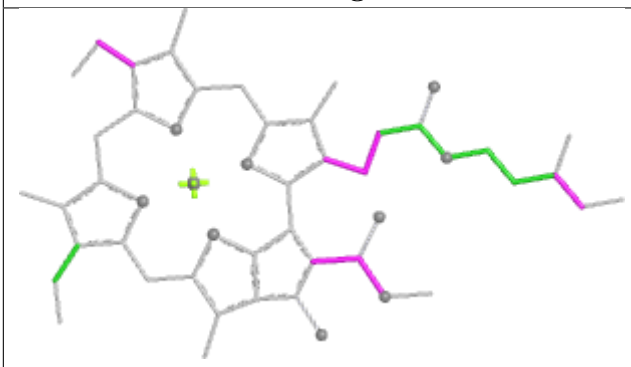
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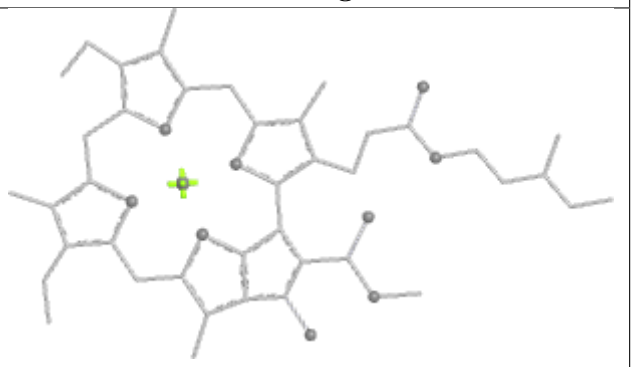
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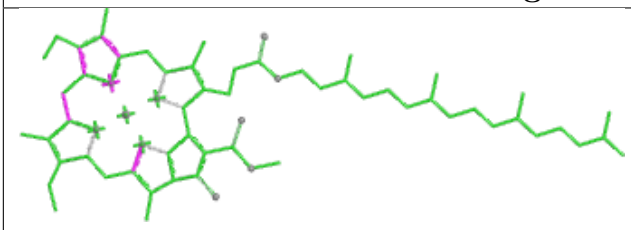


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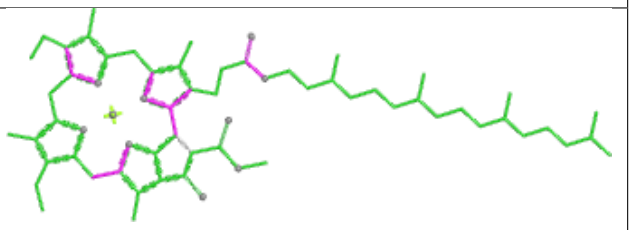


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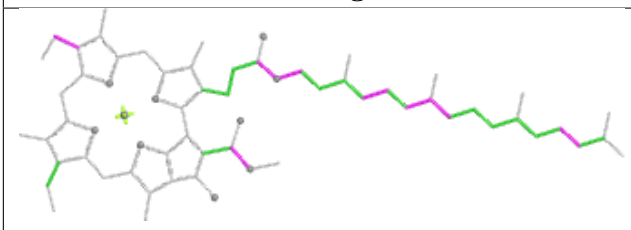
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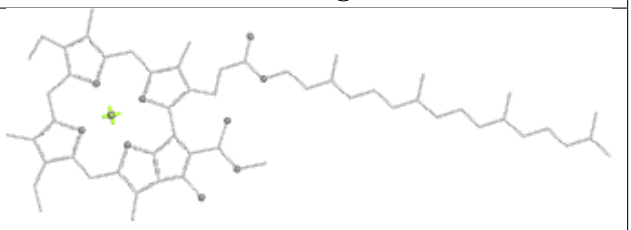
Bond lengths



Bond angles

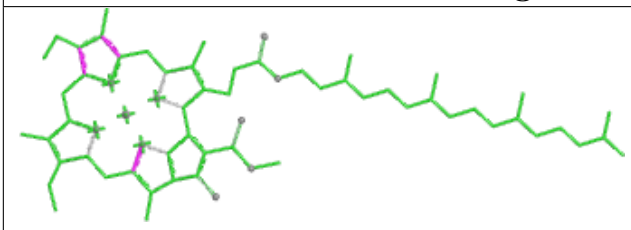


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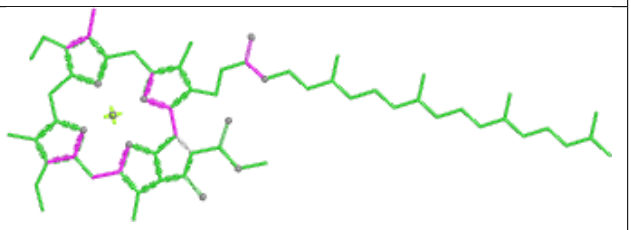


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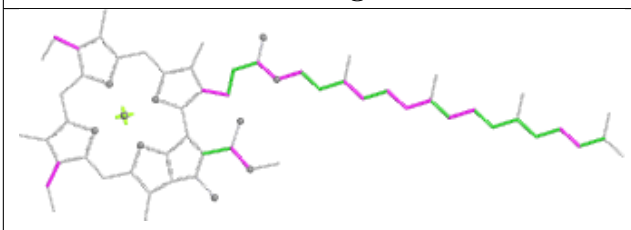
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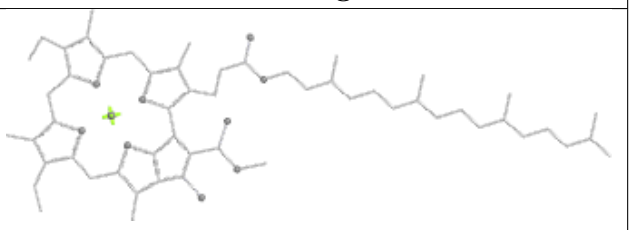
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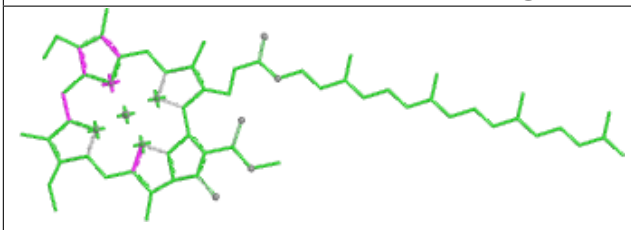


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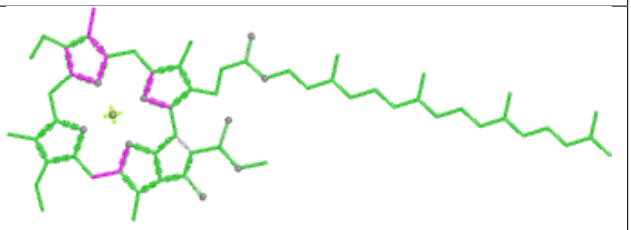


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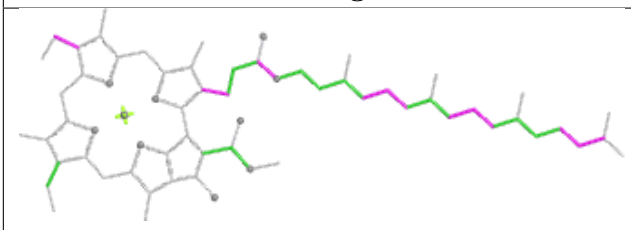
Ligand CLA a 1140



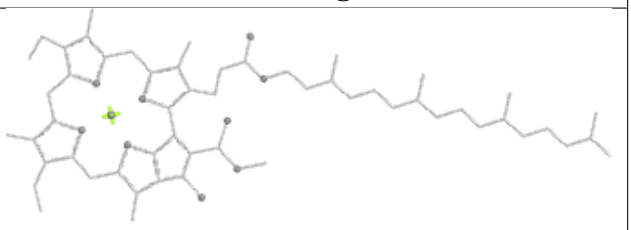
Bond lengths



Bond angles

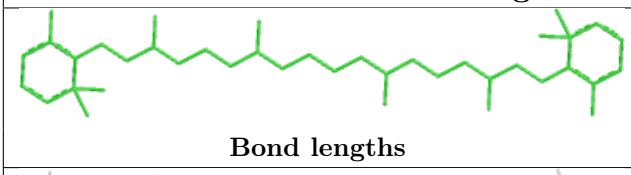


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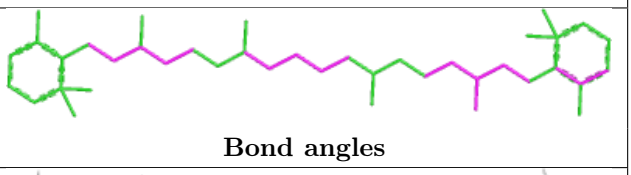


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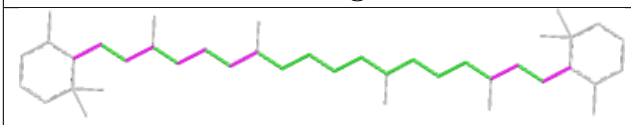
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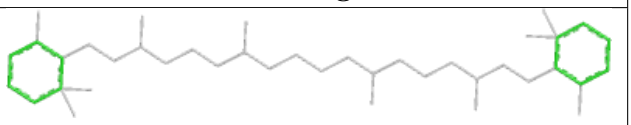
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Bond angles

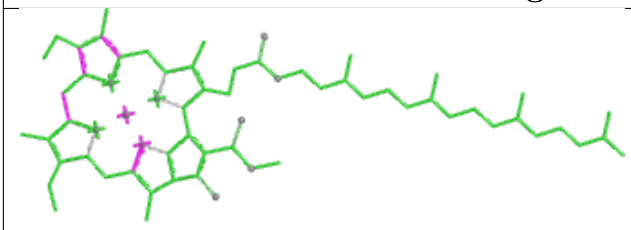


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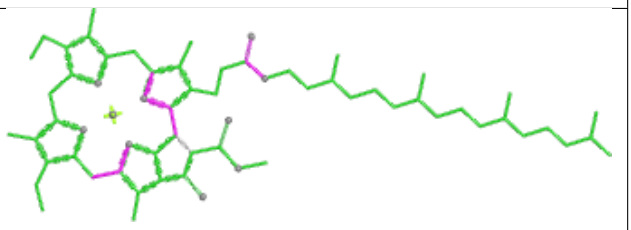


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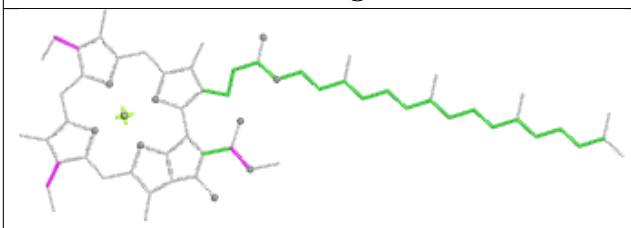
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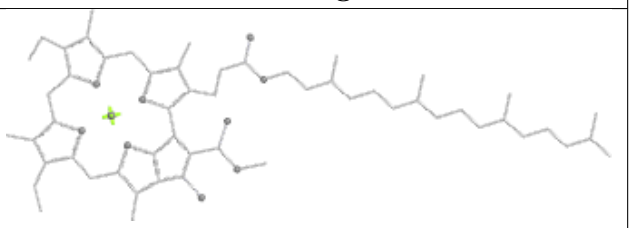
Bond lengths



Bond angles

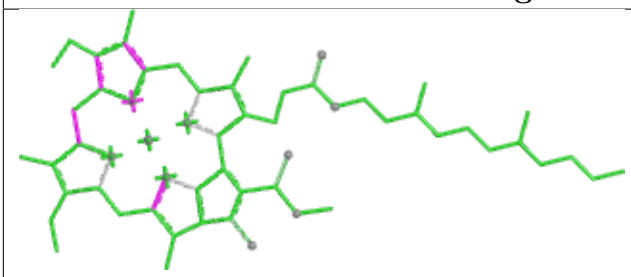


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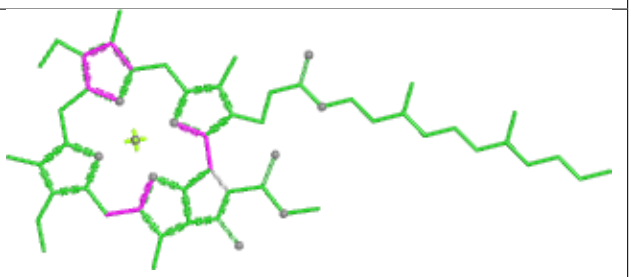


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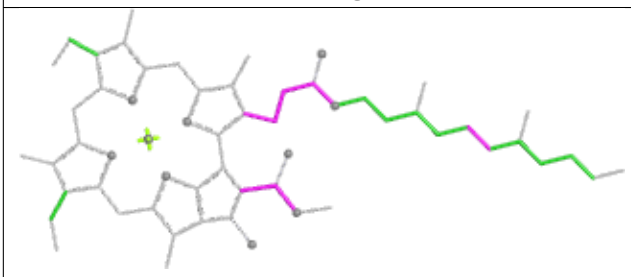
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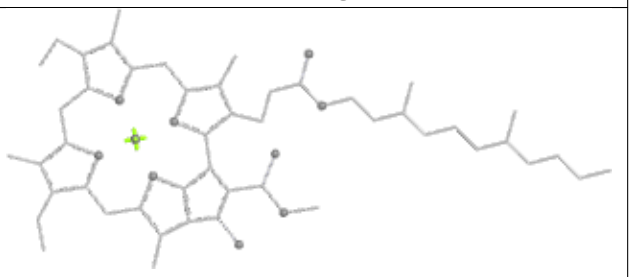
Bond lengths



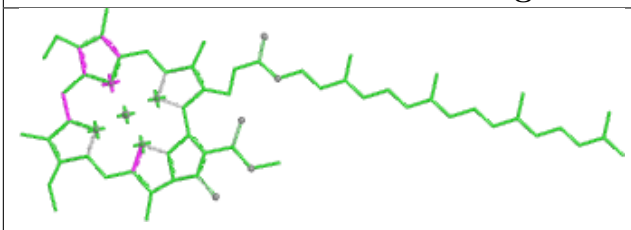
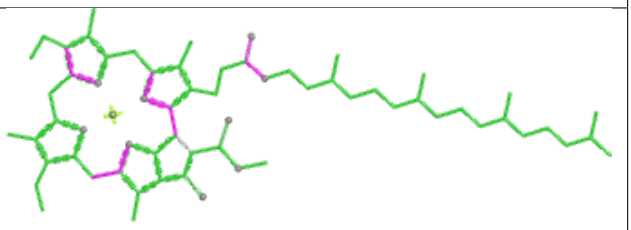
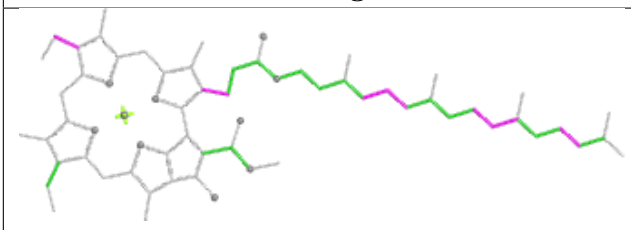
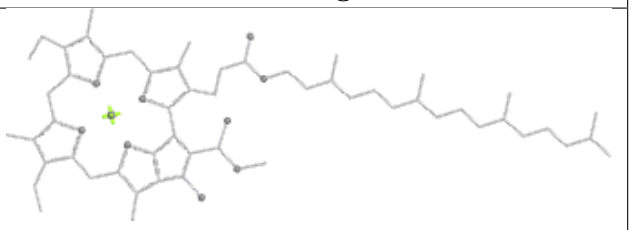
Bond angles

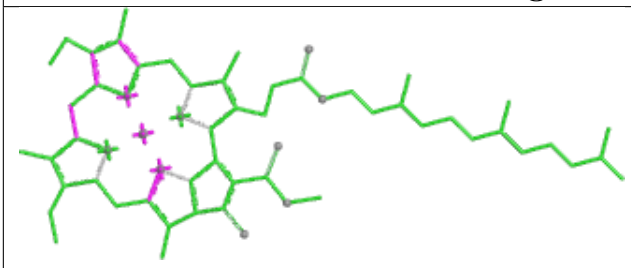
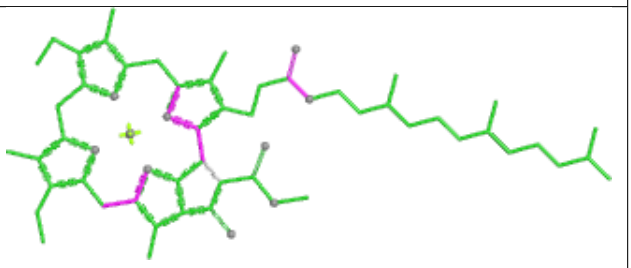
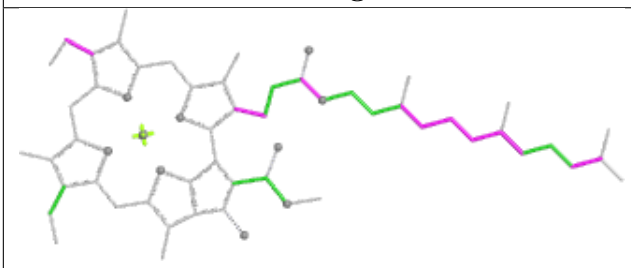
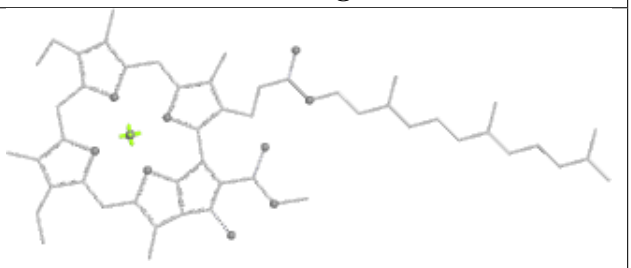


Torsions

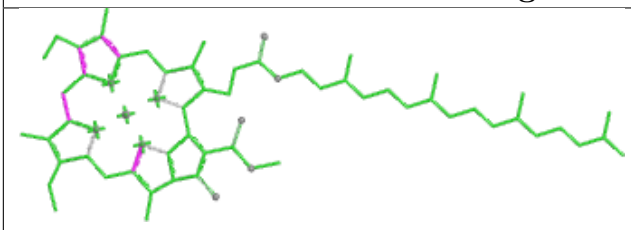


Rings

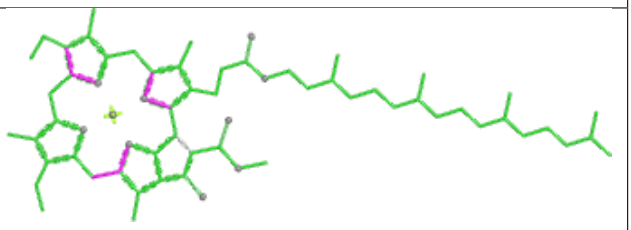
Ligand CLA A 1109	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA x 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

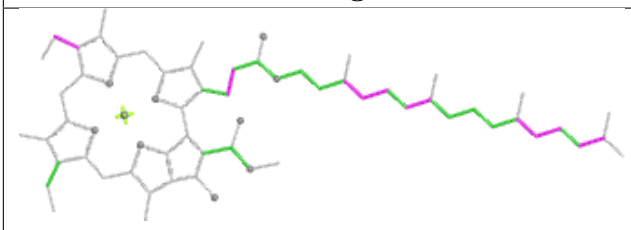
Ligand CLA b 1204



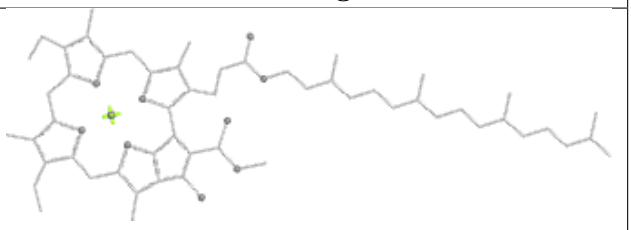
Bond lengths



Bond angles

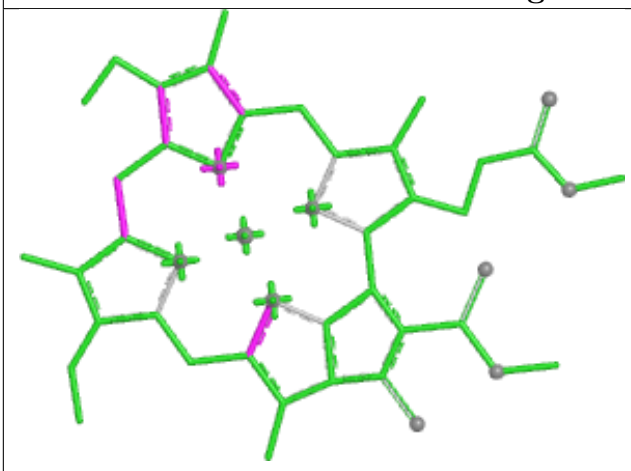


Torsions

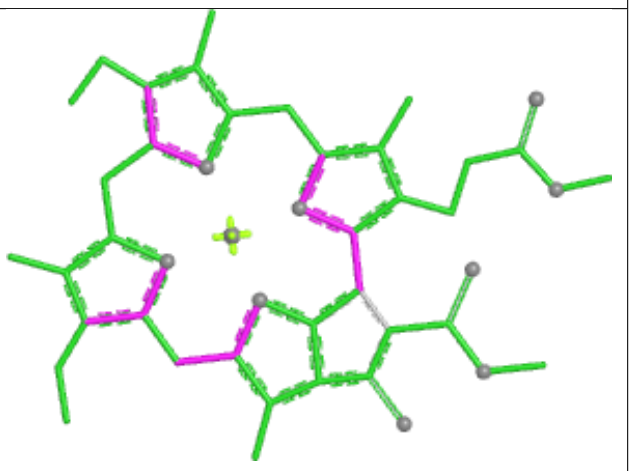


Rings

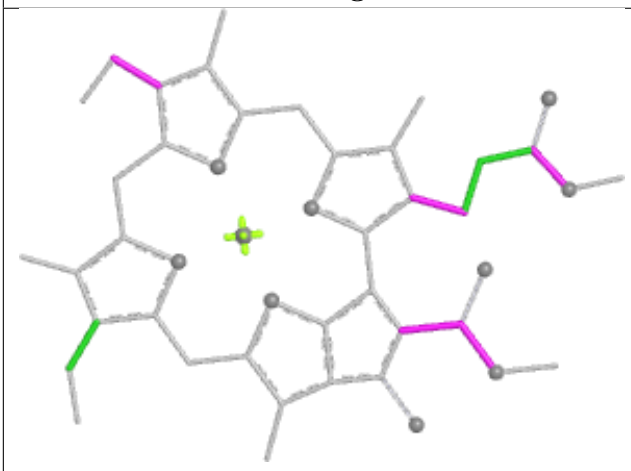
Ligand CLA n 503



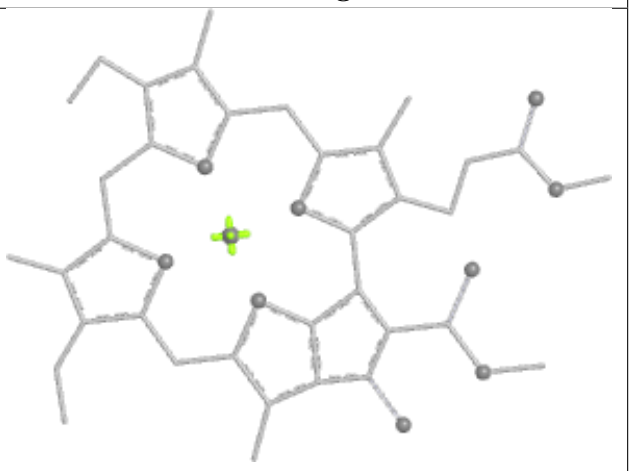
Bond lengths



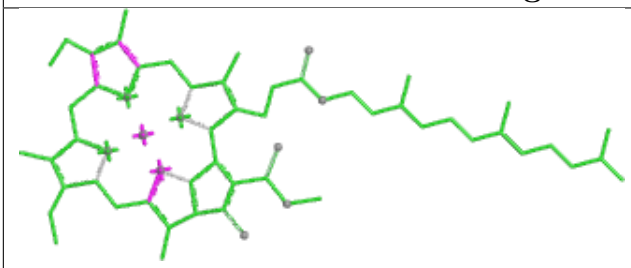
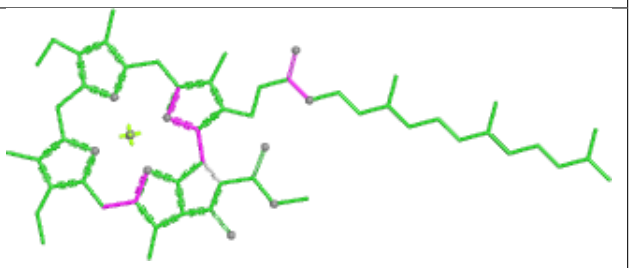
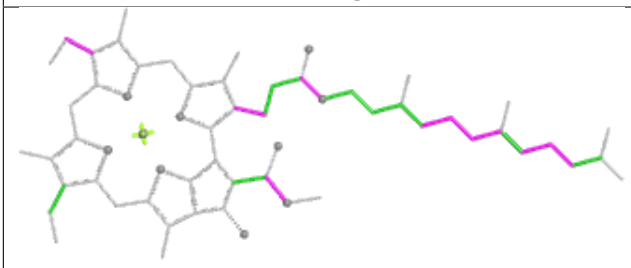
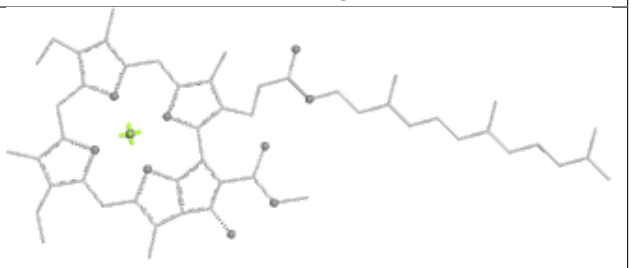
Bond angles

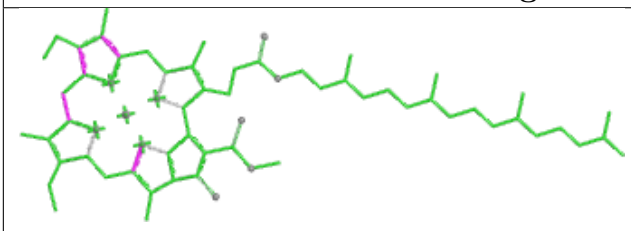
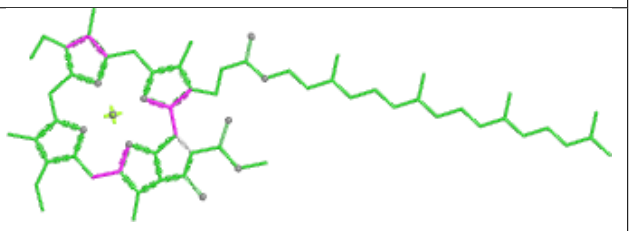
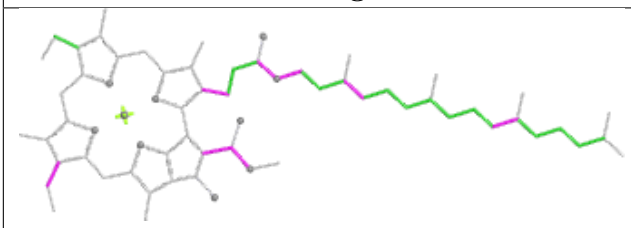
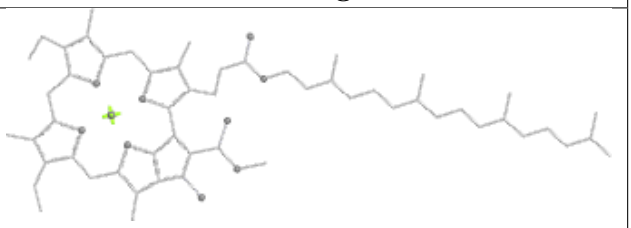


Torsions

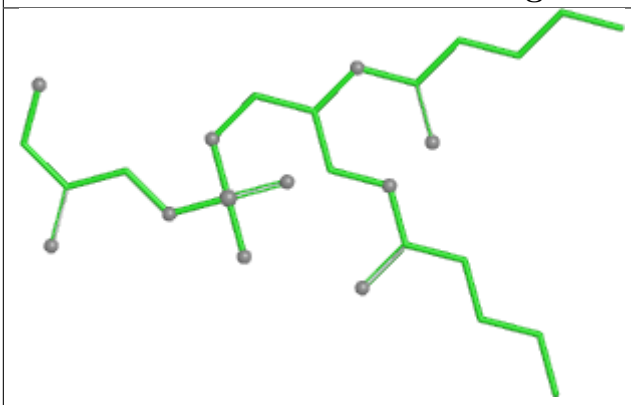


Rings

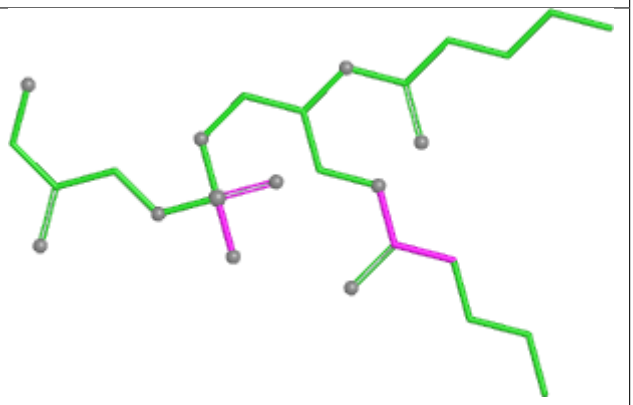
Ligand CLA X 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

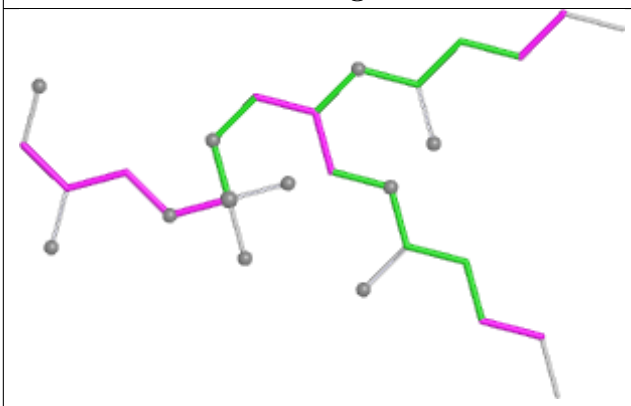
Ligand LHG u 605



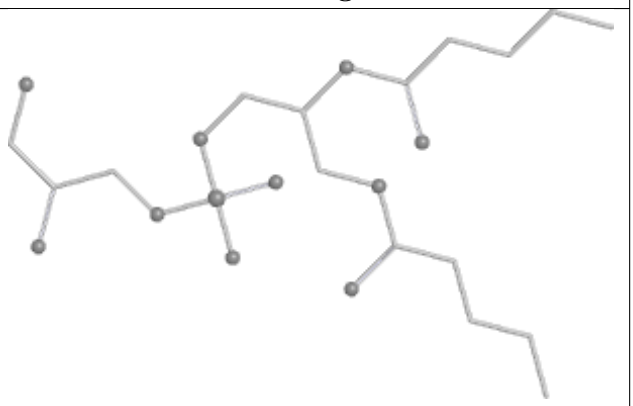
Bond lengths



Bond angles

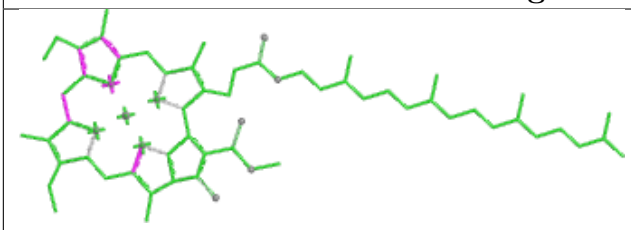


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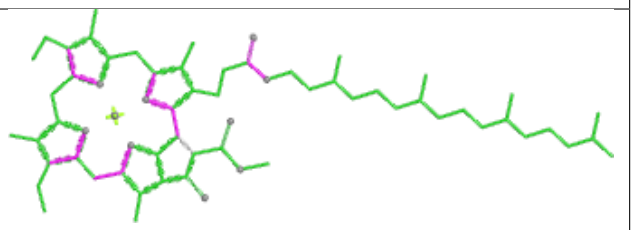


Rings

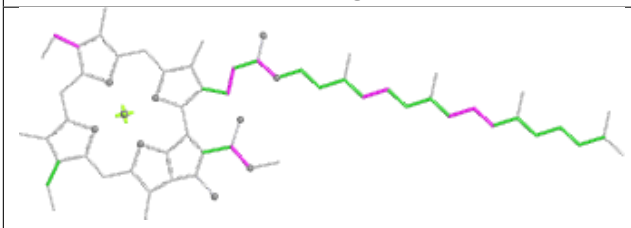
Ligand CLA x 505



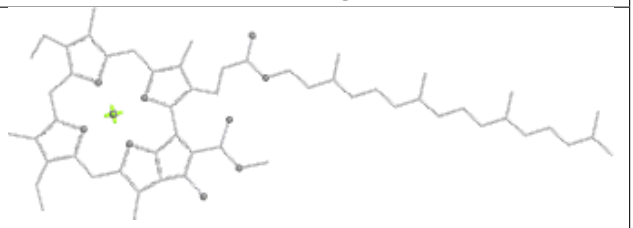
Bond lengths



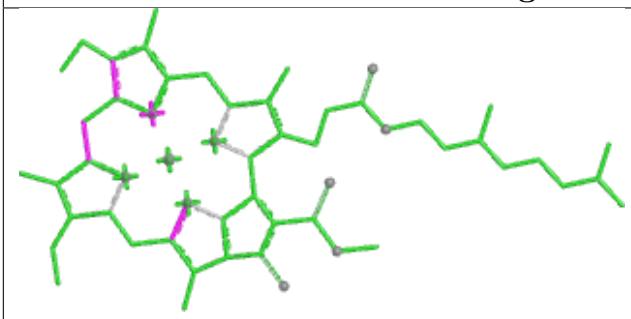
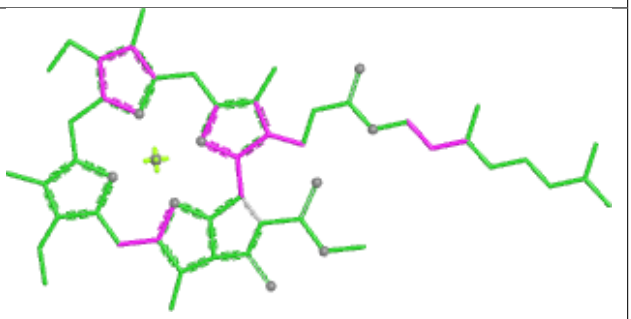
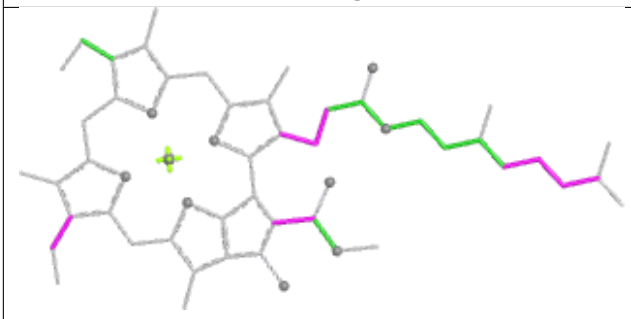
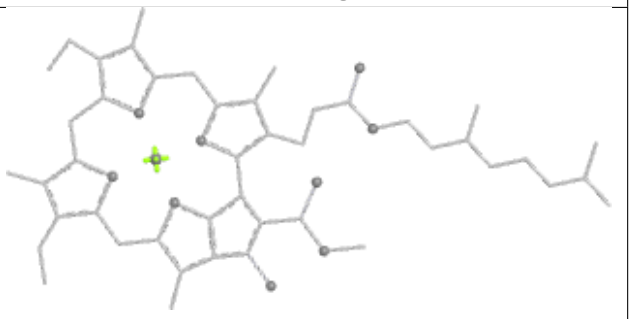
Bond angles

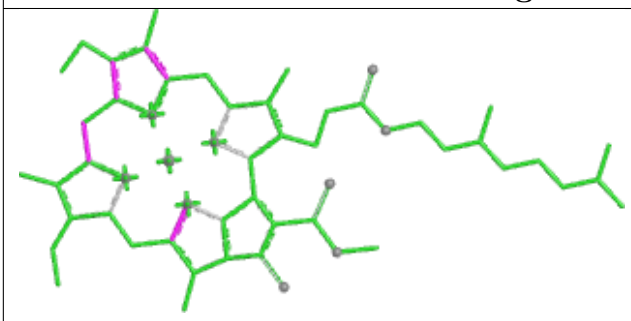
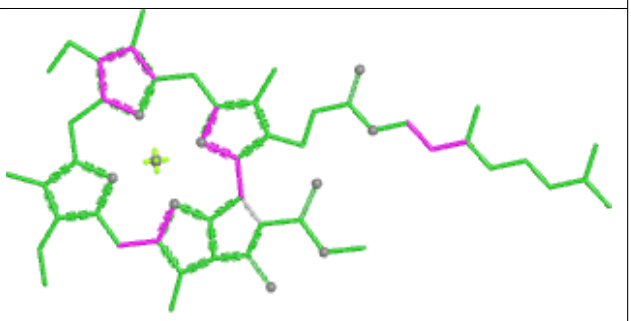
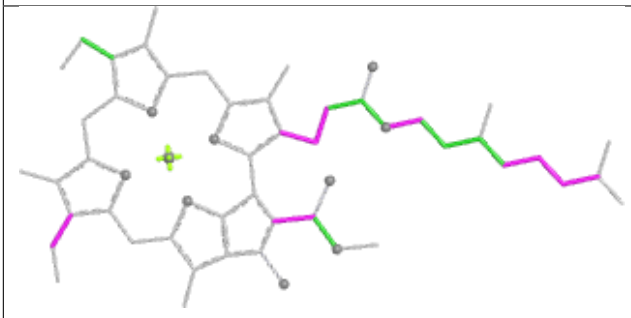
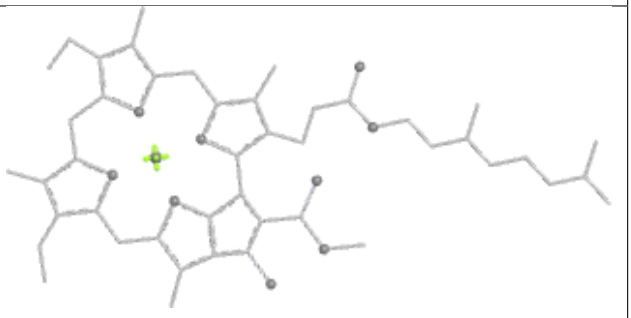


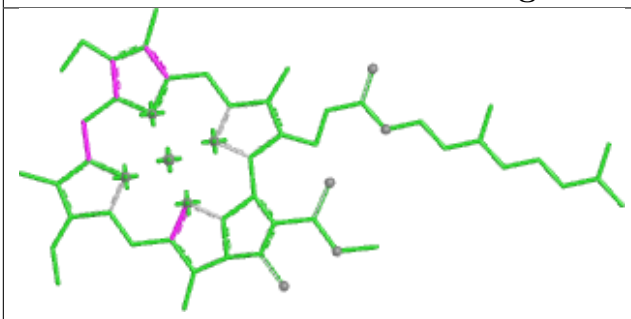
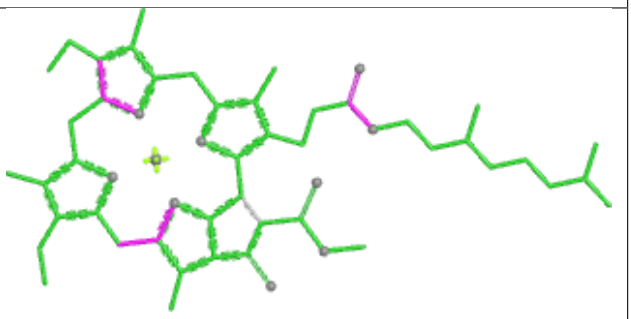
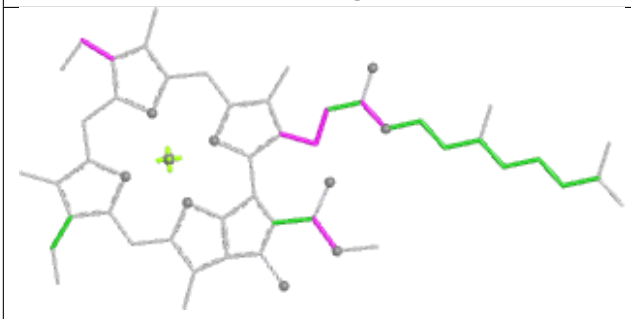
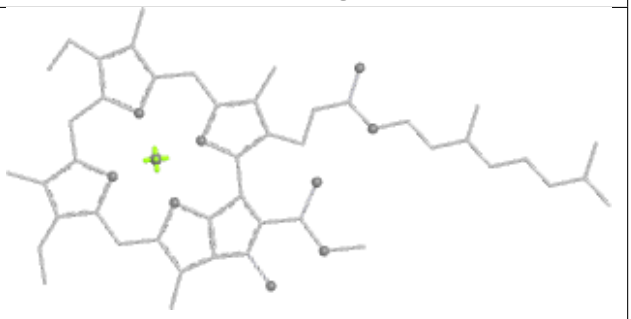
Torsions

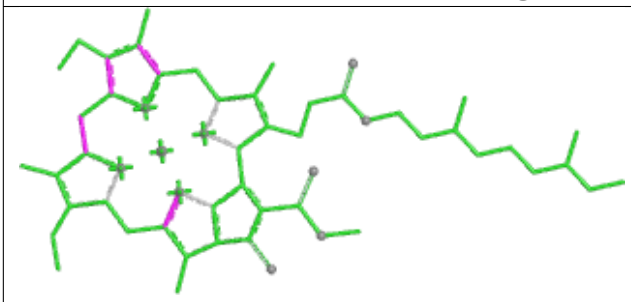
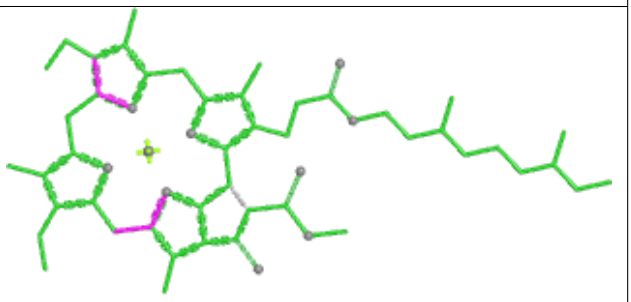
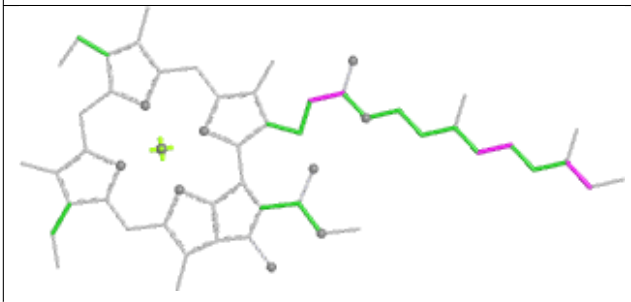
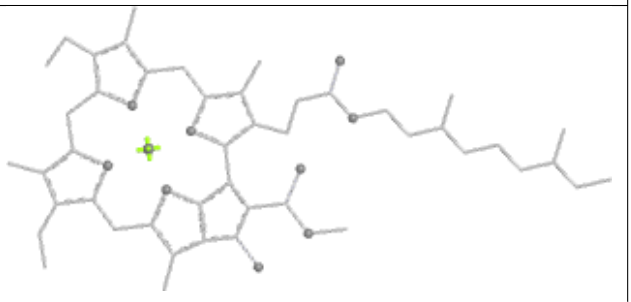


Rings

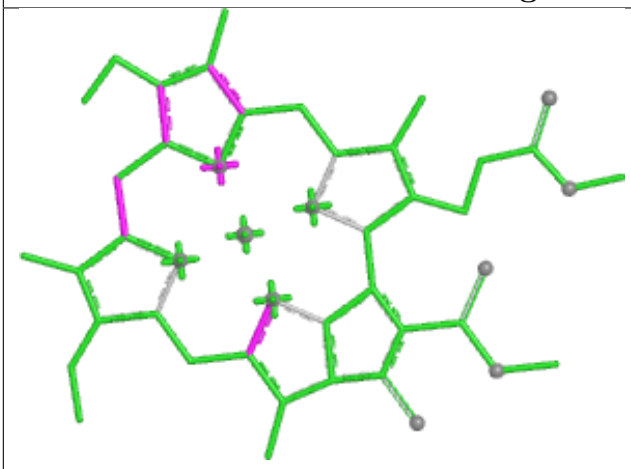
Ligand CLA b 1012	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1012	
	
Bond lengths	Bond angles
	
Torsions	Rings

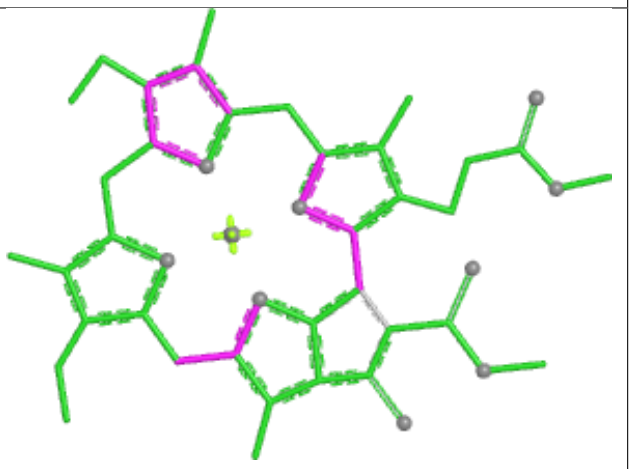
Ligand CLA W 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

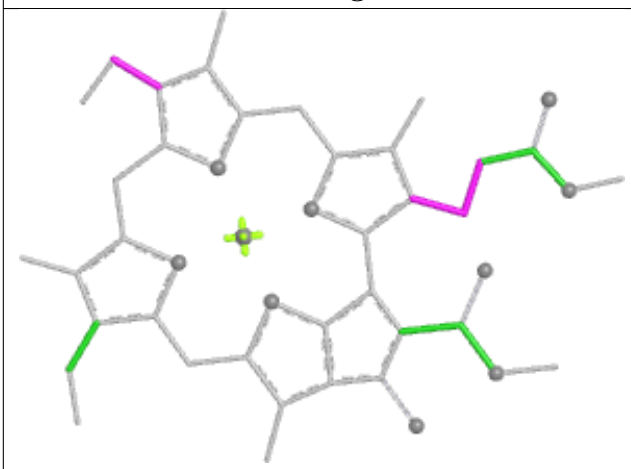
Ligand CLA a 1129



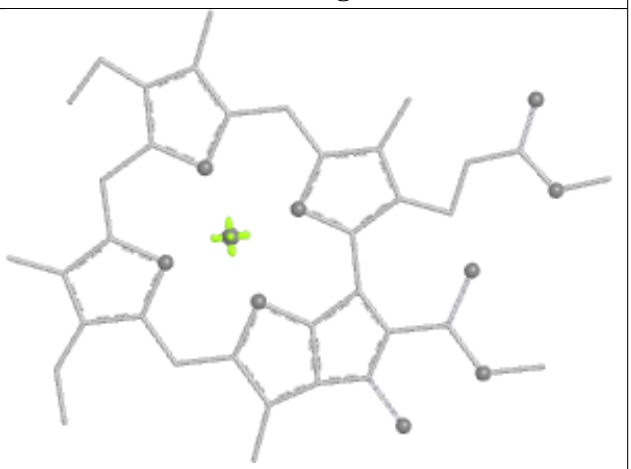
Bond lengths



Bond angles

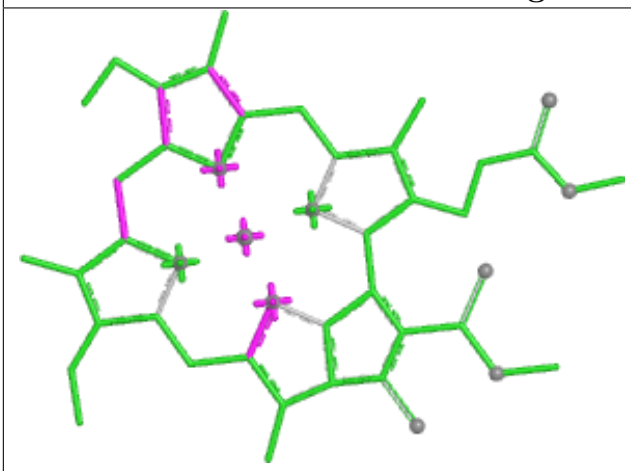


Torsions

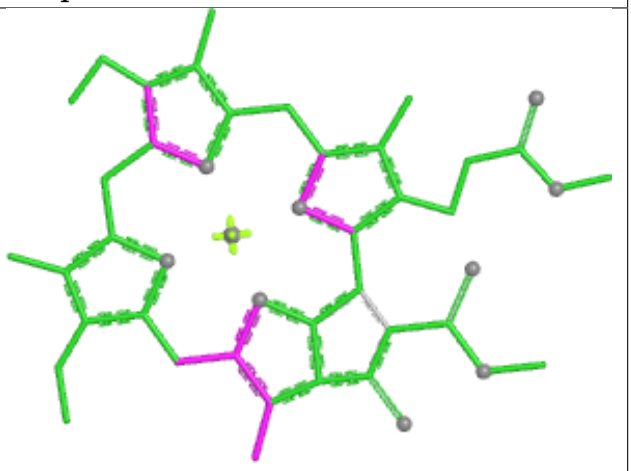


Rings

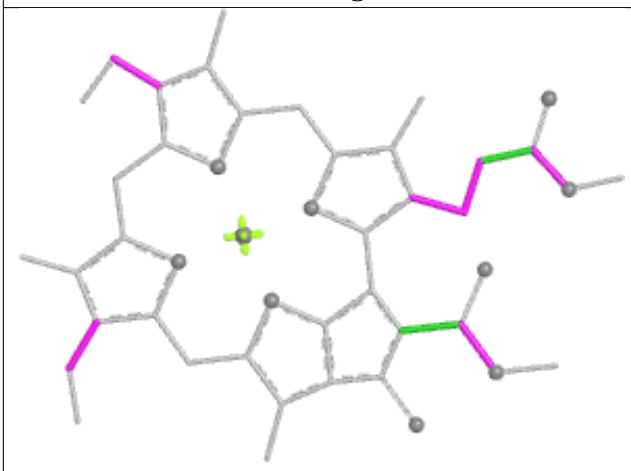
Ligand CLA q 503



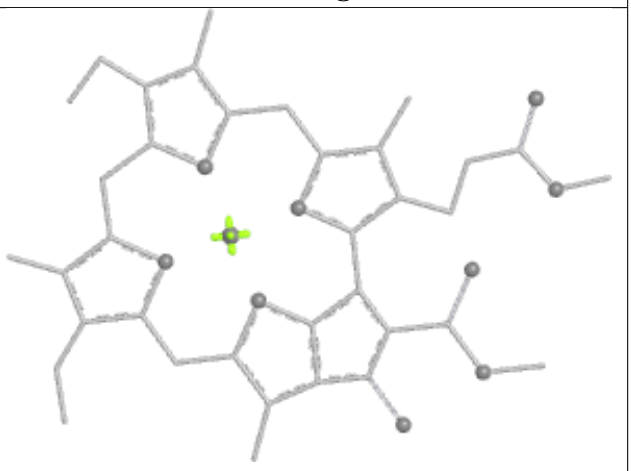
Bond lengths



Bond angles

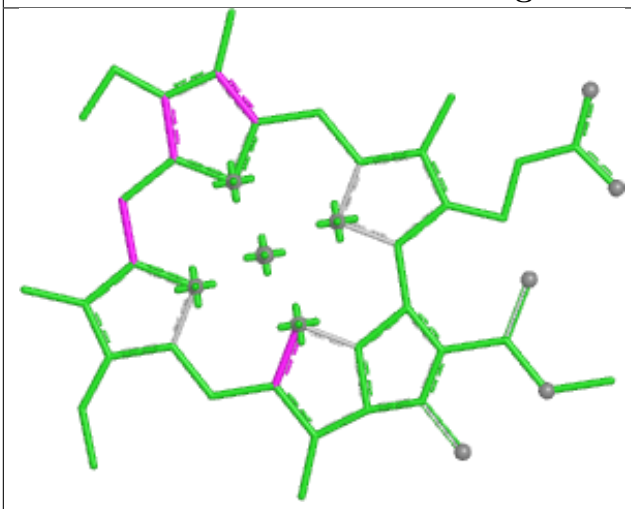


Torsions

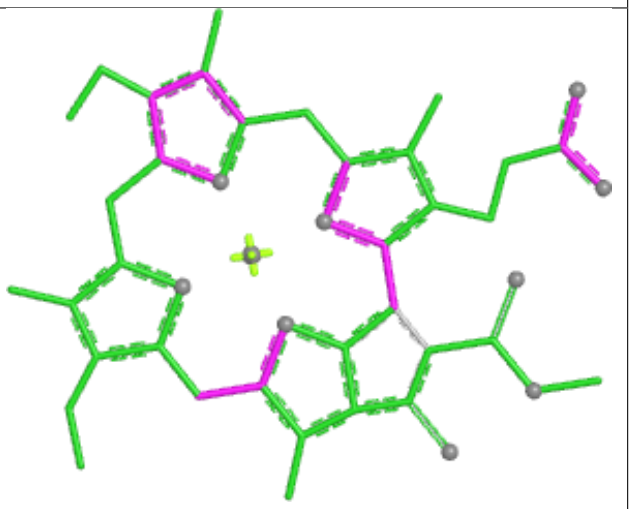


Rings

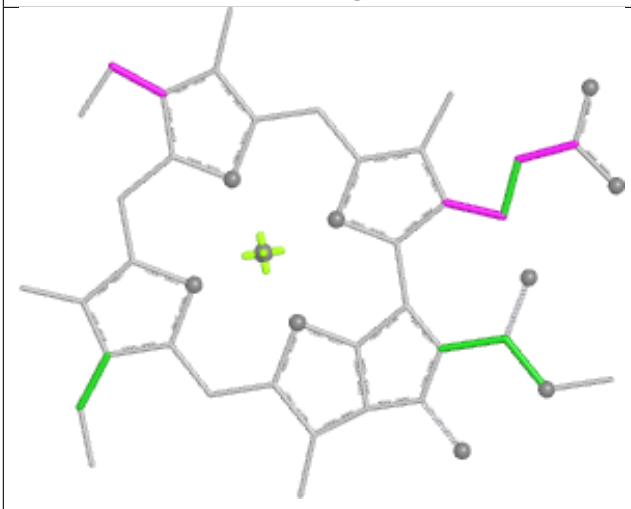
Ligand CLA B 1208



Bond lengths



Bond angles

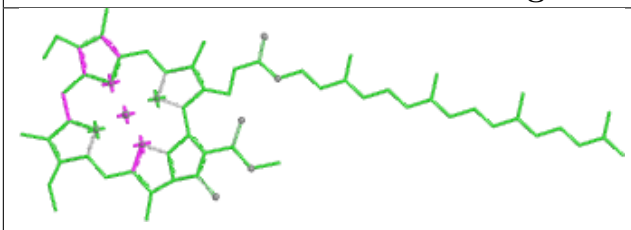


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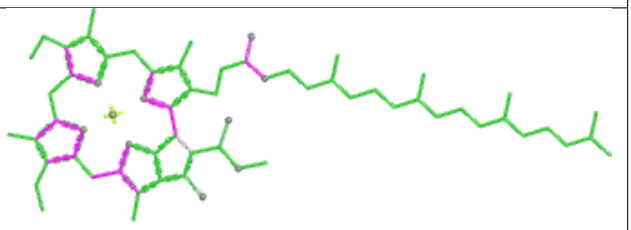


Rings

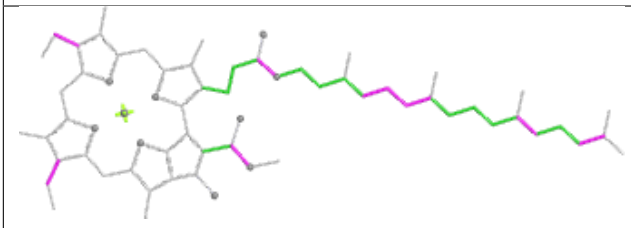
Ligand CLA h 511



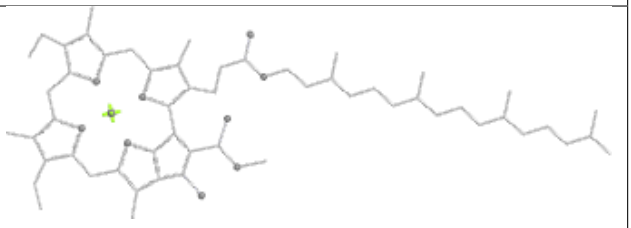
Bond lengths



Bond angles

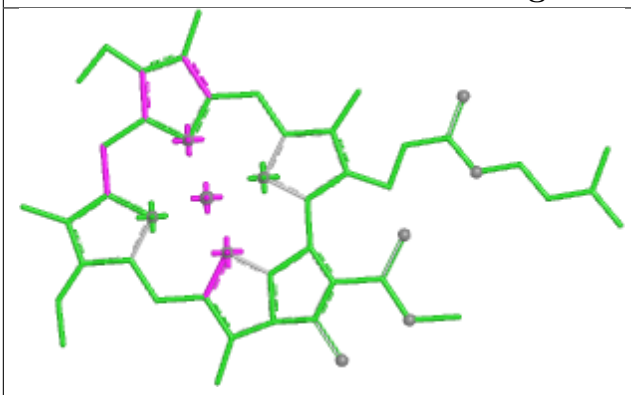


Torsions

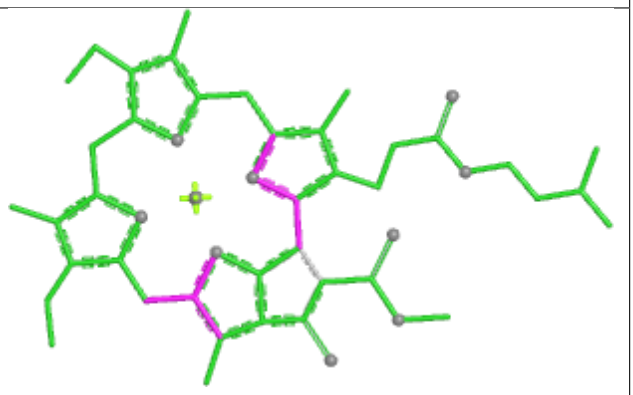


Rings

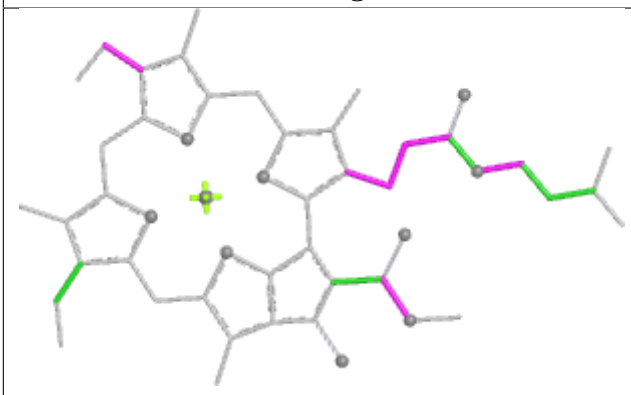
Ligand CLA o 514



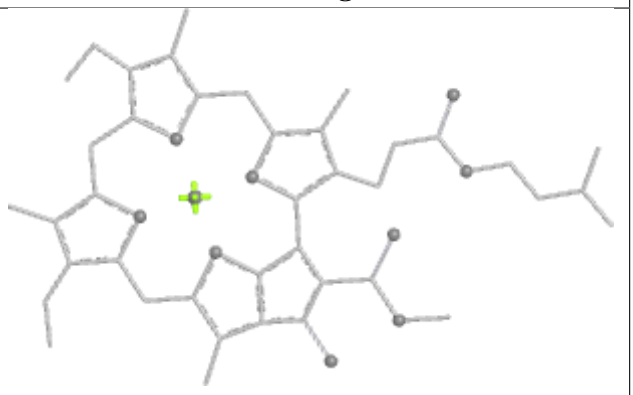
Bond lengths



Bond angles



Torsions

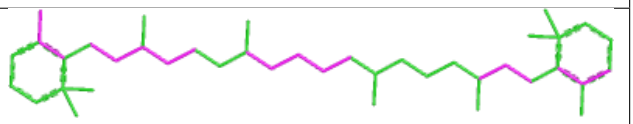


Rings

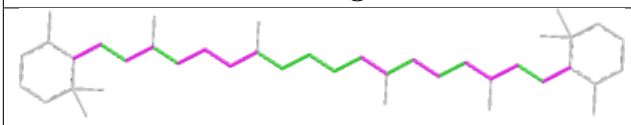
Ligand BCR r 601



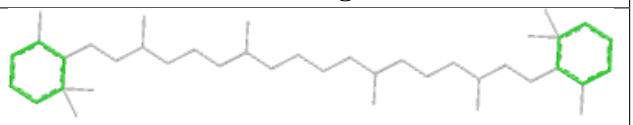
Bond lengths



Bond angles

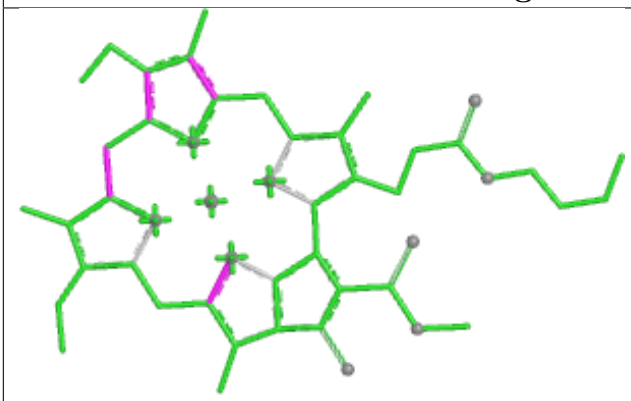


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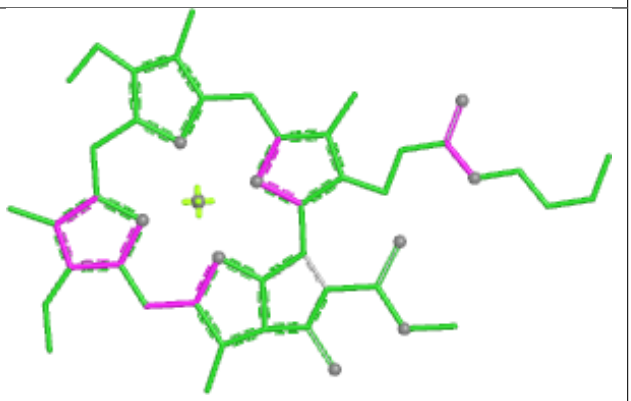


Rings

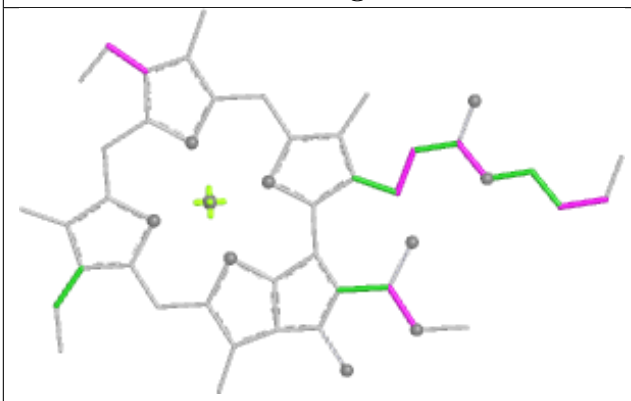
Ligand CLA A 1120



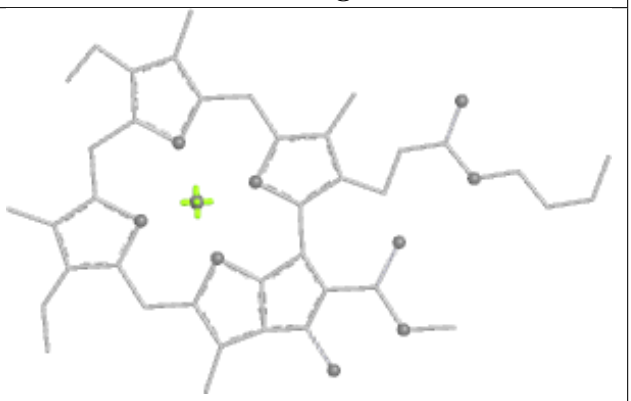
Bond lengths



Bond angles



Torsions

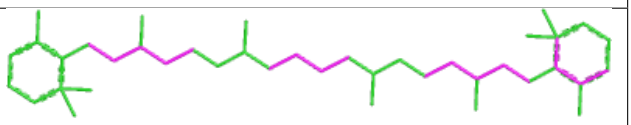


Rings

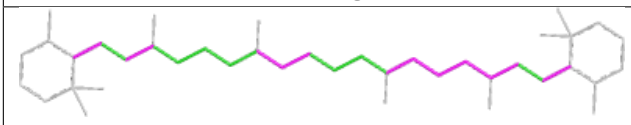
Ligand BCR G 4014



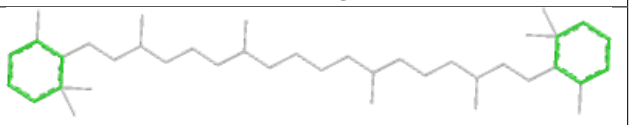
Bond lengths



Bond angles

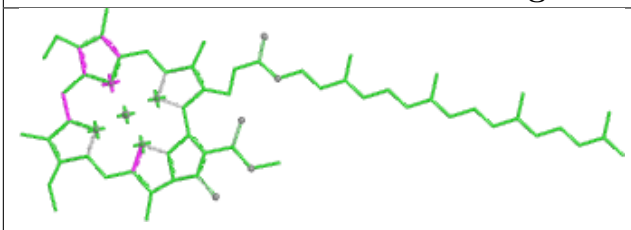


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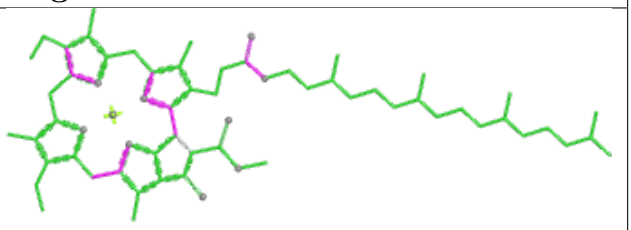


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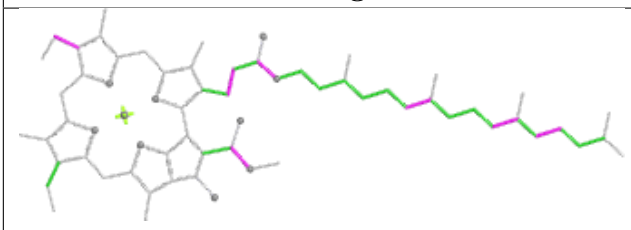
Ligand CLA g 510



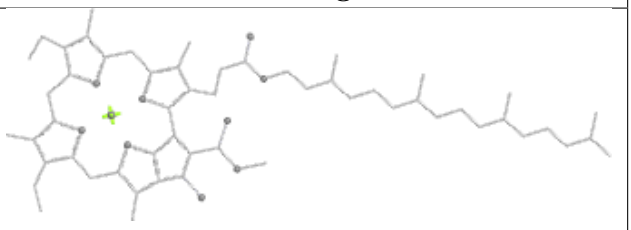
Bond lengths



Bond angles

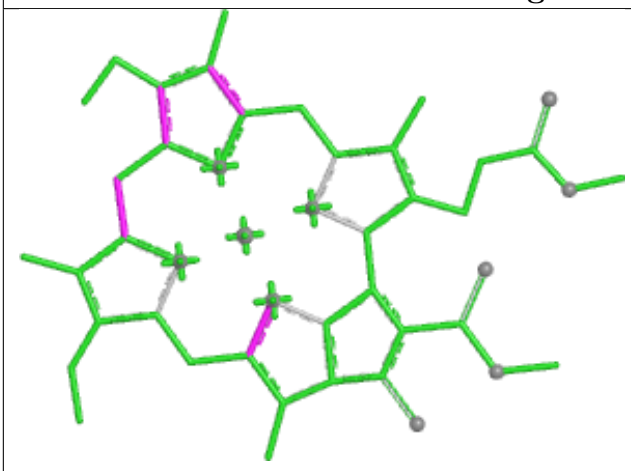


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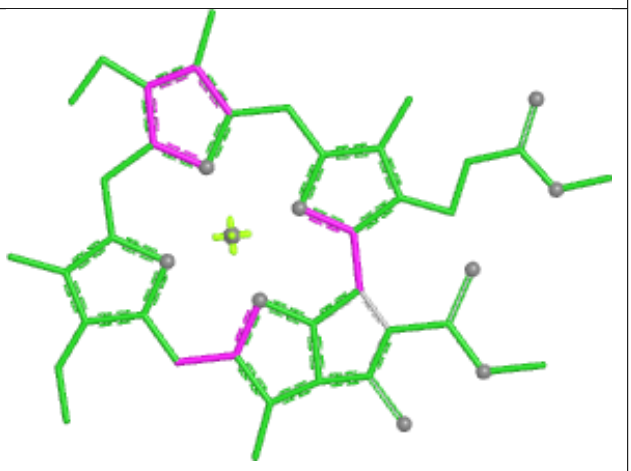


Rings

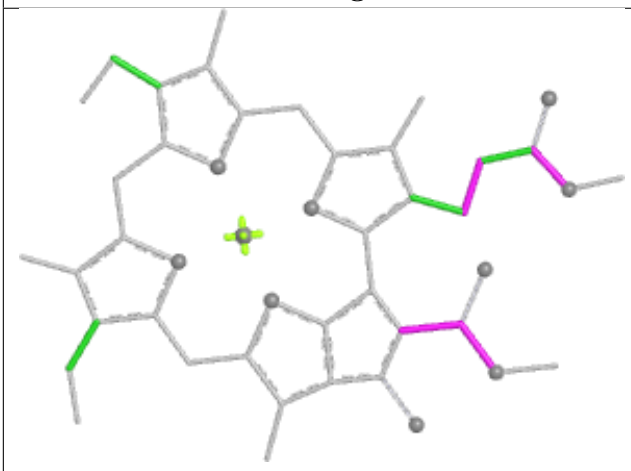
Ligand CLA h 513



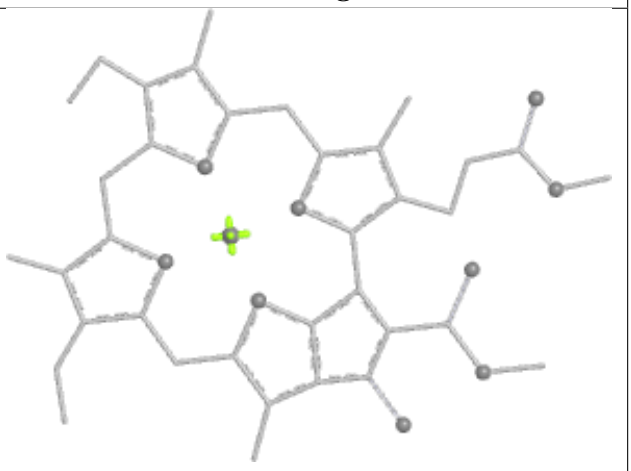
Bond lengths



Bond angles

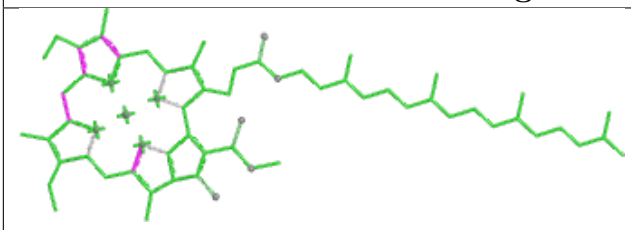


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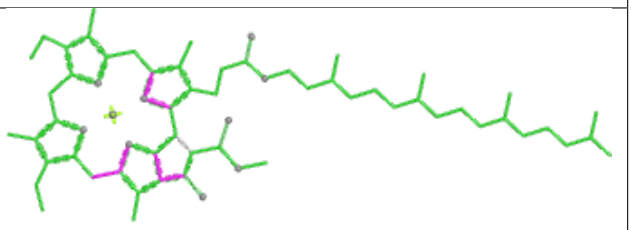


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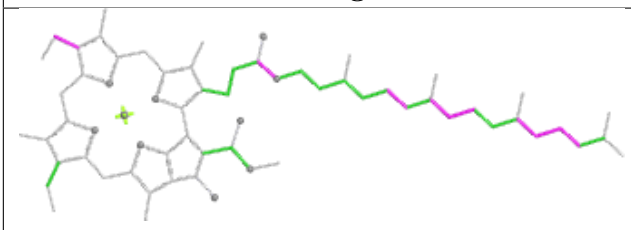
Ligand CLA A 1125



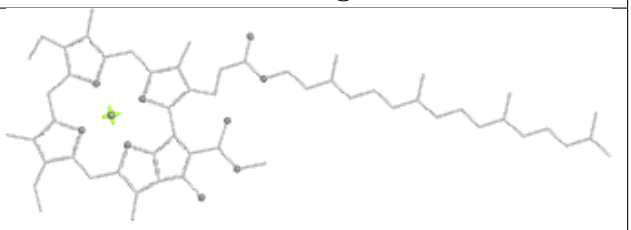
Bond lengths



Bond angles

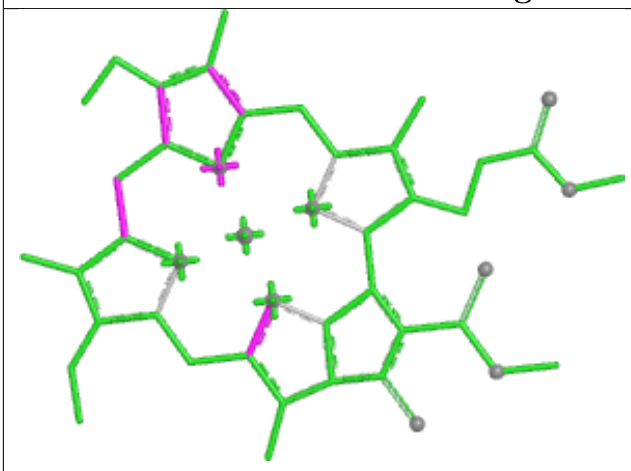


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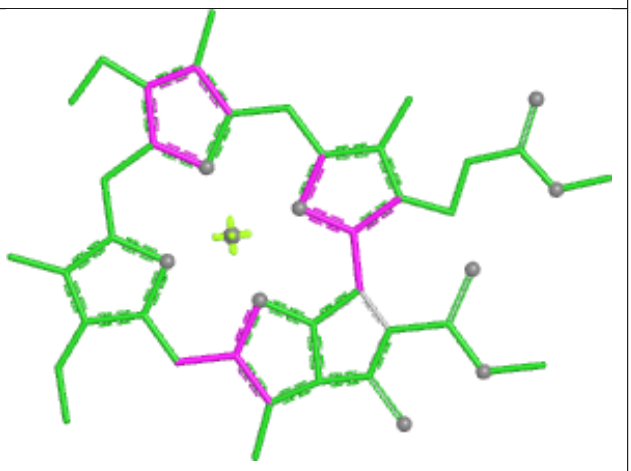


Rings

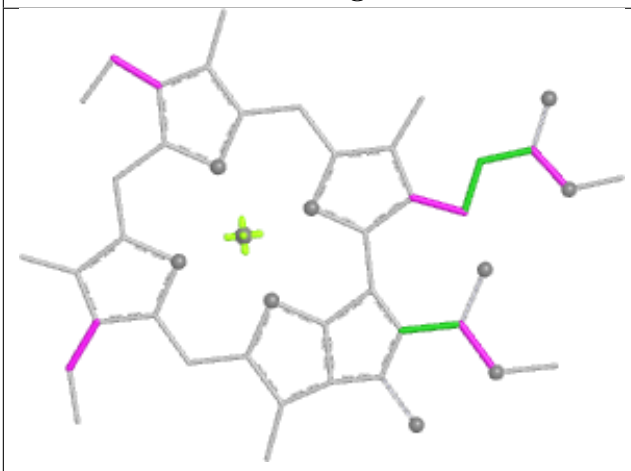
Ligand CLA H 1114



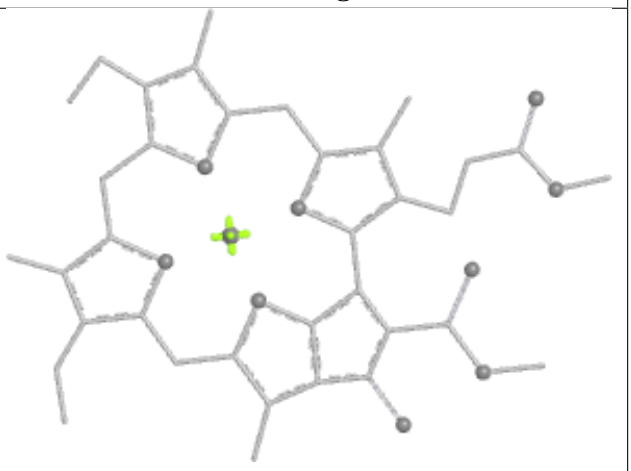
Bond lengths



Bond angles

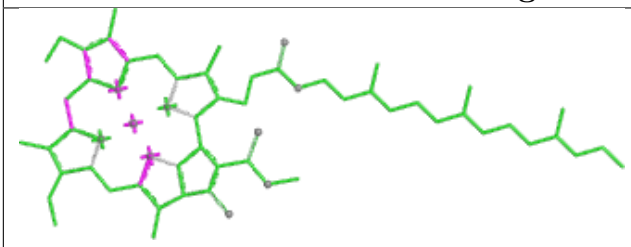


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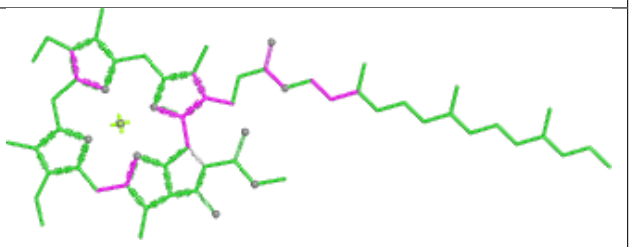


Rings

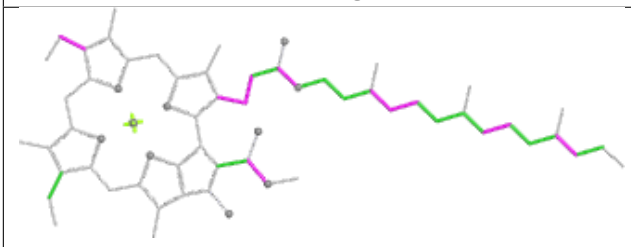
Ligand CLA b 1235



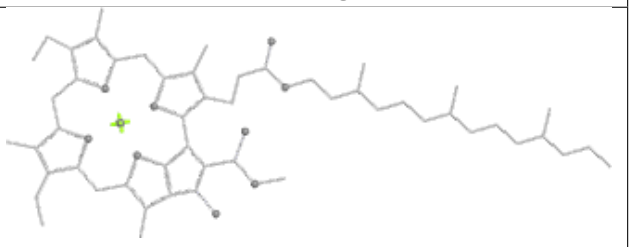
Bond lengths



Bond angles

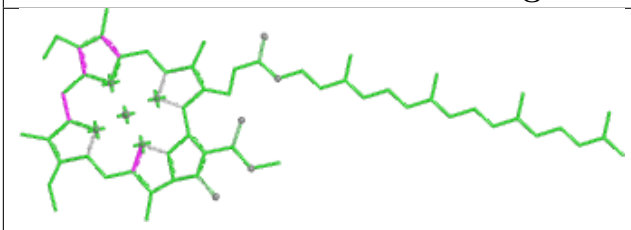


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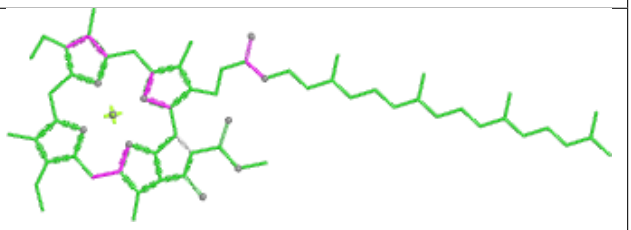


Rings

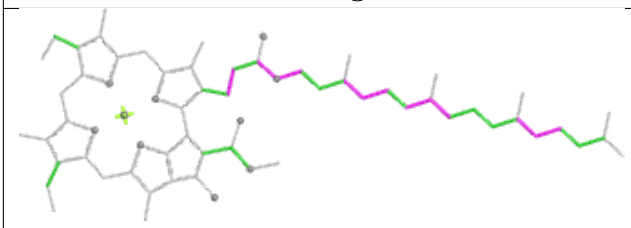
Ligand CLA l 1503



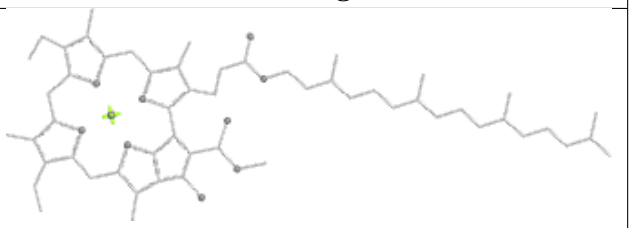
Bond lengths



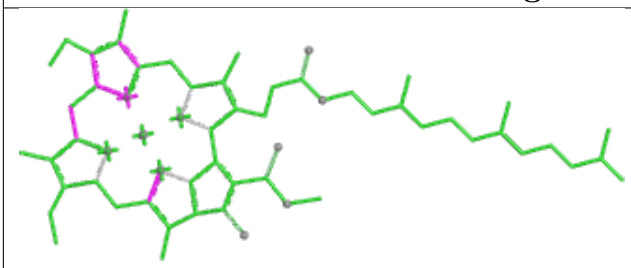
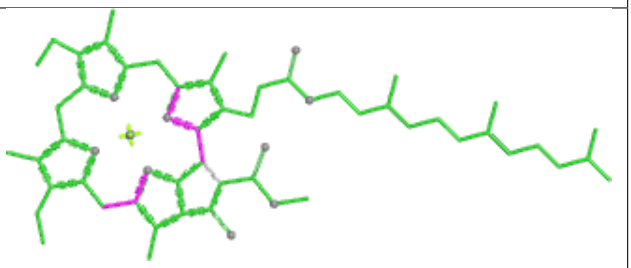
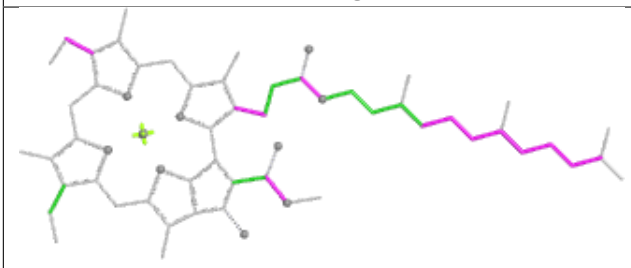
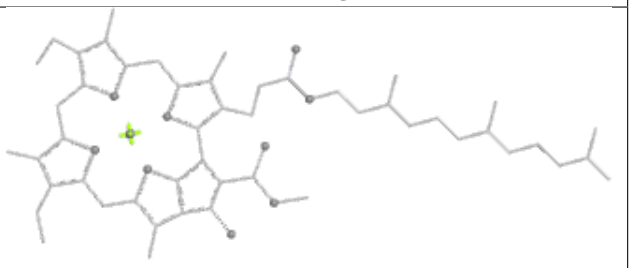
Bond angles

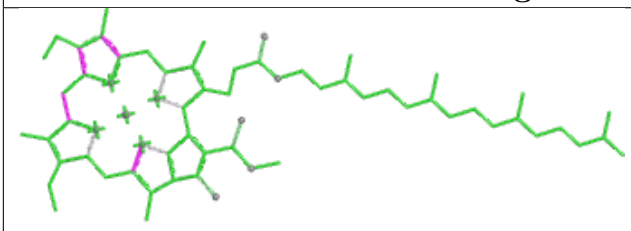
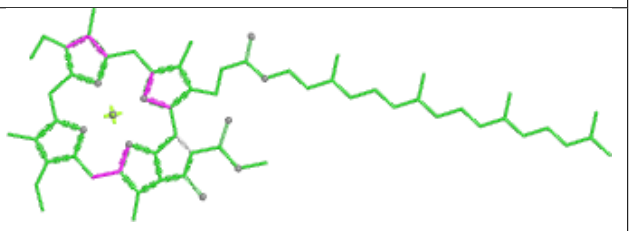
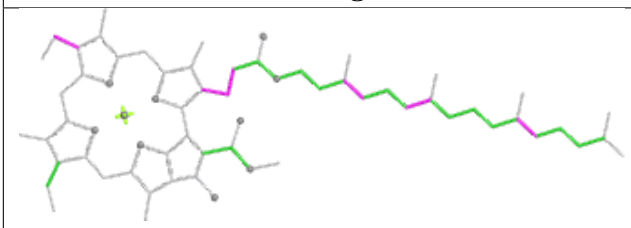
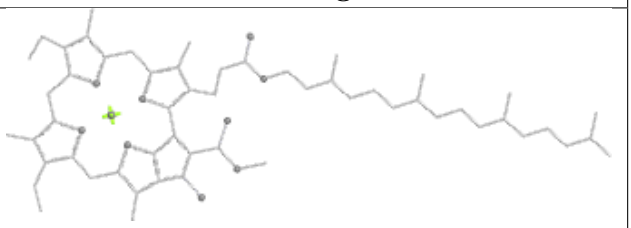


Torsions

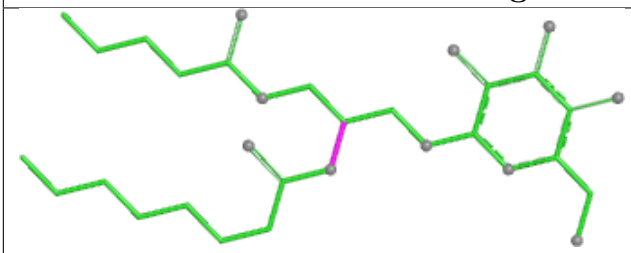


Rings

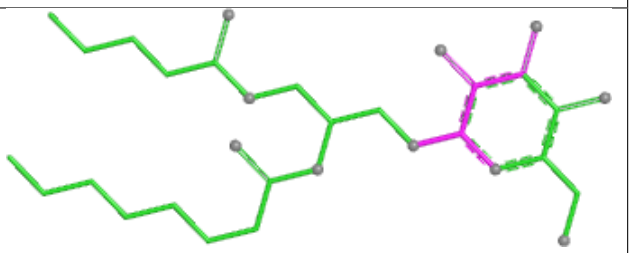
Ligand CLA X 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1204	
 Bond lengths	 Bond angles
 Torsions	 Rings

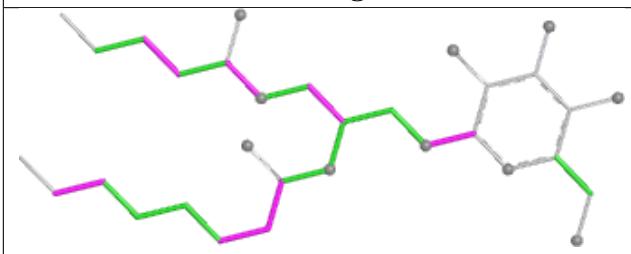
Ligand LMG H 4201



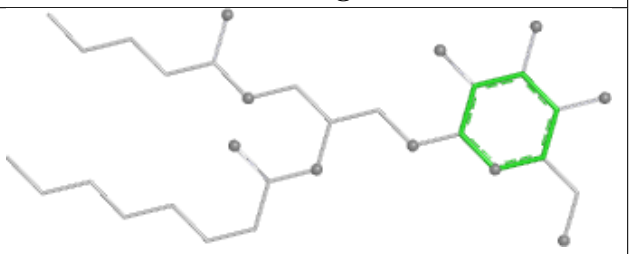
Bond lengths



Bond angles

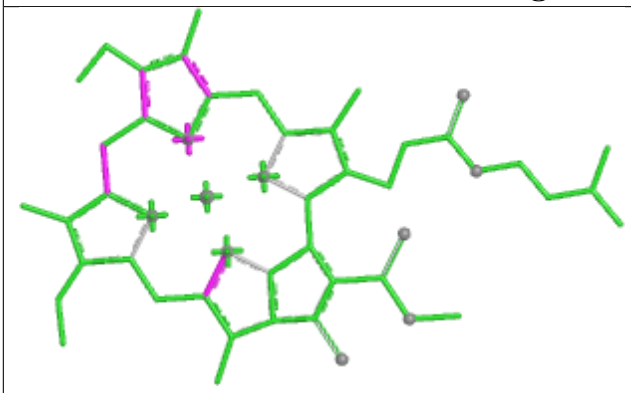


Torsions

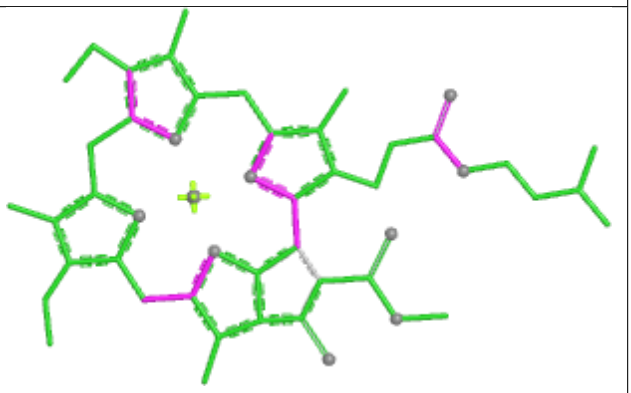


Rings

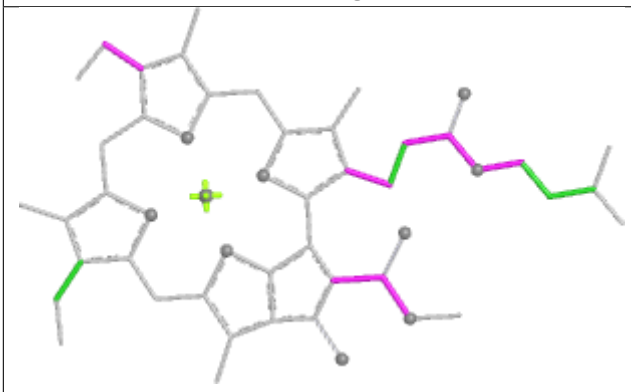
Ligand CLA r 514



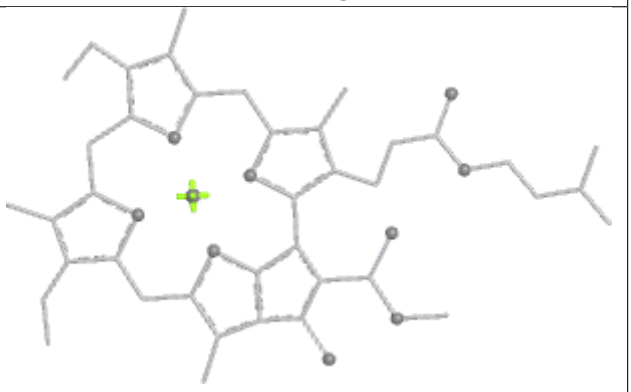
Bond lengths



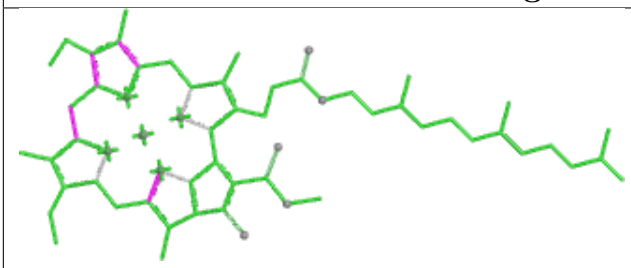
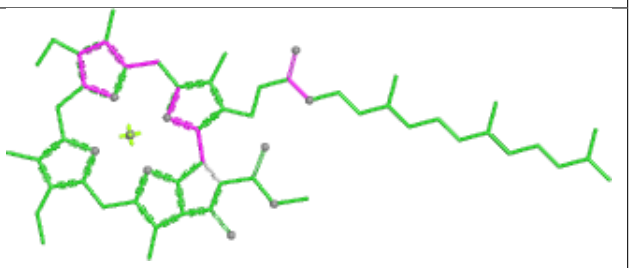
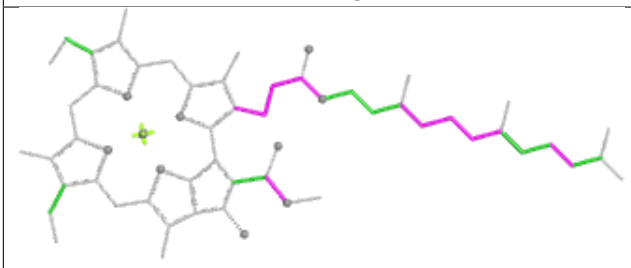
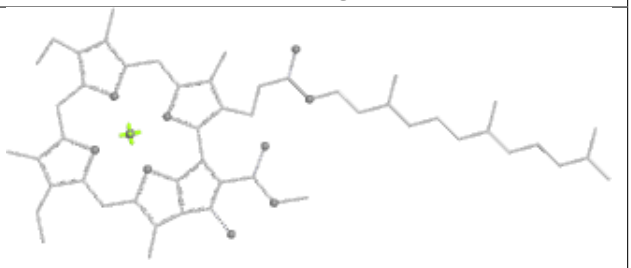
Bond angles

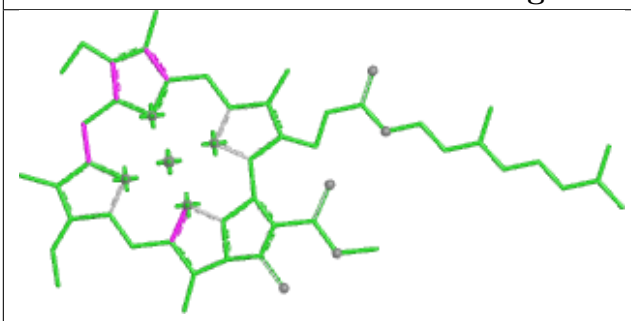
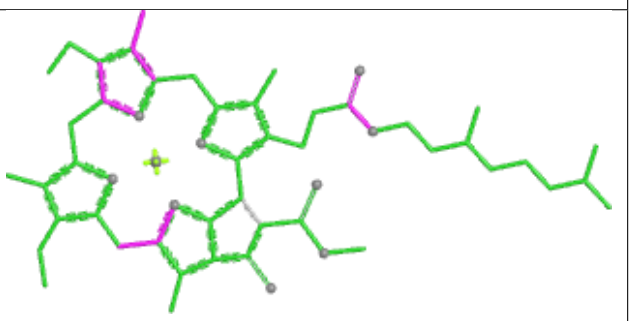
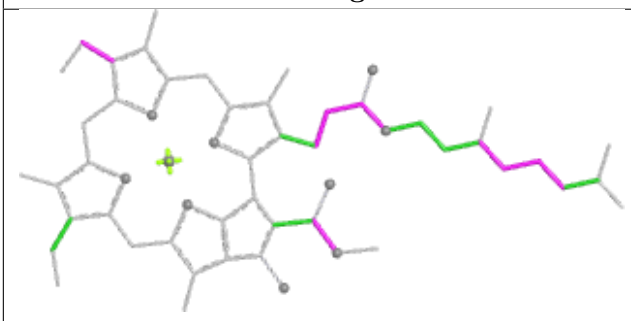
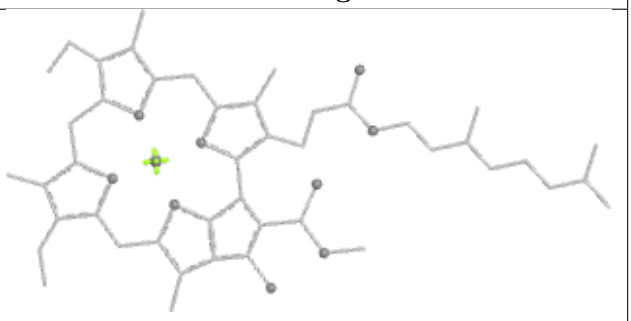


Torsions

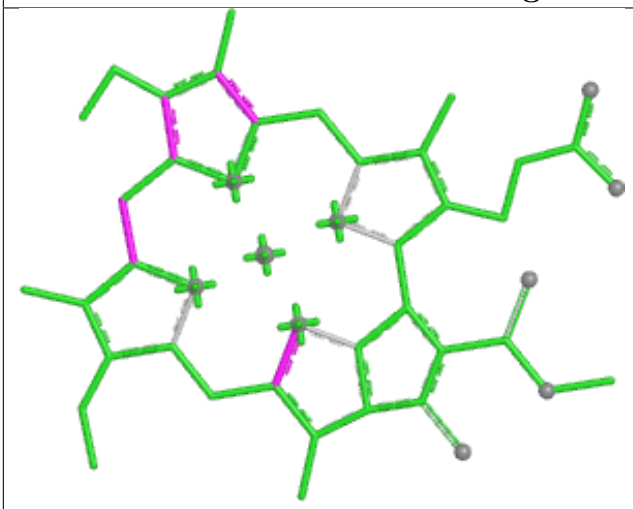


Rings

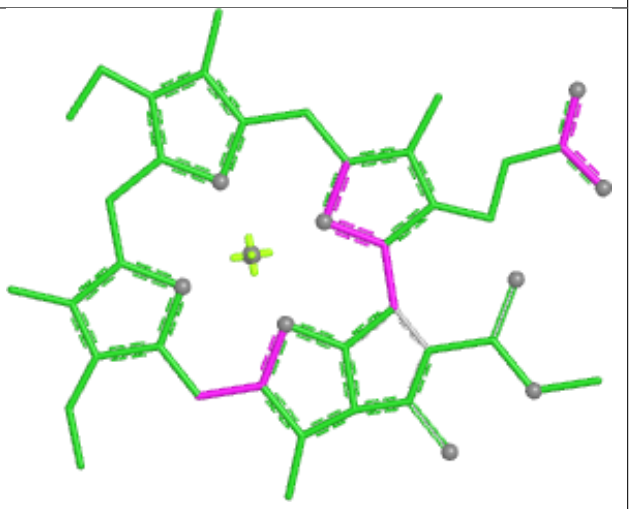
Ligand CLA Y 509	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA u 508	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

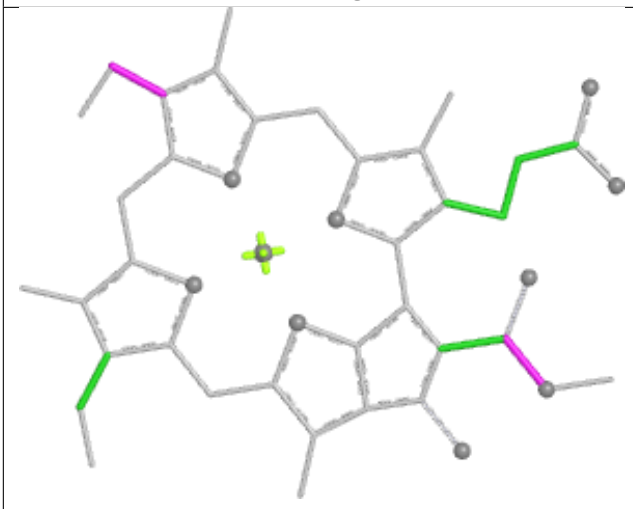
Ligand CLA f 1301



Bond lengths



Bond angles

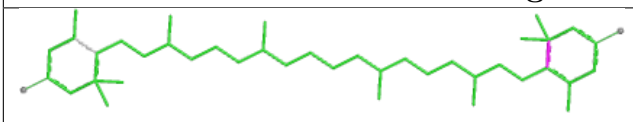


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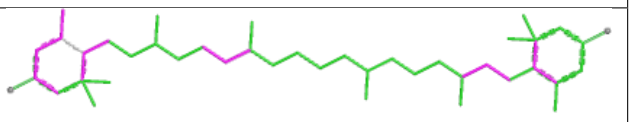


Rings

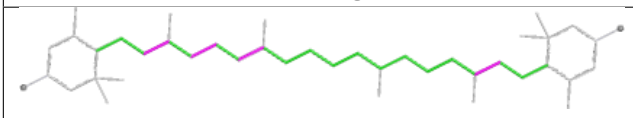
Ligand LUT Z 601



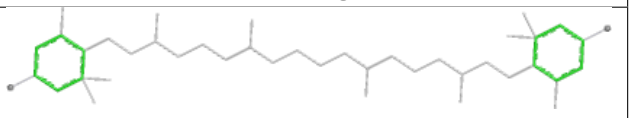
Bond lengths



Bond angles

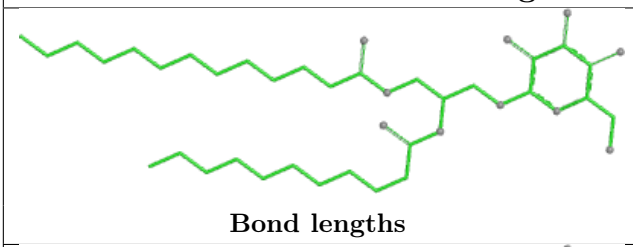


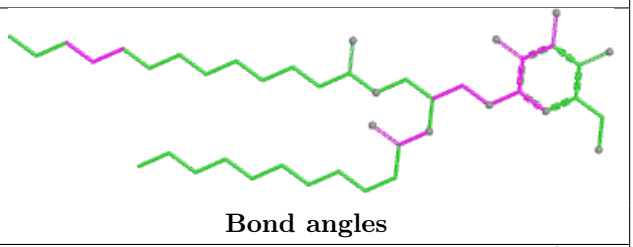
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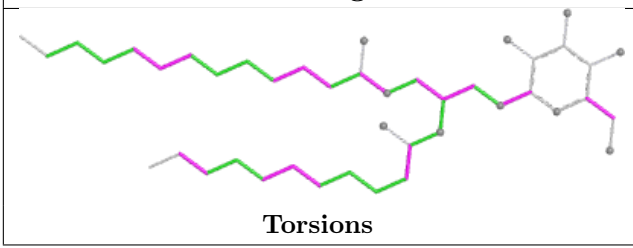


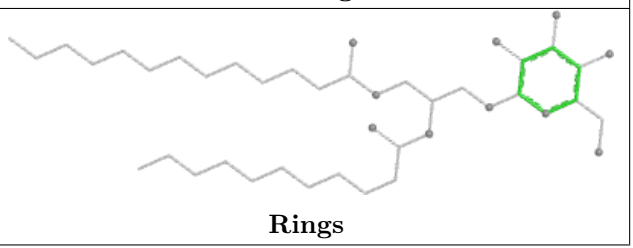
Rings

Ligand LMG G 848

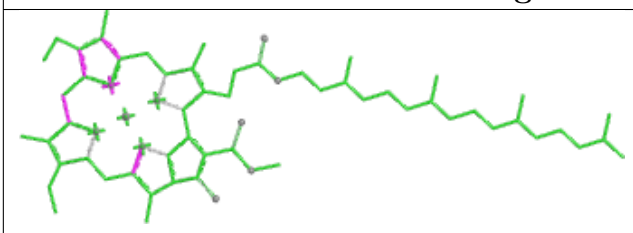

Bond lengths

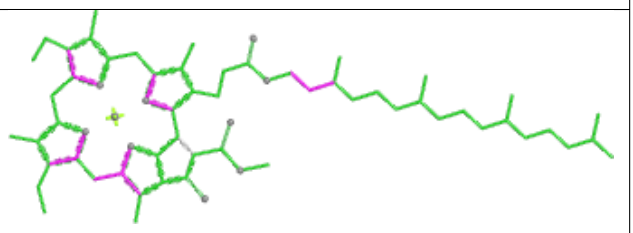

Bond angles

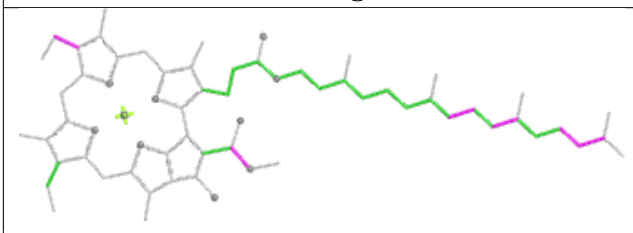

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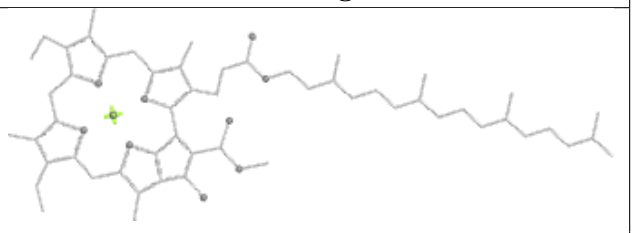

Rings

Ligand CLA H 1117

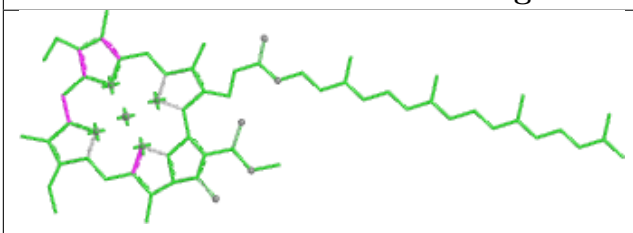

Bond lengths

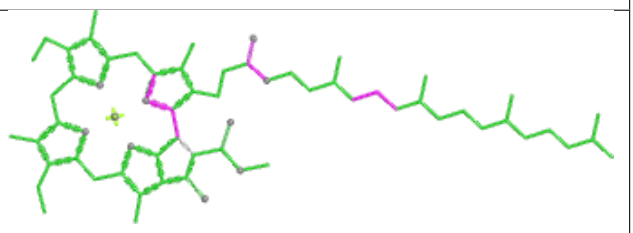

Bond angles

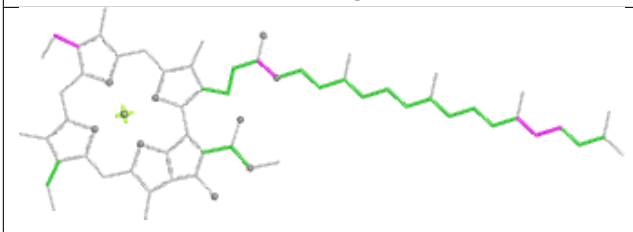

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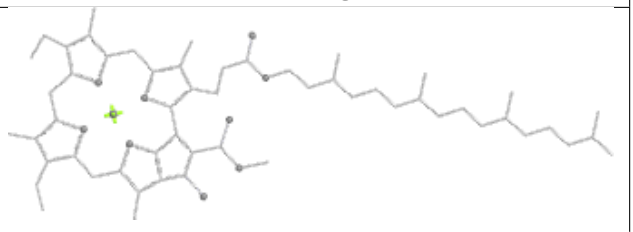

Rings

Ligand CLA G 1223

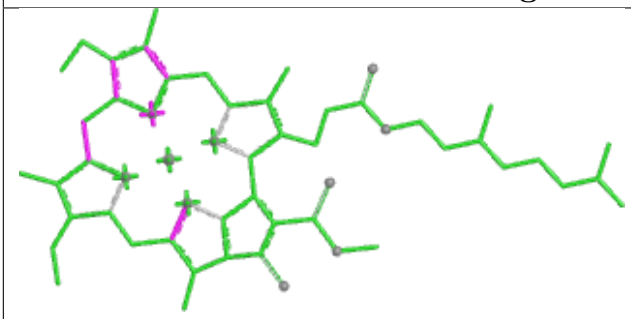

Bond lengths


Bond angles

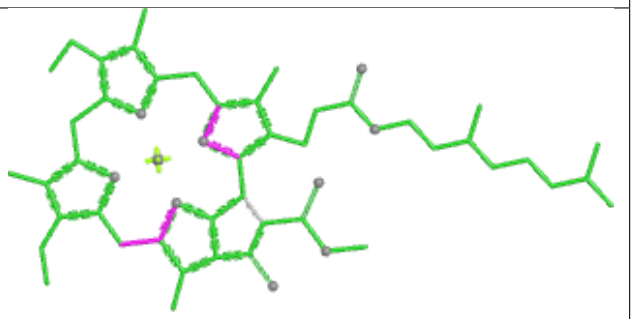

Torsions


Rings

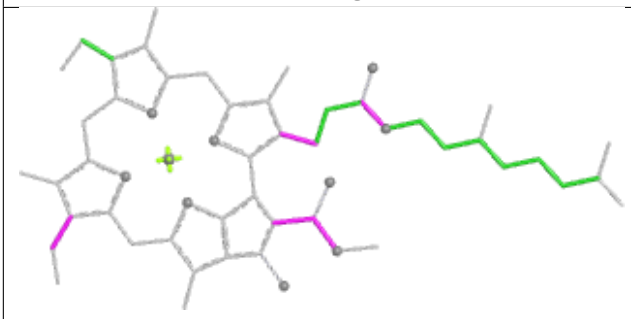
Ligand CLA a 1111



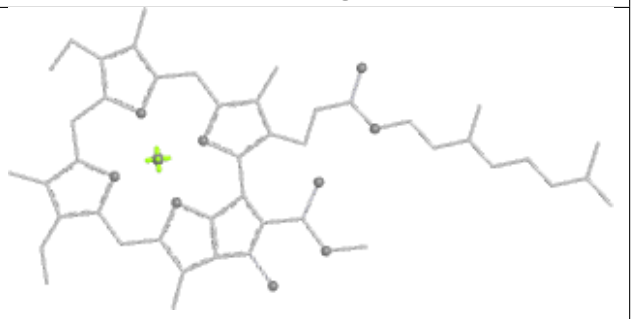
Bond lengths



Bond angles

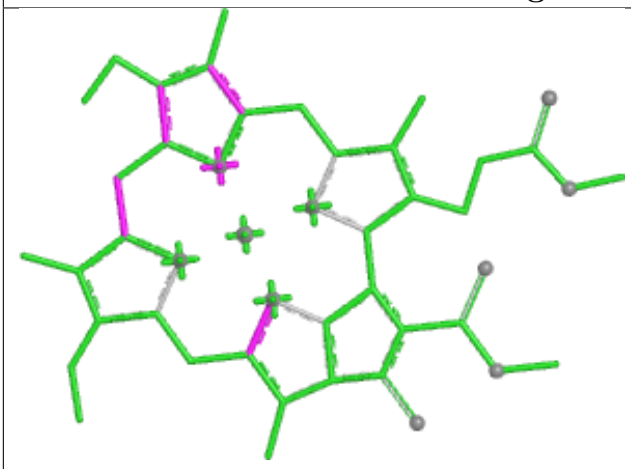


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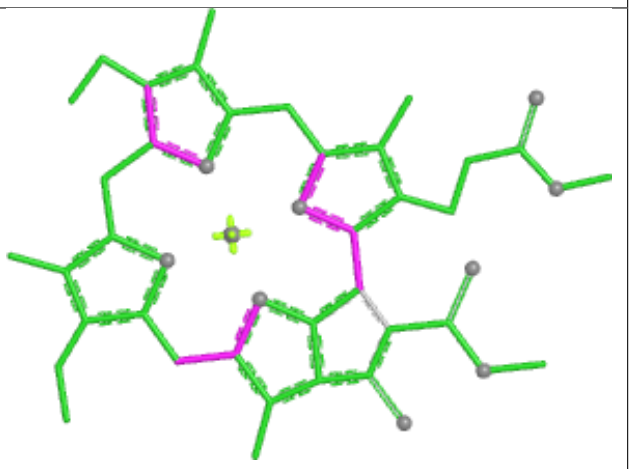


Rings

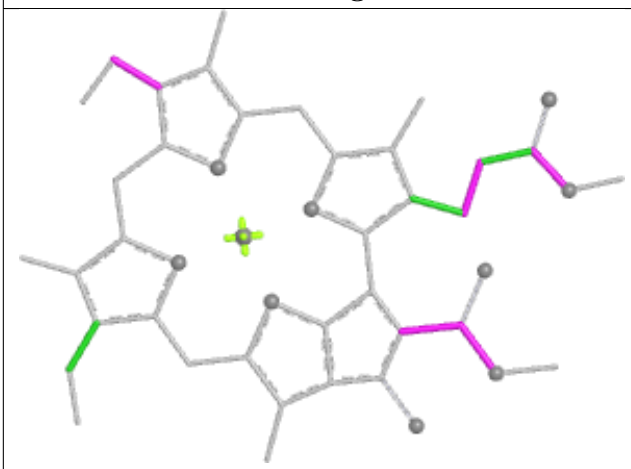
Ligand CLA u 516



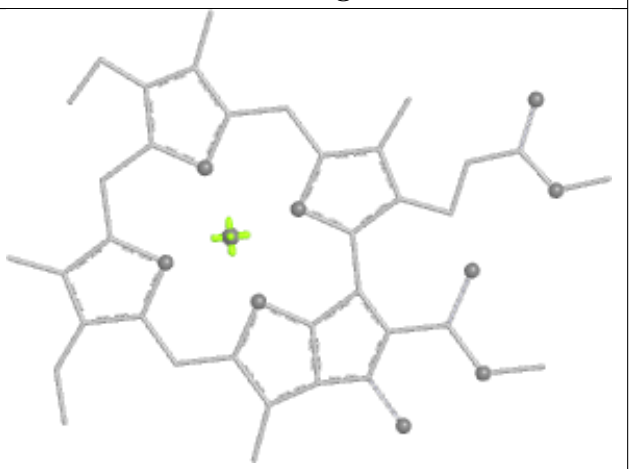
Bond lengths



Bond angles

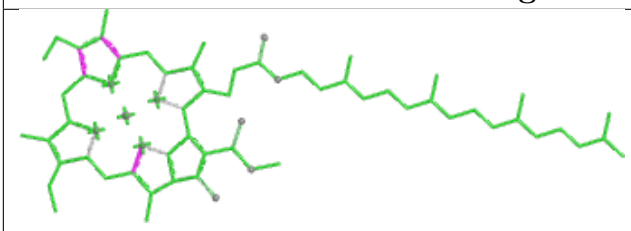


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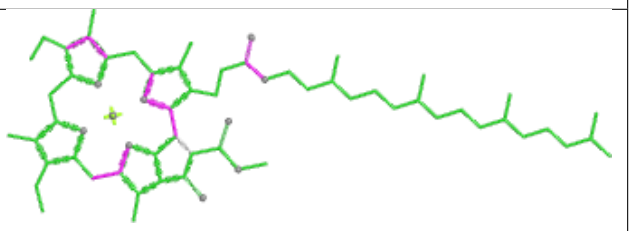


Rings

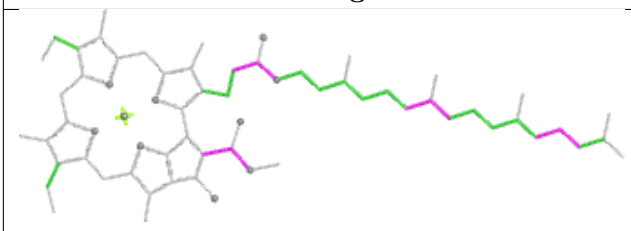
Ligand CLA W 510



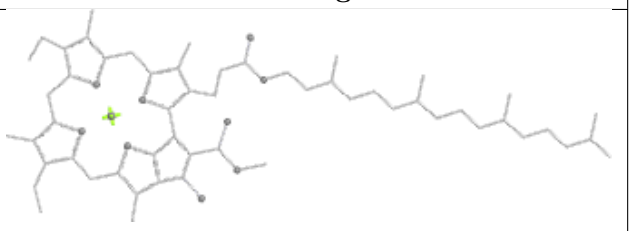
Bond lengths



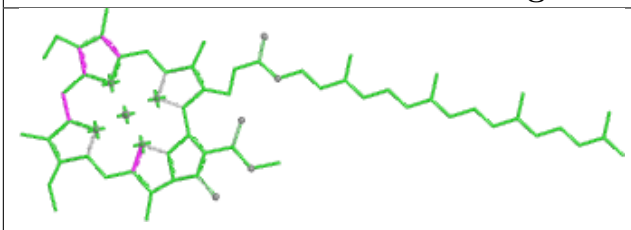
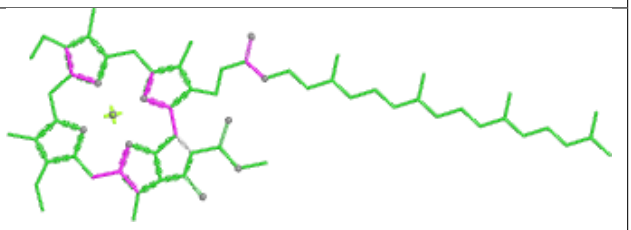
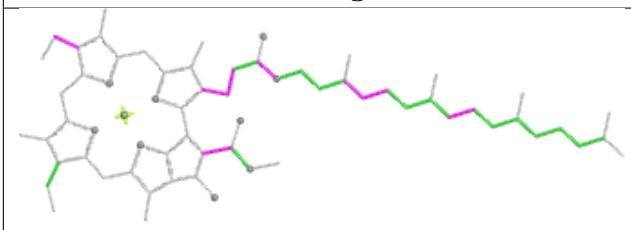
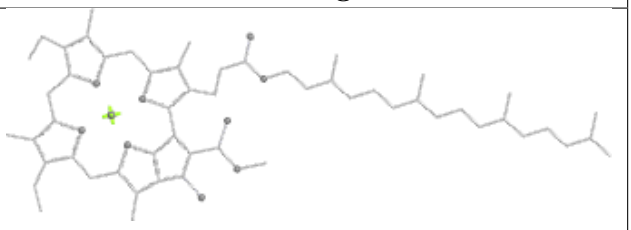
Bond angles

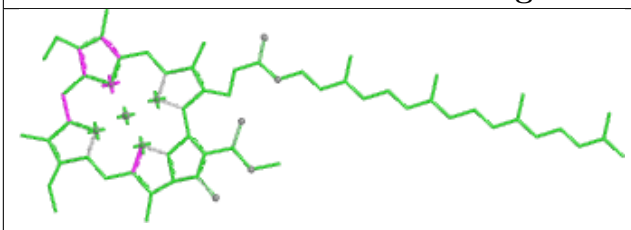
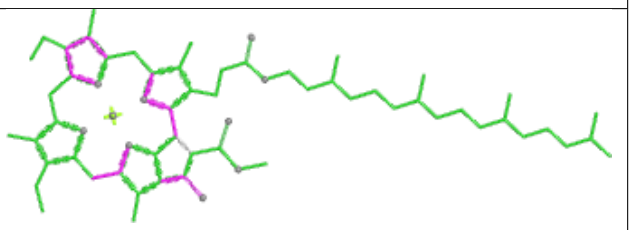
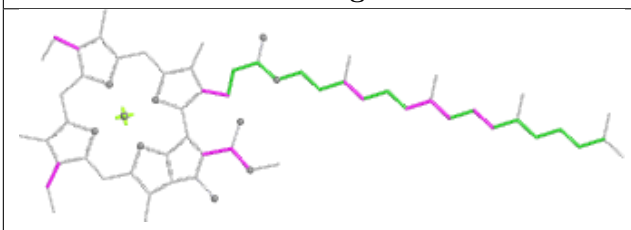
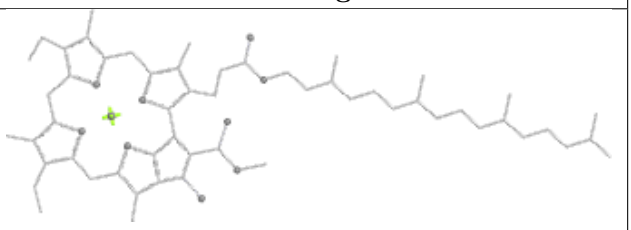


Torsions

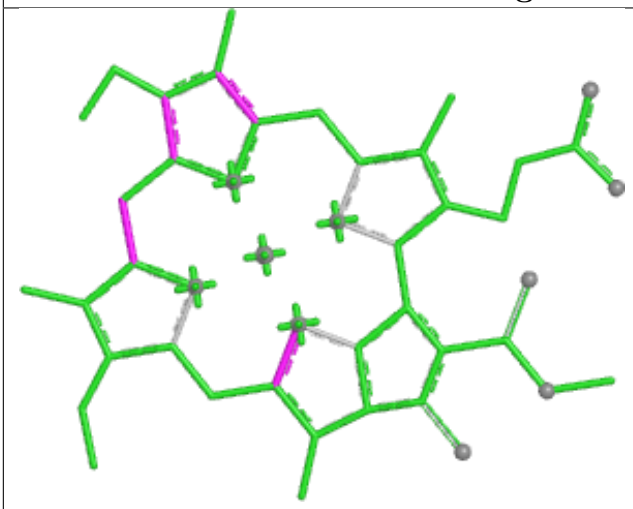


Rings

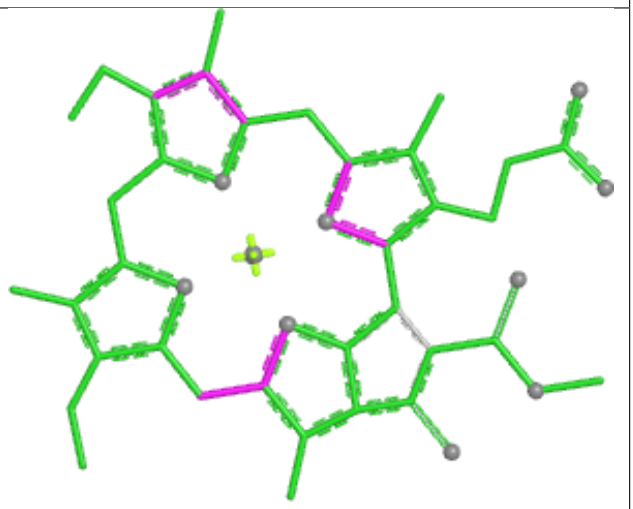
Ligand CLA x 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1210	
 Bond lengths	 Bond angles
 Torsions	 Rings

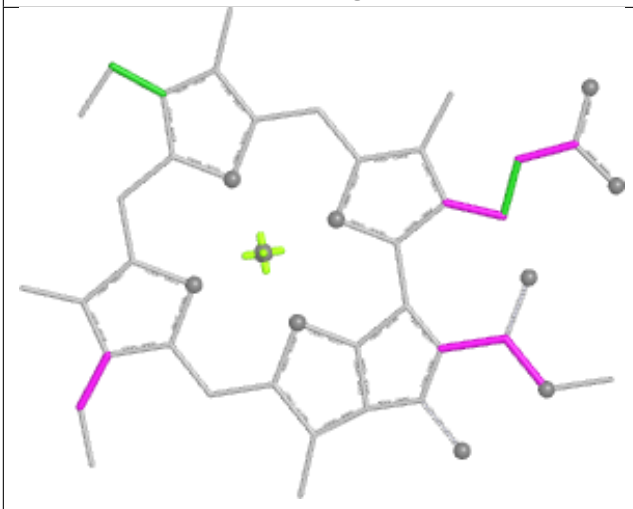
Ligand CLA T 4003



Bond lengths



Bond angles

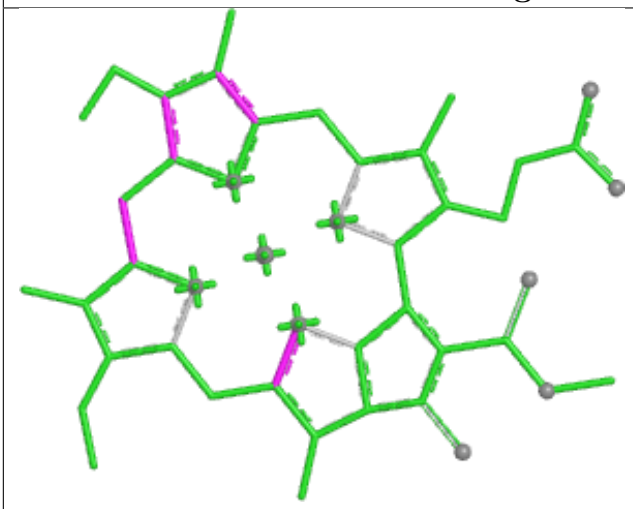


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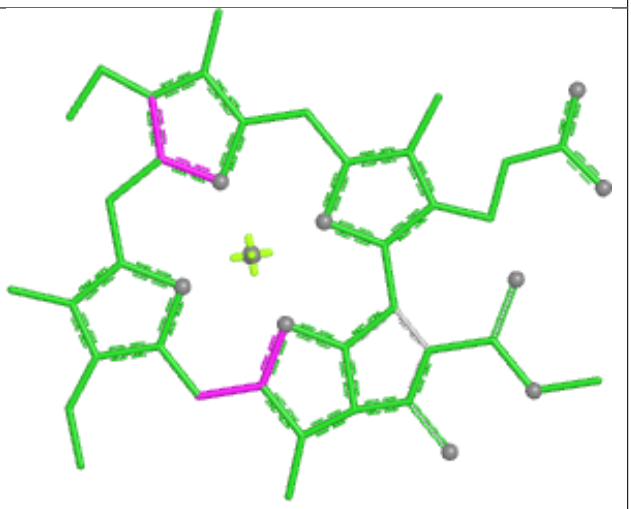


Rings

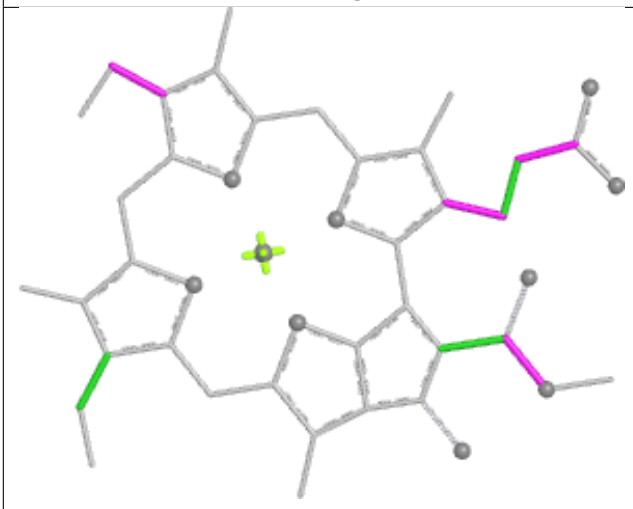
Ligand CLA G 1230



Bond lengths



Bond angles

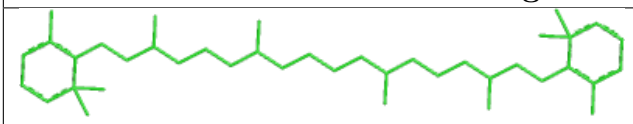


Torsions

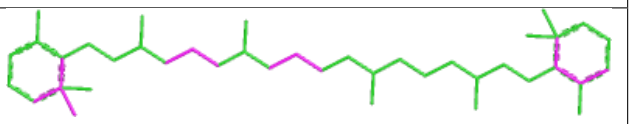


Rings

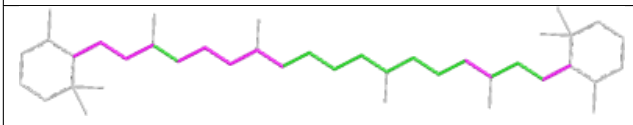
Ligand BCR w 603



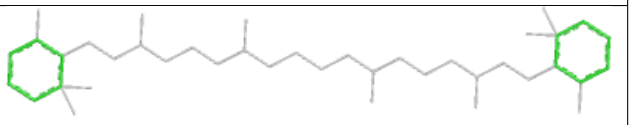
Bond lengths



Bond angles

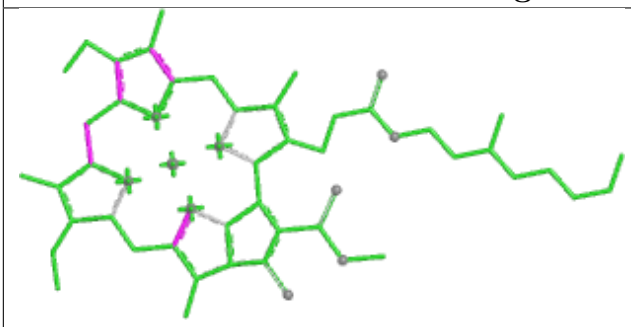


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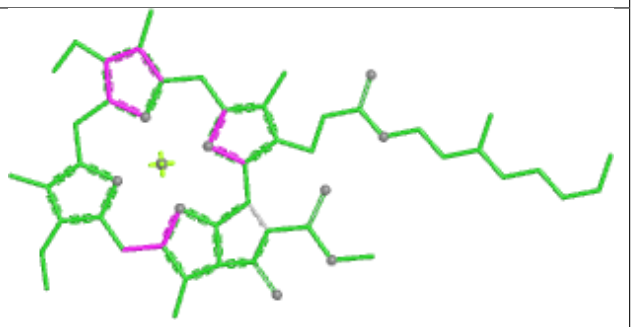


Rings

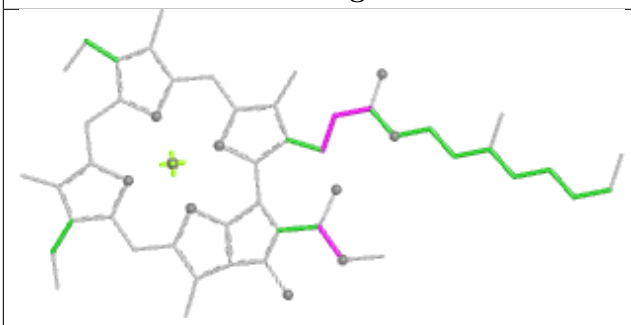
Ligand CLA G 1201



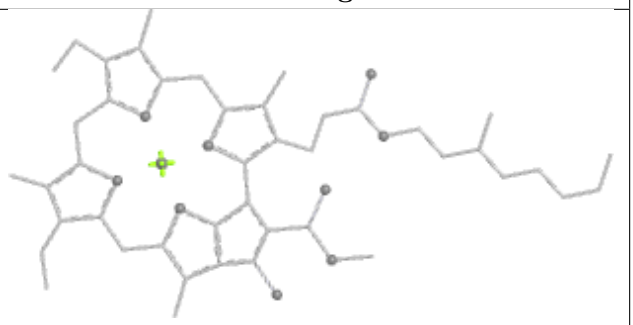
Bond lengths



Bond angles

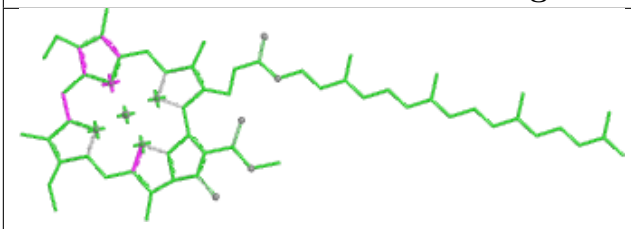


Torsions

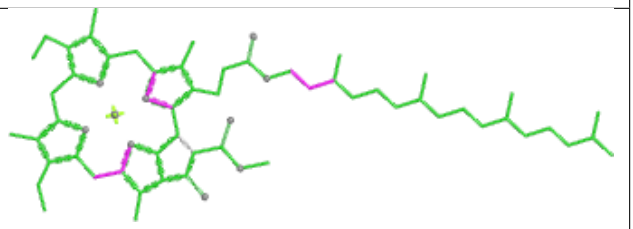


Rings

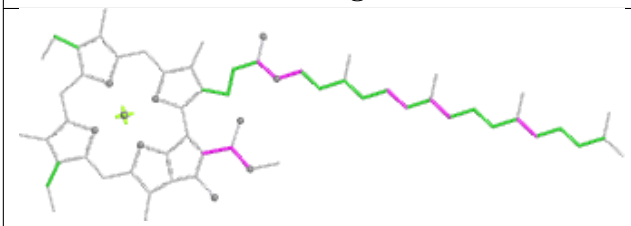
Ligand CLA r 507



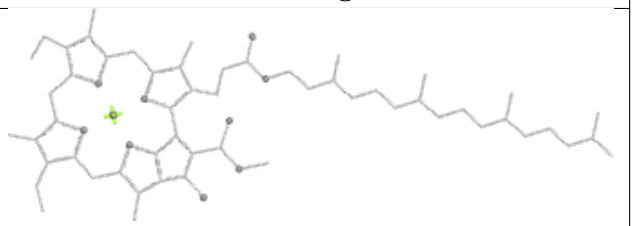
Bond lengths



Bond angles

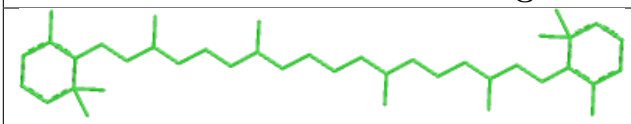


Torsions

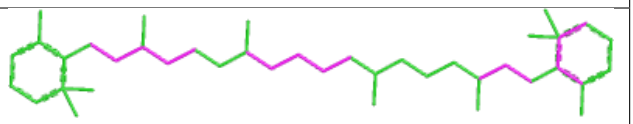


Rings

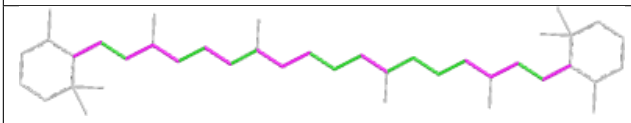
Ligand BCR b 4014



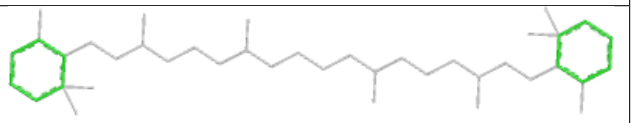
Bond lengths



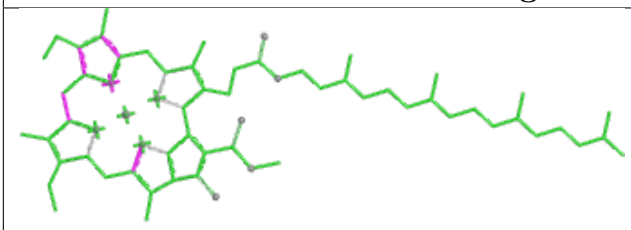
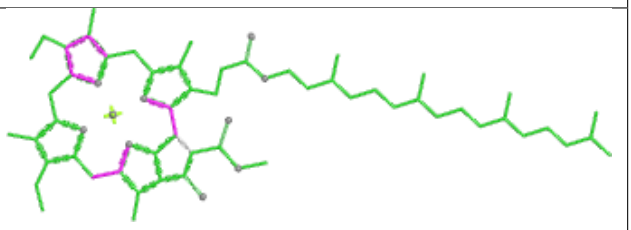
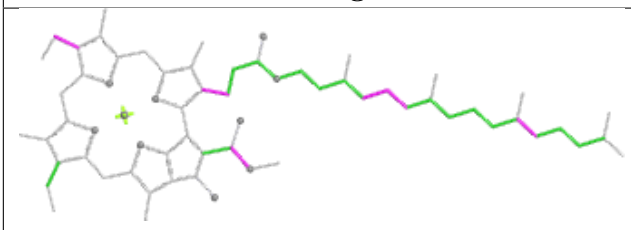
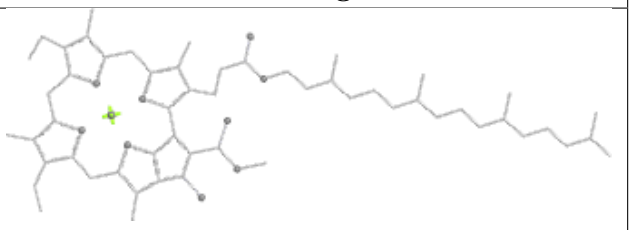
Bond angles

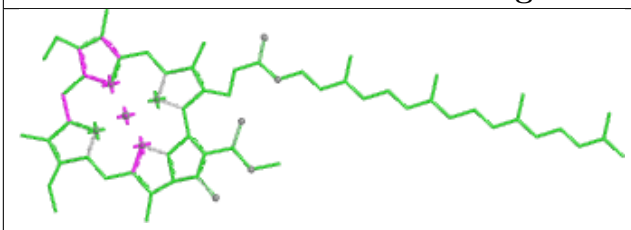
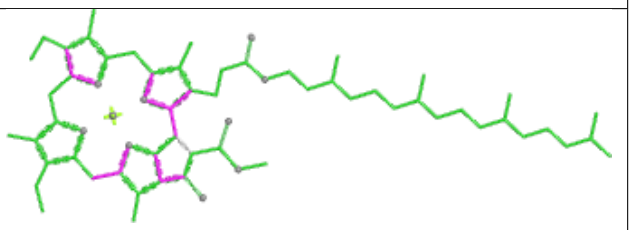
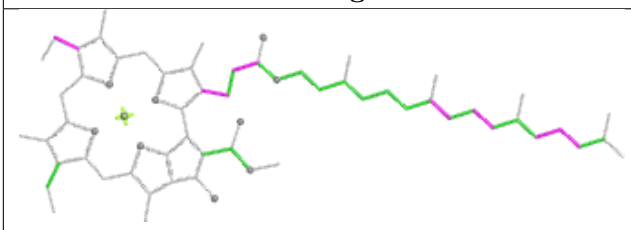
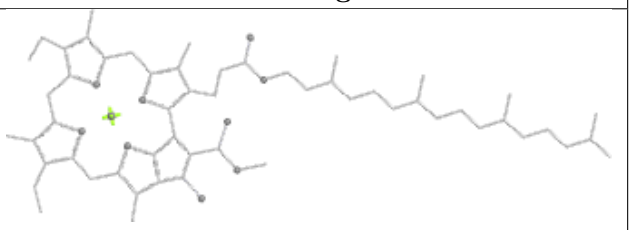


Torsions

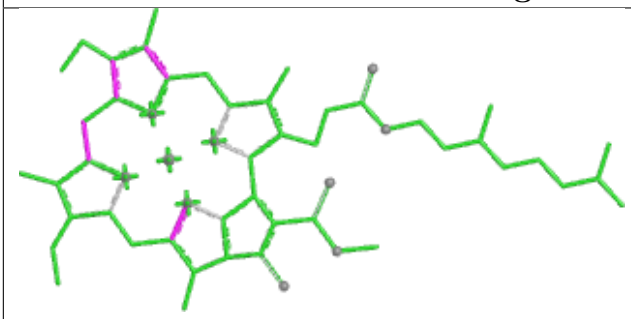


Rings

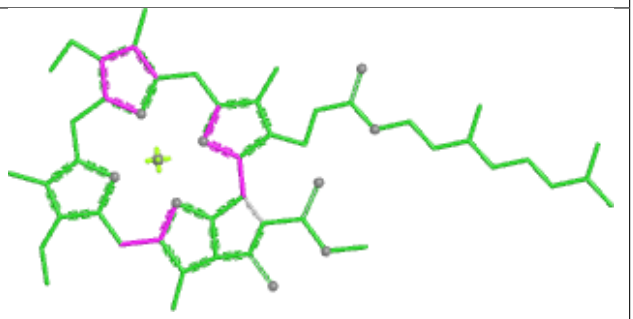
Ligand CLA a 1119	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1023	
 Bond lengths	 Bond angles
 Torsions	 Rings

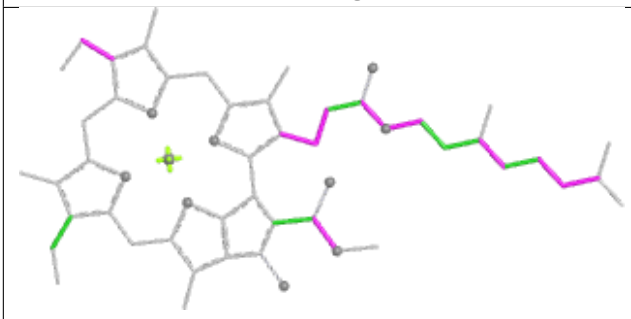
Ligand CLA G 1228



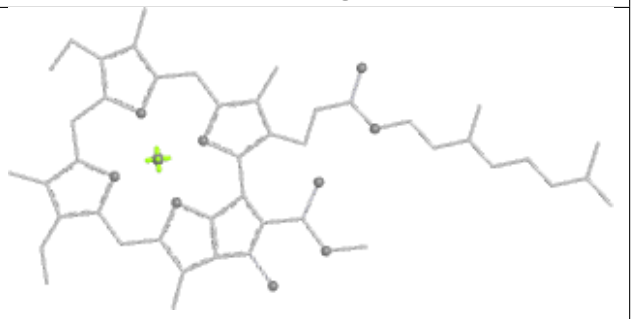
Bond lengths



Bond angles

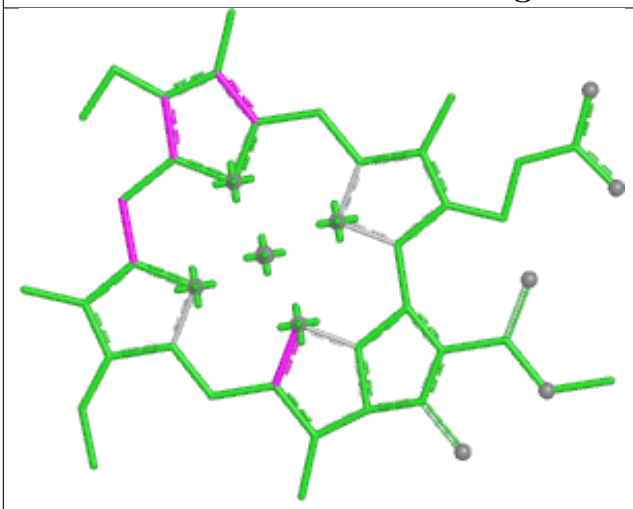


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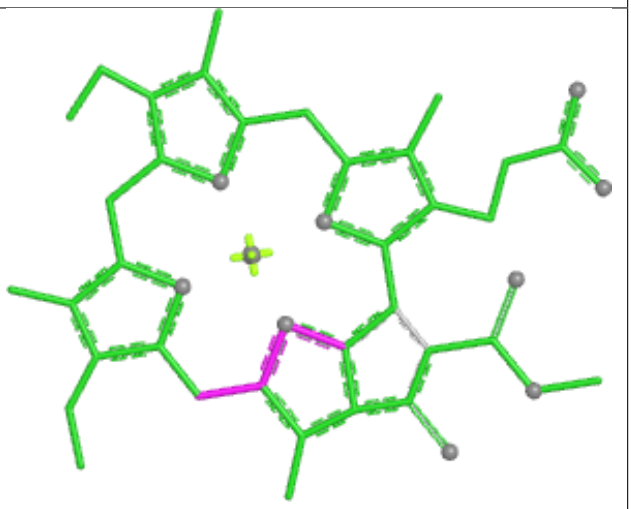


Rings

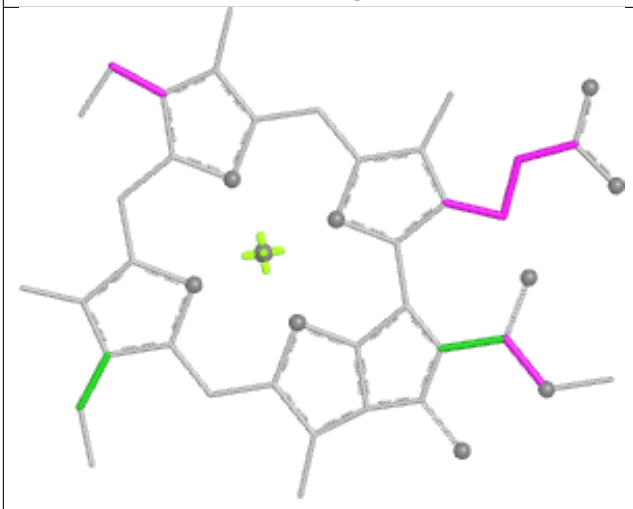
Ligand CLA G 1217



Bond lengths



Bond angles

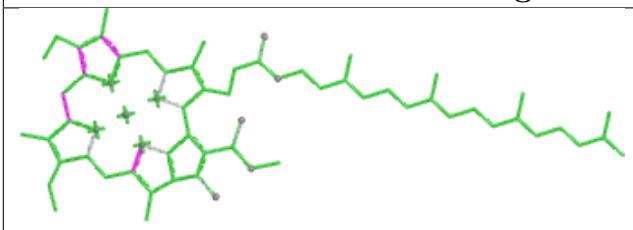


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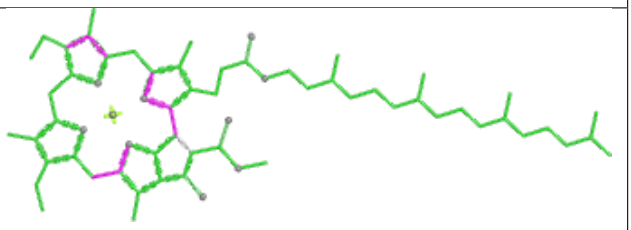


Rings

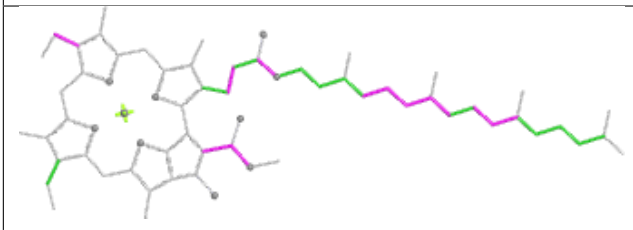
Ligand CLA H 1106



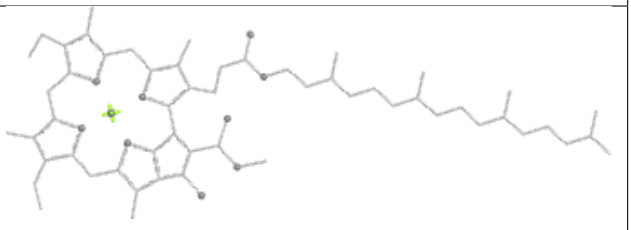
Bond lengths



Bond angles

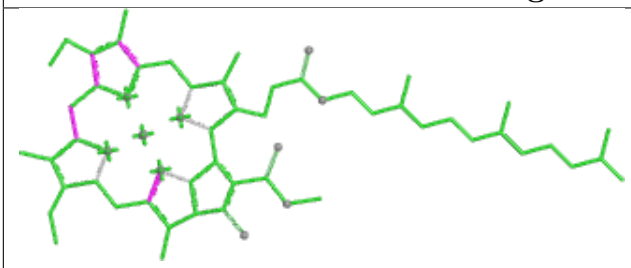


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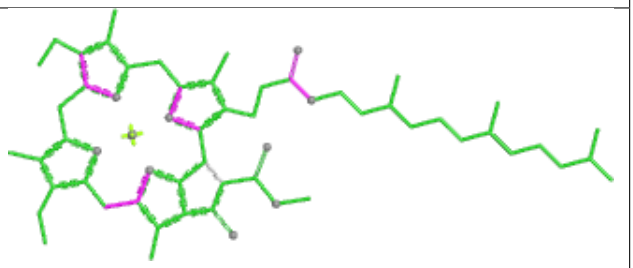


Rings

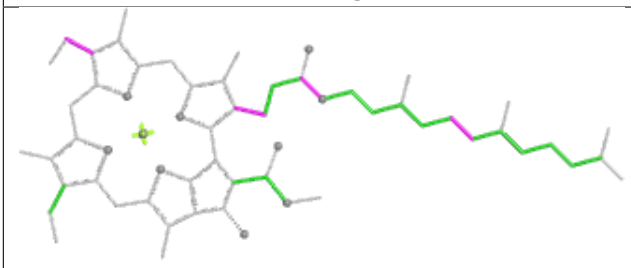
Ligand CLA n 504



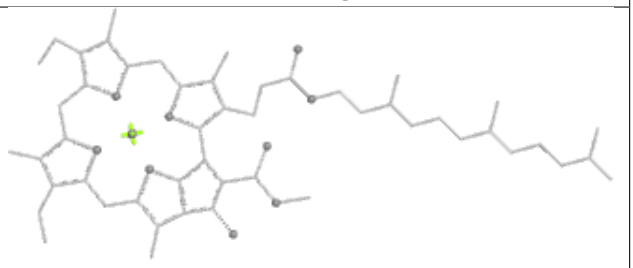
Bond lengths



Bond angles

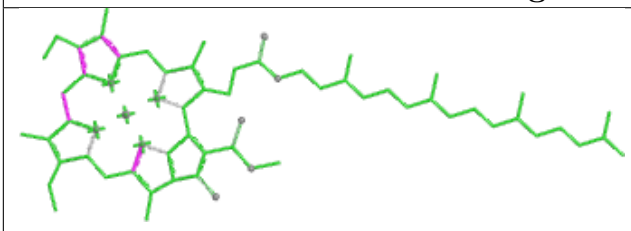


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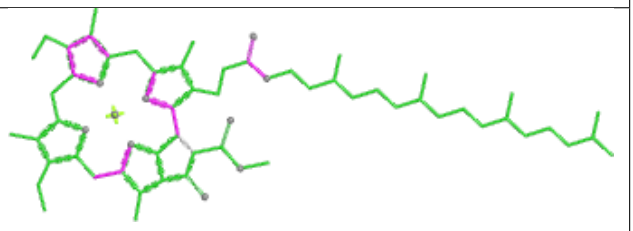


Rings

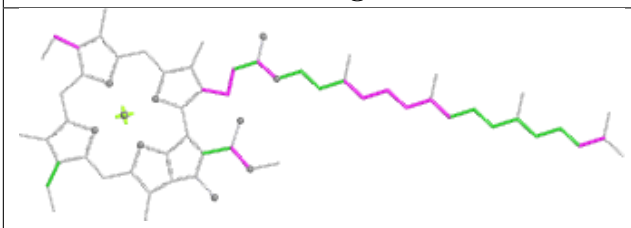
Ligand CLA o 515



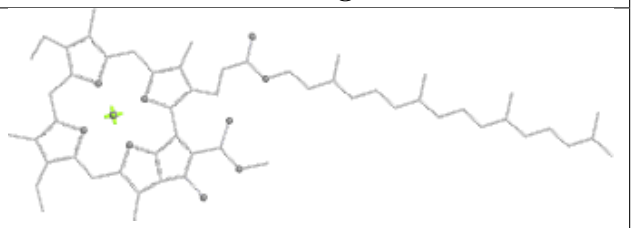
Bond lengths



Bond angles

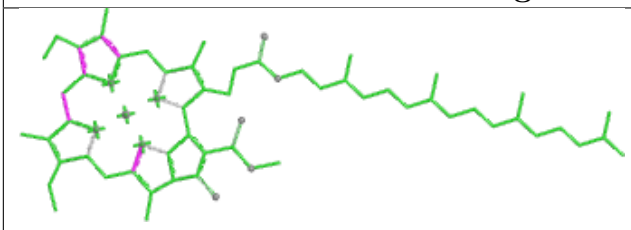


Torsions

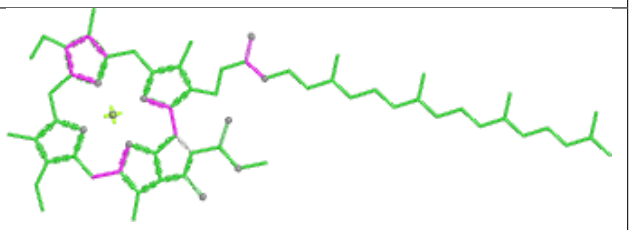


Rings

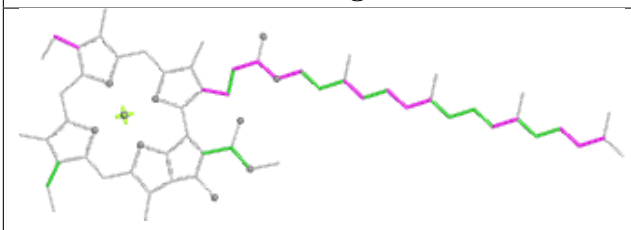
Ligand CLA G 1202



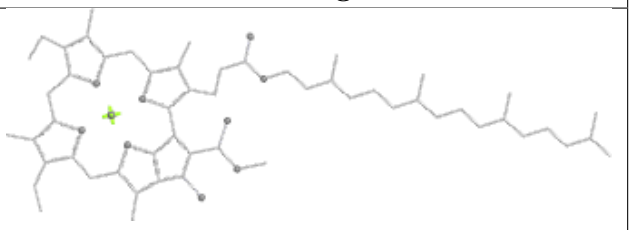
Bond lengths



Bond angles

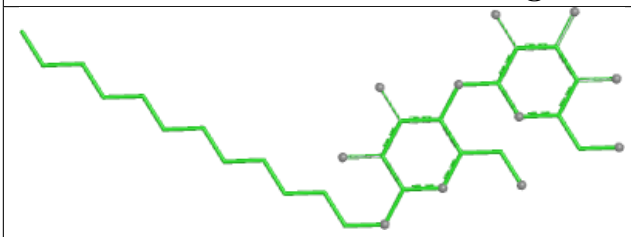


Torsions

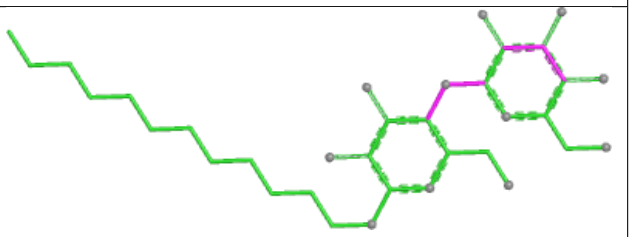


Rings

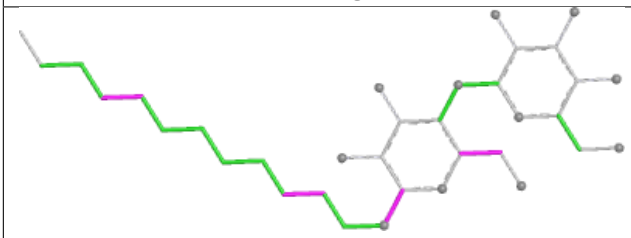
Ligand LMU r 606



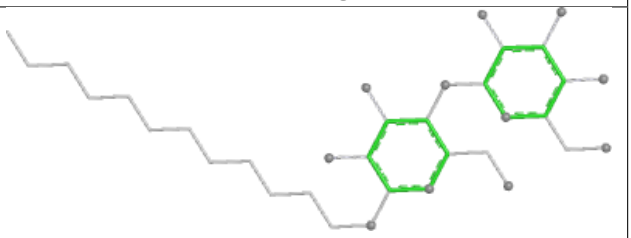
Bond lengths



Bond angles



Torsions

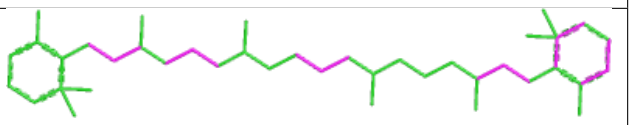


Rings

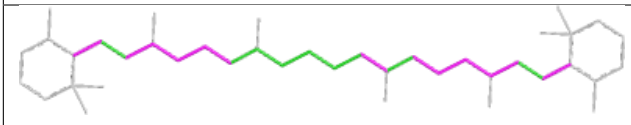
Ligand BCR H 4011



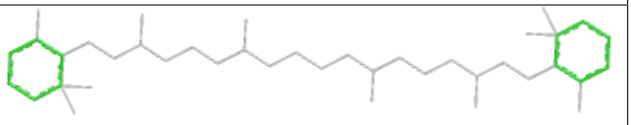
Bond lengths



Bond angles

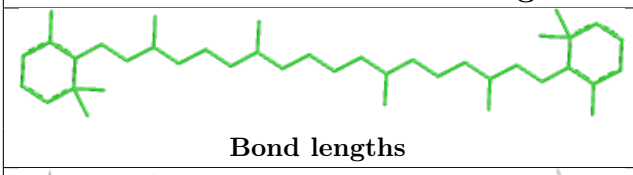


Torsions

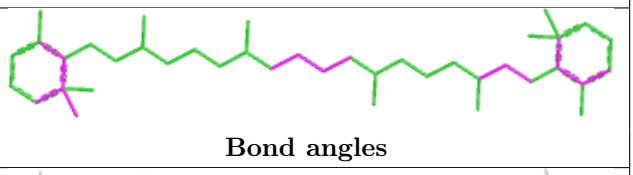


Rings

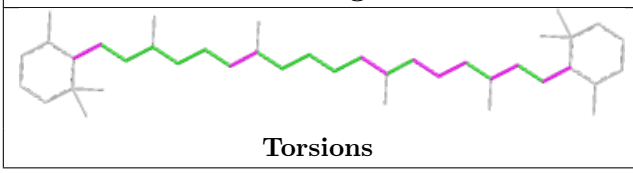
Ligand BCR J 4013



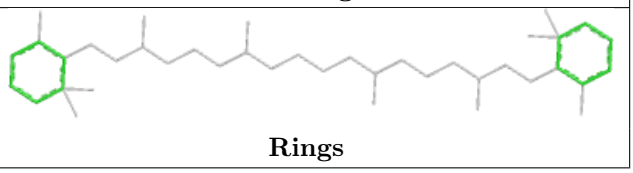
Bond lengths



Bond angles

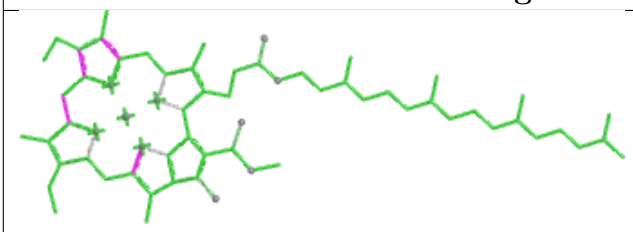


Torsions

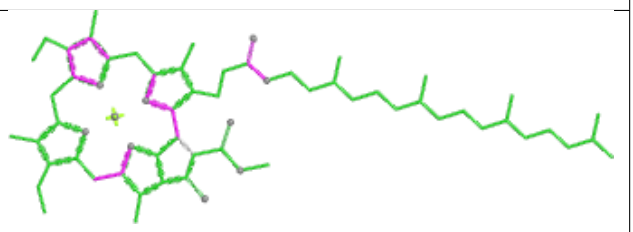


Rings

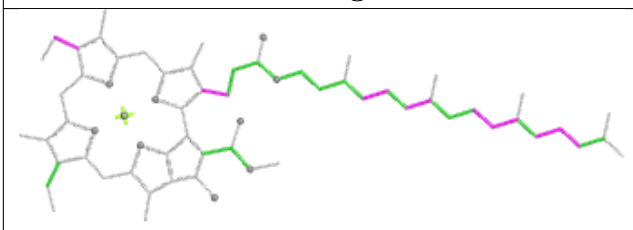
Ligand CLA H 1109



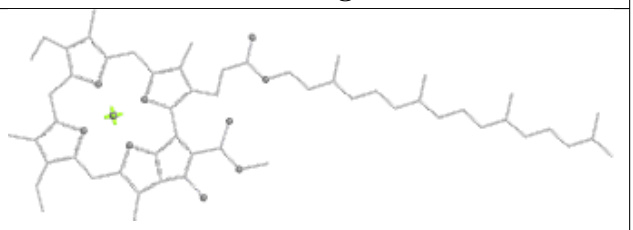
Bond lengths



Bond angles

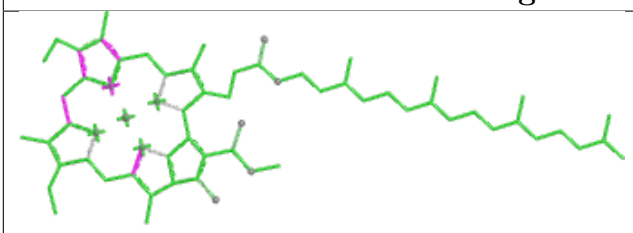


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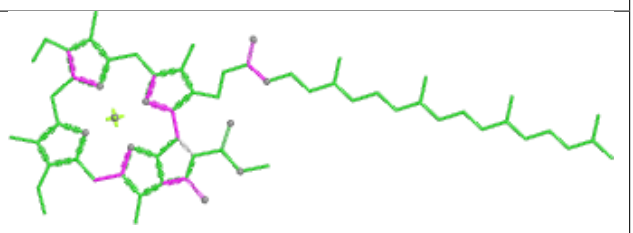


Rings

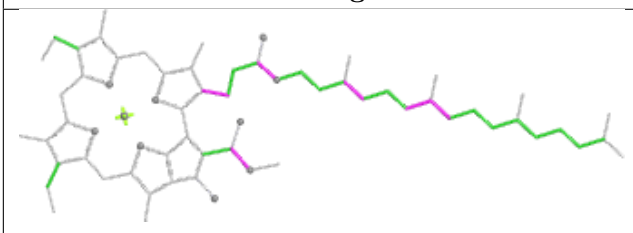
Ligand CLA b 1210



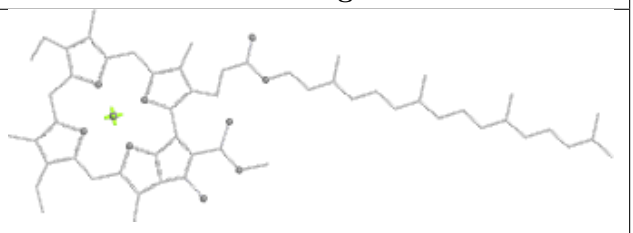
Bond lengths



Bond angles

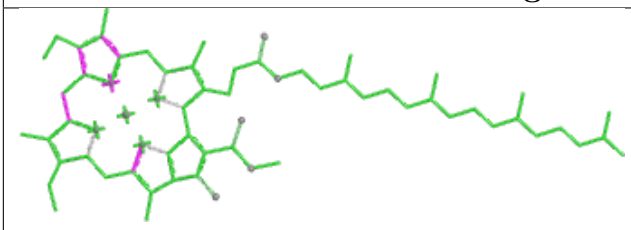


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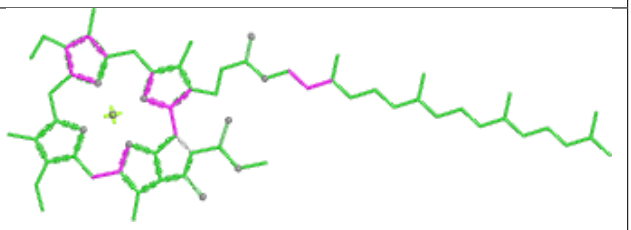


Rings

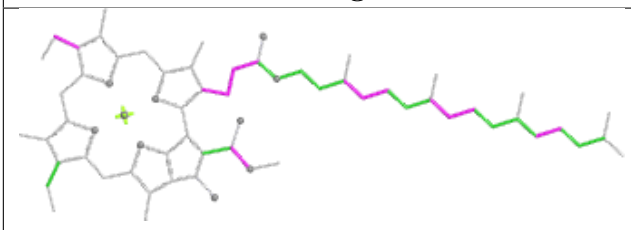
Ligand CLA Y 505



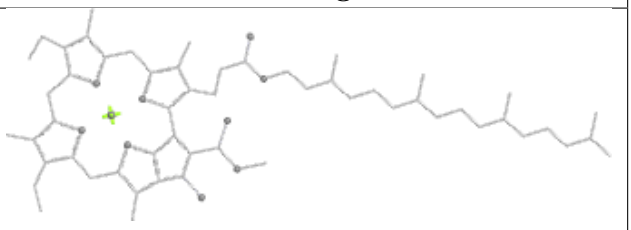
Bond lengths



Bond angles

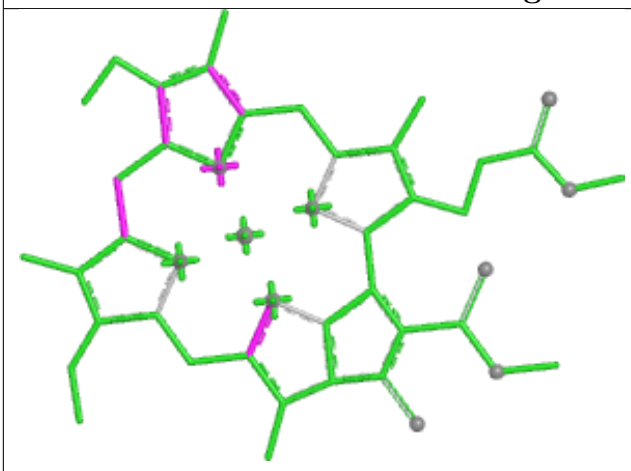


Torsions

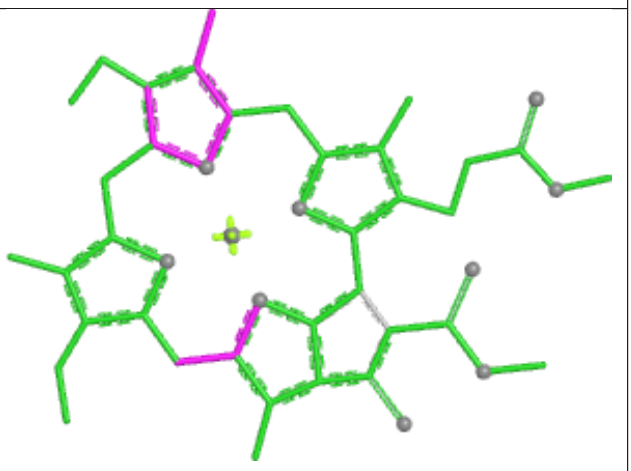


Rings

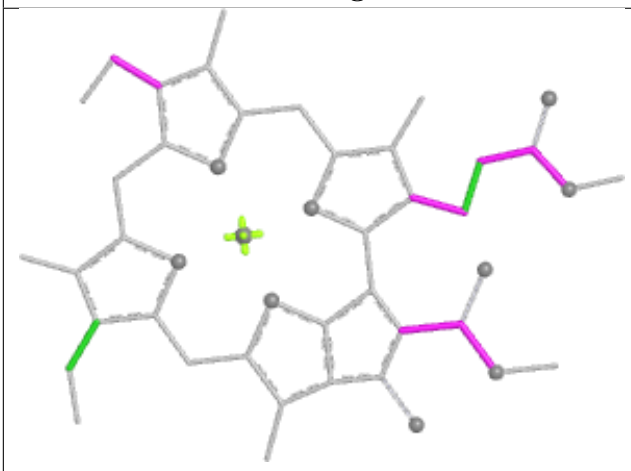
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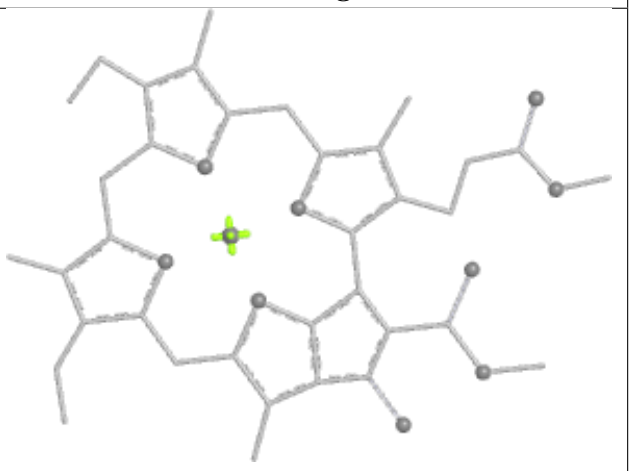
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Bond angles

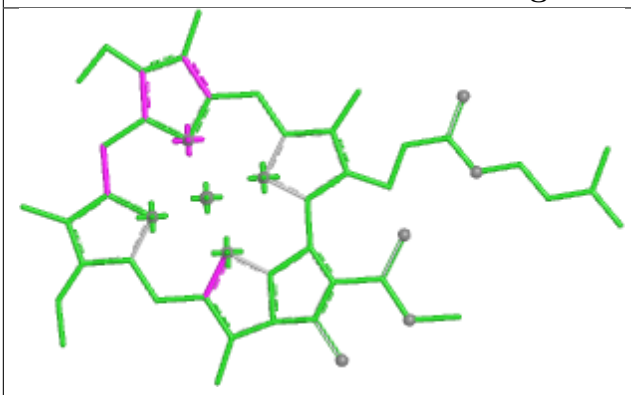


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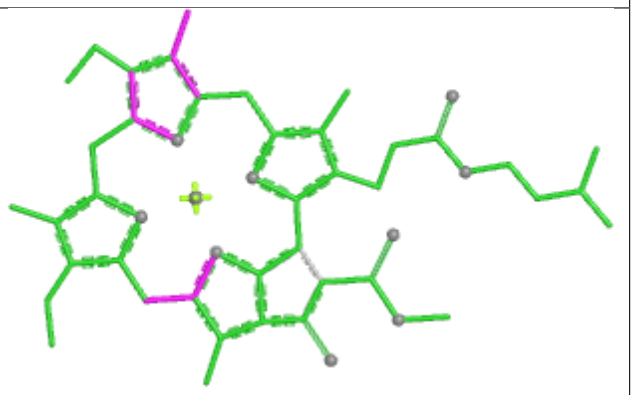


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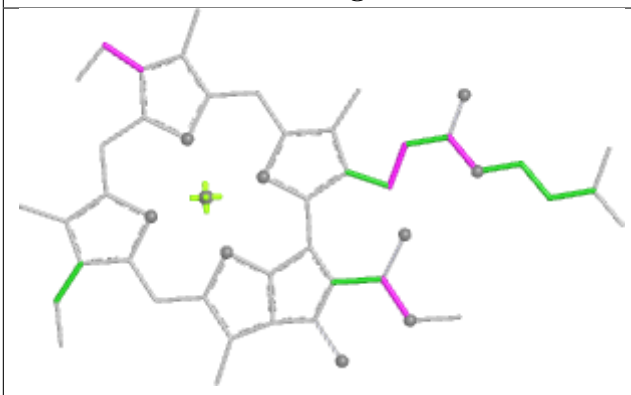
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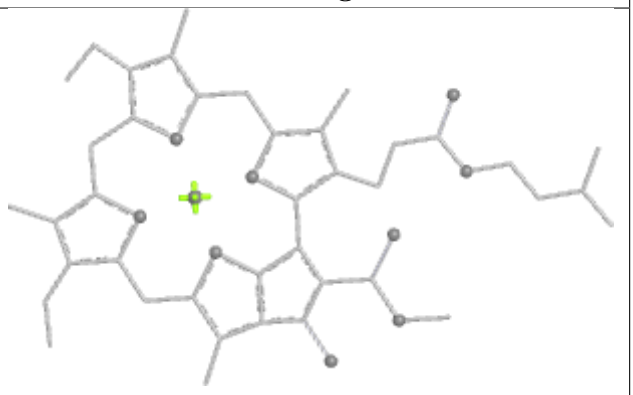
Bond lengths



Bond angles

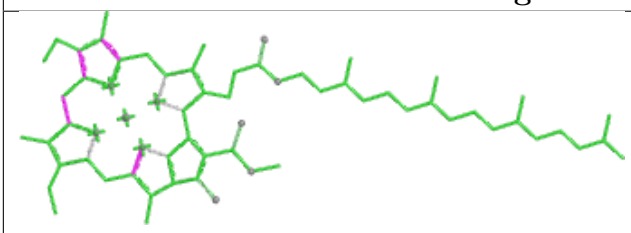


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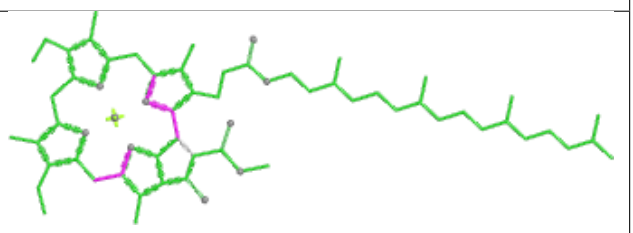


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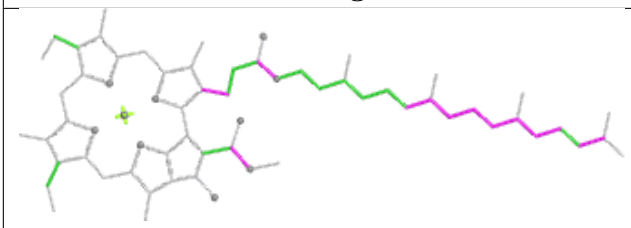
Ligand CLA G 1221



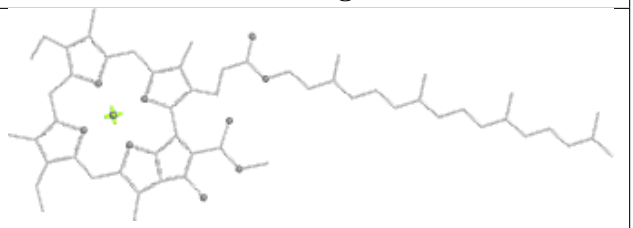
Bond lengths



Bond angles

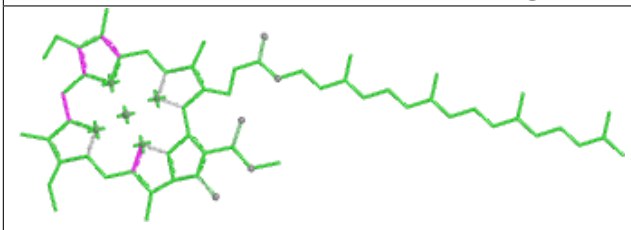


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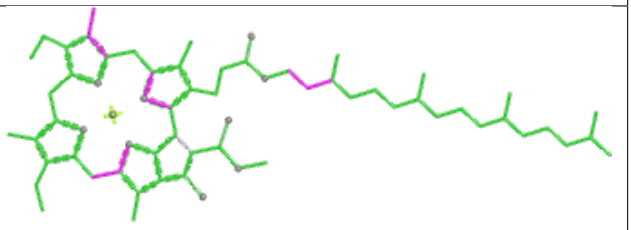


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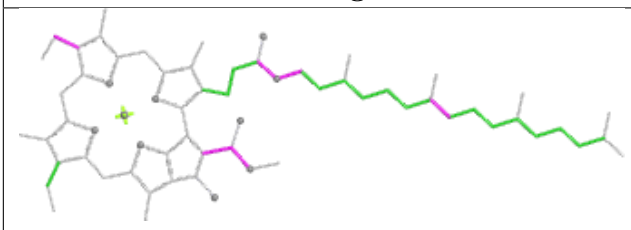
Ligand CLA X 507



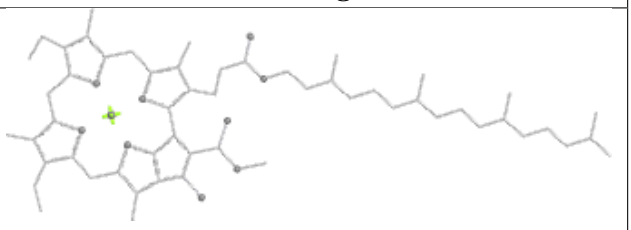
Bond lengths



Bond angles

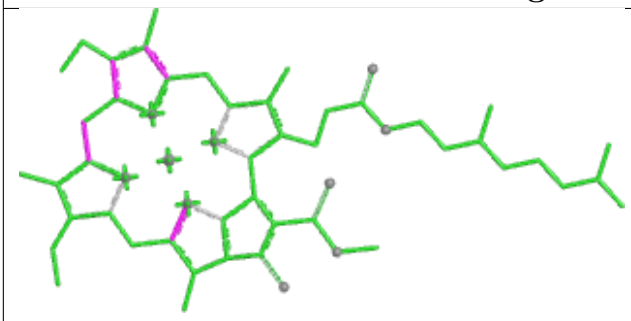


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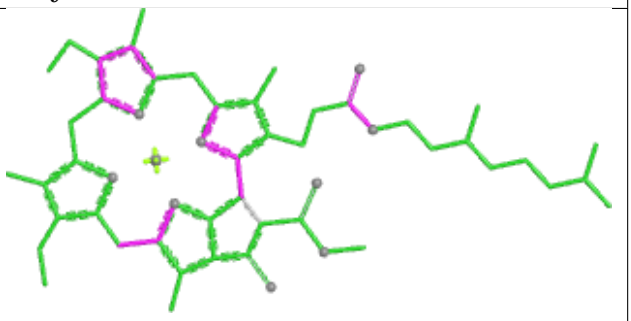


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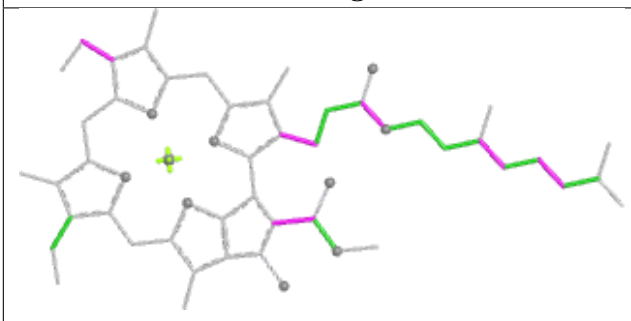
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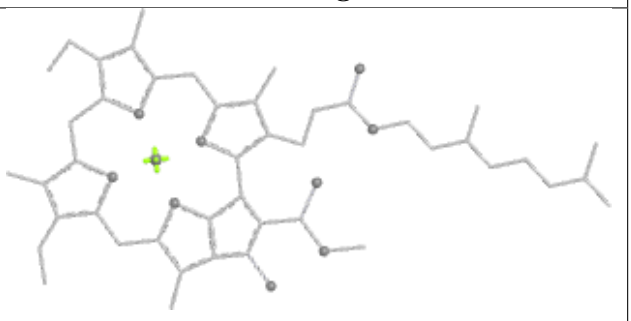
Bond lengths



Bond angles

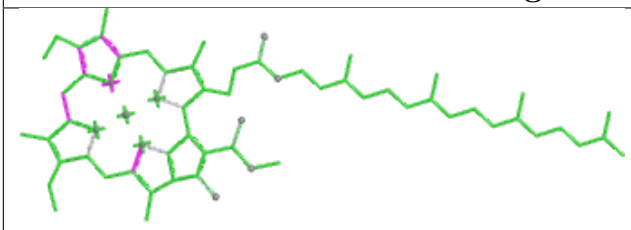


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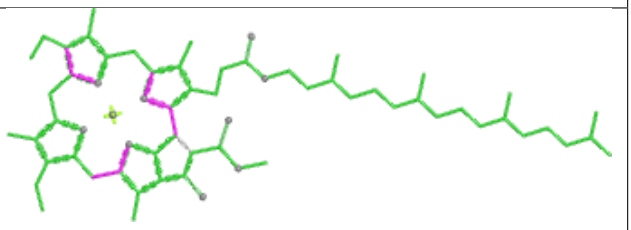


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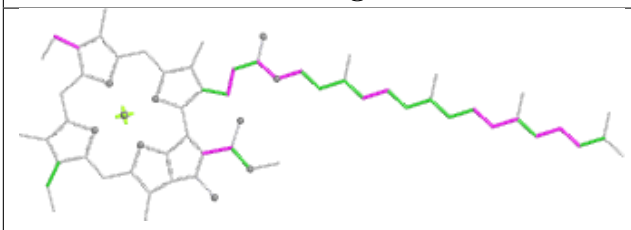
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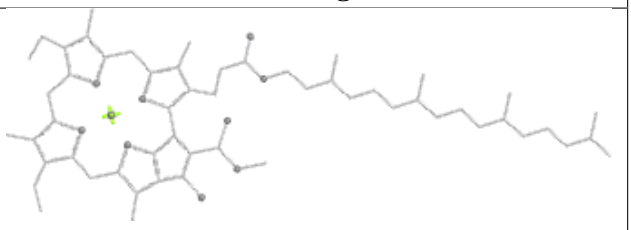
Bond lengths



Bond angles

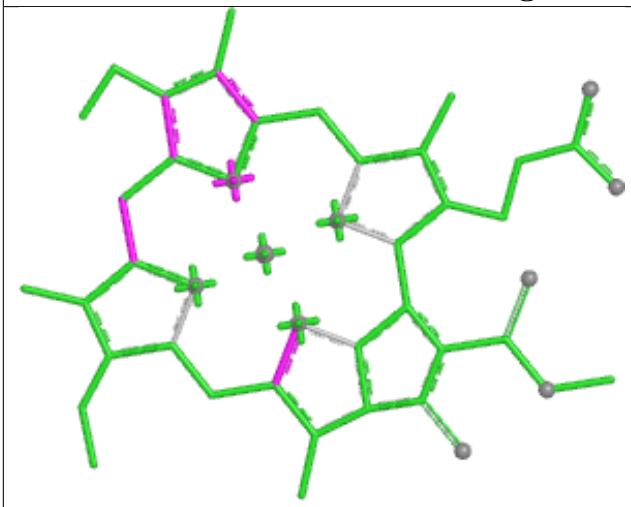


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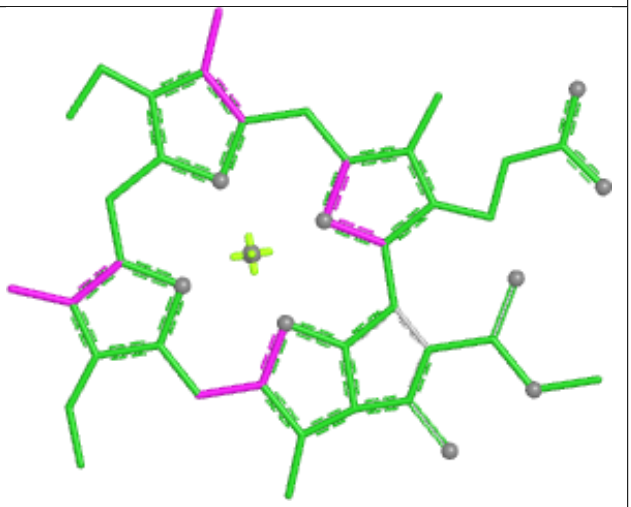


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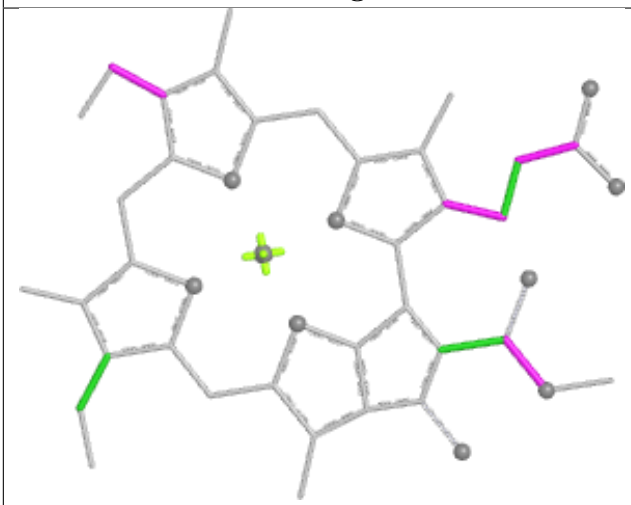
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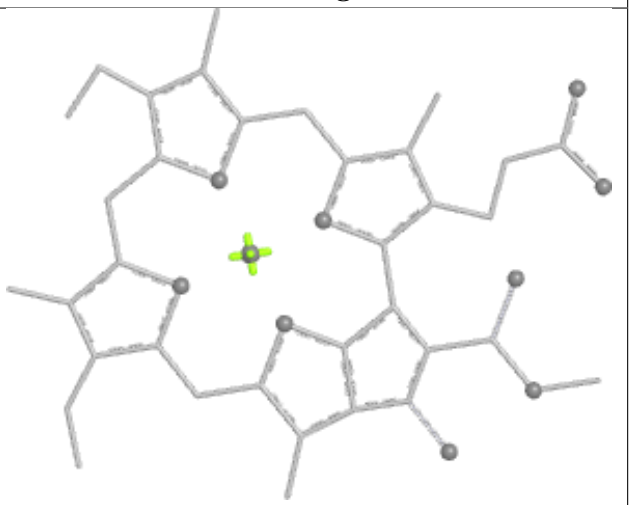
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Bond angles

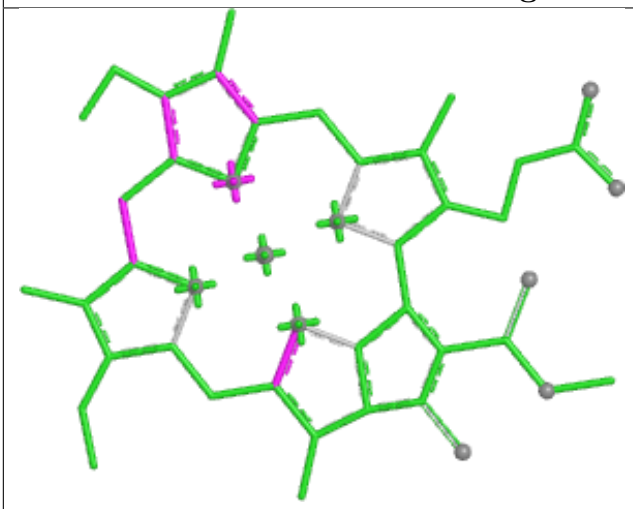


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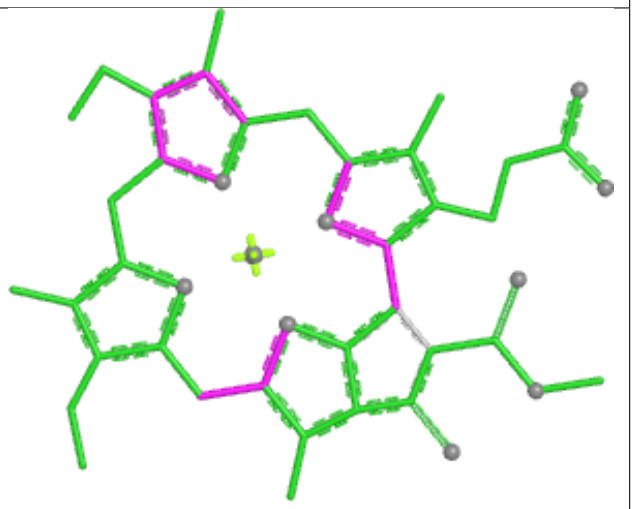


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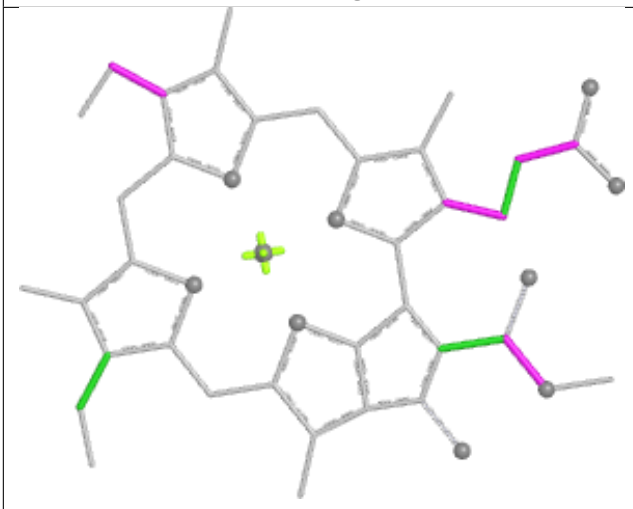
Ligand CLA a 1108



Bond lengths



Bond angles

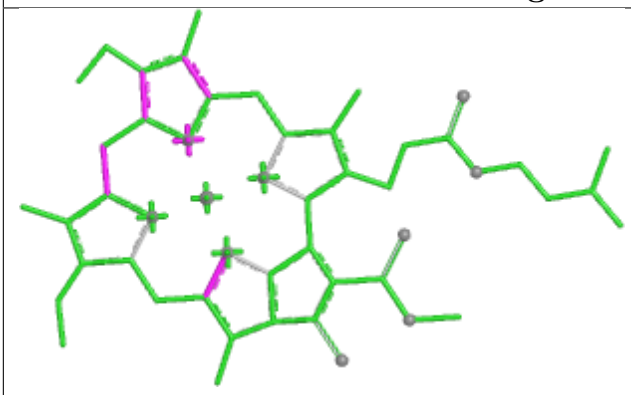


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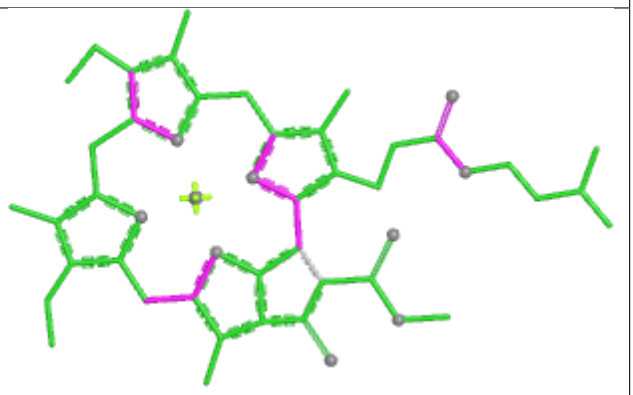


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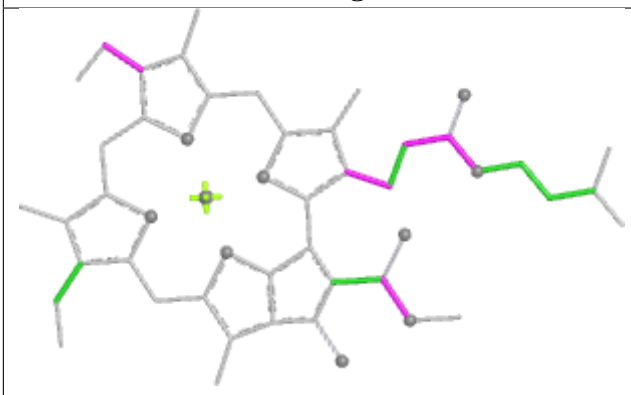
Ligand CLA x 514



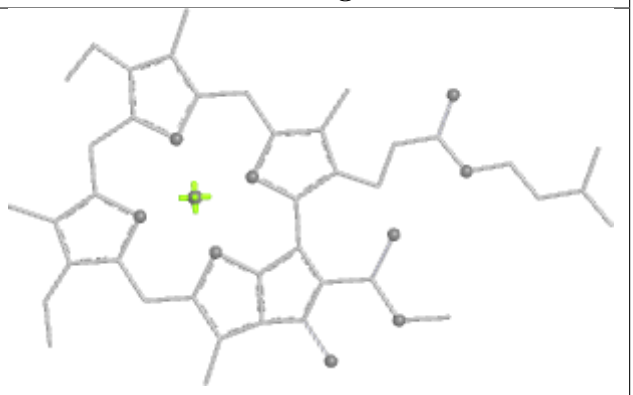
Bond lengths



Bond angles

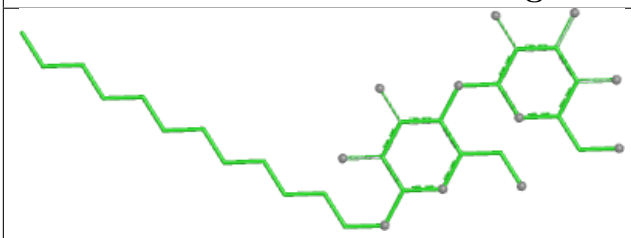


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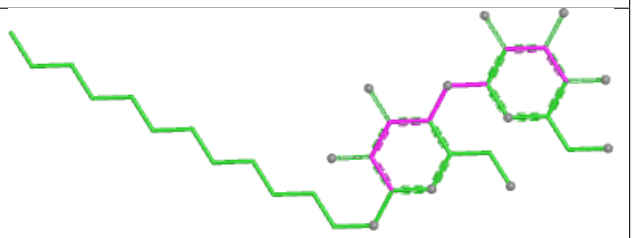


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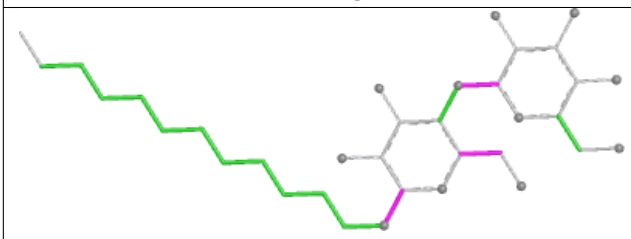
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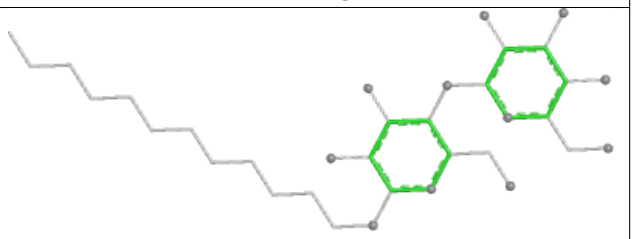
Bond lengths



Bond angles

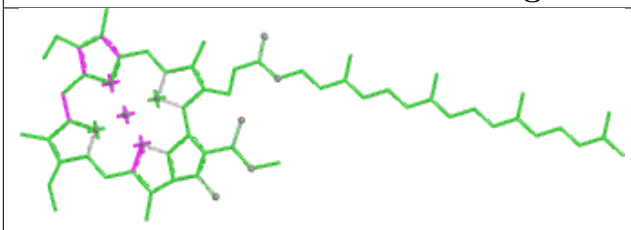


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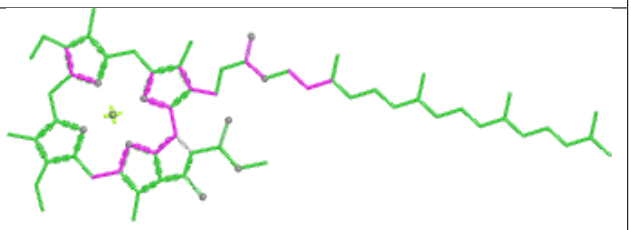


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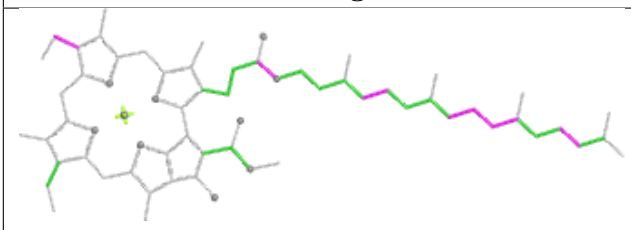
Ligand CLA Y 512



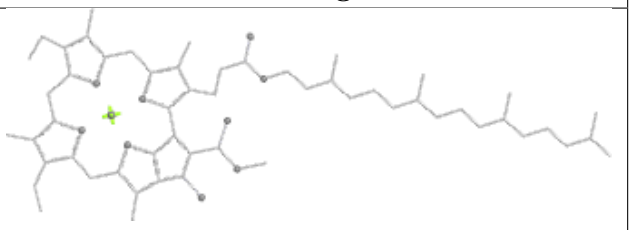
Bond lengths



Bond angles

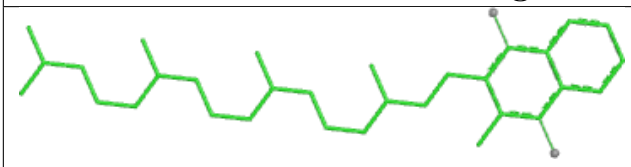


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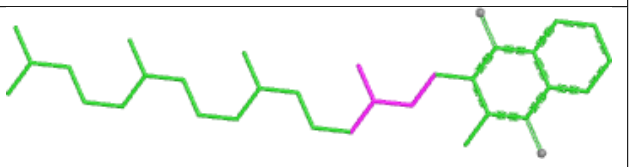


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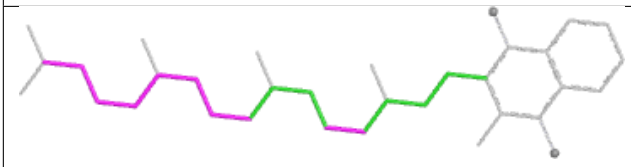
Ligand PQN G 2002



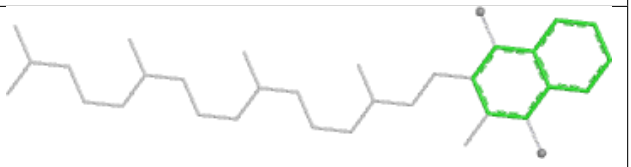
Bond lengths



Bond angles

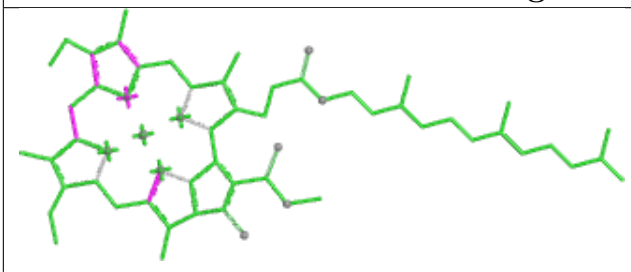


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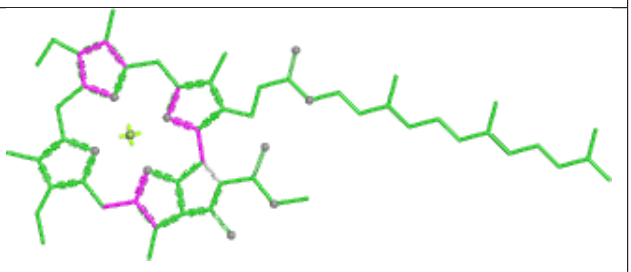


Rings

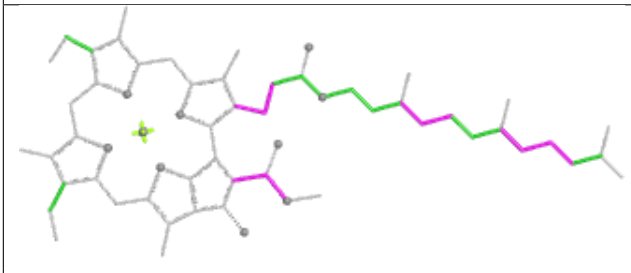
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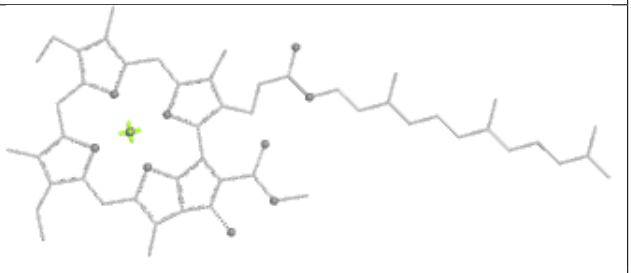
Bond lengths



Bond angles

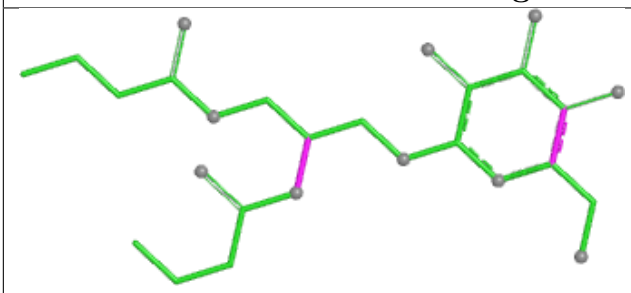


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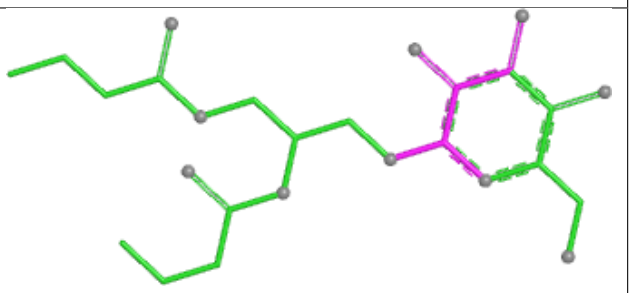


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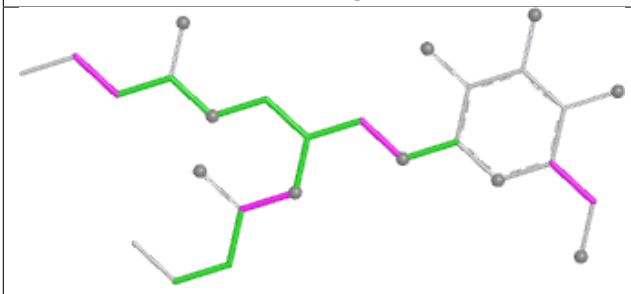
Ligand LMG F 4017



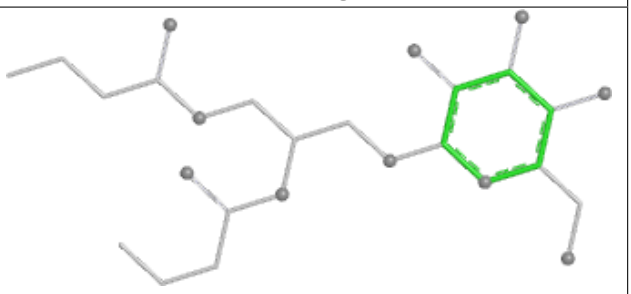
Bond lengths



Bond angles

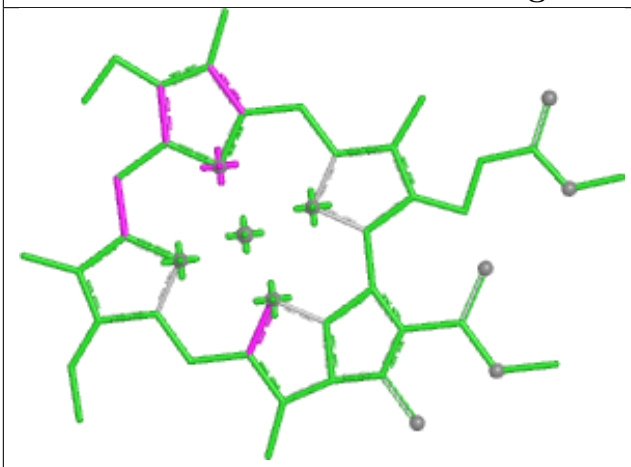


Torsions

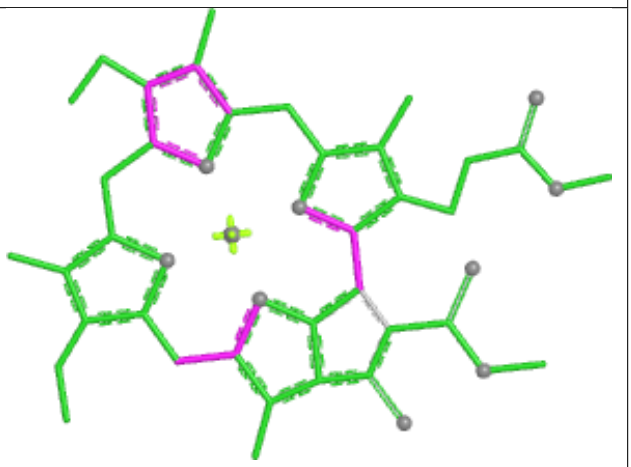


Rings

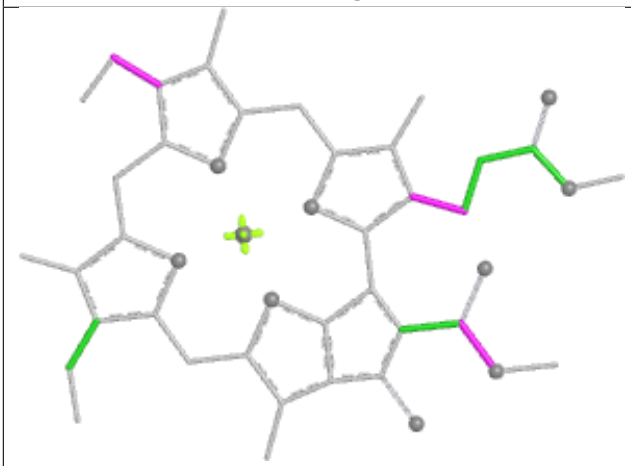
Ligand CLA o 503



Bond lengths



Bond angles

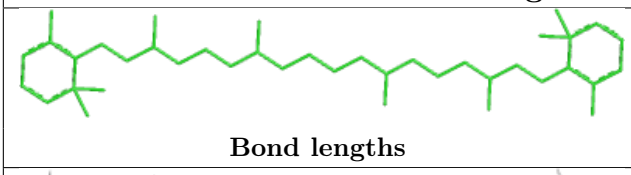


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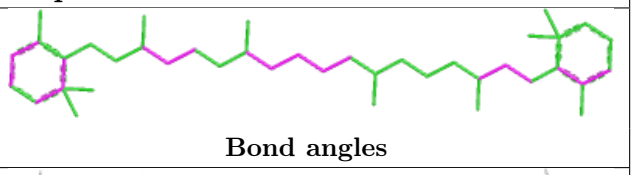


Rings

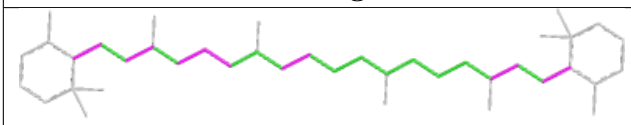
Ligand BCR p 602



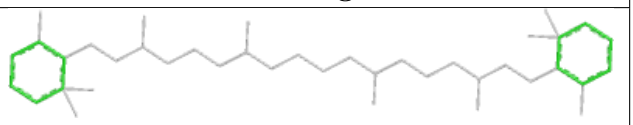
Bond lengths



Bond angles

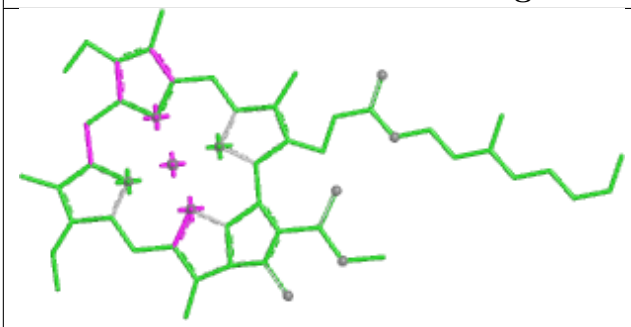


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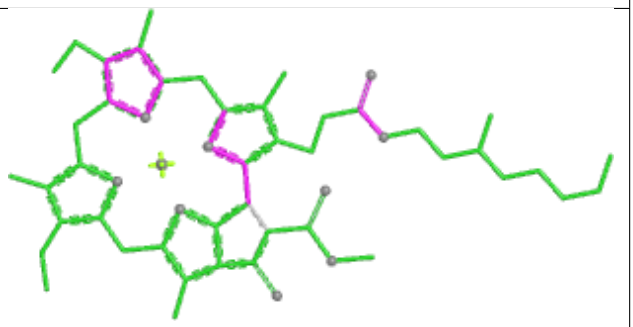


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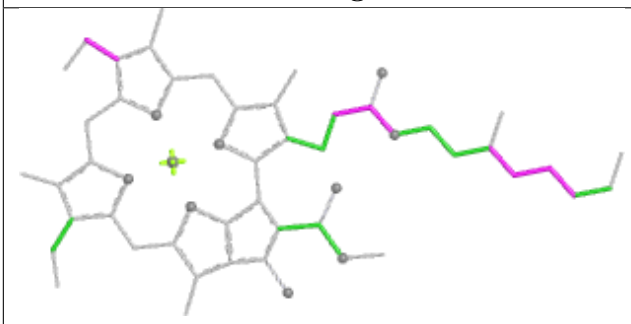
Ligand CLA H 1133



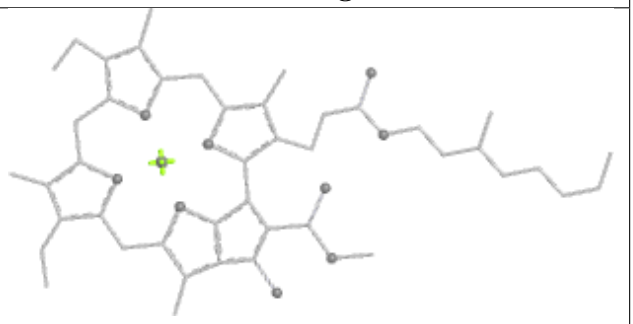
Bond lengths



Bond angles

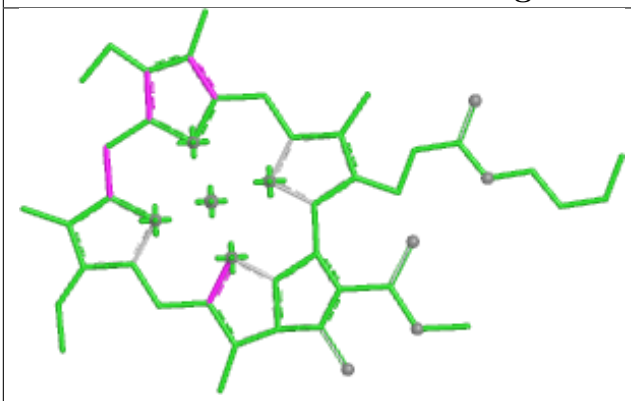


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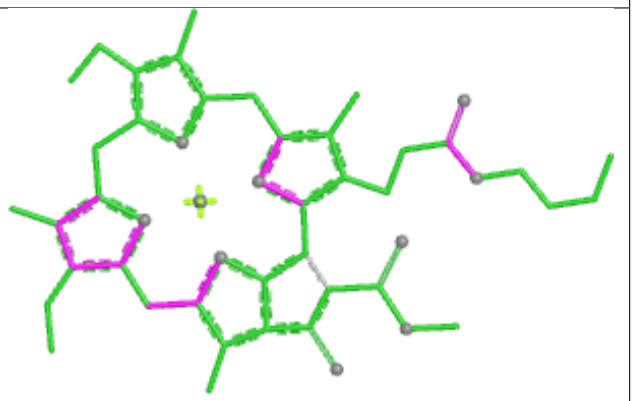


Rings

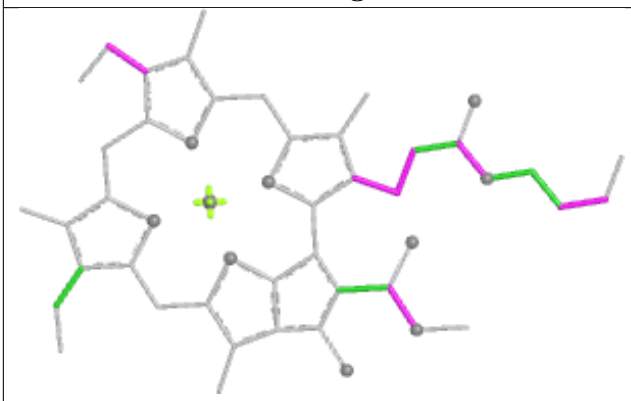
Ligand CLA H 1120



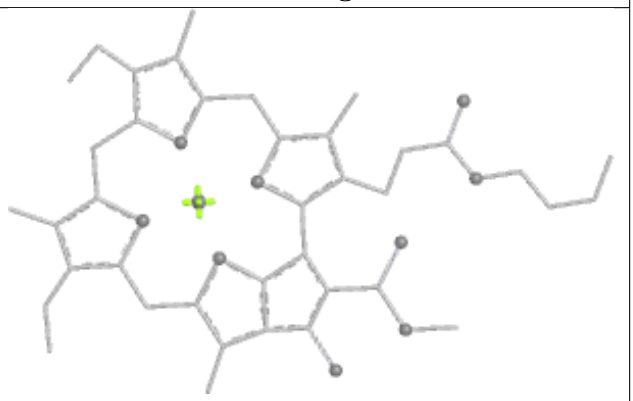
Bond lengths



Bond angles

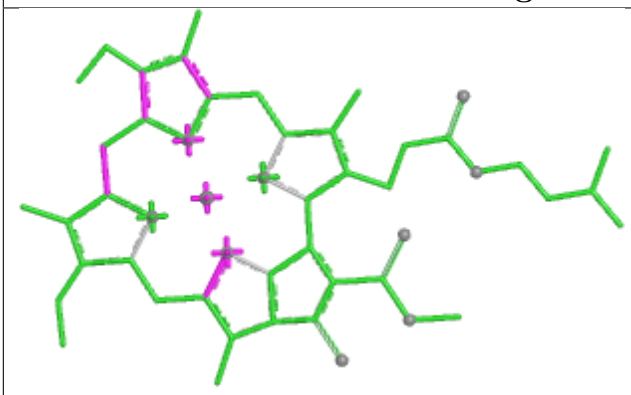


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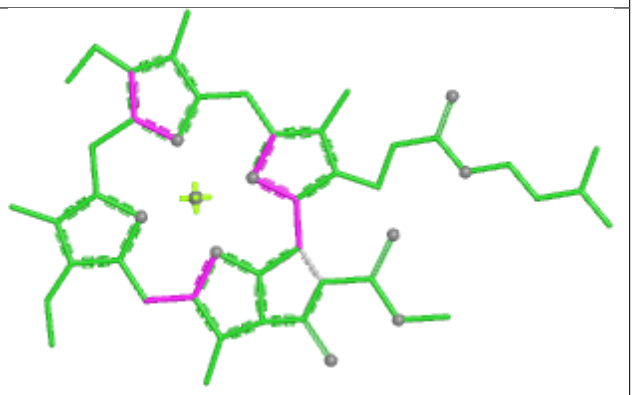


Rings

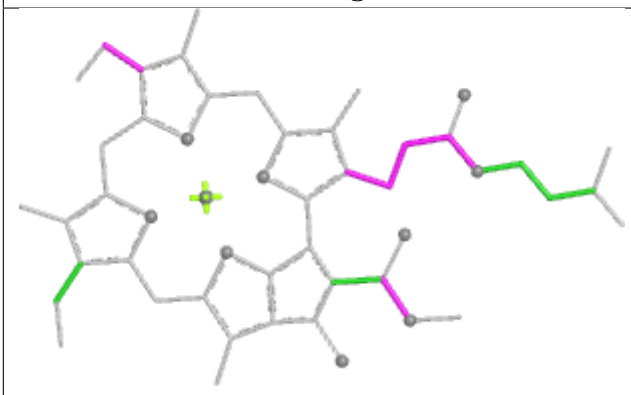
Ligand CLA B 1236



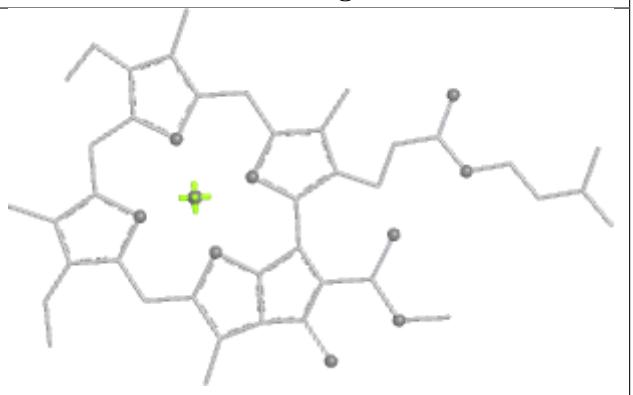
Bond lengths



Bond angles

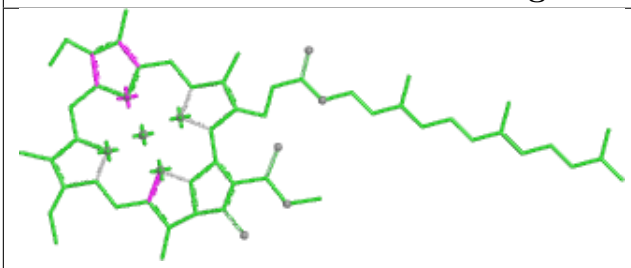


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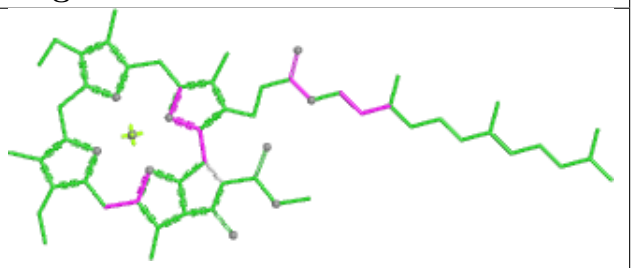


Rings

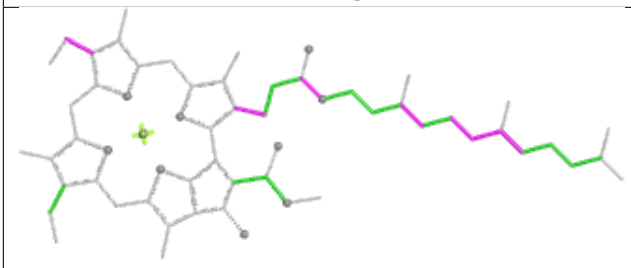
Ligand CLA g 506



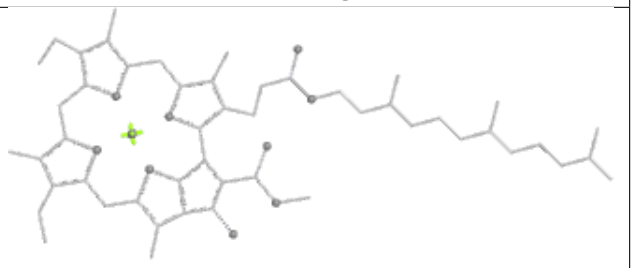
Bond lengths



Bond angles

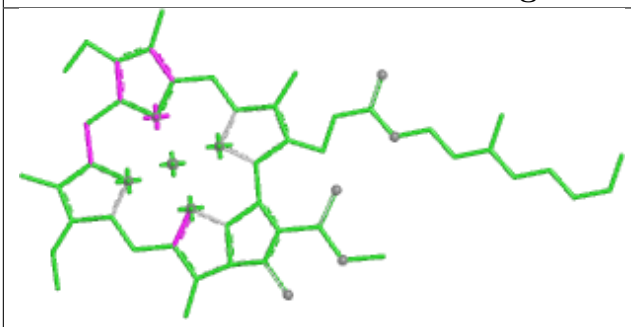


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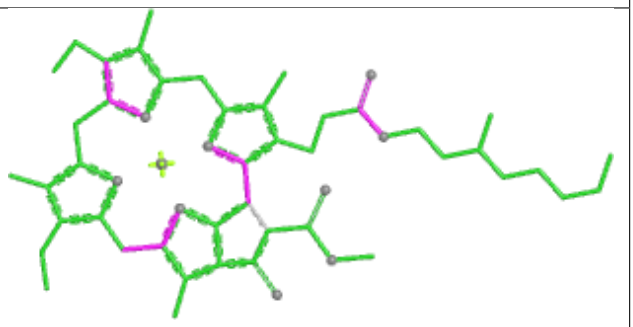


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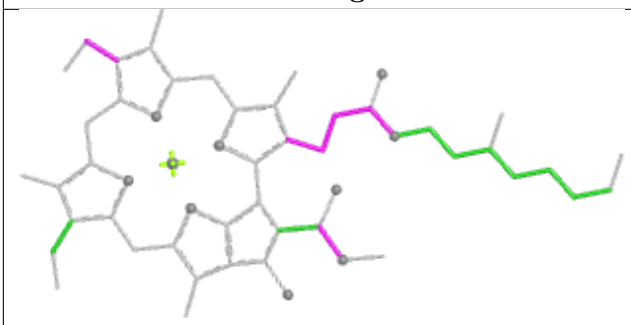
Ligand CLA a 1116



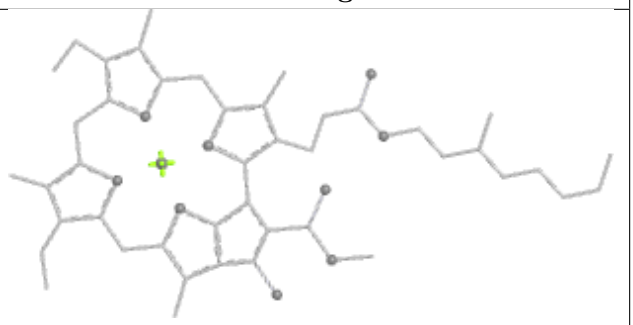
Bond lengths



Bond angles

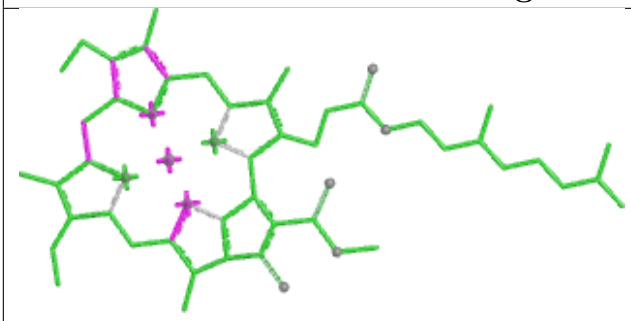


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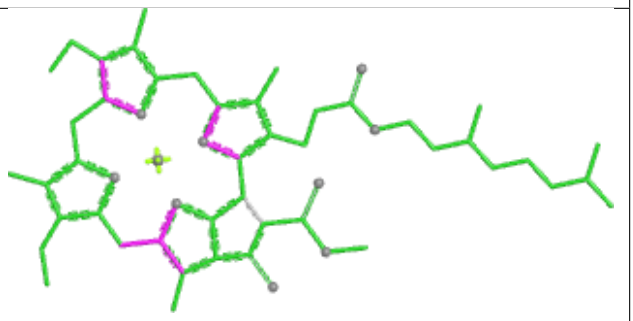


Rings

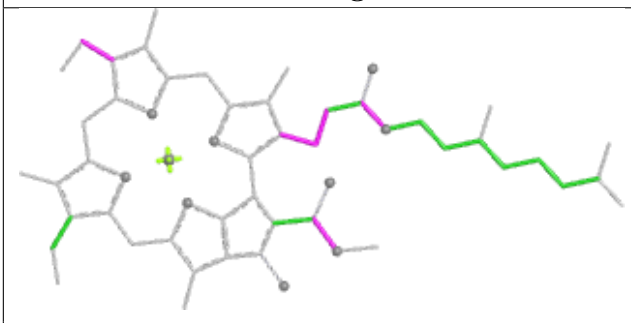
Ligand CLA B 1213



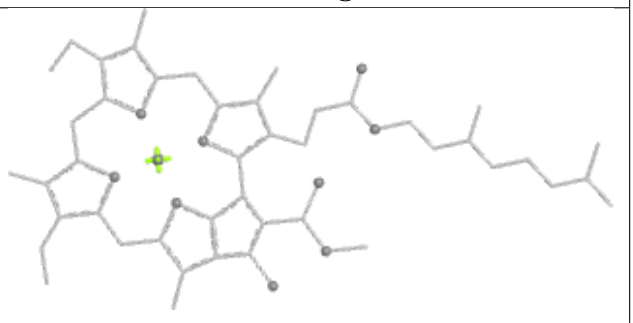
Bond lengths



Bond angles

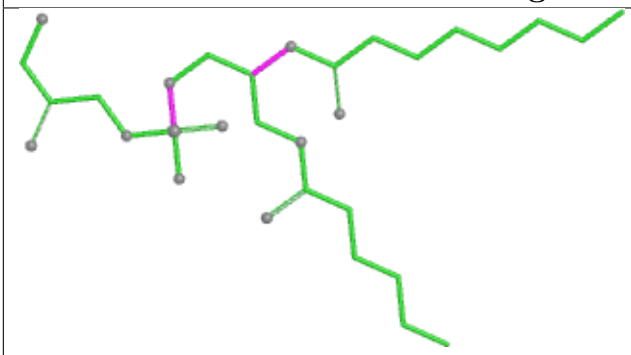


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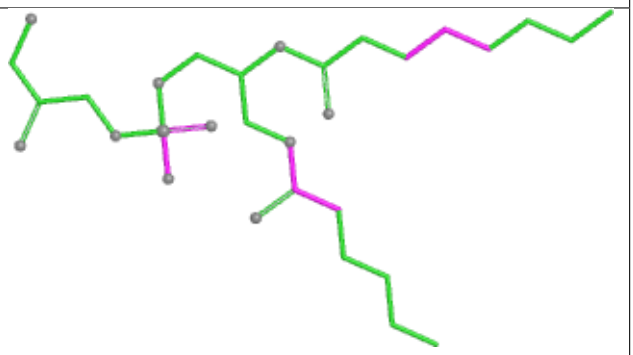


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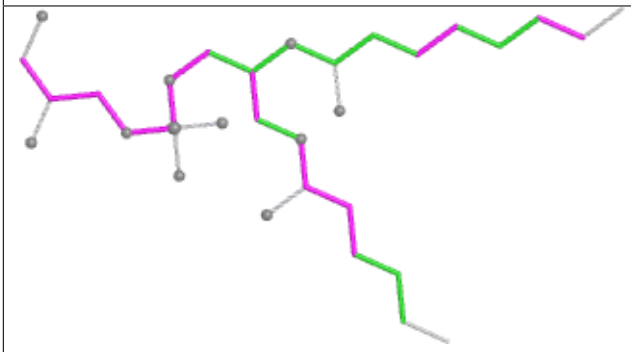
Ligand LHG r 605



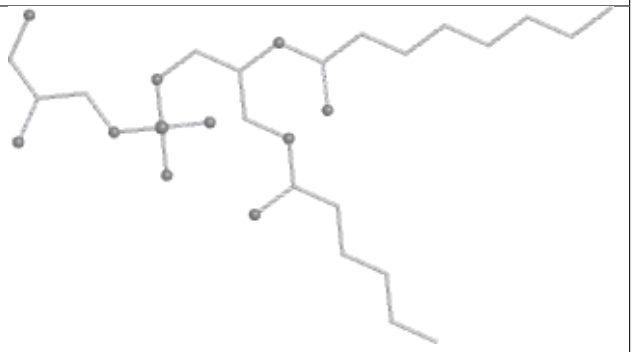
Bond lengths



Bond angles

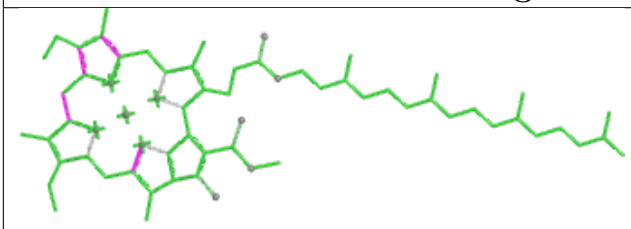


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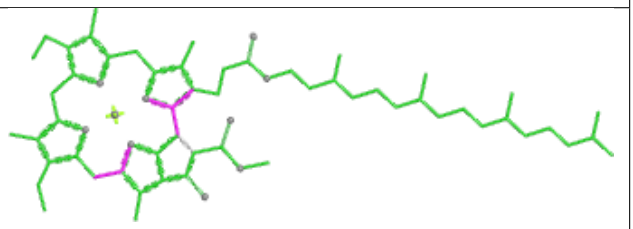


Rings

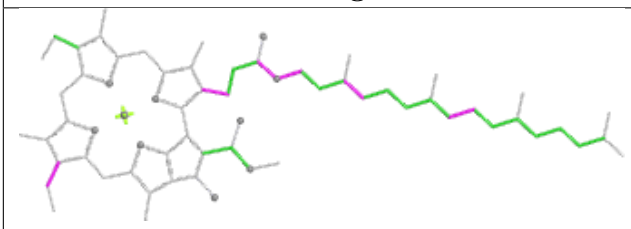
Ligand CLA H 1123



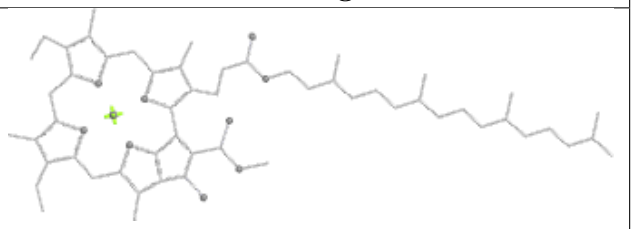
Bond lengths



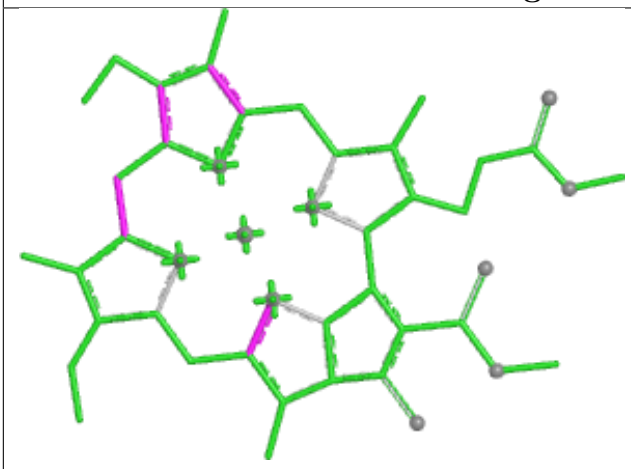
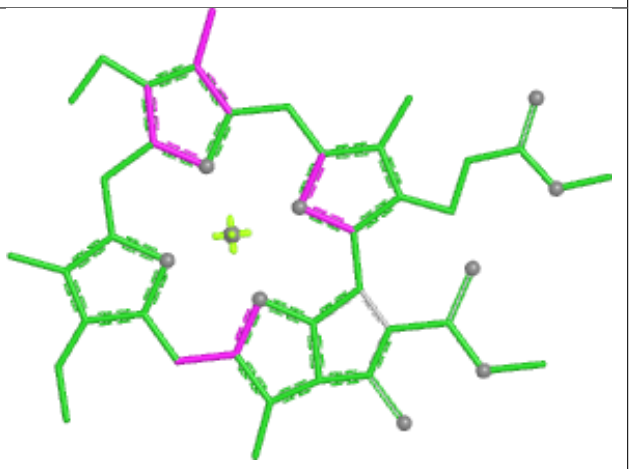
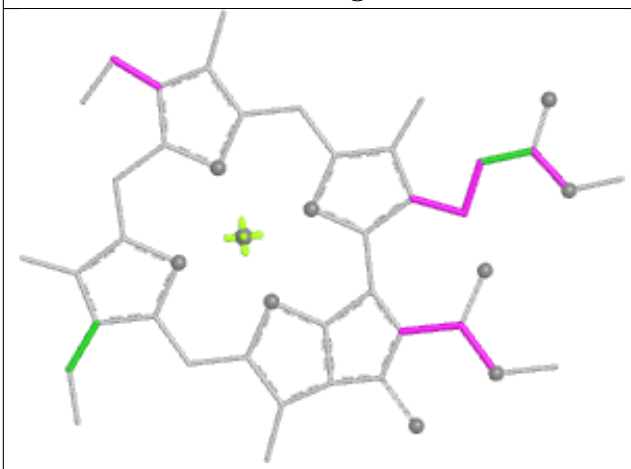
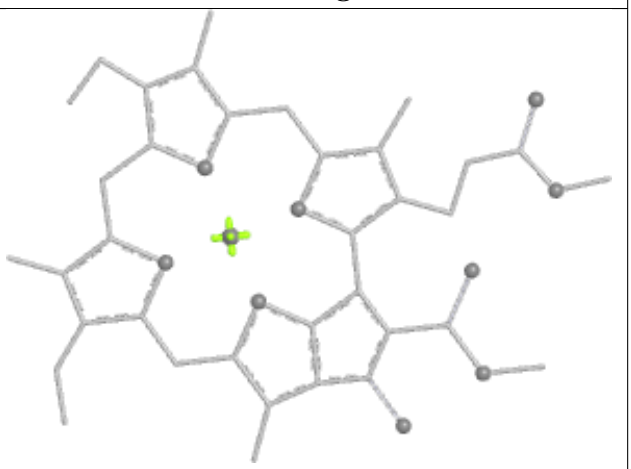
Bond angles



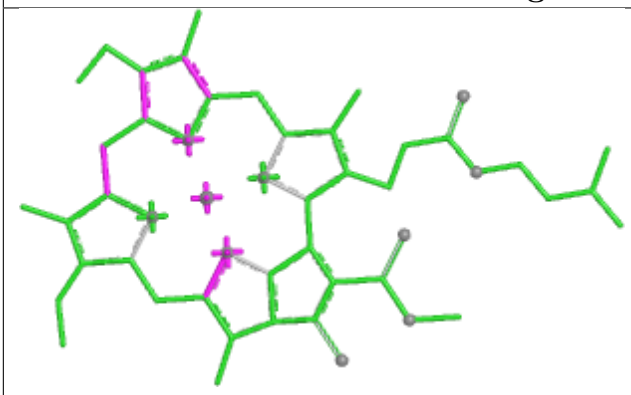
Torsions



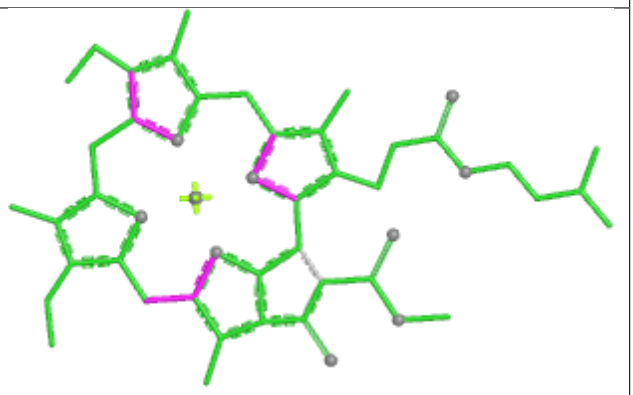
Rings

Ligand CLA Y 516	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

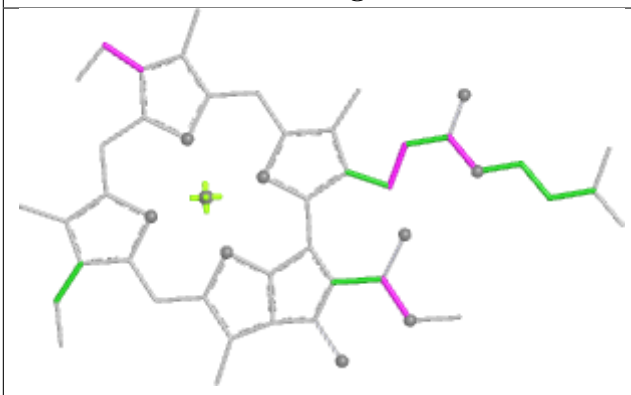
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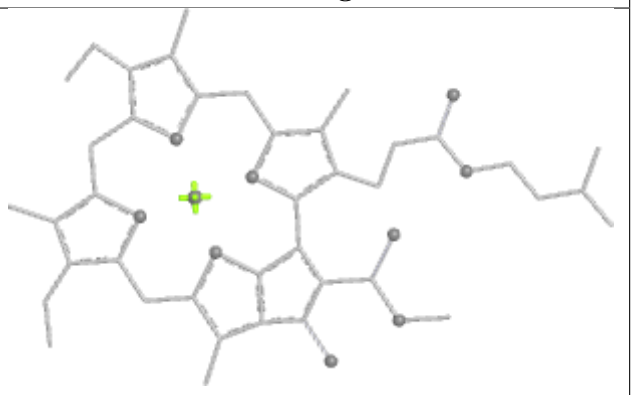
Bond lengths



Bond angles



Torsions

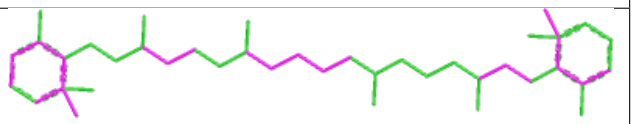


Rings

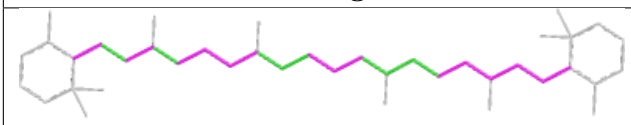
Ligand BCR u 604



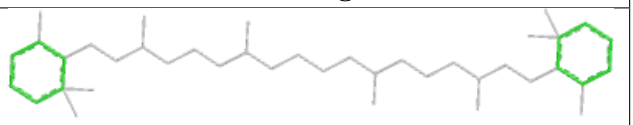
Bond lengths



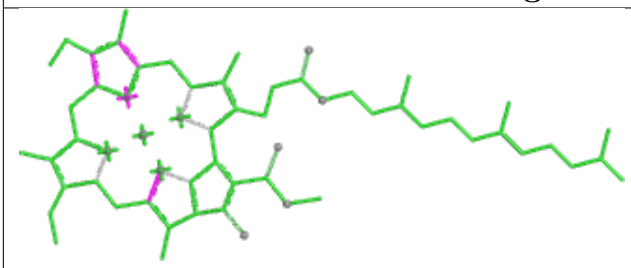
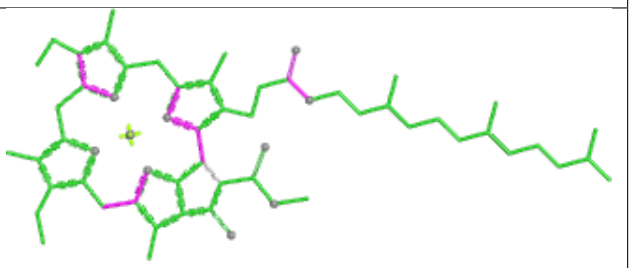
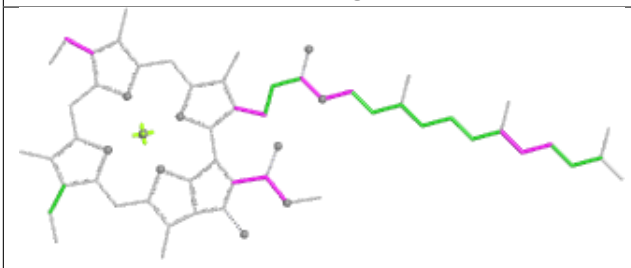
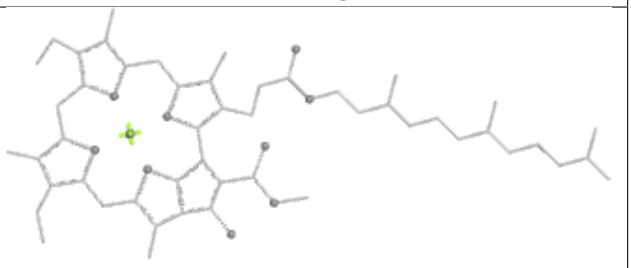
Bond angles

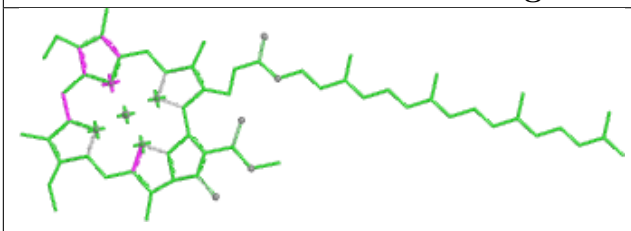
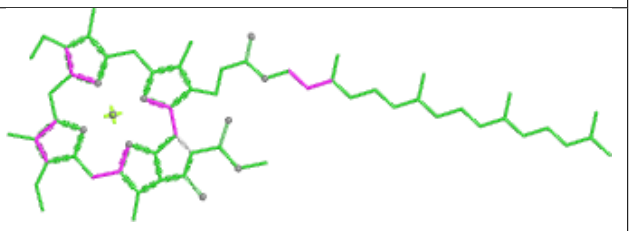
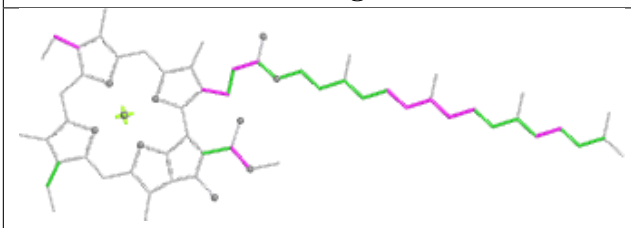
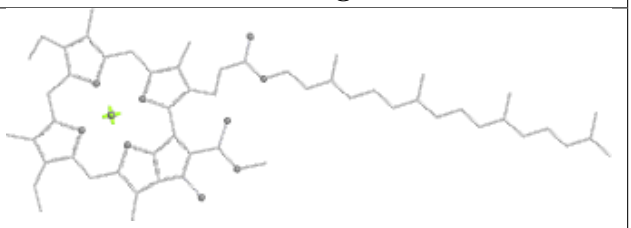


Torsions

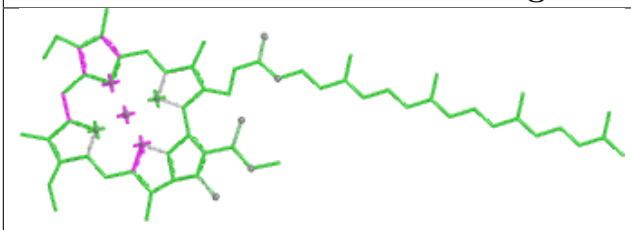


Rings

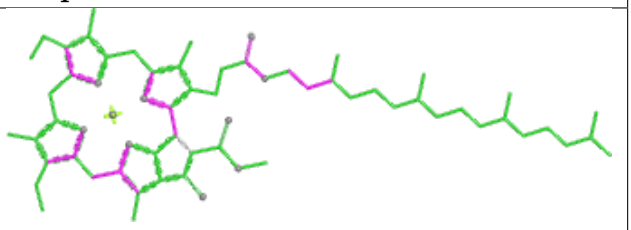
Ligand CLA Y 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA w 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

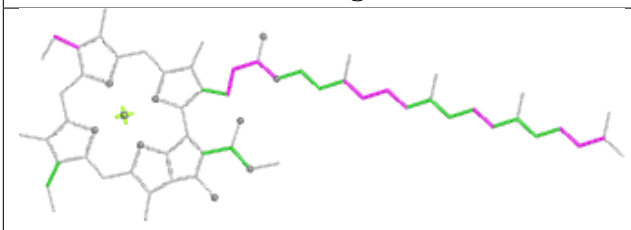
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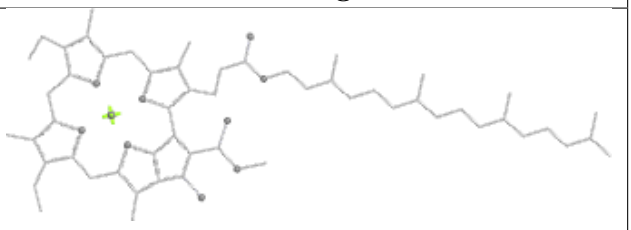
Bond lengths



Bond angles

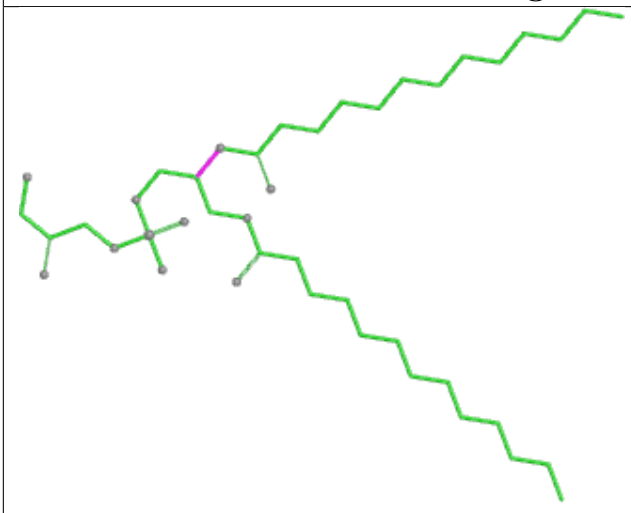


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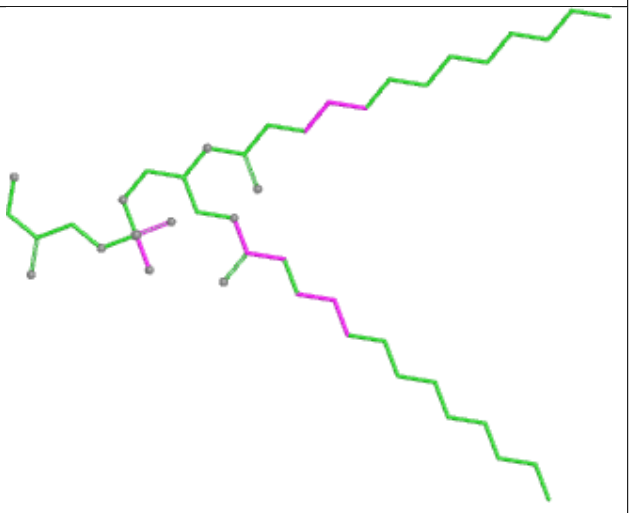


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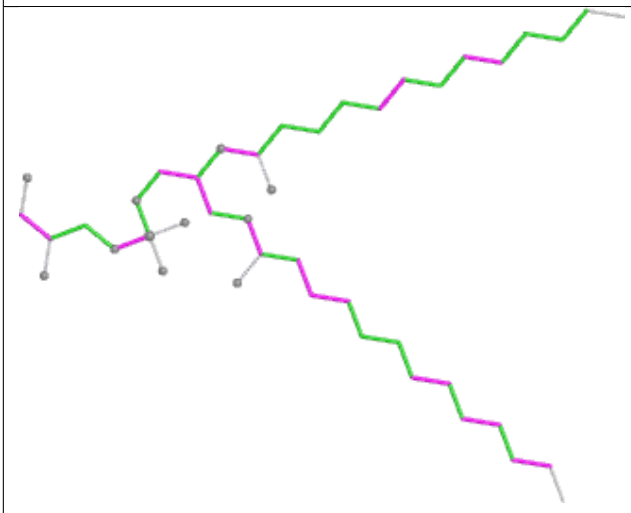
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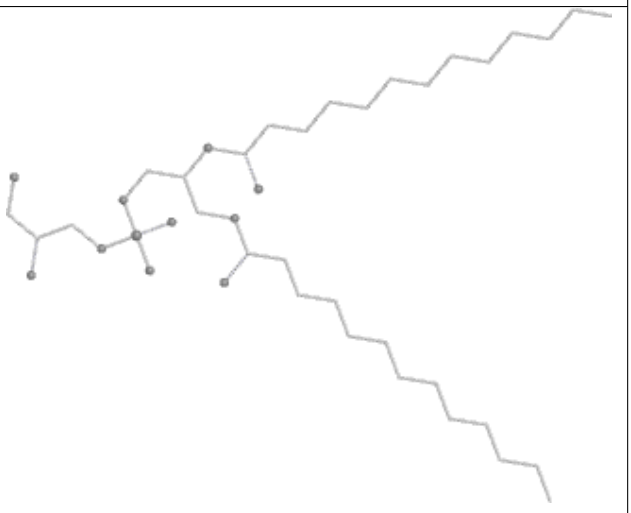
Bond lengths



Bond angles

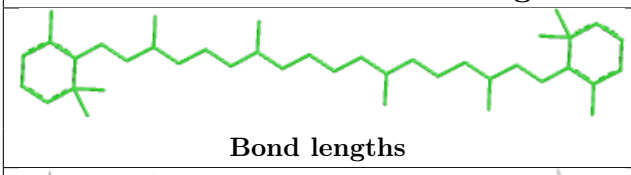


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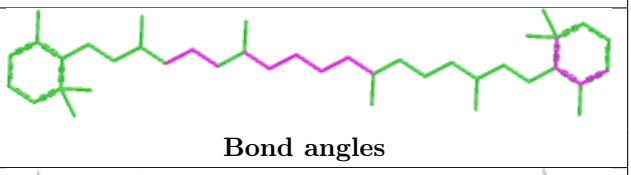


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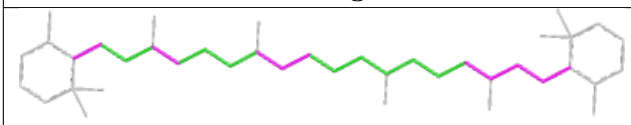
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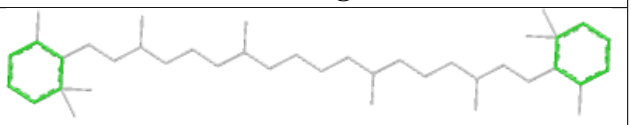
Bond lengths



Bond angles

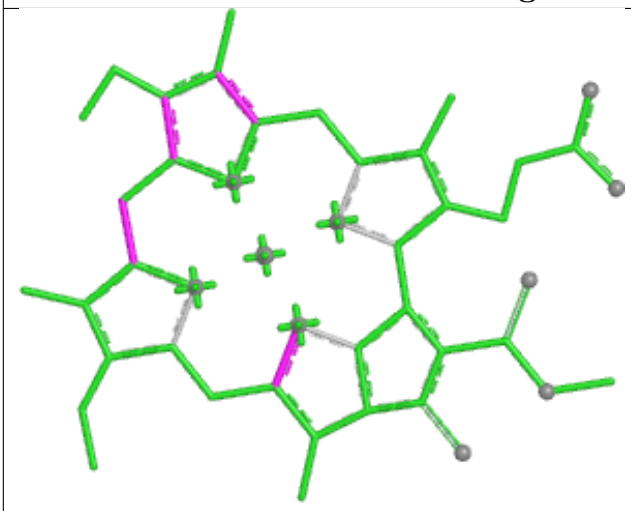


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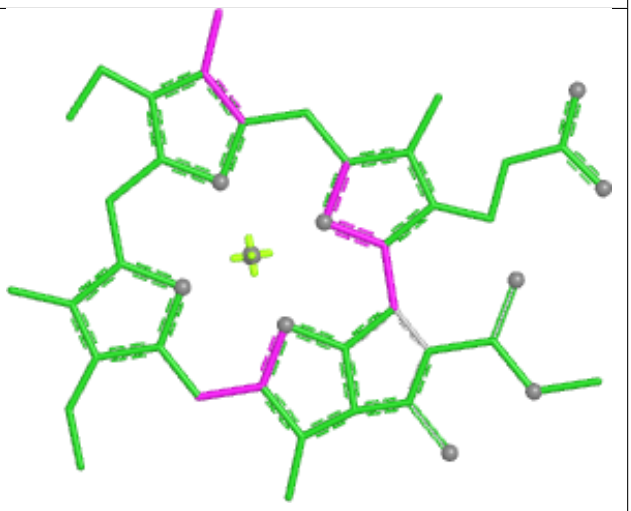


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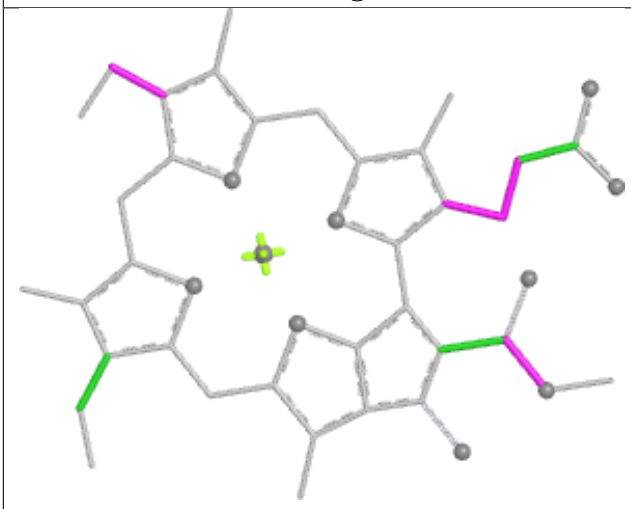
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Bond lengths



Bond angles

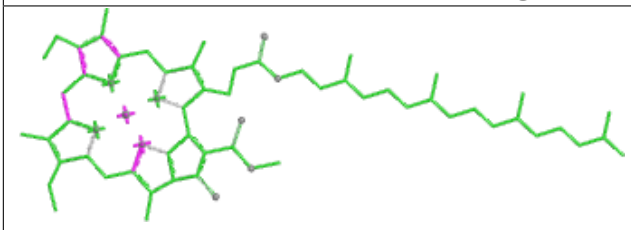


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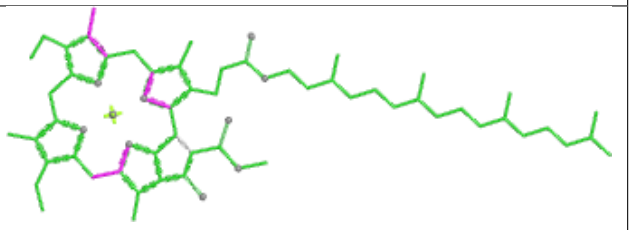


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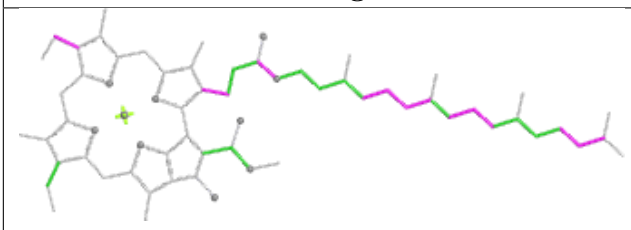
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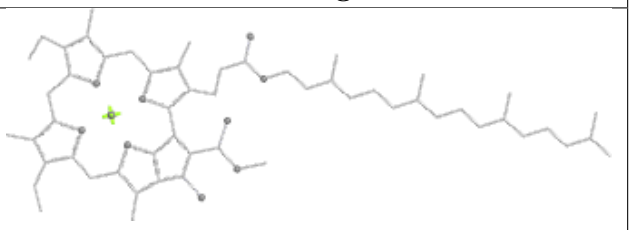
Bond lengths



Bond angles

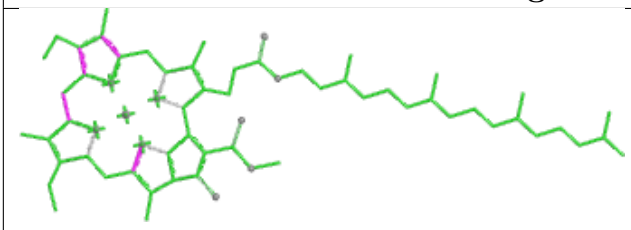


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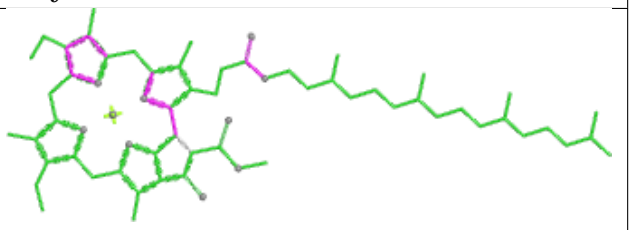


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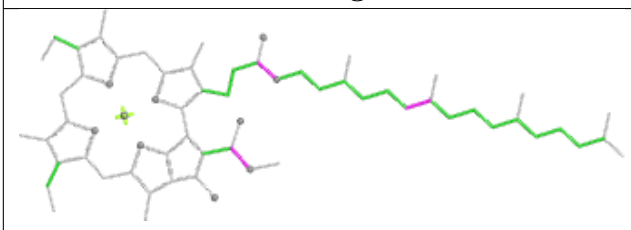
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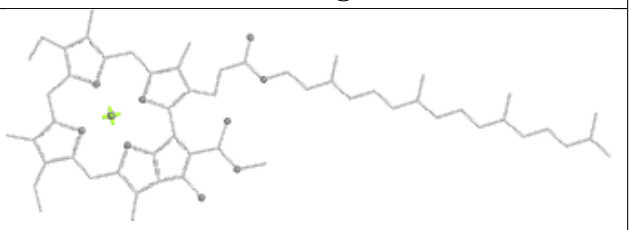
Bond lengths



Bond angles

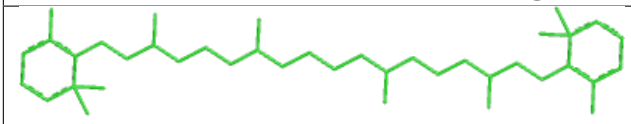


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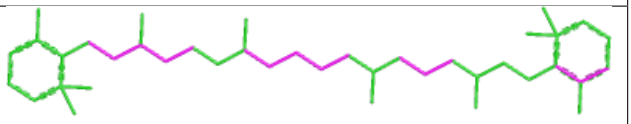


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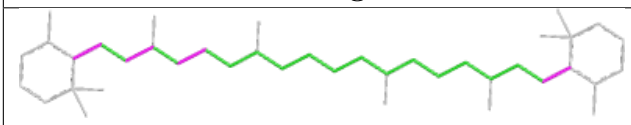
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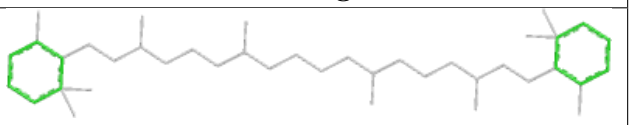
Bond lengths



Bond angles

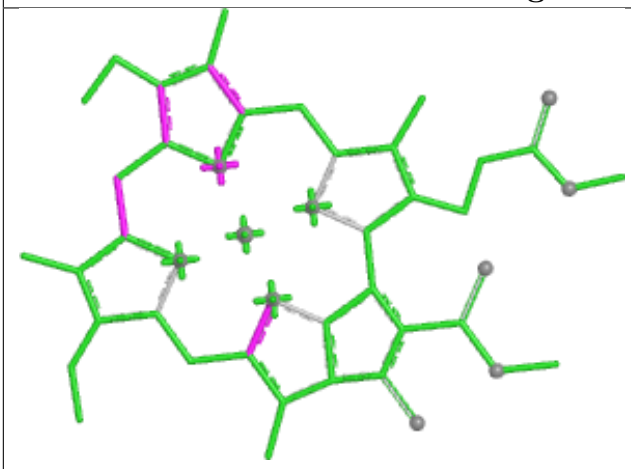


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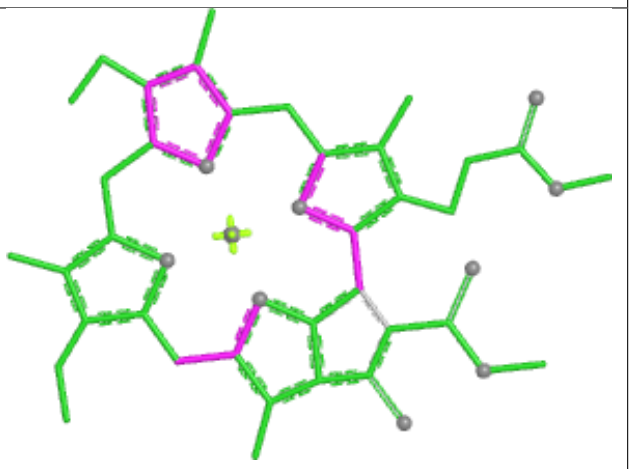


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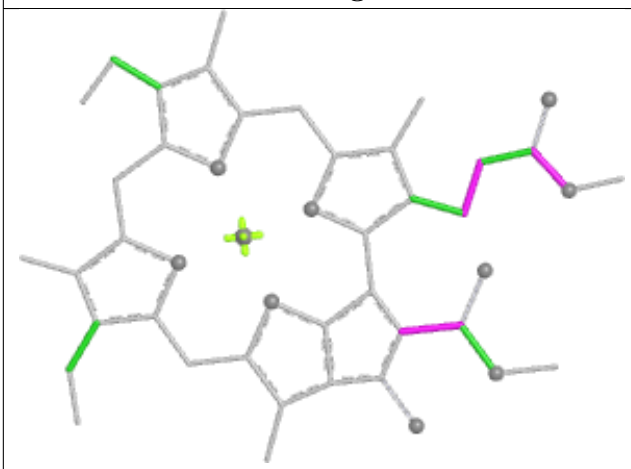
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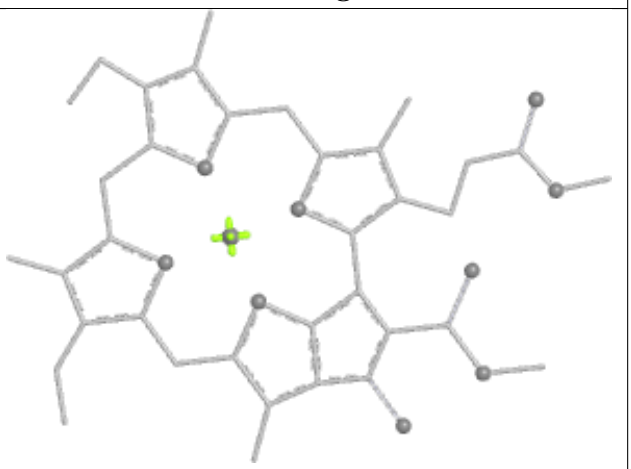
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Bond angles

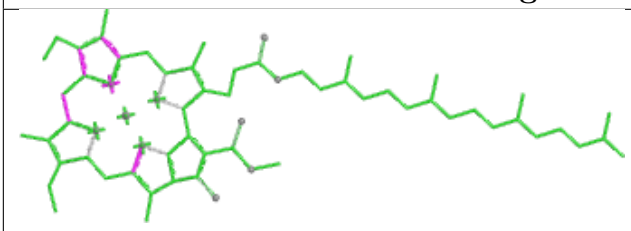


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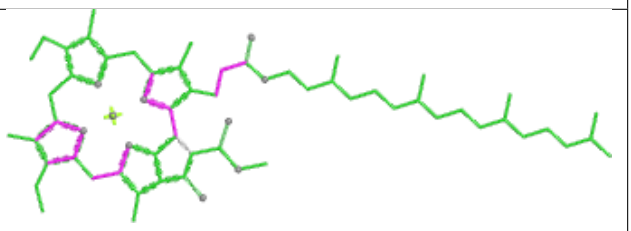


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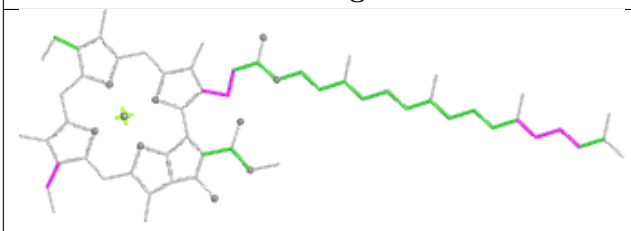
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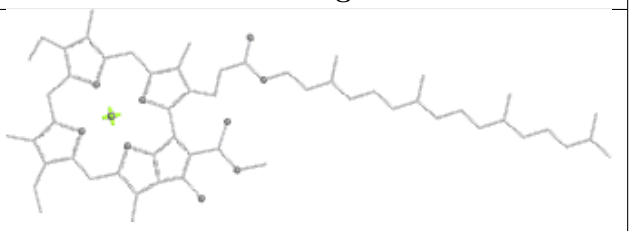
Bond lengths



Bond angles

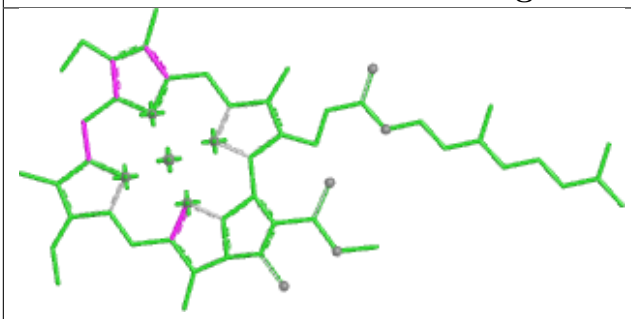


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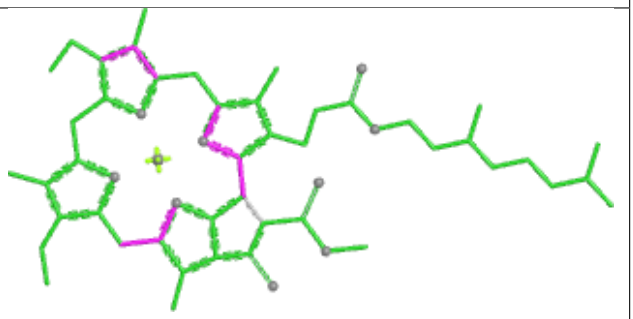


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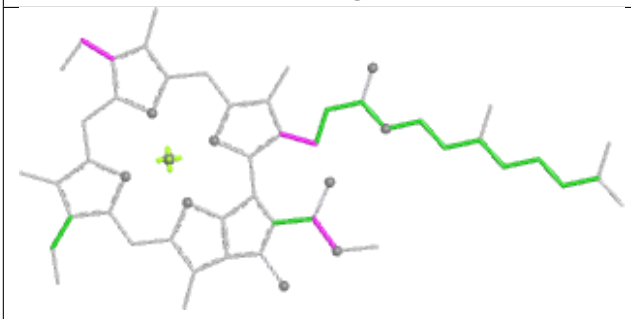
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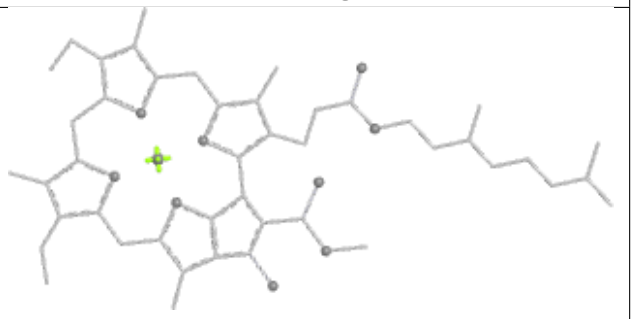
Bond lengths



Bond angles

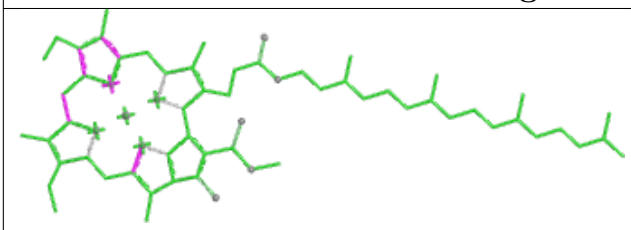


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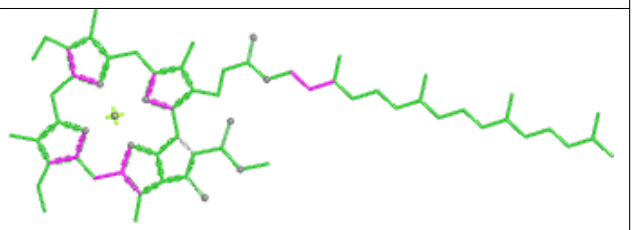


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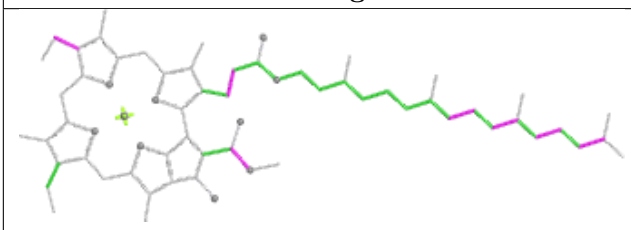
Ligand CLA a 1117



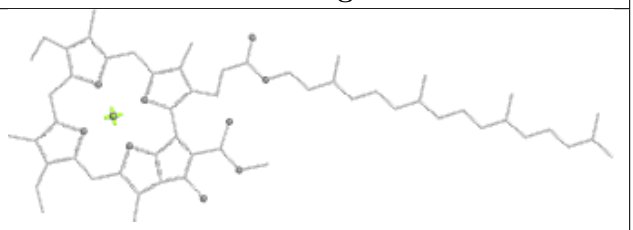
Bond lengths



Bond angles

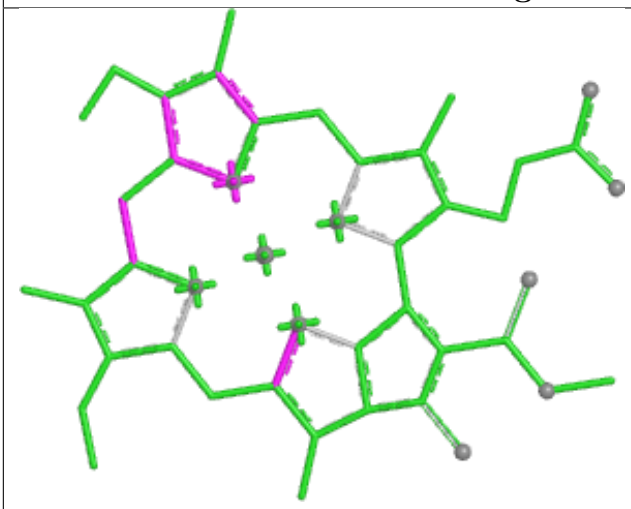


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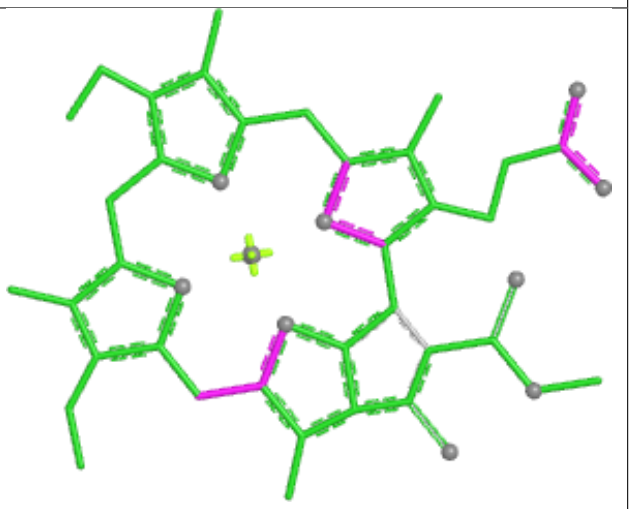


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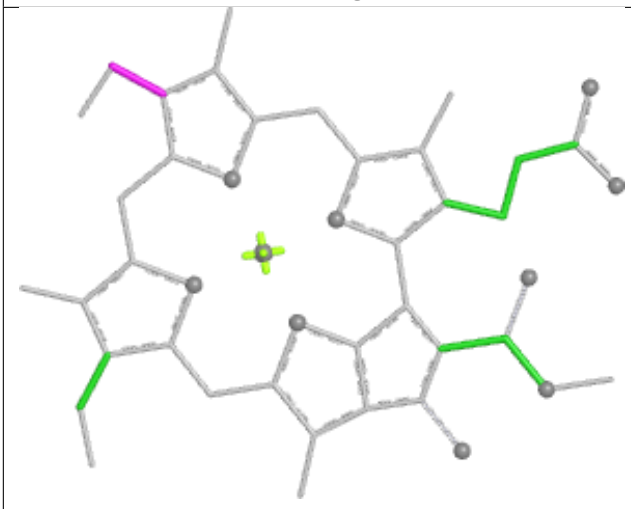
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Bond lengths



Bond angles

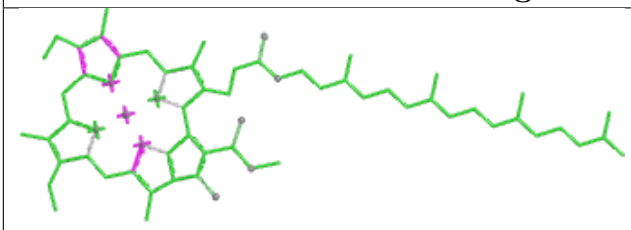


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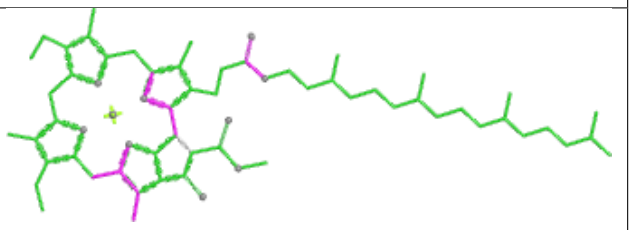


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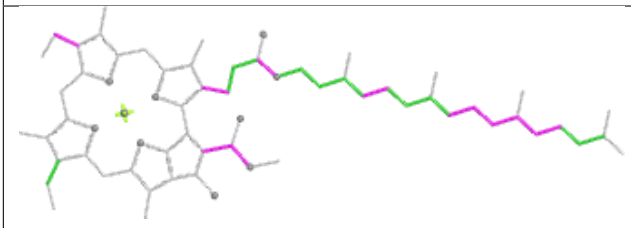
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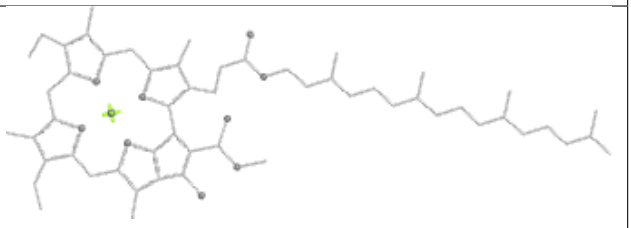
Bond lengths



Bond angles

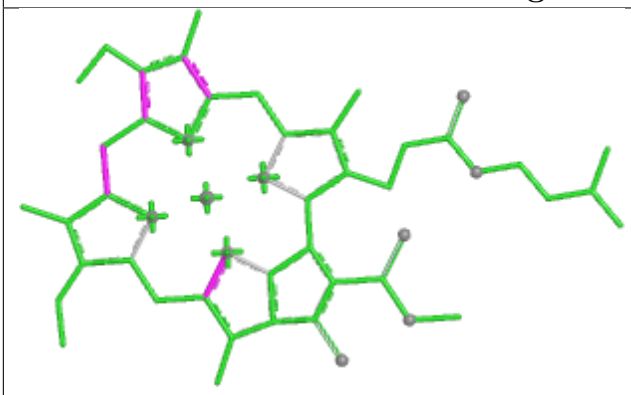


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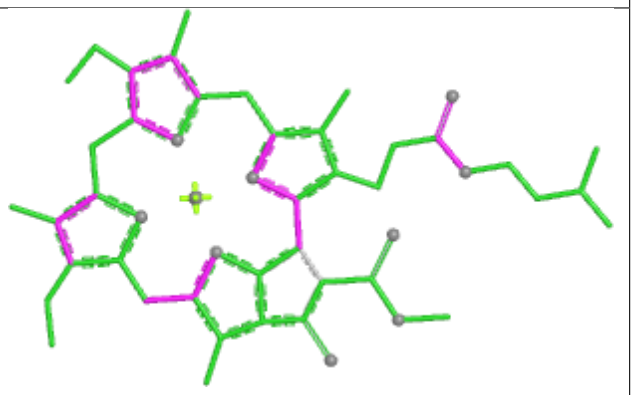


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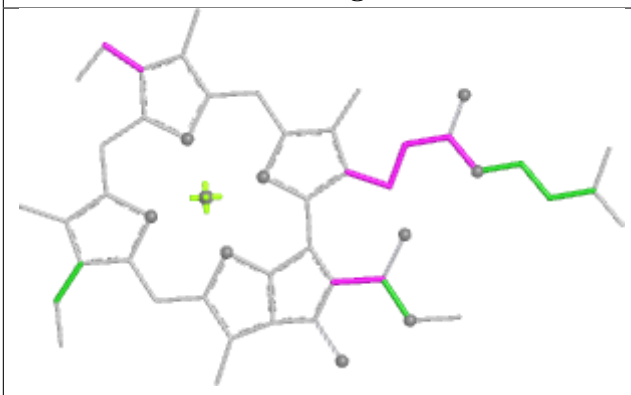
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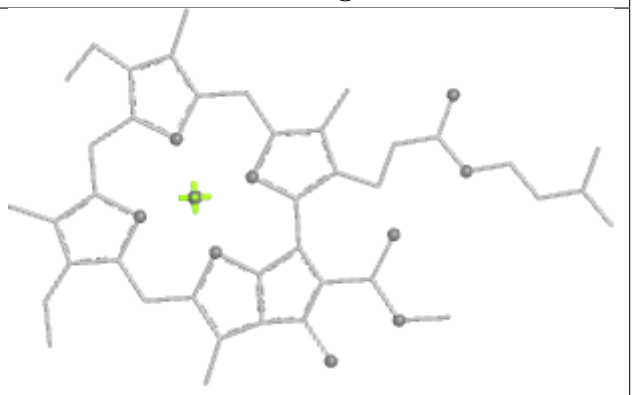
Bond lengths



Bond angles

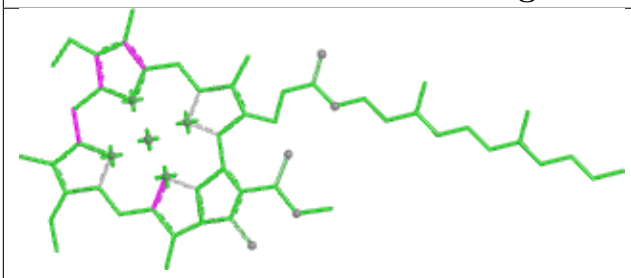


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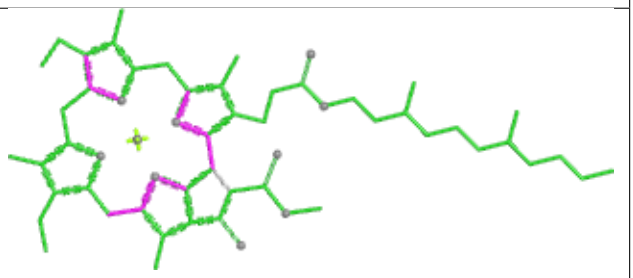


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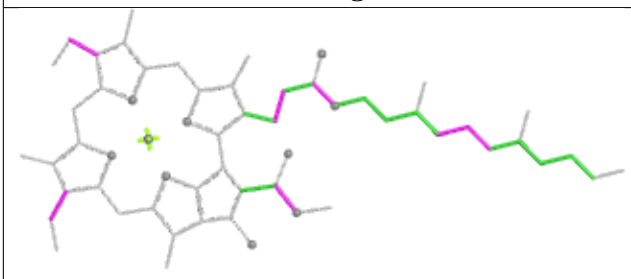
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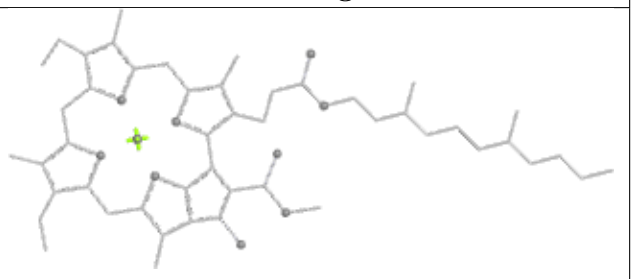
Bond lengths



Bond angles

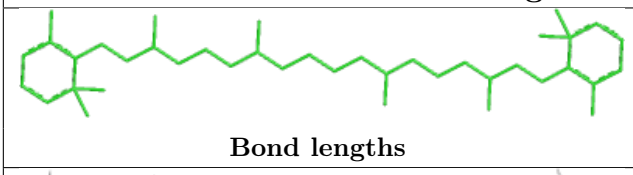


Torsions

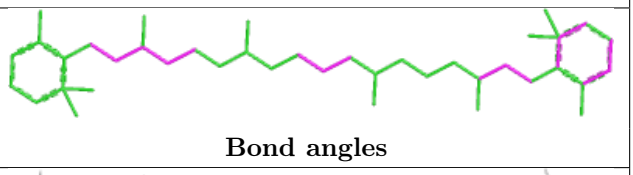


Rings

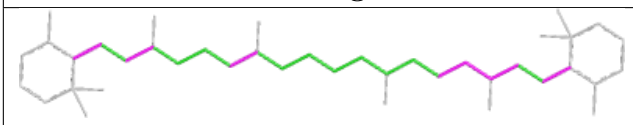
Ligand BCR n 601



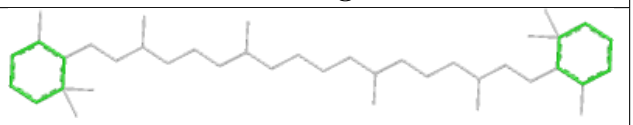
Bond lengths



Bond angles

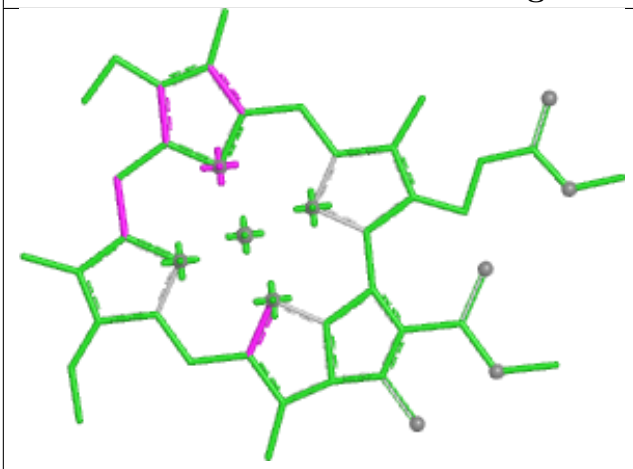


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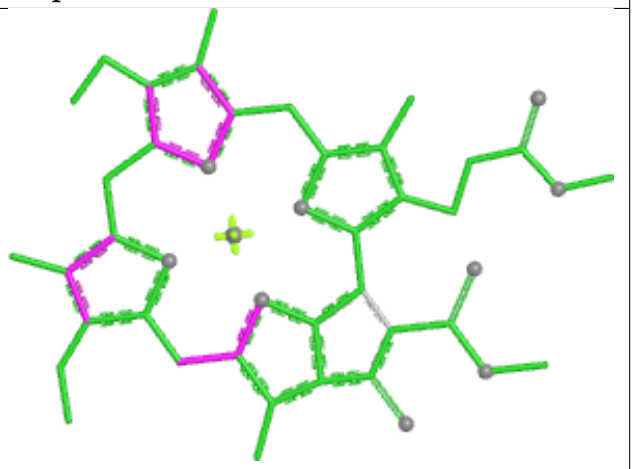


Rings

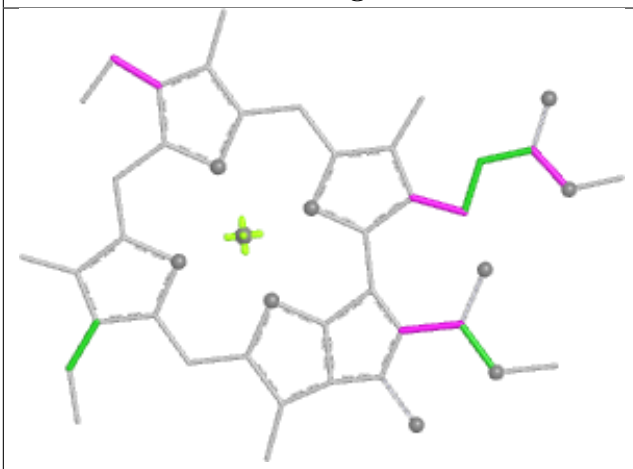
Ligand CLA p 513



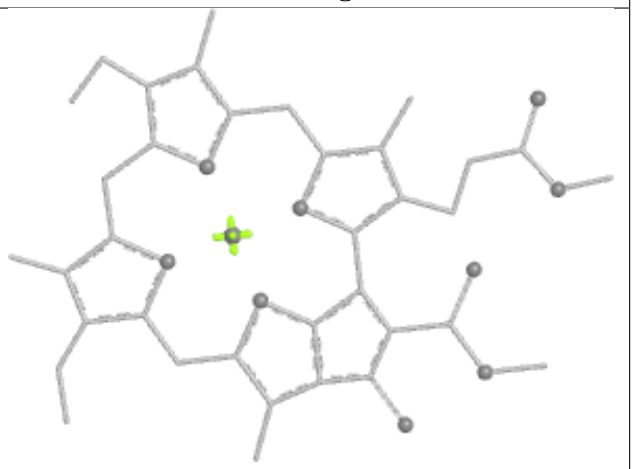
Bond lengths



Bond angles

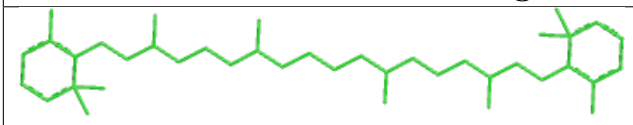


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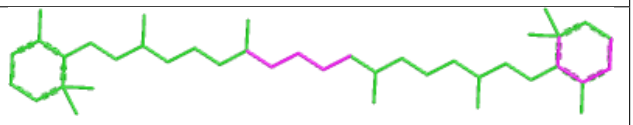


Rings

Ligand BCR B 4005



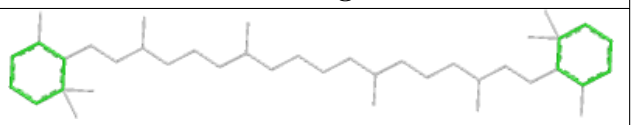
Bond lengths



Bond angles

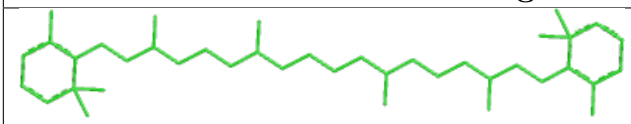


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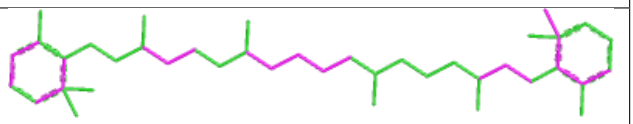


Rings

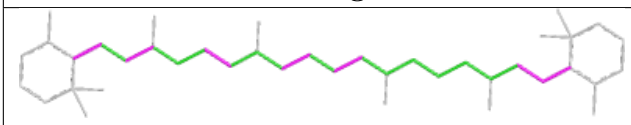
Ligand BCR W 604



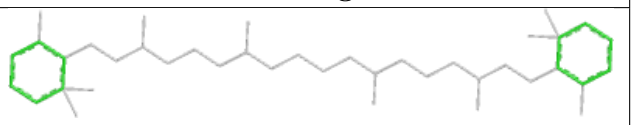
Bond lengths



Bond angles

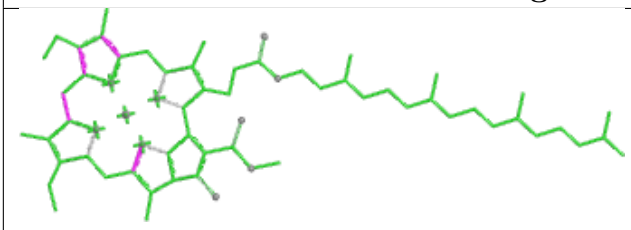


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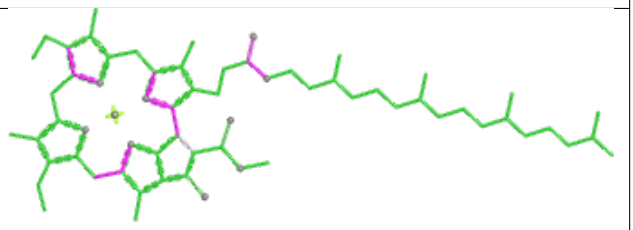


Rings

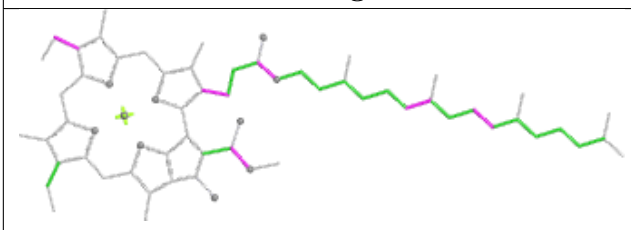
Ligand CLA t 511



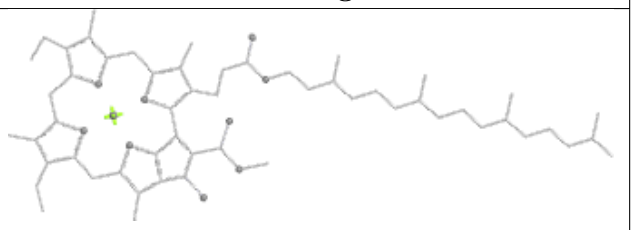
Bond lengths



Bond angles

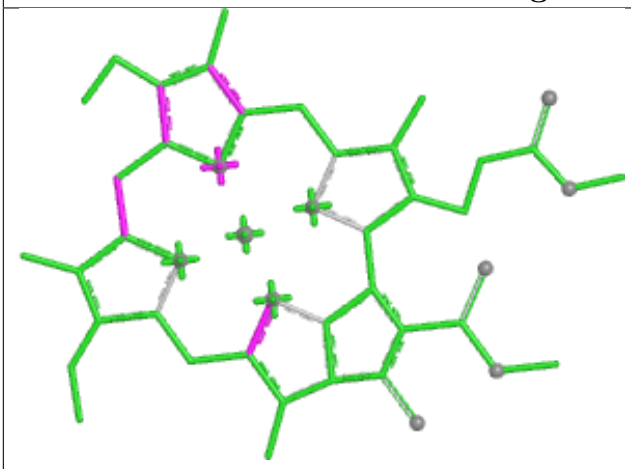


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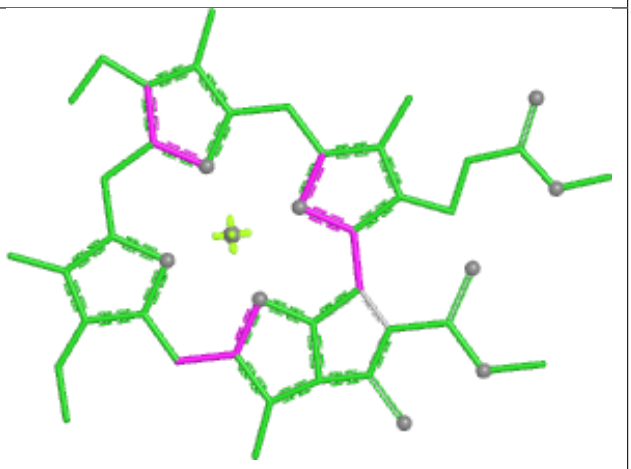


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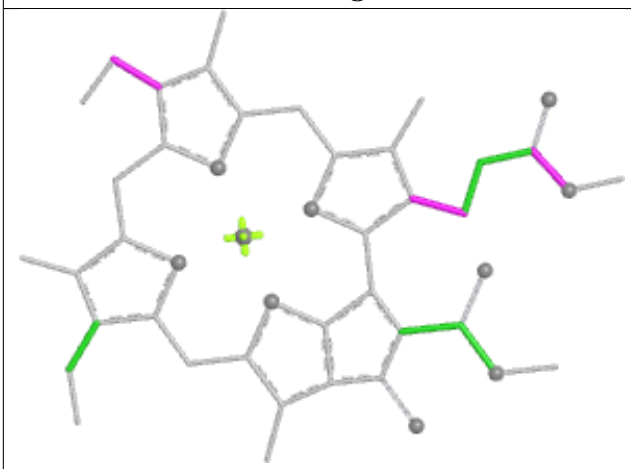
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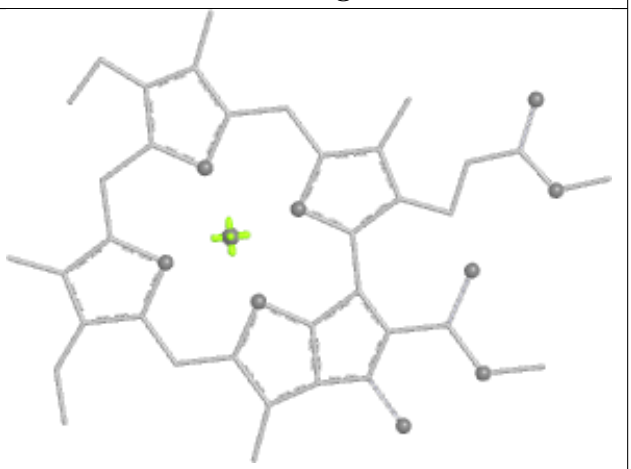
Bond lengths



Bond angles



Torsions

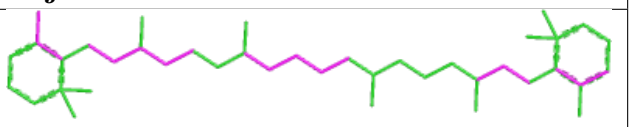


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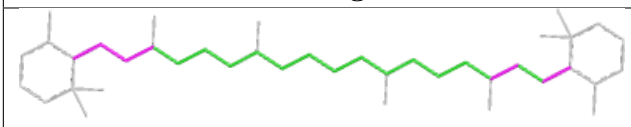
Ligand BCR j 4012



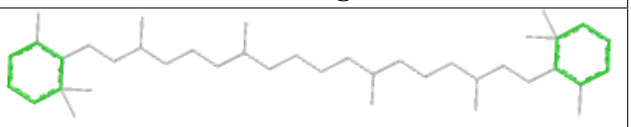
Bond lengths



Bond angles

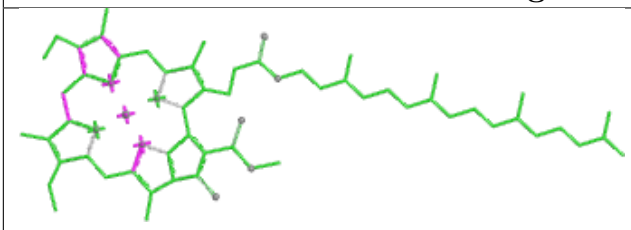


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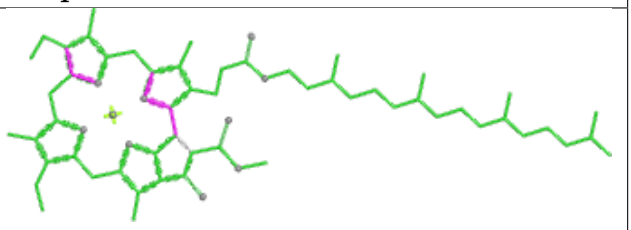


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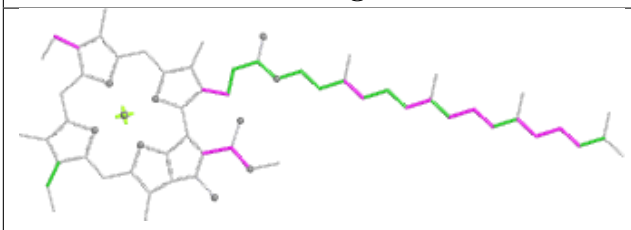
Ligand CLA q 512



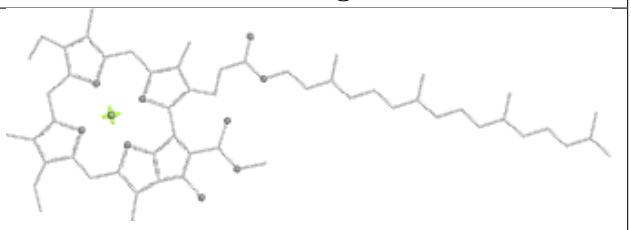
Bond lengths



Bond angles

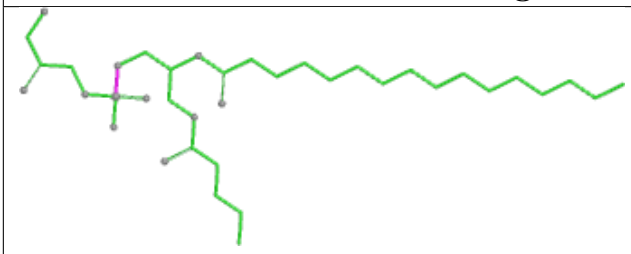


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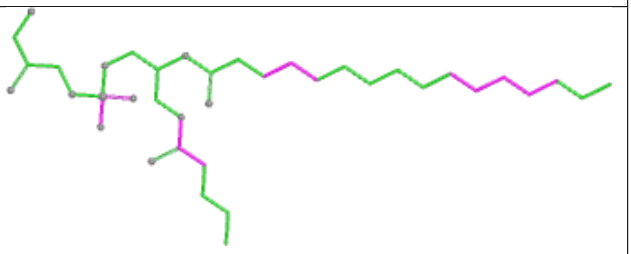


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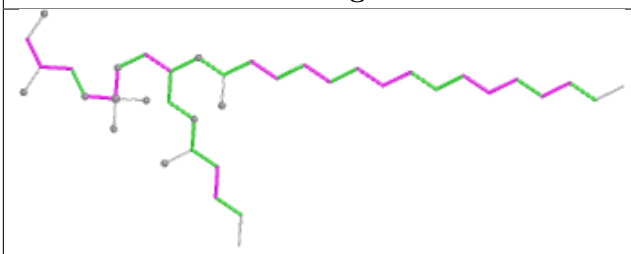
Ligand LHG B 4018



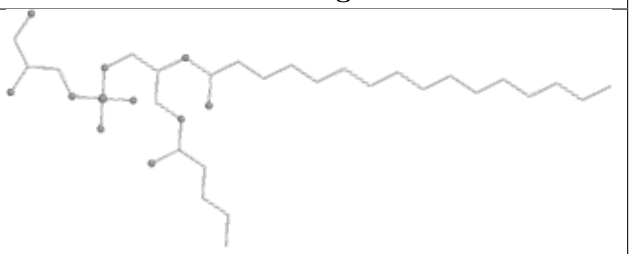
Bond lengths



Bond angles

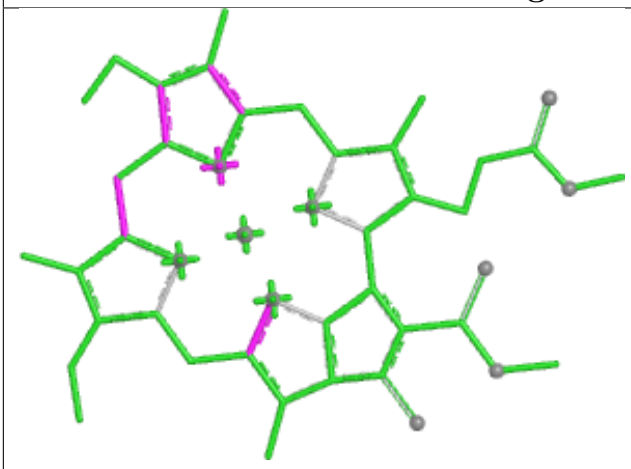


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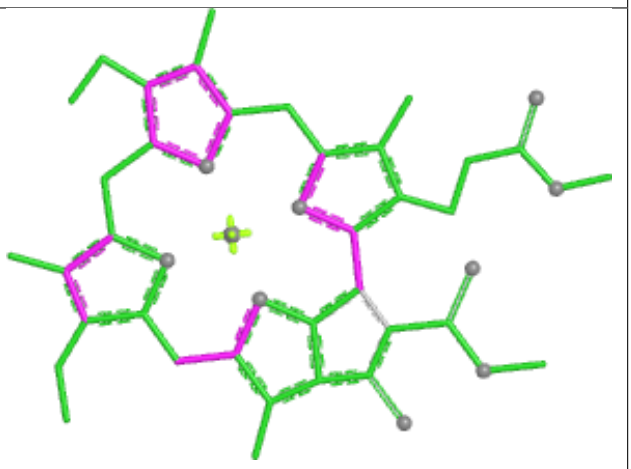


Rings

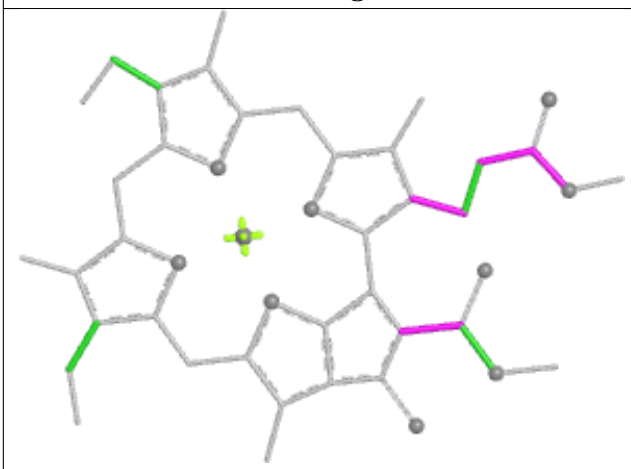
Ligand CLA v 501



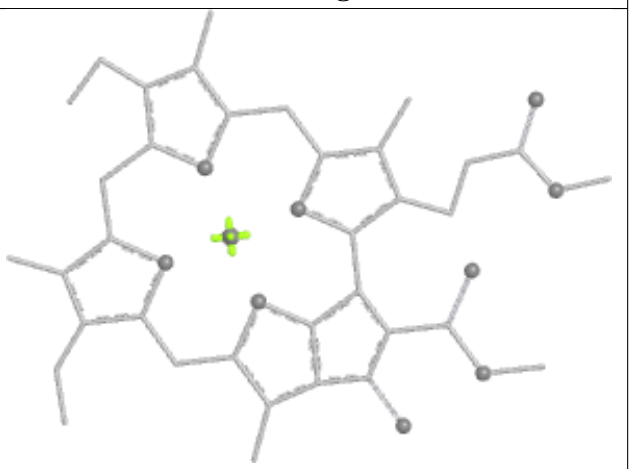
Bond lengths



Bond angles

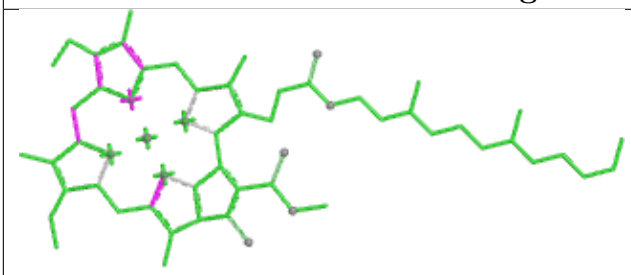


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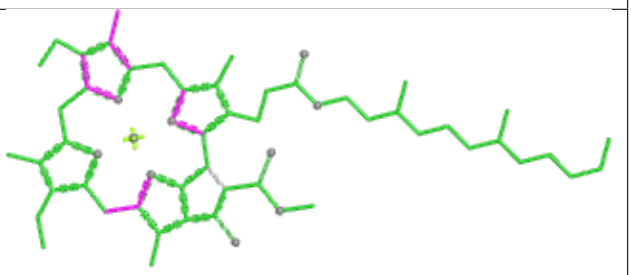


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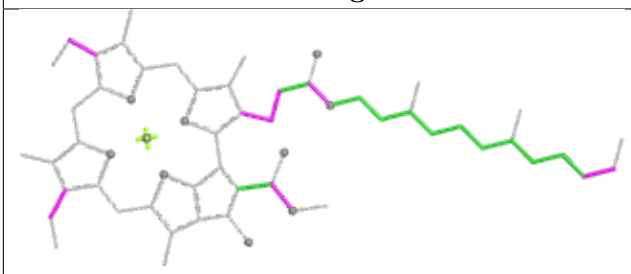
Ligand CLA a 1122



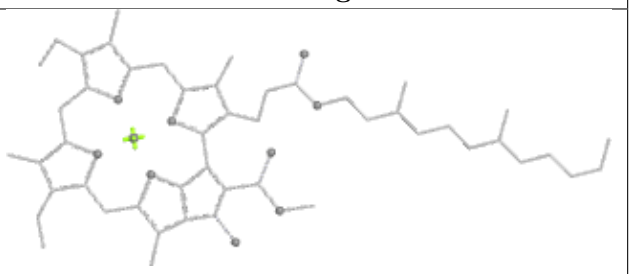
Bond lengths



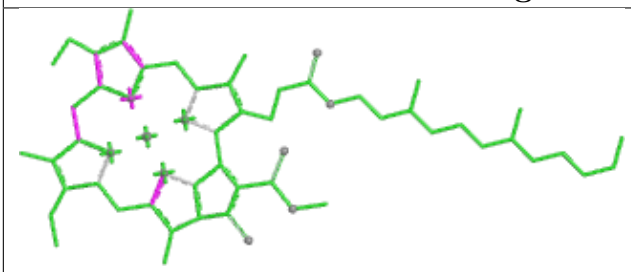
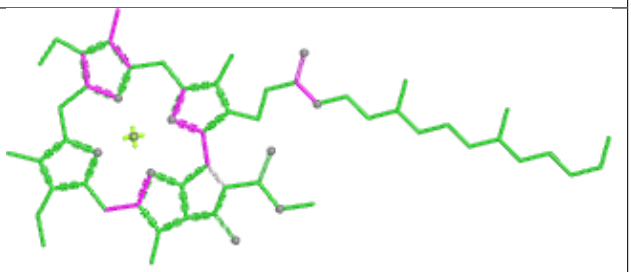
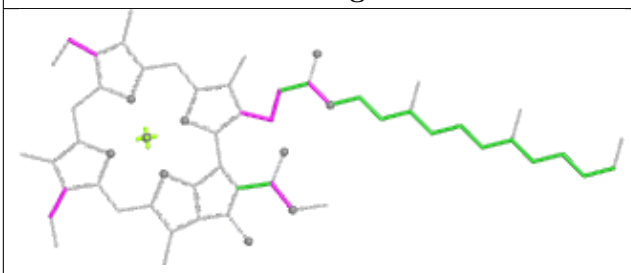
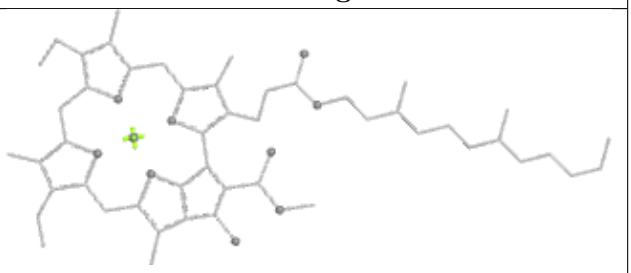
Bond angles

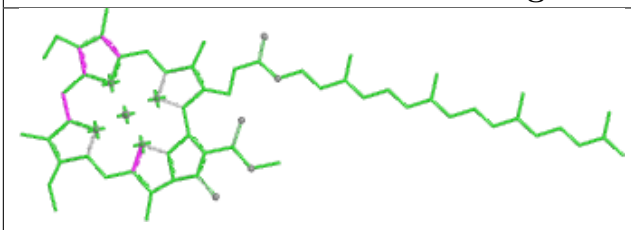
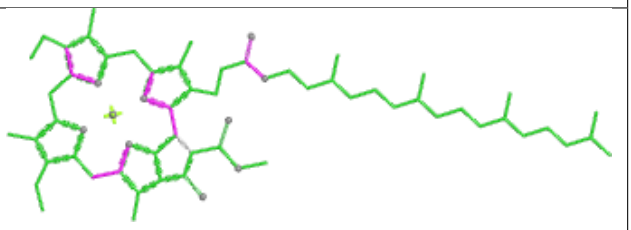
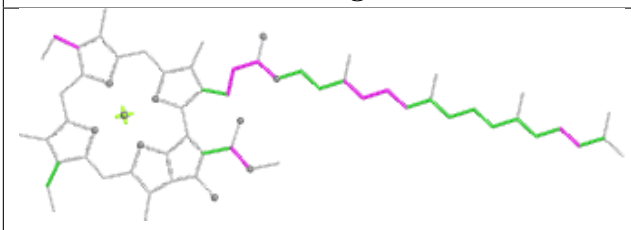
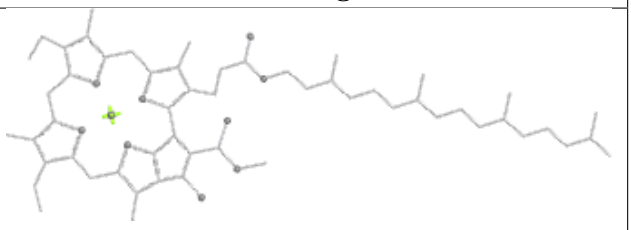


Torsions

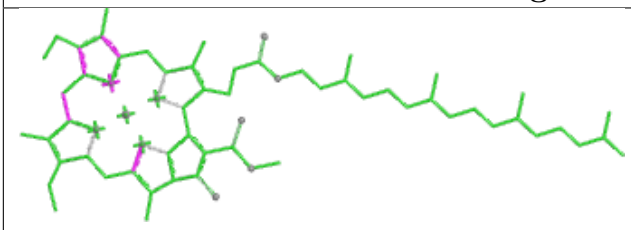


Rings

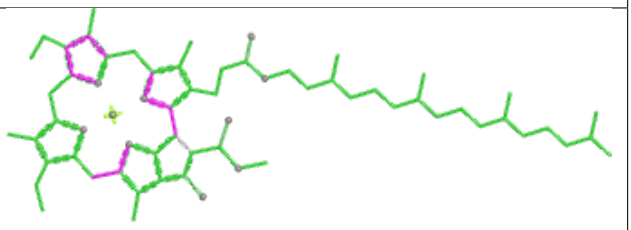
Ligand CLA A 1122	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

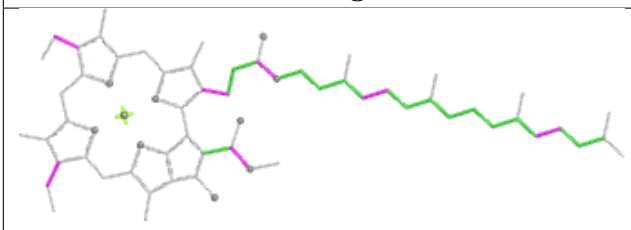
Ligand CLA r 509



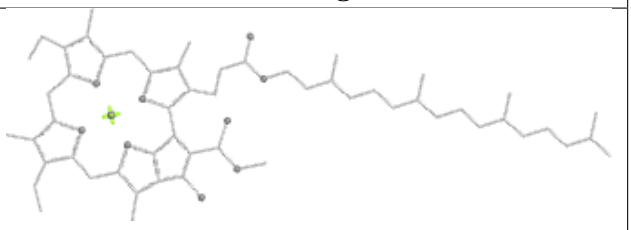
Bond lengths



Bond angles

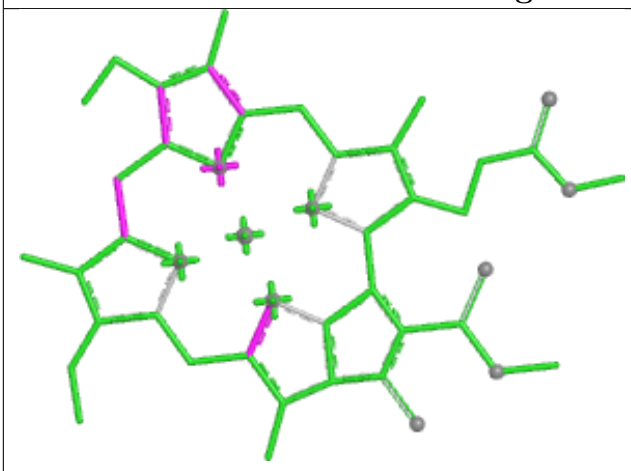


Torsions

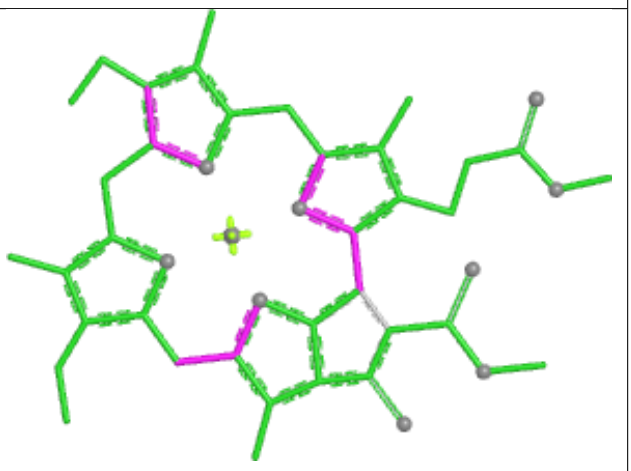


Rings

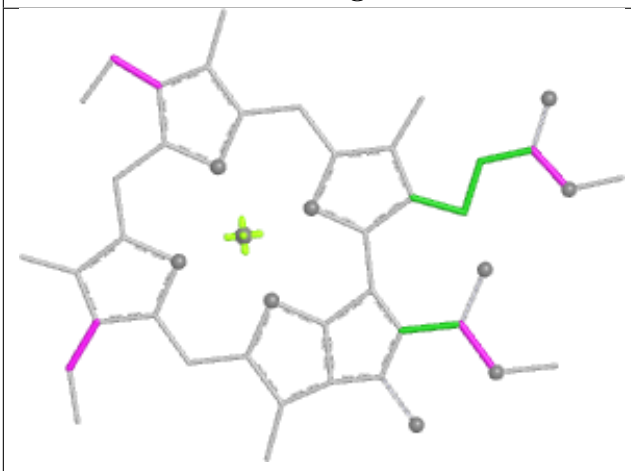
Ligand CLA B 1240



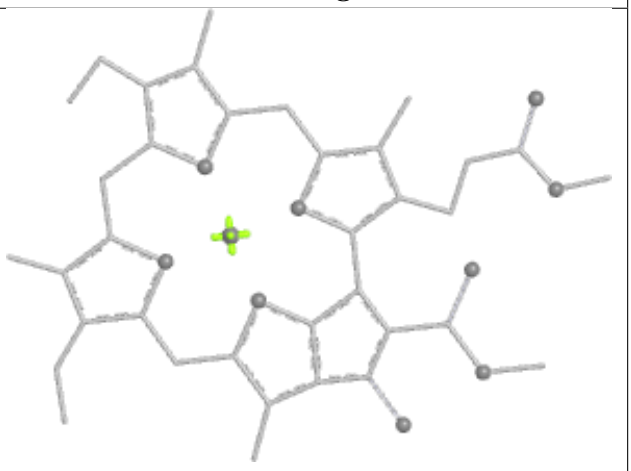
Bond lengths



Bond angles

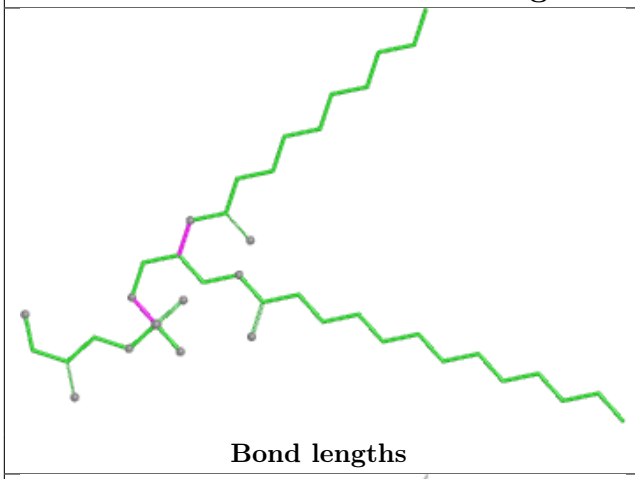


Torsions

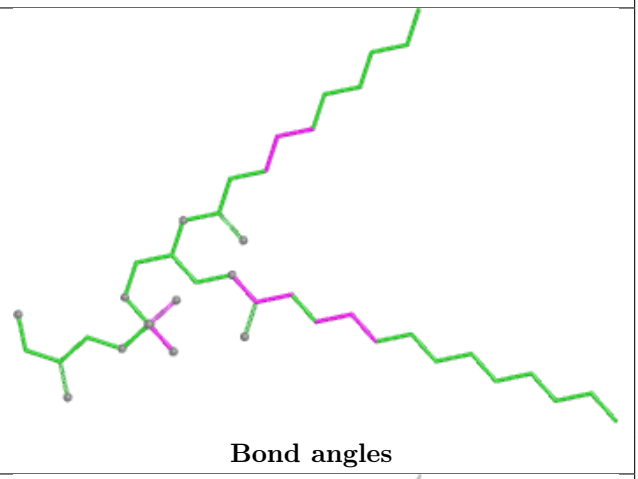


Rings

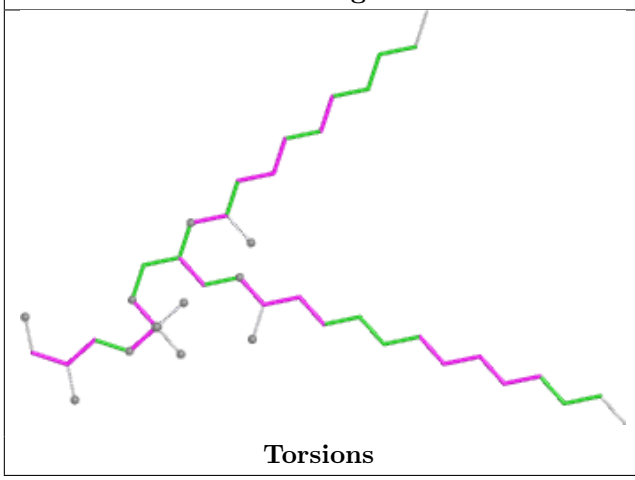
Ligand LHG I 103



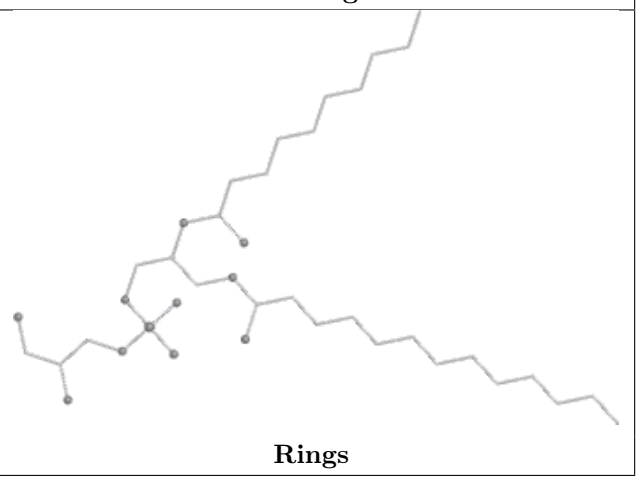
Bond lengths



Bond angles

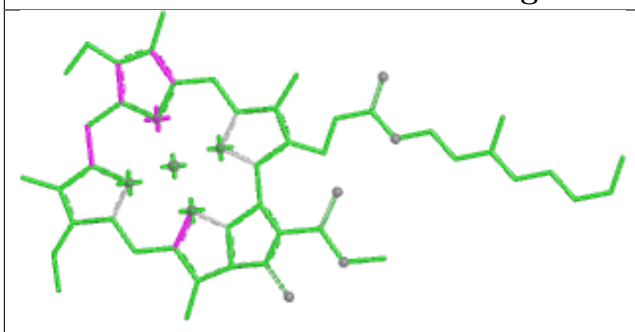


Torsions

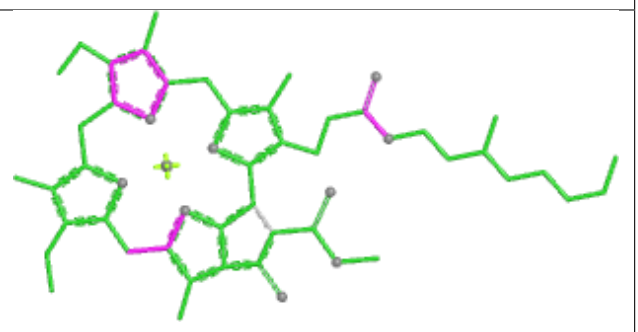


Rings

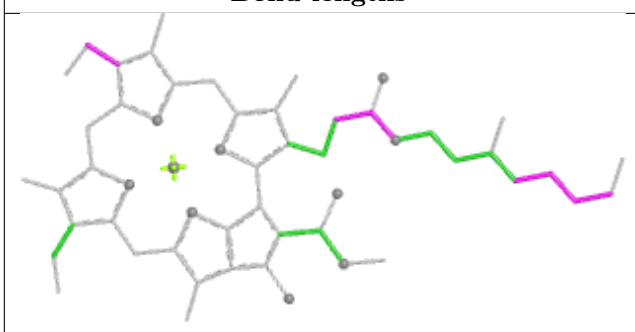
Ligand CLA a 1133



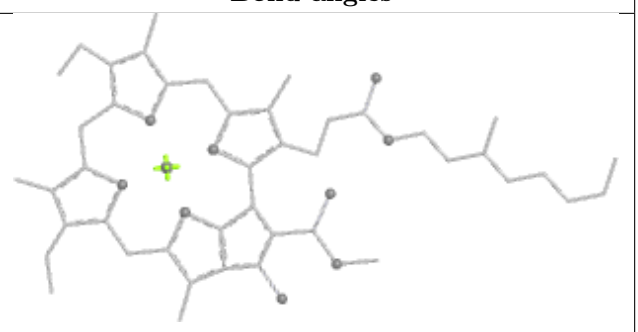
Bond lengths



Bond angles

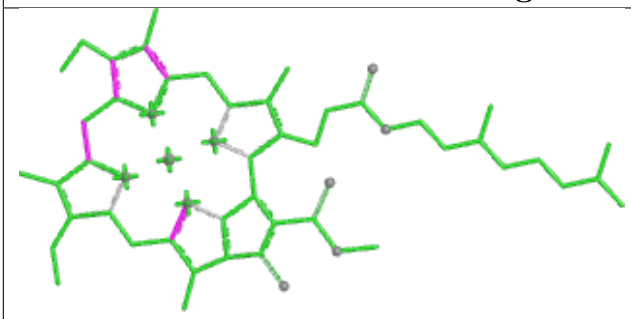


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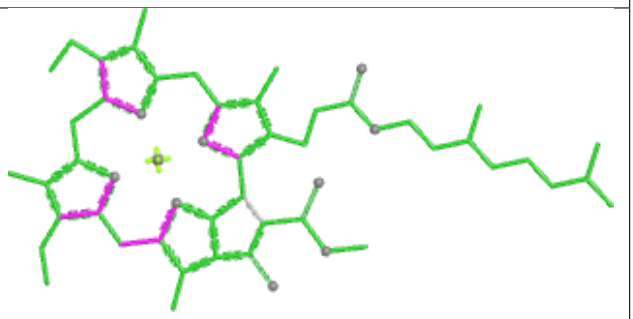


Rings

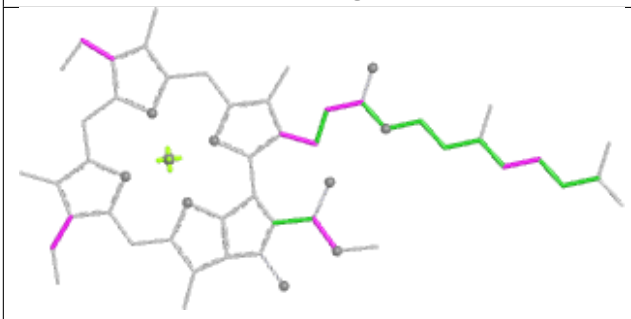
Ligand CLA B 1214



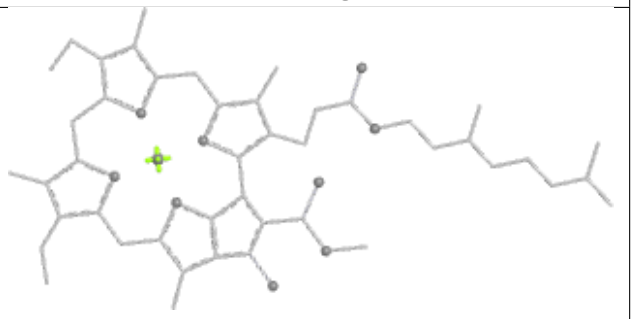
Bond lengths



Bond angles

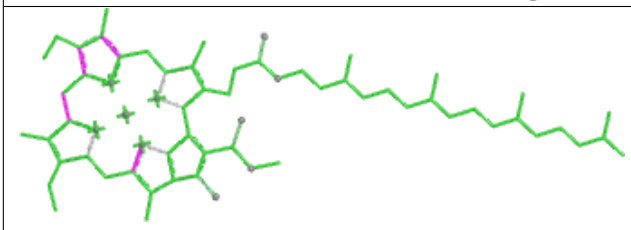


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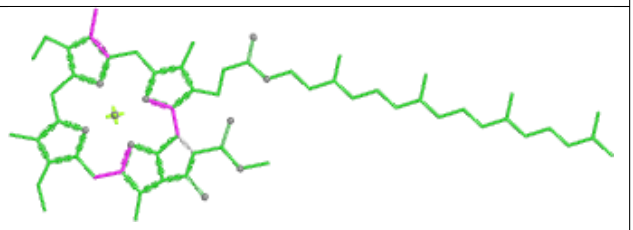


Rings

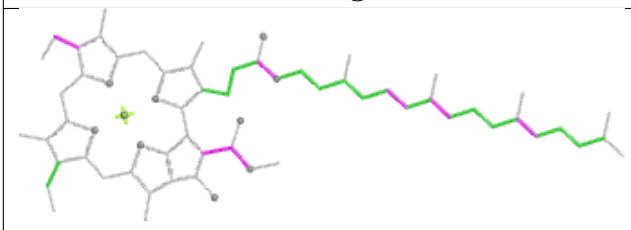
Ligand CLA w 507



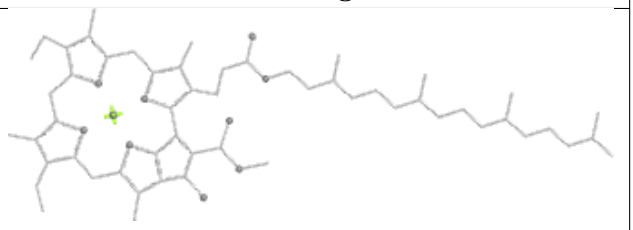
Bond lengths



Bond angles

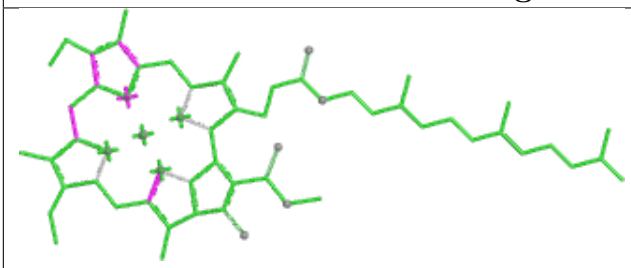


Torsions

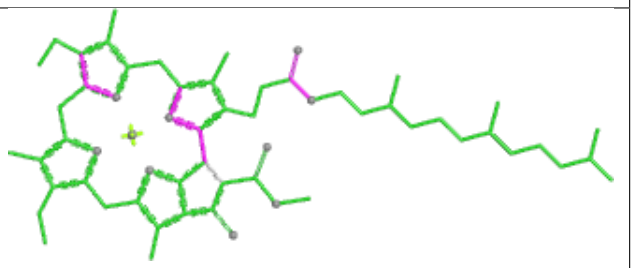


Rings

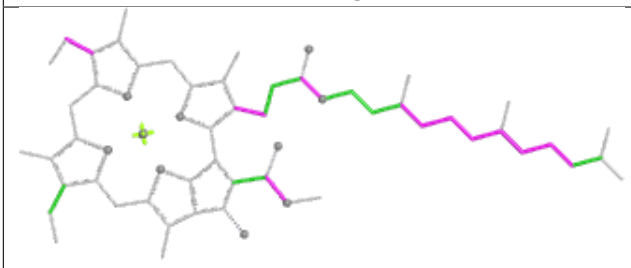
Ligand CLA A 1139



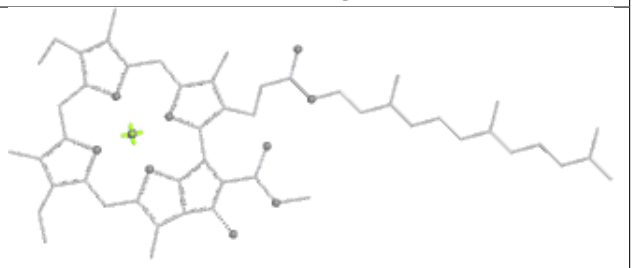
Bond lengths



Bond angles

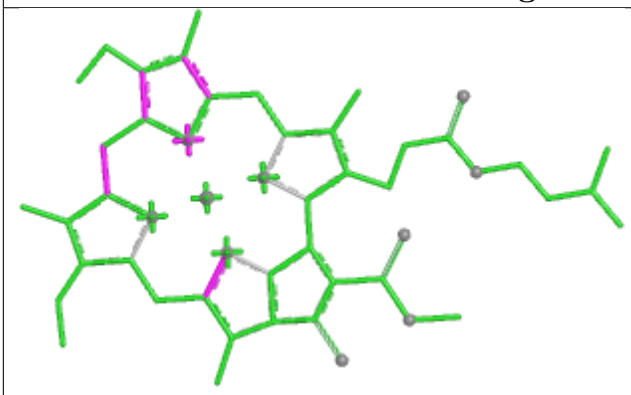


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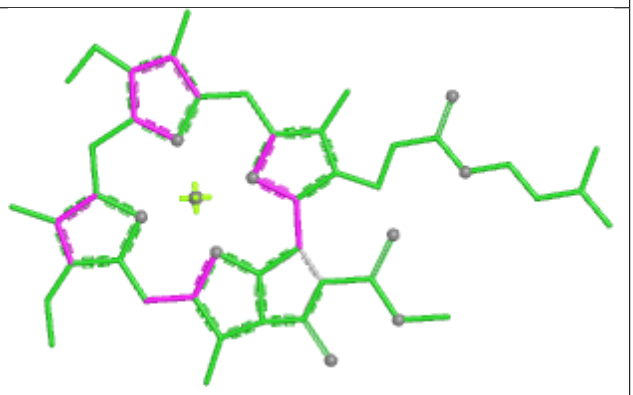


Rings

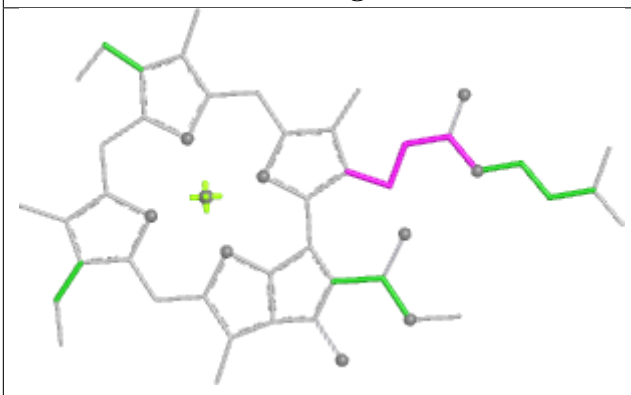
Ligand CLA b 1236



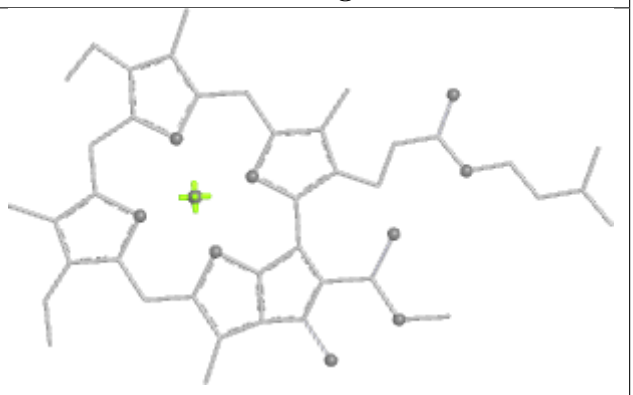
Bond lengths



Bond angles

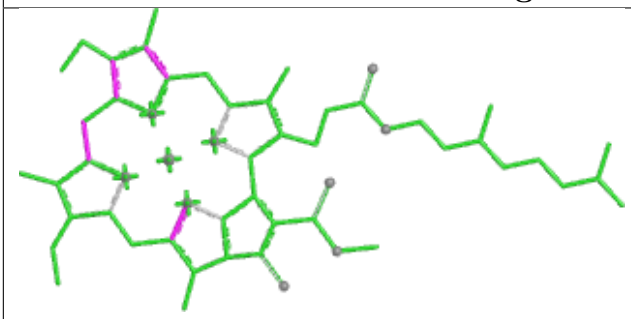


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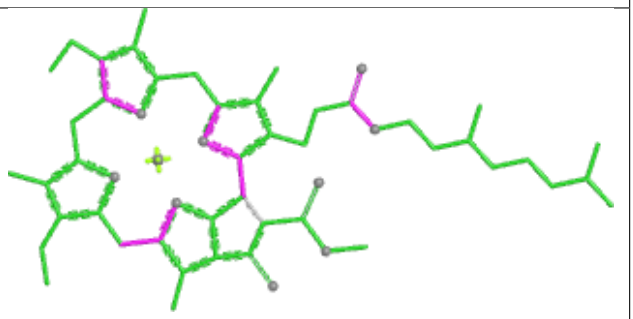


Rings

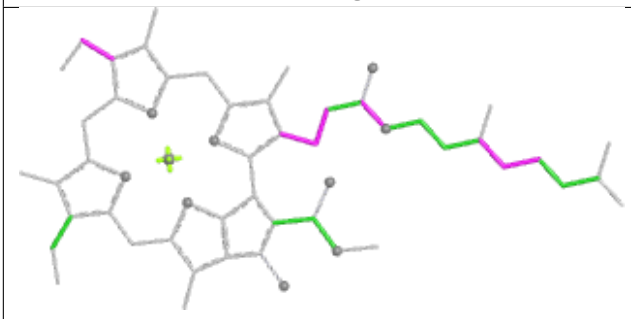
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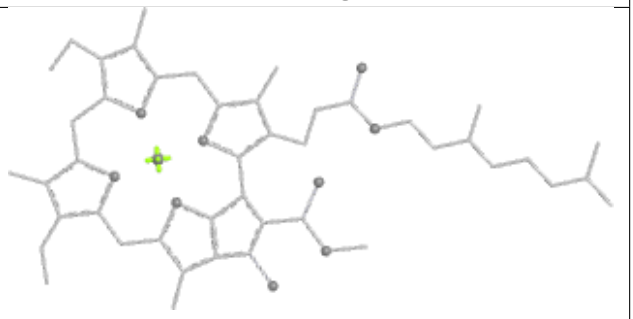
Bond lengths



Bond angles

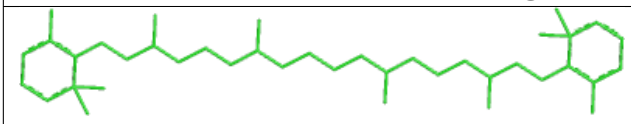


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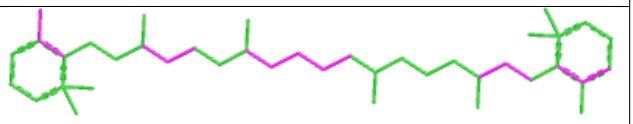


Rings

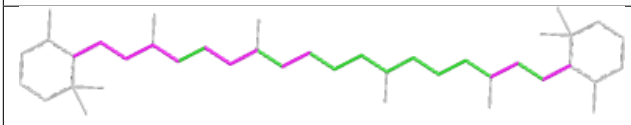
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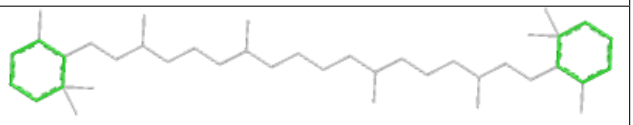
Bond lengths



Bond angles

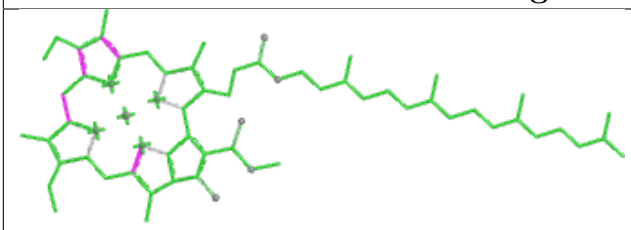


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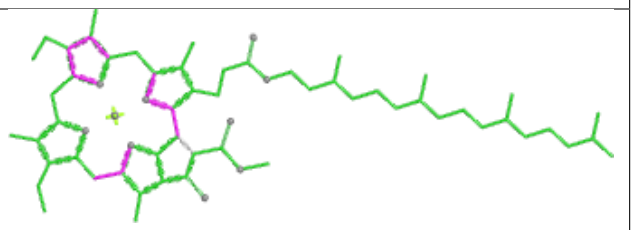


Rings

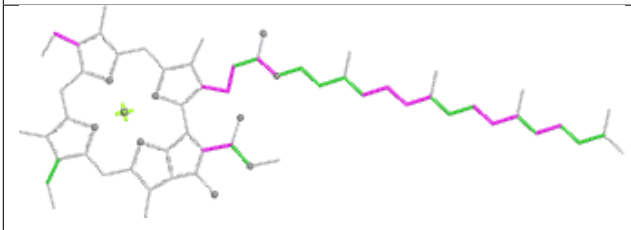
Ligand CLA t 515



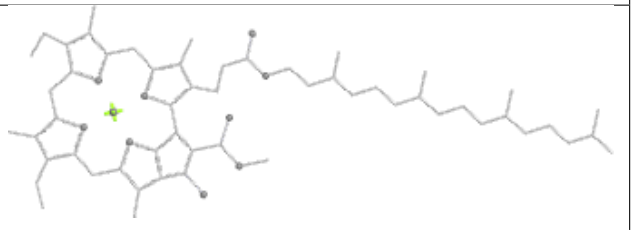
Bond lengths



Bond angles

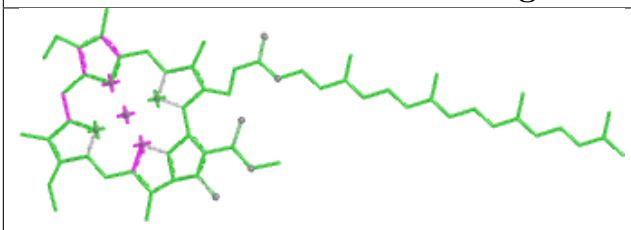


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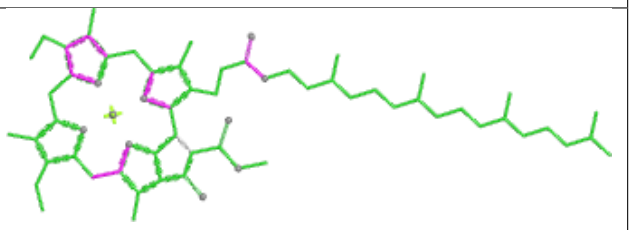


Rings

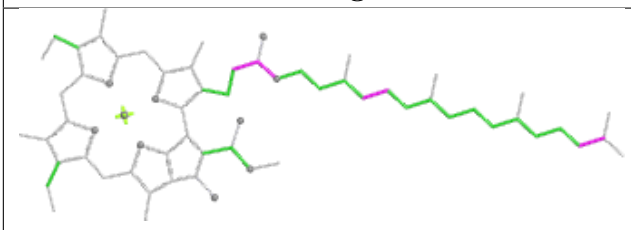
Ligand CL0 H 1011



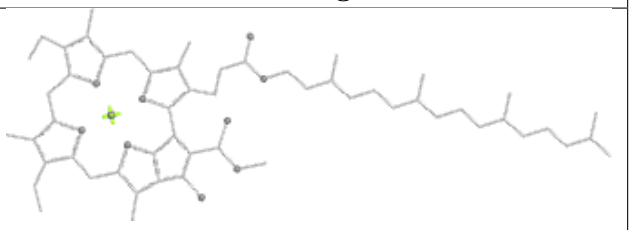
Bond lengths



Bond angles

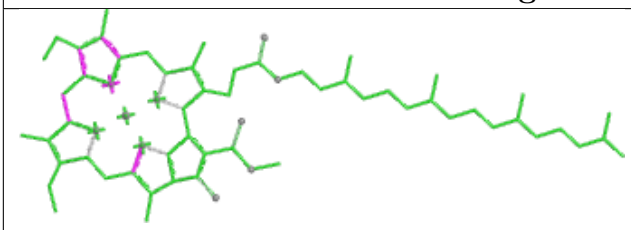


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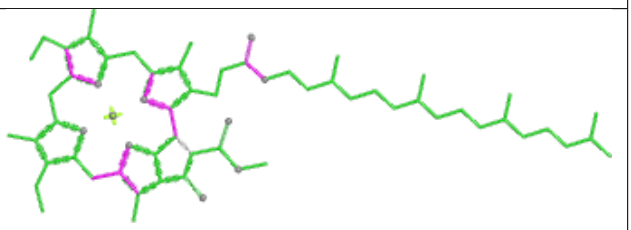


Rings

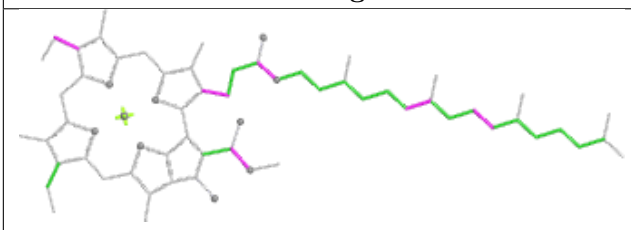
Ligand CLA W 511



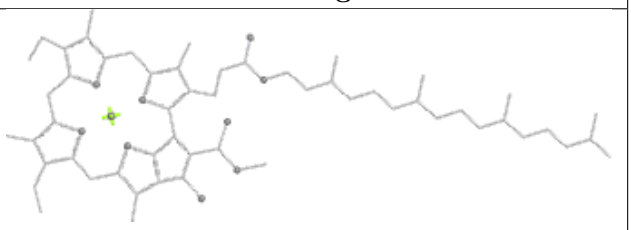
Bond lengths



Bond angles

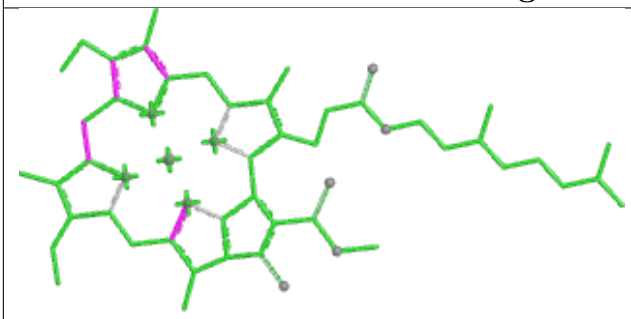


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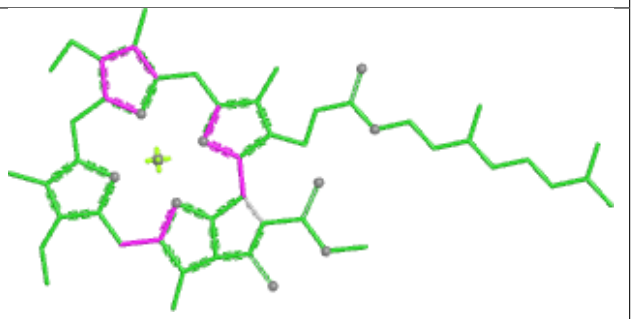


Rings

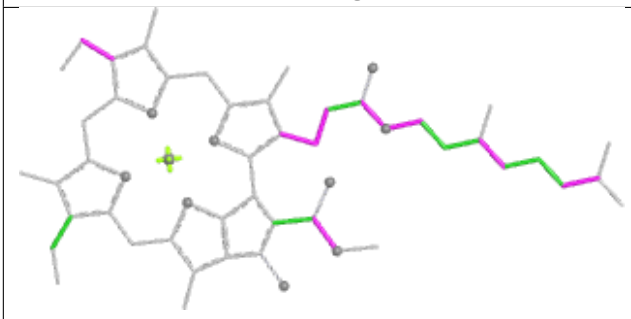
Ligand CLA b 1228



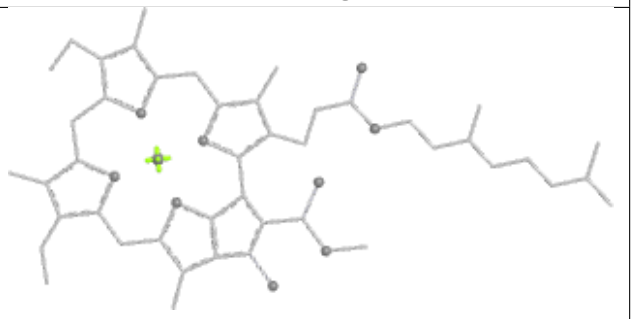
Bond lengths



Bond angles

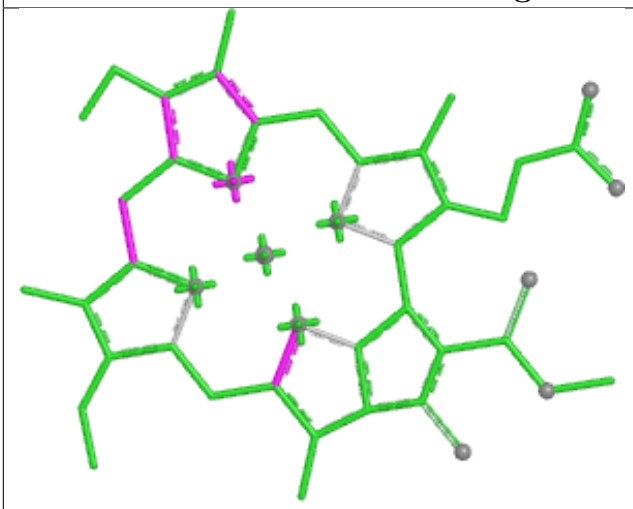


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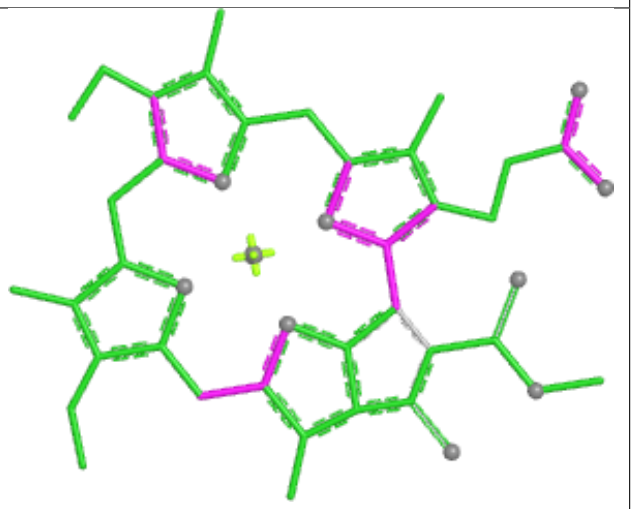


Rings

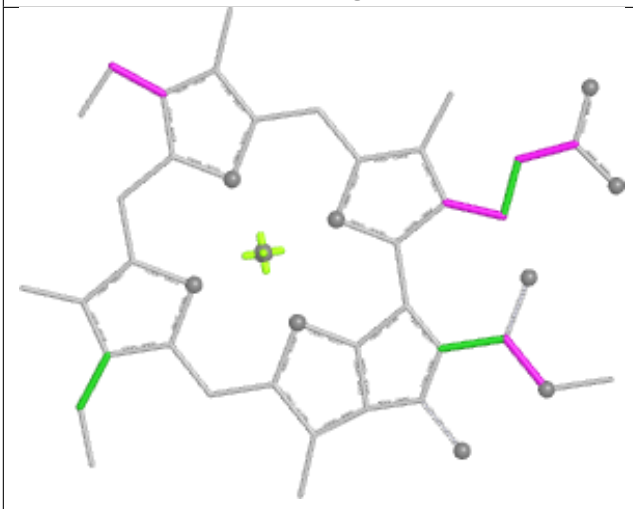
Ligand CLA G 1232



Bond lengths



Bond angles

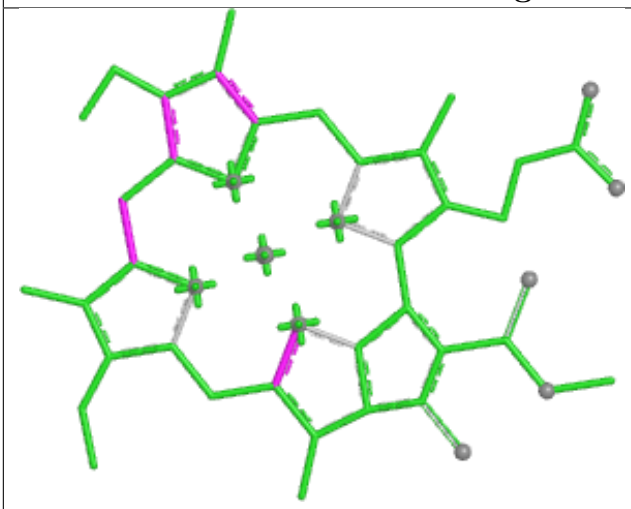


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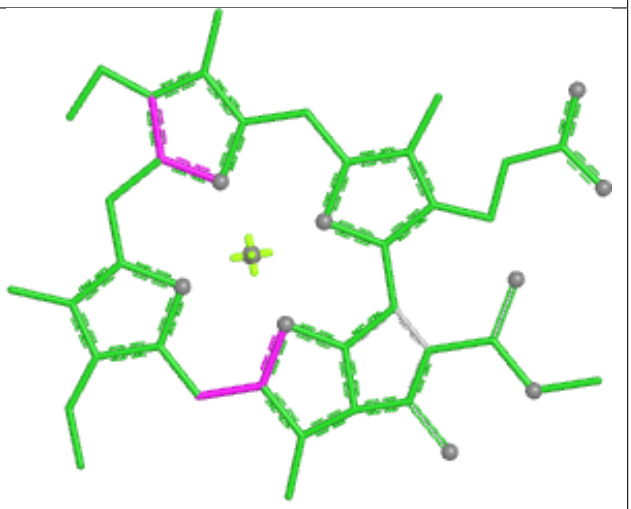


Rings

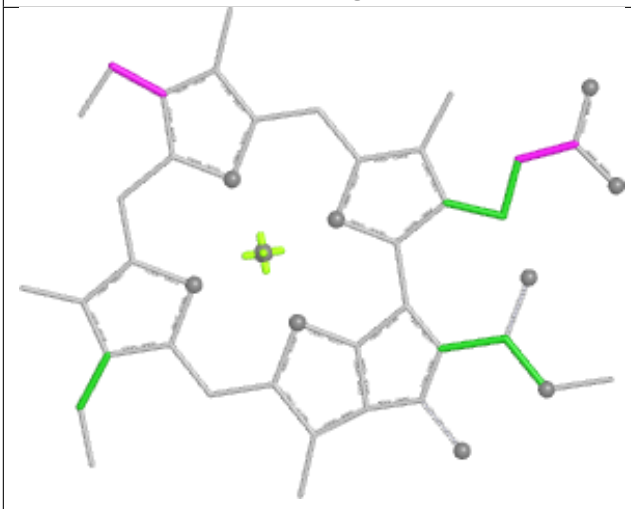
Ligand CLA H 1134



Bond lengths



Bond angles

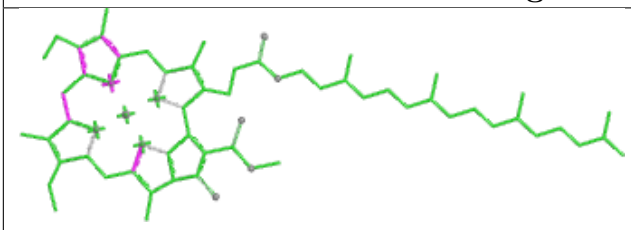


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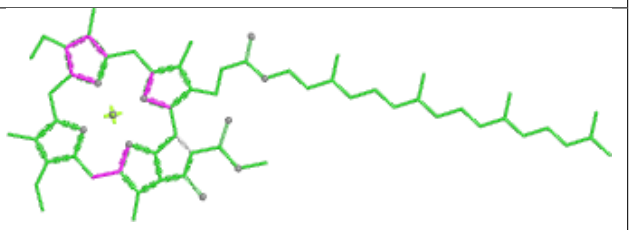


Rings

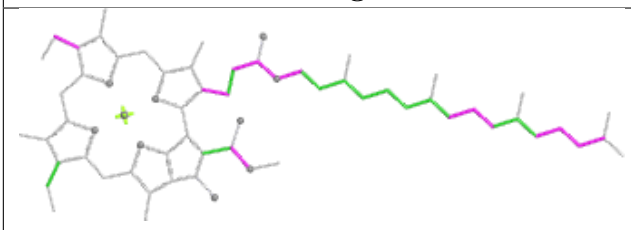
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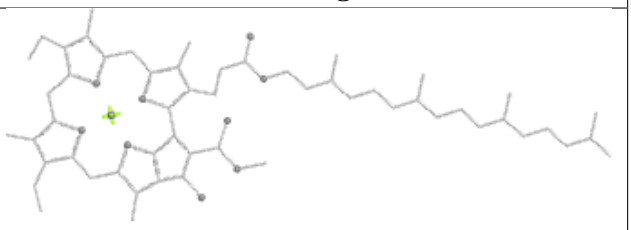
Bond lengths



Bond angles

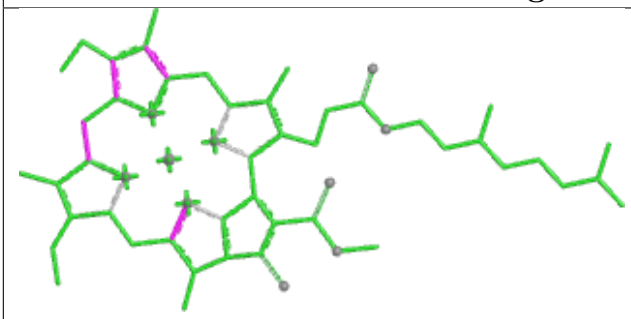


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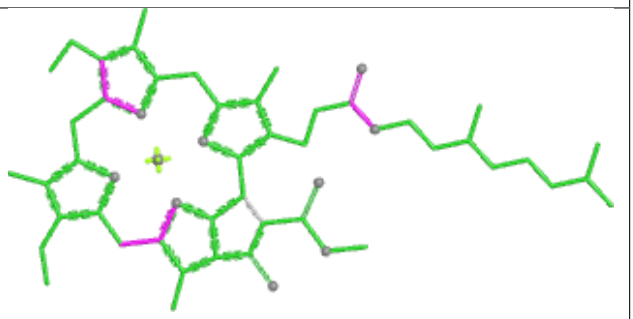


Rings

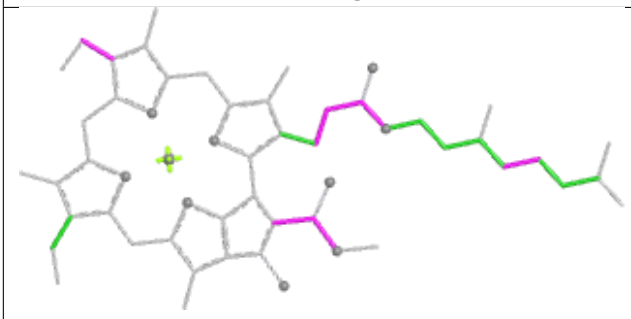
Ligand CLA x 508



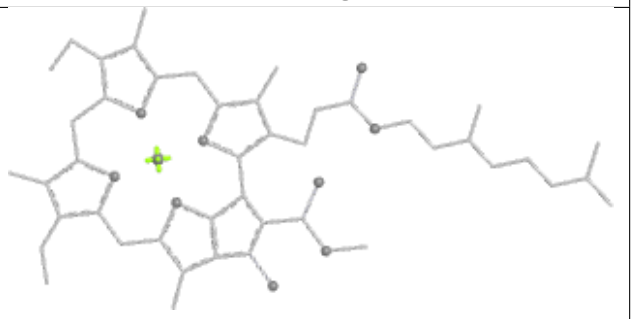
Bond lengths



Bond angles

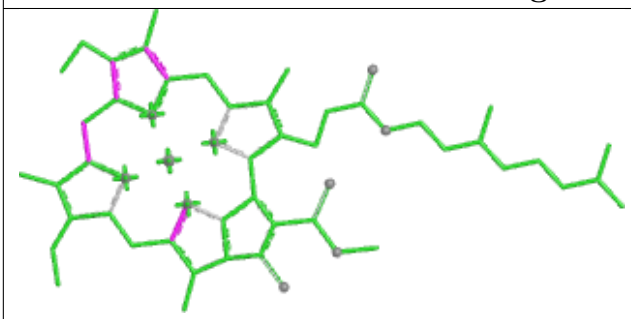


Torsions

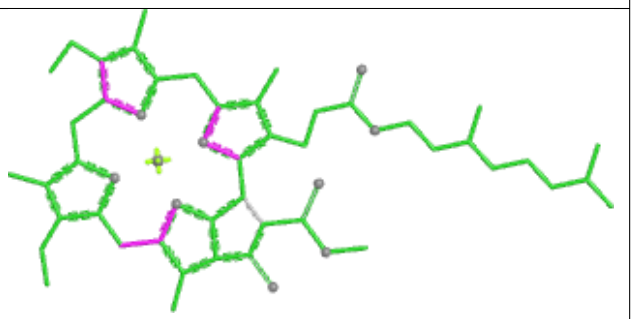


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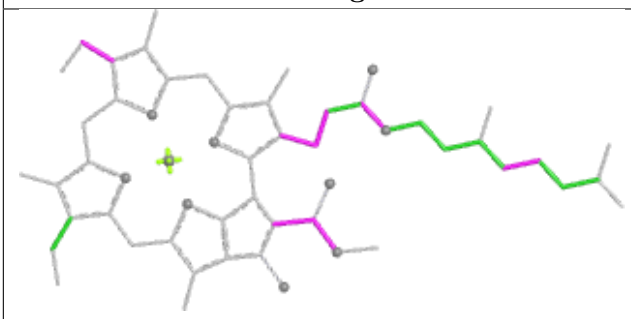
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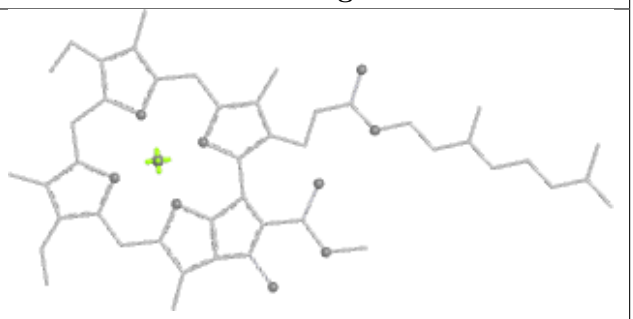
Bond lengths



Bond angles

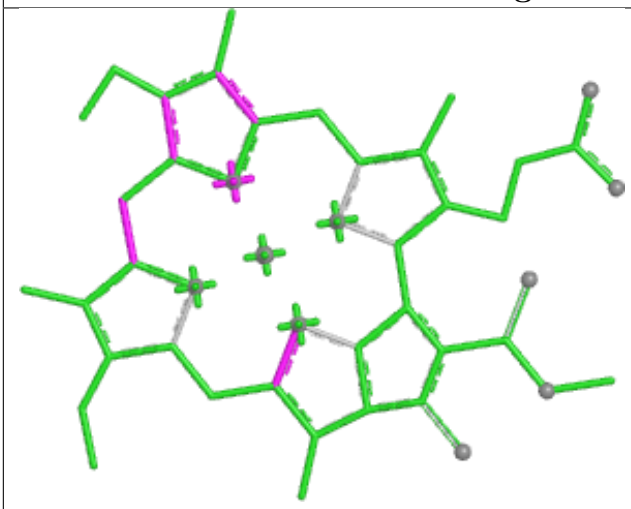


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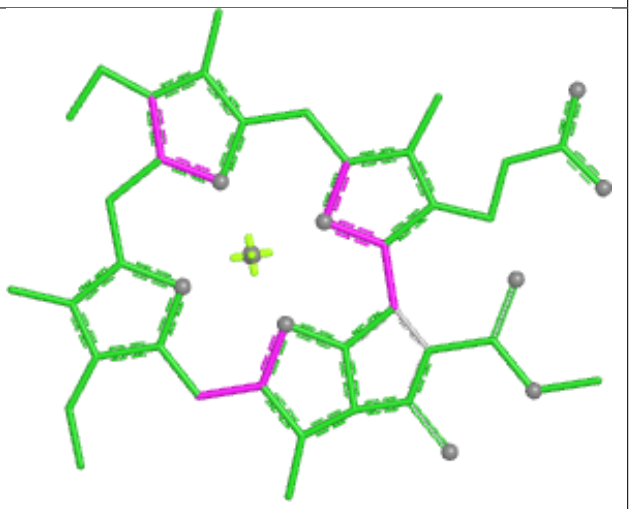


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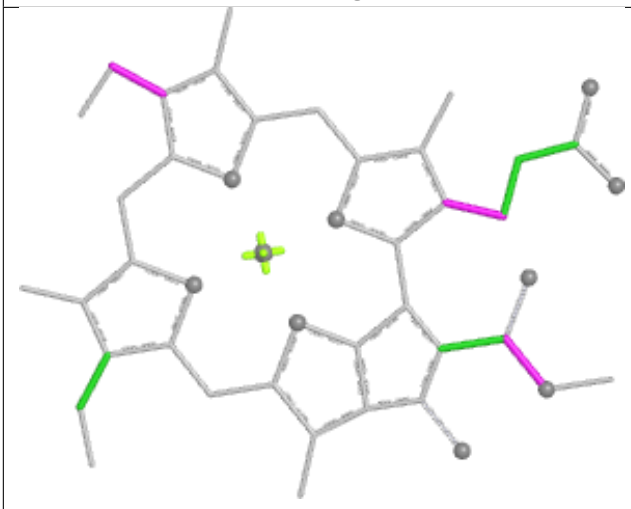
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Bond lengths



Bond angles

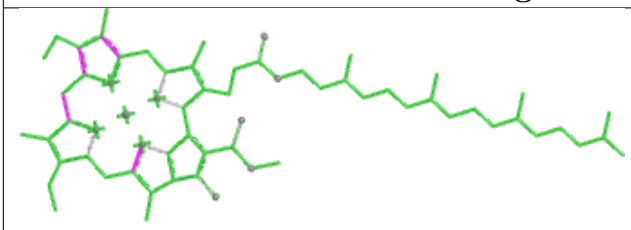


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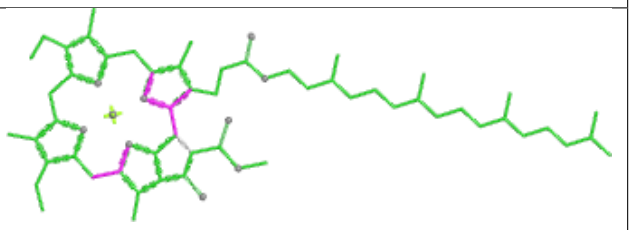


Rings

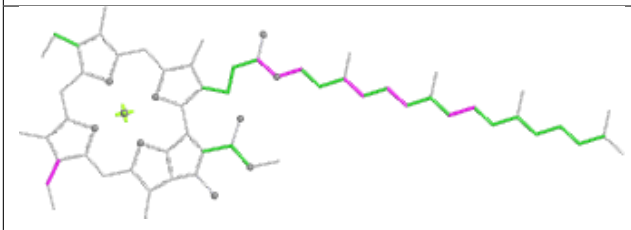
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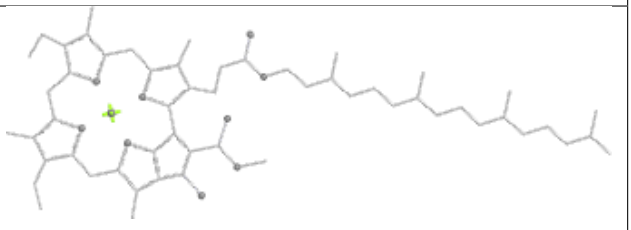
Bond lengths



Bond angles

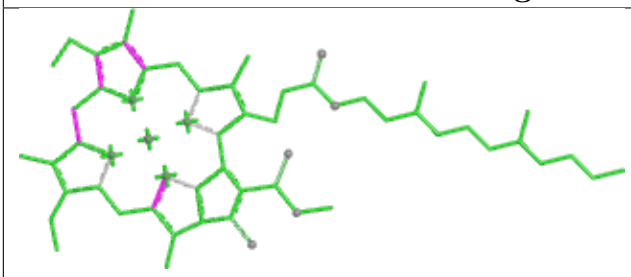


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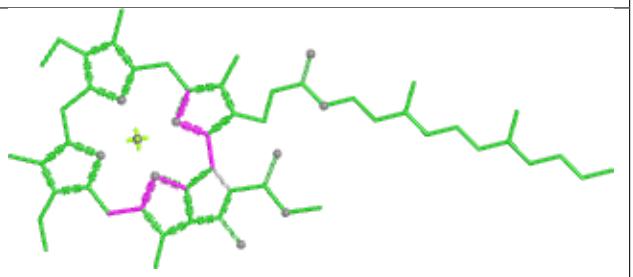


Rings

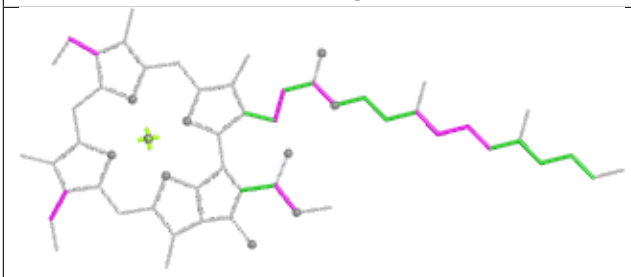
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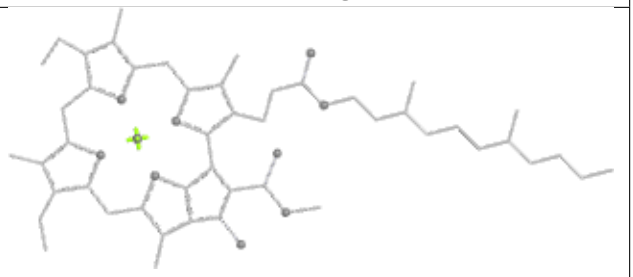
Bond lengths



Bond angles

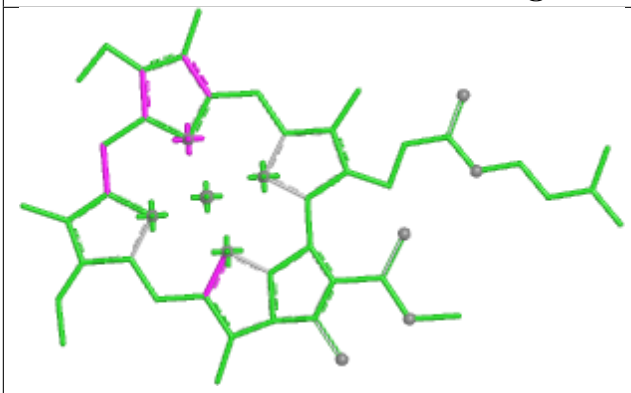


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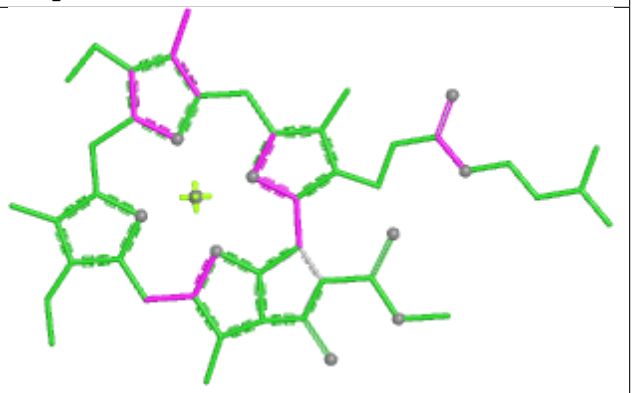


Rings

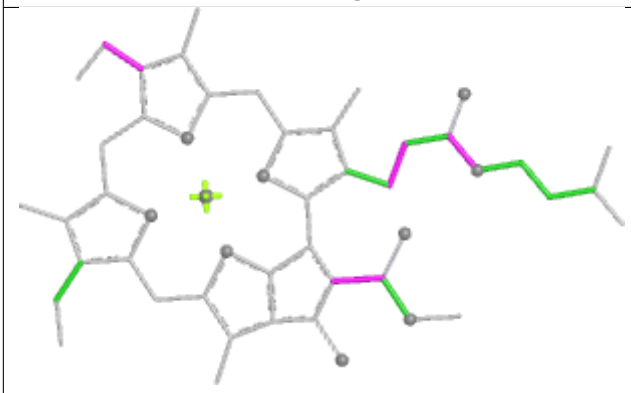
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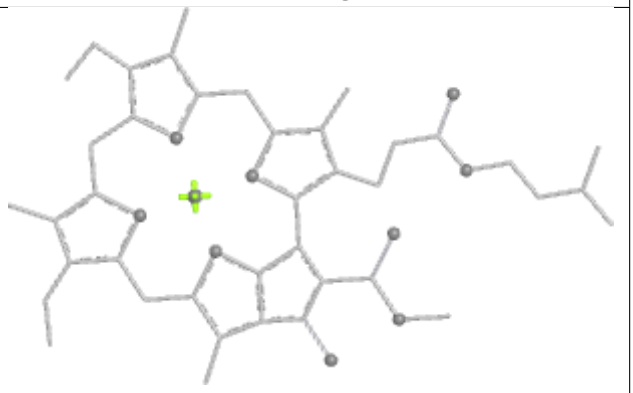
Bond lengths



Bond angles

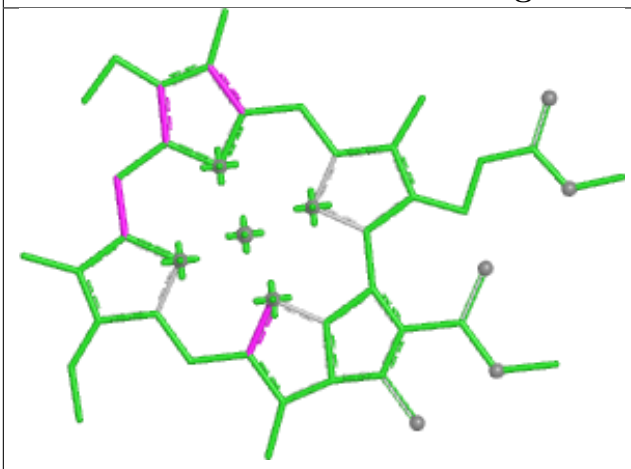


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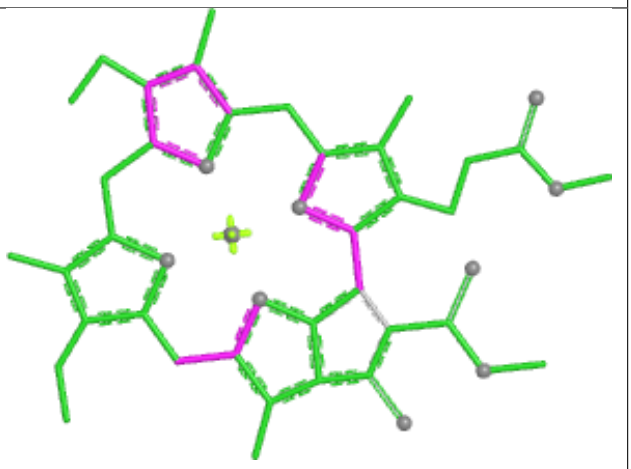


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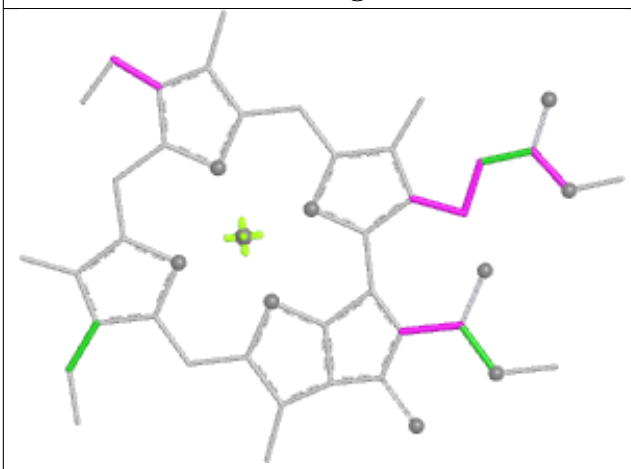
Ligand CLA A 1129



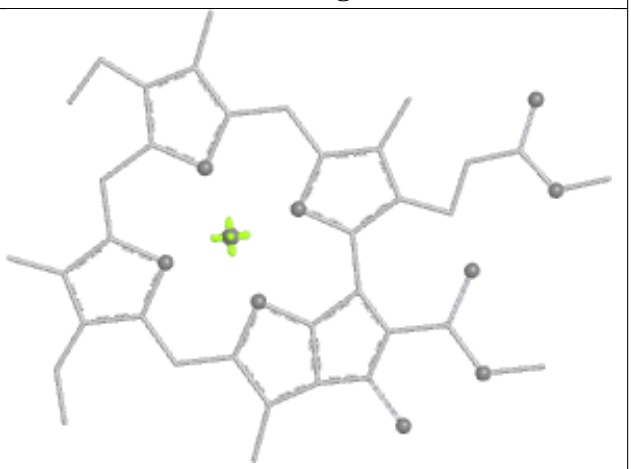
Bond lengths



Bond angles

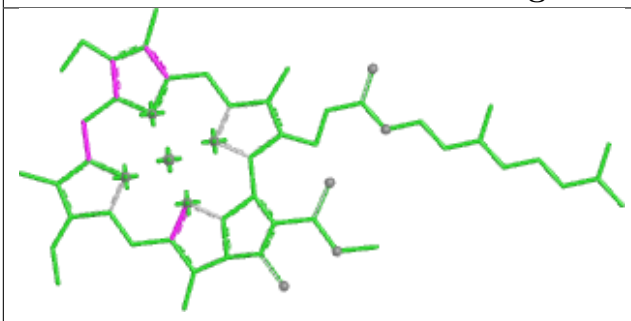


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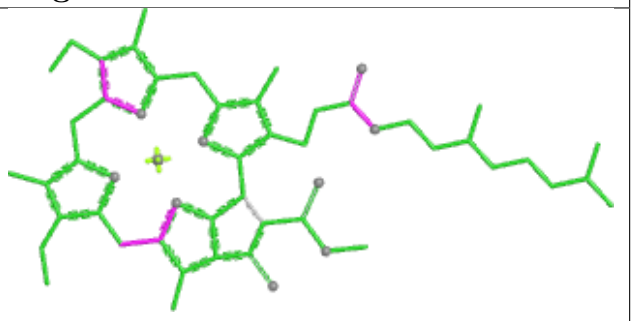


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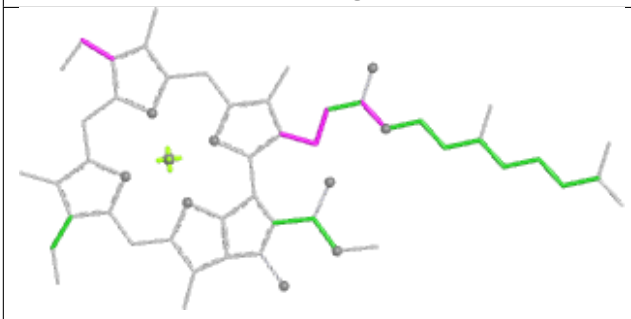
Ligand CLA g 508



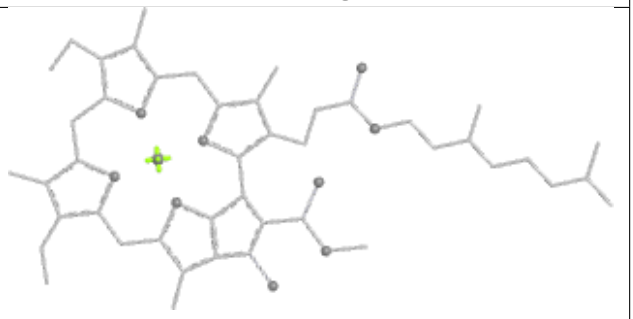
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Bond angles

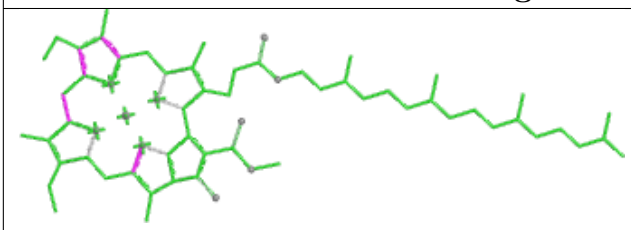


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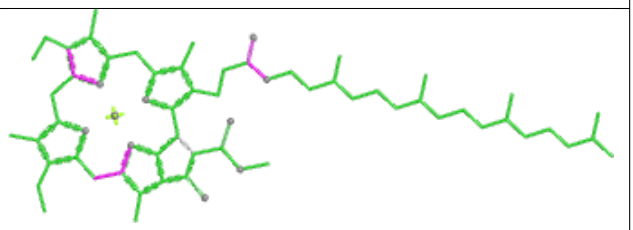


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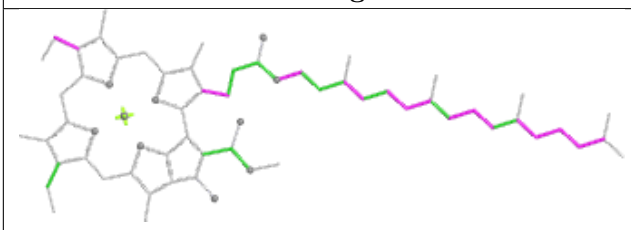
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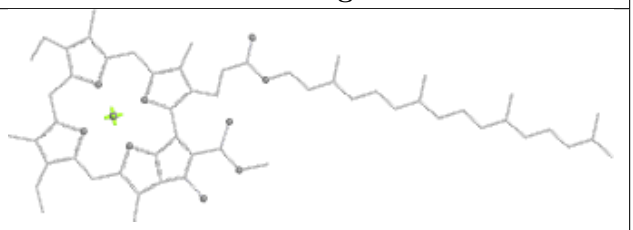
Bond lengths



Bond angles



Torsions

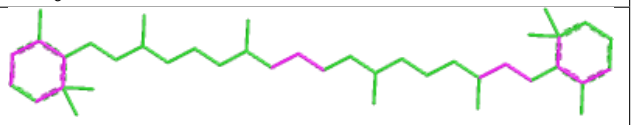


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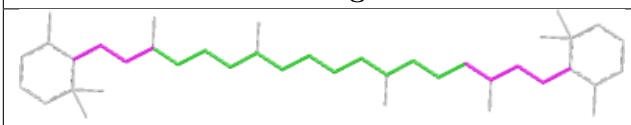
Ligand BCR y 604



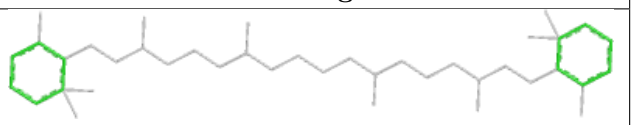
Bond lengths



Bond angles

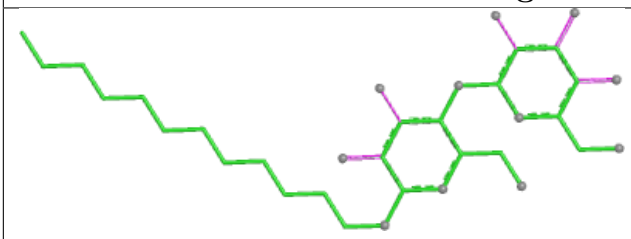


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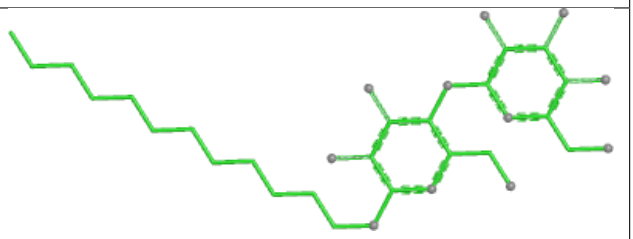


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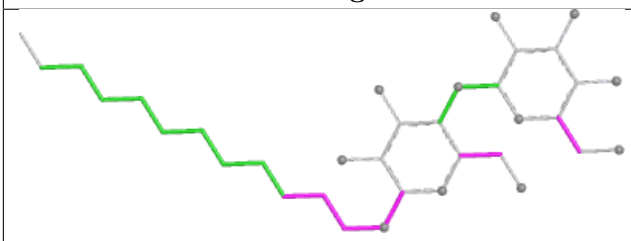
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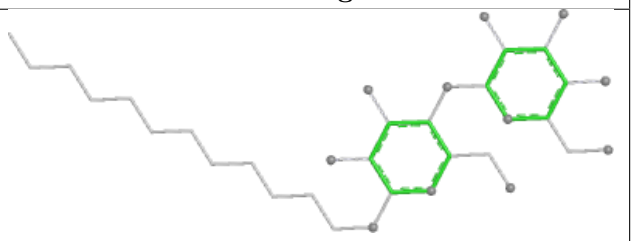
Bond lengths



Bond angles

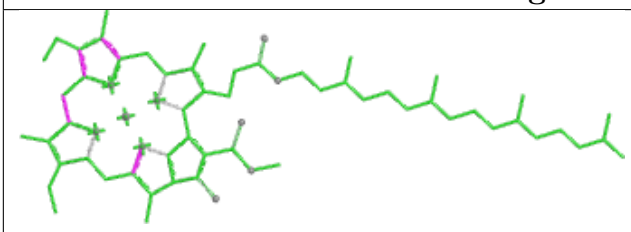


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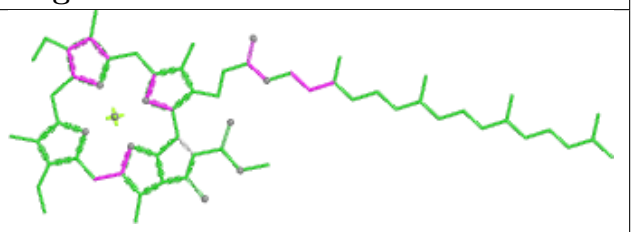


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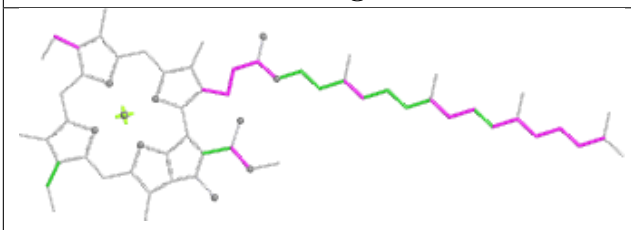
Ligand CLA g 504



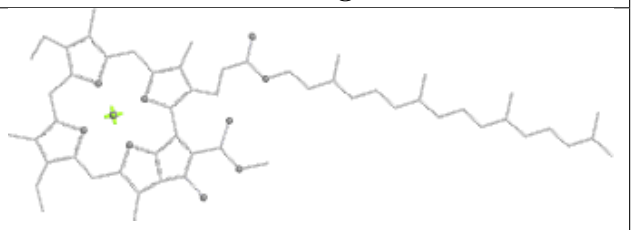
Bond lengths



Bond angles

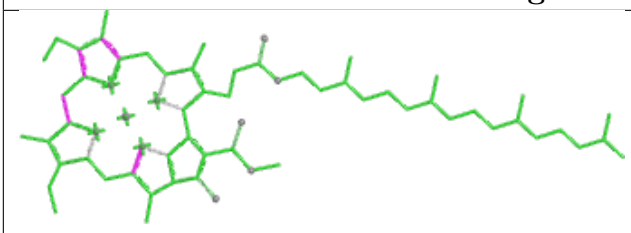


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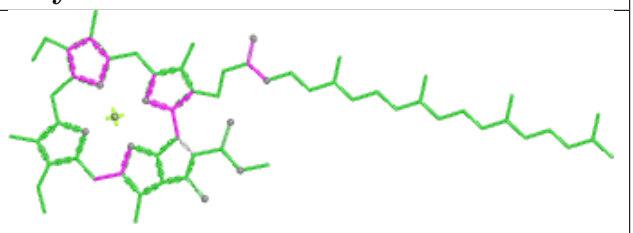


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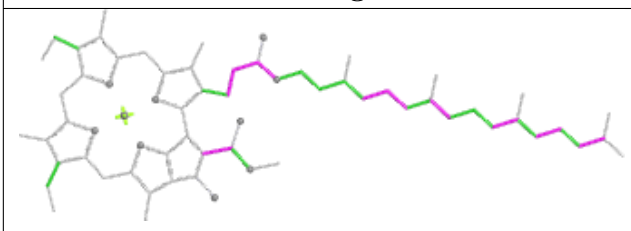
Ligand CLA y 515



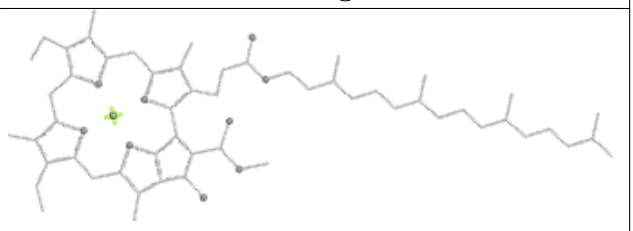
Bond lengths



Bond angles

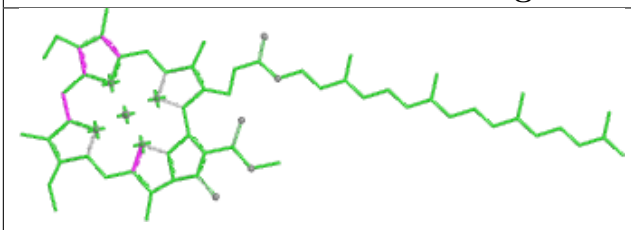


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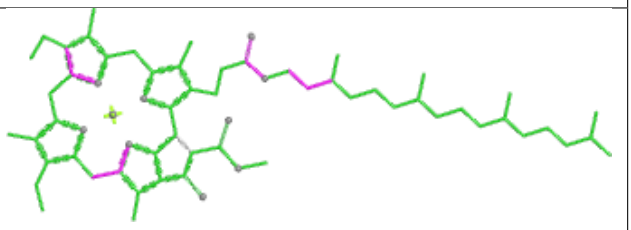


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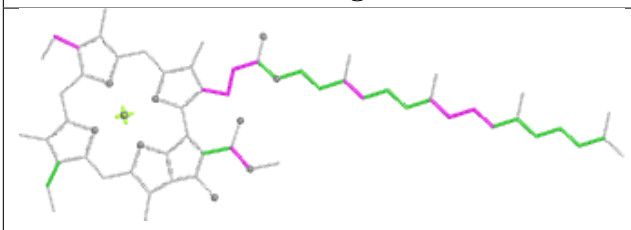
Ligand CLA A 1138



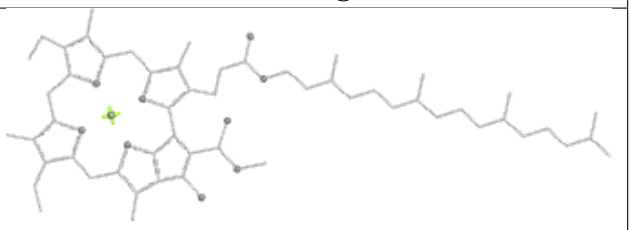
Bond lengths



Bond angles

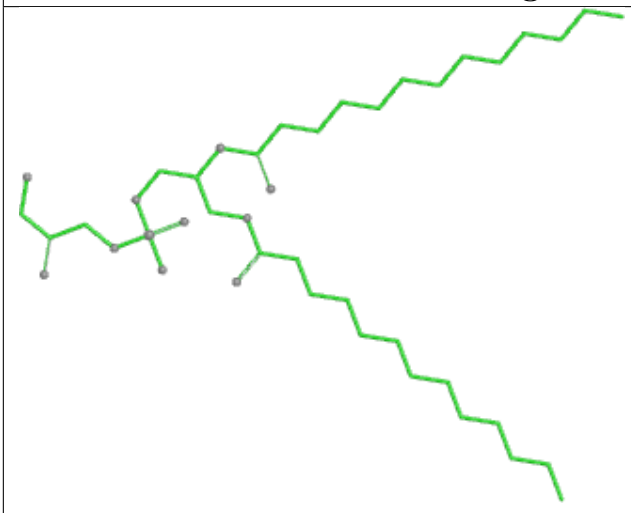


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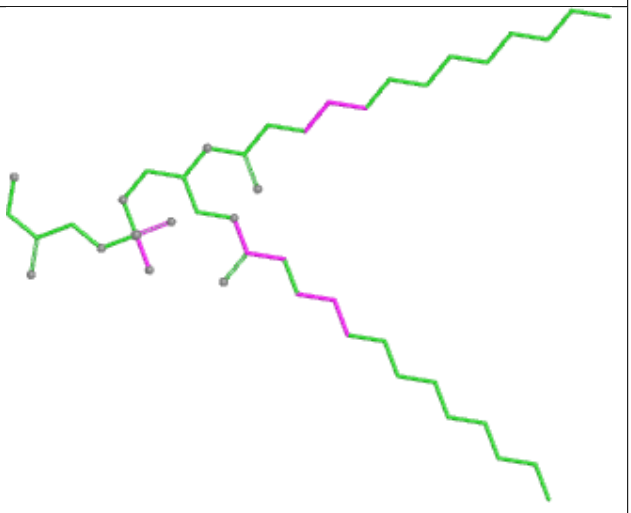


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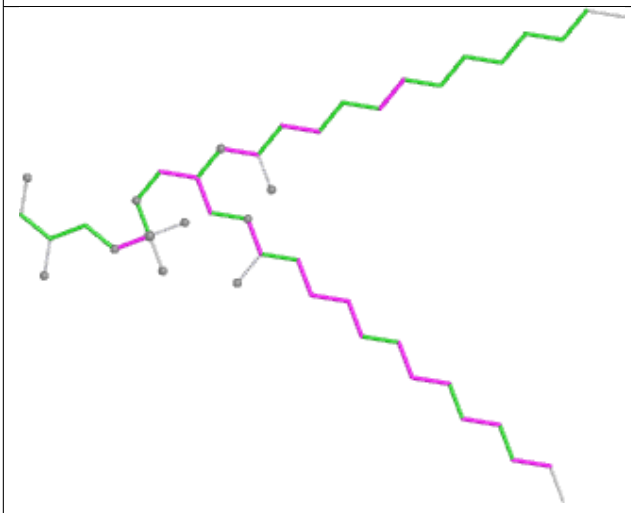
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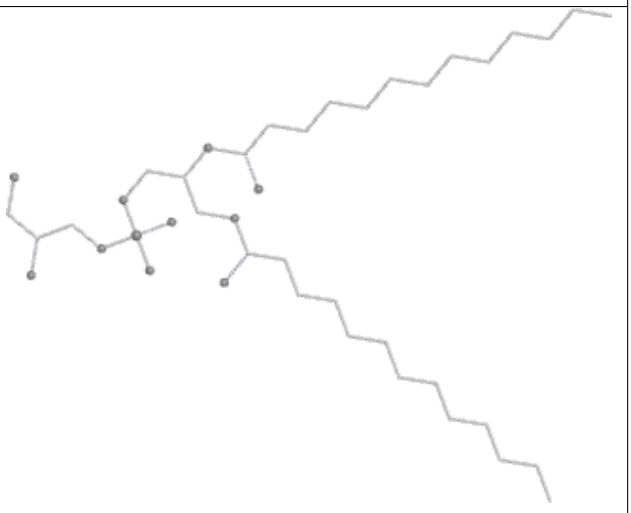
Bond lengths



Bond angles

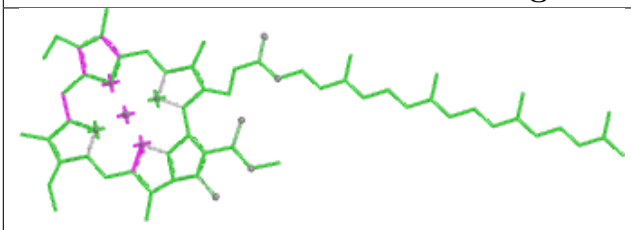


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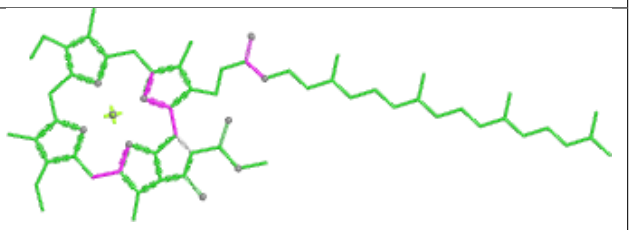


Rings

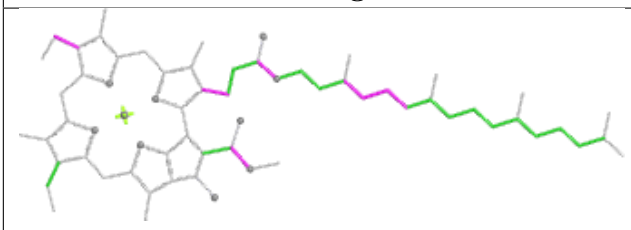
Ligand CLA r 512



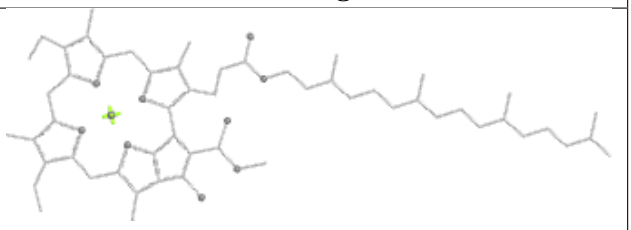
Bond lengths



Bond angles

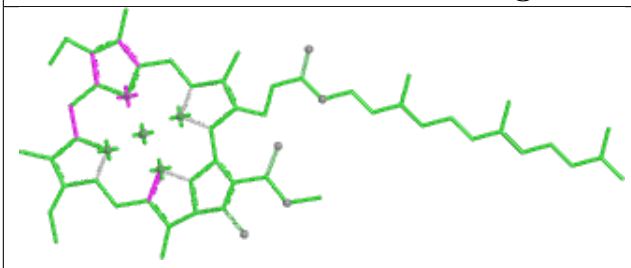


Torsions

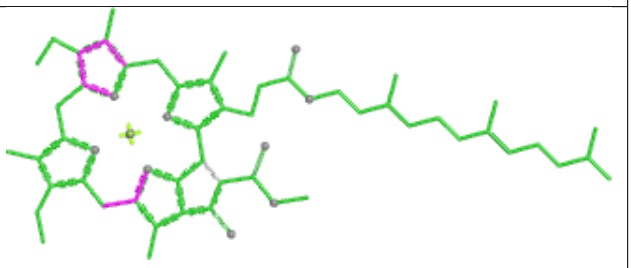


Rings

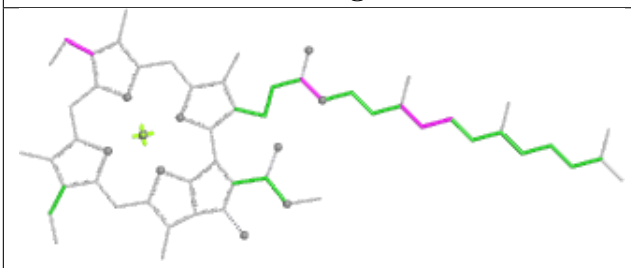
Ligand CLA H 1124



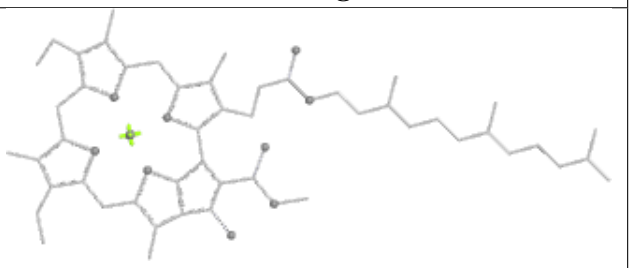
Bond lengths



Bond angles



Torsions

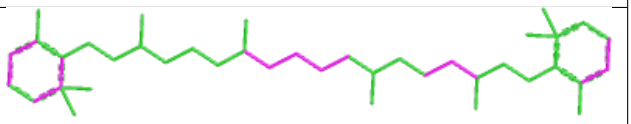


Rings

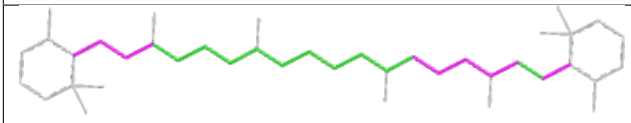
Ligand BCR u 602



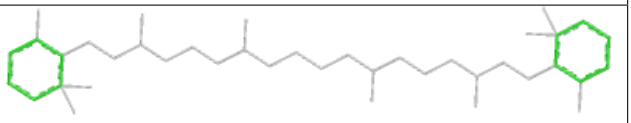
Bond lengths



Bond angles

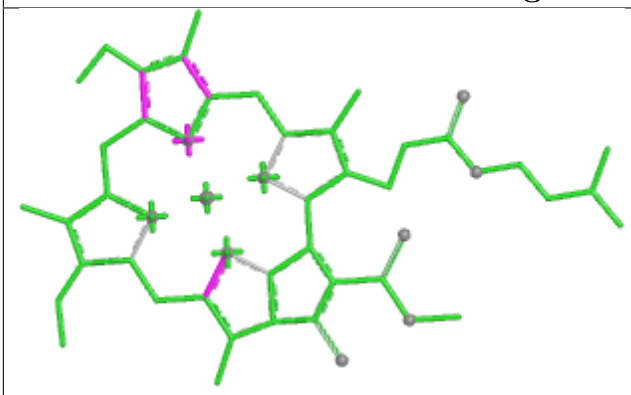


Torsions

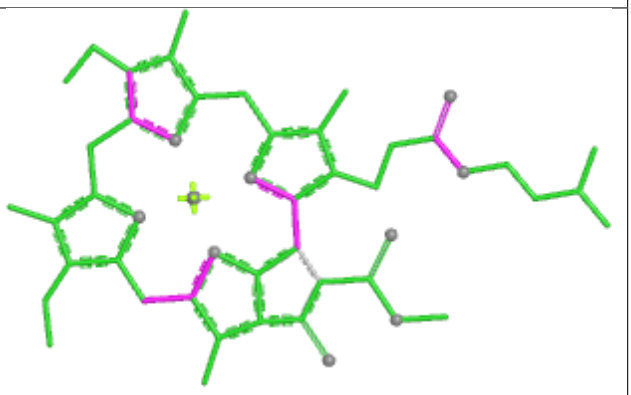


Rings

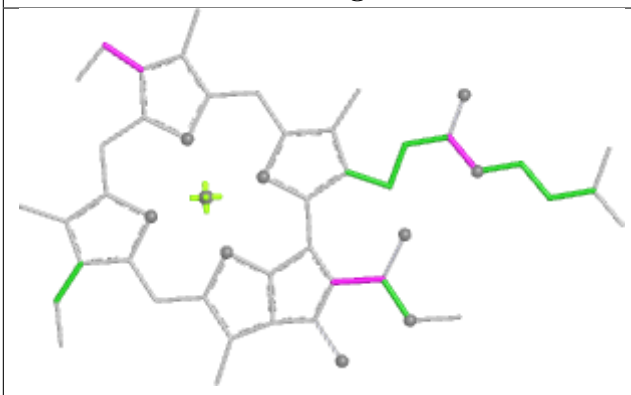
Ligand CLA Y 502



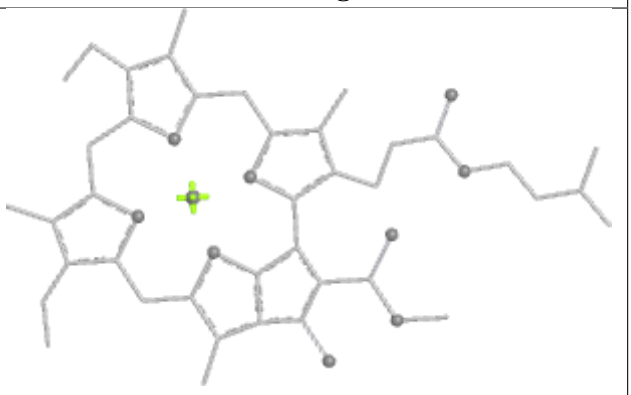
Bond lengths



Bond angles



Torsions

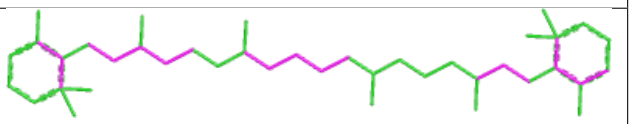


Rings

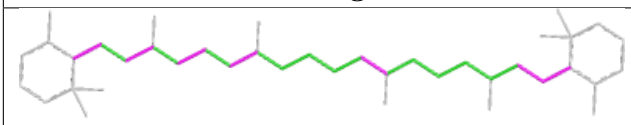
Ligand BCR S 4015



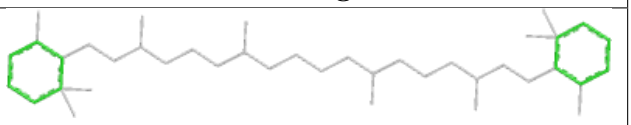
Bond lengths



Bond angles

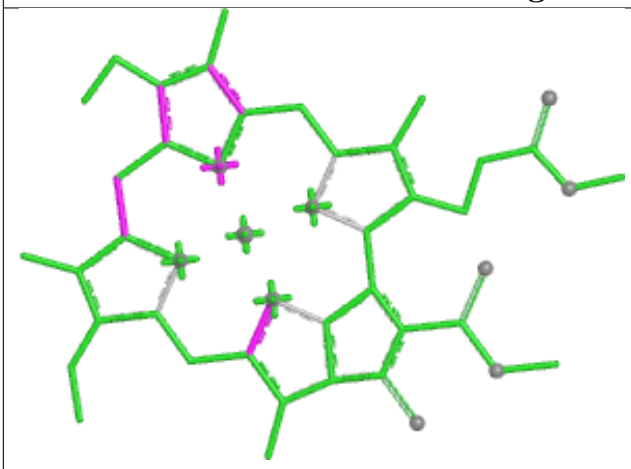


Torsions

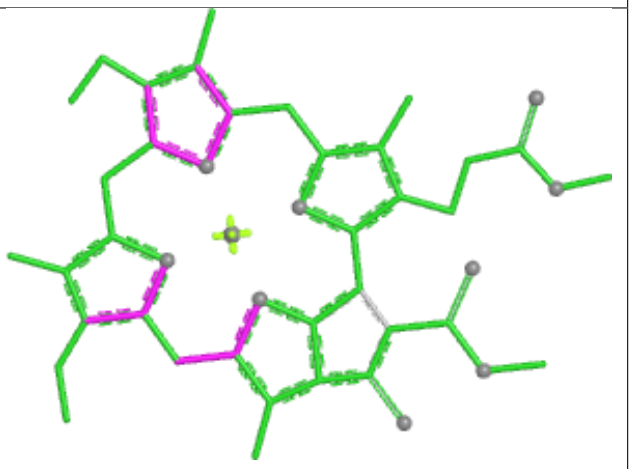


Rings

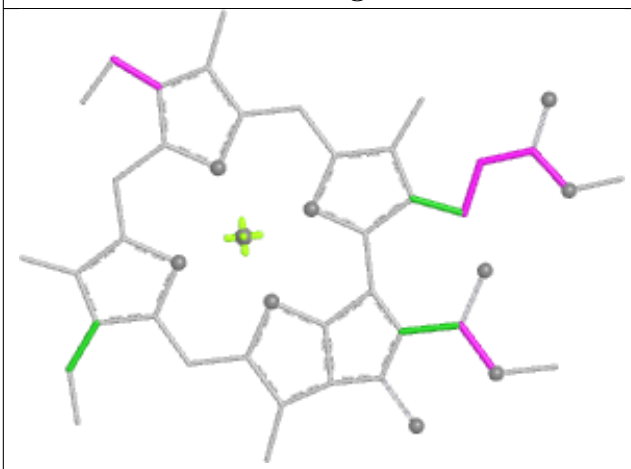
Ligand CLA x 503



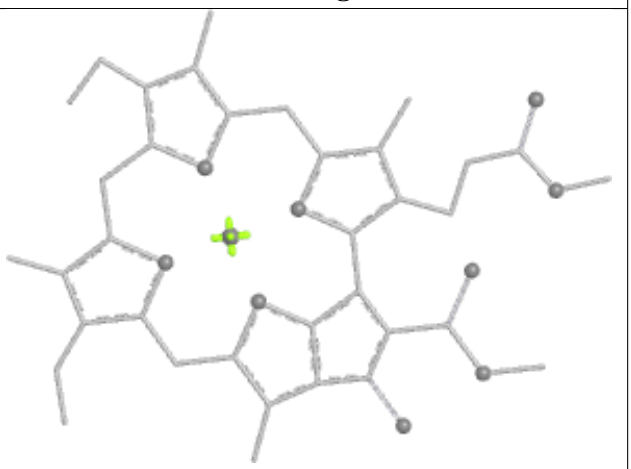
Bond lengths



Bond angles

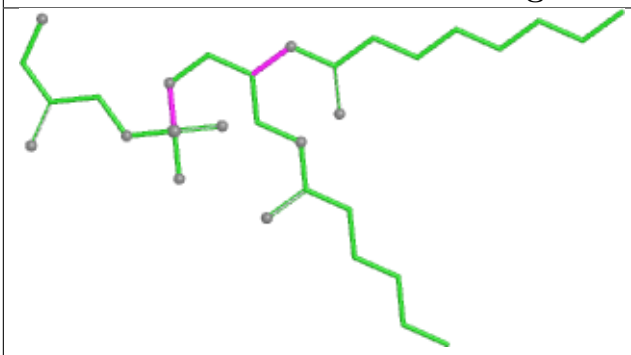


Torsions

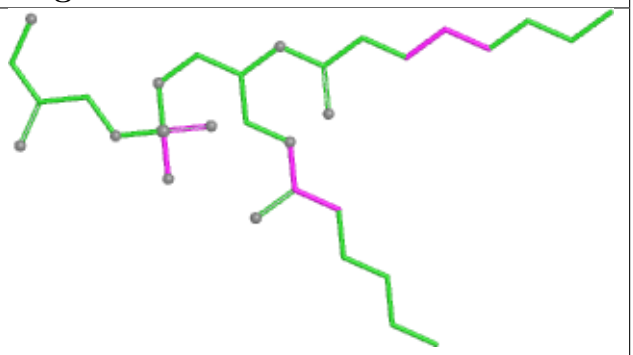


Rings

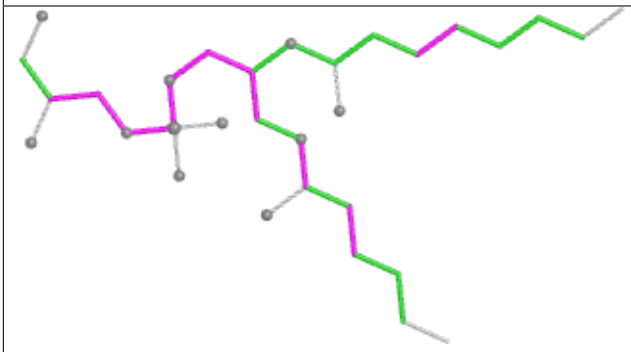
Ligand LHG g 605



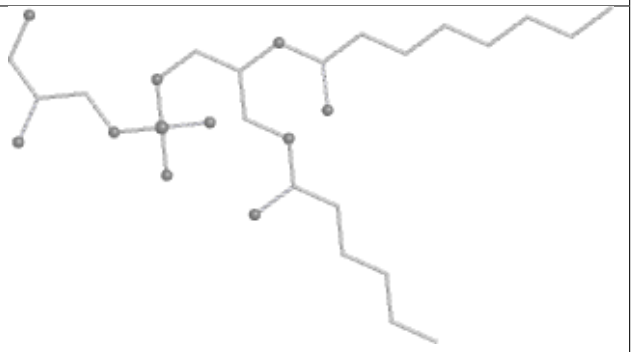
Bond lengths



Bond angles

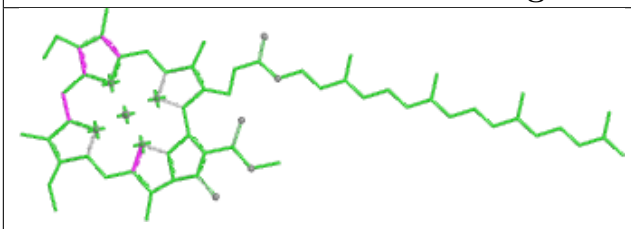


Torsions

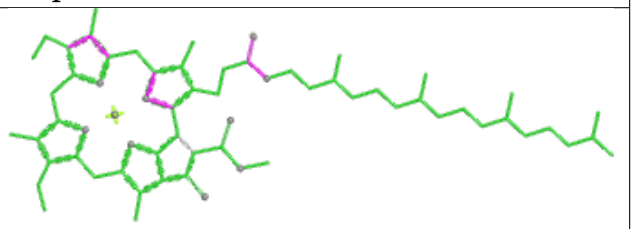


Rings

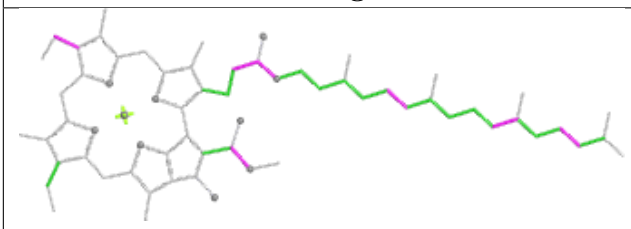
Ligand CLA p 510



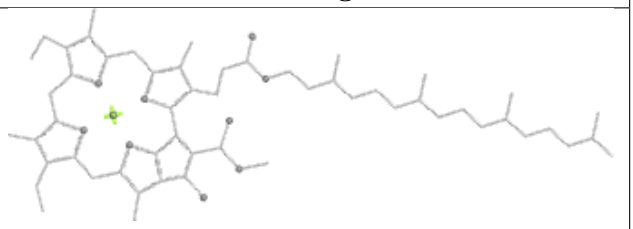
Bond lengths



Bond angles

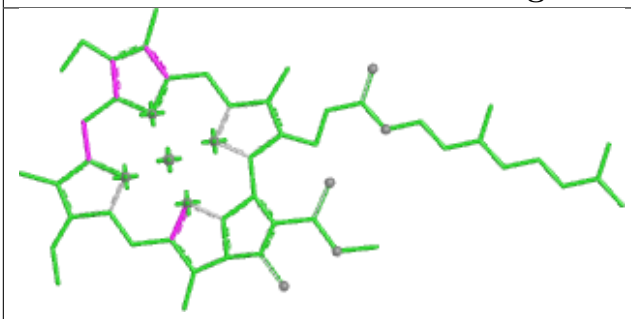


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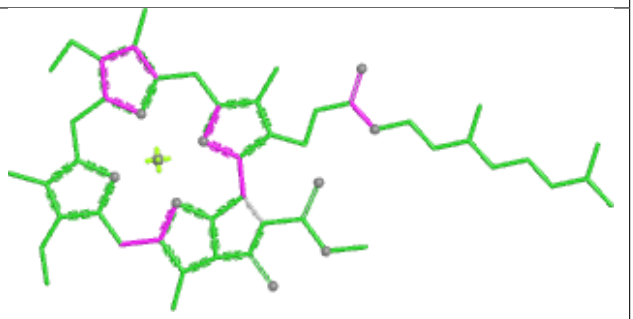


Rings

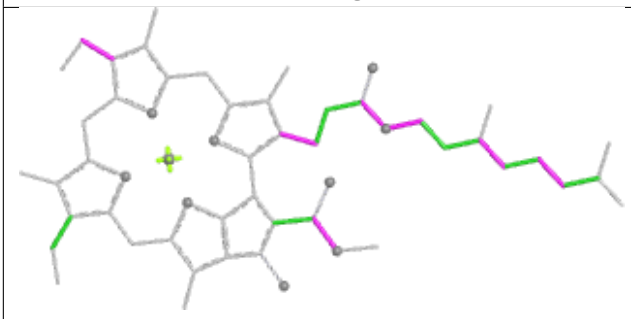
Ligand CLA h 508



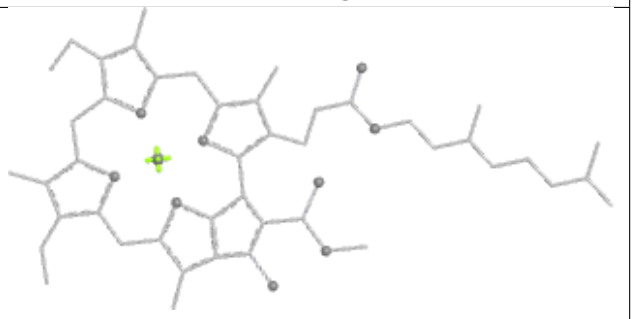
Bond lengths



Bond angles

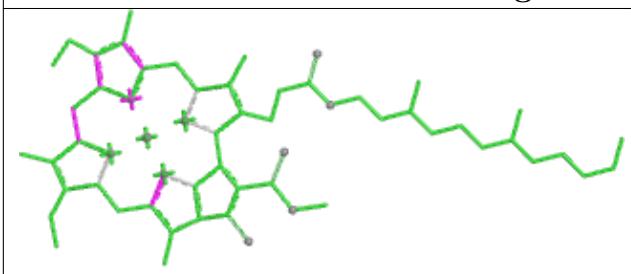


Torsions

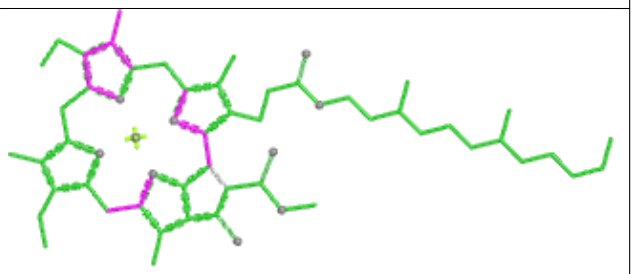


Rings

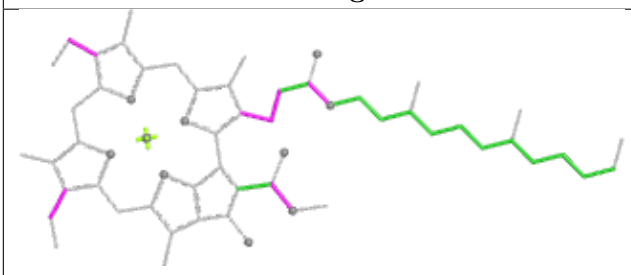
Ligand CLA H 1122



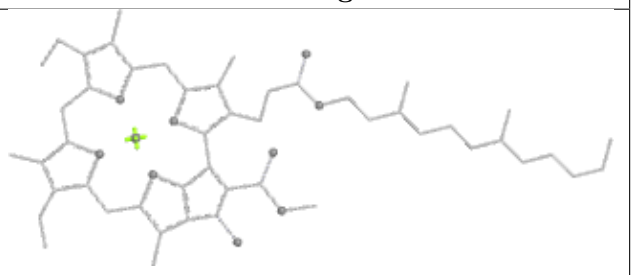
Bond lengths



Bond angles

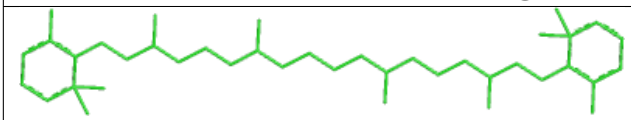


Torsions

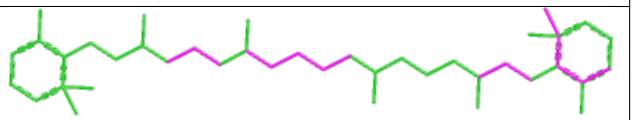


Rings

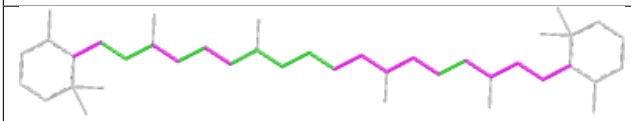
Ligand BCR b 4010



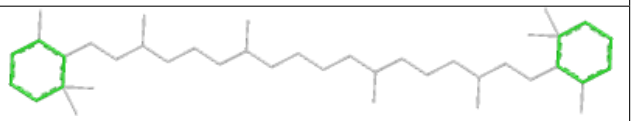
Bond lengths



Bond angles

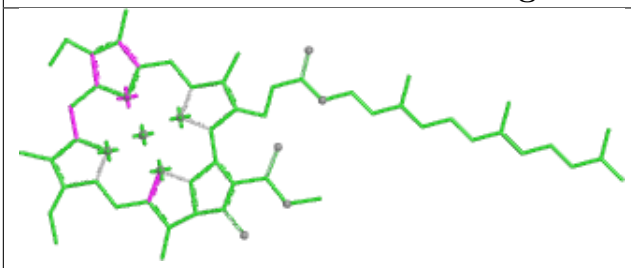


Torsions

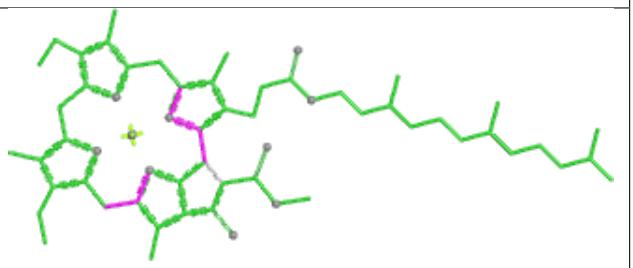


Rings

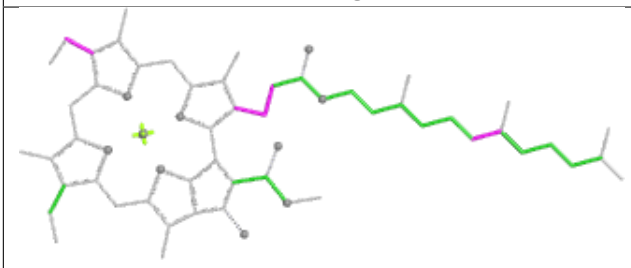
Ligand CLA W 504



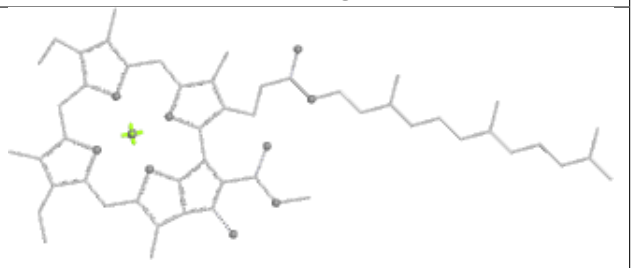
Bond lengths



Bond angles

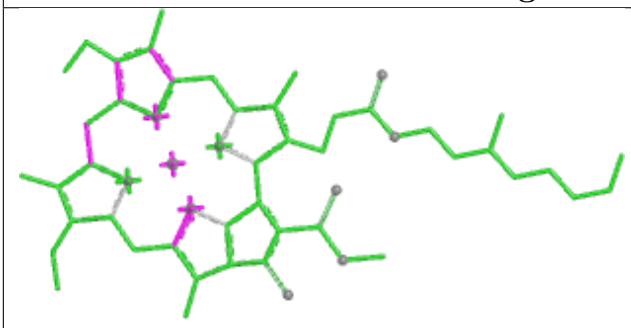


Torsions

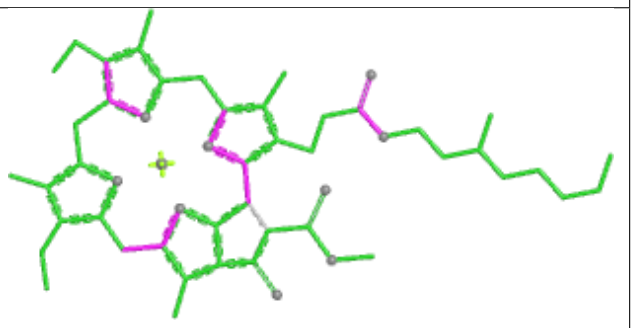


Rings

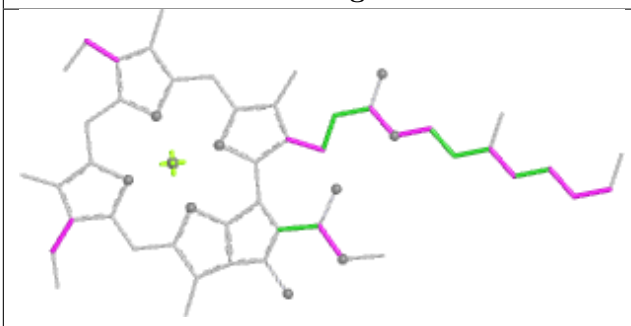
Ligand CLA b 1220



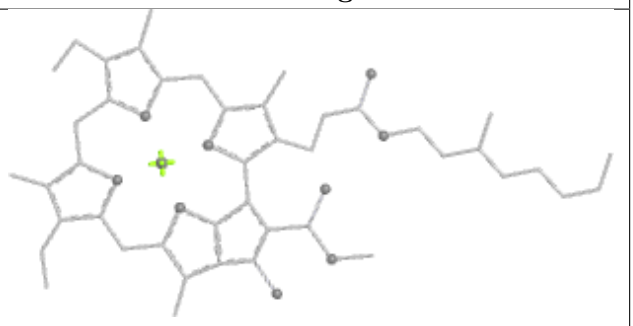
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

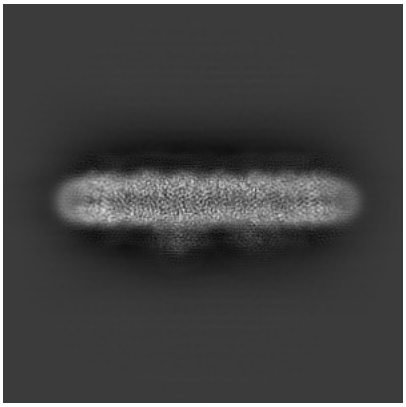
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26601. These allow visual inspection of the internal detail of the map and identification of artifacts.

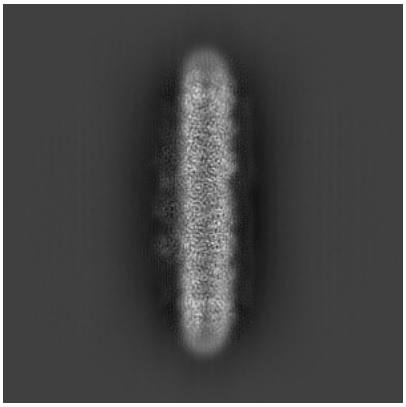
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

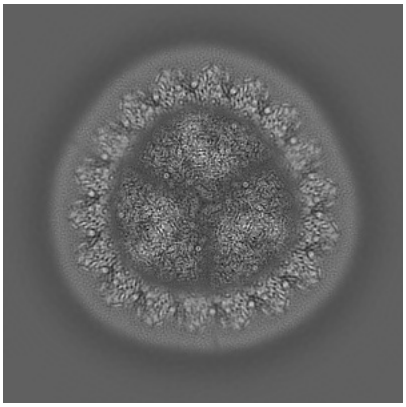
6.1.1 Primary map



X



Y

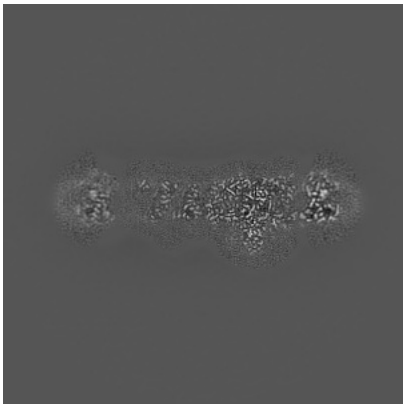


Z

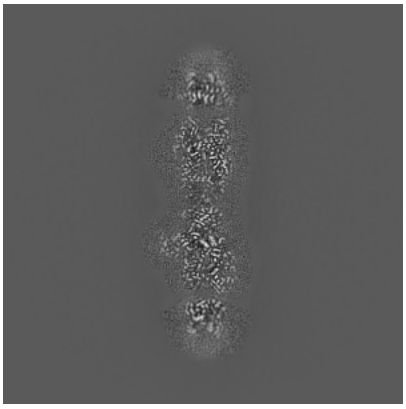
The images above show the map projected in three orthogonal directions.

6.2 Central slices

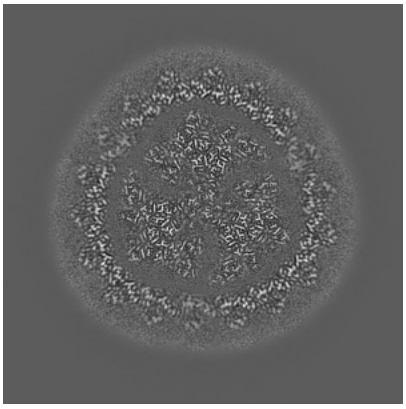
6.2.1 Primary map



X Index: 200



Y Index: 200

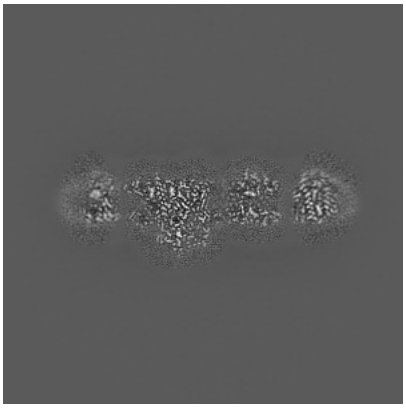


Z Index: 200

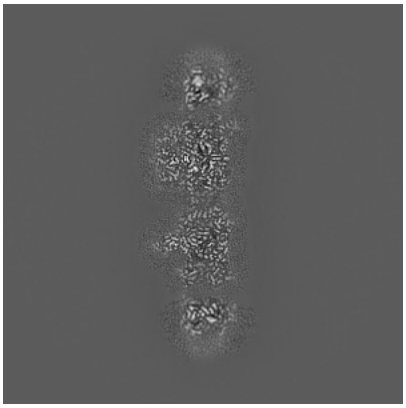
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

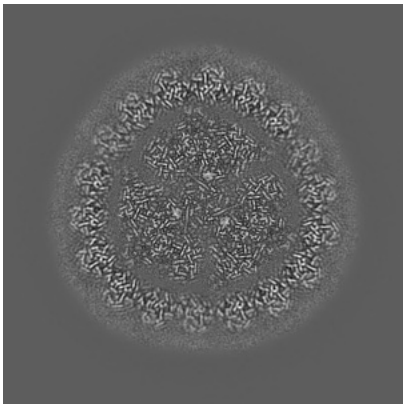
6.3.1 Primary map



X Index: 160



Y Index: 177

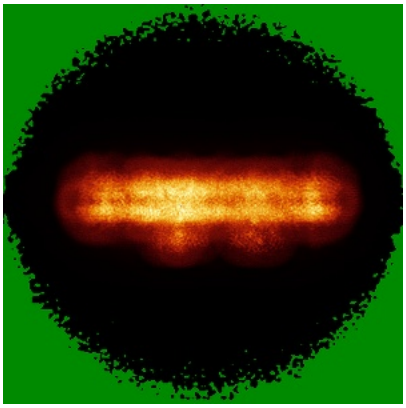


Z Index: 193

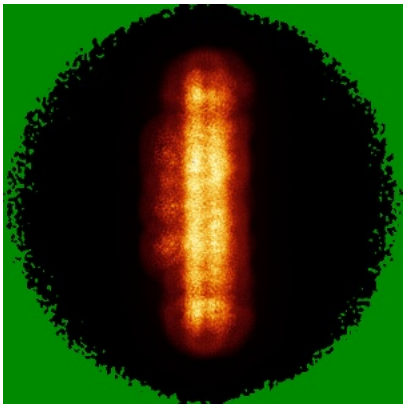
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

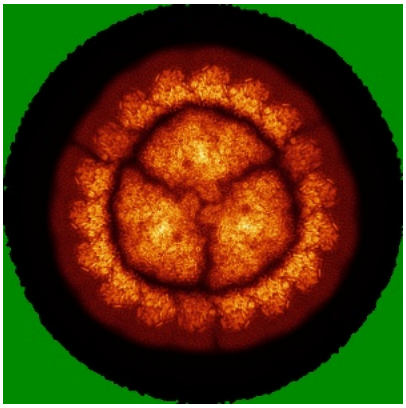
6.4.1 Primary map



X



Y

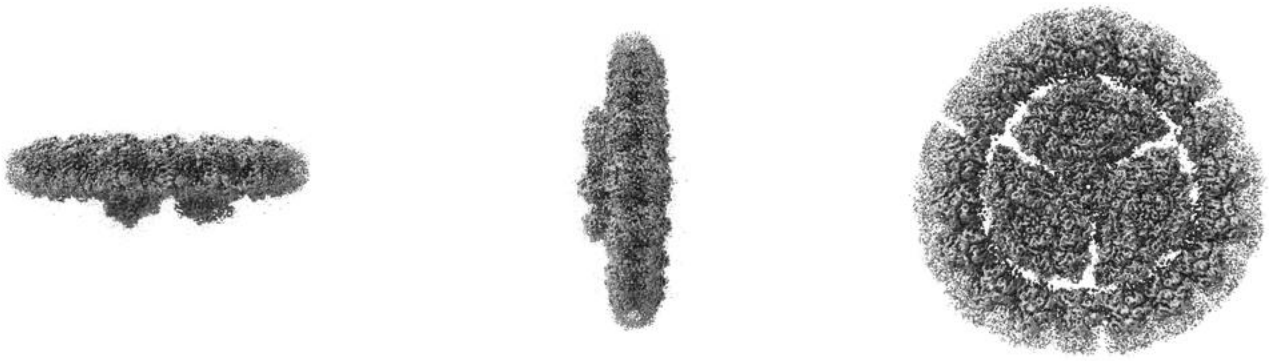


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 9.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

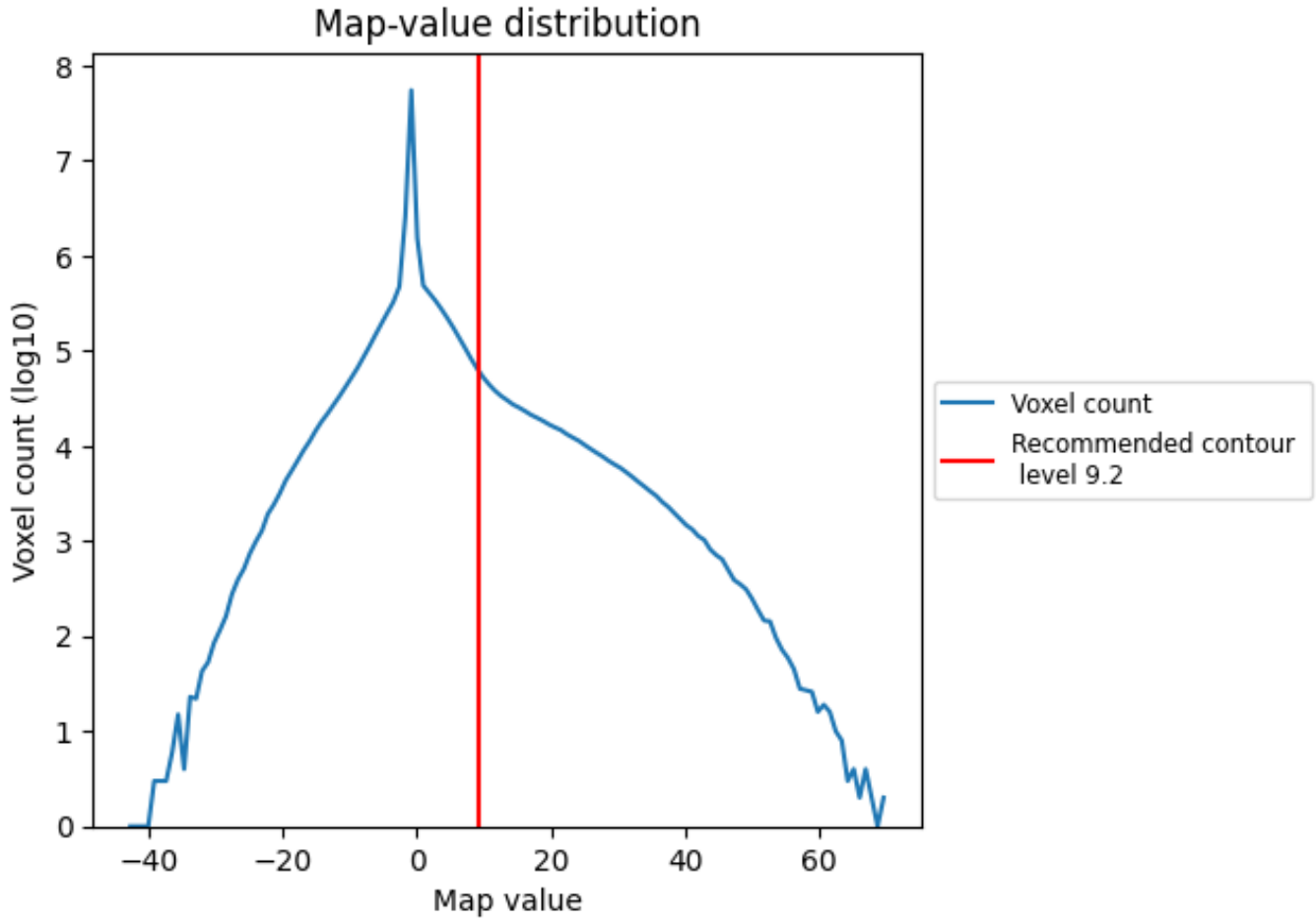
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

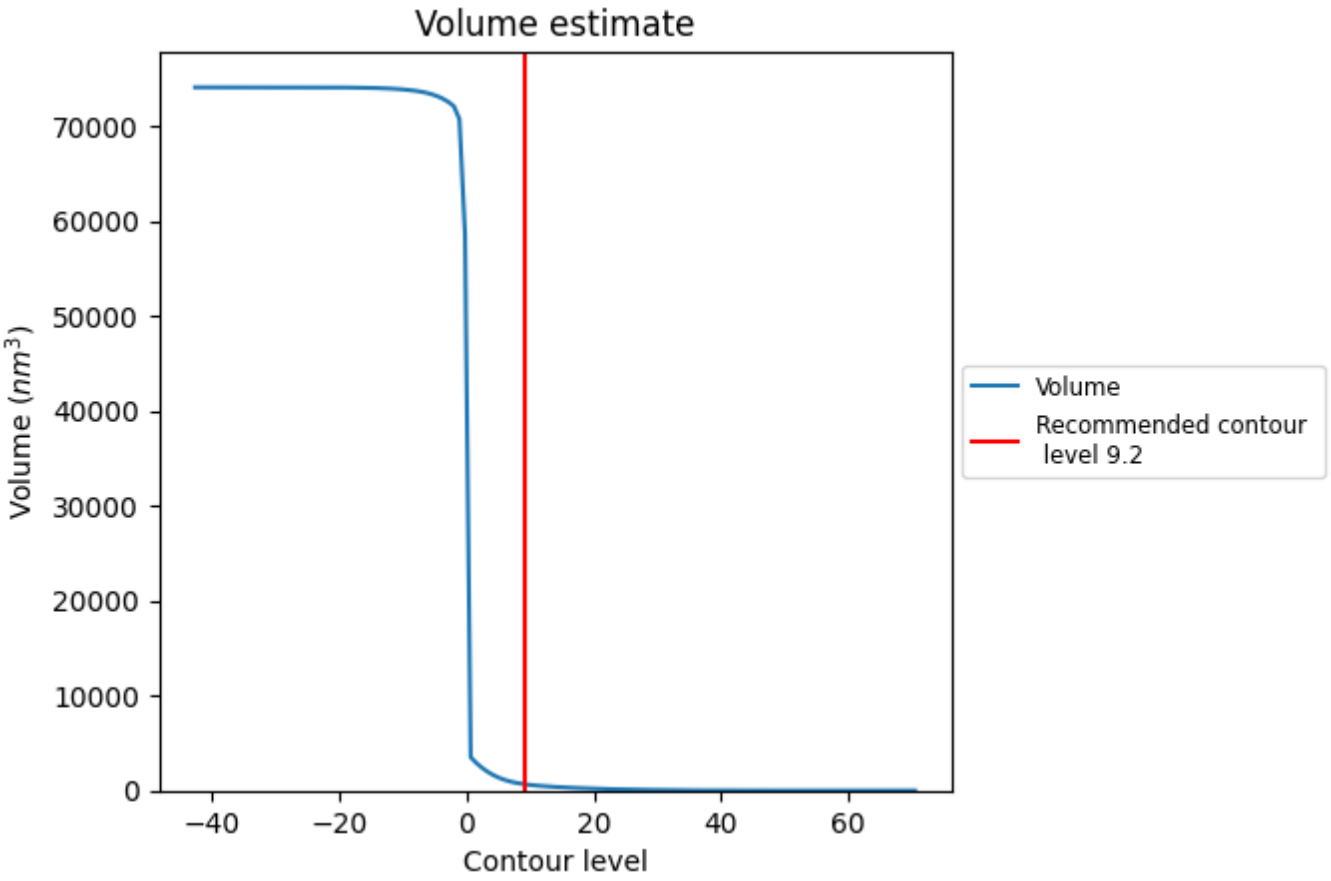
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

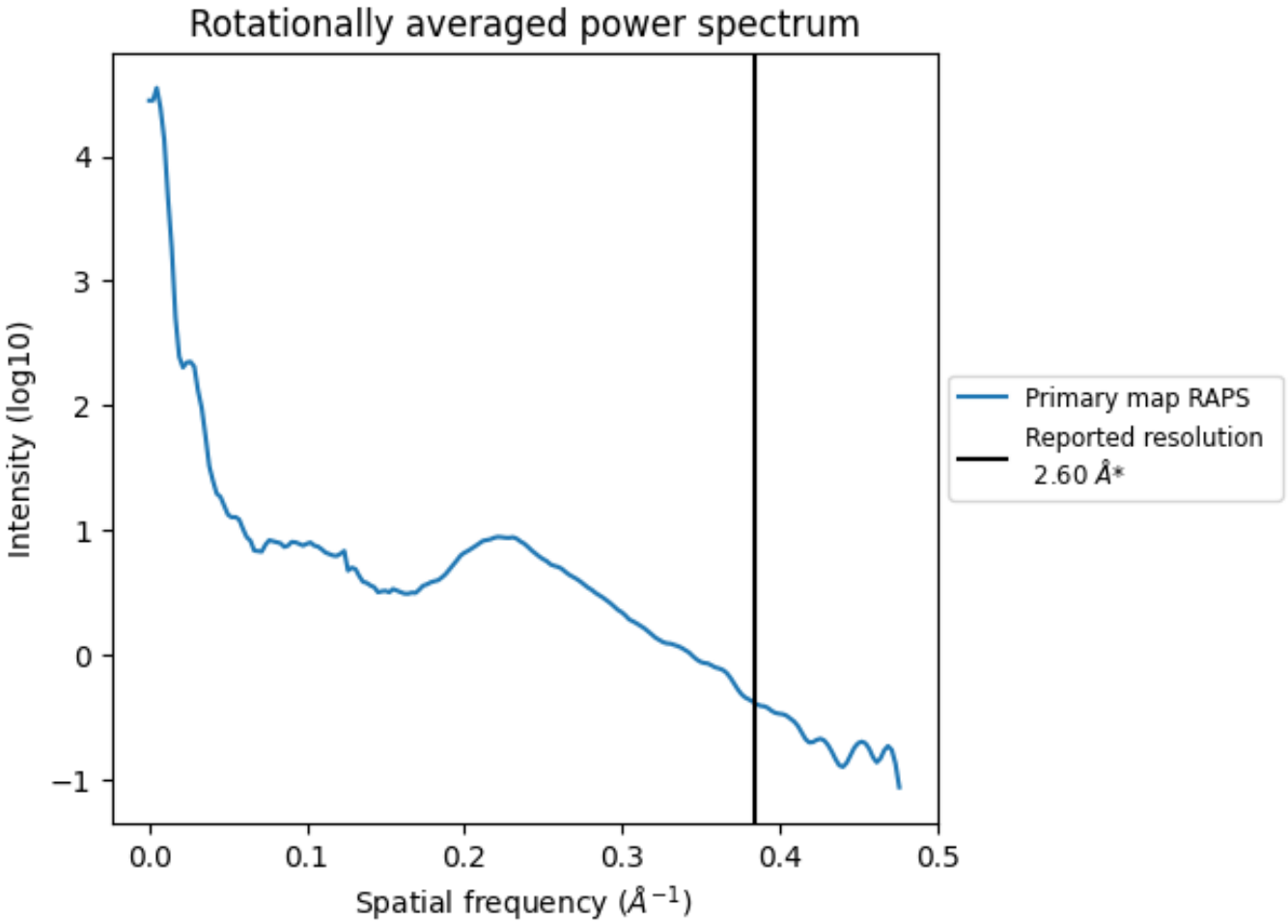
7.2 Volume estimate (i)



The volume at the recommended contour level is 657 nm^3; this corresponds to an approximate mass of 594 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

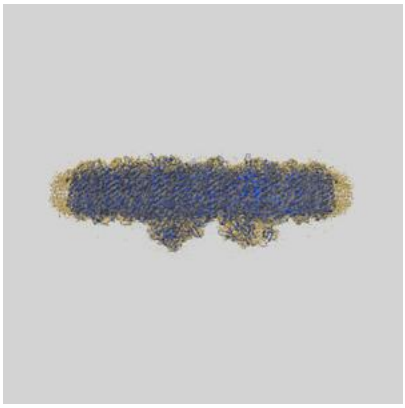
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

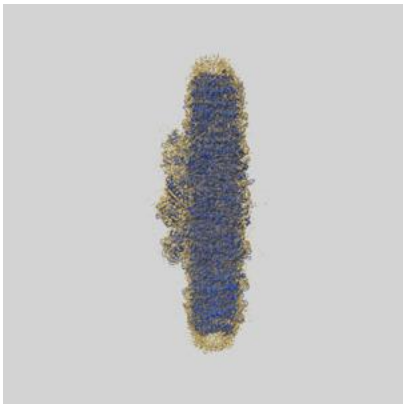
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26601 and PDB model 7UMH. Per-residue inclusion information can be found in section 3 on page 54.

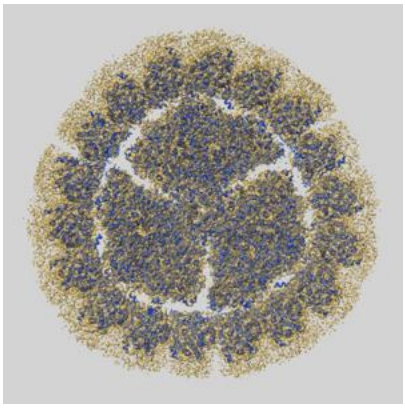
9.1 Map-model overlay



X



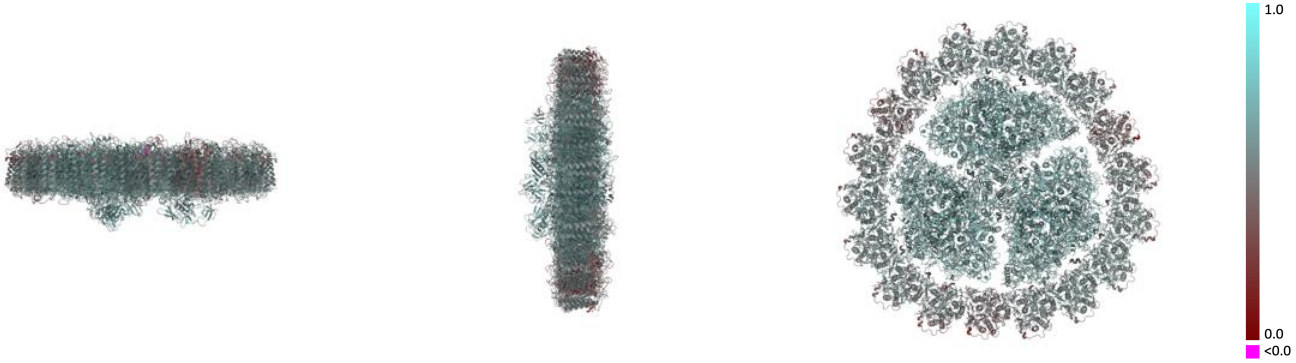
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

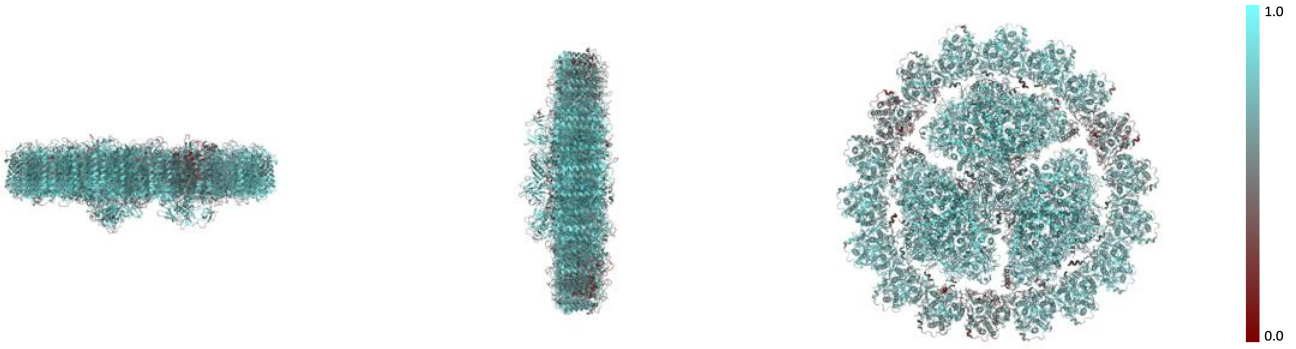
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

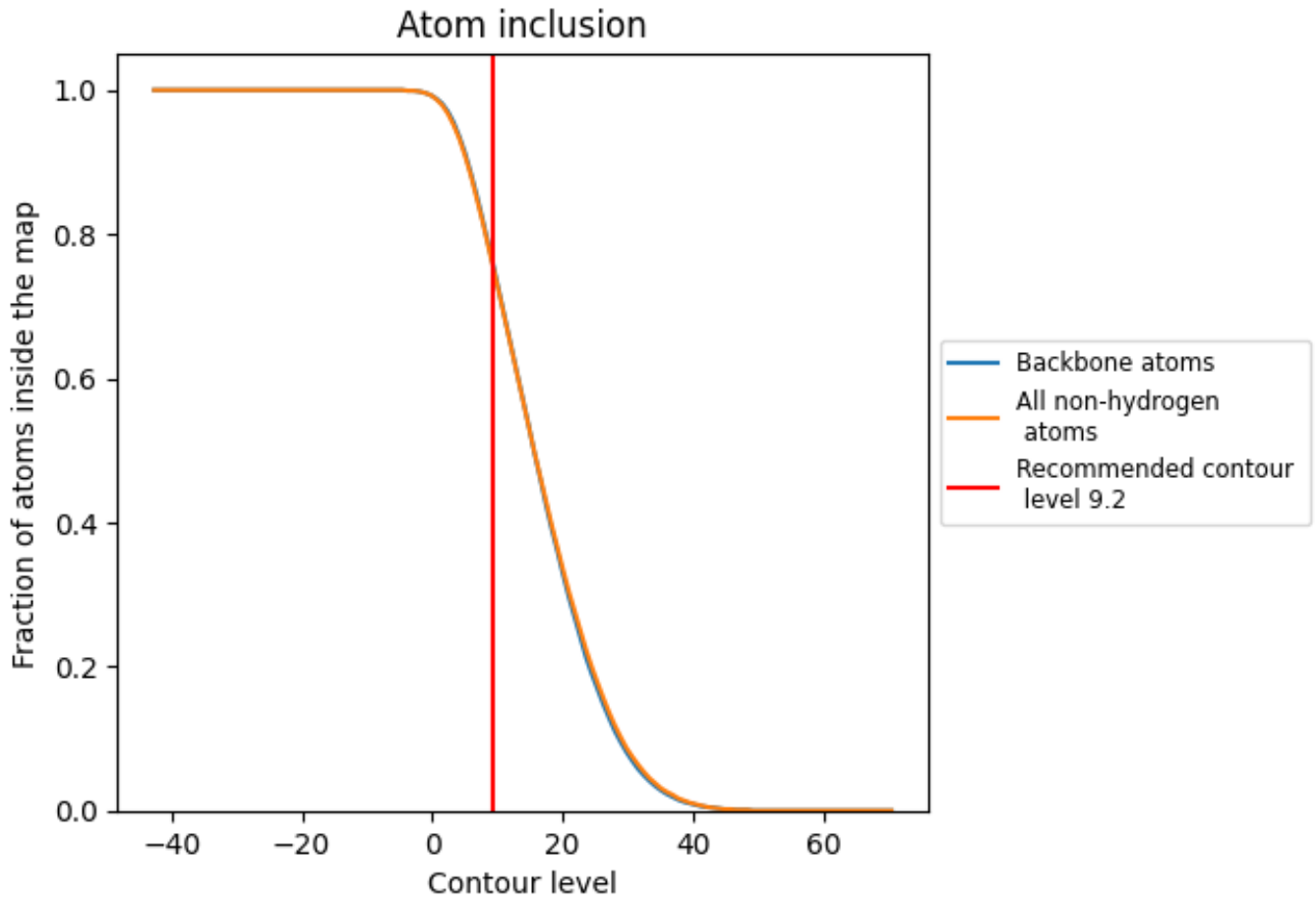
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (9.2).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (9.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.5830
A	0.8500	0.6590
B	0.8530	0.6580
C	0.8720	0.6440
D	0.7320	0.6010
E	0.7110	0.5910
F	0.6610	0.6030
G	0.8570	0.6580
H	0.8550	0.6590
I	0.7320	0.6300
J	0.7310	0.6300
K	0.5930	0.5910
L	0.7710	0.6360
M	0.7140	0.6350
N	0.8740	0.6450
O	0.6800	0.5860
P	0.7240	0.6040
Q	0.6700	0.6070
R	0.7320	0.6350
S	0.7270	0.6340
T	0.6090	0.5850
U	0.7720	0.6400
V	0.6770	0.6170
W	0.6650	0.5000
X	0.7490	0.5360
Y	0.7840	0.5560
Z	0.7720	0.5460
a	0.8490	0.6620
b	0.8570	0.6610
c	0.8700	0.6500
d	0.7210	0.6020
e	0.6720	0.5800
f	0.6720	0.6070
g	0.7050	0.5260
h	0.5270	0.4200



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Chain	Atom inclusion	Q-score
i	0.7370	0.6290
j	0.7590	0.6360
k	0.6030	0.5890
l	0.7650	0.6350
m	0.7140	0.6350
n	0.6720	0.5010
o	0.7400	0.5370
p	0.7770	0.5570
q	0.7590	0.5430
r	0.6990	0.5170
s	0.7750	0.5550
t	0.6620	0.4980
u	0.7400	0.5300
v	0.5460	0.4350
w	0.7620	0.5450
x	0.6830	0.5150
y	0.5320	0.4260