wwPDB EM Validation Summary Report (i)

Sep 30, 2026 – 03:19 AM JST

PDB ID	:	9WD5 / pdb_00009wd5
EMDB ID	:	EMD-65883
Title	:	Cryo-EM structure of PSI-CpcL
Authors	:	Mao, Z.Y.; Li, Z.H.; Han, G.Y.
Deposited on	:	2025-08-18
Resolution	:	2.98 Å(reported)

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:

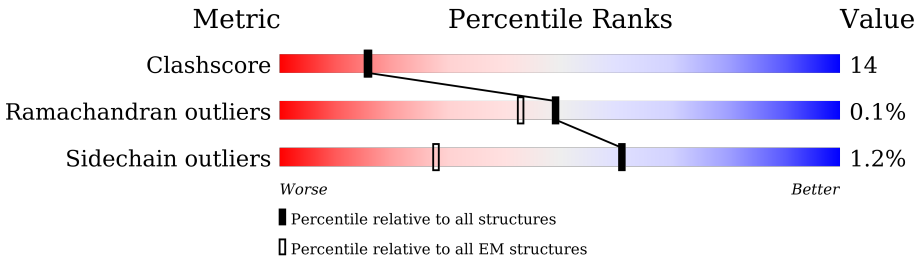
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

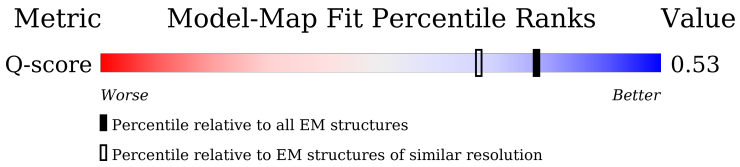
1 Overall quality at a glance

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

The reported resolution of this entry is 2.98 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	13236 (2.48 - 3.48)

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	1	237	9% 86%
2	A	752	73% 25%
2	G	752	73% 25%
2	a	752	74% 24%

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Mol	Chain	Length	Quality of chain
2	g	752	73% 25%
3	H	44	50% 20% 30%
3	X	44	61% 9% 30%
3	h	44	52% 16% 32%
3	x	44	55% 16% 30%
4	B	741	77% 22%
4	N	741	78% 21%
4	b	741	76% 24%
4	n	741	76% 23%
5	C	81	72% 26%
5	P	81	85% 14%
5	c	81	79% 20%
5	p	81	78% 21%
6	D	139	80% 17%
6	Q	139	81% 17%
6	d	139	83% 14%
6	q	139	90% 8%
7	E	70	70% 17% 13%
7	R	70	64% 23% 13%
7	e	70	70% 16% 13%
7	r	70	59% 27% 14%
8	F	164	71% 15% 14%
8	S	164	73% 13% 14%
8	f	164	71% 15% 14%
8	s	164	70% 16% 14%

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Mol	Chain	Length	Quality of chain
9	J	49	73% 18% 8%
9	T	49	65% 24% 10%
9	j	49	73% 18% 8%
9	t	49	76% 16% 8%
10	K	86	10% 59% 24% 15%
10	U	86	7% 62% 23% 15%
10	k	86	10% 69% 21% 9%
10	u	86	12% 56% 35% 9%
11	I	46	57% 17% 26%
11	V	46	61% 11% 28%
11	i	46	59% 15% 26%
11	v	46	7% 48% 26% 26%
12	L	172	72% 17% 10%
12	W	172	72% 18% 10%
12	l	172	73% 17% 10%
12	w	172	72% 19% 10%
13	M	32	9% 66% 31%
13	Y	32	6% 75% 22%
13	m	32	6% 75% 22%
13	y	32	81% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	855	-	-	X	-
14	CLA	G	852	-	-	X	-
17	BCR	N	852	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 98661 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-associated linker protein CpcL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	33	Total	C	N	O	S	0	0
			247	166	36	44	1		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	741	Total	C	N	O	S	0	0
			5814	3814	1001	978	21		
2	g	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		
2	A	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		
2	a	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		

- Molecule 3 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	31	Total	C	N	O	0	0
			257	179	40	38		
3	h	30	Total	C	N	O	0	0
			248	174	38	36		
3	X	31	Total	C	N	O	0	0
			257	179	40	38		
3	x	31	Total	C	N	O	0	0
			257	179	40	38		

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	739	Total	C	N	O	S	0	0
			5913	3902	990	1003	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	738	Total	C	N	O	S	0	0
			5906	3898	989	1001	18		
4	B	740	Total	C	N	O	S	0	0
			5918	3905	991	1004	18		
4	b	740	Total	C	N	O	S	0	0
			5918	3905	991	1004	18		

- Molecule 5 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
5	p	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
5	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
5	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	135	Total	C	N	O	S	0	0
			1040	666	179	194	1		
6	q	136	Total	C	N	O	S	0	0
			1047	670	180	196	1		
6	D	135	Total	C	N	O	S	0	0
			1040	666	179	194	1		
6	d	136	Total	C	N	O	S	0	0
			1047	670	180	196	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	61	Total	C	N	O	0	0
			490	313	84	93		
7	r	60	Total	C	N	O	0	0
			481	308	83	90		
7	E	61	Total	C	N	O	0	0
			490	313	84	93		
7	e	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
8	s	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
8	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
8	f	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	44	Total	C	N	O	0	0
			354	241	53	60		
9	t	45	Total	C	N	O	0	0
			359	244	54	61		
9	J	45	Total	C	N	O	0	0
			359	244	54	61		
9	j	45	Total	C	N	O	0	0
			359	244	54	61		

- Molecule 10 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	73	Total	C	N	O	S	0	0
			537	357	89	90	1		
10	u	78	Total	C	N	O	S	0	0
			568	376	94	97	1		
10	K	73	Total	C	N	O	S	0	0
			537	357	89	90	1		
10	k	78	Total	C	N	O	S	0	0
			568	376	94	97	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	33	Total	C	N	O	0	0
			268	184	37	47		
11	v	34	Total	C	N	O	0	0
			275	189	38	48		
11	I	34	Total	C	N	O	0	0
			275	189	38	48		

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	i	34	Total 275	C 189	N 38	O 48	0	0

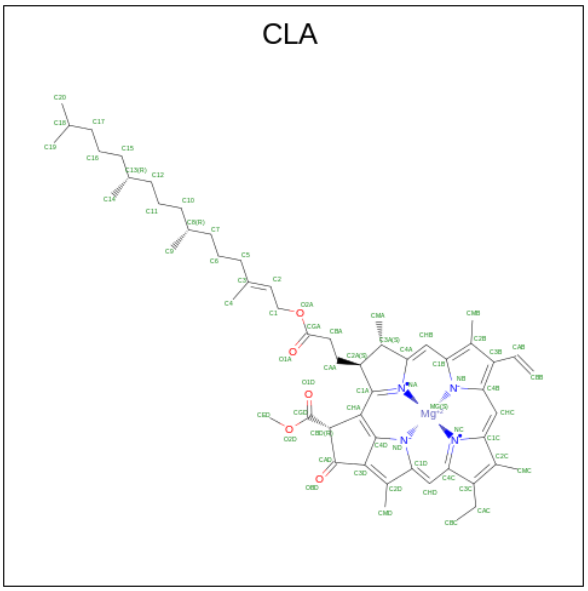
- Molecule 12 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	155	Total 1163	C 763	N 197	O 202	S 1	0	0
12	w	155	Total 1163	C 763	N 197	O 202	S 1	0	0
12	L	155	Total 1163	C 763	N 197	O 202	S 1	0	0
12	l	155	Total 1163	C 763	N 197	O 202	S 1	0	0

- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	31	Total 241	C 160	N 37	O 44	0	0
13	y	31	Total 241	C 160	N 37	O 44	0	0
13	M	31	Total 241	C 160	N 37	O 44	0	0
13	m	31	Total 241	C 160	N 37	O 44	0	0

- Molecule 14 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
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	U	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	W	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	h	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	t	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	u	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	u	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	w	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	w	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	X	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	x	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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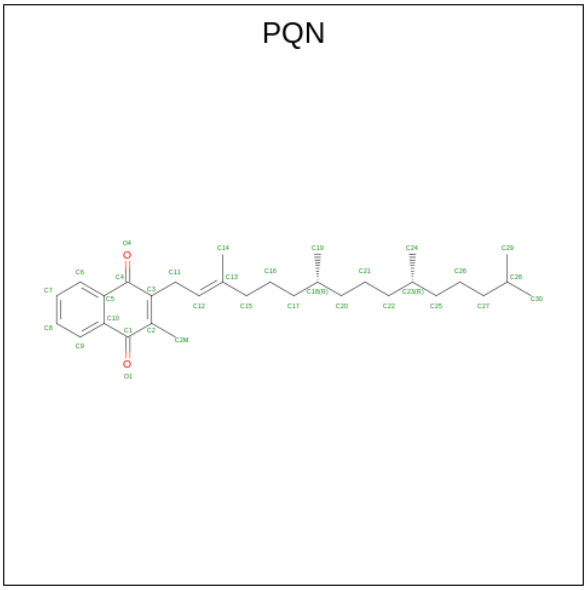
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



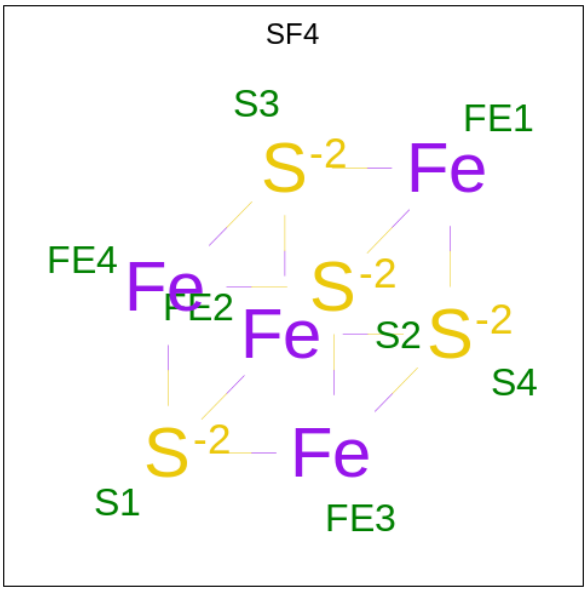
Mol	Chain	Residues	Atoms			AltConf
15	G	1	Total	C	O	0
			33	31	2	
15	N	1	Total	C	O	0
			33	31	2	
15	g	1	Total	C	O	0
			33	31	2	
15	n	1	Total	C	O	0
			33	31	2	
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	

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Mol	Chain	Residues	Atoms	AltConf
15	a	1	Total C O 33 31 2	0
15	b	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



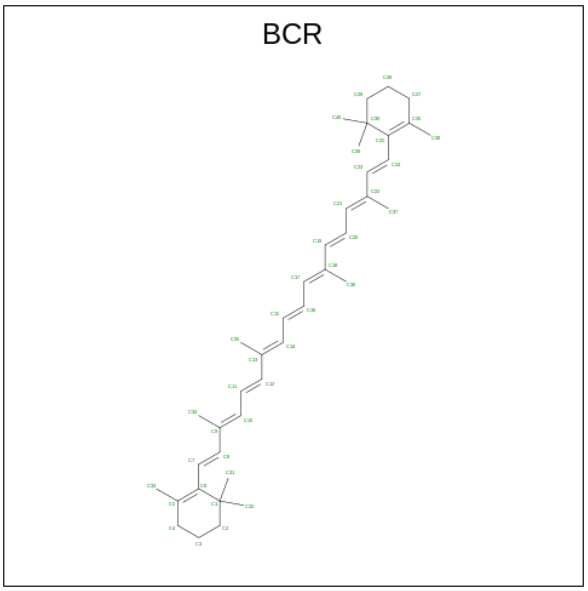
Mol	Chain	Residues	Atoms	AltConf
16	G	1	Total Fe S 8 4 4	0
16	P	1	Total Fe S 8 4 4	0
16	P	1	Total Fe S 8 4 4	0
16	g	1	Total Fe S 8 4 4	0
16	p	1	Total Fe S 8 4 4	0
16	p	1	Total Fe S 8 4 4	0
16	A	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
16	a	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	N	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	N	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	Y	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	s	1	Total C 40 40	0
17	t	1	Total C 40 40	0
17	t	1	Total C 40 40	0
17	u	1	Total C 40 40	0
17	v	1	Total C 40 40	0
17	w	1	Total C 40 40	0
17	w	1	Total C 40 40	0
17	w	1	Total C 40 40	0
17	y	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0

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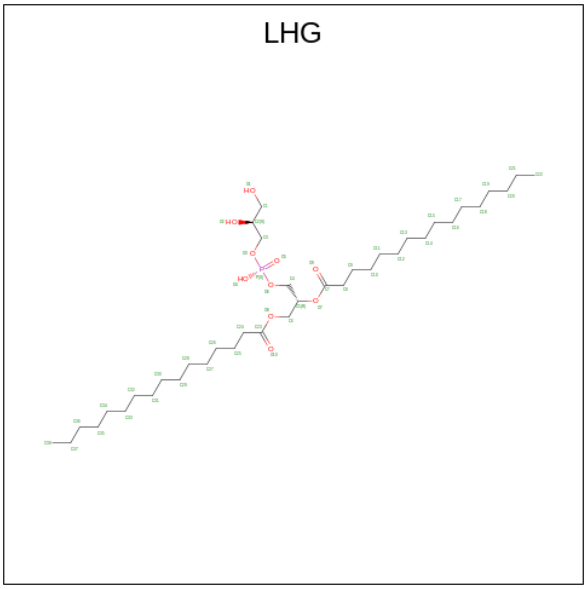
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0

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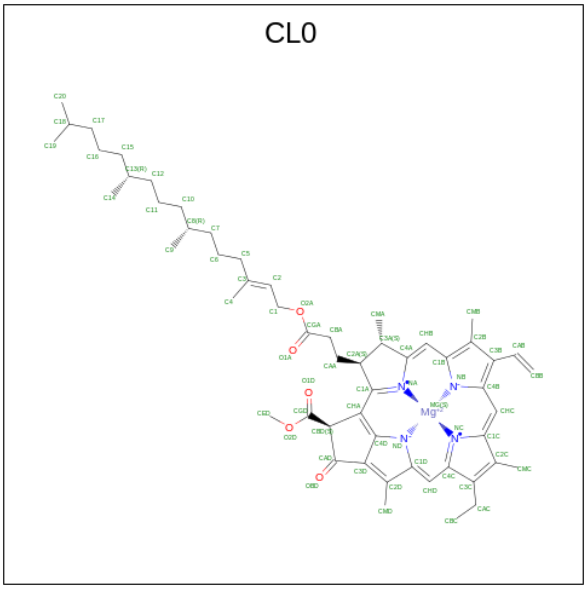
Mol	Chain	Residues	Atoms	AltConf
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	m	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



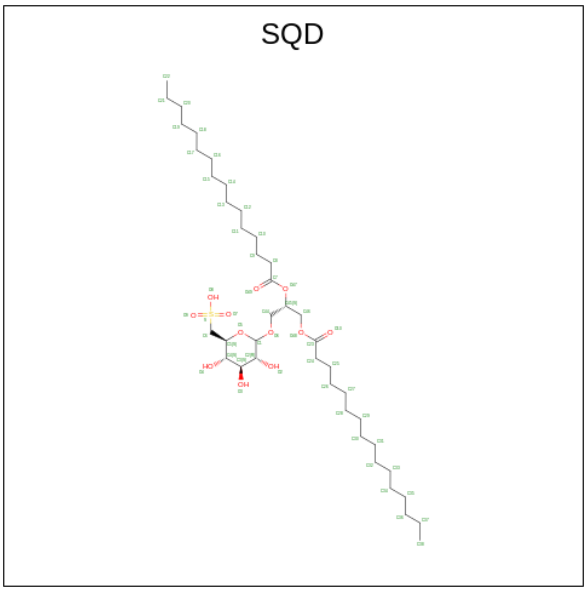
Mol	Chain	Residues	Atoms				AltConf
18	G	1	Total	C	O	P	0
			49	38	10	1	
18	G	1	Total	C	O	P	0
			49	38	10	1	
18	S	1	Total	C	O	P	0
			43	32	10	1	
18	g	1	Total	C	O	P	0
			49	38	10	1	
18	g	1	Total	C	O	P	0
			49	38	10	1	
18	v	1	Total	C	O	P	0
			43	32	10	1	
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	X	1	Total	C	O	P	0
			43	32	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	m	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



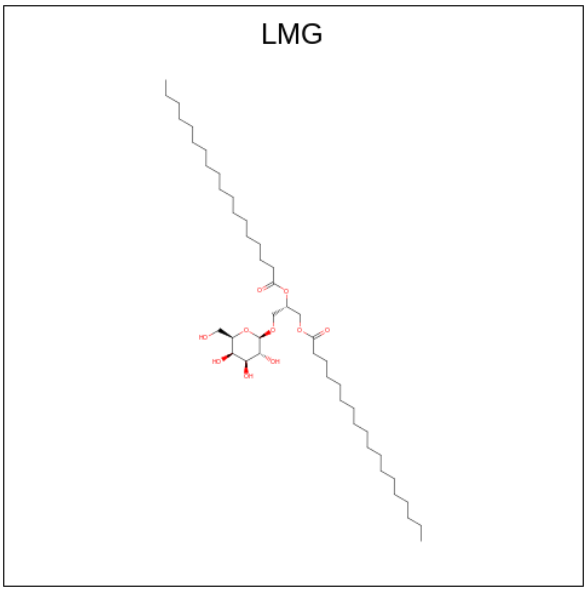
Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	H	1	Total	C	O	S	0
			54	41	12	1	
20	h	1	Total	C	O	S	0
			54	41	12	1	
20	n	1	Total	C	O	S	0
			54	41	12	1	
20	w	1	Total	C	O	S	0
			54	41	12	1	
20	B	1	Total	C	O	S	0
			54	41	12	1	
20	x	1	Total	C	O	S	0
			54	41	12	1	
20	b	1	Total	C	O	S	0
			54	41	12	1	
20	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



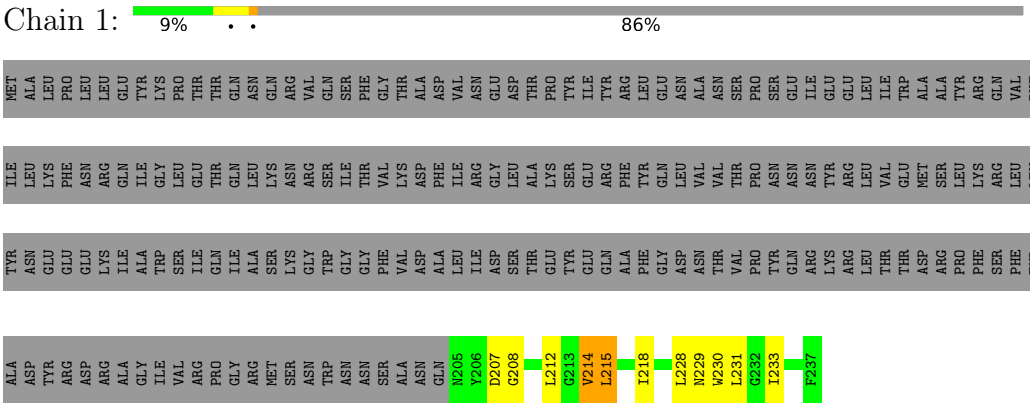
Mol	Chain	Residues	Atoms	AltConf
21	N	1	Total C O 35 25 10	0
21	N	1	Total C O 55 45 10	0
21	n	1	Total C O 55 45 10	0
21	B	1	Total C O 35 25 10	0
21	B	1	Total C O 55 45 10	0
21	b	1	Total C O 55 45 10	0

3 Residue-property plots (i)

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.

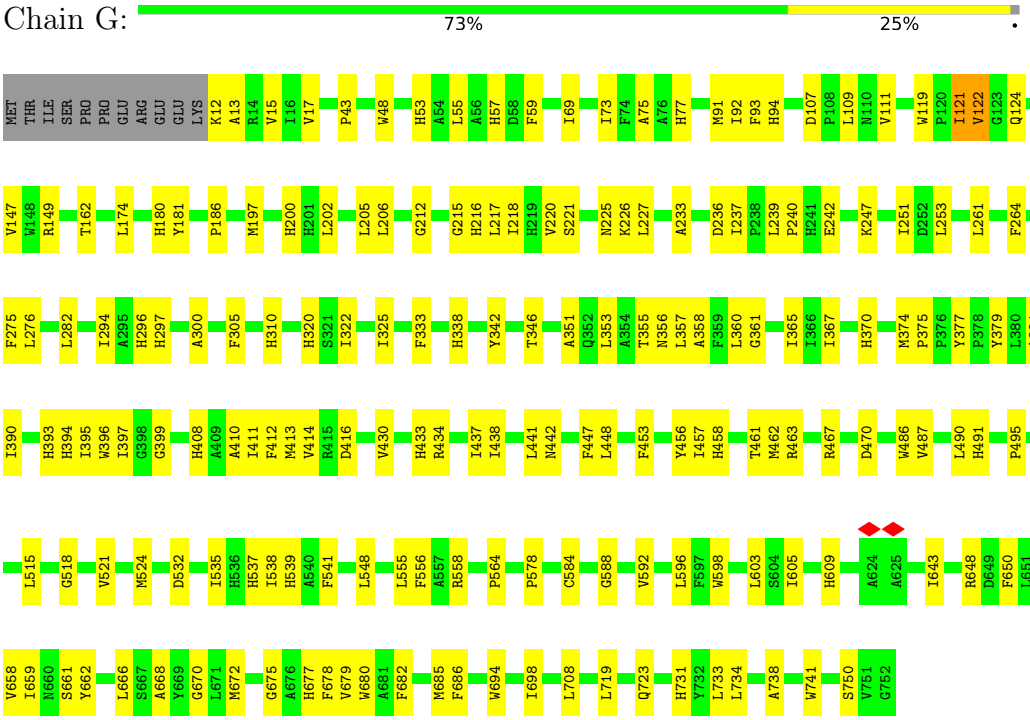
• Molecule 1: Photosystem I-associated linker protein CpcL

Chain 1:



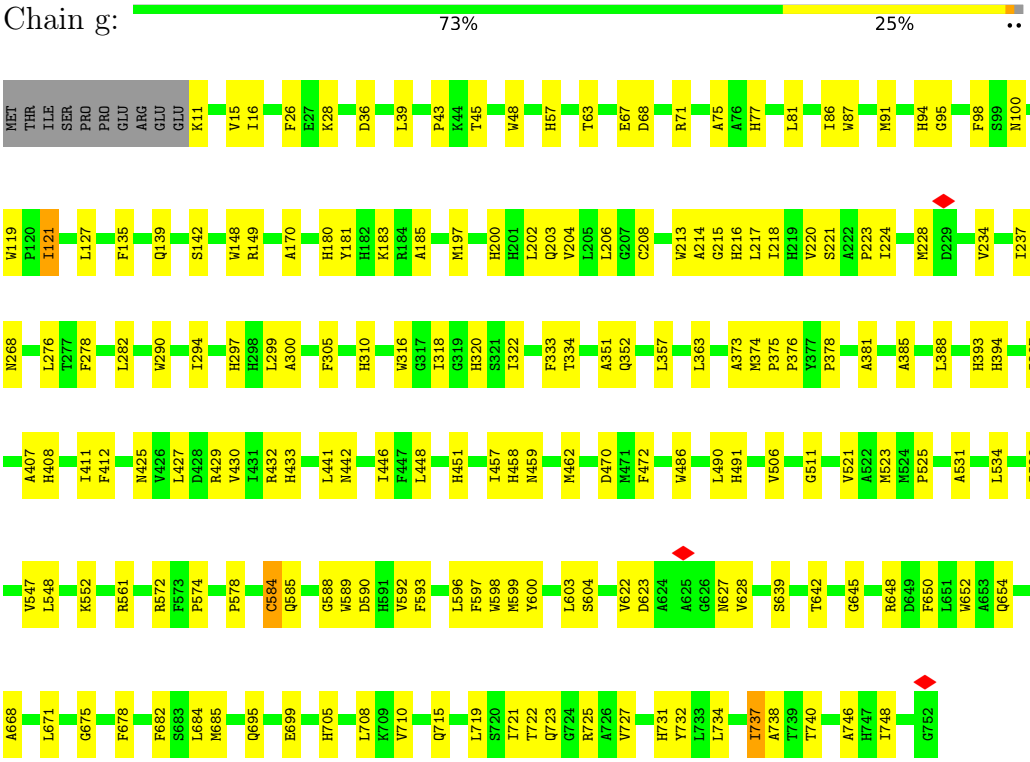
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1

Chain G:



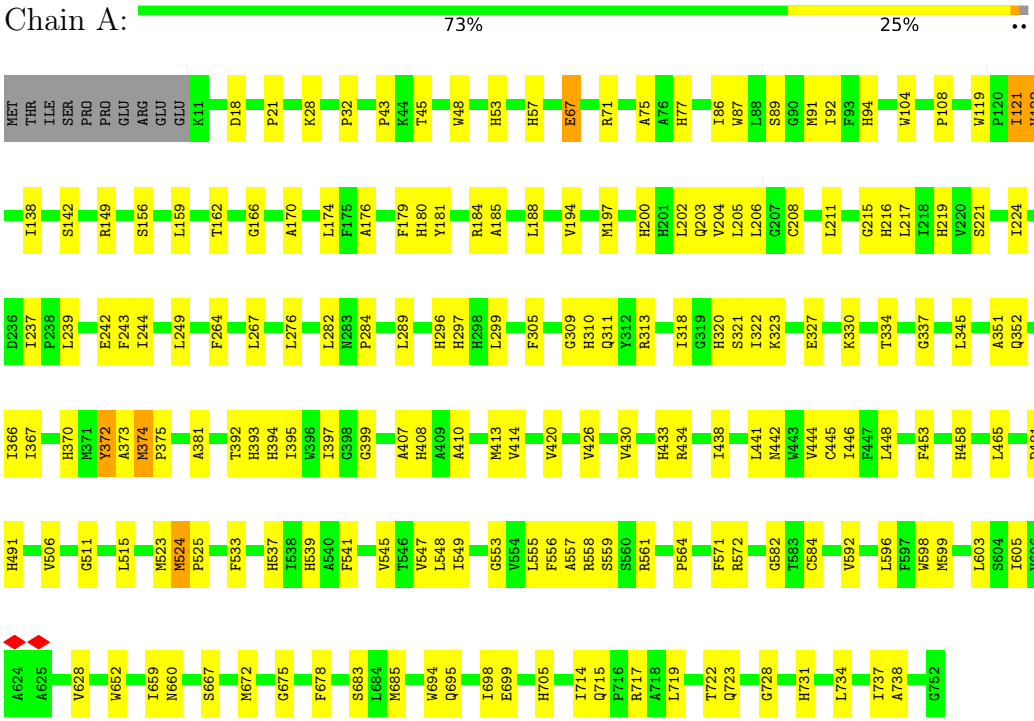
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1

Chain g:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1

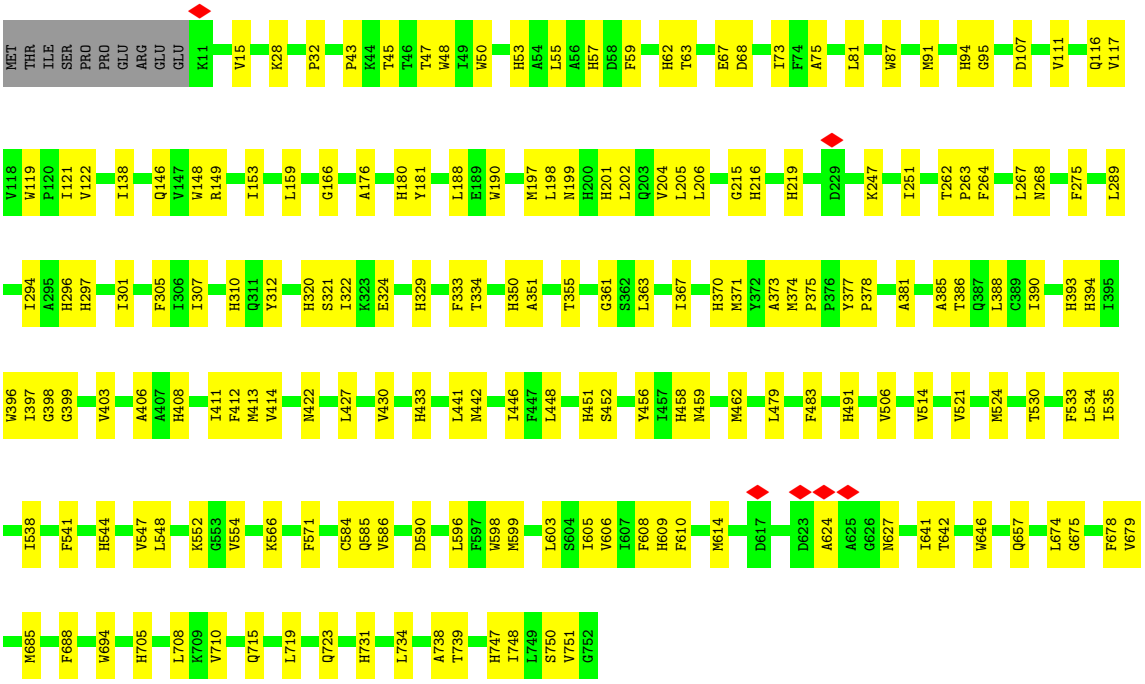
Chain A:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:

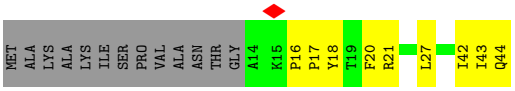




• Molecule 3: Photosystem I 4.8 kDa protein

Chain H:

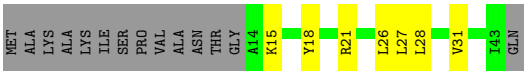




• Molecule 3: Photosystem I 4.8 kDa protein

Chain h:

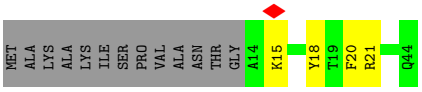




• Molecule 3: Photosystem I 4.8 kDa protein

Chain X:

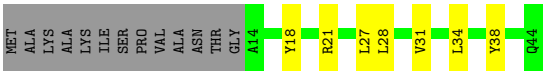




• Molecule 3: Photosystem I 4.8 kDa protein

Chain x:

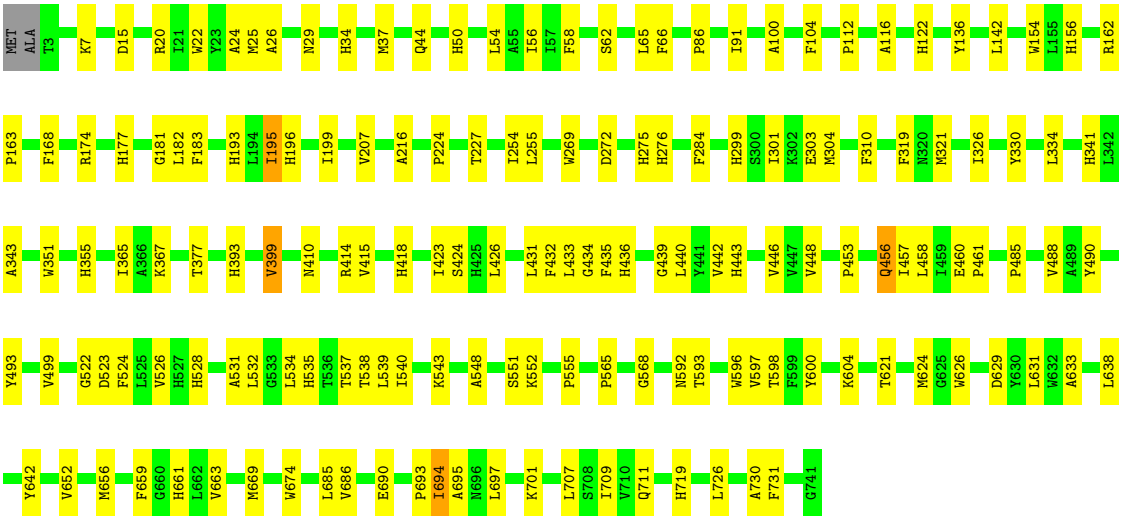




• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain N:

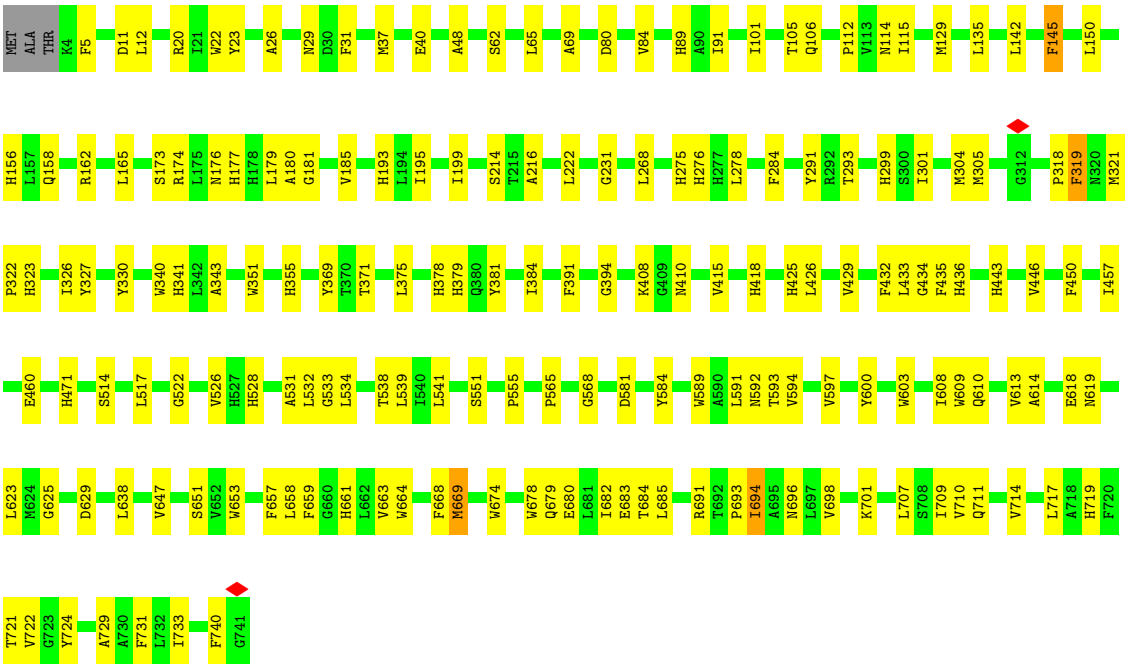




• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain n:

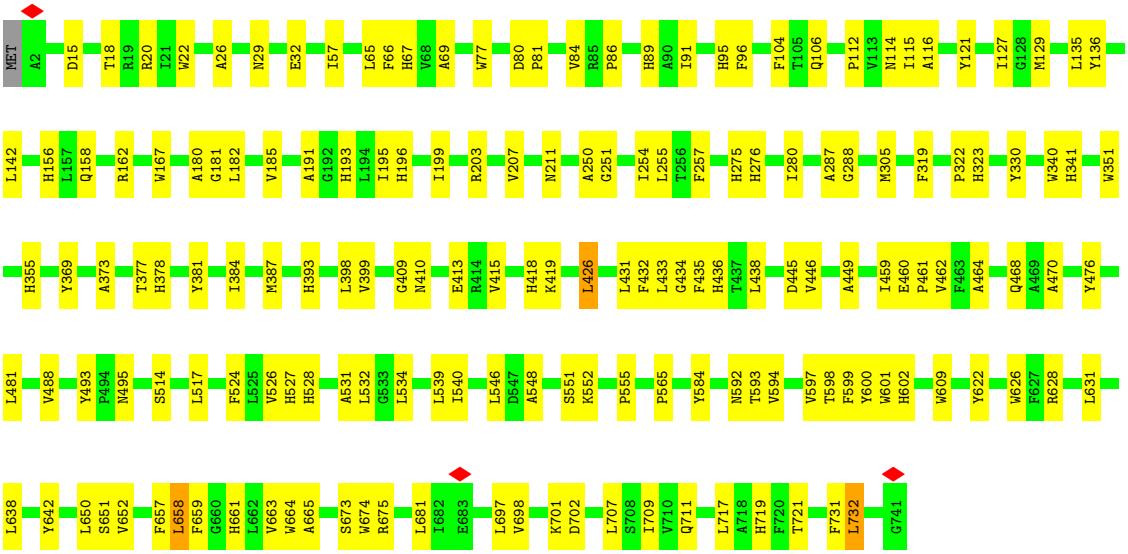




• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B:

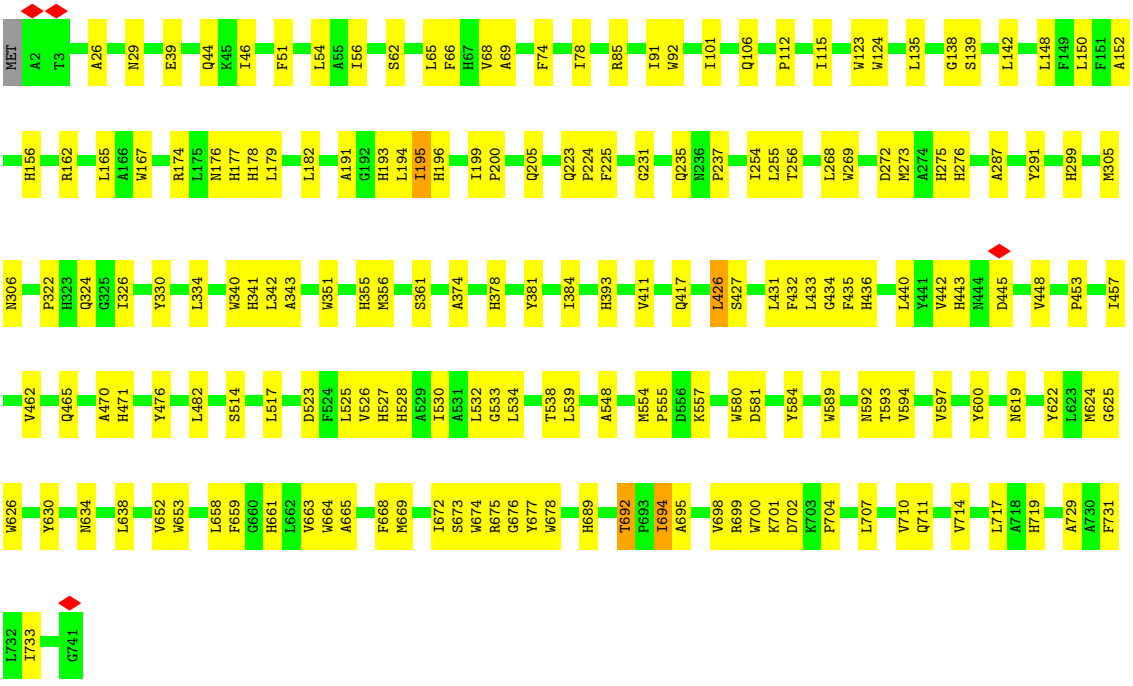




• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain b:

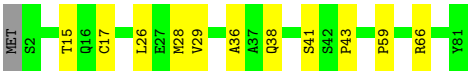




• Molecule 5: Photosystem I iron-sulfur center

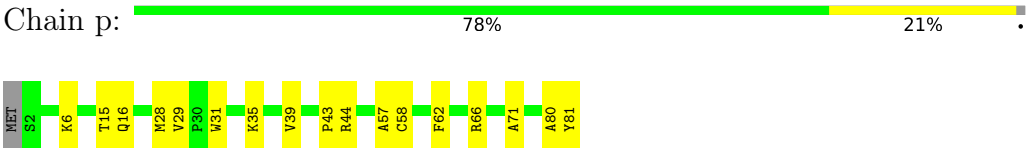
Chain P:





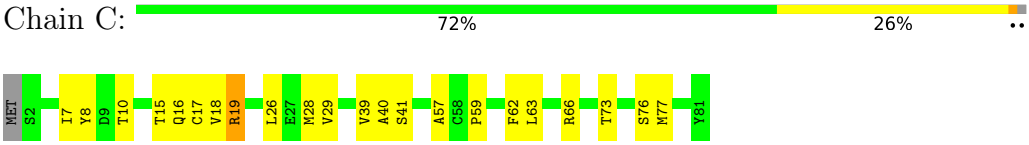
• Molecule 5: Photosystem I iron-sulfur center

Chain p:



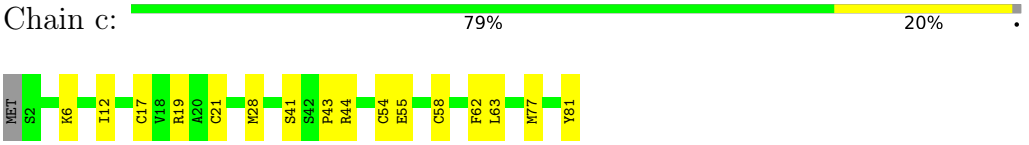
• Molecule 5: Photosystem I iron-sulfur center

Chain C:



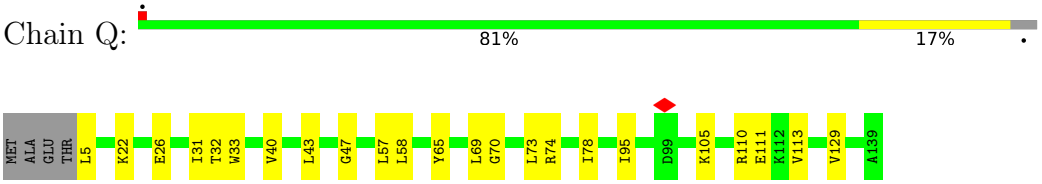
• Molecule 5: Photosystem I iron-sulfur center

Chain c:



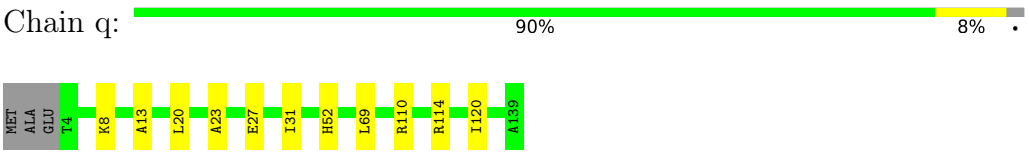
• Molecule 6: Photosystem I reaction center subunit II

Chain Q:



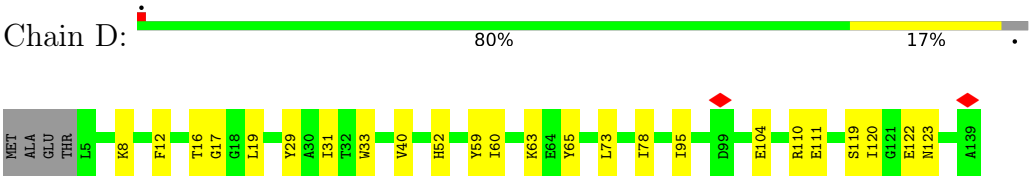
• Molecule 6: Photosystem I reaction center subunit II

Chain q:



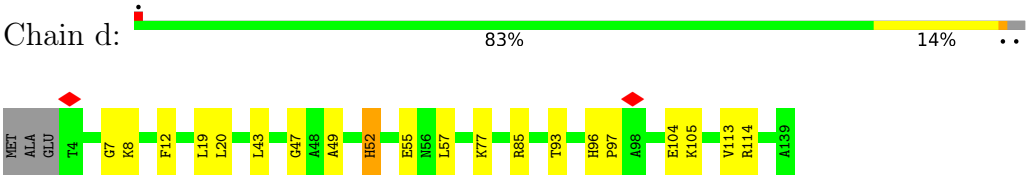
• Molecule 6: Photosystem I reaction center subunit II

Chain D:



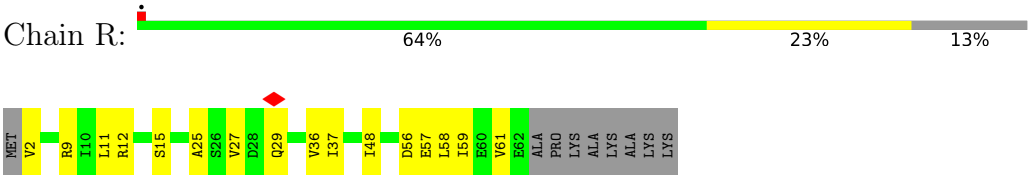
• Molecule 6: Photosystem I reaction center subunit II

Chain d:



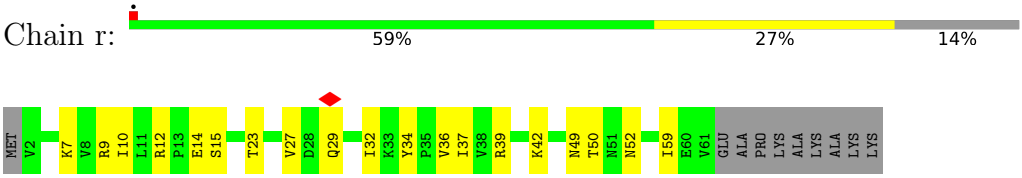
• Molecule 7: Photosystem I reaction center subunit IV

Chain R:



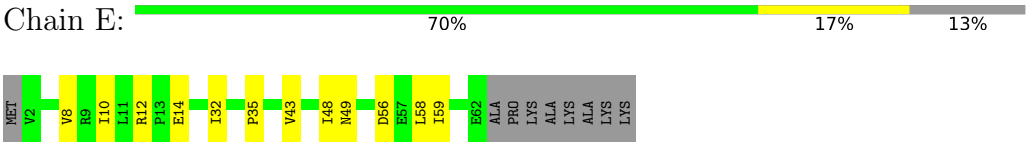
• Molecule 7: Photosystem I reaction center subunit IV

Chain r:



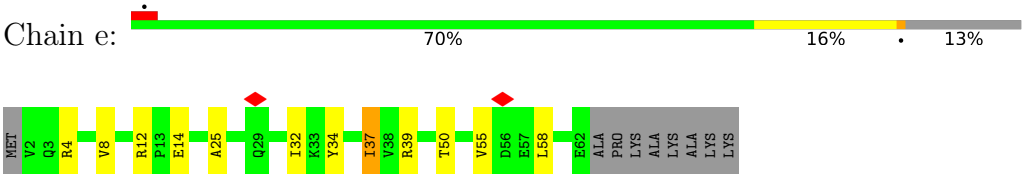
• Molecule 7: Photosystem I reaction center subunit IV

Chain E:



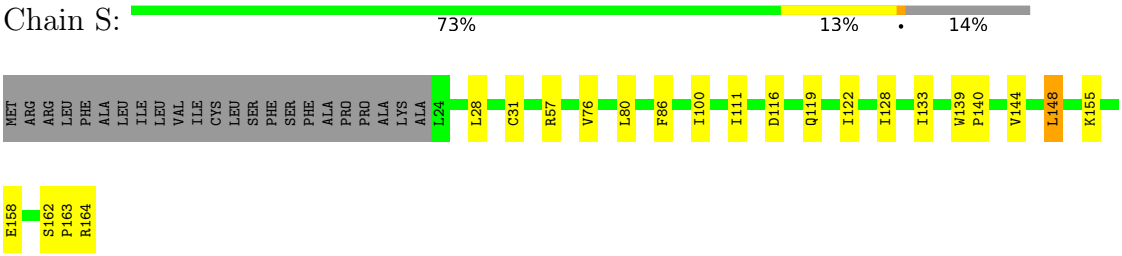
• Molecule 7: Photosystem I reaction center subunit IV

Chain e:



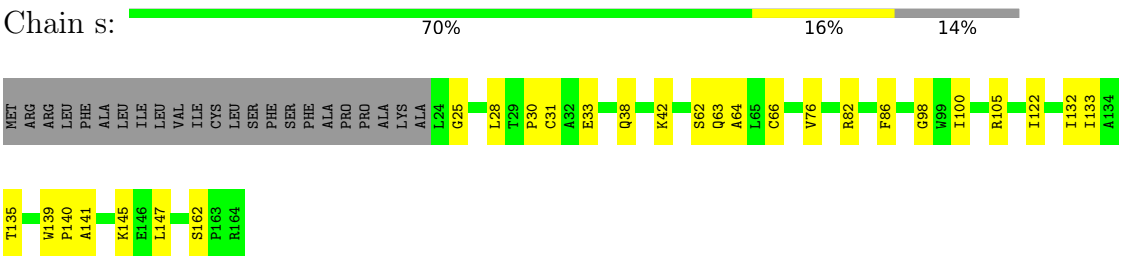
• Molecule 8: Photosystem I reaction center subunit III

Chain S:



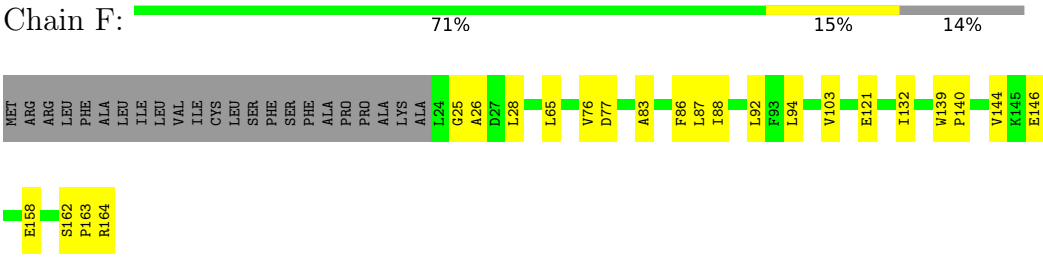
• Molecule 8: Photosystem I reaction center subunit III

Chain s:



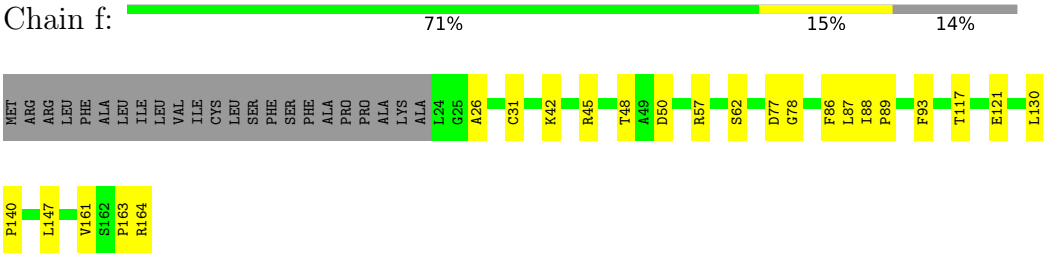
• Molecule 8: Photosystem I reaction center subunit III

Chain F:



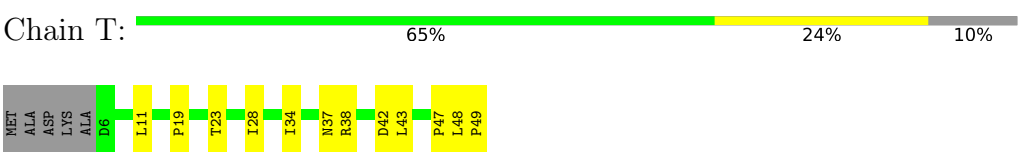
• Molecule 8: Photosystem I reaction center subunit III

Chain f:



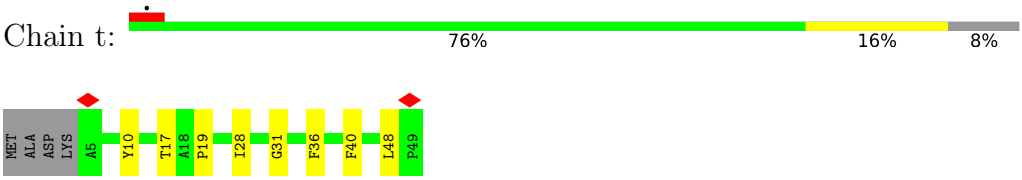
• Molecule 9: Photosystem I reaction center subunit IX

Chain T:



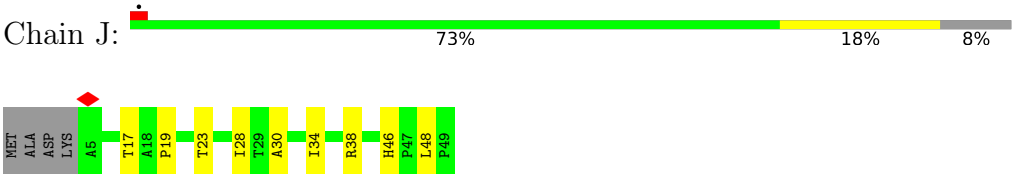
• Molecule 9: Photosystem I reaction center subunit IX

Chain t:



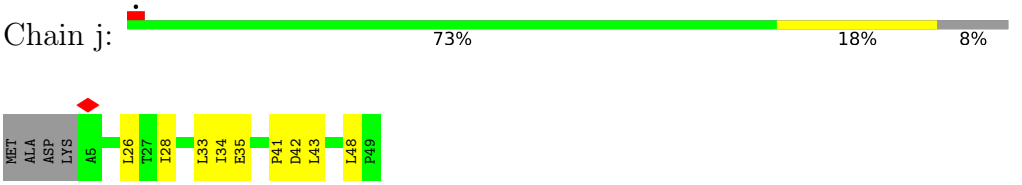
• Molecule 9: Photosystem I reaction center subunit IX

Chain J:



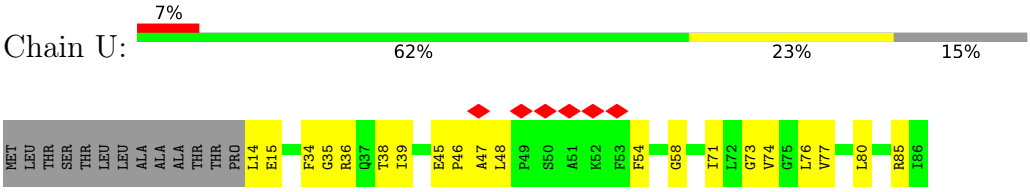
• Molecule 9: Photosystem I reaction center subunit IX

Chain j:



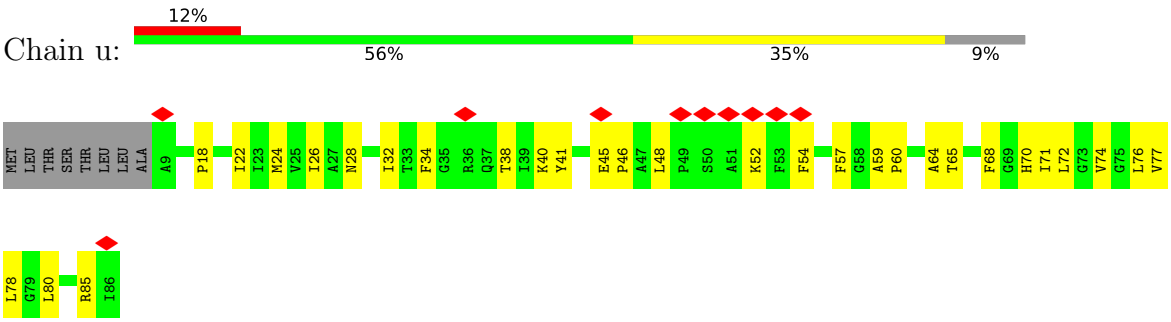
• Molecule 10: Photosystem I reaction center subunit PsaK 1

Chain U:



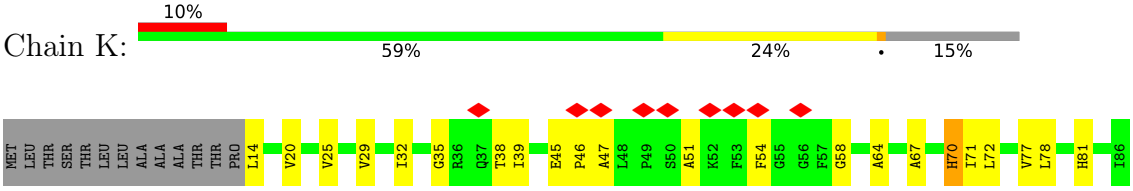
• Molecule 10: Photosystem I reaction center subunit PsaK 1

Chain u:



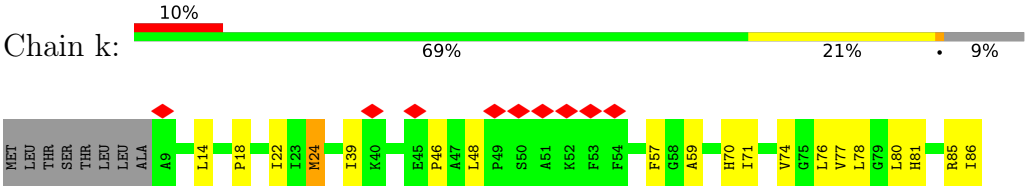
• Molecule 10: Photosystem I reaction center subunit PsaK 1

Chain K:



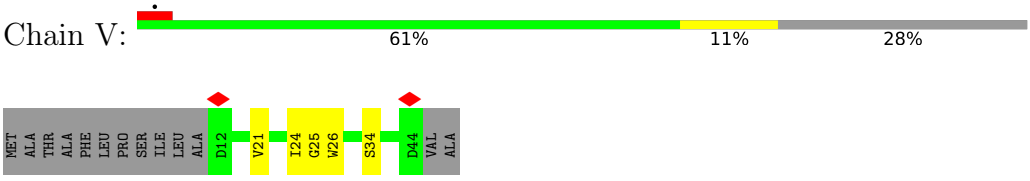
• Molecule 10: Photosystem I reaction center subunit PsaK 1

Chain k:



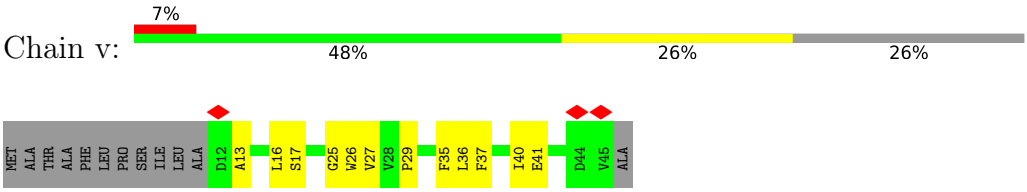
• Molecule 11: Photosystem I reaction center subunit VIII

Chain V:



• Molecule 11: Photosystem I reaction center subunit VIII

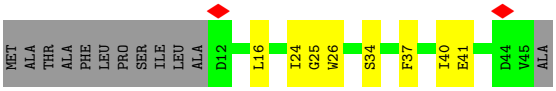
Chain v:



• Molecule 11: Photosystem I reaction center subunit VIII

Chain I:

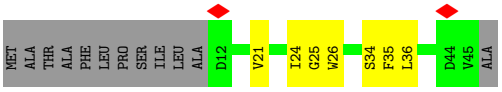




• Molecule 11: Photosystem I reaction center subunit VIII

Chain i:

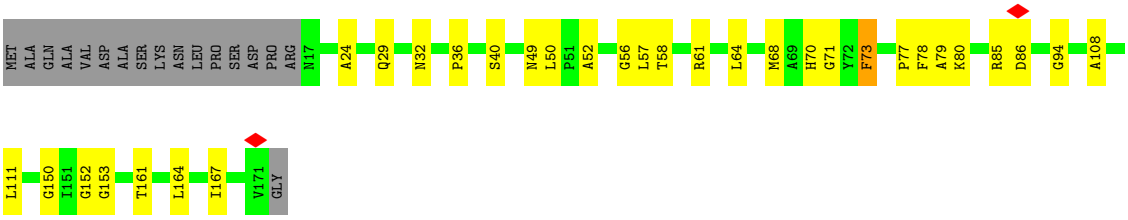




• Molecule 12: Photosystem I reaction center subunit XI

Chain W:

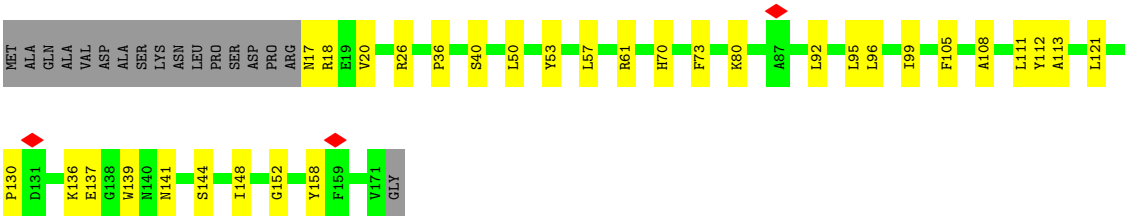




• Molecule 12: Photosystem I reaction center subunit XI

Chain w:





• Molecule 12: Photosystem I reaction center subunit XI

Chain L:

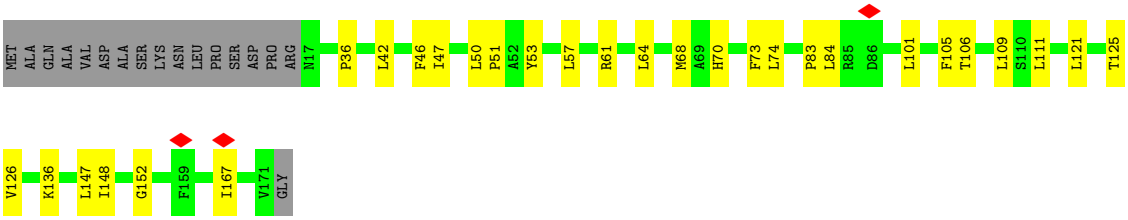




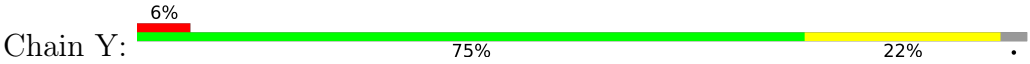
• Molecule 12: Photosystem I reaction center subunit XI

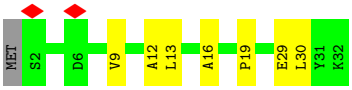
Chain l:



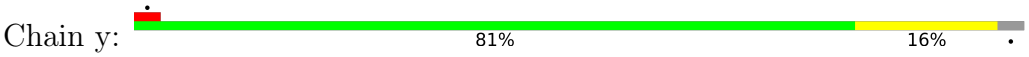


• Molecule 13: Photosystem I reaction center subunit XII





• Molecule 13: Photosystem I reaction center subunit XII





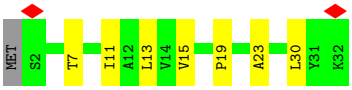
• Molecule 13: Photosystem I reaction center subunit XII





• Molecule 13: Photosystem I reaction center subunit XII





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120345	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.126	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.185	Depositor
Map size (Å)	686.39996, 686.39996, 686.39996	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: CLA, PQN, SQD, SF4, LMG, CL0, LHG, BCR

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	1	0.14	0/252	0.43	0/341
2	A	0.13	0/6022	0.28	0/8214
2	G	0.15	0/6013	0.31	0/8203
2	a	0.13	0/6022	0.29	0/8214
2	g	0.13	0/6022	0.29	0/8214
3	H	0.14	0/267	0.36	0/366
3	X	0.16	0/267	0.39	0/366
3	h	0.14	0/258	0.31	0/354
3	x	0.13	0/267	0.32	0/366
4	B	0.14	0/6142	0.31	0/8396
4	N	0.13	0/6137	0.29	0/8389
4	b	0.12	0/6142	0.28	0/8396
4	n	0.13	0/6130	0.28	0/8379
5	C	0.14	0/608	0.32	0/825
5	P	0.14	0/608	0.31	0/825
5	c	0.14	0/608	0.39	0/825
5	p	0.13	0/608	0.28	0/825
6	D	0.10	0/1064	0.26	0/1436
6	Q	0.15	0/1064	0.31	0/1436
6	d	0.12	0/1071	0.38	0/1446
6	q	0.10	0/1071	0.26	0/1446
7	E	0.20	0/499	0.35	0/677
7	R	0.12	0/499	0.28	0/677
7	e	0.12	0/499	0.28	0/677
7	r	0.11	0/490	0.30	0/665
8	F	0.14	0/1104	0.31	0/1500
8	S	0.12	0/1104	0.29	0/1500
8	f	0.12	0/1104	0.33	0/1500
8	s	0.12	0/1104	0.30	0/1500
9	J	0.10	0/371	0.23	0/509
9	T	0.12	0/366	0.27	0/502
9	j	0.13	0/371	0.28	0/509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
9	t	0.12	0/371	0.26	0/509
10	K	0.14	0/551	0.40	0/750
10	U	0.18	0/551	0.46	0/750
10	k	0.15	0/583	0.41	0/796
10	u	0.23	0/583	0.54	0/796
11	I	0.14	0/284	0.31	0/388
11	V	0.16	0/277	0.37	0/378
11	i	0.15	0/284	0.28	0/388
11	v	0.14	0/284	0.29	0/388
12	L	0.13	0/1198	0.30	0/1642
12	W	0.12	0/1198	0.27	0/1642
12	l	0.11	0/1198	0.26	0/1642
12	w	0.14	0/1198	0.32	0/1642
13	M	0.10	0/245	0.23	0/334
13	Y	0.13	0/245	0.27	0/334
13	m	0.12	0/245	0.24	0/334
13	y	0.13	0/245	0.23	0/334
All	All	0.13	0/73694	0.30	0/100525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	247	0	250	11	0
2	A	5823	0	5696	188	0
2	G	5814	0	5684	176	0
2	a	5823	0	5696	180	0
2	g	5823	0	5697	180	0
3	H	257	0	261	11	0
3	X	257	0	261	5	0
3	h	248	0	253	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	x	257	0	261	6	0
4	B	5918	0	5671	159	0
4	N	5913	0	5666	157	0
4	b	5918	0	5671	171	0
4	n	5906	0	5659	165	0
5	C	598	0	574	16	0
5	P	598	0	574	9	0
5	c	598	0	574	12	0
5	p	598	0	574	13	0
6	D	1040	0	1043	18	0
6	Q	1040	0	1043	15	0
6	d	1047	0	1050	13	0
6	q	1047	0	1050	9	0
7	E	490	0	484	8	0
7	R	490	0	484	8	0
7	e	490	0	484	9	0
7	r	481	0	478	13	0
8	F	1080	0	1078	20	0
8	S	1080	0	1078	16	0
8	f	1080	0	1078	20	0
8	s	1080	0	1078	20	0
9	J	359	0	364	11	0
9	T	354	0	359	9	0
9	j	359	0	364	10	0
9	t	359	0	364	6	0
10	K	537	0	562	19	0
10	U	537	0	562	15	0
10	k	568	0	593	15	0
10	u	568	0	593	23	0
11	I	275	0	268	6	0
11	V	268	0	259	4	0
11	i	275	0	268	9	0
11	v	275	0	268	13	0
12	L	1163	0	1166	29	0
12	W	1163	0	1166	28	0
12	l	1163	0	1166	23	0
12	w	1163	0	1166	32	0
13	M	241	0	256	8	0
13	Y	241	0	256	7	0
13	m	241	0	256	7	0
13	y	241	0	256	4	0
14	A	2631	0	2625	202	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	2345	0	2344	156	0
14	F	104	0	91	1	0
14	G	2451	0	2445	197	0
14	H	49	0	39	3	0
14	J	82	0	58	3	0
14	K	41	0	29	2	0
14	L	156	0	133	8	0
14	N	2495	0	2526	179	0
14	S	104	0	91	3	0
14	T	82	0	58	2	0
14	U	90	0	68	1	0
14	W	156	0	133	17	0
14	X	49	0	39	3	0
14	a	2566	0	2555	199	0
14	b	2430	0	2456	171	0
14	f	104	0	91	7	0
14	g	2542	0	2562	182	0
14	h	49	0	39	4	0
14	j	82	0	58	6	0
14	k	41	0	29	0	0
14	l	150	0	125	11	0
14	n	2430	0	2450	177	0
14	s	104	0	91	3	0
14	t	82	0	58	2	0
14	u	90	0	68	0	0
14	w	150	0	125	11	0
14	x	49	0	39	2	0
15	A	33	0	46	5	0
15	B	33	0	46	5	0
15	G	33	0	46	10	0
15	N	33	0	46	6	0
15	a	33	0	46	4	0
15	b	33	0	46	4	0
15	g	33	0	46	4	0
15	n	33	0	46	4	0
16	A	8	0	0	0	0
16	C	16	0	0	1	0
16	G	8	0	0	0	0
16	P	16	0	0	1	0
16	a	8	0	0	0	0
16	c	16	0	0	1	0
16	g	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	p	16	0	0	1	0
17	A	280	0	392	45	0
17	B	320	0	448	51	0
17	F	40	0	56	1	0
17	G	240	0	336	35	0
17	I	120	0	168	21	0
17	J	40	0	56	6	0
17	K	40	0	56	3	0
17	L	40	0	56	5	0
17	M	40	0	56	4	0
17	N	320	0	448	63	0
17	S	40	0	56	4	0
17	T	80	0	112	12	0
17	U	40	0	56	2	0
17	V	40	0	56	2	0
17	W	120	0	168	18	0
17	Y	40	0	56	4	0
17	a	240	0	336	33	0
17	b	320	0	448	49	0
17	f	40	0	56	4	0
17	g	240	0	336	35	0
17	i	80	0	112	15	0
17	j	80	0	112	8	0
17	k	40	0	56	2	0
17	l	80	0	112	9	0
17	m	40	0	56	3	0
17	n	320	0	448	52	0
17	s	40	0	56	4	0
17	t	80	0	112	14	0
17	u	40	0	56	2	0
17	v	40	0	56	7	0
17	w	120	0	168	19	0
17	y	40	0	56	2	0
18	A	98	0	148	7	0
18	G	98	0	148	10	0
18	S	43	0	59	4	0
18	X	43	0	59	2	0
18	a	98	0	148	14	0
18	g	98	0	148	8	0
18	m	43	0	59	6	0
18	v	43	0	59	3	0
19	A	45	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	G	65	0	72	7	0
19	a	65	0	70	4	0
19	g	65	0	72	7	0
20	B	54	0	78	4	0
20	H	54	0	78	3	0
20	b	54	0	78	6	0
20	h	54	0	78	7	0
20	l	54	0	78	4	0
20	n	54	0	78	0	0
20	w	54	0	78	3	0
20	x	54	0	78	4	0
21	B	90	0	126	6	0
21	N	90	0	126	8	0
21	b	55	0	86	3	0
21	n	55	0	86	3	0
All	All	98661	0	99030	2867	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 14.

The worst 5 of 2867 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)
14:G:852:CLA:CED	17:N:852:BCR:H401	1.27	1.58
14:G:852:CLA:CED	17:N:852:BCR:C40	2.02	1.37
14:G:852:CLA:HED2	17:N:852:BCR:C40	1.54	1.33
2:A:442:ASN:OD1	14:A:855:CLA:HED1	1.35	1.25
2:A:541:PHE:CZ	14:A:855:CLA:O1A	1.79	1.25

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	1	31/237 (13%)	30 (97%)	1 (3%)	0	100	100
2	A	740/752 (98%)	707 (96%)	32 (4%)	1 (0%)	48	78
2	G	739/752 (98%)	707 (96%)	31 (4%)	1 (0%)	48	78
2	a	740/752 (98%)	701 (95%)	39 (5%)	0	100	100
2	g	740/752 (98%)	711 (96%)	29 (4%)	0	100	100
3	H	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
3	X	29/44 (66%)	29 (100%)	0	0	100	100
3	h	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
3	x	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
4	B	738/741 (100%)	702 (95%)	36 (5%)	0	100	100
4	N	737/741 (100%)	718 (97%)	18 (2%)	1 (0%)	48	78
4	b	738/741 (100%)	705 (96%)	32 (4%)	1 (0%)	48	78
4	n	736/741 (99%)	706 (96%)	29 (4%)	1 (0%)	48	78
5	C	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
5	P	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
5	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
5	p	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
6	D	133/139 (96%)	127 (96%)	6 (4%)	0	100	100
6	Q	133/139 (96%)	127 (96%)	6 (4%)	0	100	100
6	d	134/139 (96%)	123 (92%)	11 (8%)	0	100	100
6	q	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
7	E	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
7	R	59/70 (84%)	55 (93%)	4 (7%)	0	100	100
7	e	59/70 (84%)	55 (93%)	4 (7%)	0	100	100
7	r	58/70 (83%)	54 (93%)	4 (7%)	0	100	100
8	F	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
8	S	139/164 (85%)	130 (94%)	9 (6%)	0	100	100
8	f	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
8	s	139/164 (85%)	136 (98%)	3 (2%)	0	100	100
9	J	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
9	T	42/49 (86%)	42 (100%)	0	0	100	100
9	j	43/49 (88%)	43 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	t	43/49 (88%)	43 (100%)	0	0	100	100
10	K	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
10	U	71/86 (83%)	67 (94%)	4 (6%)	0	100	100
10	k	76/86 (88%)	72 (95%)	4 (5%)	0	100	100
10	u	76/86 (88%)	74 (97%)	2 (3%)	0	100	100
11	I	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
11	V	31/46 (67%)	30 (97%)	1 (3%)	0	100	100
11	i	32/46 (70%)	32 (100%)	0	0	100	100
11	v	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
12	L	153/172 (89%)	149 (97%)	4 (3%)	0	100	100
12	W	153/172 (89%)	148 (97%)	5 (3%)	0	100	100
12	l	153/172 (89%)	146 (95%)	7 (5%)	0	100	100
12	w	153/172 (89%)	148 (97%)	5 (3%)	0	100	100
13	M	29/32 (91%)	29 (100%)	0	0	100	100
13	Y	29/32 (91%)	29 (100%)	0	0	100	100
13	m	29/32 (91%)	29 (100%)	0	0	100	100
13	y	29/32 (91%)	29 (100%)	0	0	100	100
All	All	9011/9741 (92%)	8630 (96%)	376 (4%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	122	VAL
4	N	694	ILE
2	A	122	VAL
4	b	694	ILE
4	n	694	ILE

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	1	26/206 (13%)	23 (88%)	3 (12%)	5 22
2	A	595/605 (98%)	587 (99%)	8 (1%)	61 81
2	G	594/605 (98%)	591 (100%)	3 (0%)	81 89
2	a	595/605 (98%)	592 (100%)	3 (0%)	81 89
2	g	595/605 (98%)	586 (98%)	9 (2%)	57 79
3	H	25/34 (74%)	25 (100%)	0	100 100
3	X	25/34 (74%)	25 (100%)	0	100 100
3	h	24/34 (71%)	23 (96%)	1 (4%)	26 59
3	x	25/34 (74%)	25 (100%)	0	100 100
4	B	600/602 (100%)	595 (99%)	5 (1%)	73 86
4	N	600/602 (100%)	595 (99%)	5 (1%)	73 86
4	b	600/602 (100%)	594 (99%)	6 (1%)	68 83
4	n	599/602 (100%)	595 (99%)	4 (1%)	76 87
5	C	67/69 (97%)	63 (94%)	4 (6%)	17 48
5	P	67/69 (97%)	67 (100%)	0	100 100
5	c	67/69 (97%)	65 (97%)	2 (3%)	36 67
5	p	67/69 (97%)	66 (98%)	1 (2%)	57 79
6	D	107/110 (97%)	106 (99%)	1 (1%)	70 85
6	Q	107/110 (97%)	104 (97%)	3 (3%)	38 69
6	d	108/110 (98%)	106 (98%)	2 (2%)	50 75
6	q	108/110 (98%)	108 (100%)	0	100 100
7	E	54/60 (90%)	54 (100%)	0	100 100
7	R	54/60 (90%)	52 (96%)	2 (4%)	30 62
7	e	54/60 (90%)	53 (98%)	1 (2%)	50 75
7	r	53/60 (88%)	53 (100%)	0	100 100
8	F	110/129 (85%)	108 (98%)	2 (2%)	51 76
8	S	110/129 (85%)	107 (97%)	3 (3%)	39 70
8	f	110/129 (85%)	110 (100%)	0	100 100
8	s	110/129 (85%)	110 (100%)	0	100 100
9	J	39/42 (93%)	39 (100%)	0	100 100
9	T	39/42 (93%)	37 (95%)	2 (5%)	21 53
9	j	39/42 (93%)	39 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	t	39/42 (93%)	37 (95%)	2 (5%)	21 53
10	K	54/64 (84%)	53 (98%)	1 (2%)	50 75
10	U	54/64 (84%)	54 (100%)	0	100 100
10	k	57/64 (89%)	55 (96%)	2 (4%)	32 63
10	u	57/64 (89%)	56 (98%)	1 (2%)	51 76
11	I	31/39 (80%)	30 (97%)	1 (3%)	34 65
11	V	30/39 (77%)	30 (100%)	0	100 100
11	i	31/39 (80%)	31 (100%)	0	100 100
11	v	31/39 (80%)	30 (97%)	1 (3%)	34 65
12	L	118/131 (90%)	115 (98%)	3 (2%)	42 71
12	W	118/131 (90%)	116 (98%)	2 (2%)	53 77
12	l	118/131 (90%)	116 (98%)	2 (2%)	53 77
12	w	118/131 (90%)	116 (98%)	2 (2%)	53 77
13	M	26/27 (96%)	26 (100%)	0	100 100
13	Y	26/27 (96%)	26 (100%)	0	100 100
13	m	26/27 (96%)	26 (100%)	0	100 100
13	y	26/27 (96%)	26 (100%)	0	100 100
All	All	7333/7854 (93%)	7246 (99%)	87 (1%)	61 82

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	10	THR
2	a	710	VAL
5	C	63	LEU
11	I	16	LEU
4	b	426	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	16	GLN
4	b	335	HIS
9	J	37	ASN
2	a	180	HIS

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Mol	Chain	Res	Type
4	b	425	HIS

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)

518 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
14	CLA	g	820	2	49,53,73	1.49	9 (18%)	59,89,113	1.47	8 (13%)
14	CLA	b	839	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
17	BCR	L	1504	-	41,41,41	0.73	0	56,56,56	1.95	17 (30%)
14	CLA	n	821	4	49,53,73	1.50	7 (14%)	59,89,113	1.43	4 (6%)
14	CLA	G	814	2	49,53,73	1.49	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	g	822	2	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	B	812	4	58,62,73	1.36	8 (13%)	69,99,113	1.38	6 (8%)
17	BCR	A	848	-	41,41,41	0.76	0	56,56,56	1.93	17 (30%)
14	CLA	a	831	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	9 (10%)
14	CLA	h	1701	3	53,57,73	1.43	8 (15%)	62,93,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	837	4	64,68,73	1.31	9 (14%)	77,107,113	1.30	9 (11%)
14	CLA	a	807	2	69,73,73	1.26	9 (13%)	83,113,113	1.35	6 (7%)
16	SF4	P	102	5	0,12,12	-	-	-		
14	CLA	G	815	-	49,53,73	1.50	7 (14%)	59,89,113	1.39	5 (8%)
17	BCR	j	103	-	41,41,41	0.75	0	56,56,56	2.02	15 (26%)
14	CLA	b	833	4	58,62,73	1.36	8 (13%)	69,99,113	1.38	7 (10%)
14	CLA	g	840	-	54,58,73	1.41	8 (14%)	65,95,113	1.44	9 (13%)
17	BCR	g	843	-	41,41,41	0.72	0	56,56,56	2.08	19 (33%)
14	CLA	b	814	4	54,58,73	1.40	8 (14%)	65,95,113	1.42	9 (13%)
14	CLA	g	823	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
14	CLA	B	810	4	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
14	CLA	b	810	4	64,68,73	1.31	9 (14%)	77,107,113	1.29	6 (7%)
14	CLA	n	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
16	SF4	A	843	2,4	0,12,12	-	-	-		
20	SQD	x	1702	-	53,54,54	1.53	7 (13%)	62,65,65	1.36	6 (9%)
14	CLA	N	803	-	69,73,73	1.26	7 (10%)	83,113,113	1.23	5 (6%)
14	CLA	A	840	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
18	LHG	a	849	-	48,48,48	1.10	6 (12%)	51,54,54	0.88	2 (3%)
14	CLA	A	829	2	69,73,73	1.25	9 (13%)	83,113,113	1.32	8 (9%)
14	CLA	T	101	9	49,53,73	1.50	8 (16%)	59,89,113	1.45	5 (8%)
14	CLA	N	836	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
14	CLA	g	807	2	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
17	BCR	B	846	-	41,41,41	0.73	0	56,56,56	2.27	18 (32%)
14	CLA	G	801	-	69,73,73	1.26	9 (13%)	83,113,113	1.23	5 (6%)
17	BCR	S	204	-	41,41,41	0.74	0	56,56,56	2.02	17 (30%)
14	CLA	g	830	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
14	CLA	N	842	4	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
14	CLA	b	838	4	51,55,73	1.45	7 (13%)	61,91,113	1.39	5 (8%)
14	CLA	L	1502	12	64,68,73	1.30	9 (14%)	77,107,113	1.31	7 (9%)
17	BCR	N	845	-	41,41,41	0.73	0	56,56,56	1.99	14 (25%)
21	LMG	N	802	-	35,35,55	0.58	0	43,43,63	0.69	0
14	CLA	b	850	4	62,66,73	1.33	10 (16%)	74,104,113	1.35	4 (5%)
20	SQD	B	801	-	53,54,54	1.53	7 (13%)	62,65,65	1.40	6 (9%)
14	CLA	u	101	10	46,49,73	1.53	9 (19%)	55,83,113	1.40	5 (9%)
14	CLA	b	836	4	64,68,73	1.31	7 (10%)	77,107,113	1.32	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	b	842	-	41,41,41	0.74	0	56,56,56	2.06	16 (28%)
14	CLA	a	823	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
14	CLA	J	101	9	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
14	CLA	b	818	4	69,73,73	1.26	8 (11%)	83,113,113	1.25	4 (4%)
14	CLA	b	815	4	53,57,73	1.42	8 (15%)	62,93,113	1.40	5 (8%)
14	CLA	A	833	2	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
14	CLA	A	815	-	49,53,73	1.48	7 (14%)	59,89,113	1.45	6 (10%)
14	CLA	k	101	10	46,49,73	1.53	9 (19%)	55,83,113	1.41	5 (9%)
17	BCR	B	847	-	41,41,41	0.72	0	56,56,56	2.07	14 (25%)
17	BCR	a	848	-	41,41,41	0.73	0	56,56,56	2.27	21 (37%)
14	CLA	A	814	2	49,53,73	1.48	7 (14%)	59,89,113	1.45	4 (6%)
14	CLA	N	821	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	6 (7%)
14	CLA	b	819	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
14	CLA	w	205	-	49,53,73	1.49	8 (16%)	59,89,113	1.42	4 (6%)
14	CLA	A	819	2	58,62,73	1.37	9 (15%)	69,99,113	1.38	5 (7%)
14	CLA	n	815	4	53,57,73	1.42	8 (15%)	62,93,113	1.41	7 (11%)
14	CLA	B	803	-	69,73,73	1.25	9 (13%)	83,113,113	1.18	3 (3%)
14	CLA	N	827	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	10 (12%)
14	CLA	N	818	4	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
20	SQD	h	1702	-	53,54,54	1.54	7 (13%)	62,65,65	1.33	6 (9%)
14	CLA	g	812	2	58,62,73	1.38	8 (13%)	69,99,113	1.38	6 (8%)
14	CLA	a	803	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	7 (8%)
14	CLA	A	834	2	58,62,73	1.37	9 (15%)	69,99,113	1.35	6 (8%)
14	CLA	N	819	4	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
14	CLA	N	825	4	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
14	CLA	j	101	9	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
17	BCR	G	843	-	41,41,41	0.76	0	56,56,56	2.08	14 (25%)
14	CLA	G	806	2	63,67,73	1.32	6 (9%)	75,105,113	1.32	6 (8%)
14	CLA	N	832	4	58,62,73	1.37	9 (15%)	69,99,113	1.34	6 (8%)
14	CLA	B	806	4	69,73,73	1.25	8 (11%)	83,113,113	1.27	8 (9%)
14	CLA	G	829	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	8 (9%)
14	CLA	T	102	9	42,45,73	1.56	9 (21%)	50,78,113	1.44	4 (8%)
14	CLA	G	822	2	58,62,73	1.36	8 (13%)	69,99,113	1.39	8 (11%)
18	LHG	X	1702	-	42,42,48	1.18	6 (14%)	45,48,54	0.96	2 (4%)
14	CLA	A	821	2	49,53,73	1.49	8 (16%)	59,89,113	1.45	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	G	835	2	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
14	CLA	g	852	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	10 (12%)
14	CLA	n	826	4	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
21	LMG	B	802	-	35,35,55	0.58	0	43,43,63	0.68	0
21	LMG	B	849	-	55,55,55	0.48	0	63,63,63	0.55	0
14	CLA	B	834	4	58,62,73	1.37	8 (13%)	69,99,113	1.39	8 (11%)
14	CLA	a	837	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	4 (4%)
19	CL0	G	851	2	69,73,73	1.95	21 (30%)	83,113,113	1.74	21 (25%)
14	CLA	b	826	4	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
14	CLA	A	818	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	9 (10%)
14	CLA	b	805	4	69,73,73	1.25	8 (11%)	83,113,113	1.30	9 (10%)
14	CLA	g	836	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
14	CLA	b	820	4	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
14	CLA	n	813	4	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
14	CLA	a	812	2	58,62,73	1.37	7 (12%)	69,99,113	1.39	6 (8%)
17	BCR	g	847	-	41,41,41	0.82	2 (4%)	56,56,56	2.07	16 (28%)
14	CLA	g	817	2	69,73,73	1.26	8 (11%)	83,113,113	1.27	8 (9%)
14	CLA	A	836	2	55,59,73	1.43	8 (14%)	66,96,113	1.38	5 (7%)
14	CLA	N	804	4	69,73,73	1.24	9 (13%)	83,113,113	1.23	5 (6%)
14	CLA	N	829	4	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
17	BCR	T	104	-	41,41,41	0.72	0	56,56,56	2.09	15 (26%)
17	BCR	i	102	-	41,41,41	0.77	0	56,56,56	2.03	17 (30%)
14	CLA	g	801	2	69,73,73	1.26	8 (11%)	83,113,113	1.30	5 (6%)
14	CLA	G	853	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	8 (9%)
17	BCR	w	207	-	41,41,41	0.72	0	56,56,56	2.14	18 (32%)
14	CLA	t	102	9	42,45,73	1.57	8 (19%)	50,78,113	1.44	5 (10%)
14	CLA	a	827	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
14	CLA	g	808	2	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
17	BCR	N	853	-	41,41,41	0.74	1 (2%)	56,56,56	2.09	16 (28%)
18	LHG	S	202	-	42,42,48	1.17	6 (14%)	45,48,54	0.96	2 (4%)
14	CLA	b	808	4	69,73,73	1.24	10 (14%)	83,113,113	1.30	7 (8%)
14	CLA	A	826	2	69,73,73	1.28	7 (10%)	83,113,113	1.39	7 (8%)
14	CLA	A	838	2	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
14	CLA	B	815	4	54,58,73	1.41	8 (14%)	65,95,113	1.43	8 (12%)
14	CLA	a	817	2	69,73,73	1.25	9 (13%)	83,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	N	852	-	41,41,41	0.77	0	56,56,56	2.03	17 (30%)
14	CLA	g	832	2	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	a	805	2	64,68,73	1.31	8 (12%)	77,107,113	1.31	6 (7%)
14	CLA	A	822	2	58,62,73	1.35	7 (12%)	69,99,113	1.37	5 (7%)
14	CLA	a	853	-	69,73,73	1.27	9 (13%)	83,113,113	1.21	6 (7%)
14	CLA	a	806	2	69,73,73	1.24	9 (13%)	83,113,113	1.31	6 (7%)
17	BCR	B	851	-	41,41,41	0.75	0	56,56,56	2.28	16 (28%)
14	CLA	G	812	2	64,68,73	1.32	8 (12%)	77,107,113	1.31	7 (9%)
17	BCR	b	843	-	41,41,41	0.73	0	56,56,56	2.04	17 (30%)
14	CLA	A	802	2	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
17	BCR	N	846	-	41,41,41	0.72	0	56,56,56	2.09	16 (28%)
16	SF4	P	101	5	0,12,12	-	-	-		
14	CLA	n	810	4	64,68,73	1.31	9 (14%)	77,107,113	1.30	5 (6%)
17	BCR	M	101	-	41,41,41	0.69	0	56,56,56	1.98	17 (30%)
14	CLA	G	810	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
14	CLA	n	822	-	59,63,73	1.35	7 (11%)	71,101,113	1.32	6 (8%)
17	BCR	n	851	-	41,41,41	0.73	0	56,56,56	2.04	16 (28%)
16	SF4	g	842	2,4	0,12,12	-	-	-		
14	CLA	g	827	2	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
16	SF4	c	102	5	0,12,12	-	-	-		
14	CLA	b	852	4	59,63,73	1.36	7 (11%)	71,101,113	1.33	6 (8%)
14	CLA	b	821	4	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
14	CLA	b	830	4	58,62,73	1.37	9 (15%)	69,99,113	1.36	7 (10%)
14	CLA	N	831	4	69,73,73	1.24	8 (11%)	83,113,113	1.32	5 (6%)
17	BCR	y	101	-	41,41,41	0.70	0	56,56,56	1.98	16 (28%)
14	CLA	N	812	4	64,68,73	1.30	9 (14%)	77,107,113	1.30	6 (7%)
17	BCR	N	847	-	41,41,41	0.71	0	56,56,56	2.17	17 (30%)
14	CLA	g	811	2	64,68,73	1.31	10 (15%)	77,107,113	1.29	7 (9%)
14	CLA	n	836	4	64,68,73	1.30	8 (12%)	77,107,113	1.37	9 (11%)
17	BCR	n	842	-	41,41,41	0.75	0	56,56,56	2.12	15 (26%)
14	CLA	W	204	-	49,53,73	1.48	8 (16%)	59,89,113	1.41	4 (6%)
14	CLA	g	819	-	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
14	CLA	g	831	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
14	CLA	n	818	4	69,73,73	1.26	8 (11%)	83,113,113	1.27	5 (6%)
14	CLA	U	101	10	46,49,73	1.53	10 (21%)	55,83,113	1.40	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	816	-	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
14	CLA	b	831	4	64,68,73	1.30	8 (12%)	77,107,113	1.32	6 (7%)
14	CLA	b	807	4	69,73,73	1.25	8 (11%)	83,113,113	1.25	6 (7%)
17	BCR	a	846	-	41,41,41	0.74	0	56,56,56	2.77	22 (39%)
14	CLA	A	810	2,14	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
14	CLA	N	828	4	69,73,73	1.26	7 (10%)	83,113,113	1.32	5 (6%)
14	CLA	G	811	2	63,67,73	1.32	7 (11%)	75,105,113	1.32	5 (6%)
14	CLA	n	816	4	49,53,73	1.49	7 (14%)	59,89,113	1.46	5 (8%)
14	CLA	A	812	2	64,68,73	1.32	10 (15%)	77,107,113	1.30	7 (9%)
14	CLA	N	820	4	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
14	CLA	g	809	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	7 (8%)
14	CLA	A	830	2	58,62,73	1.38	9 (15%)	69,99,113	1.38	7 (10%)
17	BCR	g	844	-	41,41,41	0.73	0	56,56,56	2.10	15 (26%)
14	CLA	U	102	-	53,57,73	1.43	8 (15%)	62,93,113	1.43	6 (9%)
14	CLA	G	830	2	58,62,73	1.37	9 (15%)	69,99,113	1.37	6 (8%)
14	CLA	N	823	4	49,53,73	1.49	7 (14%)	59,89,113	1.46	4 (6%)
14	CLA	a	839	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	5 (6%)
14	CLA	B	820	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
18	LHG	v	102	-	42,42,48	1.17	6 (14%)	45,48,54	0.99	3 (6%)
14	CLA	G	832	2	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
14	CLA	G	827	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
17	BCR	a	847	-	41,41,41	0.82	2 (4%)	56,56,56	2.06	17 (30%)
14	CLA	n	839	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
14	CLA	N	807	4	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
14	CLA	g	853	-	69,73,73	1.27	9 (13%)	83,113,113	1.24	6 (7%)
14	CLA	n	838	4	51,55,73	1.45	8 (15%)	61,91,113	1.38	6 (9%)
14	CLA	g	826	2	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
14	CLA	g	804	2	69,73,73	1.26	9 (13%)	83,113,113	1.25	7 (8%)
14	CLA	b	832	4	69,73,73	1.26	8 (11%)	83,113,113	1.27	8 (9%)
17	BCR	G	848	-	41,41,41	0.72	0	56,56,56	2.19	20 (35%)
14	CLA	b	802	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	8 (9%)
14	CLA	n	834	-	49,53,73	1.49	9 (18%)	59,89,113	1.44	6 (10%)
14	CLA	g	816	2	64,68,73	1.31	9 (14%)	77,107,113	1.31	4 (5%)
17	BCR	v	101	-	41,41,41	0.73	0	56,56,56	2.25	18 (32%)
14	CLA	b	834	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	B	843	-	41,41,41	0.70	0	56,56,56	2.06	16 (28%)
17	BCR	V	101	-	41,41,41	0.74	0	56,56,56	2.15	14 (25%)
16	SF4	p	101	5	0,12,12	-	-	-		
20	SQD	H	1702	-	53,54,54	1.53	7 (13%)	62,65,65	1.39	7 (11%)
14	CLA	a	820	2	49,53,73	1.48	8 (16%)	59,89,113	1.48	6 (10%)
14	CLA	N	837	-	49,53,73	1.49	9 (18%)	59,89,113	1.42	4 (6%)
17	BCR	n	843	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)
15	PQN	B	842	-	34,34,34	1.57	2 (5%)	42,45,45	1.14	3 (7%)
14	CLA	B	832	4	64,68,73	1.30	8 (12%)	77,107,113	1.28	4 (5%)
14	CLA	a	826	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
14	CLA	a	804	2	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
14	CLA	b	827	4	69,73,73	1.25	8 (11%)	83,113,113	1.24	7 (8%)
14	CLA	W	203	12	64,68,73	1.29	8 (12%)	77,107,113	1.36	8 (10%)
14	CLA	g	837	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	7 (8%)
16	SF4	c	101	5	0,12,12	-	-	-		
14	CLA	A	839	2	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
14	CLA	G	817	2	64,68,73	1.31	9 (14%)	77,107,113	1.30	4 (5%)
14	CLA	B	811	4	64,68,73	1.30	9 (14%)	77,107,113	1.32	5 (6%)
14	CLA	n	814	4	54,58,73	1.41	8 (14%)	65,95,113	1.44	7 (10%)
15	PQN	A	842	-	34,34,34	1.58	2 (5%)	42,45,45	1.15	4 (9%)
14	CLA	A	832	2	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
14	CLA	n	819	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	8 (9%)
17	BCR	W	201	-	41,41,41	0.73	0	56,56,56	2.60	21 (37%)
16	SF4	C	102	5	0,12,12	-	-	-		
14	CLA	a	840	18	49,53,73	1.50	9 (18%)	59,89,113	1.44	5 (8%)
14	CLA	G	818	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	8 (9%)
14	CLA	S	203	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
18	LHG	g	850	-	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
14	CLA	f	201	-	63,67,73	1.30	8 (12%)	75,105,113	1.35	8 (10%)
17	BCR	m	102	-	41,41,41	0.70	0	56,56,56	2.05	16 (28%)
21	LMG	b	848	-	55,55,55	0.50	0	63,63,63	0.60	0
14	CLA	B	807	4	69,73,73	1.26	7 (10%)	83,113,113	1.31	7 (8%)
17	BCR	W	205	-	41,41,41	0.74	0	56,56,56	1.69	13 (23%)
14	CLA	n	823	4	69,73,73	1.26	9 (13%)	83,113,113	1.26	7 (8%)
14	CLA	N	830	4	69,73,73	1.26	9 (13%)	83,113,113	1.27	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	t	103	-	41,41,41	0.71	0	56,56,56	2.02	14 (25%)
14	CLA	N	813	4	58,62,73	1.36	7 (12%)	69,99,113	1.37	6 (8%)
14	CLA	N	815	4	69,73,73	1.26	9 (13%)	83,113,113	1.32	5 (6%)
17	BCR	B	852	-	41,41,41	0.74	0	56,56,56	2.01	15 (26%)
14	CLA	B	835	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
14	CLA	g	821	2	58,62,73	1.37	9 (15%)	69,99,113	1.33	6 (8%)
14	CLA	G	816	2	63,67,73	1.31	9 (14%)	75,105,113	1.31	6 (8%)
18	LHG	g	849	-	48,48,48	1.10	6 (12%)	51,54,54	0.90	2 (3%)
14	CLA	A	801	-	69,73,73	1.27	8 (11%)	83,113,113	1.20	5 (6%)
14	CLA	N	817	4	53,57,73	1.42	7 (13%)	62,93,113	1.41	6 (9%)
14	CLA	l	204	-	49,53,73	1.50	8 (16%)	59,89,113	1.41	6 (10%)
14	CLA	t	101	9	49,53,73	1.48	7 (14%)	59,89,113	1.44	4 (6%)
14	CLA	A	828	2	69,73,73	1.25	9 (13%)	83,113,113	1.25	6 (7%)
14	CLA	N	841	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	7 (8%)
14	CLA	G	804	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	6 (7%)
18	LHG	m	101	-	42,42,48	1.17	6 (14%)	45,48,54	0.94	3 (6%)
14	CLA	N	805	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
17	BCR	T	103	-	41,41,41	0.70	0	56,56,56	1.96	16 (28%)
14	CLA	N	801	-	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
14	CLA	A	805	2	69,73,73	1.26	9 (13%)	83,113,113	1.23	6 (7%)
15	PQN	g	841	-	34,34,34	1.57	2 (5%)	42,45,45	1.17	5 (11%)
14	CLA	N	806	4	59,63,73	1.36	9 (15%)	71,101,113	1.31	7 (9%)
14	CLA	G	838	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	4 (4%)
14	CLA	A	811	2	63,67,73	1.32	9 (14%)	75,105,113	1.32	6 (8%)
14	CLA	N	822	4	49,53,73	1.48	8 (16%)	59,89,113	1.42	4 (6%)
14	CLA	G	820	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	8 (9%)
14	CLA	n	837	4	69,73,73	1.25	8 (11%)	83,113,113	1.28	6 (7%)
14	CLA	g	824	-	58,62,73	1.37	8 (13%)	69,99,113	1.36	7 (10%)
14	CLA	A	831	2	69,73,73	1.26	7 (10%)	83,113,113	1.27	8 (9%)
14	CLA	g	806	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	7 (8%)
14	CLA	a	852	-	49,53,73	1.47	9 (18%)	59,89,113	1.41	4 (6%)
14	CLA	b	823	4	69,73,73	1.27	8 (11%)	83,113,113	1.27	8 (9%)
14	CLA	a	830	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
18	LHG	G	849	-	48,48,48	1.10	6 (12%)	51,54,54	0.93	2 (3%)
14	CLA	n	840	4	69,73,73	1.26	8 (11%)	83,113,113	1.33	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	a	845	-	41,41,41	0.75	0	56,56,56	2.12	18 (32%)
14	CLA	b	822	-	59,63,73	1.36	6 (10%)	71,101,113	1.33	5 (7%)
14	CLA	n	807	4	69,73,73	1.24	7 (10%)	83,113,113	1.27	6 (7%)
14	CLA	N	808	4	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
14	CLA	n	852	4	59,63,73	1.36	9 (15%)	71,101,113	1.32	7 (9%)
21	LMG	n	848	-	55,55,55	0.49	0	63,63,63	0.58	0
14	CLA	n	830	4	58,62,73	1.38	9 (15%)	69,99,113	1.37	6 (8%)
16	SF4	C	101	5	0,12,12	-	-	-		
17	BCR	G	845	-	41,41,41	0.75	0	56,56,56	2.11	15 (26%)
21	LMG	N	850	-	55,55,55	0.49	0	63,63,63	0.60	0
14	CLA	g	829	2	58,62,73	1.37	8 (13%)	69,99,113	1.35	7 (10%)
14	CLA	B	850	4	69,73,73	1.27	8 (11%)	83,113,113	1.25	8 (9%)
14	CLA	n	820	4	49,53,73	1.49	8 (16%)	59,89,113	1.44	4 (6%)
15	PQN	a	841	-	34,34,34	1.58	2 (5%)	42,45,45	1.13	4 (9%)
14	CLA	b	809	4	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
14	CLA	A	809	2	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
14	CLA	J	102	9	42,45,73	1.56	9 (21%)	50,78,113	1.47	5 (10%)
14	CLA	H	1701	3	53,57,73	1.43	9 (16%)	62,93,113	1.40	4 (6%)
17	BCR	b	846	-	41,41,41	0.73	0	56,56,56	2.06	15 (26%)
17	BCR	A	846	-	41,41,41	0.73	0	56,56,56	2.07	16 (28%)
14	CLA	G	839	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
14	CLA	N	810	4	69,73,73	1.23	8 (11%)	83,113,113	1.31	6 (7%)
14	CLA	a	818	2	58,62,73	1.36	9 (15%)	69,99,113	1.38	7 (10%)
14	CLA	B	839	4	51,55,73	1.46	9 (17%)	61,91,113	1.38	6 (9%)
14	CLA	X	1701	3	53,57,73	1.43	8 (15%)	62,93,113	1.39	4 (6%)
14	CLA	n	850	4	62,66,73	1.32	10 (16%)	74,104,113	1.33	5 (6%)
14	CLA	B	836	-	49,53,73	1.49	8 (16%)	59,89,113	1.41	5 (8%)
20	SQD	w	202	-	53,54,54	1.53	7 (13%)	62,65,65	1.37	6 (9%)
14	CLA	N	816	4	54,58,73	1.41	8 (14%)	65,95,113	1.43	7 (10%)
14	CLA	a	822	2	49,53,73	1.48	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	B	816	4	53,57,73	1.42	8 (15%)	62,93,113	1.42	5 (8%)
17	BCR	F	203	-	41,41,41	0.73	0	56,56,56	2.03	16 (28%)
14	CLA	a	832	2	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
14	CLA	b	837	4	69,73,73	1.25	9 (13%)	83,113,113	1.29	8 (9%)
14	CLA	A	823	2	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	804	-	69,73,73	1.26	6 (8%)	83,113,113	1.29	9 (10%)
14	CLA	j	102	9	42,45,73	1.57	9 (21%)	50,78,113	1.44	5 (10%)
17	BCR	f	203	-	41,41,41	0.73	0	56,56,56	2.11	16 (28%)
14	CLA	g	833	2	58,62,73	1.37	9 (15%)	69,99,113	1.36	6 (8%)
15	PQN	N	843	-	34,34,34	1.57	2 (5%)	42,45,45	1.20	4 (9%)
14	CLA	n	832	4	69,73,73	1.26	7 (10%)	83,113,113	1.29	9 (10%)
17	BCR	l	206	-	41,41,41	0.71	0	56,56,56	2.10	17 (30%)
17	BCR	t	104	-	41,41,41	0.72	0	56,56,56	2.26	18 (32%)
14	CLA	A	807	2	69,73,73	1.25	9 (13%)	83,113,113	1.32	7 (8%)
14	CLA	G	819	2	58,62,73	1.37	8 (13%)	69,99,113	1.37	5 (7%)
14	CLA	G	831	2	69,73,73	1.25	9 (13%)	83,113,113	1.28	9 (10%)
14	CLA	A	816	2	63,67,73	1.31	9 (14%)	75,105,113	1.34	5 (6%)
14	CLA	b	824	4	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
14	CLA	a	808	2	49,53,73	1.49	8 (16%)	59,89,113	1.42	4 (6%)
14	CLA	G	807	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	9 (10%)
14	CLA	A	853	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
14	CLA	N	839	4	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)
14	CLA	B	813	4	58,62,73	1.38	7 (12%)	69,99,113	1.36	6 (8%)
14	CLA	B	838	4	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
14	CLA	n	806	4	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
14	CLA	L	1503	-	49,53,73	1.49	9 (18%)	59,89,113	1.42	5 (8%)
14	CLA	G	826	2	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
14	CLA	a	825	2	69,73,73	1.26	9 (13%)	83,113,113	1.27	4 (4%)
17	BCR	l	205	-	41,41,41	0.73	0	56,56,56	1.98	13 (23%)
19	CL0	g	851	2	69,73,73	1.97	21 (30%)	83,113,113	1.77	19 (22%)
14	CLA	B	805	4	59,63,73	1.36	9 (15%)	71,101,113	1.36	6 (8%)
14	CLA	A	837	2	69,73,73	1.26	9 (13%)	83,113,113	1.27	5 (6%)
17	BCR	B	848	-	41,41,41	0.75	0	56,56,56	2.12	18 (32%)
14	CLA	n	828	4	69,73,73	1.25	9 (13%)	83,113,113	1.27	8 (9%)
14	CLA	g	813	2	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
17	BCR	b	847	-	41,41,41	0.76	0	56,56,56	1.87	14 (25%)
14	CLA	b	813	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
15	PQN	n	841	-	34,34,34	1.55	2 (5%)	42,45,45	1.15	4 (9%)
14	CLA	b	817	4	69,73,73	1.25	8 (11%)	83,113,113	1.23	4 (4%)
17	BCR	Y	101	-	41,41,41	0.70	0	56,56,56	2.01	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	PQN	b	841	-	34,34,34	1.56	2 (5%)	42,45,45	1.17	3 (7%)
14	CLA	G	840	18	49,53,73	1.50	10 (20%)	59,89,113	1.39	4 (6%)
14	CLA	n	805	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)
14	CLA	A	824	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
17	BCR	j	104	-	41,41,41	0.70	0	56,56,56	2.42	21 (37%)
17	BCR	g	845	-	41,41,41	0.75	0	56,56,56	2.14	16 (28%)
14	CLA	N	835	4	58,62,73	1.35	8 (13%)	69,99,113	1.35	5 (7%)
14	CLA	u	102	-	53,57,73	1.43	8 (15%)	62,93,113	1.41	7 (11%)
14	CLA	B	804	4	49,53,73	1.49	7 (14%)	59,89,113	1.34	4 (6%)
14	CLA	b	829	4	69,73,73	1.26	9 (13%)	83,113,113	1.30	9 (10%)
18	LHG	A	850	-	48,48,48	1.10	6 (12%)	51,54,54	0.89	2 (3%)
14	CLA	g	854	-	69,73,73	1.27	9 (13%)	83,113,113	1.26	5 (6%)
14	CLA	B	830	4	69,73,73	1.23	8 (11%)	83,113,113	1.29	5 (6%)
14	CLA	n	829	4	69,73,73	1.24	7 (10%)	83,113,113	1.27	5 (6%)
16	SF4	a	842	2,4	0,12,12	-	-	-		
14	CLA	b	806	4	69,73,73	1.25	8 (11%)	83,113,113	1.30	8 (9%)
14	CLA	w	204	12	64,68,73	1.29	9 (14%)	77,107,113	1.32	6 (7%)
14	CLA	G	809	2	49,53,73	1.49	9 (18%)	59,89,113	1.44	5 (8%)
14	CLA	N	811	4	69,73,73	1.26	9 (13%)	83,113,113	1.31	7 (8%)
14	CLA	N	834	4	62,66,73	1.31	9 (14%)	74,104,113	1.36	5 (6%)
14	CLA	G	821	2	49,53,73	1.48	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	a	813	2	49,53,73	1.49	8 (16%)	59,89,113	1.44	4 (6%)
14	CLA	g	803	2	69,73,73	1.25	9 (13%)	83,113,113	1.26	7 (8%)
14	CLA	a	815	2	63,67,73	1.31	9 (14%)	75,105,113	1.32	6 (8%)
20	SQD	l	201	-	53,54,54	1.54	7 (13%)	62,65,65	1.39	7 (11%)
14	CLA	N	840	4	51,55,73	1.45	8 (15%)	61,91,113	1.40	6 (9%)
17	BCR	A	847	-	41,41,41	0.73	0	56,56,56	2.29	20 (35%)
14	CLA	g	825	2	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
14	CLA	A	813	2	58,62,73	1.37	7 (12%)	69,99,113	1.38	6 (8%)
14	CLA	B	819	4	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
14	CLA	B	831	4	58,62,73	1.37	9 (15%)	69,99,113	1.35	4 (5%)
14	CLA	A	817	2	64,68,73	1.30	8 (12%)	77,107,113	1.30	4 (5%)
14	CLA	n	802	-	69,73,73	1.25	8 (11%)	83,113,113	1.19	3 (3%)
14	CLA	a	854	-	53,57,73	1.43	8 (15%)	62,93,113	1.40	6 (9%)
14	CLA	n	817	4	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	g	828	2	69,73,73	1.25	9 (13%)	83,113,113	1.33	6 (7%)
14	CLA	A	841	18	49,53,73	1.49	7 (14%)	59,89,113	1.46	4 (6%)
14	CLA	G	833	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
14	CLA	a	801	2	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
17	BCR	B	845	-	41,41,41	0.70	0	56,56,56	2.10	14 (25%)
17	BCR	g	848	-	41,41,41	0.75	0	56,56,56	2.14	18 (32%)
14	CLA	N	809	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	10 (12%)
14	CLA	a	835	2	55,59,73	1.41	8 (14%)	66,96,113	1.40	5 (7%)
17	BCR	n	847	-	41,41,41	0.79	1 (2%)	56,56,56	1.99	15 (26%)
14	CLA	A	854	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
18	LHG	a	850	14	48,48,48	1.11	6 (12%)	51,54,54	0.95	2 (3%)
14	CLA	A	806	2	64,68,73	1.31	8 (12%)	77,107,113	1.31	6 (7%)
14	CLA	x	1701	3	53,57,73	1.42	7 (13%)	62,93,113	1.41	5 (8%)
17	BCR	B	844	-	41,41,41	0.73	0	56,56,56	2.11	20 (35%)
14	CLA	N	814	4	58,62,73	1.37	8 (13%)	69,99,113	1.38	7 (10%)
14	CLA	B	824	4	69,73,73	1.26	8 (11%)	83,113,113	1.27	5 (6%)
14	CLA	S	201	-	63,67,73	1.31	10 (15%)	75,105,113	1.33	7 (9%)
17	BCR	a	844	-	41,41,41	0.74	0	56,56,56	2.15	18 (32%)
17	BCR	b	845	-	41,41,41	0.75	0	56,56,56	2.29	19 (33%)
14	CLA	a	824	-	58,62,73	1.36	9 (15%)	69,99,113	1.37	7 (10%)
14	CLA	K	101	10	46,49,73	1.53	10 (21%)	55,83,113	1.39	3 (5%)
17	BCR	I	102	-	41,41,41	0.84	1 (2%)	56,56,56	2.84	22 (39%)
14	CLA	n	808	4	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
14	CLA	a	811	2	64,68,73	1.30	8 (12%)	77,107,113	1.32	6 (7%)
14	CLA	N	851	4	69,73,73	1.26	7 (10%)	83,113,113	1.28	8 (9%)
14	CLA	n	827	4	69,73,73	1.26	8 (11%)	83,113,113	1.25	7 (8%)
14	CLA	G	852	-	49,53,73	1.45	11 (22%)	59,89,113	1.37	4 (6%)
17	BCR	n	844	-	41,41,41	0.70	0	56,56,56	2.07	15 (26%)
14	CLA	n	824	4	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
14	CLA	G	825	-	58,62,73	1.37	8 (13%)	69,99,113	1.35	6 (8%)
14	CLA	a	855	19	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
14	CLA	N	833	4	64,68,73	1.31	7 (10%)	77,107,113	1.29	6 (7%)
17	BCR	b	849	-	41,41,41	0.71	0	56,56,56	1.99	13 (23%)
14	CLA	A	857	-	53,57,73	1.43	8 (15%)	62,93,113	1.43	5 (8%)
14	CLA	A	820	-	69,73,73	1.27	8 (11%)	83,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	W	206	-	41,41,41	0.70	0	56,56,56	2.10	18 (32%)
14	CLA	s	202	-	49,53,73	1.50	8 (16%)	59,89,113	1.44	6 (10%)
17	BCR	w	206	-	41,41,41	0.74	0	56,56,56	2.13	13 (23%)
14	CLA	B	818	4	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
17	BCR	k	102	-	41,41,41	0.72	0	56,56,56	2.08	16 (28%)
14	CLA	G	828	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
14	CLA	B	828	4	69,73,73	1.25	7 (10%)	83,113,113	1.25	6 (7%)
14	CLA	b	828	4	69,73,73	1.24	9 (13%)	83,113,113	1.28	7 (8%)
17	BCR	N	849	-	41,41,41	0.76	0	56,56,56	1.86	17 (30%)
14	CLA	s	201	-	63,67,73	1.32	9 (14%)	75,105,113	1.33	7 (9%)
14	CLA	G	836	2	55,59,73	1.40	8 (14%)	66,96,113	1.42	6 (9%)
14	CLA	a	809	2,14	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
14	CLA	w	203	12	49,53,73	1.49	9 (18%)	59,89,113	1.47	7 (11%)
14	CLA	n	831	4	64,68,73	1.31	8 (12%)	77,107,113	1.29	6 (7%)
14	CLA	B	841	4	69,73,73	1.27	9 (13%)	83,113,113	1.30	7 (8%)
14	CLA	G	805	2	69,73,73	1.25	7 (10%)	83,113,113	1.27	8 (9%)
17	BCR	A	845	-	41,41,41	0.73	0	56,56,56	2.11	17 (30%)
19	CL0	A	852	-	49,53,73	2.33	21 (42%)	59,89,113	2.02	19 (32%)
17	BCR	w	201	-	41,41,41	0.72	0	56,56,56	2.03	14 (25%)
14	CLA	g	810	2	63,67,73	1.32	9 (14%)	75,105,113	1.33	6 (8%)
14	CLA	F	201	-	63,67,73	1.32	9 (14%)	75,105,113	1.32	6 (8%)
14	CLA	B	825	4	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
17	BCR	A	849	-	41,41,41	0.73	0	56,56,56	2.24	20 (35%)
17	BCR	u	103	-	41,41,41	0.70	0	56,56,56	2.09	16 (28%)
14	CLA	B	833	4	62,66,73	1.33	9 (14%)	74,104,113	1.34	5 (6%)
14	CLA	B	814	4	69,73,73	1.25	9 (13%)	83,113,113	1.32	7 (8%)
17	BCR	i	101	-	41,41,41	0.74	0	56,56,56	2.23	17 (30%)
14	CLA	n	835	-	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
14	CLA	a	836	2	69,73,73	1.26	9 (13%)	83,113,113	1.25	6 (7%)
14	CLA	B	840	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
14	CLA	G	808	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
14	CLA	n	803	4	69,73,73	1.24	8 (11%)	83,113,113	1.23	7 (8%)
17	BCR	J	103	-	41,41,41	0.71	0	56,56,56	1.99	16 (28%)
14	CLA	A	827	2	69,73,73	1.24	7 (10%)	83,113,113	1.25	7 (8%)
14	CLA	B	826	-	69,73,73	1.24	7 (10%)	83,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	n	811	4	58,62,73	1.37	9 (15%)	69,99,113	1.35	4 (5%)
14	CLA	A	855	-	49,53,73	1.46	9 (18%)	59,89,113	1.42	6 (10%)
14	CLA	n	804	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
14	CLA	b	816	4	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
17	BCR	I	103	-	41,41,41	0.75	0	56,56,56	1.79	13 (23%)
14	CLA	N	826	4	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
14	CLA	B	823	-	59,63,73	1.35	8 (13%)	71,101,113	1.33	6 (8%)
17	BCR	G	846	-	41,41,41	0.71	0	56,56,56	2.06	16 (28%)
14	CLA	b	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
14	CLA	b	811	4	58,62,73	1.38	9 (15%)	69,99,113	1.36	6 (8%)
14	CLA	n	812	4	58,62,73	1.38	7 (12%)	69,99,113	1.36	6 (8%)
14	CLA	B	809	4	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
14	CLA	a	810	2	63,67,73	1.32	7 (11%)	75,105,113	1.33	6 (8%)
14	CLA	B	821	4	49,53,73	1.48	8 (16%)	59,89,113	1.44	4 (6%)
14	CLA	a	821	2	58,62,73	1.38	9 (15%)	69,99,113	1.34	6 (8%)
17	BCR	s	203	-	41,41,41	0.73	0	56,56,56	2.07	16 (28%)
14	CLA	A	835	2	49,53,73	1.48	7 (14%)	59,89,113	1.42	4 (6%)
14	CLA	b	840	4	69,73,73	1.27	8 (11%)	83,113,113	1.30	6 (7%)
14	CLA	G	802	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	g	835	2	55,59,73	1.40	7 (12%)	66,96,113	1.42	7 (10%)
17	BCR	G	844	-	41,41,41	0.72	0	56,56,56	2.07	18 (32%)
18	LHG	A	851	14	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
14	CLA	n	809	4	69,73,73	1.25	10 (14%)	83,113,113	1.27	4 (4%)
16	SF4	G	842	2,4	0,12,12	-	-	-		
17	BCR	g	846	-	41,41,41	0.75	0	56,56,56	2.52	18 (32%)
17	BCR	n	846	-	41,41,41	0.72	0	56,56,56	2.15	16 (28%)
14	CLA	A	808	2	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
14	CLA	g	838	2	69,73,73	1.26	9 (13%)	83,113,113	1.29	8 (9%)
14	CLA	b	803	4	69,73,73	1.24	9 (13%)	83,113,113	1.20	6 (7%)
14	CLA	A	803	2,14	58,62,73	1.37	7 (12%)	69,99,113	1.36	5 (7%)
17	BCR	n	845	-	41,41,41	0.76	0	56,56,56	2.48	17 (30%)
17	BCR	N	848	-	41,41,41	0.76	0	56,56,56	2.10	15 (26%)
17	BCR	U	103	-	41,41,41	0.71	0	56,56,56	2.03	14 (25%)
14	CLA	A	804	2	69,73,73	1.26	10 (14%)	83,113,113	1.32	6 (7%)
17	BCR	K	102	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	834	2	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
14	CLA	a	828	2	69,73,73	1.24	7 (10%)	83,113,113	1.27	6 (7%)
14	CLA	A	825	-	58,62,73	1.37	8 (13%)	69,99,113	1.40	7 (10%)
14	CLA	g	814	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
20	SQD	n	801	-	53,54,54	1.54	8 (15%)	62,65,65	1.37	6 (9%)
14	CLA	g	839	2	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
14	CLA	a	838	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
17	BCR	A	856	-	41,41,41	0.68	0	56,56,56	2.19	17 (30%)
14	CLA	N	838	4	64,68,73	1.31	9 (14%)	77,107,113	1.29	5 (6%)
14	CLA	W	202	12	55,59,73	1.40	9 (16%)	66,96,113	1.45	4 (6%)
14	CLA	g	834	2	49,53,73	1.48	7 (14%)	59,89,113	1.44	5 (8%)
20	SQD	b	801	-	53,54,54	1.55	8 (15%)	62,65,65	1.32	7 (11%)
14	CLA	B	829	4	69,73,73	1.25	9 (13%)	83,113,113	1.25	9 (10%)
15	PQN	G	841	-	34,34,34	1.57	2 (5%)	42,45,45	1.16	4 (9%)
14	CLA	g	802	2	58,62,73	1.37	8 (13%)	69,99,113	1.36	7 (10%)
14	CLA	B	827	4	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
14	CLA	a	829	2	58,62,73	1.37	9 (15%)	69,99,113	1.35	7 (10%)
14	CLA	l	203	12	64,68,73	1.30	9 (14%)	77,107,113	1.32	6 (7%)
17	BCR	G	847	-	41,41,41	0.77	1 (2%)	56,56,56	2.01	15 (26%)
18	LHG	G	850	14	48,48,48	1.10	6 (12%)	51,54,54	0.92	2 (3%)
17	BCR	b	844	-	41,41,41	0.69	0	56,56,56	2.04	14 (25%)
14	CLA	b	812	4	58,62,73	1.36	8 (13%)	69,99,113	1.39	6 (8%)
14	CLA	G	824	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	6 (7%)
14	CLA	l	202	12	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
14	CLA	f	202	-	49,53,73	1.50	8 (16%)	59,89,113	1.42	6 (10%)
19	CL0	a	851	2,14	69,73,73	1.99	19 (27%)	83,113,113	1.72	20 (24%)
14	CLA	a	814	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
17	BCR	b	851	-	41,41,41	0.73	0	56,56,56	2.00	15 (26%)
14	CLA	B	817	4	49,53,73	1.49	10 (20%)	59,89,113	1.45	6 (10%)
14	CLA	a	819	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	8 (9%)
14	CLA	g	818	2	58,62,73	1.38	7 (12%)	69,99,113	1.37	4 (5%)
14	CLA	G	813	2	58,62,73	1.36	7 (12%)	69,99,113	1.37	6 (8%)
16	SF4	p	102	5	0,12,12	-	-	-		
14	CLA	G	803	2	58,62,73	1.37	8 (13%)	69,99,113	1.35	7 (10%)
17	BCR	n	849	-	41,41,41	0.73	0	56,56,56	1.97	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	A	844	-	41,41,41	0.73	0	56,56,56	2.03	15 (26%)
14	CLA	g	815	2	63,67,73	1.31	7 (11%)	75,105,113	1.31	7 (9%)
14	CLA	a	802	2,14	58,62,73	1.37	8 (13%)	69,99,113	1.40	7 (10%)
14	CLA	a	833	2	58,62,73	1.37	9 (15%)	69,99,113	1.35	6 (8%)
14	CLA	g	805	2	64,68,73	1.32	8 (12%)	77,107,113	1.30	6 (7%)
14	CLA	G	834	2	58,62,73	1.36	9 (15%)	69,99,113	1.35	6 (8%)
17	BCR	a	843	-	41,41,41	0.72	0	56,56,56	2.01	15 (26%)
17	BCR	N	844	-	41,41,41	0.75	0	56,56,56	2.09	11 (19%)
14	CLA	N	824	-	59,63,73	1.36	9 (15%)	71,101,113	1.33	4 (5%)
14	CLA	G	823	2	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	G	837	2	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
14	CLA	n	833	4	58,62,73	1.37	7 (12%)	69,99,113	1.36	6 (8%)
14	CLA	L	1501	12	55,59,73	1.40	9 (16%)	66,96,113	1.43	7 (10%)
14	CLA	B	808	4	69,73,73	1.25	8 (11%)	83,113,113	1.26	7 (8%)
14	CLA	b	835	-	49,53,73	1.49	7 (14%)	59,89,113	1.40	5 (8%)
14	CLA	B	822	4	49,53,73	1.49	8 (16%)	59,89,113	1.46	4 (6%)
14	CLA	F	202	-	49,53,73	1.49	9 (18%)	59,89,113	1.44	6 (10%)
17	BCR	I	101	-	41,41,41	0.75	0	56,56,56	2.20	16 (28%)

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
14	CLA	g	820	2	-	9/15/91/115	-
14	CLA	b	839	-	-	10/39/115/115	-
17	BCR	L	1504	-	-	2/29/63/63	0/2/2/2
14	CLA	n	821	4	-	5/15/91/115	-
14	CLA	G	814	2	-	8/15/91/115	-
14	CLA	g	822	2	-	4/15/91/115	-
14	CLA	B	812	4	-	8/26/102/115	-
17	BCR	A	848	-	-	2/29/63/63	0/2/2/2
14	CLA	a	831	2	-	7/39/115/115	-
14	CLA	h	1701	3	-	10/20/96/115	-
14	CLA	B	837	4	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	807	2	-	7/39/115/115	-
16	SF4	P	102	5	-	-	0/6/5/5
14	CLA	G	815	-	-	3/15/91/115	-
17	BCR	j	103	-	-	2/29/63/63	0/2/2/2
14	CLA	b	833	4	-	6/26/102/115	-
14	CLA	g	840	-	-	6/21/97/115	-
17	BCR	g	843	-	-	2/29/63/63	0/2/2/2
14	CLA	b	814	4	-	10/21/97/115	-
14	CLA	g	823	-	-	10/39/115/115	-
14	CLA	B	810	4	-	20/39/115/115	-
14	CLA	b	810	4	-	16/33/109/115	-
14	CLA	n	825	-	-	14/39/115/115	-
20	SQD	x	1702	-	-	29/49/69/69	0/1/1/1
16	SF4	A	843	2,4	-	-	0/6/5/5
14	CLA	N	803	-	-	15/39/115/115	-
14	CLA	A	840	-	-	13/39/115/115	-
18	LHG	a	849	-	-	27/53/53/53	-
14	CLA	A	829	2	-	8/39/115/115	-
14	CLA	T	101	9	-	11/15/91/115	-
14	CLA	N	836	-	-	2/15/91/115	-
14	CLA	g	807	2	-	19/39/115/115	-
17	BCR	B	846	-	-	7/29/63/63	0/2/2/2
14	CLA	G	801	-	-	8/39/115/115	-
17	BCR	S	204	-	-	2/29/63/63	0/2/2/2
14	CLA	g	830	2	-	16/39/115/115	-
14	CLA	N	842	4	-	15/39/115/115	-
14	CLA	b	838	4	-	4/18/94/115	-
14	CLA	L	1502	12	-	12/33/109/115	-
17	BCR	N	845	-	-	3/29/63/63	0/2/2/2
21	LMG	N	802	-	-	9/30/50/70	0/1/1/1
14	CLA	b	850	4	-	9/31/107/115	-
20	SQD	B	801	-	-	22/49/69/69	0/1/1/1
14	CLA	u	101	10	-	5/9/81/115	-
14	CLA	b	836	4	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	842	-	-	4/29/63/63	0/2/2/2
14	CLA	a	823	-	-	14/39/115/115	-
14	CLA	J	101	9	-	11/15/91/115	-
14	CLA	b	818	4	-	8/39/115/115	-
14	CLA	b	815	4	-	5/20/96/115	-
14	CLA	A	833	2	-	14/39/115/115	-
14	CLA	A	815	-	-	4/15/91/115	-
14	CLA	k	101	10	-	5/9/81/115	-
17	BCR	B	847	-	-	2/29/63/63	0/2/2/2
17	BCR	a	848	-	-	12/29/63/63	0/2/2/2
14	CLA	A	814	2	-	5/15/91/115	-
14	CLA	N	821	-	-	17/39/115/115	-
14	CLA	b	819	-	-	9/39/115/115	-
14	CLA	w	205	-	-	6/15/91/115	-
14	CLA	A	819	2	-	14/26/102/115	-
14	CLA	n	815	4	-	7/20/96/115	-
14	CLA	B	803	-	-	14/39/115/115	-
14	CLA	N	827	-	-	15/39/115/115	-
14	CLA	N	818	4	-	4/15/91/115	-
20	SQD	h	1702	-	-	28/49/69/69	0/1/1/1
14	CLA	g	812	2	-	9/26/102/115	-
14	CLA	a	803	2	-	17/39/115/115	-
14	CLA	A	834	2	-	6/26/102/115	-
14	CLA	N	819	4	-	13/39/115/115	-
14	CLA	N	825	4	-	14/39/115/115	-
14	CLA	j	101	9	-	10/15/91/115	-
17	BCR	G	843	-	-	2/29/63/63	0/2/2/2
14	CLA	G	806	2	-	10/32/108/115	-
14	CLA	N	832	4	-	7/26/102/115	-
14	CLA	B	806	4	-	15/39/115/115	-
14	CLA	G	829	2	-	7/39/115/115	-
14	CLA	T	102	9	-	0/4/76/115	-
14	CLA	G	822	2	-	8/26/102/115	-
18	LHG	X	1702	-	-	28/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	821	2	-	7/15/91/115	-
14	CLA	G	835	2	-	9/15/91/115	-
14	CLA	g	852	-	-	13/39/115/115	-
14	CLA	n	826	4	-	7/39/115/115	-
21	LMG	B	802	-	-	10/30/50/70	0/1/1/1
21	LMG	B	849	-	-	20/50/70/70	0/1/1/1
14	CLA	B	834	4	-	11/26/102/115	-
14	CLA	a	837	2	-	17/39/115/115	-
19	CL0	G	851	2	-	9/39/115/115	-
14	CLA	b	826	4	-	9/39/115/115	-
14	CLA	A	818	2	-	16/39/115/115	-
14	CLA	b	805	4	-	14/39/115/115	-
14	CLA	g	836	2	-	15/39/115/115	-
14	CLA	b	820	4	-	8/15/91/115	-
14	CLA	n	813	4	-	10/39/115/115	-
14	CLA	a	812	2	-	7/26/102/115	-
17	BCR	g	847	-	-	4/29/63/63	0/2/2/2
14	CLA	g	817	2	-	10/39/115/115	-
14	CLA	A	836	2	-	8/23/99/115	-
14	CLA	N	804	4	-	19/39/115/115	-
14	CLA	N	829	4	-	10/39/115/115	-
17	BCR	T	104	-	-	8/29/63/63	0/2/2/2
17	BCR	i	102	-	-	6/29/63/63	0/2/2/2
14	CLA	g	801	2	-	6/39/115/115	-
14	CLA	G	853	2	-	9/39/115/115	-
17	BCR	w	207	-	-	4/29/63/63	0/2/2/2
14	CLA	t	102	9	-	0/4/76/115	-
14	CLA	a	827	2	-	10/39/115/115	-
14	CLA	g	808	2	-	7/15/91/115	-
17	BCR	N	853	-	-	0/29/63/63	0/2/2/2
18	LHG	S	202	-	-	24/47/47/53	-
14	CLA	b	808	4	-	11/39/115/115	-
14	CLA	A	826	2	-	11/39/115/115	-
14	CLA	A	838	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	815	4	-	5/21/97/115	-
14	CLA	a	817	2	-	10/39/115/115	-
17	BCR	N	852	-	-	3/29/63/63	0/2/2/2
14	CLA	g	832	2	-	13/39/115/115	-
14	CLA	a	805	2	-	5/33/109/115	-
14	CLA	A	822	2	-	12/26/102/115	-
14	CLA	a	853	-	-	7/39/115/115	-
14	CLA	a	806	2	-	15/39/115/115	-
17	BCR	B	851	-	-	3/29/63/63	0/2/2/2
14	CLA	G	812	2	-	9/33/109/115	-
17	BCR	b	843	-	-	6/29/63/63	0/2/2/2
14	CLA	A	802	2	-	15/39/115/115	-
17	BCR	N	846	-	-	4/29/63/63	0/2/2/2
16	SF4	P	101	5	-	-	0/6/5/5
14	CLA	n	810	4	-	18/33/109/115	-
17	BCR	M	101	-	-	2/29/63/63	0/2/2/2
14	CLA	G	810	2	-	18/39/115/115	-
14	CLA	n	822	-	-	11/27/103/115	-
17	BCR	n	851	-	-	4/29/63/63	0/2/2/2
16	SF4	g	842	2,4	-	-	0/6/5/5
14	CLA	g	827	2	-	11/39/115/115	-
16	SF4	c	102	5	-	-	0/6/5/5
14	CLA	b	852	4	-	10/27/103/115	-
14	CLA	b	821	4	-	5/15/91/115	-
14	CLA	b	830	4	-	9/26/102/115	-
14	CLA	N	831	4	-	11/39/115/115	-
17	BCR	y	101	-	-	5/29/63/63	0/2/2/2
14	CLA	N	812	4	-	14/33/109/115	-
17	BCR	N	847	-	-	8/29/63/63	0/2/2/2
14	CLA	g	811	2	-	5/33/109/115	-
14	CLA	n	836	4	-	2/33/109/115	-
17	BCR	n	842	-	-	2/29/63/63	0/2/2/2
14	CLA	W	204	-	-	6/15/91/115	-
14	CLA	g	819	-	-	14/39/115/115	-
14	CLA	g	831	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	n	818	4	-	10/39/115/115	-
14	CLA	U	101	10	-	7/9/81/115	-
14	CLA	a	816	-	-	10/33/109/115	-
14	CLA	b	831	4	-	4/33/109/115	-
14	CLA	b	807	4	-	5/39/115/115	-
17	BCR	a	846	-	-	11/29/63/63	0/2/2/2
14	CLA	A	810	2,14	-	12/39/115/115	-
14	CLA	N	828	4	-	10/39/115/115	-
14	CLA	G	811	2	-	9/32/108/115	-
14	CLA	n	816	4	-	6/15/91/115	-
14	CLA	A	812	2	-	12/33/109/115	-
14	CLA	N	820	4	-	10/39/115/115	-
14	CLA	g	809	2	-	12/39/115/115	-
14	CLA	A	830	2	-	11/26/102/115	-
17	BCR	g	844	-	-	3/29/63/63	0/2/2/2
14	CLA	U	102	-	-	3/20/96/115	-
14	CLA	G	830	2	-	9/26/102/115	-
14	CLA	N	823	4	-	4/15/91/115	-
14	CLA	a	839	2	-	4/39/115/115	-
14	CLA	B	820	-	-	8/39/115/115	-
18	LHG	v	102	-	-	28/47/47/53	-
14	CLA	G	832	2	-	16/39/115/115	-
14	CLA	G	827	2	-	14/39/115/115	-
17	BCR	a	847	-	-	4/29/63/63	0/2/2/2
14	CLA	n	839	-	-	4/39/115/115	-
14	CLA	N	807	4	-	12/39/115/115	-
14	CLA	g	853	-	-	6/39/115/115	-
14	CLA	n	838	4	-	4/18/94/115	-
14	CLA	g	826	2	-	16/39/115/115	-
14	CLA	g	804	2	-	14/39/115/115	-
14	CLA	b	832	4	-	14/39/115/115	-
17	BCR	G	848	-	-	12/29/63/63	0/2/2/2
14	CLA	b	802	-	-	10/39/115/115	-
14	CLA	n	834	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	g	816	2	-	15/33/109/115	-
17	BCR	v	101	-	-	2/29/63/63	0/2/2/2
14	CLA	b	834	-	-	4/15/91/115	-
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
17	BCR	V	101	-	-	2/29/63/63	0/2/2/2
16	SF4	p	101	5	-	-	0/6/5/5
20	SQD	H	1702	-	-	22/49/69/69	0/1/1/1
14	CLA	a	820	2	-	7/15/91/115	-
14	CLA	N	837	-	-	10/15/91/115	-
17	BCR	n	843	-	-	6/29/63/63	0/2/2/2
15	PQN	B	842	-	-	6/23/43/43	0/2/2/2
14	CLA	B	832	4	-	14/33/109/115	-
14	CLA	a	826	2	-	15/39/115/115	-
14	CLA	a	804	2	-	19/39/115/115	-
14	CLA	b	827	4	-	13/39/115/115	-
14	CLA	W	203	12	-	9/33/109/115	-
14	CLA	g	837	2	-	18/39/115/115	-
16	SF4	c	101	5	-	-	0/6/5/5
14	CLA	A	839	2	-	18/39/115/115	-
14	CLA	G	817	2	-	11/33/109/115	-
14	CLA	B	811	4	-	14/33/109/115	-
14	CLA	n	814	4	-	4/21/97/115	-
15	PQN	A	842	-	-	6/23/43/43	0/2/2/2
14	CLA	A	832	2	-	11/39/115/115	-
14	CLA	n	819	-	-	9/39/115/115	-
17	BCR	W	201	-	-	11/29/63/63	0/2/2/2
16	SF4	C	102	5	-	-	0/6/5/5
14	CLA	a	840	18	-	9/15/91/115	-
14	CLA	G	818	2	-	8/39/115/115	-
14	CLA	S	203	-	-	5/15/91/115	-
18	LHG	g	850	-	-	22/53/53/53	-
14	CLA	f	201	-	-	10/32/108/115	-
17	BCR	m	102	-	-	4/29/63/63	0/2/2/2
21	LMG	b	848	-	-	20/50/70/70	0/1/1/1
14	CLA	B	807	4	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	W	205	-	-	4/29/63/63	0/2/2/2
14	CLA	n	823	4	-	15/39/115/115	-
14	CLA	N	830	4	-	9/39/115/115	-
17	BCR	t	103	-	-	2/29/63/63	0/2/2/2
14	CLA	N	813	4	-	6/26/102/115	-
14	CLA	N	815	4	-	12/39/115/115	-
17	BCR	B	852	-	-	0/29/63/63	0/2/2/2
14	CLA	B	835	-	-	9/15/91/115	-
14	CLA	g	821	2	-	13/26/102/115	-
14	CLA	G	816	2	-	11/32/108/115	-
18	LHG	g	849	-	-	30/53/53/53	-
14	CLA	A	801	-	-	7/39/115/115	-
14	CLA	N	817	4	-	6/20/96/115	-
14	CLA	l	204	-	-	9/15/91/115	-
14	CLA	t	101	9	-	6/15/91/115	-
14	CLA	A	828	2	-	8/39/115/115	-
14	CLA	N	841	-	-	6/39/115/115	-
14	CLA	G	804	2	-	20/39/115/115	-
18	LHG	m	101	-	-	25/47/47/53	-
14	CLA	N	805	-	-	16/39/115/115	-
17	BCR	T	103	-	-	2/29/63/63	0/2/2/2
14	CLA	N	801	-	-	15/39/115/115	-
14	CLA	A	805	2	-	20/39/115/115	-
15	PQN	g	841	-	-	2/23/43/43	0/2/2/2
14	CLA	N	806	4	-	9/27/103/115	-
14	CLA	G	838	2	-	13/39/115/115	-
14	CLA	A	811	2	-	18/32/108/115	-
14	CLA	N	822	4	-	8/15/91/115	-
14	CLA	G	820	-	-	14/39/115/115	-
14	CLA	n	837	4	-	16/39/115/115	-
14	CLA	g	824	-	-	3/26/102/115	-
14	CLA	A	831	2	-	17/39/115/115	-
14	CLA	g	806	2	-	16/39/115/115	-
14	CLA	a	852	-	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	823	4	-	14/39/115/115	-
14	CLA	a	830	2	-	15/39/115/115	-
18	LHG	G	849	-	-	28/53/53/53	-
14	CLA	n	840	4	-	15/39/115/115	-
17	BCR	a	845	-	-	0/29/63/63	0/2/2/2
14	CLA	b	822	-	-	12/27/103/115	-
14	CLA	n	807	4	-	7/39/115/115	-
14	CLA	N	808	4	-	13/39/115/115	-
14	CLA	n	852	4	-	7/27/103/115	-
21	LMG	n	848	-	-	13/50/70/70	0/1/1/1
14	CLA	n	830	4	-	9/26/102/115	-
17	BCR	G	845	-	-	1/29/63/63	0/2/2/2
16	SF4	C	101	5	-	-	0/6/5/5
21	LMG	N	850	-	-	16/50/70/70	0/1/1/1
14	CLA	g	829	2	-	5/26/102/115	-
14	CLA	B	850	4	-	17/39/115/115	-
14	CLA	n	820	4	-	10/15/91/115	-
15	PQN	a	841	-	-	3/23/43/43	0/2/2/2
14	CLA	b	809	4	-	13/39/115/115	-
14	CLA	A	809	2	-	6/15/91/115	-
14	CLA	J	102	9	-	0/4/76/115	-
14	CLA	H	1701	3	-	11/20/96/115	-
17	BCR	b	846	-	-	4/29/63/63	0/2/2/2
17	BCR	A	846	-	-	2/29/63/63	0/2/2/2
14	CLA	G	839	2	-	13/39/115/115	-
14	CLA	N	810	4	-	14/39/115/115	-
14	CLA	a	818	2	-	9/26/102/115	-
14	CLA	B	839	4	-	7/18/94/115	-
14	CLA	X	1701	3	-	11/20/96/115	-
14	CLA	n	850	4	-	15/31/107/115	-
14	CLA	B	836	-	-	9/15/91/115	-
20	SQD	w	202	-	-	27/49/69/69	0/1/1/1
14	CLA	N	816	4	-	3/21/97/115	-
14	CLA	a	822	2	-	8/15/91/115	-
14	CLA	B	816	4	-	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	F	203	-	-	2/29/63/63	0/2/2/2
14	CLA	a	832	2	-	11/39/115/115	-
14	CLA	b	837	4	-	6/39/115/115	-
14	CLA	A	823	2	-	5/15/91/115	-
14	CLA	b	804	-	-	11/39/115/115	-
14	CLA	j	102	9	-	2/4/76/115	-
17	BCR	f	203	-	-	2/29/63/63	0/2/2/2
14	CLA	g	833	2	-	5/26/102/115	-
15	PQN	N	843	-	-	1/23/43/43	0/2/2/2
14	CLA	n	832	4	-	15/39/115/115	-
17	BCR	l	206	-	-	4/29/63/63	0/2/2/2
17	BCR	t	104	-	-	7/29/63/63	0/2/2/2
14	CLA	A	807	2	-	18/39/115/115	-
14	CLA	G	819	2	-	7/26/102/115	-
14	CLA	G	831	2	-	11/39/115/115	-
14	CLA	A	816	2	-	10/32/108/115	-
14	CLA	b	824	4	-	9/39/115/115	-
14	CLA	a	808	2	-	7/15/91/115	-
14	CLA	G	807	2	-	15/39/115/115	-
14	CLA	A	853	-	-	14/39/115/115	-
14	CLA	N	839	4	-	7/39/115/115	-
14	CLA	B	813	4	-	11/26/102/115	-
14	CLA	B	838	4	-	5/39/115/115	-
14	CLA	n	806	4	-	16/39/115/115	-
14	CLA	L	1503	-	-	3/15/91/115	-
14	CLA	G	826	2	-	12/39/115/115	-
14	CLA	a	825	2	-	7/39/115/115	-
17	BCR	l	205	-	-	4/29/63/63	0/2/2/2
19	CL0	g	851	2	-	5/39/115/115	-
14	CLA	B	805	4	-	12/27/103/115	-
14	CLA	A	837	2	-	11/39/115/115	-
17	BCR	B	848	-	-	2/29/63/63	0/2/2/2
14	CLA	n	828	4	-	14/39/115/115	-
14	CLA	g	813	2	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	847	-	-	0/29/63/63	0/2/2/2
14	CLA	b	813	4	-	13/39/115/115	-
15	PQN	n	841	-	-	2/23/43/43	0/2/2/2
14	CLA	b	817	4	-	13/39/115/115	-
17	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
15	PQN	b	841	-	-	1/23/43/43	0/2/2/2
14	CLA	G	840	18	-	10/15/91/115	-
14	CLA	n	805	4	-	11/39/115/115	-
14	CLA	A	824	-	-	8/39/115/115	-
17	BCR	j	104	-	-	11/29/63/63	0/2/2/2
17	BCR	g	845	-	-	2/29/63/63	0/2/2/2
14	CLA	N	835	4	-	7/26/102/115	-
14	CLA	u	102	-	-	7/20/96/115	-
14	CLA	B	804	4	-	7/15/91/115	-
14	CLA	b	829	4	-	11/39/115/115	-
18	LHG	A	850	-	-	25/53/53/53	-
14	CLA	g	854	-	-	22/39/115/115	-
14	CLA	B	830	4	-	9/39/115/115	-
14	CLA	n	829	4	-	10/39/115/115	-
16	SF4	a	842	2,4	-	-	0/6/5/5
14	CLA	b	806	4	-	9/39/115/115	-
14	CLA	w	204	12	-	11/33/109/115	-
14	CLA	G	809	2	-	4/15/91/115	-
14	CLA	N	811	4	-	14/39/115/115	-
14	CLA	N	834	4	-	11/31/107/115	-
14	CLA	G	821	2	-	7/15/91/115	-
14	CLA	a	813	2	-	8/15/91/115	-
14	CLA	g	803	2	-	20/39/115/115	-
14	CLA	a	815	2	-	10/32/108/115	-
20	SQD	l	201	-	-	19/49/69/69	0/1/1/1
14	CLA	N	840	4	-	6/18/94/115	-
17	BCR	A	847	-	-	2/29/63/63	0/2/2/2
14	CLA	g	825	2	-	13/39/115/115	-
14	CLA	A	813	2	-	7/26/102/115	-
14	CLA	B	819	4	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	831	4	-	9/26/102/115	-
14	CLA	A	817	2	-	13/33/109/115	-
14	CLA	n	802	-	-	15/39/115/115	-
14	CLA	a	854	-	-	5/20/96/115	-
14	CLA	n	817	4	-	11/39/115/115	-
14	CLA	g	828	2	-	9/39/115/115	-
14	CLA	A	841	18	-	9/15/91/115	-
14	CLA	G	833	2	-	13/39/115/115	-
14	CLA	a	801	2	-	9/39/115/115	-
17	BCR	B	845	-	-	4/29/63/63	0/2/2/2
17	BCR	g	848	-	-	12/29/63/63	0/2/2/2
14	CLA	N	809	4	-	7/39/115/115	-
14	CLA	a	835	2	-	7/23/99/115	-
17	BCR	n	847	-	-	2/29/63/63	0/2/2/2
14	CLA	A	854	2	-	16/39/115/115	-
18	LHG	a	850	14	-	32/53/53/53	-
14	CLA	A	806	2	-	8/33/109/115	-
14	CLA	x	1701	3	-	11/20/96/115	-
17	BCR	B	844	-	-	11/29/63/63	0/2/2/2
14	CLA	N	814	4	-	9/26/102/115	-
14	CLA	B	824	4	-	16/39/115/115	-
14	CLA	S	201	-	-	11/32/108/115	-
17	BCR	a	844	-	-	3/29/63/63	0/2/2/2
17	BCR	b	845	-	-	11/29/63/63	0/2/2/2
14	CLA	a	824	-	-	8/26/102/115	-
14	CLA	K	101	10	-	7/9/81/115	-
17	BCR	I	102	-	-	14/29/63/63	0/2/2/2
14	CLA	n	808	4	-	12/39/115/115	-
14	CLA	a	811	2	-	15/33/109/115	-
14	CLA	N	851	4	-	17/39/115/115	-
14	CLA	n	827	4	-	17/39/115/115	-
14	CLA	G	852	-	-	7/15/91/115	-
17	BCR	n	844	-	-	6/29/63/63	0/2/2/2
14	CLA	n	824	4	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	825	-	-	4/26/102/115	-
14	CLA	a	855	19	-	17/39/115/115	-
14	CLA	N	833	4	-	15/33/109/115	-
17	BCR	b	849	-	-	6/29/63/63	0/2/2/2
14	CLA	A	857	-	-	4/20/96/115	-
14	CLA	A	820	-	-	15/39/115/115	-
17	BCR	W	206	-	-	6/29/63/63	0/2/2/2
14	CLA	s	202	-	-	5/15/91/115	-
17	BCR	w	206	-	-	5/29/63/63	0/2/2/2
14	CLA	B	818	4	-	23/39/115/115	-
17	BCR	k	102	-	-	0/29/63/63	0/2/2/2
14	CLA	G	828	2	-	12/39/115/115	-
14	CLA	B	828	4	-	10/39/115/115	-
14	CLA	b	828	4	-	14/39/115/115	-
17	BCR	N	849	-	-	0/29/63/63	0/2/2/2
14	CLA	s	201	-	-	16/32/108/115	-
14	CLA	G	836	2	-	3/23/99/115	-
14	CLA	a	809	2,14	-	15/39/115/115	-
14	CLA	w	203	12	-	8/15/91/115	-
14	CLA	n	831	4	-	7/33/109/115	-
14	CLA	B	841	4	-	17/39/115/115	-
14	CLA	G	805	2	-	16/39/115/115	-
17	BCR	A	845	-	-	2/29/63/63	0/2/2/2
19	CL0	A	852	-	-	2/15/91/115	-
17	BCR	w	201	-	-	5/29/63/63	0/2/2/2
14	CLA	g	810	2	-	11/32/108/115	-
14	CLA	F	201	-	-	8/32/108/115	-
14	CLA	B	825	4	-	9/39/115/115	-
17	BCR	A	849	-	-	12/29/63/63	0/2/2/2
17	BCR	u	103	-	-	0/29/63/63	0/2/2/2
14	CLA	B	833	4	-	12/31/107/115	-
14	CLA	B	814	4	-	14/39/115/115	-
17	BCR	i	101	-	-	3/29/63/63	0/2/2/2
14	CLA	n	835	-	-	8/15/91/115	-
14	CLA	a	836	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	840	-	-	11/39/115/115	-
14	CLA	G	808	2	-	17/39/115/115	-
14	CLA	n	803	4	-	15/39/115/115	-
17	BCR	J	103	-	-	2/29/63/63	0/2/2/2
14	CLA	A	827	2	-	8/39/115/115	-
14	CLA	B	826	-	-	14/39/115/115	-
14	CLA	n	811	4	-	11/26/102/115	-
14	CLA	A	855	-	-	9/15/91/115	-
14	CLA	n	804	-	-	12/39/115/115	-
14	CLA	b	816	4	-	4/15/91/115	-
17	BCR	I	103	-	-	8/29/63/63	0/2/2/2
14	CLA	N	826	4	-	13/39/115/115	-
14	CLA	B	823	-	-	12/27/103/115	-
17	BCR	G	846	-	-	4/29/63/63	0/2/2/2
14	CLA	b	825	-	-	16/39/115/115	-
14	CLA	b	811	4	-	11/26/102/115	-
14	CLA	n	812	4	-	5/26/102/115	-
14	CLA	B	809	4	-	8/39/115/115	-
14	CLA	a	810	2	-	11/32/108/115	-
14	CLA	B	821	4	-	10/15/91/115	-
14	CLA	a	821	2	-	14/26/102/115	-
17	BCR	s	203	-	-	2/29/63/63	0/2/2/2
14	CLA	A	835	2	-	9/15/91/115	-
14	CLA	b	840	4	-	18/39/115/115	-
14	CLA	G	802	2	-	8/39/115/115	-
14	CLA	g	835	2	-	7/23/99/115	-
17	BCR	G	844	-	-	3/29/63/63	0/2/2/2
18	LHG	A	851	14	-	25/53/53/53	-
14	CLA	n	809	4	-	15/39/115/115	-
16	SF4	G	842	2,4	-	-	0/6/5/5
17	BCR	g	846	-	-	9/29/63/63	0/2/2/2
17	BCR	n	846	-	-	3/29/63/63	0/2/2/2
14	CLA	A	808	2	-	11/39/115/115	-
14	CLA	g	838	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	803	4	-	18/39/115/115	-
14	CLA	A	803	2,14	-	6/26/102/115	-
17	BCR	n	845	-	-	3/29/63/63	0/2/2/2
17	BCR	N	848	-	-	2/29/63/63	0/2/2/2
17	BCR	U	103	-	-	0/29/63/63	0/2/2/2
14	CLA	A	804	2	-	16/39/115/115	-
17	BCR	K	102	-	-	2/29/63/63	0/2/2/2
14	CLA	a	834	2	-	9/15/91/115	-
14	CLA	a	828	2	-	9/39/115/115	-
14	CLA	A	825	-	-	8/26/102/115	-
14	CLA	g	814	-	-	4/15/91/115	-
20	SQD	n	801	-	-	21/49/69/69	0/1/1/1
14	CLA	g	839	2	-	7/39/115/115	-
14	CLA	a	838	2	-	7/39/115/115	-
17	BCR	A	856	-	-	7/29/63/63	0/2/2/2
14	CLA	N	838	4	-	14/33/109/115	-
14	CLA	W	202	12	-	7/23/99/115	-
14	CLA	g	834	2	-	7/15/91/115	-
20	SQD	b	801	-	-	18/49/69/69	0/1/1/1
14	CLA	B	829	4	-	10/39/115/115	-
15	PQN	G	841	-	-	5/23/43/43	0/2/2/2
14	CLA	g	802	2	-	8/26/102/115	-
14	CLA	B	827	4	-	10/39/115/115	-
14	CLA	a	829	2	-	5/26/102/115	-
14	CLA	l	203	12	-	11/33/109/115	-
17	BCR	G	847	-	-	2/29/63/63	0/2/2/2
18	LHG	G	850	14	-	29/53/53/53	-
17	BCR	b	844	-	-	6/29/63/63	0/2/2/2
14	CLA	b	812	4	-	8/26/102/115	-
14	CLA	G	824	-	-	13/39/115/115	-
14	CLA	l	202	12	-	6/15/91/115	-
14	CLA	f	202	-	-	5/15/91/115	-
19	CL0	a	851	2,14	-	10/39/115/115	-
14	CLA	a	814	-	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	851	-	-	1/29/63/63	0/2/2/2
14	CLA	B	817	4	-	9/15/91/115	-
14	CLA	a	819	-	-	14/39/115/115	-
14	CLA	g	818	2	-	9/26/102/115	-
14	CLA	G	813	2	-	7/26/102/115	-
16	SF4	p	102	5	-	-	0/6/5/5
14	CLA	G	803	2	-	5/26/102/115	-
17	BCR	n	849	-	-	3/29/63/63	0/2/2/2
17	BCR	A	844	-	-	2/29/63/63	0/2/2/2
14	CLA	g	815	2	-	9/32/108/115	-
14	CLA	a	802	2,14	-	8/26/102/115	-
14	CLA	a	833	2	-	4/26/102/115	-
14	CLA	g	805	2	-	5/33/109/115	-
14	CLA	G	834	2	-	1/26/102/115	-
17	BCR	a	843	-	-	2/29/63/63	0/2/2/2
17	BCR	N	844	-	-	2/29/63/63	0/2/2/2
14	CLA	N	824	-	-	4/27/103/115	-
14	CLA	G	823	2	-	10/15/91/115	-
14	CLA	G	837	2	-	19/39/115/115	-
14	CLA	n	833	4	-	13/26/102/115	-
14	CLA	L	1501	12	-	8/23/99/115	-
14	CLA	B	808	4	-	12/39/115/115	-
14	CLA	b	835	-	-	8/15/91/115	-
14	CLA	B	822	4	-	5/15/91/115	-
14	CLA	F	202	-	-	5/15/91/115	-
17	BCR	I	101	-	-	4/29/63/63	0/2/2/2

The worst 5 of 3362 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	841	PQN	C3-C2	7.56	1.49	1.35
15	g	841	PQN	C3-C2	7.51	1.48	1.35
15	A	842	PQN	C3-C2	7.50	1.48	1.35
15	N	843	PQN	C3-C2	7.48	1.48	1.35
15	b	841	PQN	C3-C2	7.47	1.48	1.35

The worst 5 of 3967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	102	BCR	C16-C17-C18	-10.26	112.67	127.31
17	a	846	BCR	C24-C23-C22	-9.63	111.68	126.23
17	I	102	BCR	C24-C23-C22	-9.44	111.97	126.23
17	a	846	BCR	C16-C17-C18	-9.07	114.36	127.31
17	W	201	BCR	C20-C21-C22	-8.72	114.86	127.31

There are no chirality outliers.

5 of 4851 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	803	CLA	C1A-C2A-CAA-CBA
14	G	803	CLA	C3A-C2A-CAA-CBA
14	G	803	CLA	O1A-CGA-O2A-C1
14	G	804	CLA	C1A-C2A-CAA-CBA
14	G	805	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

486 monomers are involved in 1938 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	g	820	CLA	4	0
14	b	839	CLA	2	0
17	L	1504	BCR	5	0
14	n	821	CLA	1	0
14	G	814	CLA	6	0
14	g	822	CLA	4	0
14	B	812	CLA	4	0
17	A	848	BCR	3	0
14	a	831	CLA	10	0
14	h	1701	CLA	4	0
14	B	837	CLA	7	0
14	a	807	CLA	8	0
16	P	102	SF4	1	0
17	j	103	BCR	5	0
14	b	833	CLA	1	0
14	g	840	CLA	3	0
17	g	843	BCR	8	0
14	b	814	CLA	4	0
14	g	823	CLA	3	0
14	B	810	CLA	5	0
14	b	810	CLA	4	0
14	n	825	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	x	1702	SQD	4	0
14	N	803	CLA	14	0
14	A	840	CLA	3	0
18	a	849	LHG	5	0
14	A	829	CLA	4	0
14	T	101	CLA	1	0
14	N	836	CLA	2	0
14	g	807	CLA	12	0
17	B	846	BCR	6	0
14	G	801	CLA	7	0
17	S	204	BCR	4	0
14	g	830	CLA	8	0
14	N	842	CLA	8	0
14	b	838	CLA	3	0
14	L	1502	CLA	6	0
17	N	845	BCR	5	0
21	N	802	LMG	2	0
20	B	801	SQD	4	0
14	b	836	CLA	8	0
17	b	842	BCR	5	0
14	a	823	CLA	4	0
14	J	101	CLA	1	0
14	b	818	CLA	3	0
14	b	815	CLA	1	0
14	A	833	CLA	3	0
17	B	847	BCR	7	0
17	a	848	BCR	11	0
14	A	814	CLA	1	0
14	N	821	CLA	3	0
14	b	819	CLA	6	0
14	A	819	CLA	3	0
14	n	815	CLA	3	0
14	B	803	CLA	7	0
14	N	827	CLA	8	0
14	N	818	CLA	3	0
20	h	1702	SQD	7	0
14	g	812	CLA	4	0
14	a	803	CLA	5	0
14	A	834	CLA	3	0
14	N	819	CLA	7	0
14	N	825	CLA	2	0
14	j	101	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	843	BCR	12	0
14	G	806	CLA	6	0
14	N	832	CLA	5	0
14	B	806	CLA	3	0
14	G	829	CLA	6	0
14	T	102	CLA	1	0
14	G	822	CLA	1	0
18	X	1702	LHG	2	0
14	A	821	CLA	8	0
14	G	835	CLA	2	0
14	g	852	CLA	6	0
14	n	826	CLA	7	0
21	B	802	LMG	1	0
21	B	849	LMG	5	0
14	B	834	CLA	1	0
14	a	837	CLA	10	0
19	G	851	CL0	7	0
14	b	826	CLA	7	0
14	A	818	CLA	4	0
14	b	805	CLA	4	0
14	g	836	CLA	3	0
14	b	820	CLA	2	0
14	n	813	CLA	5	0
14	a	812	CLA	2	0
17	g	847	BCR	3	0
14	g	817	CLA	6	0
14	A	836	CLA	3	0
14	N	804	CLA	10	0
14	N	829	CLA	5	0
17	T	104	BCR	9	0
17	i	102	BCR	6	0
14	g	801	CLA	2	0
14	G	853	CLA	4	0
17	w	207	BCR	5	0
14	t	102	CLA	1	0
14	a	827	CLA	3	0
14	g	808	CLA	2	0
17	N	853	BCR	7	0
18	S	202	LHG	4	0
14	b	808	CLA	8	0
14	A	826	CLA	11	0
14	A	838	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	815	CLA	3	0
14	a	817	CLA	5	0
17	N	852	BCR	28	0
14	g	832	CLA	9	0
14	a	805	CLA	5	0
14	a	853	CLA	4	0
14	a	806	CLA	5	0
17	B	851	BCR	11	0
14	G	812	CLA	9	0
17	b	843	BCR	3	0
14	A	802	CLA	12	0
17	N	846	BCR	5	0
14	n	810	CLA	4	0
17	M	101	BCR	4	0
14	G	810	CLA	4	0
14	n	822	CLA	3	0
17	n	851	BCR	6	0
14	g	827	CLA	8	0
16	c	102	SF4	1	0
14	b	852	CLA	3	0
14	b	821	CLA	2	0
14	b	830	CLA	5	0
14	N	831	CLA	8	0
17	y	101	BCR	2	0
14	N	812	CLA	2	0
17	N	847	BCR	2	0
14	g	811	CLA	5	0
14	n	836	CLA	2	0
17	n	842	BCR	3	0
14	W	204	CLA	4	0
14	g	819	CLA	9	0
14	g	831	CLA	6	0
14	n	818	CLA	4	0
14	a	816	CLA	5	0
14	b	831	CLA	4	0
14	b	807	CLA	5	0
17	a	846	BCR	7	0
14	A	810	CLA	4	0
14	N	828	CLA	8	0
14	G	811	CLA	1	0
14	n	816	CLA	5	0
14	A	812	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	820	CLA	7	0
14	g	809	CLA	1	0
14	A	830	CLA	7	0
17	g	844	BCR	4	0
14	U	102	CLA	1	0
14	G	830	CLA	1	0
14	N	823	CLA	3	0
14	a	839	CLA	7	0
14	B	820	CLA	5	0
18	v	102	LHG	3	0
14	G	832	CLA	5	0
14	G	827	CLA	12	0
17	a	847	BCR	3	0
14	n	839	CLA	6	0
14	N	807	CLA	5	0
14	g	853	CLA	5	0
14	n	838	CLA	1	0
14	g	826	CLA	7	0
14	g	804	CLA	7	0
14	b	832	CLA	6	0
17	G	848	BCR	6	0
14	b	802	CLA	6	0
14	n	834	CLA	1	0
14	g	816	CLA	8	0
17	v	101	BCR	7	0
14	b	834	CLA	1	0
17	B	843	BCR	5	0
17	V	101	BCR	2	0
20	H	1702	SQD	3	0
14	a	820	CLA	2	0
17	n	843	BCR	2	0
15	B	842	PQN	5	0
14	B	832	CLA	3	0
14	a	826	CLA	13	0
14	a	804	CLA	5	0
14	b	827	CLA	9	0
14	W	203	CLA	12	0
14	g	837	CLA	13	0
14	A	839	CLA	4	0
14	G	817	CLA	6	0
14	B	811	CLA	3	0
14	n	814	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	842	PQN	5	0
14	A	832	CLA	4	0
14	n	819	CLA	5	0
17	W	201	BCR	6	0
16	C	102	SF4	1	0
14	a	840	CLA	2	0
14	G	818	CLA	5	0
14	S	203	CLA	3	0
18	g	850	LHG	7	0
14	f	201	CLA	3	0
17	m	102	BCR	3	0
21	b	848	LMG	3	0
14	B	807	CLA	5	0
17	W	205	BCR	6	0
14	n	823	CLA	4	0
14	N	830	CLA	3	0
17	t	103	BCR	7	0
14	N	813	CLA	4	0
14	N	815	CLA	7	0
17	B	852	BCR	8	0
14	B	835	CLA	1	0
14	g	821	CLA	2	0
14	G	816	CLA	4	0
18	g	849	LHG	1	0
14	A	801	CLA	6	0
14	N	817	CLA	5	0
14	l	204	CLA	1	0
14	t	101	CLA	1	0
14	A	828	CLA	4	0
14	N	841	CLA	4	0
14	G	804	CLA	12	0
18	m	101	LHG	6	0
14	N	805	CLA	6	0
17	T	103	BCR	3	0
14	N	801	CLA	4	0
14	A	805	CLA	5	0
15	g	841	PQN	4	0
14	N	806	CLA	4	0
14	G	838	CLA	9	0
14	A	811	CLA	6	0
14	N	822	CLA	2	0
14	G	820	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	n	837	CLA	7	0
14	g	824	CLA	3	0
14	A	831	CLA	7	0
14	g	806	CLA	4	0
14	a	852	CLA	18	0
14	b	823	CLA	4	0
14	a	830	CLA	4	0
18	G	849	LHG	6	0
14	n	840	CLA	16	0
17	a	845	BCR	3	0
14	b	822	CLA	2	0
14	n	807	CLA	4	0
14	N	808	CLA	2	0
14	n	852	CLA	2	0
21	n	848	LMG	3	0
14	n	830	CLA	3	0
17	G	845	BCR	5	0
21	N	850	LMG	6	0
14	g	829	CLA	3	0
14	B	850	CLA	5	0
14	n	820	CLA	2	0
15	a	841	PQN	4	0
14	b	809	CLA	3	0
14	A	809	CLA	2	0
14	J	102	CLA	2	0
14	H	1701	CLA	3	0
17	b	846	BCR	7	0
17	A	846	BCR	5	0
14	G	839	CLA	6	0
14	N	810	CLA	5	0
14	a	818	CLA	3	0
14	B	839	CLA	4	0
14	X	1701	CLA	3	0
14	n	850	CLA	5	0
20	w	202	SQD	3	0
14	N	816	CLA	3	0
14	a	822	CLA	2	0
14	B	816	CLA	2	0
17	F	203	BCR	1	0
14	a	832	CLA	7	0
14	b	837	CLA	3	0
14	A	823	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	804	CLA	12	0
14	j	102	CLA	3	0
17	f	203	BCR	4	0
14	g	833	CLA	5	0
15	N	843	PQN	6	0
14	n	832	CLA	5	0
17	l	206	BCR	4	0
17	t	104	BCR	7	0
14	A	807	CLA	5	0
14	G	819	CLA	1	0
14	G	831	CLA	7	0
14	A	816	CLA	3	0
14	b	824	CLA	13	0
14	a	808	CLA	3	0
14	G	807	CLA	5	0
14	A	853	CLA	12	0
14	N	839	CLA	5	0
14	B	813	CLA	3	0
14	B	838	CLA	9	0
14	n	806	CLA	7	0
14	G	826	CLA	2	0
14	a	825	CLA	5	0
17	l	205	BCR	5	0
19	g	851	CL0	7	0
14	B	805	CLA	6	0
14	A	837	CLA	4	0
17	B	848	BCR	7	0
14	n	828	CLA	6	0
14	g	813	CLA	1	0
17	b	847	BCR	6	0
14	b	813	CLA	4	0
15	n	841	PQN	4	0
14	b	817	CLA	6	0
17	Y	101	BCR	4	0
15	b	841	PQN	4	0
14	G	840	CLA	2	0
14	n	805	CLA	5	0
14	A	824	CLA	7	0
17	j	104	BCR	3	0
17	g	845	BCR	8	0
14	N	835	CLA	2	0
14	B	804	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	829	CLA	8	0
18	A	850	LHG	2	0
14	g	854	CLA	8	0
14	B	830	CLA	7	0
14	n	829	CLA	6	0
14	b	806	CLA	6	0
14	w	204	CLA	11	0
14	G	809	CLA	2	0
14	N	811	CLA	6	0
14	N	834	CLA	7	0
14	G	821	CLA	4	0
14	a	813	CLA	2	0
14	g	803	CLA	5	0
14	a	815	CLA	3	0
20	l	201	SQD	4	0
14	N	840	CLA	8	0
17	A	847	BCR	5	0
14	g	825	CLA	8	0
14	A	813	CLA	2	0
14	B	819	CLA	4	0
14	B	831	CLA	3	0
14	A	817	CLA	3	0
14	n	802	CLA	7	0
14	a	854	CLA	1	0
14	n	817	CLA	7	0
14	g	828	CLA	7	0
14	A	841	CLA	1	0
14	G	833	CLA	6	0
14	a	801	CLA	11	0
17	B	845	BCR	6	0
17	g	848	BCR	5	0
14	N	809	CLA	2	0
14	a	835	CLA	2	0
17	n	847	BCR	5	0
14	A	854	CLA	7	0
18	a	850	LHG	9	0
14	A	806	CLA	5	0
14	x	1701	CLA	2	0
17	B	844	BCR	4	0
14	N	814	CLA	5	0
14	B	824	CLA	4	0
17	a	844	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b	845	BCR	5	0
14	a	824	CLA	2	0
14	K	101	CLA	2	0
17	I	102	BCR	3	0
14	n	808	CLA	10	0
14	a	811	CLA	7	0
14	N	851	CLA	6	0
14	n	827	CLA	8	0
14	G	852	CLA	27	0
17	n	844	BCR	6	0
14	n	824	CLA	8	0
14	G	825	CLA	3	0
14	a	855	CLA	12	0
14	N	833	CLA	4	0
17	b	849	BCR	13	0
14	A	820	CLA	7	0
17	W	206	BCR	6	0
14	s	202	CLA	1	0
17	w	206	BCR	5	0
14	B	818	CLA	4	0
17	k	102	BCR	2	0
14	G	828	CLA	7	0
14	B	828	CLA	8	0
14	b	828	CLA	4	0
17	N	849	BCR	3	0
14	s	201	CLA	2	0
14	G	836	CLA	1	0
14	a	809	CLA	4	0
14	n	831	CLA	2	0
14	B	841	CLA	5	0
14	G	805	CLA	8	0
17	A	845	BCR	7	0
19	A	852	CL0	2	0
17	w	201	BCR	9	0
14	g	810	CLA	3	0
14	F	201	CLA	1	0
14	B	825	CLA	10	0
17	A	849	BCR	10	0
17	u	103	BCR	2	0
14	B	833	CLA	5	0
14	B	814	CLA	9	0
17	i	101	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	836	CLA	3	0
14	B	840	CLA	5	0
14	G	808	CLA	7	0
14	n	803	CLA	10	0
17	J	103	BCR	6	0
14	A	827	CLA	10	0
14	B	826	CLA	5	0
14	n	811	CLA	1	0
14	A	855	CLA	21	0
14	n	804	CLA	13	0
14	b	816	CLA	4	0
17	I	103	BCR	12	0
14	N	826	CLA	7	0
14	B	823	CLA	3	0
17	G	846	BCR	4	0
14	b	825	CLA	5	0
14	b	811	CLA	8	0
14	n	812	CLA	2	0
14	B	809	CLA	6	0
14	a	810	CLA	2	0
14	B	821	CLA	1	0
14	a	821	CLA	5	0
17	s	203	BCR	4	0
14	A	835	CLA	1	0
14	b	840	CLA	11	0
14	G	802	CLA	10	0
17	G	844	BCR	3	0
18	A	851	LHG	5	0
14	n	809	CLA	4	0
17	g	846	BCR	8	0
17	n	846	BCR	9	0
14	A	808	CLA	9	0
14	g	838	CLA	4	0
14	b	803	CLA	6	0
14	A	803	CLA	4	0
17	n	845	BCR	9	0
17	N	848	BCR	6	0
17	U	103	BCR	2	0
14	A	804	CLA	9	0
17	K	102	BCR	3	0
14	a	828	CLA	8	0
14	A	825	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	g	839	CLA	8	0
14	a	838	CLA	4	0
17	A	856	BCR	10	0
14	N	838	CLA	3	0
14	W	202	CLA	3	0
14	g	834	CLA	4	0
20	b	801	SQD	6	0
14	B	829	CLA	4	0
15	G	841	PQN	10	0
14	B	827	CLA	10	0
14	a	829	CLA	3	0
14	l	203	CLA	9	0
17	G	847	BCR	6	0
18	G	850	LHG	4	0
17	b	844	BCR	3	0
14	b	812	CLA	3	0
14	G	824	CLA	4	0
14	l	202	CLA	3	0
14	f	202	CLA	5	0
19	a	851	CL0	4	0
17	b	851	BCR	9	0
14	B	817	CLA	2	0
14	a	819	CLA	11	0
14	g	818	CLA	1	0
14	G	813	CLA	4	0
16	p	102	SF4	1	0
14	G	803	CLA	5	0
17	n	849	BCR	13	0
17	A	844	BCR	6	0
14	g	815	CLA	5	0
14	a	802	CLA	4	0
14	a	833	CLA	3	0
14	g	805	CLA	4	0
14	G	834	CLA	2	0
17	a	843	BCR	6	0
17	N	844	BCR	7	0
14	N	824	CLA	2	0
14	G	823	CLA	5	0
14	G	837	CLA	5	0
14	n	833	CLA	1	0
14	L	1501	CLA	2	0
14	B	808	CLA	5	0

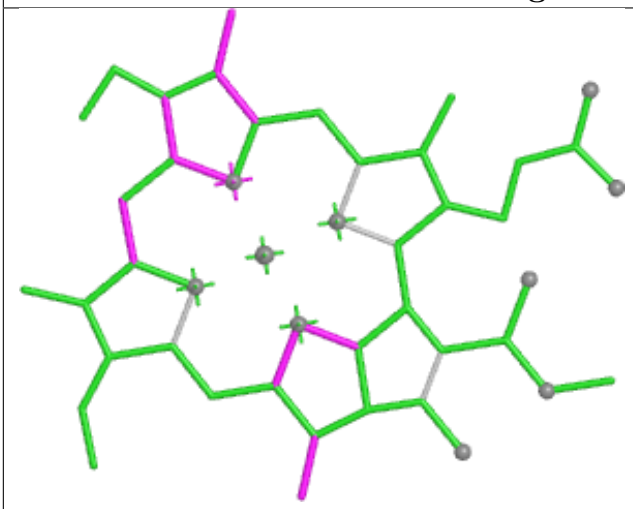
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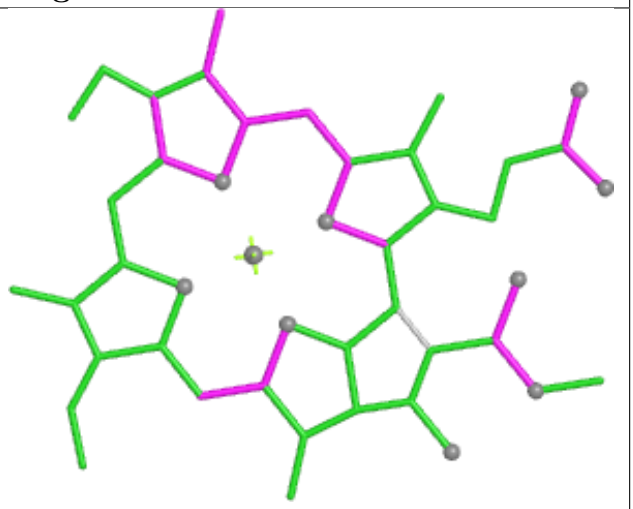
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	822	CLA	1	0
17	I	101	BCR	6	0

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.

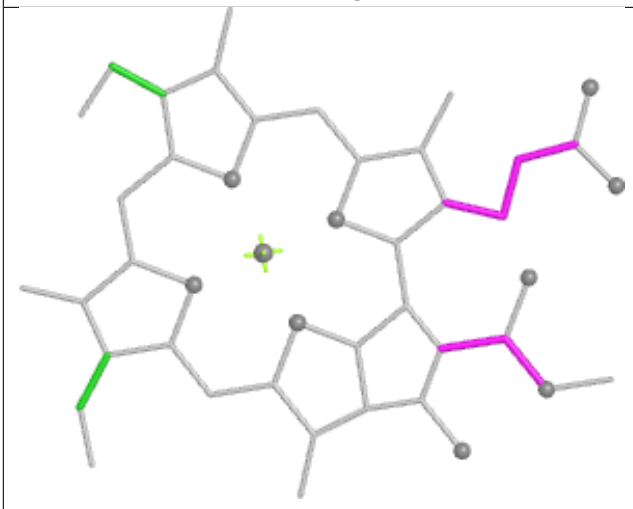
Ligand CLA g 820



Bond lengths



Bond angles

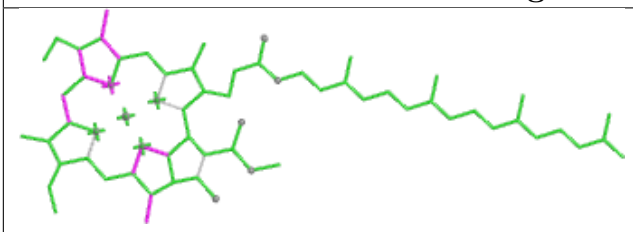


Torsions

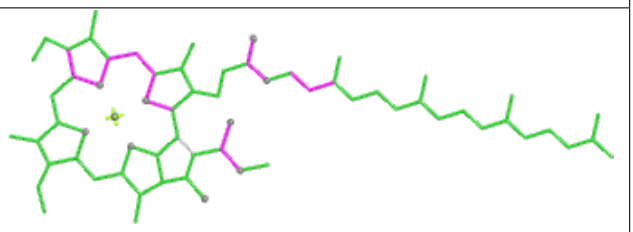


Rings

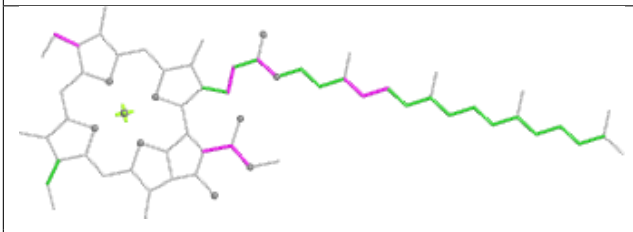
Ligand CLA b 839



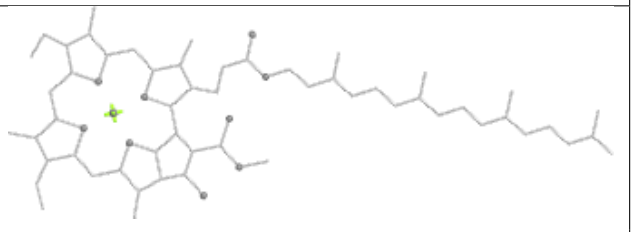
Bond lengths



Bond angles

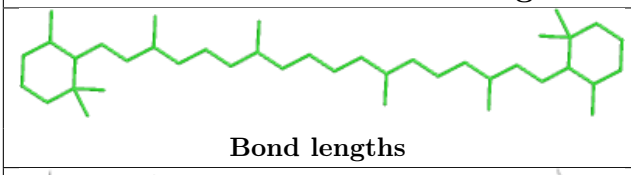


Torsions

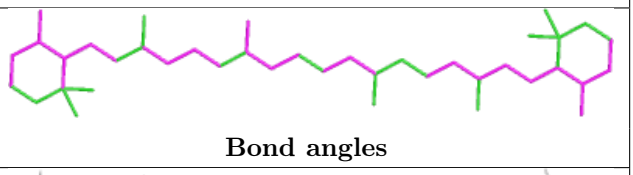


Rings

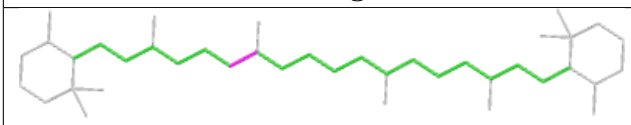
Ligand BCR L 1504



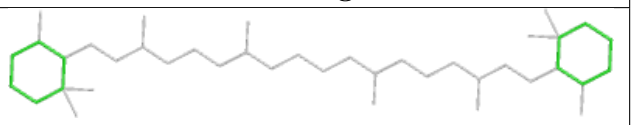
Bond lengths



Bond angles

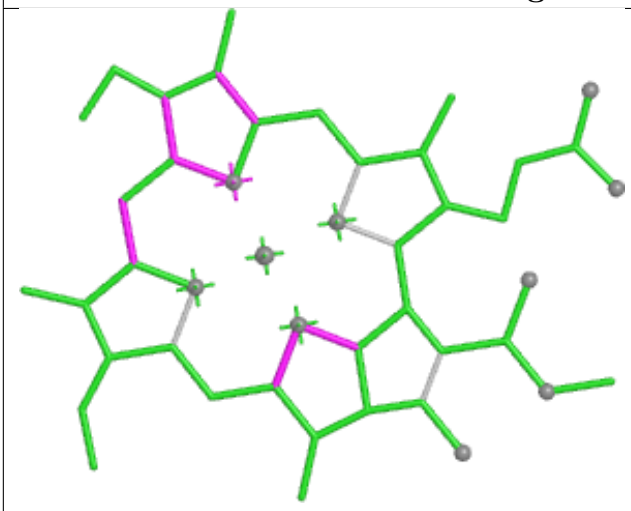


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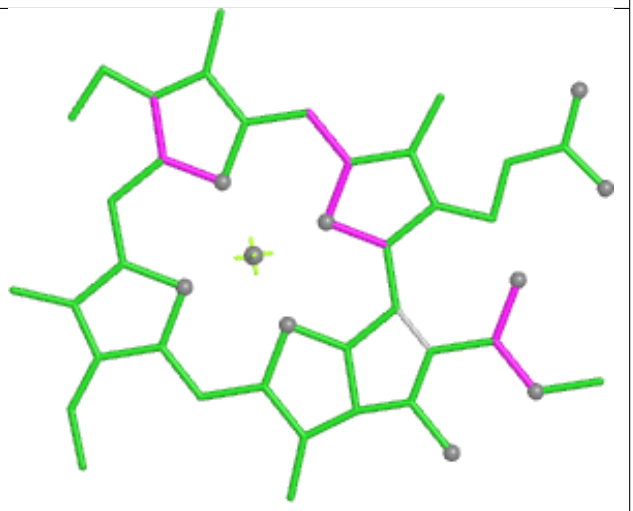


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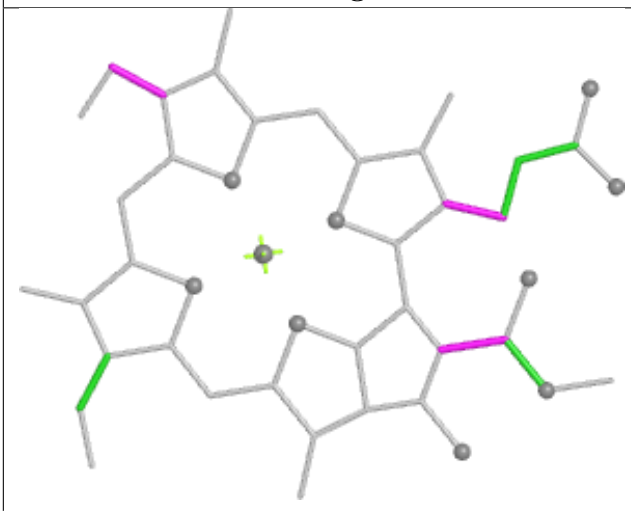
Ligand CLA n 821



Bond lengths



Bond angles

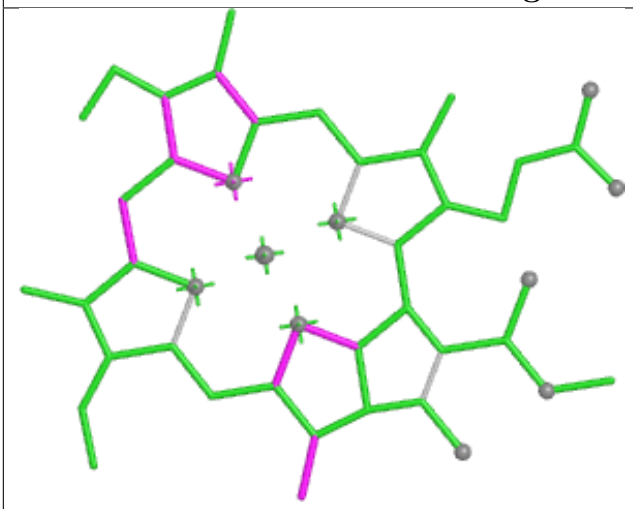


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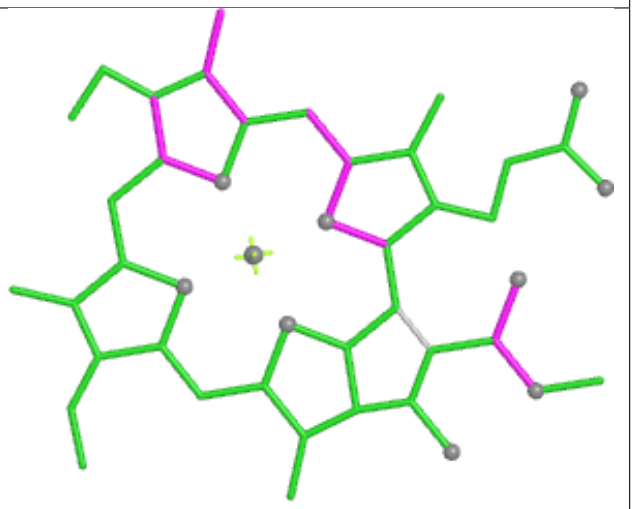


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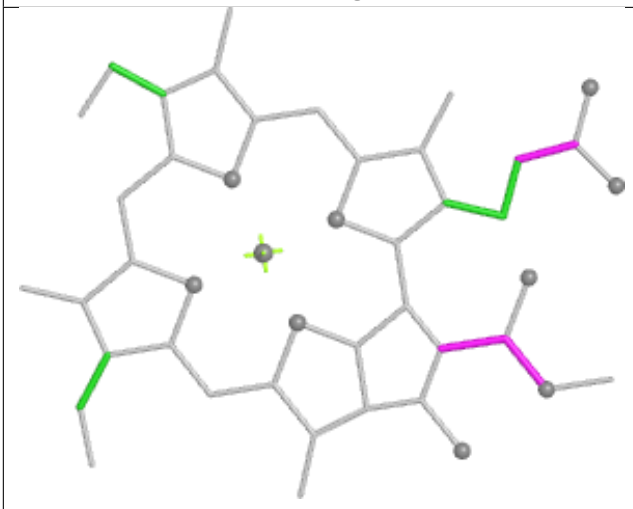
Ligand CLA G 814



Bond lengths



Bond angles

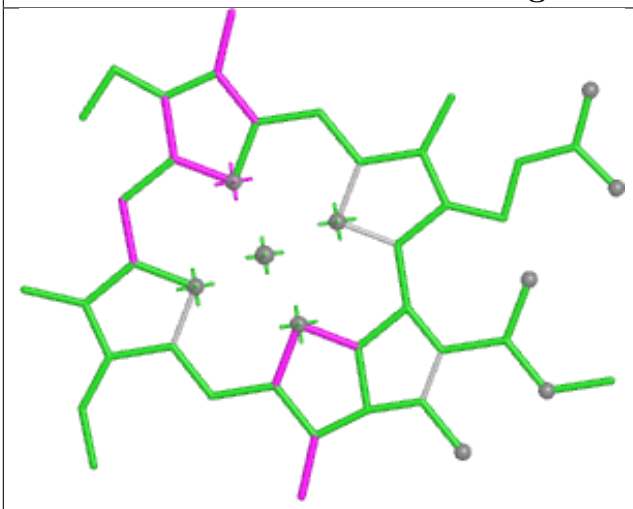


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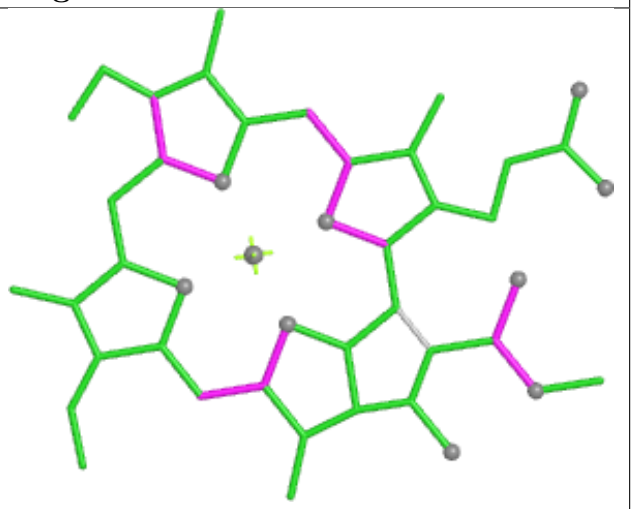


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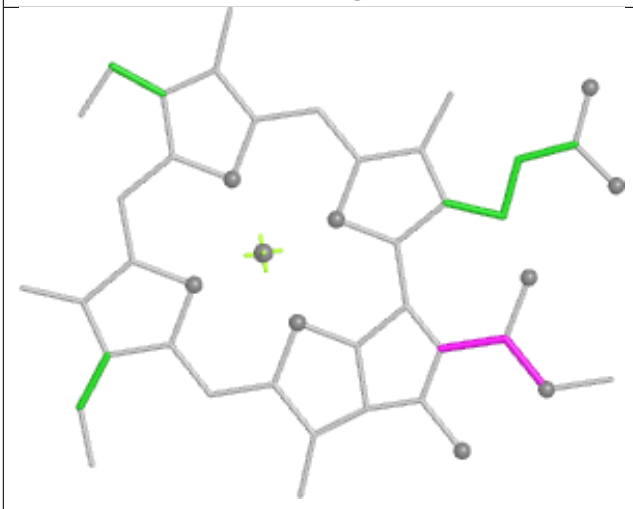
Ligand CLA g 822



Bond lengths



Bond angles

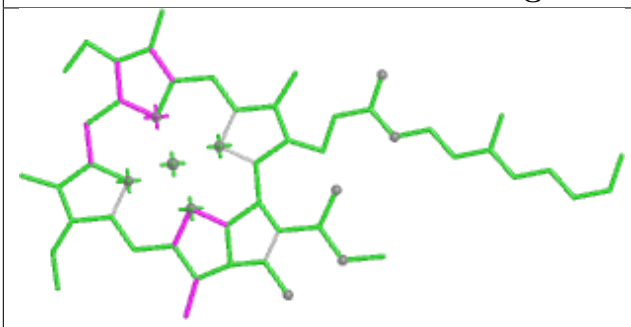


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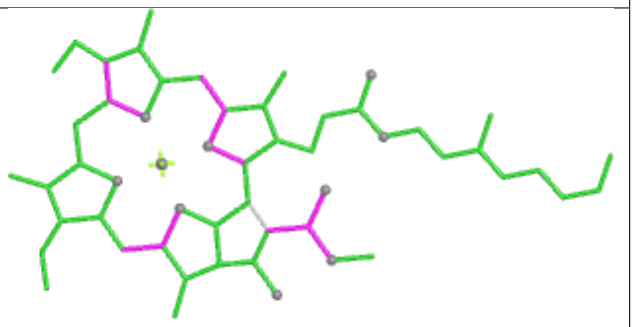


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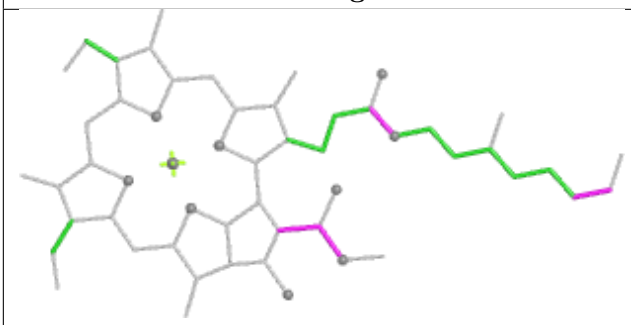
Ligand CLA B 812



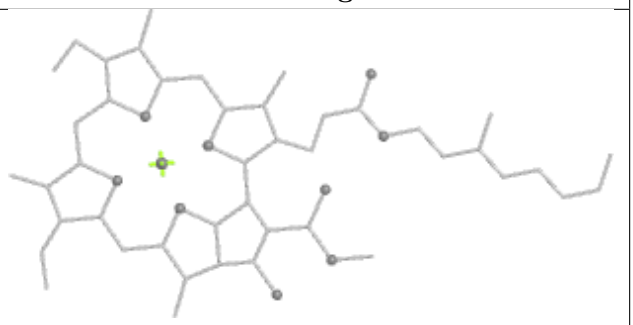
Bond lengths



Bond angles



Torsions

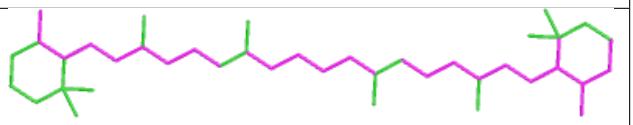


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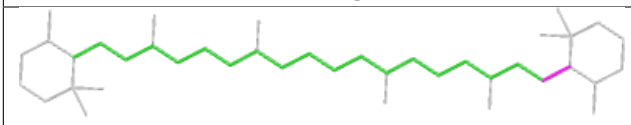
Ligand BCR A 848



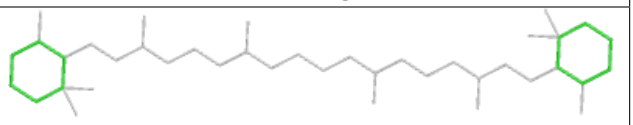
Bond lengths



Bond angles

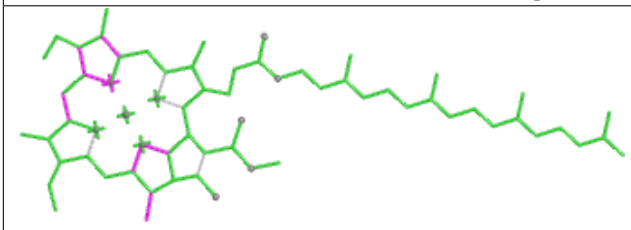


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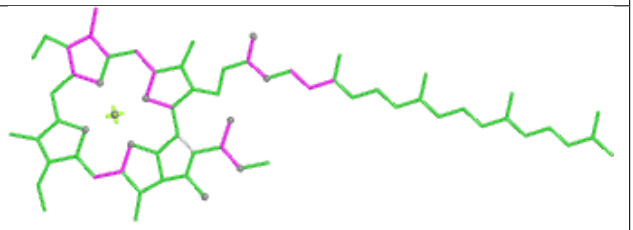


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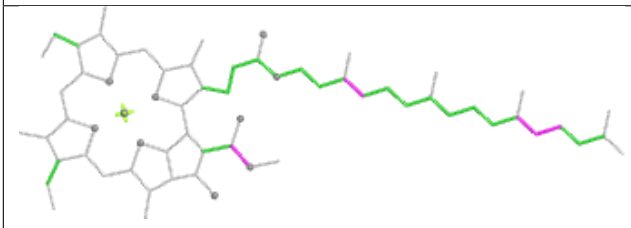
Ligand CLA a 831



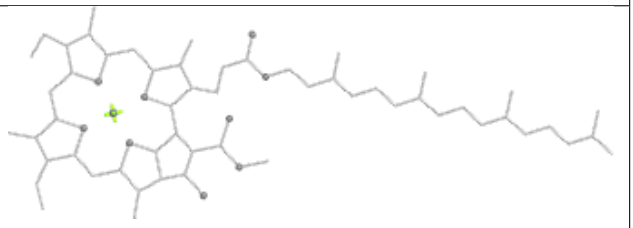
Bond lengths



Bond angles

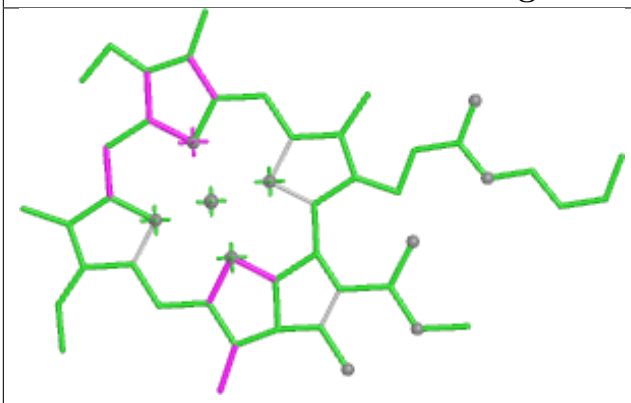


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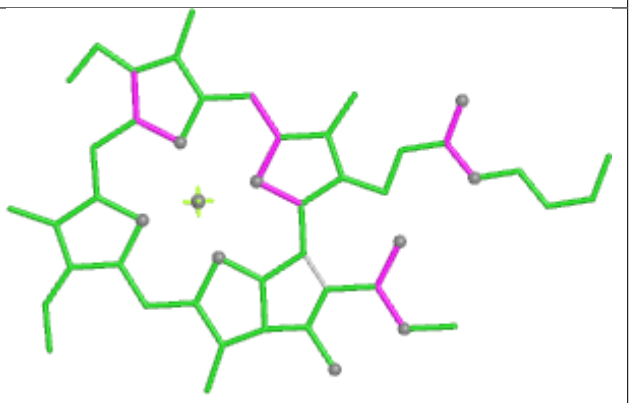


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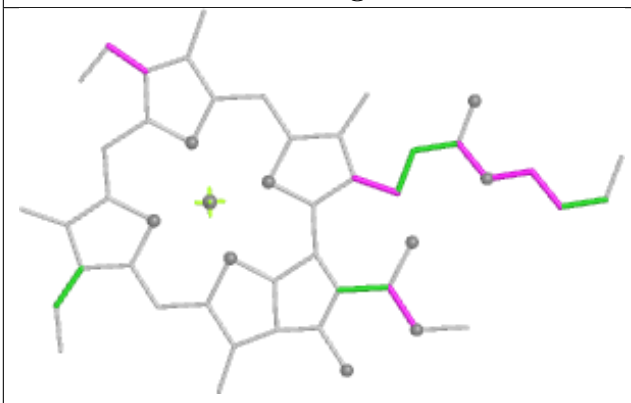
Ligand CLA h 1701



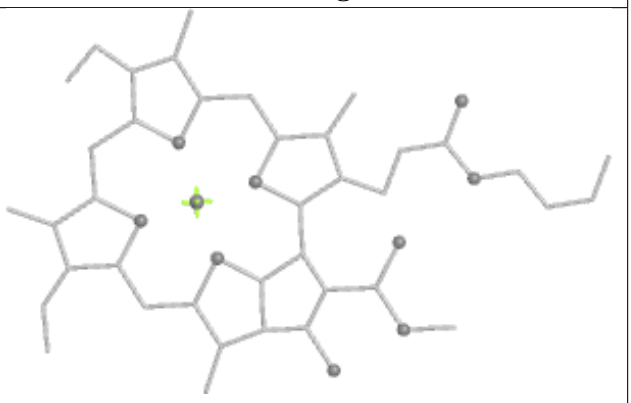
Bond lengths



Bond angles

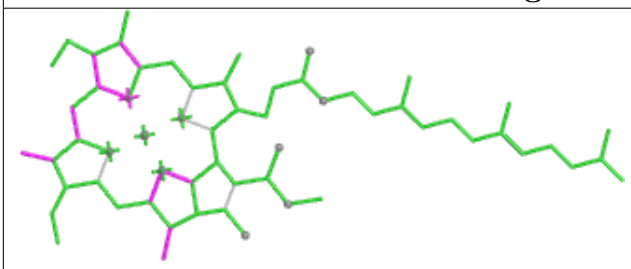


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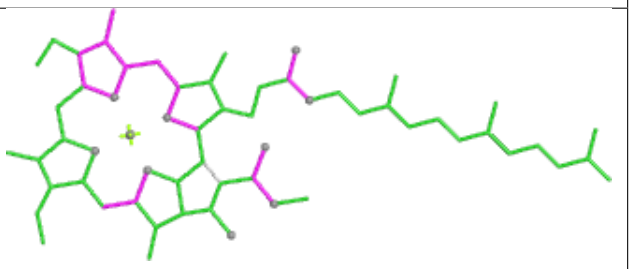


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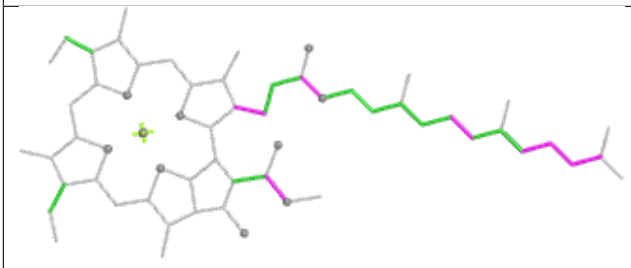
Ligand CLA B 837



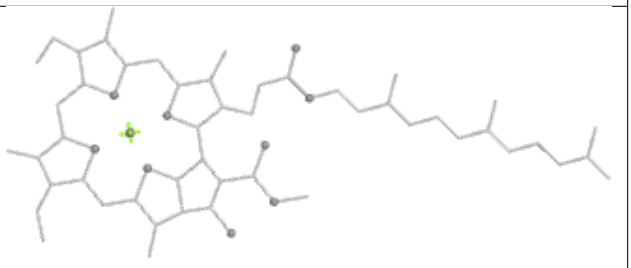
Bond lengths



Bond angles

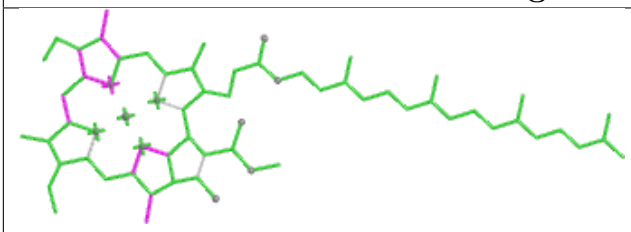


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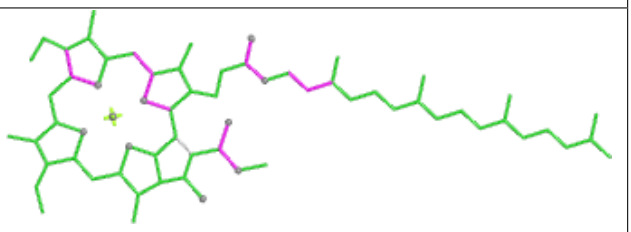


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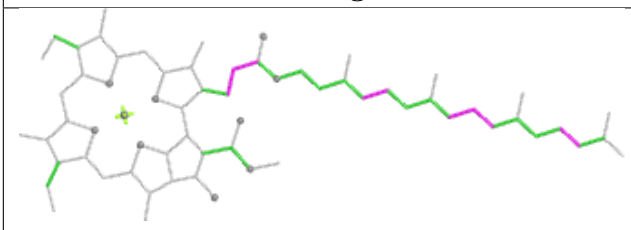
Ligand CLA a 807



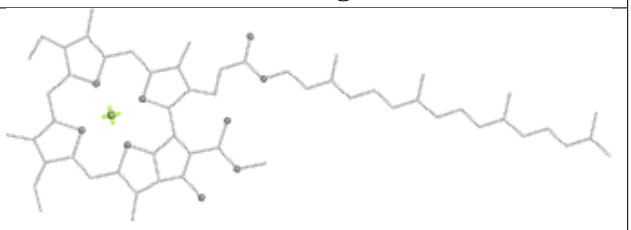
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Bond angles

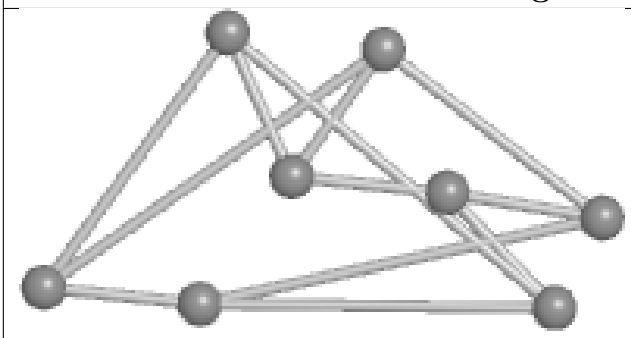


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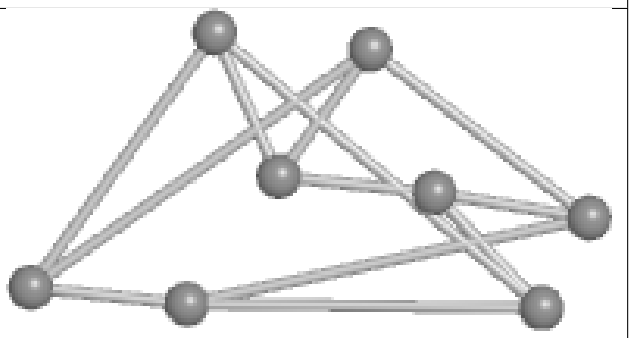


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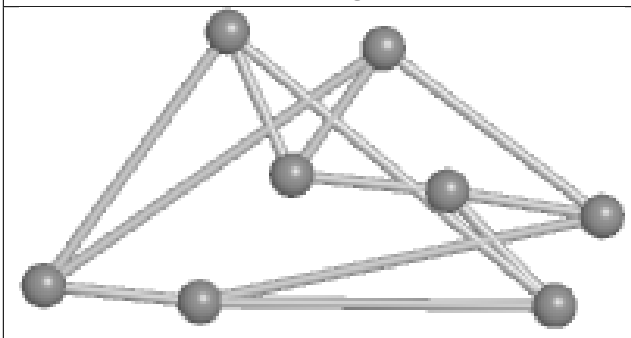
Ligand SF4 P 102



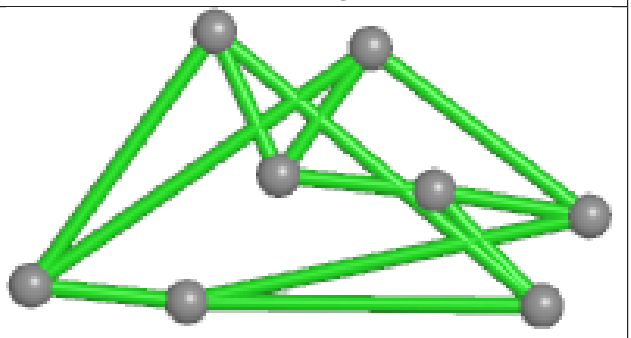
Bond lengths



Bond angles

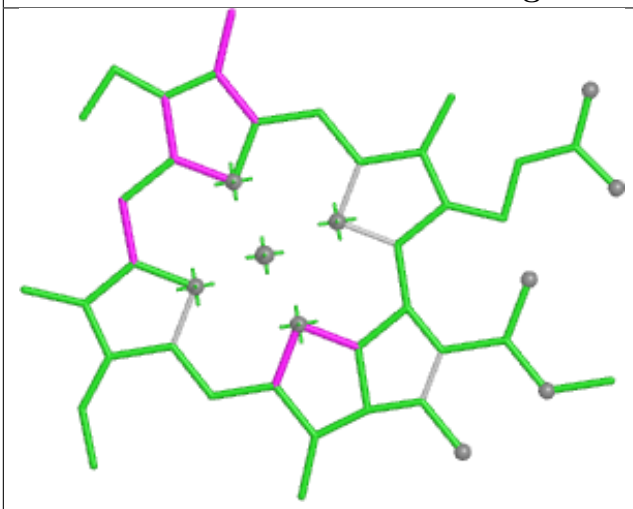


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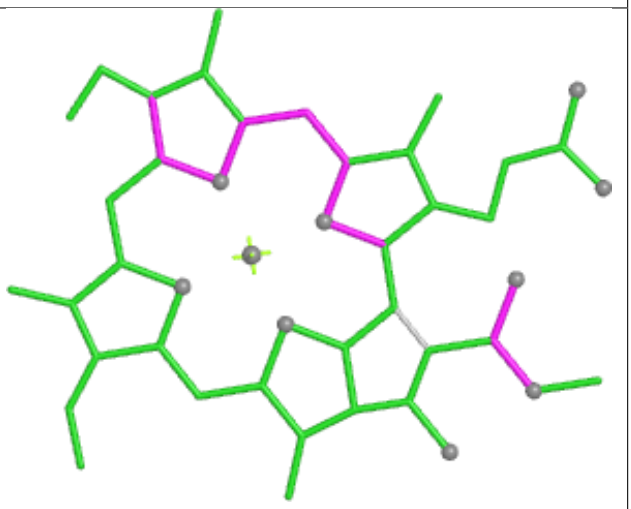


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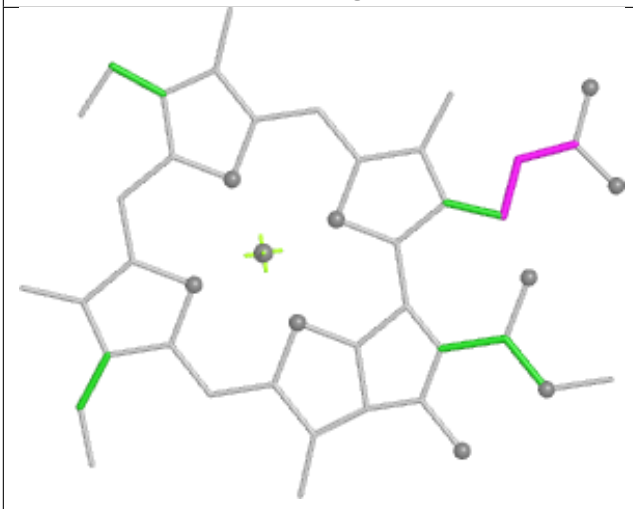
Ligand CLA G 815



Bond lengths



Bond angles

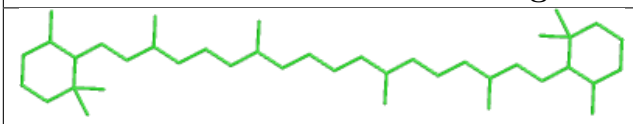


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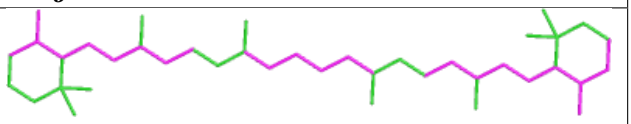


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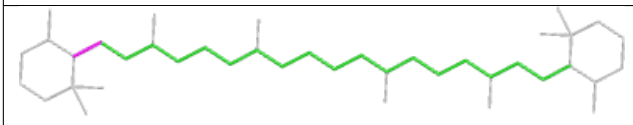
Ligand BCR j 103



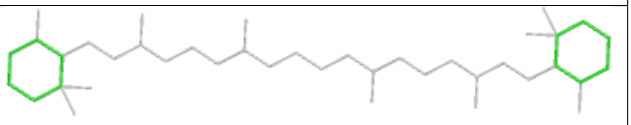
Bond lengths



Bond angles

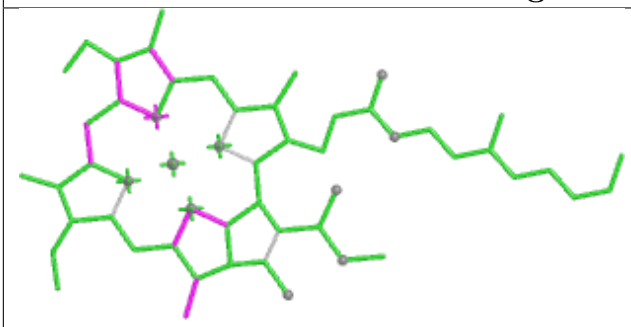


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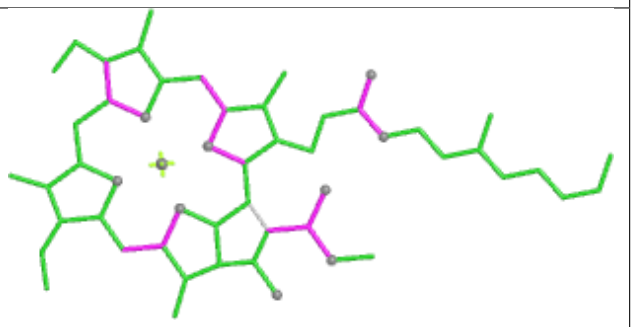


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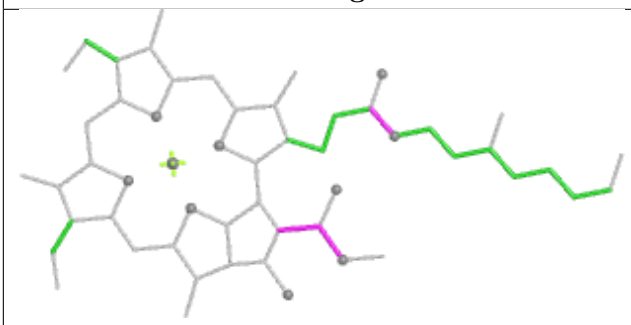
Ligand CLA b 833



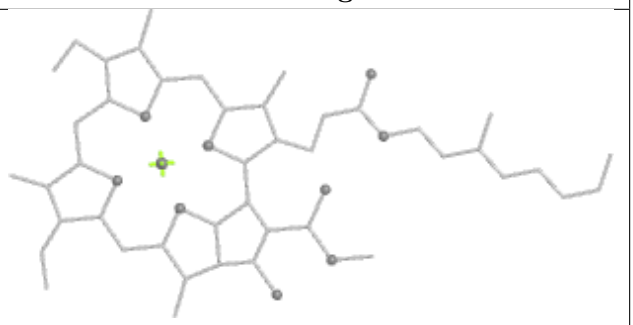
Bond lengths



Bond angles

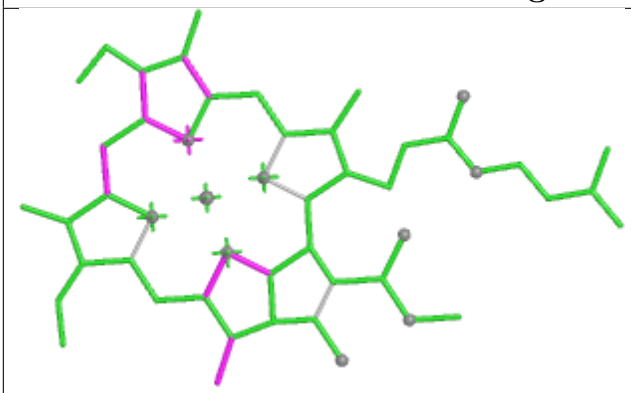


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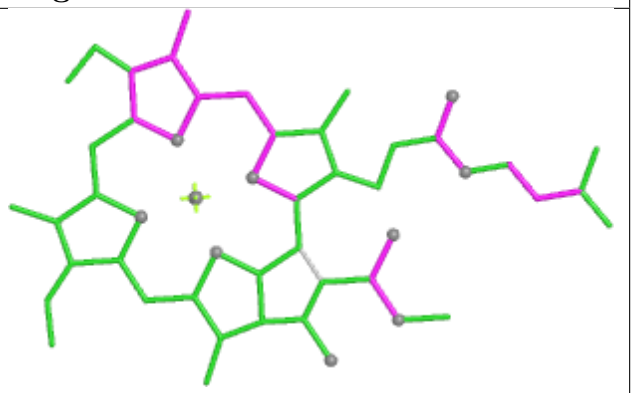


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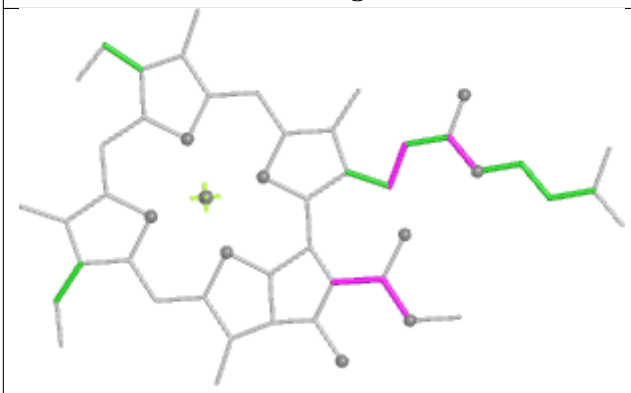
Ligand CLA g 840



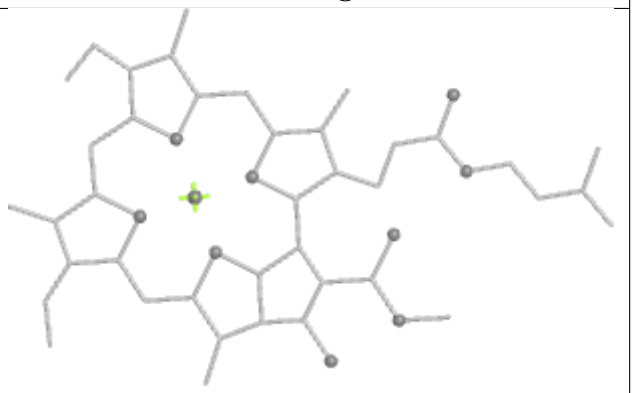
Bond lengths



Bond angles

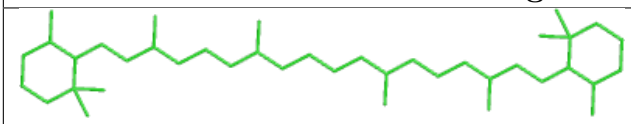


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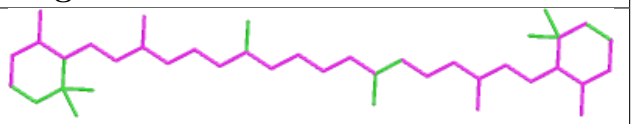


Rings

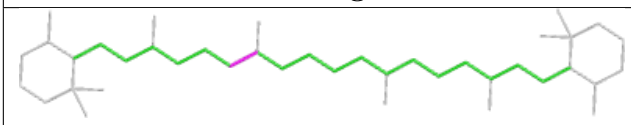
Ligand BCR g 843



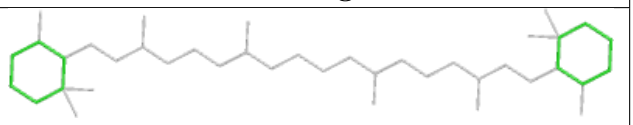
Bond lengths



Bond angles

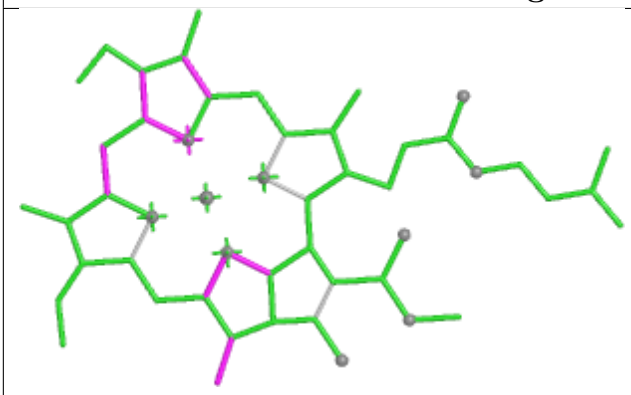


Torsions

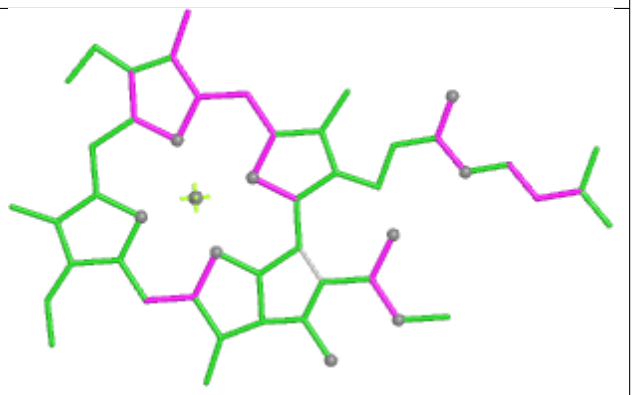


Rings

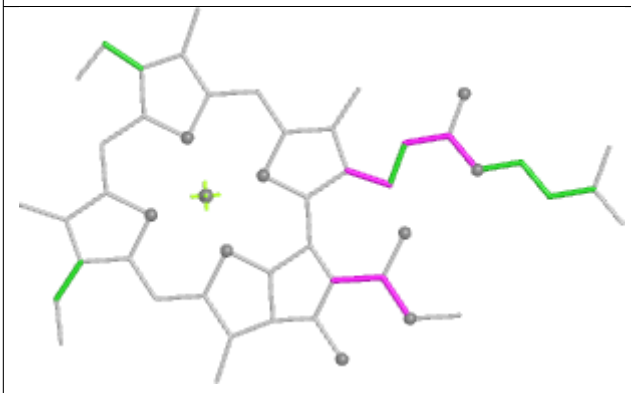
Ligand CLA b 814



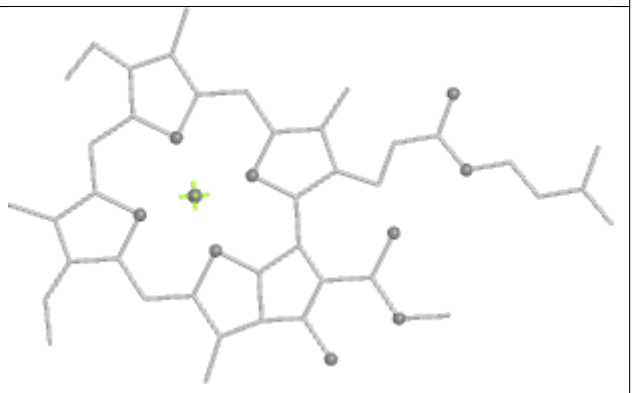
Bond lengths



Bond angles

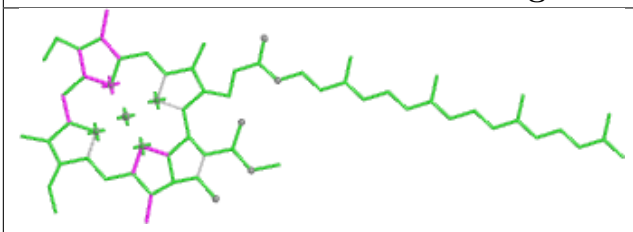


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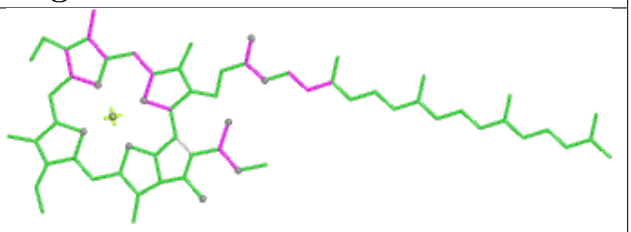


Rings

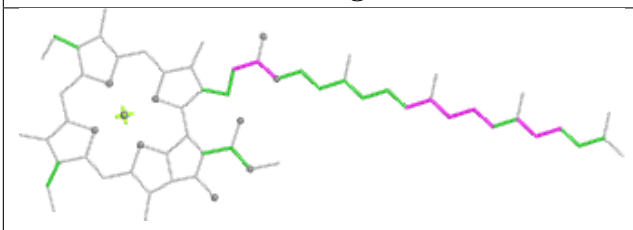
Ligand CLA g 823



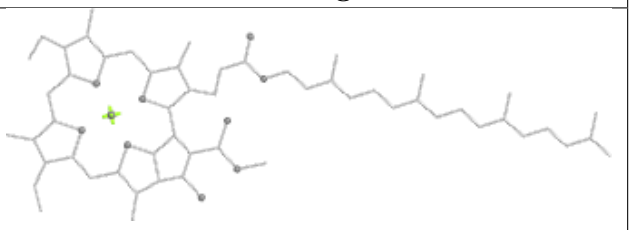
Bond lengths



Bond angles

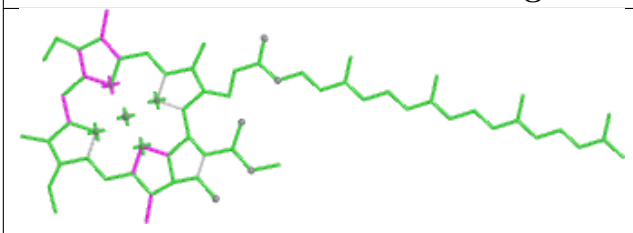


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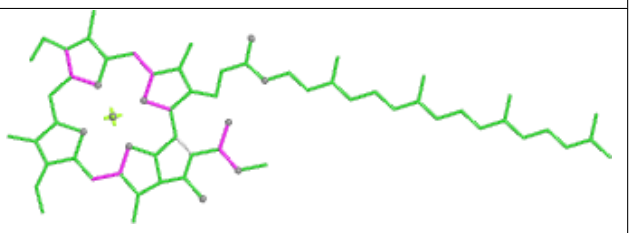


Rings

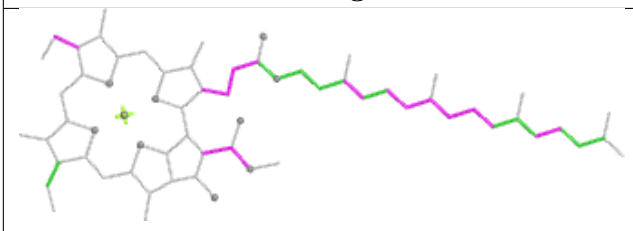
Ligand CLA B 810



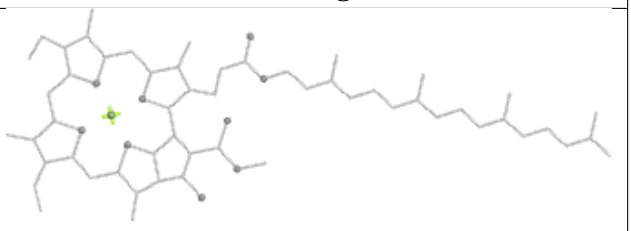
Bond lengths



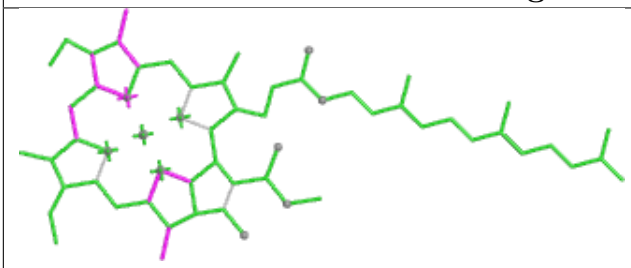
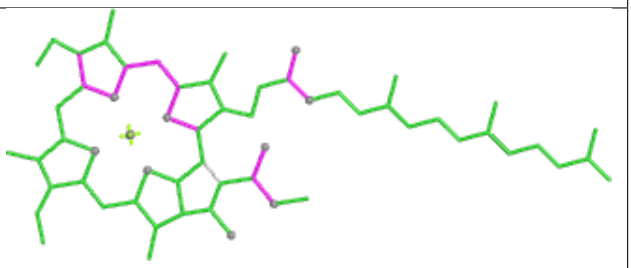
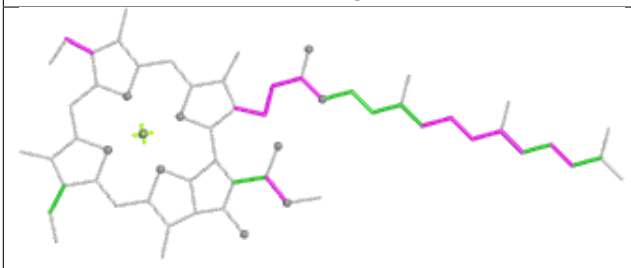
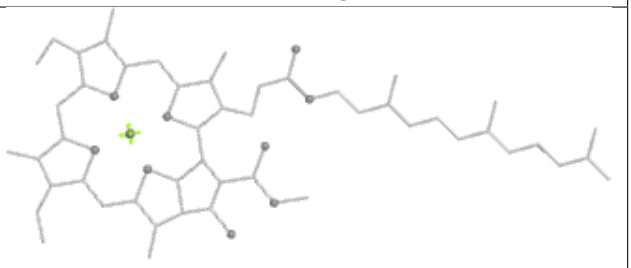
Bond angles

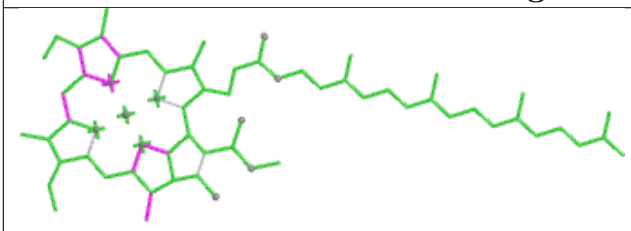
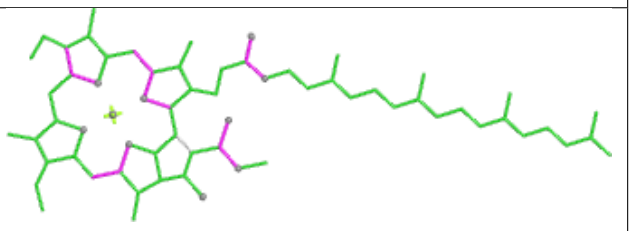
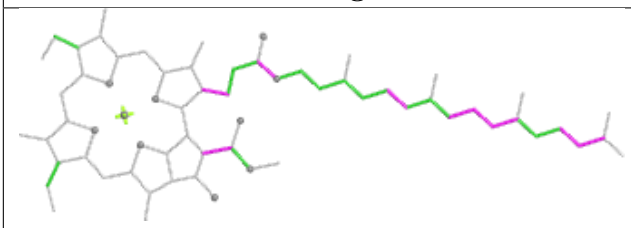
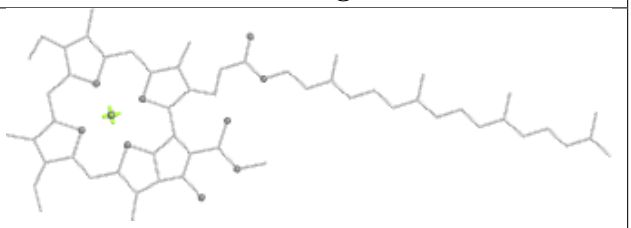


Torsions

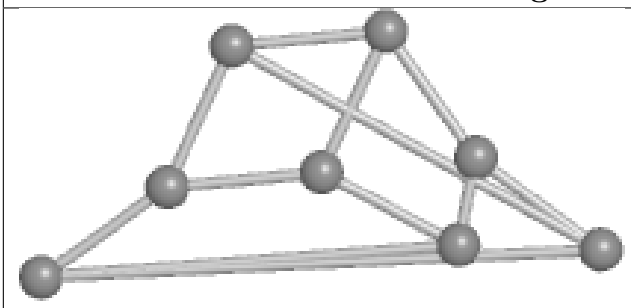


Rings

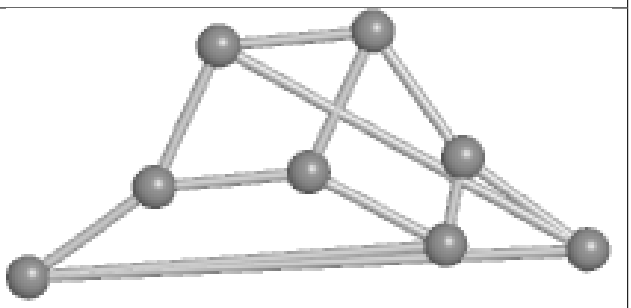
Ligand CLA b 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

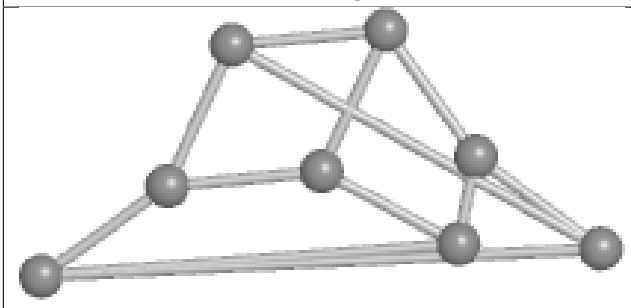
Ligand SF4 A 843



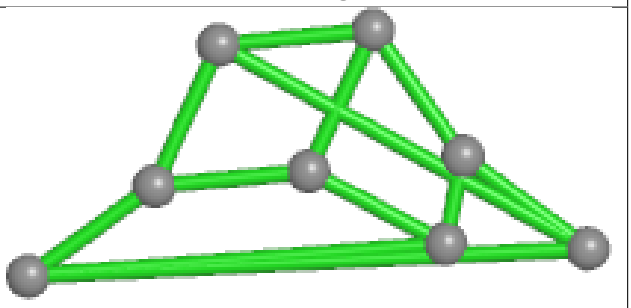
Bond lengths



Bond angles

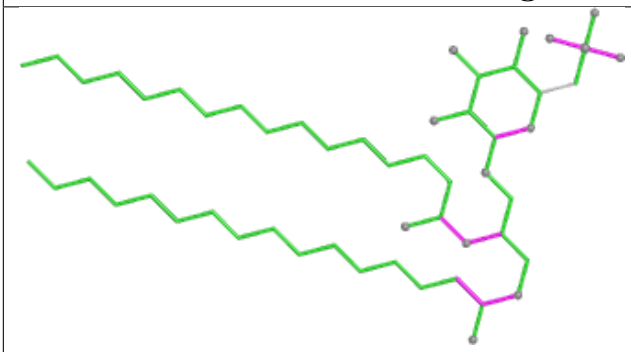


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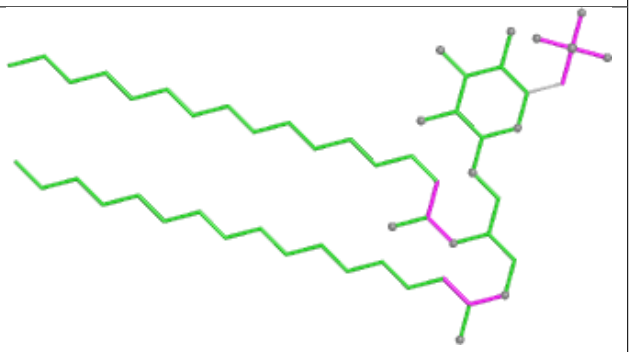


Rings

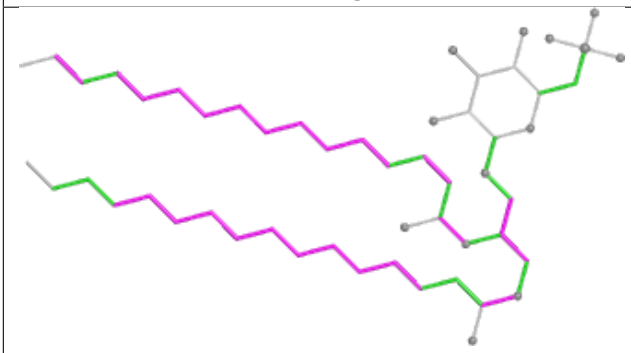
Ligand SQD x 1702



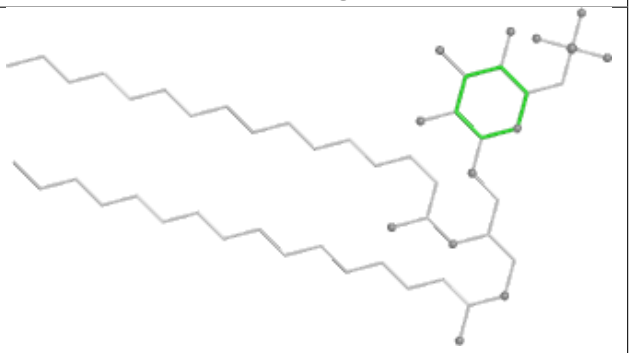
Bond lengths



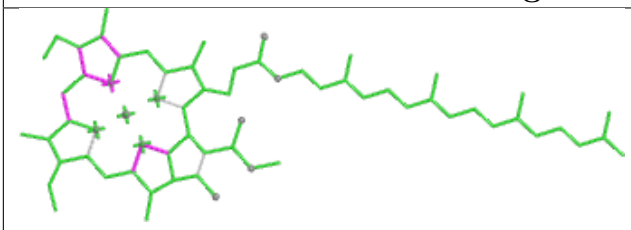
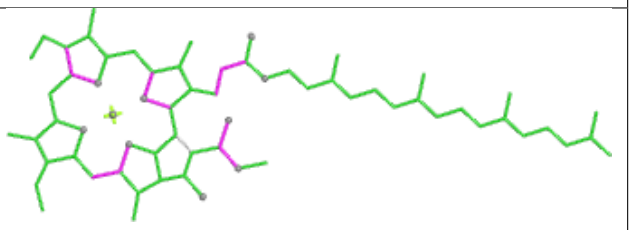
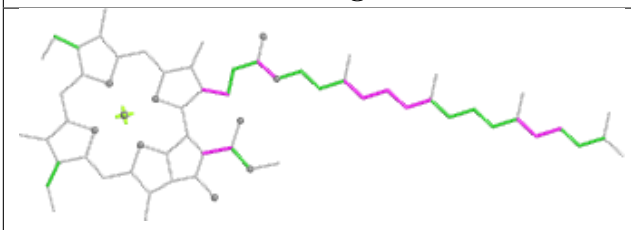
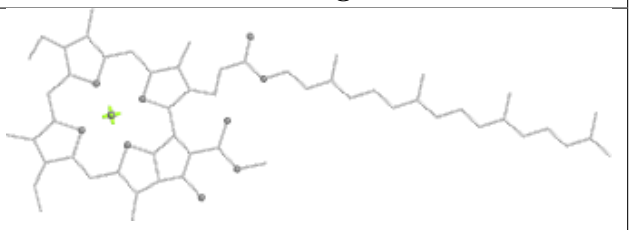
Bond angles

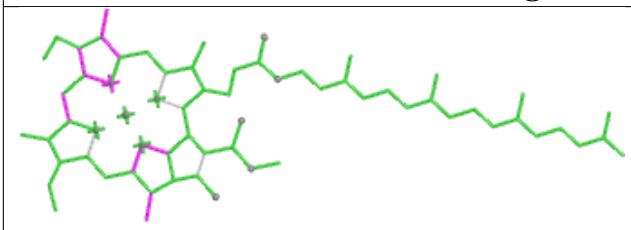
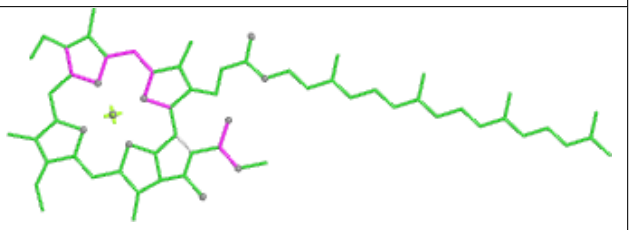
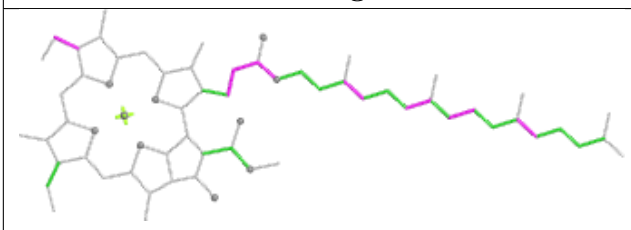
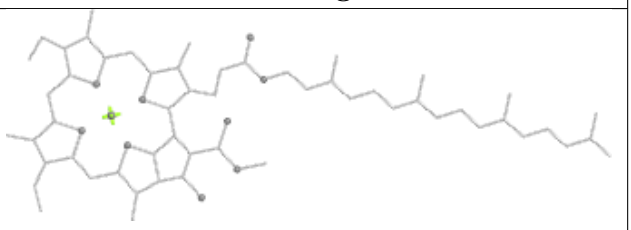


Torsions

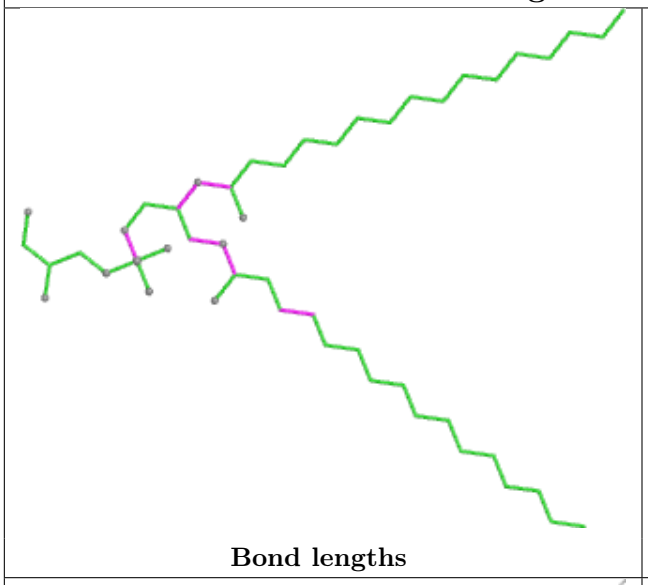


Rings

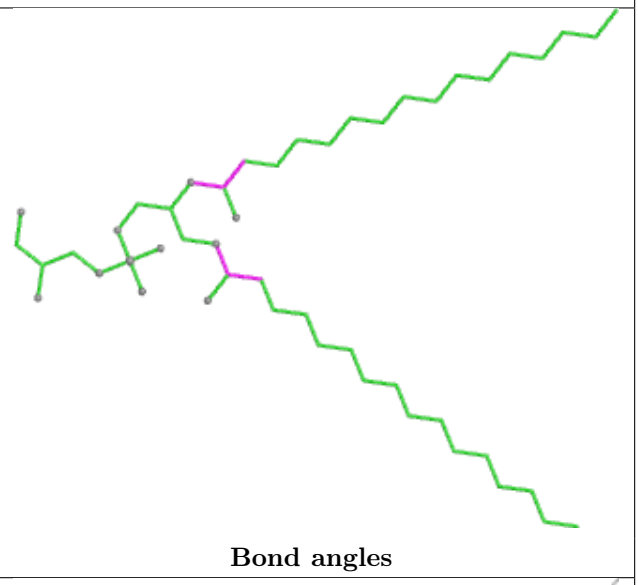
Ligand CLA N 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

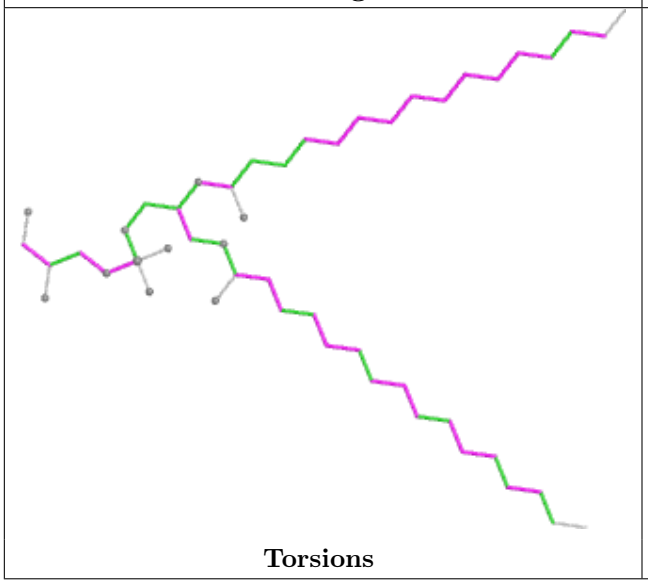
Ligand LHG a 849



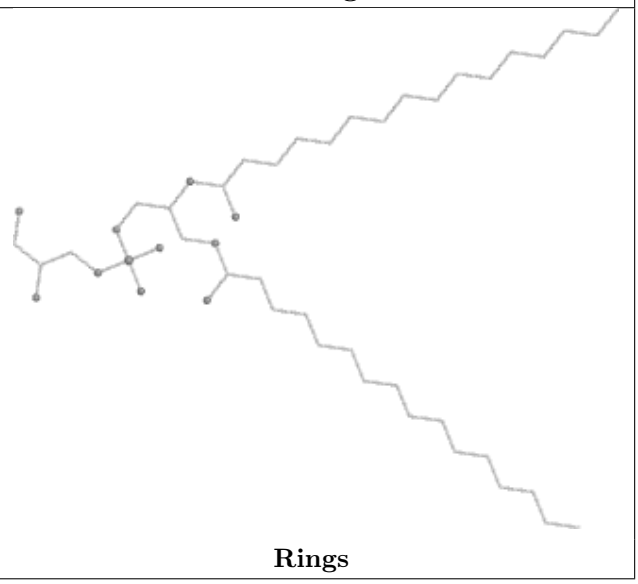
Bond lengths



Bond angles

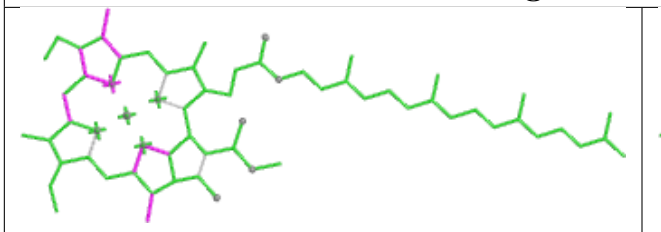


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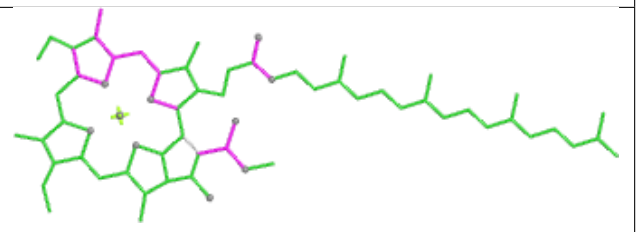


Rings

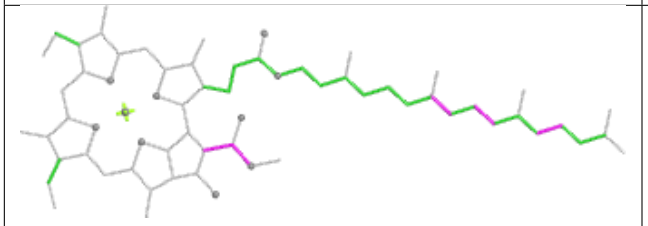
Ligand CLA A 829



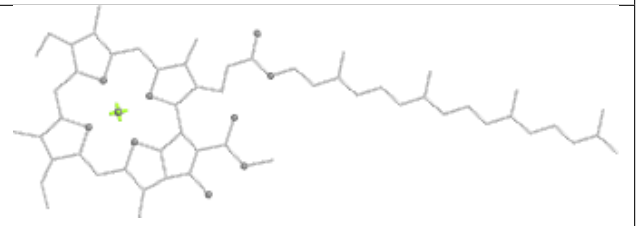
Bond lengths



Bond angles

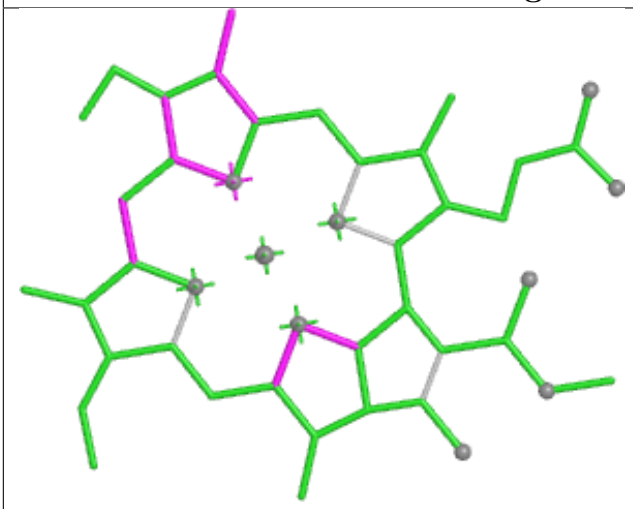


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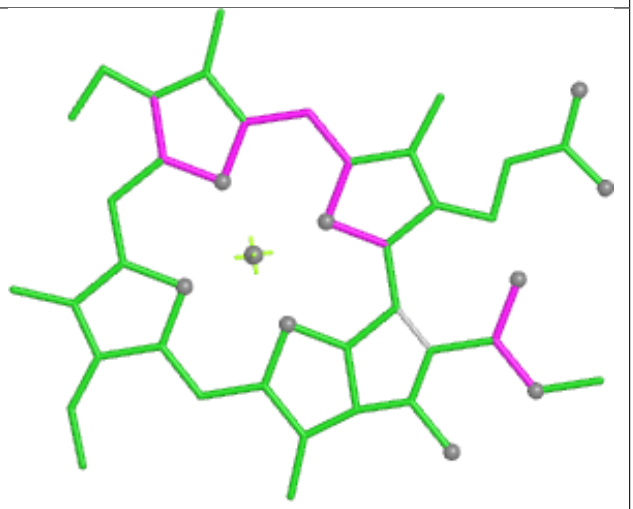


Rings

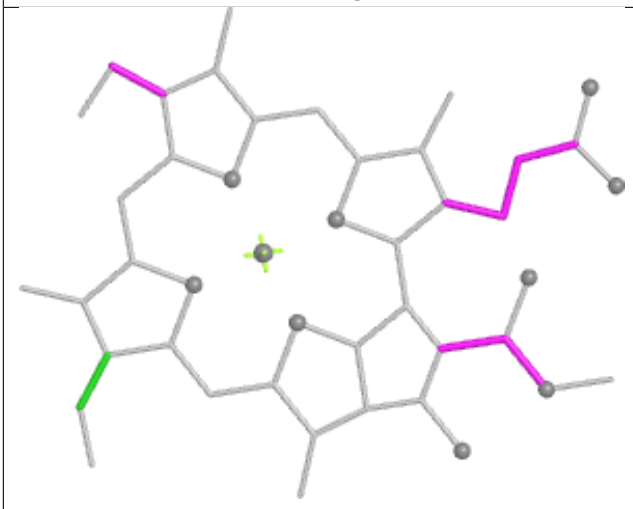
Ligand CLA T 101



Bond lengths



Bond angles

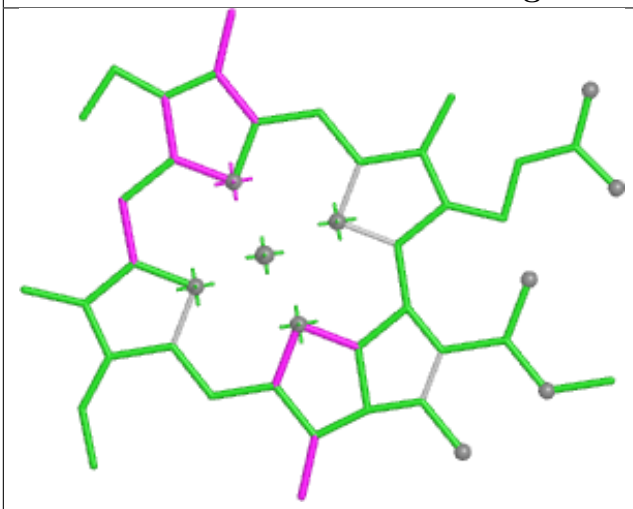


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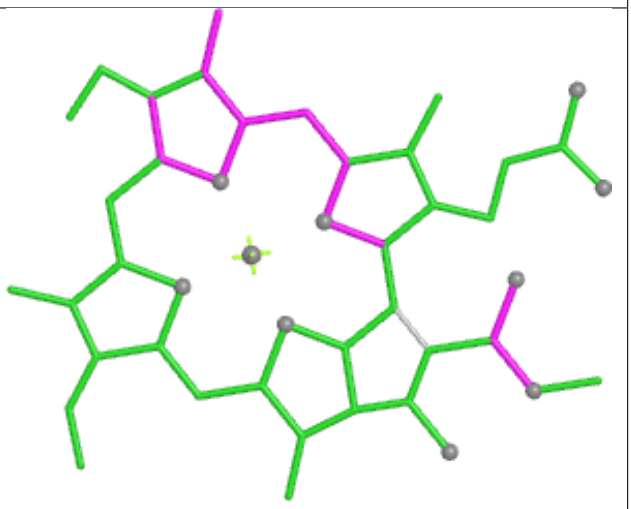


Rings

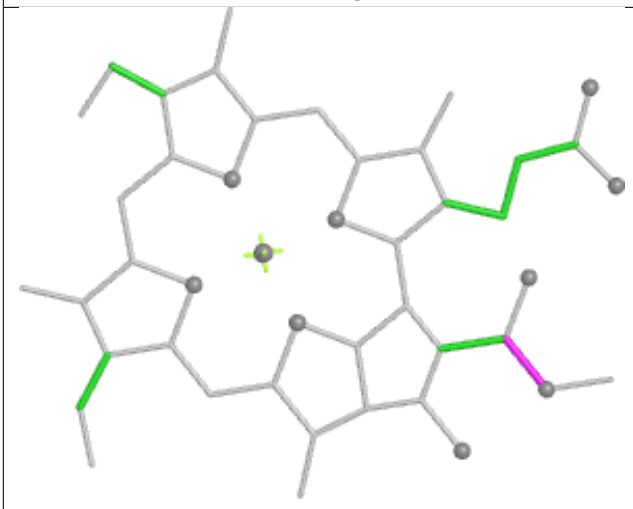
Ligand CLA N 836



Bond lengths



Bond angles

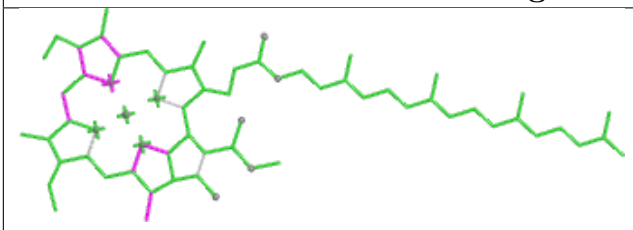


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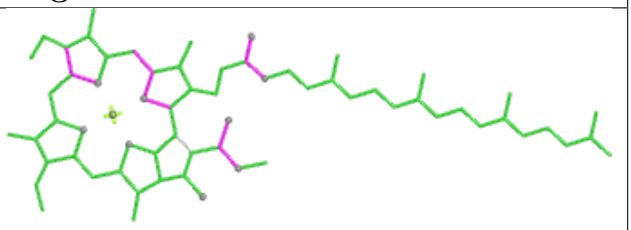


Rings

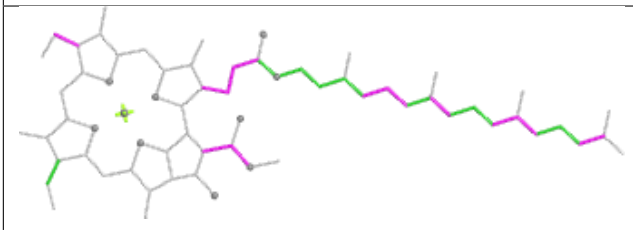
Ligand CLA g 807



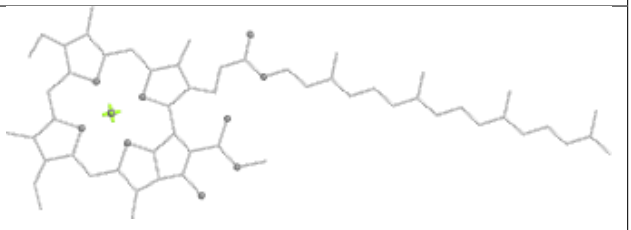
Bond lengths



Bond angles

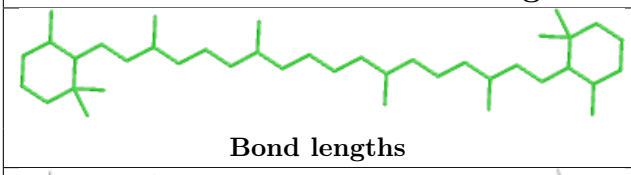


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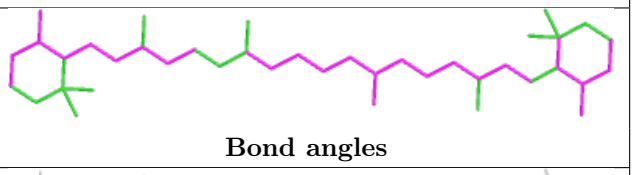


Rings

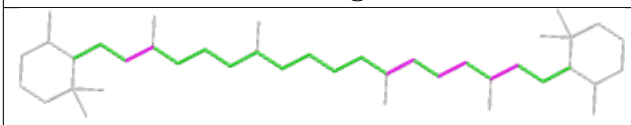
Ligand BCR B 846



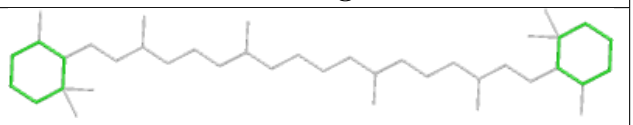
Bond lengths



Bond angles

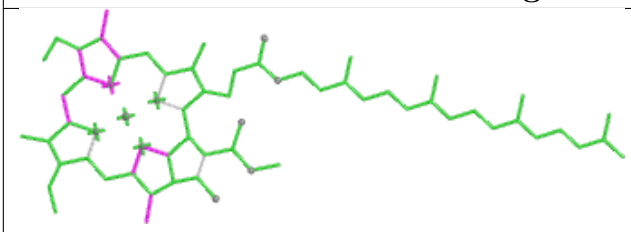


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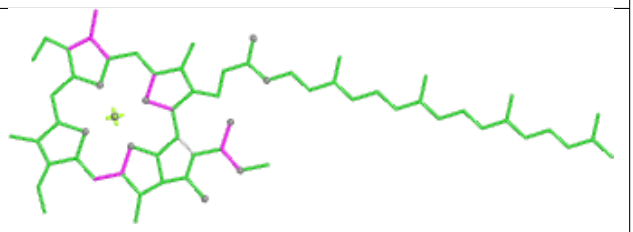


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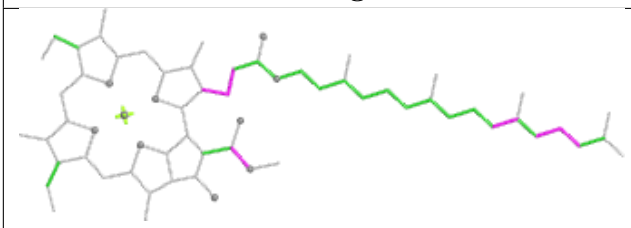
Ligand CLA G 801



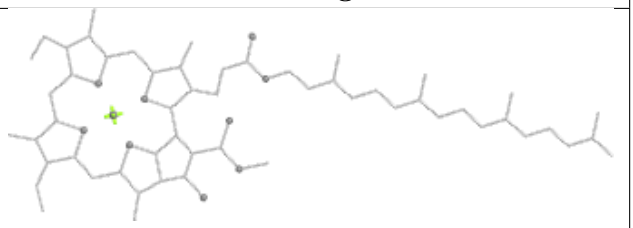
Bond lengths



Bond angles

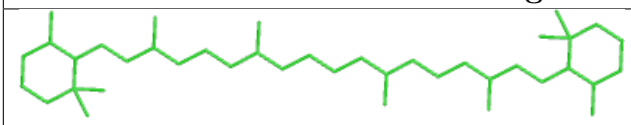


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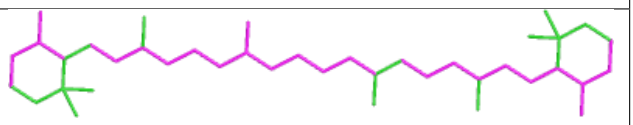


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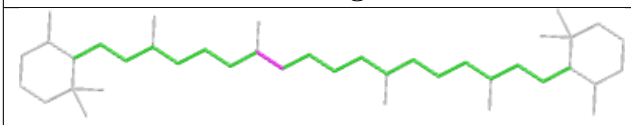
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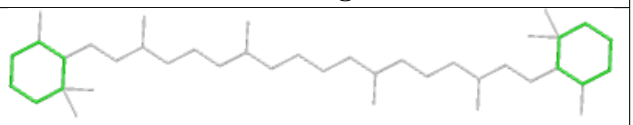
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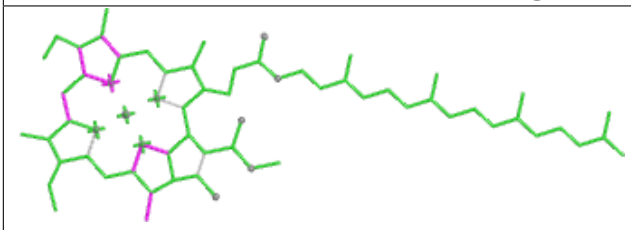


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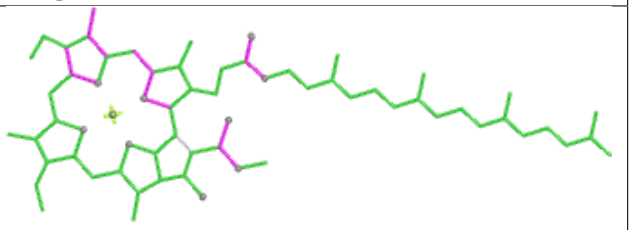


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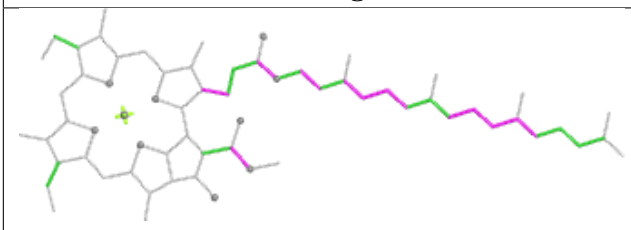
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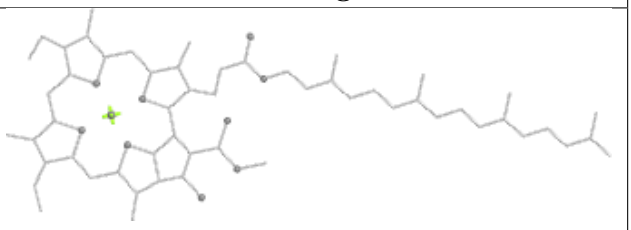
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Bond angles

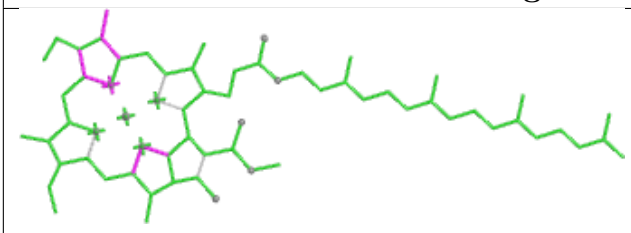


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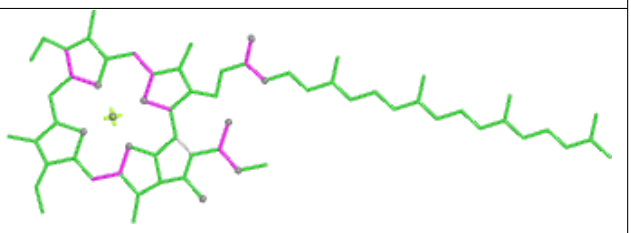


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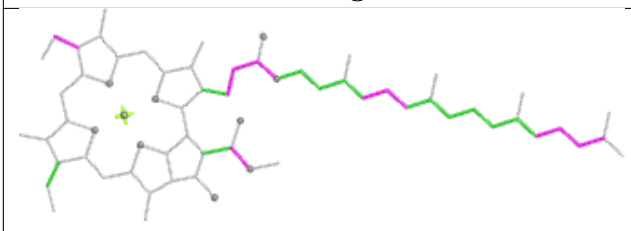
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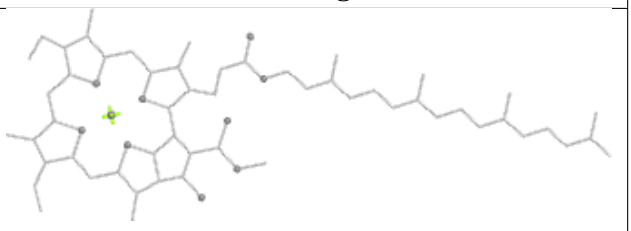
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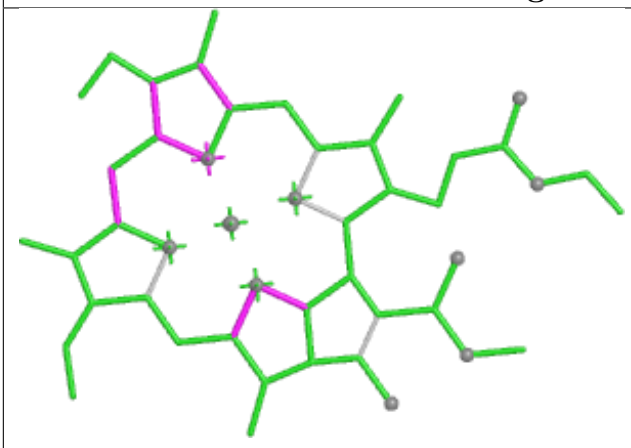


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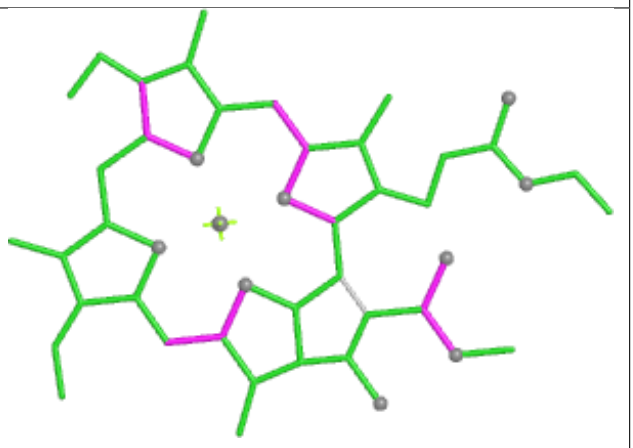


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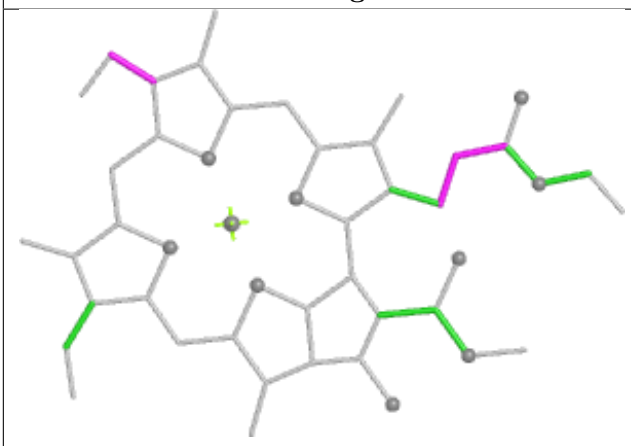
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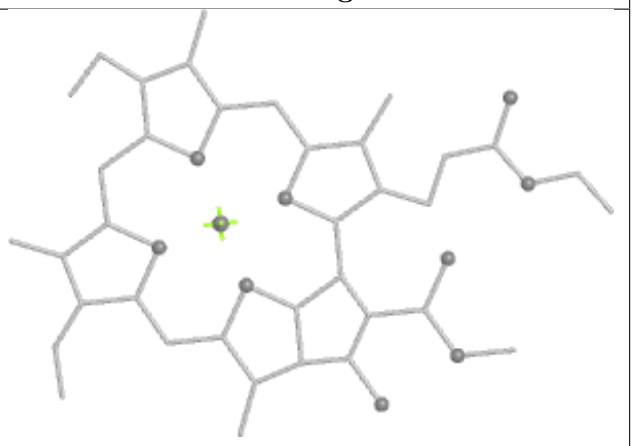
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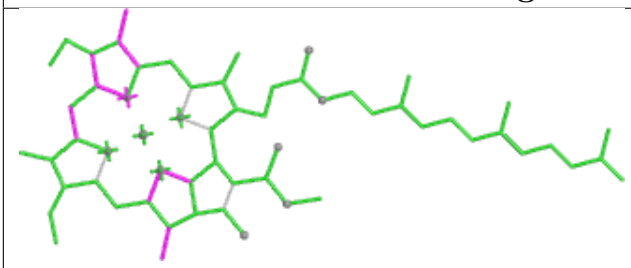


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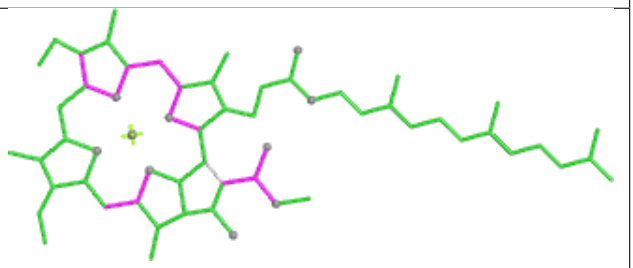


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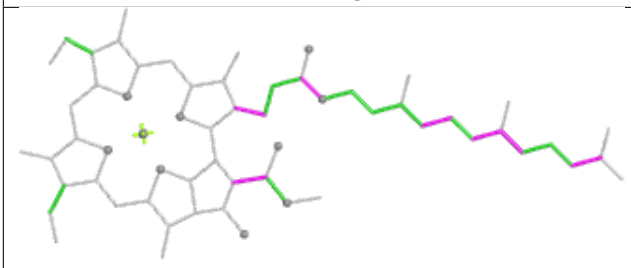
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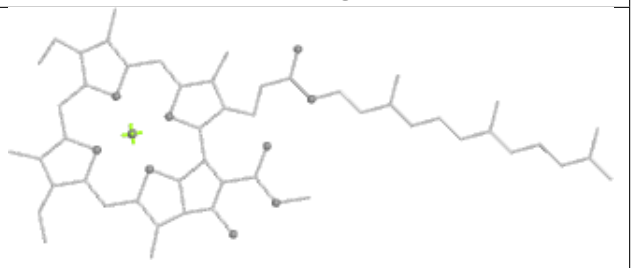
Bond lengths



Bond angles

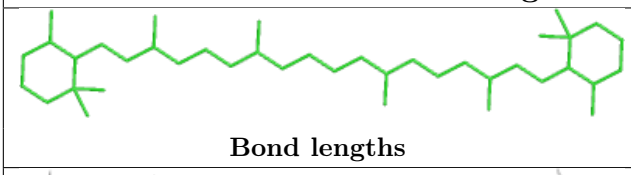


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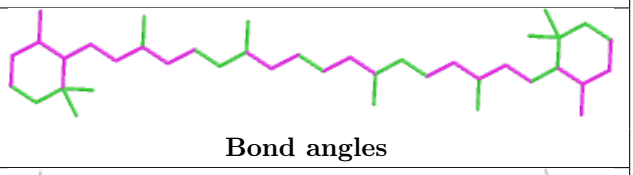


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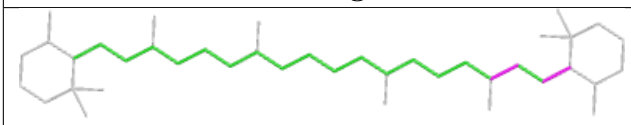
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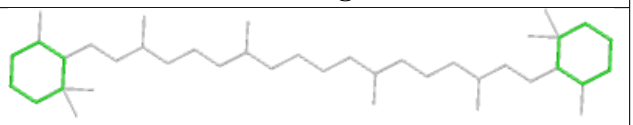
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Bond angles

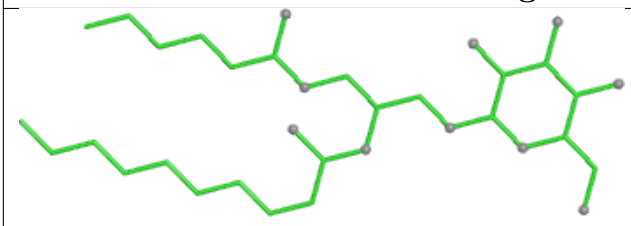


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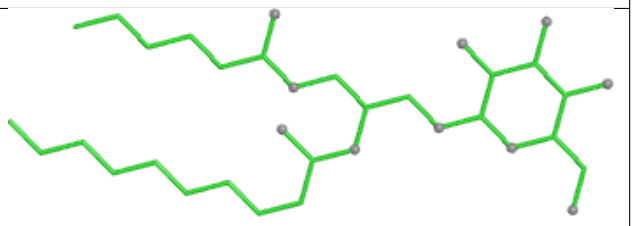


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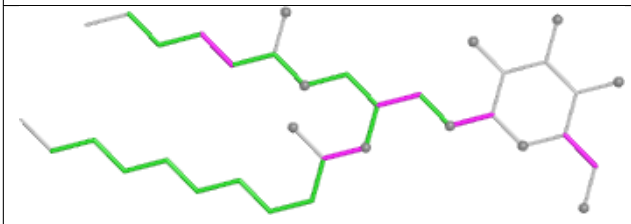
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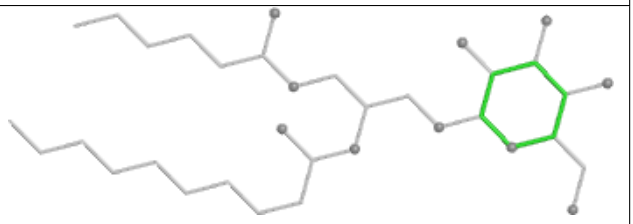
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Bond angles

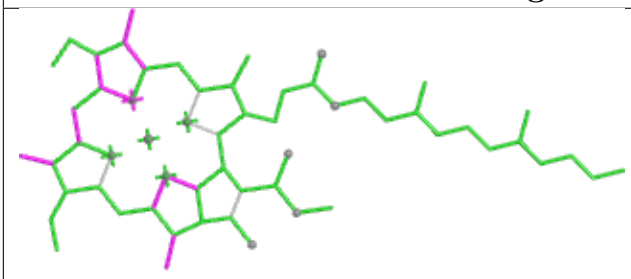


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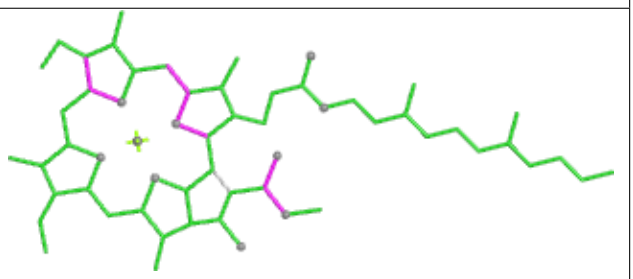


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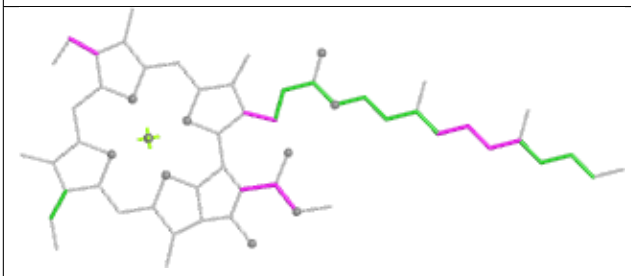
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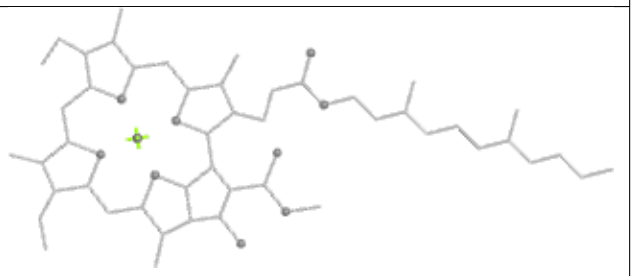
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Bond angles

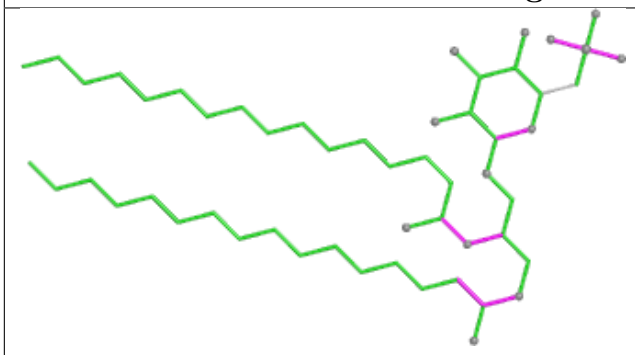


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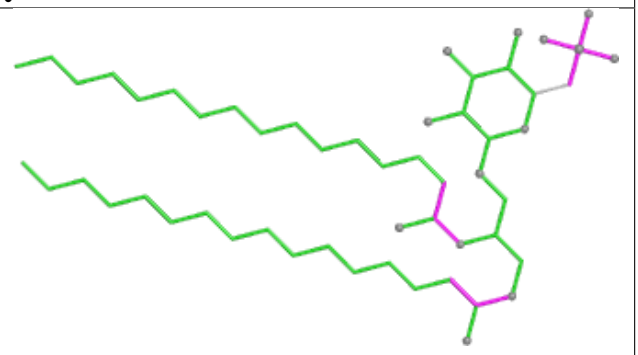


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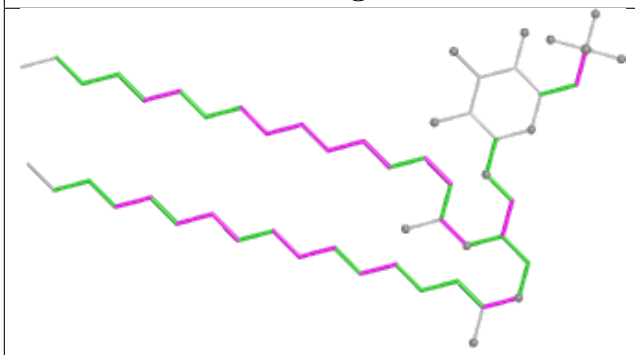
Ligand SQD B 801



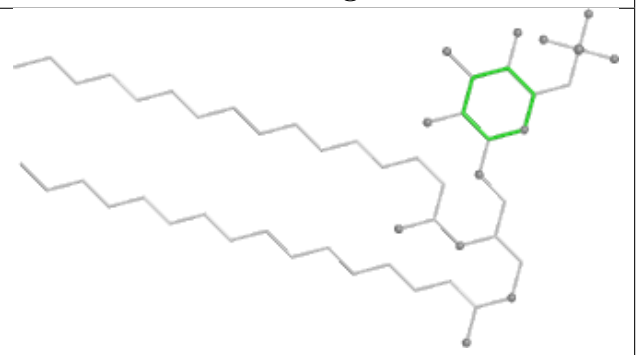
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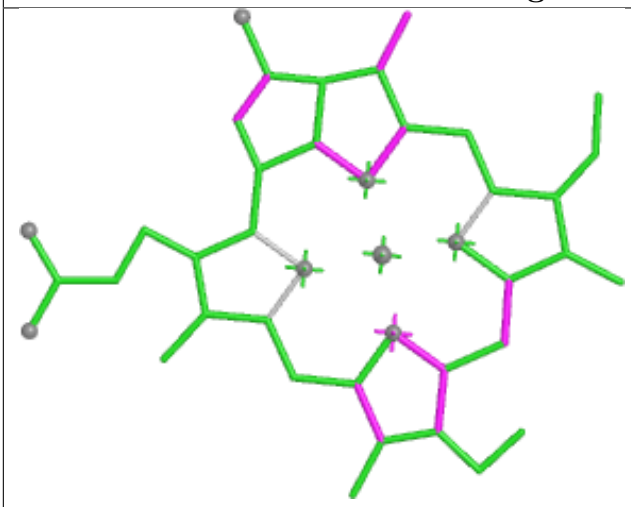


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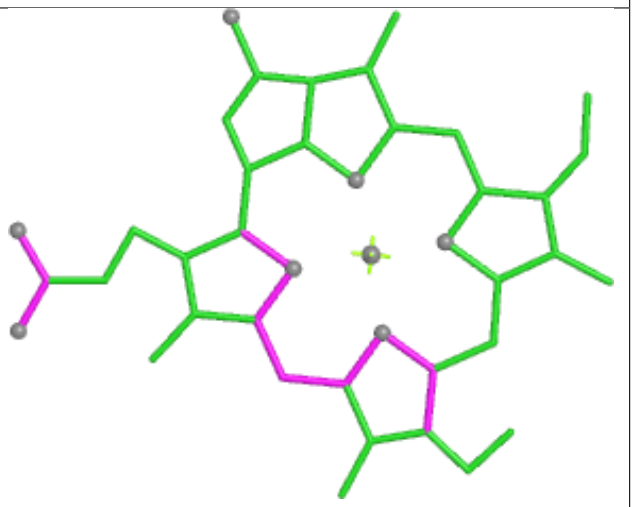


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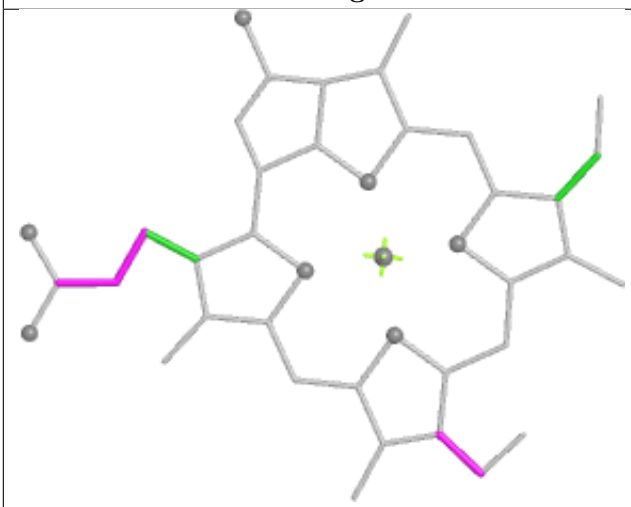
Ligand CLA u 101



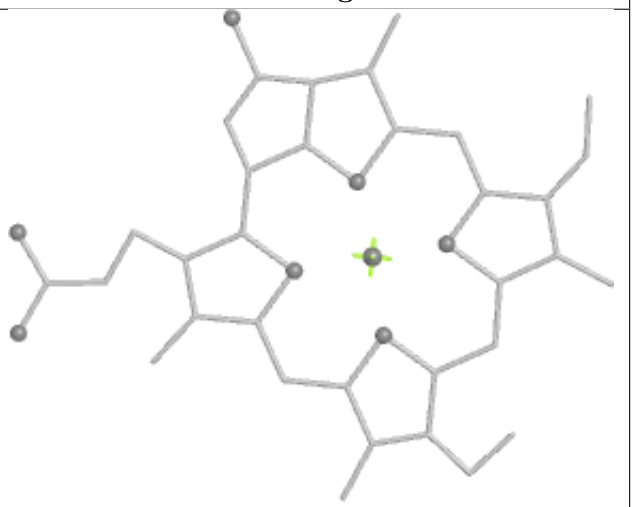
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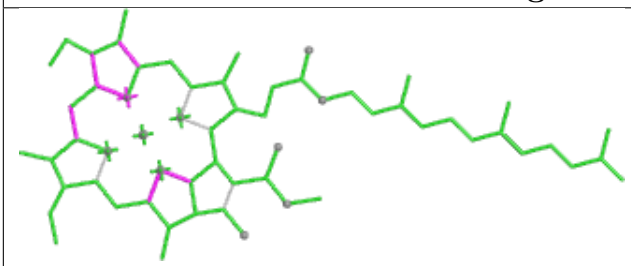


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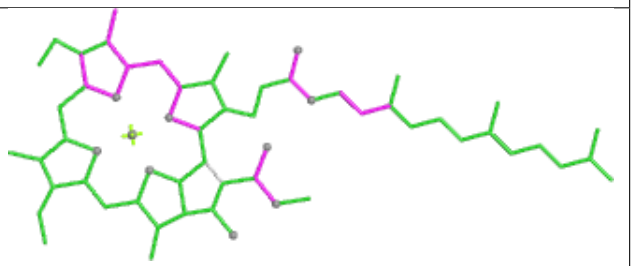


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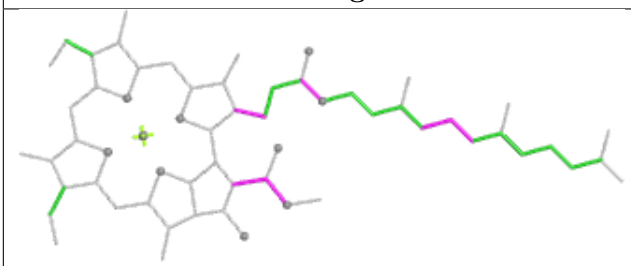
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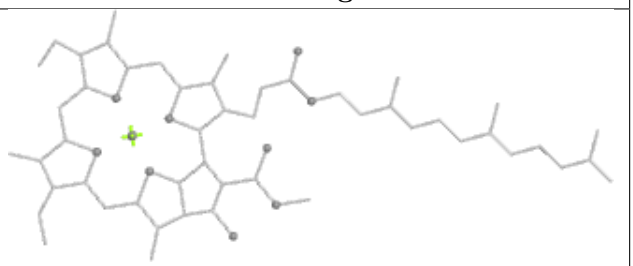
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Bond angles

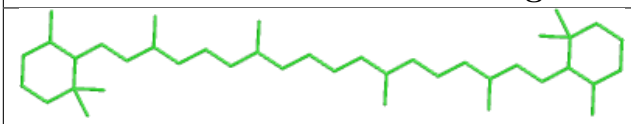


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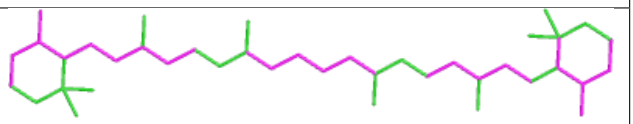


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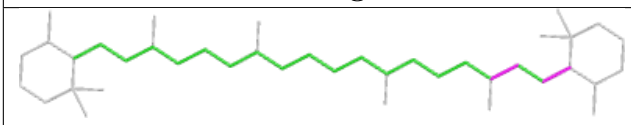
Ligand BCR b 842



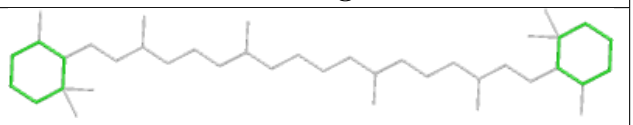
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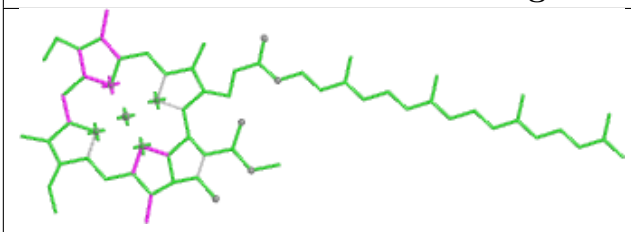


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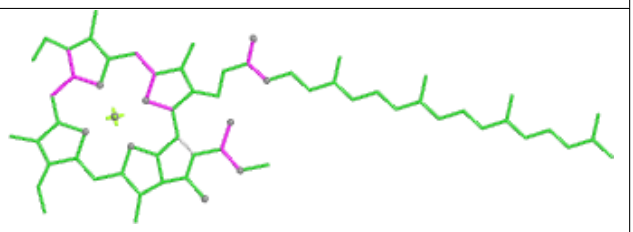


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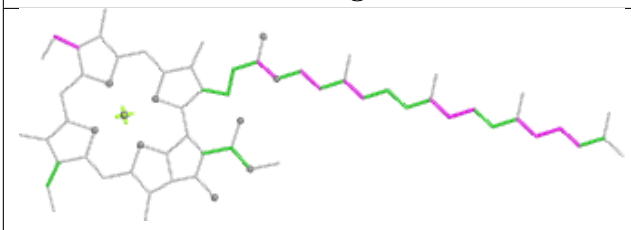
Ligand CLA a 823



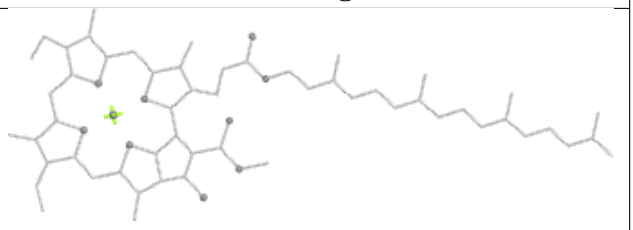
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Bond angles

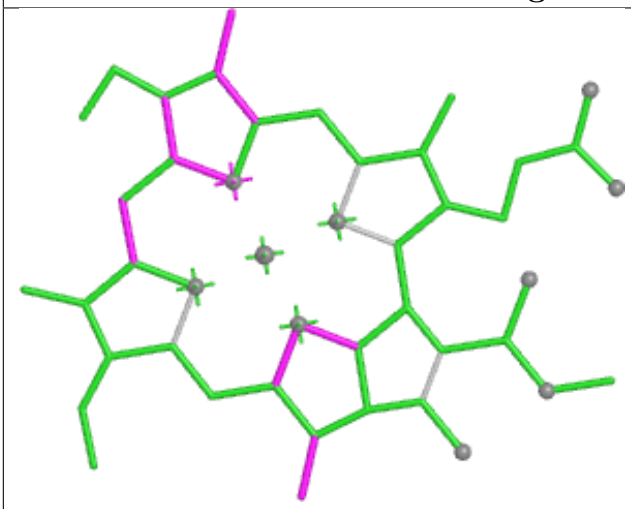


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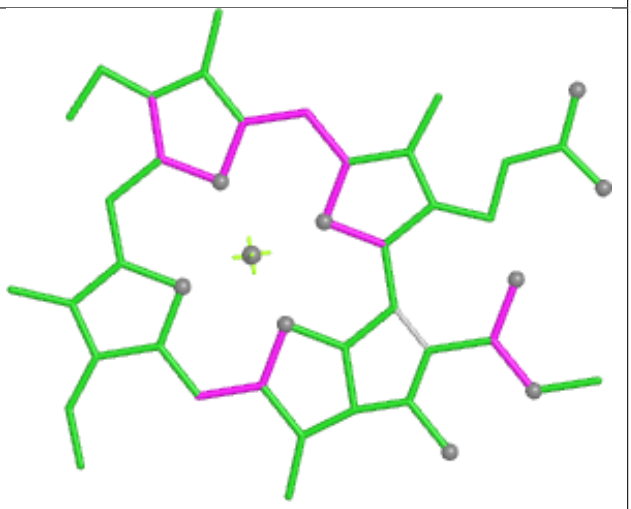


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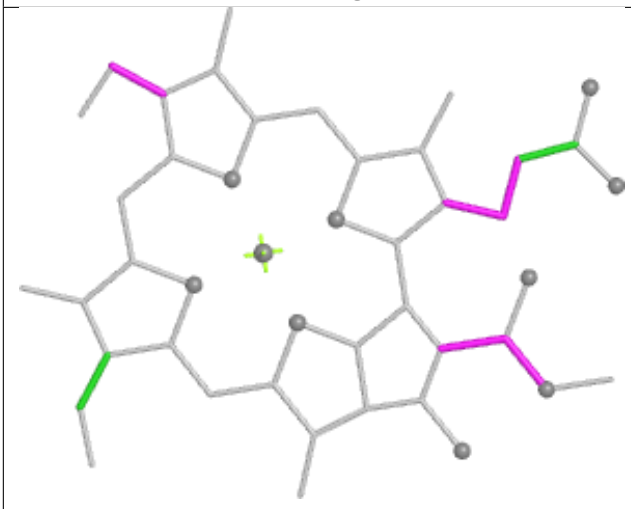
Ligand CLA J 101



Bond lengths



Bond angles

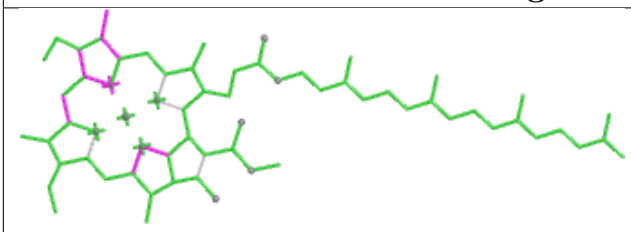


Torsions

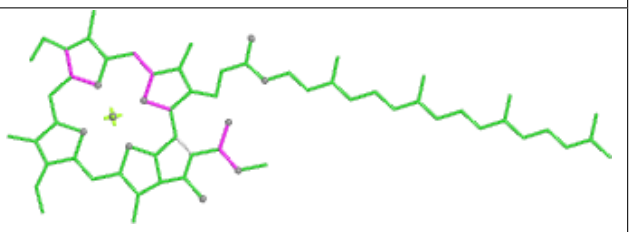


Rings

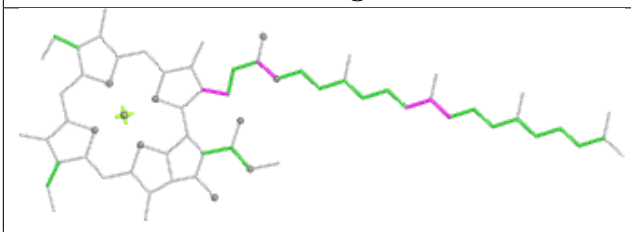
Ligand CLA b 818



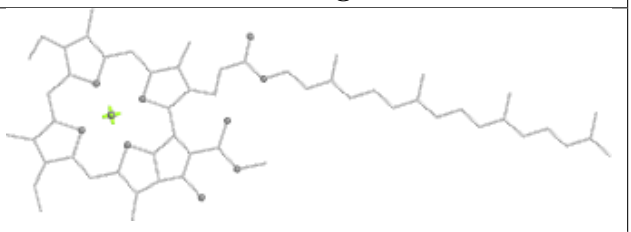
Bond lengths



Bond angles

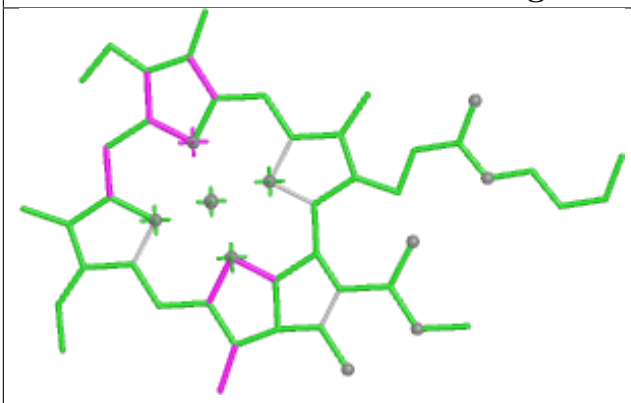


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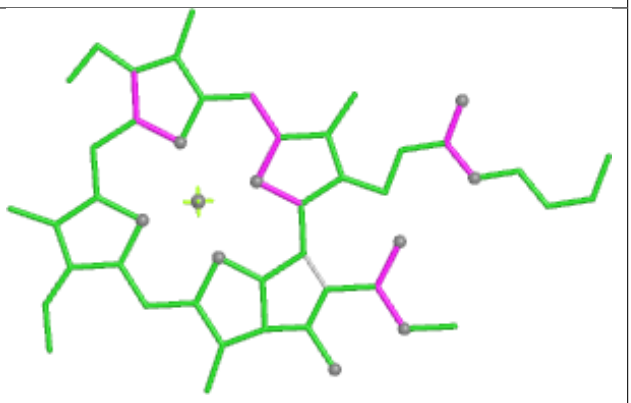


Rings

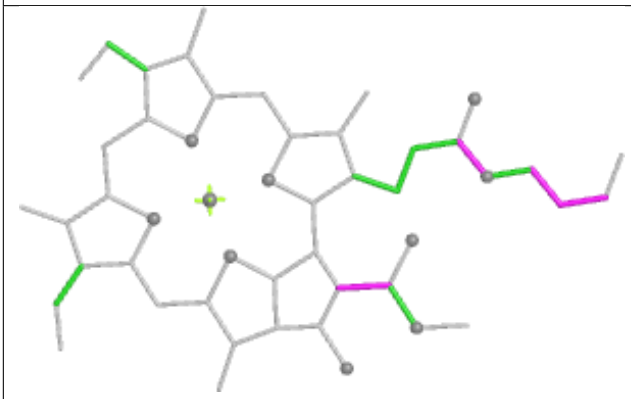
Ligand CLA b 815



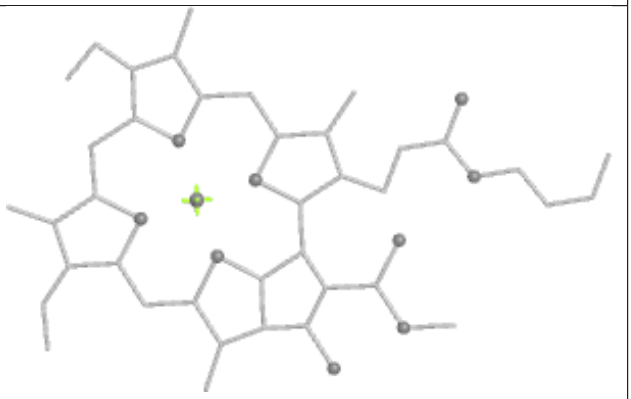
Bond lengths



Bond angles

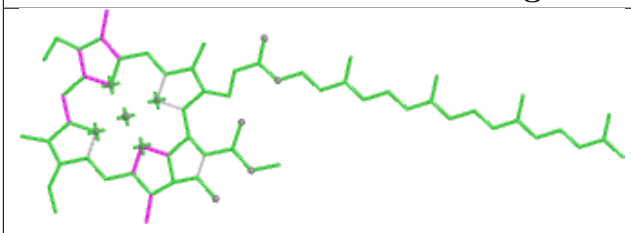


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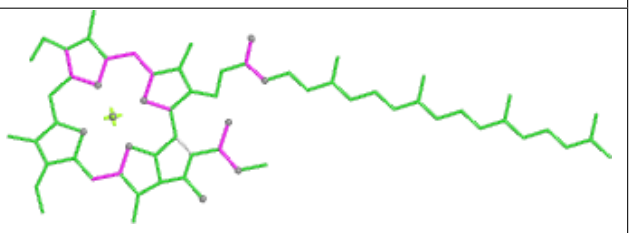


Rings

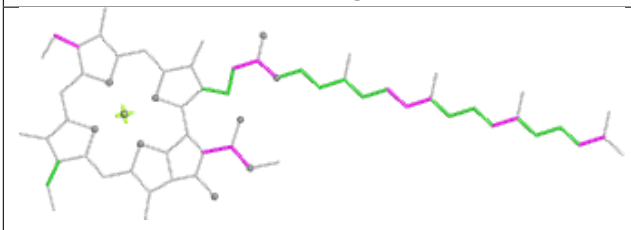
Ligand CLA A 833



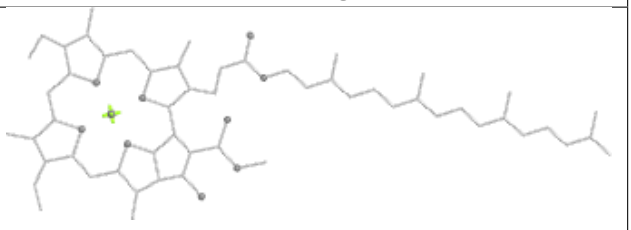
Bond lengths



Bond angles

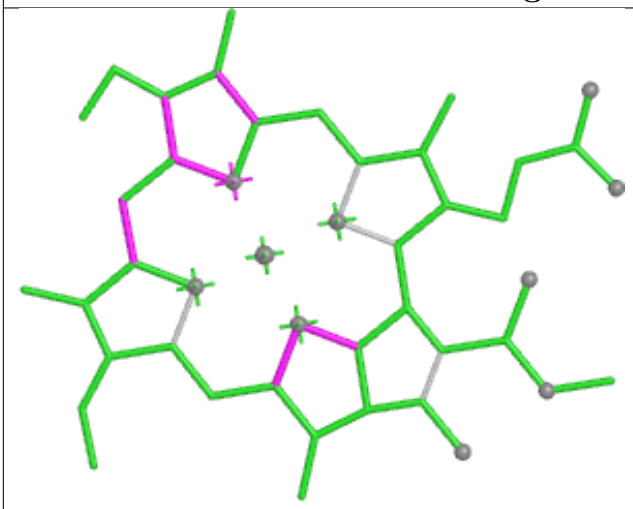


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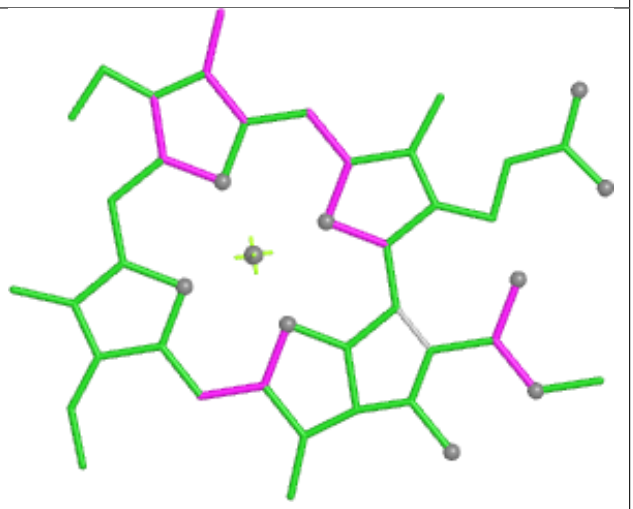


Rings

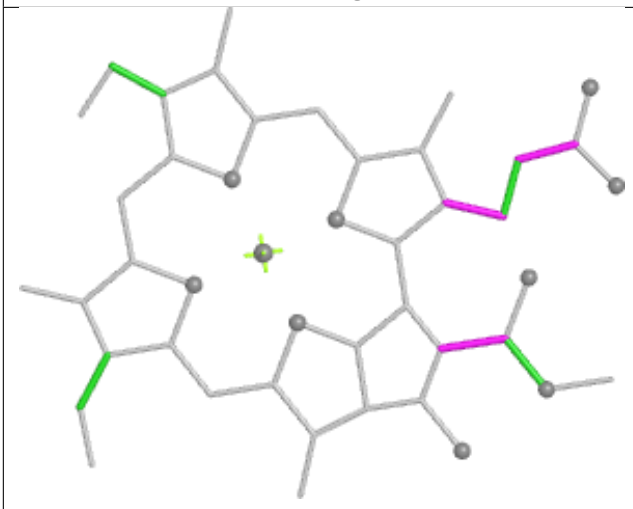
Ligand CLA A 815



Bond lengths



Bond angles

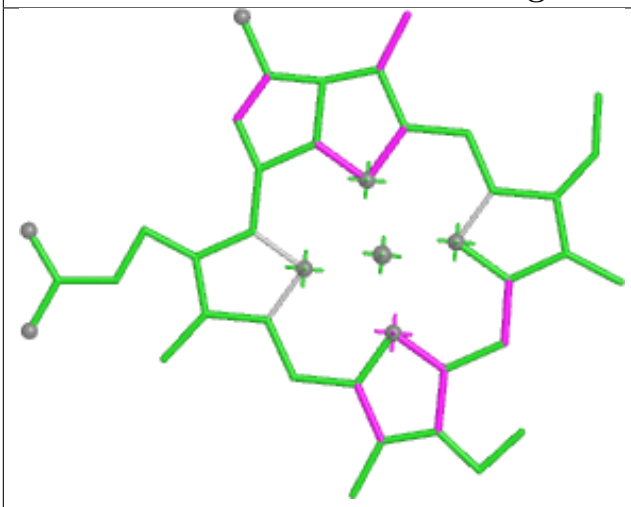


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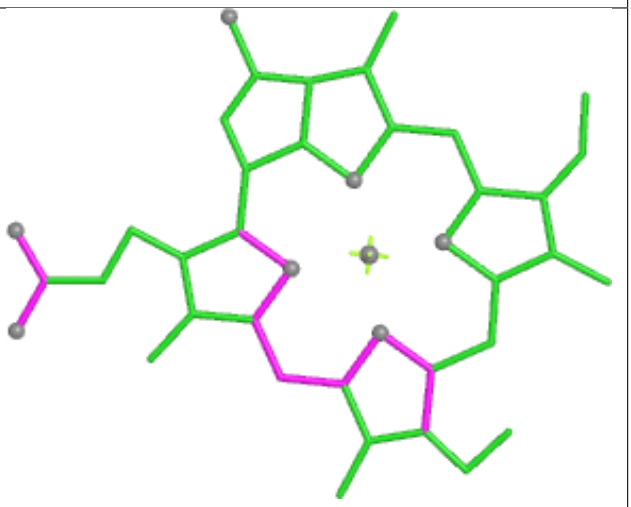


Rings

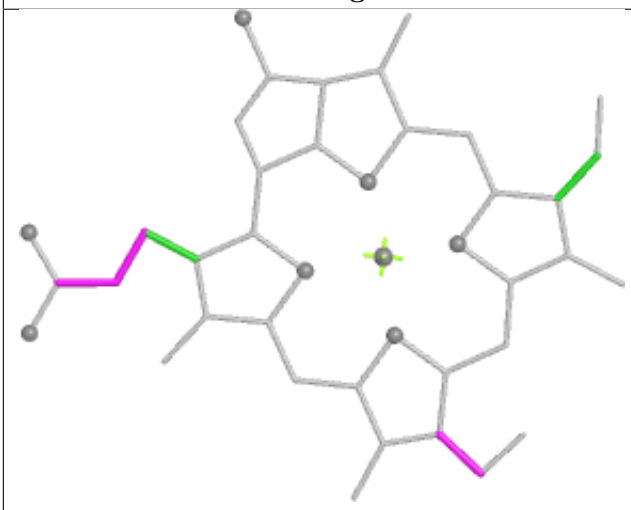
Ligand CLA k 101



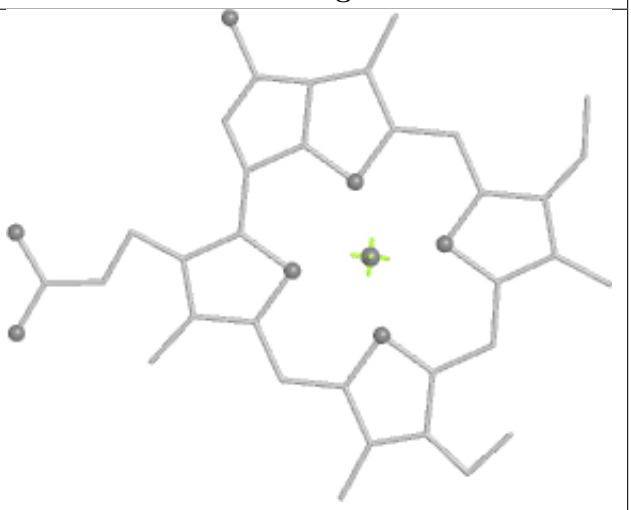
Bond lengths



Bond angles

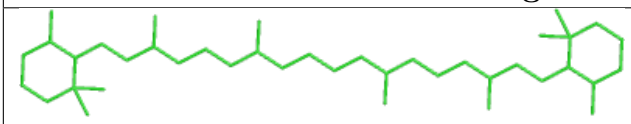


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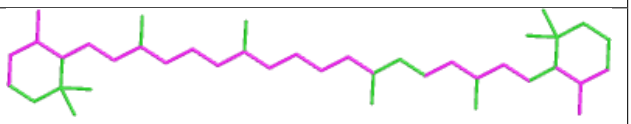


Rings

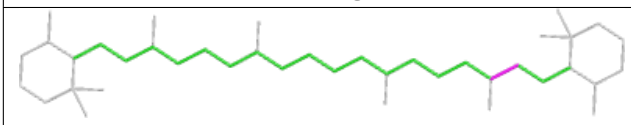
Ligand BCR B 847



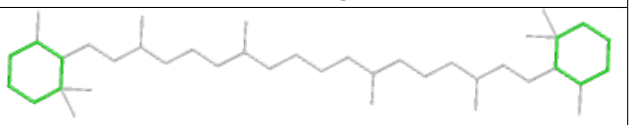
Bond lengths



Bond angles

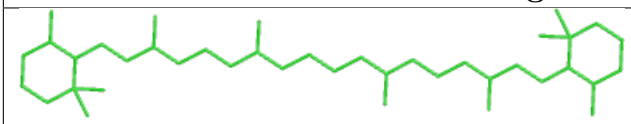


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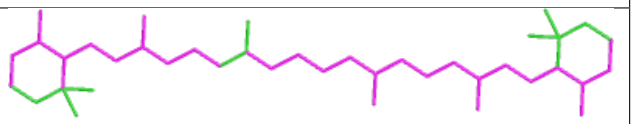


Rings

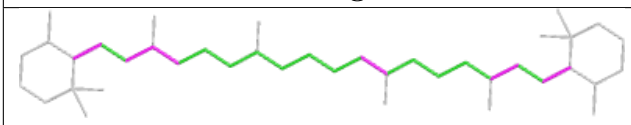
Ligand BCR a 848



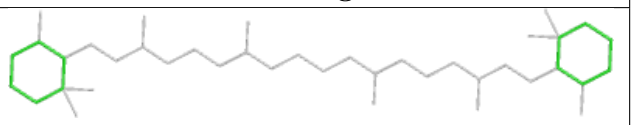
Bond lengths



Bond angles

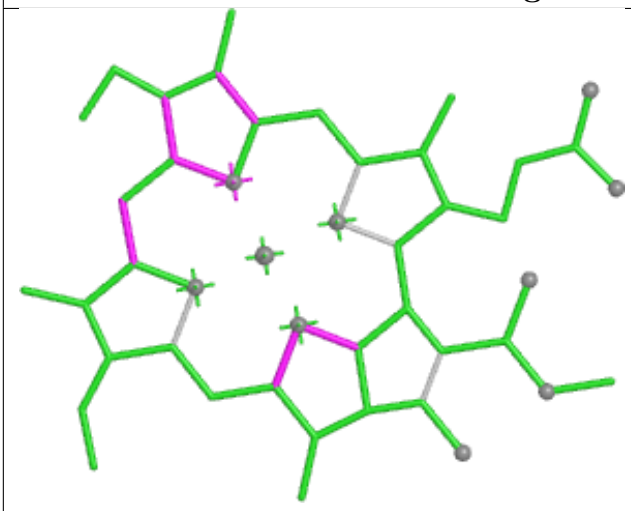


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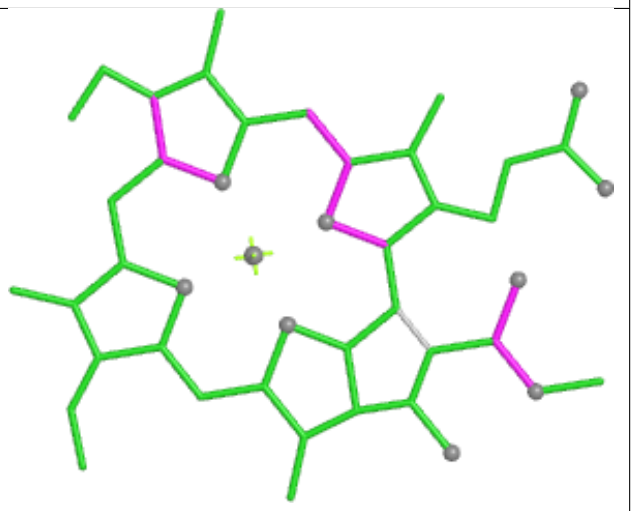


Rings

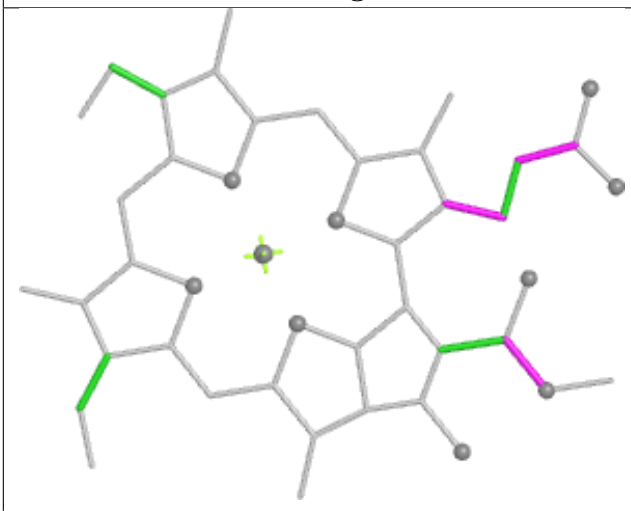
Ligand CLA A 814



Bond lengths



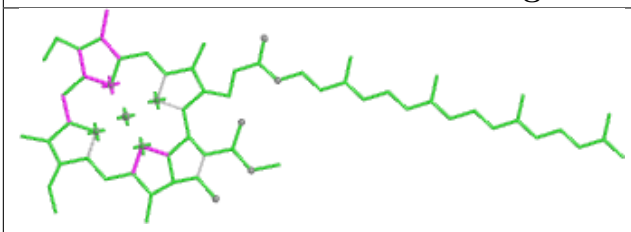
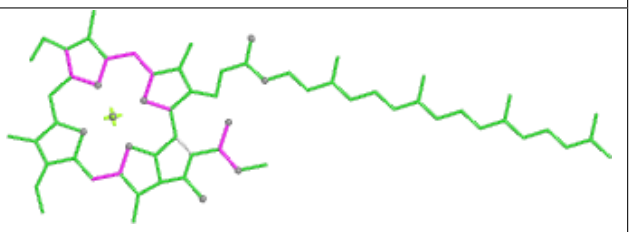
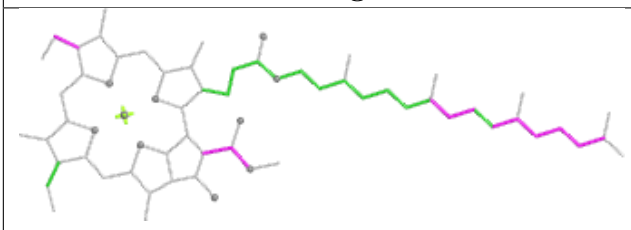
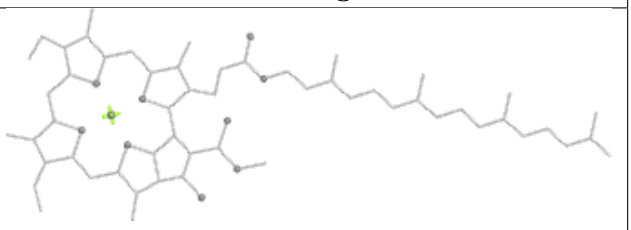
Bond angles

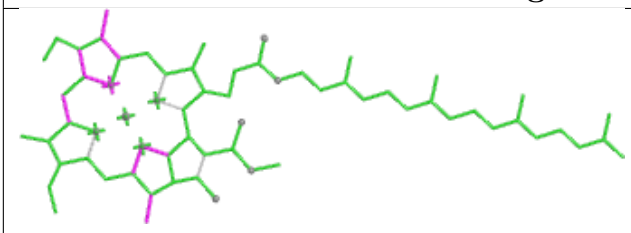
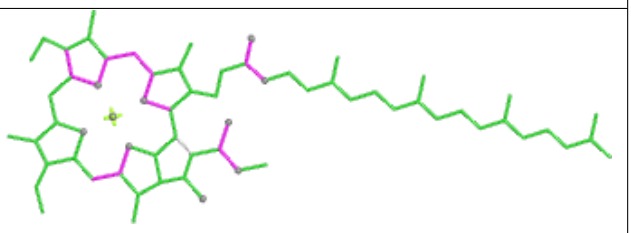
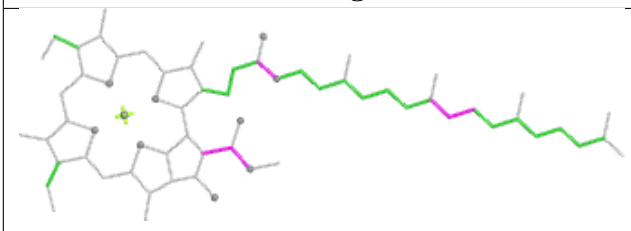
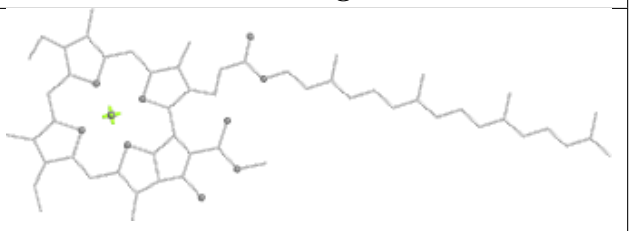


Torsions

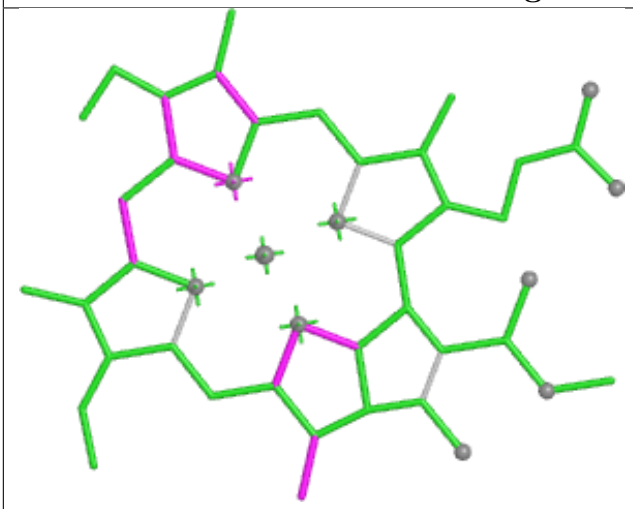


Rings

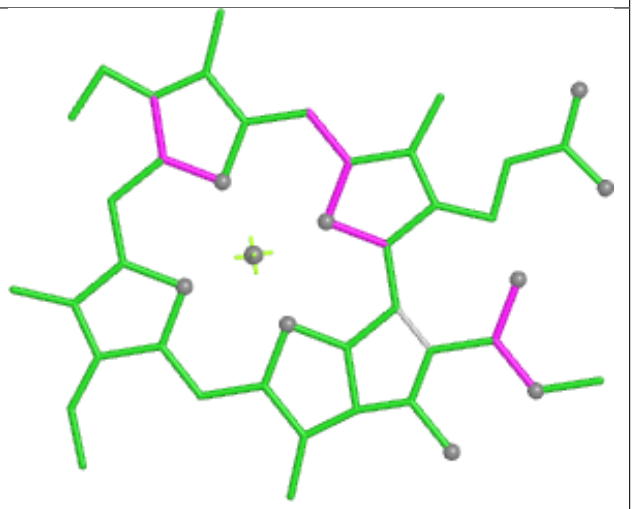
Ligand CLA N 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

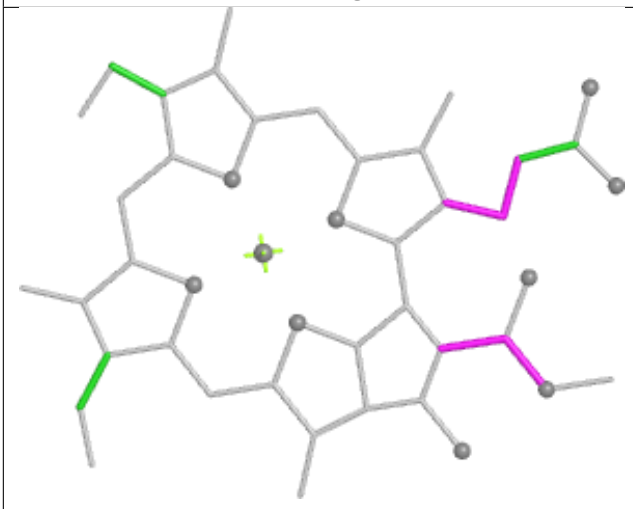
Ligand CLA w 205



Bond lengths



Bond angles

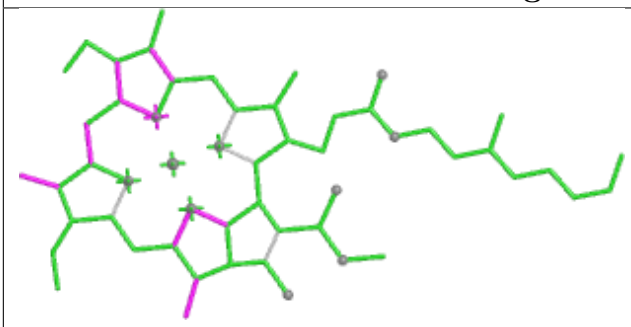


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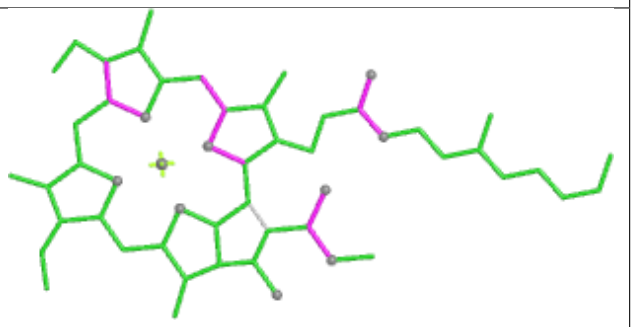


Rings

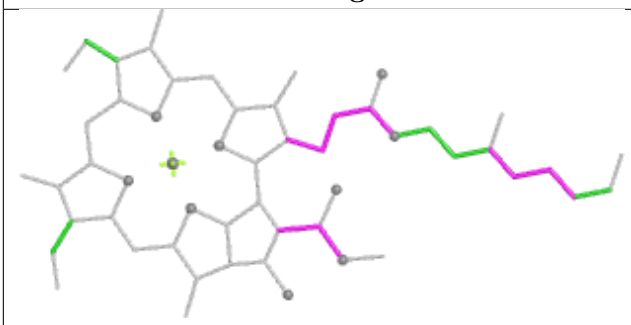
Ligand CLA A 819



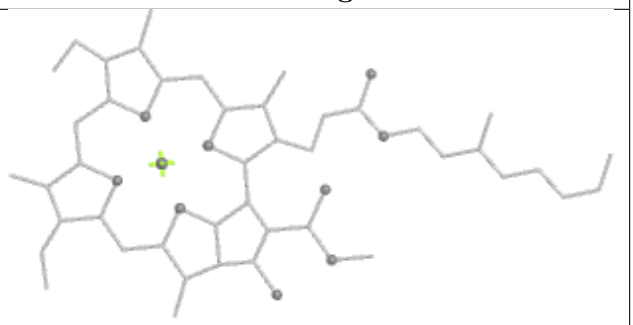
Bond lengths



Bond angles

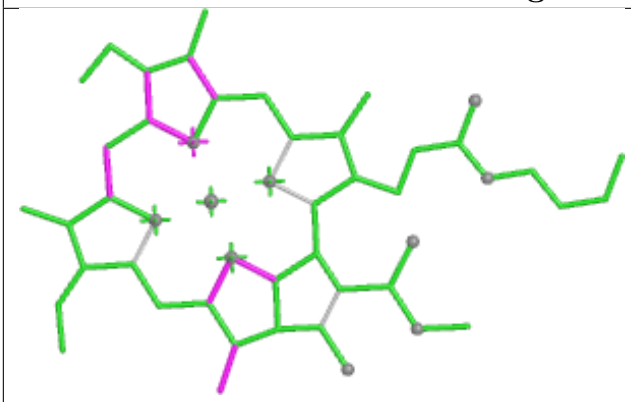


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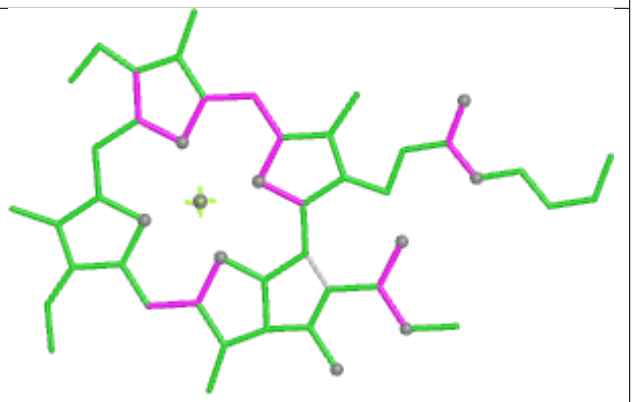


Rings

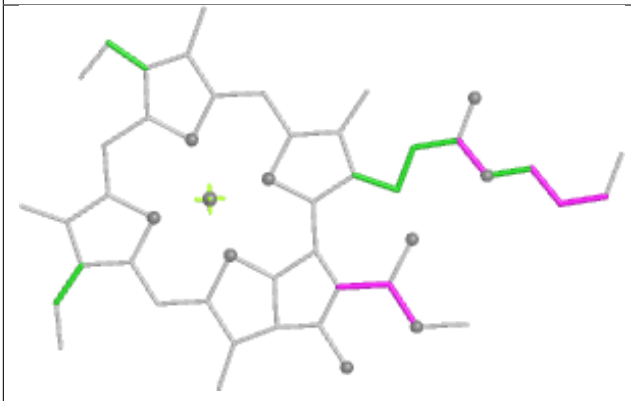
Ligand CLA n 815



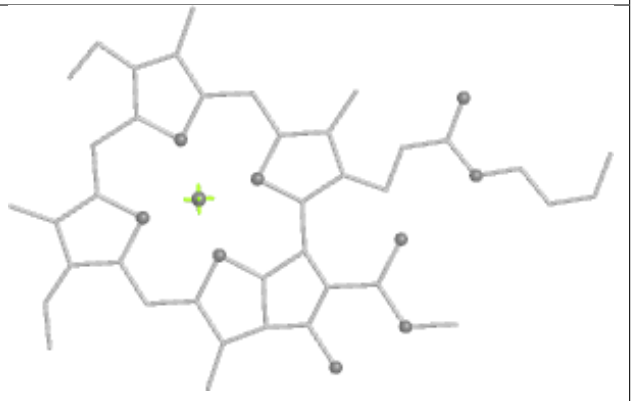
Bond lengths



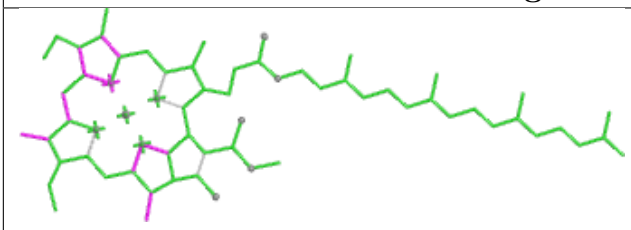
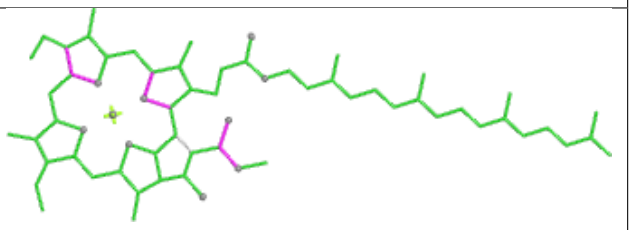
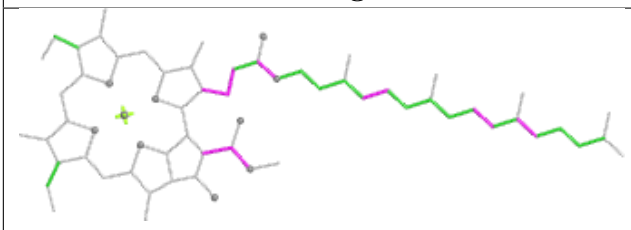
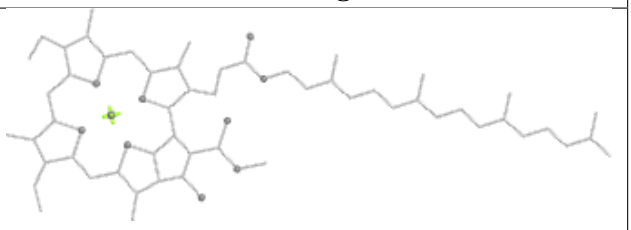
Bond angles

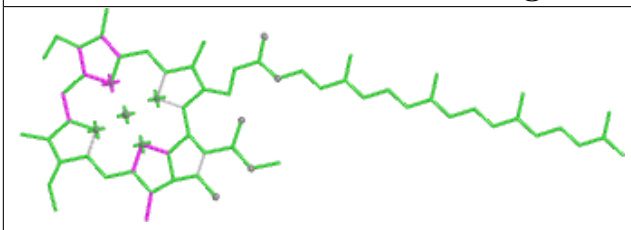
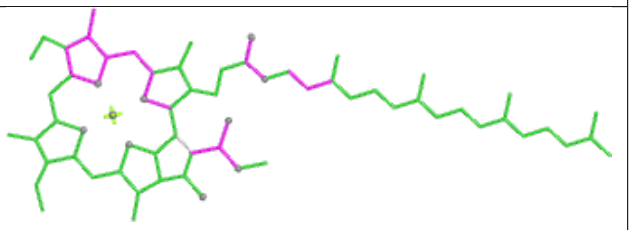
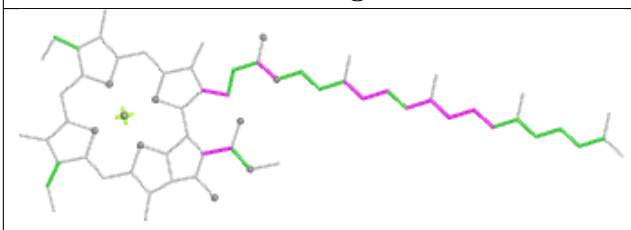
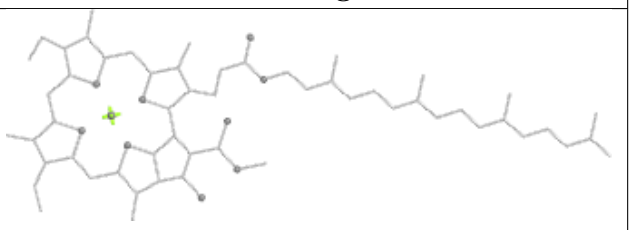


Torsions

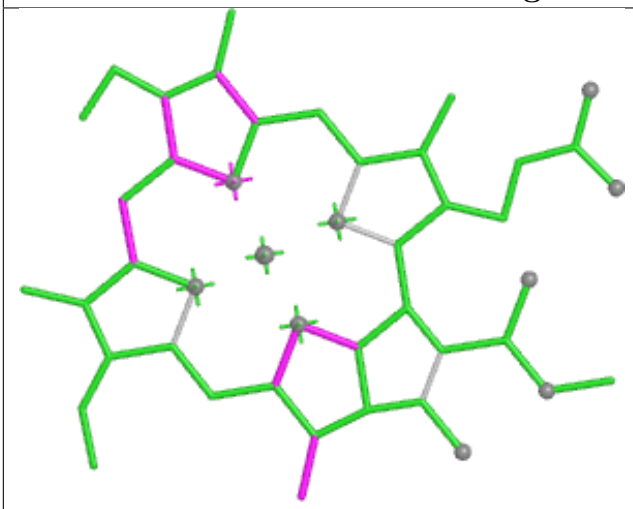


Rings

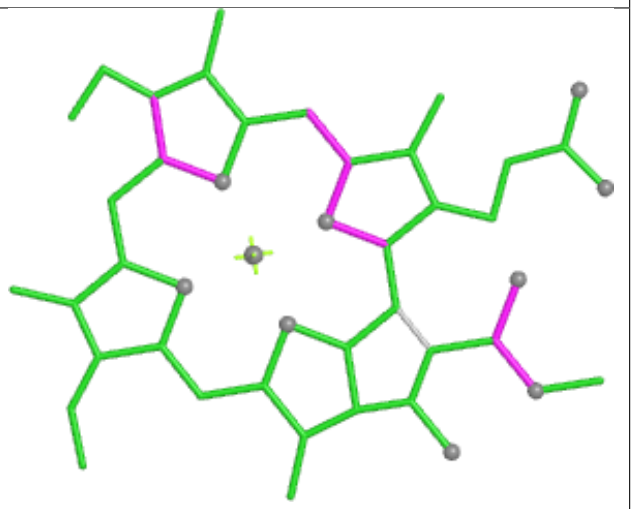
Ligand CLA B 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

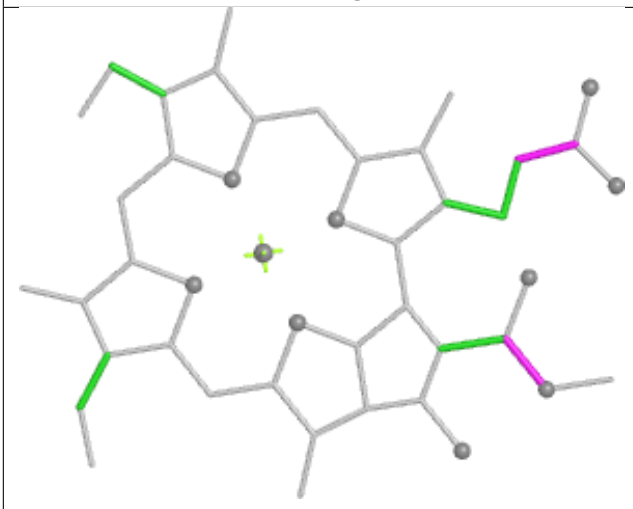
Ligand CLA N 818



Bond lengths



Bond angles

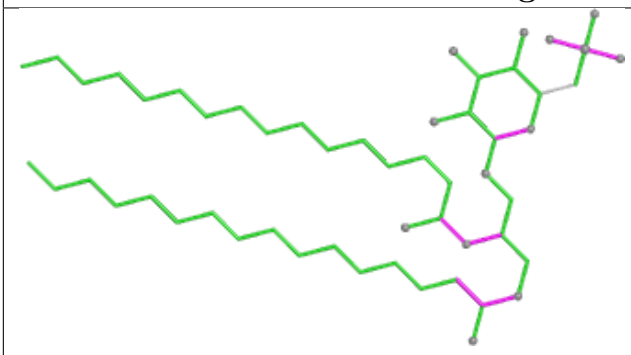


Torsions

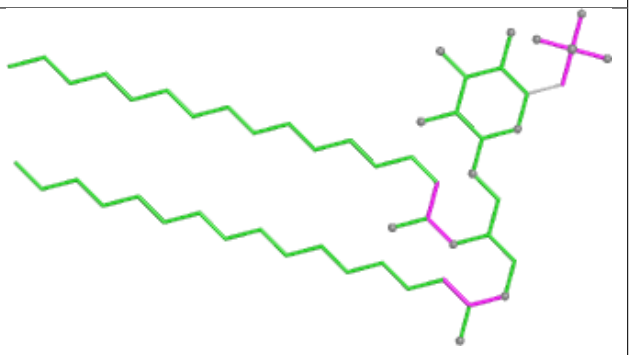


Rings

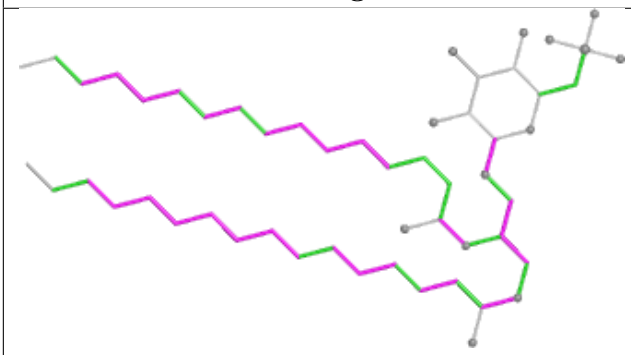
Ligand SQD h 1702



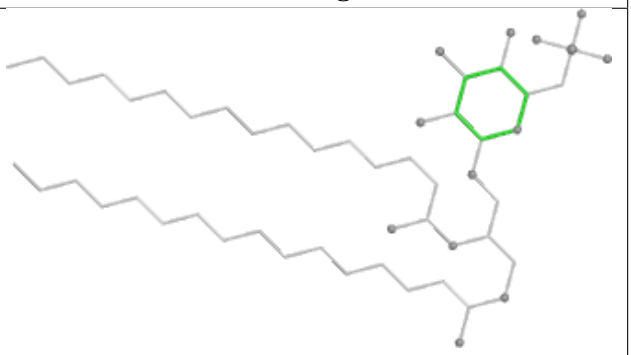
Bond lengths



Bond angles

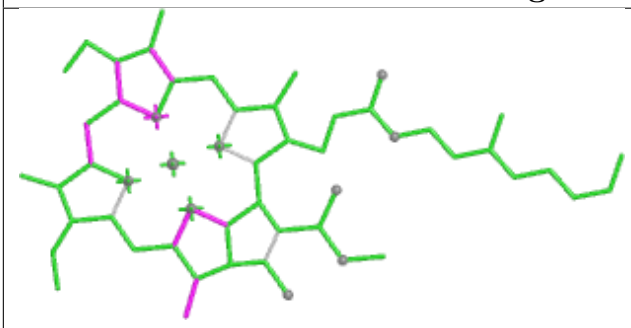


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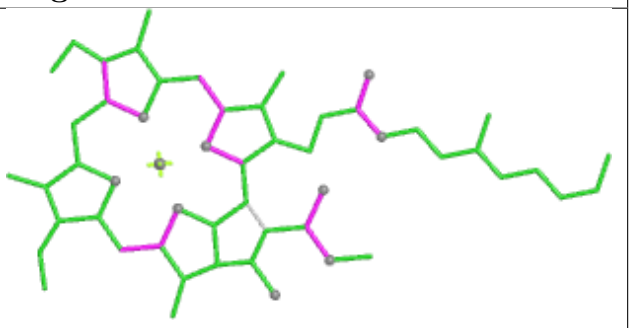


Rings

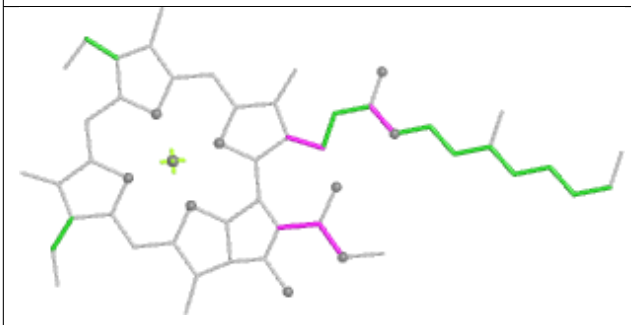
Ligand CLA g 812



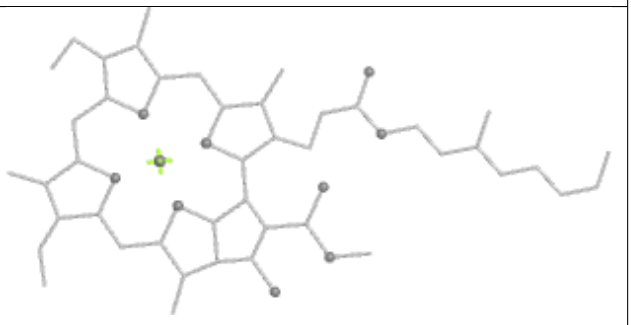
Bond lengths



Bond angles

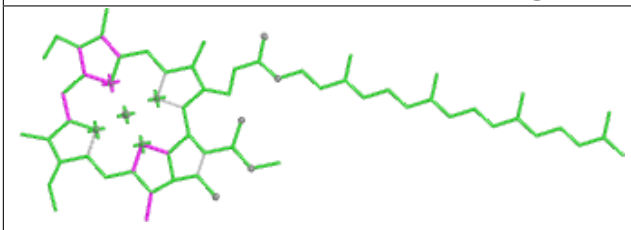


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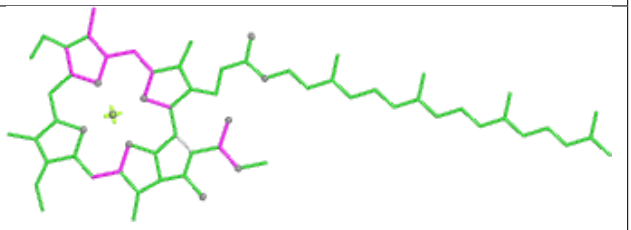


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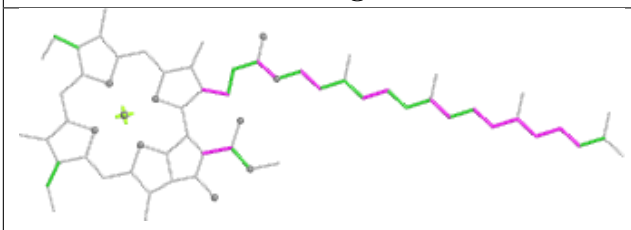
Ligand CLA a 803



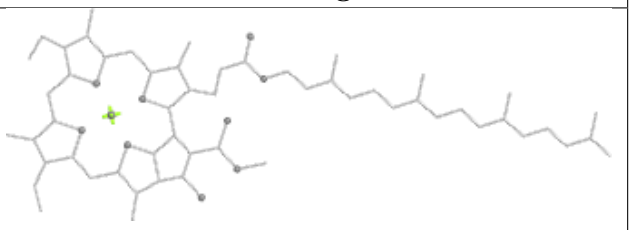
Bond lengths



Bond angles

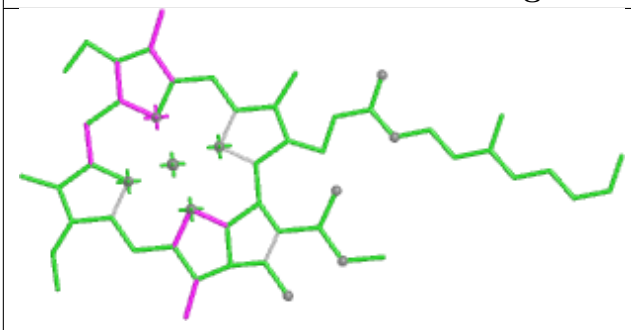


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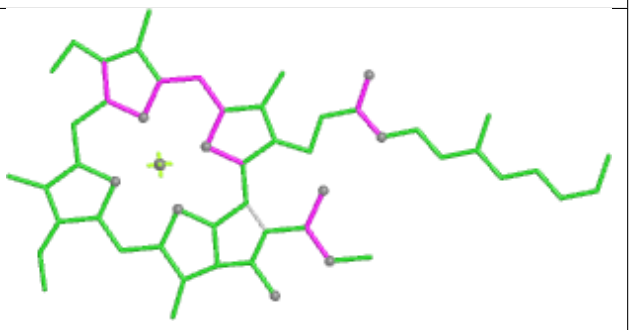


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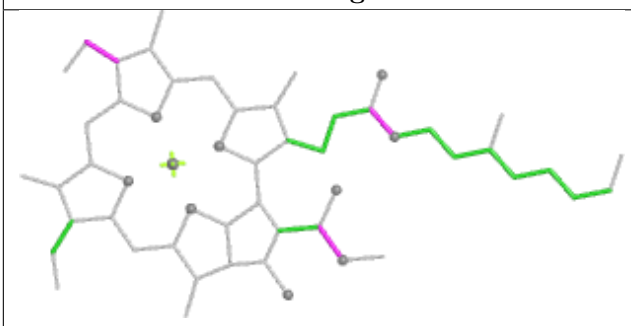
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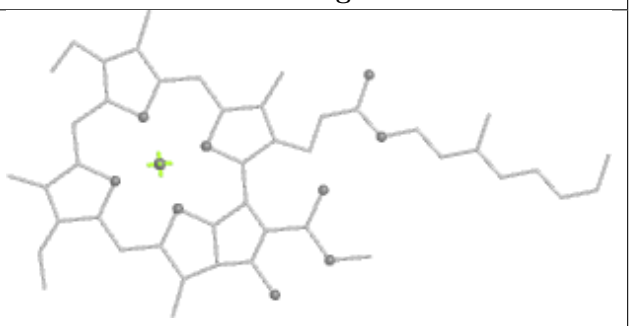
Bond lengths



Bond angles

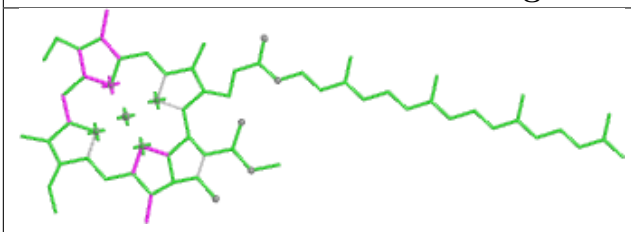


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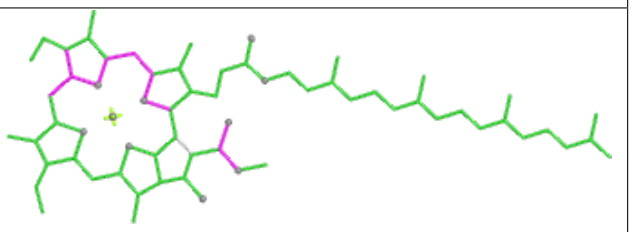


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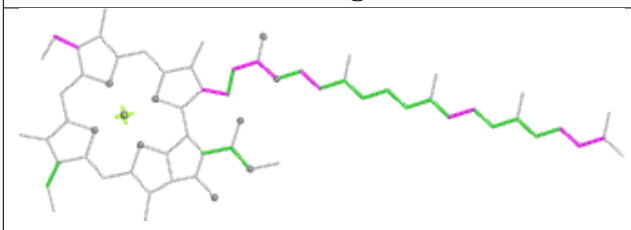
Ligand CLA N 819



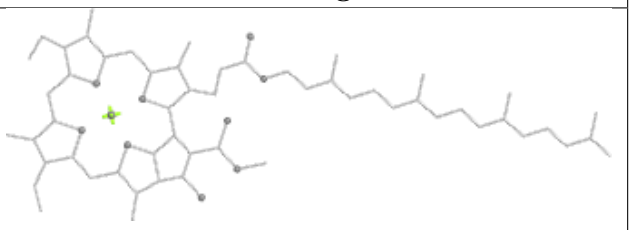
Bond lengths



Bond angles

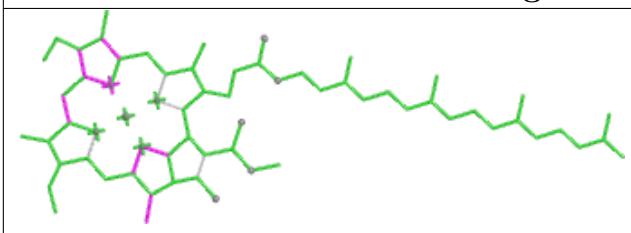


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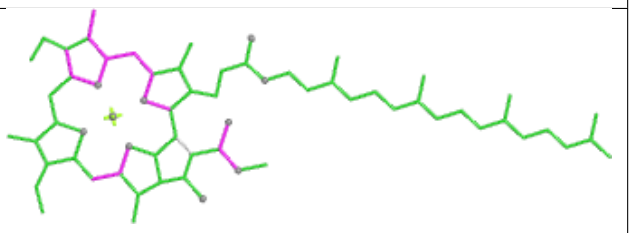


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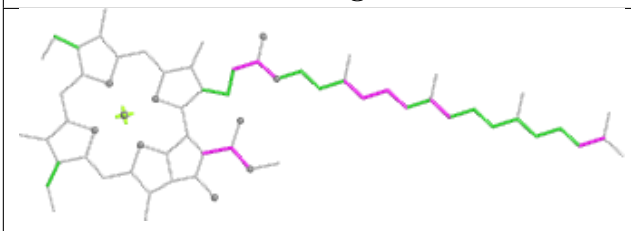
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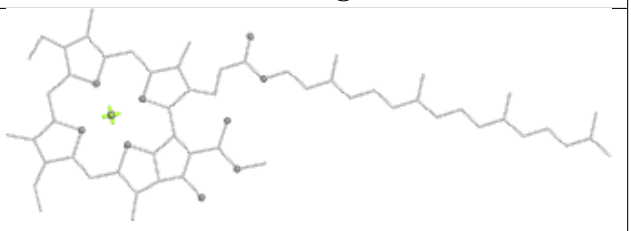
Bond lengths



Bond angles

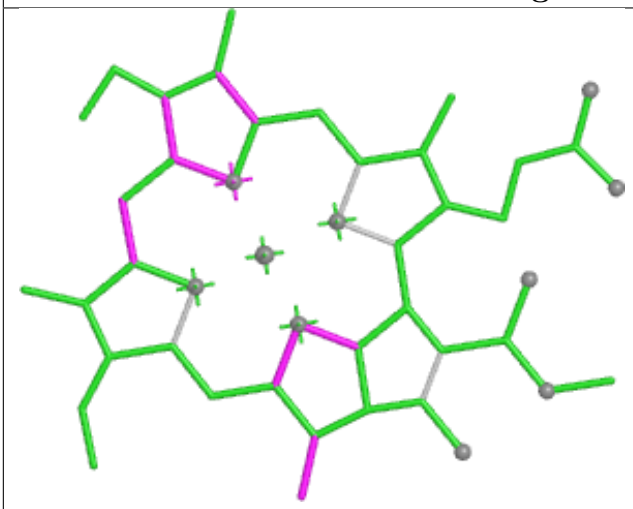


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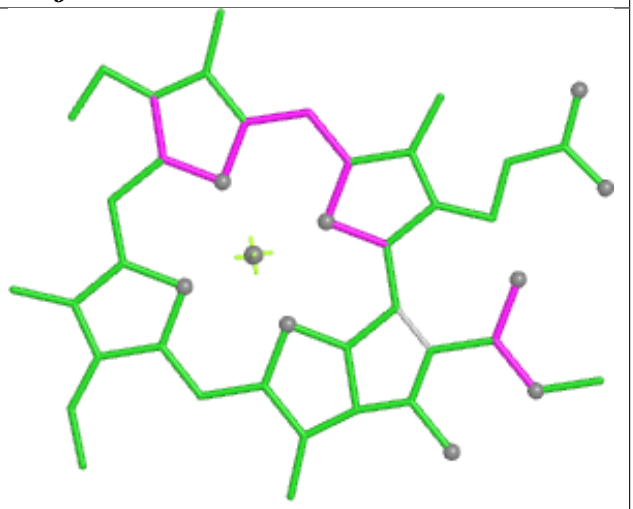


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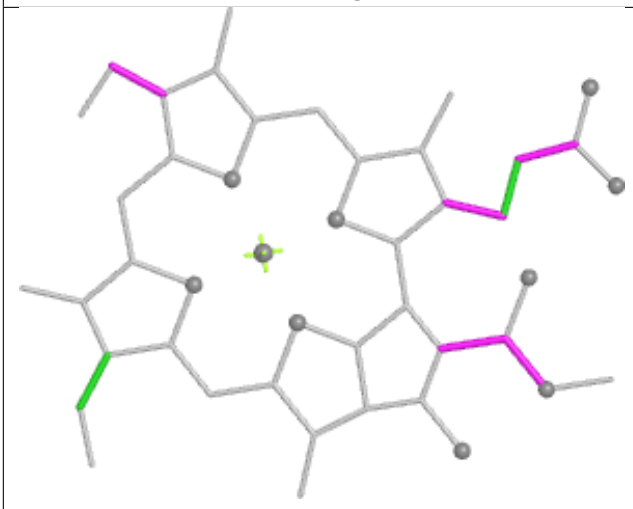
Ligand CLA j 101



Bond lengths



Bond angles

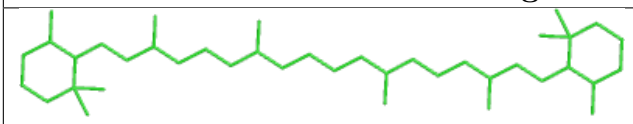


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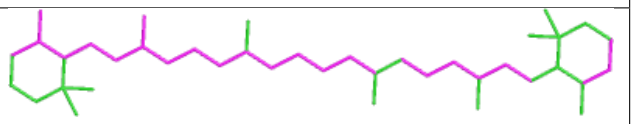


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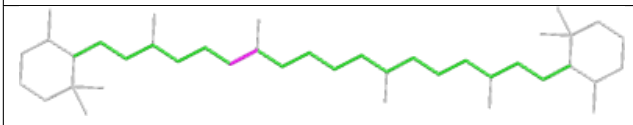
Ligand BCR G 843



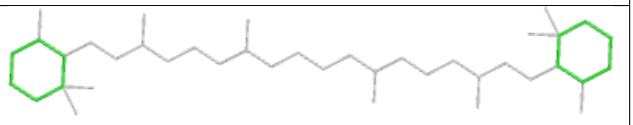
Bond lengths



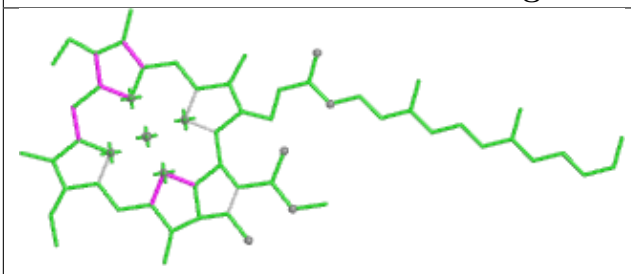
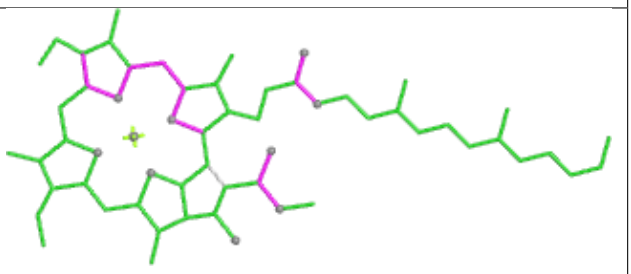
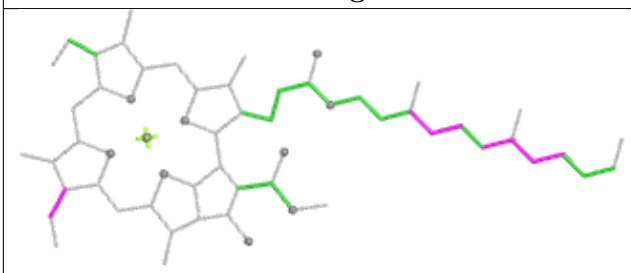
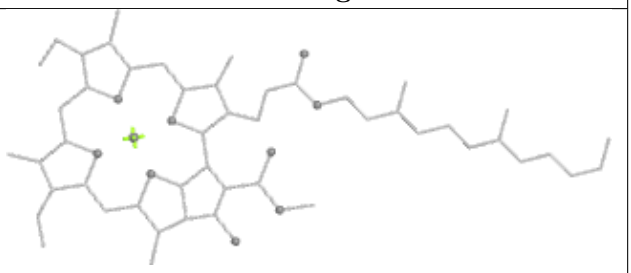
Bond angles

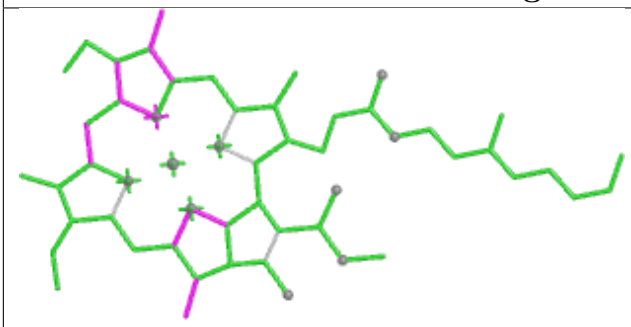
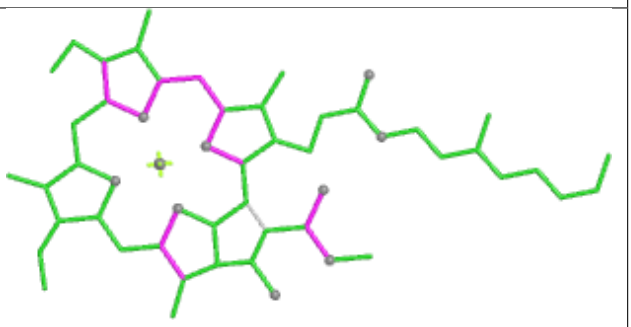
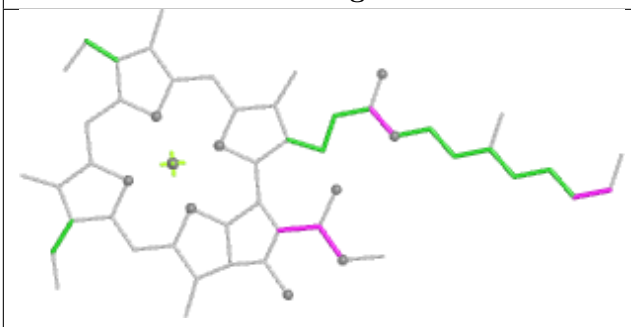
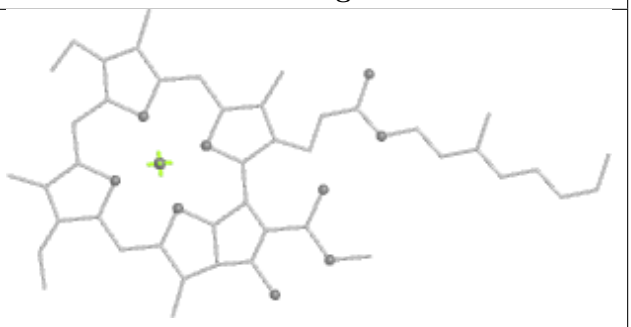


Torsions

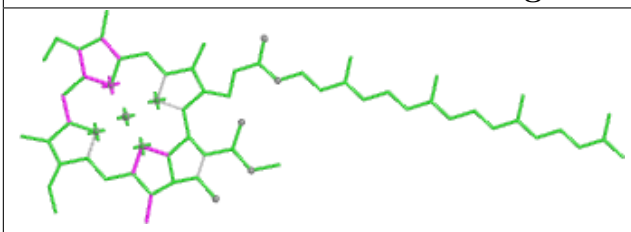


Rings

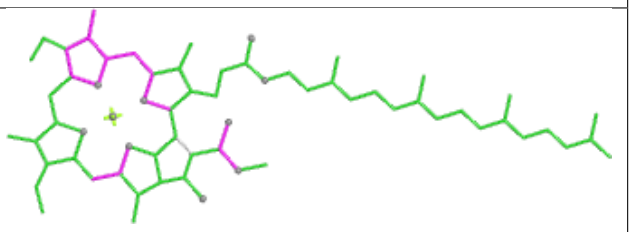
Ligand CLA G 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

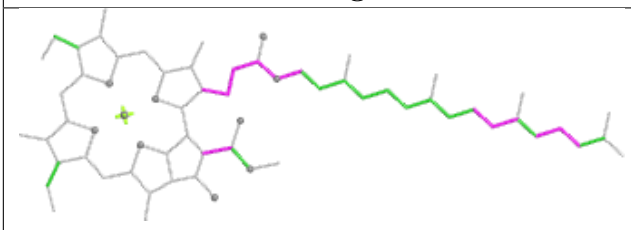
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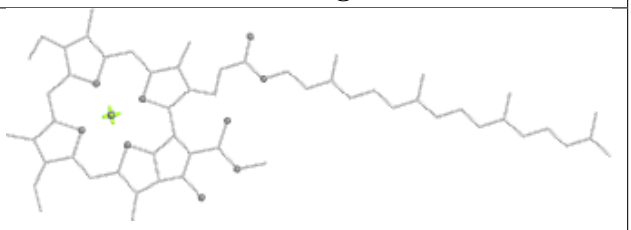
Bond lengths



Bond angles

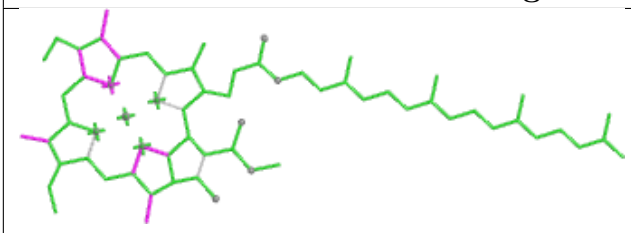


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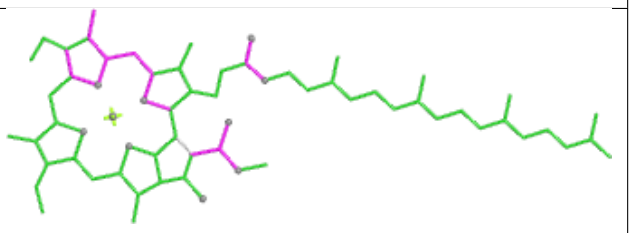


Rings

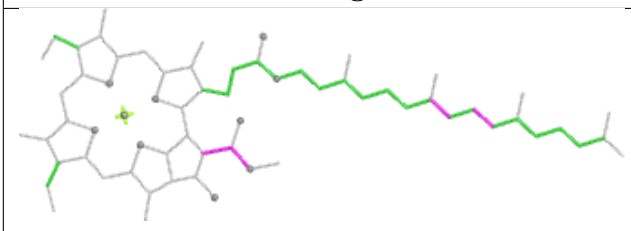
Ligand CLA G 829



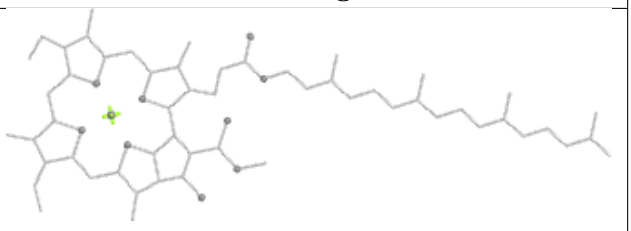
Bond lengths



Bond angles

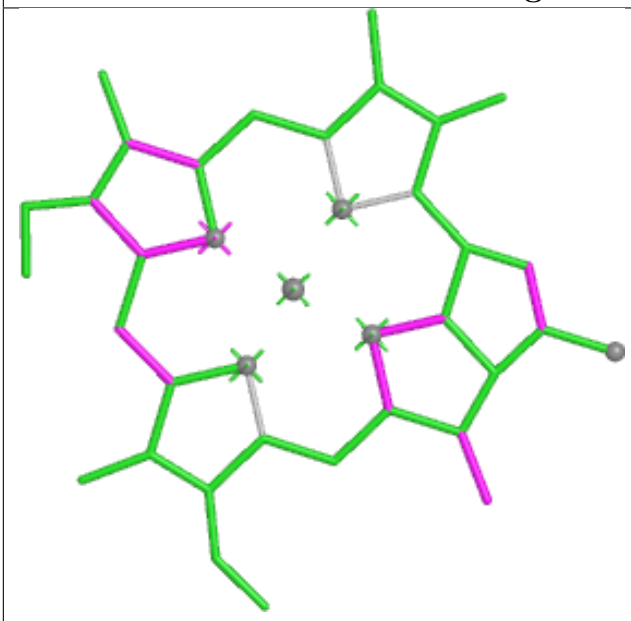


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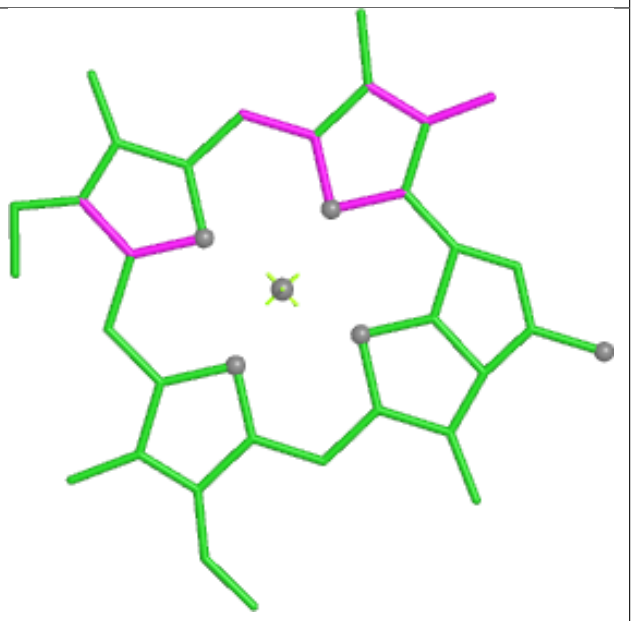


Rings

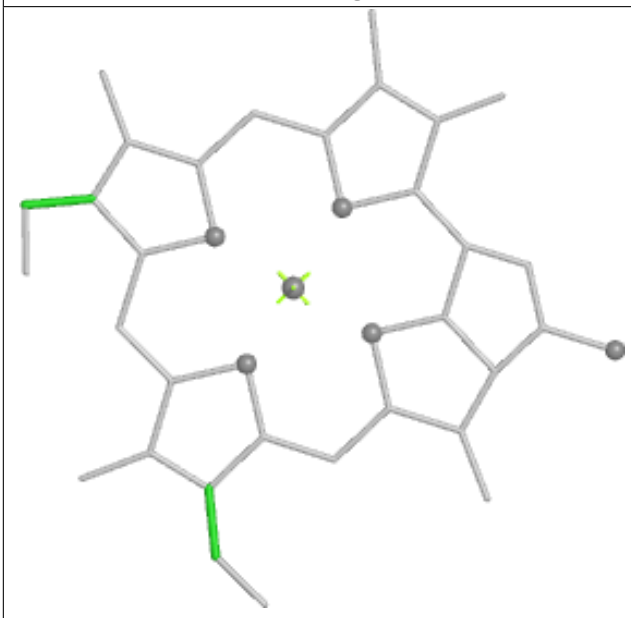
Ligand CLA T 102



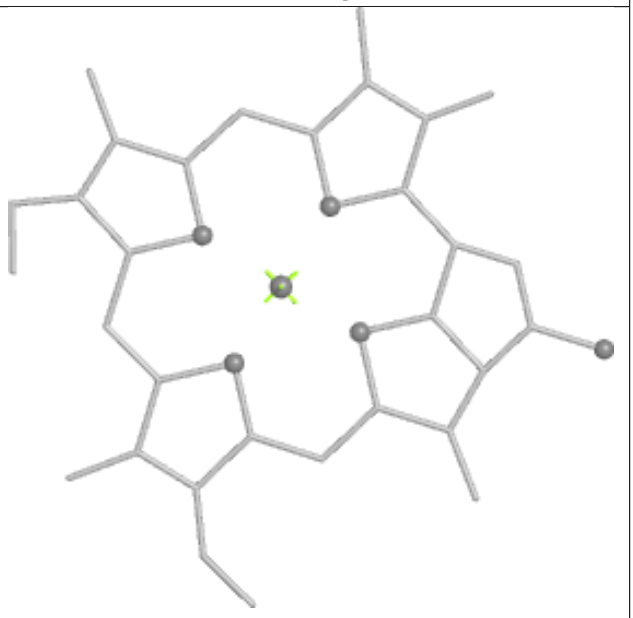
Bond lengths



Bond angles

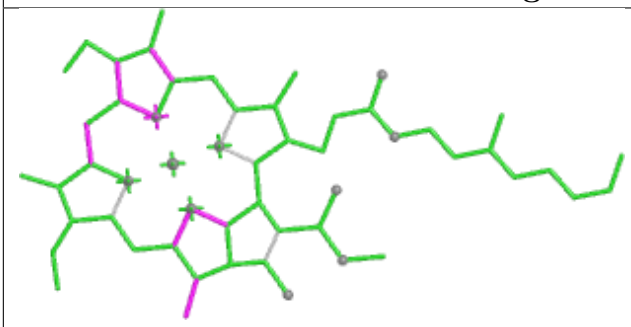


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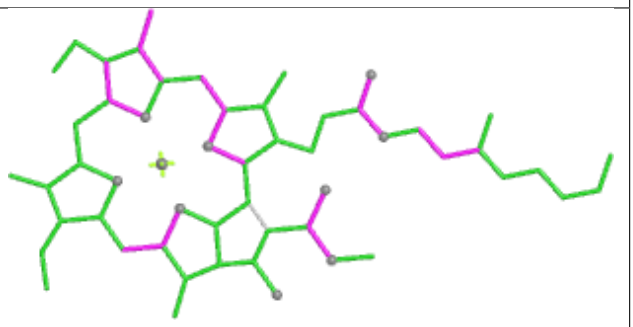


Rings

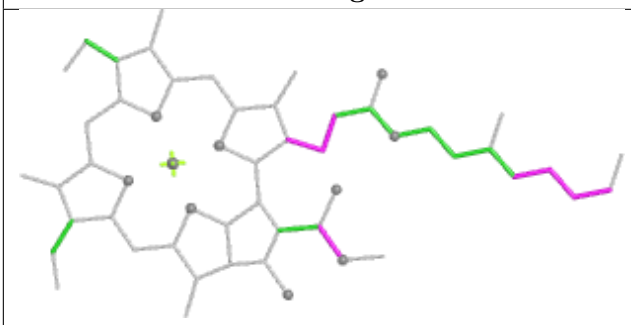
Ligand CLA G 822



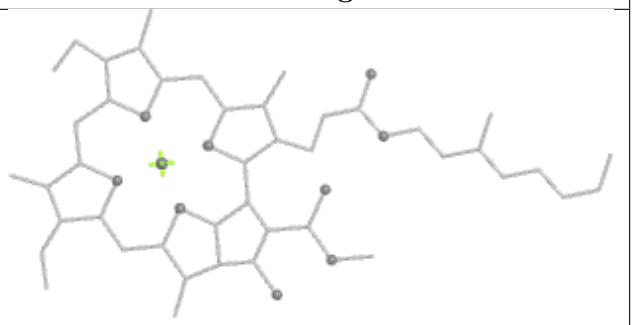
Bond lengths



Bond angles

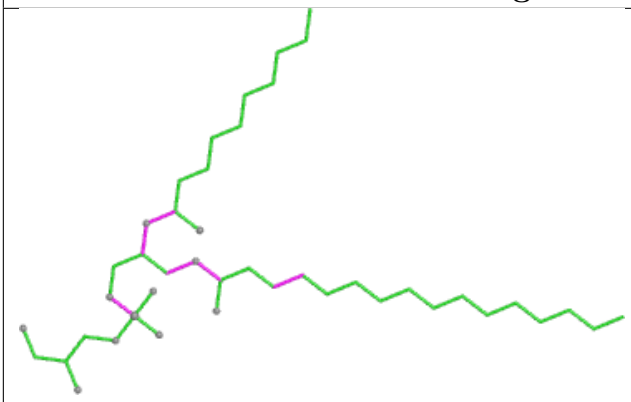


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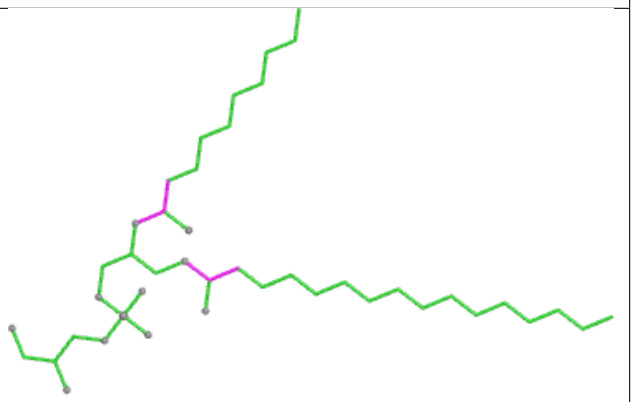


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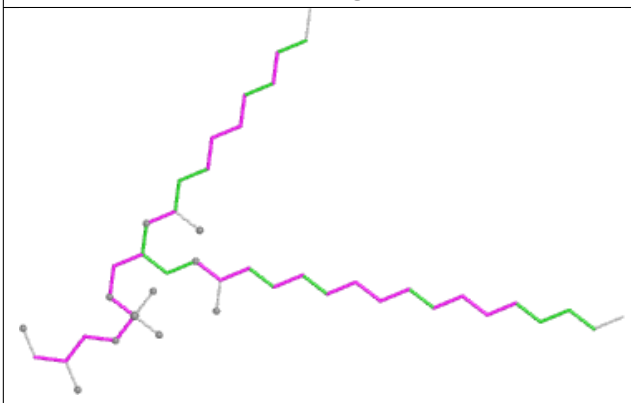
Ligand LHG X 1702



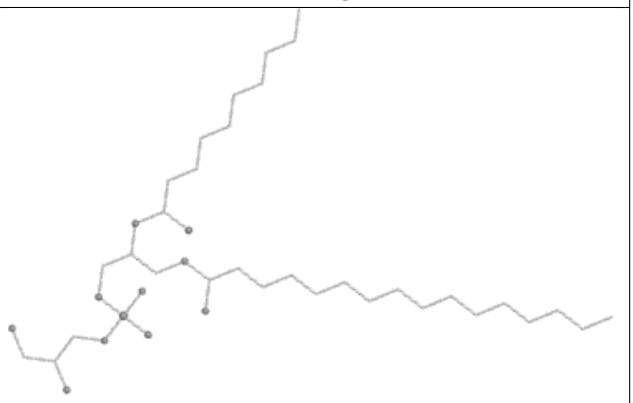
Bond lengths



Bond angles

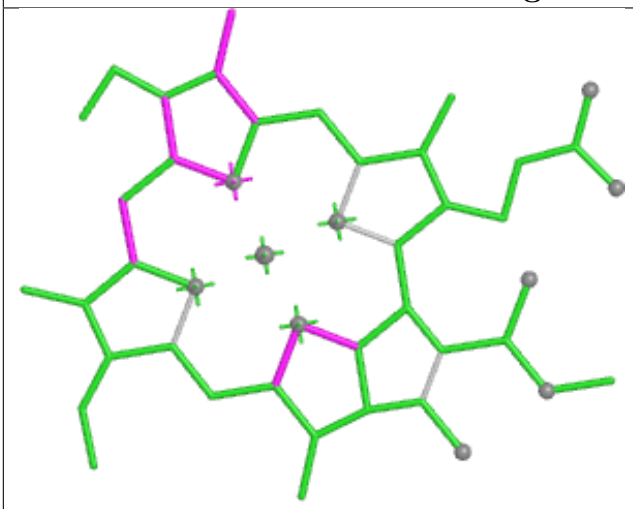


Torsions

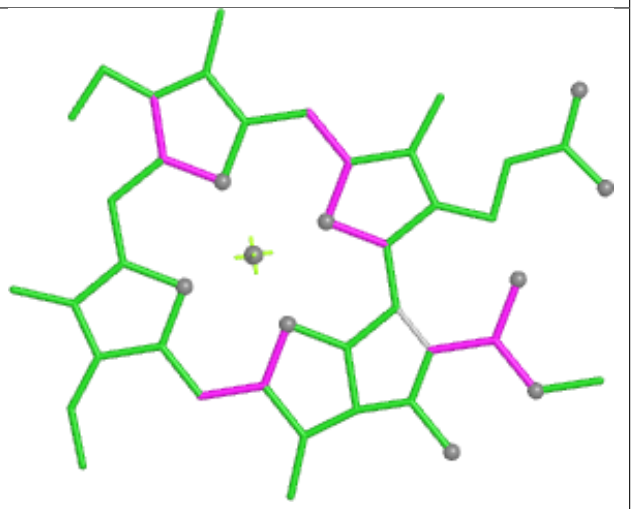


Rings

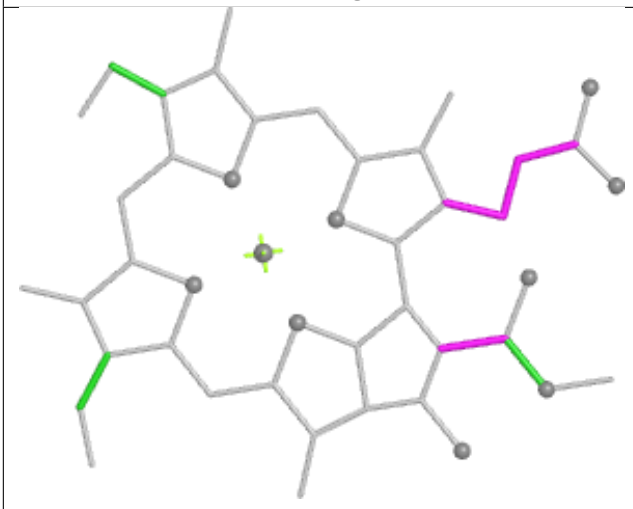
Ligand CLA A 821



Bond lengths



Bond angles

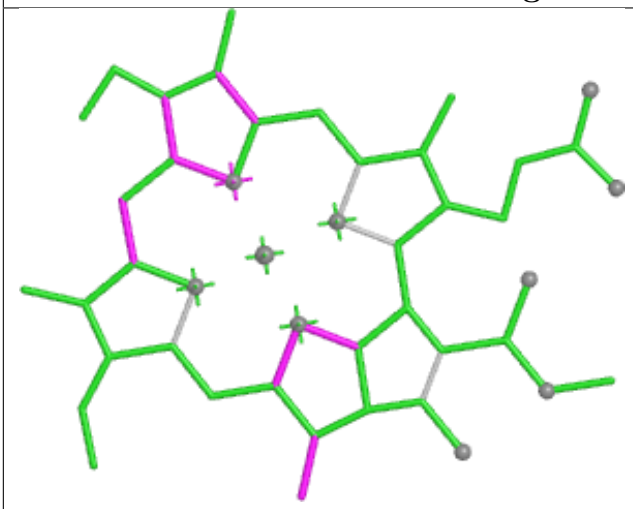


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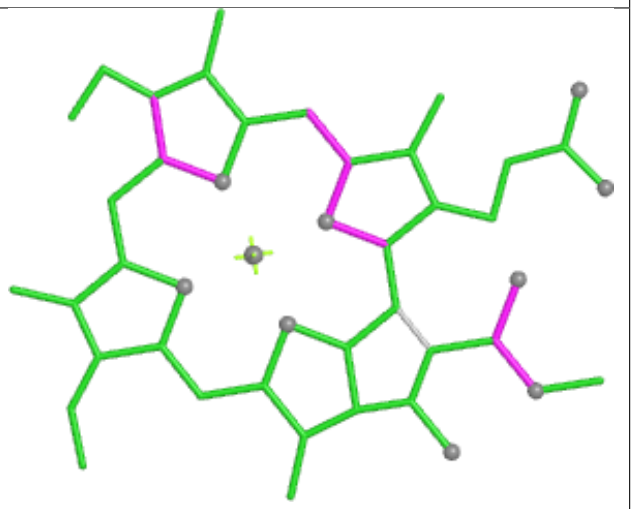


Rings

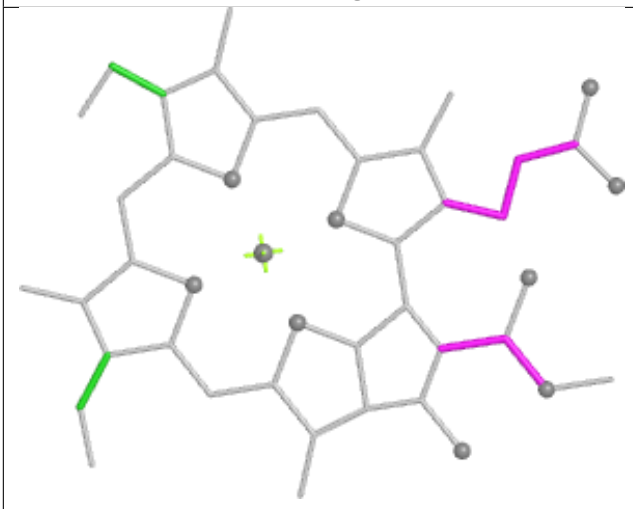
Ligand CLA G 835



Bond lengths



Bond angles

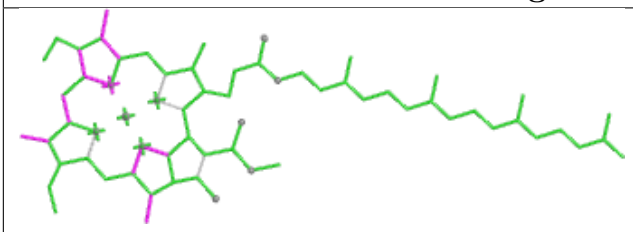


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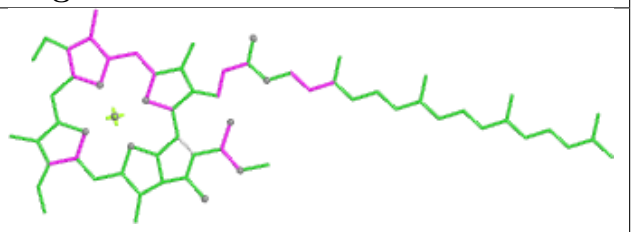


Rings

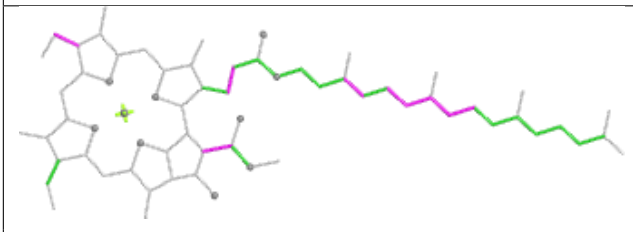
Ligand CLA g 852



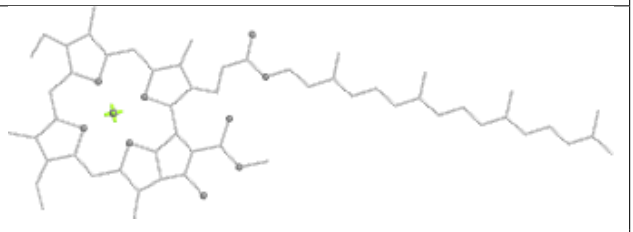
Bond lengths



Bond angles

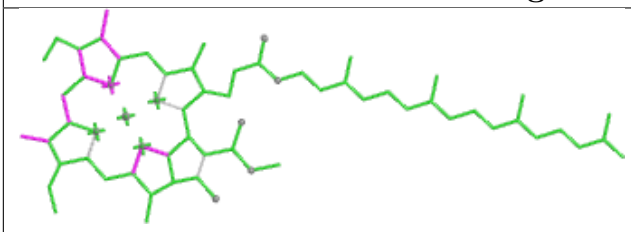


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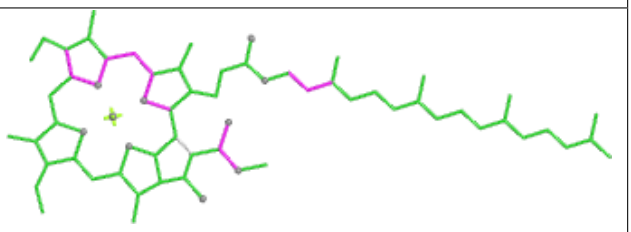


Rings

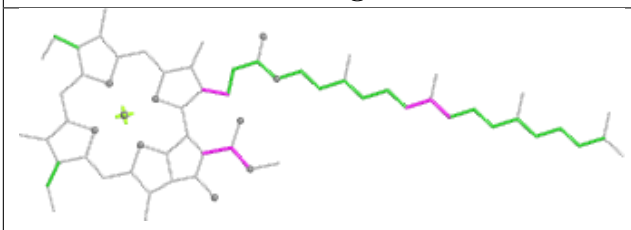
Ligand CLA n 826



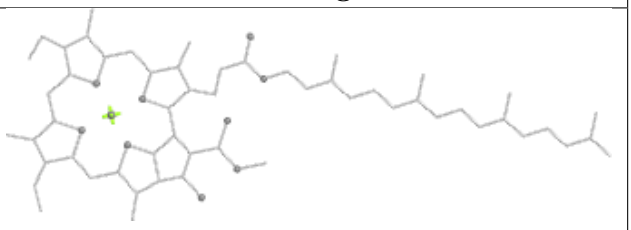
Bond lengths



Bond angles

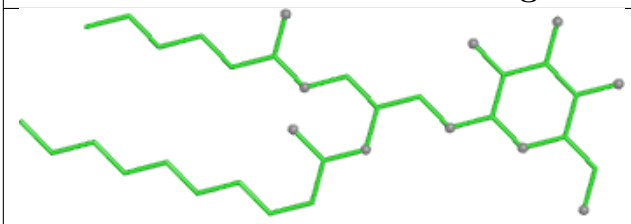


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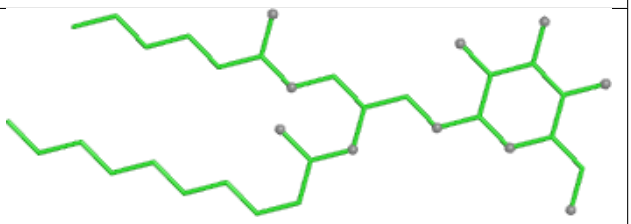


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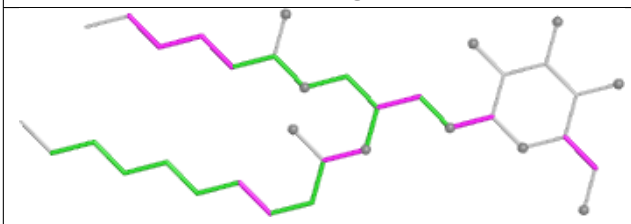
Ligand LMG B 802



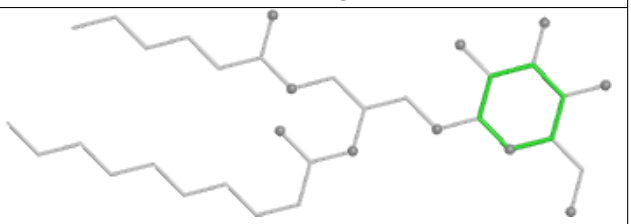
Bond lengths



Bond angles



Torsions



Rings

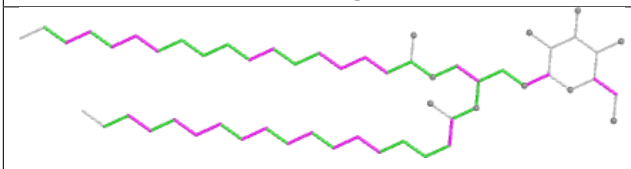
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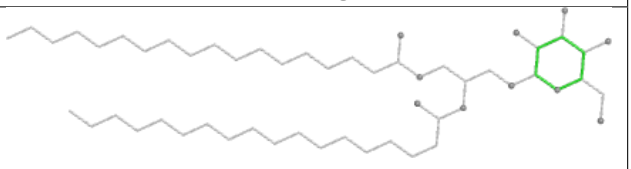
Bond lengths



Bond angles

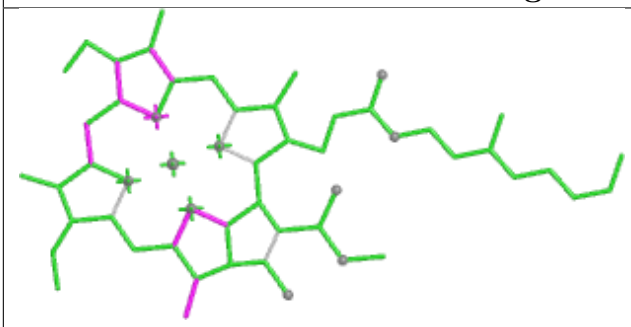


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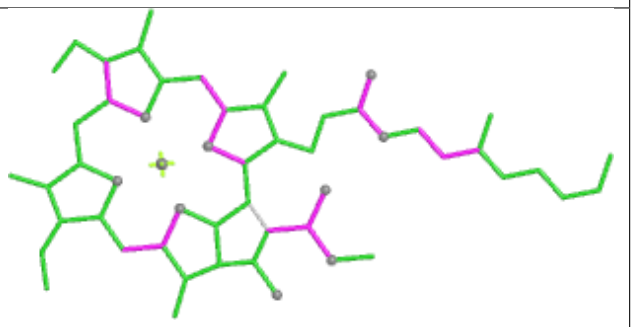


Rings

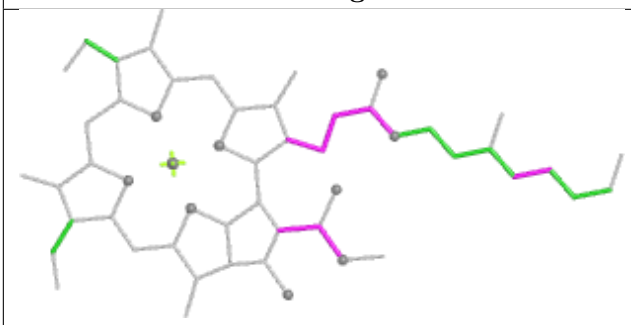
Ligand CLA B 834



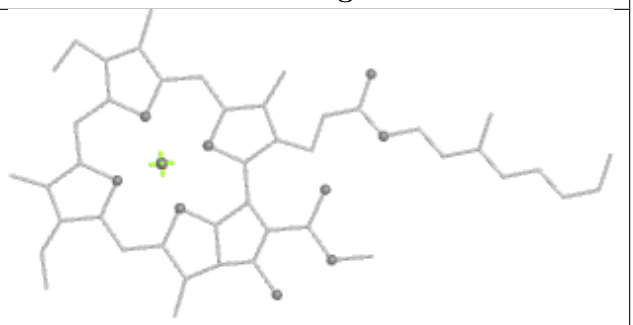
Bond lengths



Bond angles

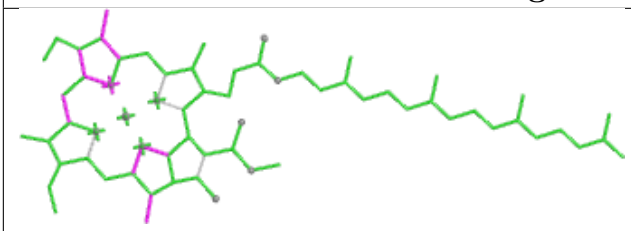


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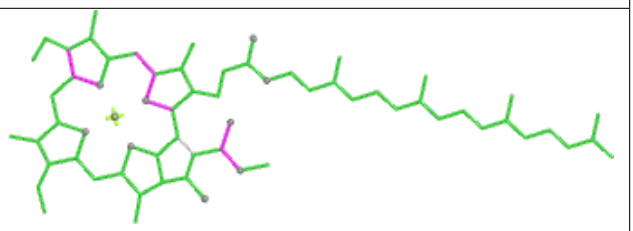


Rings

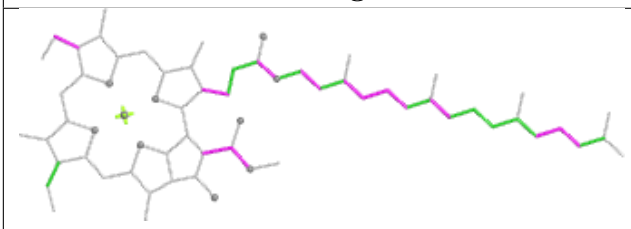
Ligand CLA a 837



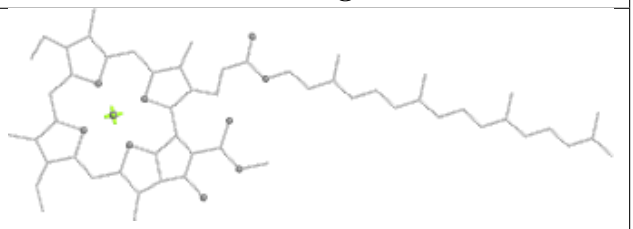
Bond lengths



Bond angles

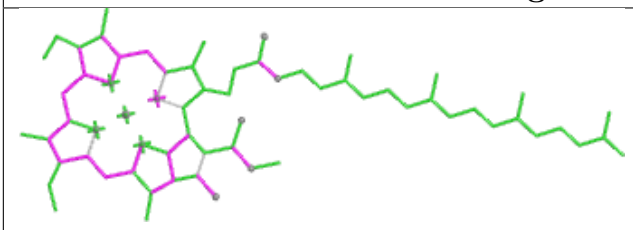


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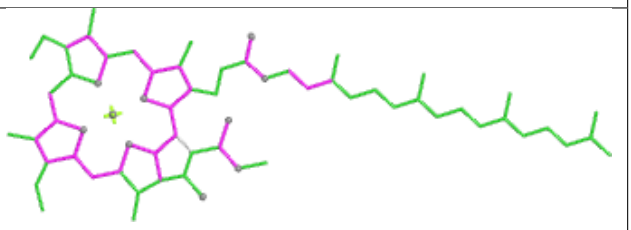


Rings

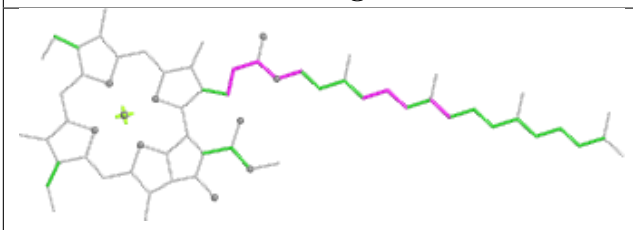
Ligand CL0 G 851



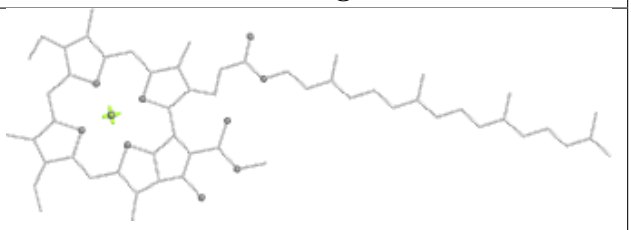
Bond lengths



Bond angles

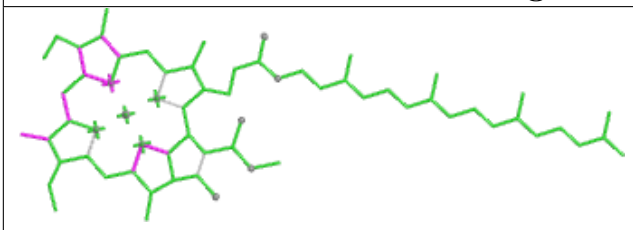


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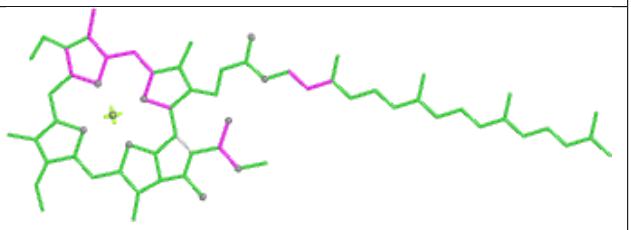


Rings

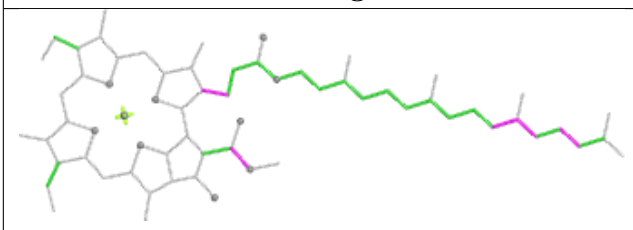
Ligand CLA b 826



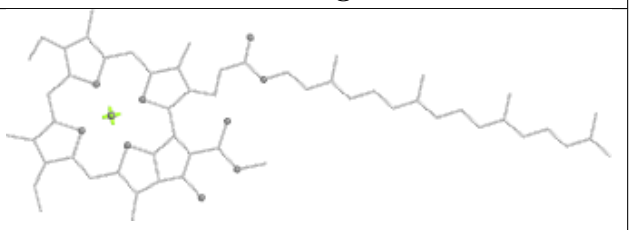
Bond lengths



Bond angles

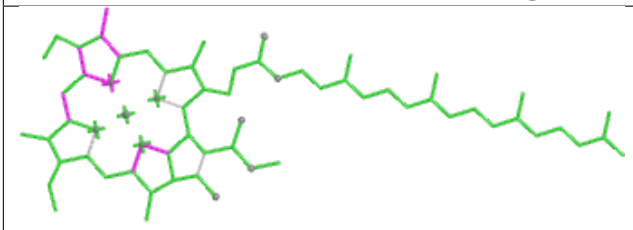


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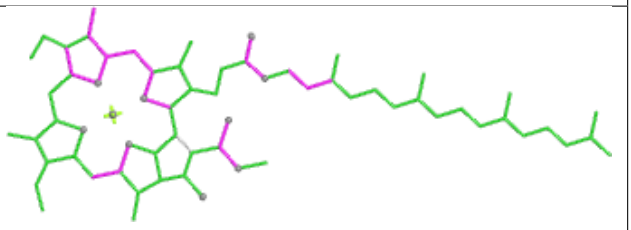


Rings

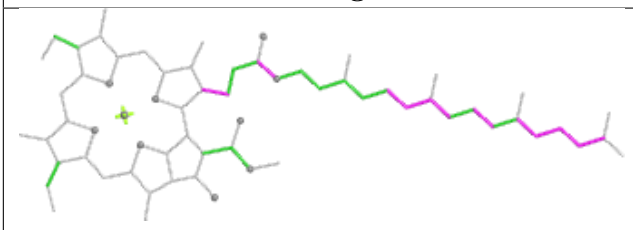
Ligand CLA A 818



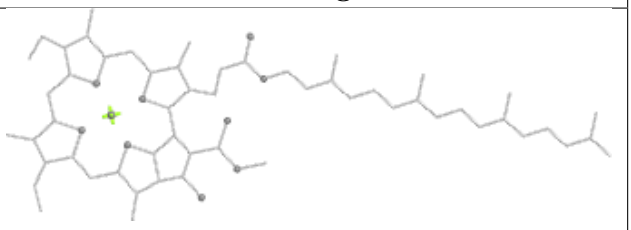
Bond lengths



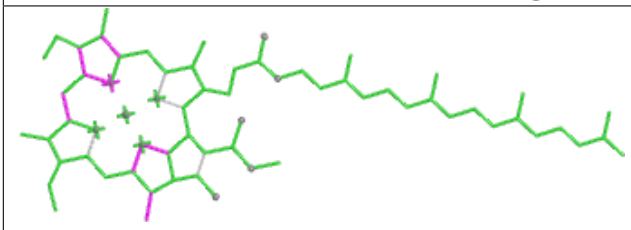
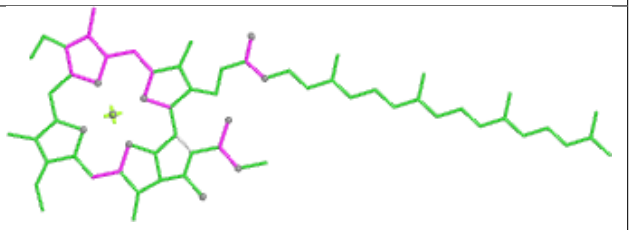
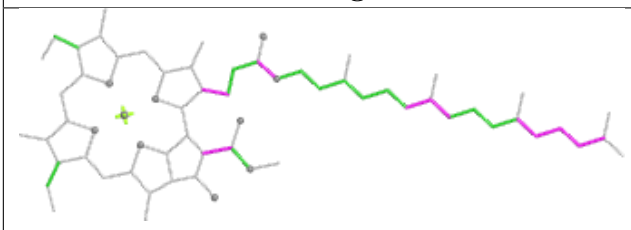
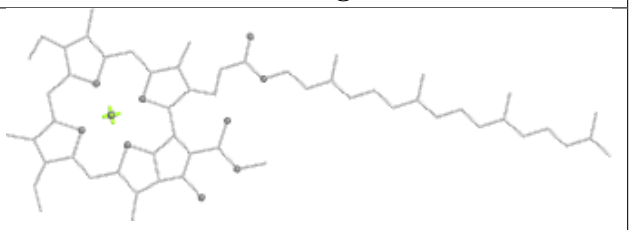
Bond angles

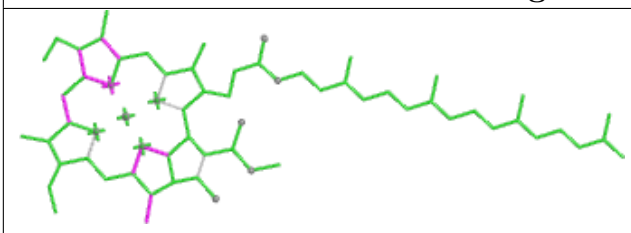
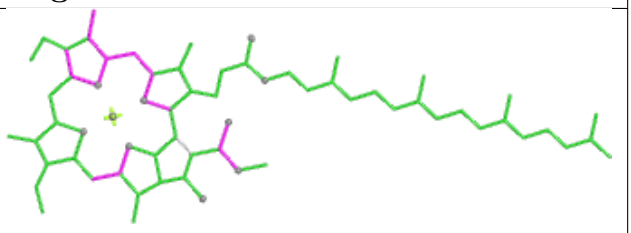
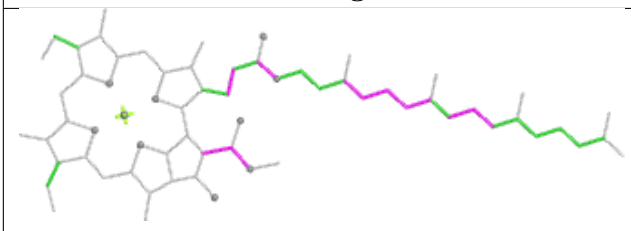
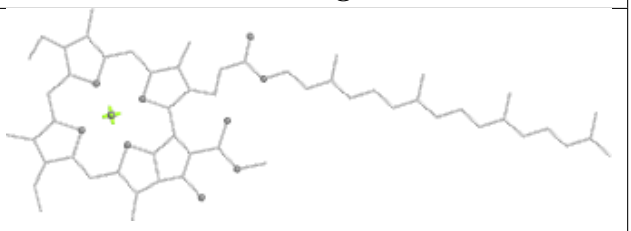


Torsions

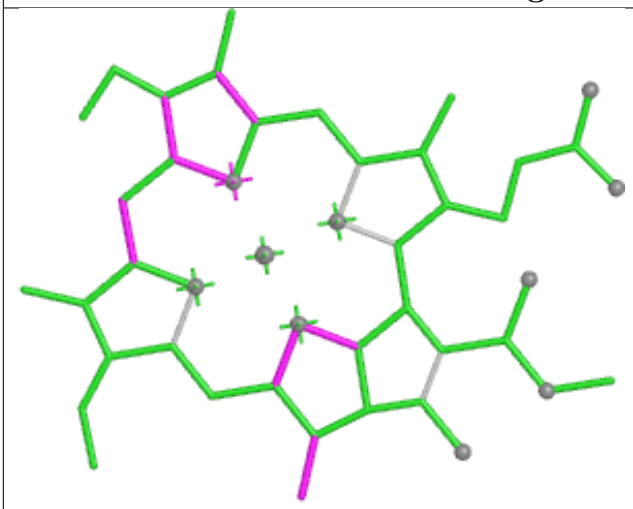


Rings

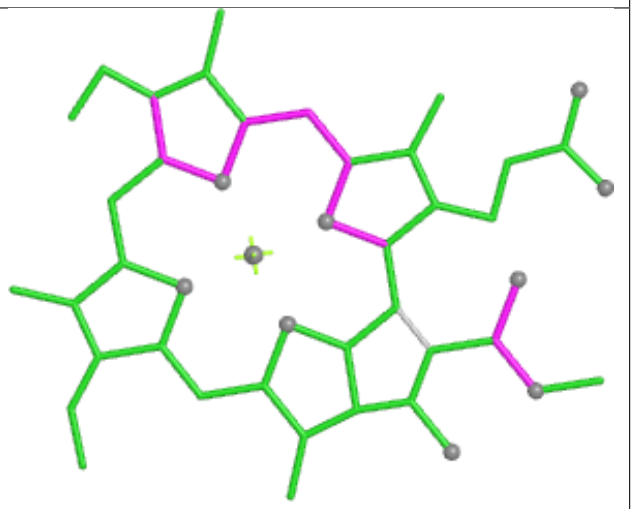
Ligand CLA b 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

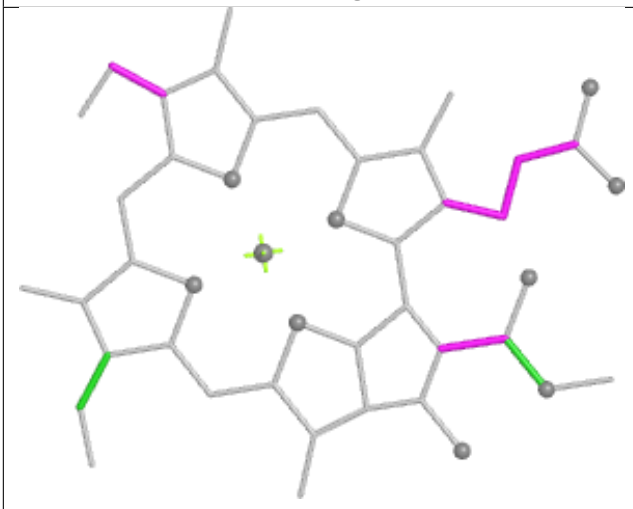
Ligand CLA b 820



Bond lengths



Bond angles

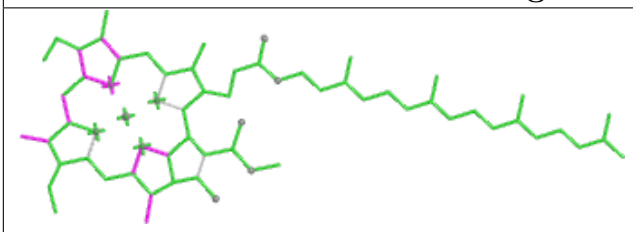


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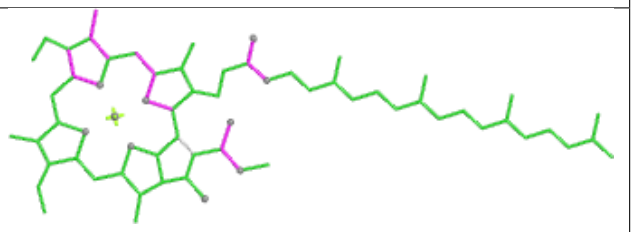


Rings

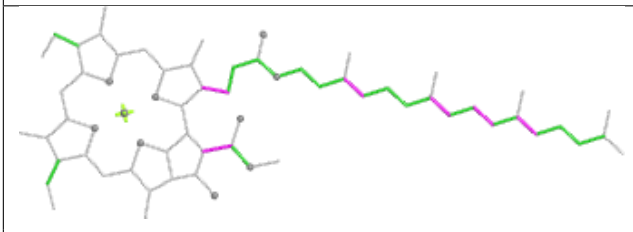
Ligand CLA n 813



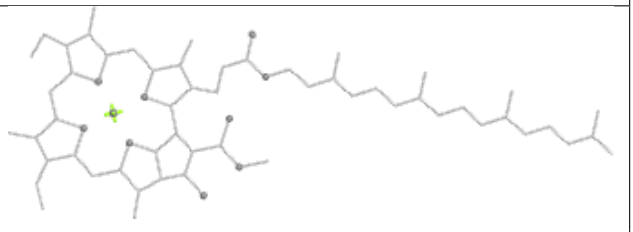
Bond lengths



Bond angles

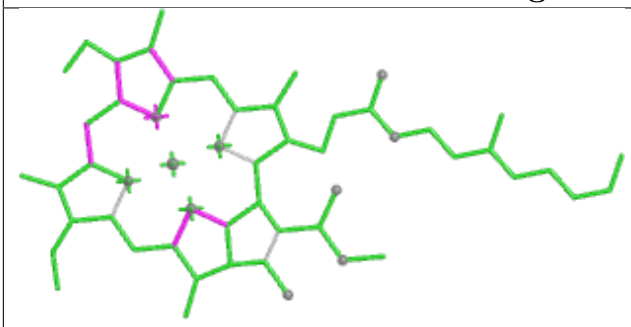


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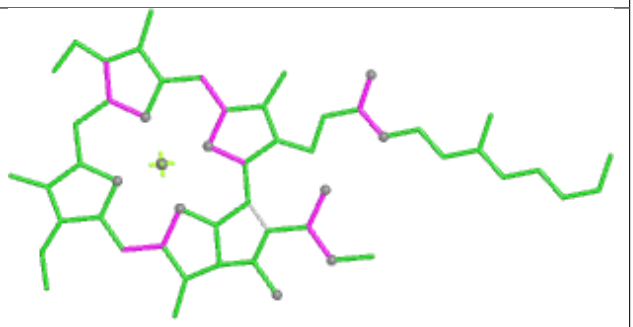


Rings

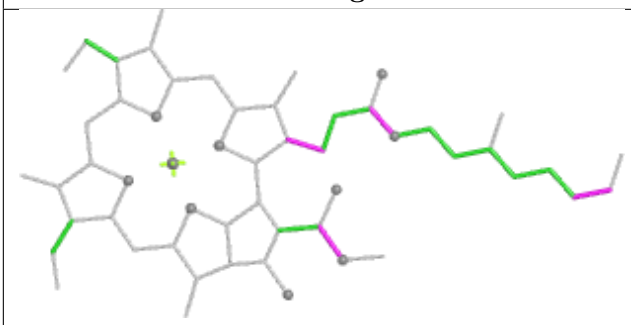
Ligand CLA a 812



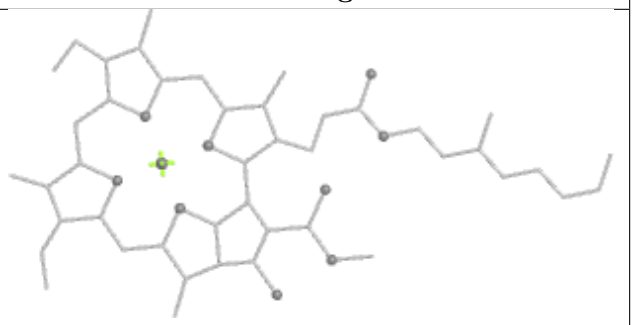
Bond lengths



Bond angles



Torsions

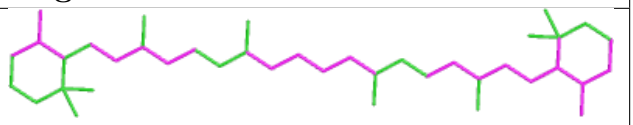


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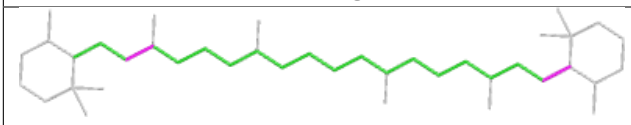
Ligand BCR g 847



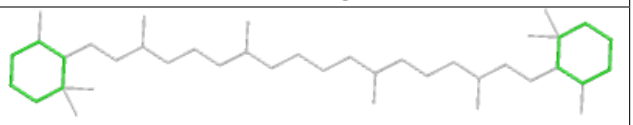
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Bond angles

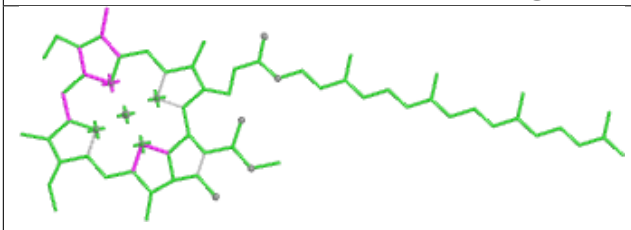


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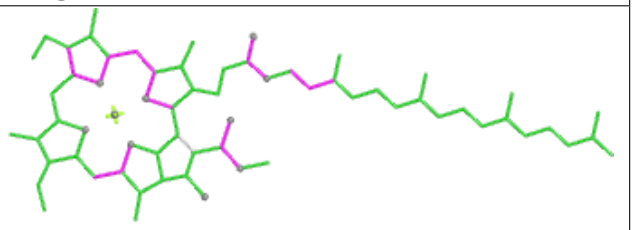


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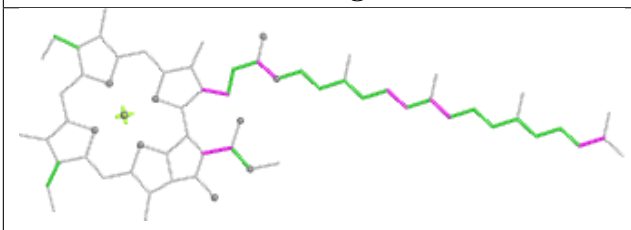
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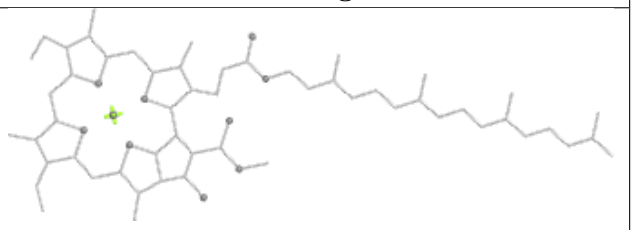
Bond lengths



Bond angles

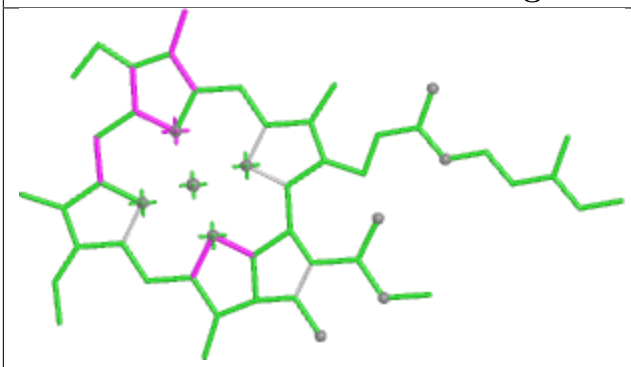


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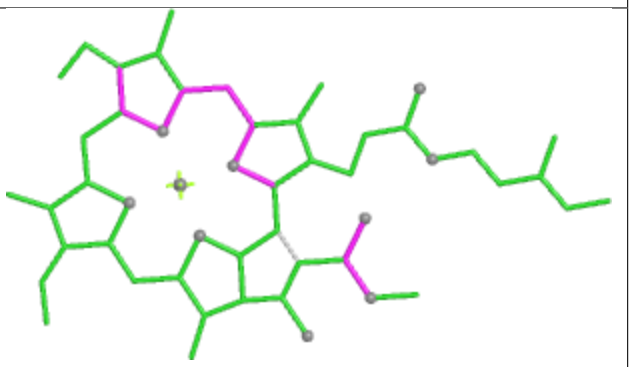


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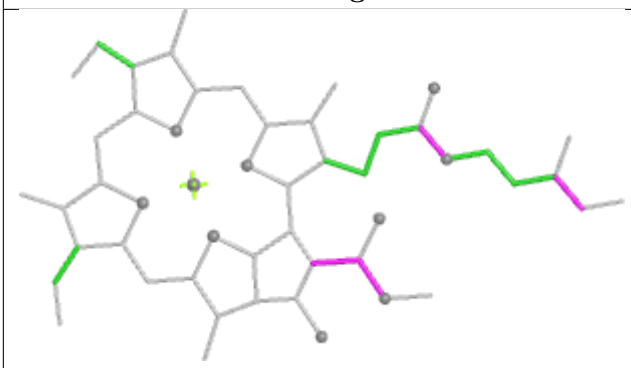
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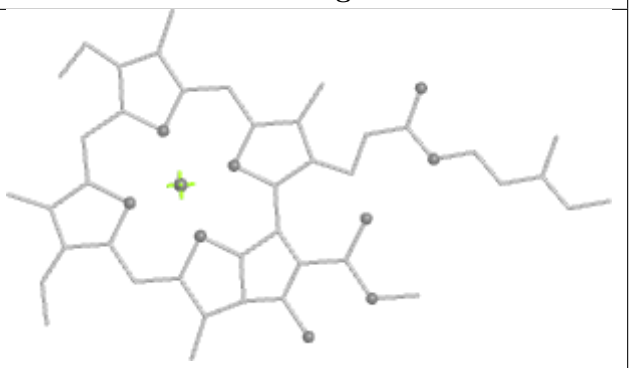
Bond lengths



Bond angles

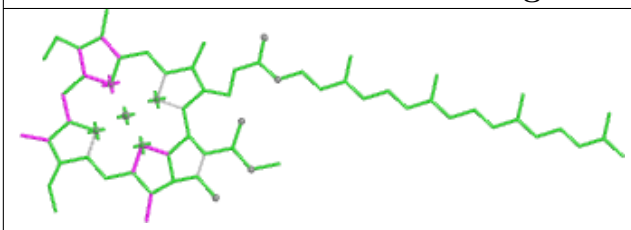


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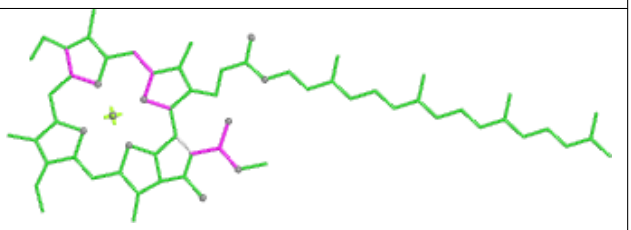


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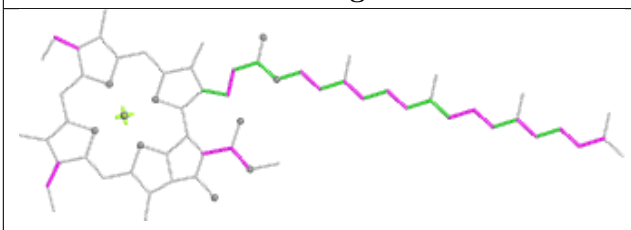
Ligand CLA N 804



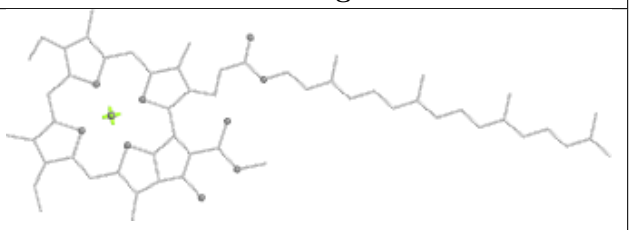
Bond lengths



Bond angles

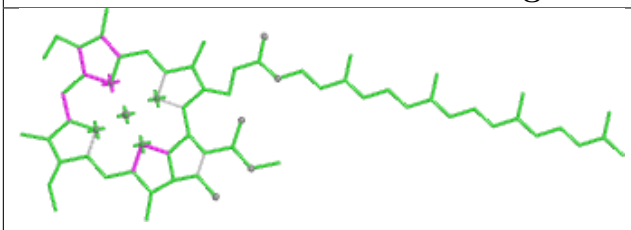


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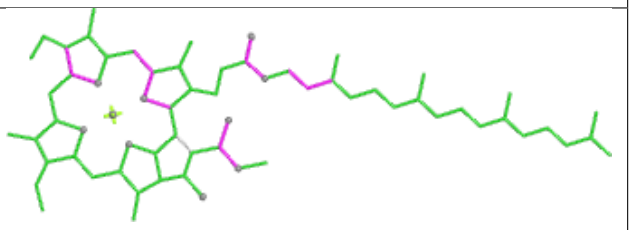


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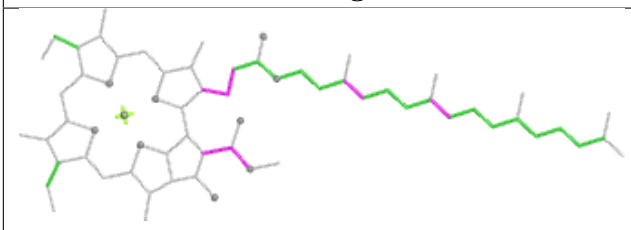
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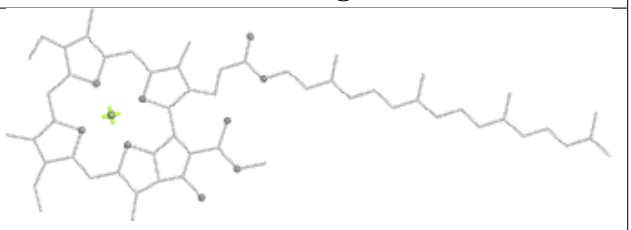
Bond lengths



Bond angles

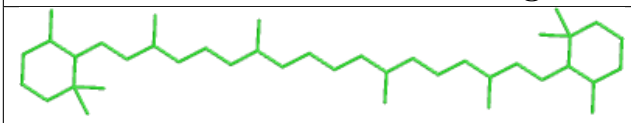


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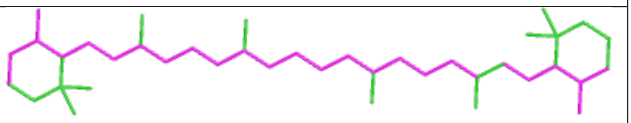


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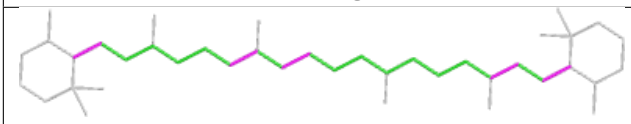
Ligand BCR T 104



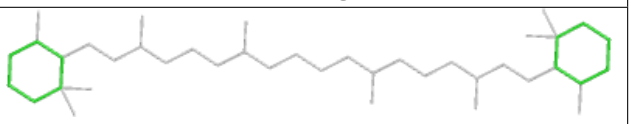
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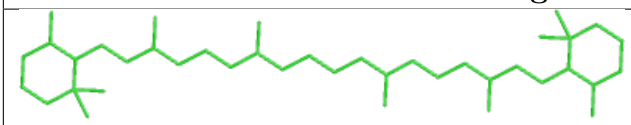


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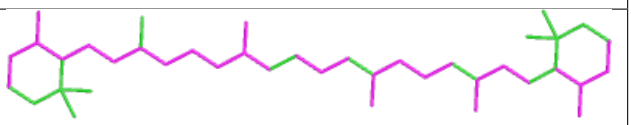


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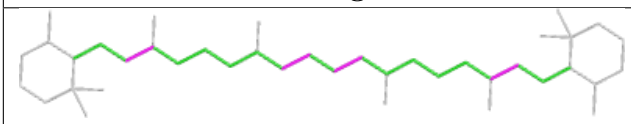
Ligand BCR i 102



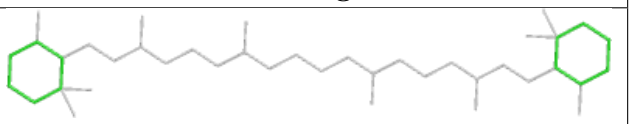
Bond lengths



Bond angles

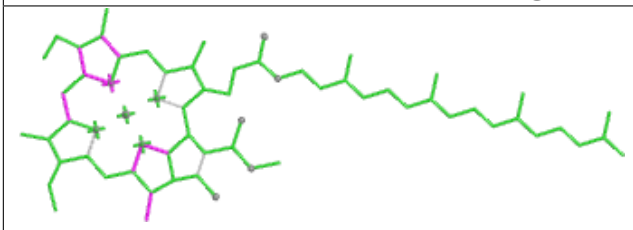


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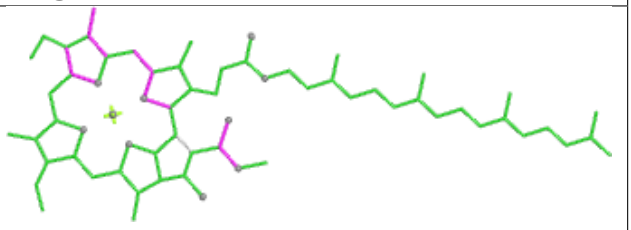


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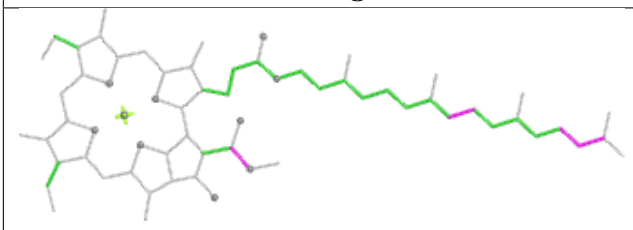
Ligand CLA g 801



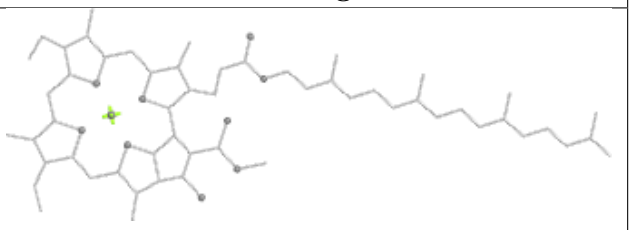
Bond lengths



Bond angles

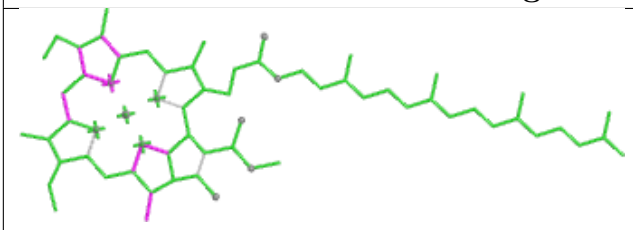


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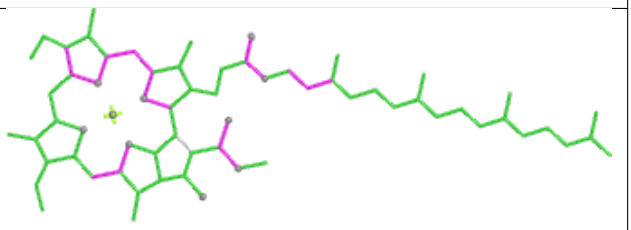


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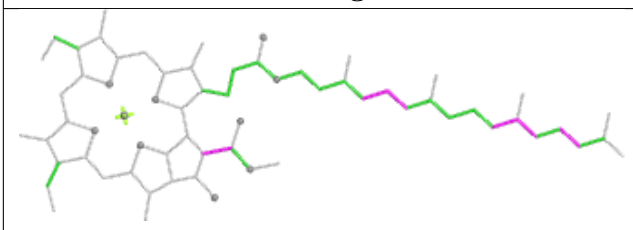
Ligand CLA G 853



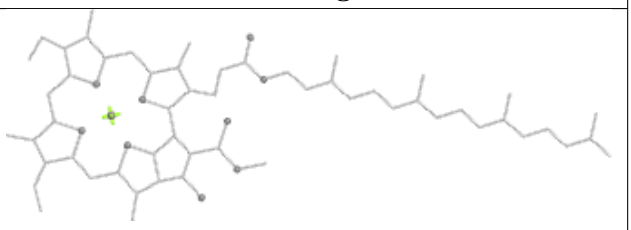
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Bond angles



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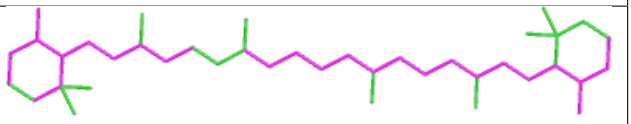


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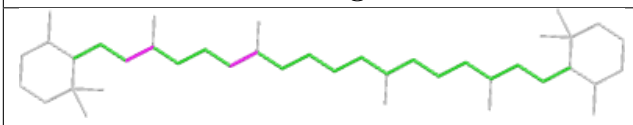
Ligand BCR w 207



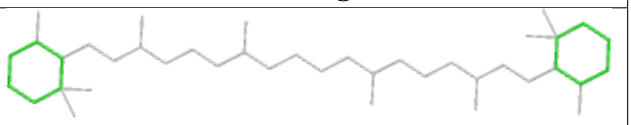
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Bond angles

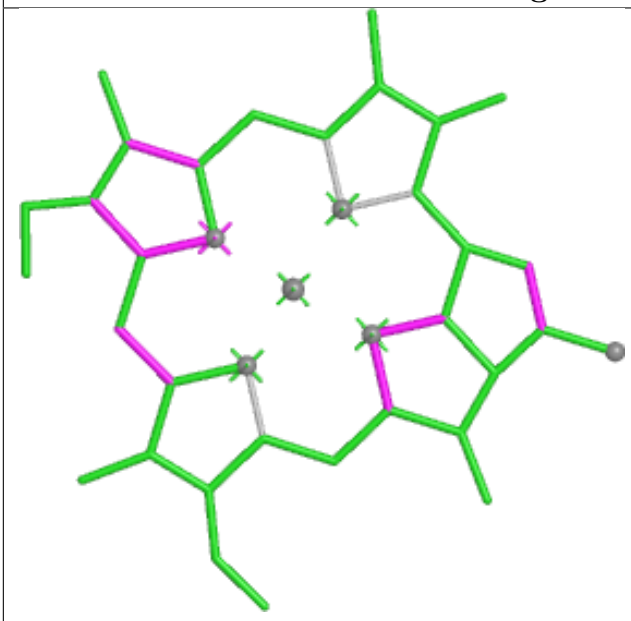


Torsions



Rings

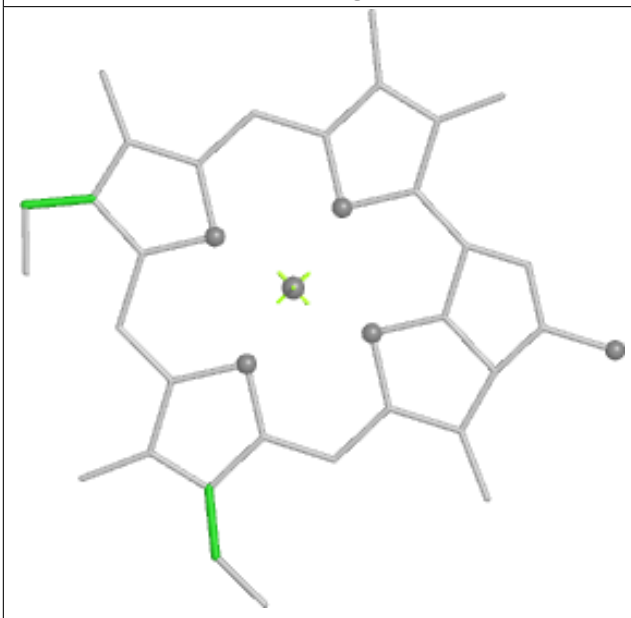
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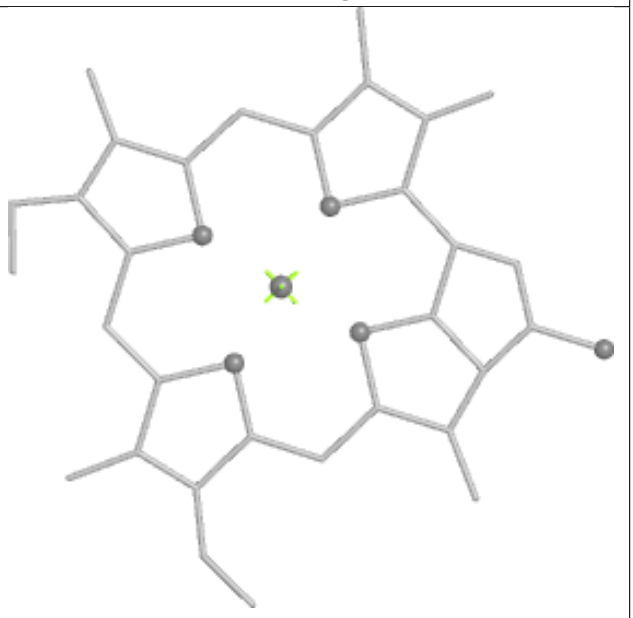
Bond lengths



Bond angles

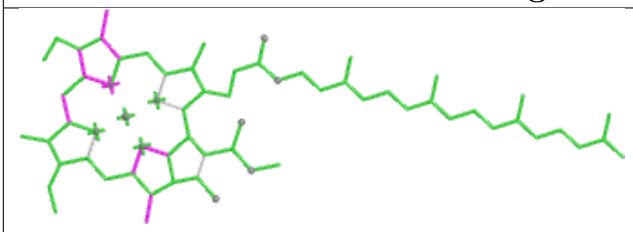


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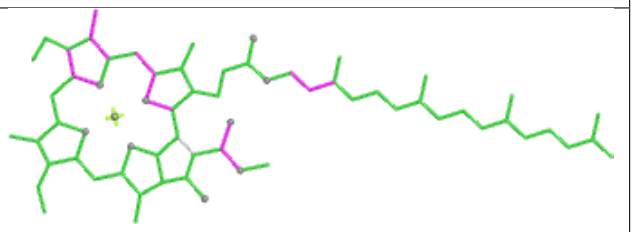


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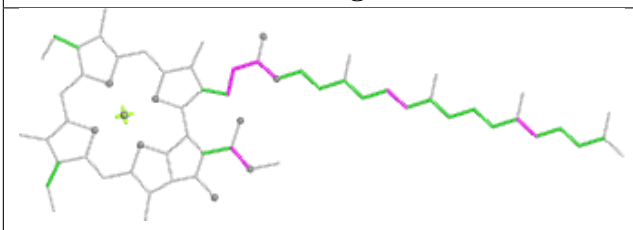
Ligand CLA a 827



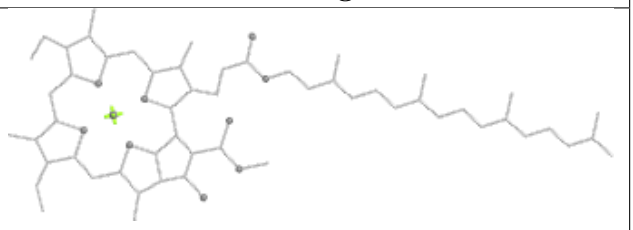
Bond lengths



Bond angles

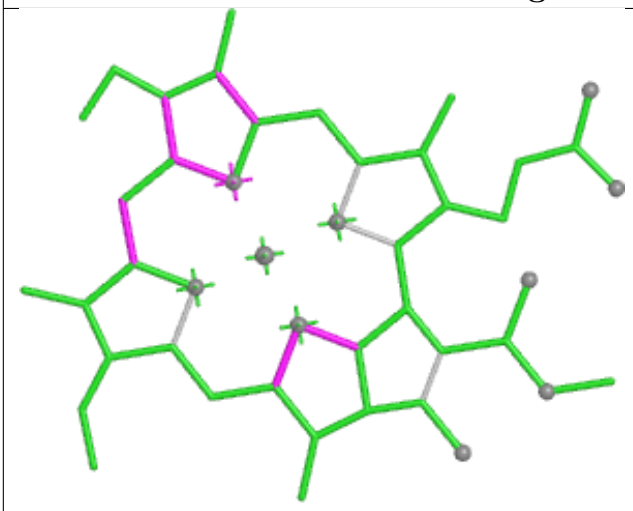


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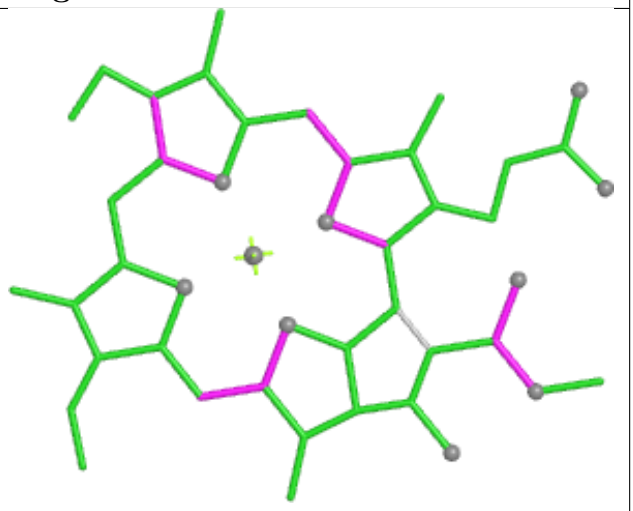


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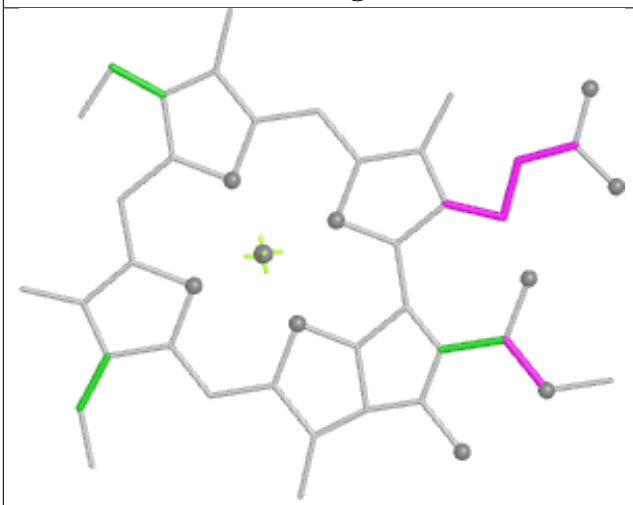
Ligand CLA g 808



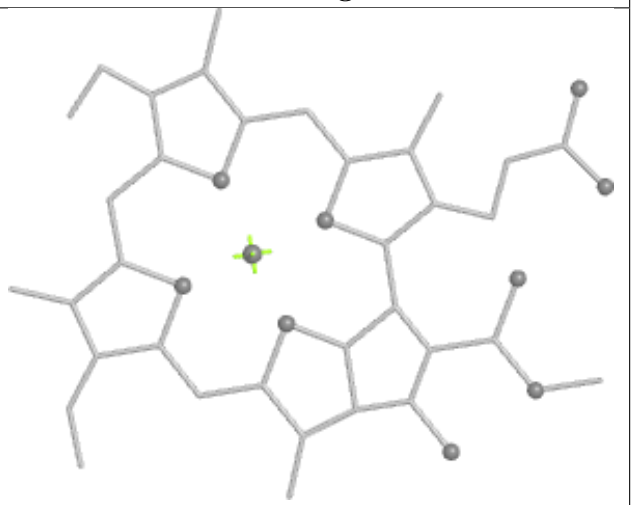
Bond lengths



Bond angles

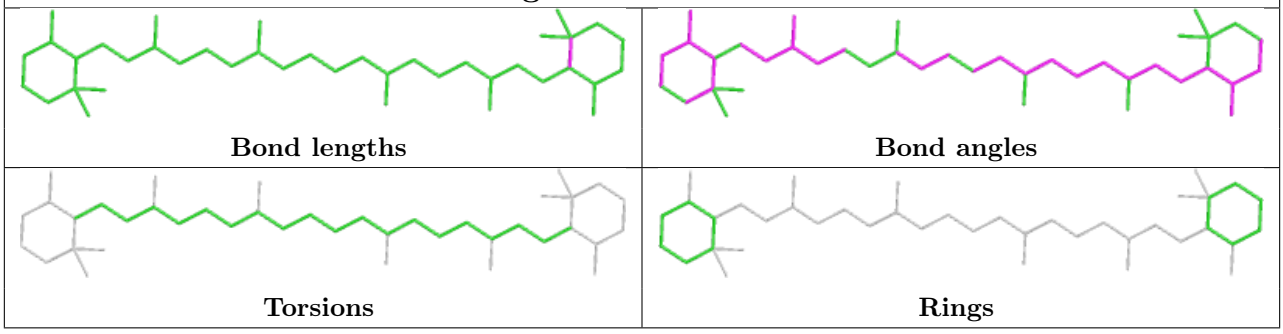


Torsions



Rings

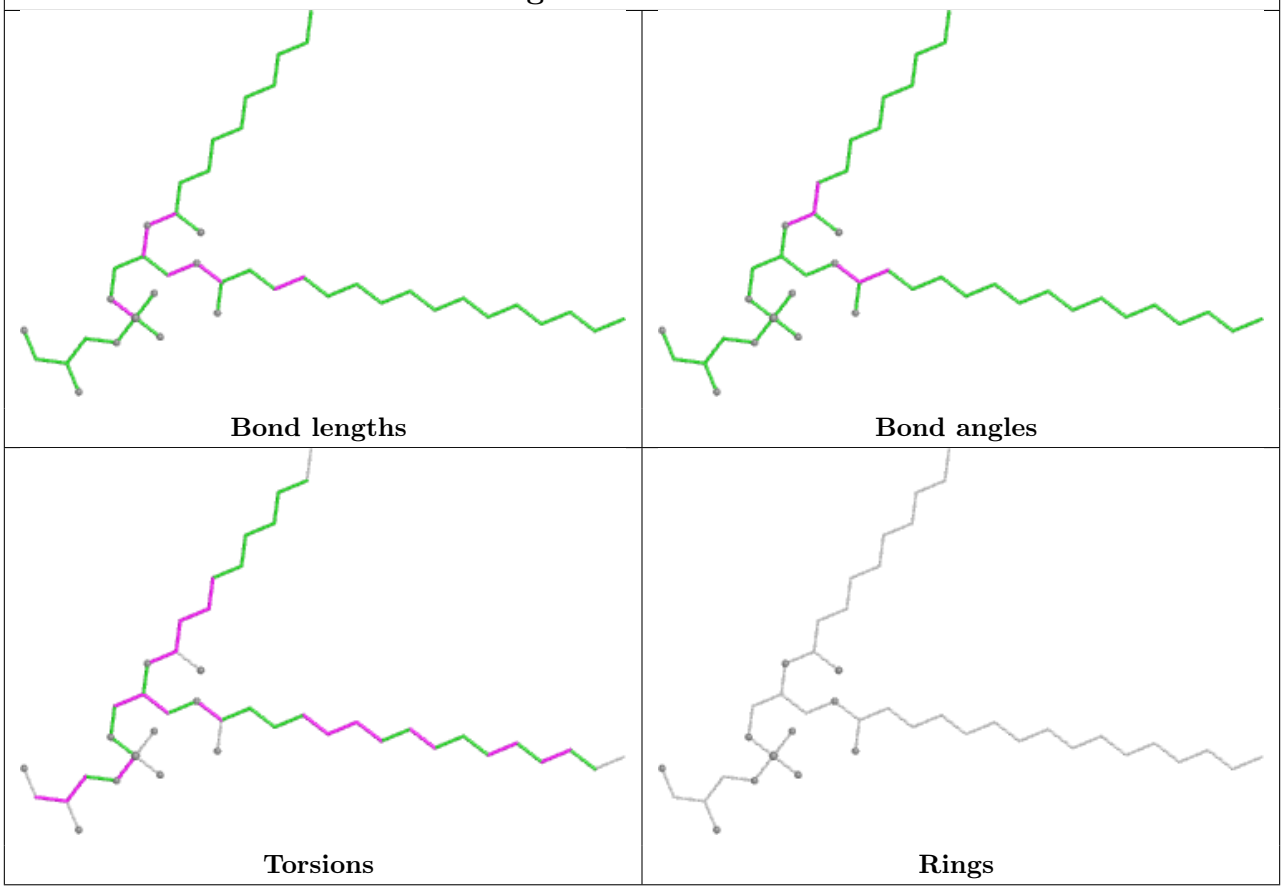
Ligand BCR N 853



Bond lengths | Bond angles

Torsions | Rings

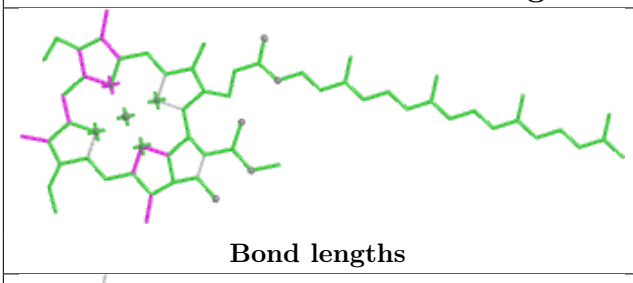
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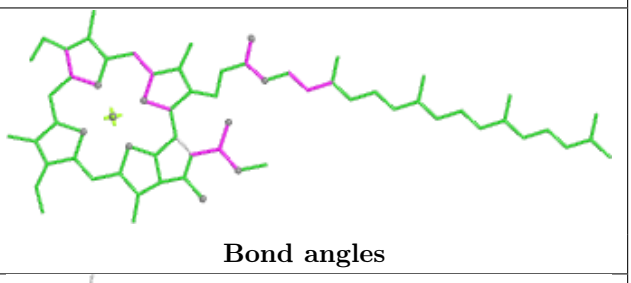
Bond lengths | Bond angles

Torsions | Rings

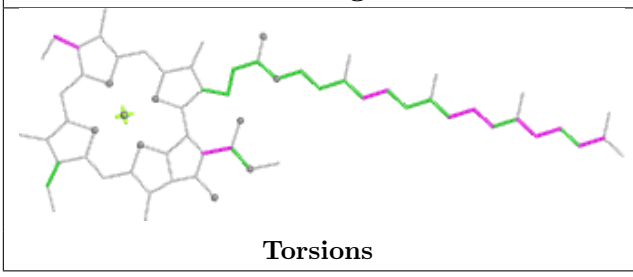
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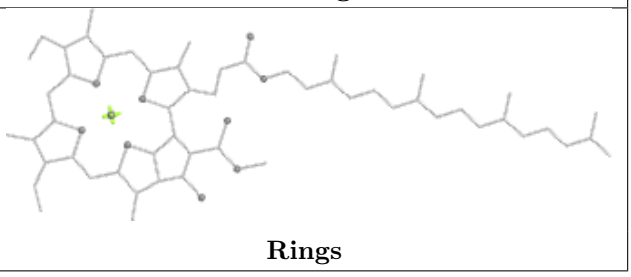
Bond lengths



Bond angles

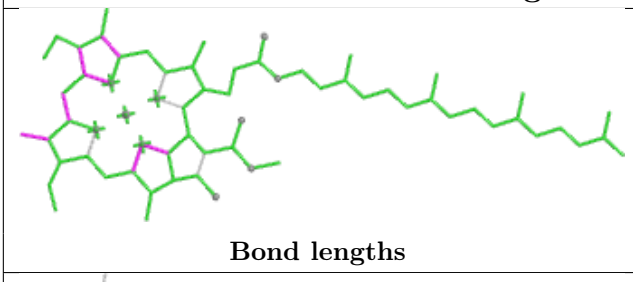


Torsions

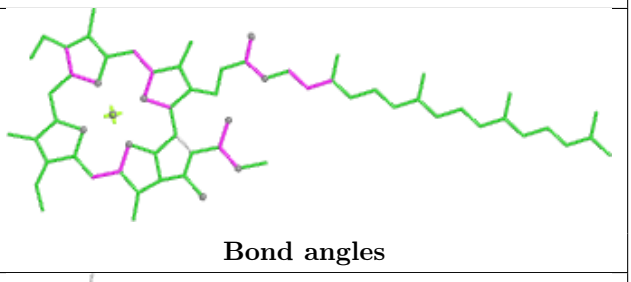


Rings

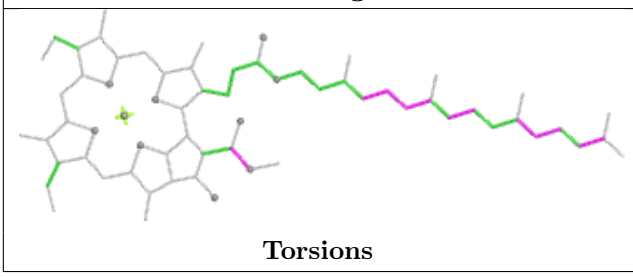
Ligand CLA A 826



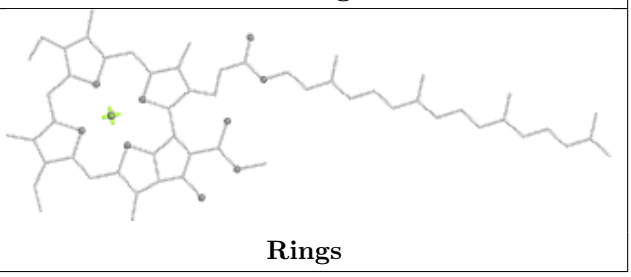
Bond lengths



Bond angles

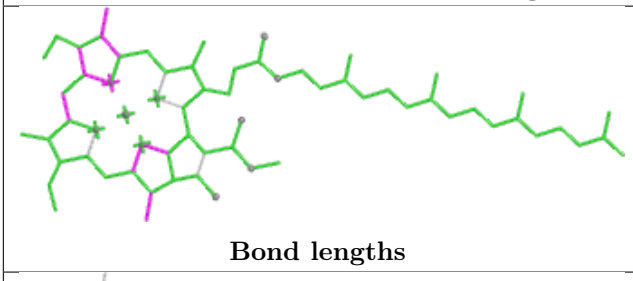


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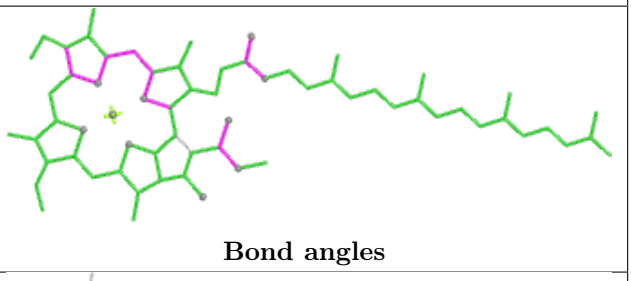


Rings

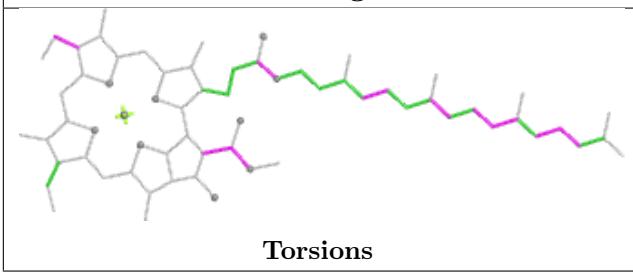
Ligand CLA A 838



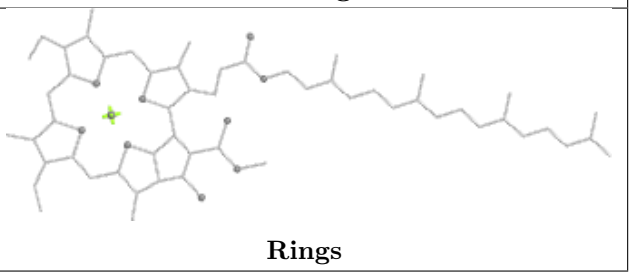
Bond lengths



Bond angles

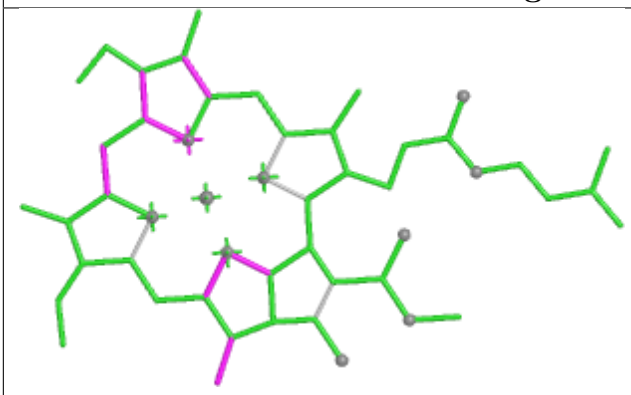


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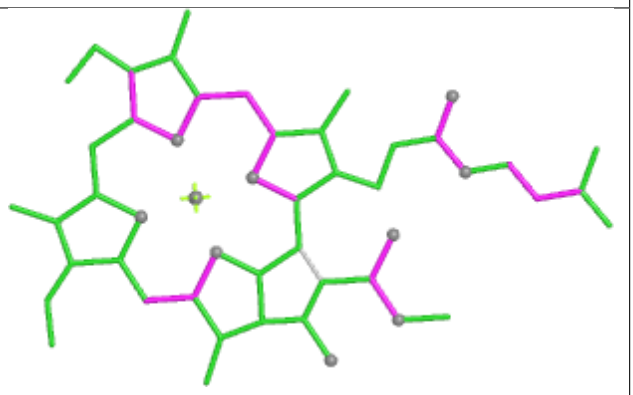


Rings

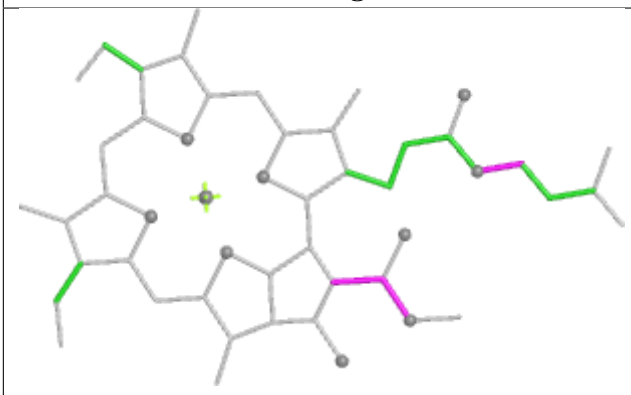
Ligand CLA B 815



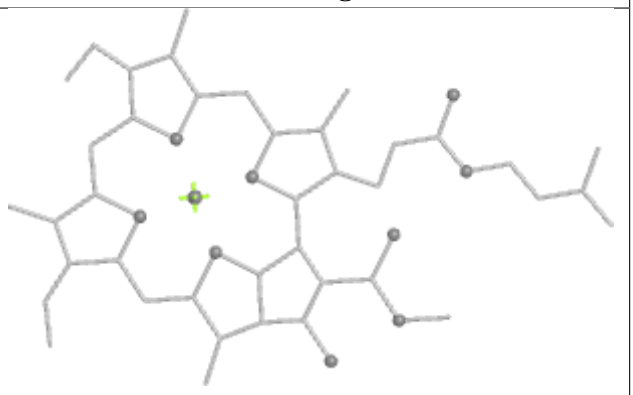
Bond lengths



Bond angles

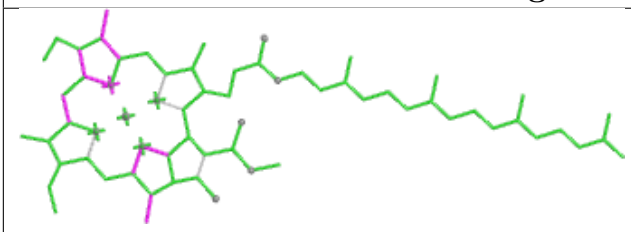


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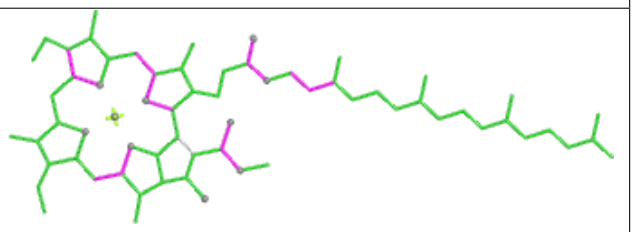


Rings

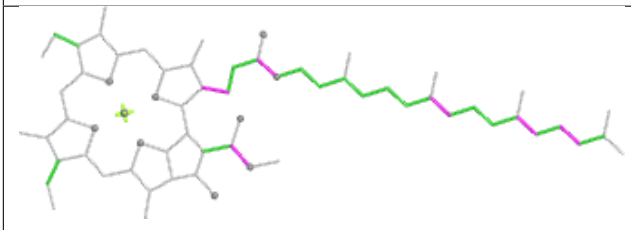
Ligand CLA a 817



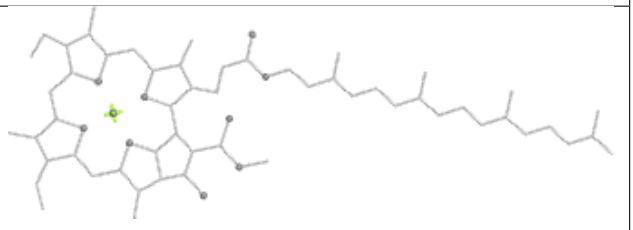
Bond lengths



Bond angles

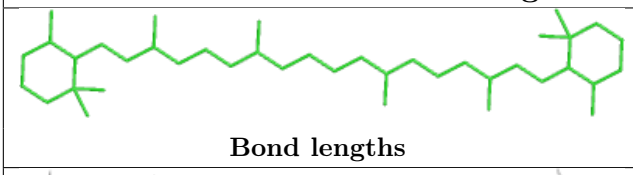


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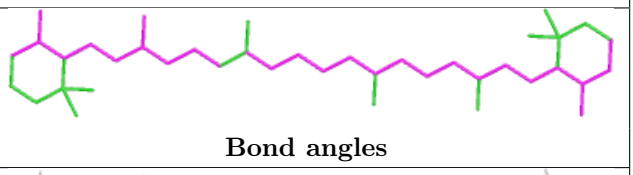


Rings

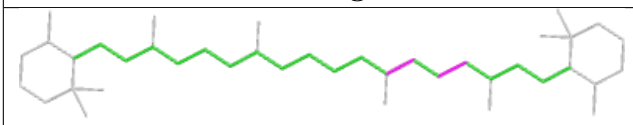
Ligand BCR N 852



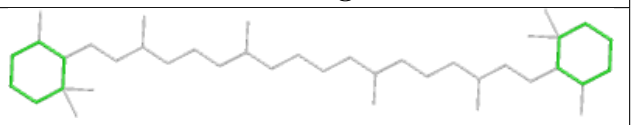
Bond lengths



Bond angles

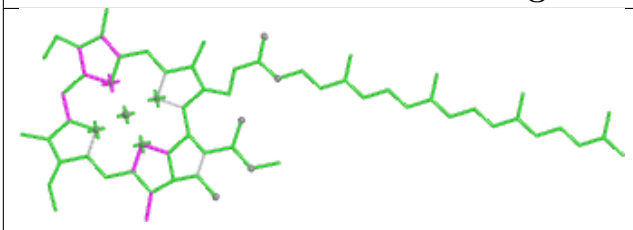


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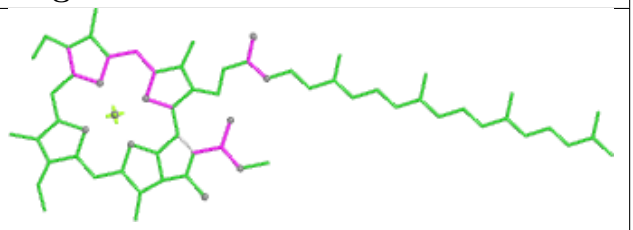


Rings

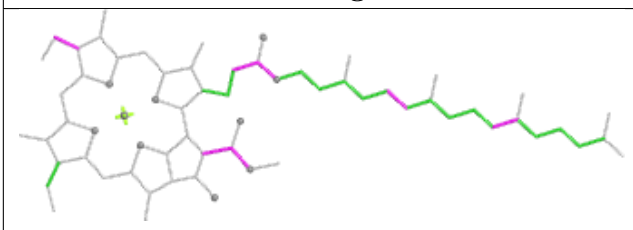
Ligand CLA g 832



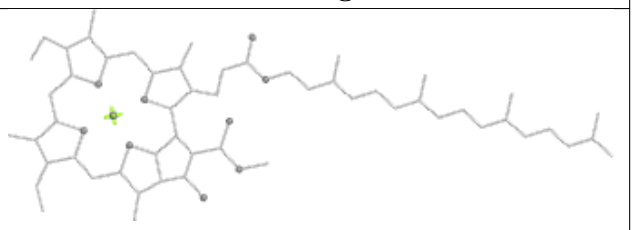
Bond lengths



Bond angles

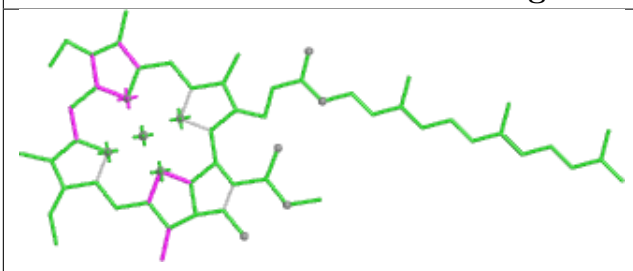


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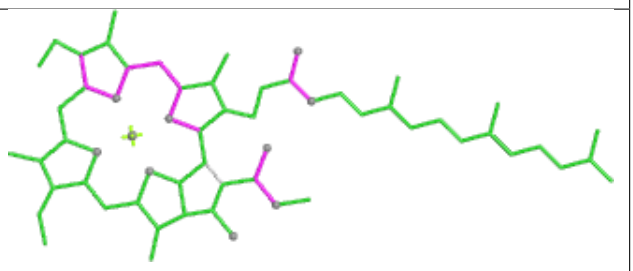


Rings

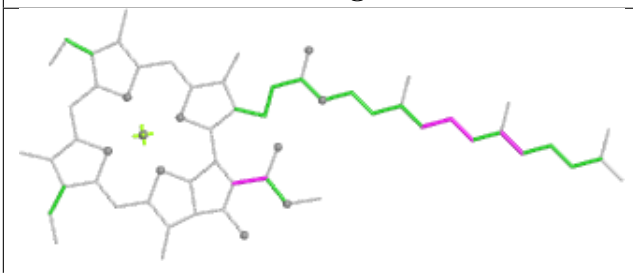
Ligand CLA a 805



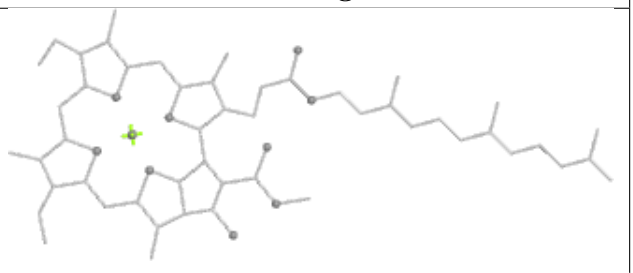
Bond lengths



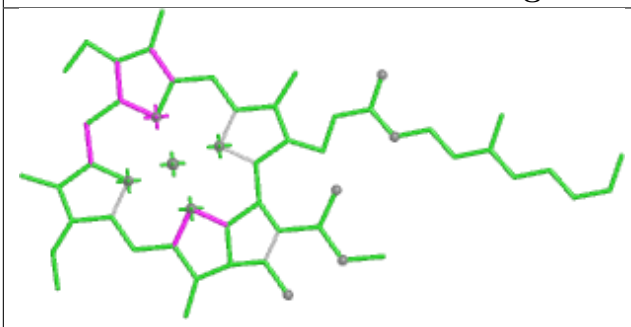
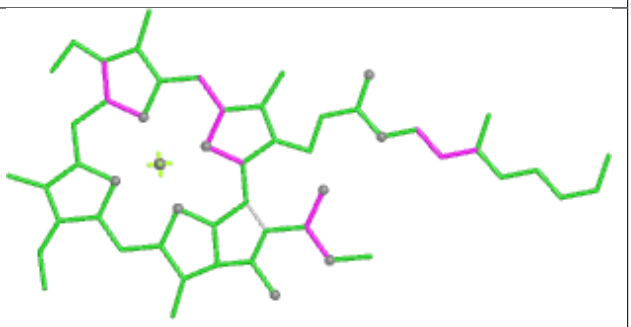
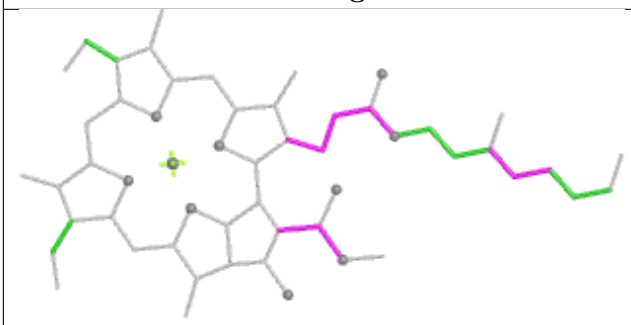
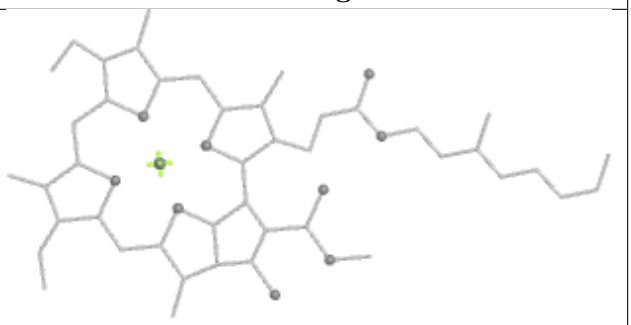
Bond angles

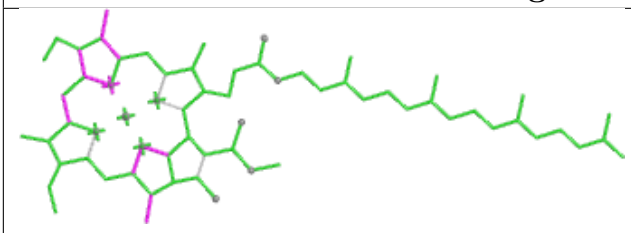
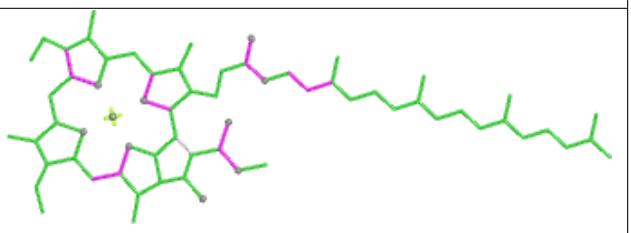
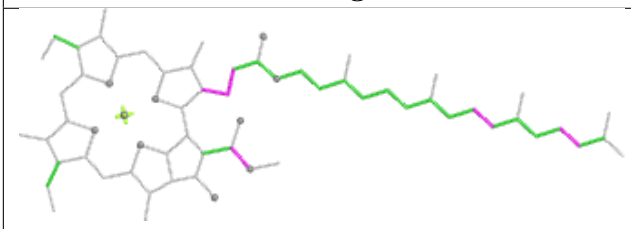
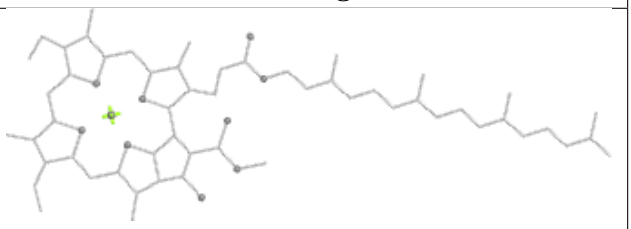


Torsions

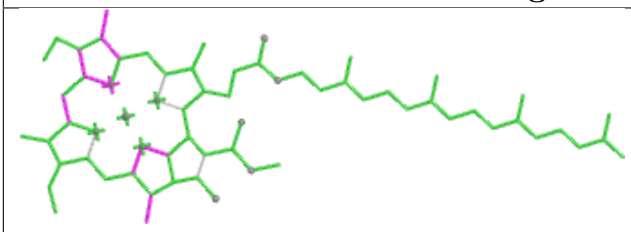


Rings

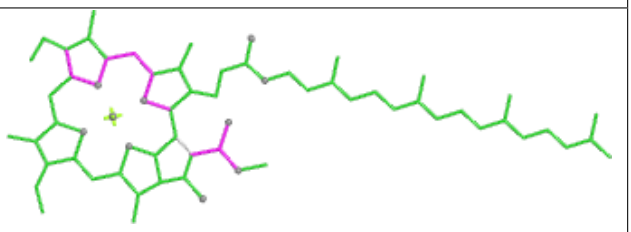
Ligand CLA A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

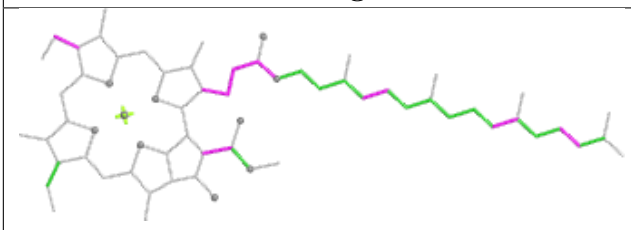
Ligand CLA a 806



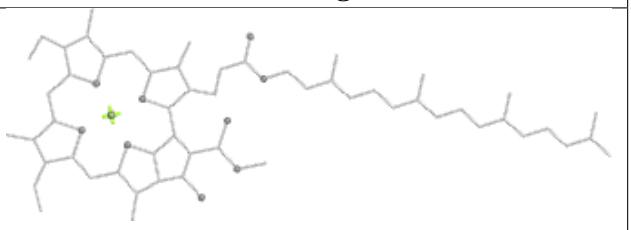
Bond lengths



Bond angles



Torsions

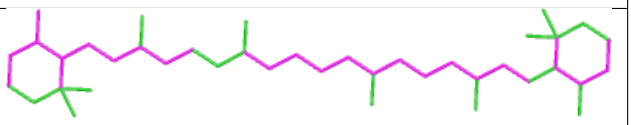


Rings

Ligand BCR B 851



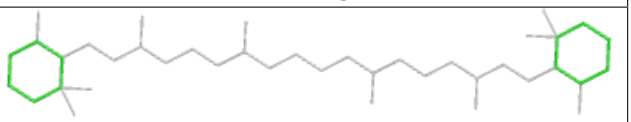
Bond lengths



Bond angles

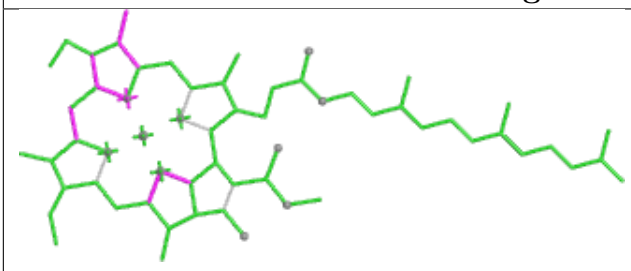


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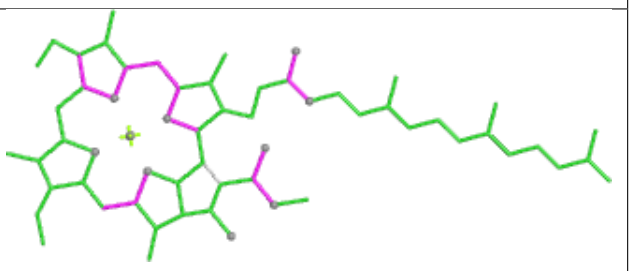


Rings

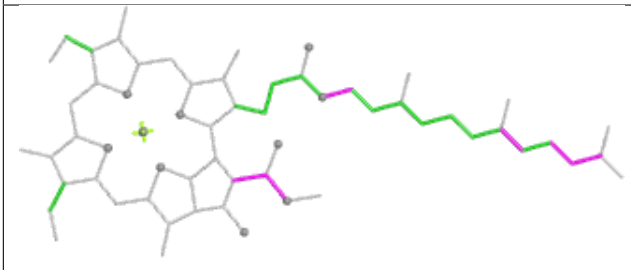
Ligand CLA G 812



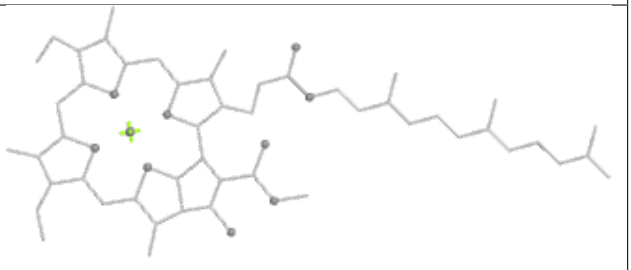
Bond lengths



Bond angles

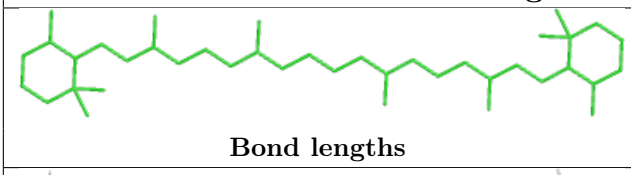


Torsions

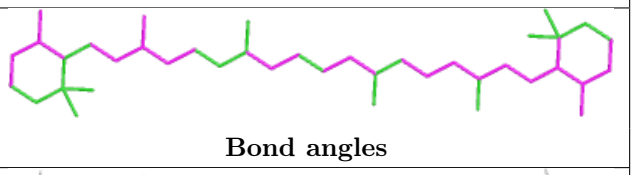


Rings

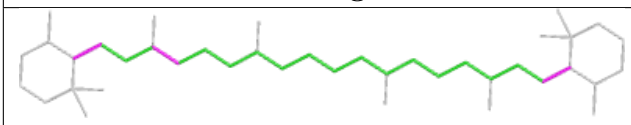
Ligand BCR b 843



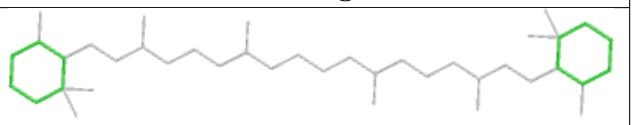
Bond lengths



Bond angles

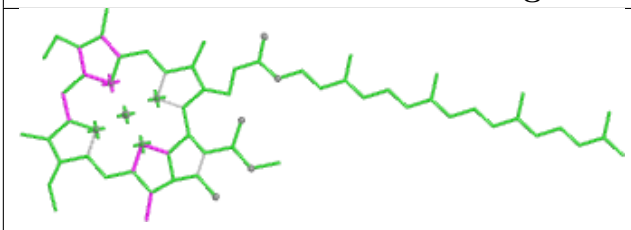


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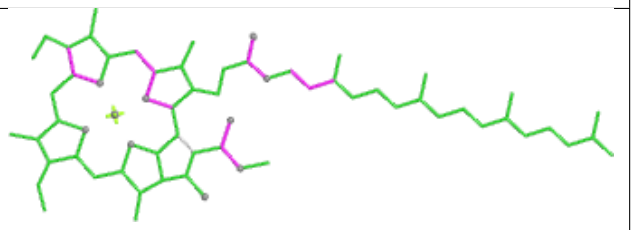


Rings

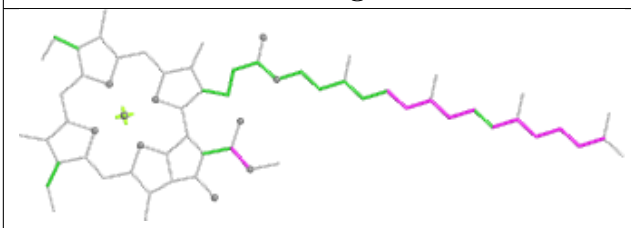
Ligand CLA A 802



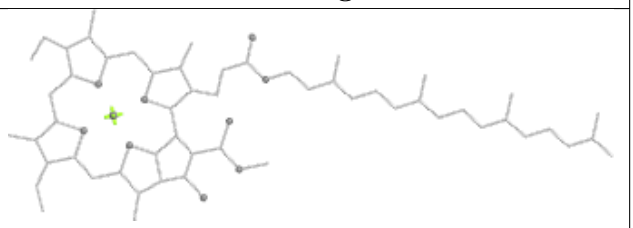
Bond lengths



Bond angles

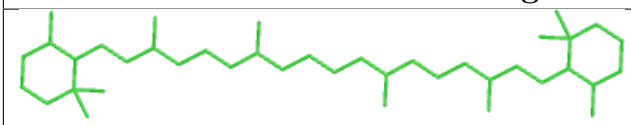


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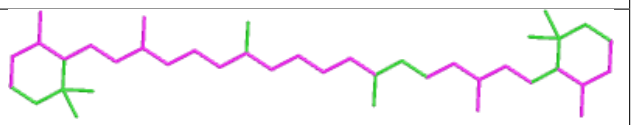


Rings

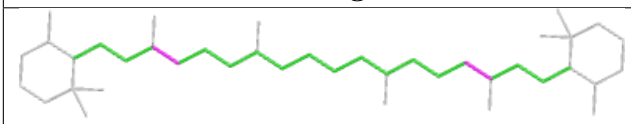
Ligand BCR N 846



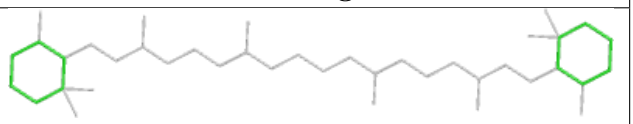
Bond lengths



Bond angles

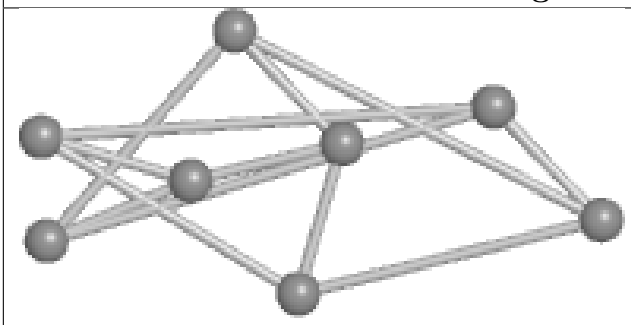


Torsions

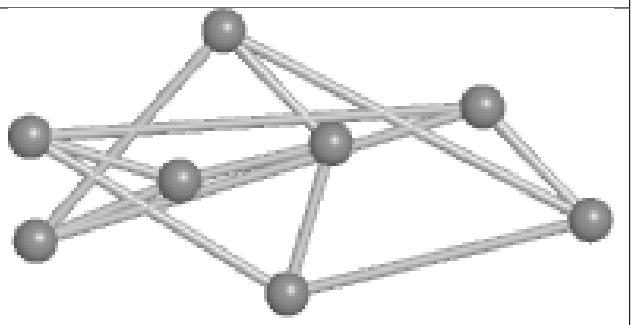


Rings

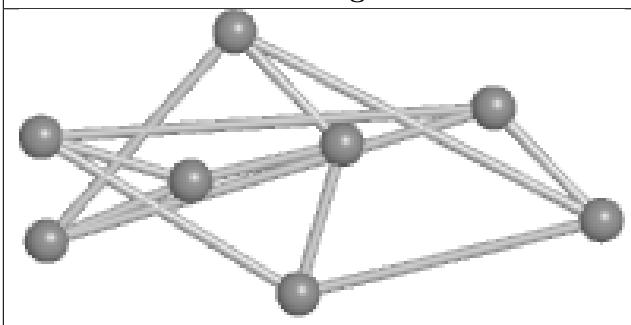
Ligand SF4 P 101



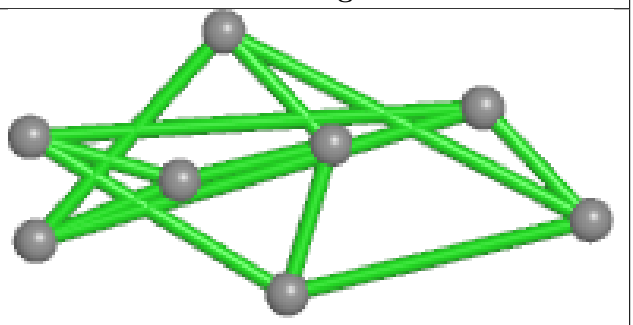
Bond lengths



Bond angles

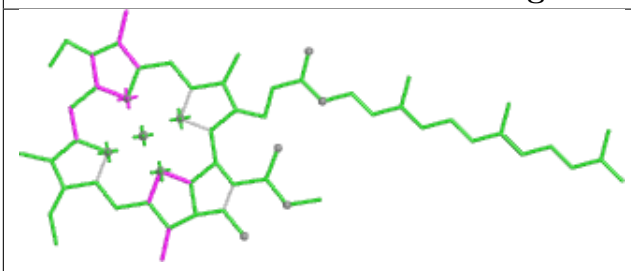


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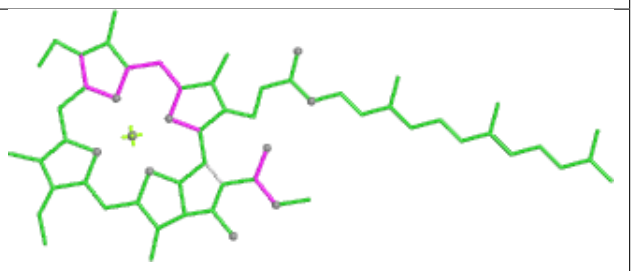


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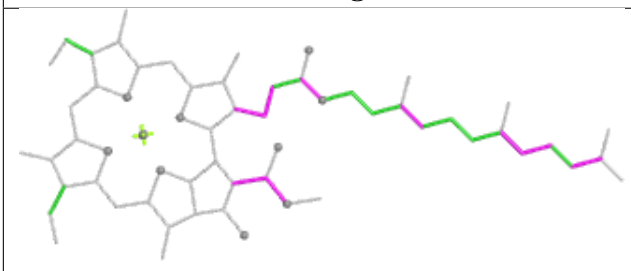
Ligand CLA n 810



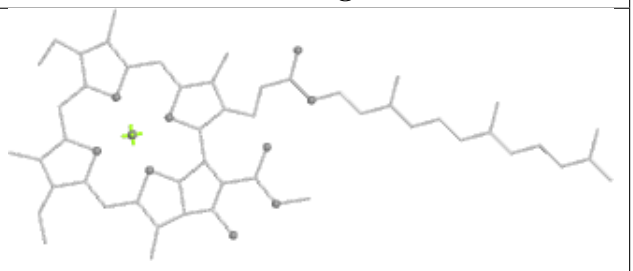
Bond lengths



Bond angles

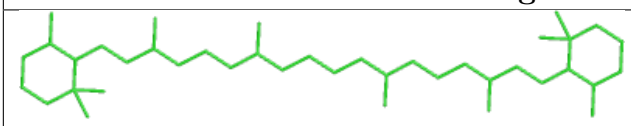


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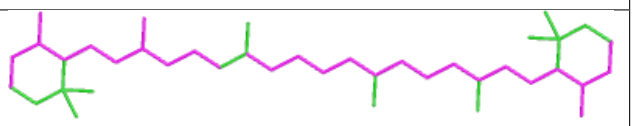


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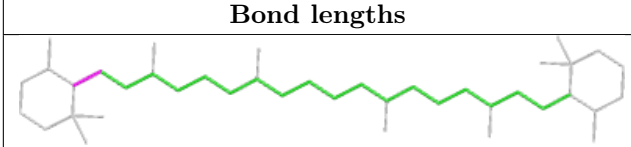
Ligand BCR M 101



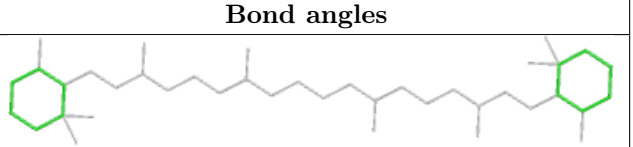
Bond lengths



Bond angles

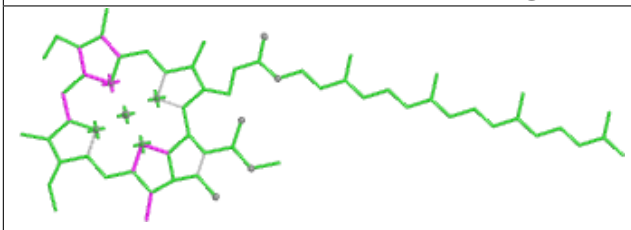


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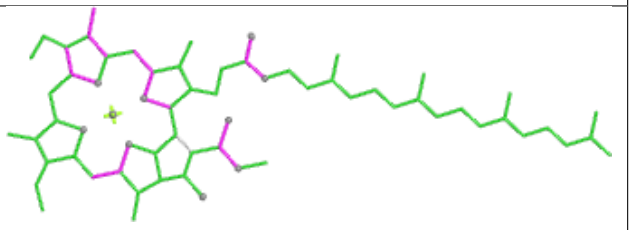


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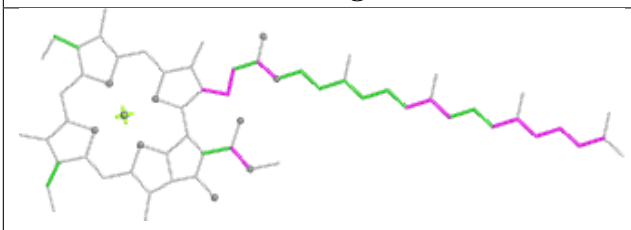
Ligand CLA G 810



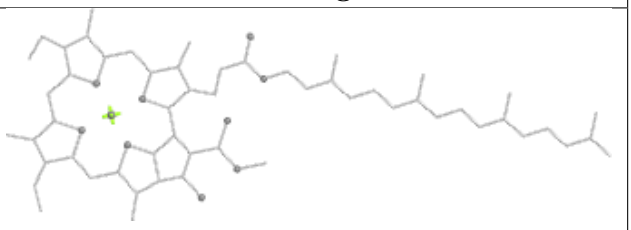
Bond lengths



Bond angles

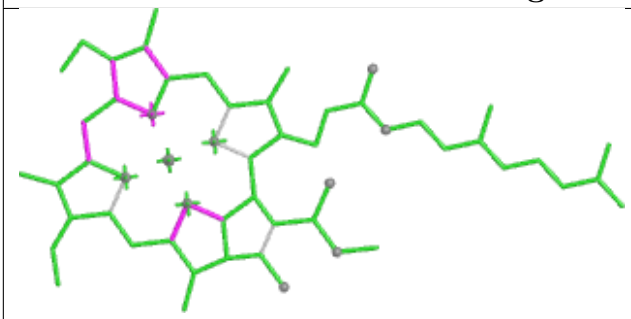


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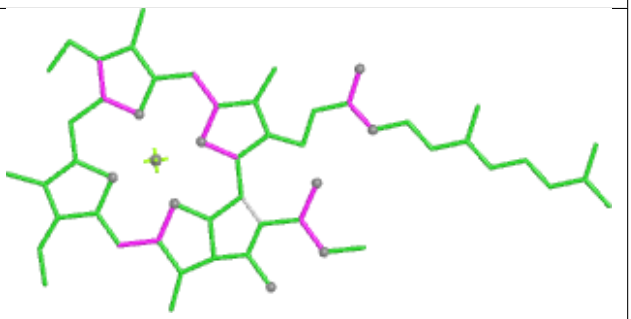


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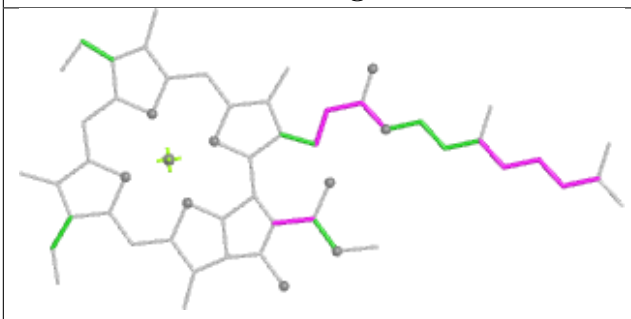
Ligand CLA n 822



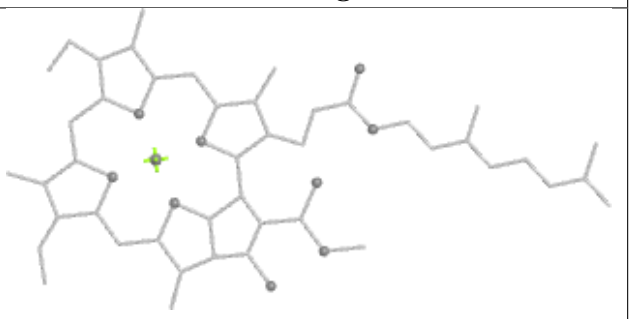
Bond lengths



Bond angles

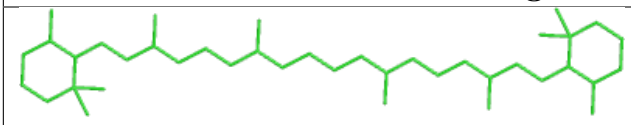


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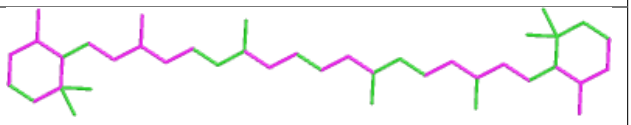


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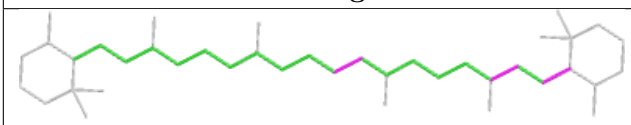
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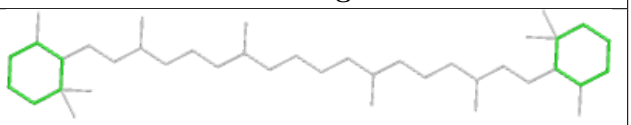
Bond lengths



Bond angles

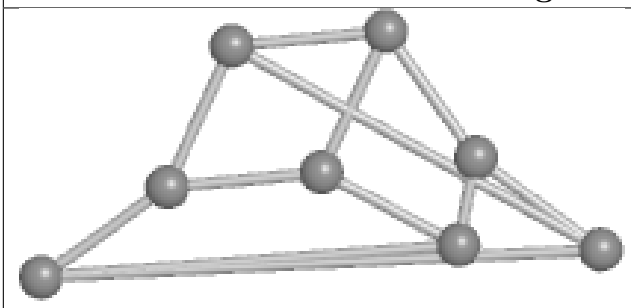


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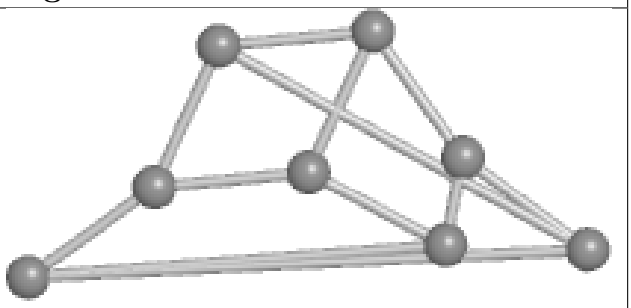


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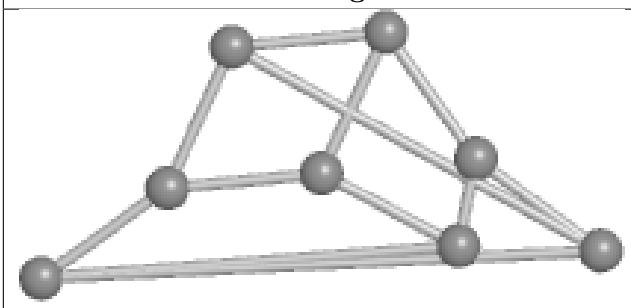
Ligand SF4 g 842



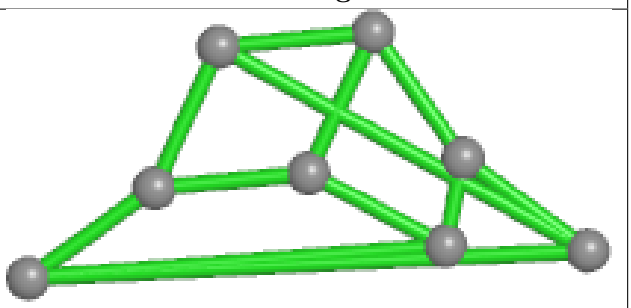
Bond lengths



Bond angles

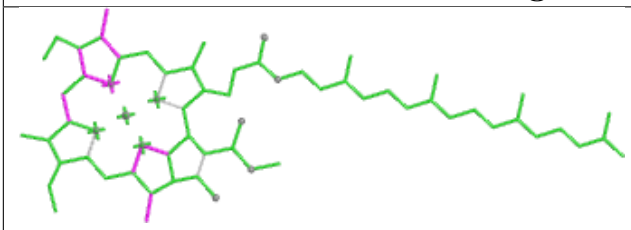


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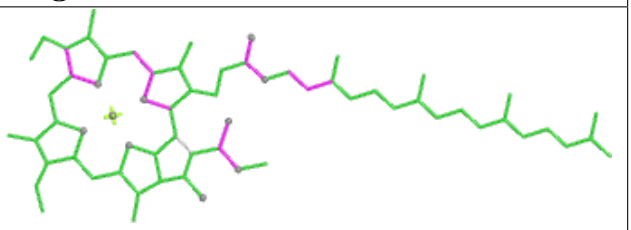


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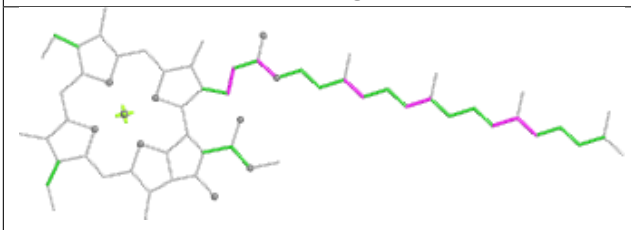
Ligand CLA g 827



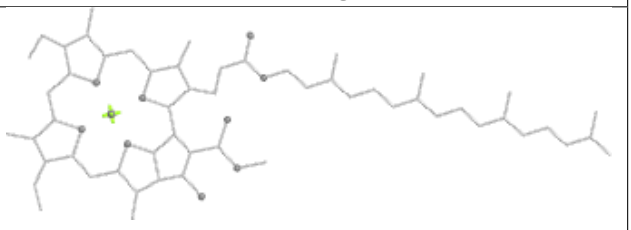
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Bond angles

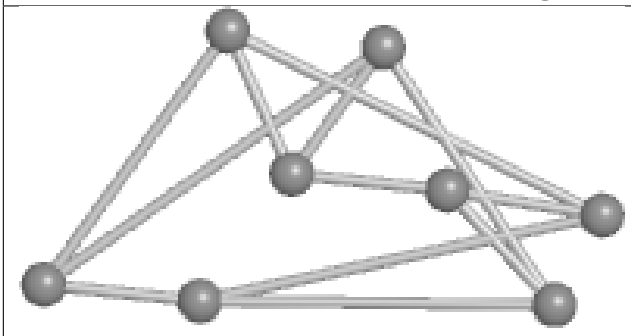


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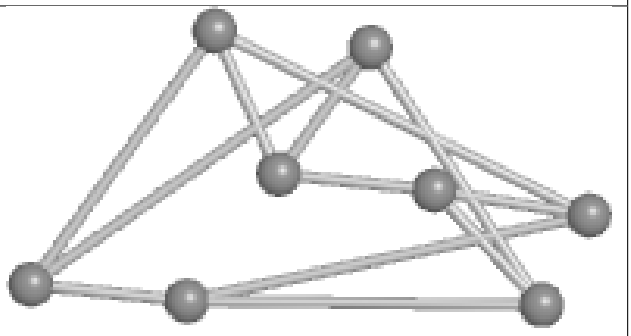


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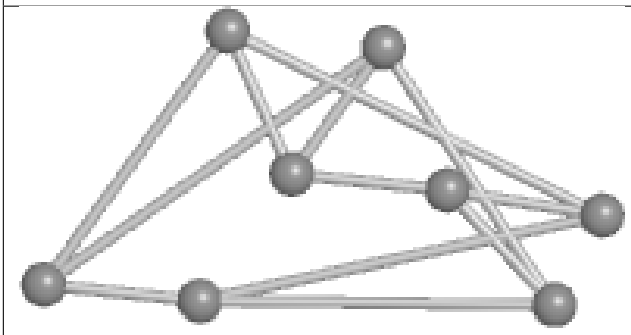
Ligand SF4 c 102



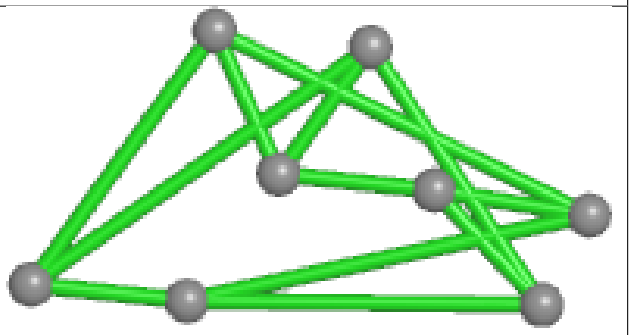
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Bond angles

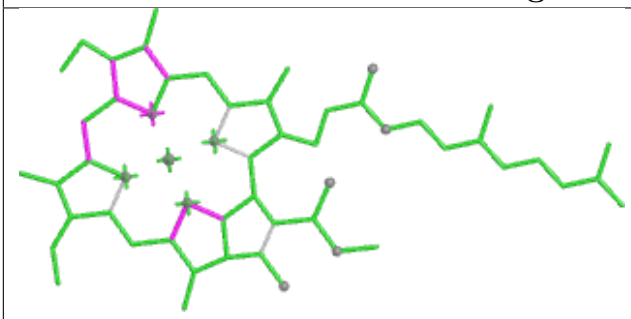


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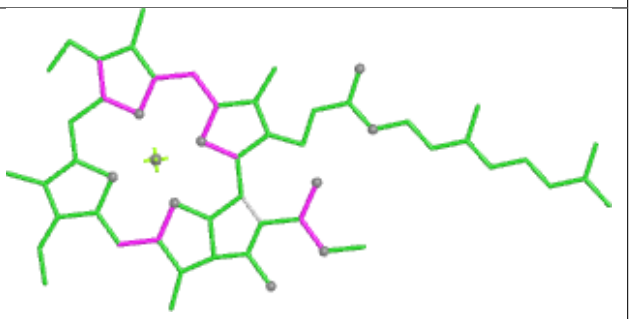


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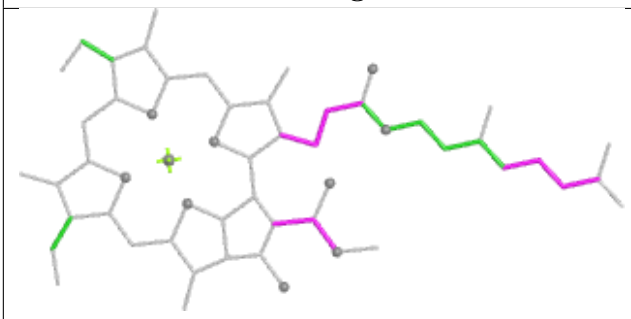
Ligand CLA b 852



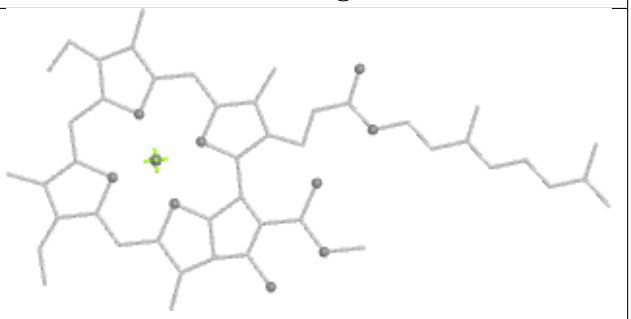
Bond lengths



Bond angles

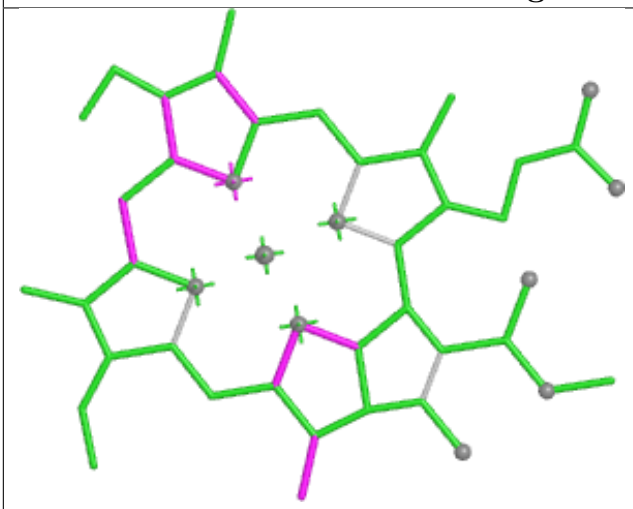


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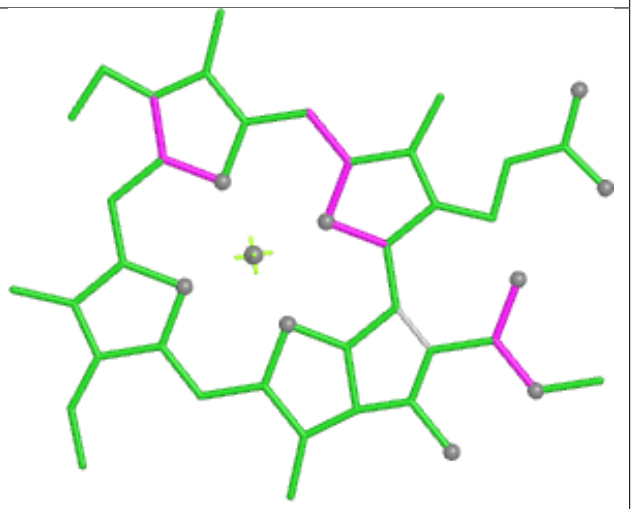


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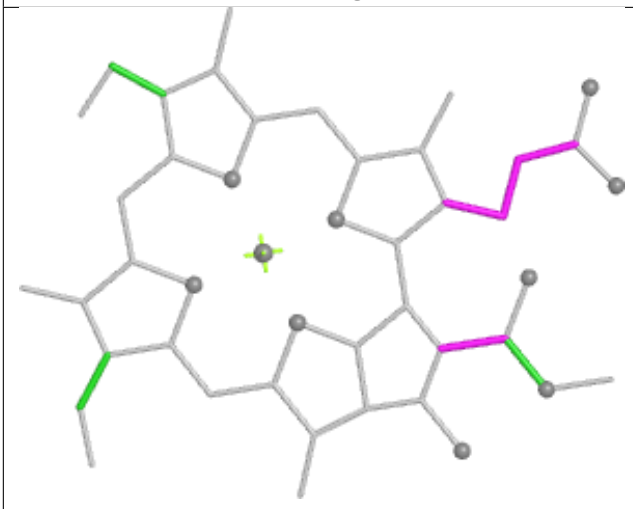
Ligand CLA b 821



Bond lengths



Bond angles

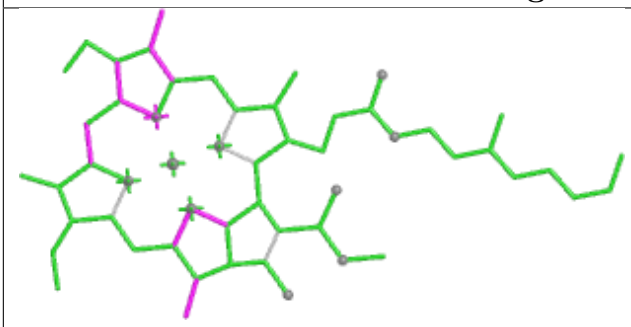


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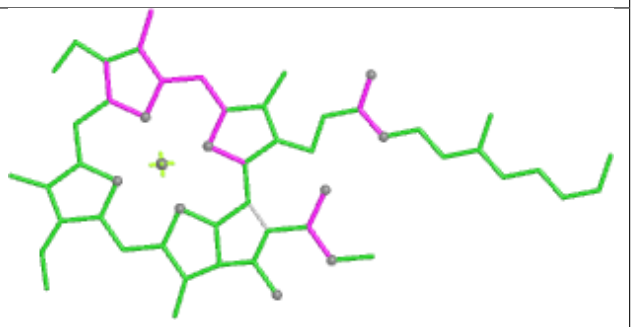


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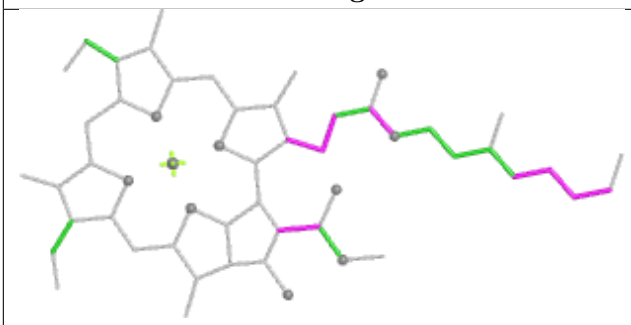
Ligand CLA b 830



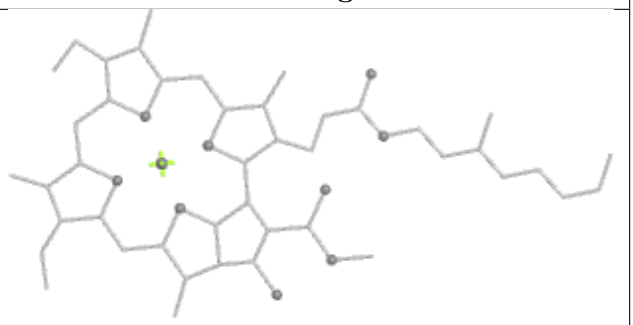
Bond lengths



Bond angles

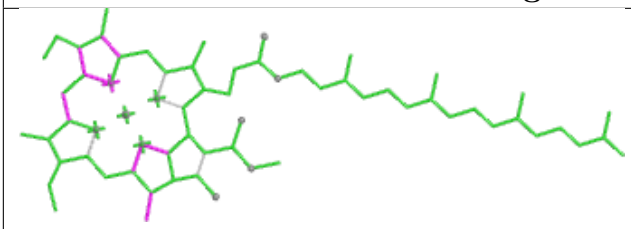


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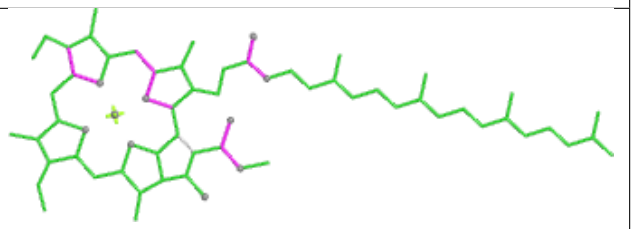


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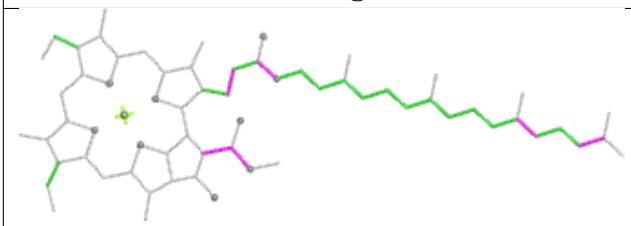
Ligand CLA N 831



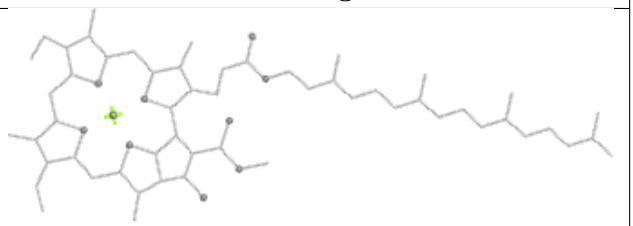
Bond lengths



Bond angles

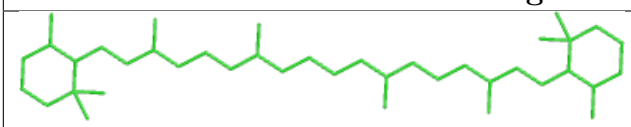


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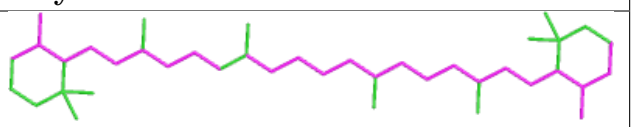


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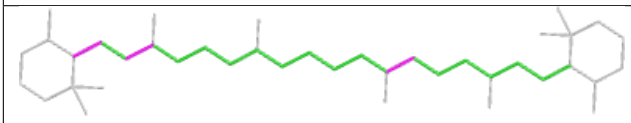
Ligand BCR y 101



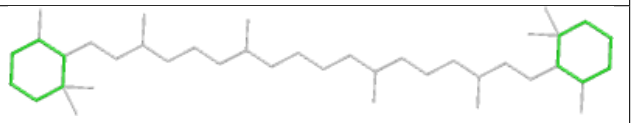
Bond lengths



Bond angles

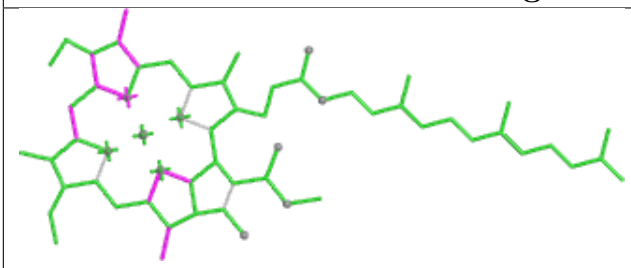


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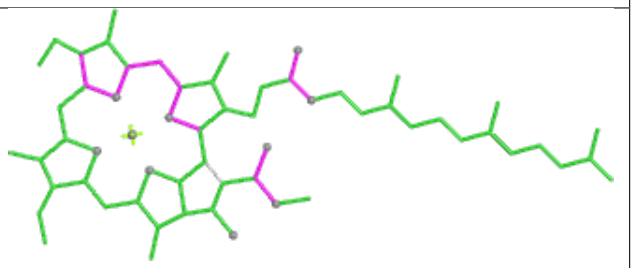


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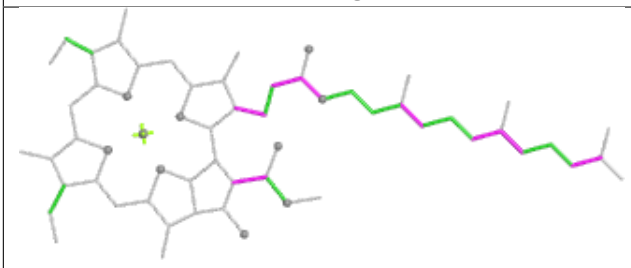
Ligand CLA N 812



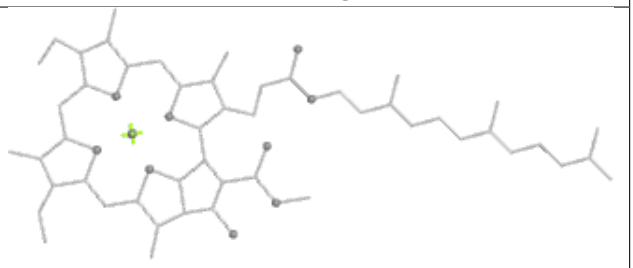
Bond lengths



Bond angles

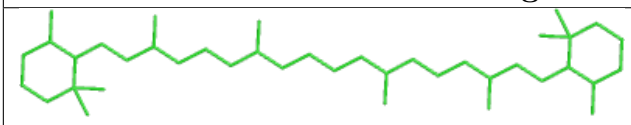


Torsions

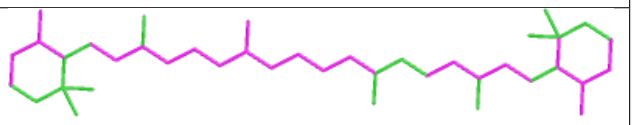


Rings

Ligand BCR N 847



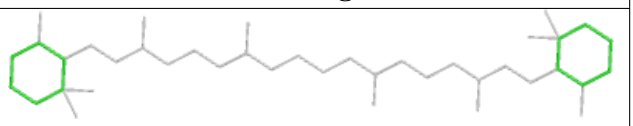
Bond lengths



Bond angles

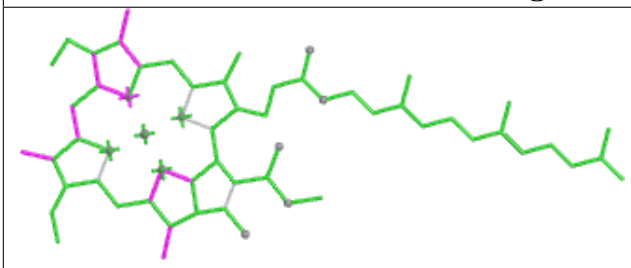


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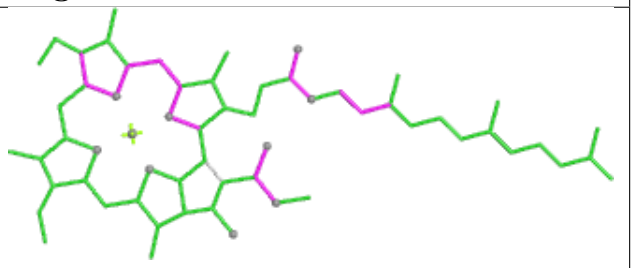


Rings

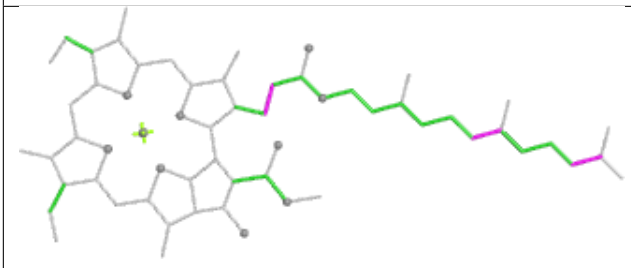
Ligand CLA g 811



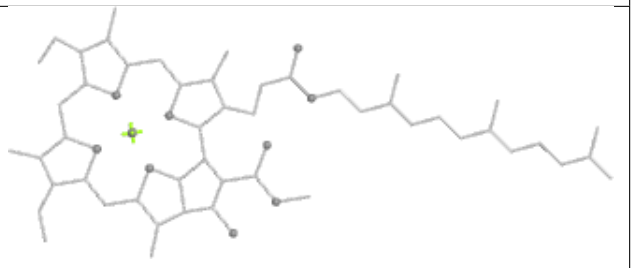
Bond lengths



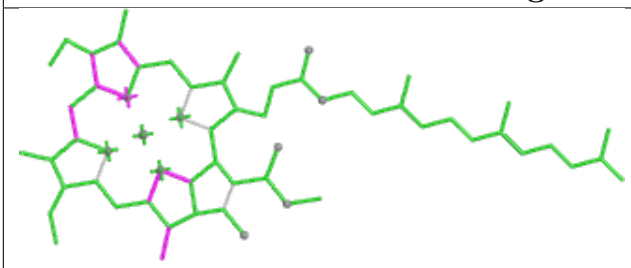
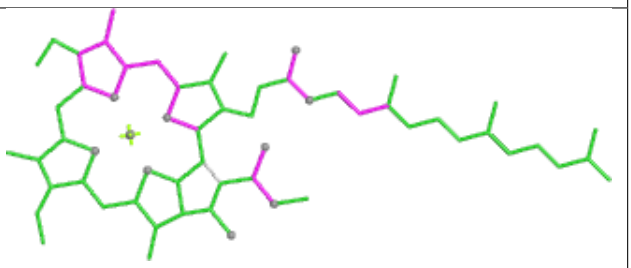
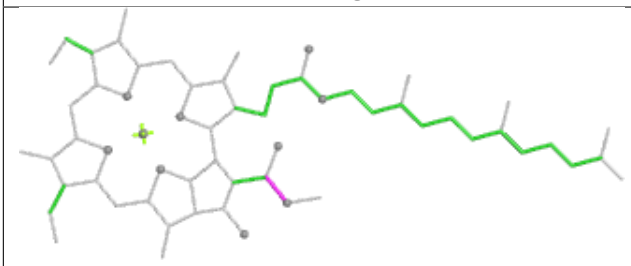
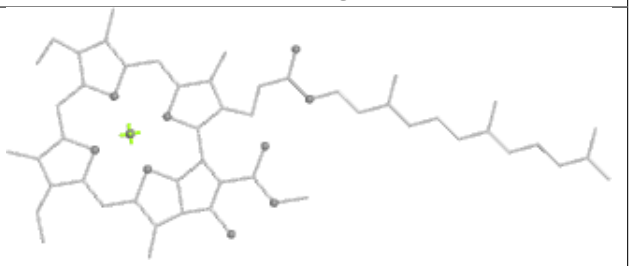
Bond angles

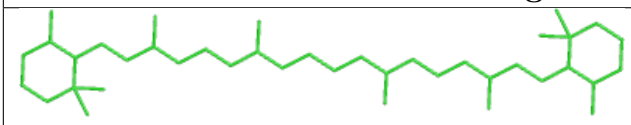
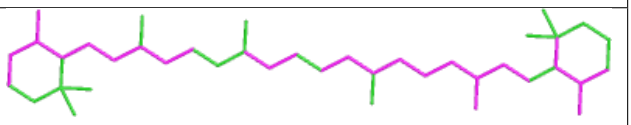
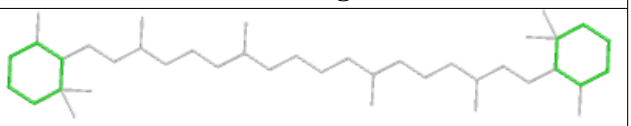


Torsions

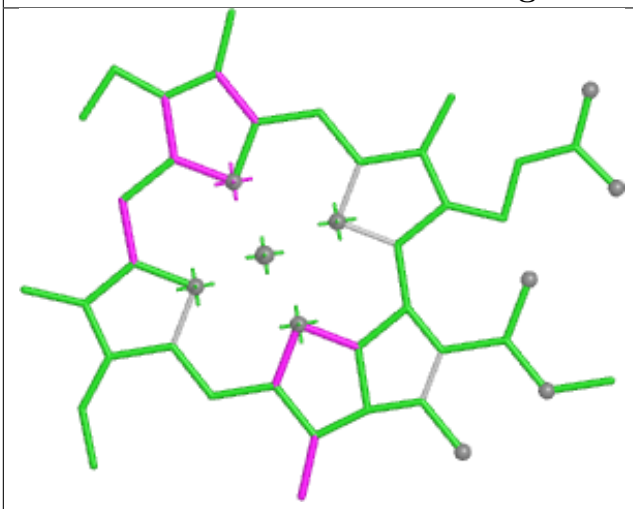


Rings

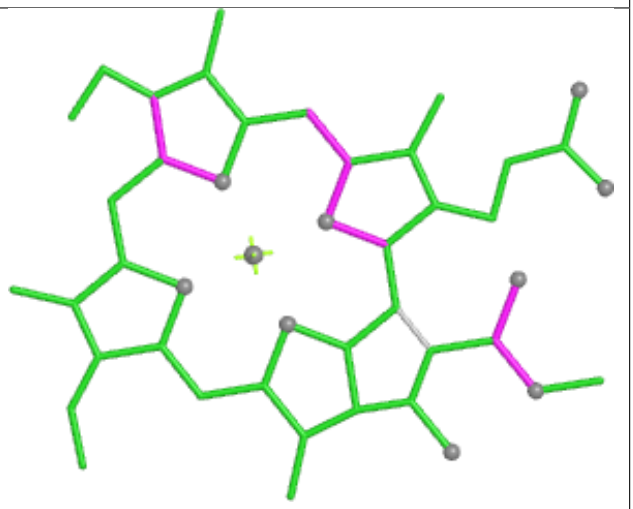
Ligand CLA n 836	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR n 842	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

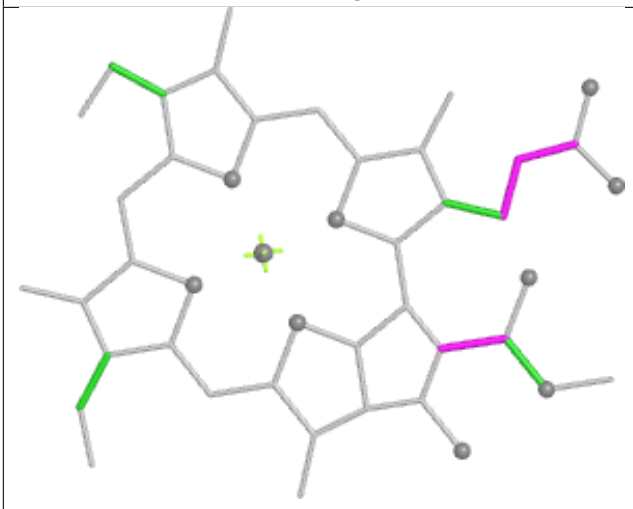
Ligand CLA W 204



Bond lengths



Bond angles

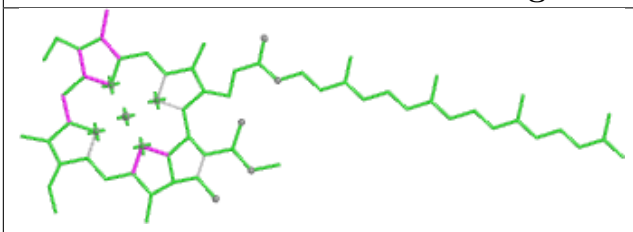


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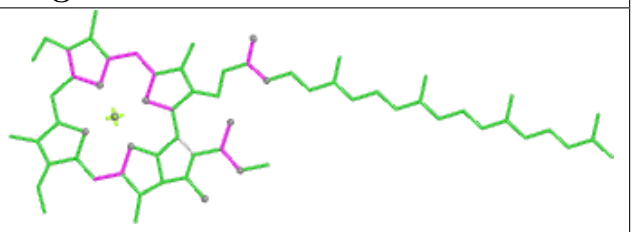


Rings

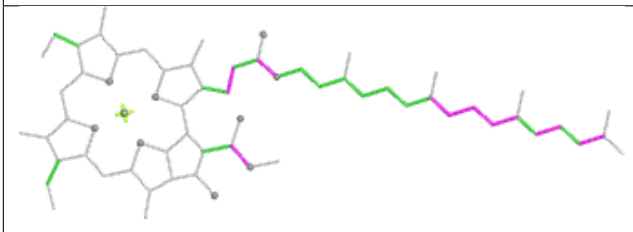
Ligand CLA g 819



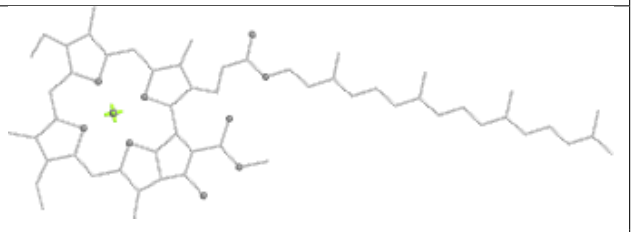
Bond lengths



Bond angles

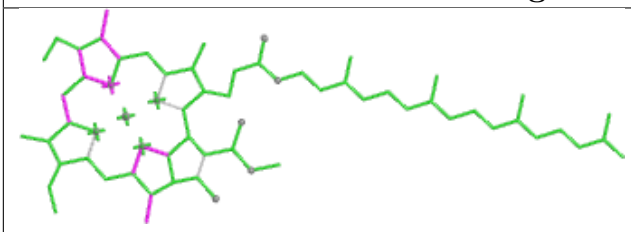


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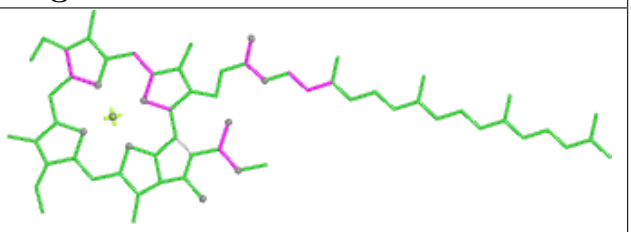


Rings

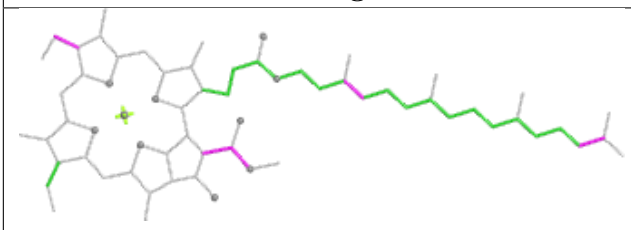
Ligand CLA g 831



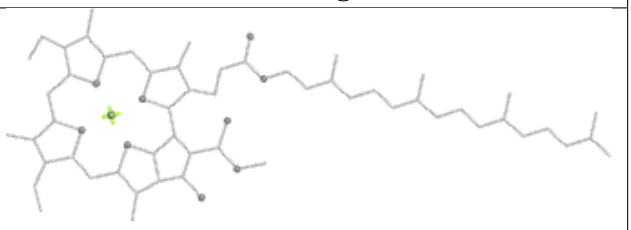
Bond lengths



Bond angles

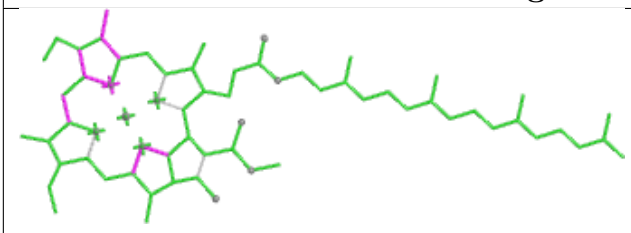


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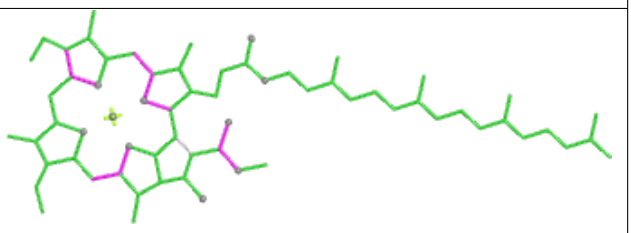


Rings

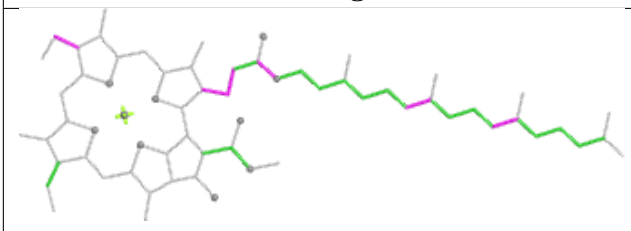
Ligand CLA n 818



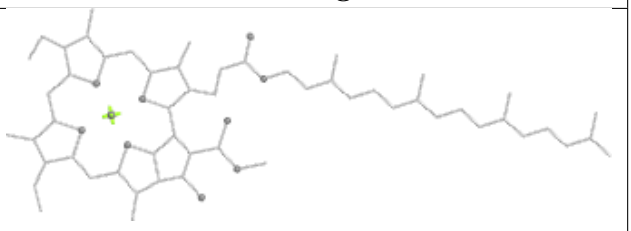
Bond lengths



Bond angles

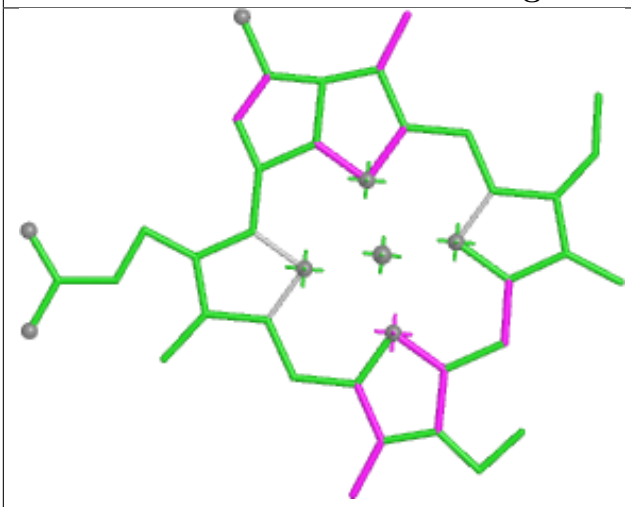


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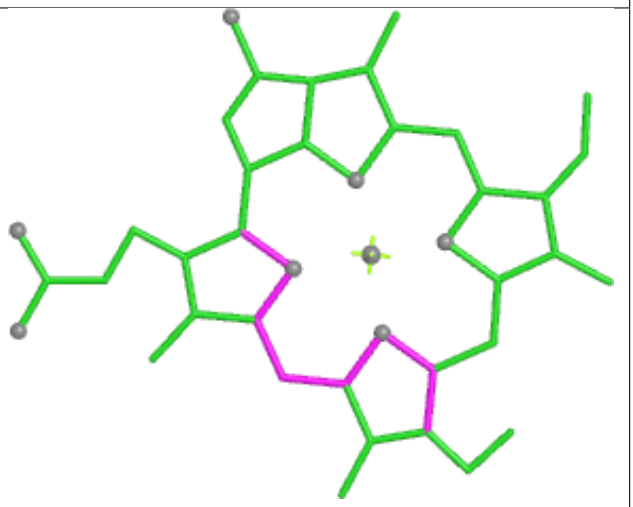


Rings

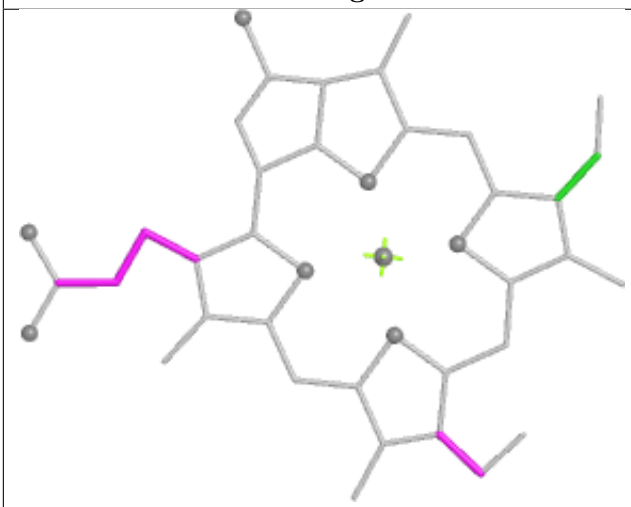
Ligand CLA U 101



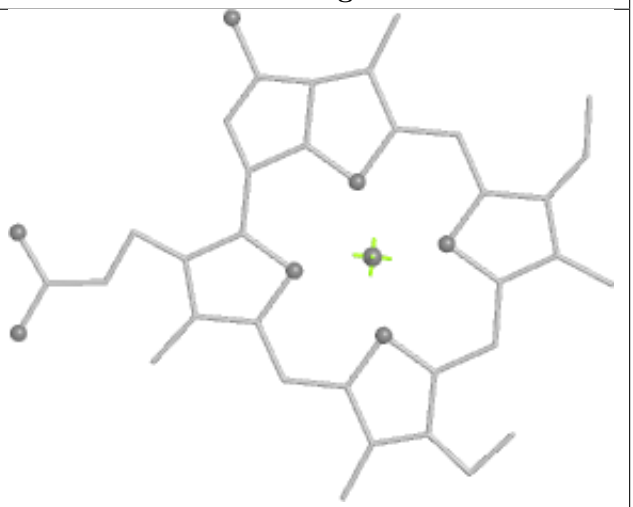
Bond lengths



Bond angles

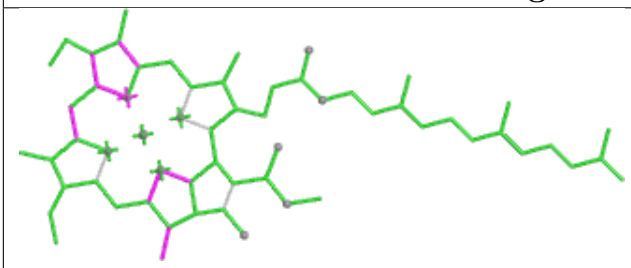


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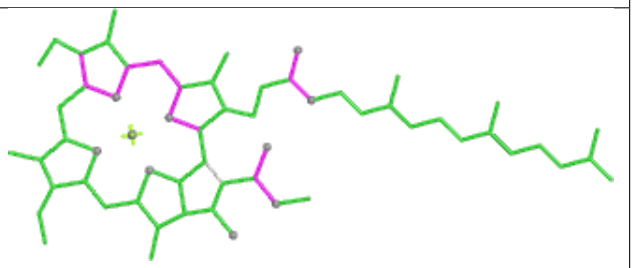


Rings

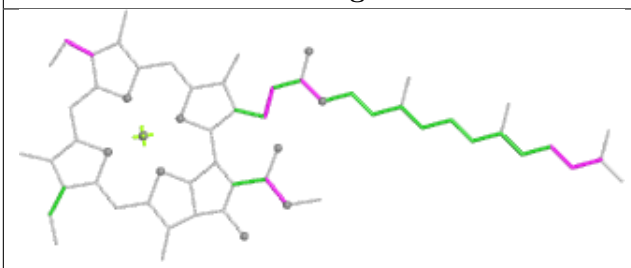
Ligand CLA a 816



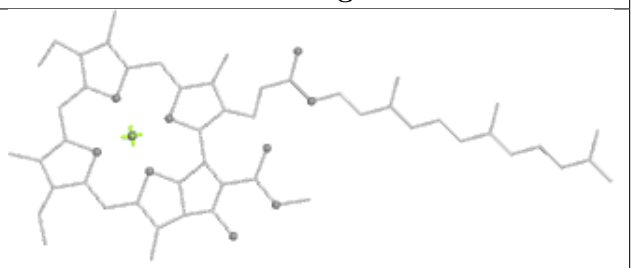
Bond lengths



Bond angles

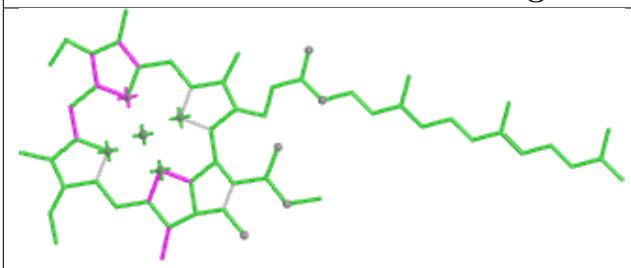


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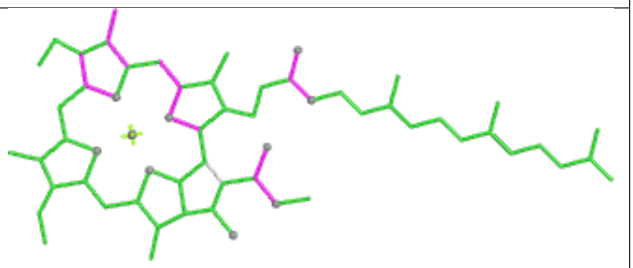


Rings

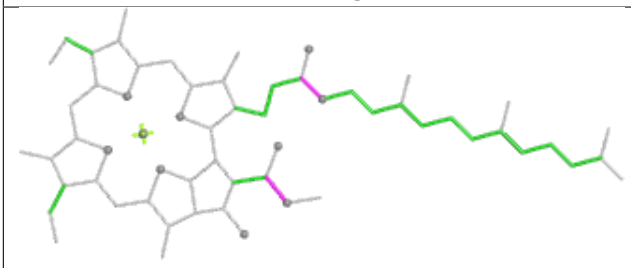
Ligand CLA b 831



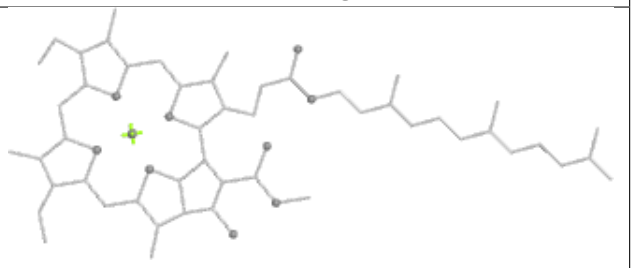
Bond lengths



Bond angles

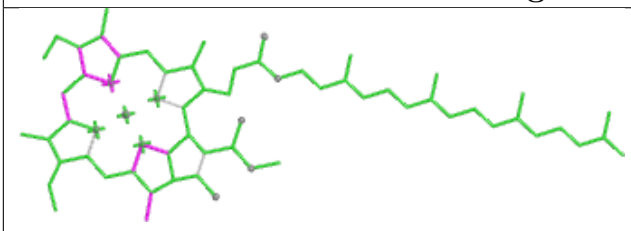


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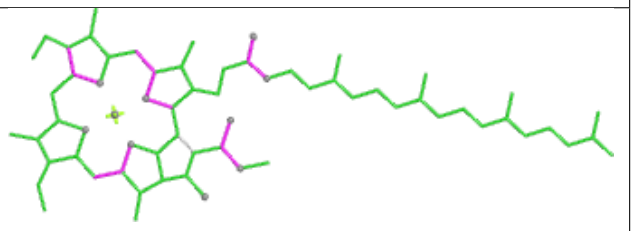


Rings

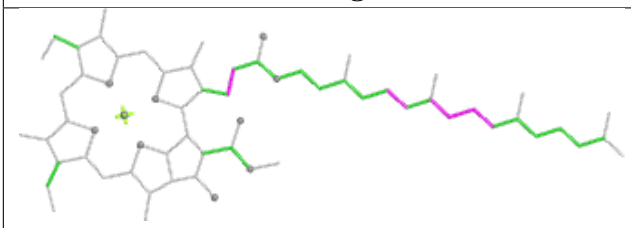
Ligand CLA b 807



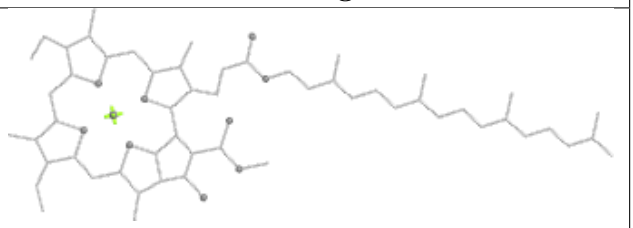
Bond lengths



Bond angles



Torsions



Rings

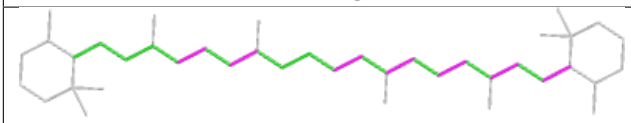
Ligand BCR a 846



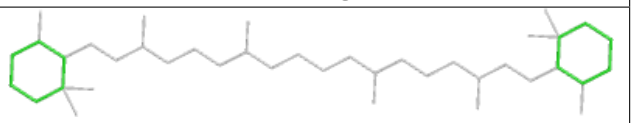
Bond lengths



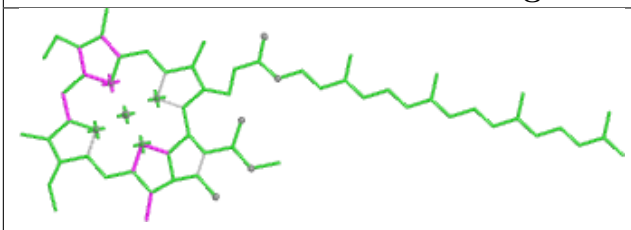
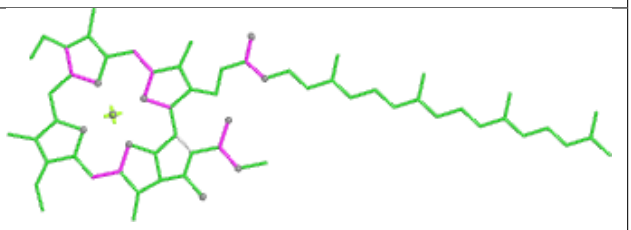
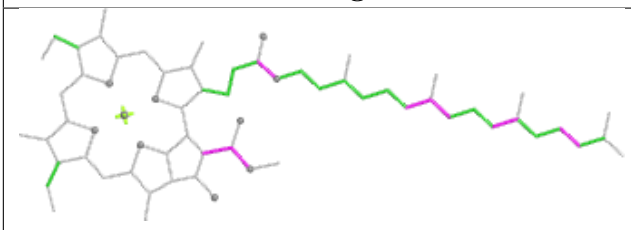
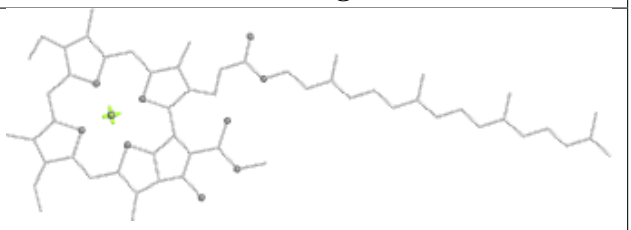
Bond angles

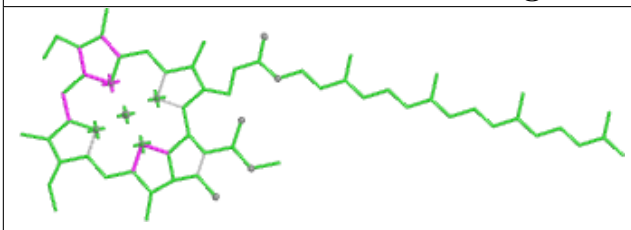
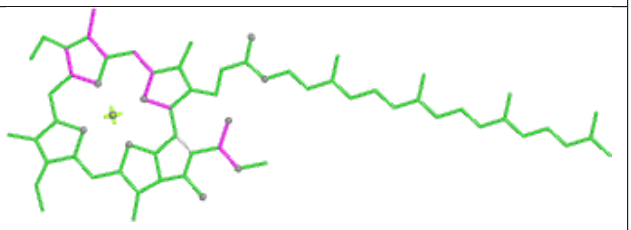
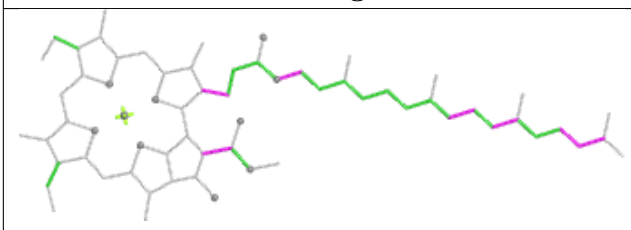
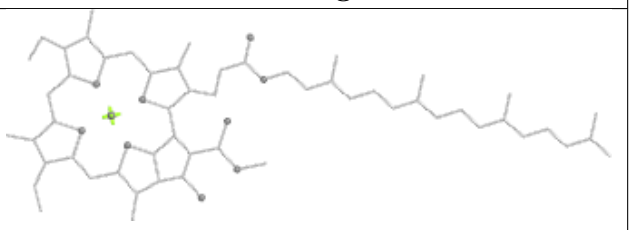


Torsions

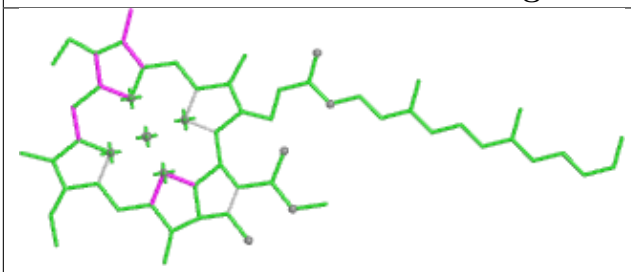


Rings

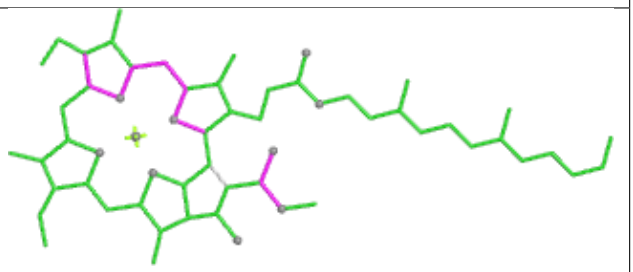
Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

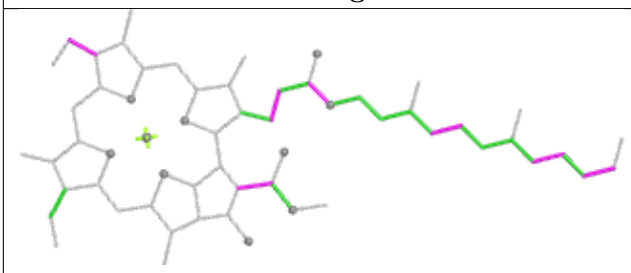
Ligand CLA G 811



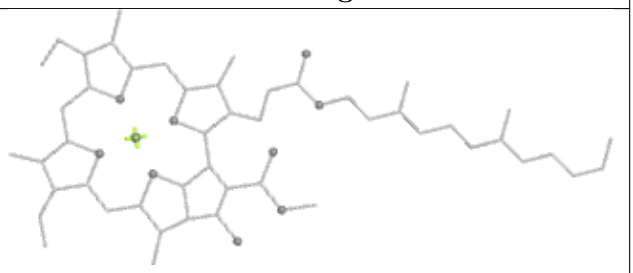
Bond lengths



Bond angles

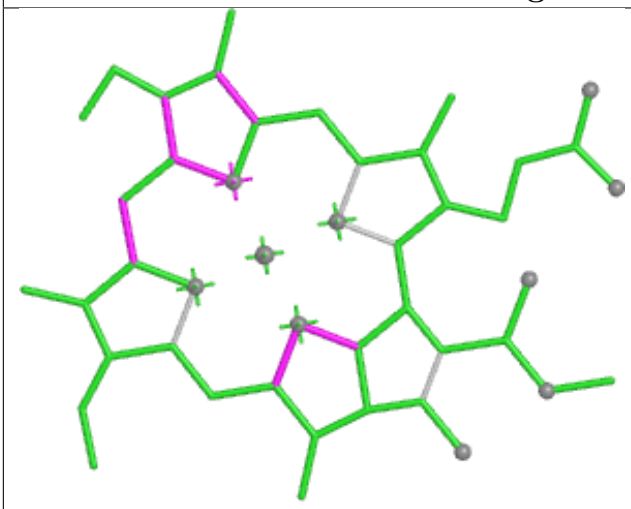


Torsions

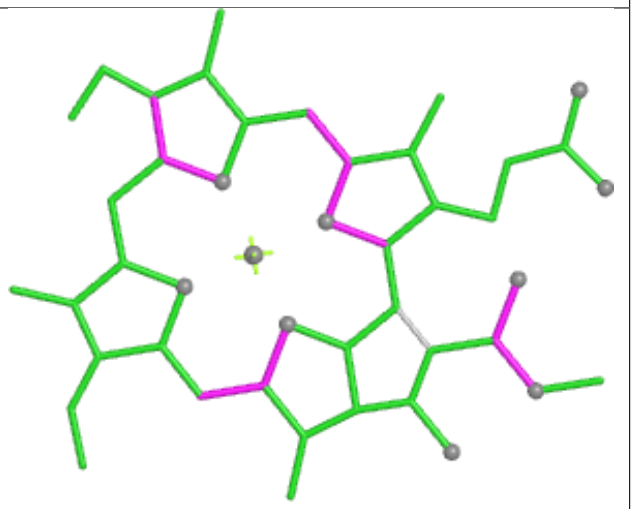


Rings

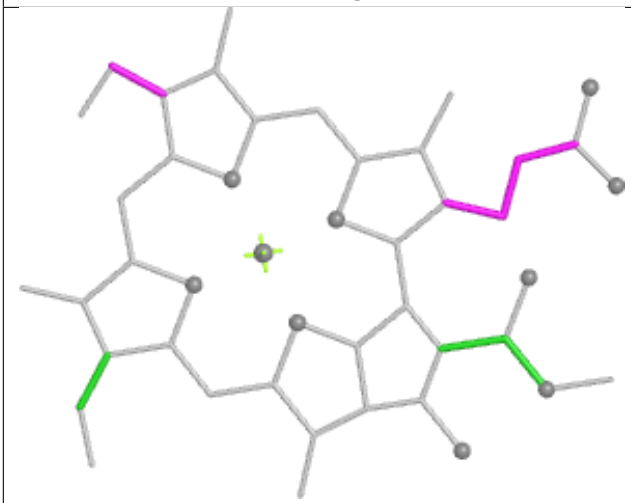
Ligand CLA n 816



Bond lengths



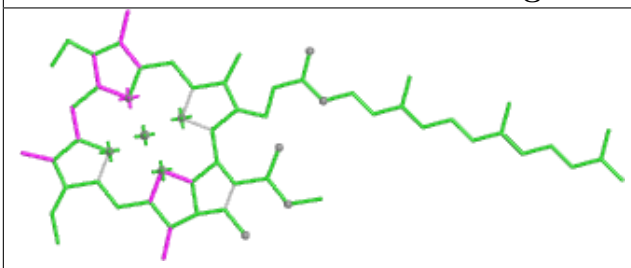
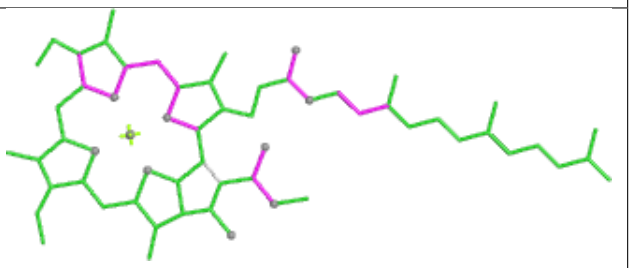
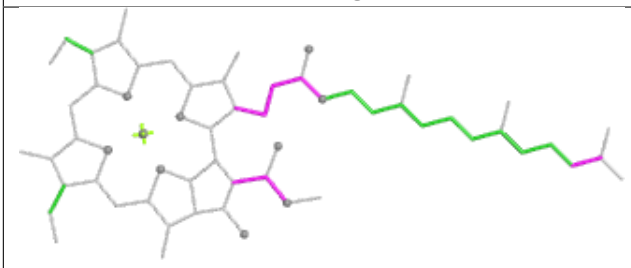
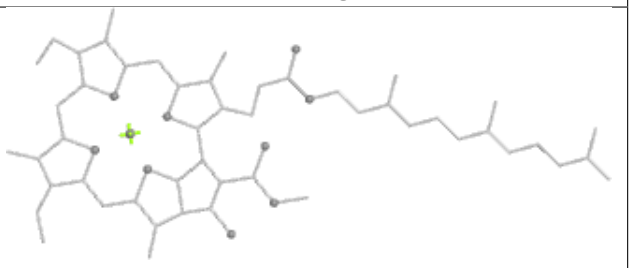
Bond angles

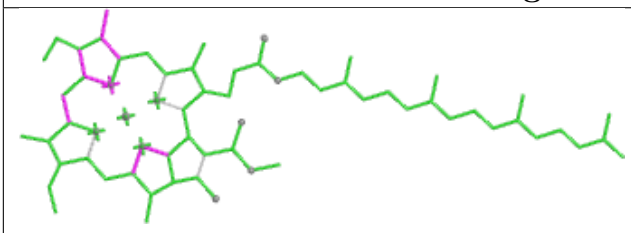
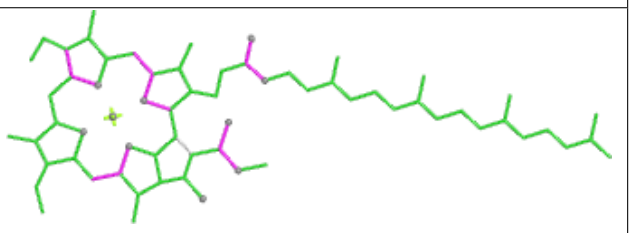
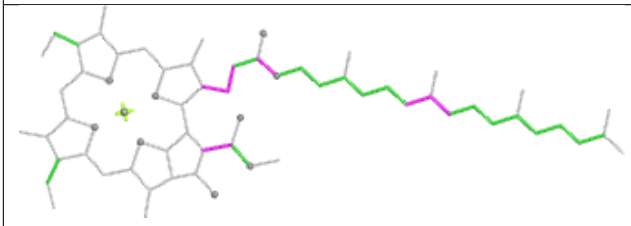
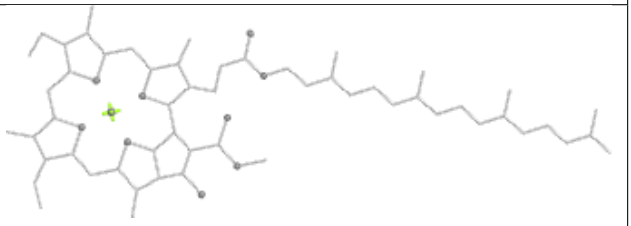


Torsions

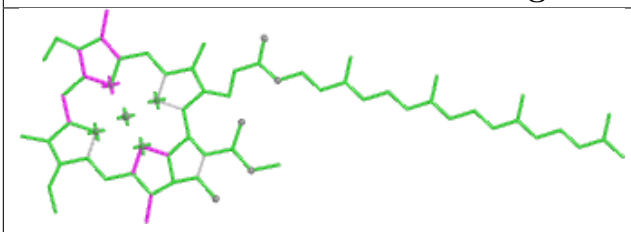


Rings

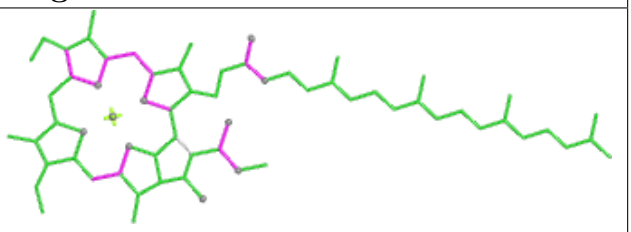
Ligand CLA A 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

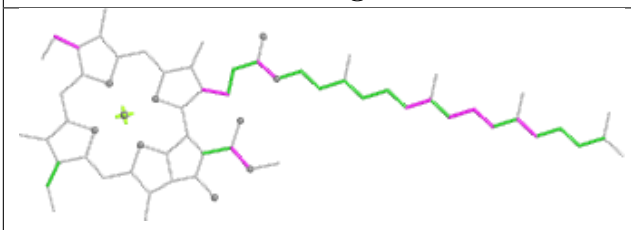
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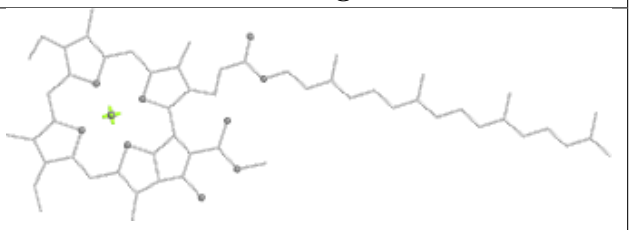
Bond lengths



Bond angles

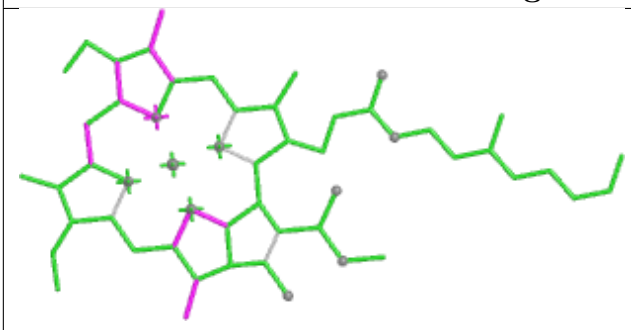


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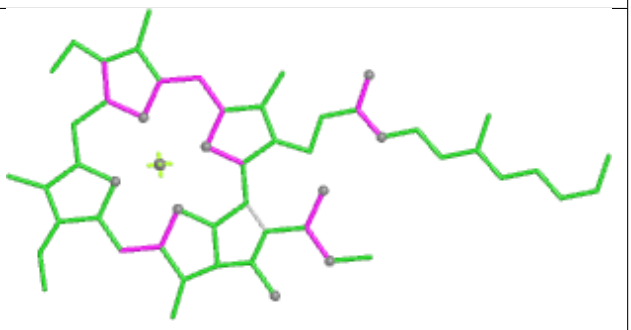


Rings

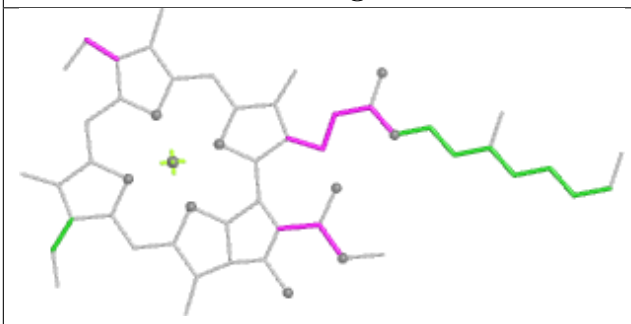
Ligand CLA A 830



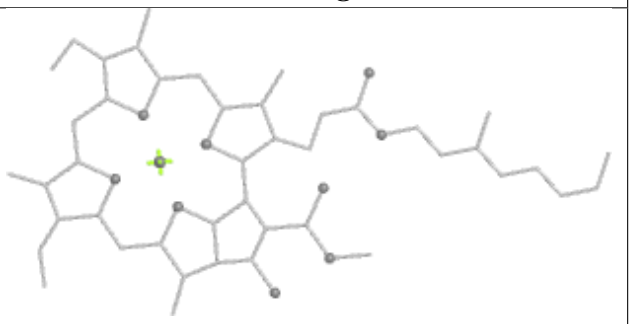
Bond lengths



Bond angles

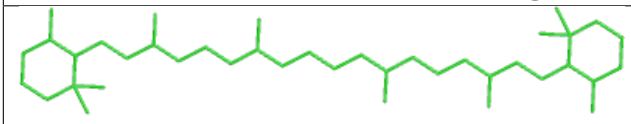


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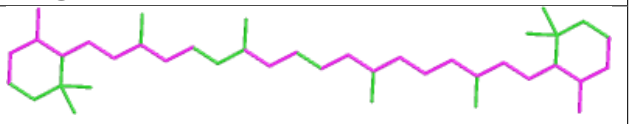


Rings

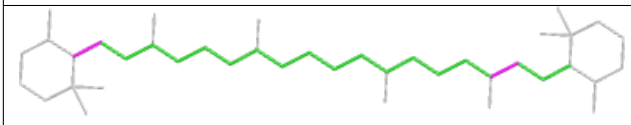
Ligand BCR g 844



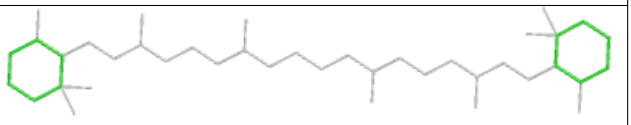
Bond lengths



Bond angles

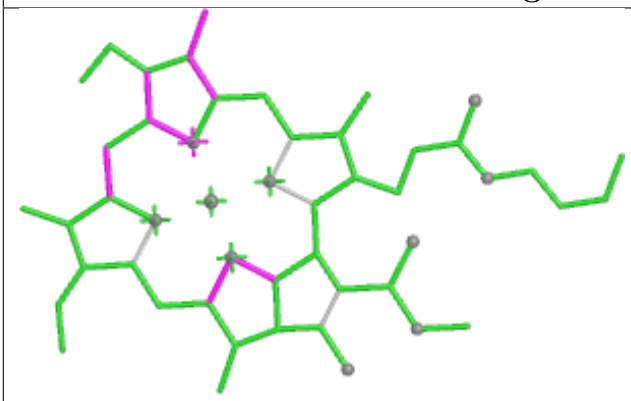


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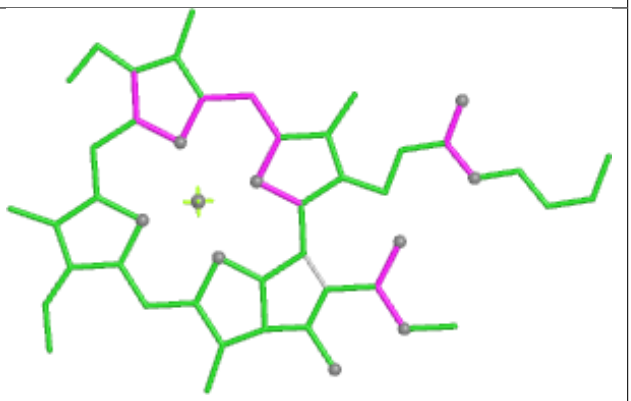


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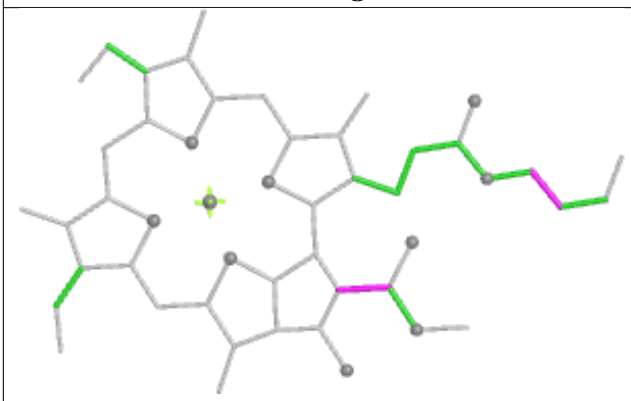
Ligand CLA U 102



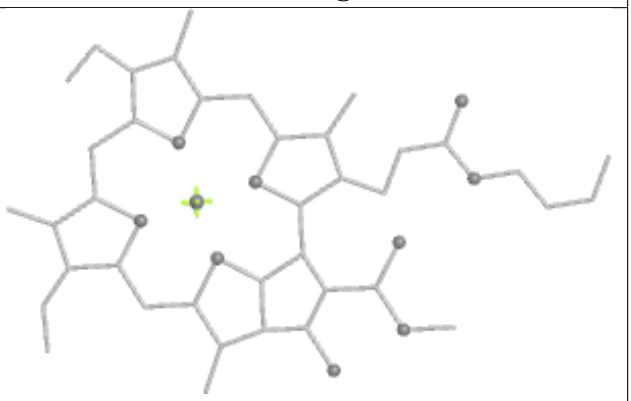
Bond lengths



Bond angles

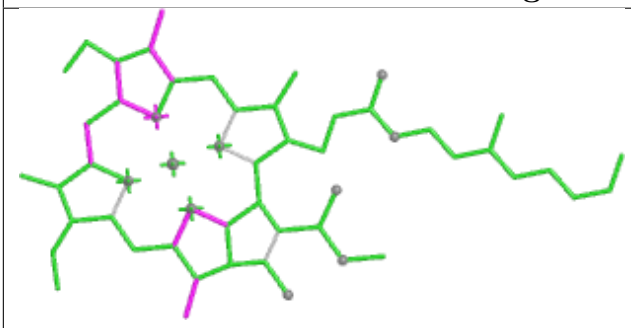


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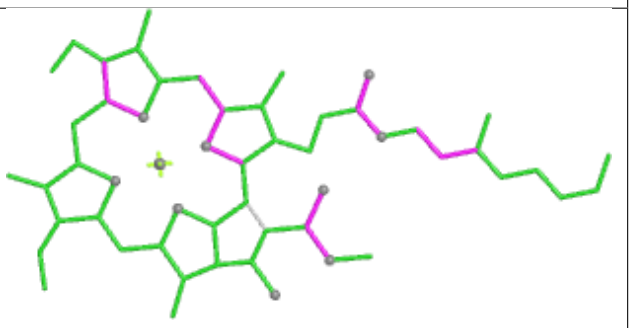


Rings

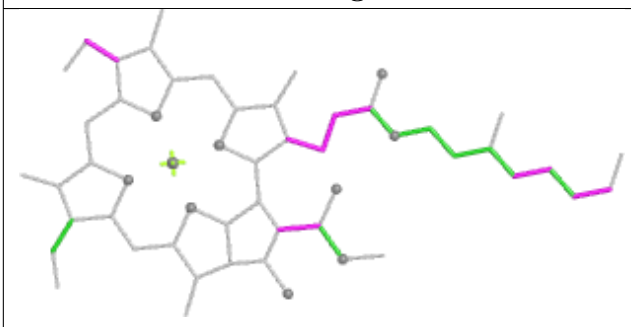
Ligand CLA G 830



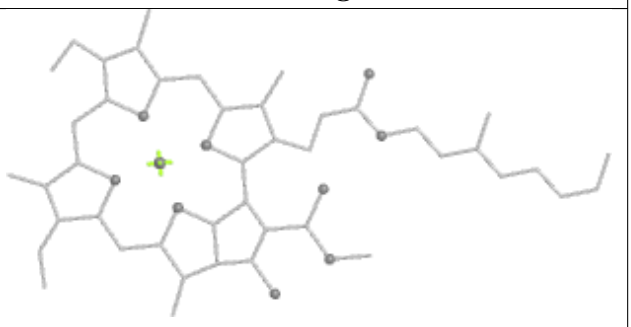
Bond lengths



Bond angles

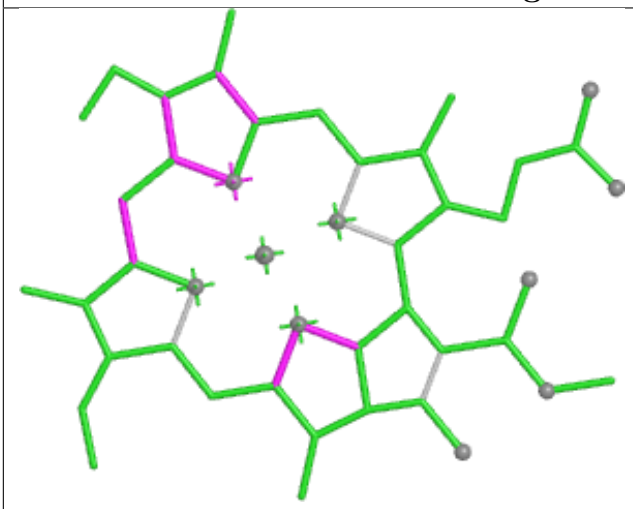


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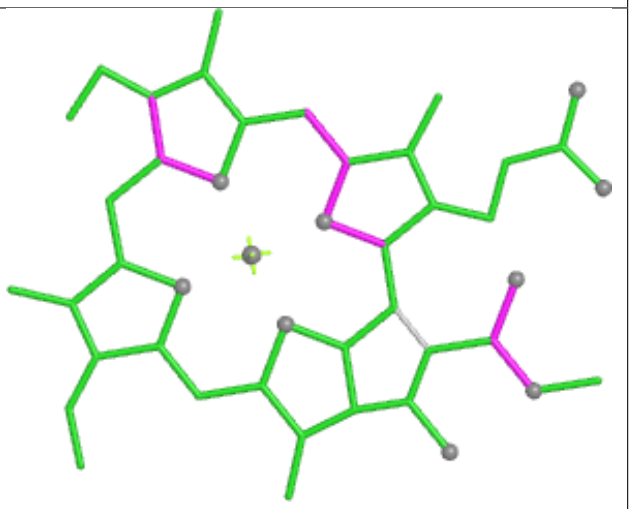


Rings

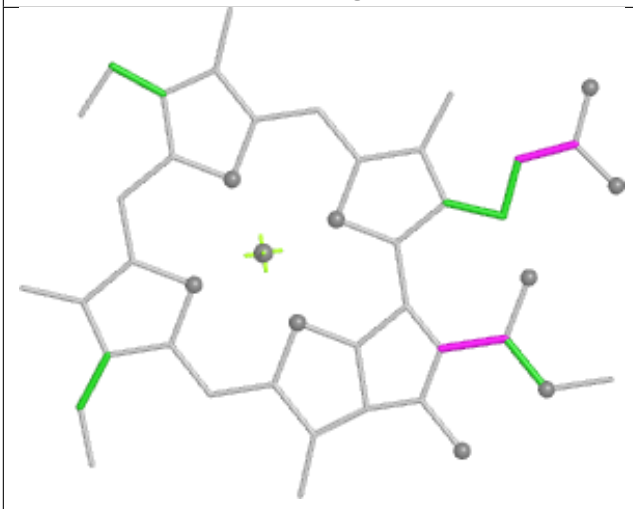
Ligand CLA N 823



Bond lengths



Bond angles

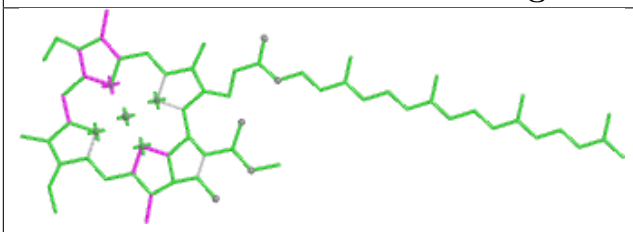


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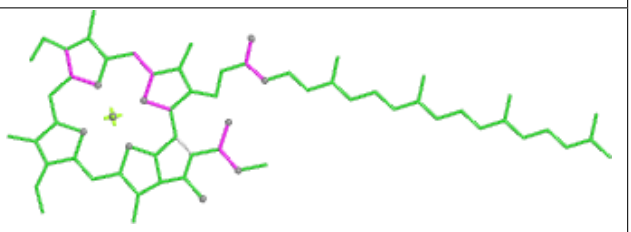


Rings

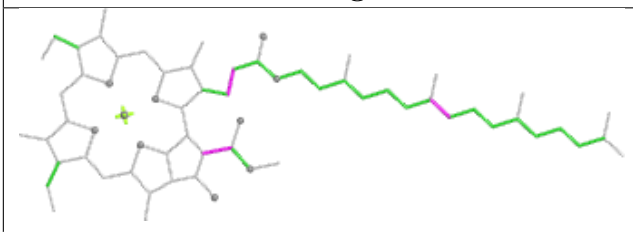
Ligand CLA a 839



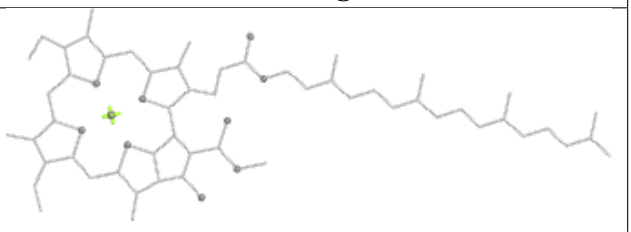
Bond lengths



Bond angles

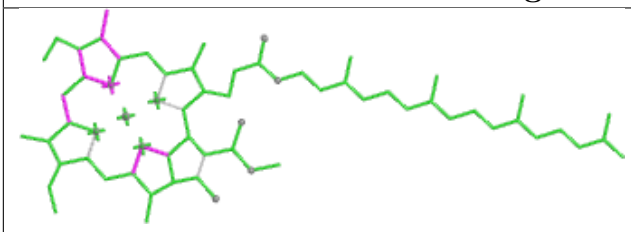


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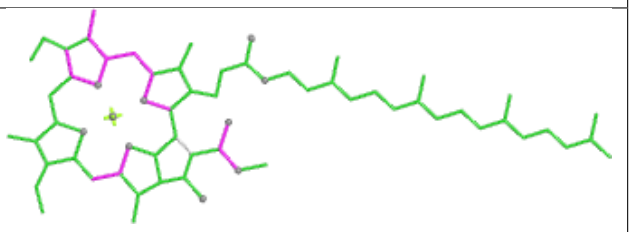


Rings

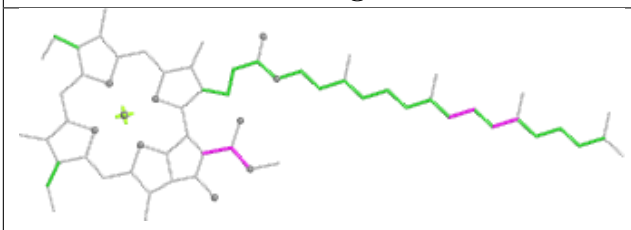
Ligand CLA B 820



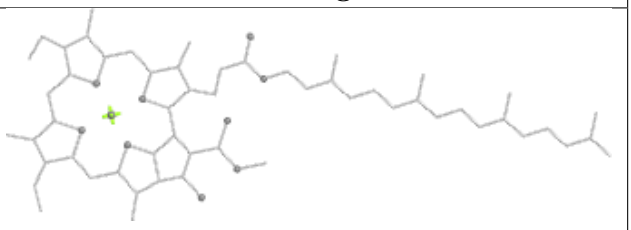
Bond lengths



Bond angles

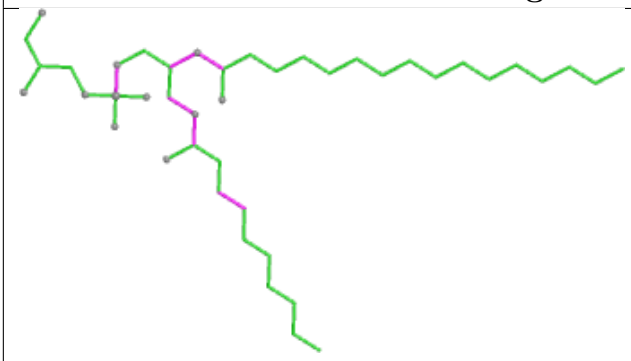


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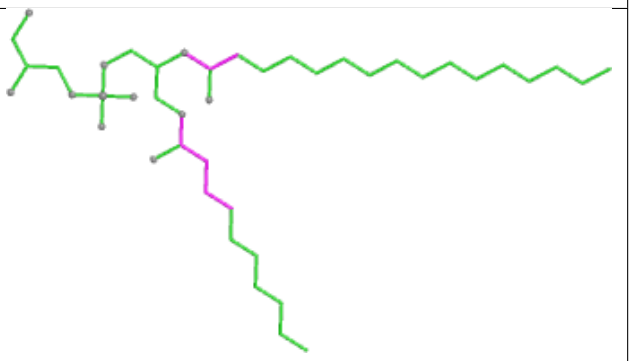


Rings

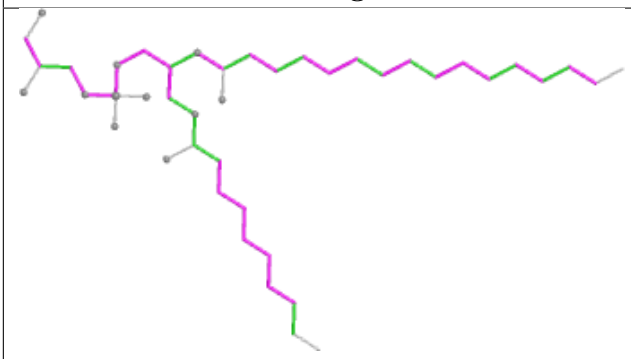
Ligand LHG v 102



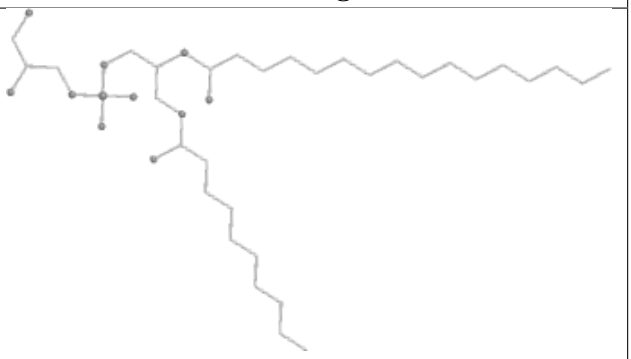
Bond lengths



Bond angles

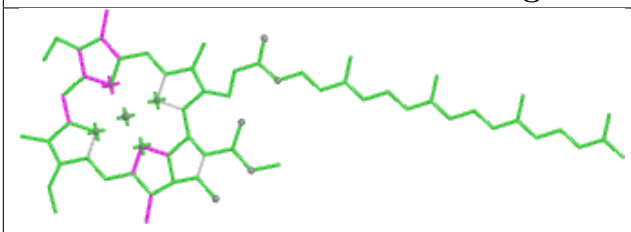


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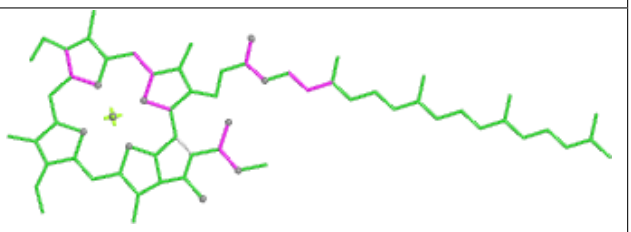


Rings

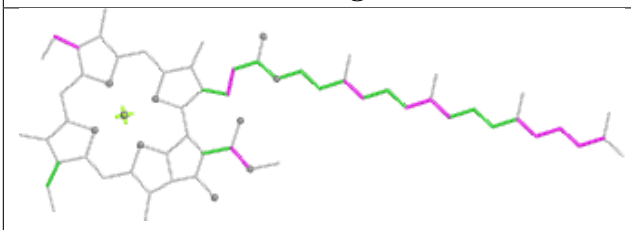
Ligand CLA G 832



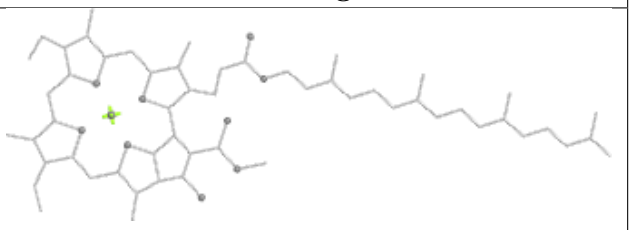
Bond lengths



Bond angles

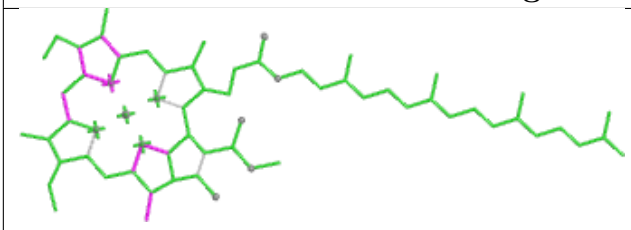


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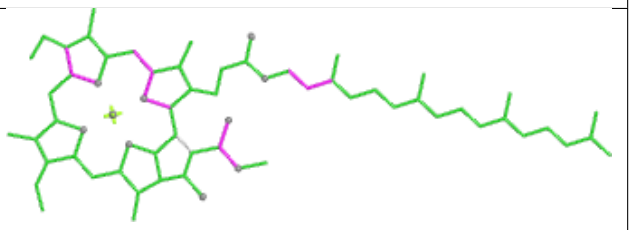


Rings

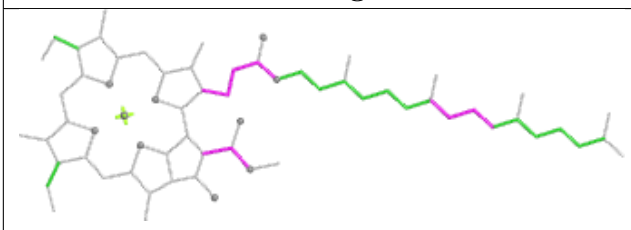
Ligand CLA G 827



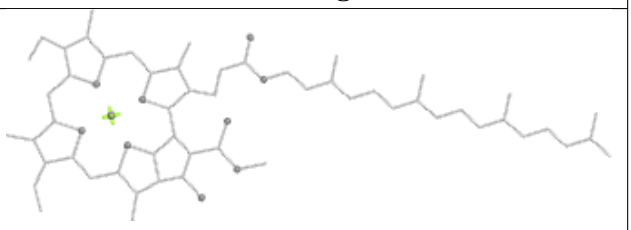
Bond lengths



Bond angles

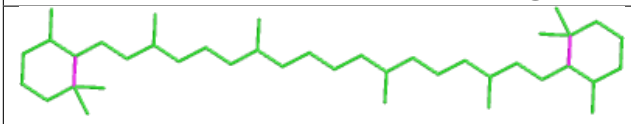


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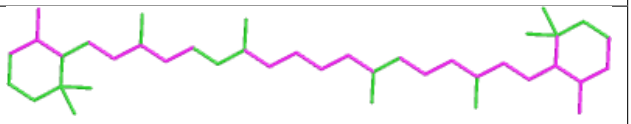


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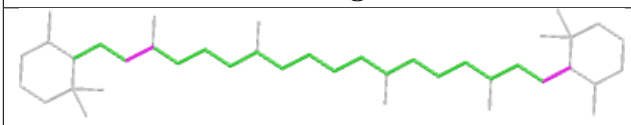
Ligand BCR a 847



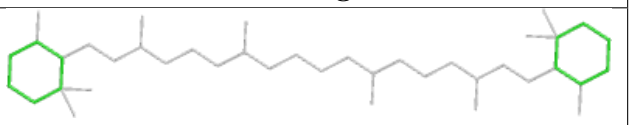
Bond lengths



Bond angles

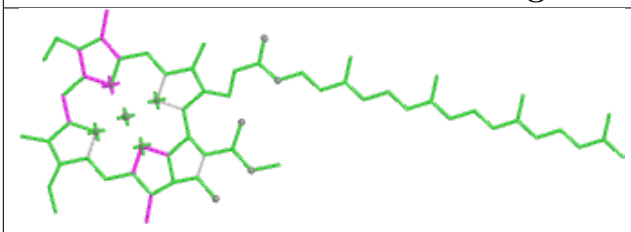


Torsions

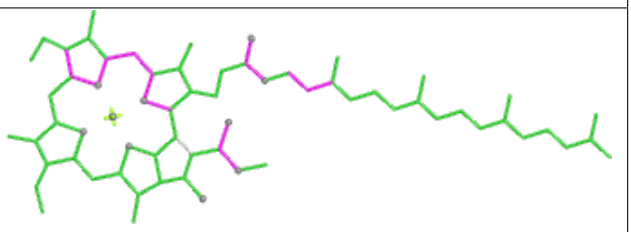


Rings

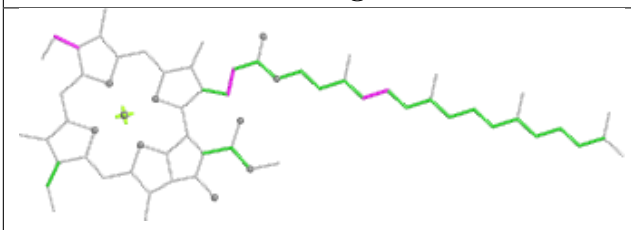
Ligand CLA n 839



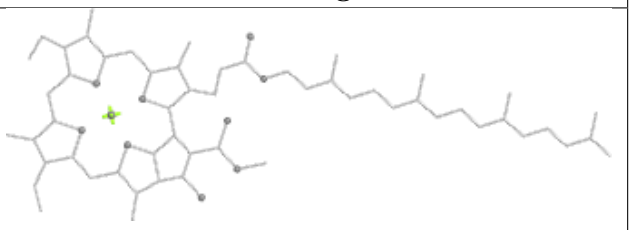
Bond lengths



Bond angles

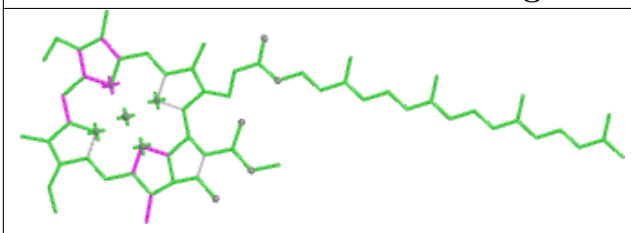


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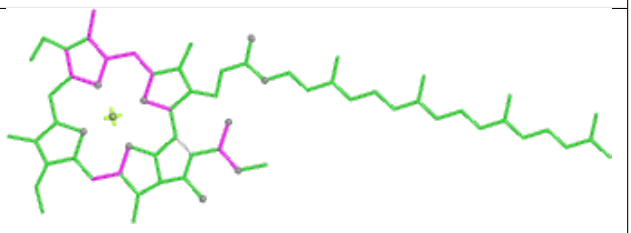


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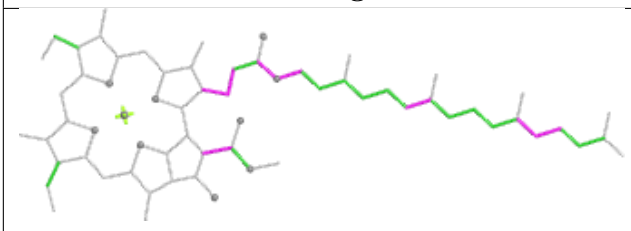
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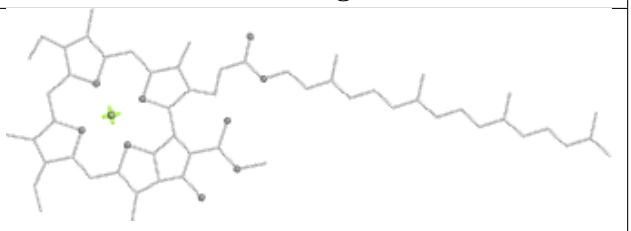
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Bond angles

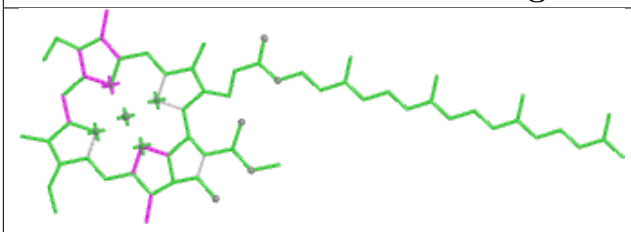


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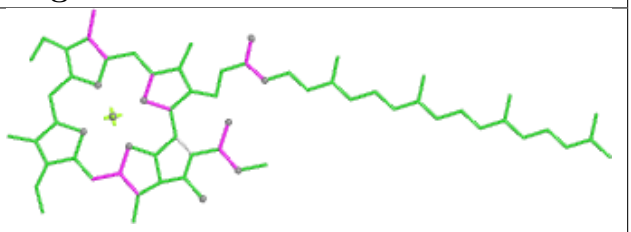


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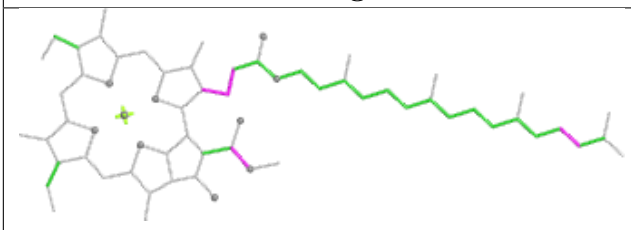
Ligand CLA g 853



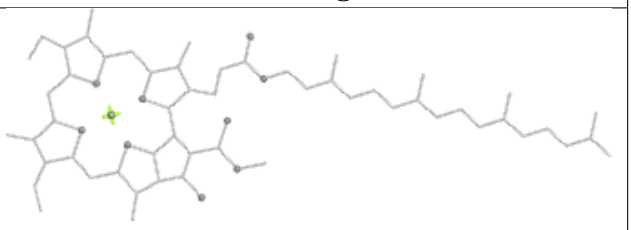
Bond lengths



Bond angles

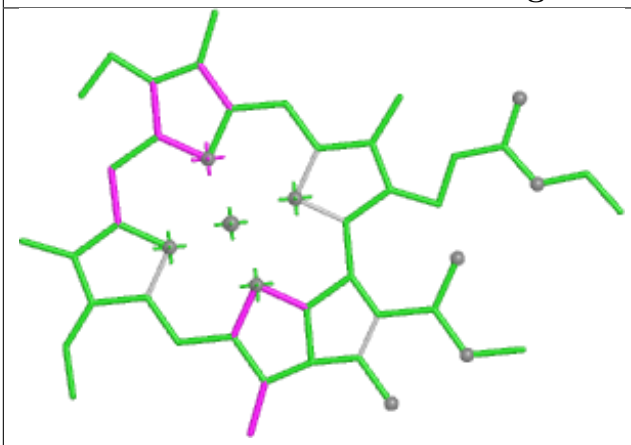


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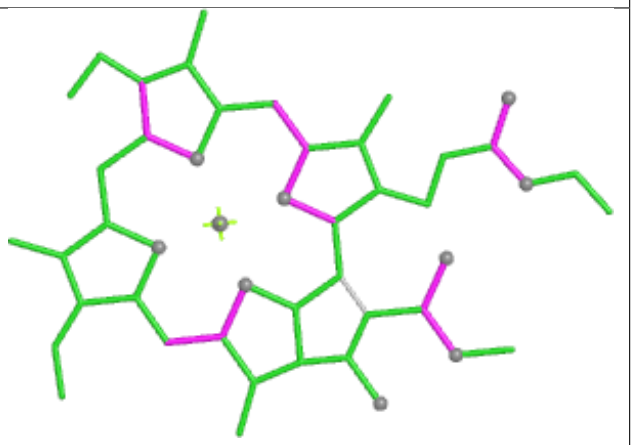


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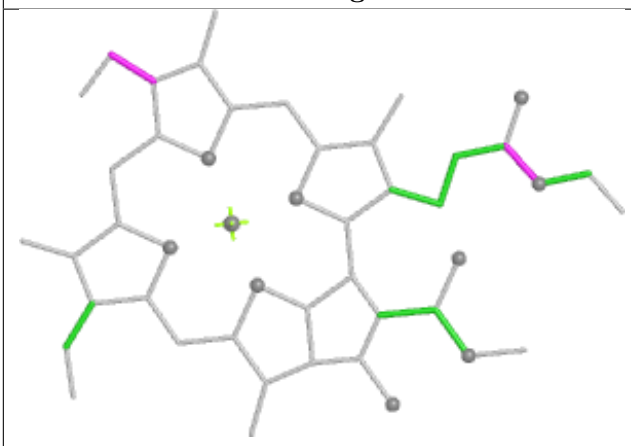
Ligand CLA n 838



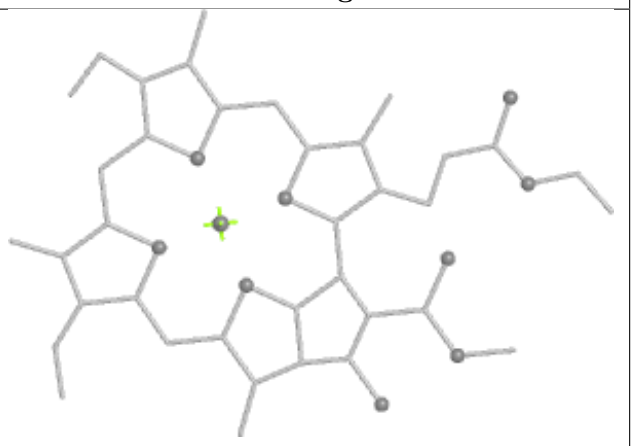
Bond lengths



Bond angles

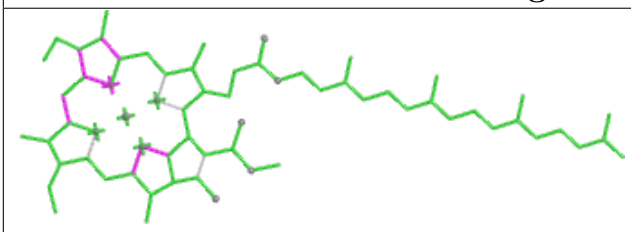


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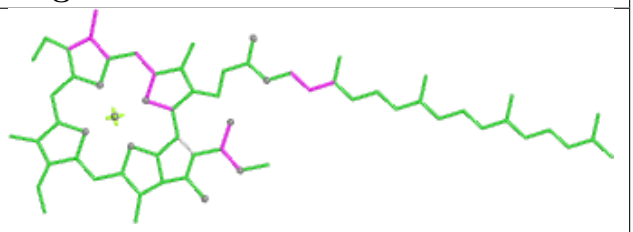


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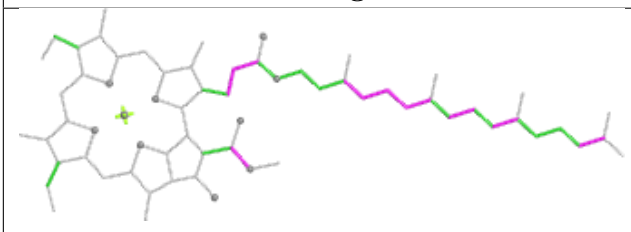
Ligand CLA g 826



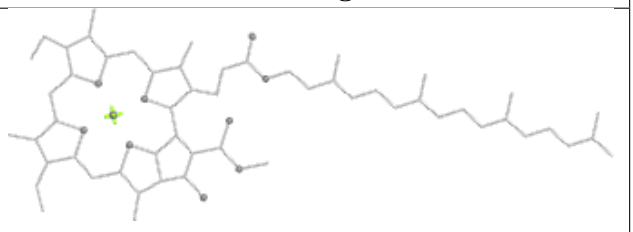
Bond lengths



Bond angles

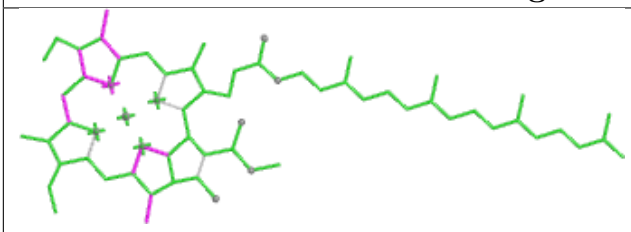


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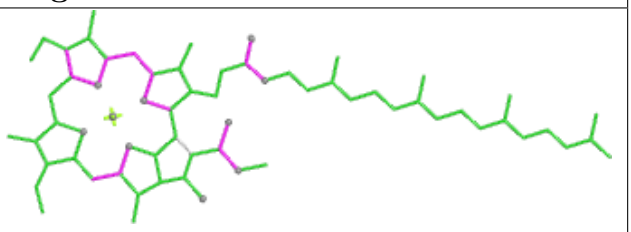


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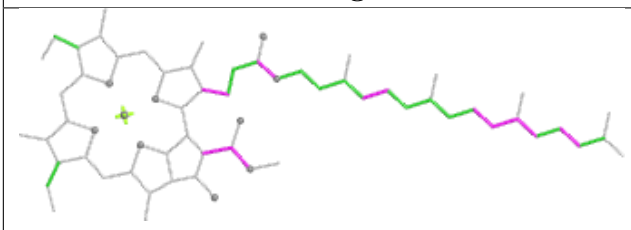
Ligand CLA g 804



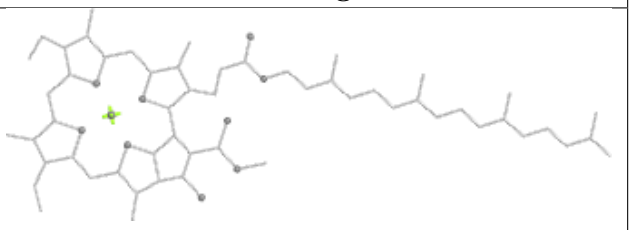
Bond lengths



Bond angles

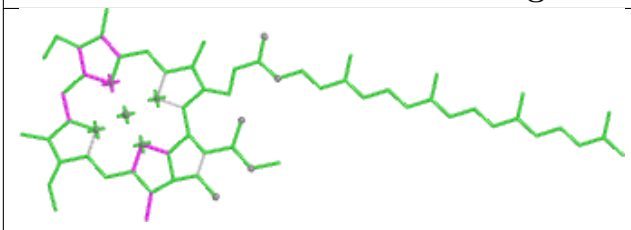


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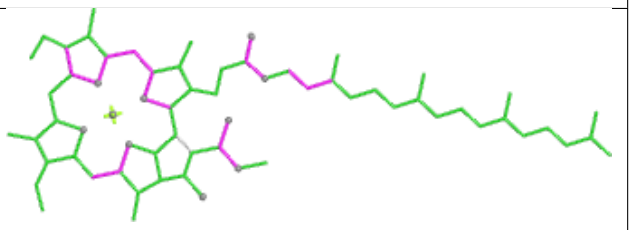


Rings

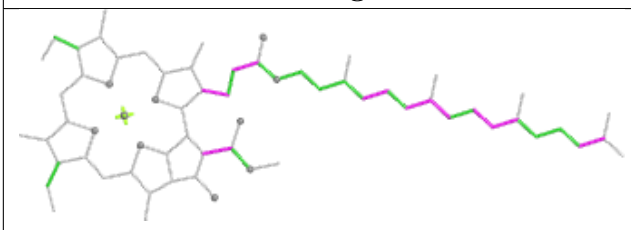
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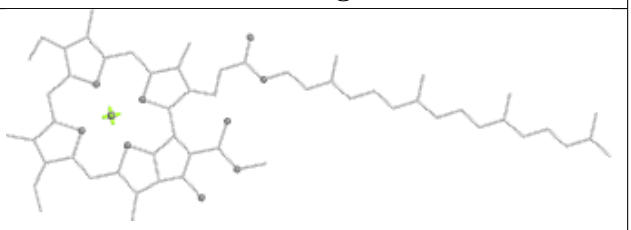
Bond lengths



Bond angles

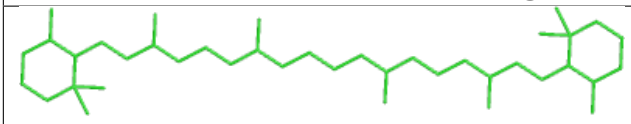


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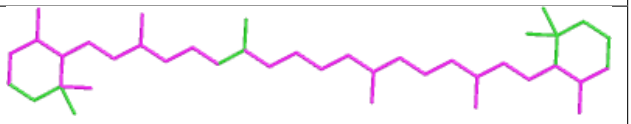


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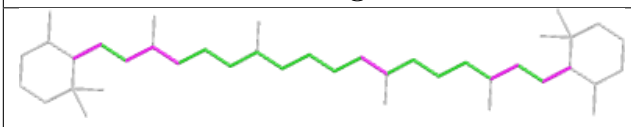
Ligand BCR G 848



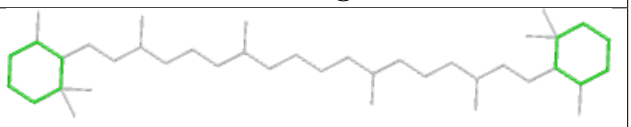
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Bond angles

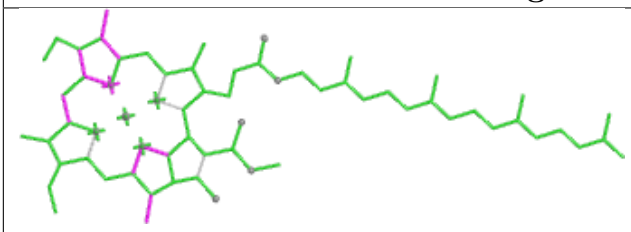


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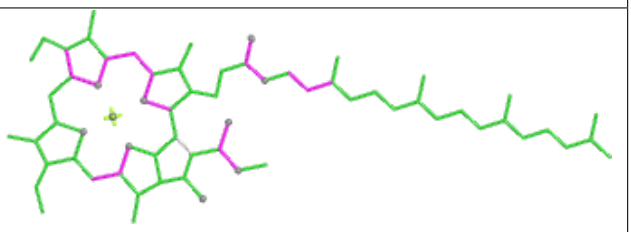


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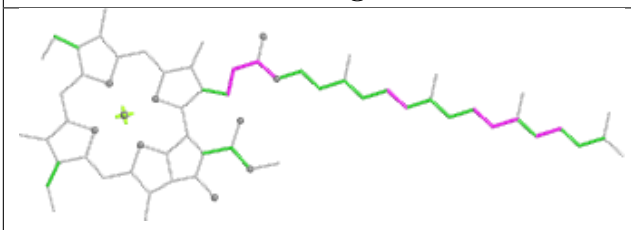
Ligand CLA b 802



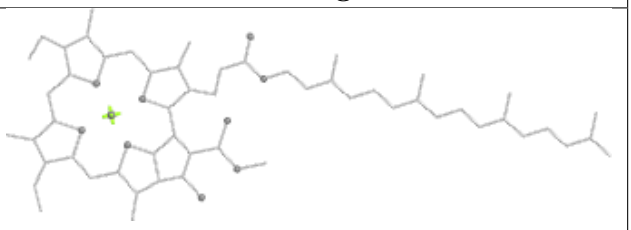
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Bond angles

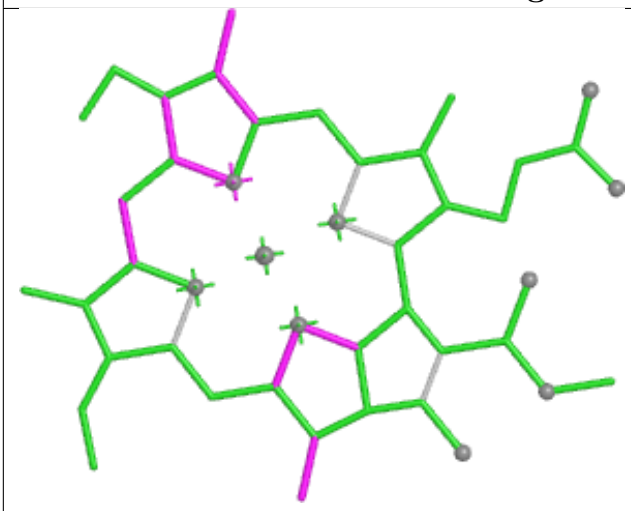


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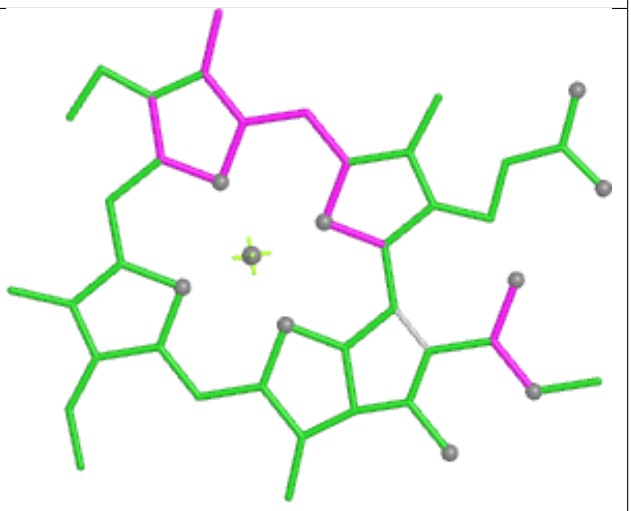


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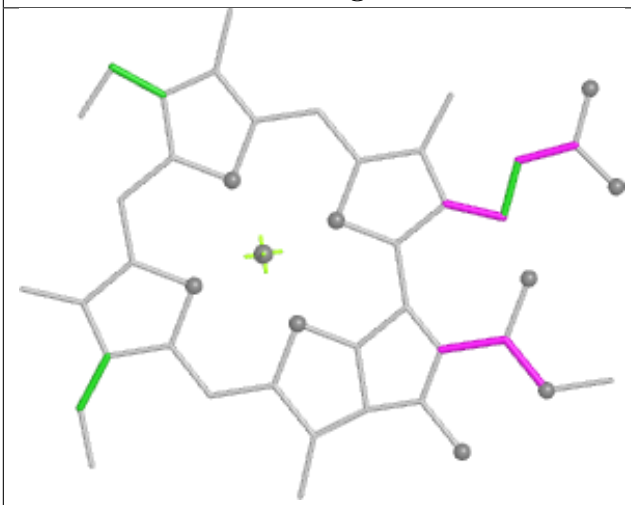
Ligand CLA n 834



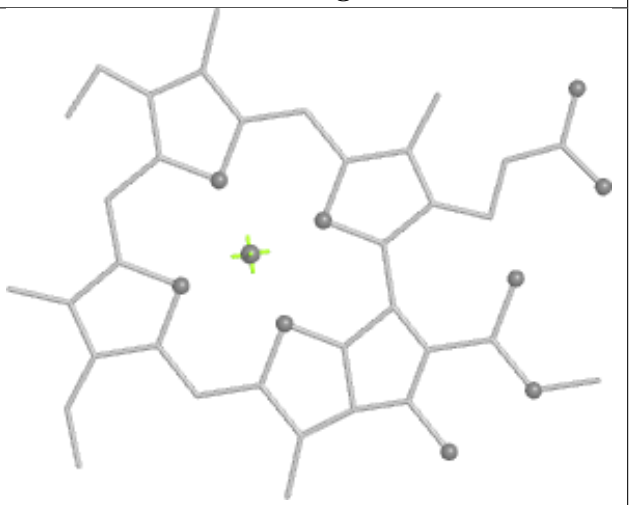
Bond lengths



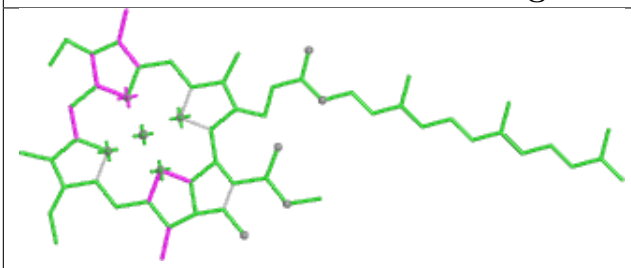
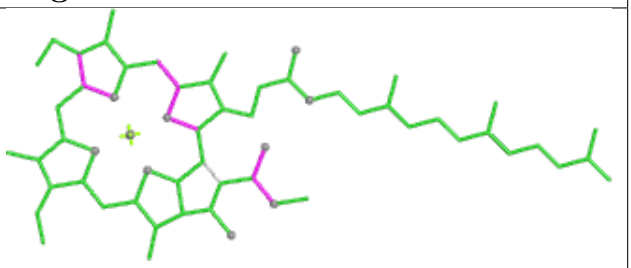
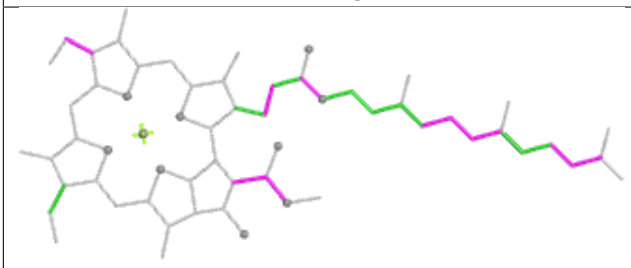
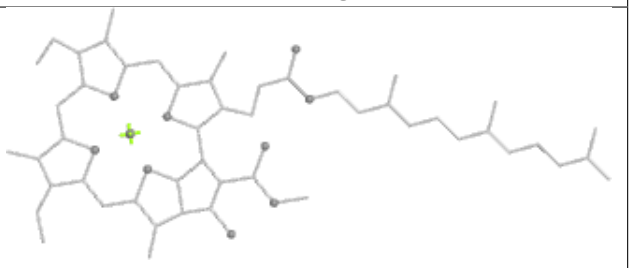
Bond angles

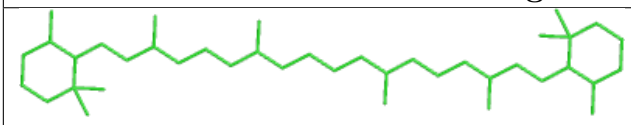
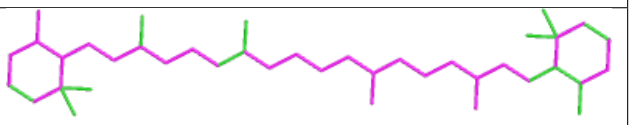
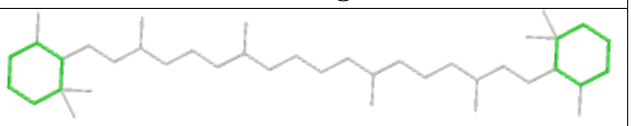


Torsions

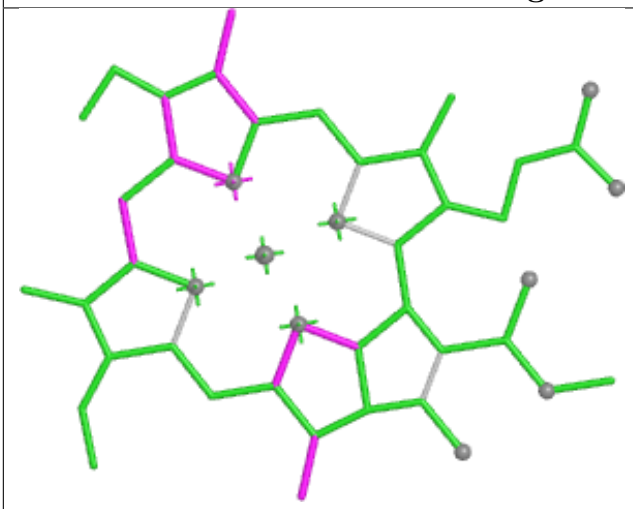


Rings

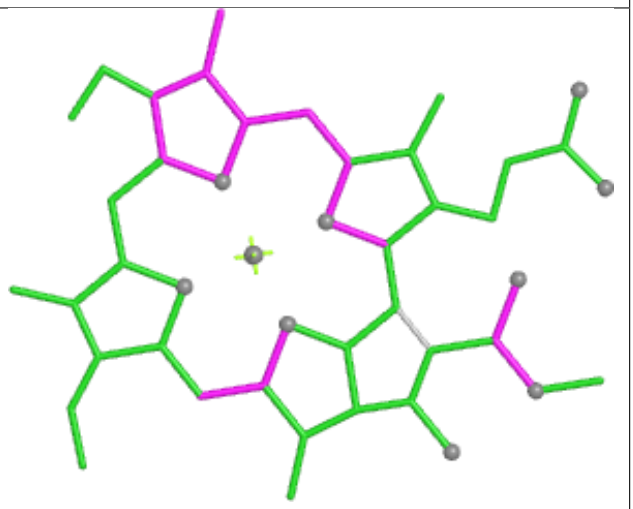
Ligand CLA g 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR v 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

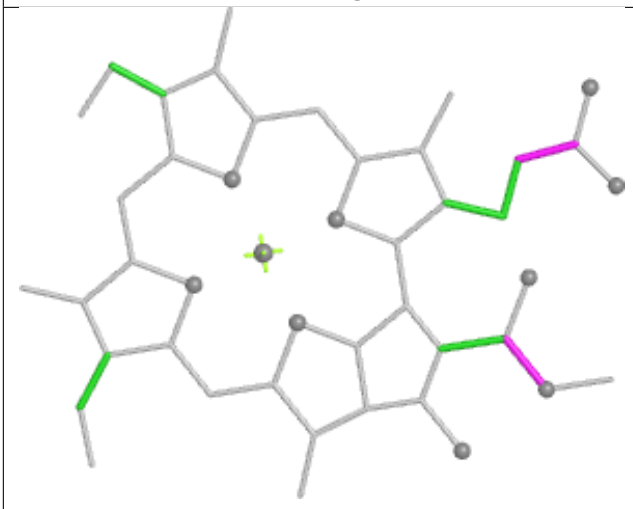
Ligand CLA b 834



Bond lengths



Bond angles

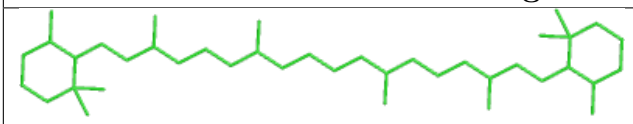


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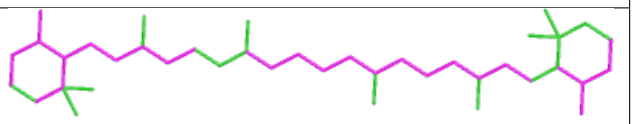


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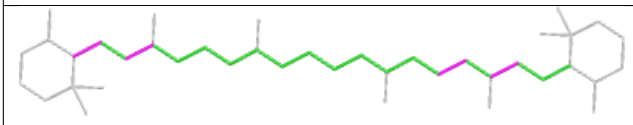
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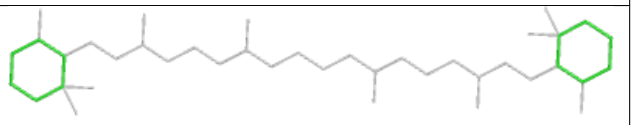
Bond lengths



Bond angles

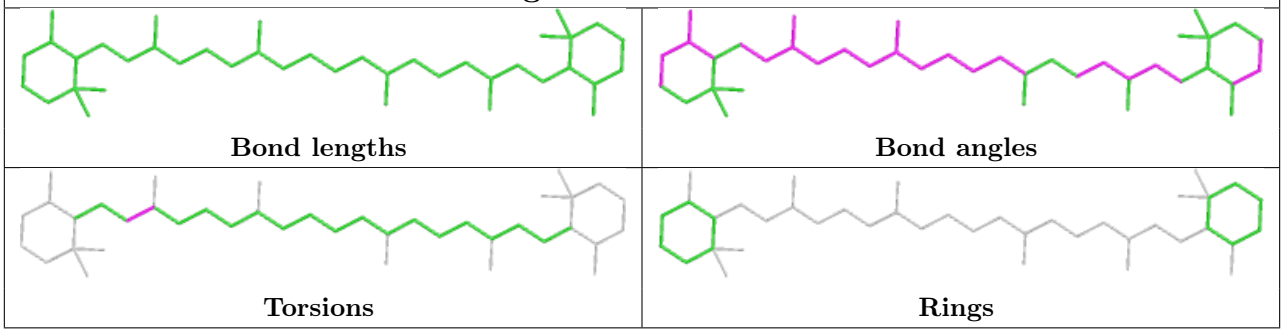


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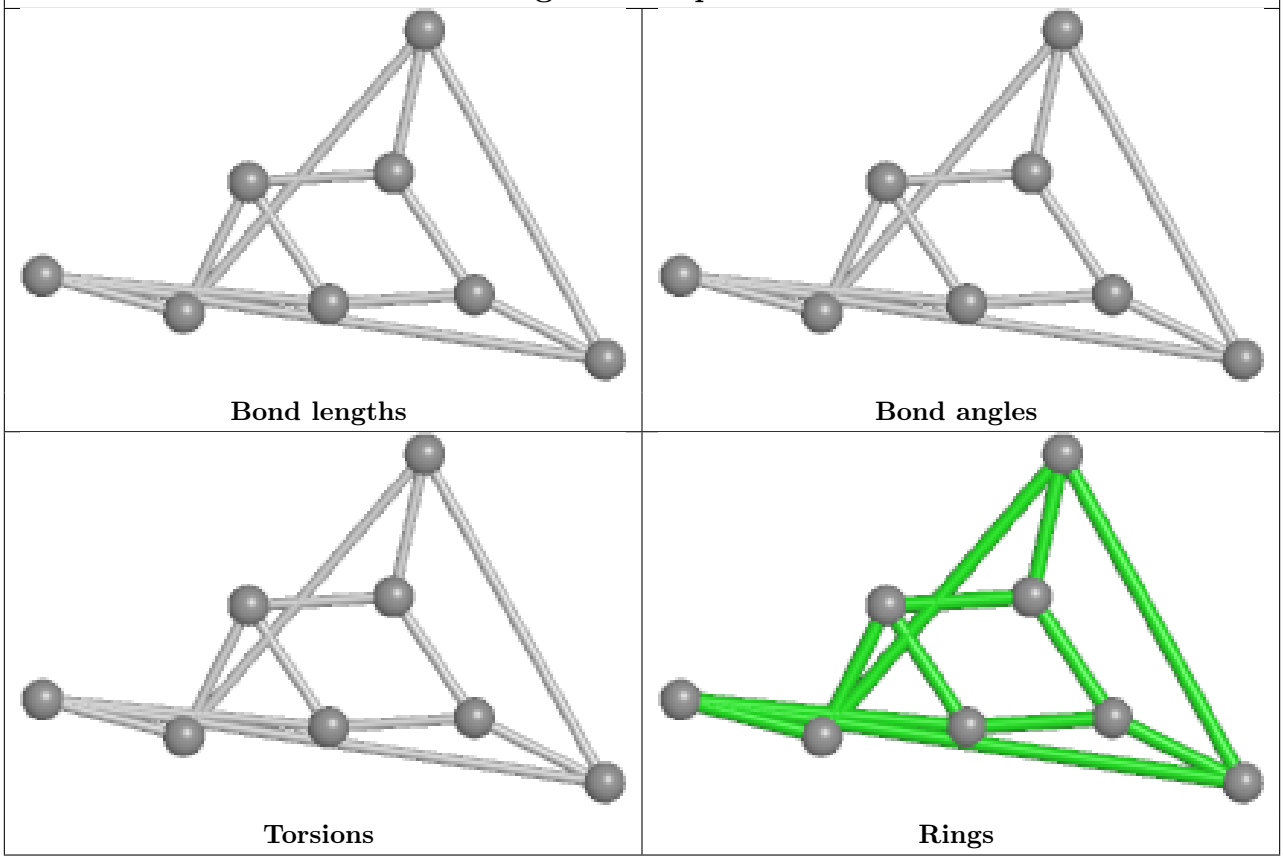


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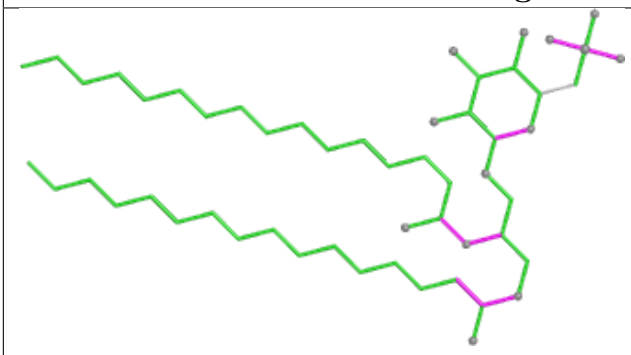
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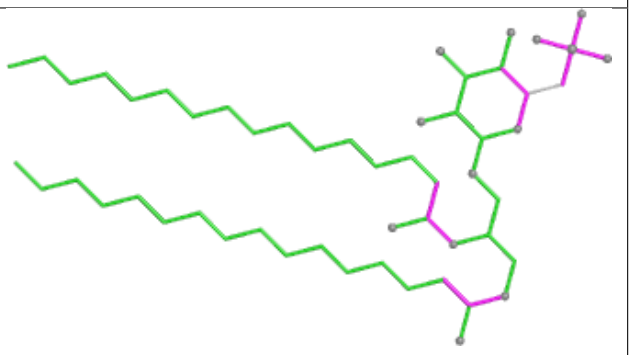
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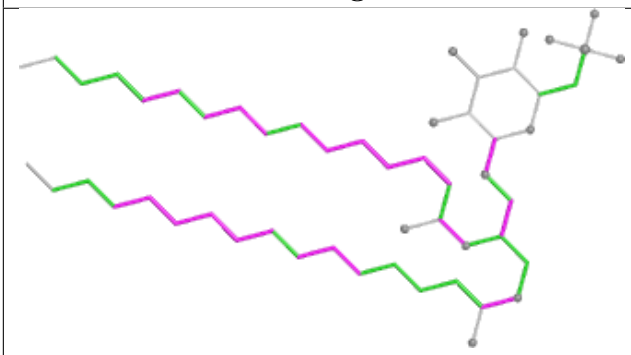
Ligand SQD H 1702



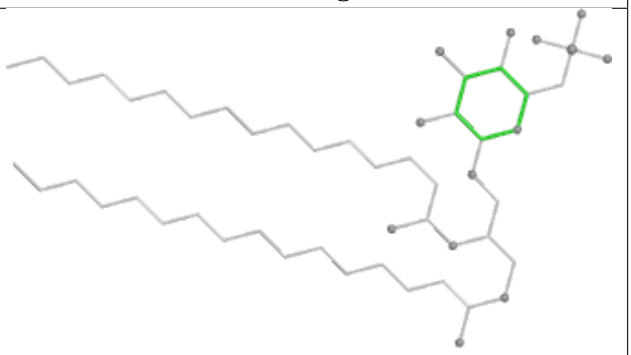
Bond lengths



Bond angles

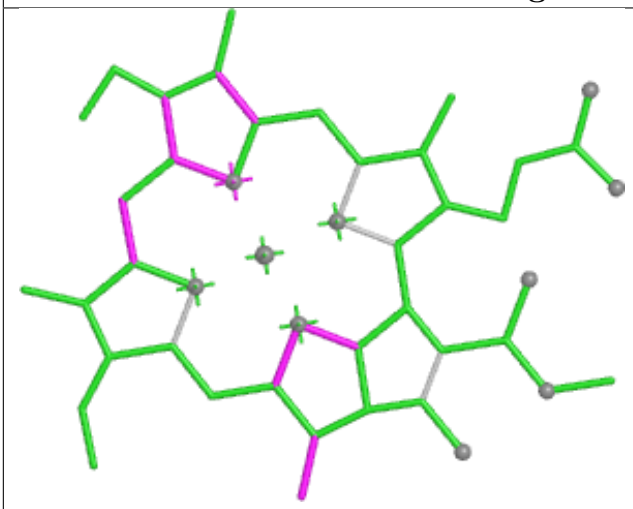


Torsions

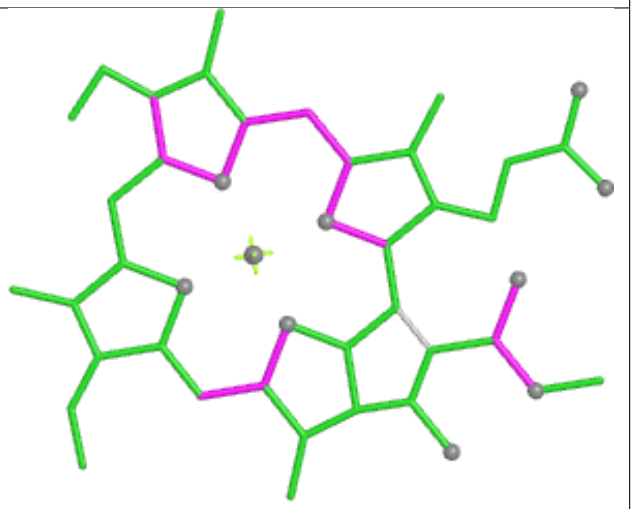


Rings

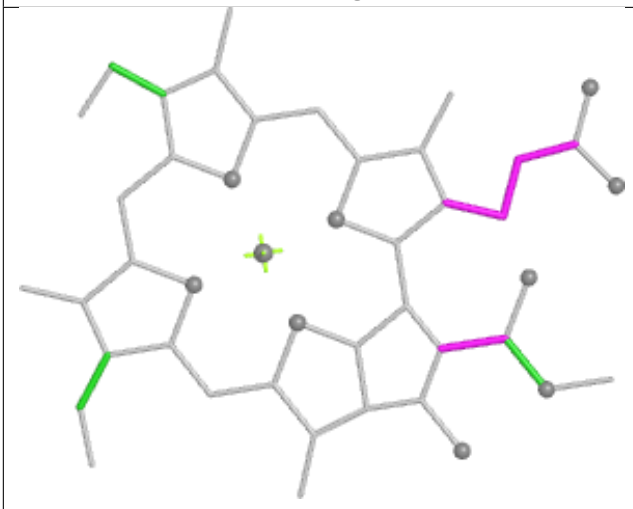
Ligand CLA a 820



Bond lengths



Bond angles

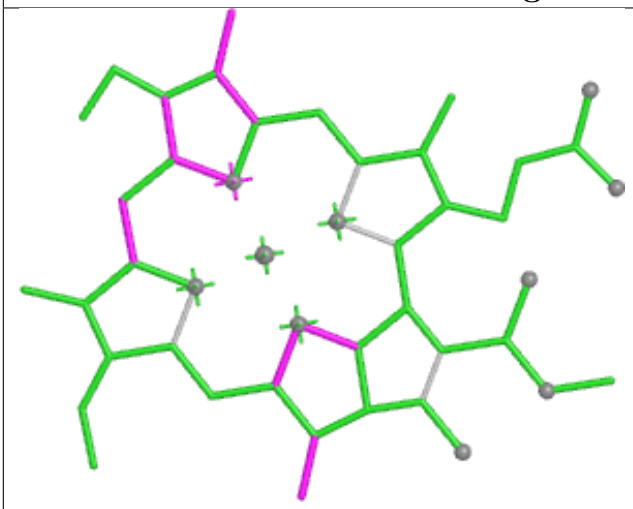


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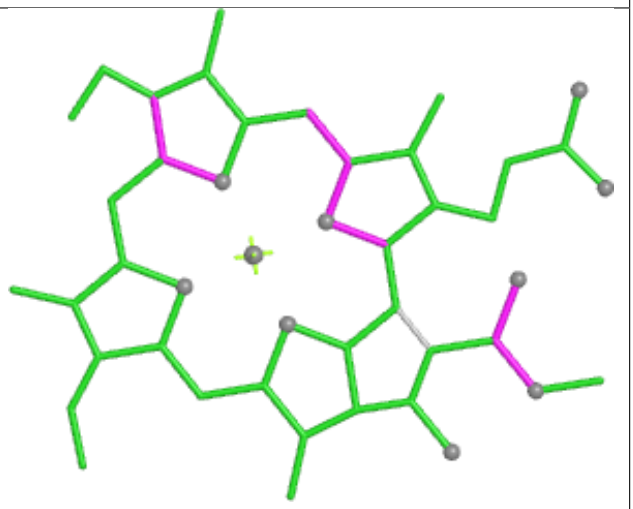


Rings

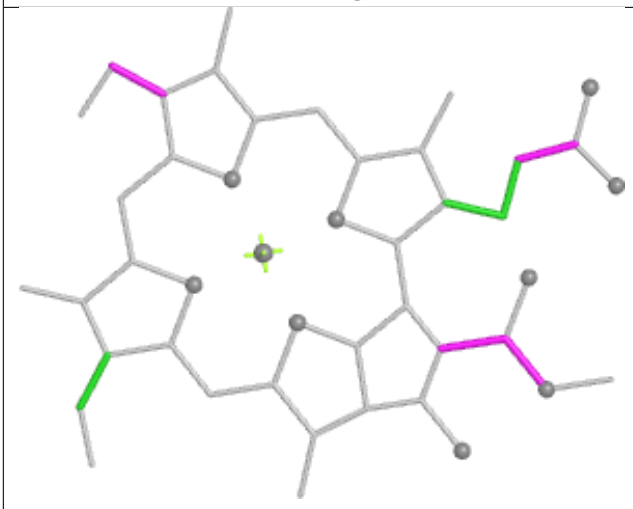
Ligand CLA N 837



Bond lengths



Bond angles

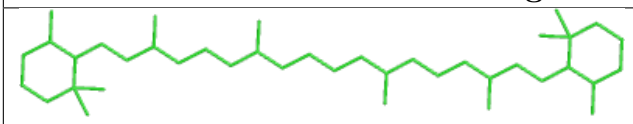


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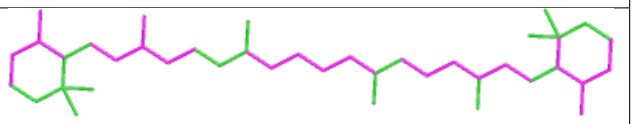


Rings

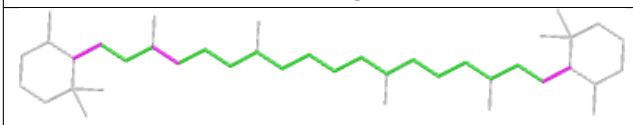
Ligand BCR n 843



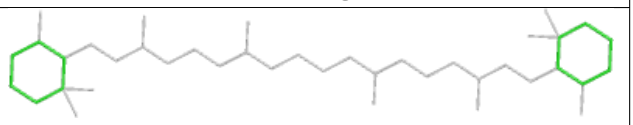
Bond lengths



Bond angles

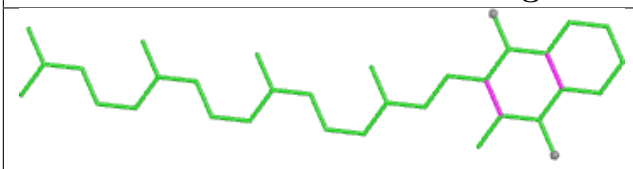


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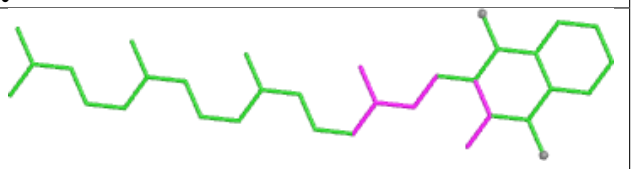


Rings

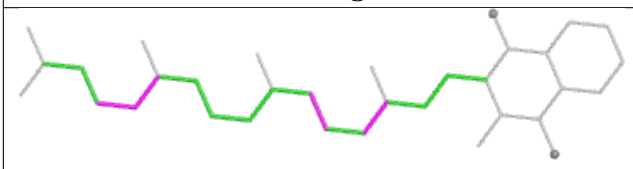
Ligand PQN B 842



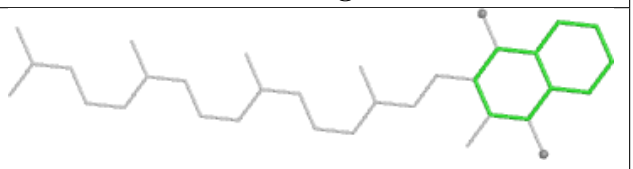
Bond lengths



Bond angles

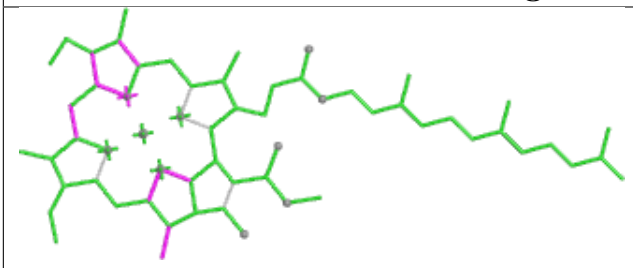


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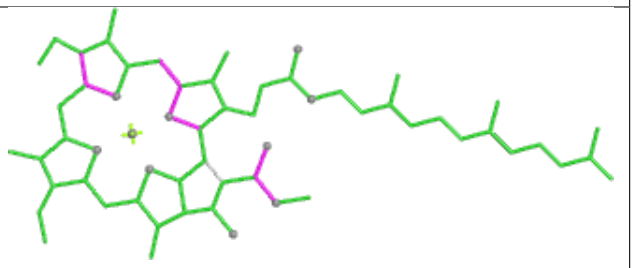


Rings

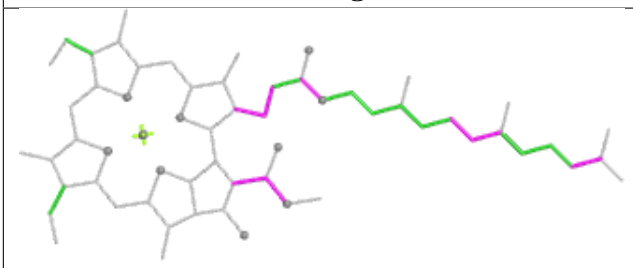
Ligand CLA B 832



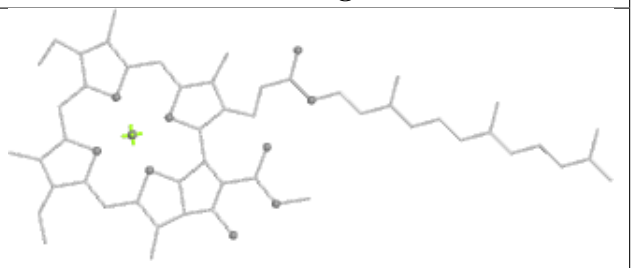
Bond lengths



Bond angles

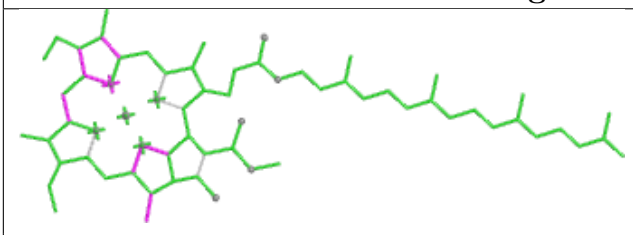


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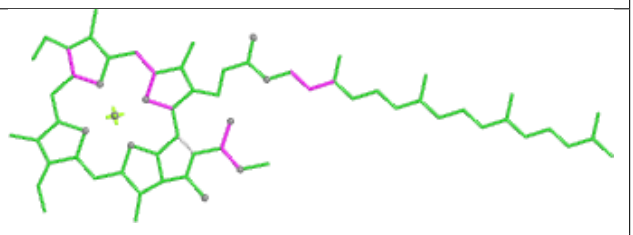


Rings

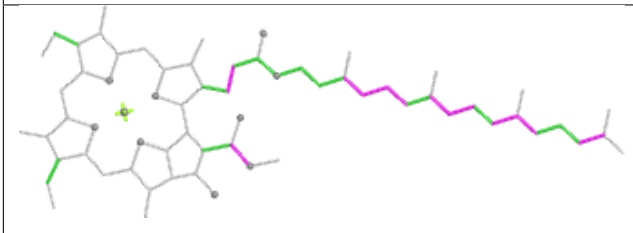
Ligand CLA a 826



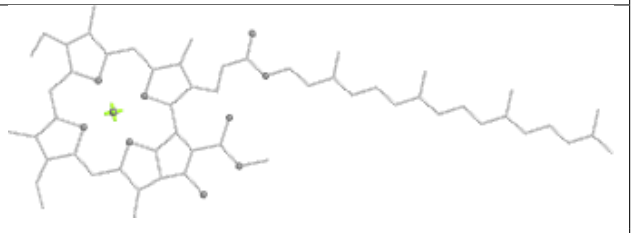
Bond lengths



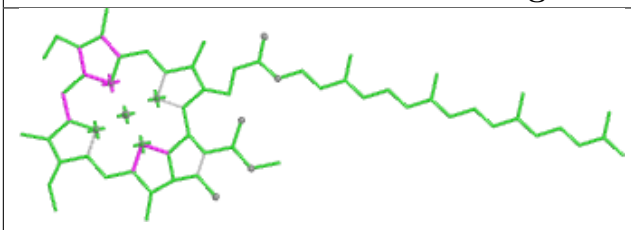
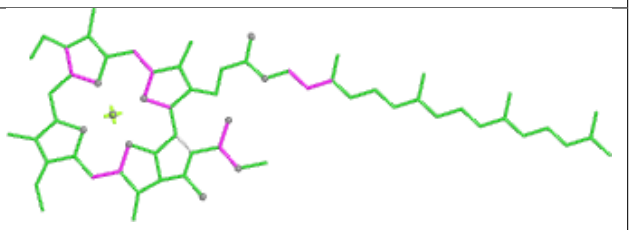
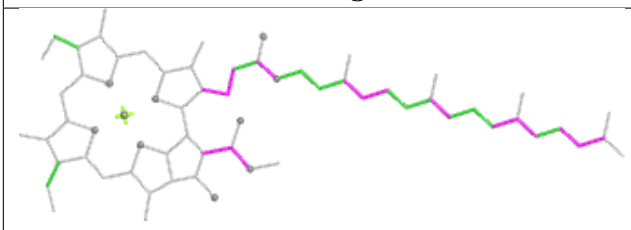
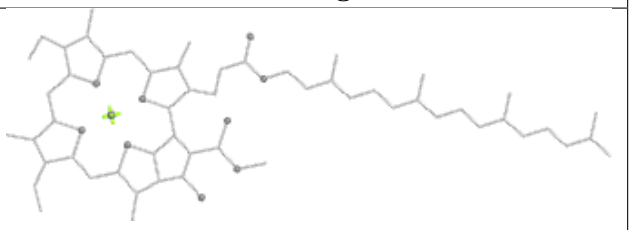
Bond angles

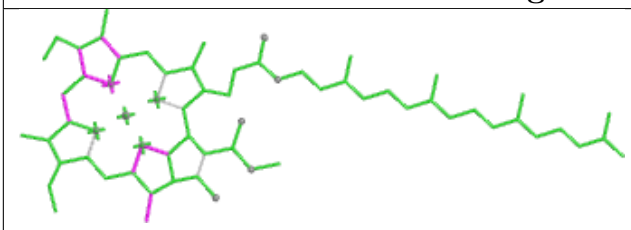
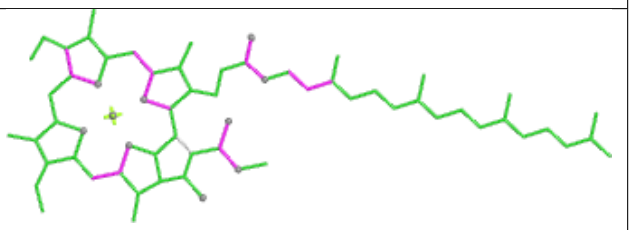
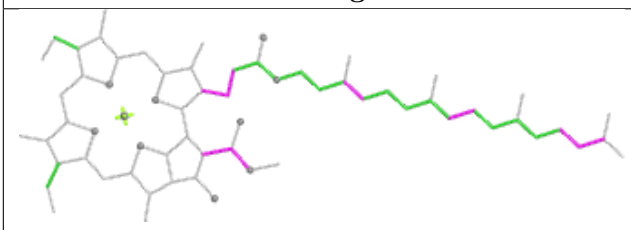
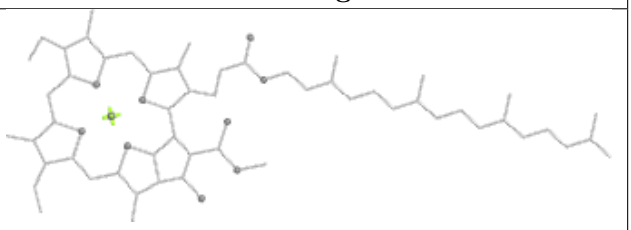


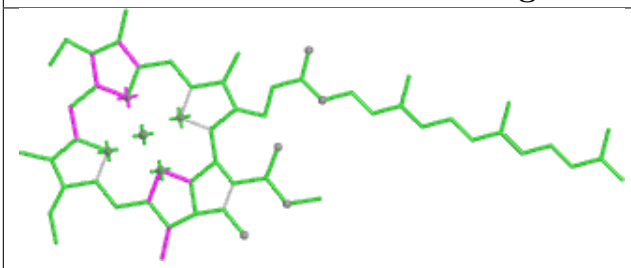
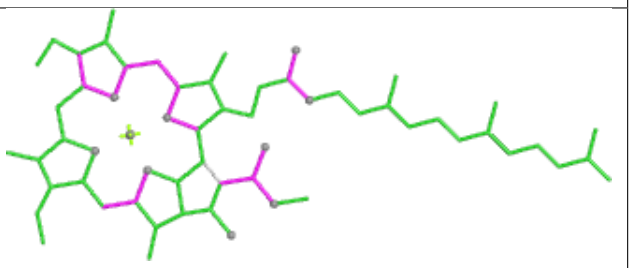
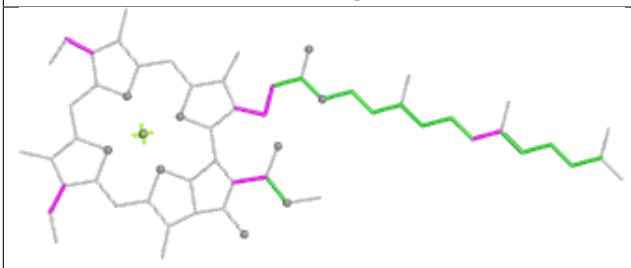
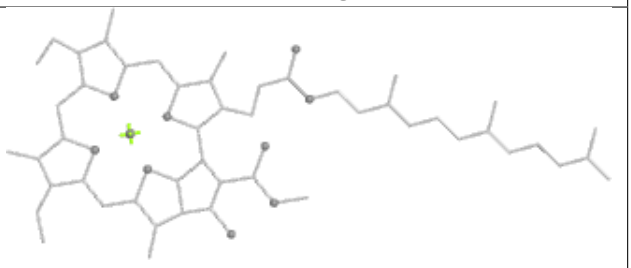
Torsions

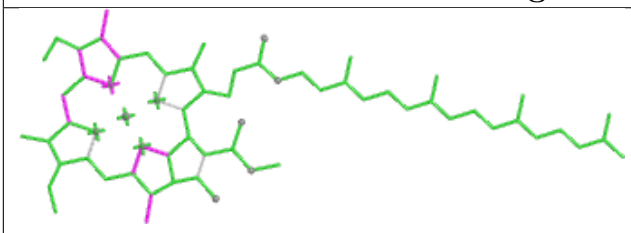
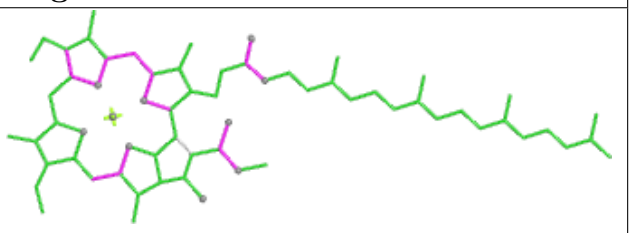
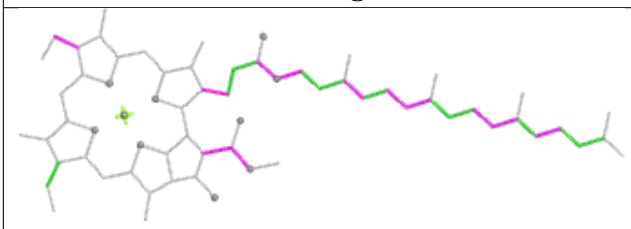
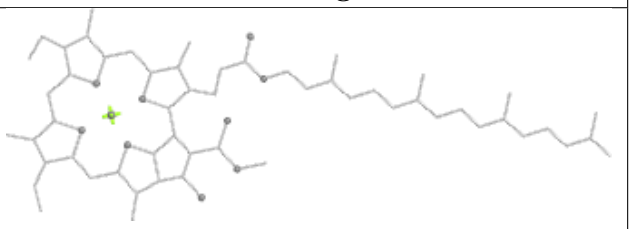


Rings

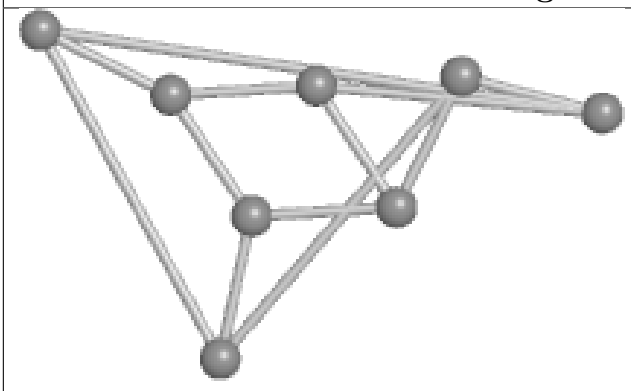
Ligand CLA a 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

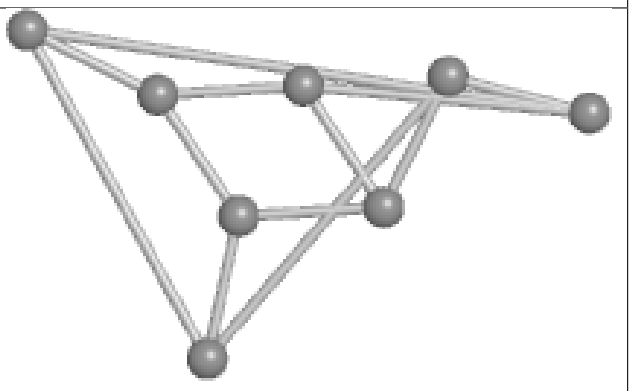
Ligand CLA W 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

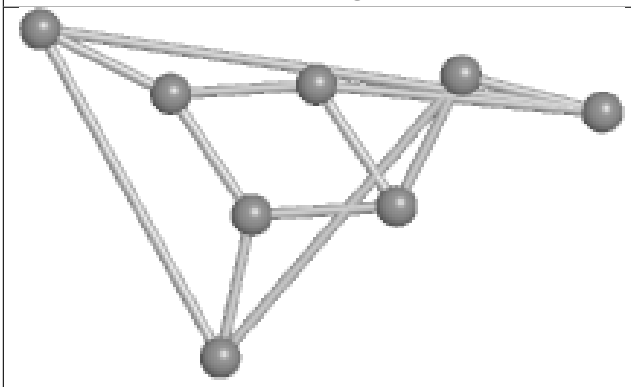
Ligand SF4 c 101



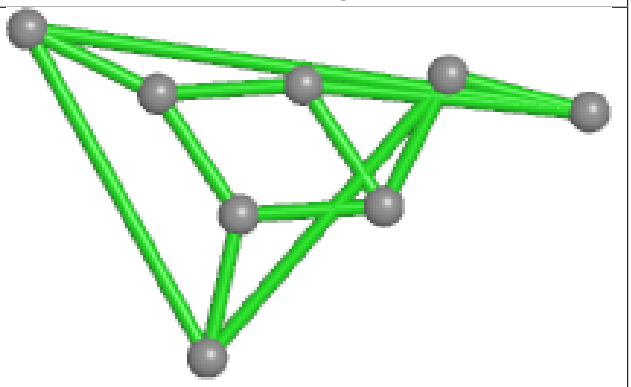
Bond lengths



Bond angles

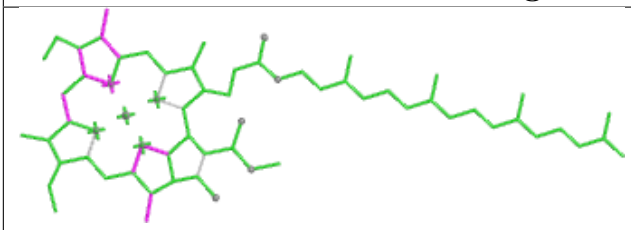


Torsions

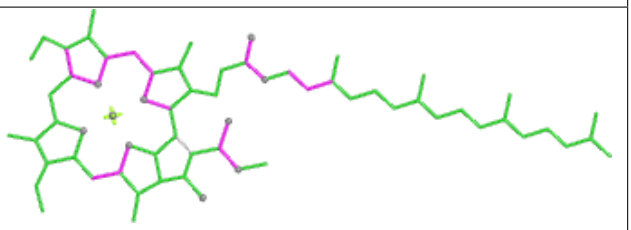


Rings

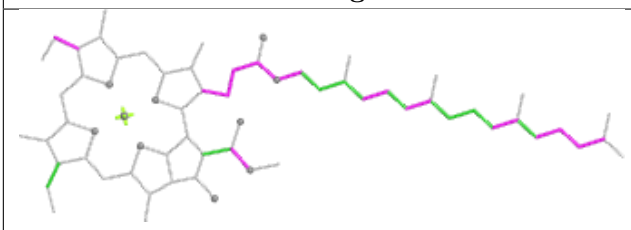
Ligand CLA A 839



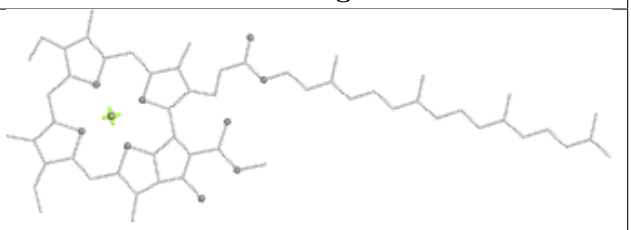
Bond lengths



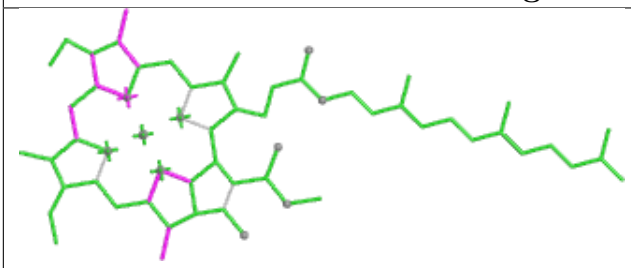
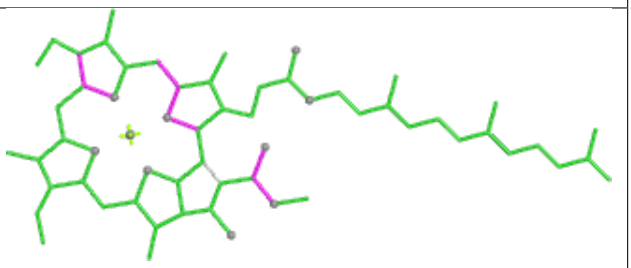
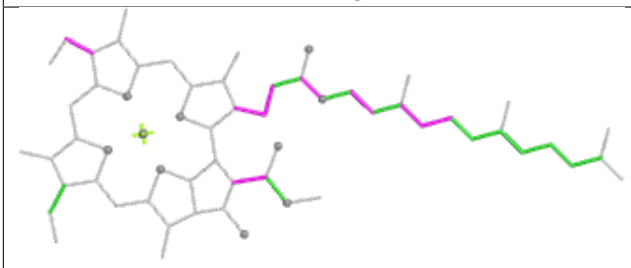
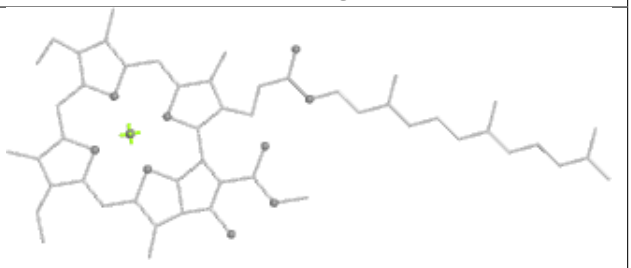
Bond angles

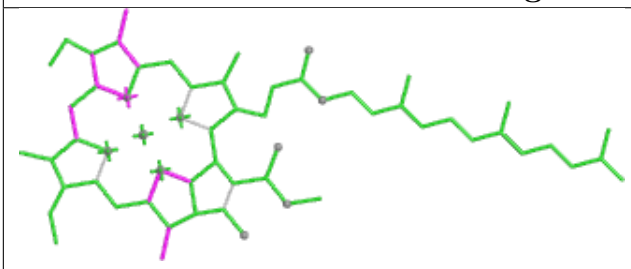
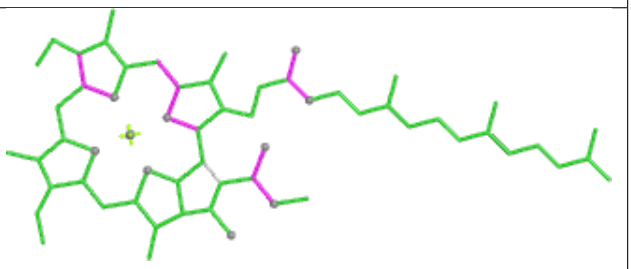
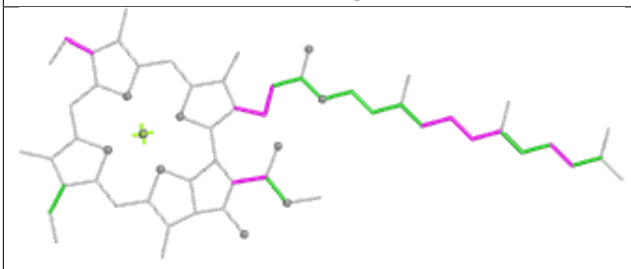
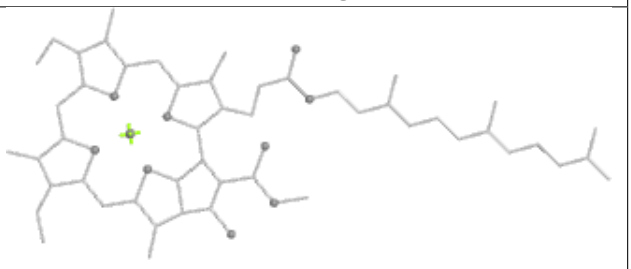


Torsions

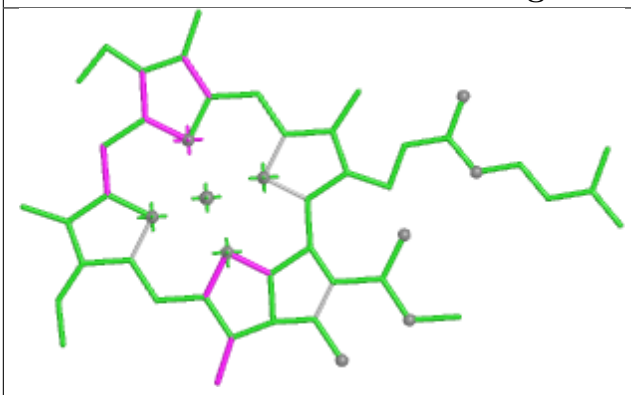


Rings

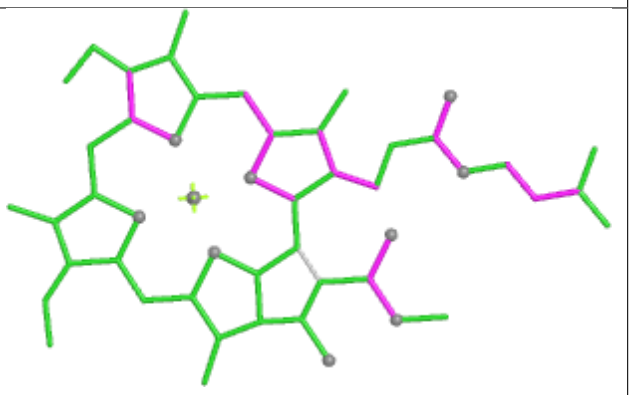
Ligand CLA G 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 811	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

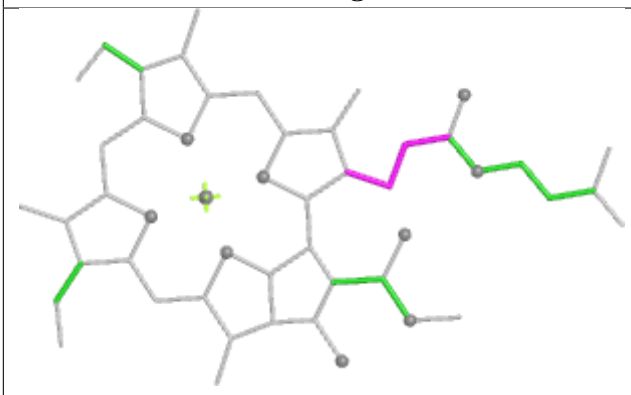
Ligand CLA n 814



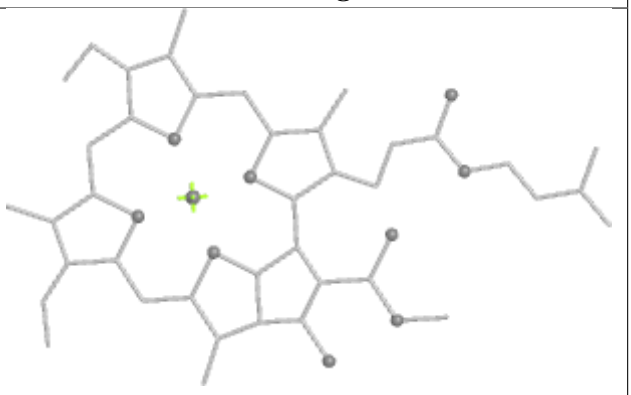
Bond lengths



Bond angles

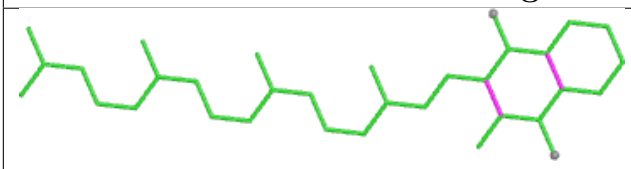


Torsions

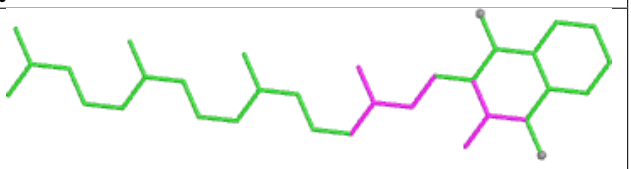


Rings

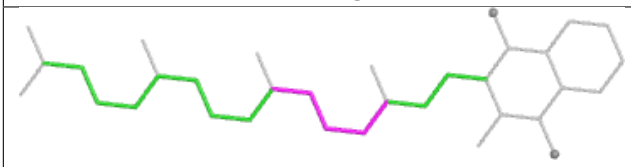
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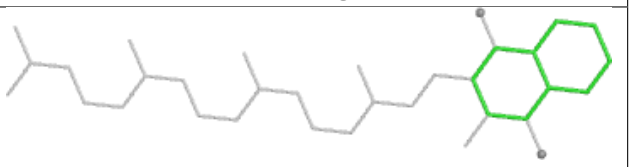
Bond lengths



Bond angles

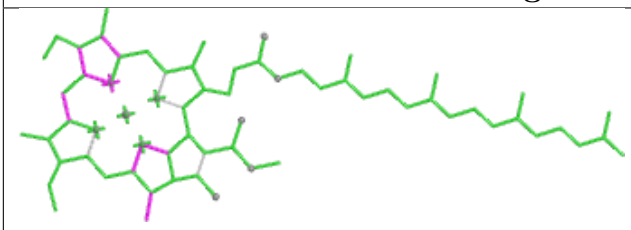


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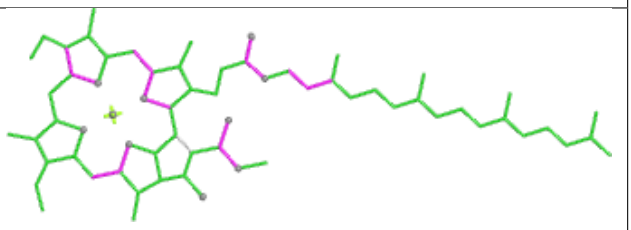


Rings

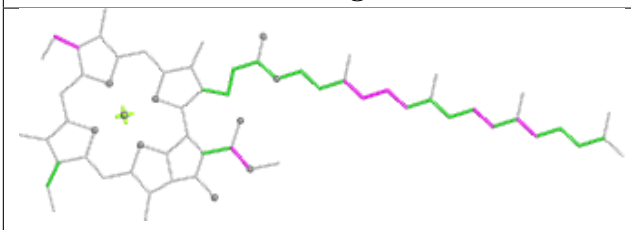
Ligand CLA A 832



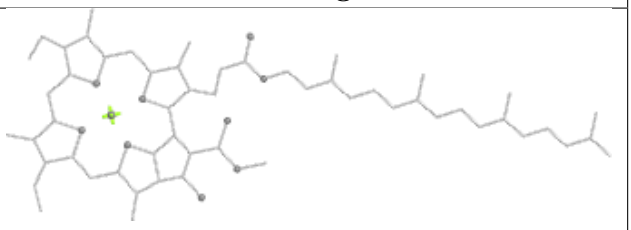
Bond lengths



Bond angles

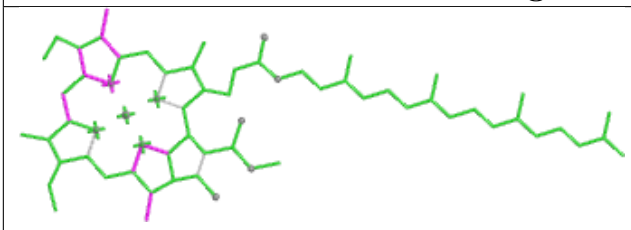


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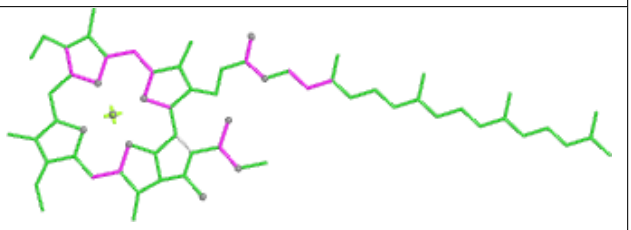


Rings

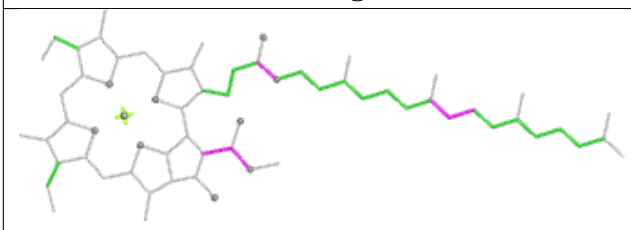
Ligand CLA n 819



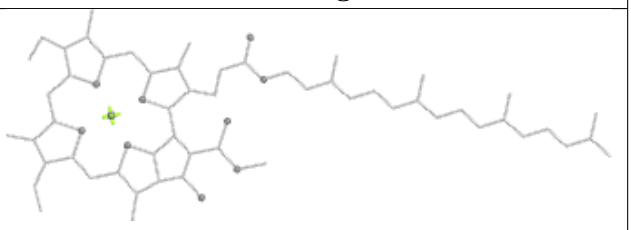
Bond lengths



Bond angles

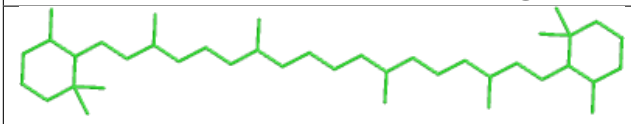


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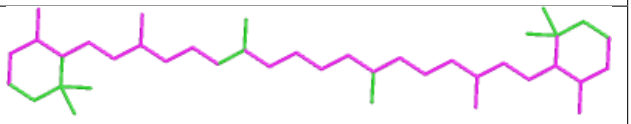


Rings

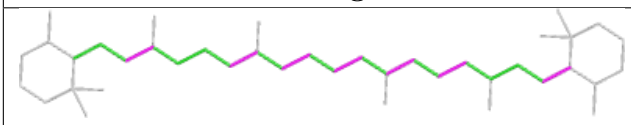
Ligand BCR W 201



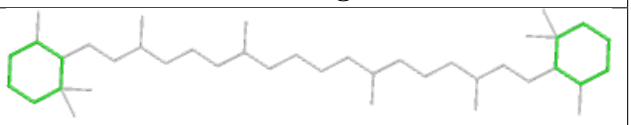
Bond lengths



Bond angles

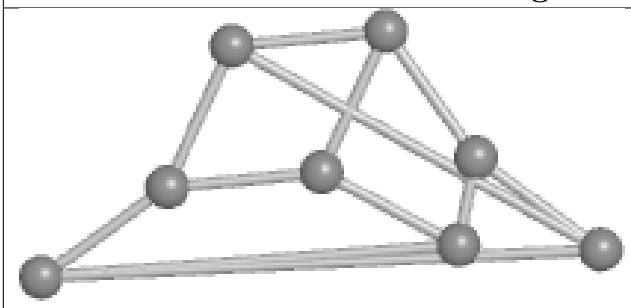


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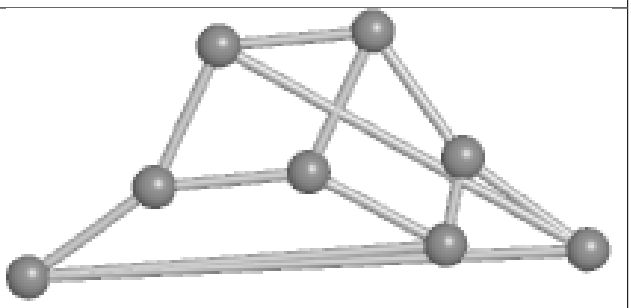


Rings

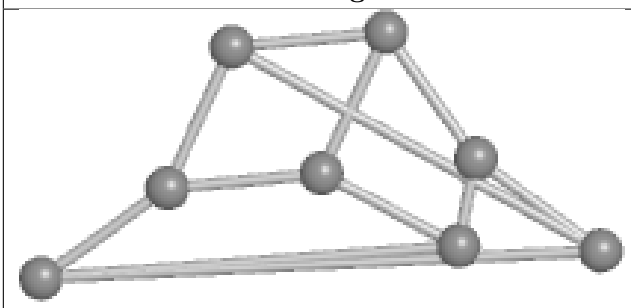
Ligand SF4 C 102



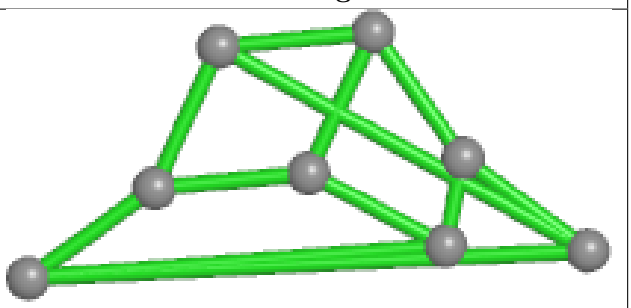
Bond lengths



Bond angles

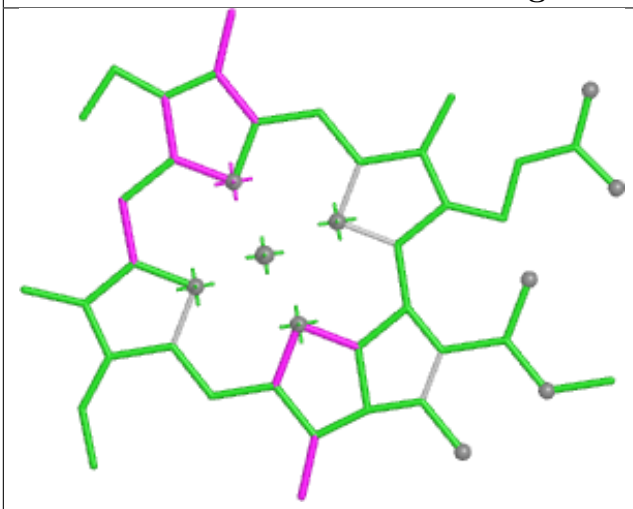


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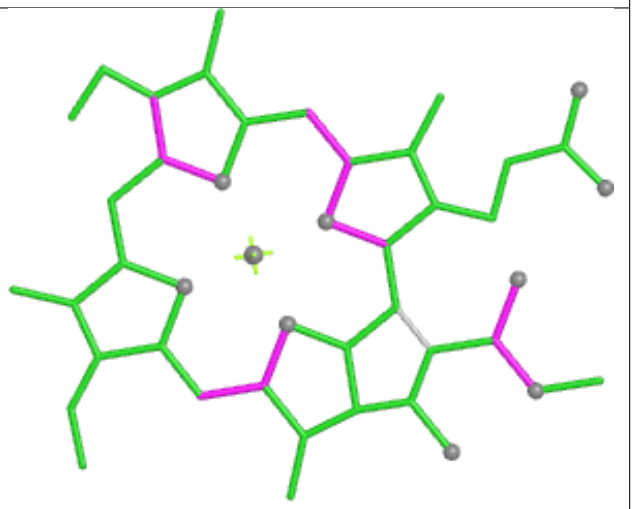


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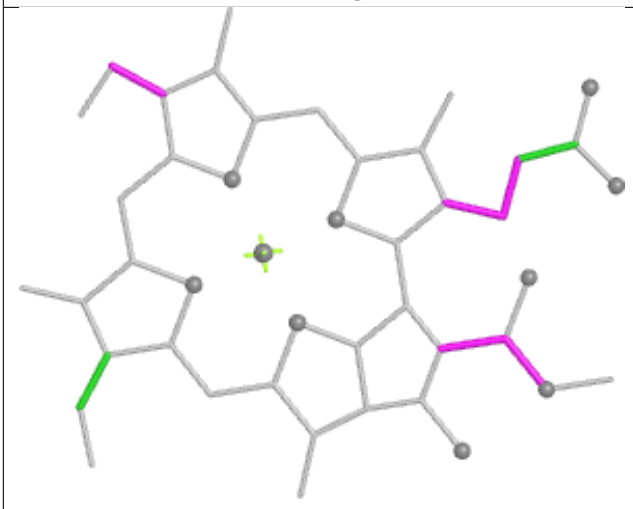
Ligand CLA a 840



Bond lengths



Bond angles

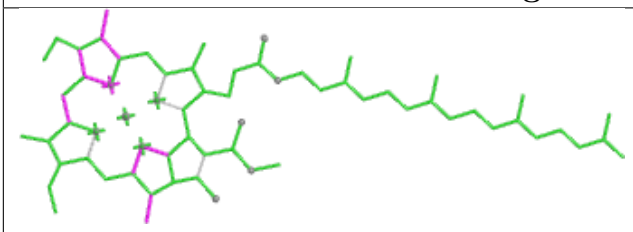


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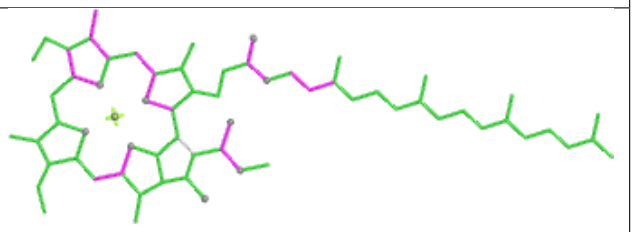


Rings

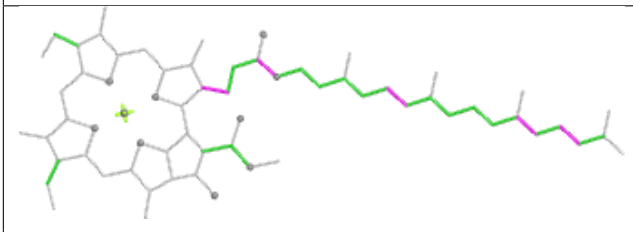
Ligand CLA G 818



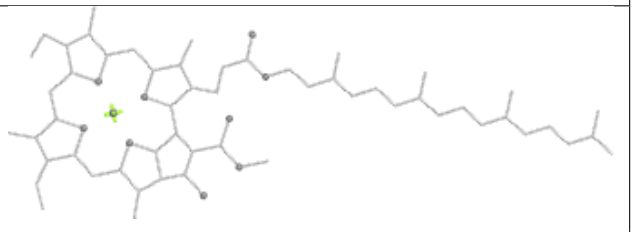
Bond lengths



Bond angles

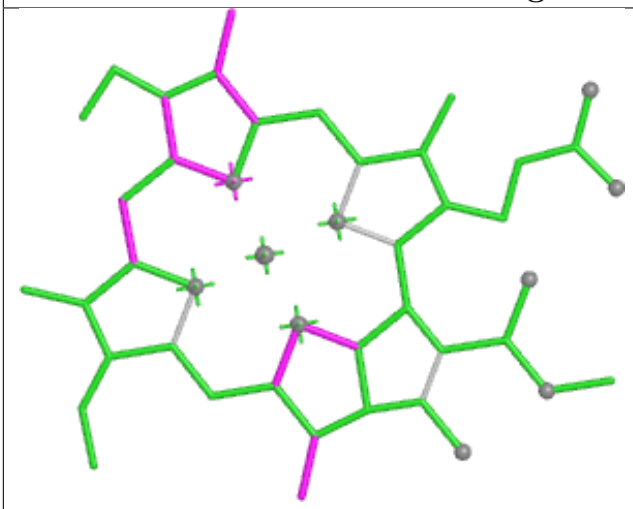


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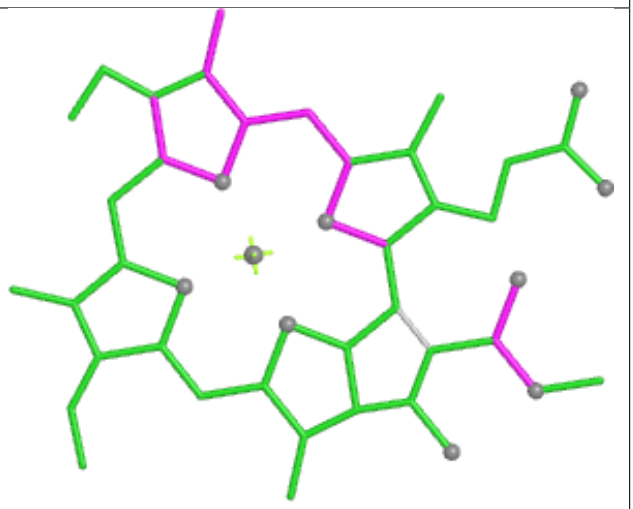


Rings

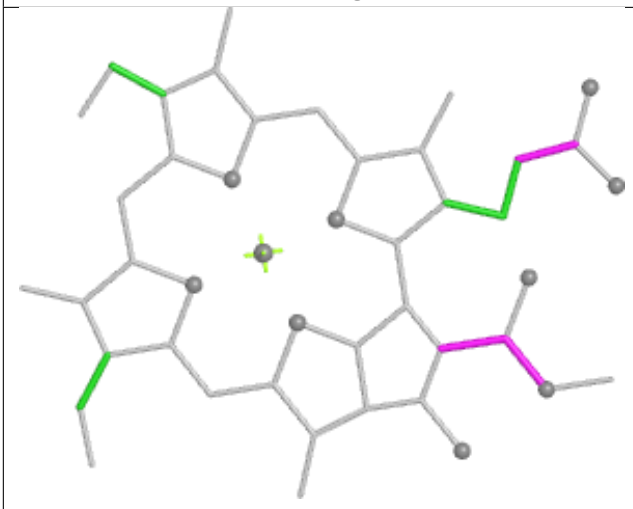
Ligand CLA S 203



Bond lengths



Bond angles

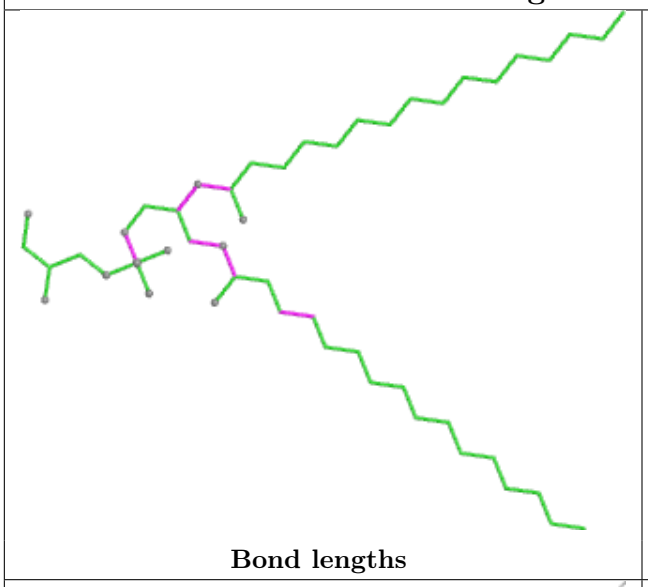


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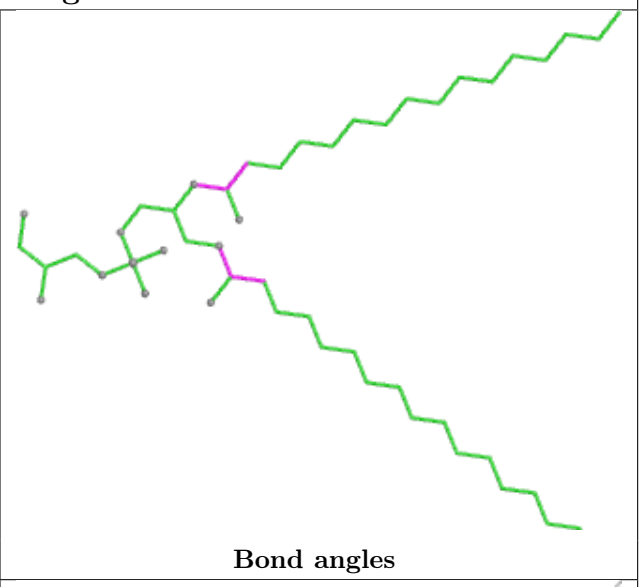


Rings

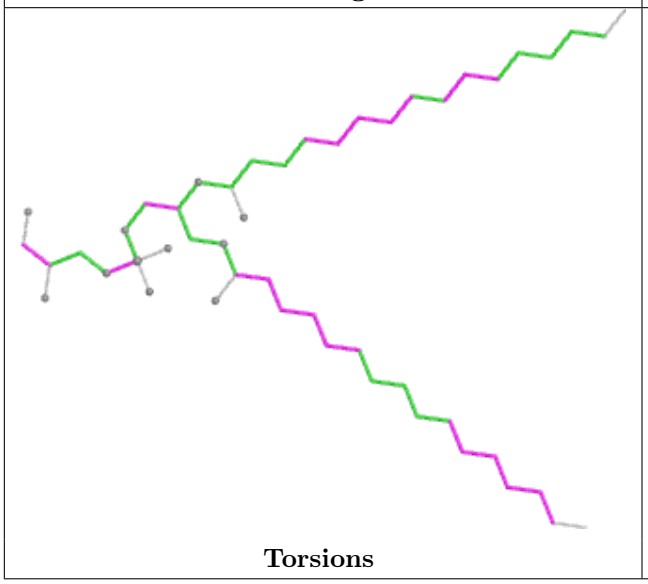
Ligand LHG g 850



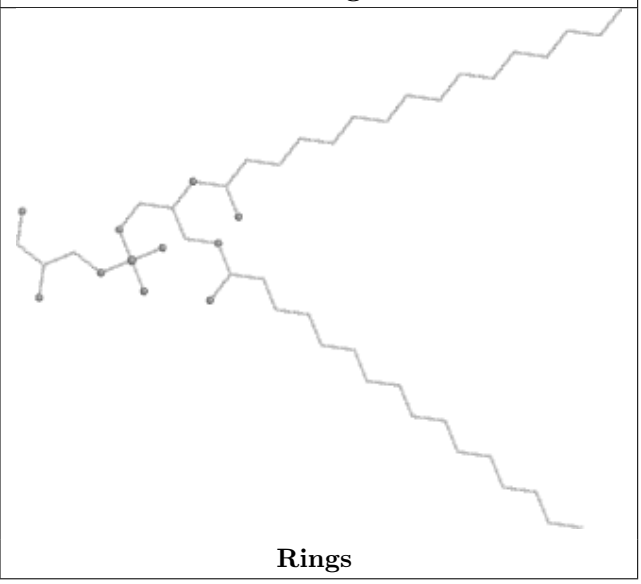
Bond lengths



Bond angles

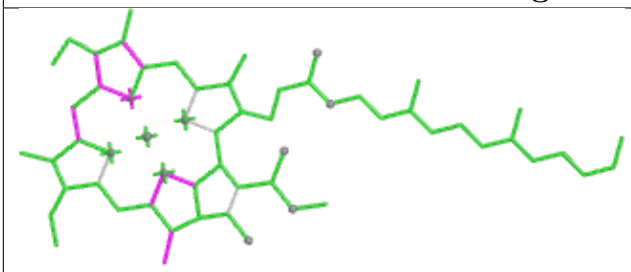


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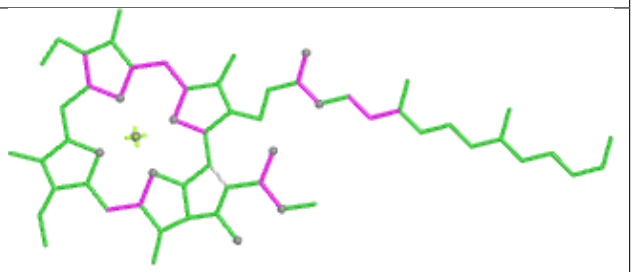


Rings

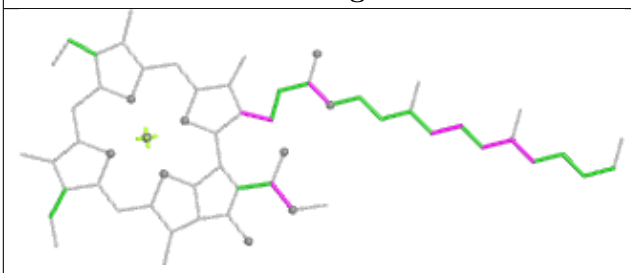
Ligand CLA f 201



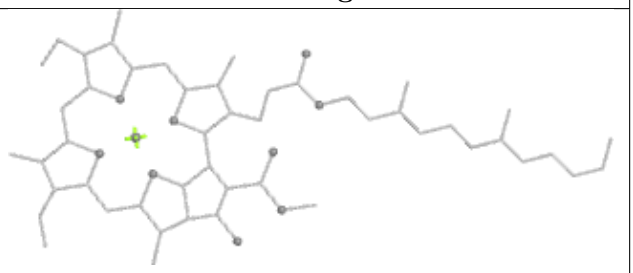
Bond lengths



Bond angles

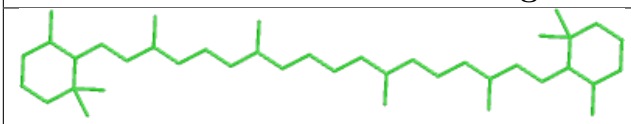


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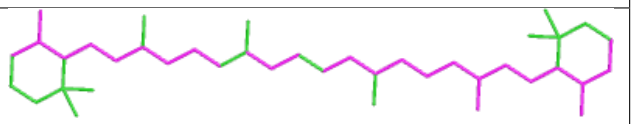


Rings

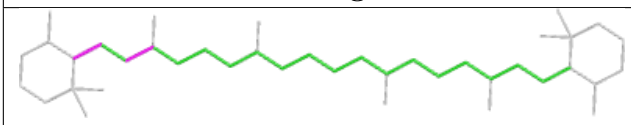
Ligand BCR m 102



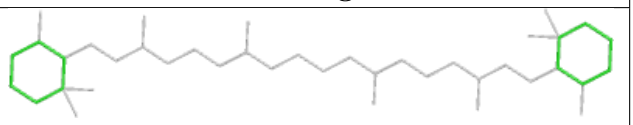
Bond lengths



Bond angles



Torsions



Rings

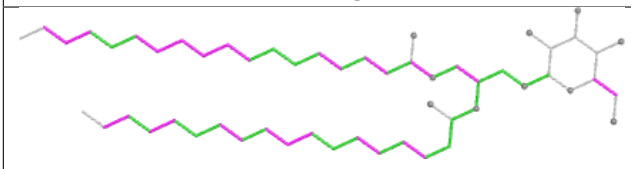
Ligand LMG b 848



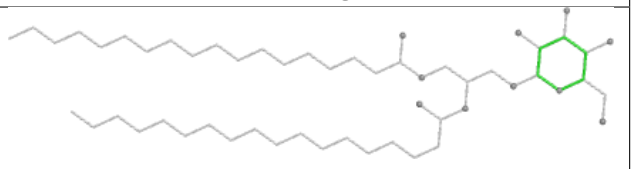
Bond lengths



Bond angles

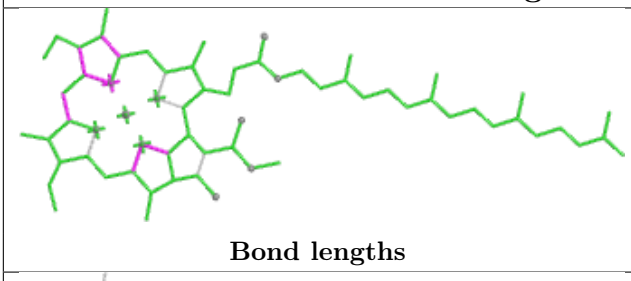


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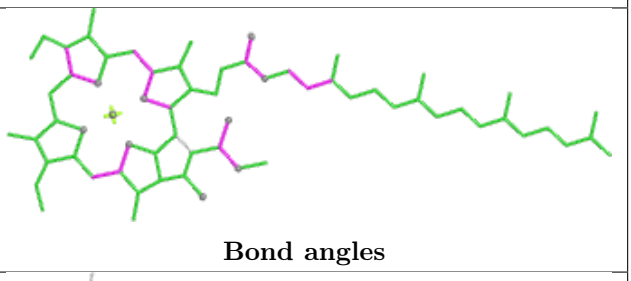


Rings

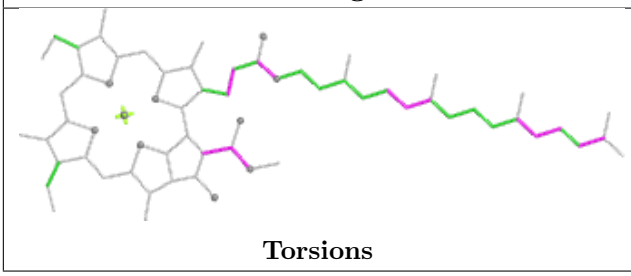
Ligand CLA B 807



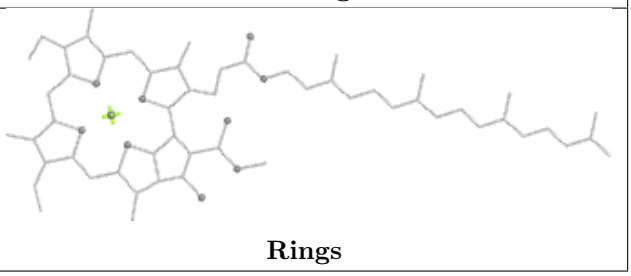
Bond lengths



Bond angles

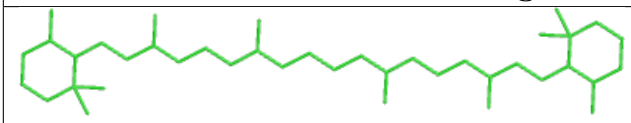


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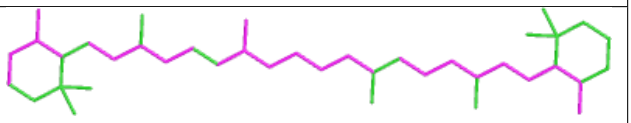


Rings

Ligand BCR W 205



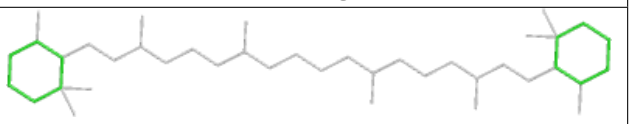
Bond lengths



Bond angles

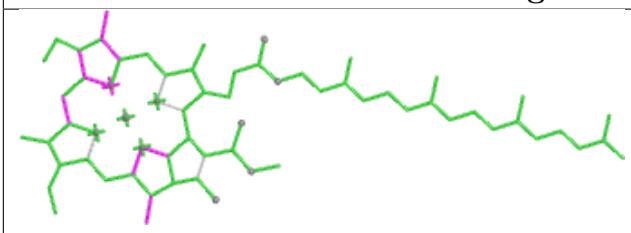


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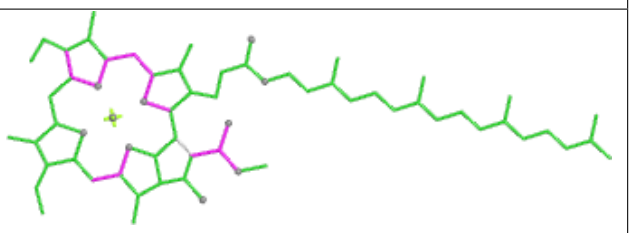


Rings

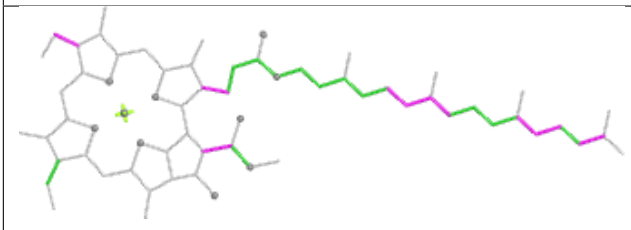
Ligand CLA n 823



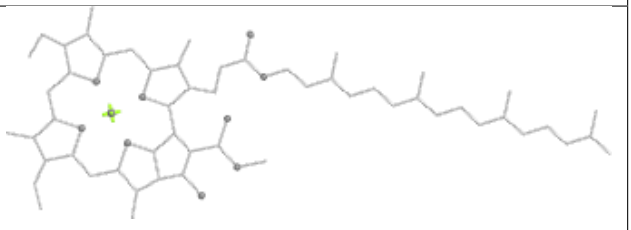
Bond lengths



Bond angles

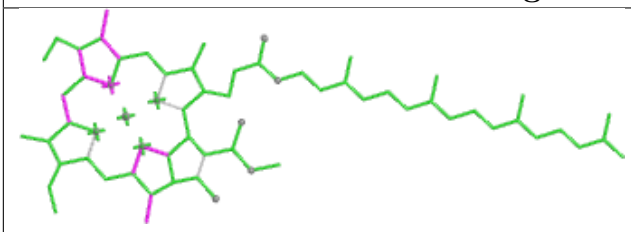


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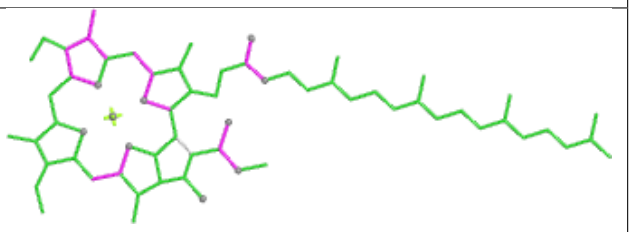


Rings

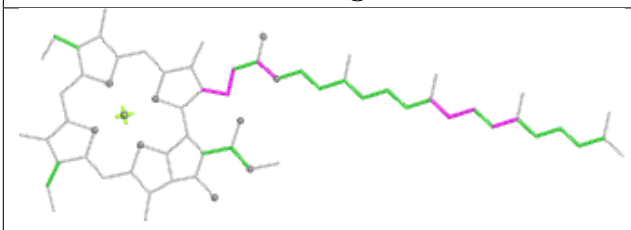
Ligand CLA N 830



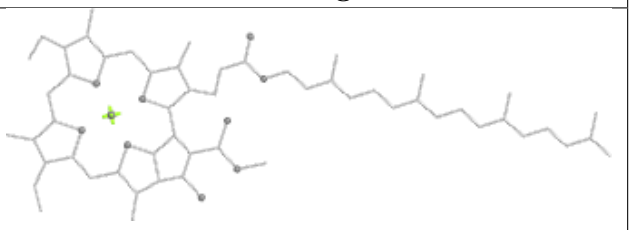
Bond lengths



Bond angles



Torsions

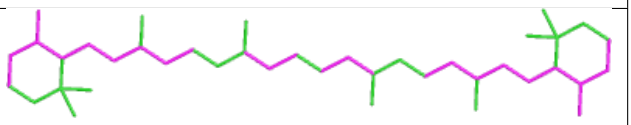


Rings

Ligand BCR t 103



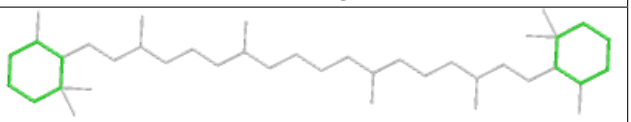
Bond lengths



Bond angles

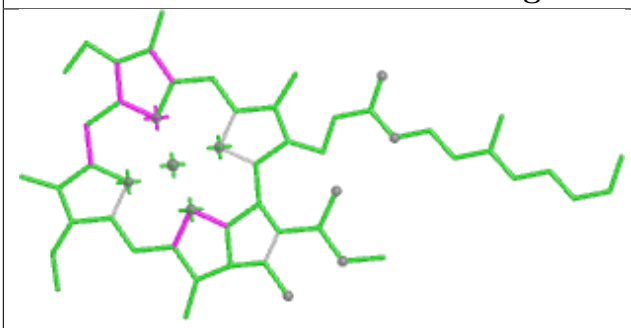


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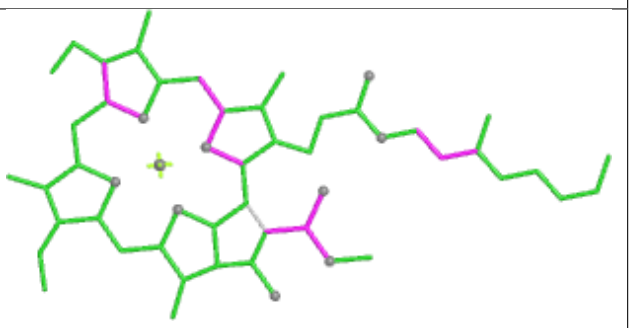


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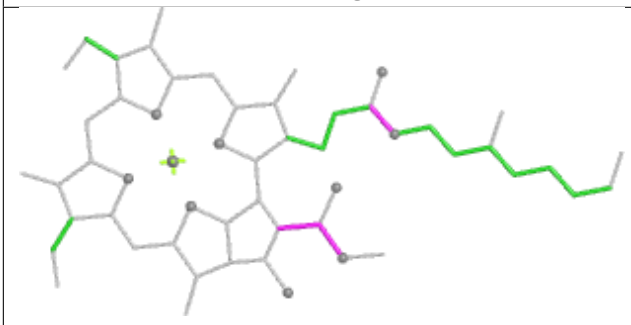
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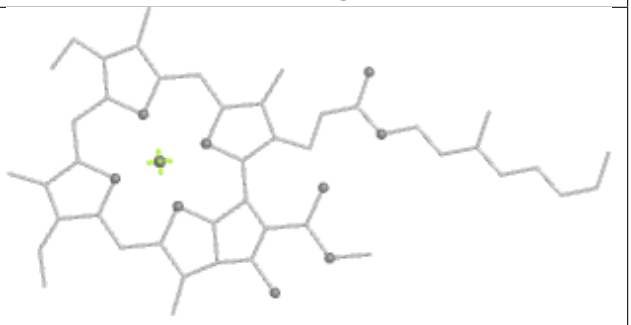
Bond lengths



Bond angles

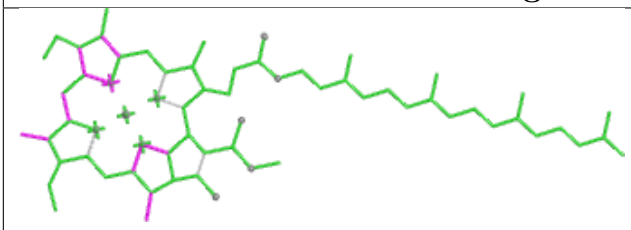


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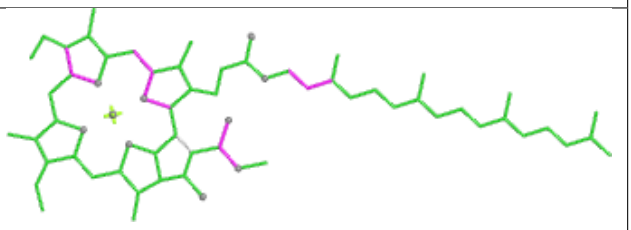


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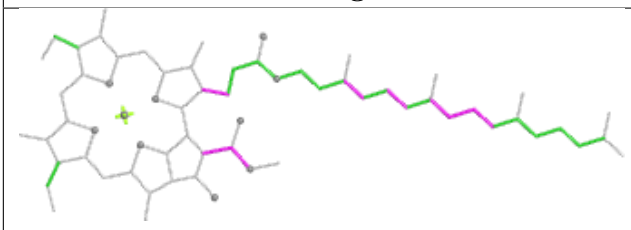
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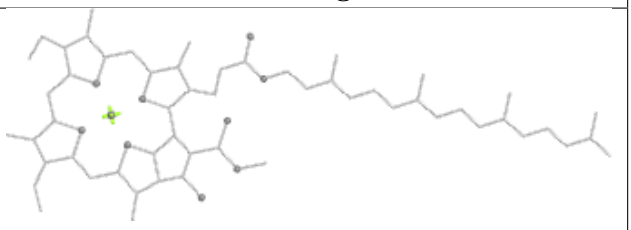
Bond lengths



Bond angles

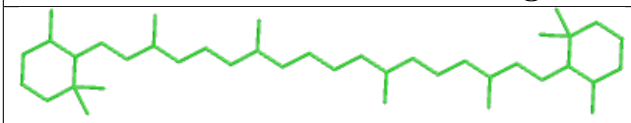


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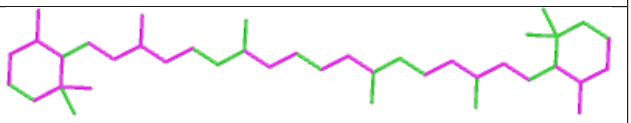


Rings

Ligand BCR B 852



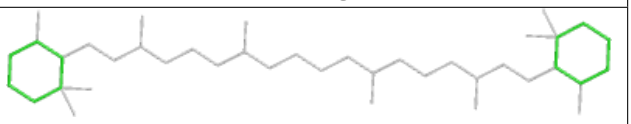
Bond lengths



Bond angles

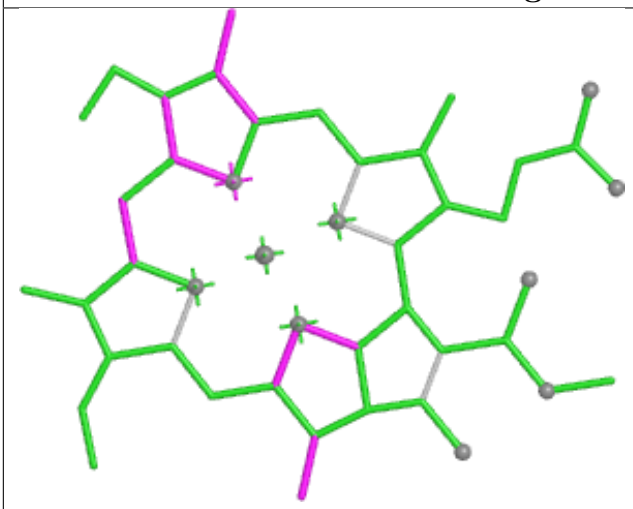


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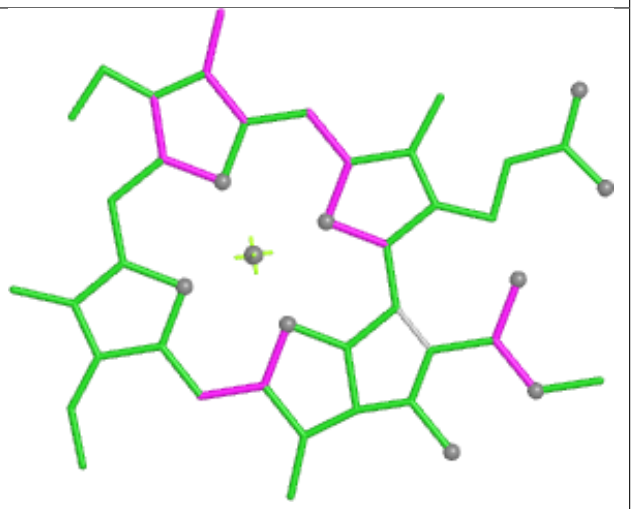


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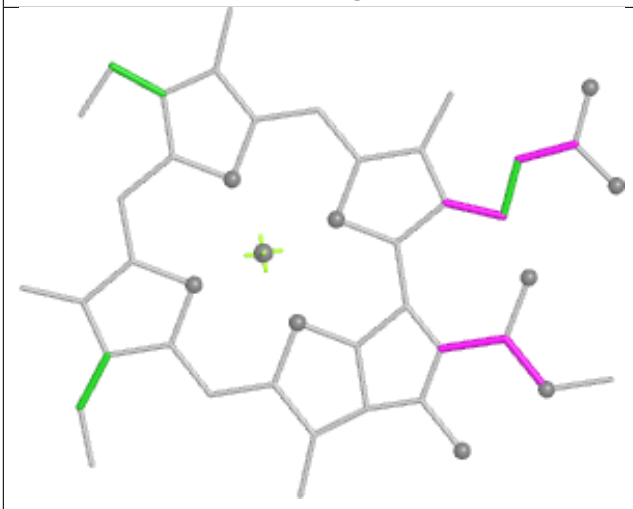
Ligand CLA B 835



Bond lengths



Bond angles

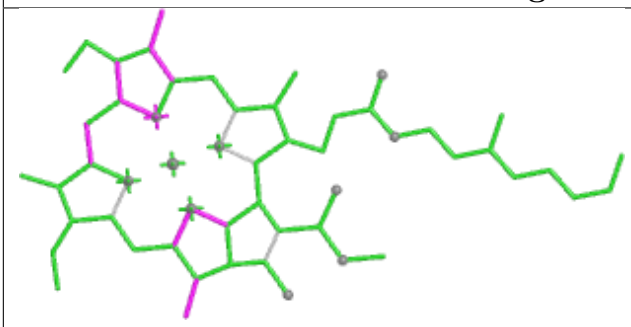


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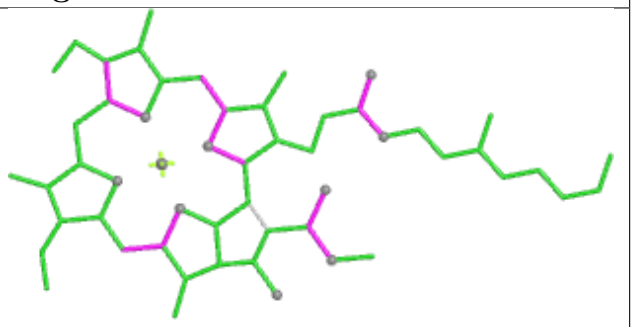


Rings

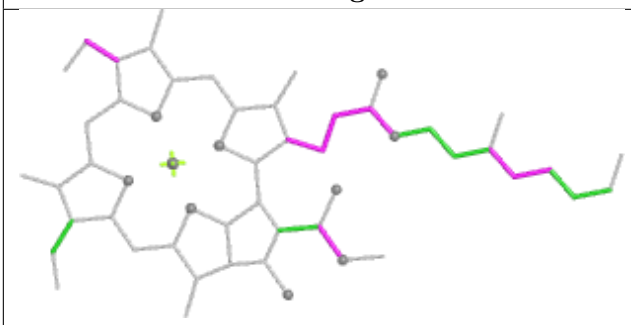
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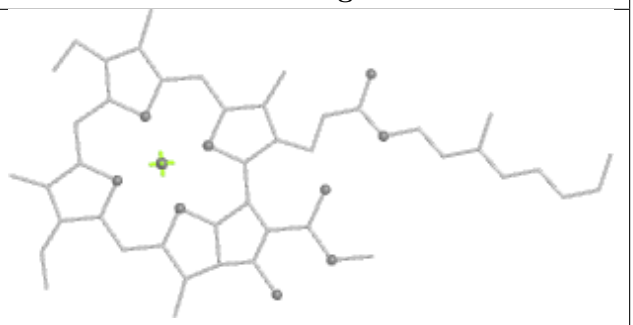
Bond lengths



Bond angles

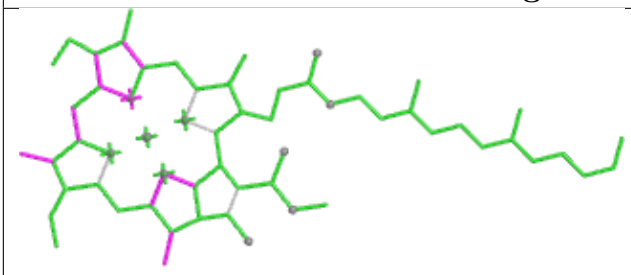


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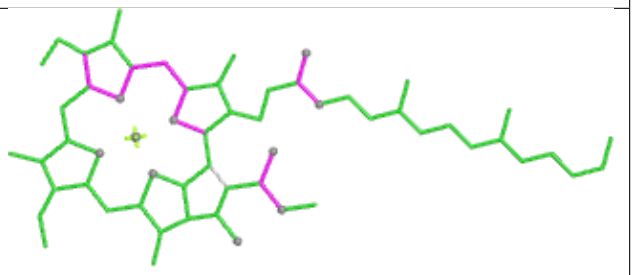


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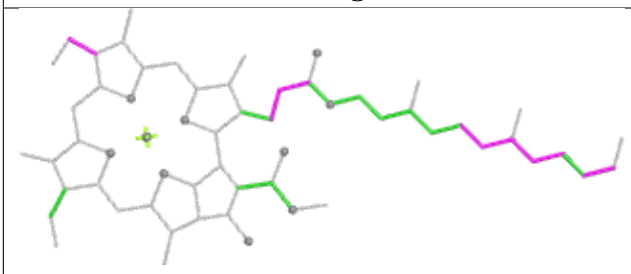
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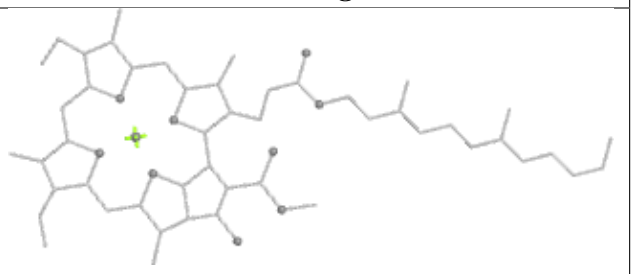
Bond lengths



Bond angles

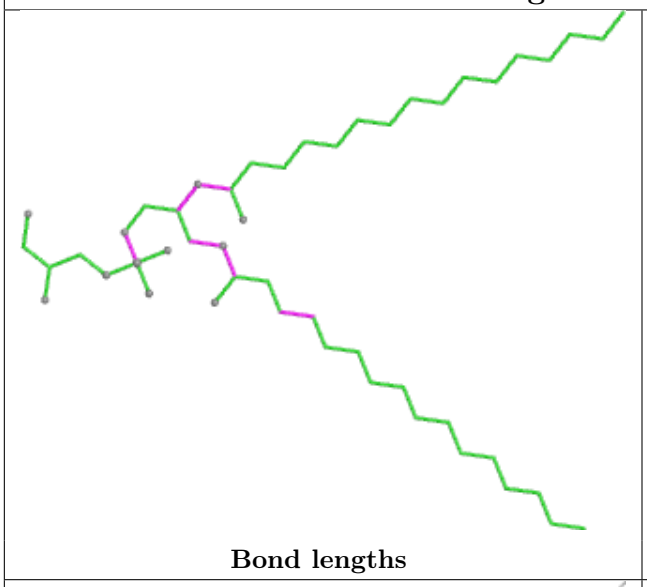


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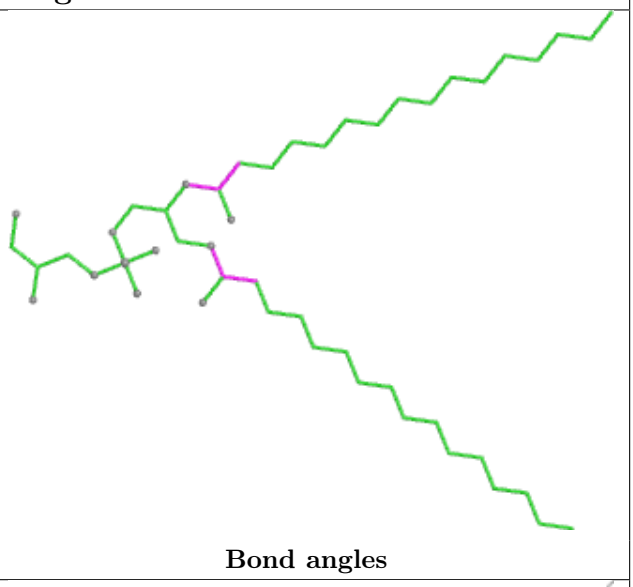


Rings

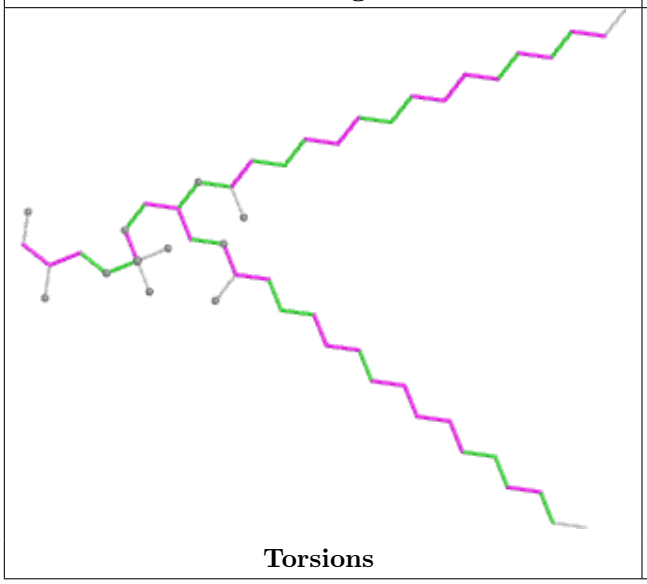
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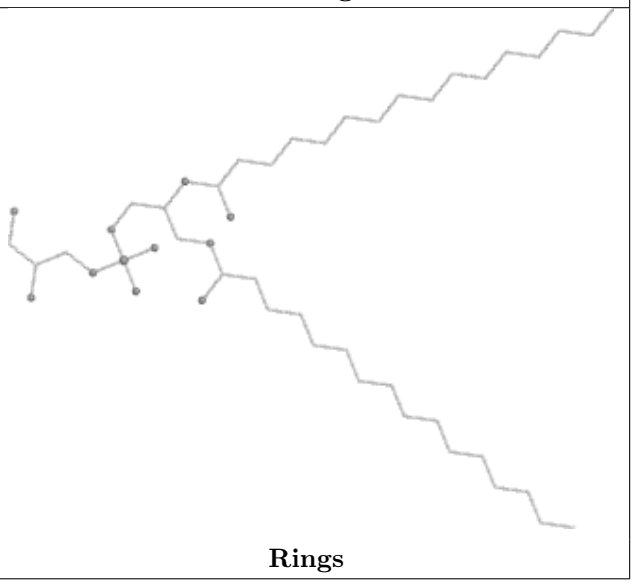
Bond lengths



Bond angles

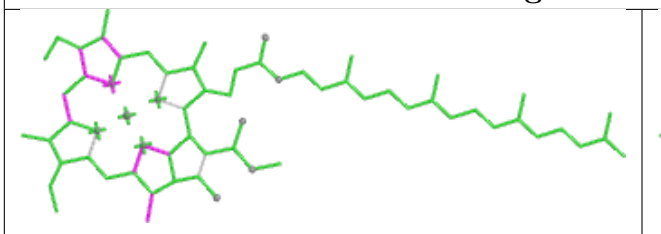


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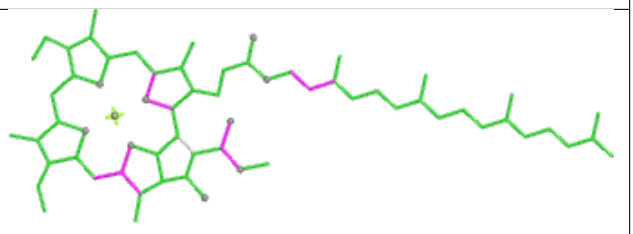


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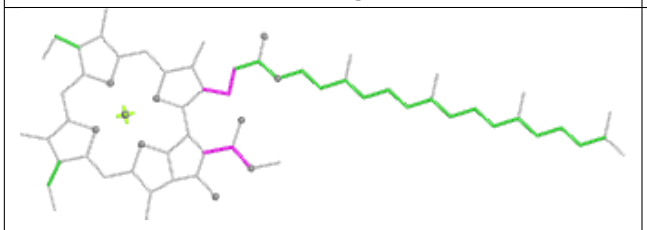
Ligand CLA A 801



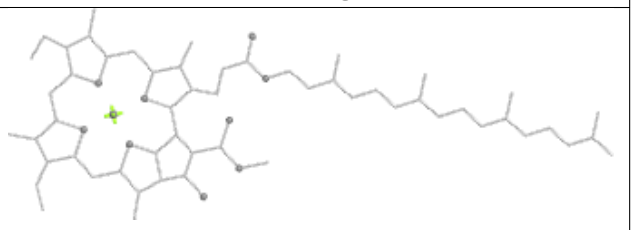
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Bond angles

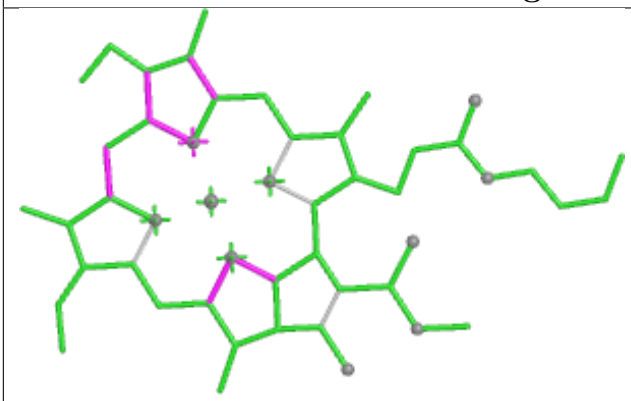


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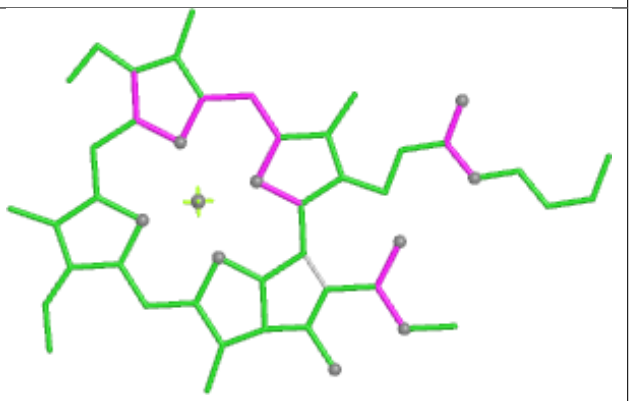


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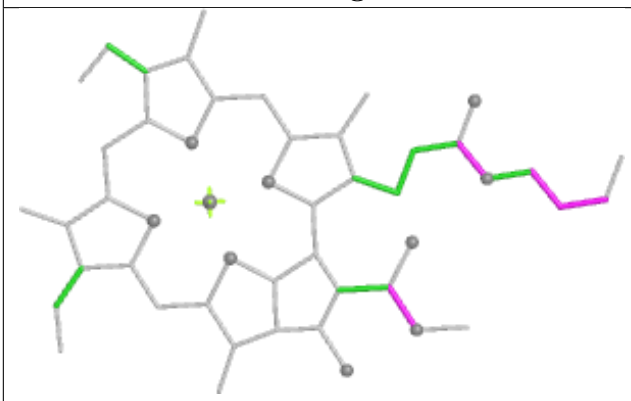
Ligand CLA N 817



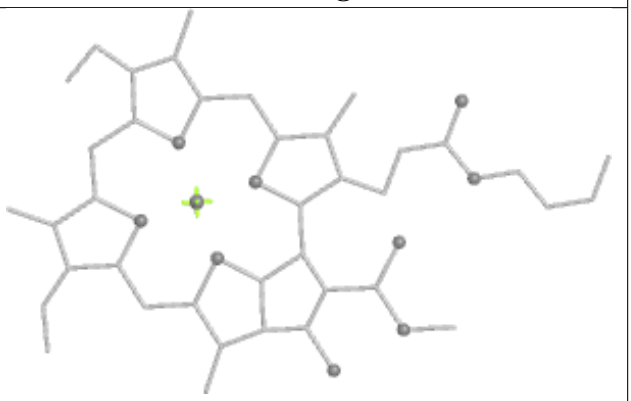
Bond lengths



Bond angles

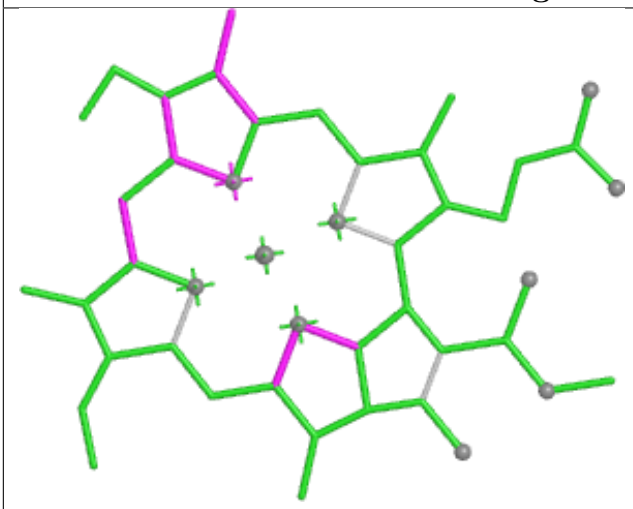


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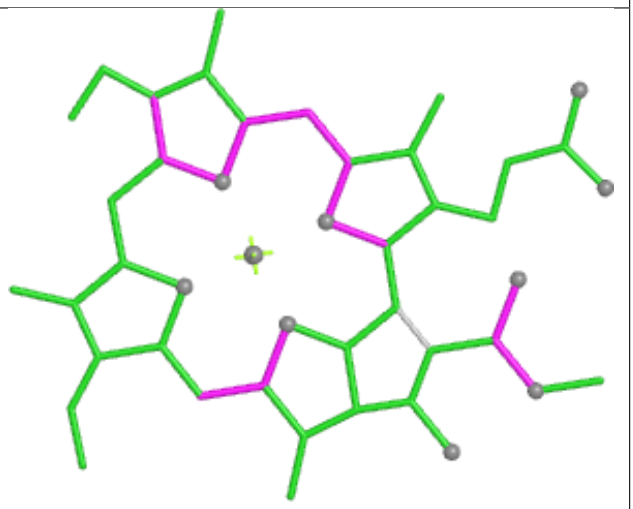


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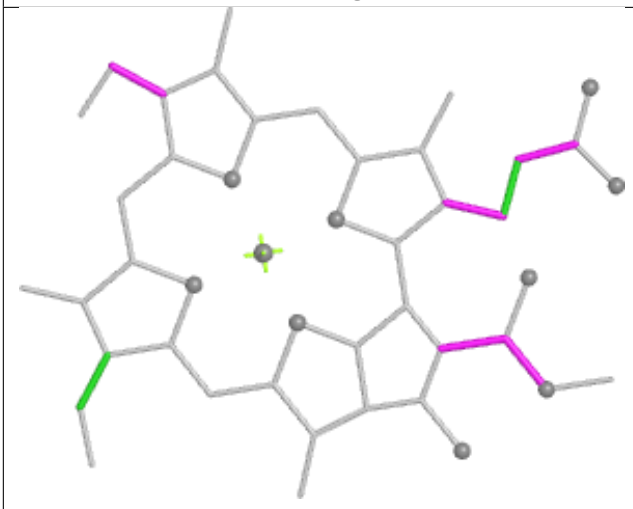
Ligand CLA l 204



Bond lengths



Bond angles

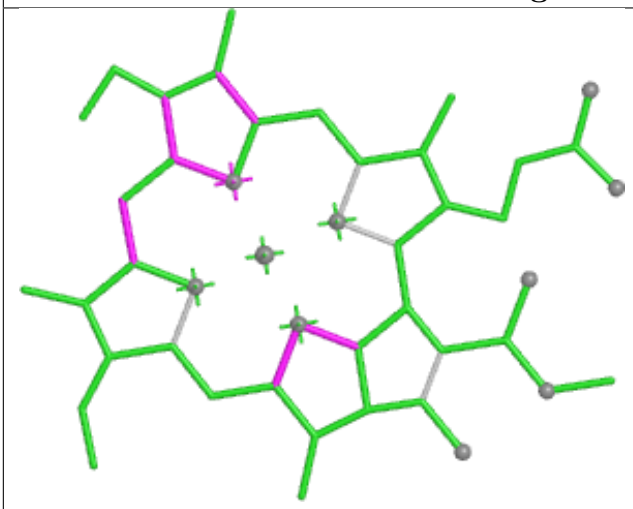


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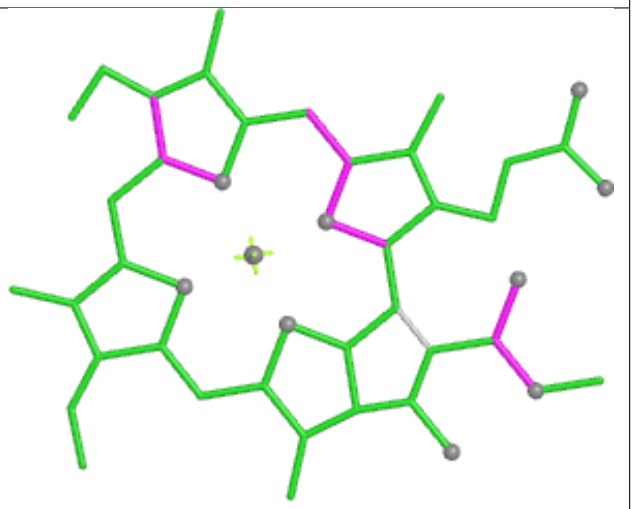


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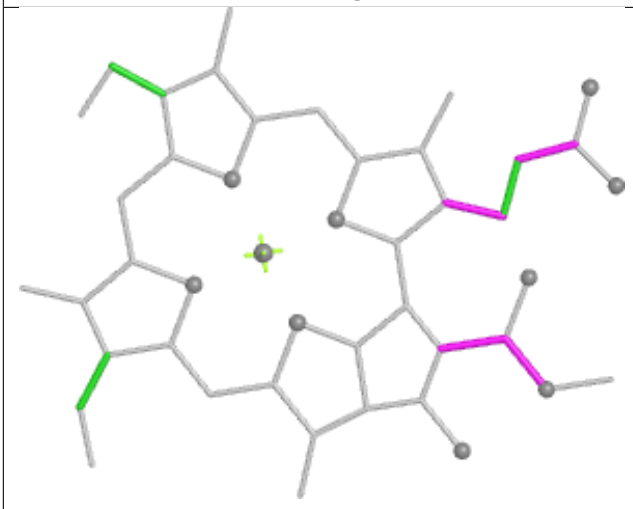
Ligand CLA t 101



Bond lengths



Bond angles

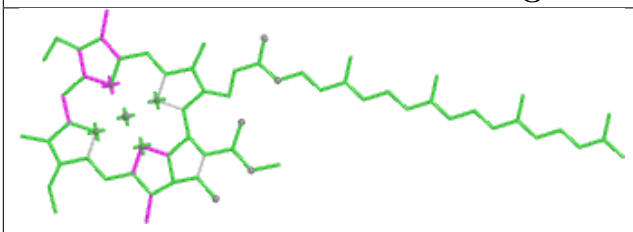


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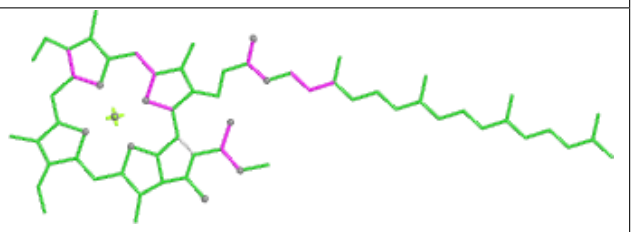


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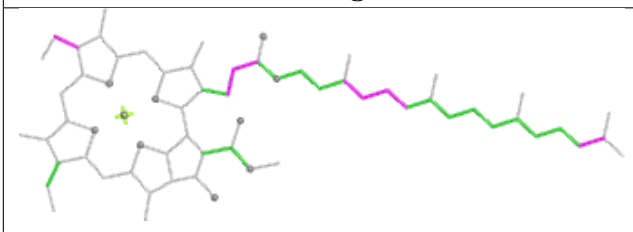
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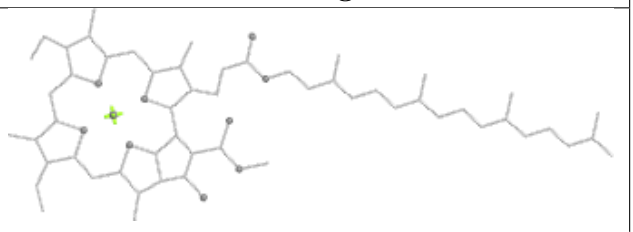
Bond lengths



Bond angles

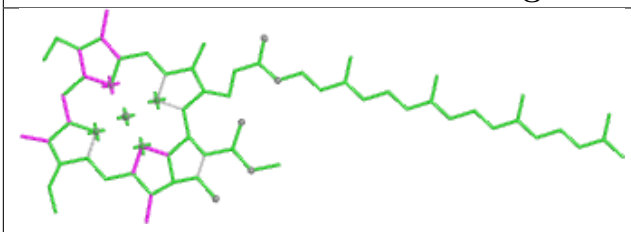


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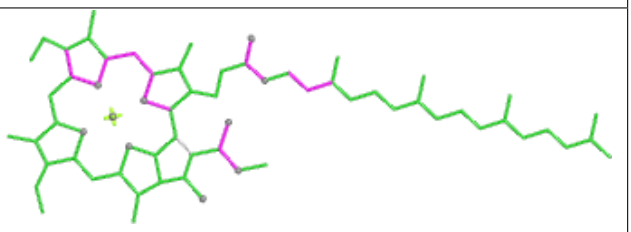


Rings

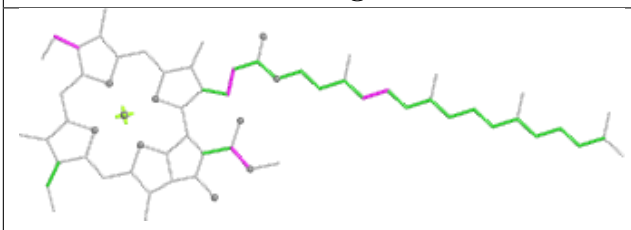
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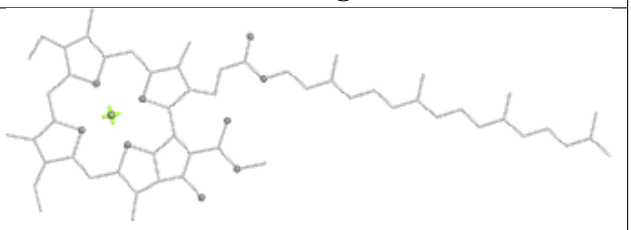
Bond lengths



Bond angles

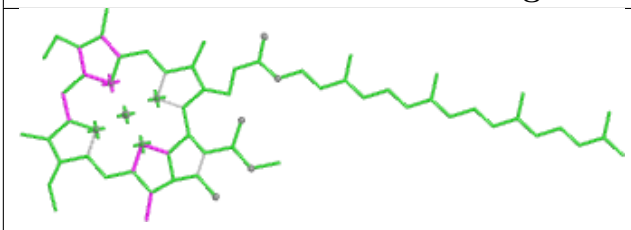


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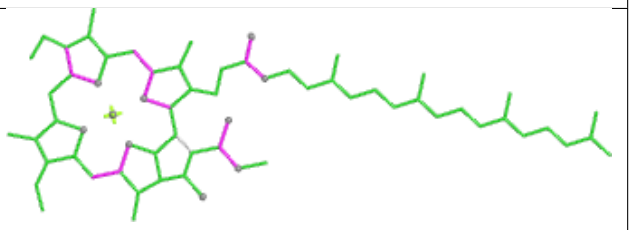


Rings

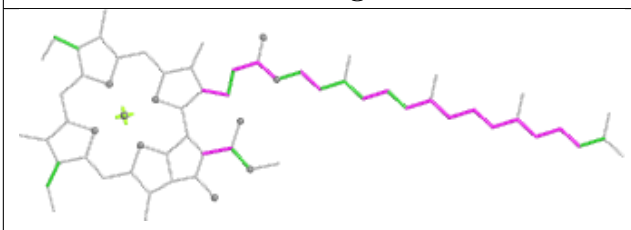
Ligand CLA G 804



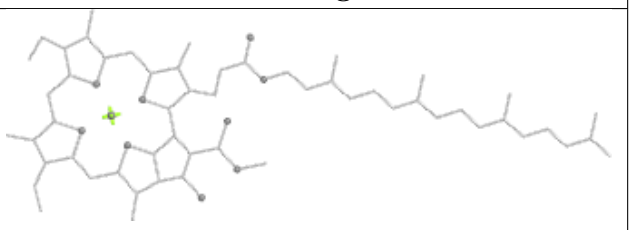
Bond lengths



Bond angles

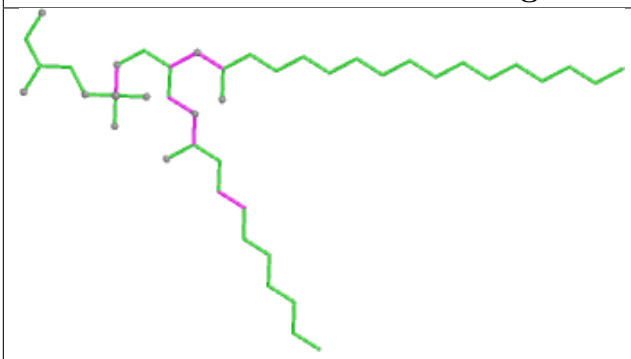


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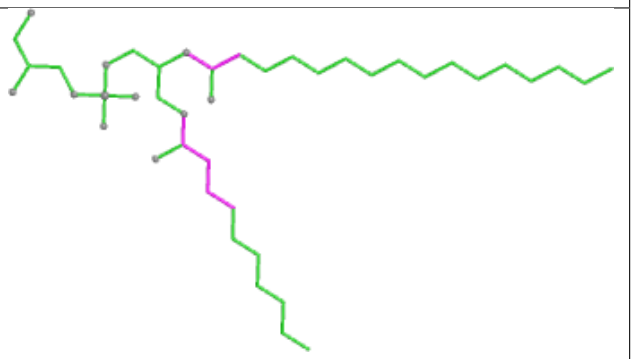


Rings

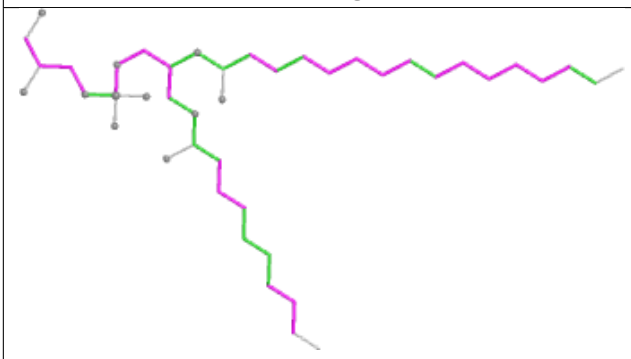
Ligand LHG m 101



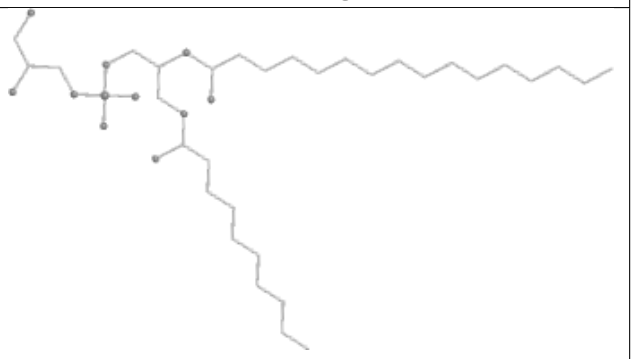
Bond lengths



Bond angles

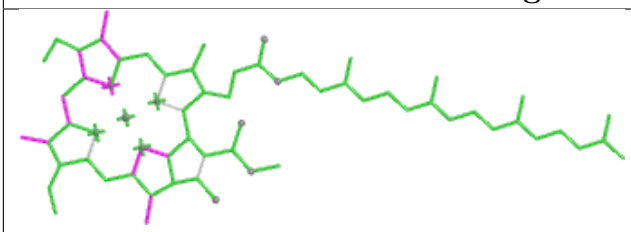


Torsions

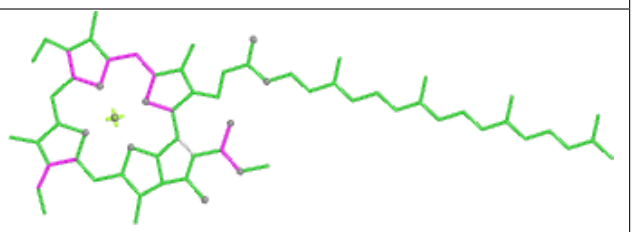


Rings

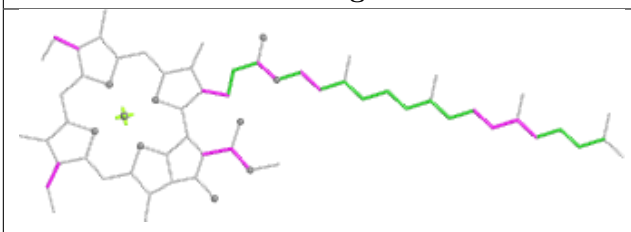
Ligand CLA N 805



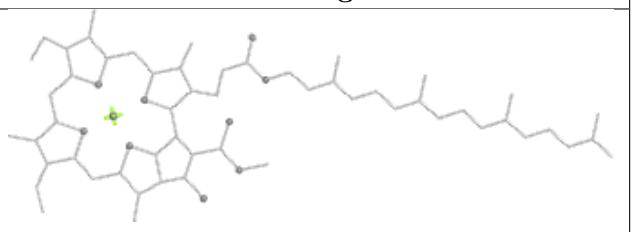
Bond lengths



Bond angles

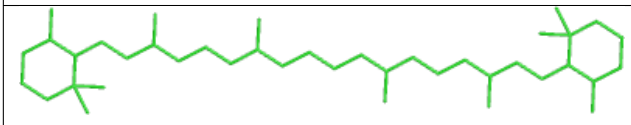


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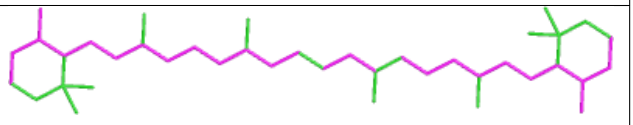


Rings

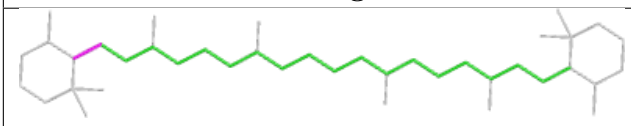
Ligand BCR T 103



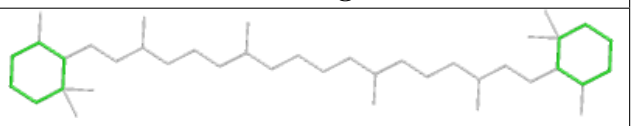
Bond lengths



Bond angles

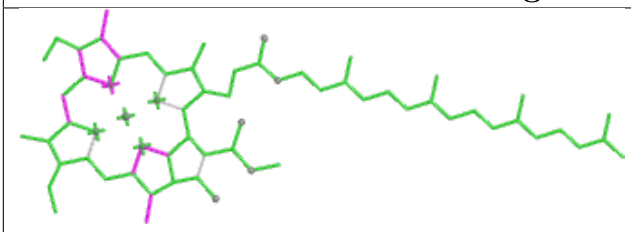


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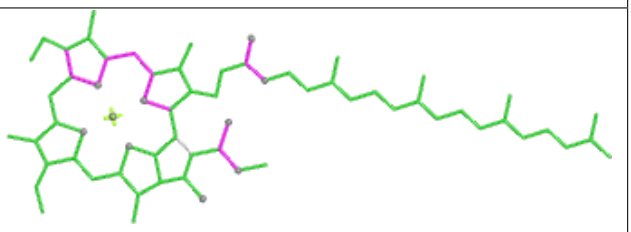


Rings

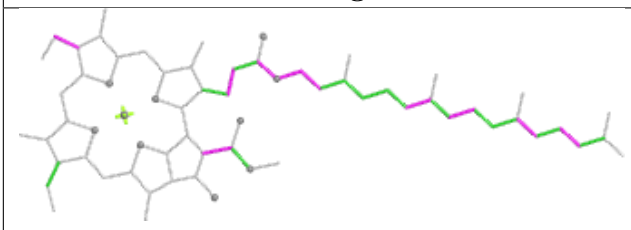
Ligand CLA N 801



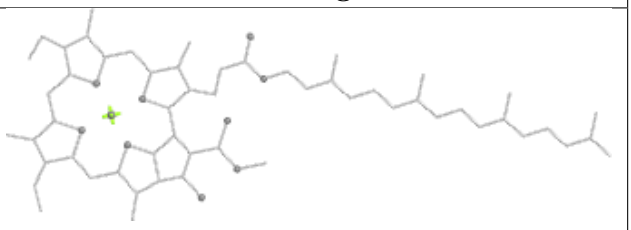
Bond lengths



Bond angles

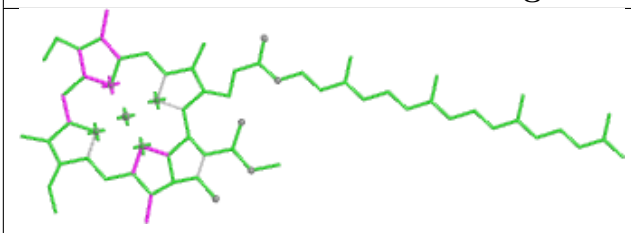


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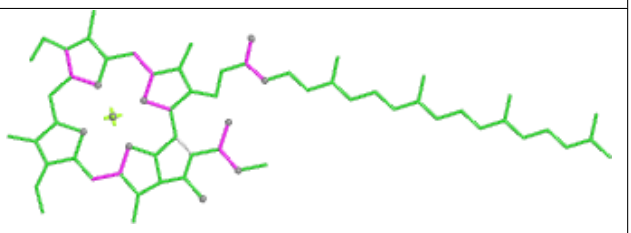


Rings

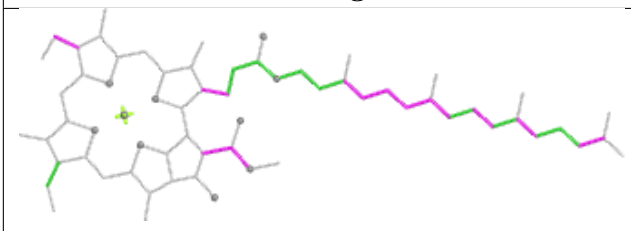
Ligand CLA A 805



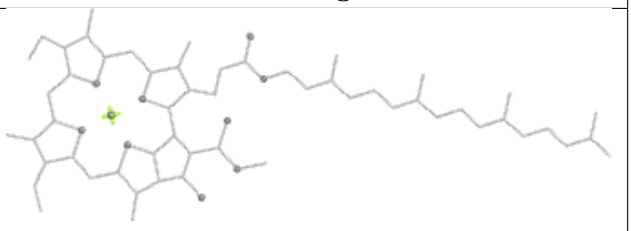
Bond lengths



Bond angles

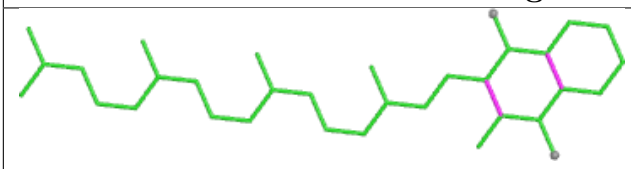


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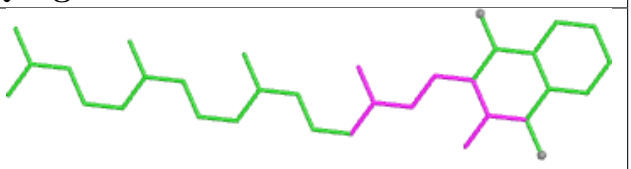


Rings

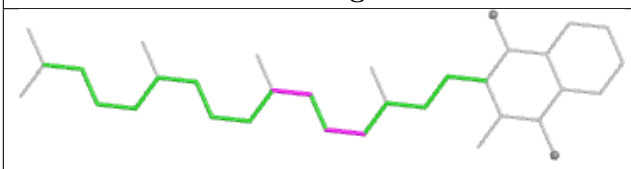
Ligand PQN g 841



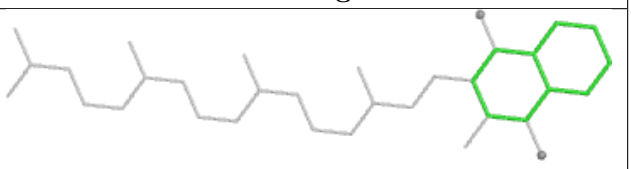
Bond lengths



Bond angles

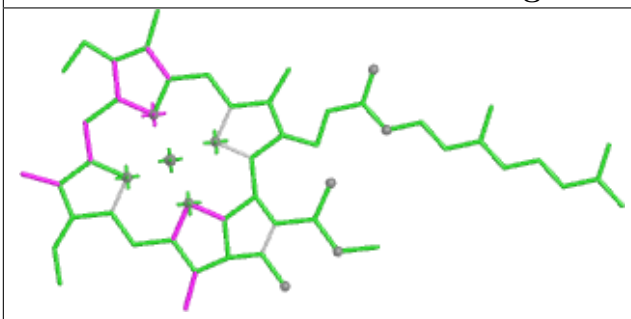


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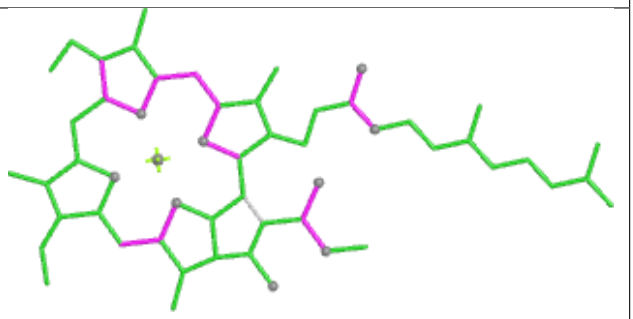


Rings

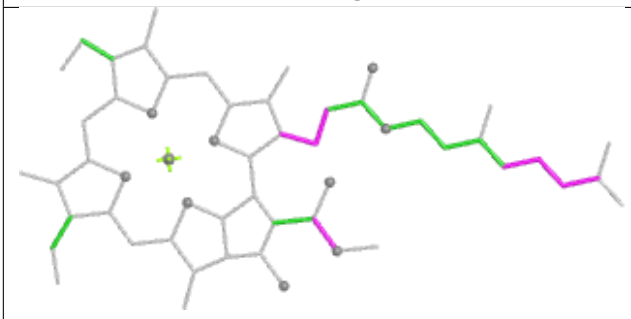
Ligand CLA N 806



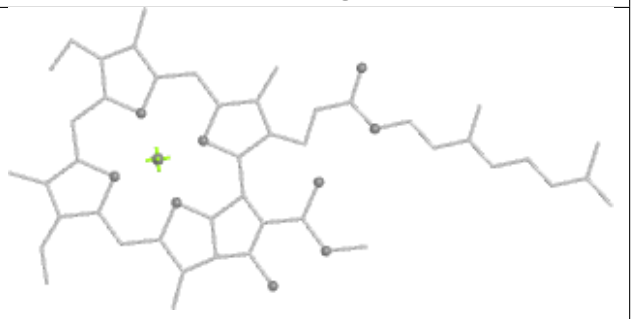
Bond lengths



Bond angles

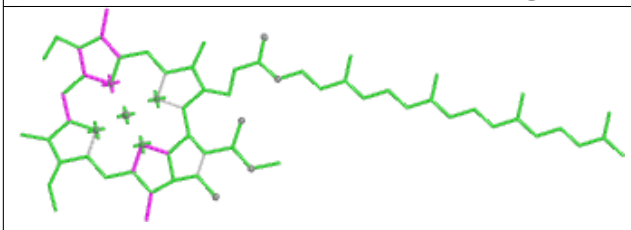


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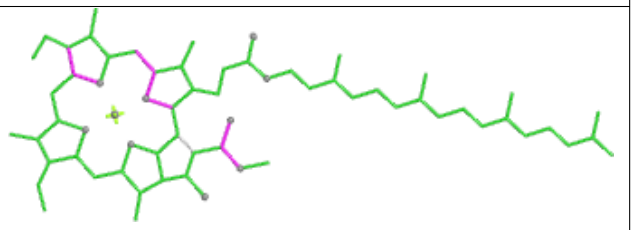


Rings

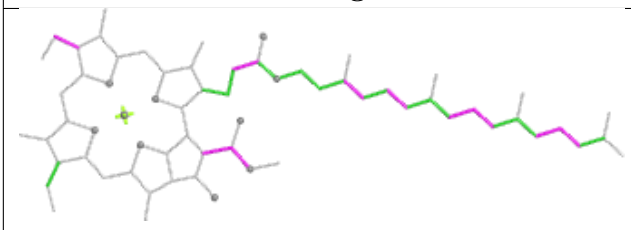
Ligand CLA G 838



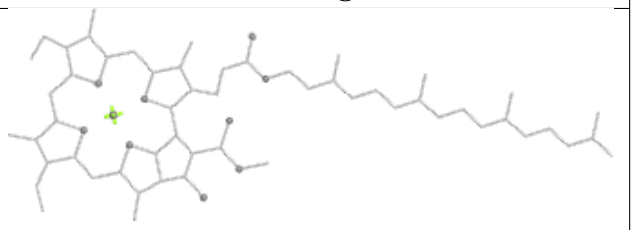
Bond lengths



Bond angles

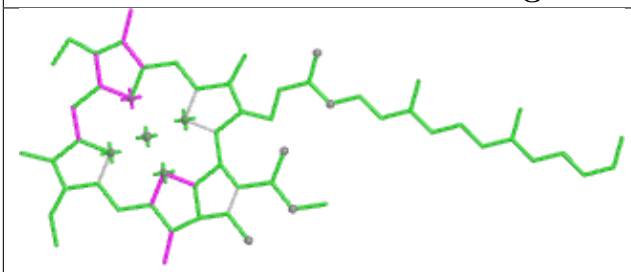


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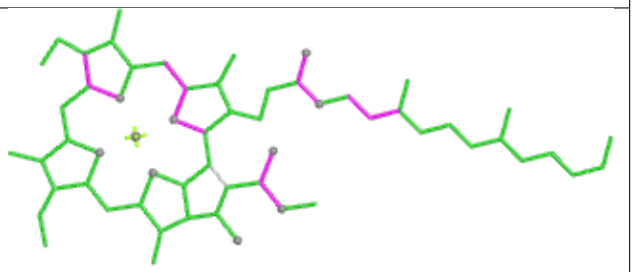


Rings

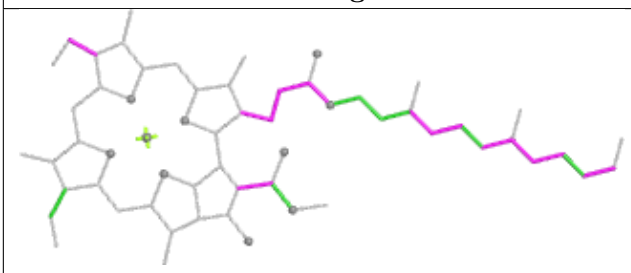
Ligand CLA A 811



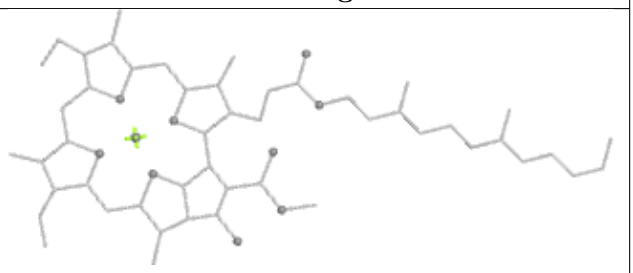
Bond lengths



Bond angles

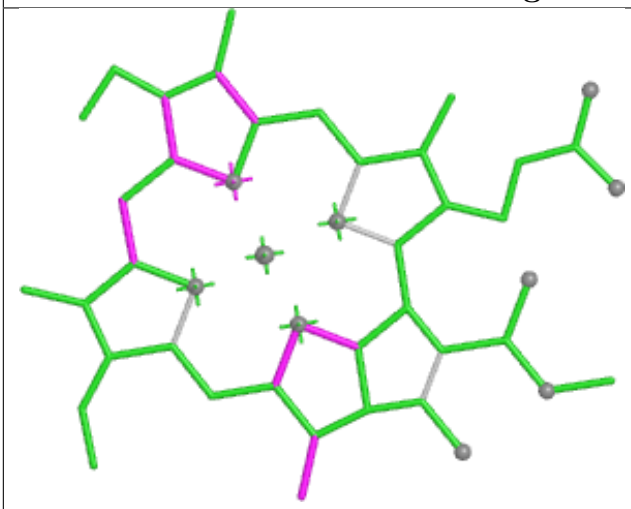


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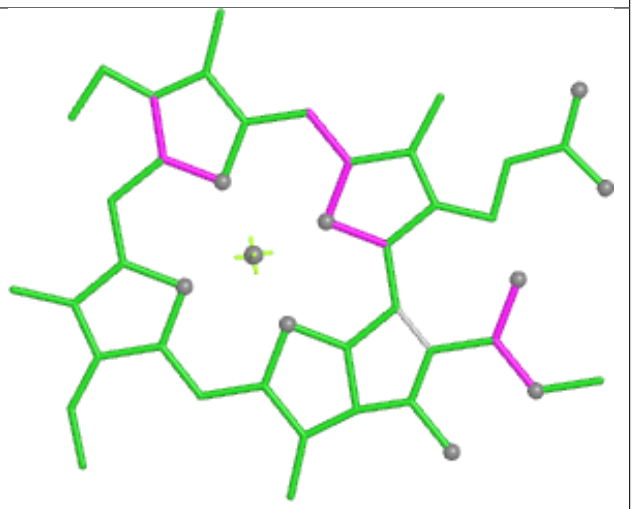


Rings

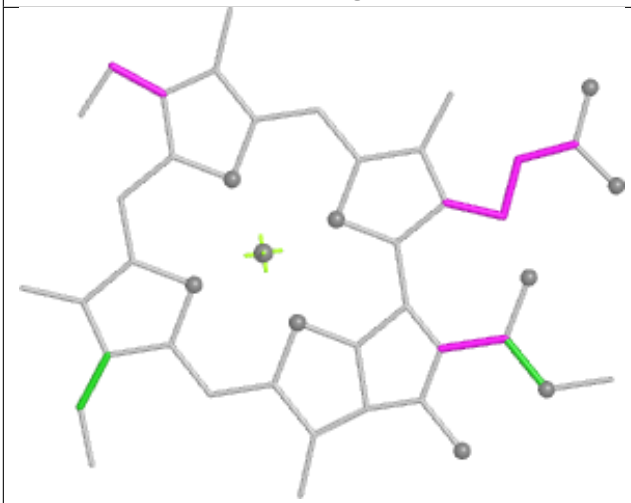
Ligand CLA N 822



Bond lengths



Bond angles

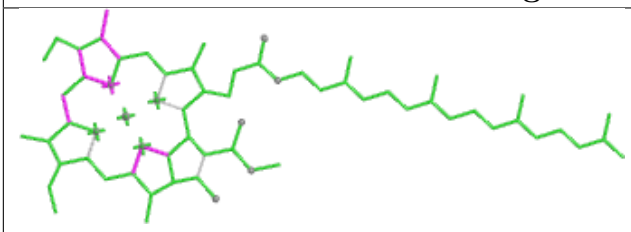


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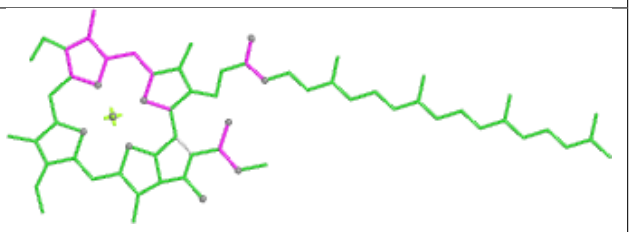


Rings

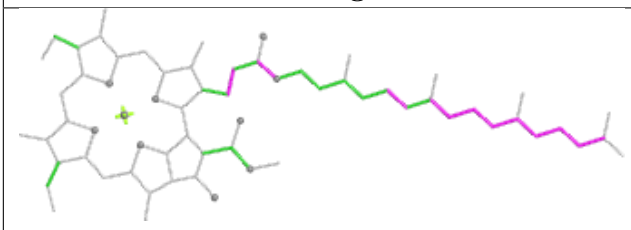
Ligand CLA G 820



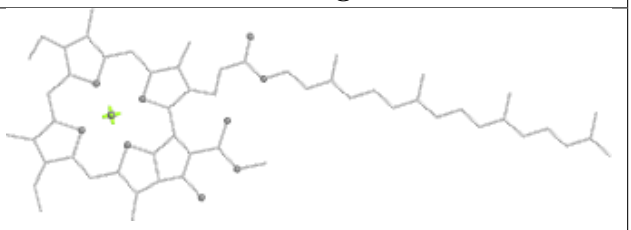
Bond lengths



Bond angles

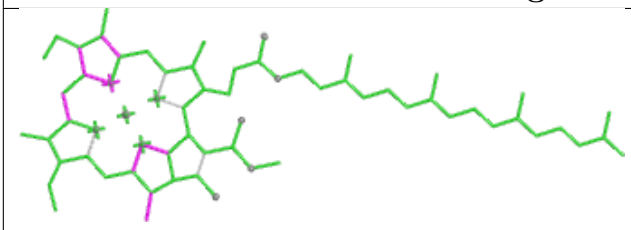


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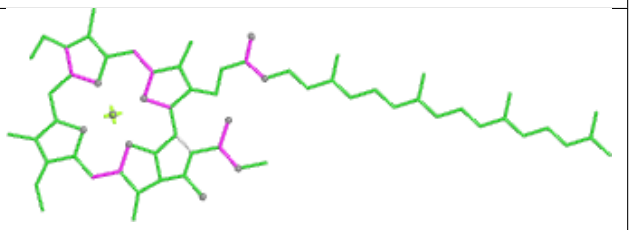


Rings

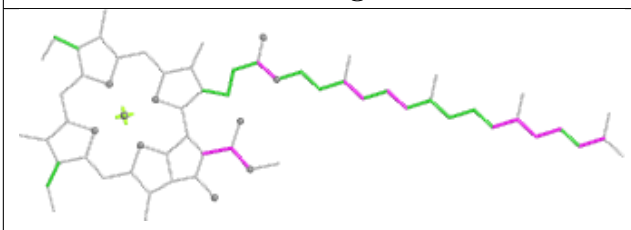
Ligand CLA n 837



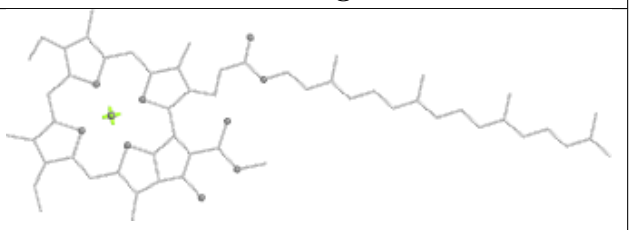
Bond lengths



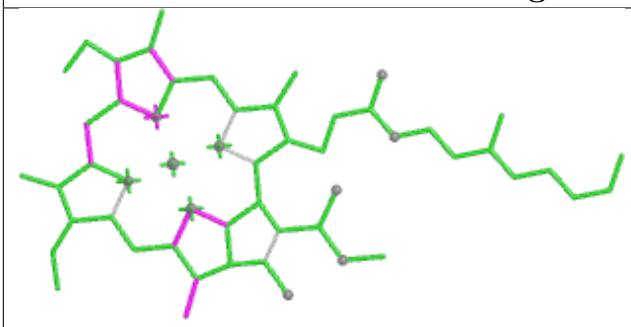
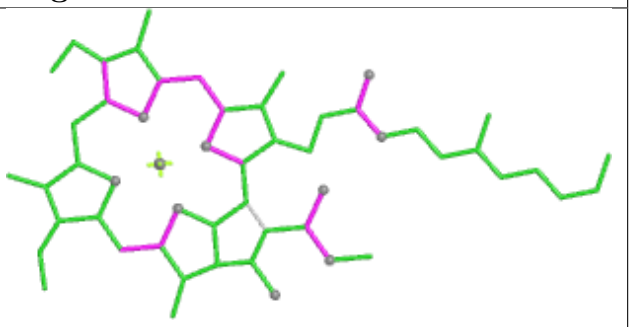
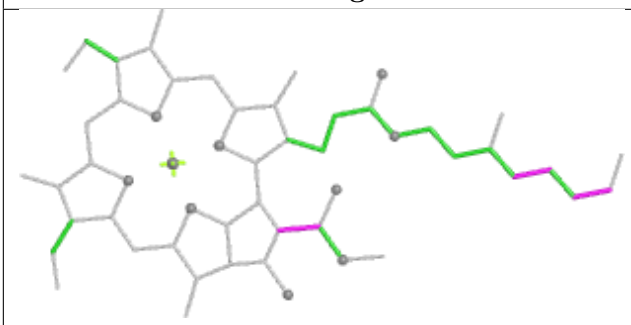
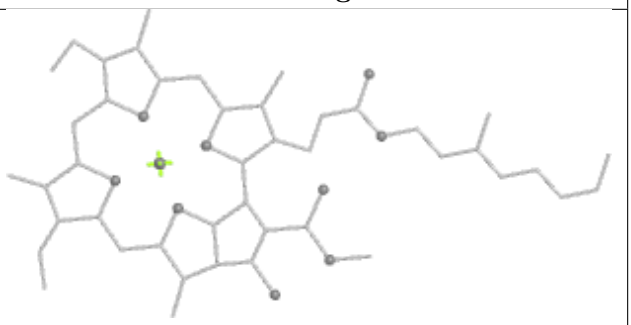
Bond angles

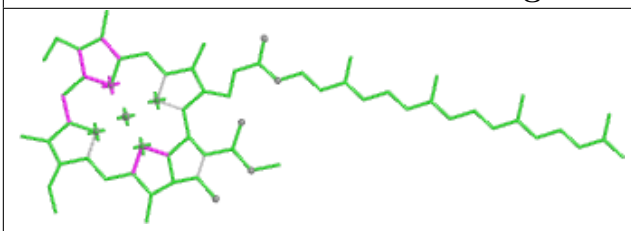
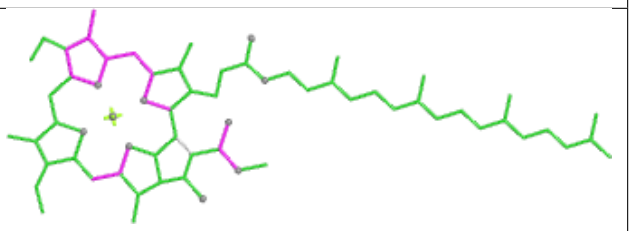
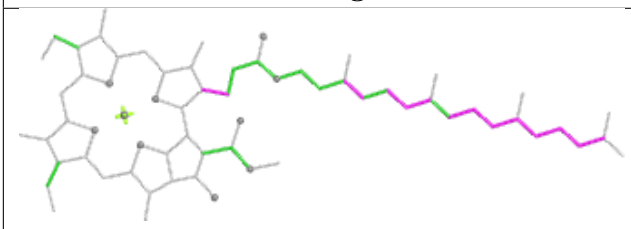
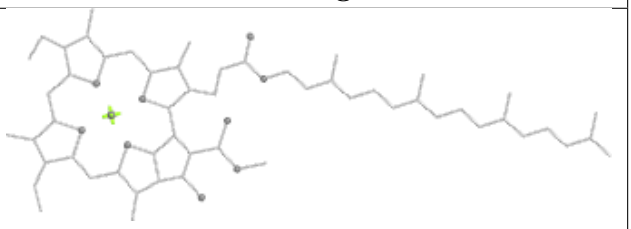


Torsions

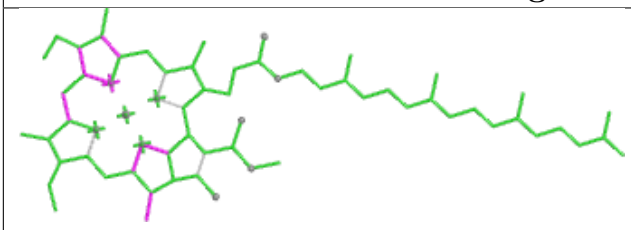


Rings

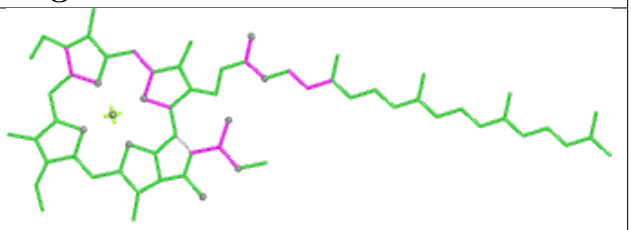
Ligand CLA g 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

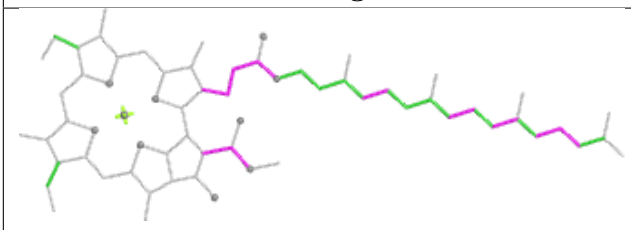
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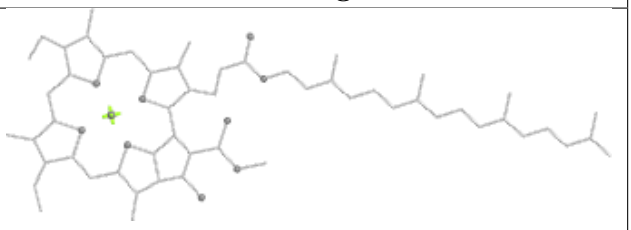
Bond lengths



Bond angles

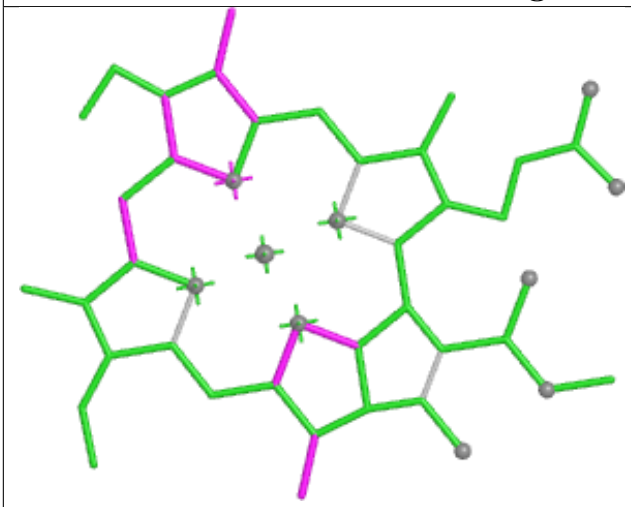


Torsions

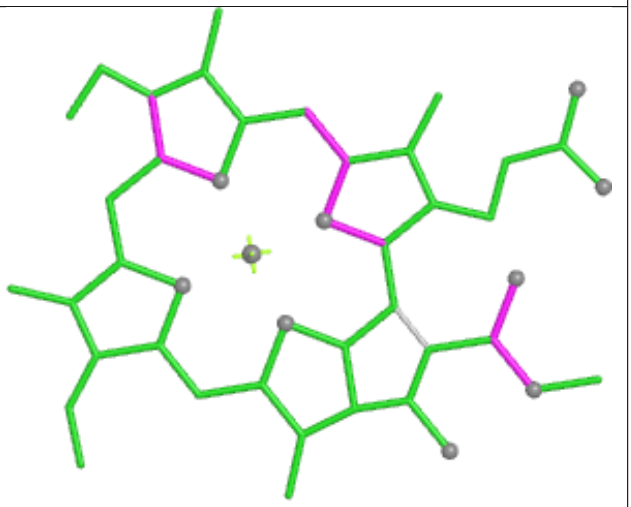


Rings

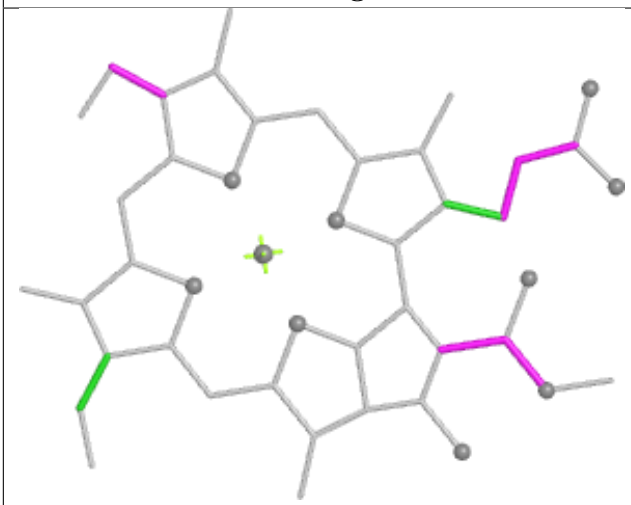
Ligand CLA a 852



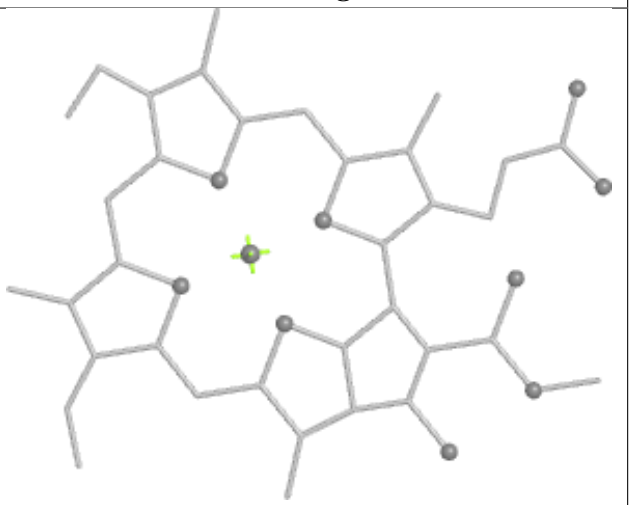
Bond lengths



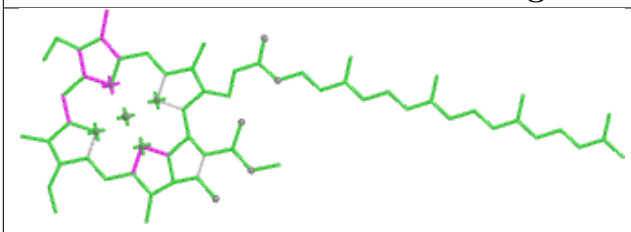
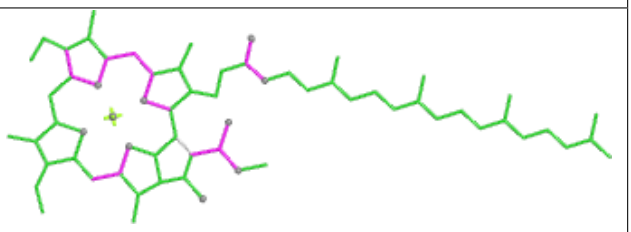
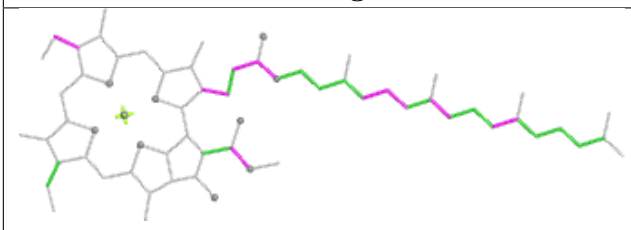
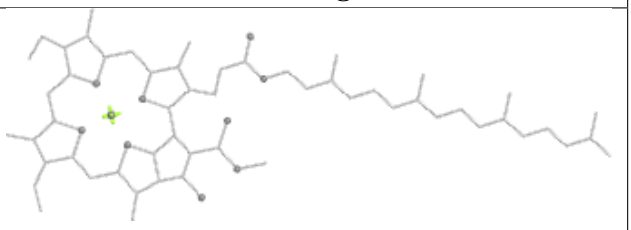
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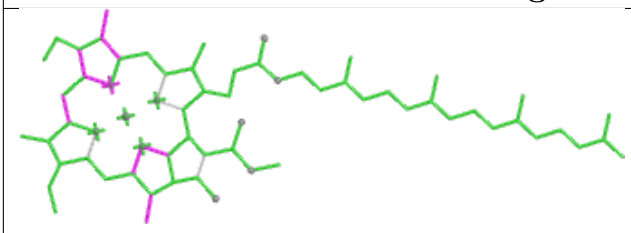
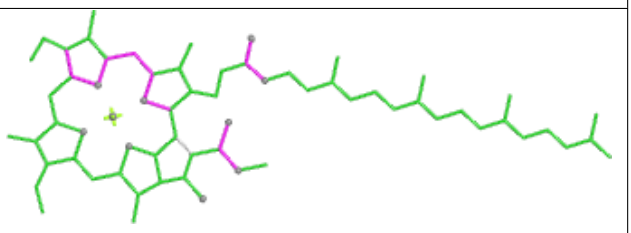
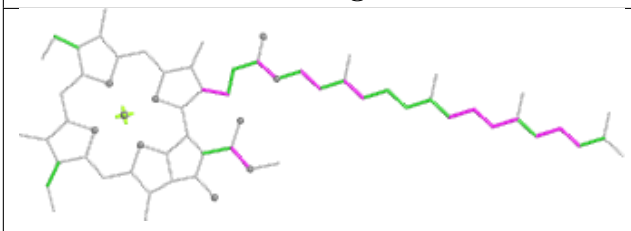
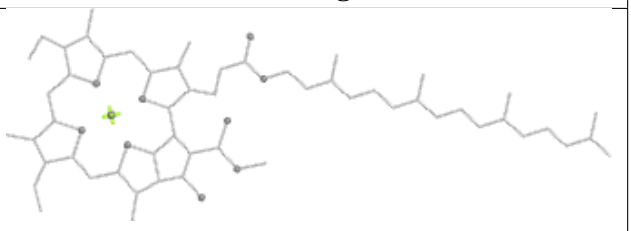


Torsions

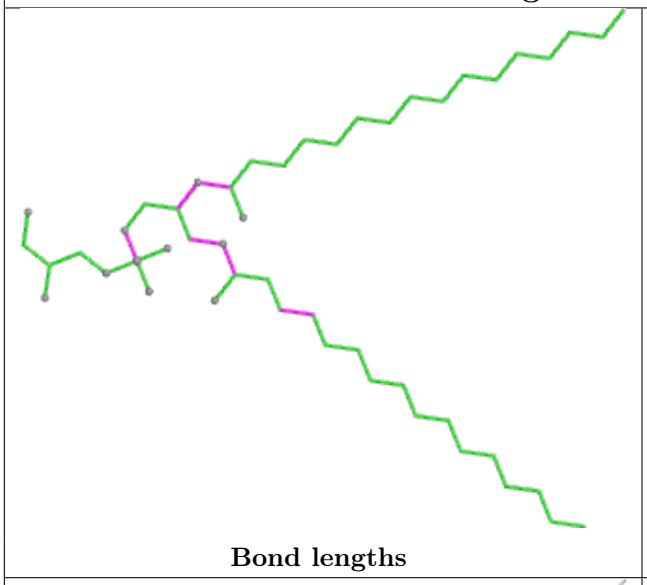


Rings

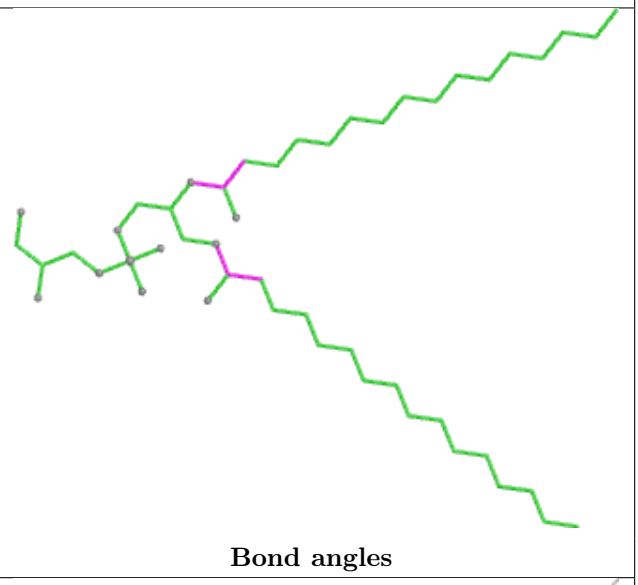
Ligand CLA b 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

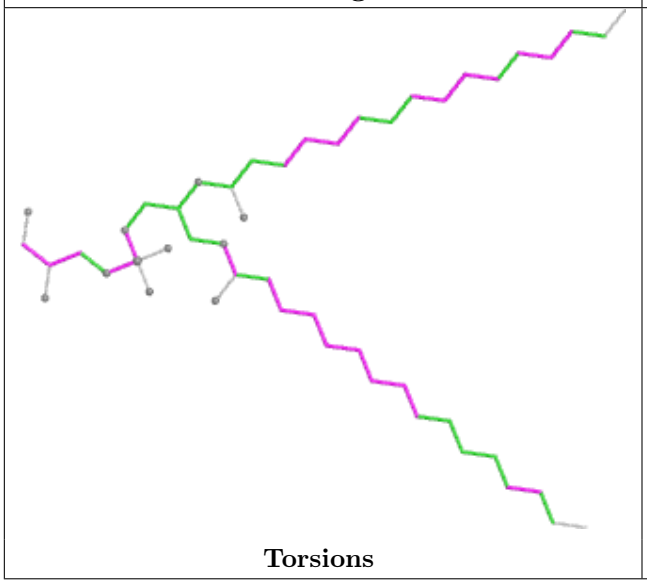
Ligand LHG G 849



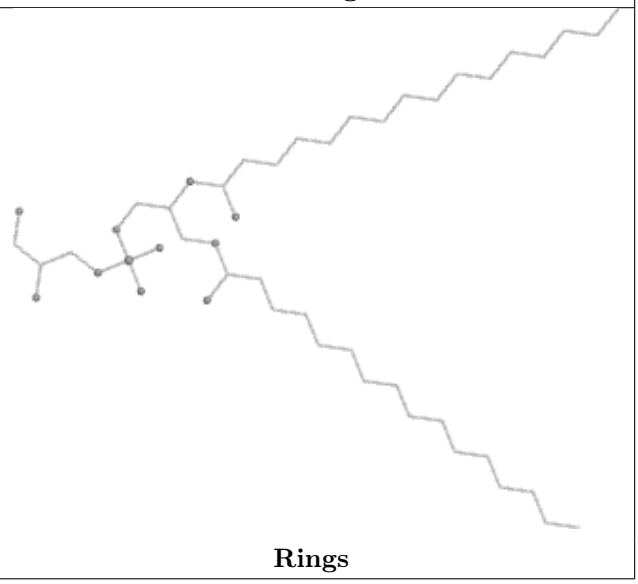
Bond lengths



Bond angles

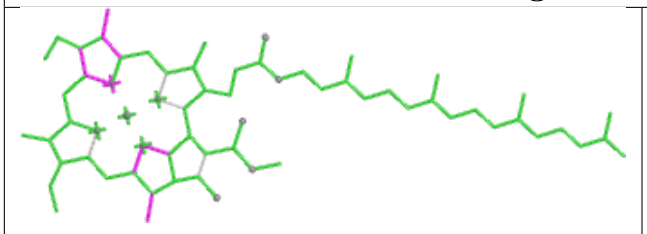


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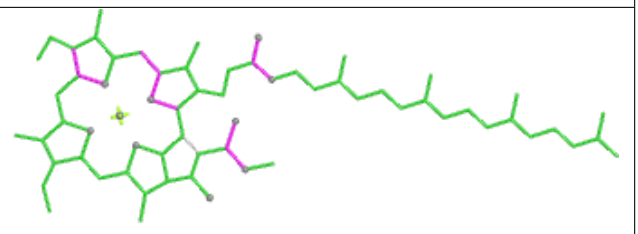


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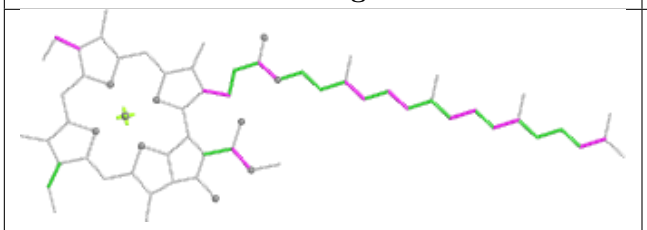
Ligand CLA n 840



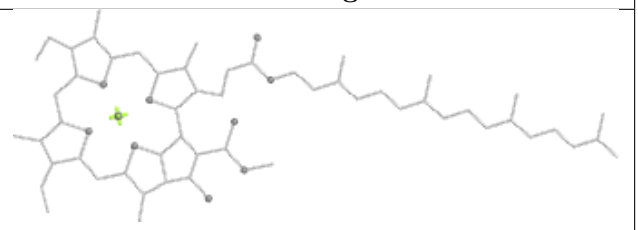
Bond lengths



Bond angles

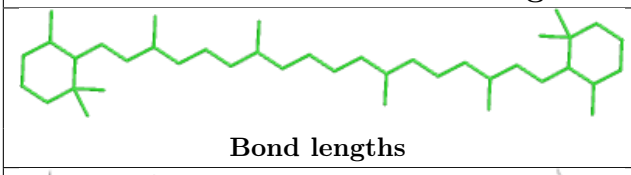


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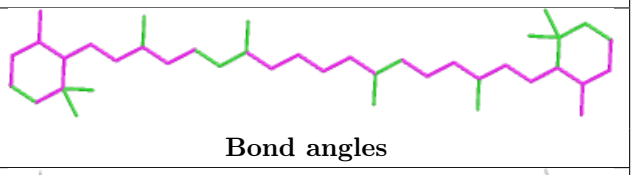


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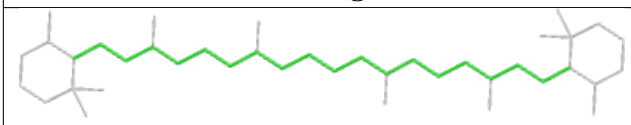
Ligand BCR a 845



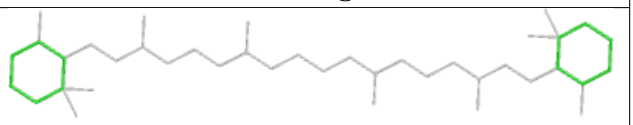
Bond lengths



Bond angles

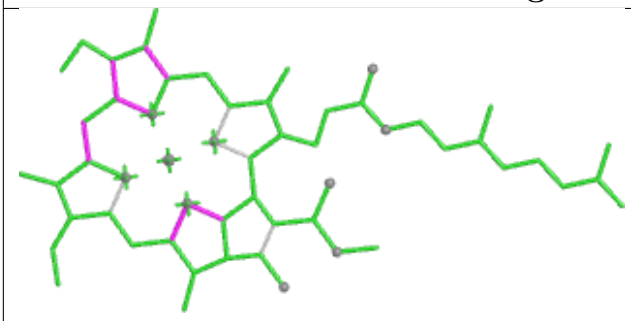


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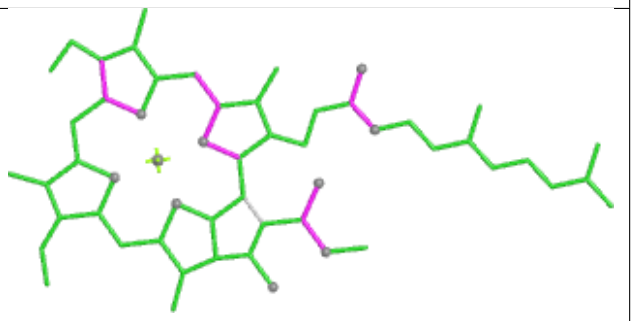


Rings

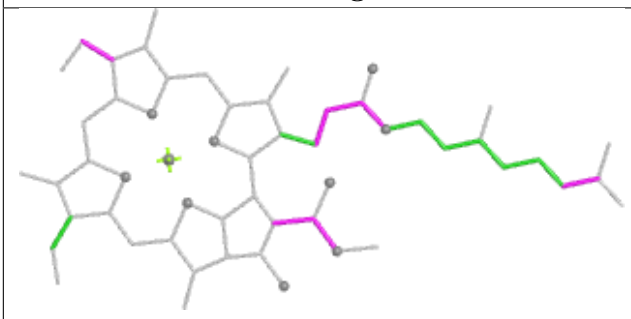
Ligand CLA b 822



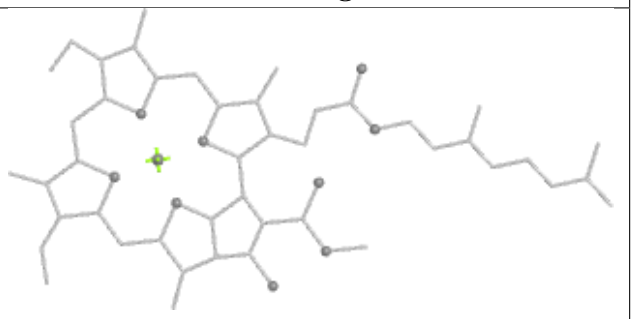
Bond lengths



Bond angles

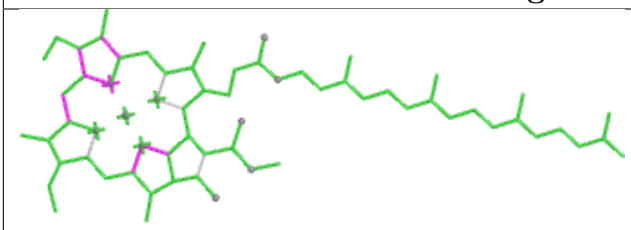


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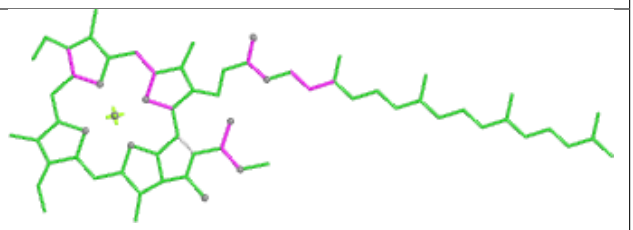


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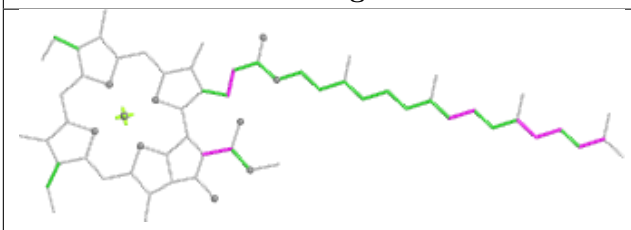
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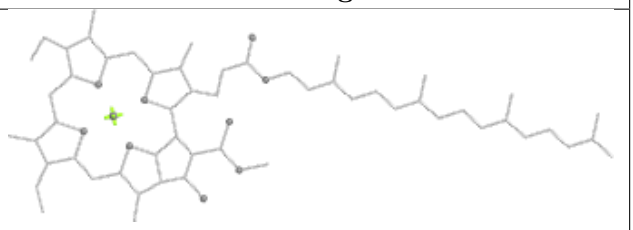
Bond lengths



Bond angles

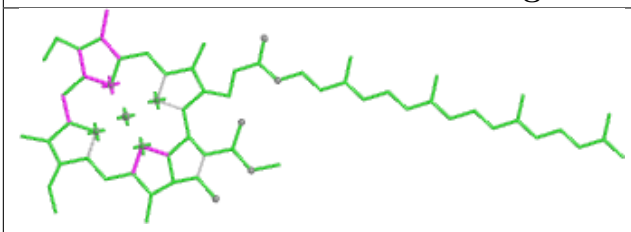


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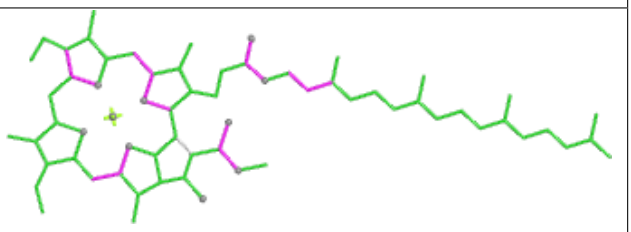


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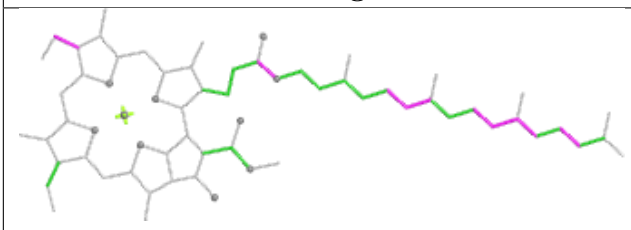
Ligand CLA N 808



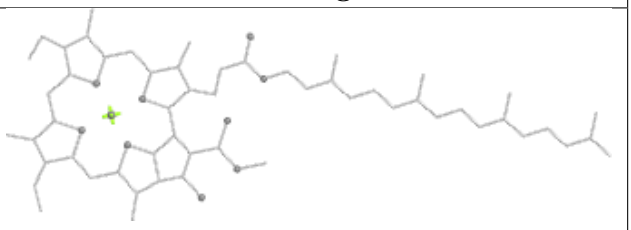
Bond lengths



Bond angles

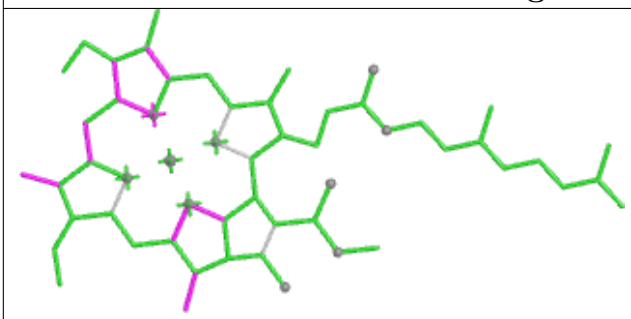


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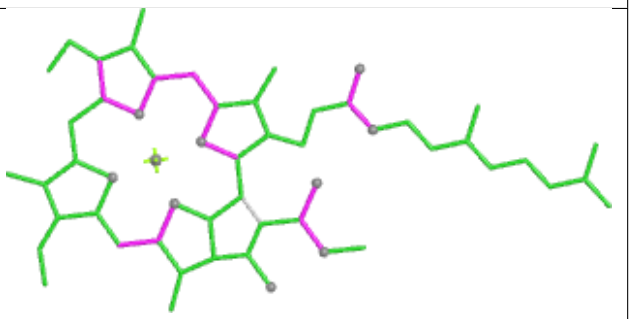


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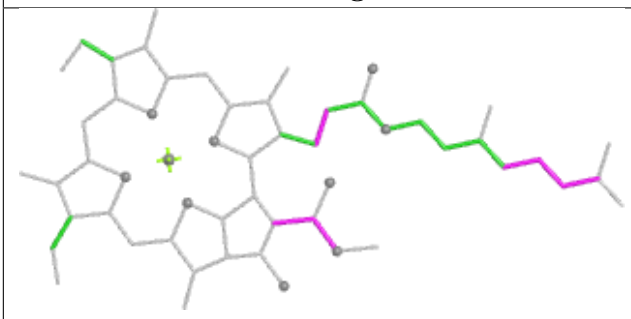
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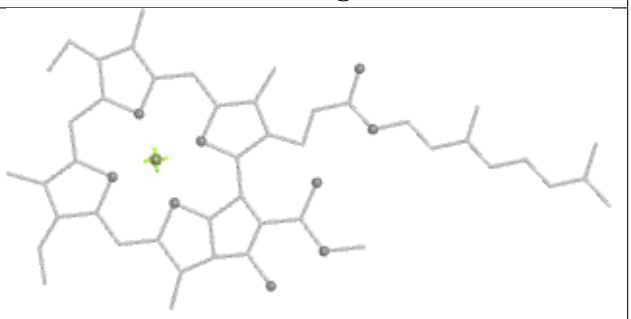
Bond lengths



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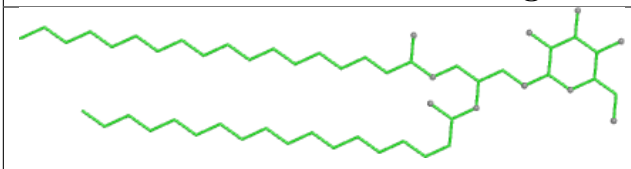


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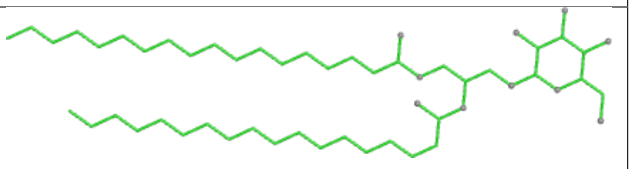


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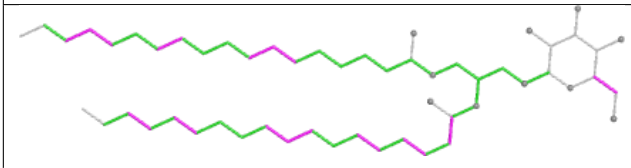
Ligand LMG n 848



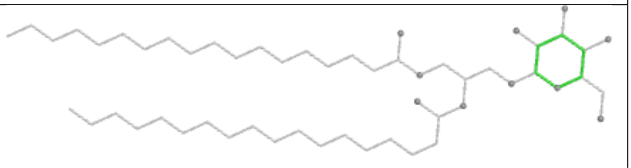
Bond lengths



Bond angles

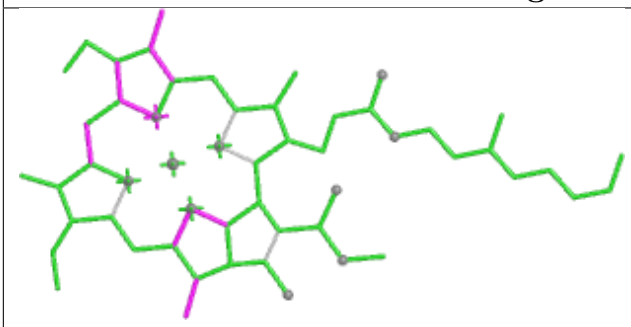


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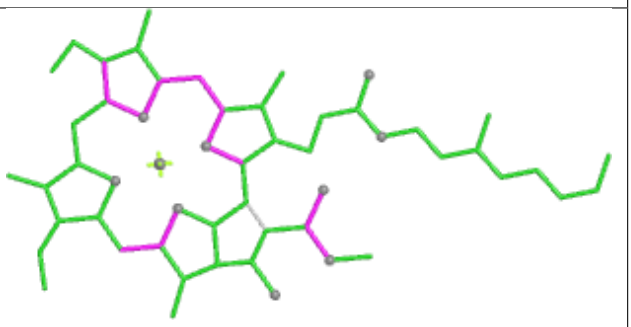


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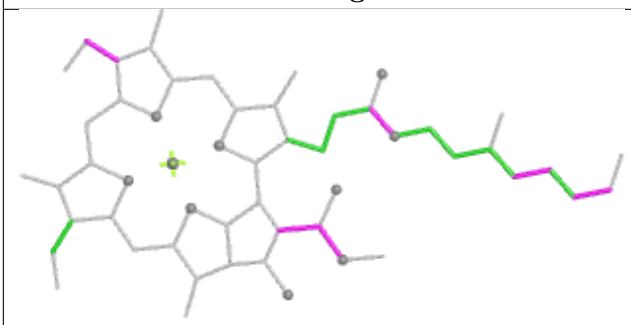
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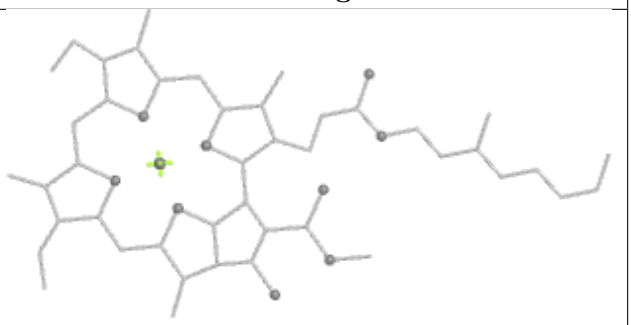
Bond lengths



Bond angles

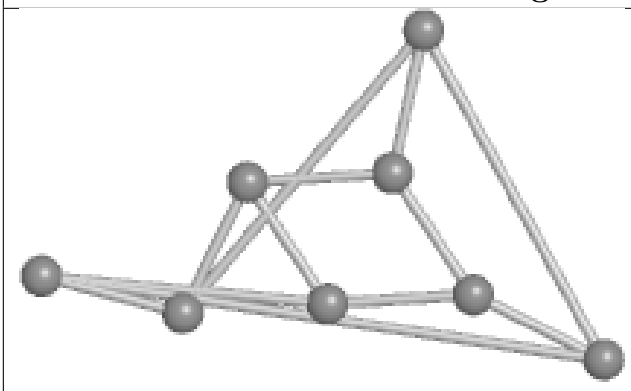


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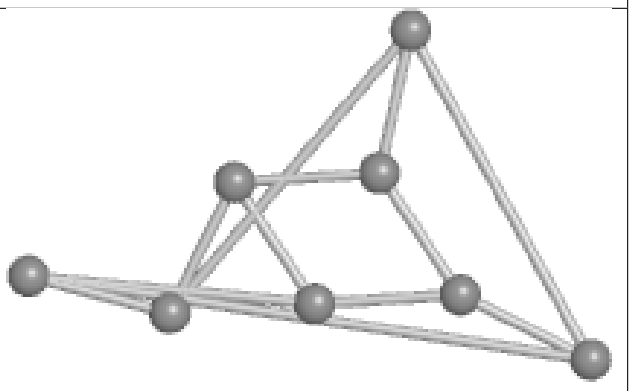


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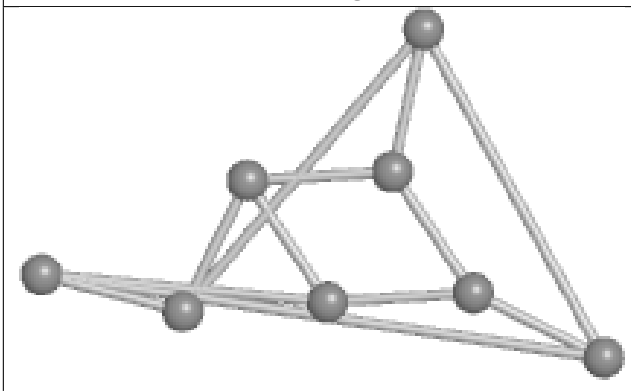
Ligand SF4 C 101



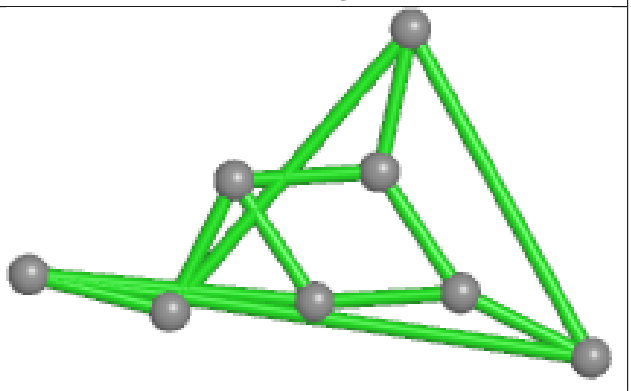
Bond lengths



Bond angles

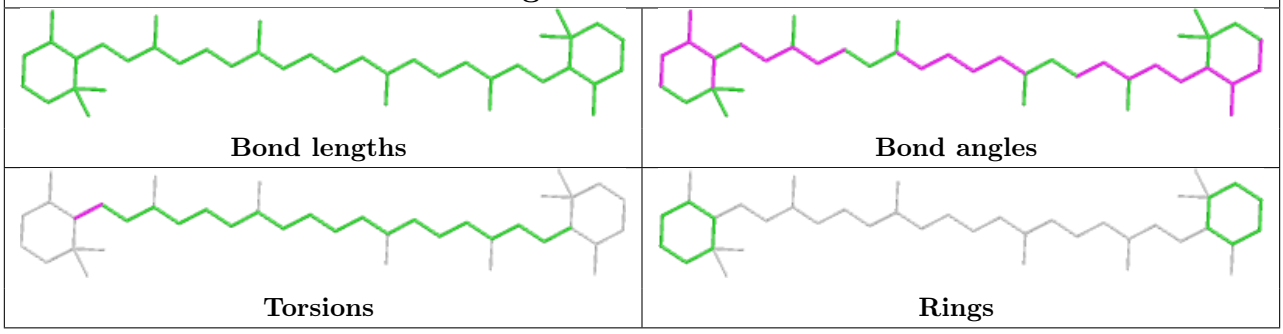


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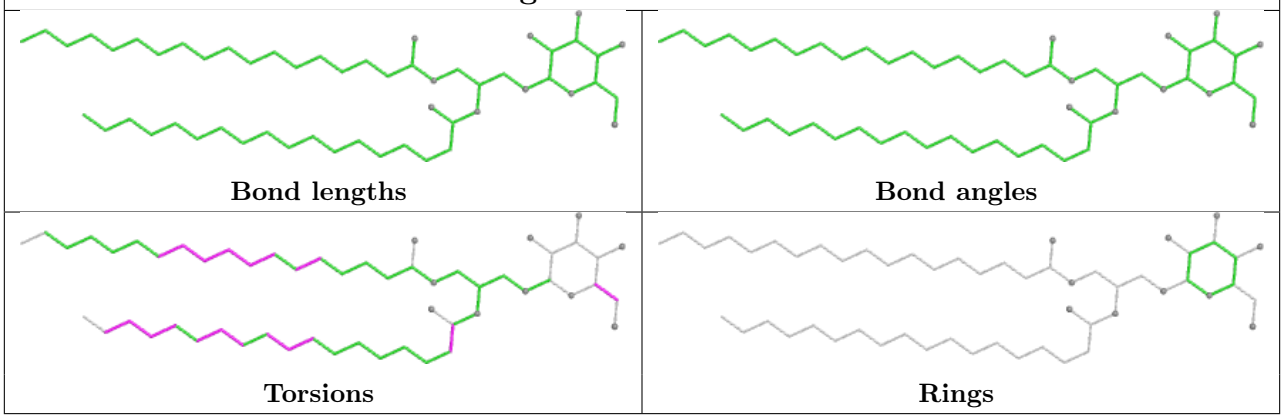


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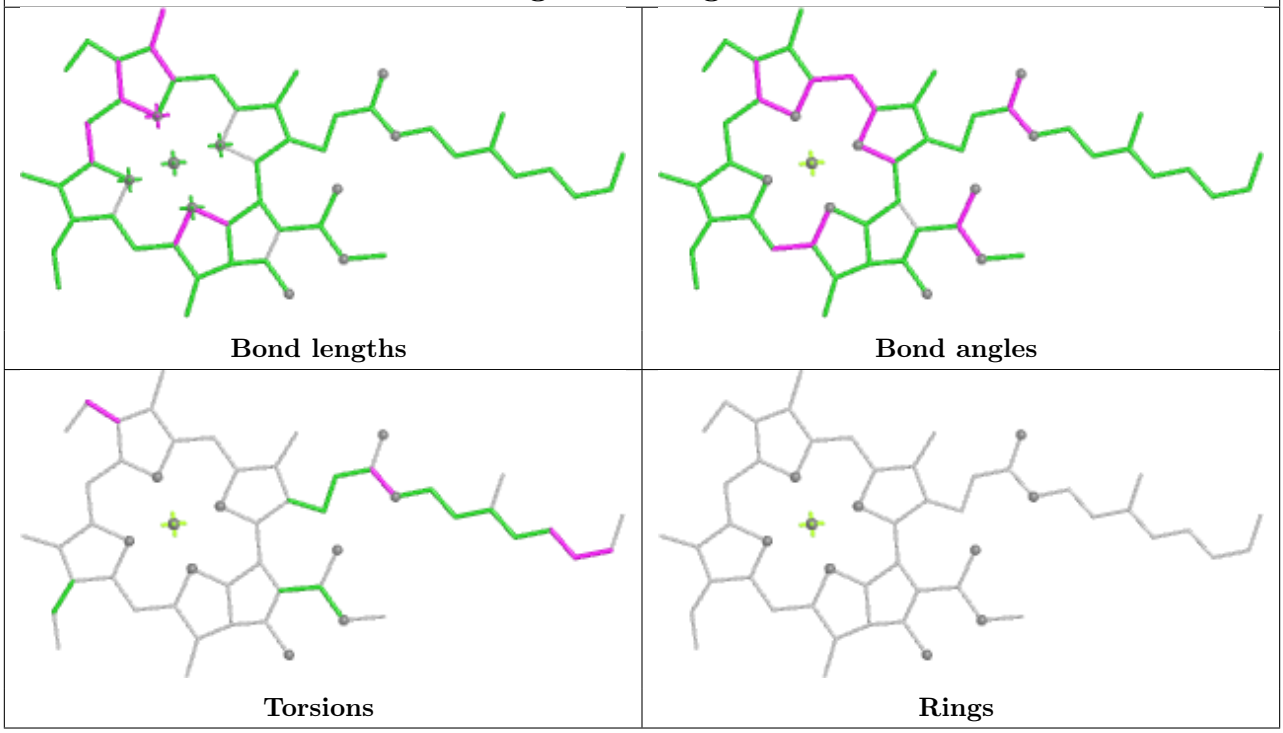
Ligand BCR G 845



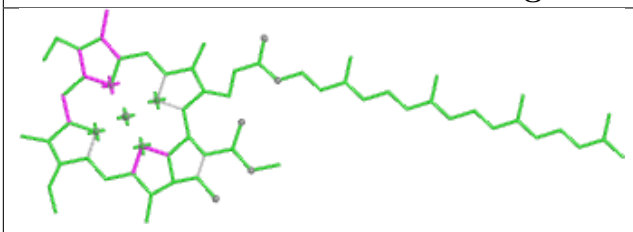
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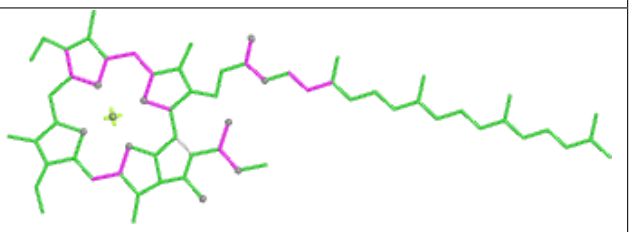
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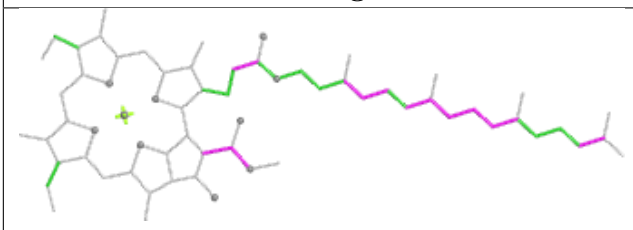
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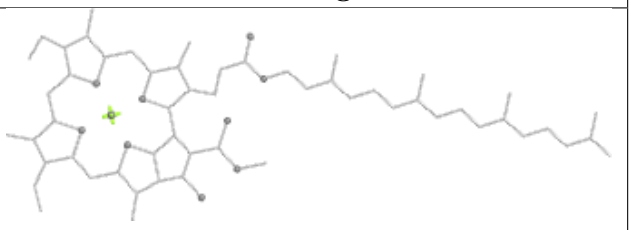
Bond lengths



Bond angles

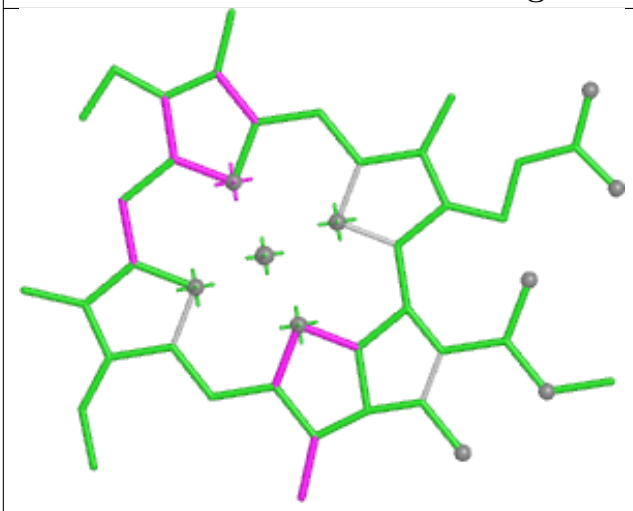


Torsions

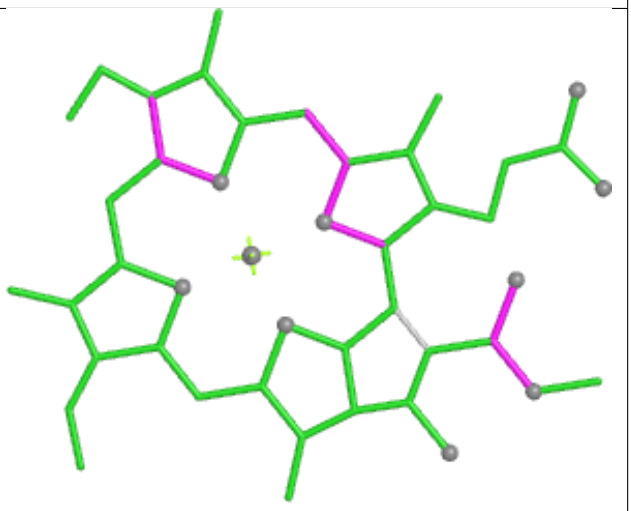


Rings

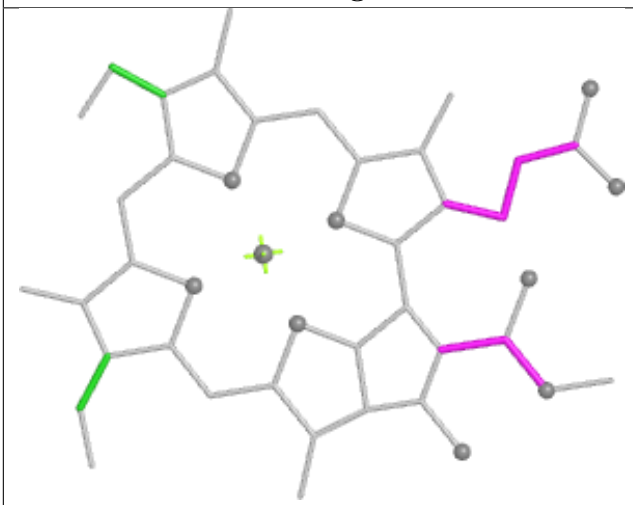
Ligand CLA n 820



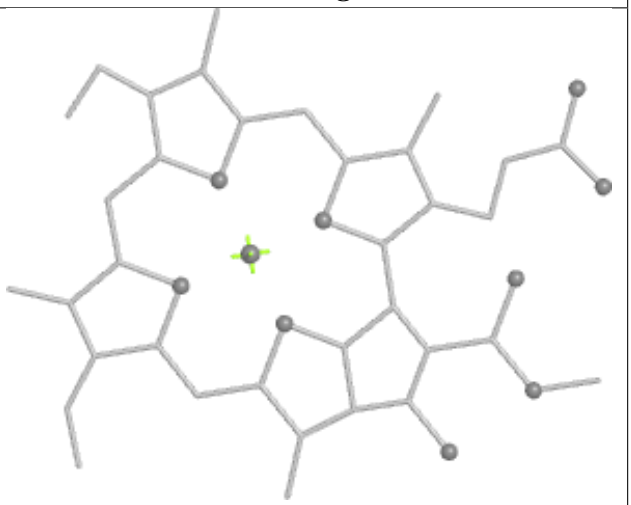
Bond lengths



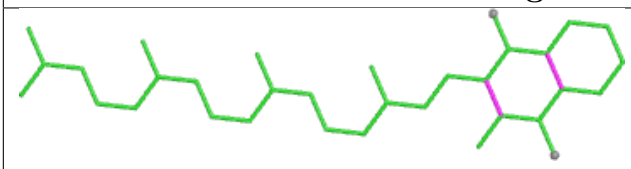
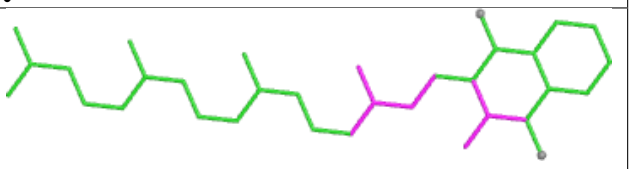
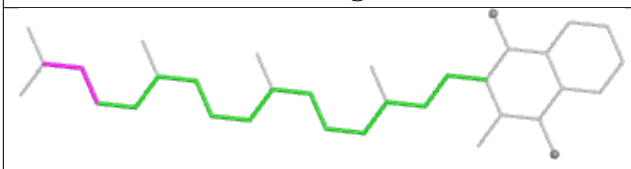
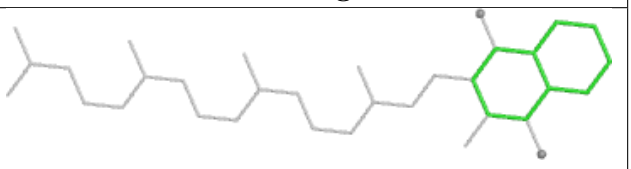
Bond angles

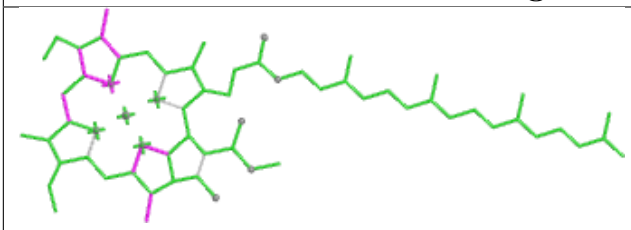
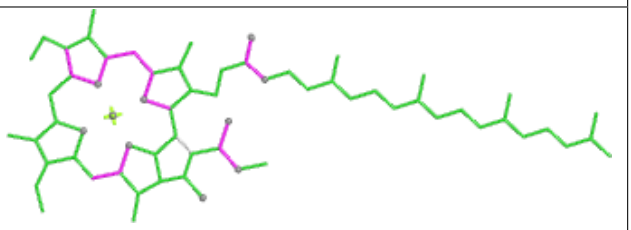
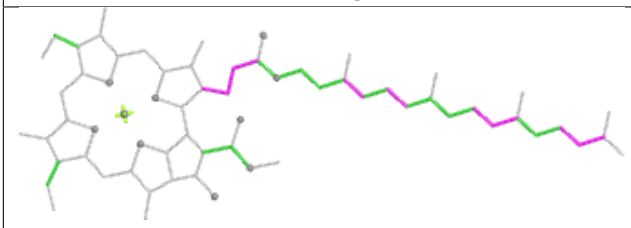
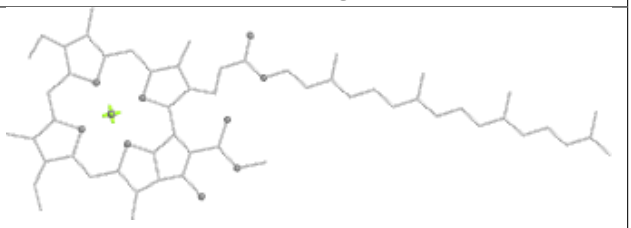


Torsions

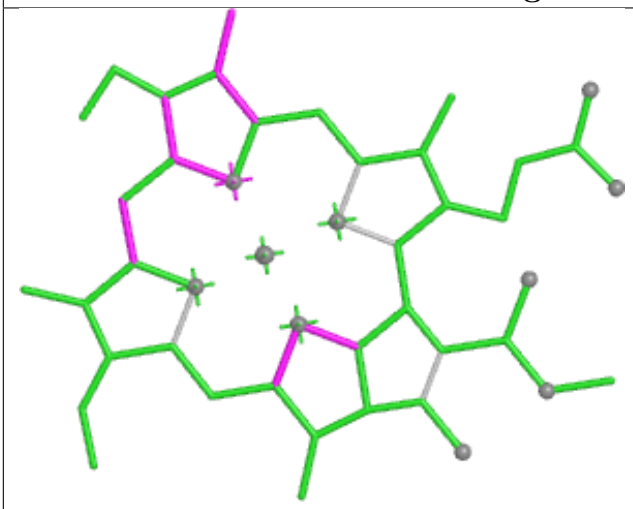


Rings

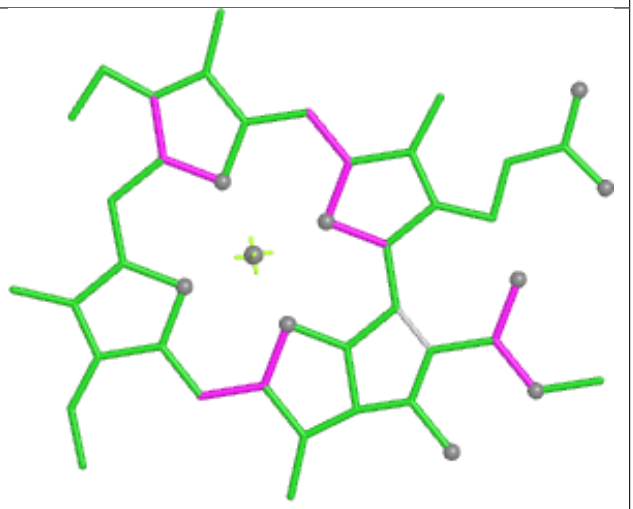
Ligand PQN a 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

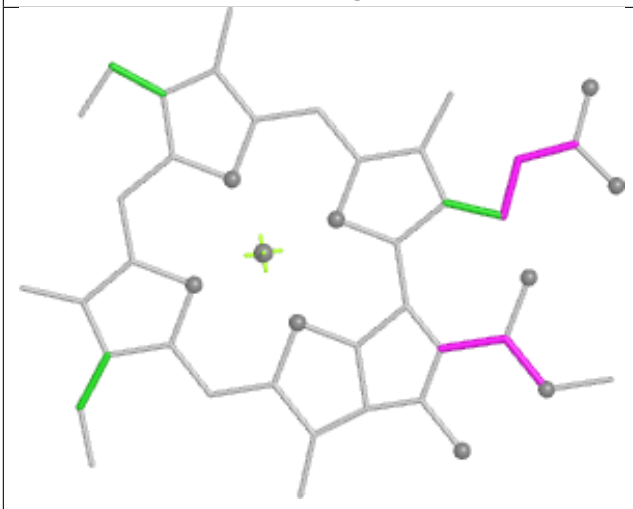
Ligand CLA A 809



Bond lengths



Bond angles

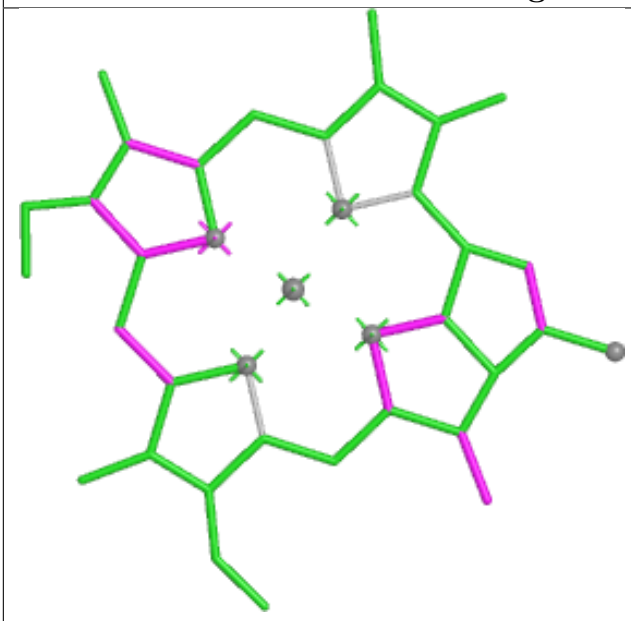


Torsions



Rings

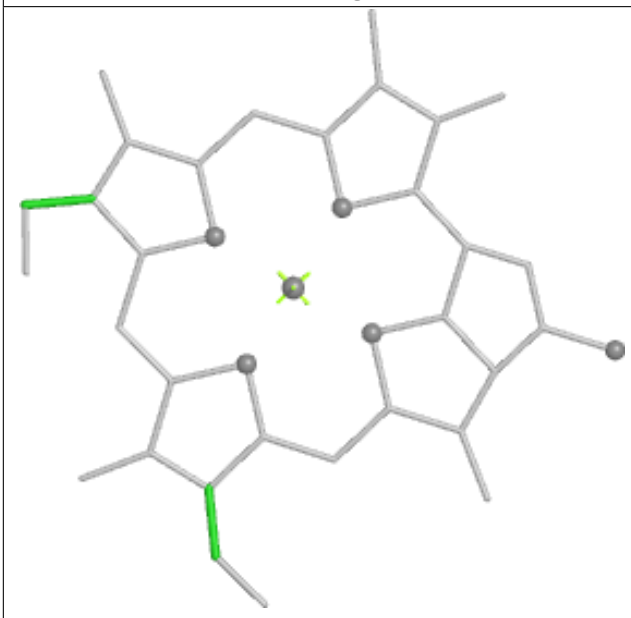
Ligand CLA J 102



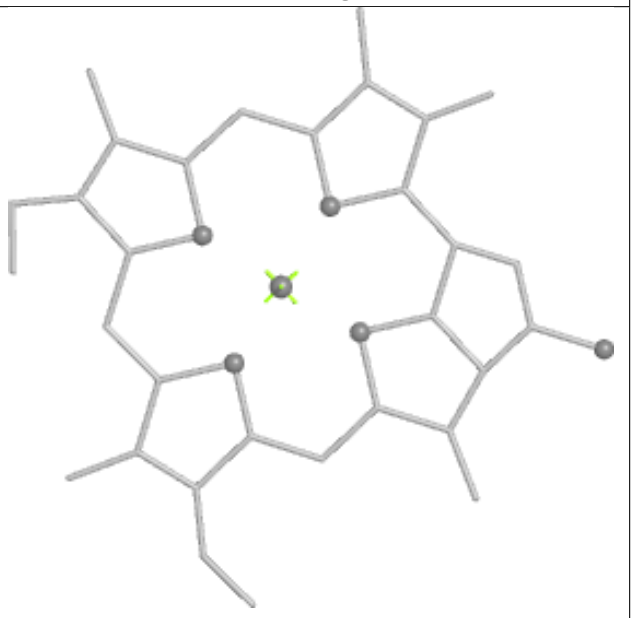
Bond lengths



Bond angles

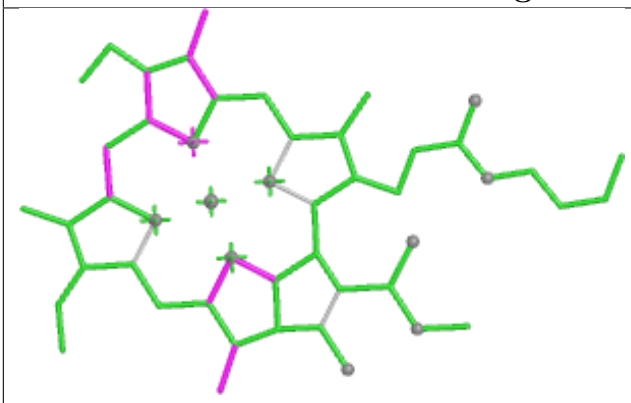


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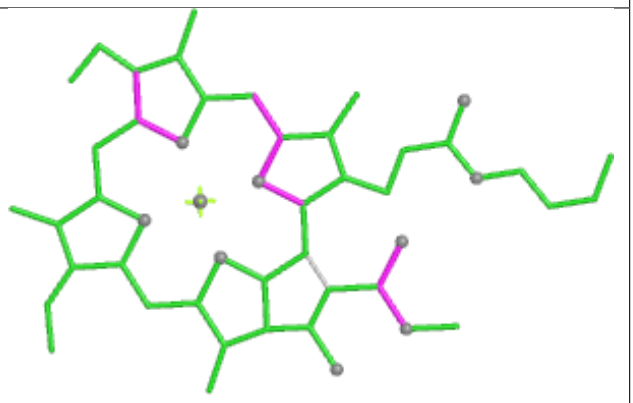


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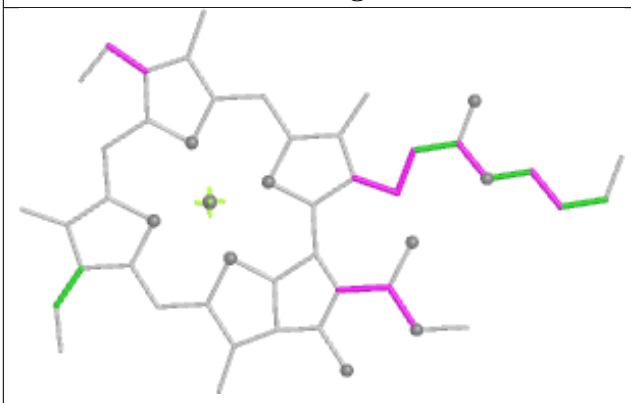
Ligand CLA H 1701



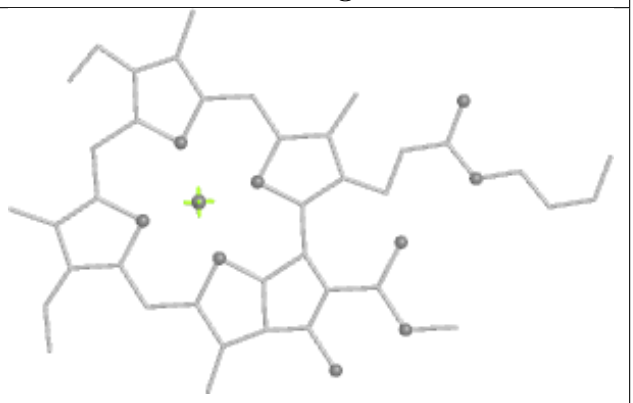
Bond lengths



Bond angles



Torsions

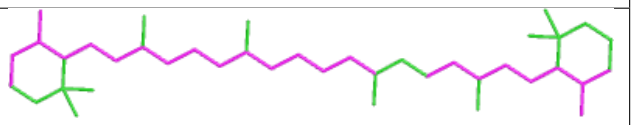


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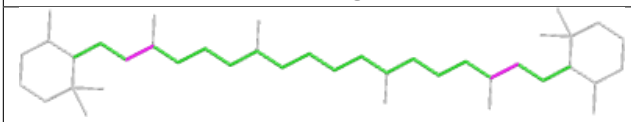
Ligand BCR b 846



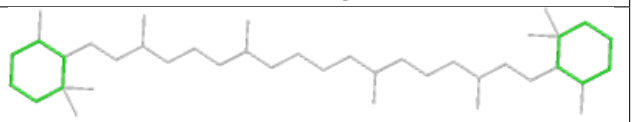
Bond lengths



Bond angles

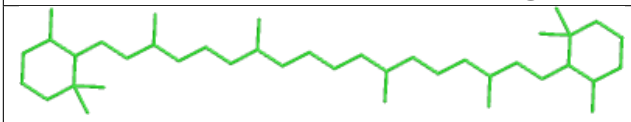


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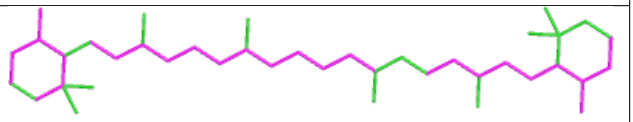


Rings

Ligand BCR A 846



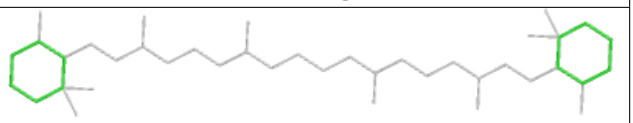
Bond lengths



Bond angles

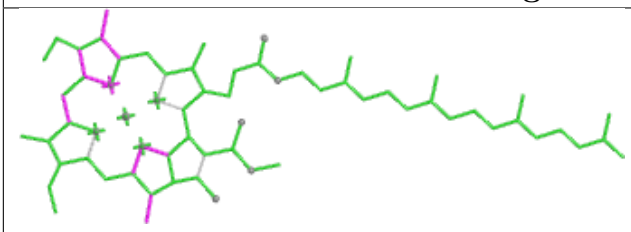


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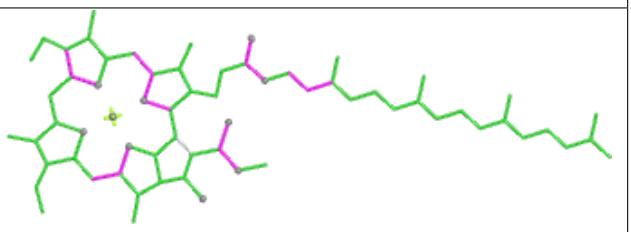


Rings

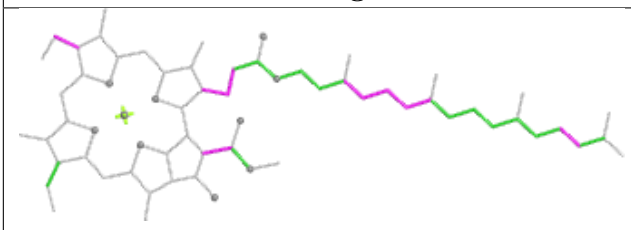
Ligand CLA G 839



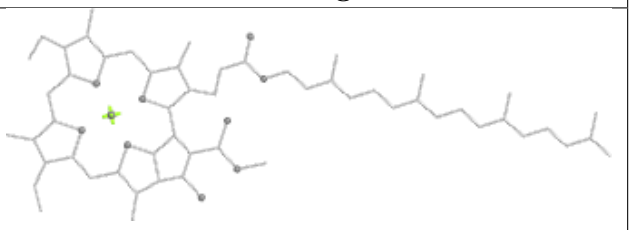
Bond lengths



Bond angles

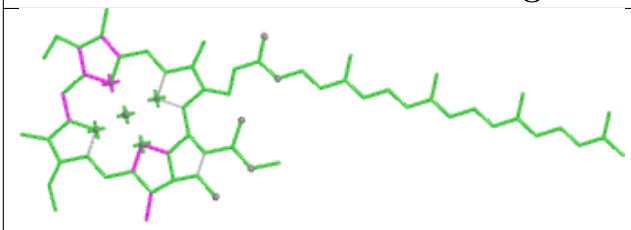


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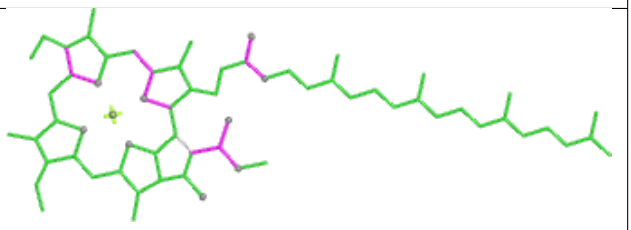


Rings

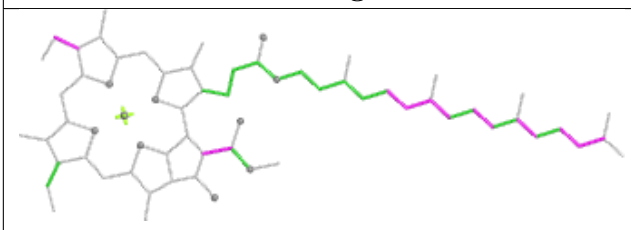
Ligand CLA N 810



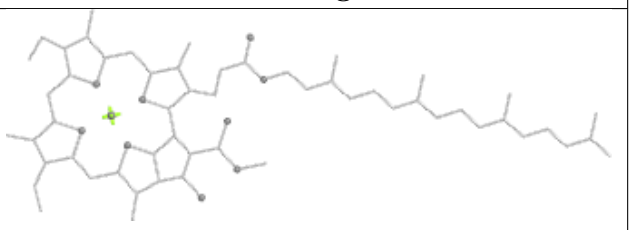
Bond lengths



Bond angles

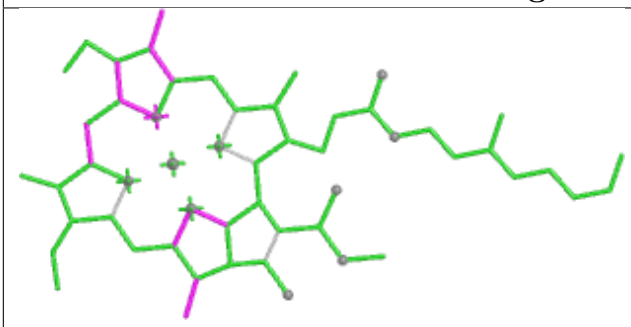


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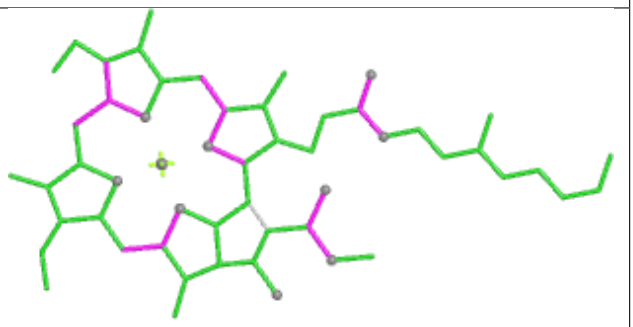


Rings

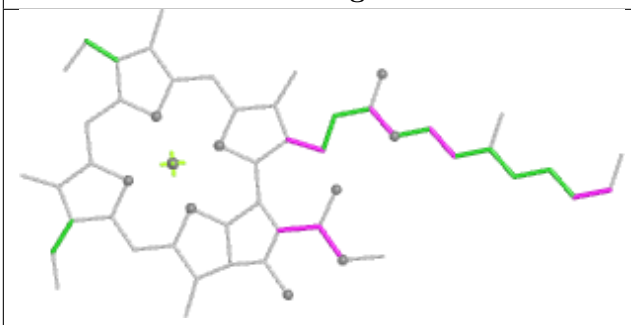
Ligand CLA a 818



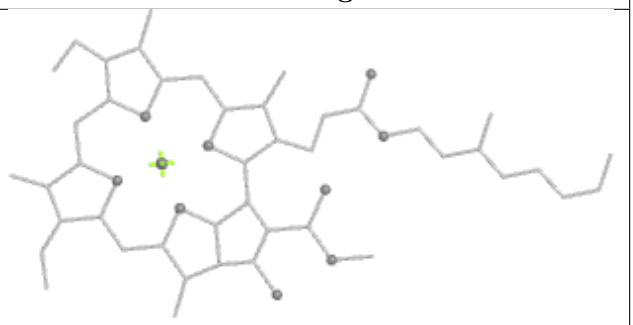
Bond lengths



Bond angles

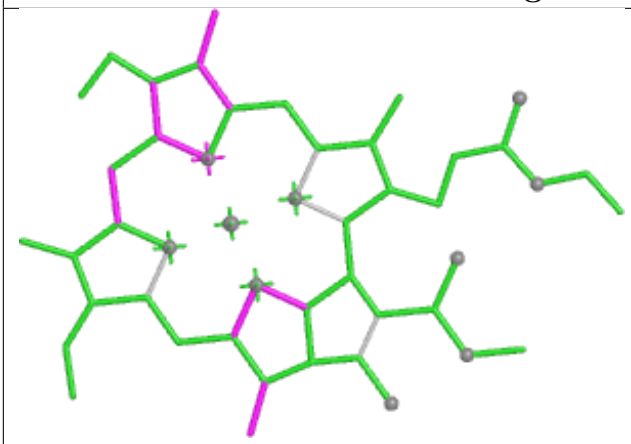


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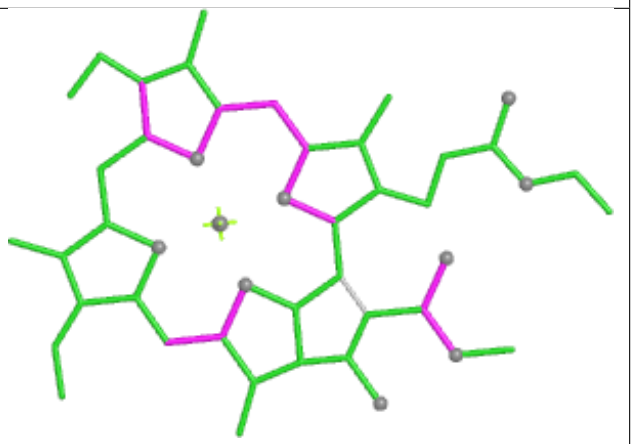


Rings

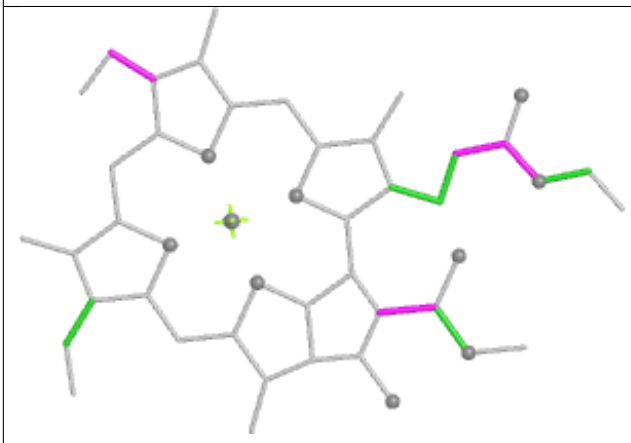
Ligand CLA B 839



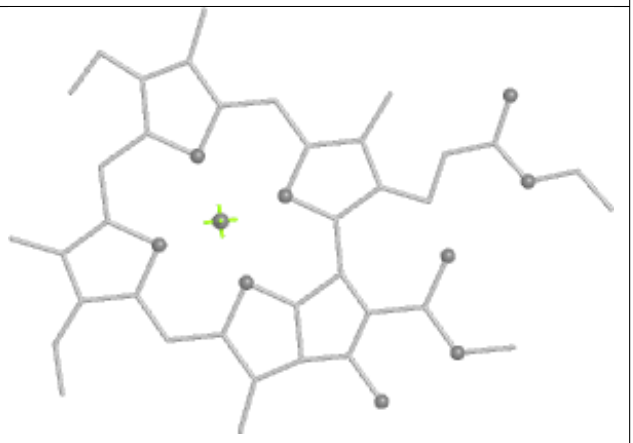
Bond lengths



Bond angles

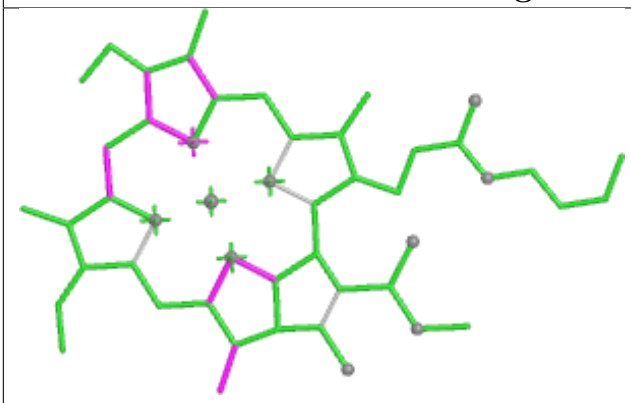


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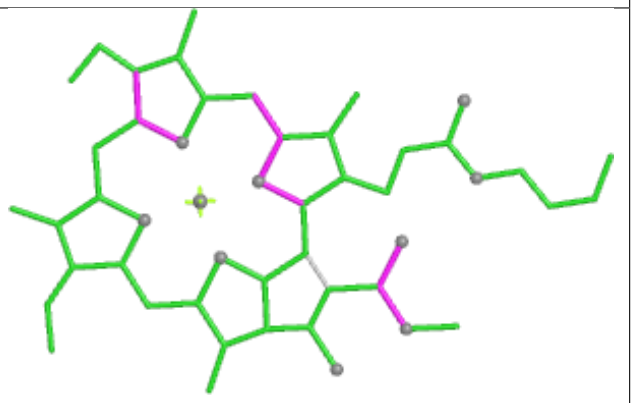


Rings

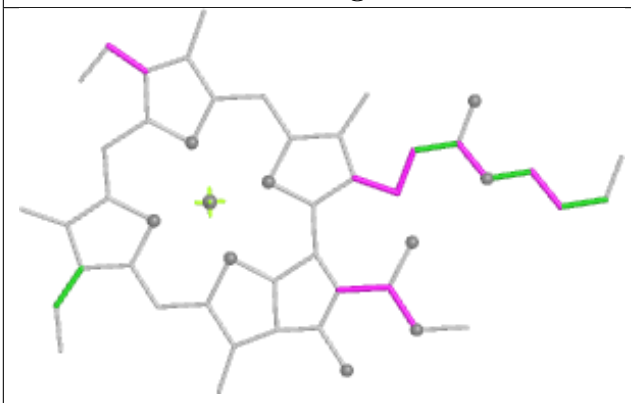
Ligand CLA X 1701



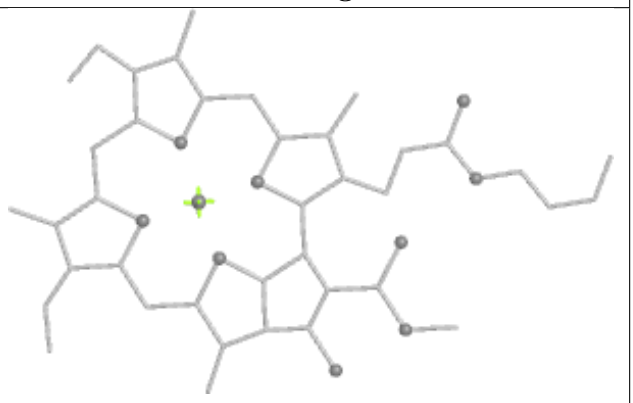
Bond lengths



Bond angles

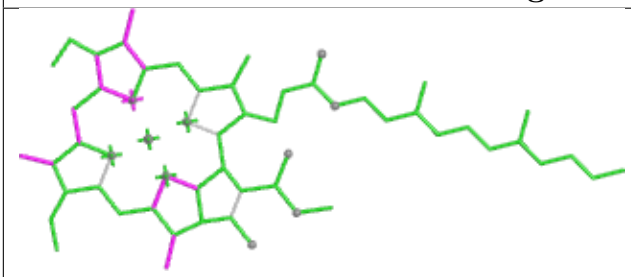


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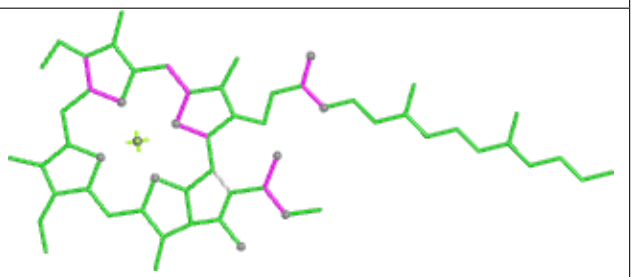


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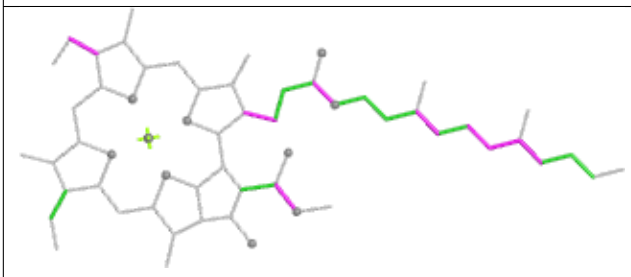
Ligand CLA n 850



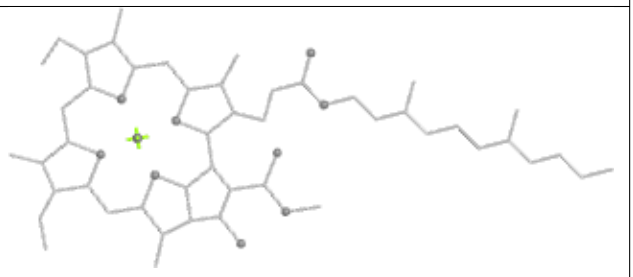
Bond lengths



Bond angles

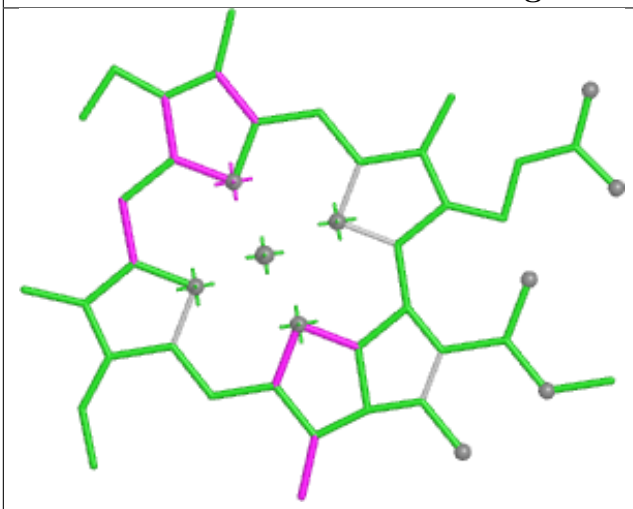


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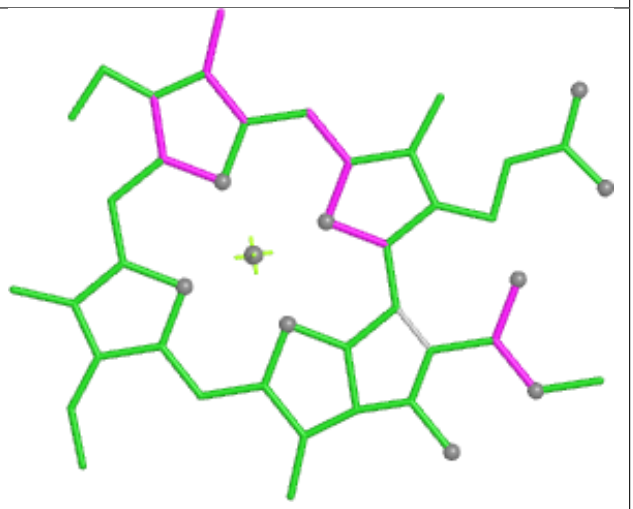


Rings

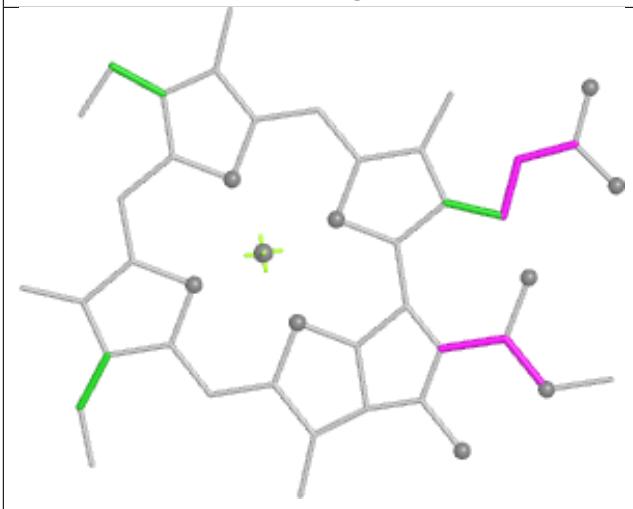
Ligand CLA B 836



Bond lengths



Bond angles

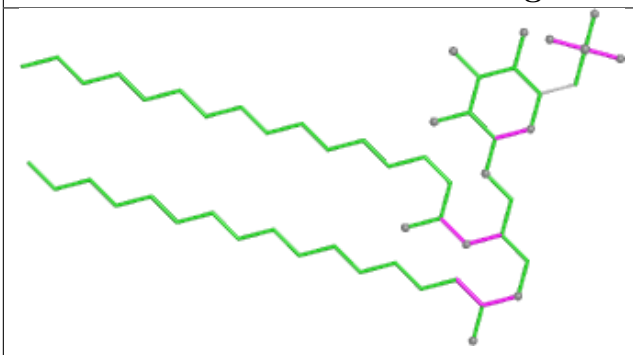


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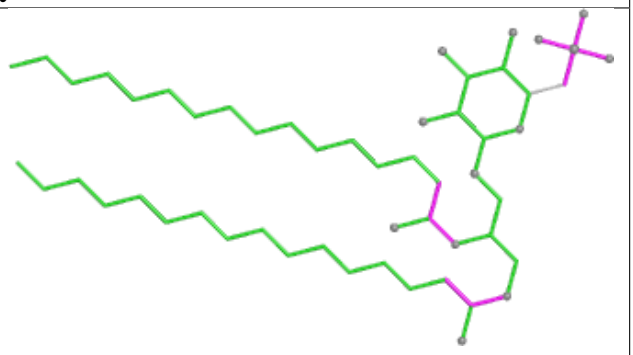


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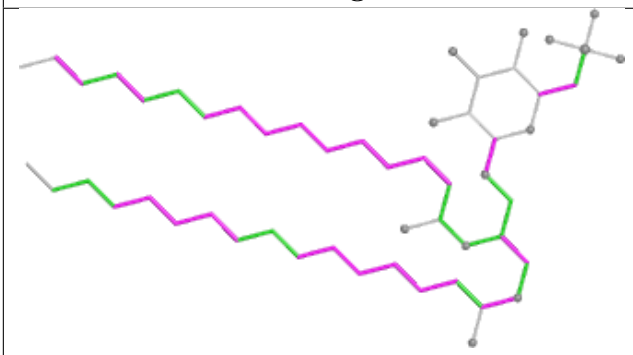
Ligand SQD w 202



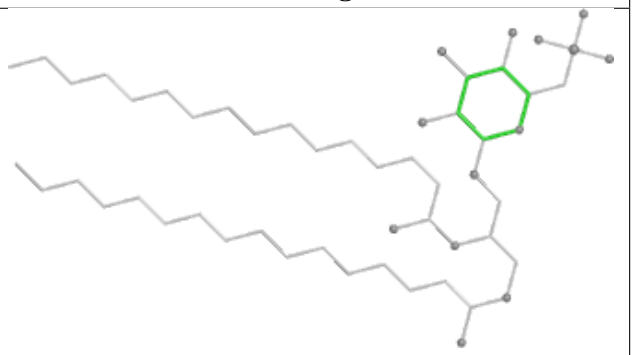
Bond lengths



Bond angles

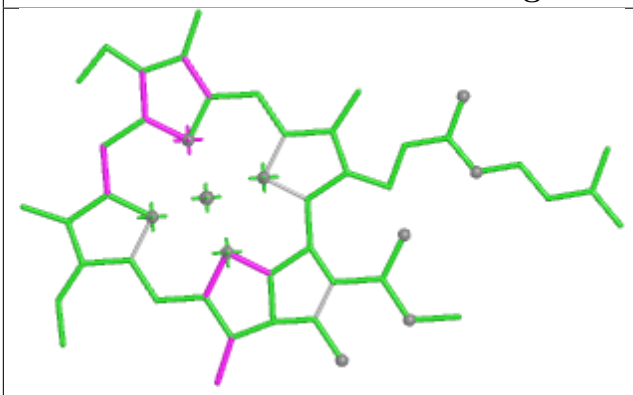


Torsions

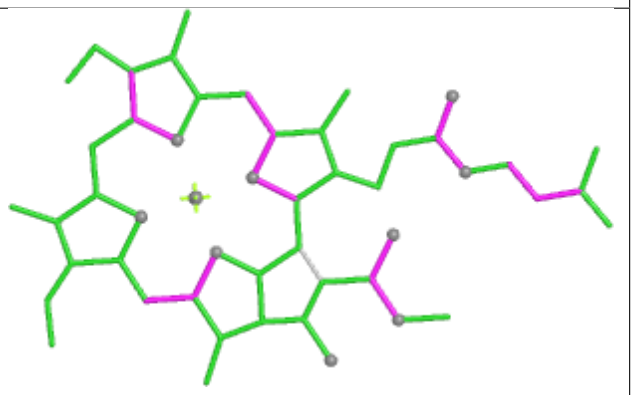


Rings

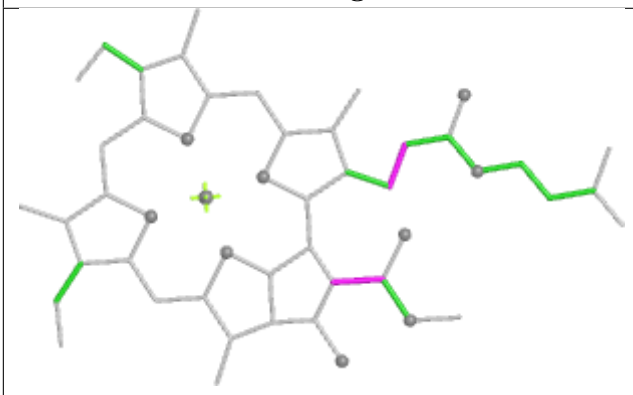
Ligand CLA N 816



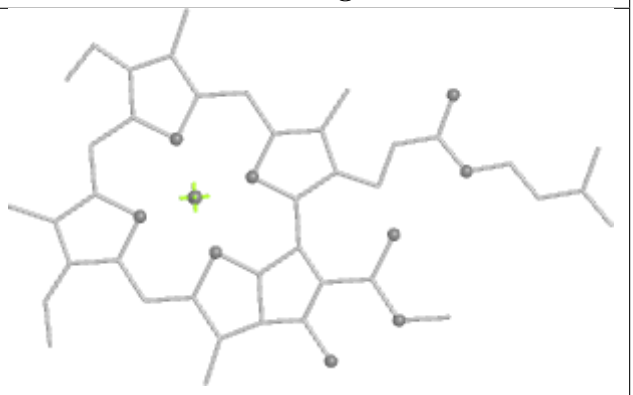
Bond lengths



Bond angles

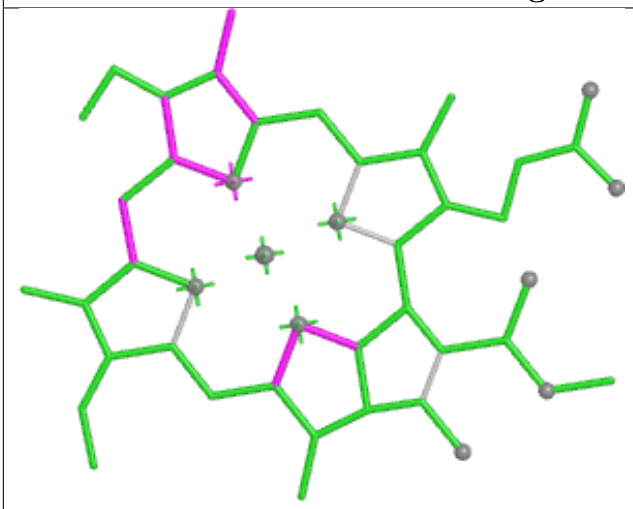


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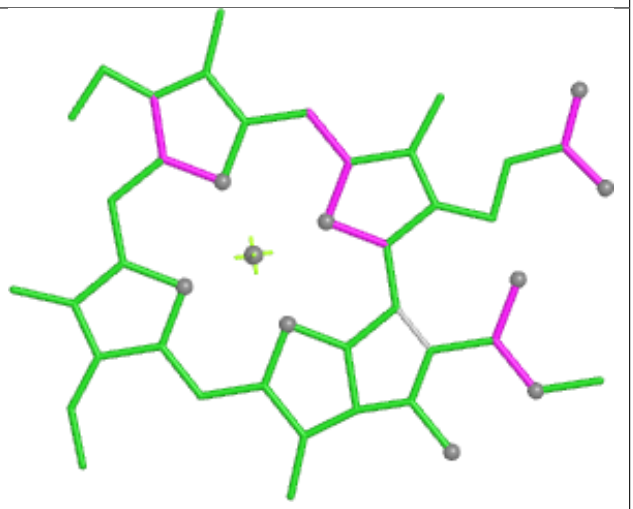


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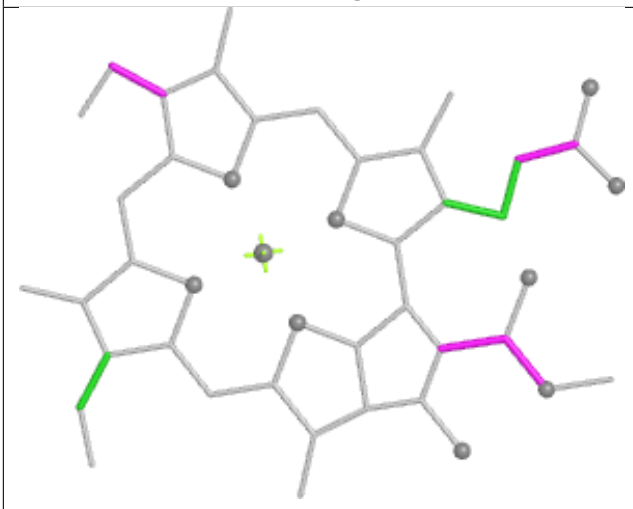
Ligand CLA a 822



Bond lengths



Bond angles

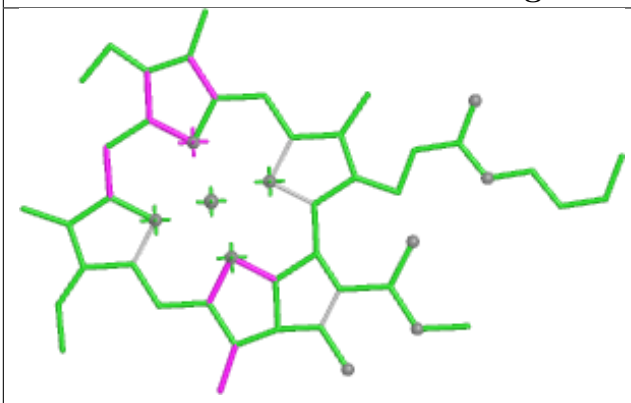


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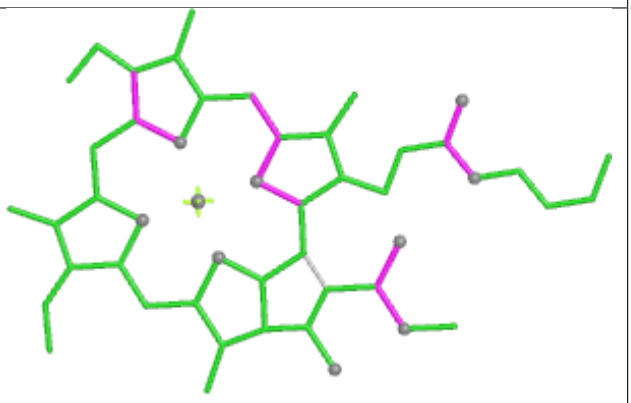


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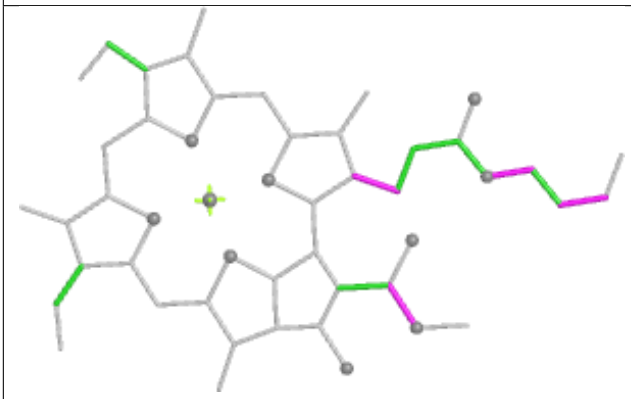
Ligand CLA B 816



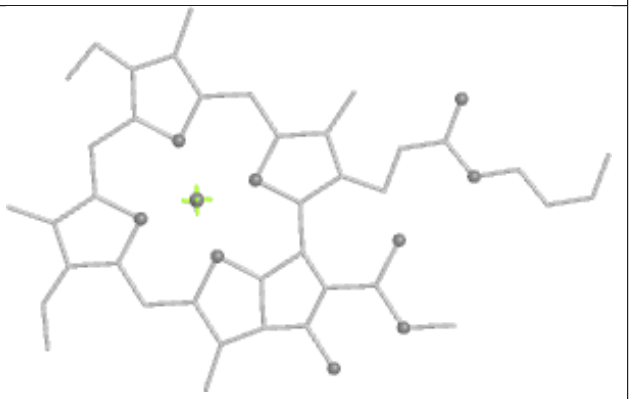
Bond lengths



Bond angles



Torsions

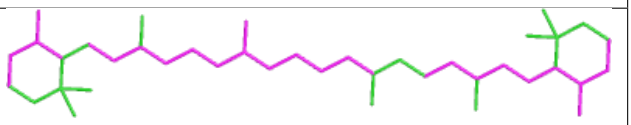


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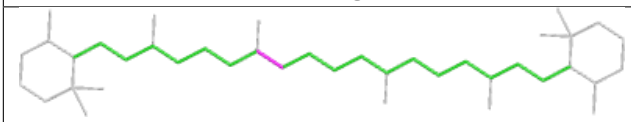
Ligand BCR F 203



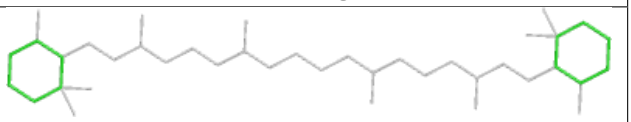
Bond lengths



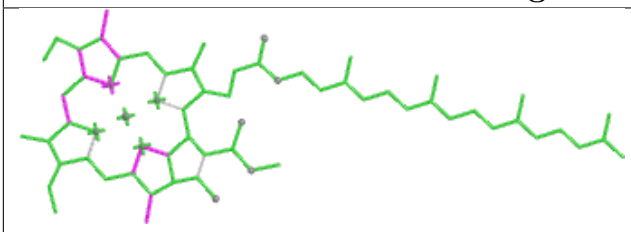
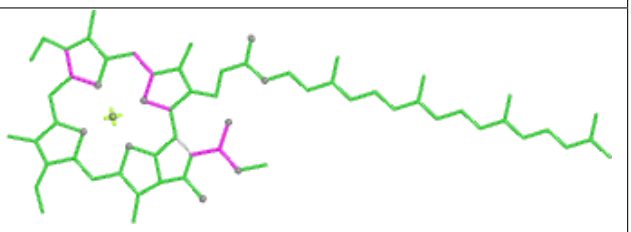
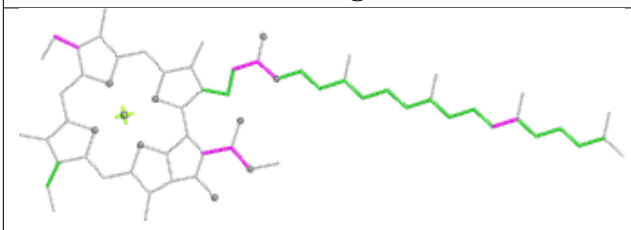
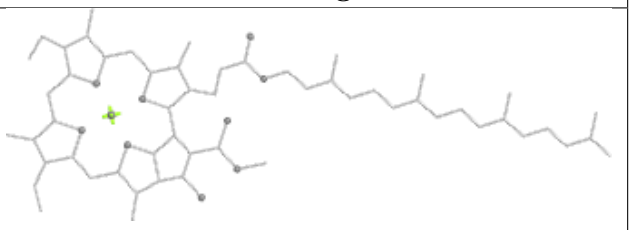
Bond angles

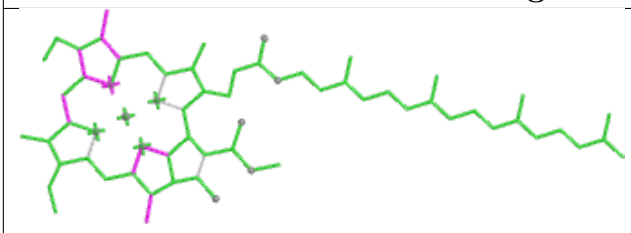
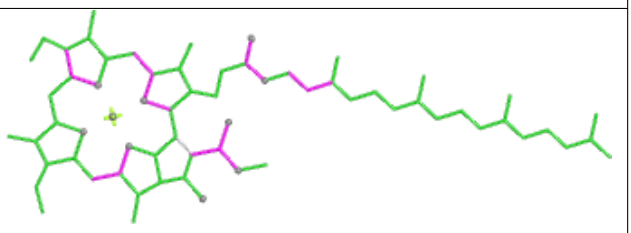
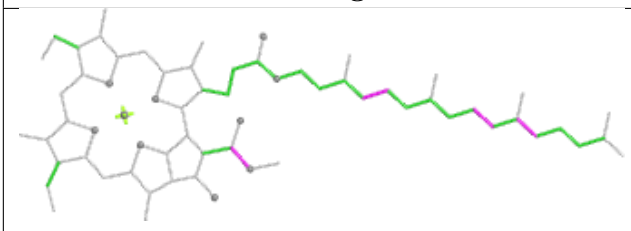
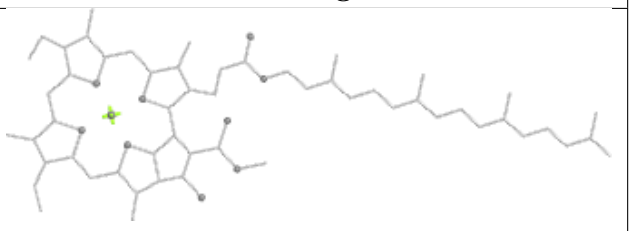


Torsions

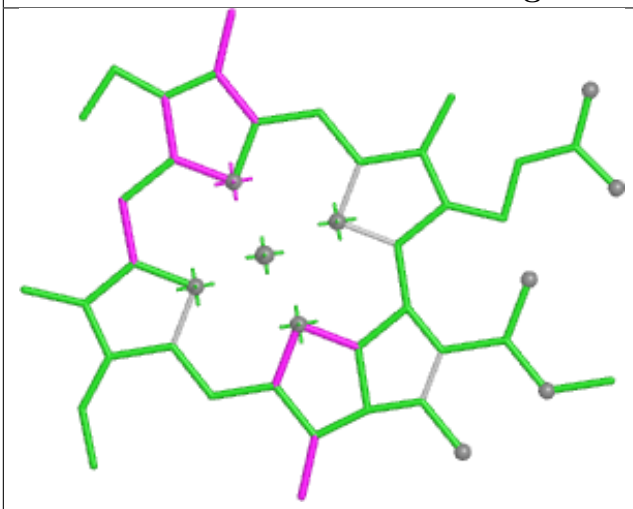


Rings

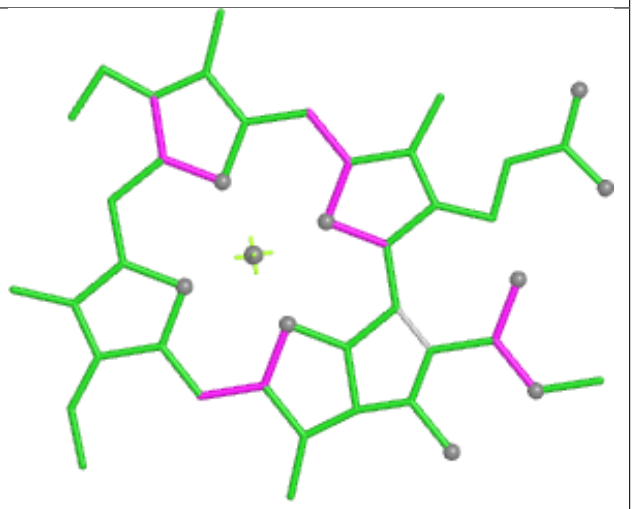
Ligand CLA a 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

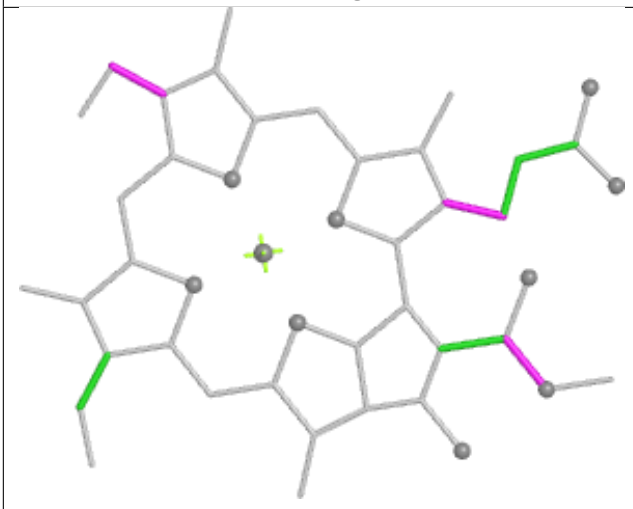
Ligand CLA A 823



Bond lengths



Bond angles

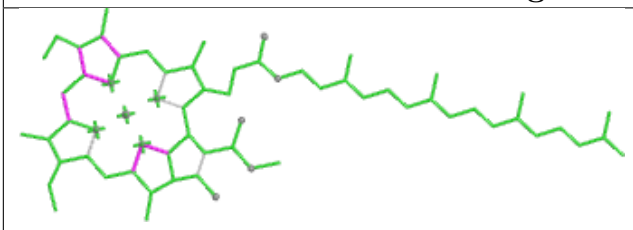


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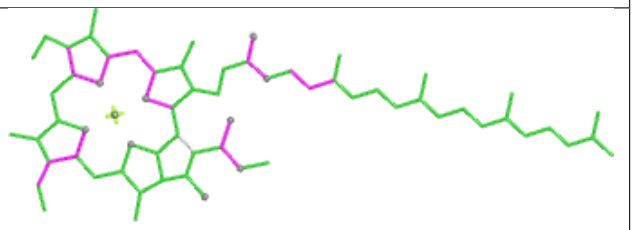


Rings

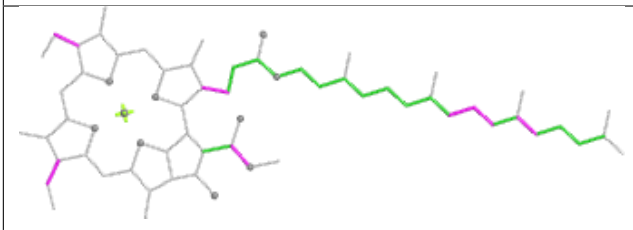
Ligand CLA b 804



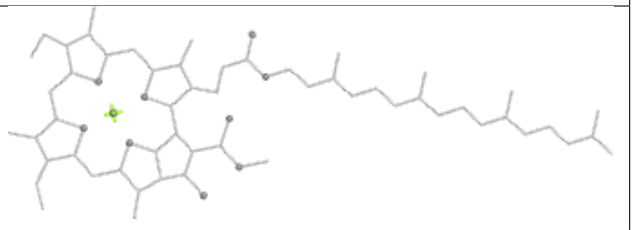
Bond lengths



Bond angles

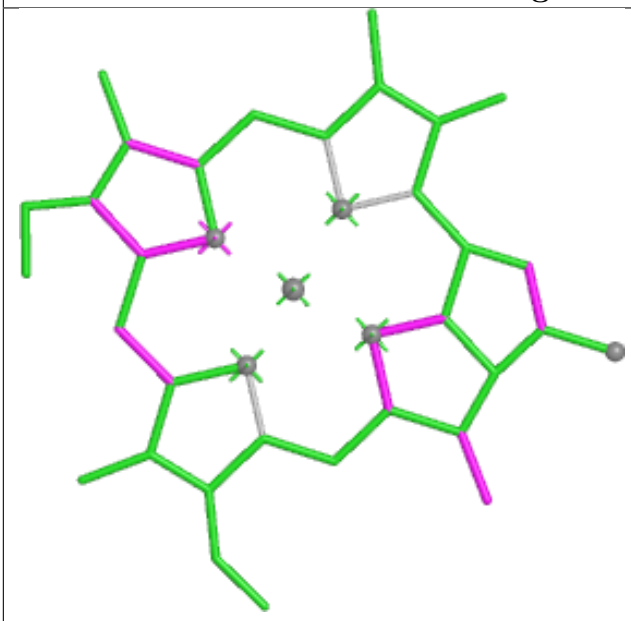


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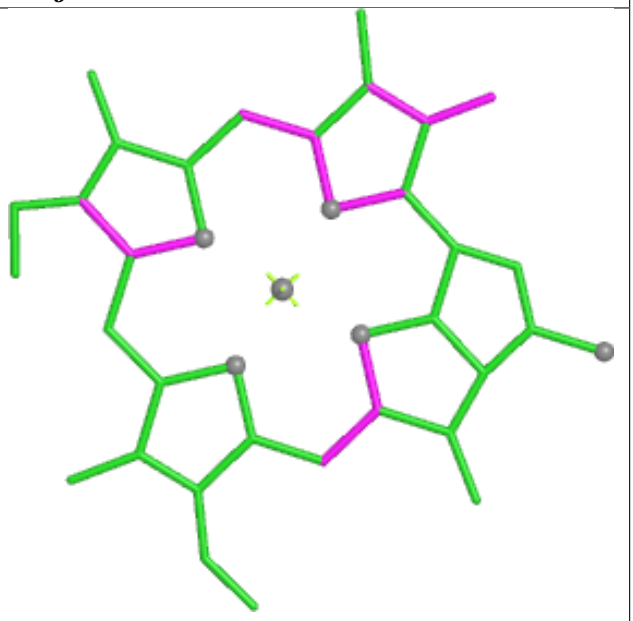


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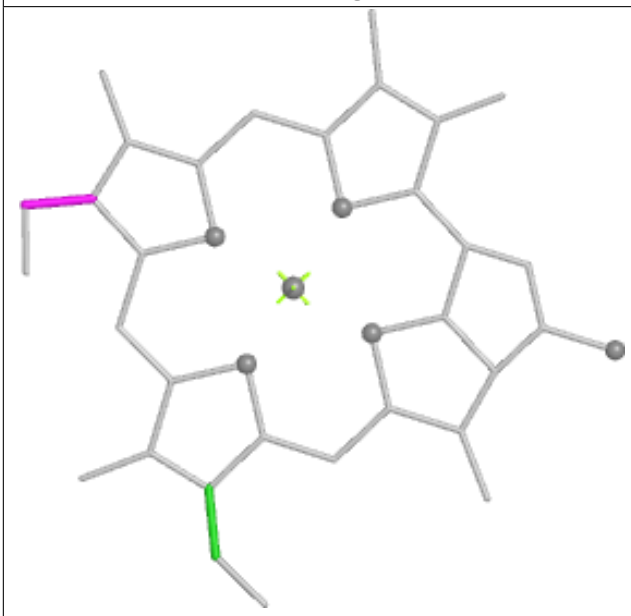
Ligand CLA j 102



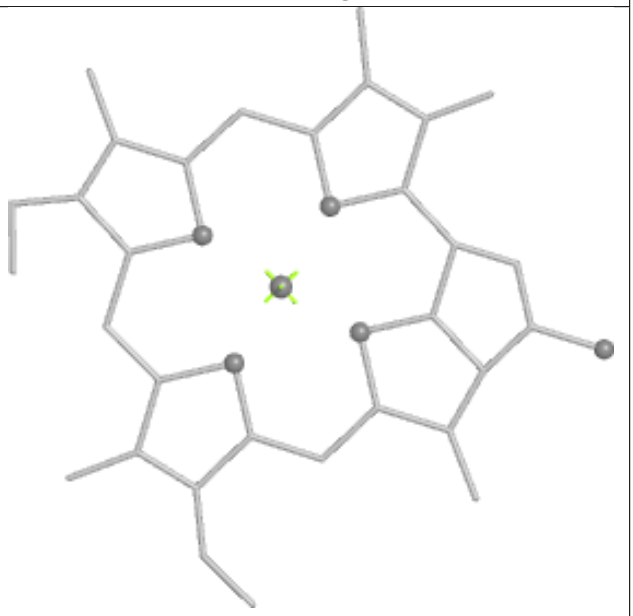
Bond lengths



Bond angles

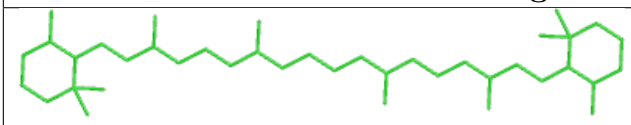


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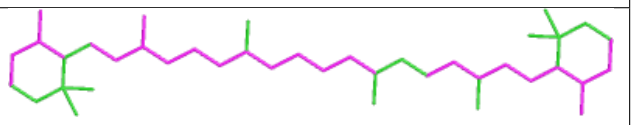


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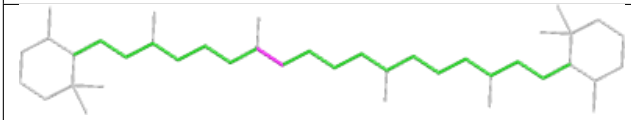
Ligand BCR f 203



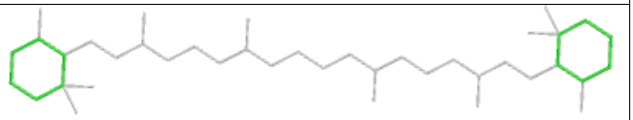
Bond lengths



Bond angles

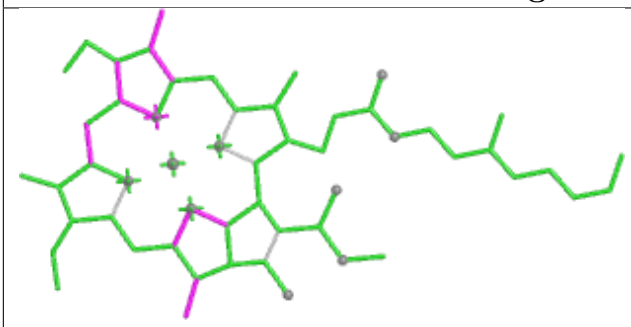


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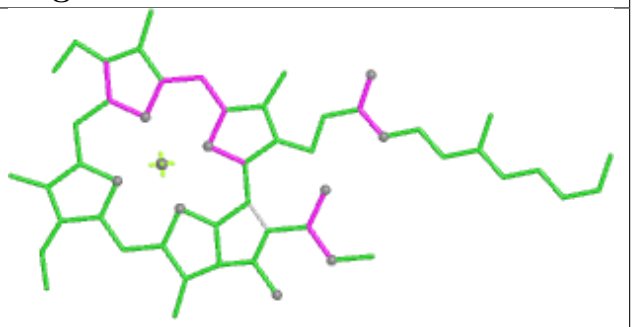


Rings

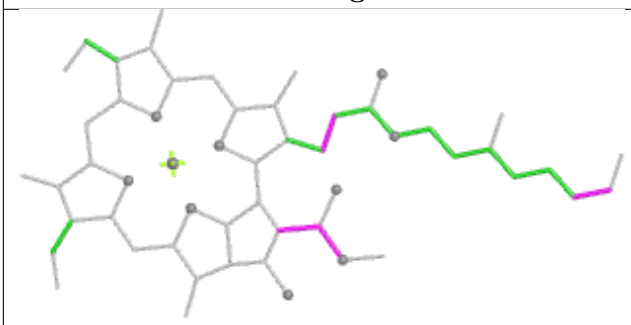
Ligand CLA g 833



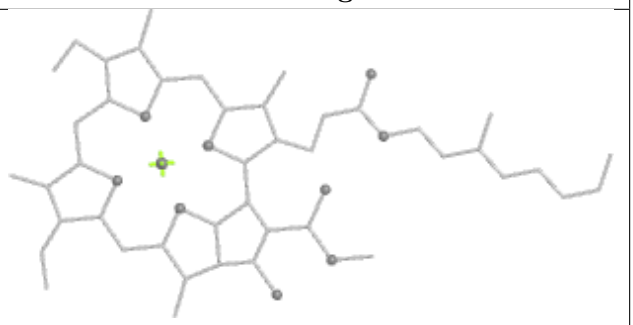
Bond lengths



Bond angles

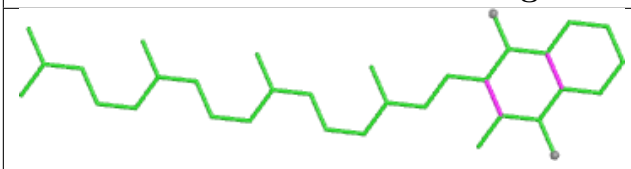


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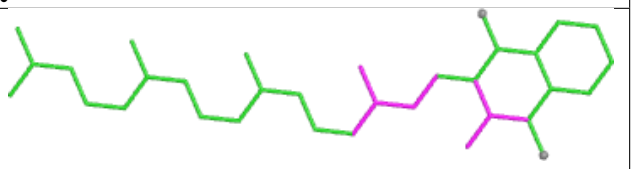


Rings

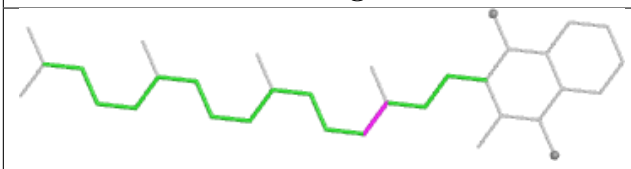
Ligand PQN N 843



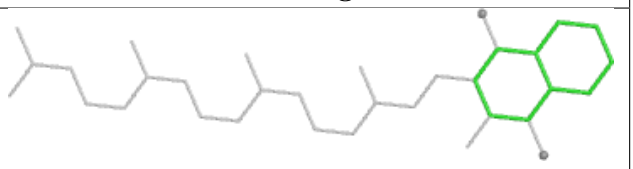
Bond lengths



Bond angles

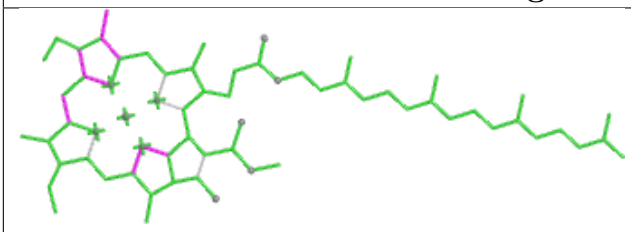


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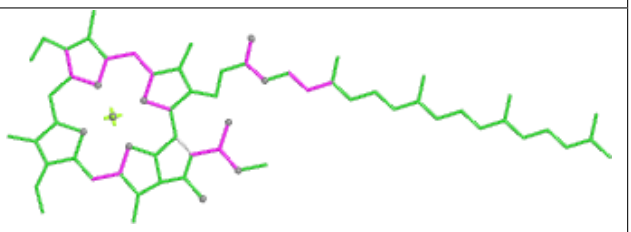


Rings

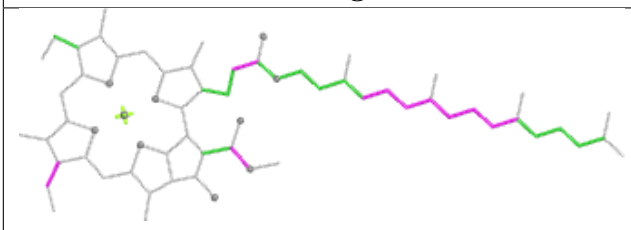
Ligand CLA n 832



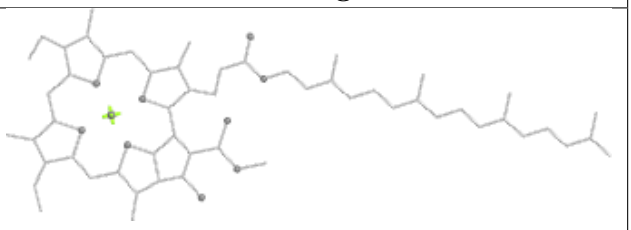
Bond lengths



Bond angles



Torsions

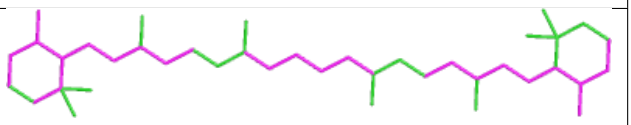


Rings

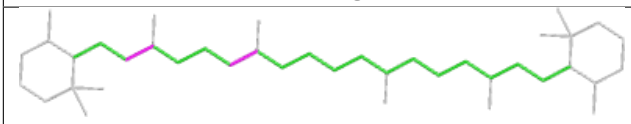
Ligand BCR l 206



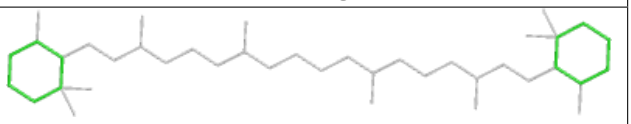
Bond lengths



Bond angles

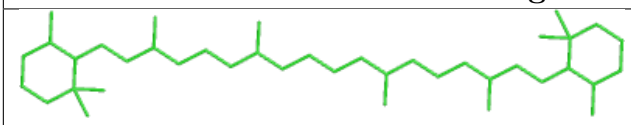


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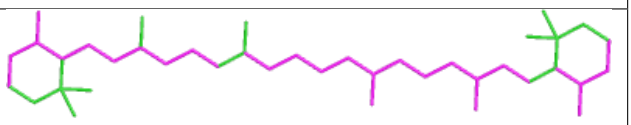


Rings

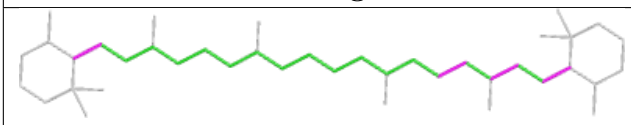
Ligand BCR t 104



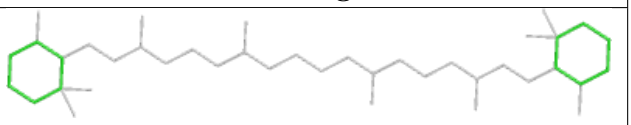
Bond lengths



Bond angles

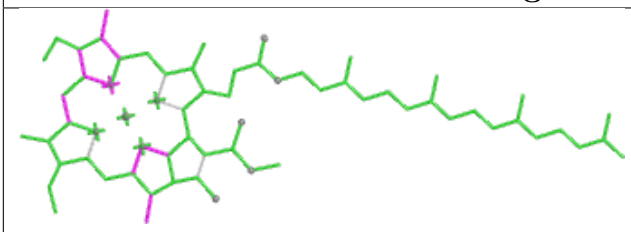


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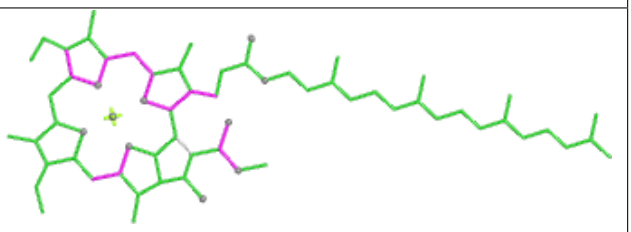


Rings

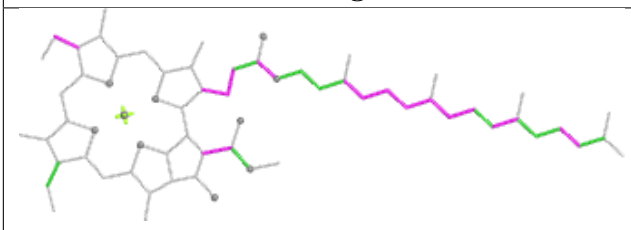
Ligand CLA A 807



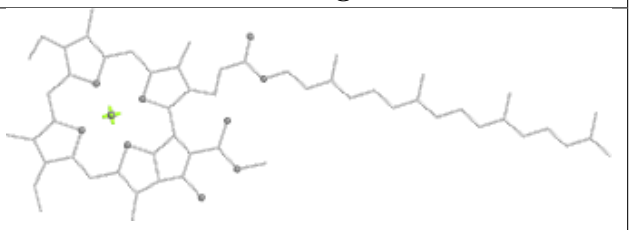
Bond lengths



Bond angles

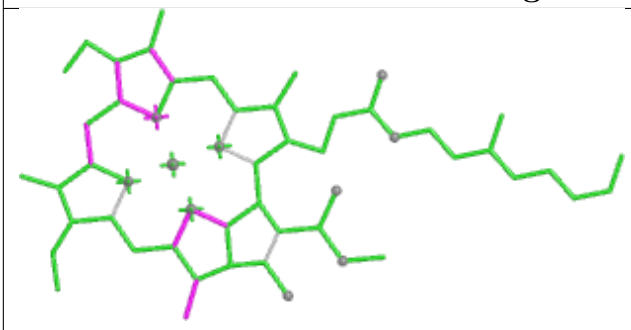


Torsions

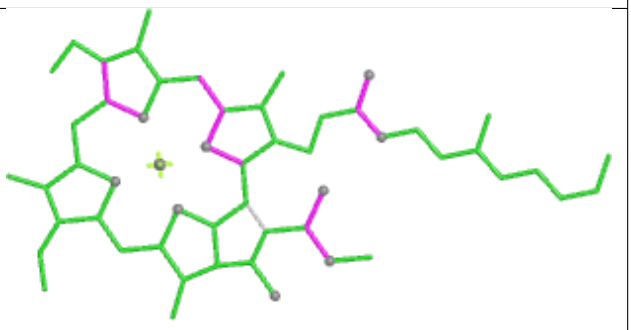


Rings

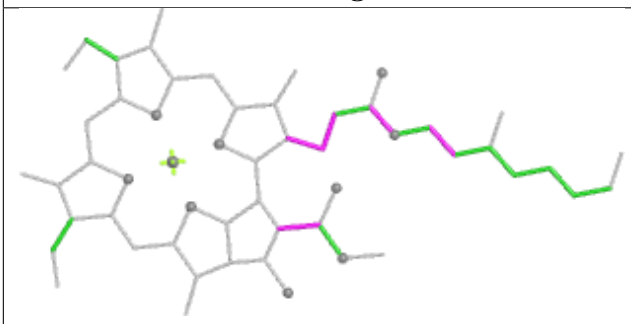
Ligand CLA G 819



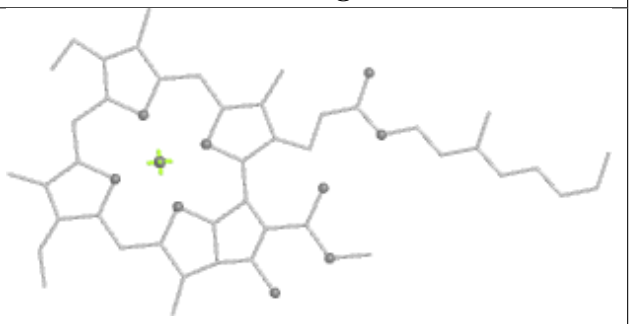
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Bond angles

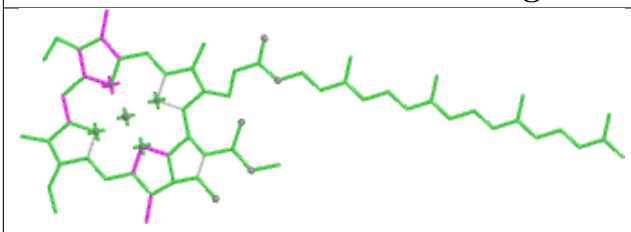


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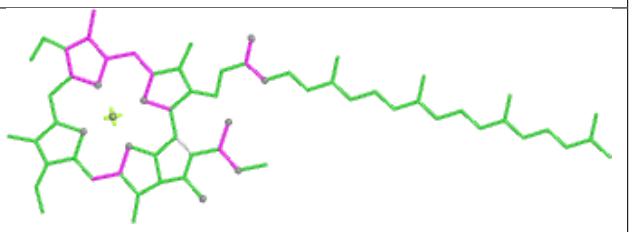


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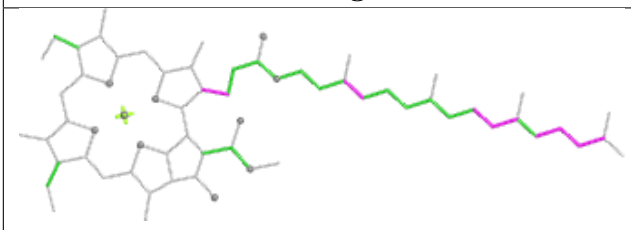
Ligand CLA G 831



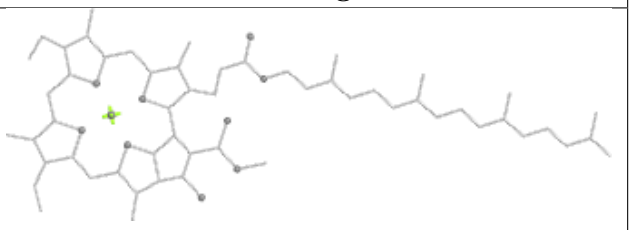
Bond lengths



Bond angles

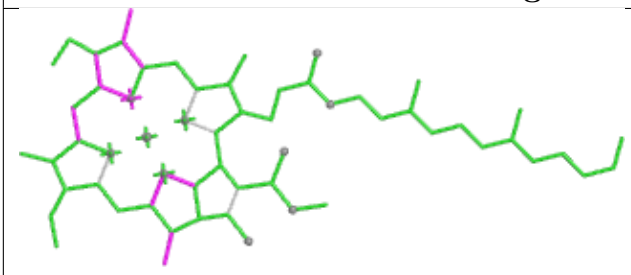


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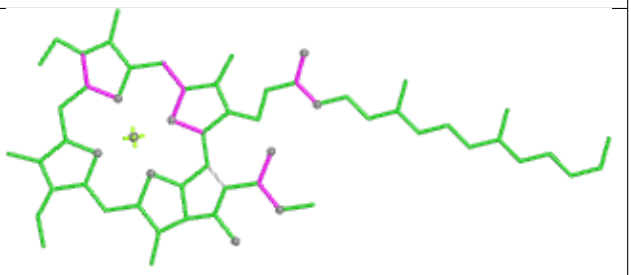


Rings

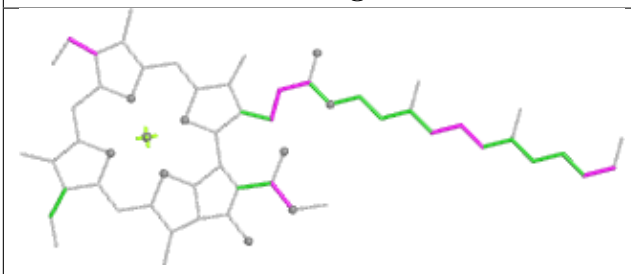
Ligand CLA A 816



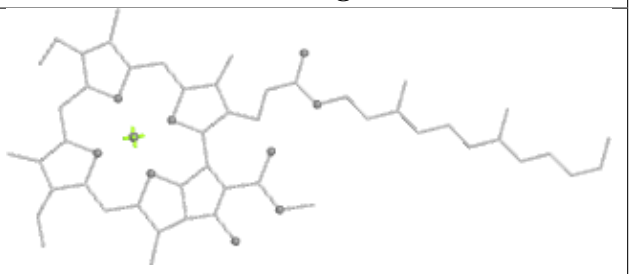
Bond lengths



Bond angles

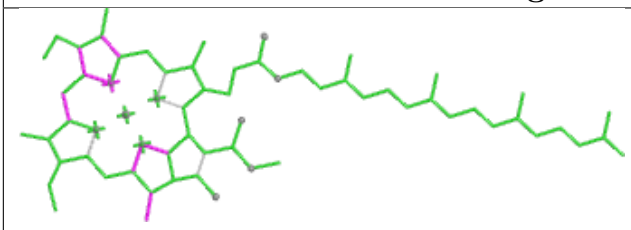


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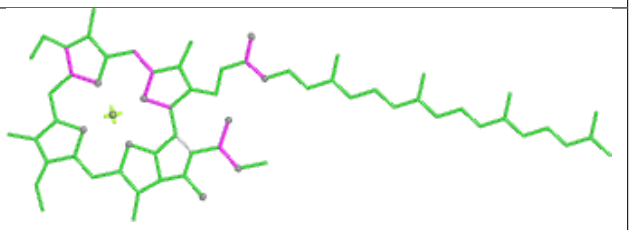


Rings

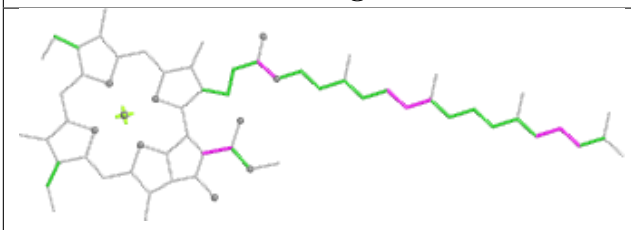
Ligand CLA b 824



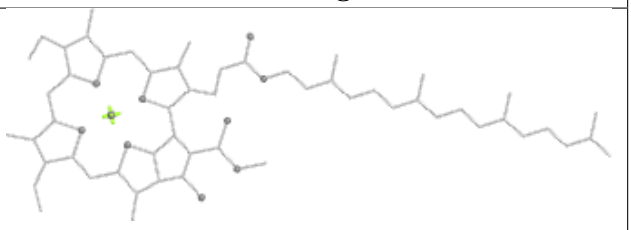
Bond lengths



Bond angles

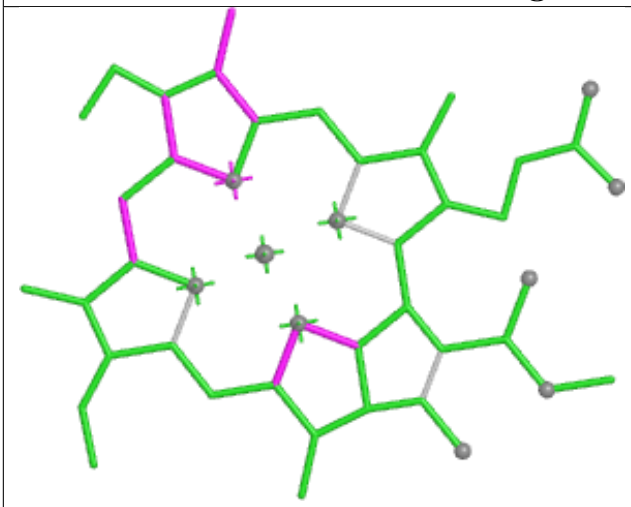


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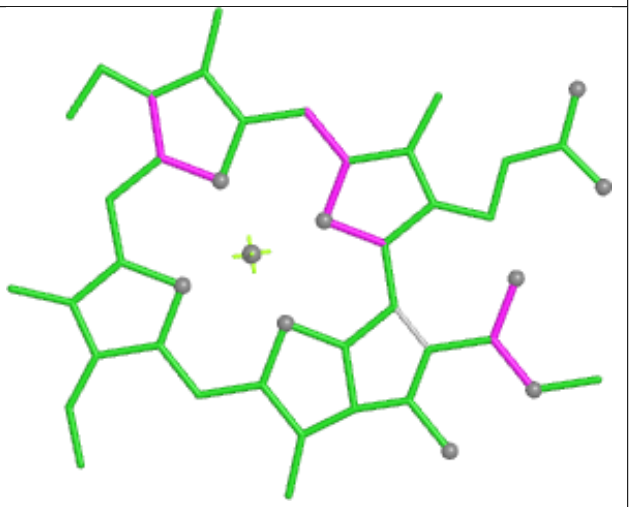


Rings

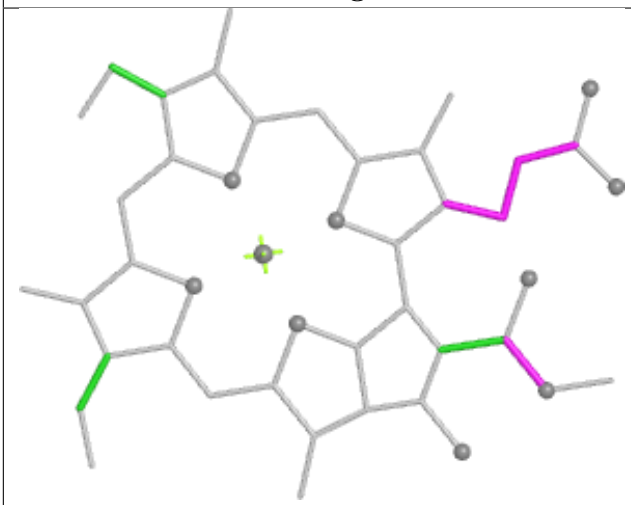
Ligand CLA a 808



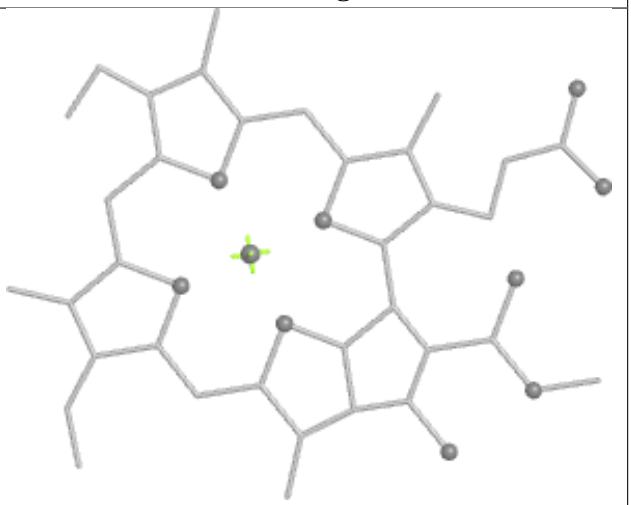
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Bond angles

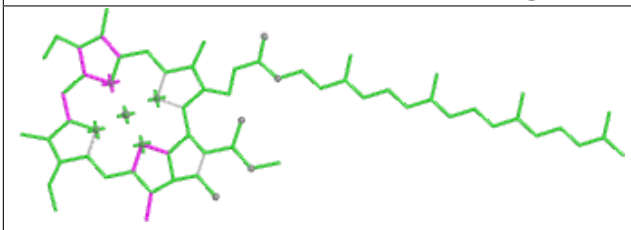


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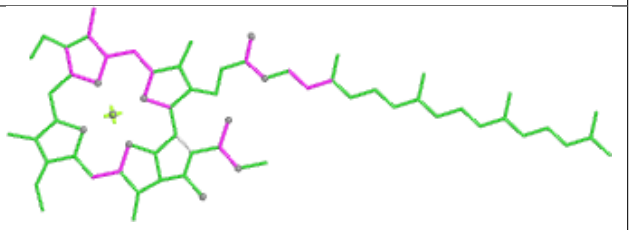


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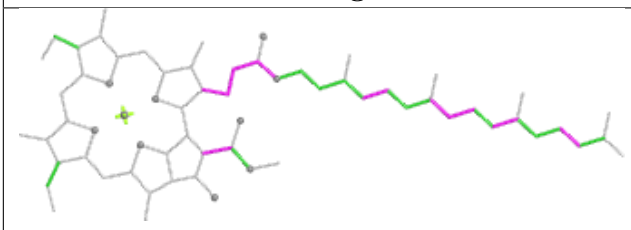
Ligand CLA G 807



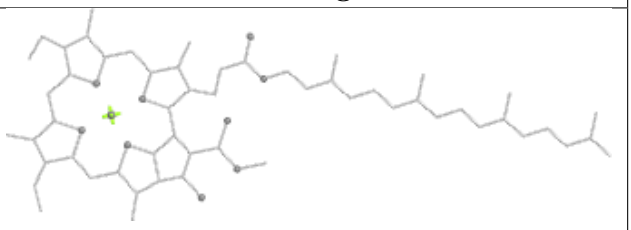
Bond lengths



Bond angles

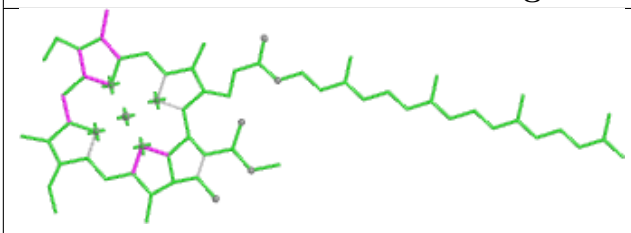


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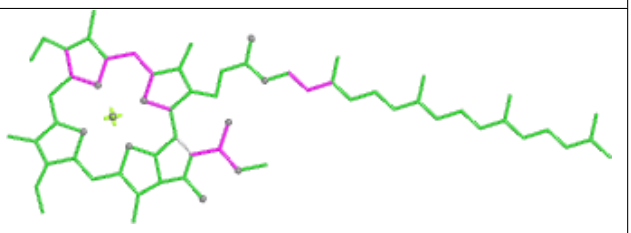


Rings

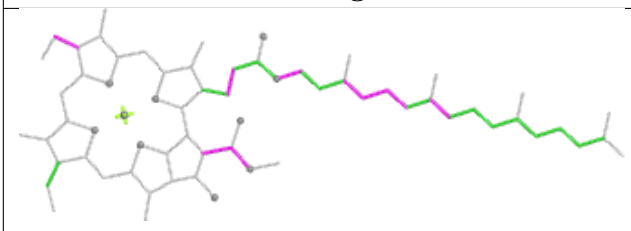
Ligand CLA A 853



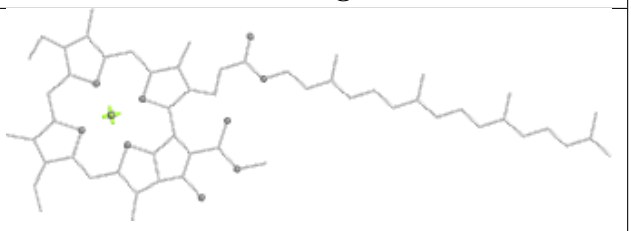
Bond lengths



Bond angles

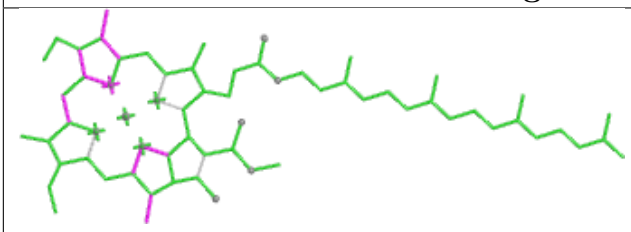


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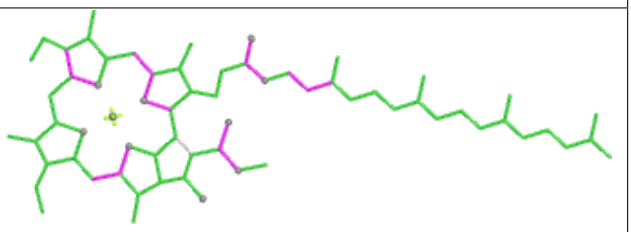


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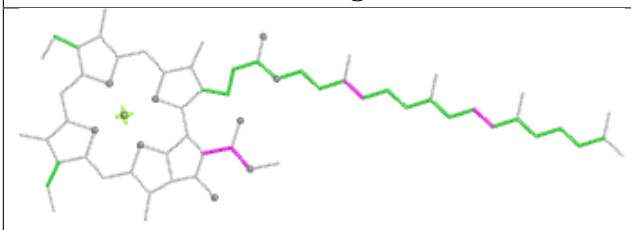
Ligand CLA N 839



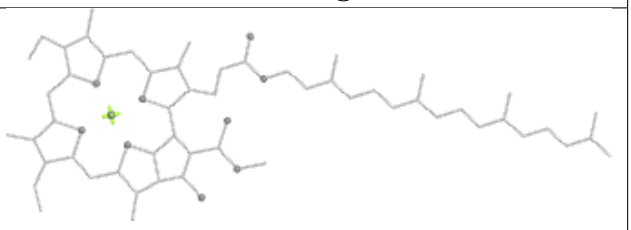
Bond lengths



Bond angles

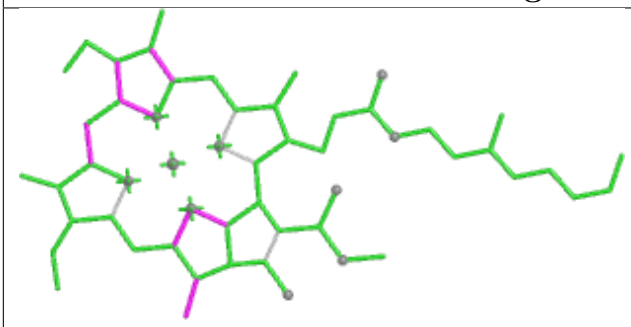


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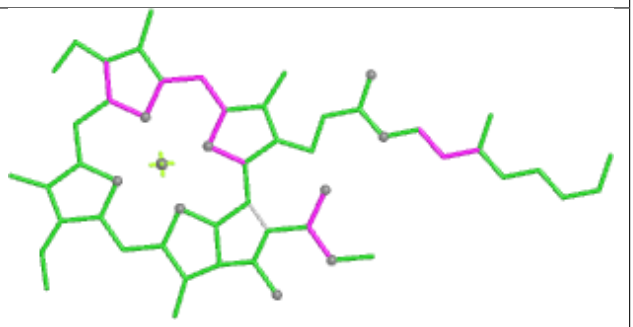


Rings

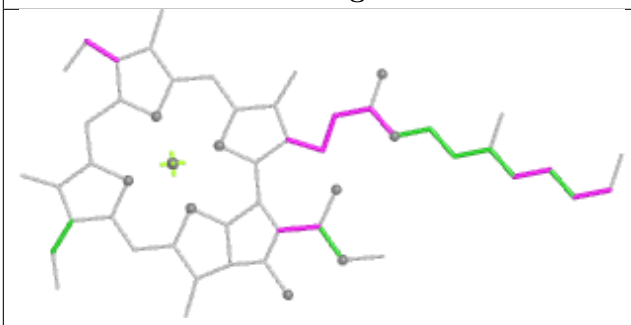
Ligand CLA B 813



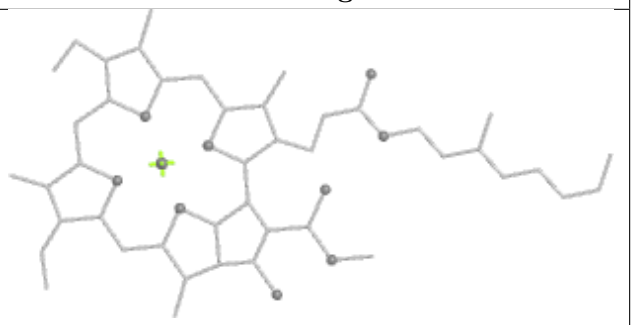
Bond lengths



Bond angles

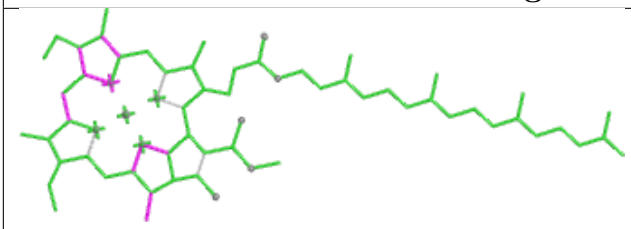


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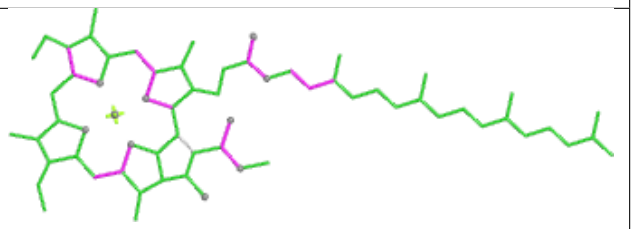


Rings

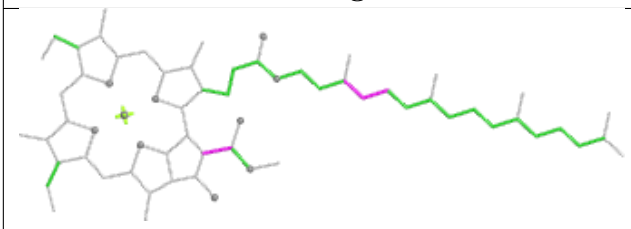
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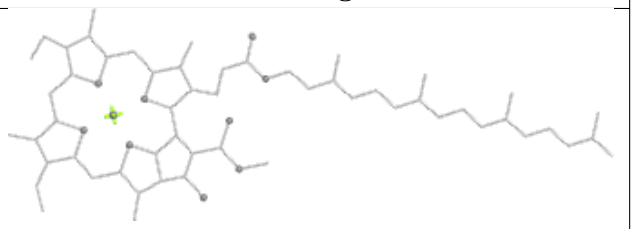
Bond lengths



Bond angles

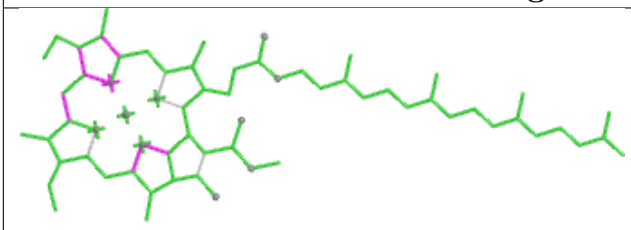


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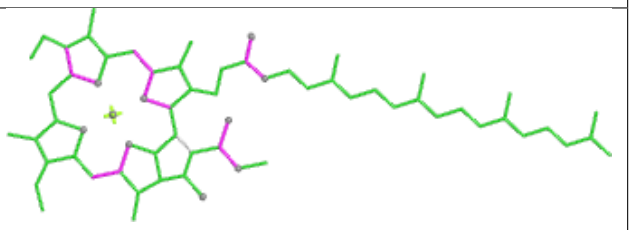


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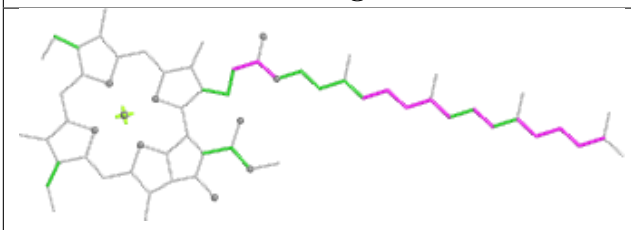
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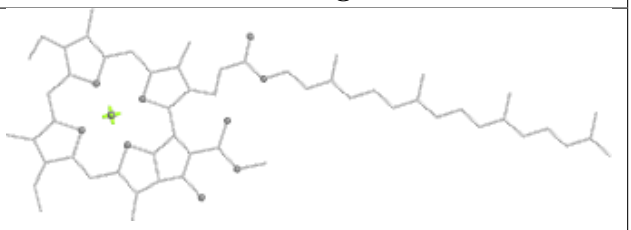
Bond lengths



Bond angles

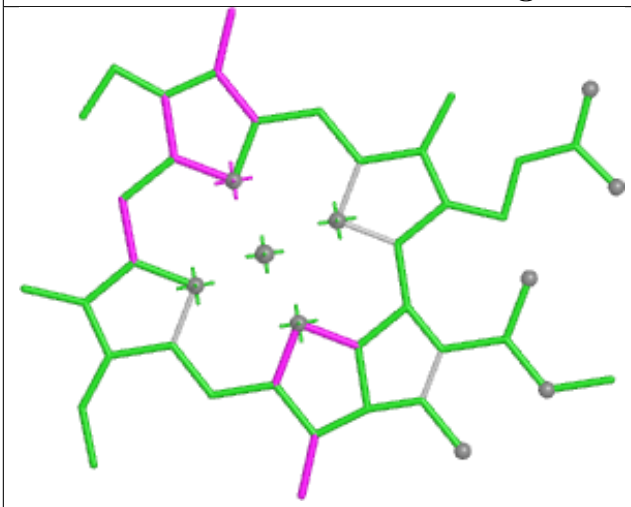


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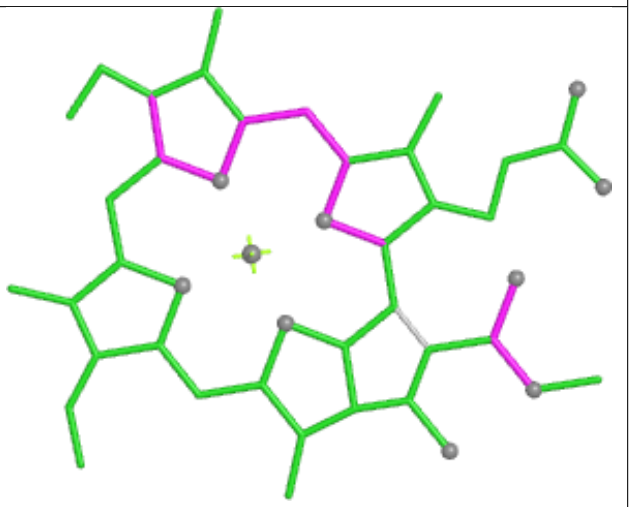


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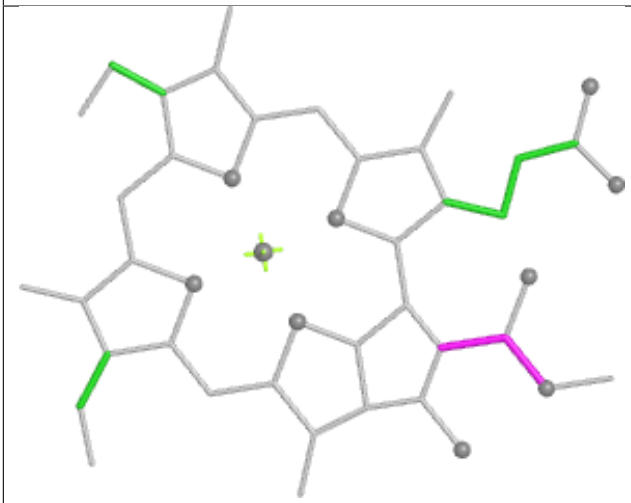
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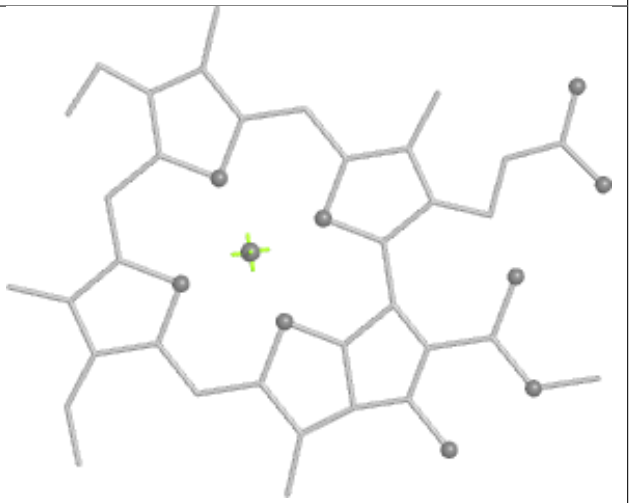
Bond lengths



Bond angles

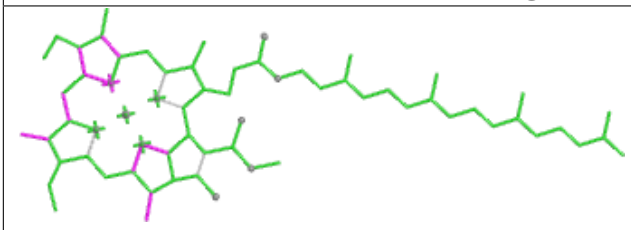


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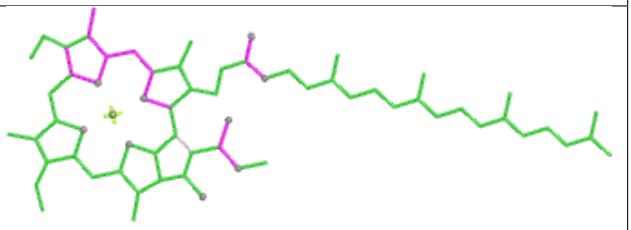


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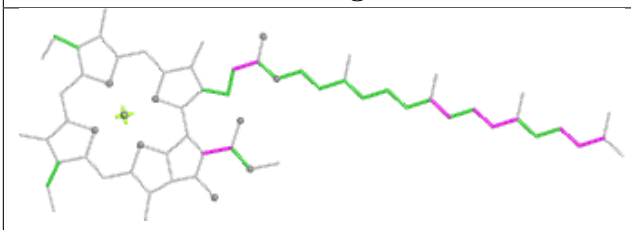
Ligand CLA G 826



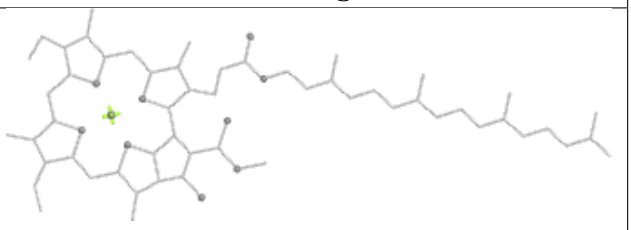
Bond lengths



Bond angles

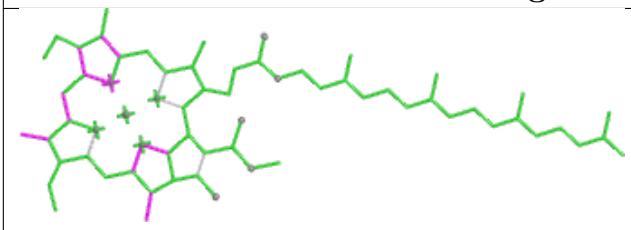


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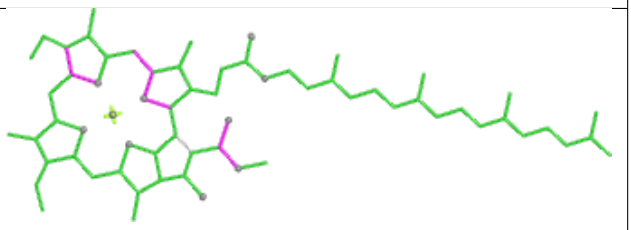


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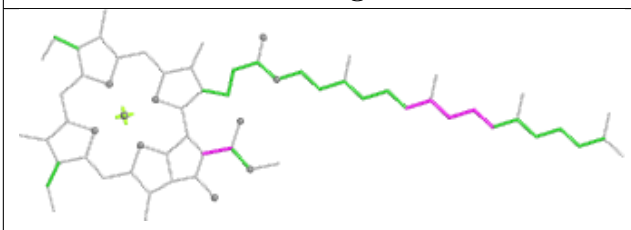
Ligand CLA a 825



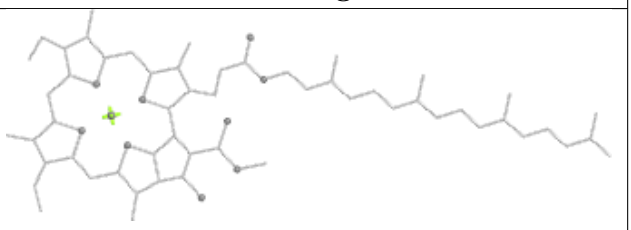
Bond lengths



Bond angles



Torsions

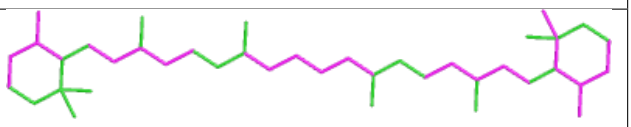


Rings

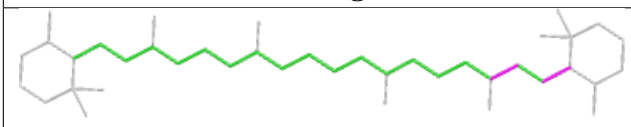
Ligand BCR l 205



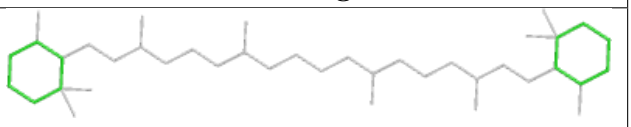
Bond lengths



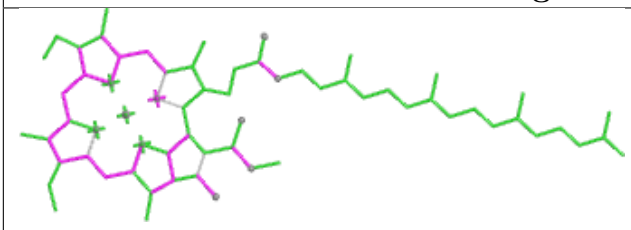
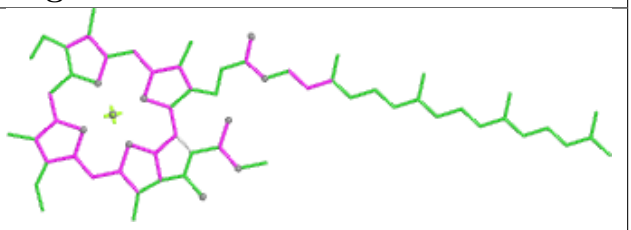
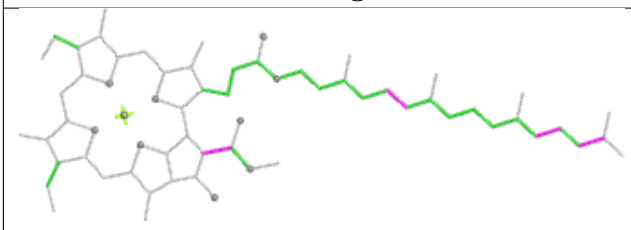
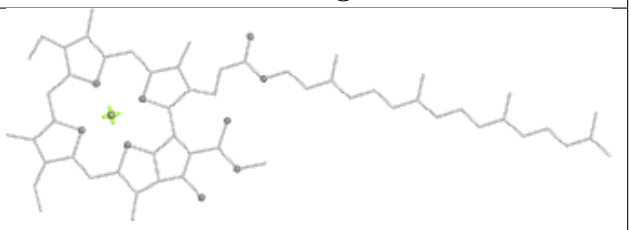
Bond angles

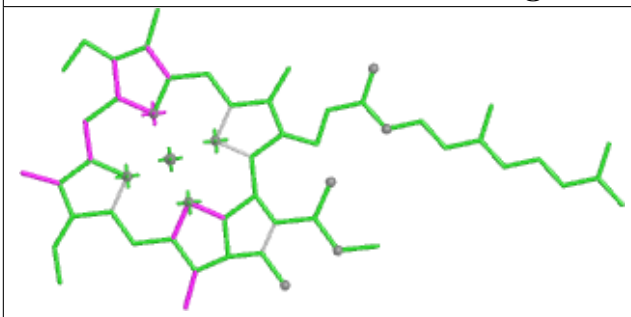
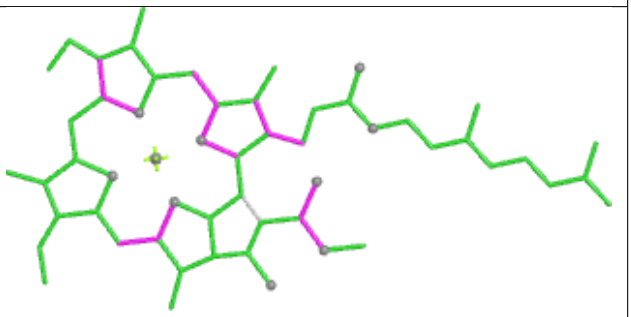
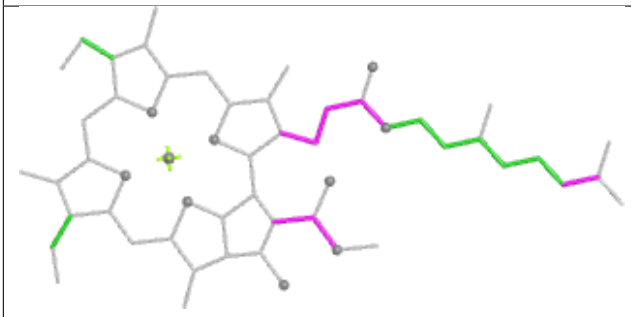
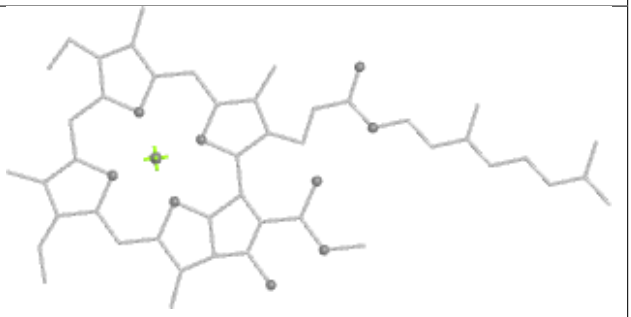


Torsions

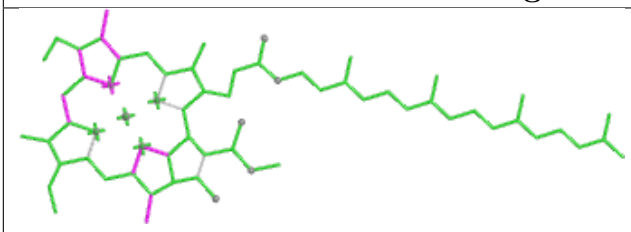


Rings

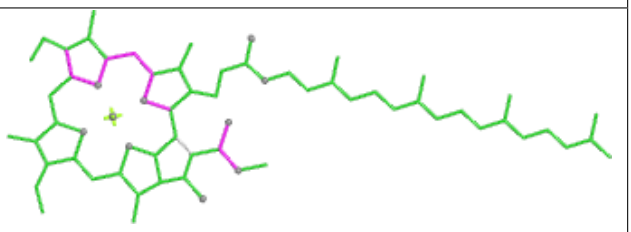
Ligand CL0 g 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

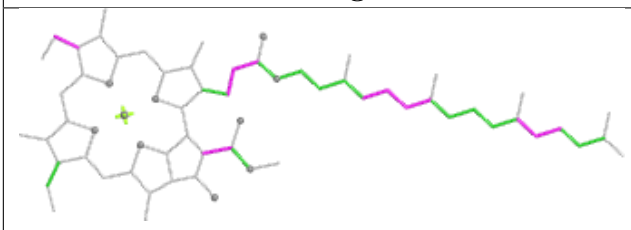
Ligand CLA A 837



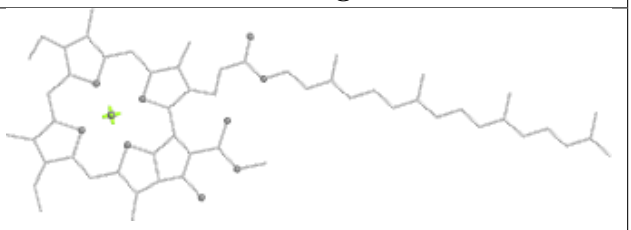
Bond lengths



Bond angles



Torsions

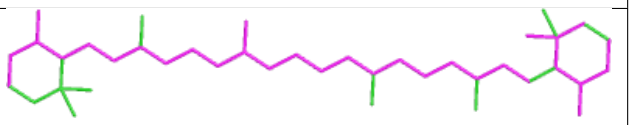


Rings

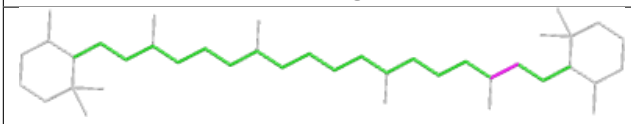
Ligand BCR B 848



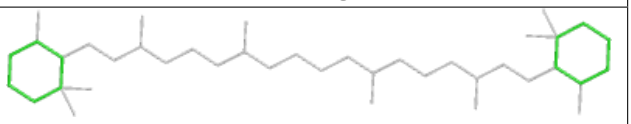
Bond lengths



Bond angles

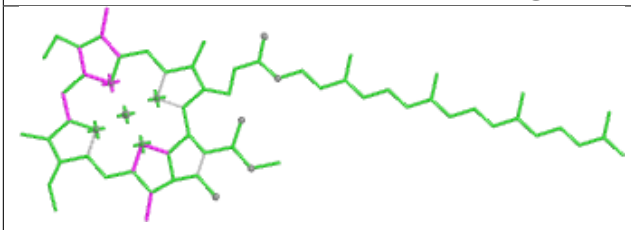


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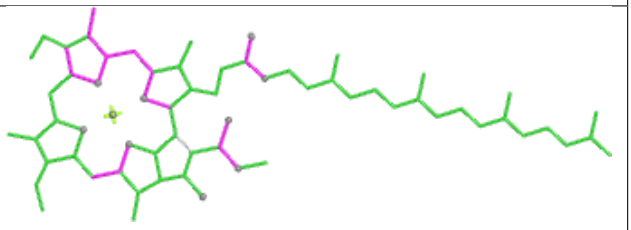


Rings

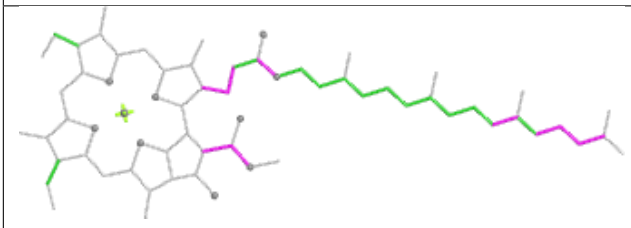
Ligand CLA n 828



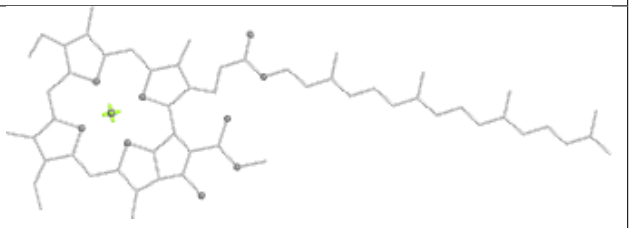
Bond lengths



Bond angles

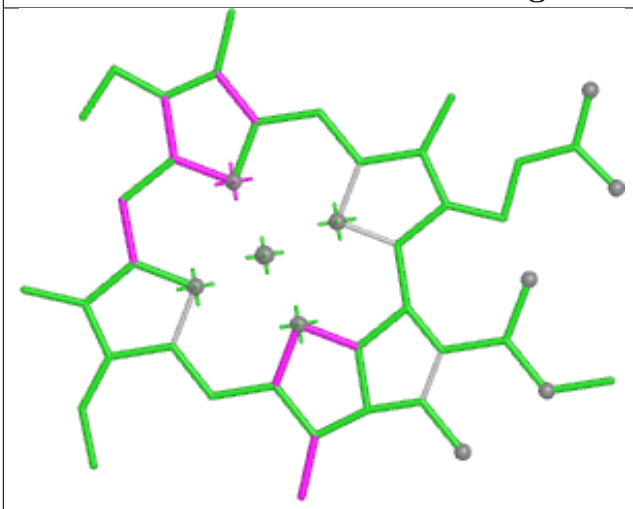


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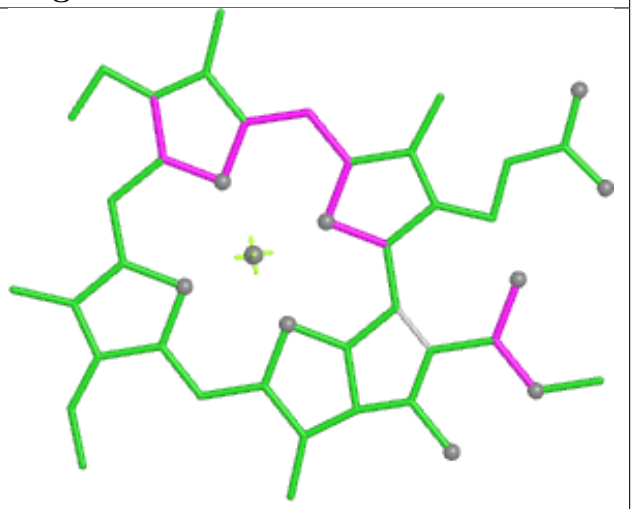


Rings

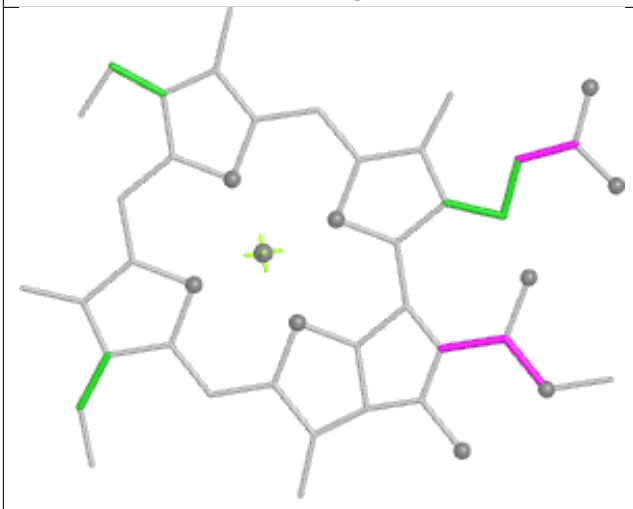
Ligand CLA g 813



Bond lengths



Bond angles

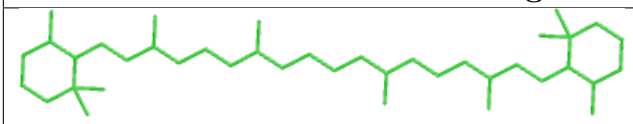


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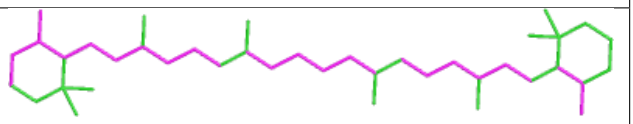


Rings

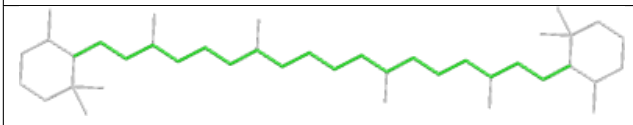
Ligand BCR b 847



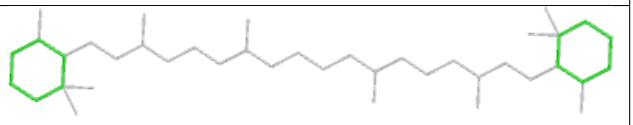
Bond lengths



Bond angles

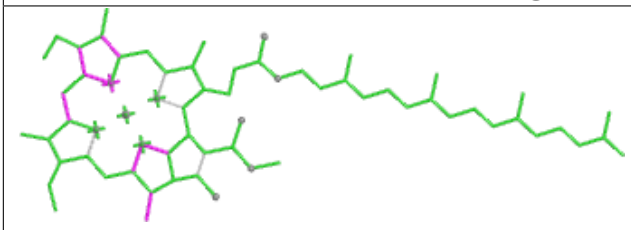


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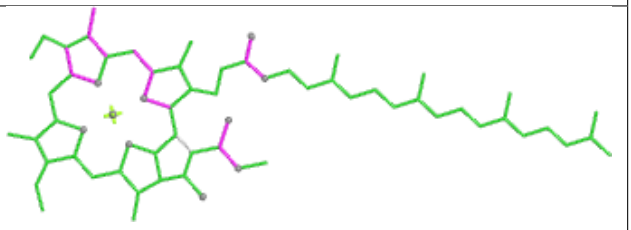


Rings

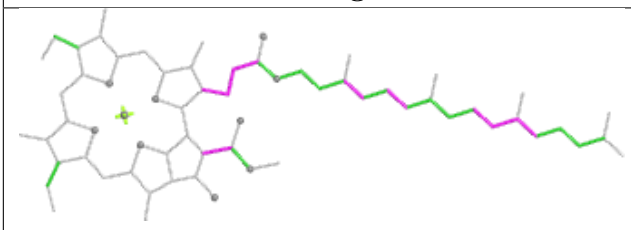
Ligand CLA b 813



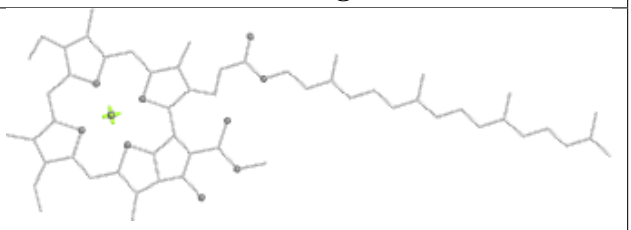
Bond lengths



Bond angles

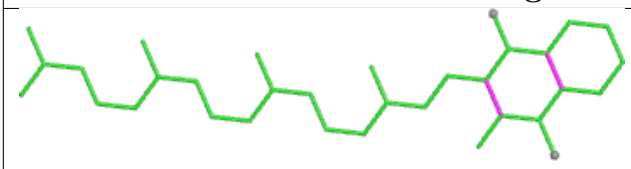


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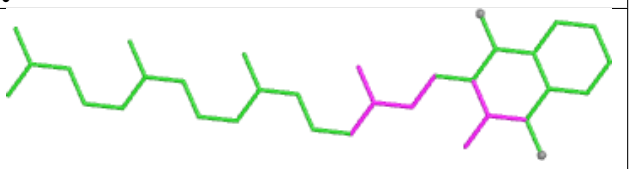


Rings

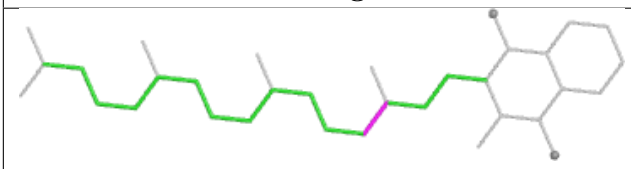
Ligand PQN n 841



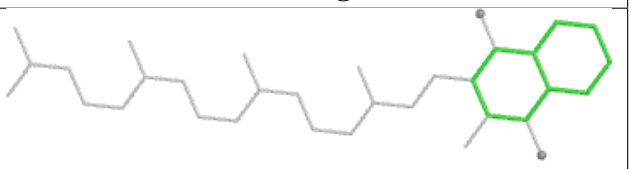
Bond lengths



Bond angles

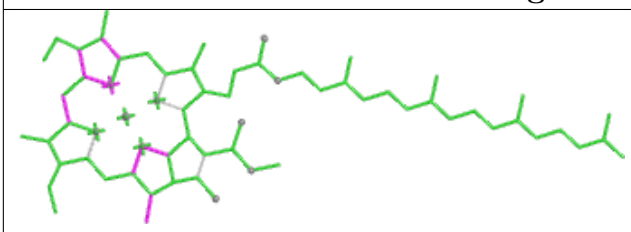


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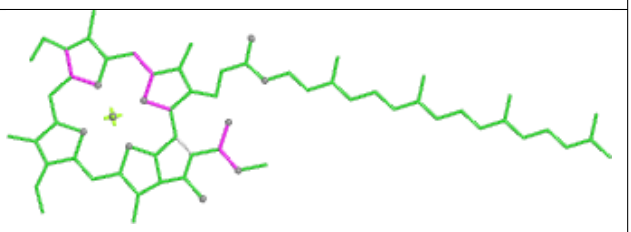


Rings

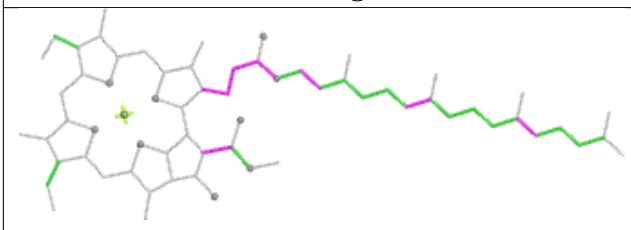
Ligand CLA b 817



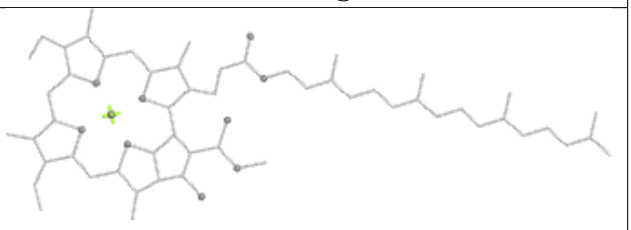
Bond lengths



Bond angles

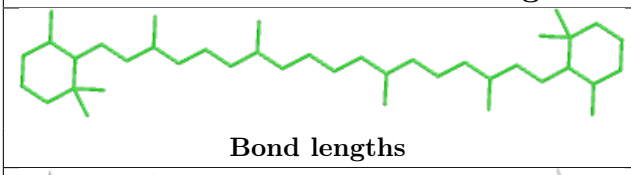


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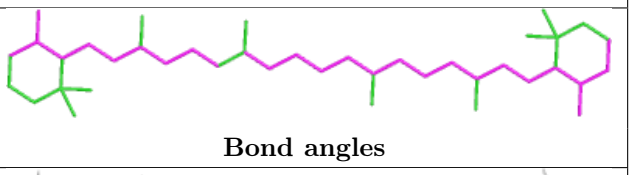


Rings

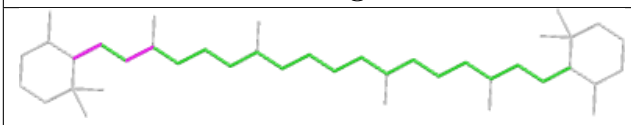
Ligand BCR Y 101



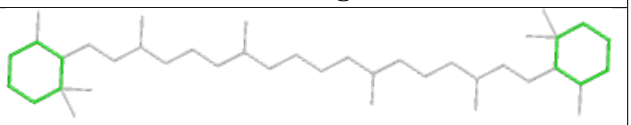
Bond lengths



Bond angles

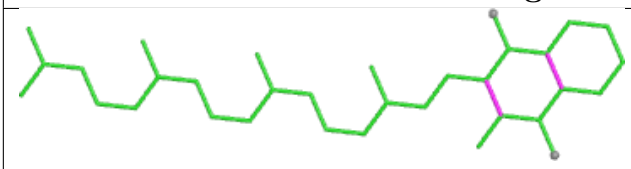


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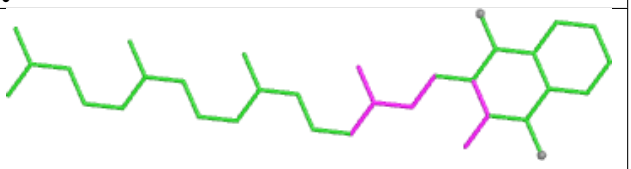


Rings

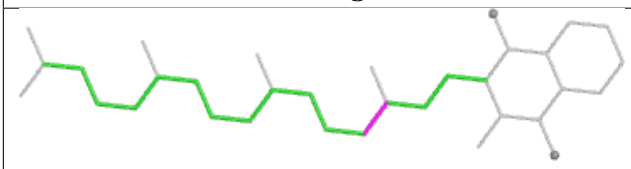
Ligand PQN b 841



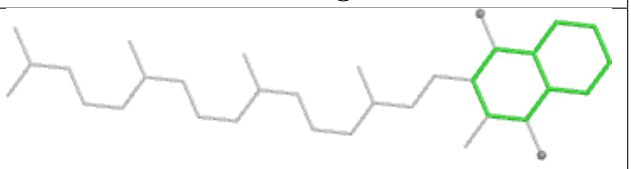
Bond lengths



Bond angles

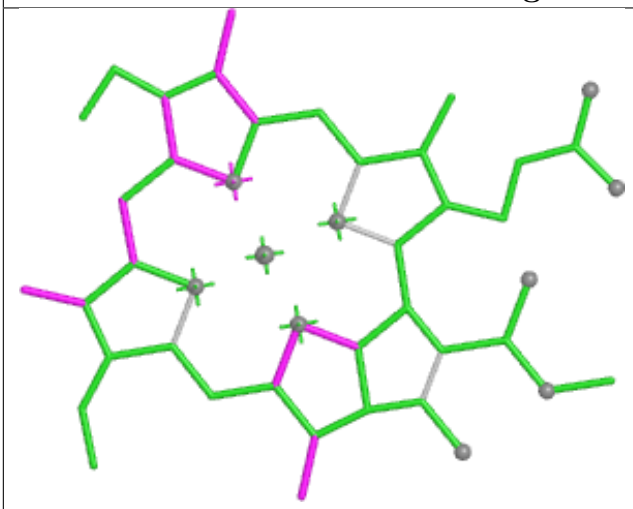


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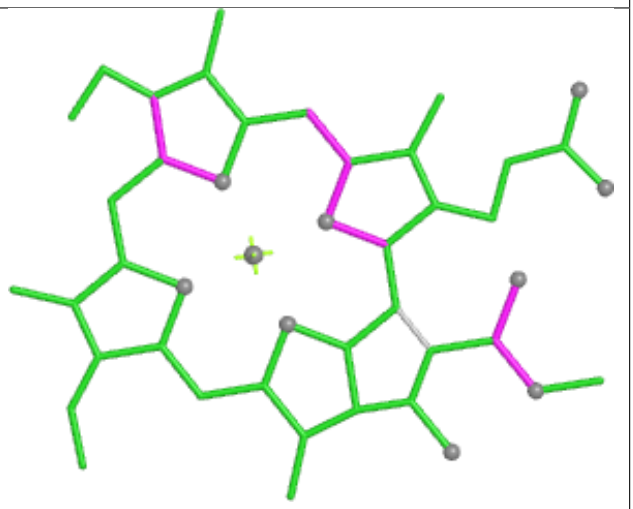


Rings

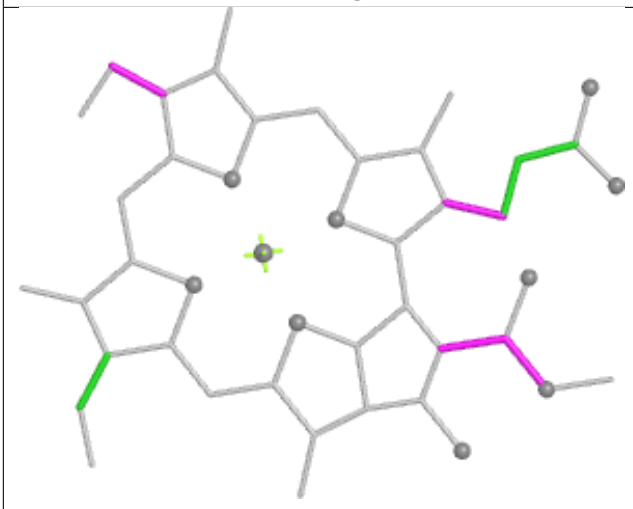
Ligand CLA G 840



Bond lengths



Bond angles

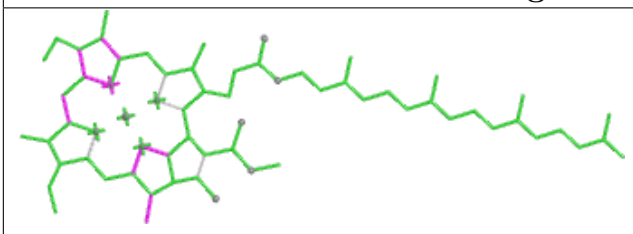


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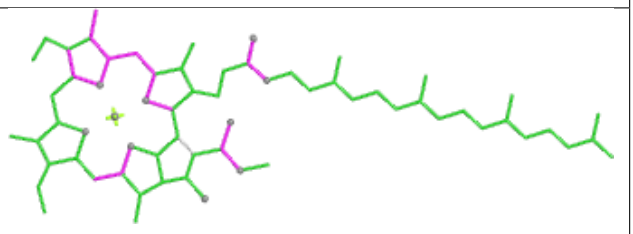


Rings

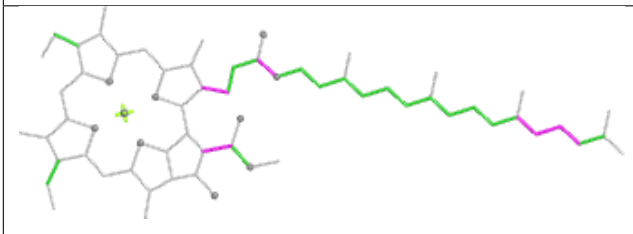
Ligand CLA n 805



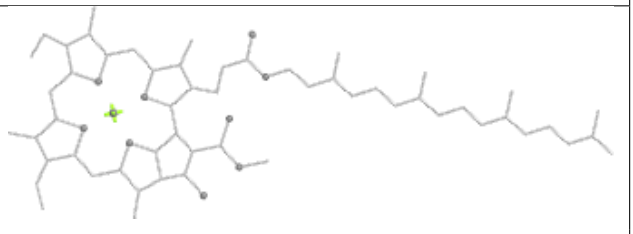
Bond lengths



Bond angles

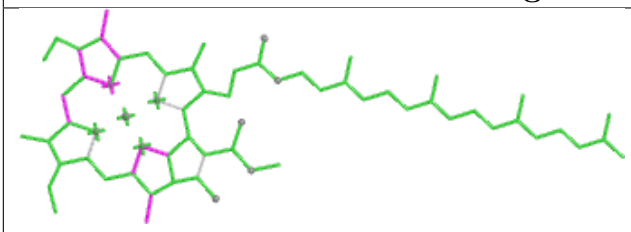


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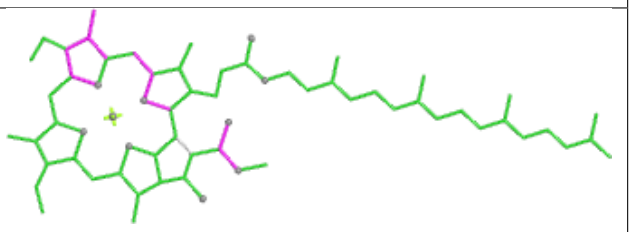


Rings

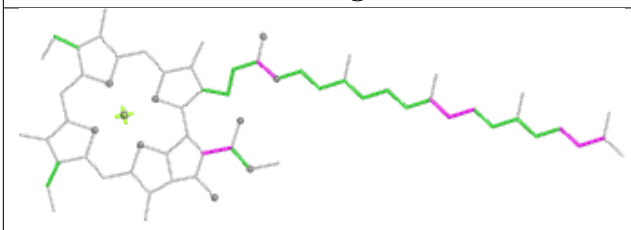
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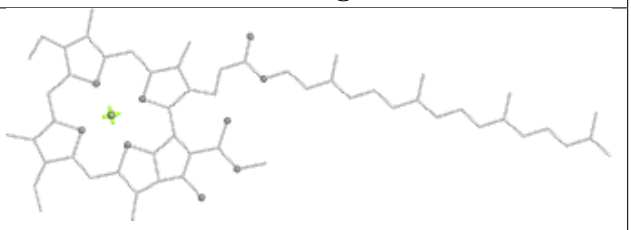
Bond lengths



Bond angles



Torsions



Rings

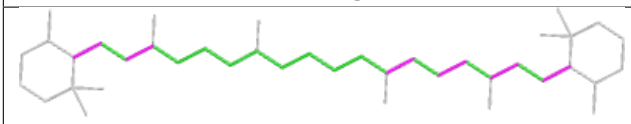
Ligand BCR j 104



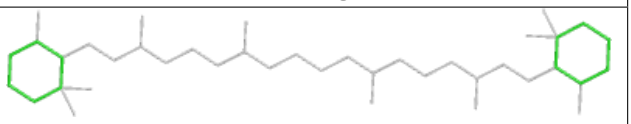
Bond lengths



Bond angles

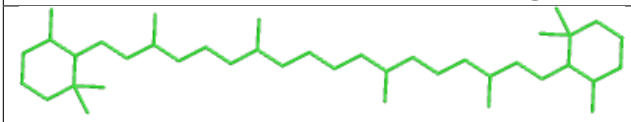


Torsions

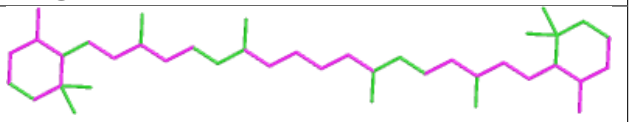


Rings

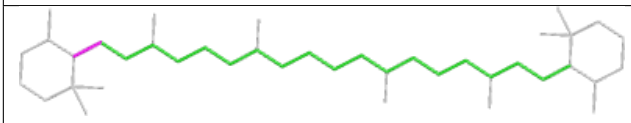
Ligand BCR g 845



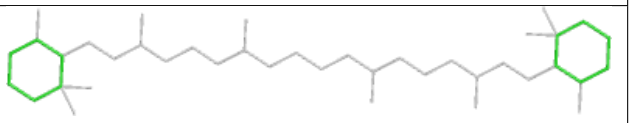
Bond lengths



Bond angles

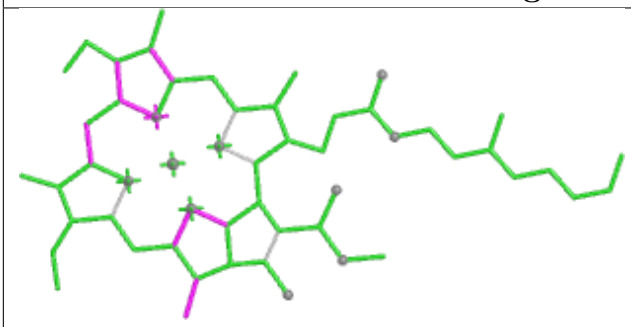


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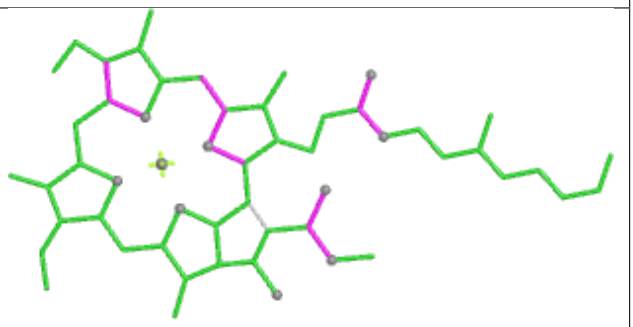


Rings

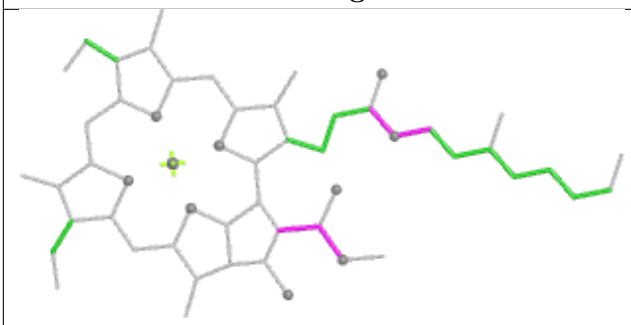
Ligand CLA N 835



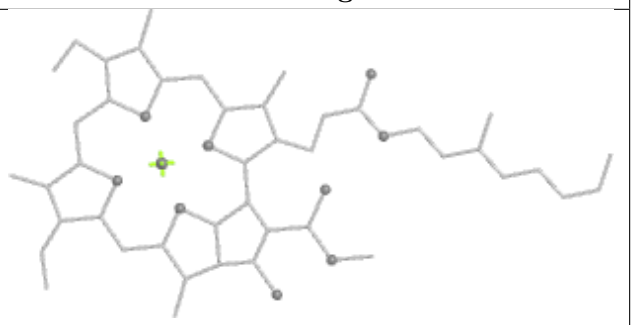
Bond lengths



Bond angles

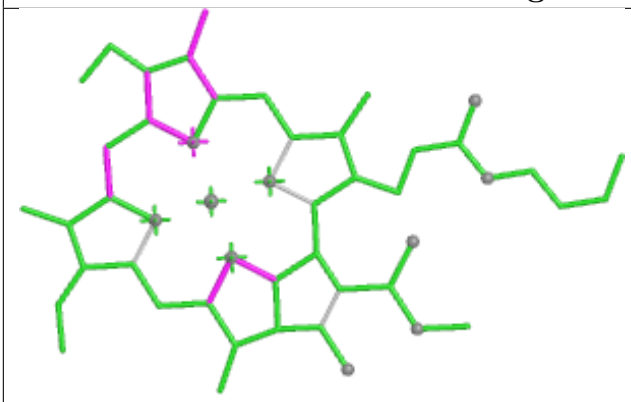


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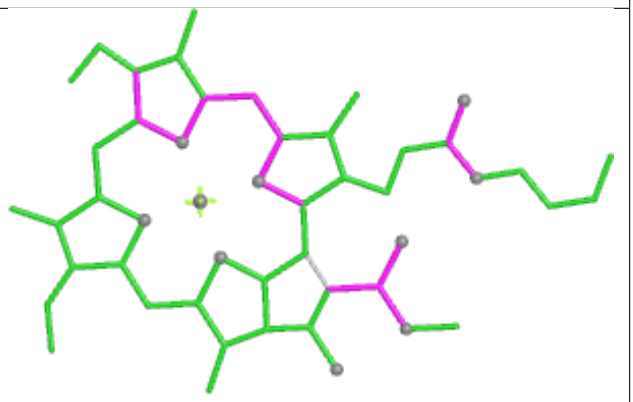


Rings

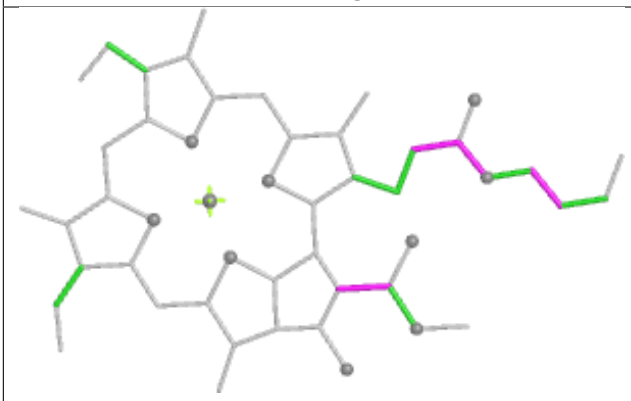
Ligand CLA u 102



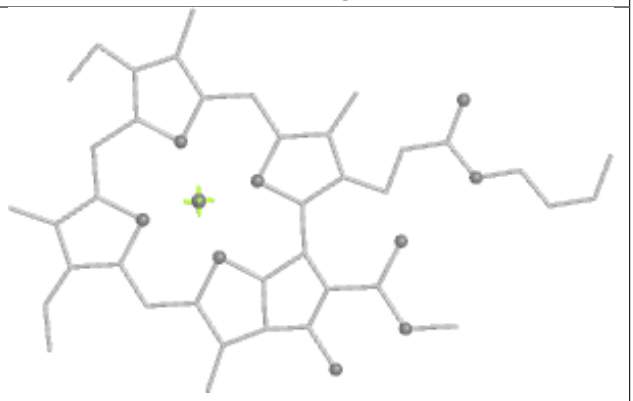
Bond lengths



Bond angles

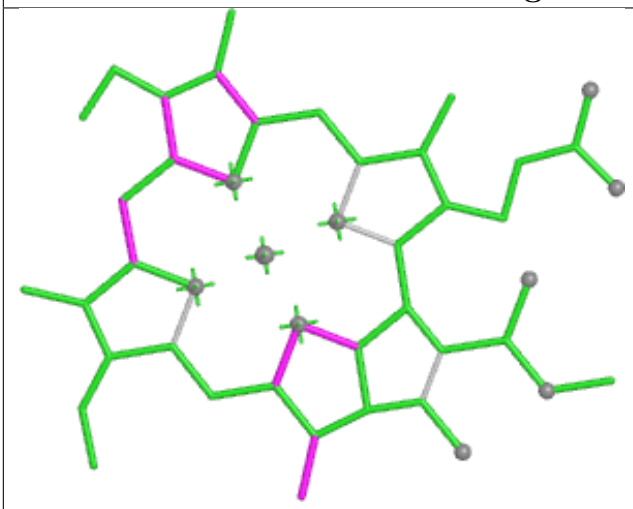


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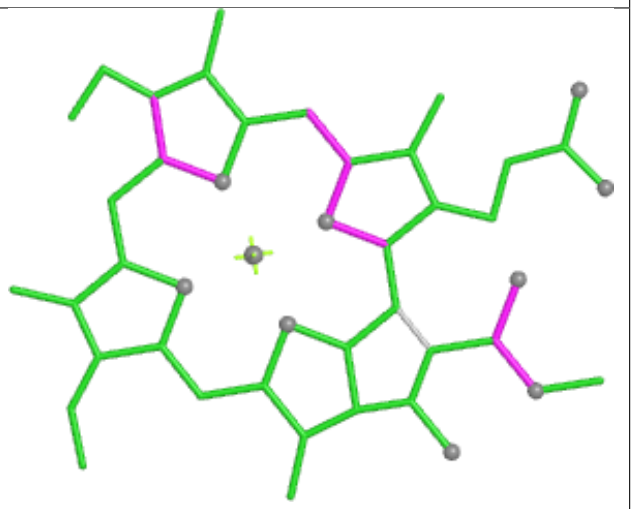


Rings

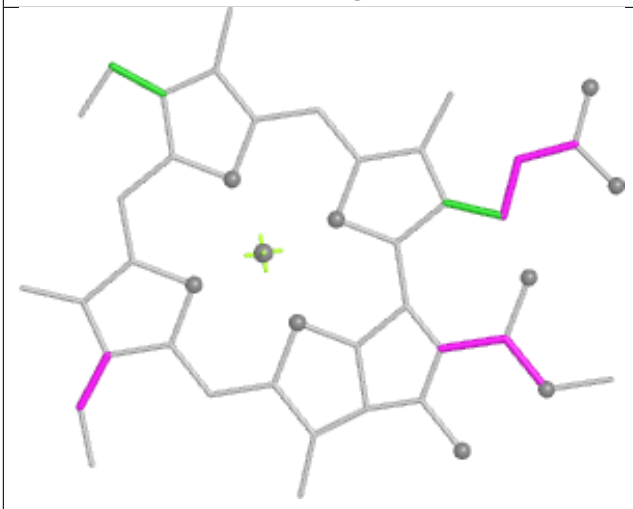
Ligand CLA B 804



Bond lengths



Bond angles

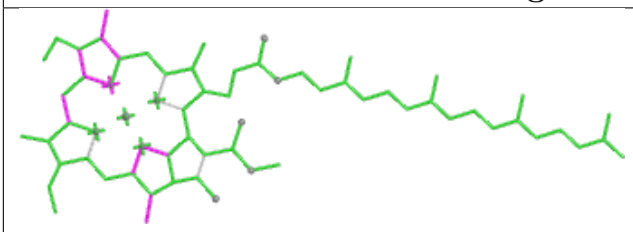


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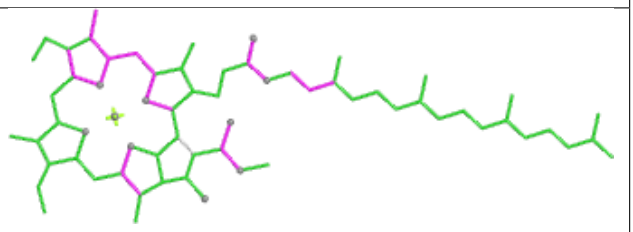


Rings

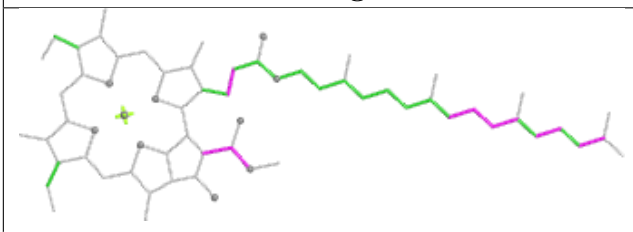
Ligand CLA b 829



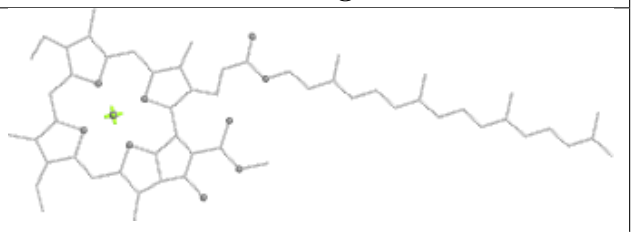
Bond lengths



Bond angles

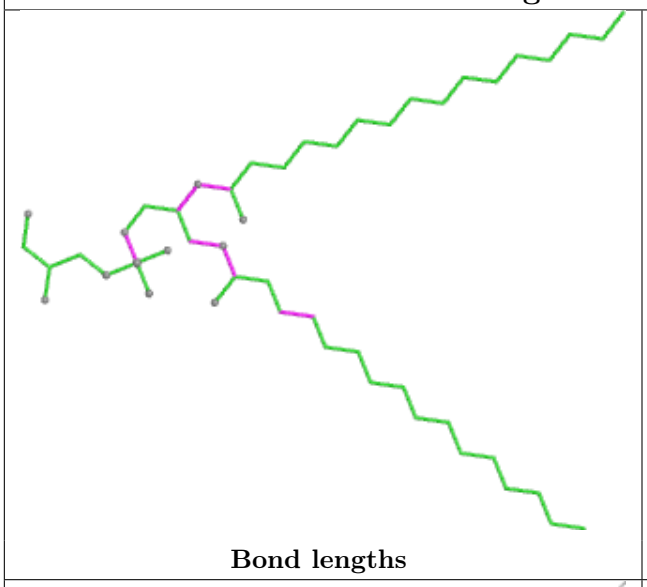


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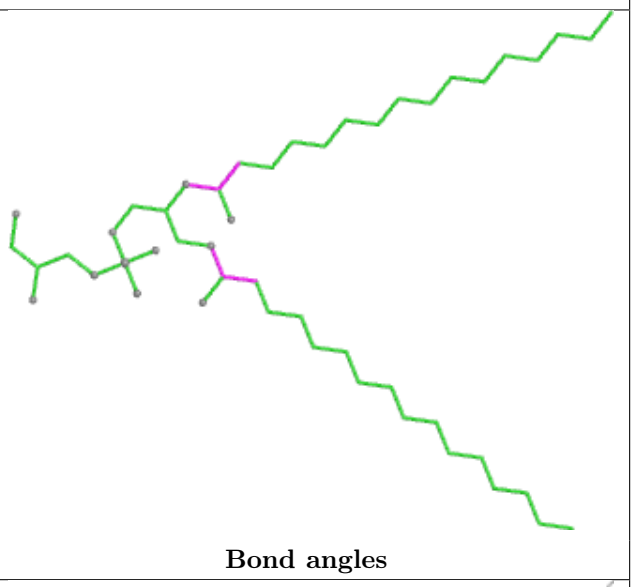


Rings

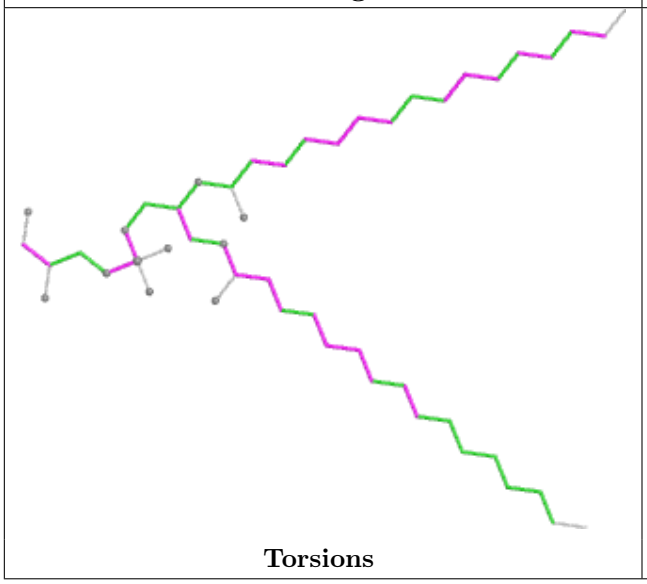
Ligand LHG A 850



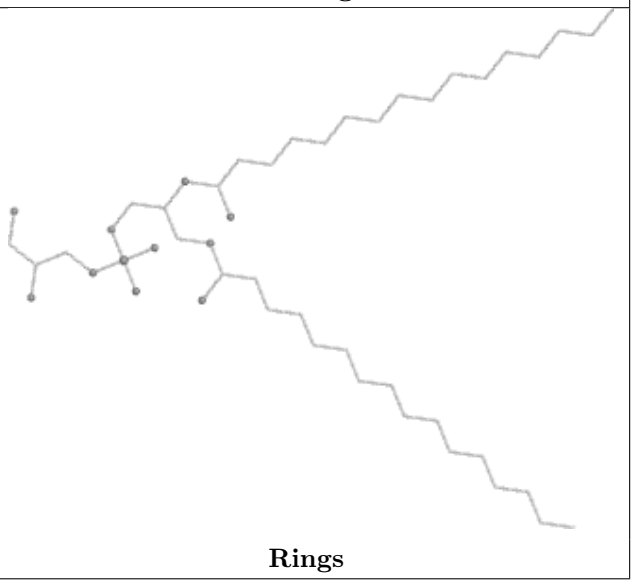
Bond lengths



Bond angles

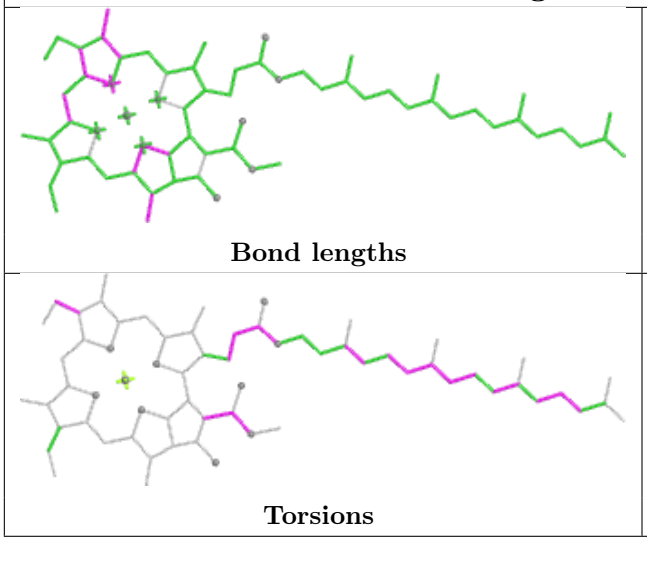


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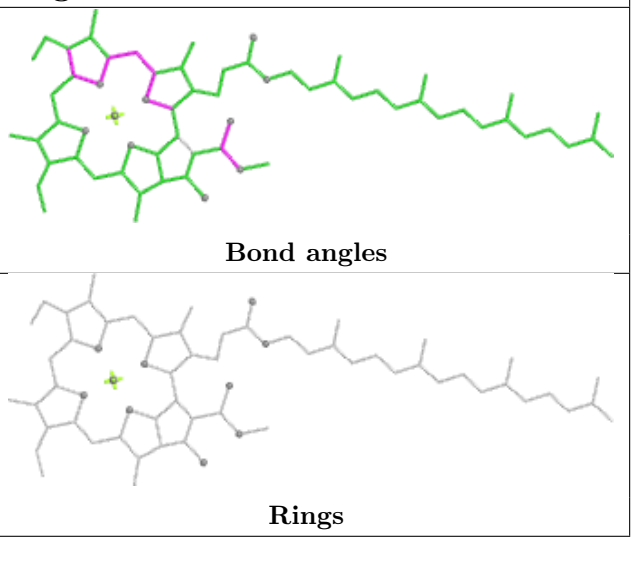


Rings

Ligand CLA g 854



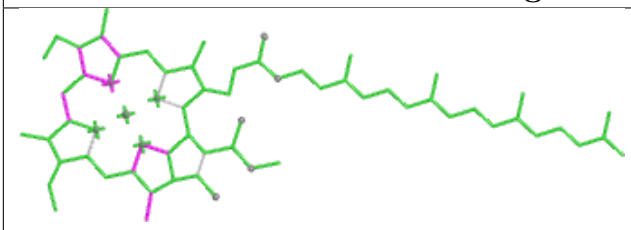
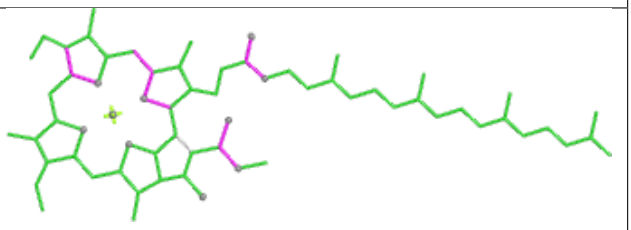
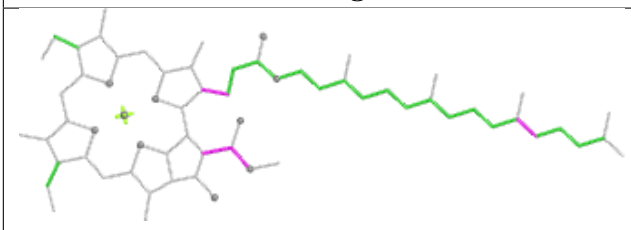
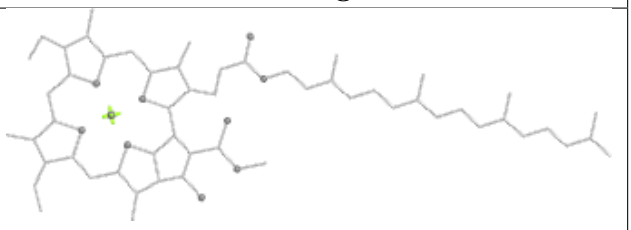
Bond lengths

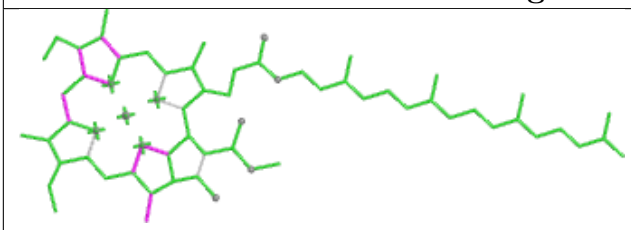
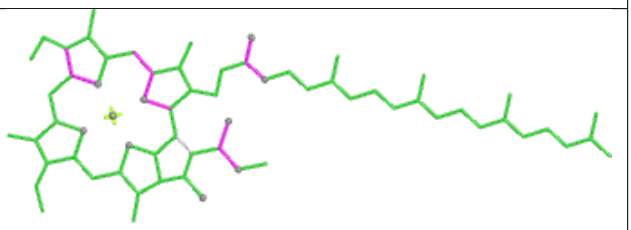
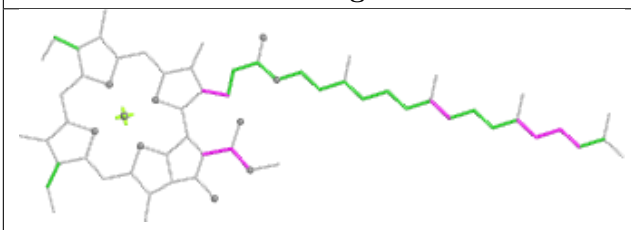
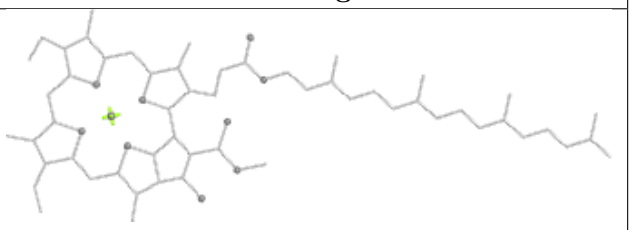


Bond angles

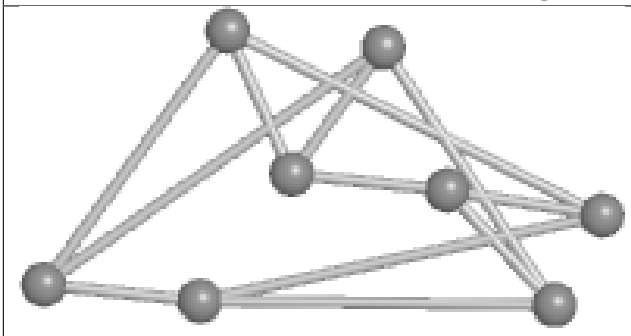
Torsions

Rings

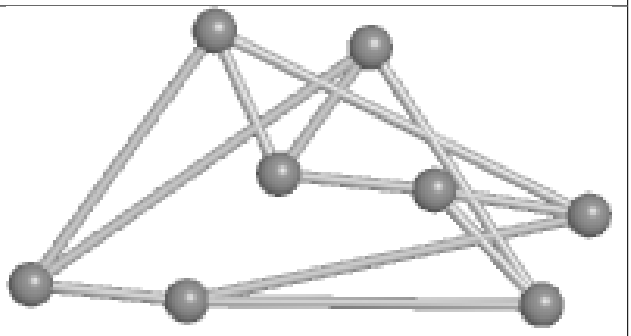
Ligand CLA B 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

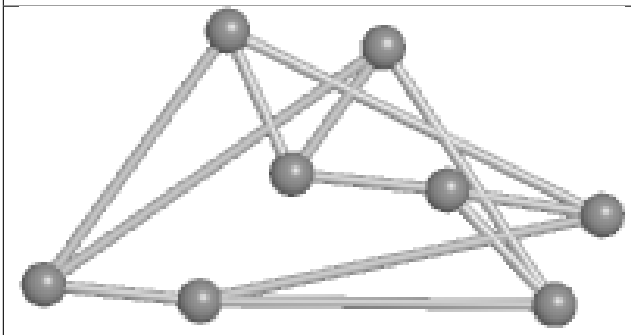
Ligand SF4 a 842



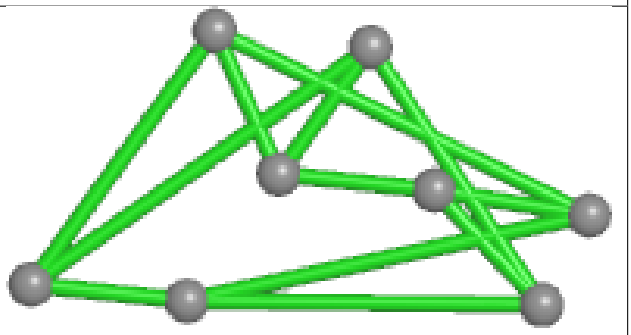
Bond lengths



Bond angles

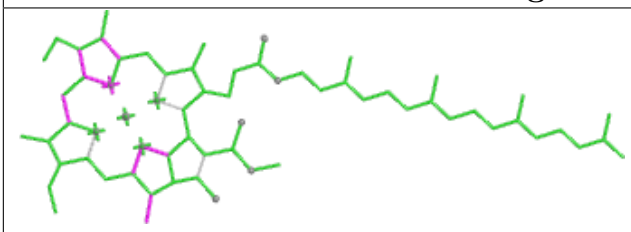


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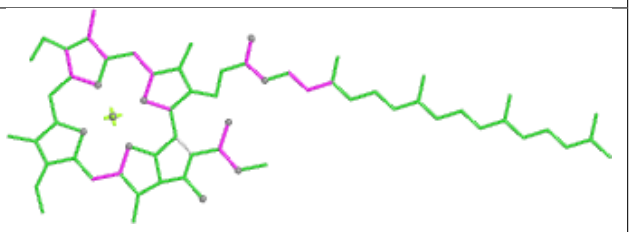


Rings

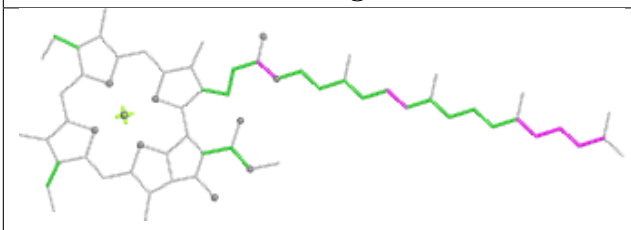
Ligand CLA b 806



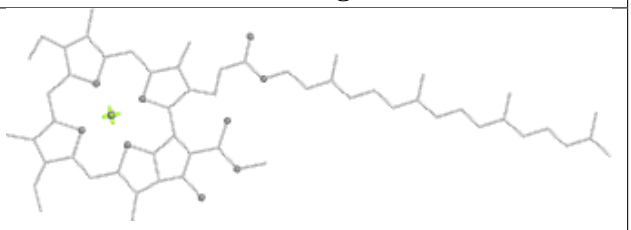
Bond lengths



Bond angles

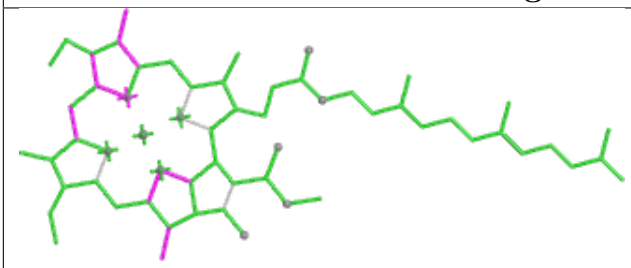


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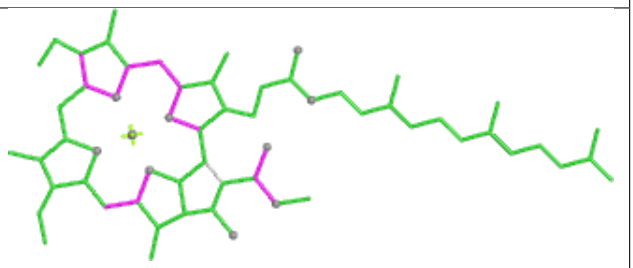


Rings

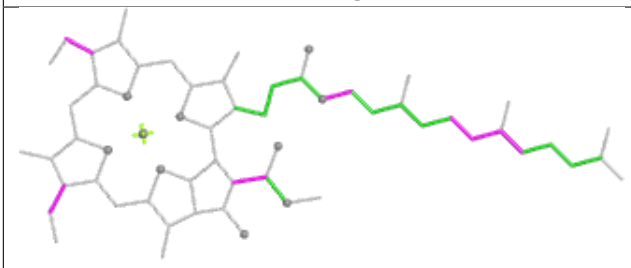
Ligand CLA w 204



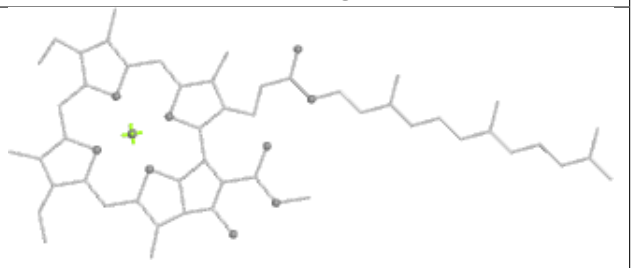
Bond lengths



Bond angles

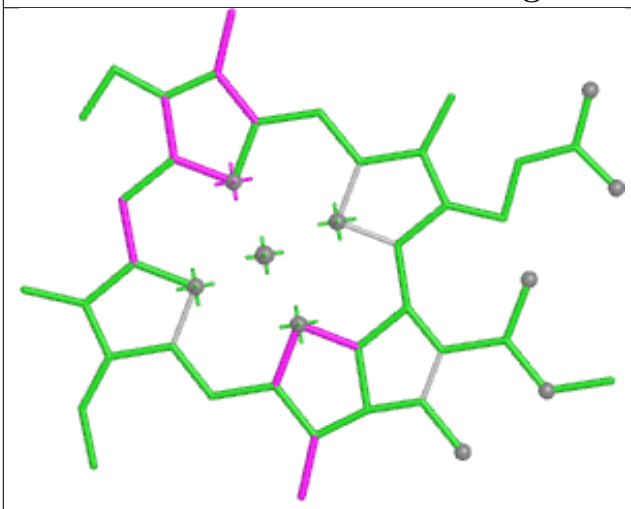


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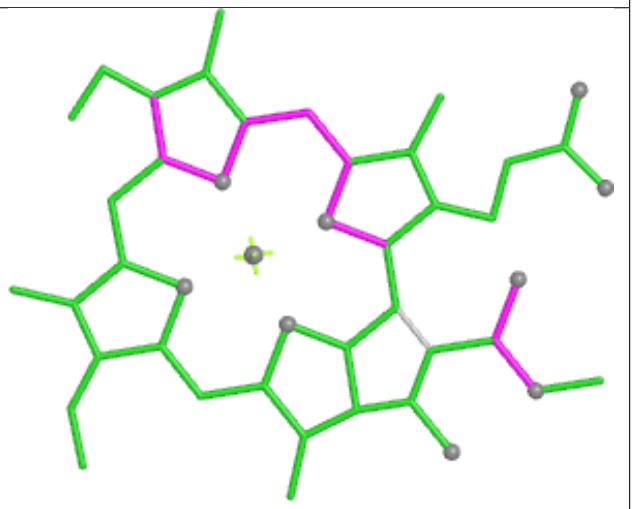


Rings

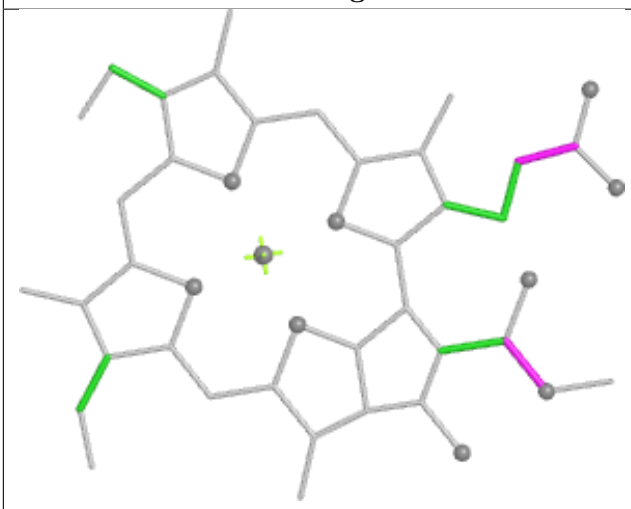
Ligand CLA G 809



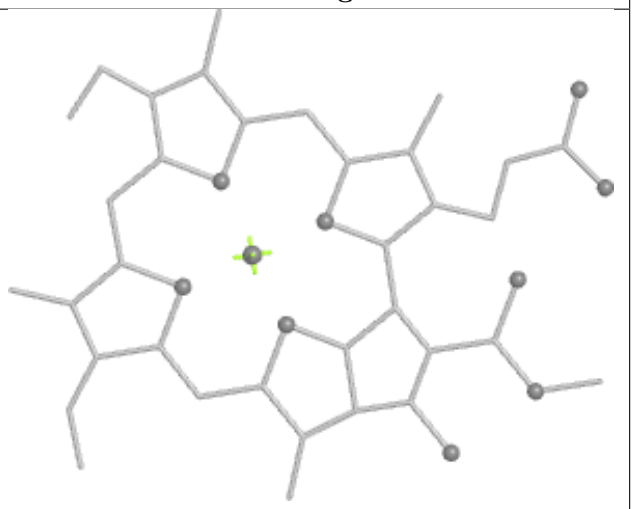
Bond lengths



Bond angles

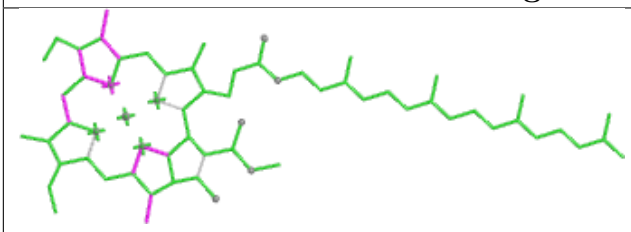


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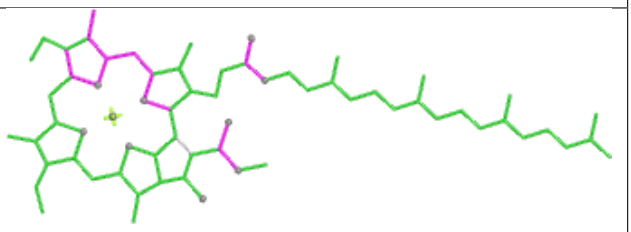


Rings

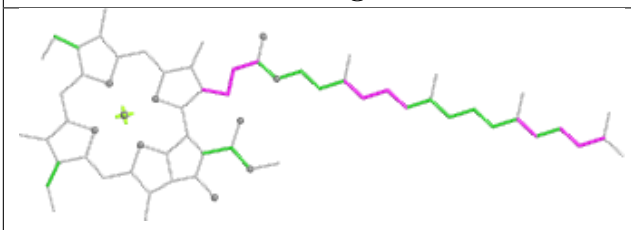
Ligand CLA N 811



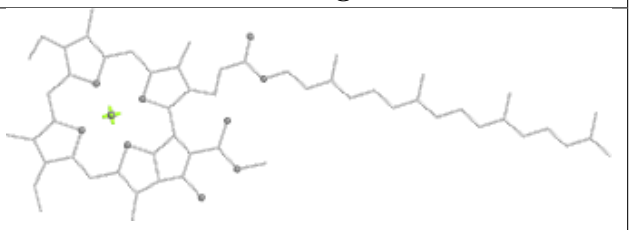
Bond lengths



Bond angles

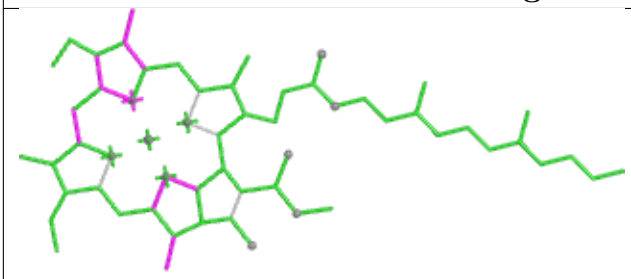


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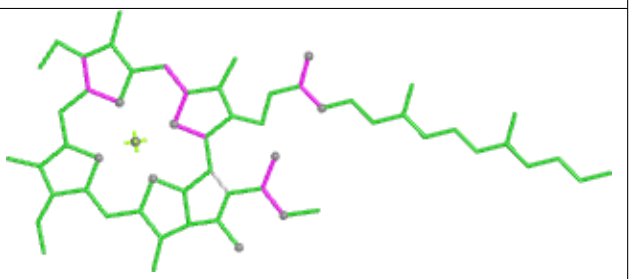


Rings

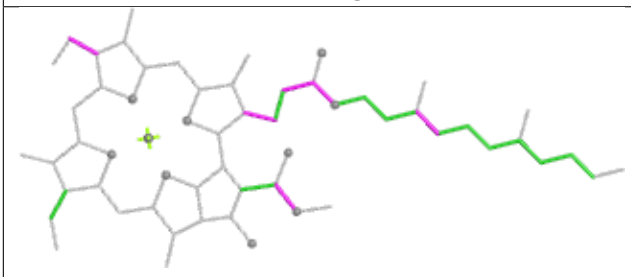
Ligand CLA N 834



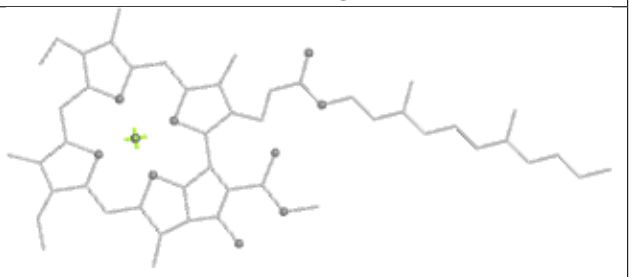
Bond lengths



Bond angles

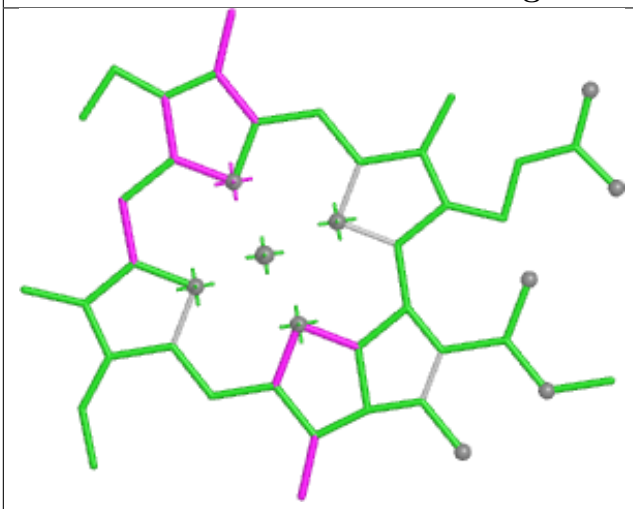


Torsions

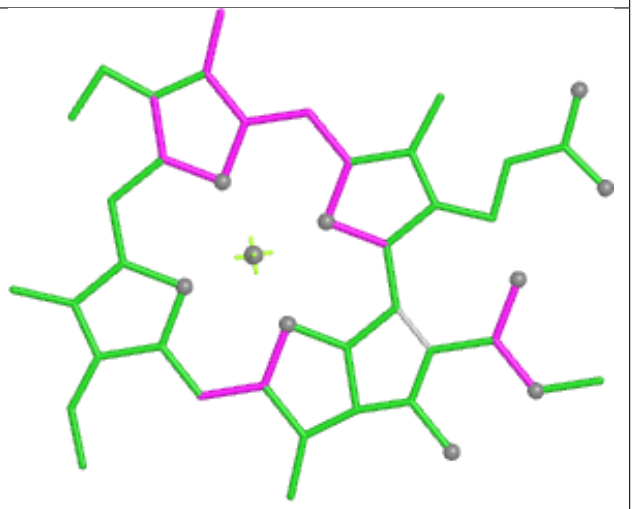


Rings

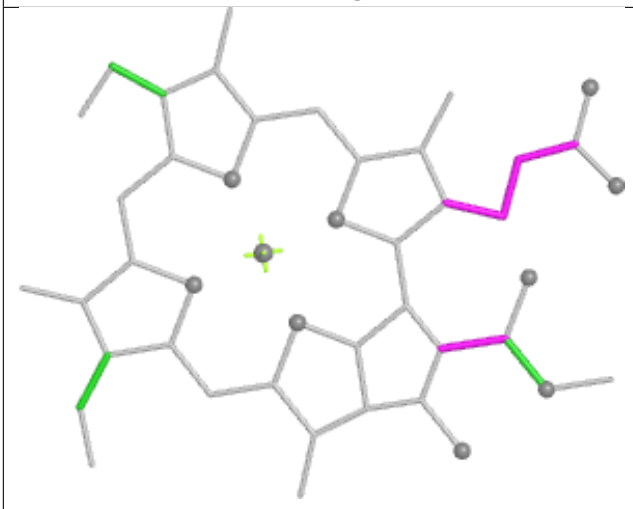
Ligand CLA G 821



Bond lengths



Bond angles

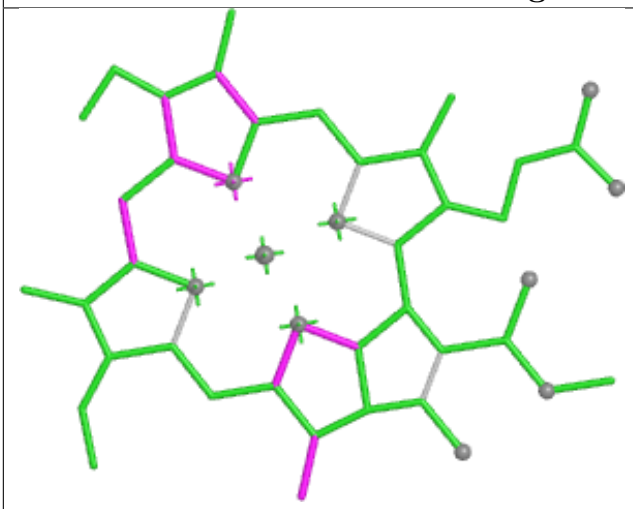


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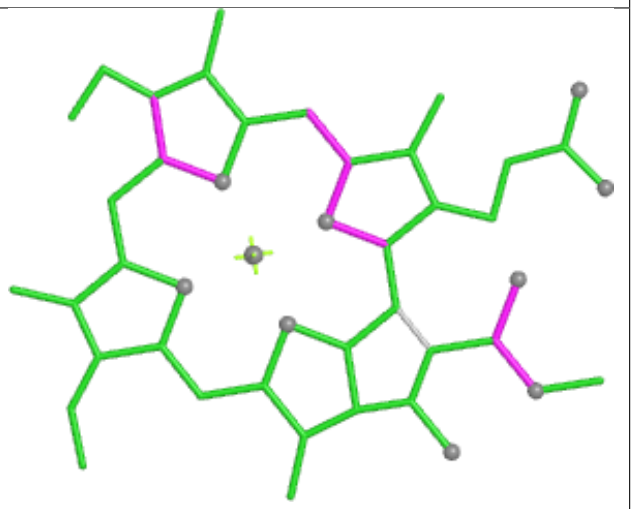


Rings

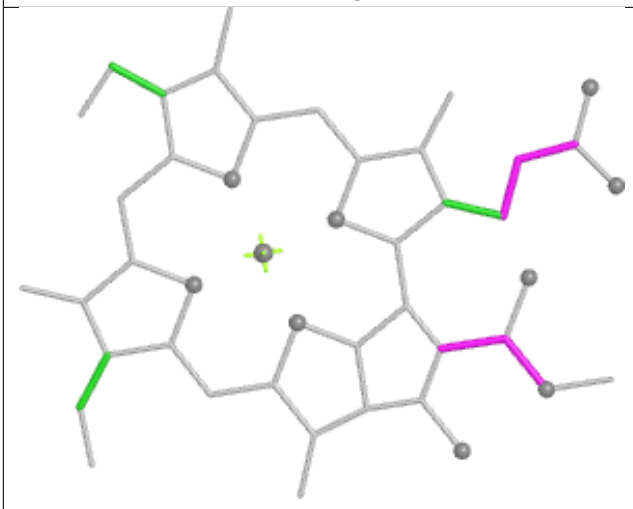
Ligand CLA a 813



Bond lengths



Bond angles

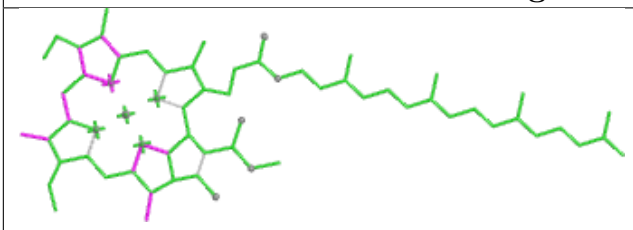


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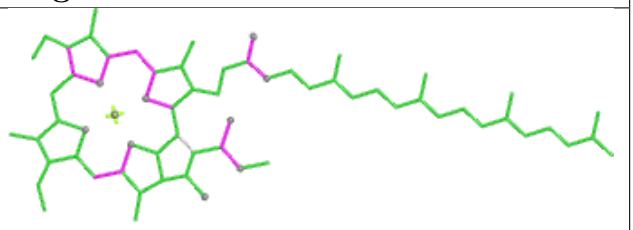


Rings

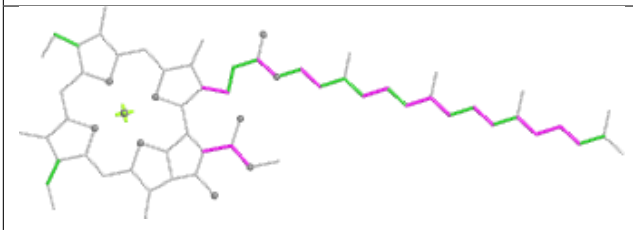
Ligand CLA g 803



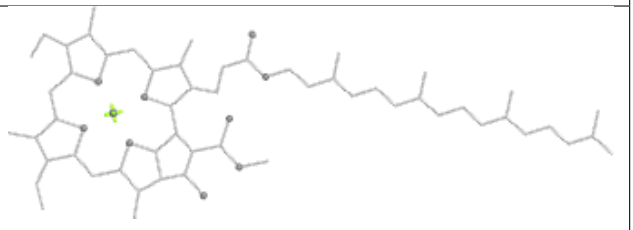
Bond lengths



Bond angles

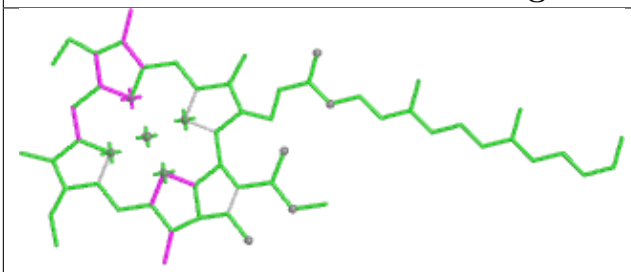


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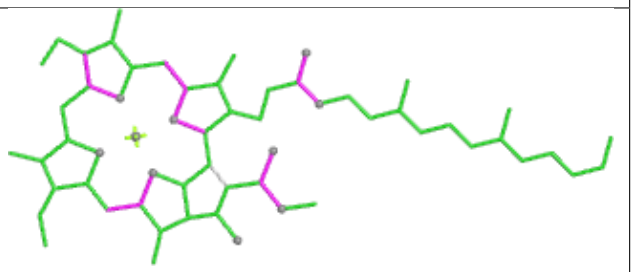


Rings

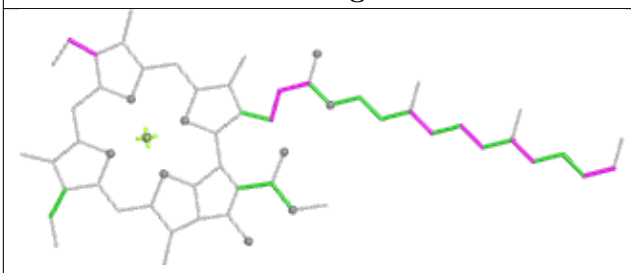
Ligand CLA a 815



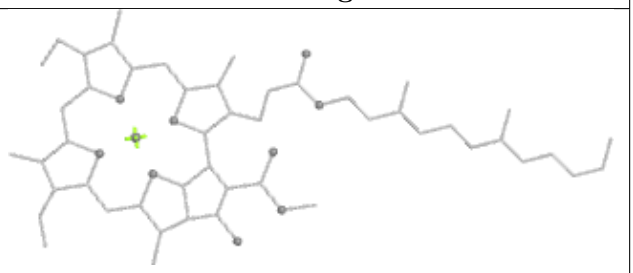
Bond lengths



Bond angles

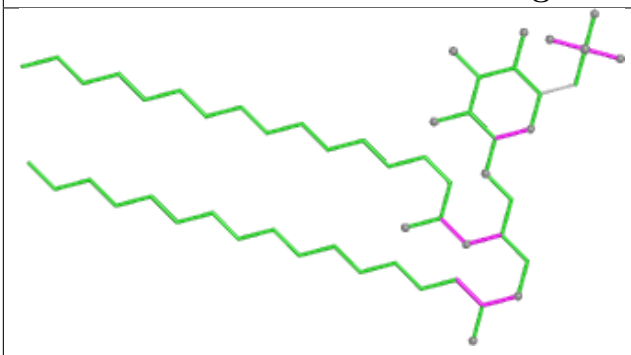


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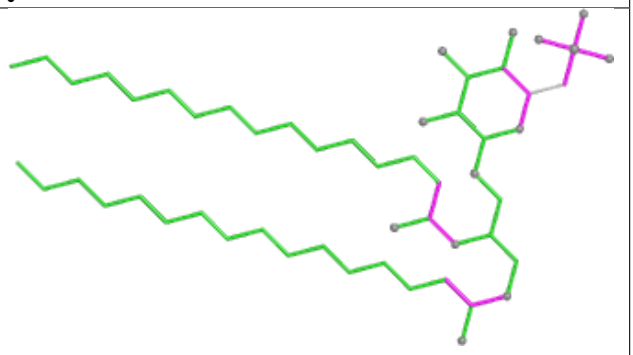


Rings

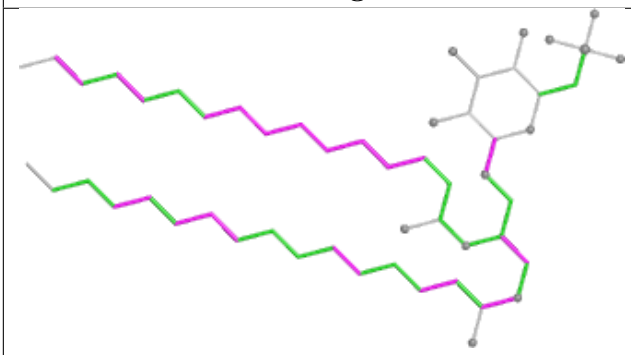
Ligand SQD l 201



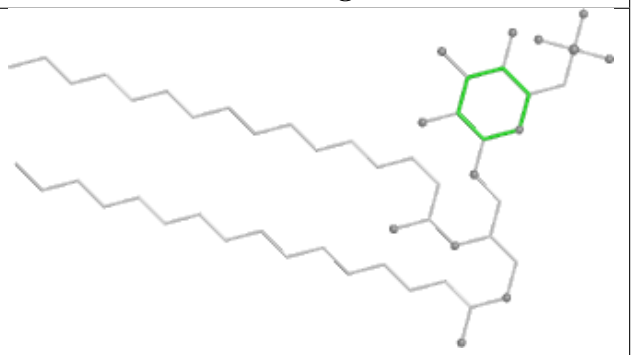
Bond lengths



Bond angles

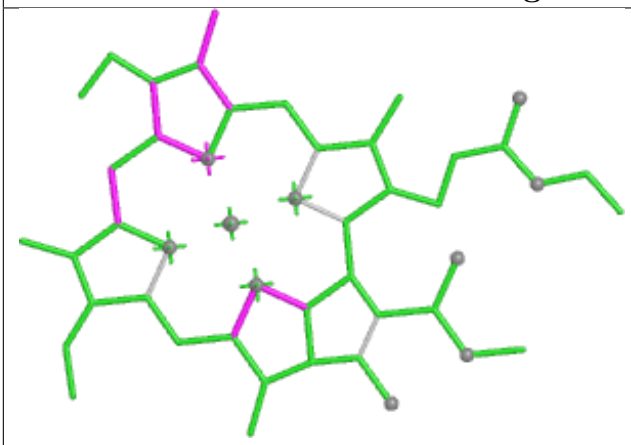


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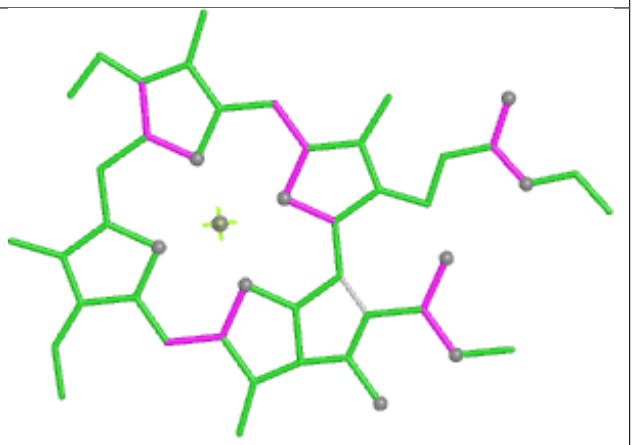


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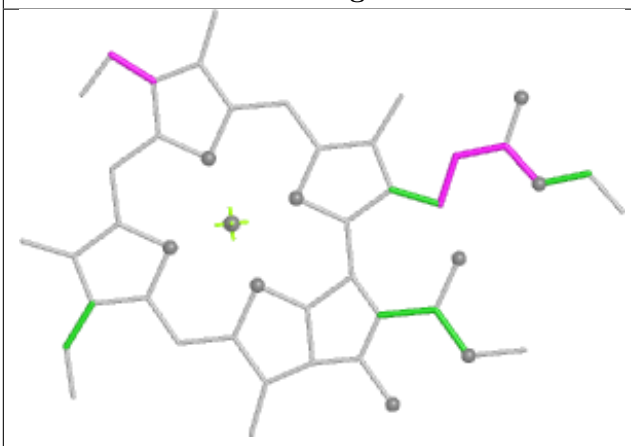
Ligand CLA N 840



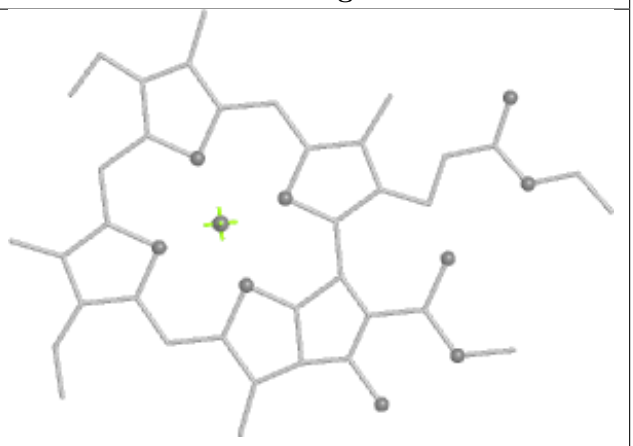
Bond lengths



Bond angles



Torsions

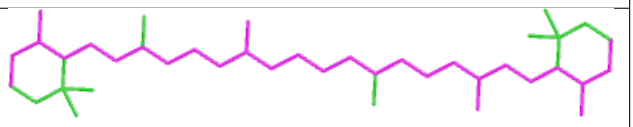


Rings

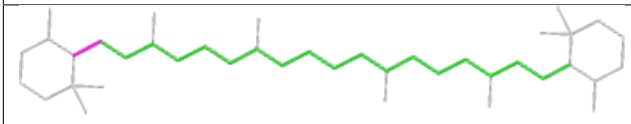
Ligand BCR A 847



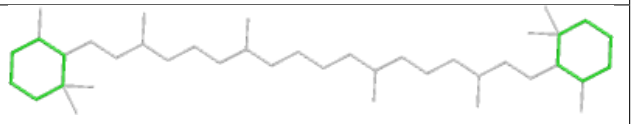
Bond lengths



Bond angles

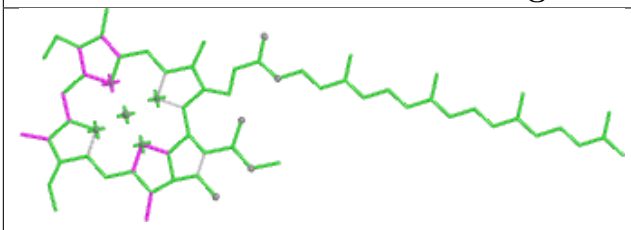


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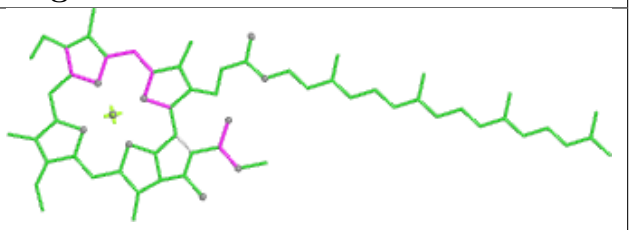


Rings

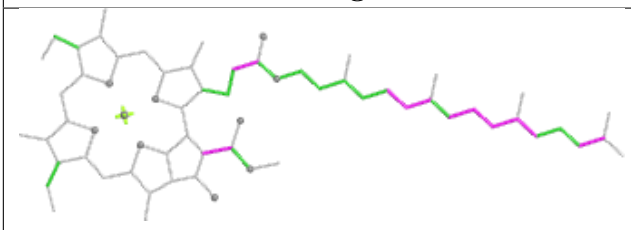
Ligand CLA g 825



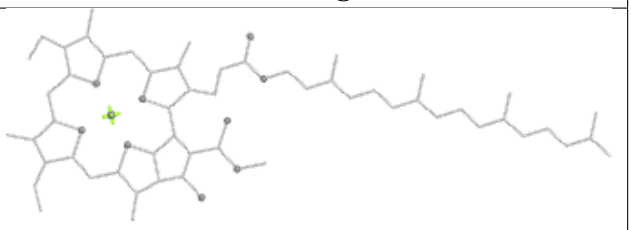
Bond lengths



Bond angles

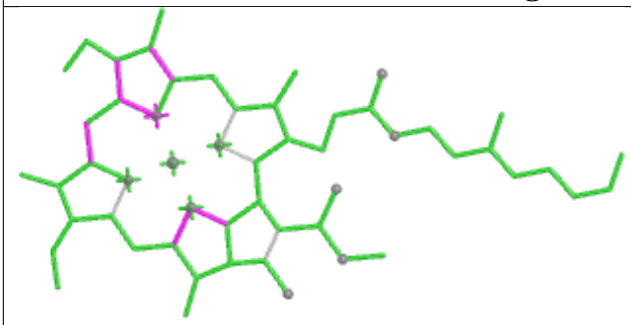


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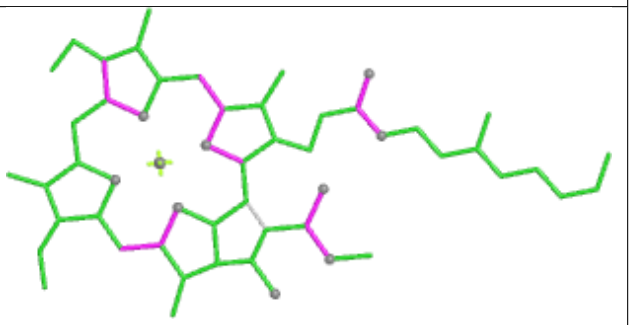


Rings

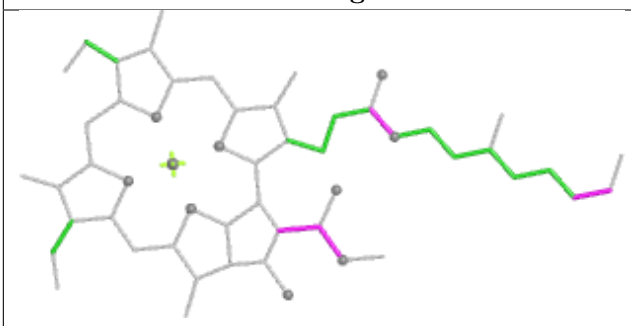
Ligand CLA A 813



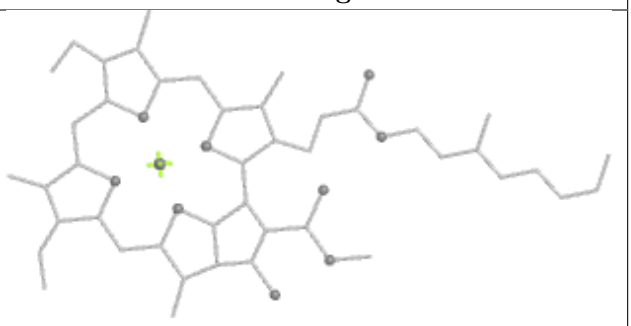
Bond lengths



Bond angles

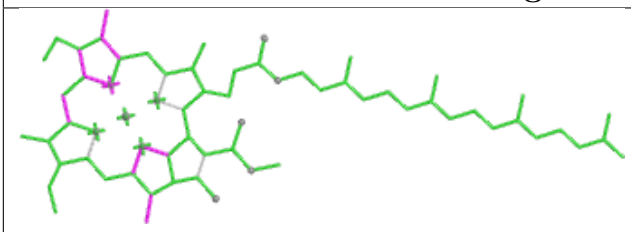


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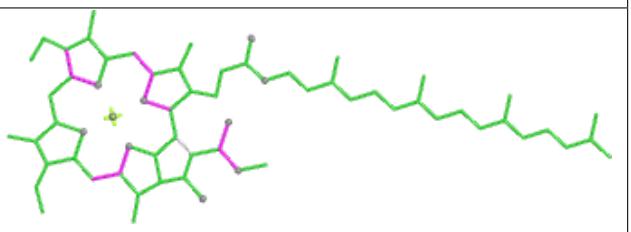


Rings

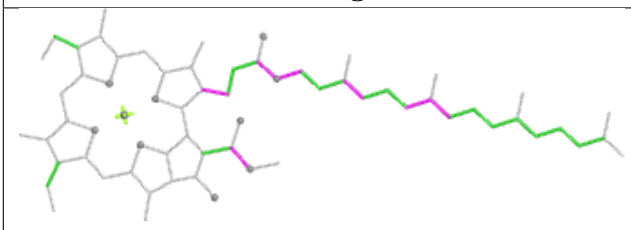
Ligand CLA B 819



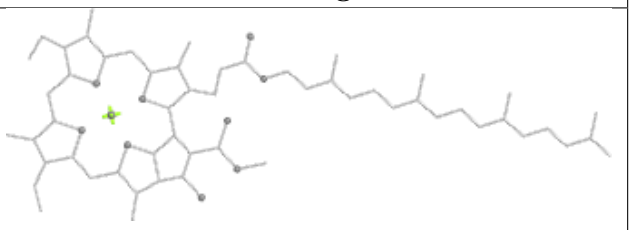
Bond lengths



Bond angles

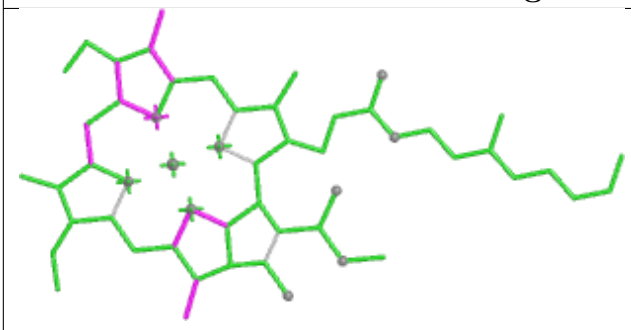


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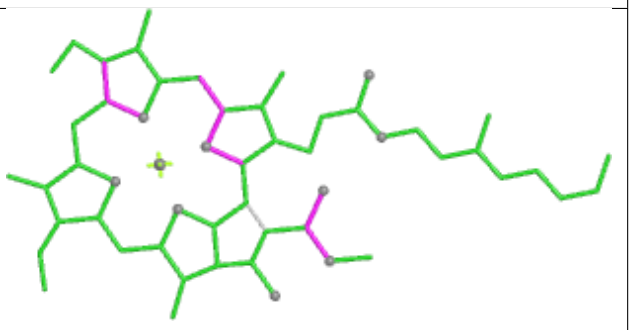


Rings

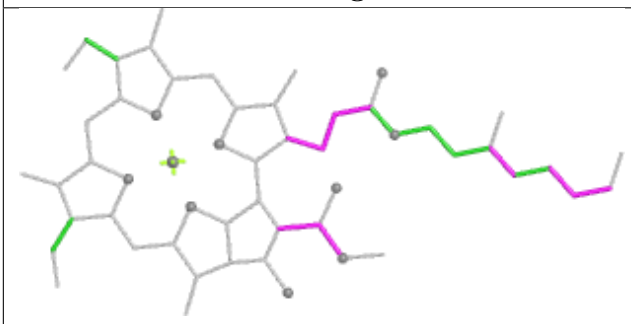
Ligand CLA B 831



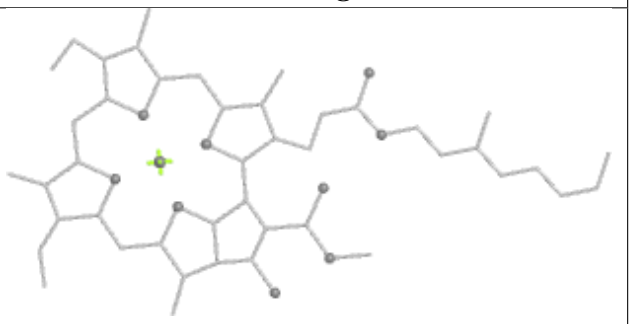
Bond lengths



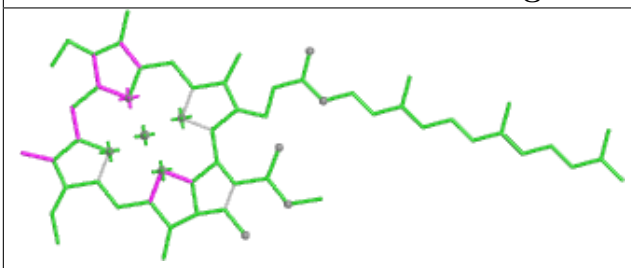
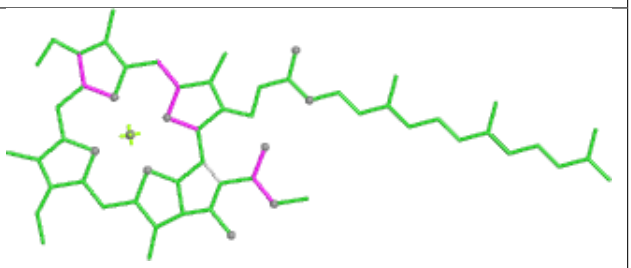
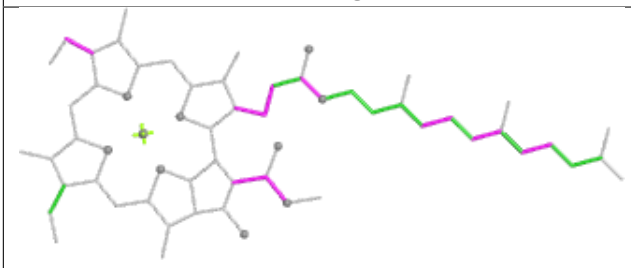
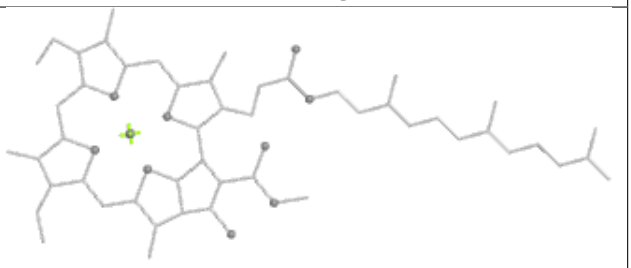
Bond angles

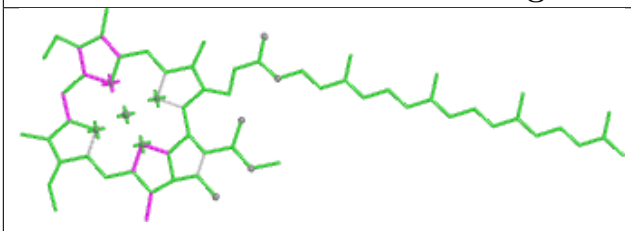
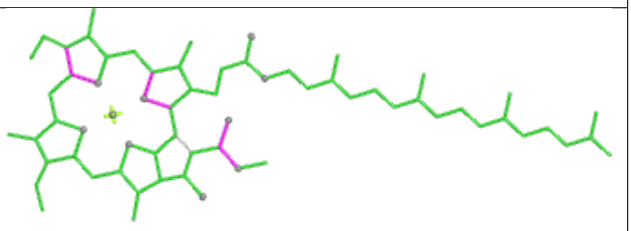
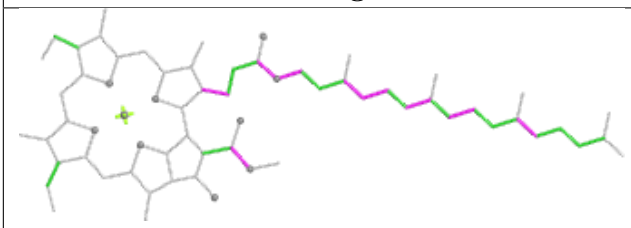
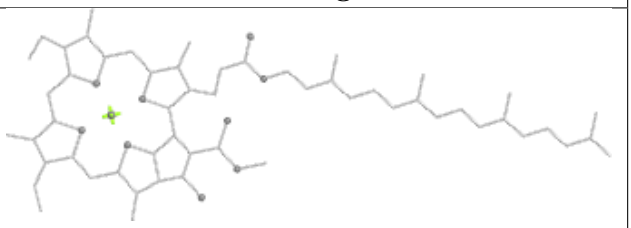


Torsions

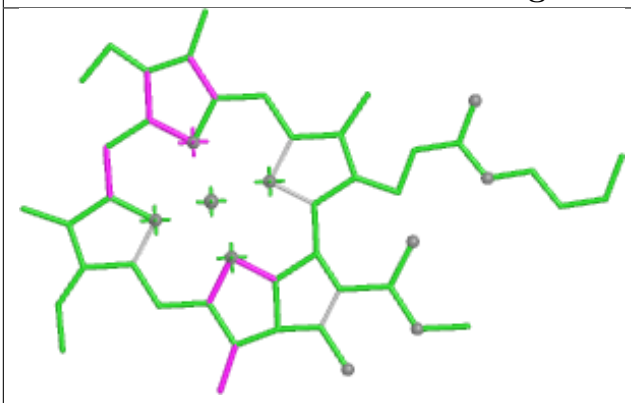


Rings

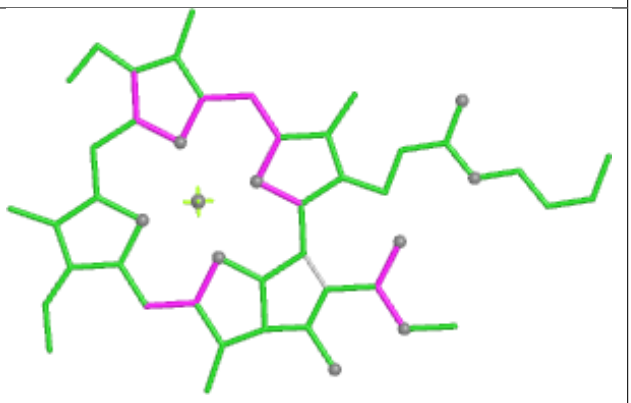
Ligand CLA A 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

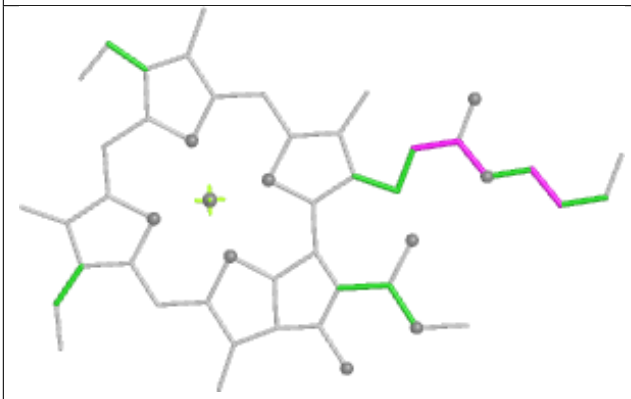
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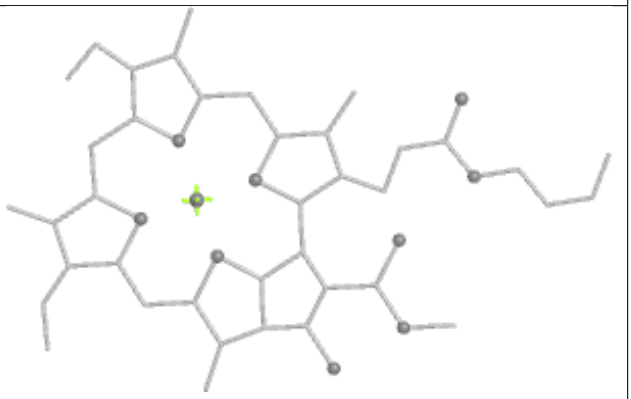
Bond lengths



Bond angles

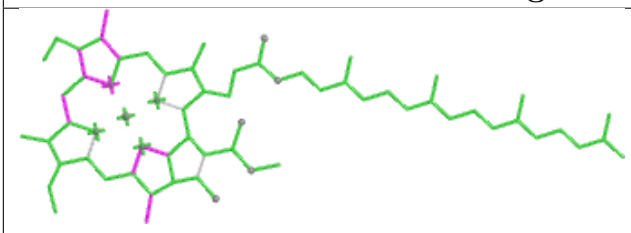


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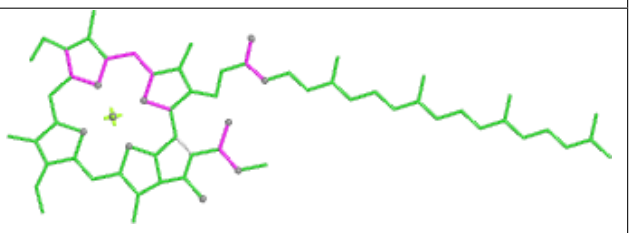


Rings

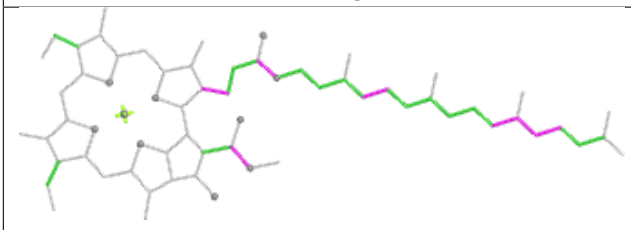
Ligand CLA n 817



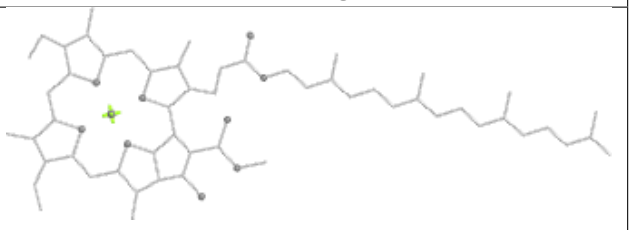
Bond lengths



Bond angles

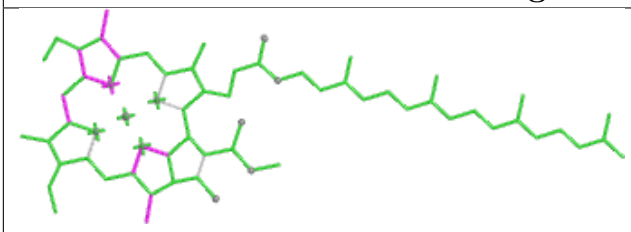


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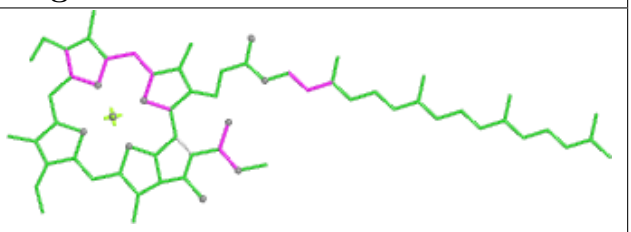


Rings

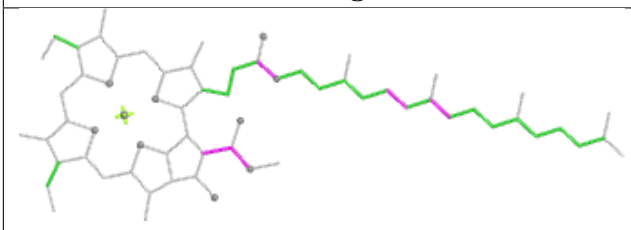
Ligand CLA g 828



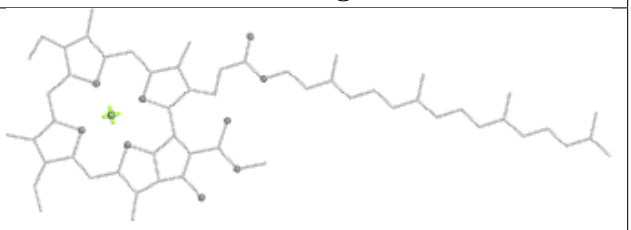
Bond lengths



Bond angles

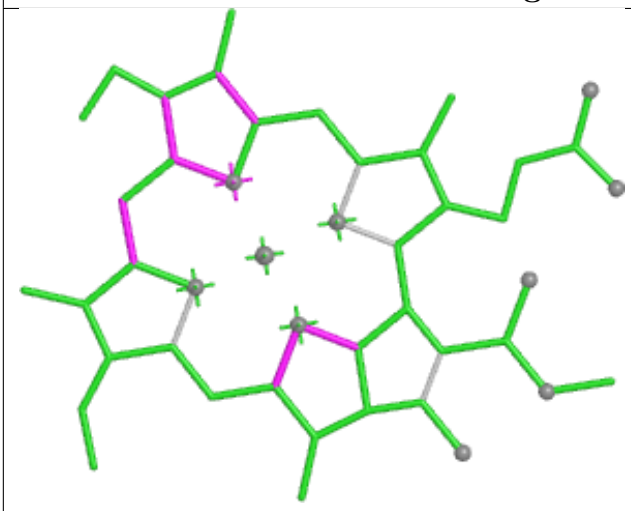


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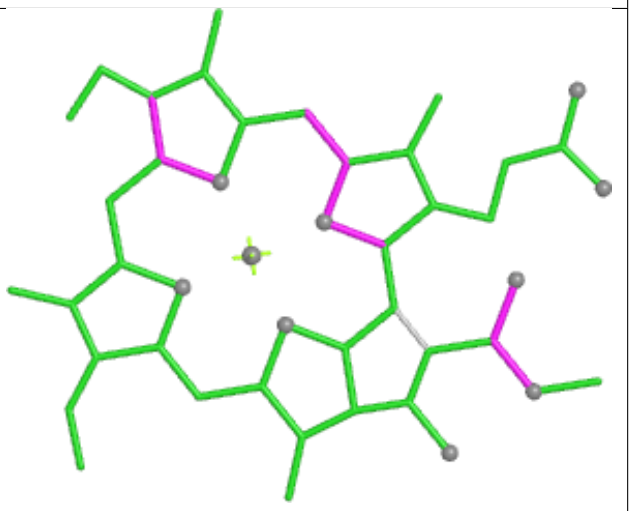


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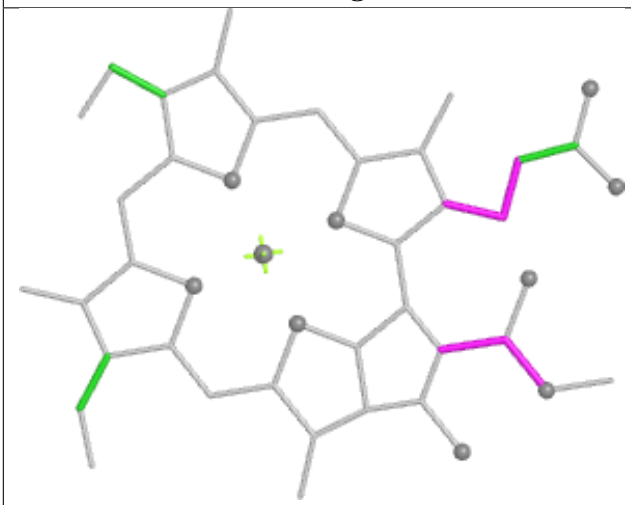
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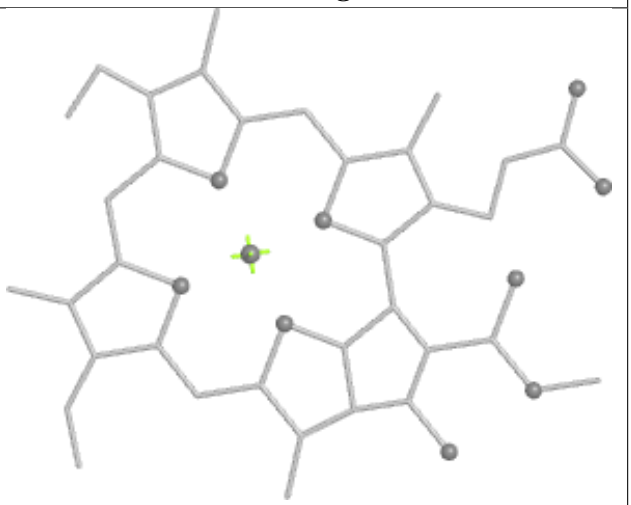
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Bond angles

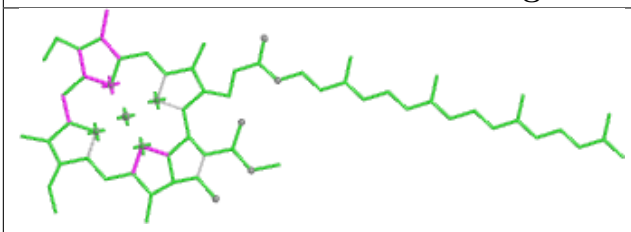


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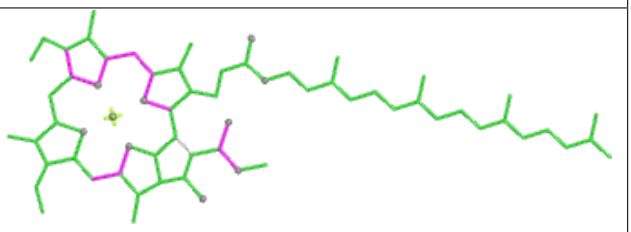


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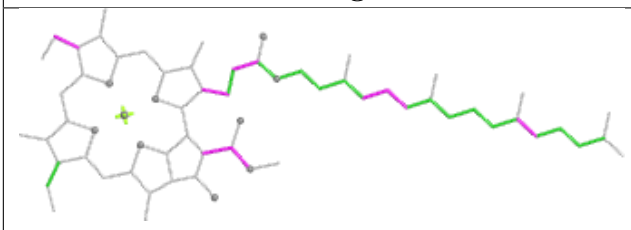
Ligand CLA G 833



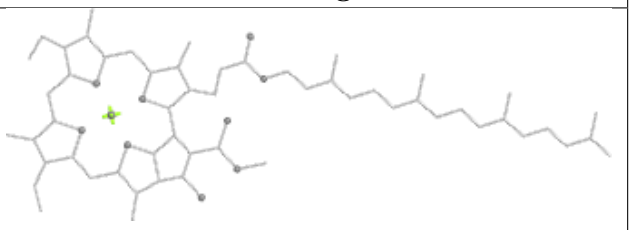
Bond lengths



Bond angles

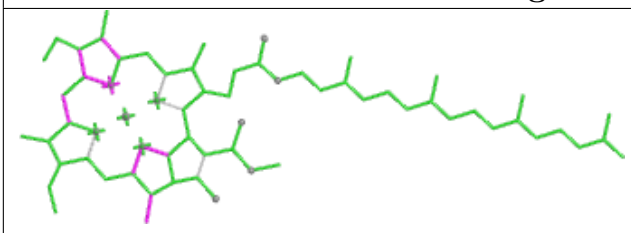


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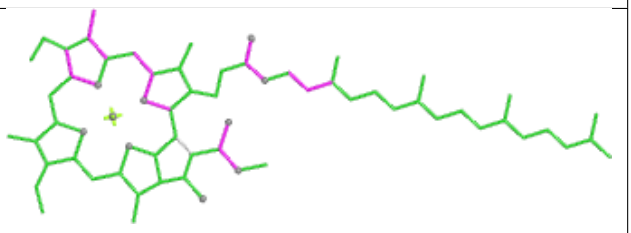


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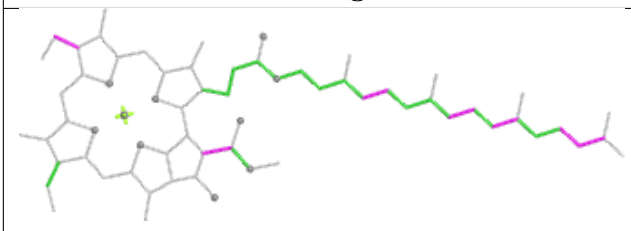
Ligand CLA a 801



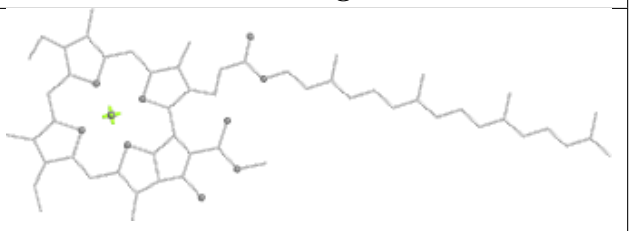
Bond lengths



Bond angles

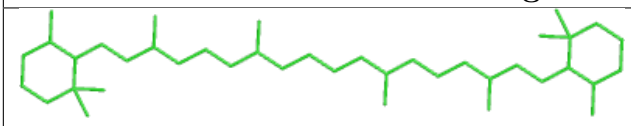


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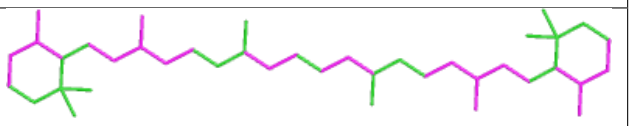


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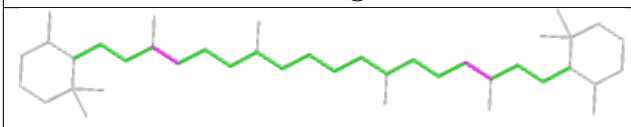
Ligand BCR B 845



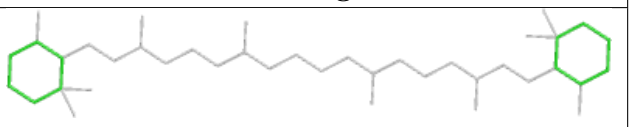
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Bond angles

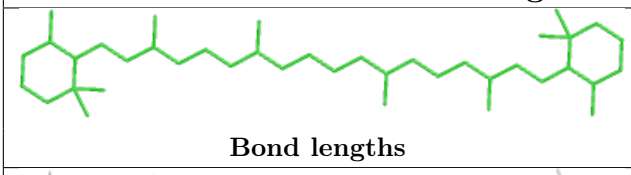


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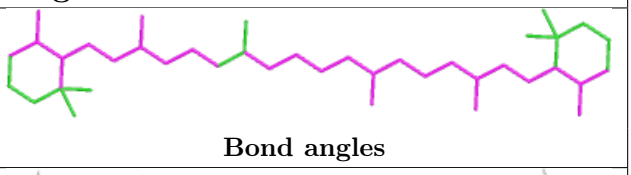


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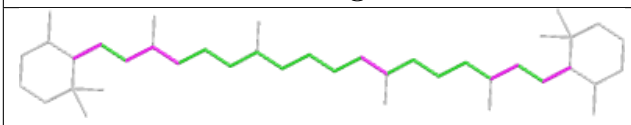
Ligand BCR g 848



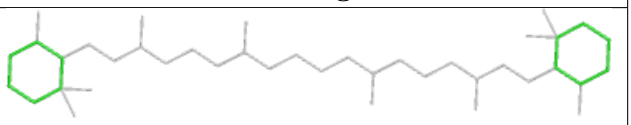
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Bond angles

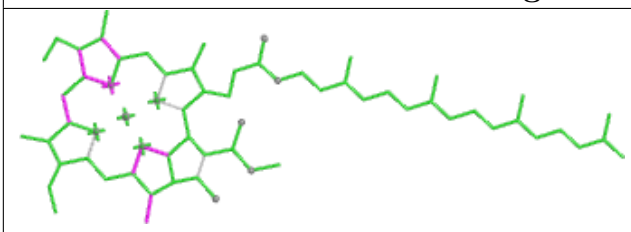


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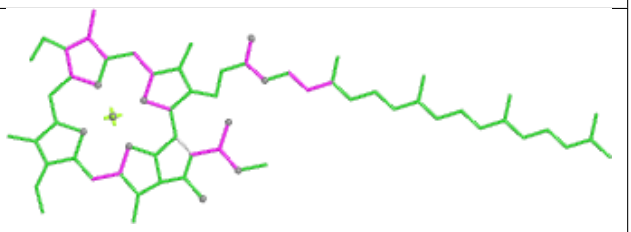


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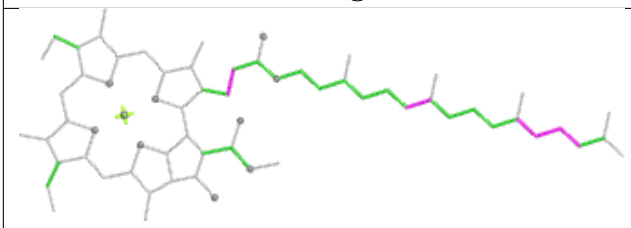
Ligand CLA N 809



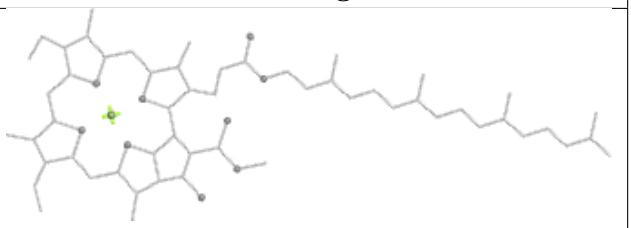
Bond lengths



Bond angles

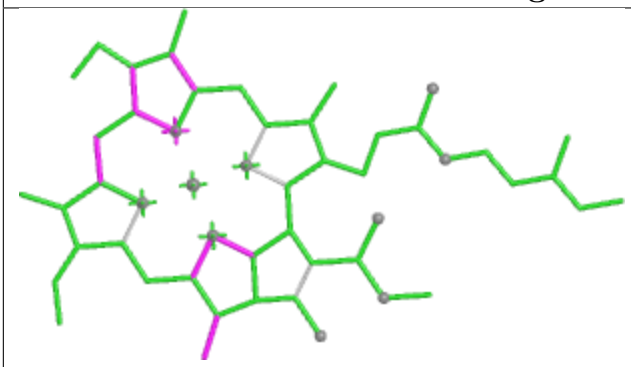


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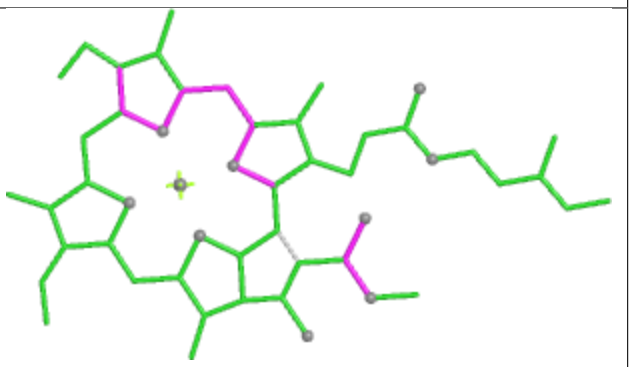


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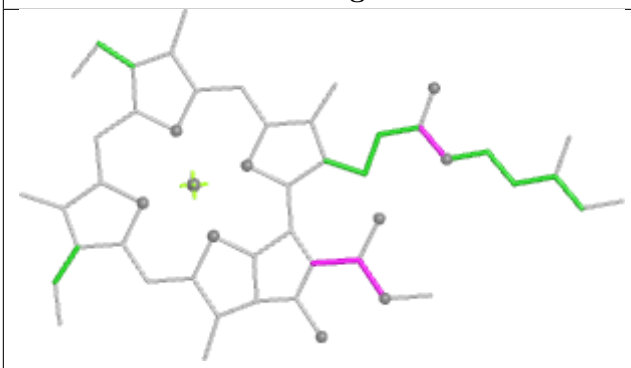
Ligand CLA a 835



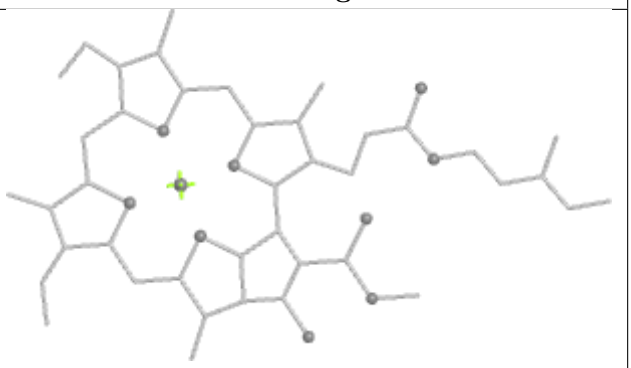
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Bond angles

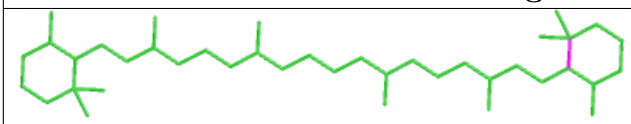


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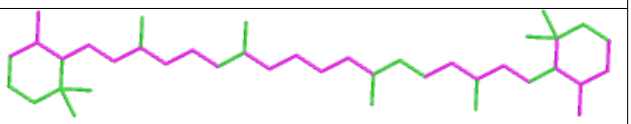


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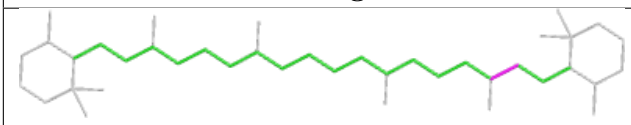
Ligand BCR n 847



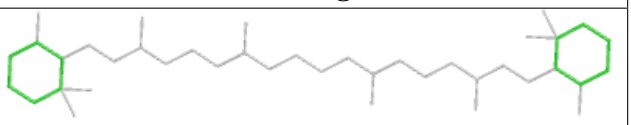
Bond lengths



Bond angles

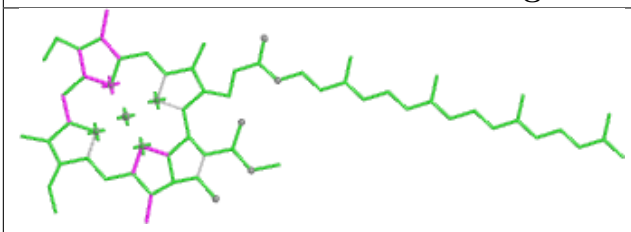


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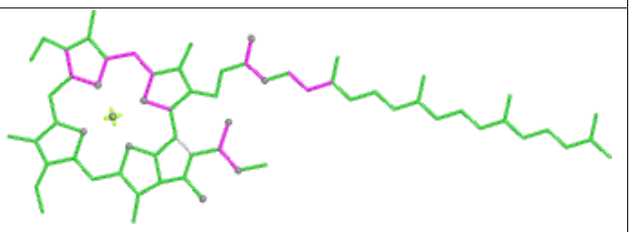


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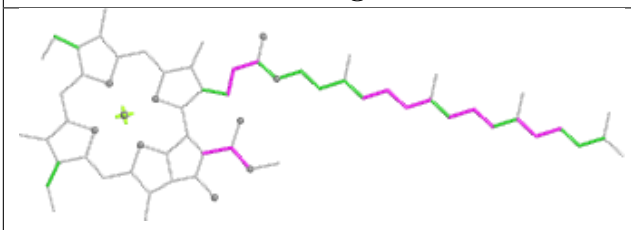
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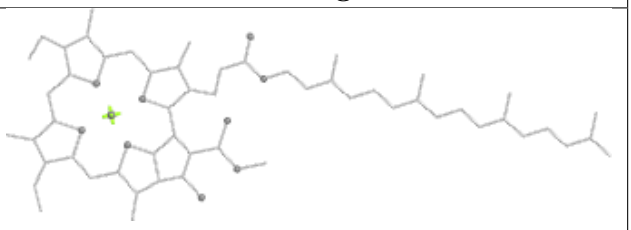
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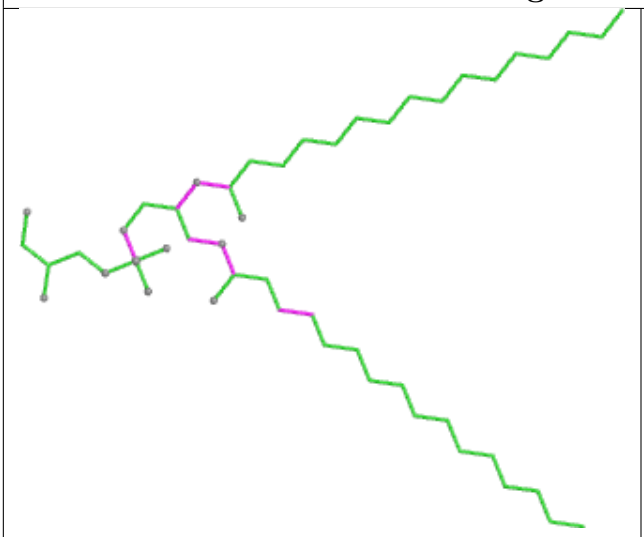


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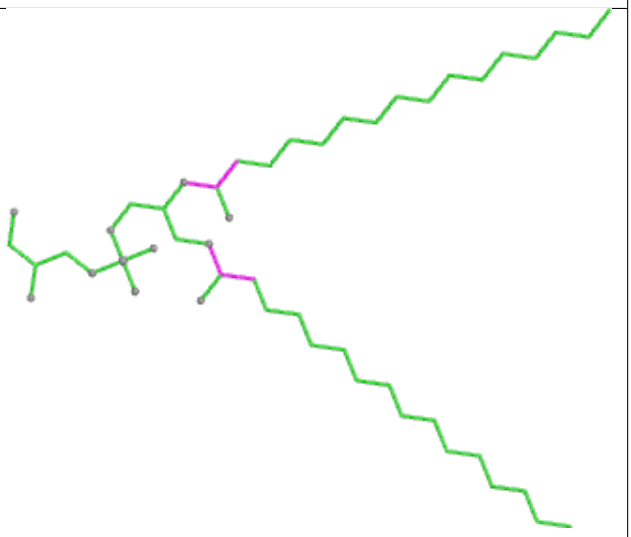


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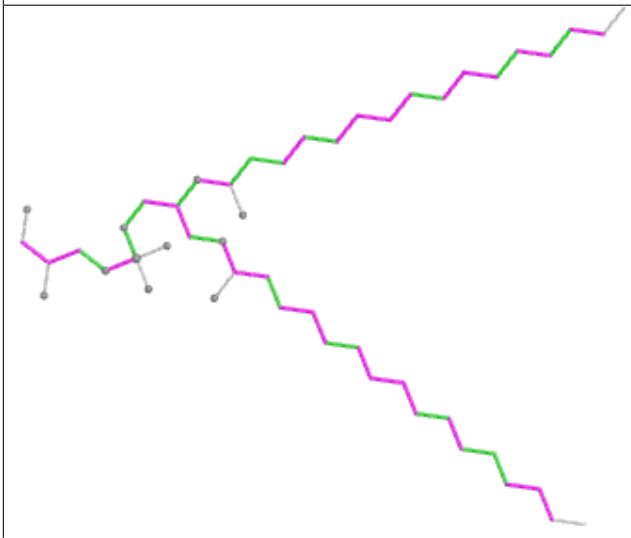
Ligand LHG a 850



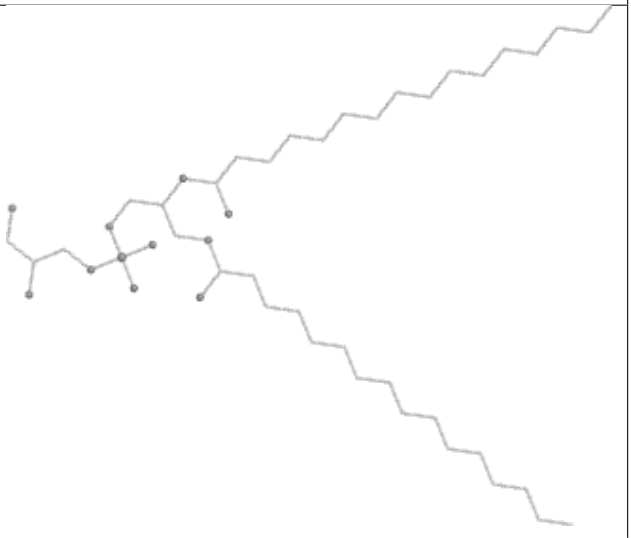
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Bond angles

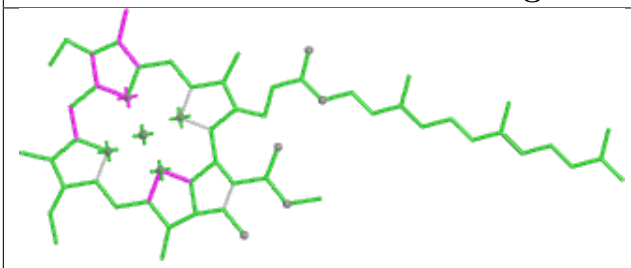


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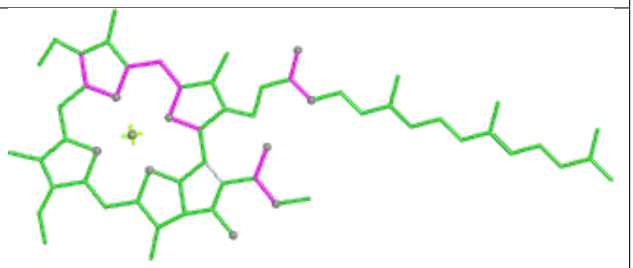


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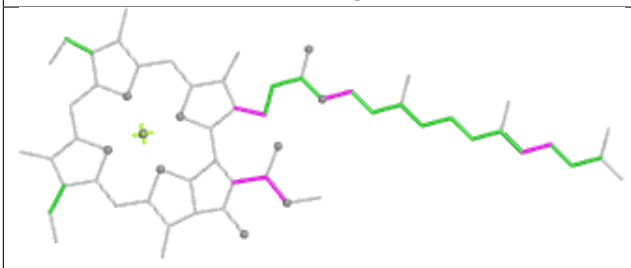
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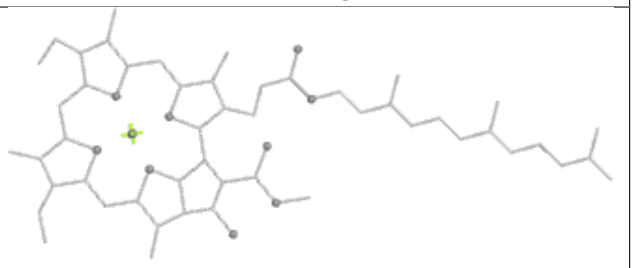
Bond lengths



Bond angles

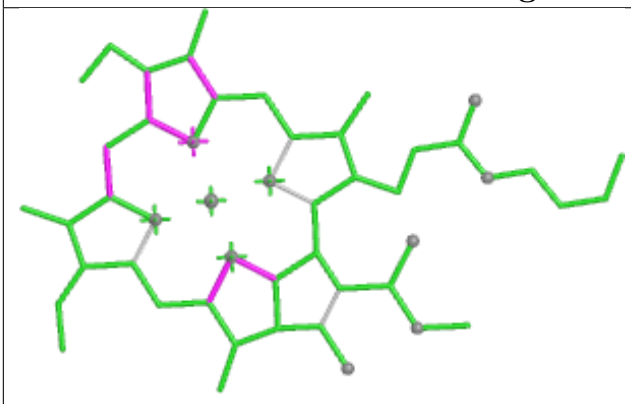


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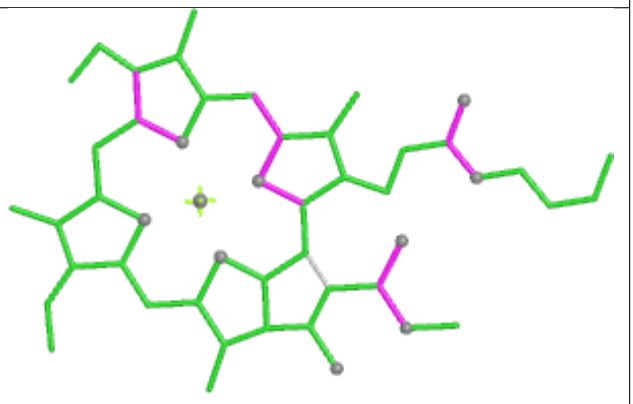


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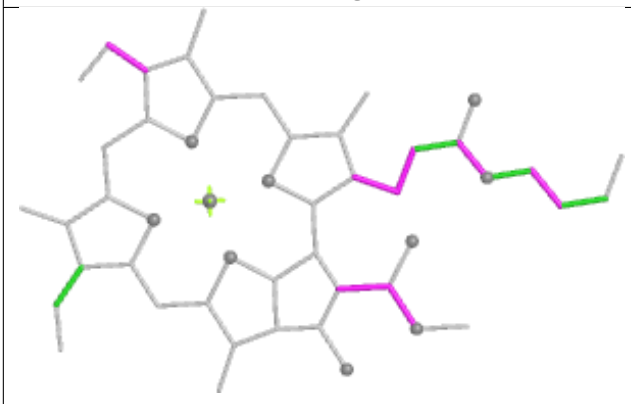
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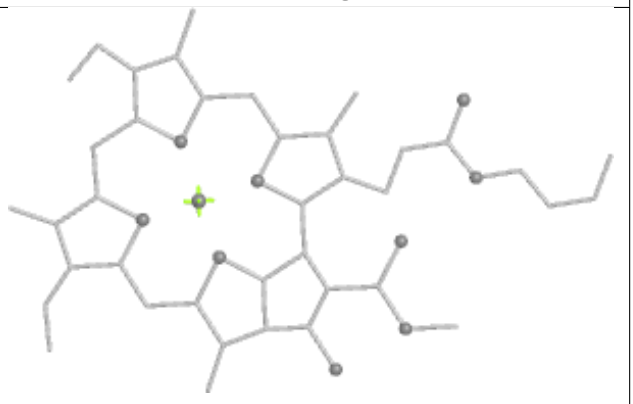
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Bond angles

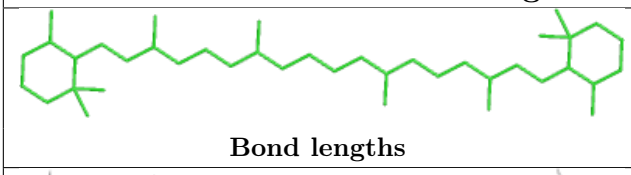


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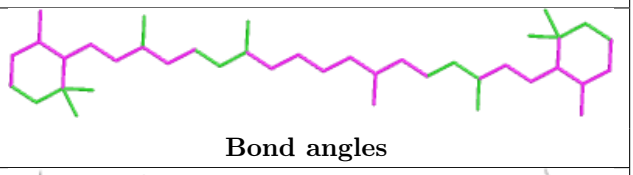


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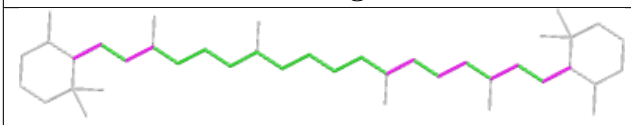
Ligand BCR B 844



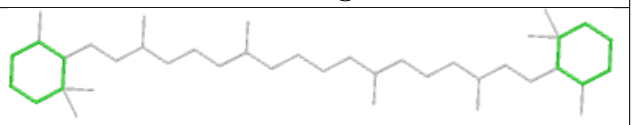
Bond lengths



Bond angles

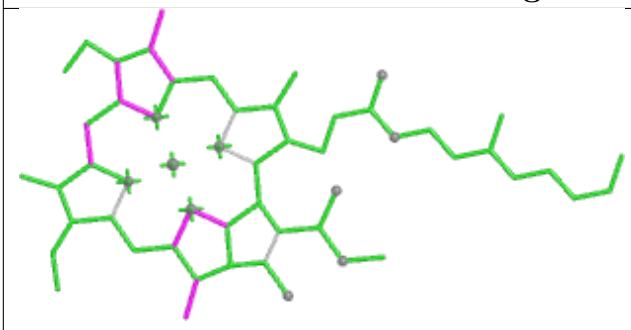


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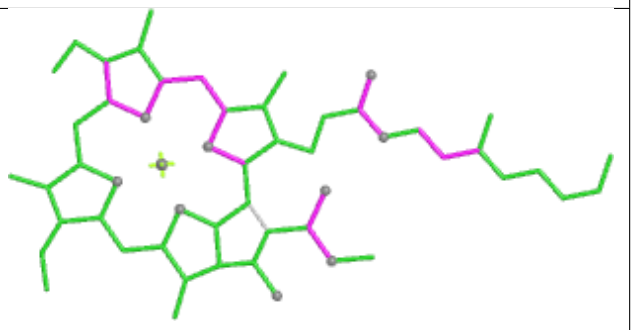


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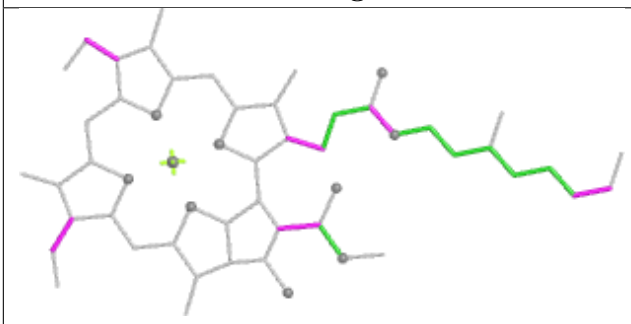
Ligand CLA N 814



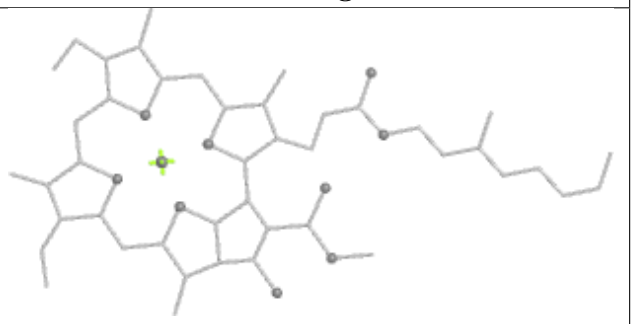
Bond lengths



Bond angles

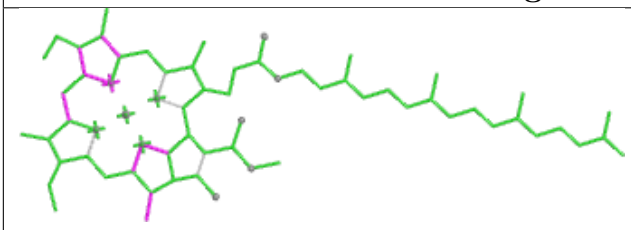


Torsions

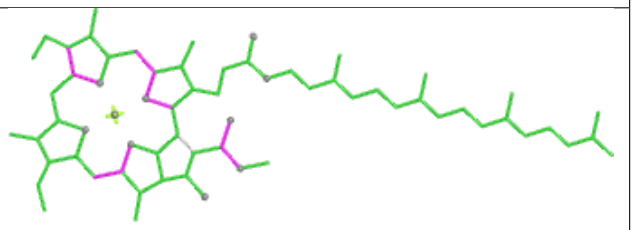


Rings

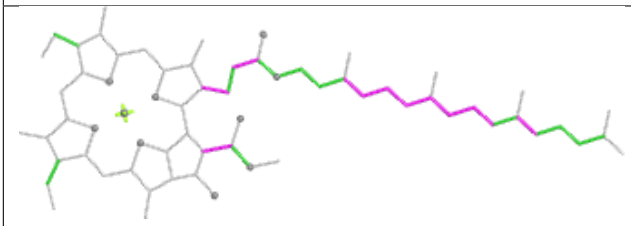
Ligand CLA B 824



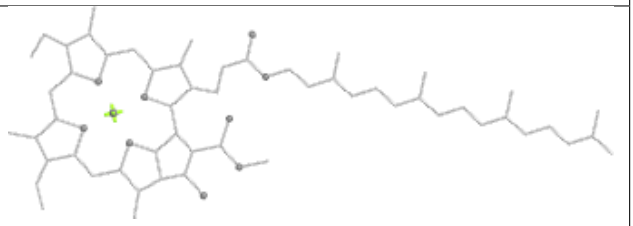
Bond lengths



Bond angles

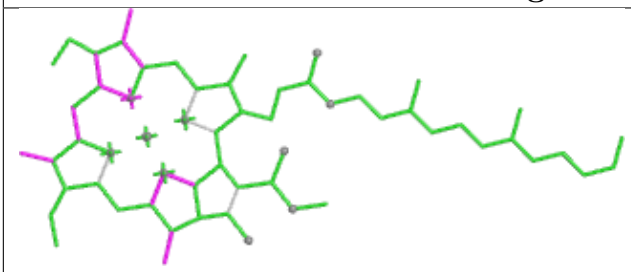


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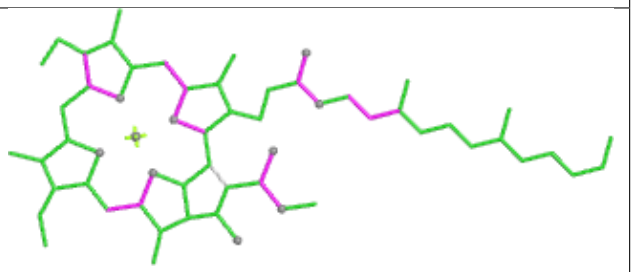


Rings

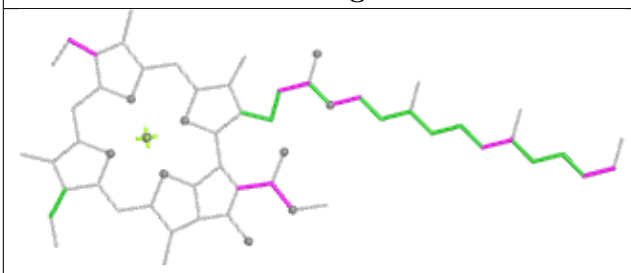
Ligand CLA S 201



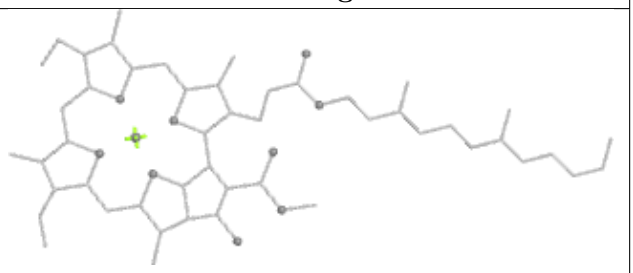
Bond lengths



Bond angles

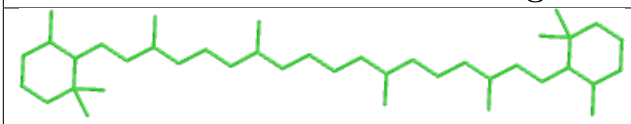


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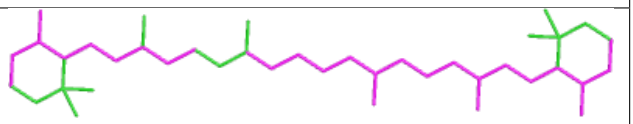


Rings

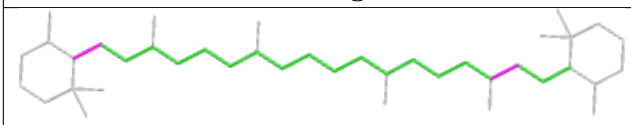
Ligand BCR a 844



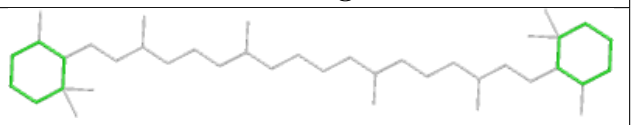
Bond lengths



Bond angles



Torsions

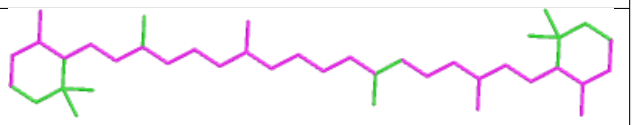


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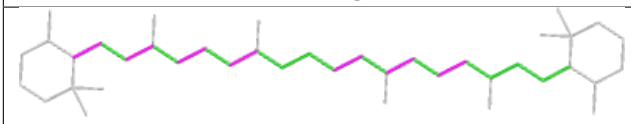
Ligand BCR b 845



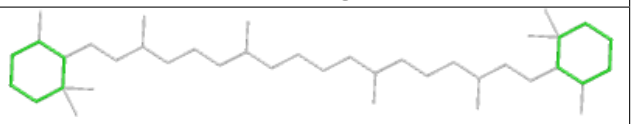
Bond lengths



Bond angles

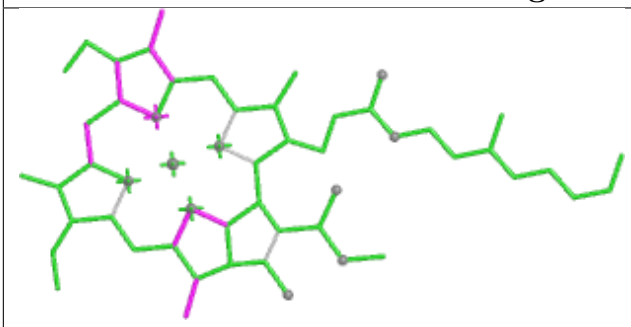


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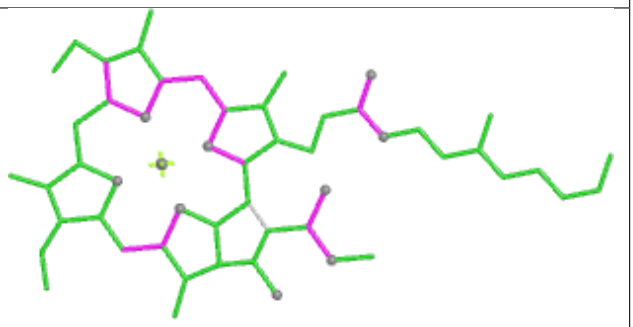


Rings

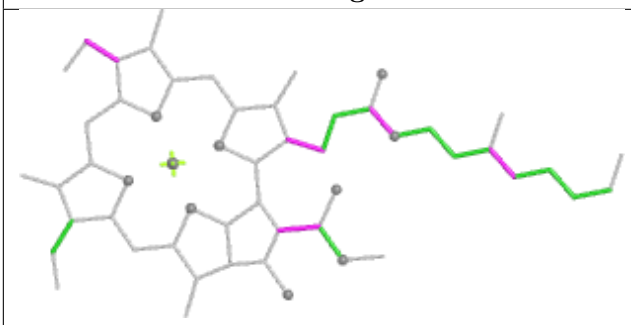
Ligand CLA a 824



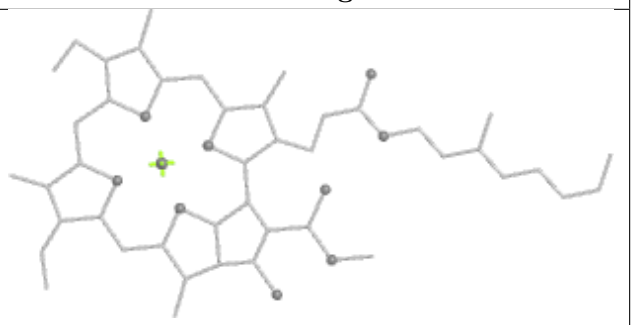
Bond lengths



Bond angles

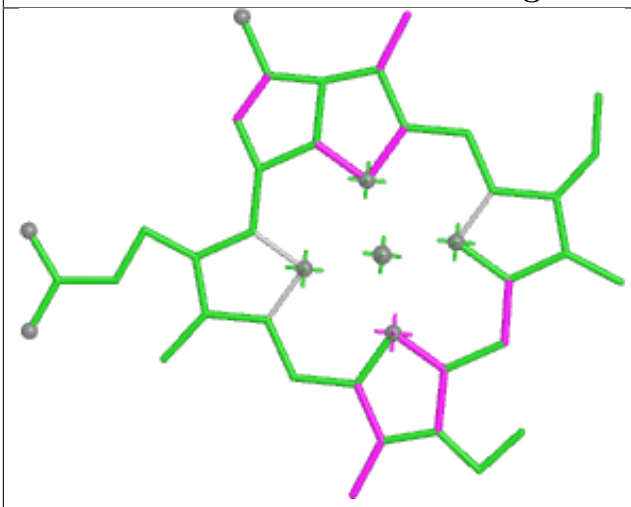


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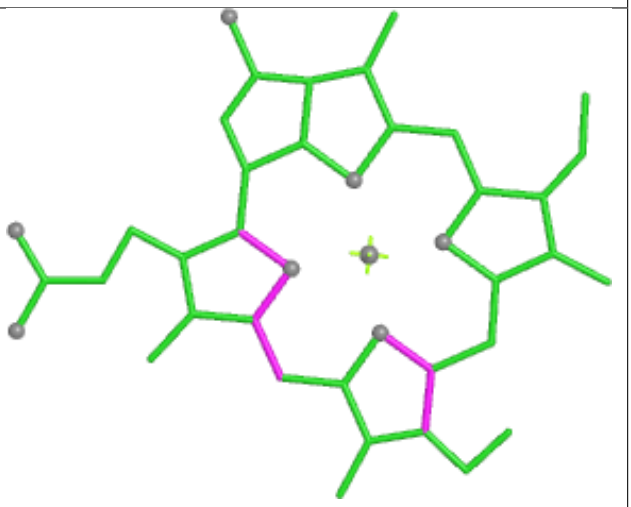


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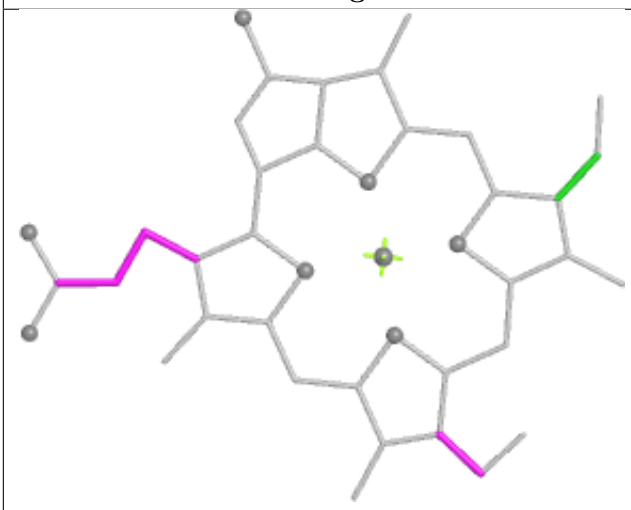
Ligand CLA K 101



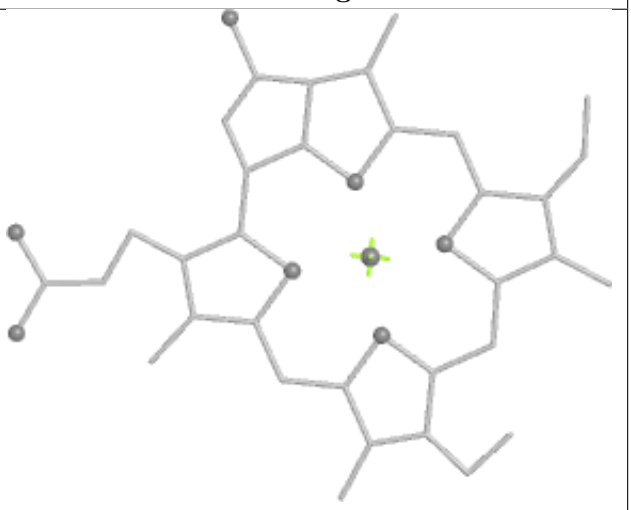
Bond lengths



Bond angles

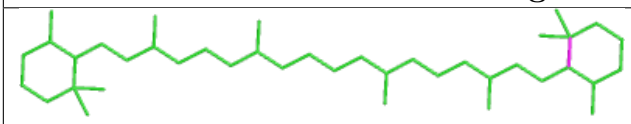


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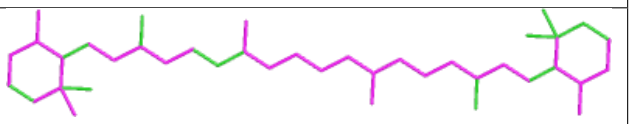


Rings

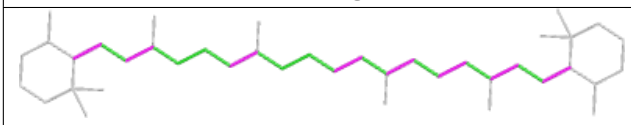
Ligand BCR I 102



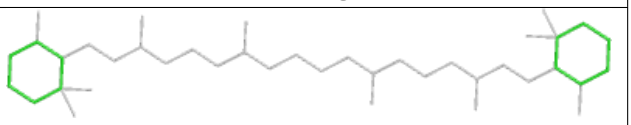
Bond lengths



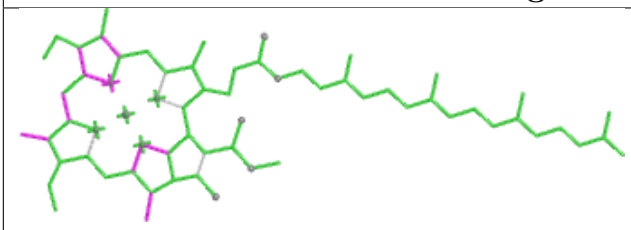
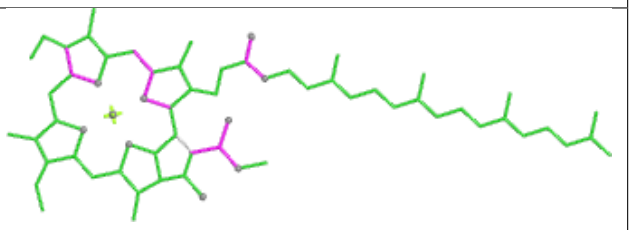
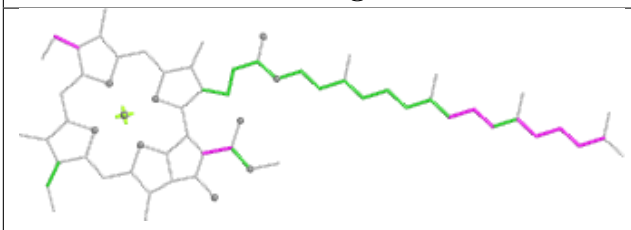
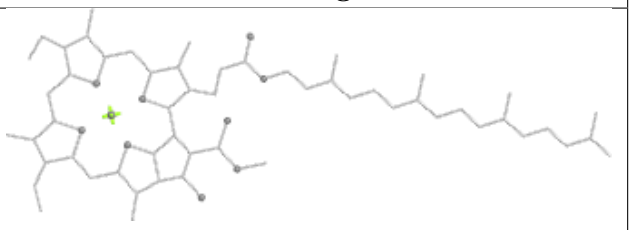
Bond angles

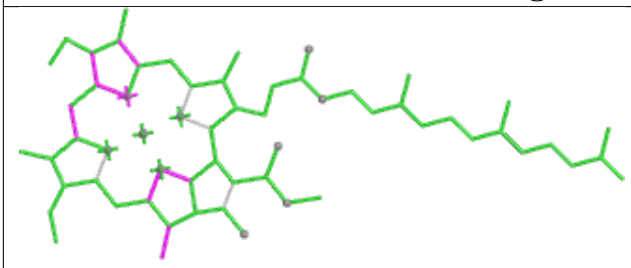
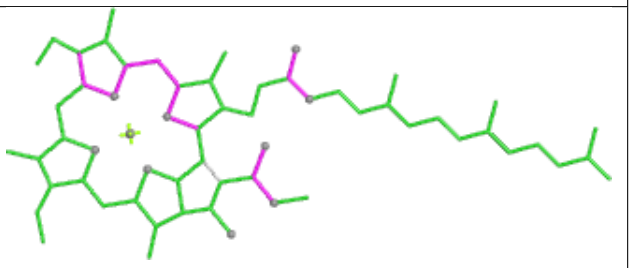
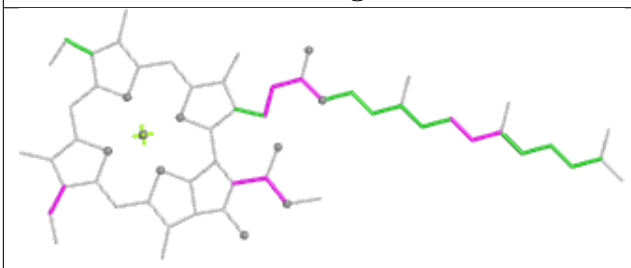
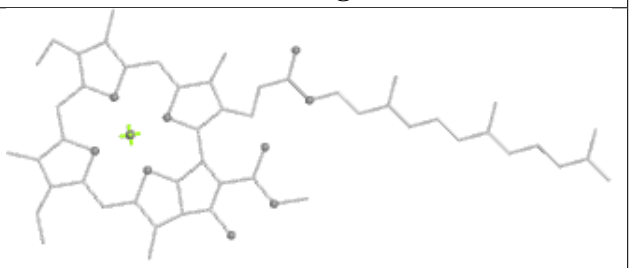


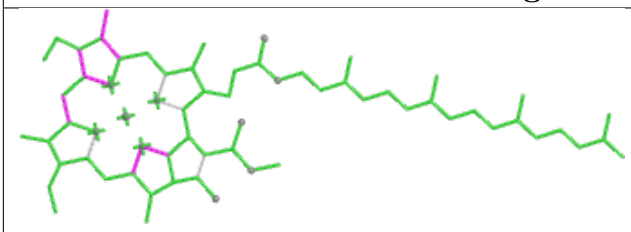
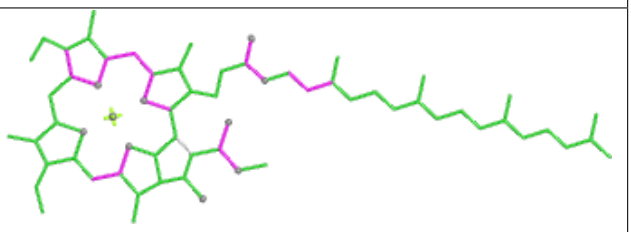
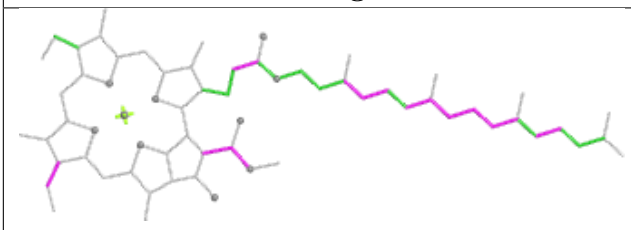
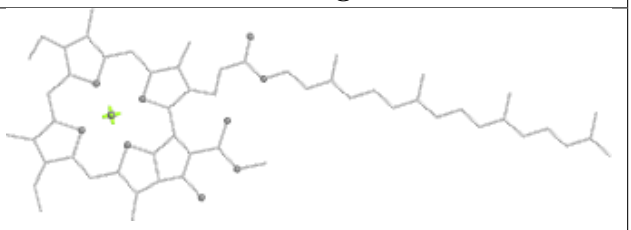
Torsions

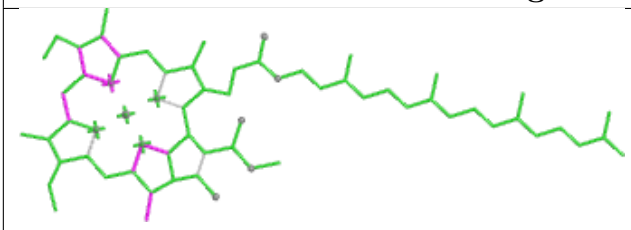
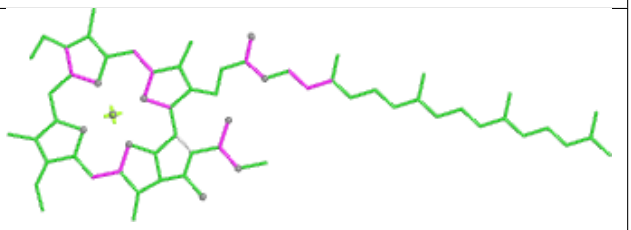
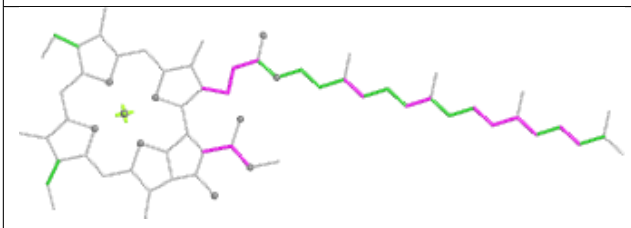
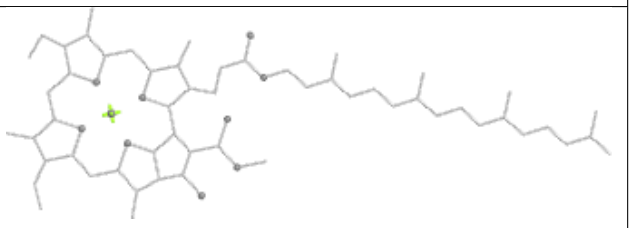


Rings

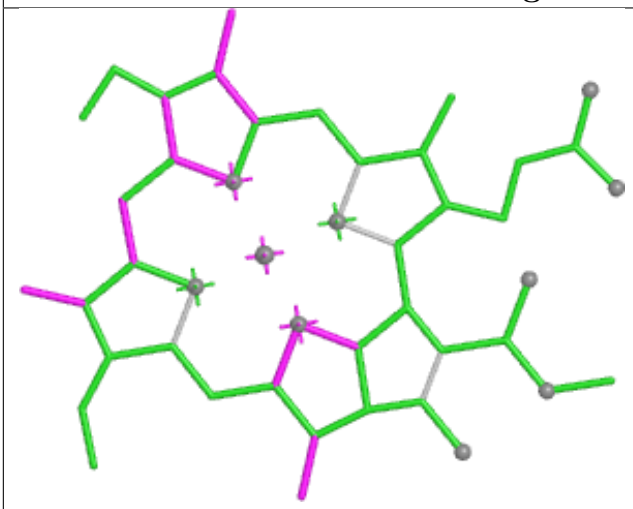
Ligand CLA n 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

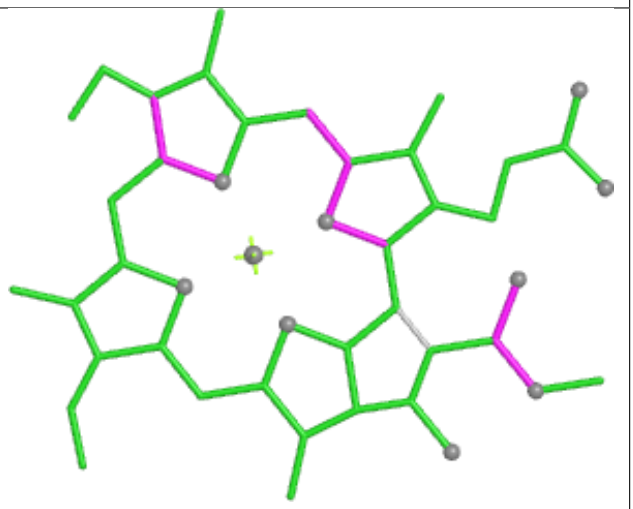
Ligand CLA N 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

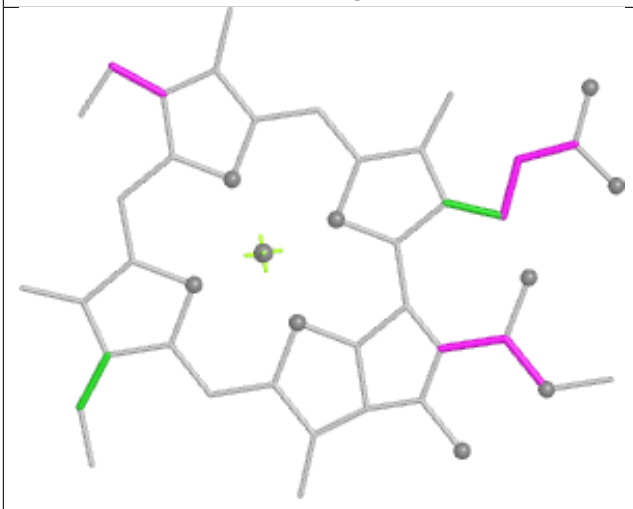
Ligand CLA G 852



Bond lengths



Bond angles

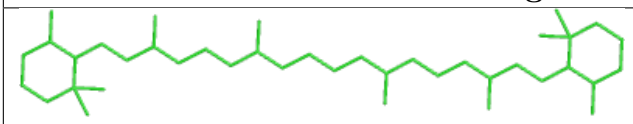


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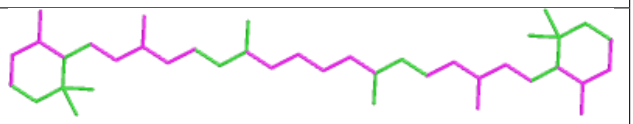


Rings

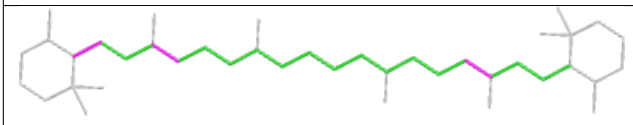
Ligand BCR n 844



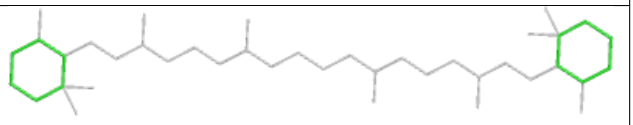
Bond lengths



Bond angles

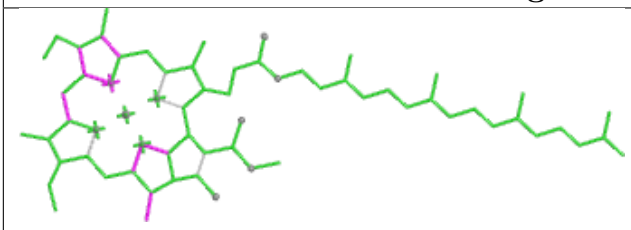


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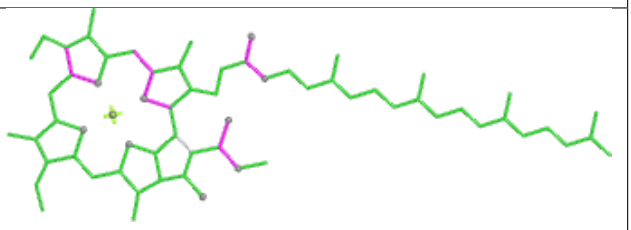


Rings

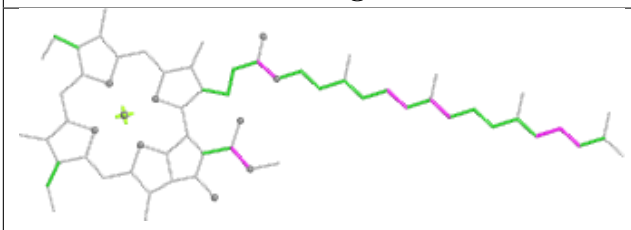
Ligand CLA n 824



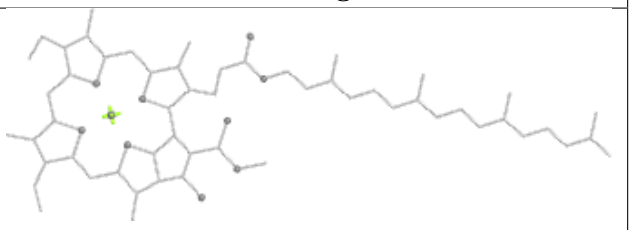
Bond lengths



Bond angles

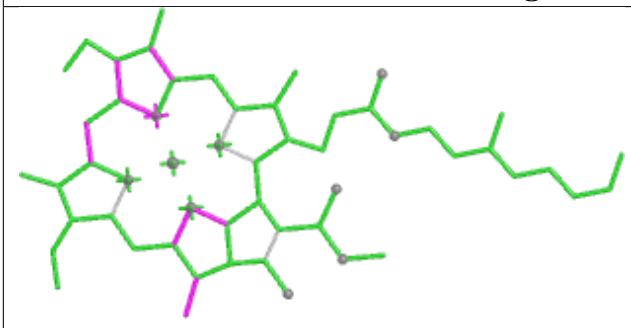


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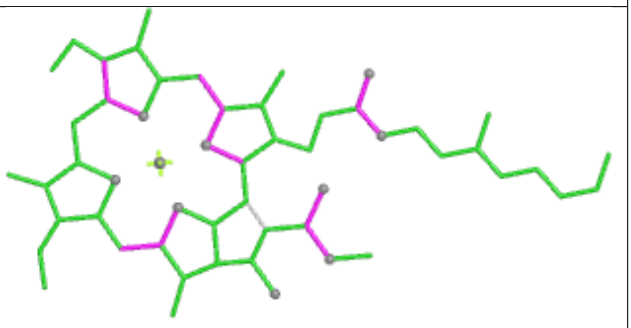


Rings

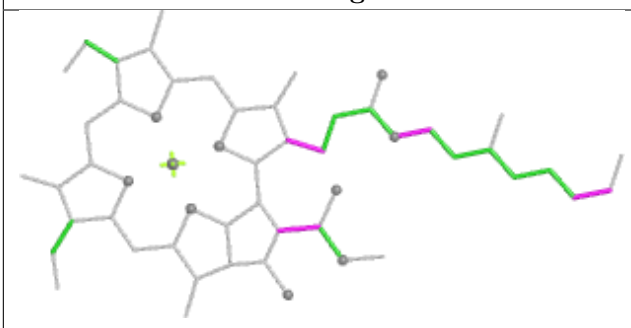
Ligand CLA G 825



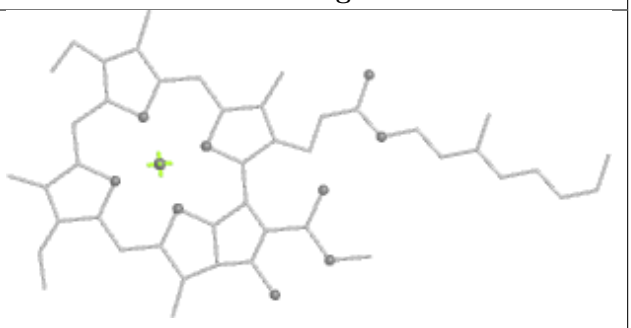
Bond lengths



Bond angles

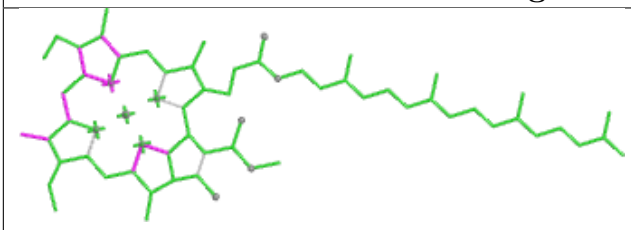


Torsions

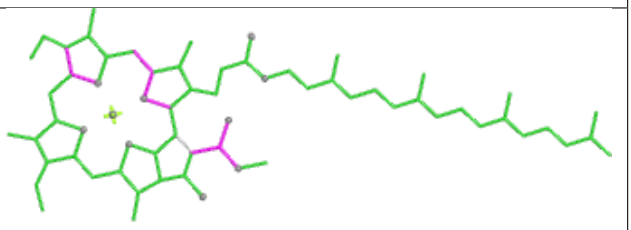


Rings

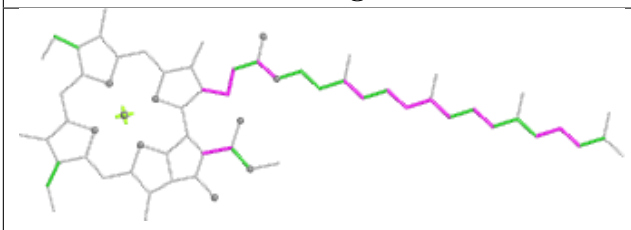
Ligand CLA a 855



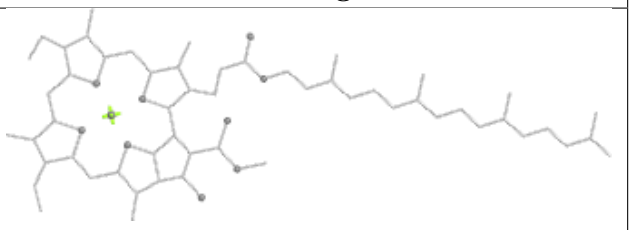
Bond lengths



Bond angles

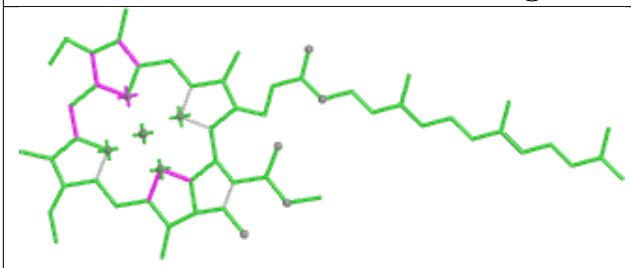


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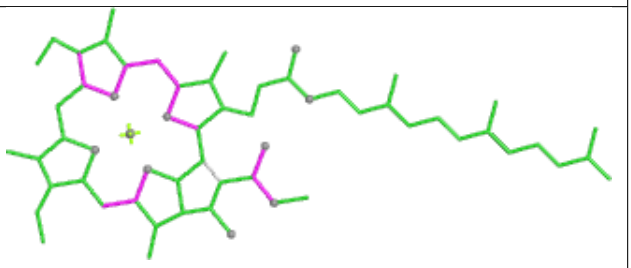


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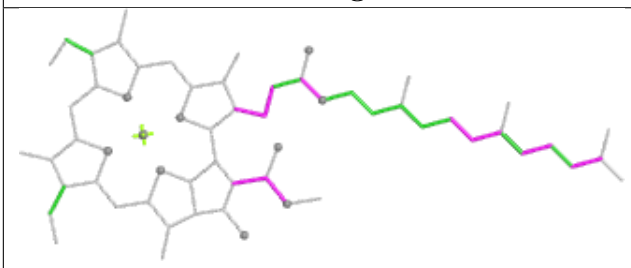
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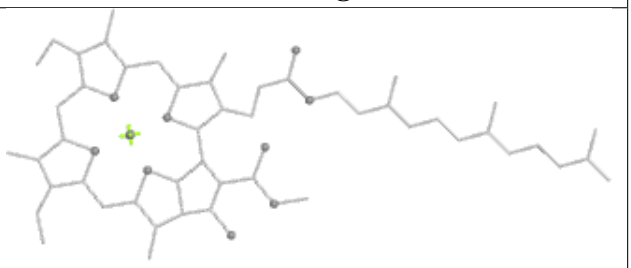
Bond lengths



Bond angles



Torsions

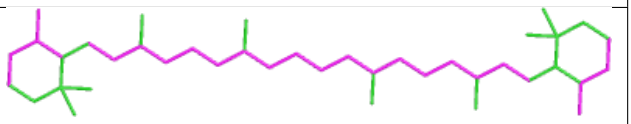


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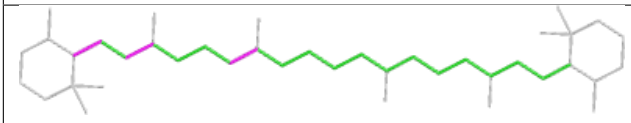
Ligand BCR b 849



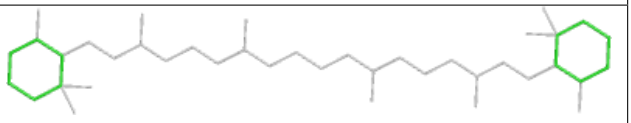
Bond lengths



Bond angles

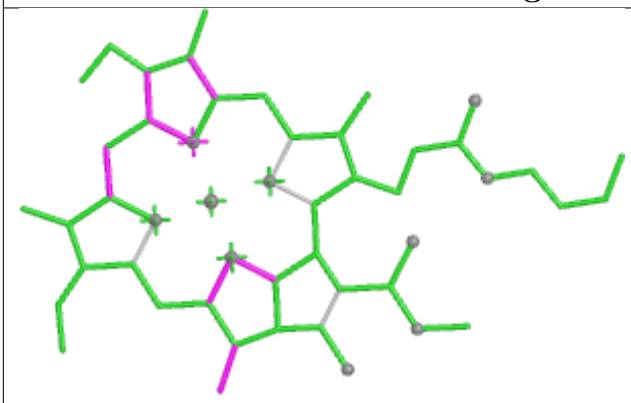


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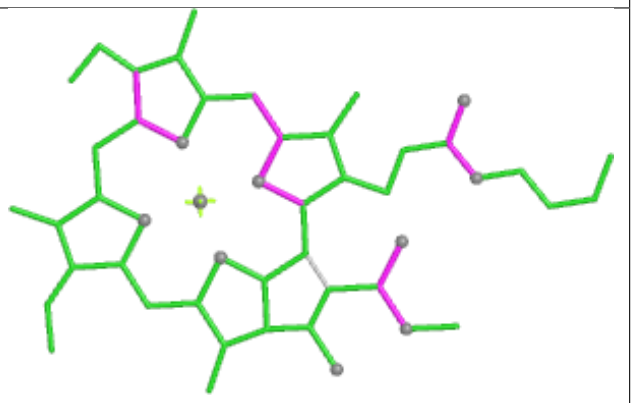


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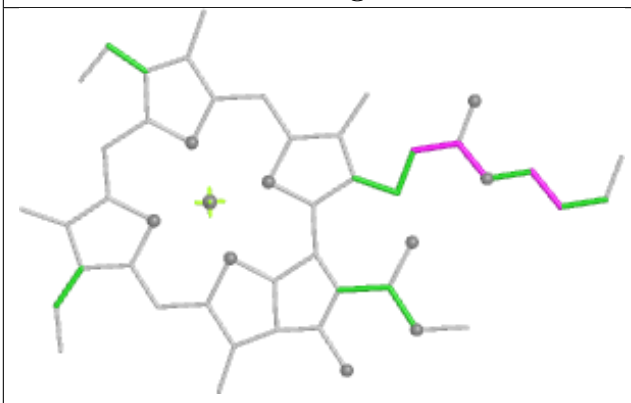
Ligand CLA A 857



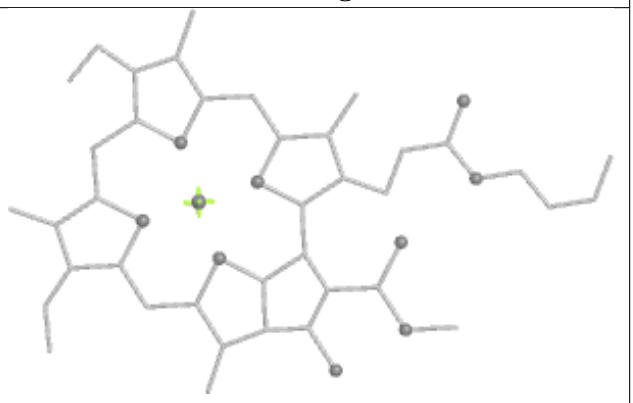
Bond lengths



Bond angles

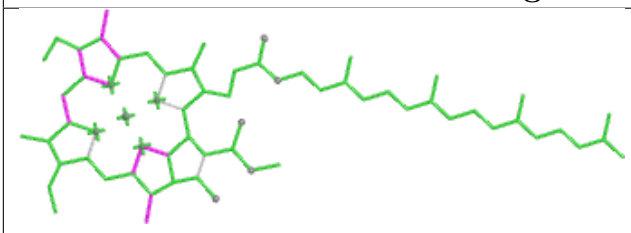


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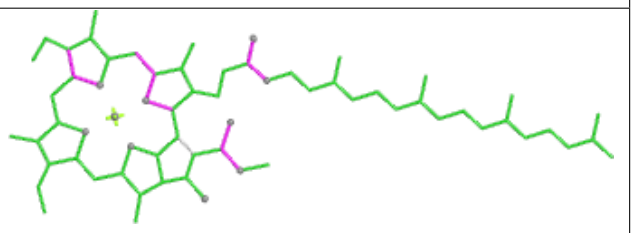


Rings

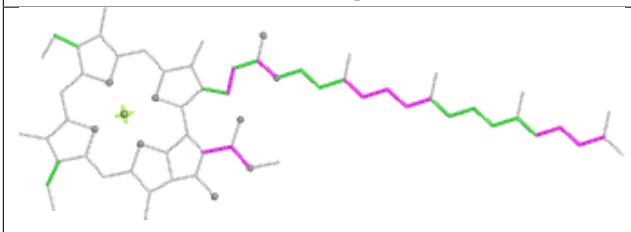
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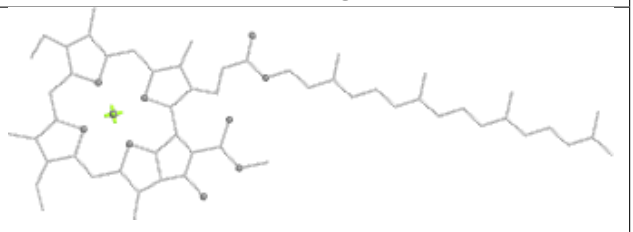
Bond lengths



Bond angles

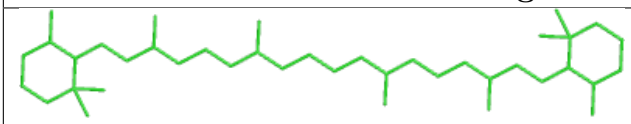


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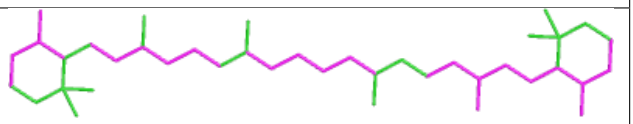


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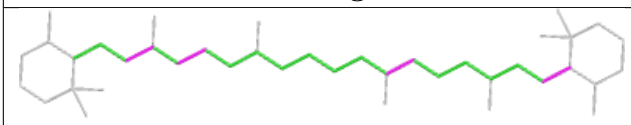
Ligand BCR W 206



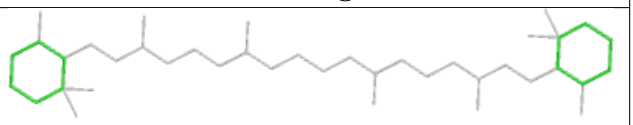
Bond lengths



Bond angles

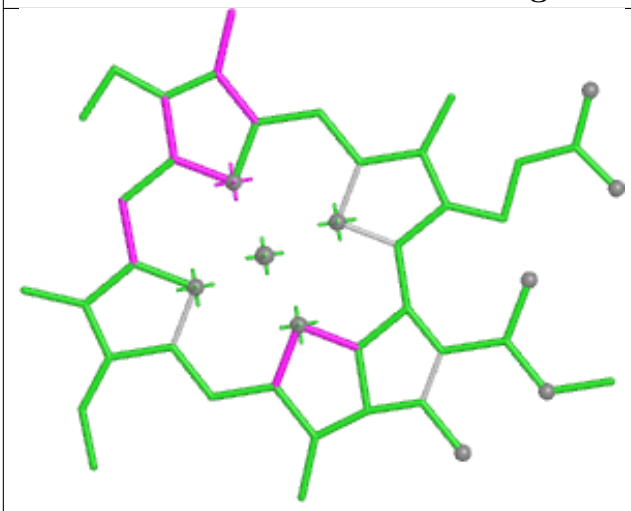


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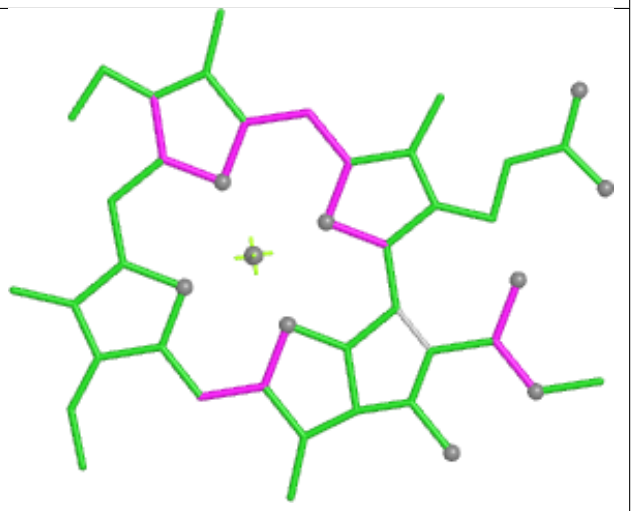


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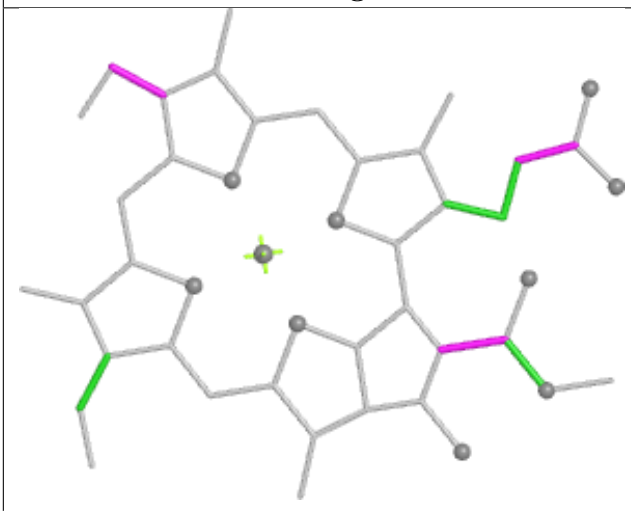
Ligand CLA s 202



Bond lengths



Bond angles

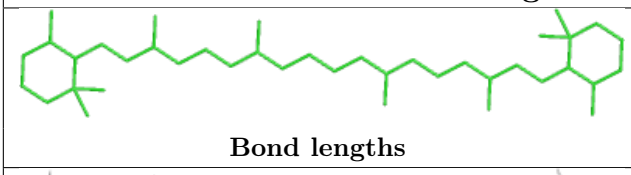


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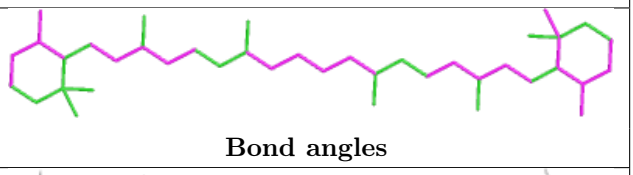


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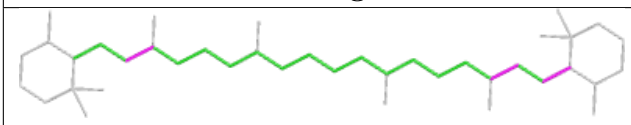
Ligand BCR w 206



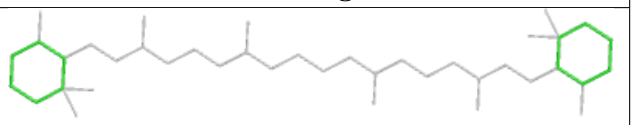
Bond lengths



Bond angles

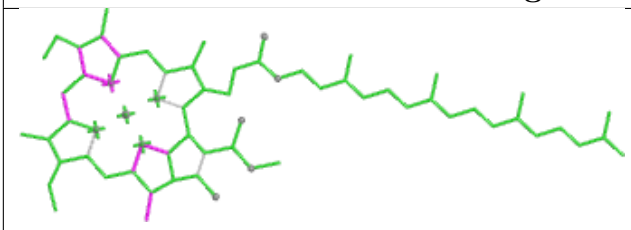


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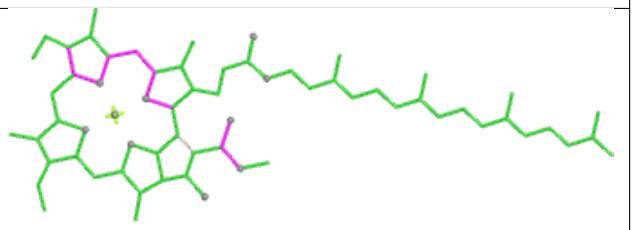


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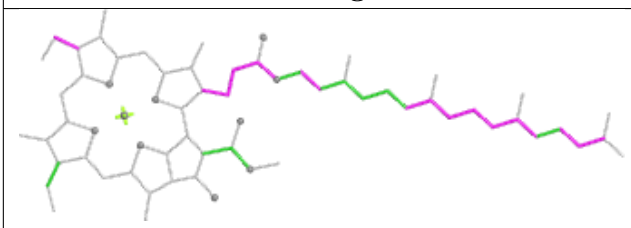
Ligand CLA B 818



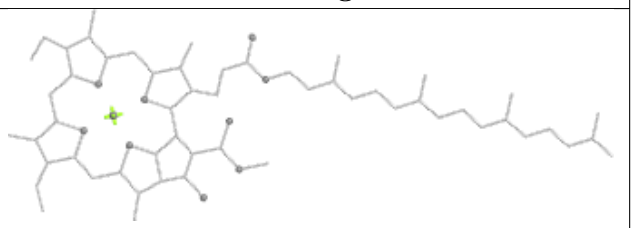
Bond lengths



Bond angles

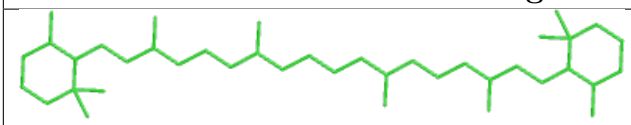


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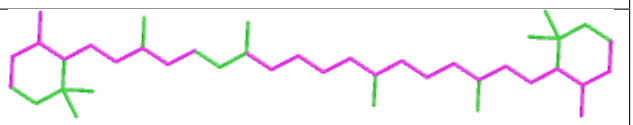


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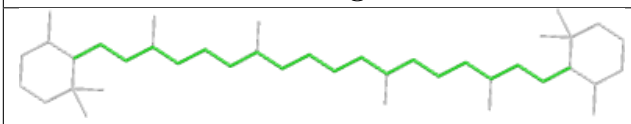
Ligand BCR k 102



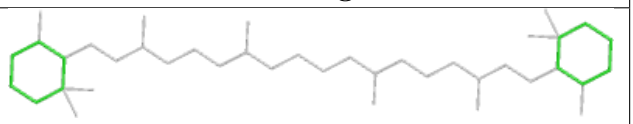
Bond lengths



Bond angles

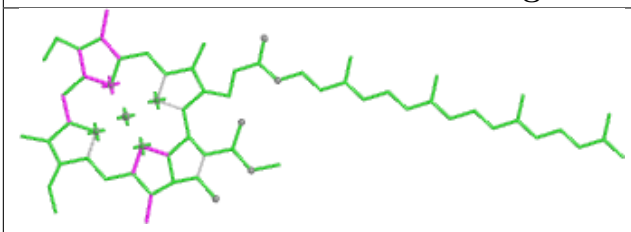


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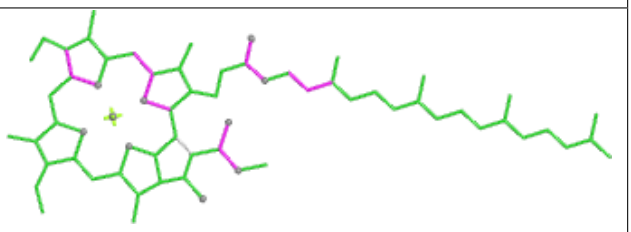


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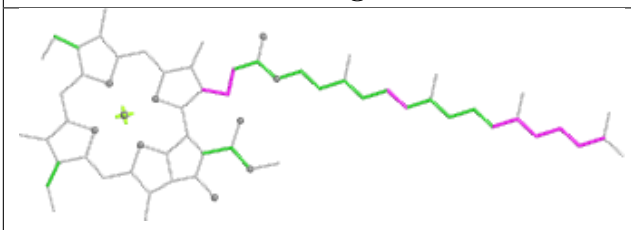
Ligand CLA G 828



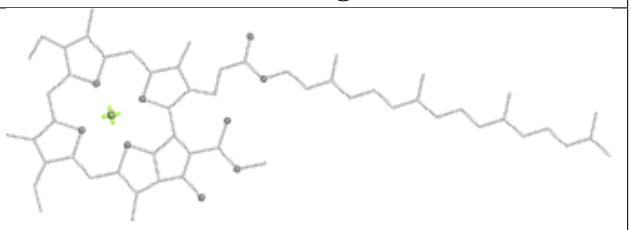
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Bond angles

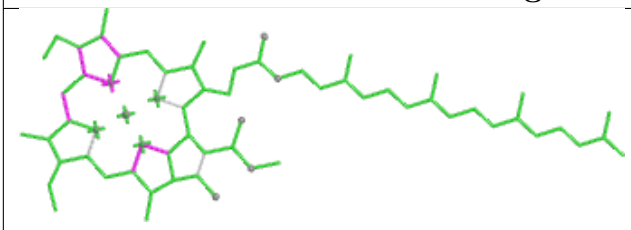


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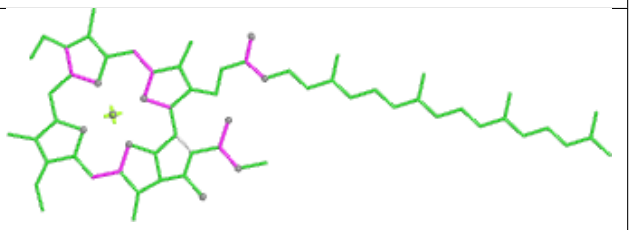


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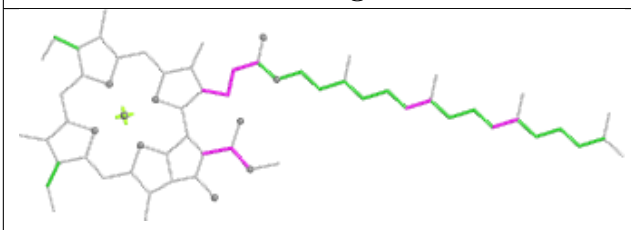
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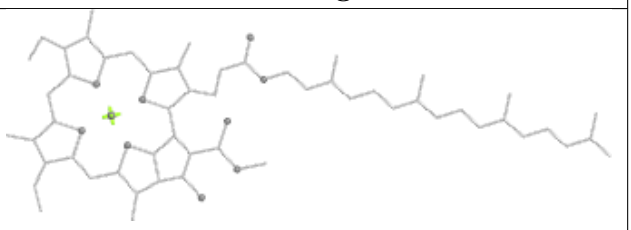
Bond lengths



Bond angles

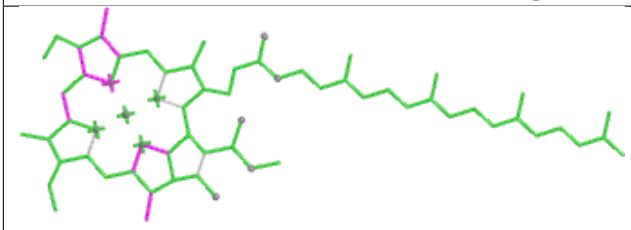


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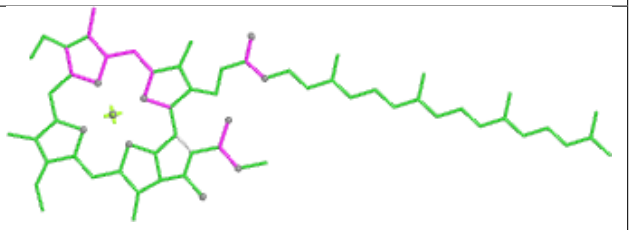


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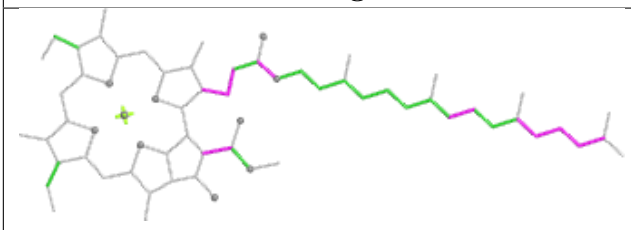
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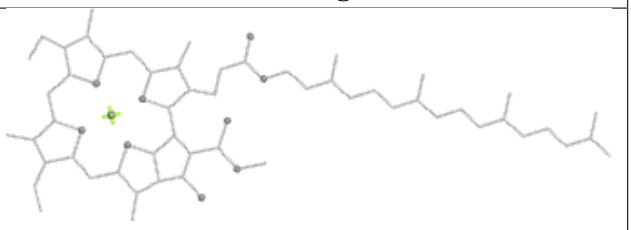
Bond lengths



Bond angles

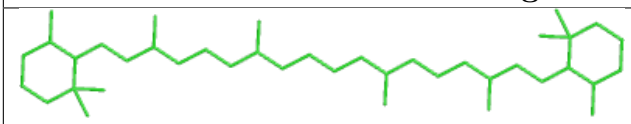


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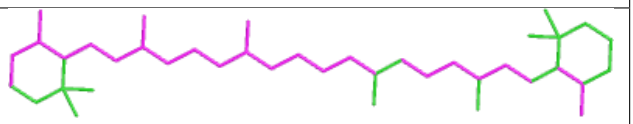


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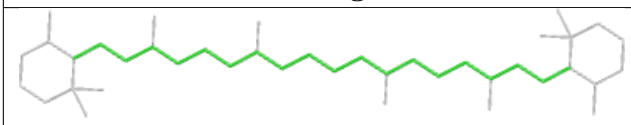
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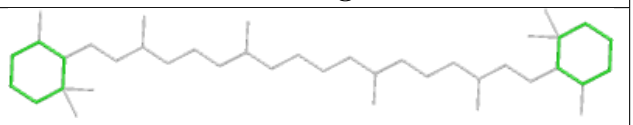
Bond lengths



Bond angles

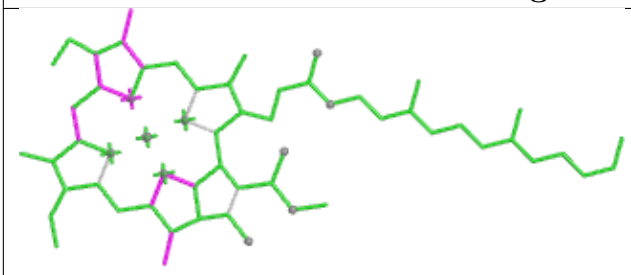


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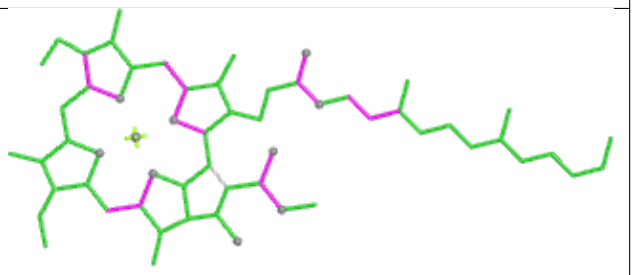


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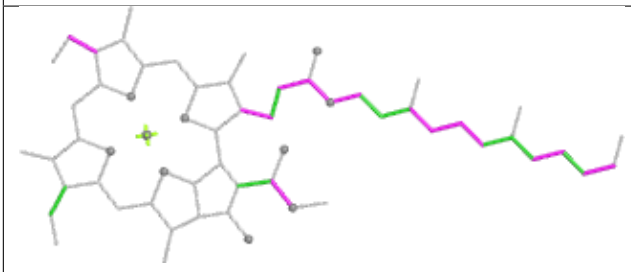
Ligand CLA s 201



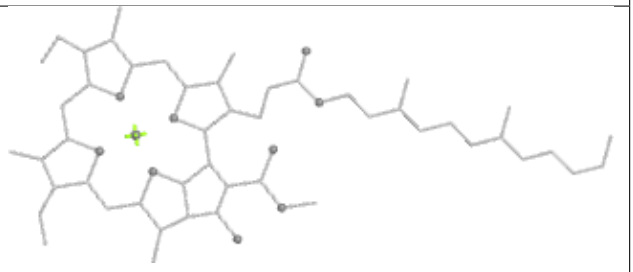
Bond lengths



Bond angles

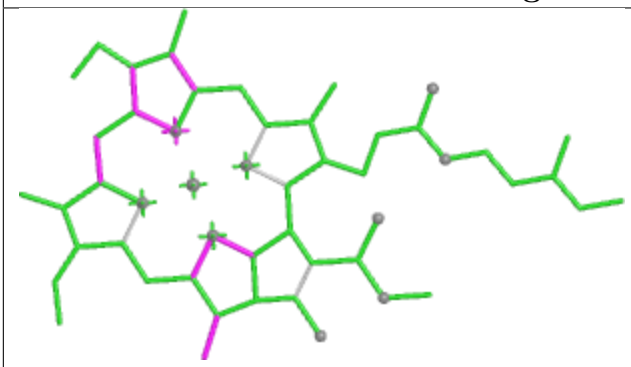


Torsions

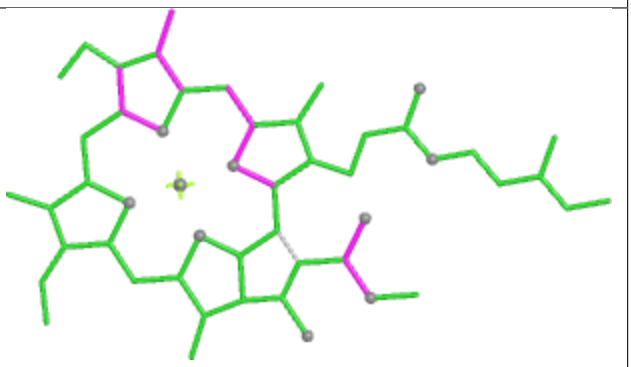


Rings

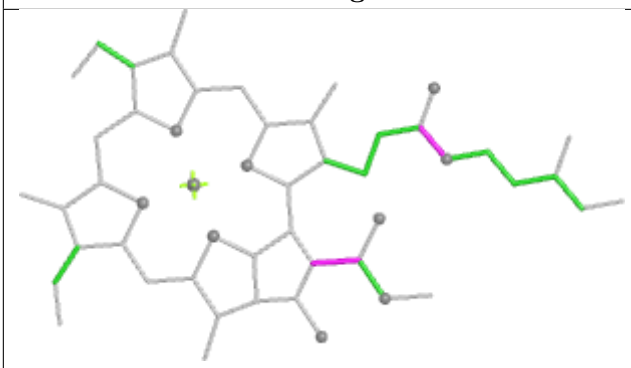
Ligand CLA G 836



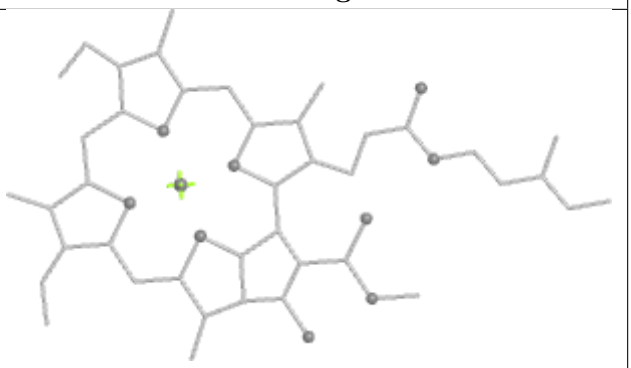
Bond lengths



Bond angles

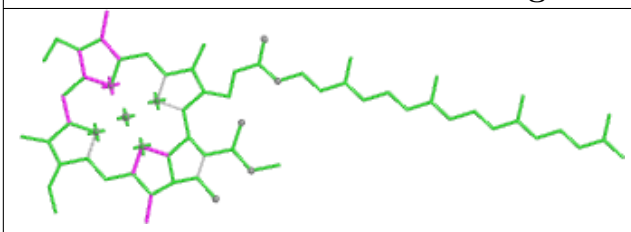


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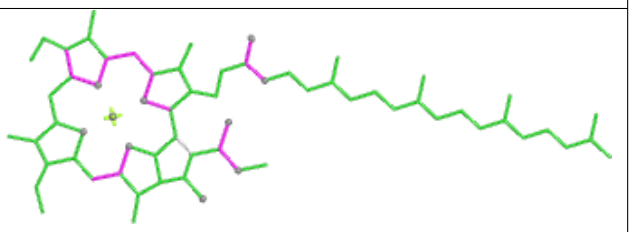


Rings

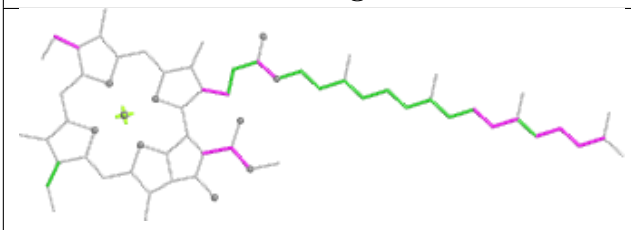
Ligand CLA a 809



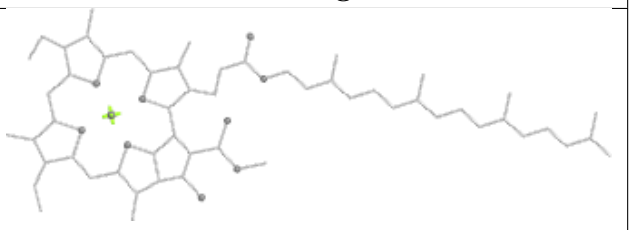
Bond lengths



Bond angles

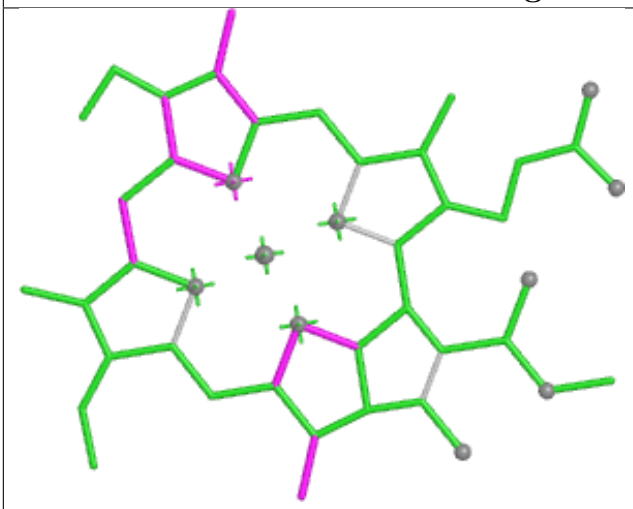


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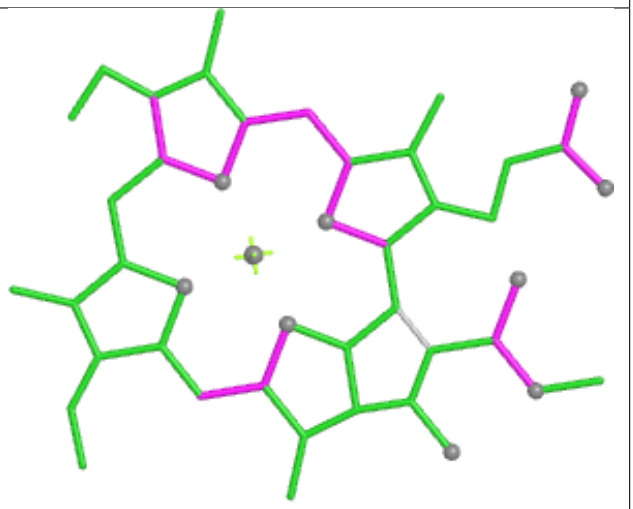


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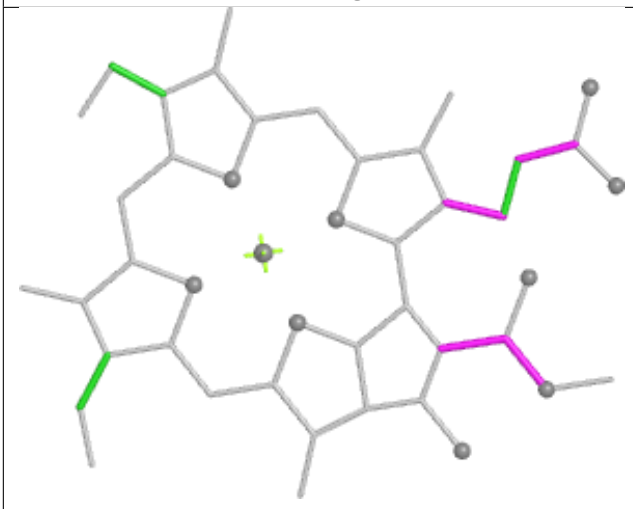
Ligand CLA w 203



Bond lengths



Bond angles

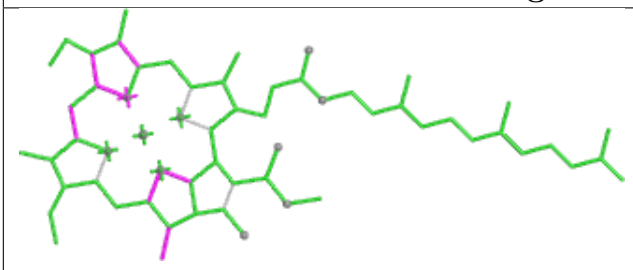


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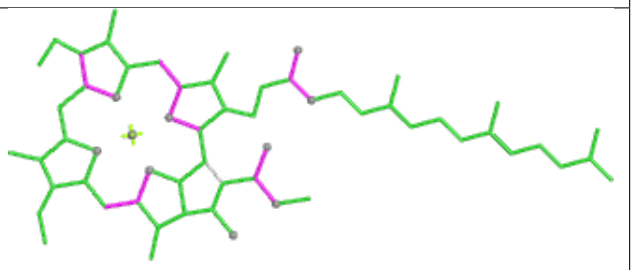


Rings

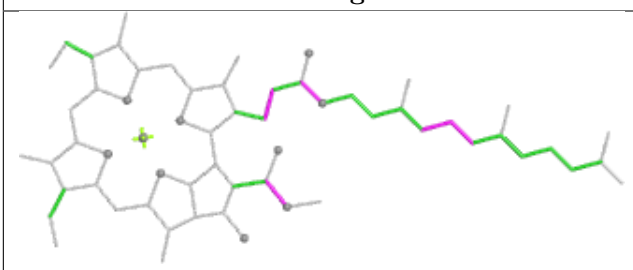
Ligand CLA n 831



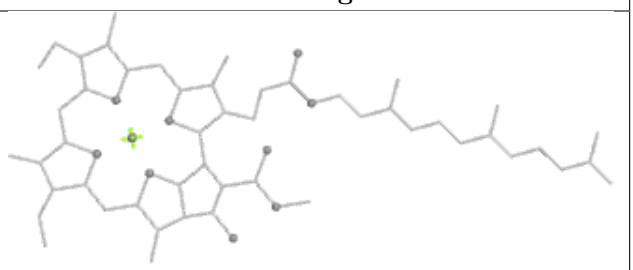
Bond lengths



Bond angles

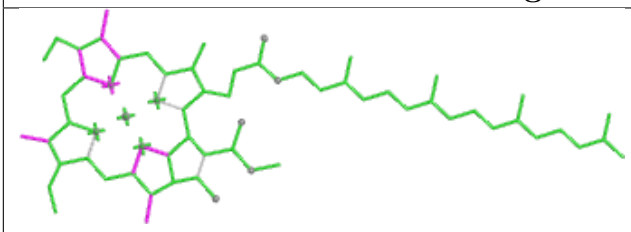


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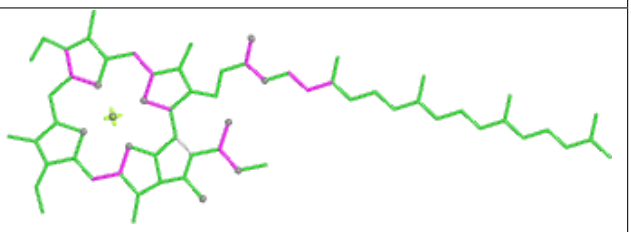


Rings

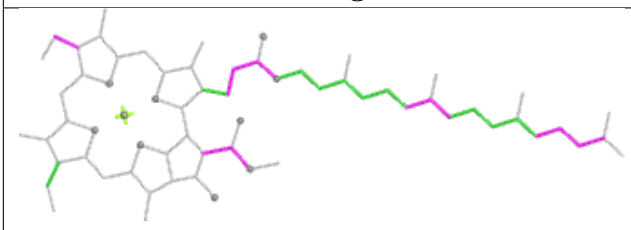
Ligand CLA B 841



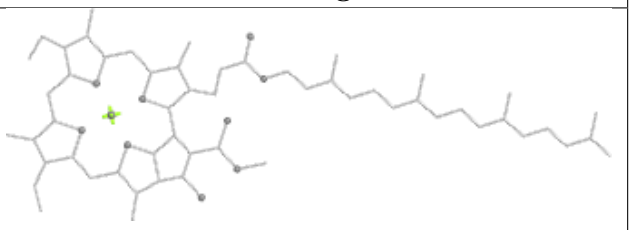
Bond lengths



Bond angles

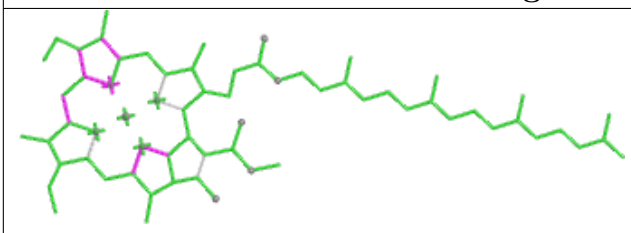


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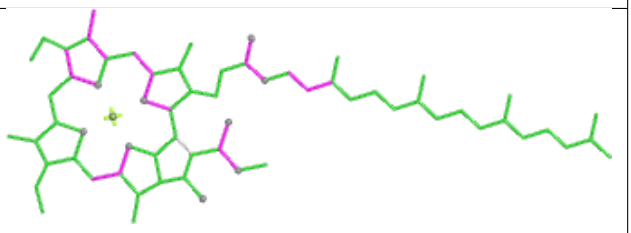


Rings

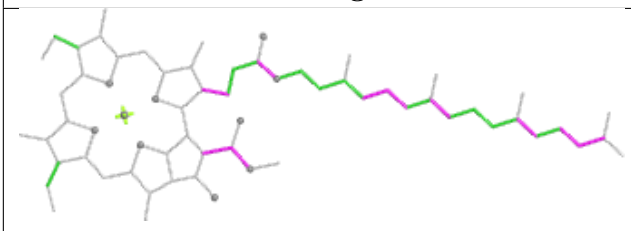
Ligand CLA G 805



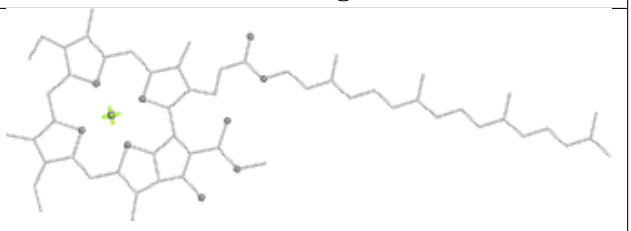
Bond lengths



Bond angles

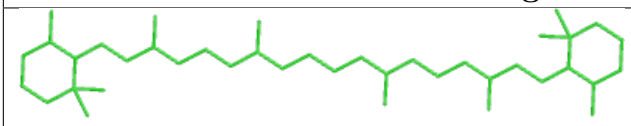


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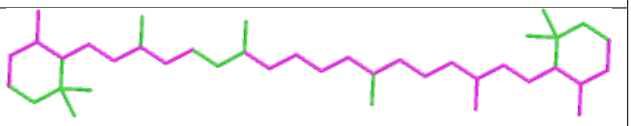


Rings

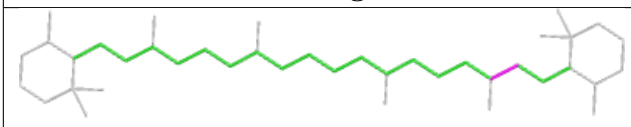
Ligand BCR A 845



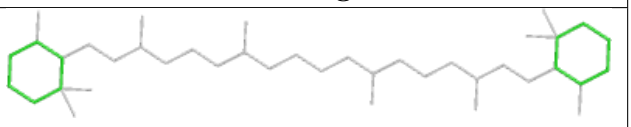
Bond lengths



Bond angles

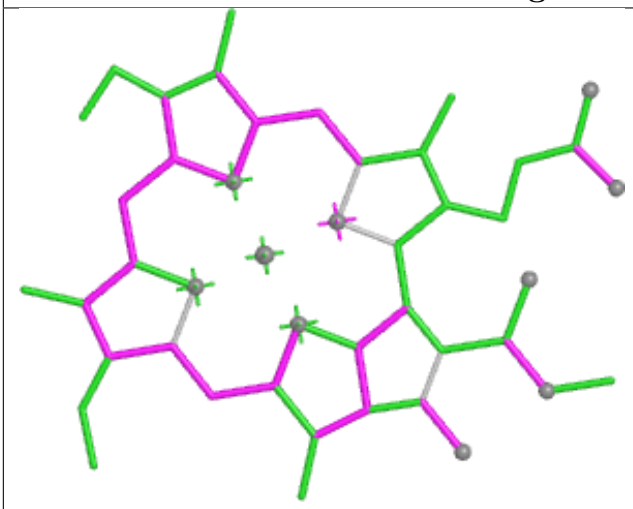


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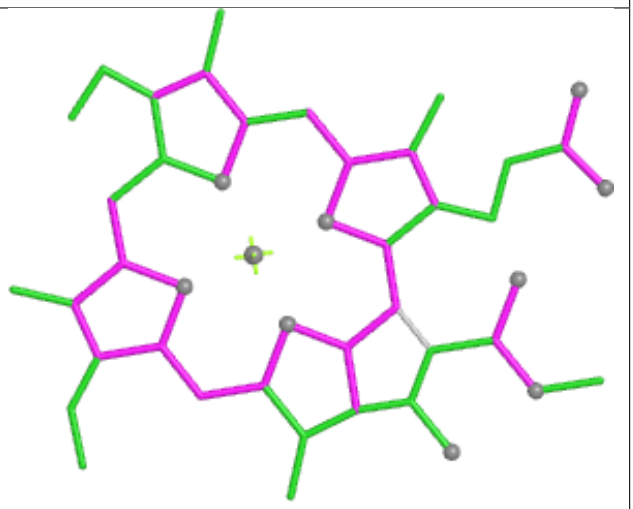


Rings

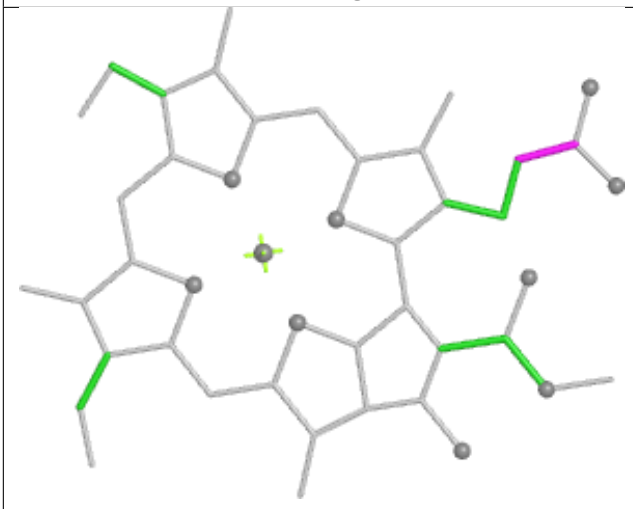
Ligand CL0 A 852



Bond lengths



Bond angles

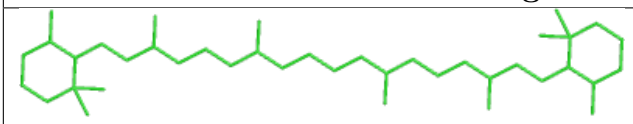


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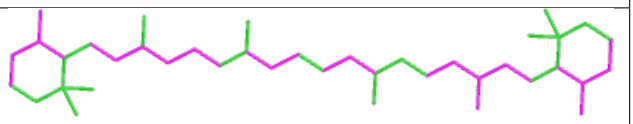


Rings

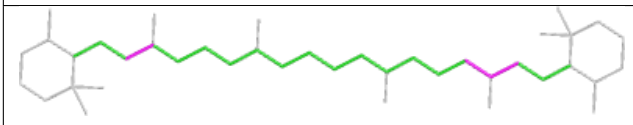
Ligand BCR w 201



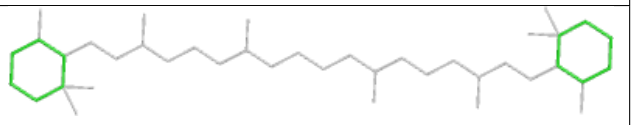
Bond lengths



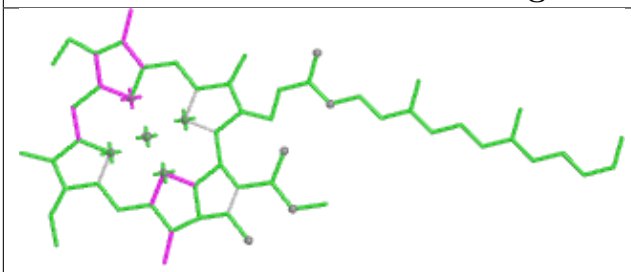
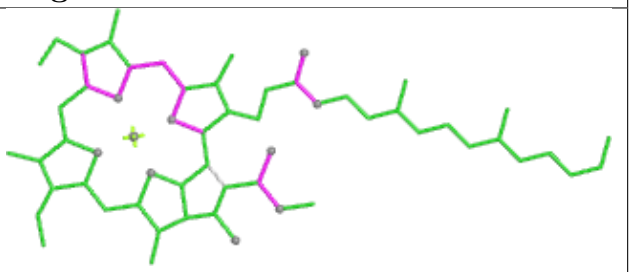
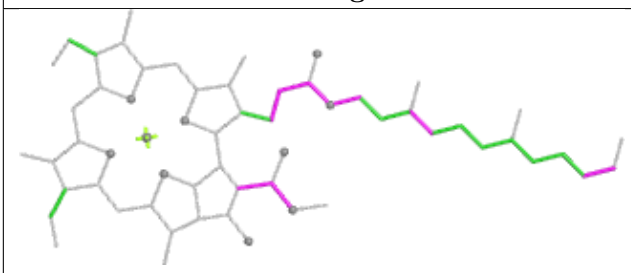
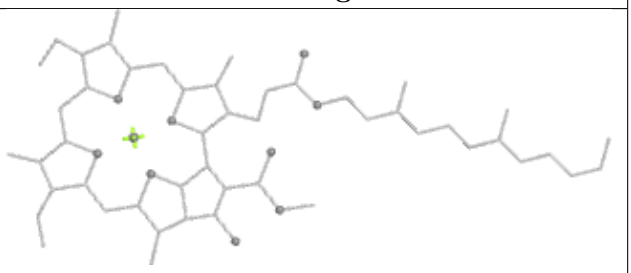
Bond angles

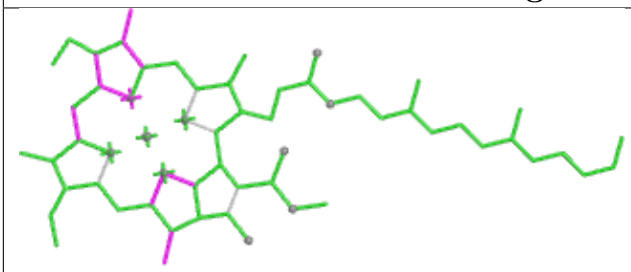
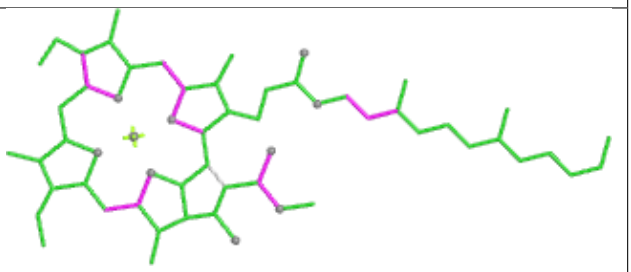
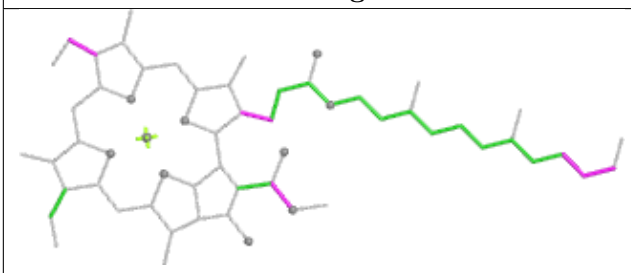
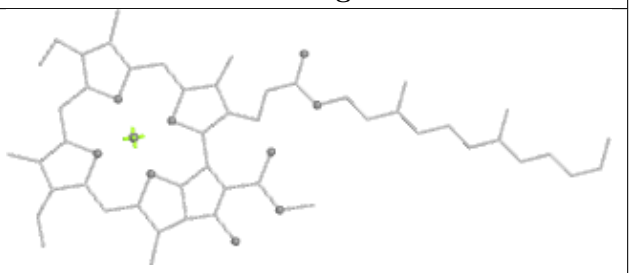


Torsions

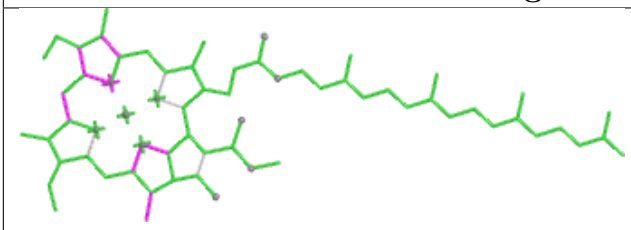


Rings

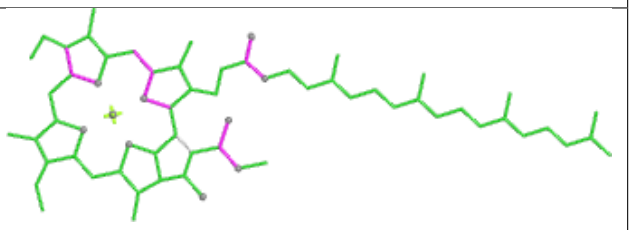
Ligand CLA g 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA F 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

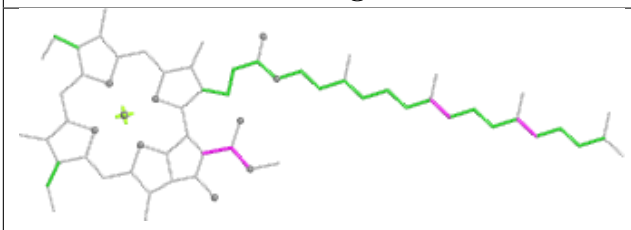
Ligand CLA B 825



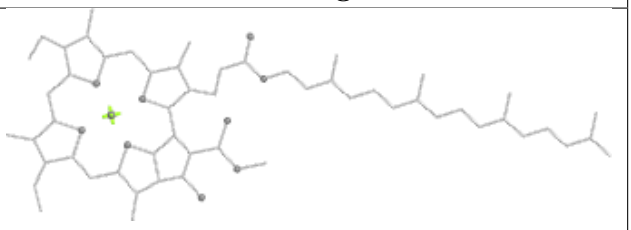
Bond lengths



Bond angles

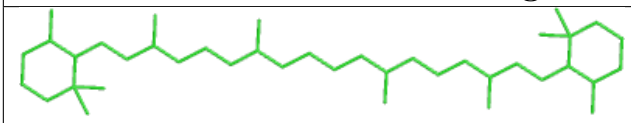


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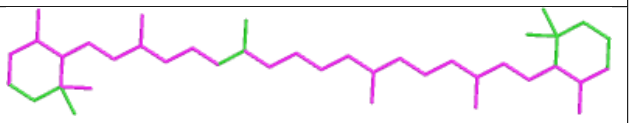


Rings

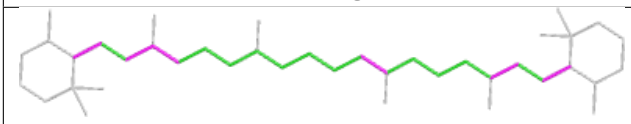
Ligand BCR A 849



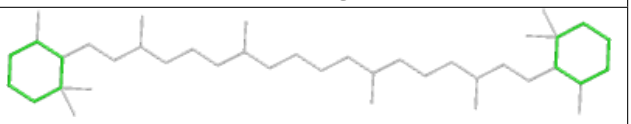
Bond lengths



Bond angles



Torsions

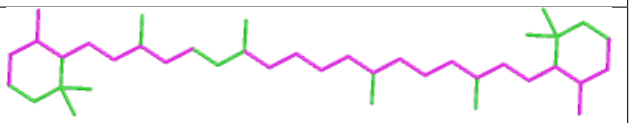


Rings

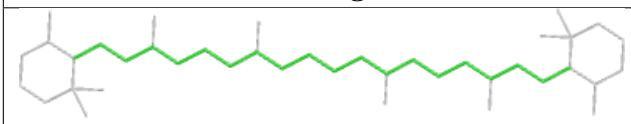
Ligand BCR u 103



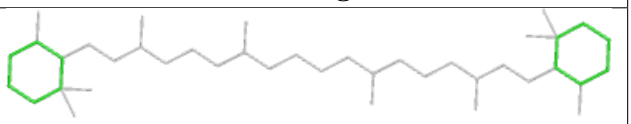
Bond lengths



Bond angles

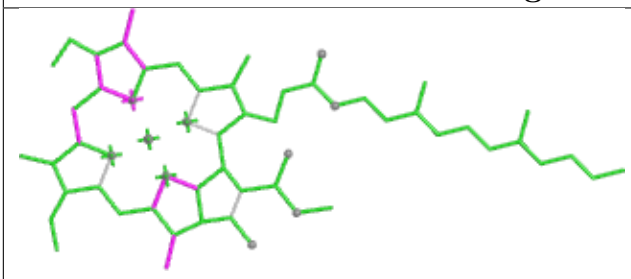


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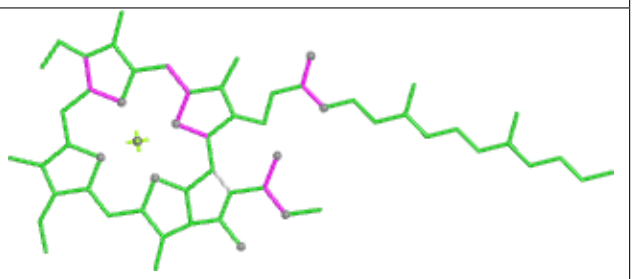


Rings

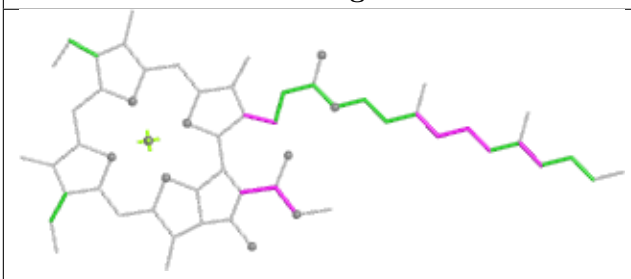
Ligand CLA B 833



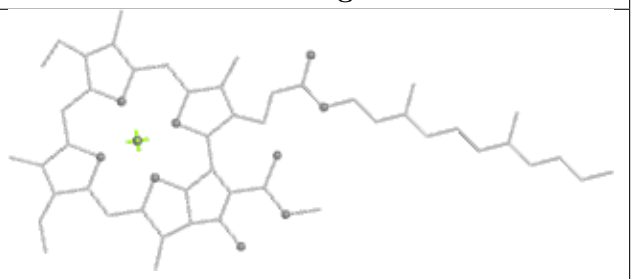
Bond lengths



Bond angles

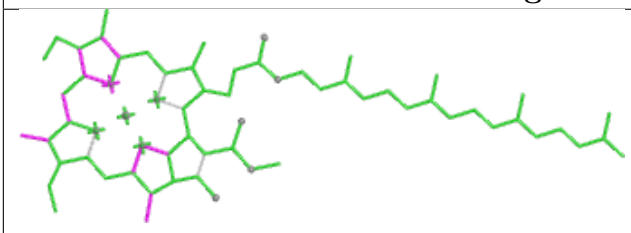


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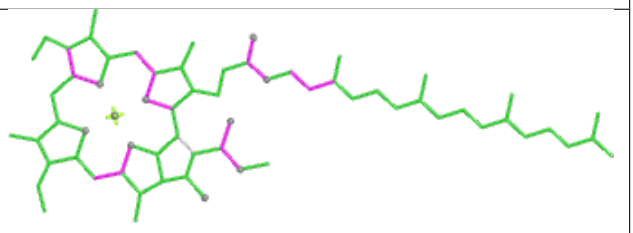


Rings

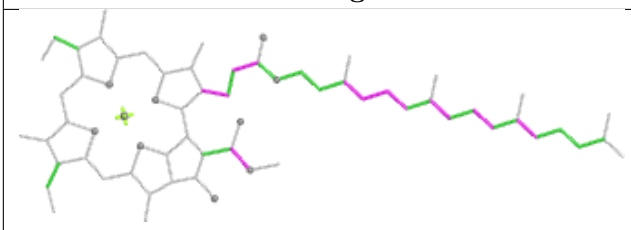
Ligand CLA B 814



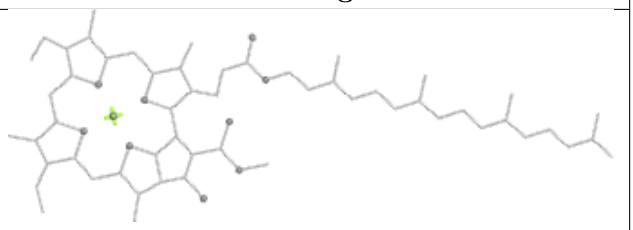
Bond lengths



Bond angles

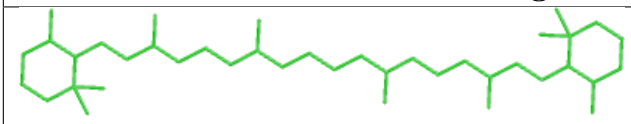


Torsions

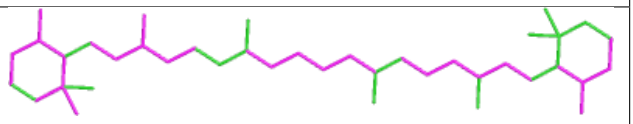


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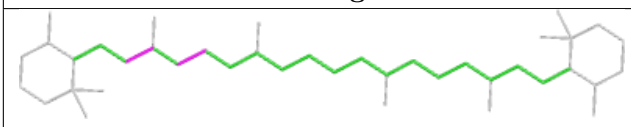
Ligand BCR i 101



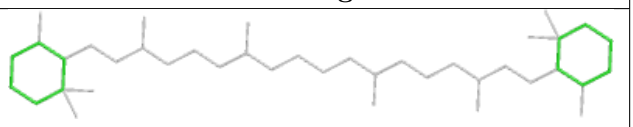
Bond lengths



Bond angles

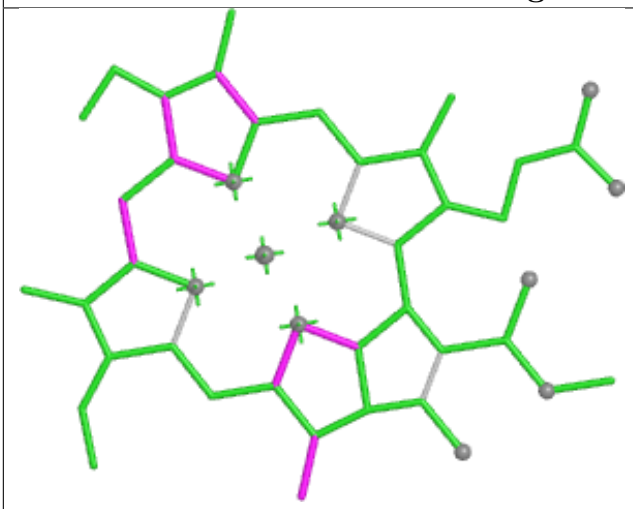


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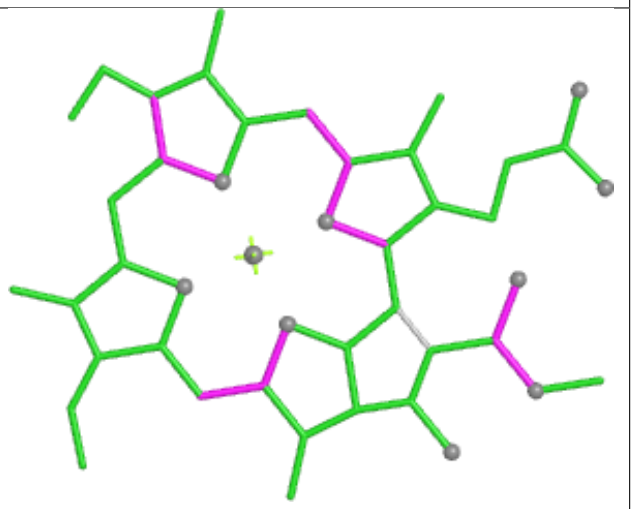


Rings

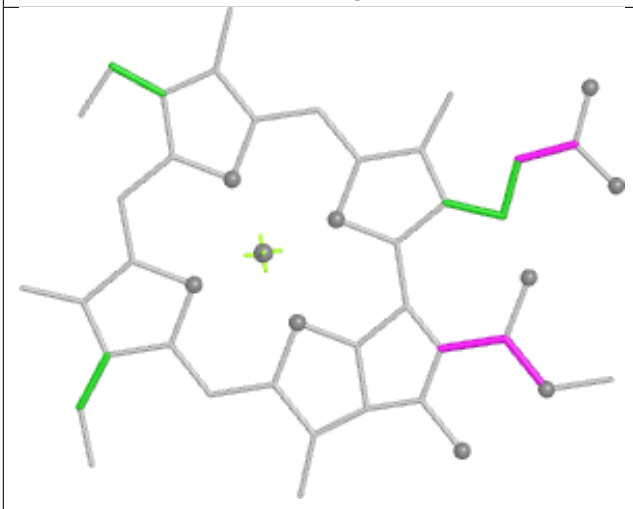
Ligand CLA n 835



Bond lengths



Bond angles

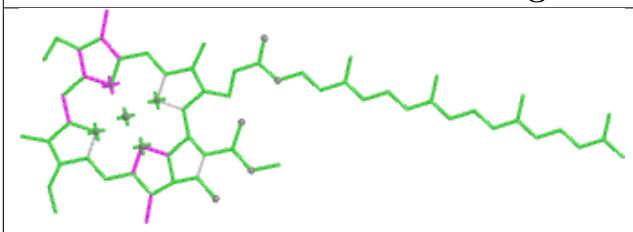


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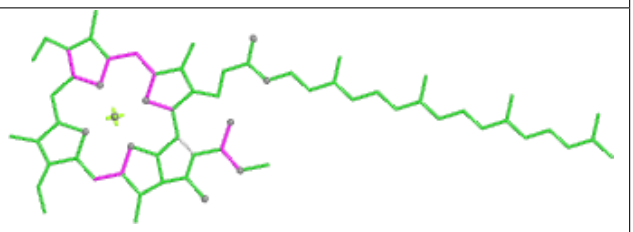


Rings

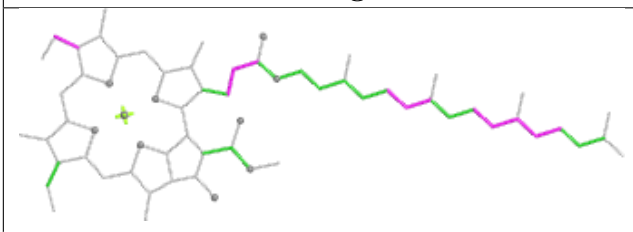
Ligand CLA a 836



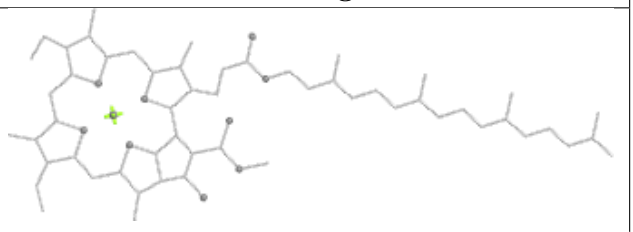
Bond lengths



Bond angles

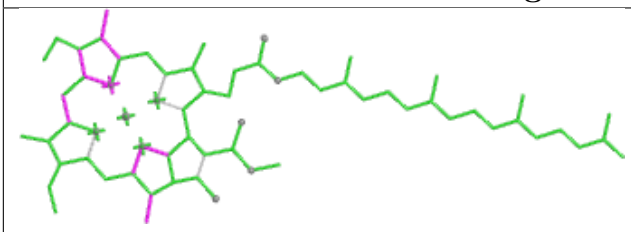


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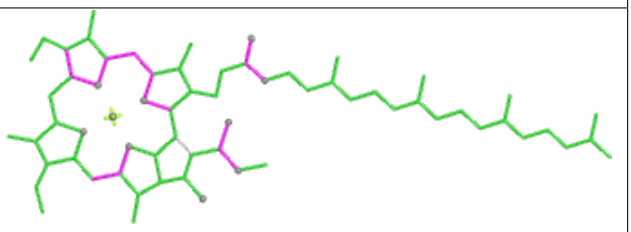


Rings

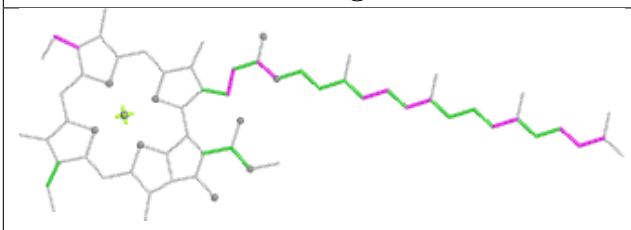
Ligand CLA B 840



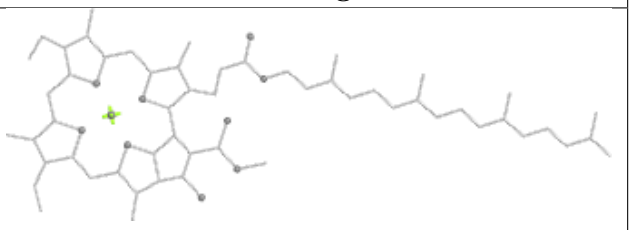
Bond lengths



Bond angles

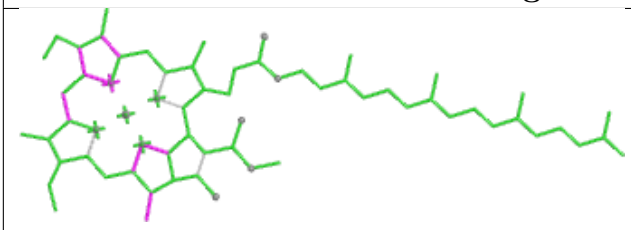


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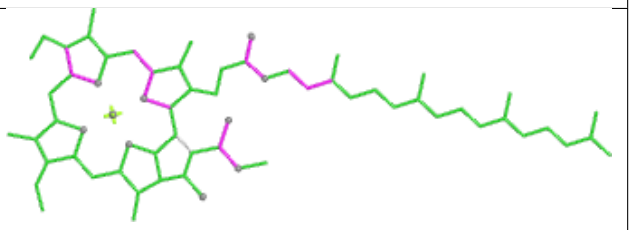


Rings

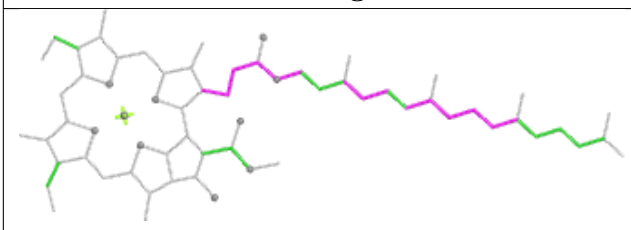
Ligand CLA G 808



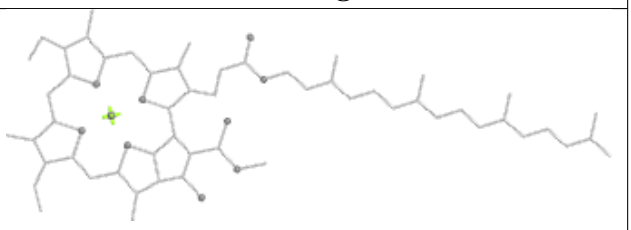
Bond lengths



Bond angles

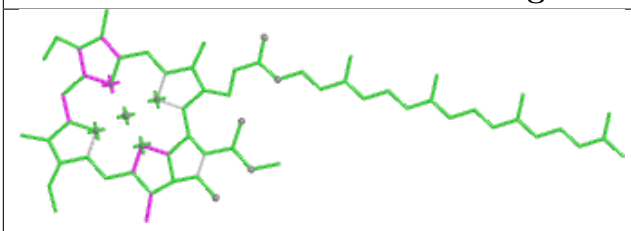


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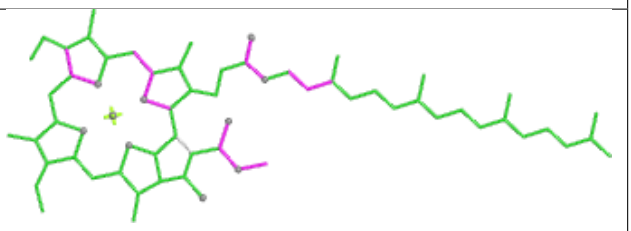


Rings

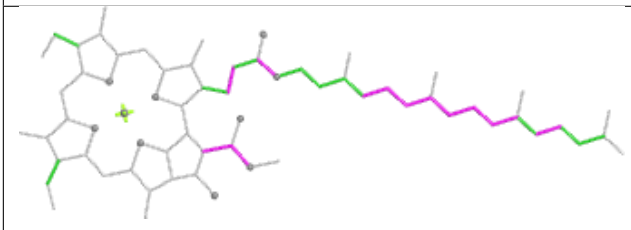
Ligand CLA n 803



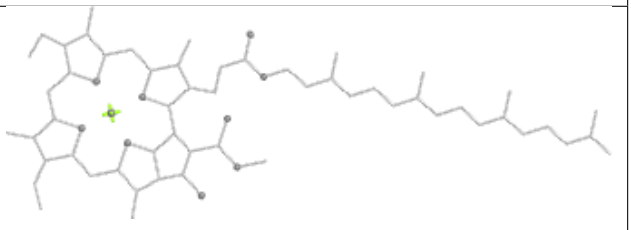
Bond lengths



Bond angles

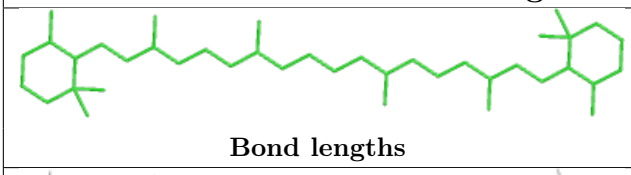


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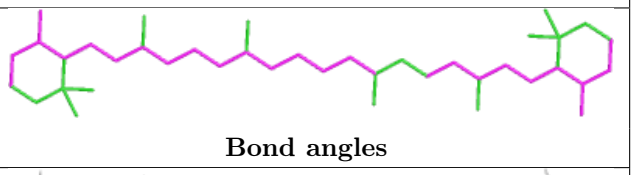


Rings

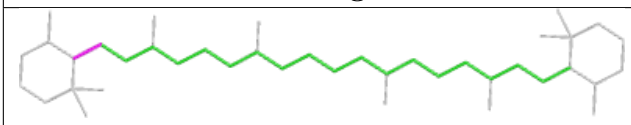
Ligand BCR J 103



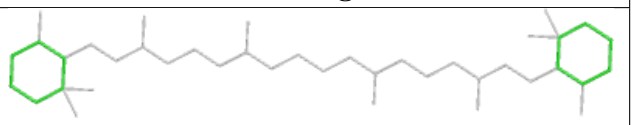
Bond lengths



Bond angles

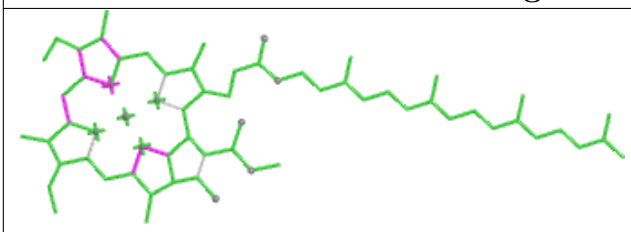


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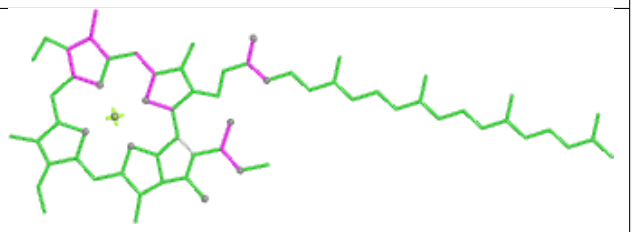


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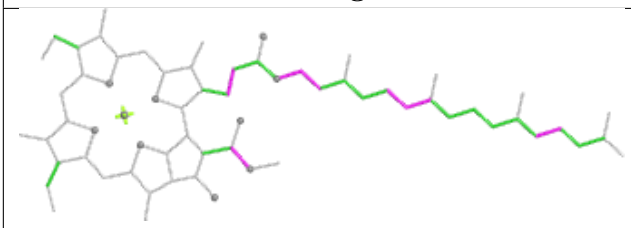
Ligand CLA A 827



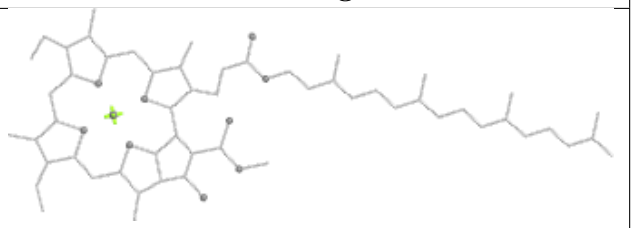
Bond lengths



Bond angles

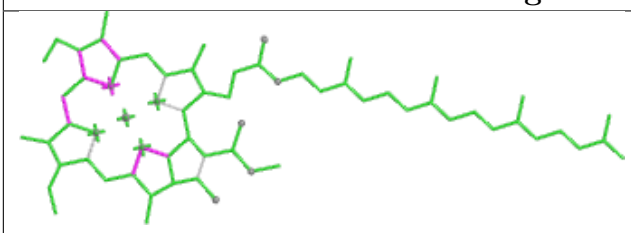


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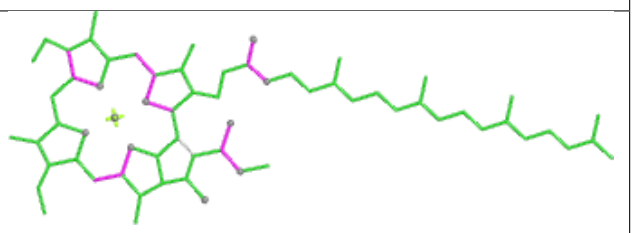


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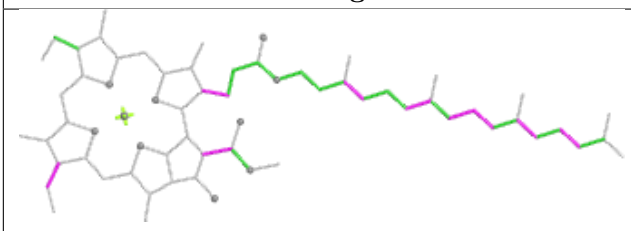
Ligand CLA B 826



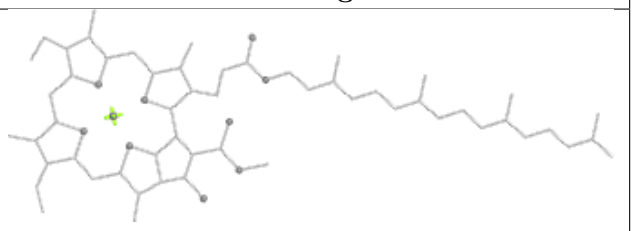
Bond lengths



Bond angles

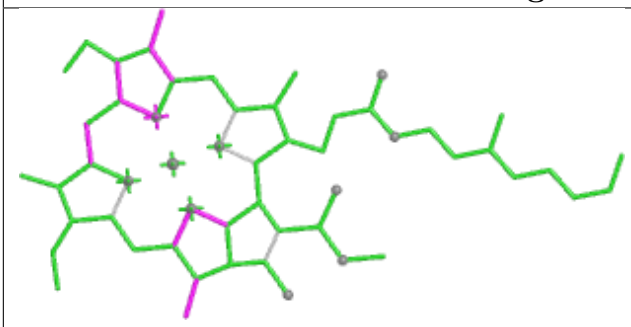


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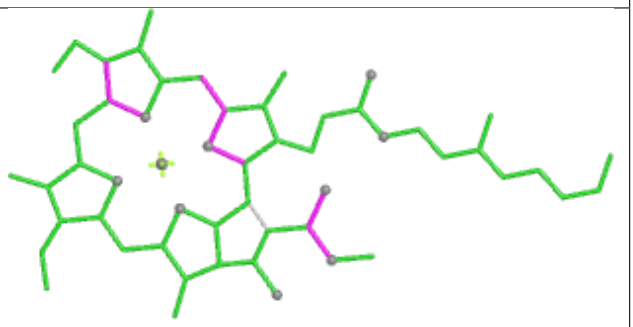


Rings

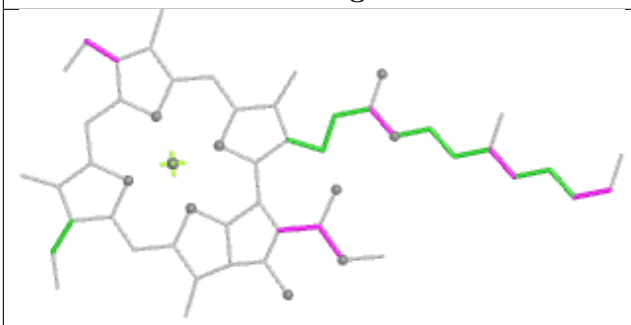
Ligand CLA n 811



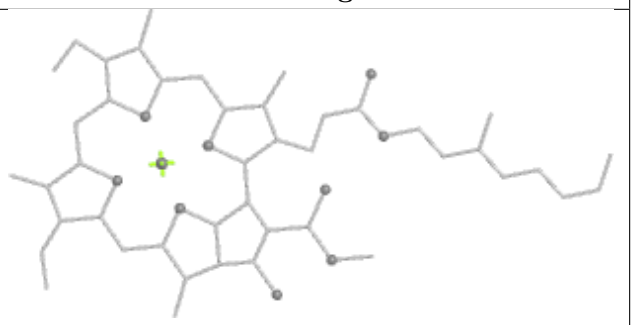
Bond lengths



Bond angles

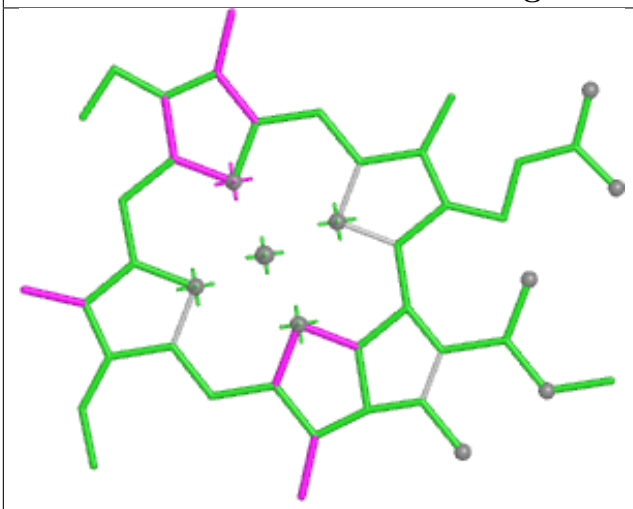


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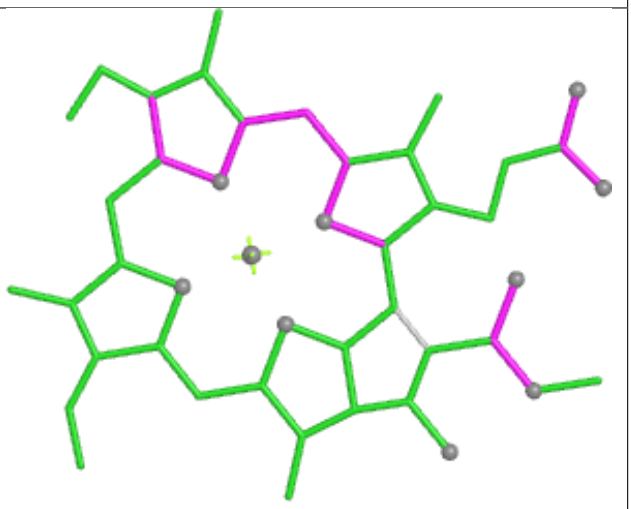


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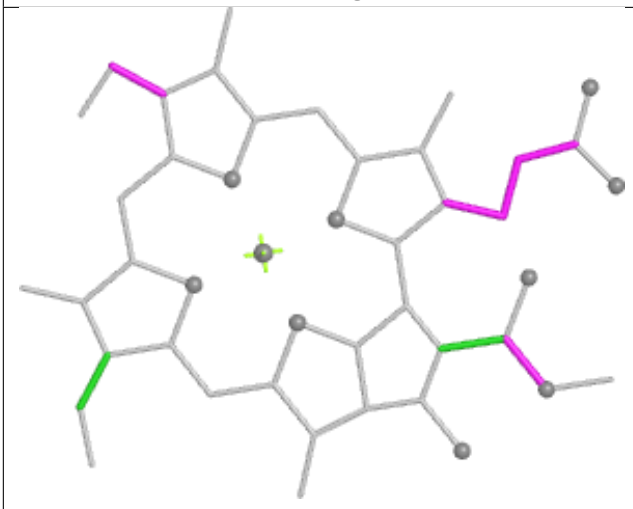
Ligand CLA A 855



Bond lengths



Bond angles

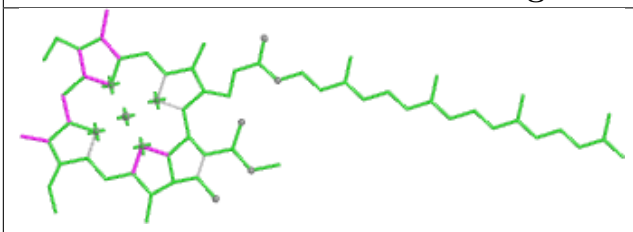


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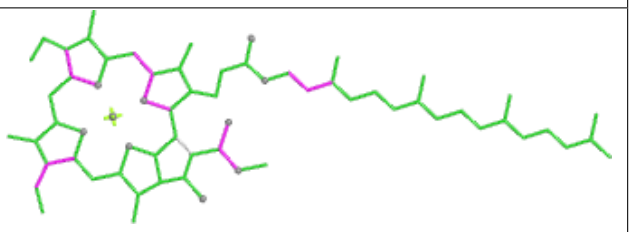


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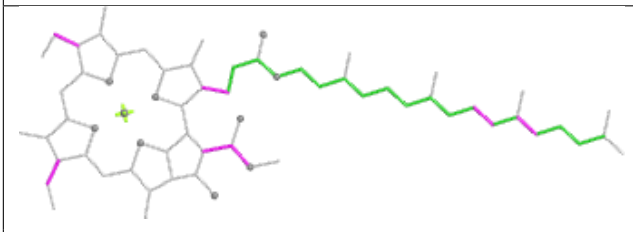
Ligand CLA n 804



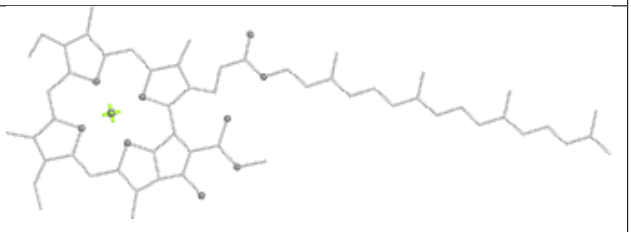
Bond lengths



Bond angles

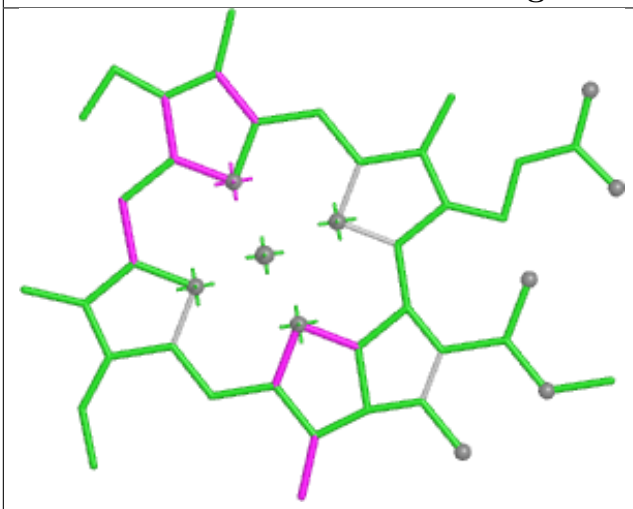


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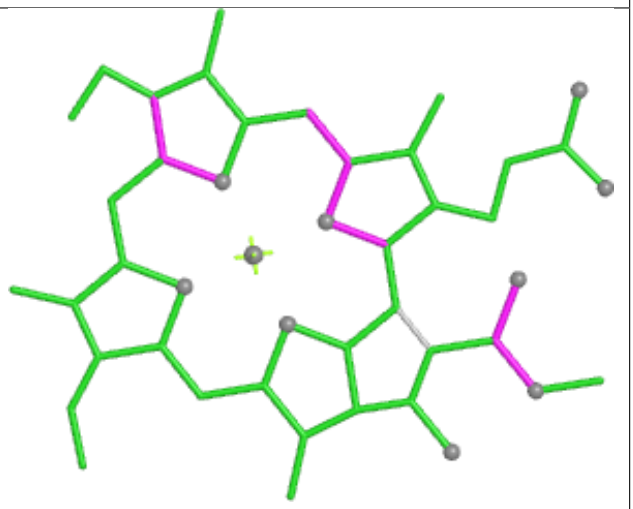


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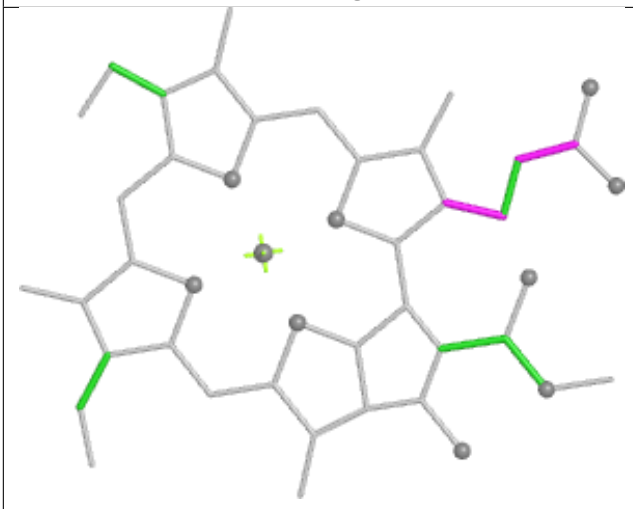
Ligand CLA b 816



Bond lengths



Bond angles

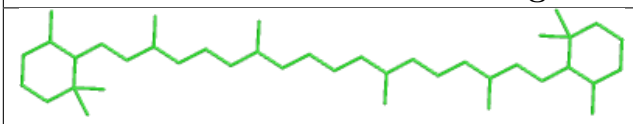


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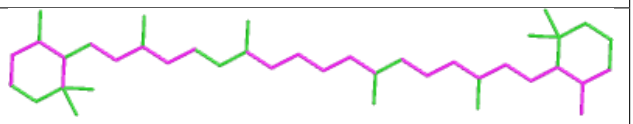


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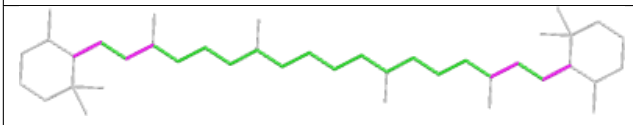
Ligand BCR I 103



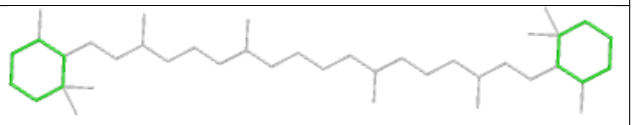
Bond lengths



Bond angles

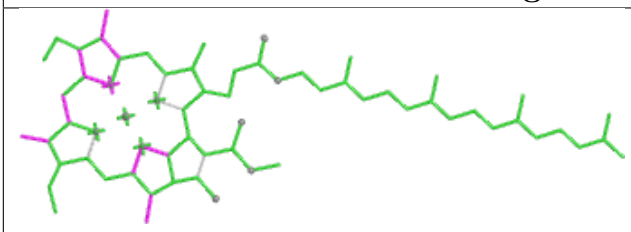


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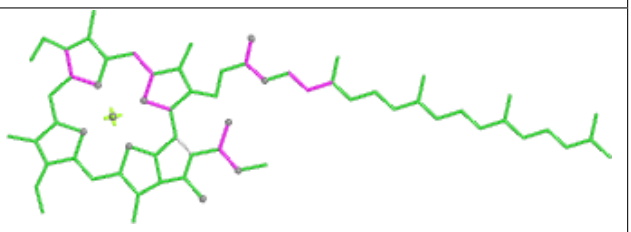


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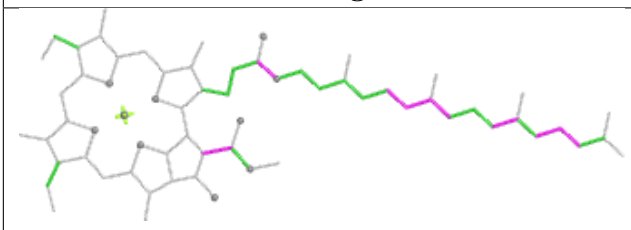
Ligand CLA N 826



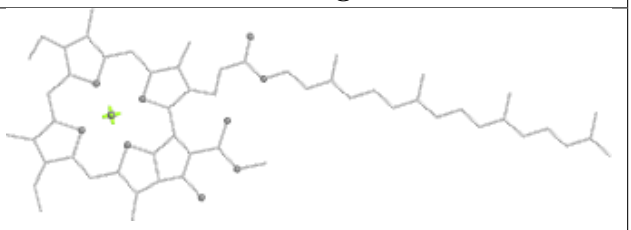
Bond lengths



Bond angles

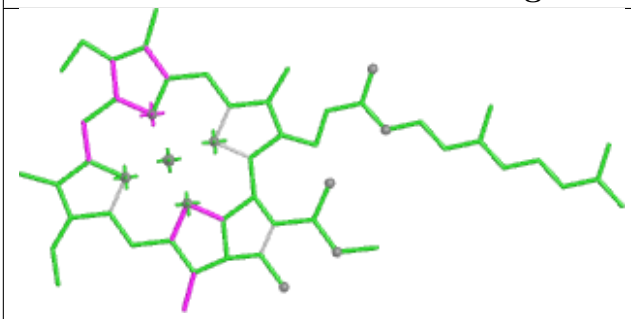


Torsions

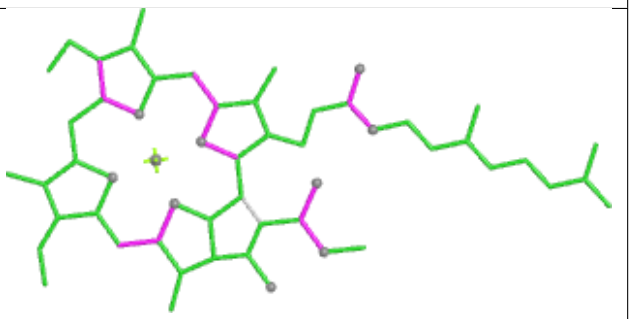


Rings

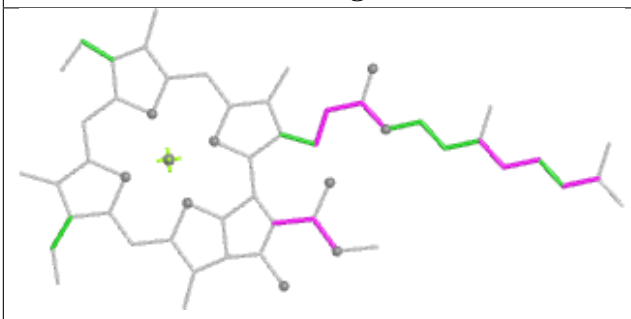
Ligand CLA B 823



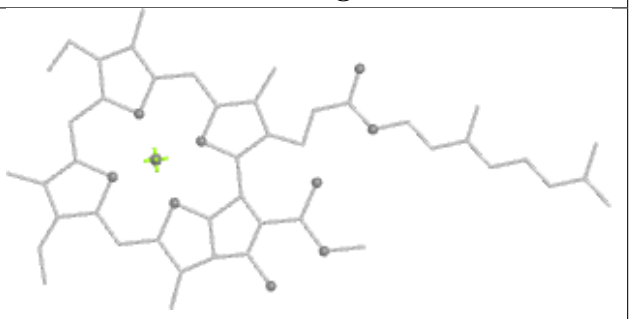
Bond lengths



Bond angles

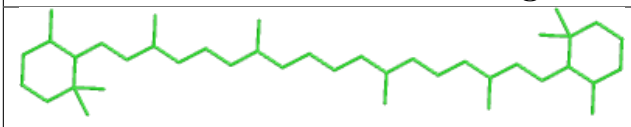


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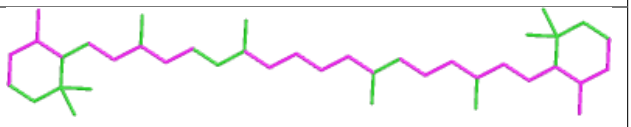


Rings

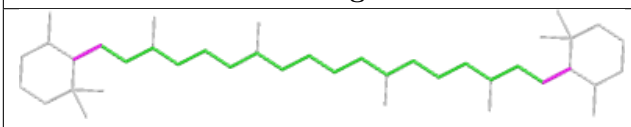
Ligand BCR G 846



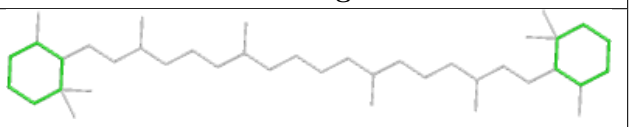
Bond lengths



Bond angles

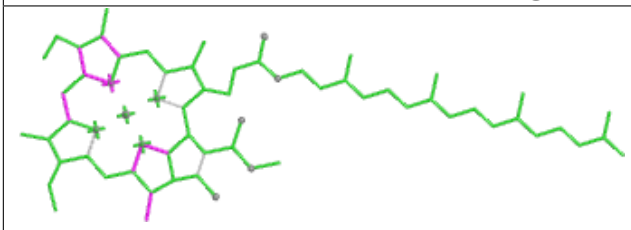


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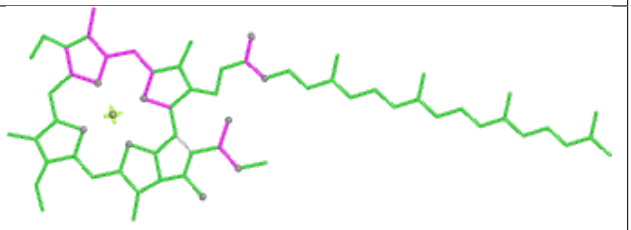


Rings

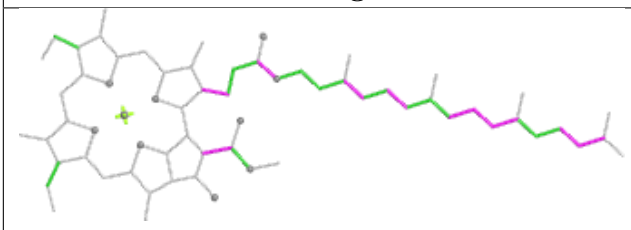
Ligand CLA b 825



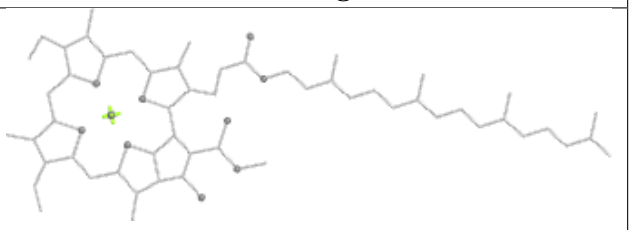
Bond lengths



Bond angles

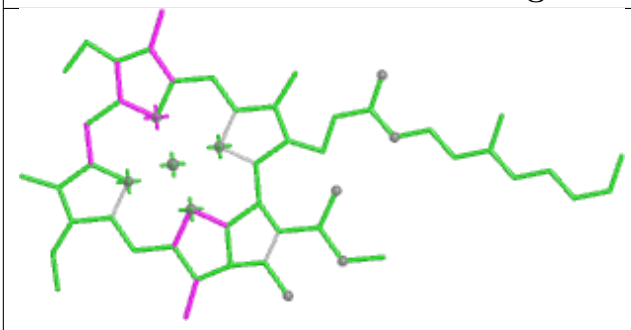


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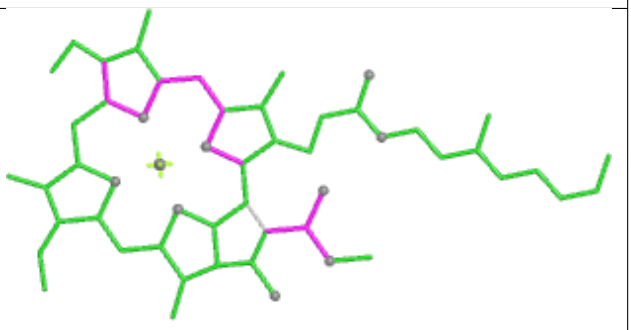


Rings

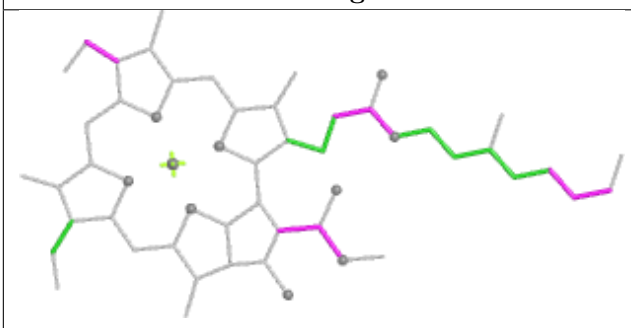
Ligand CLA b 811



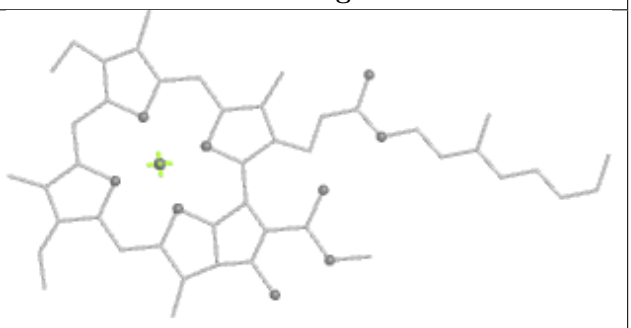
Bond lengths



Bond angles

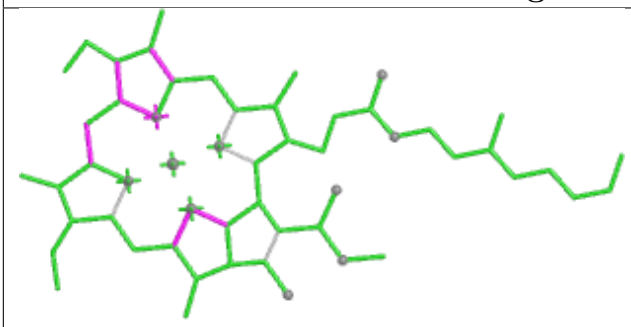


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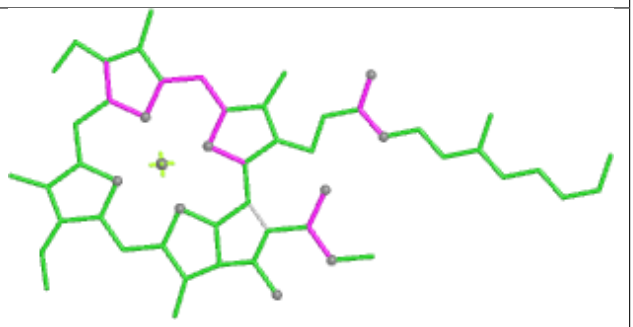


Rings

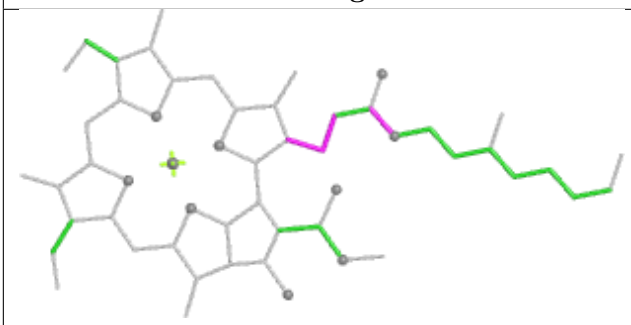
Ligand CLA n 812



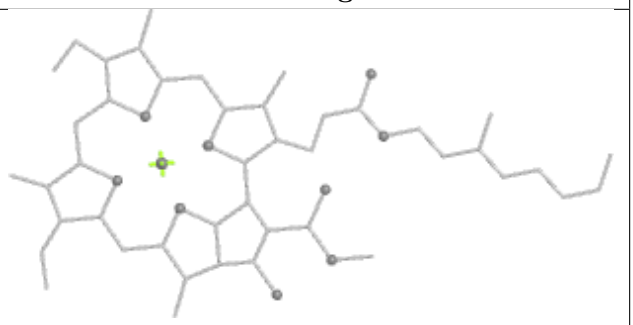
Bond lengths



Bond angles

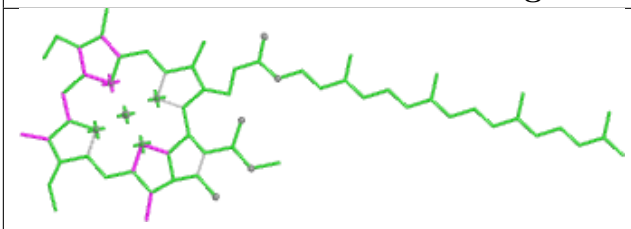


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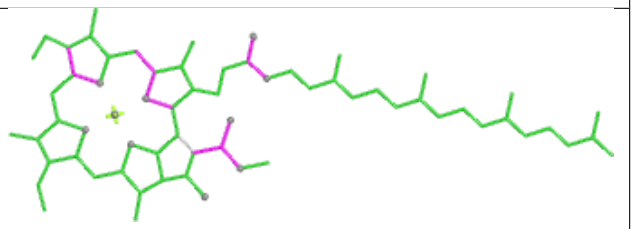


Rings

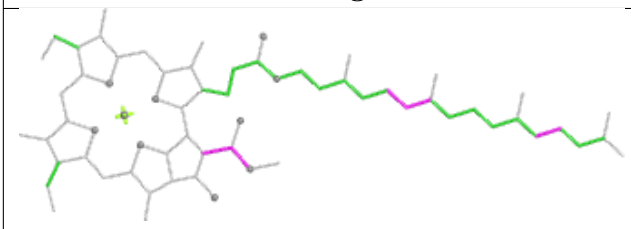
Ligand CLA B 809



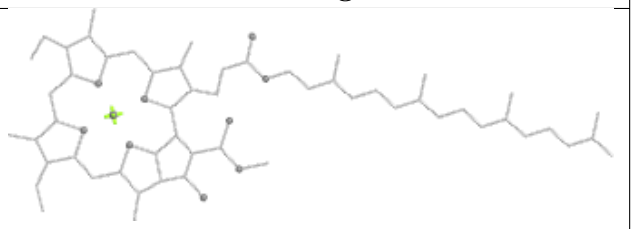
Bond lengths



Bond angles

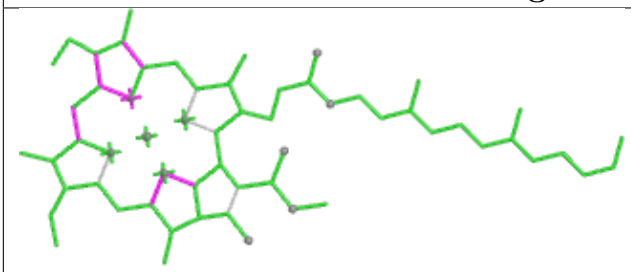


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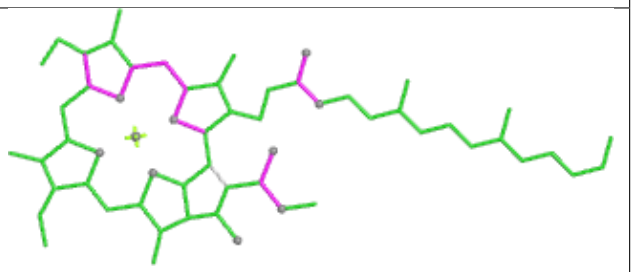


Rings

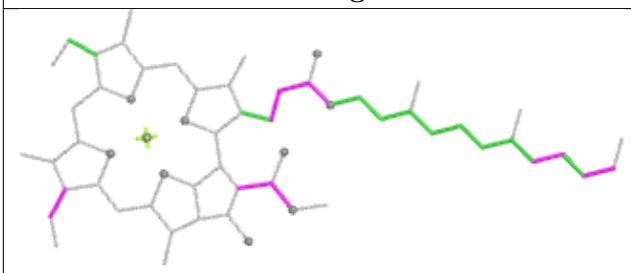
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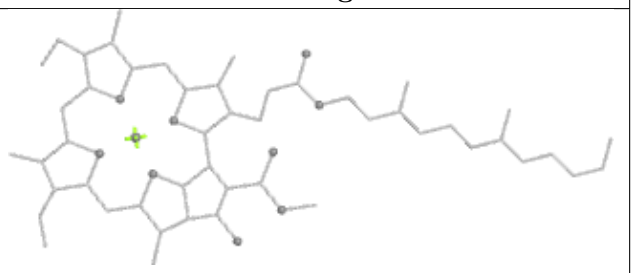
Bond lengths



Bond angles

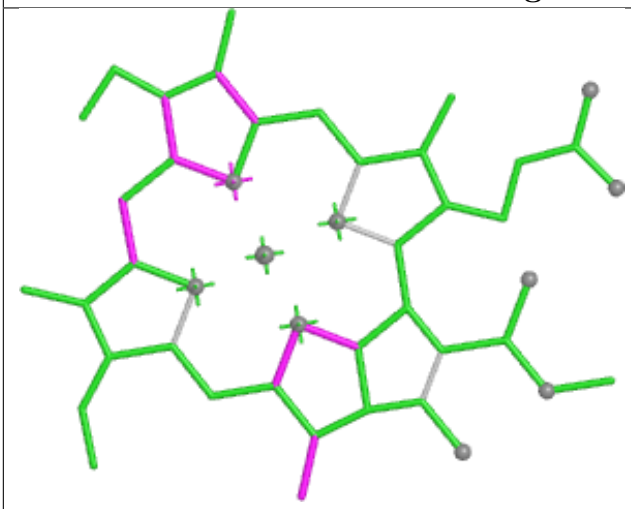


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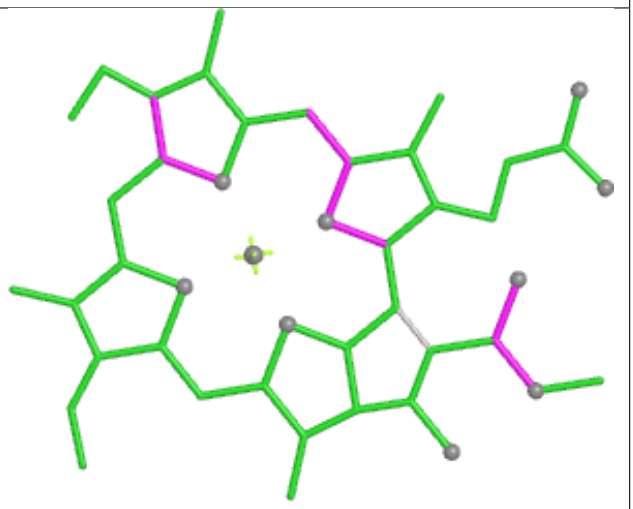


Rings

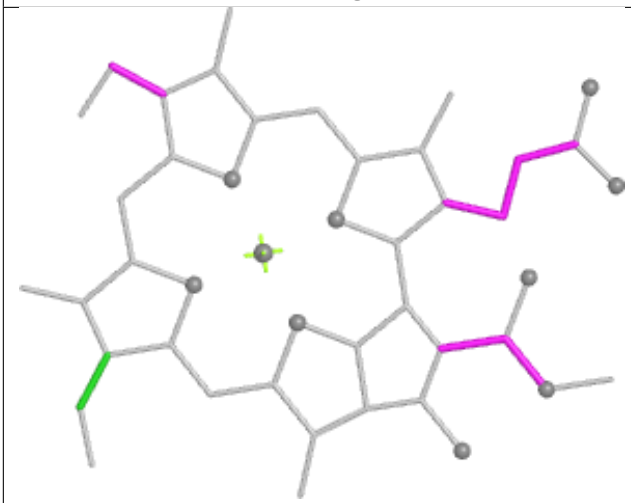
Ligand CLA B 821



Bond lengths



Bond angles

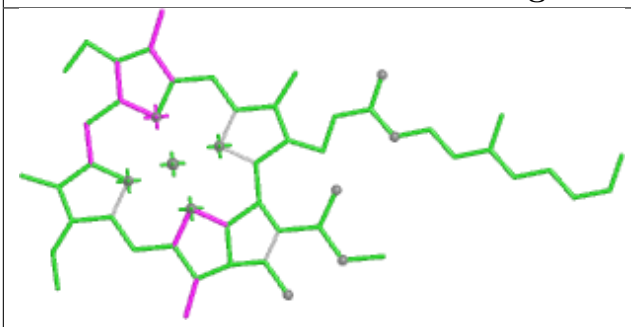


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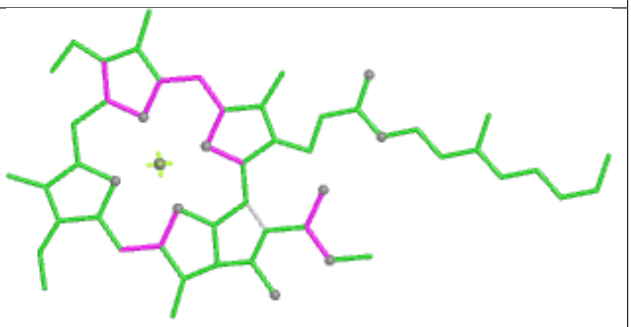


Rings

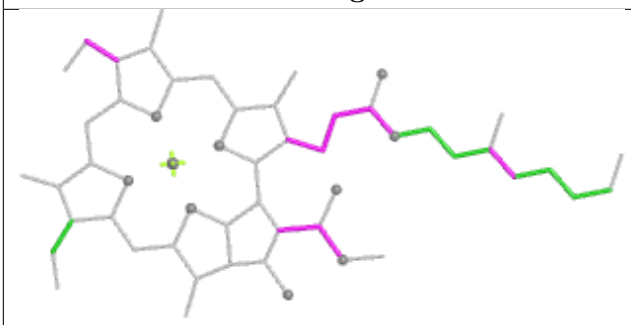
Ligand CLA a 821



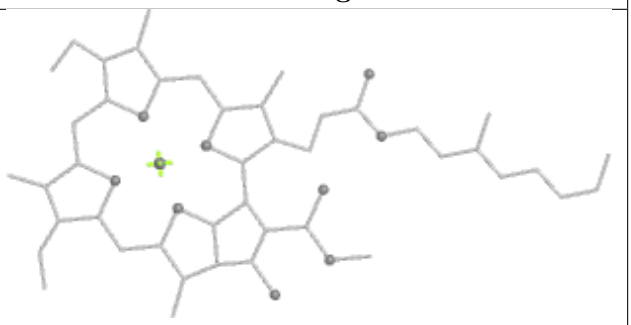
Bond lengths



Bond angles



Torsions

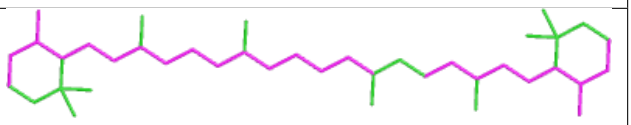


Rings

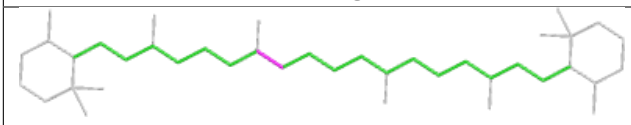
Ligand BCR s 203



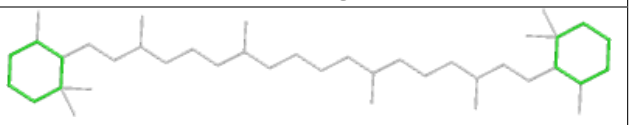
Bond lengths



Bond angles

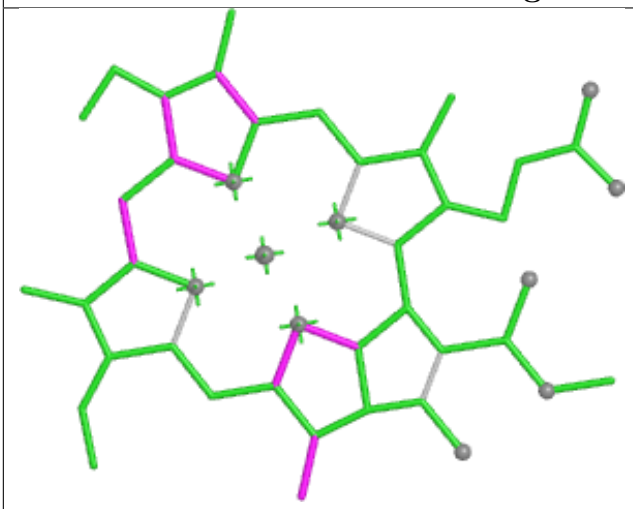


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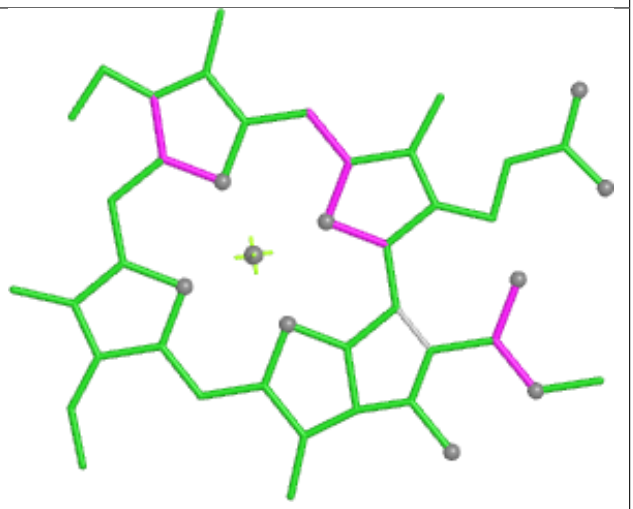


Rings

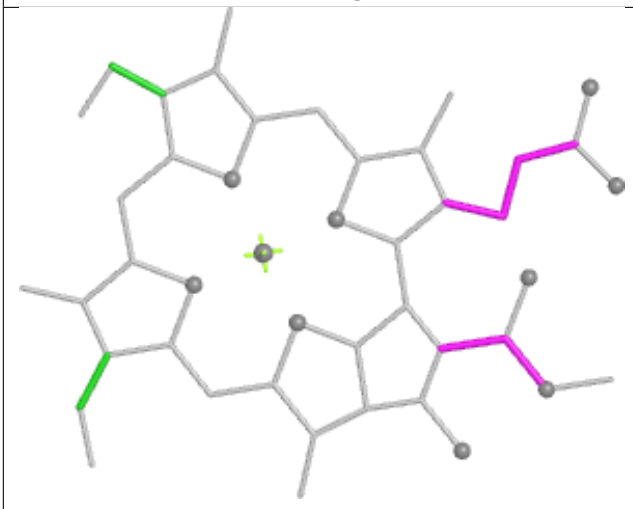
Ligand CLA A 835



Bond lengths



Bond angles

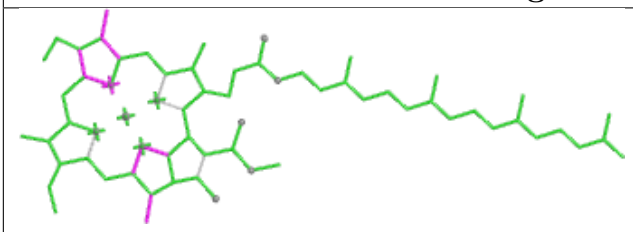


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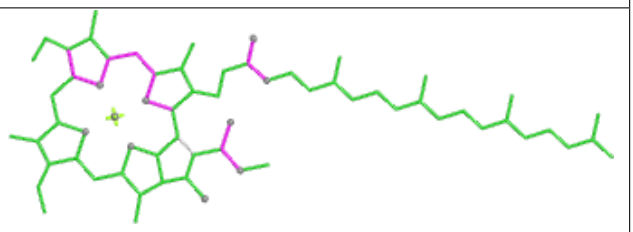


Rings

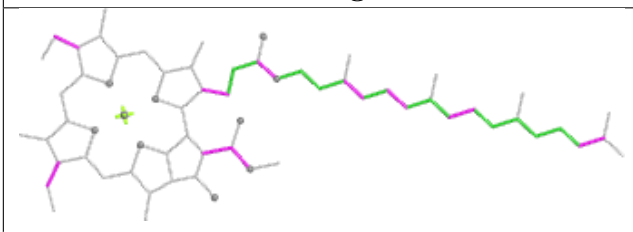
Ligand CLA b 840



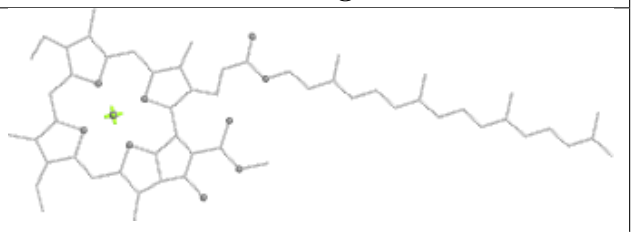
Bond lengths



Bond angles

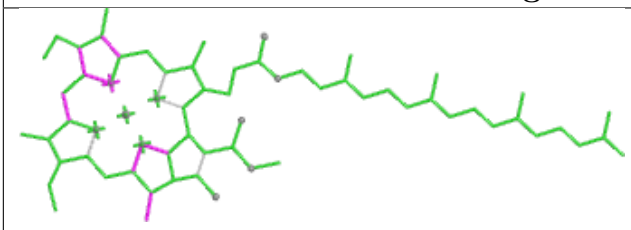


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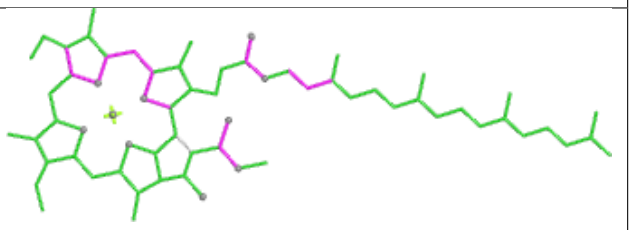


Rings

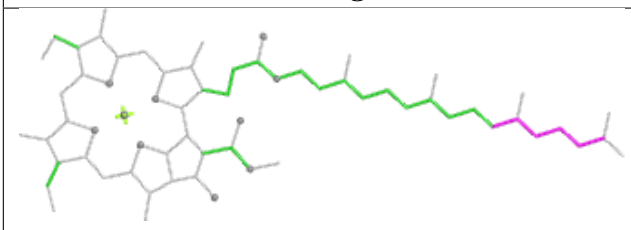
Ligand CLA G 802



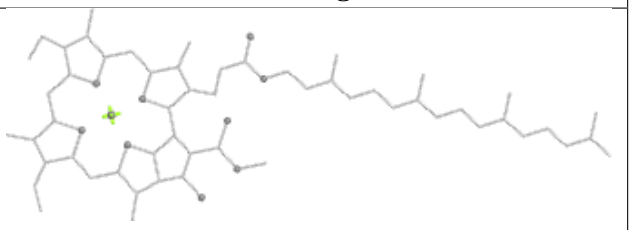
Bond lengths



Bond angles

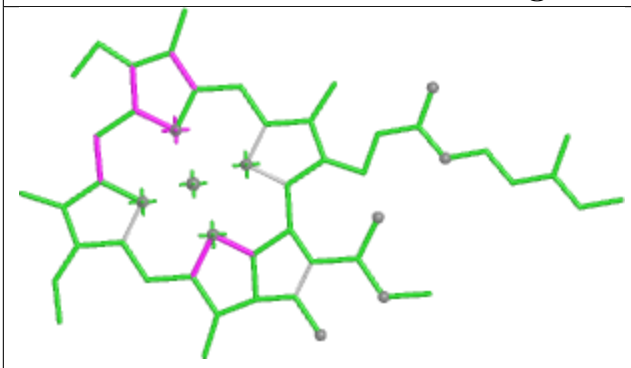


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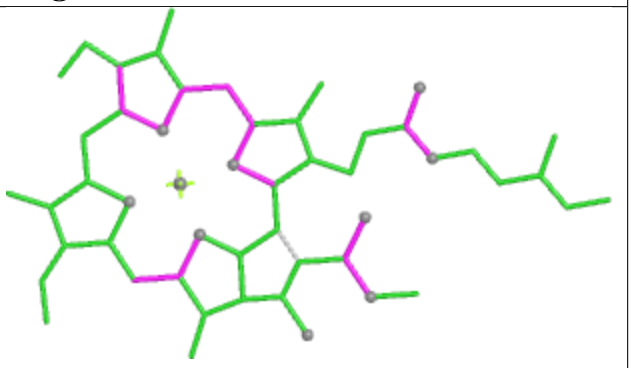


Rings

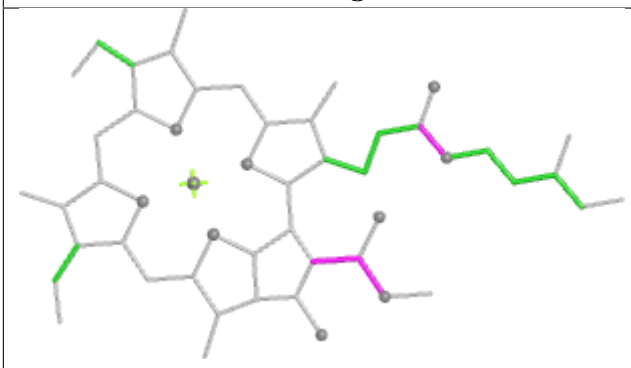
Ligand CLA g 835



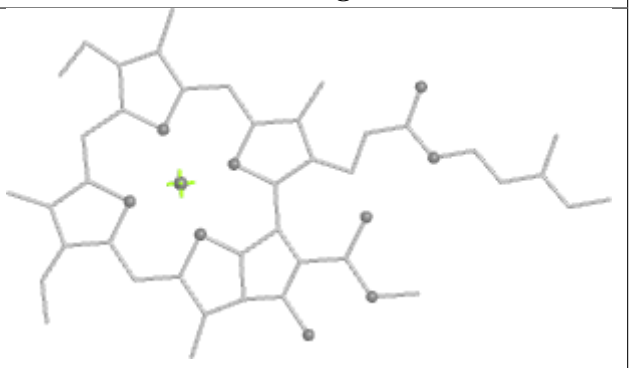
Bond lengths



Bond angles

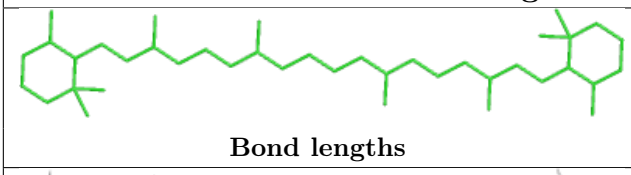


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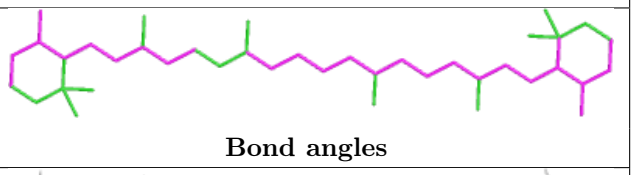


Rings

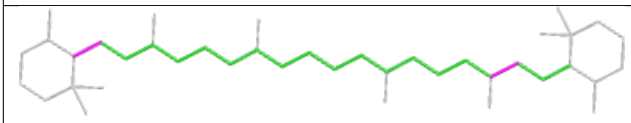
Ligand BCR G 844



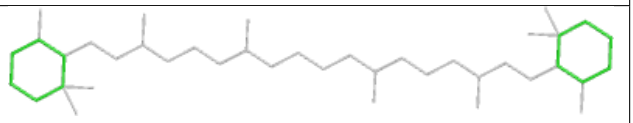
Bond lengths



Bond angles

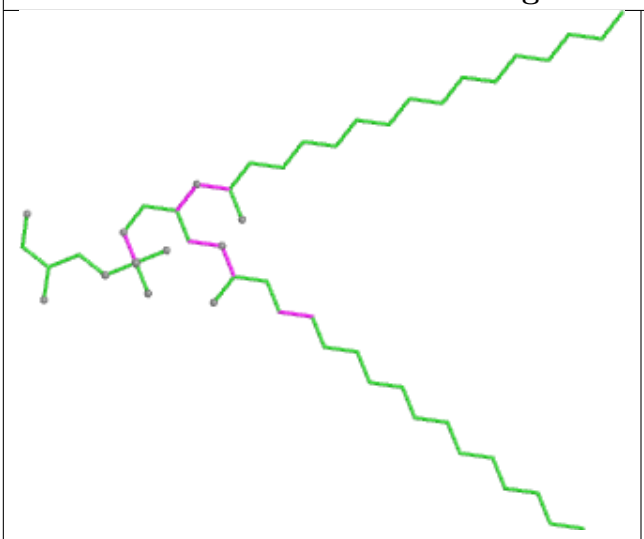


Torsions

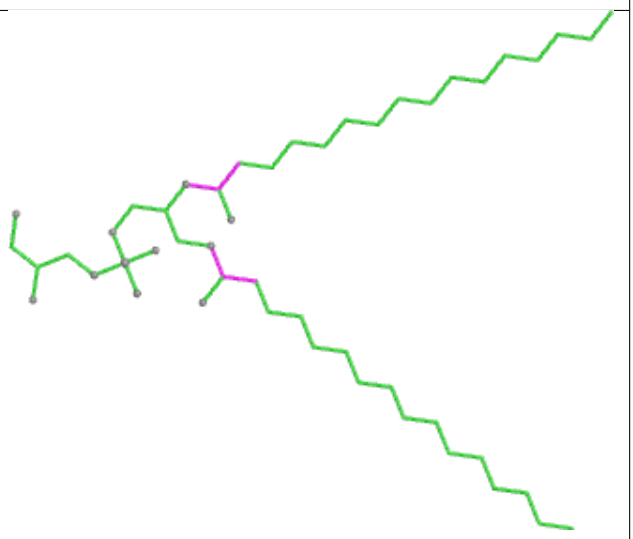


Rings

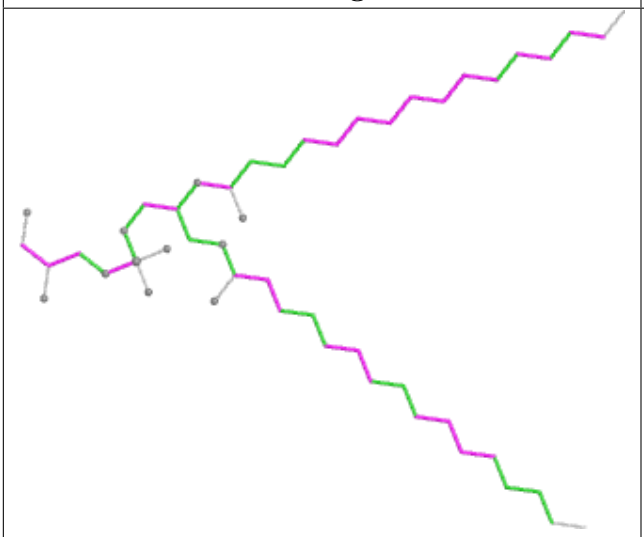
Ligand LHG A 851



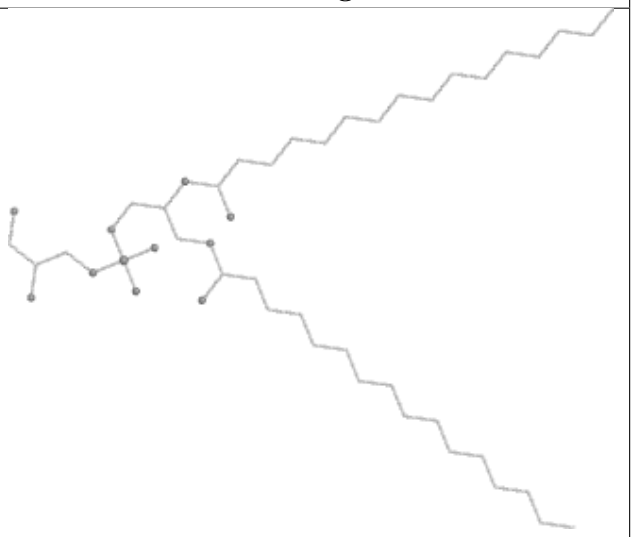
Bond lengths



Bond angles

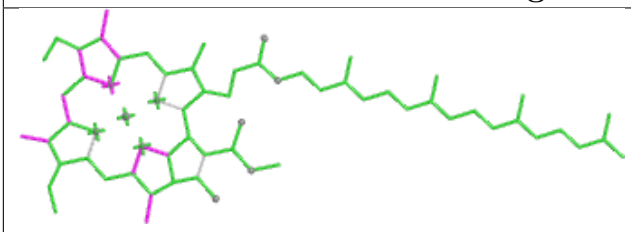


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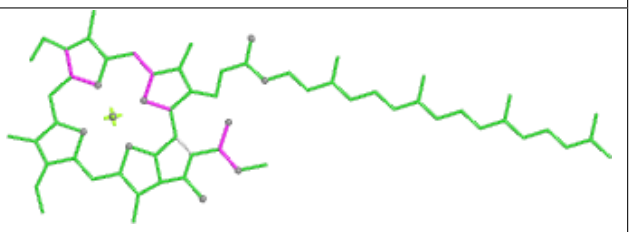


Rings

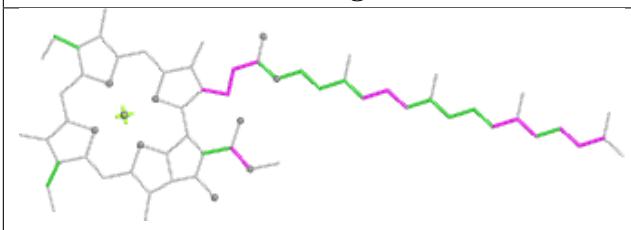
Ligand CLA n 809



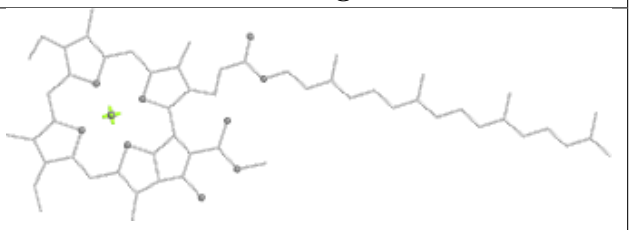
Bond lengths



Bond angles

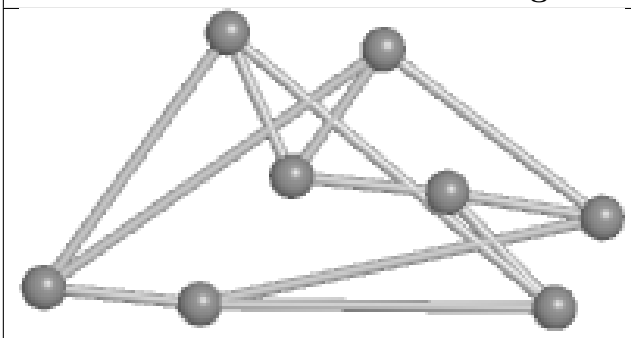


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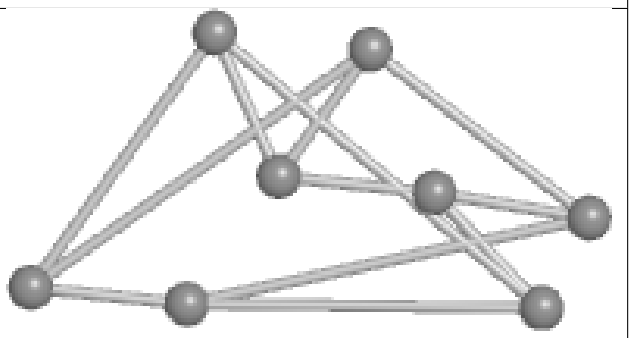


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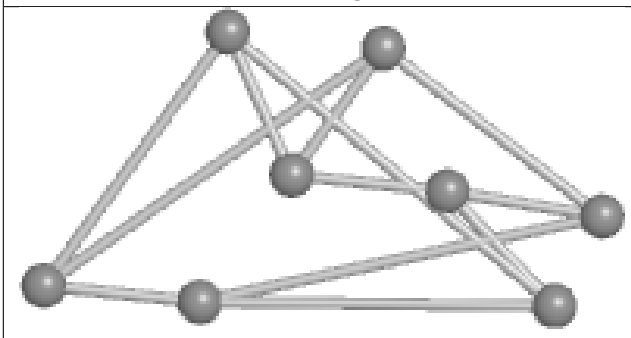
Ligand SF4 G 842



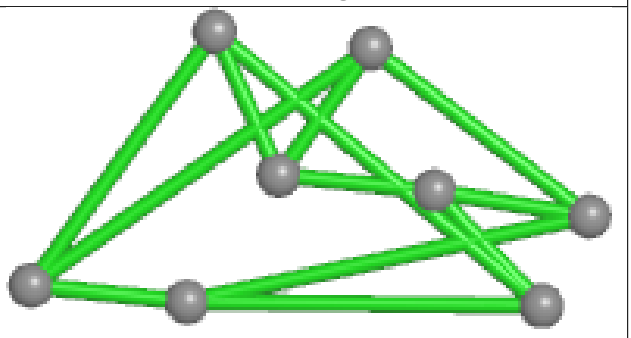
Bond lengths



Bond angles



Torsions



Rings

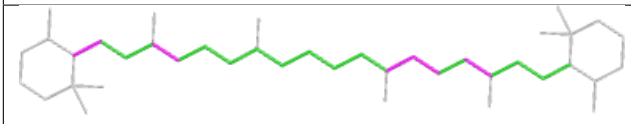
Ligand BCR g 846



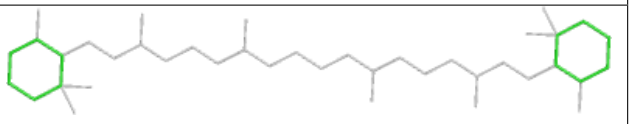
Bond lengths



Bond angles

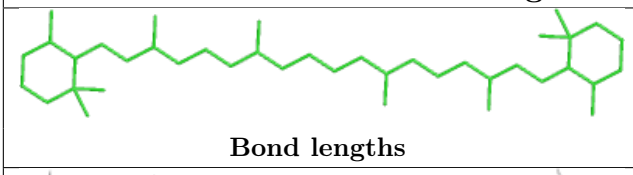


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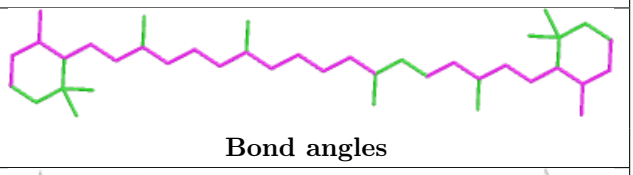


Rings

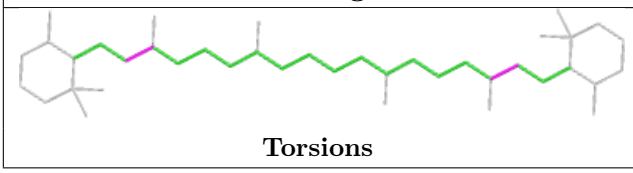
Ligand BCR n 846



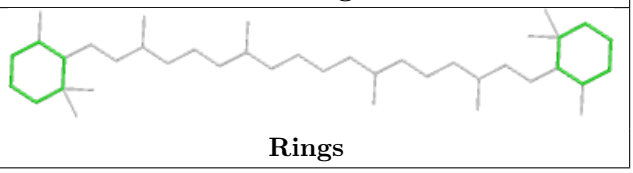
Bond lengths



Bond angles

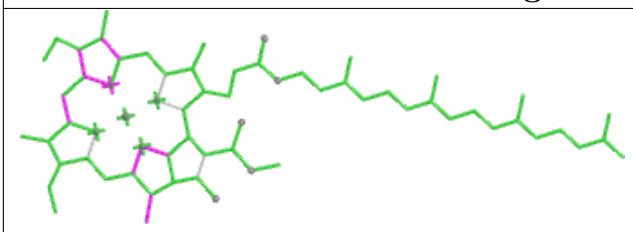


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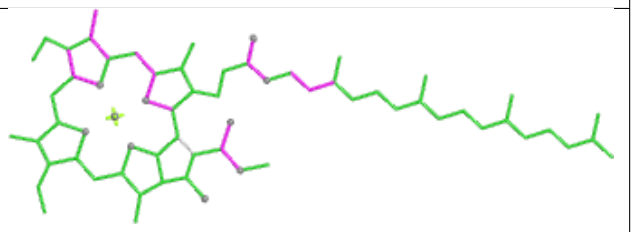


Rings

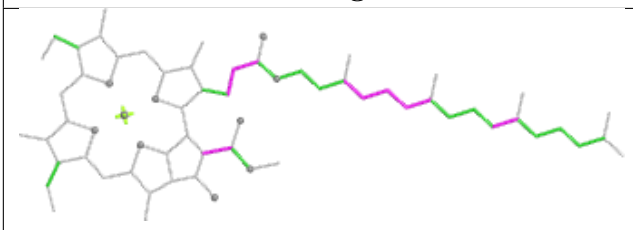
Ligand CLA A 808



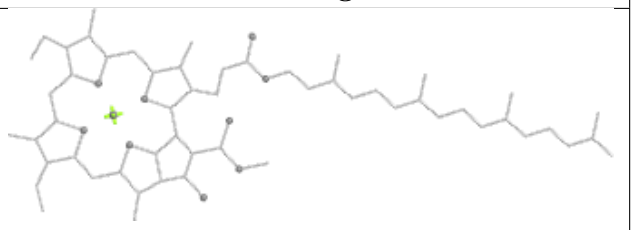
Bond lengths



Bond angles

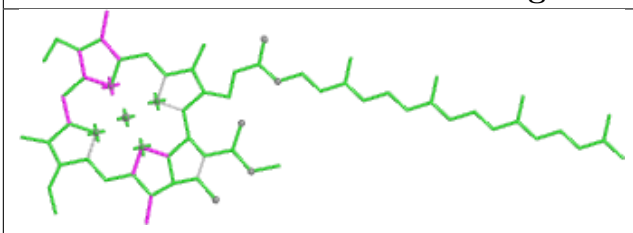


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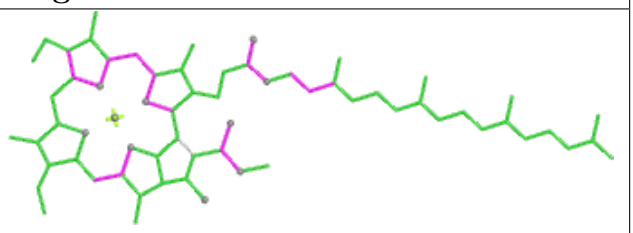


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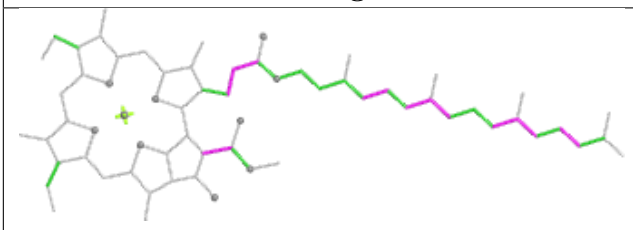
Ligand CLA g 838



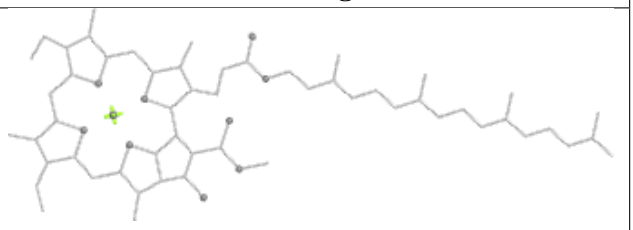
Bond lengths



Bond angles

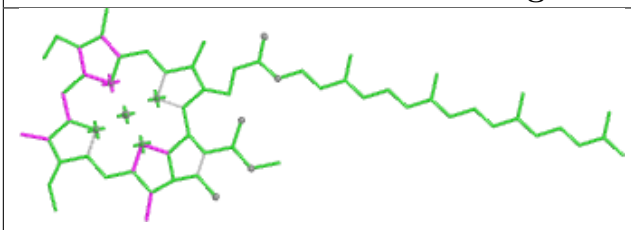


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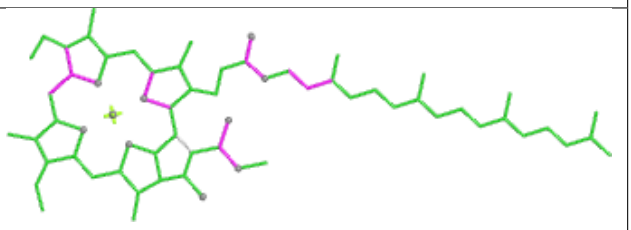


Rings

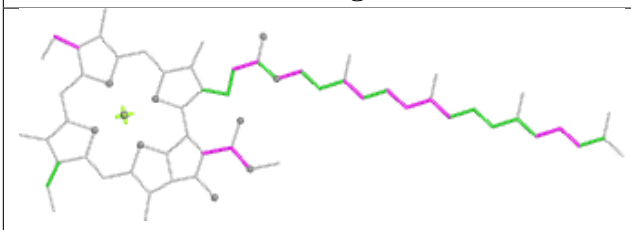
Ligand CLA b 803



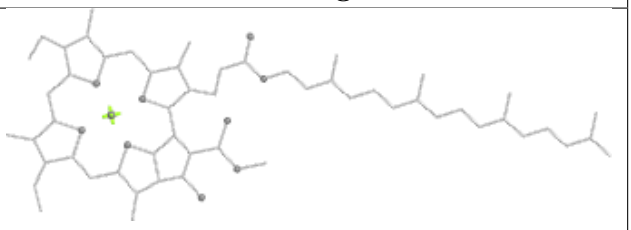
Bond lengths



Bond angles

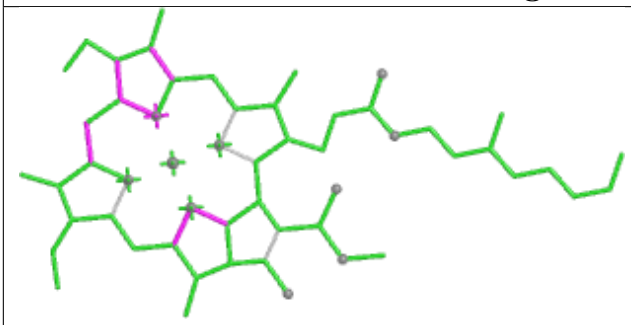


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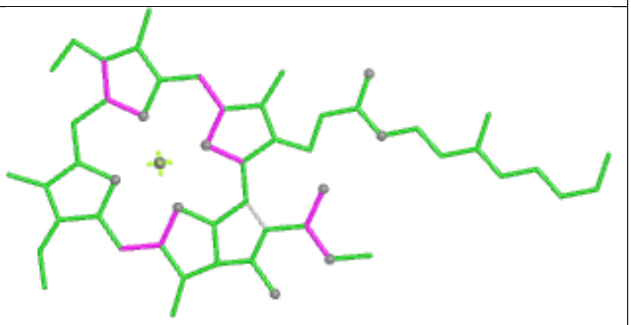


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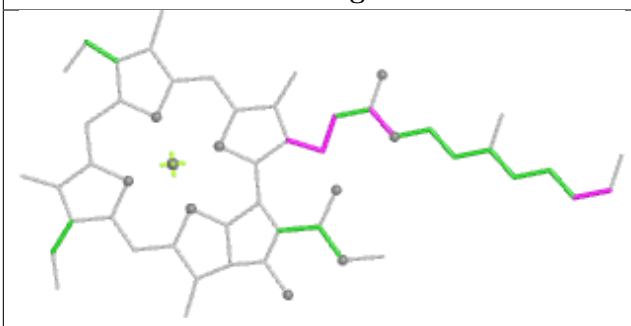
Ligand CLA A 803



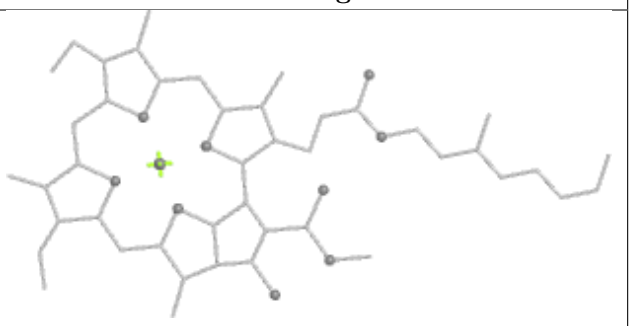
Bond lengths



Bond angles

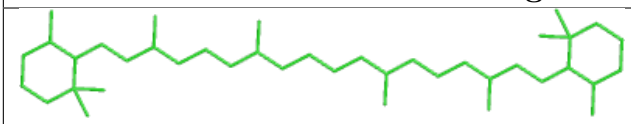


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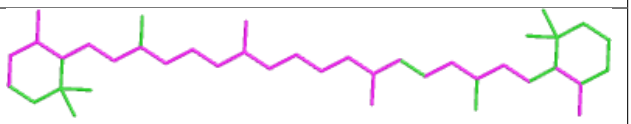


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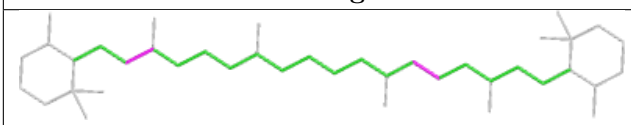
Ligand BCR n 845



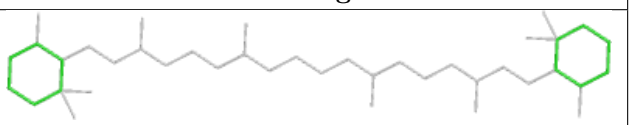
Bond lengths



Bond angles

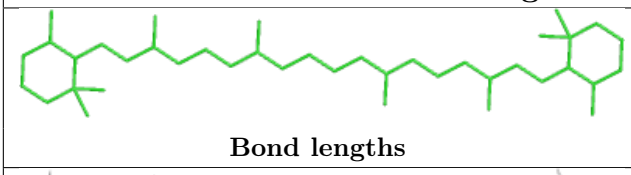


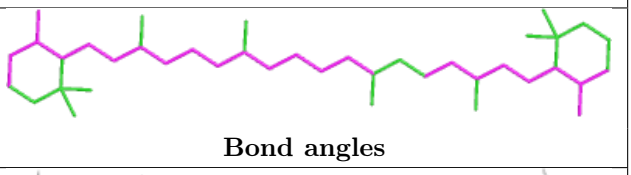
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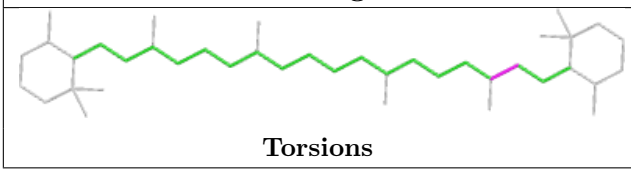


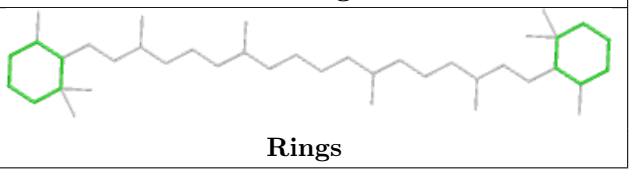
Rings

Ligand BCR N 848

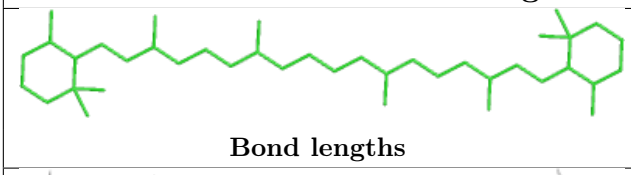

Bond lengths

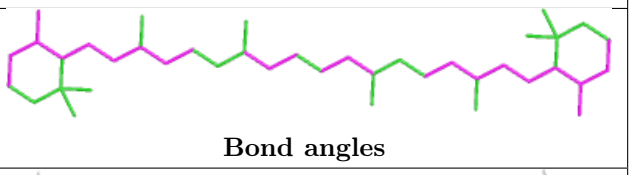

Bond angles

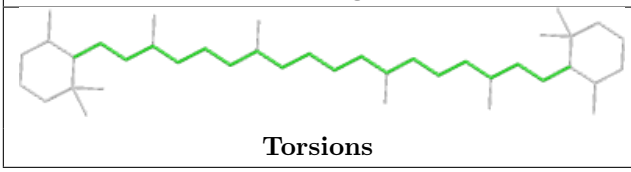

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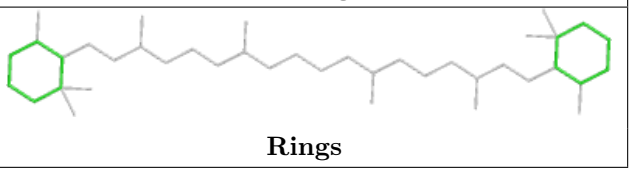

Rings

Ligand BCR U 103

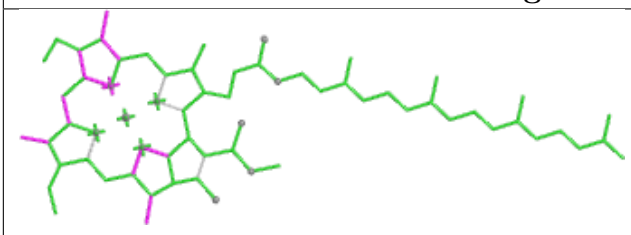

Bond lengths

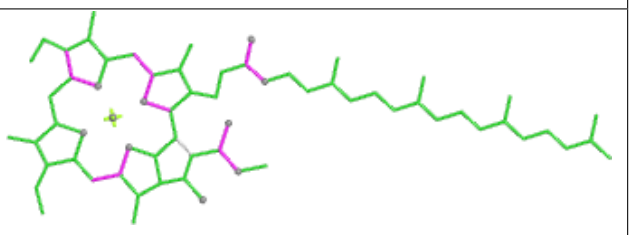

Bond angles

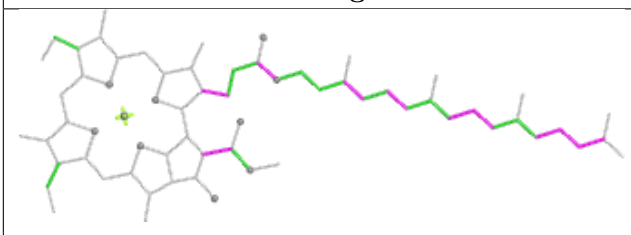

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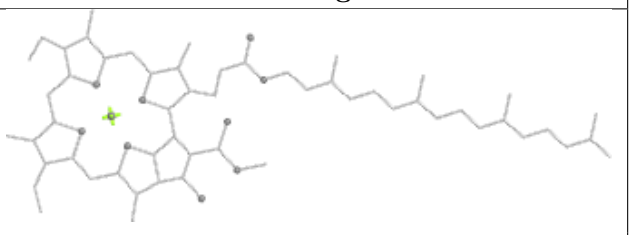

Rings

Ligand CLA A 804


Bond lengths

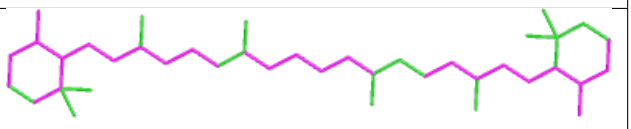

Bond angles

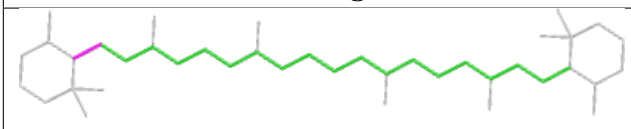

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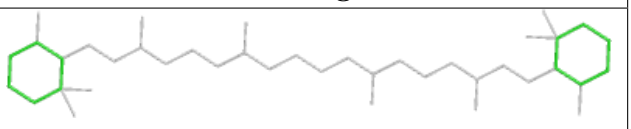

Rings

Ligand BCR K 102

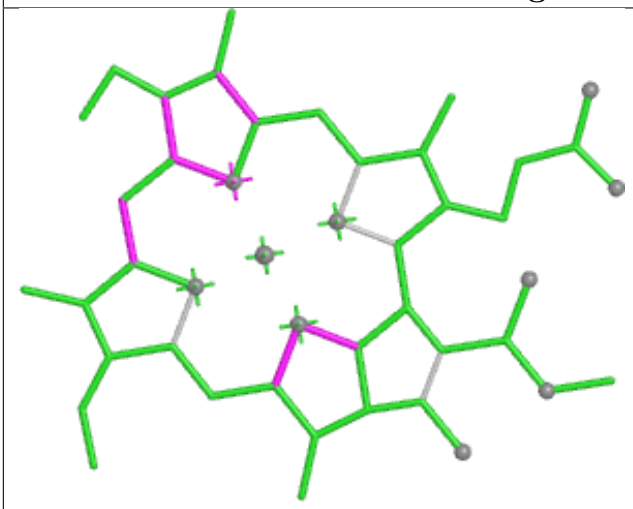

Bond lengths


Bond angles

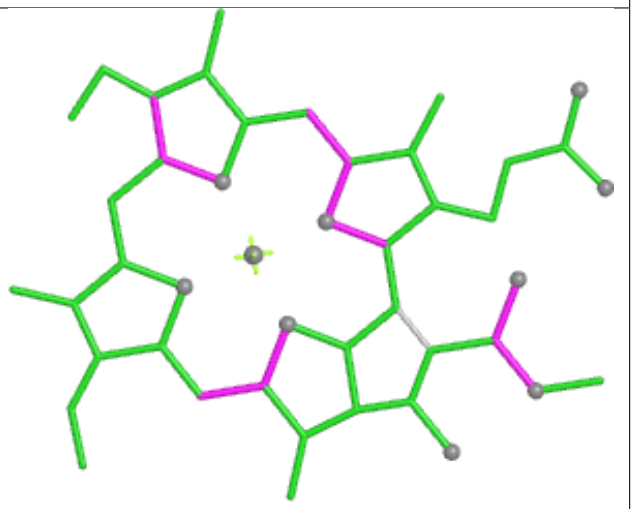

Torsions


Rings

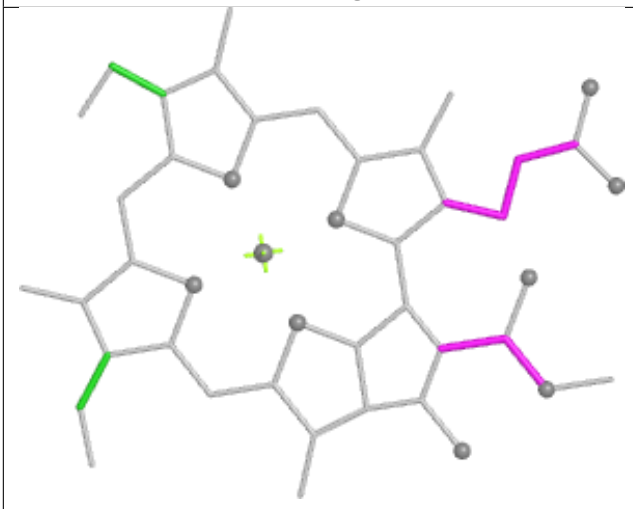
Ligand CLA a 834



Bond lengths



Bond angles

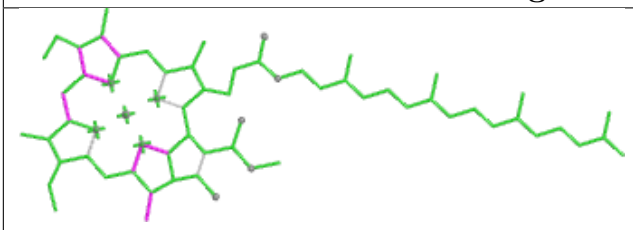


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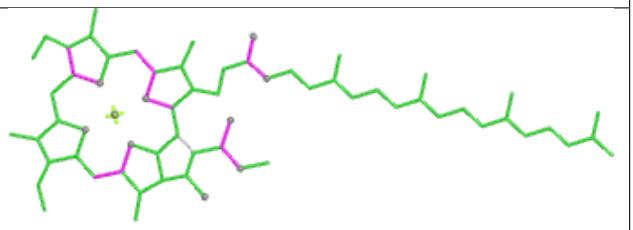


Rings

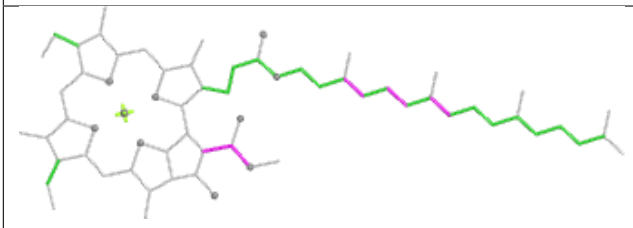
Ligand CLA a 828



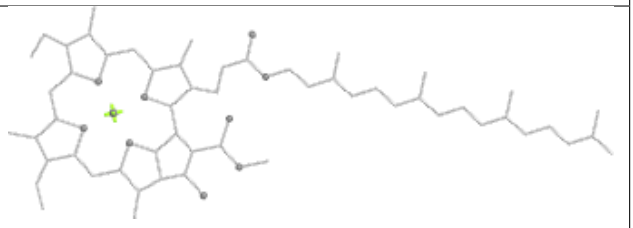
Bond lengths



Bond angles

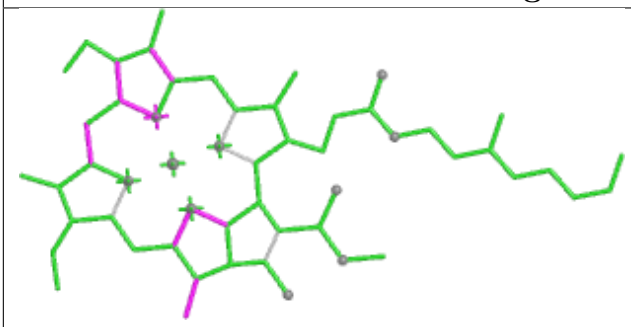


Torsions

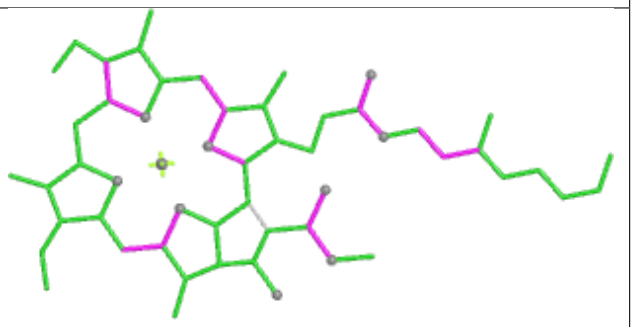


Rings

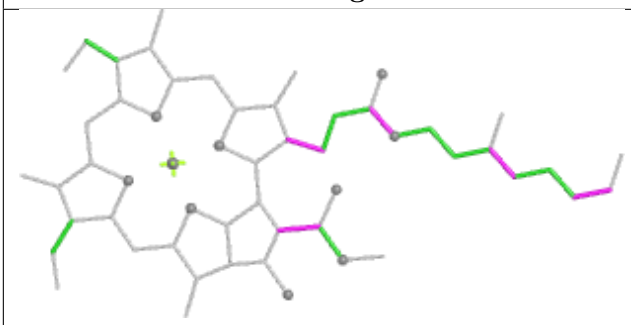
Ligand CLA A 825



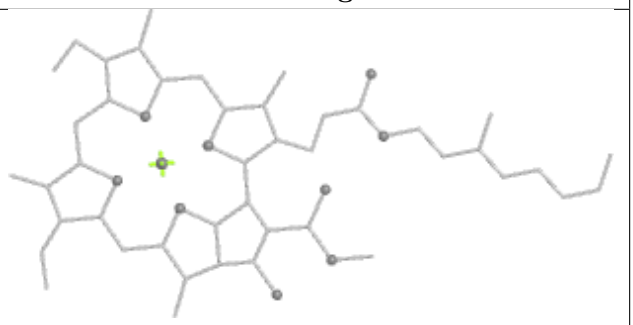
Bond lengths



Bond angles

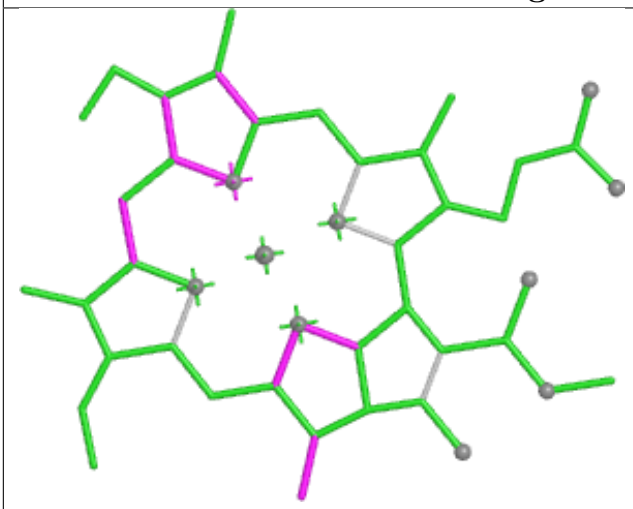


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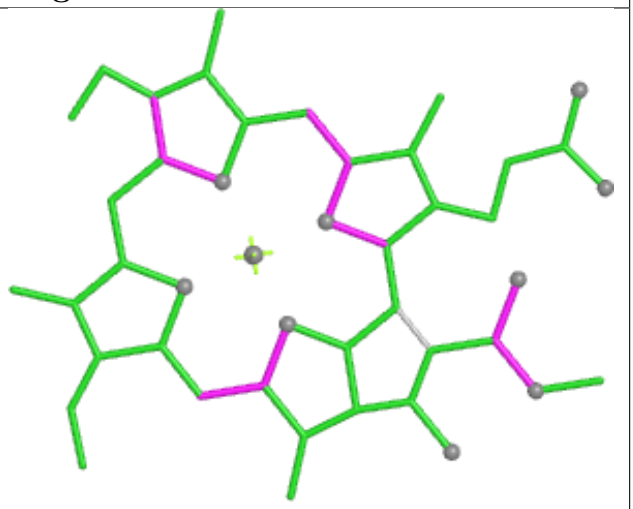


Rings

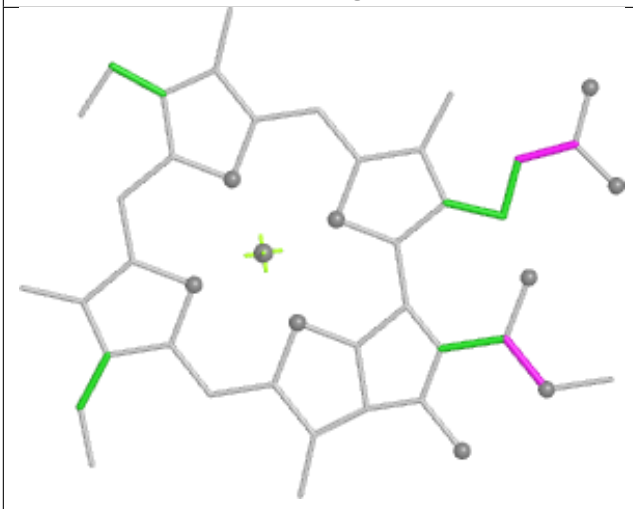
Ligand CLA g 814



Bond lengths



Bond angles

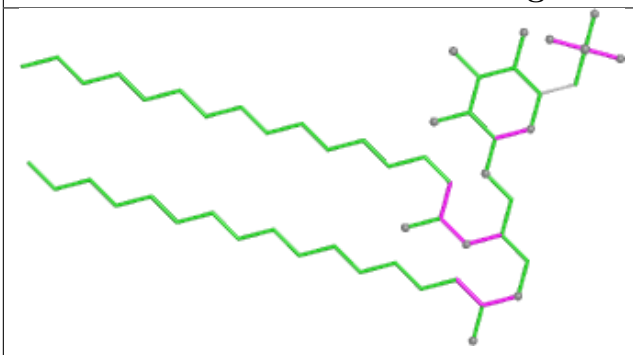


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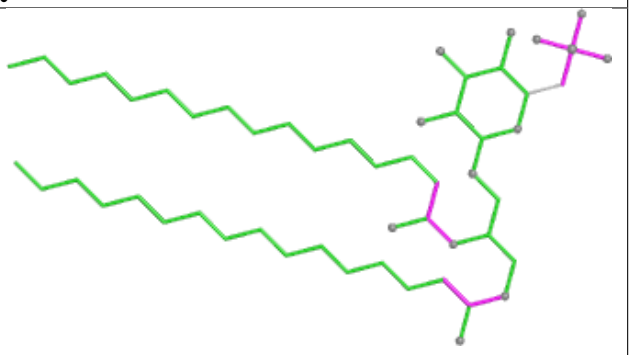


Rings

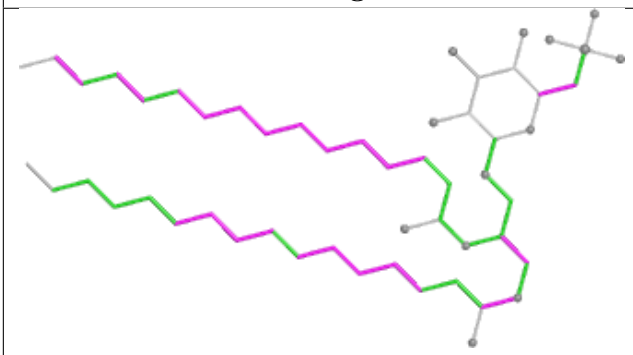
Ligand SQD n 801



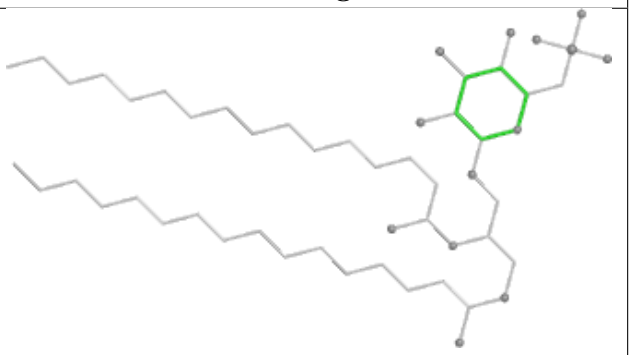
Bond lengths



Bond angles

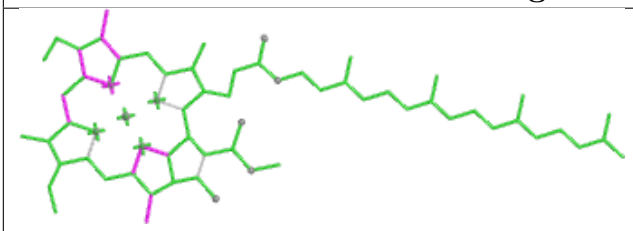


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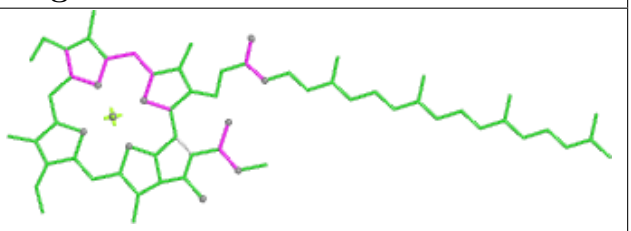


Rings

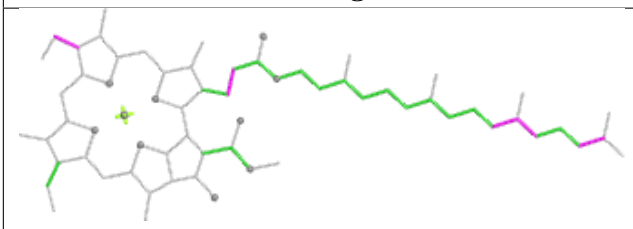
Ligand CLA g 839



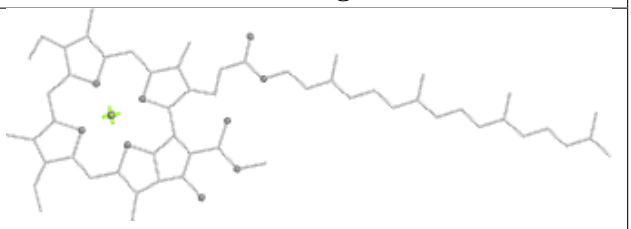
Bond lengths



Bond angles

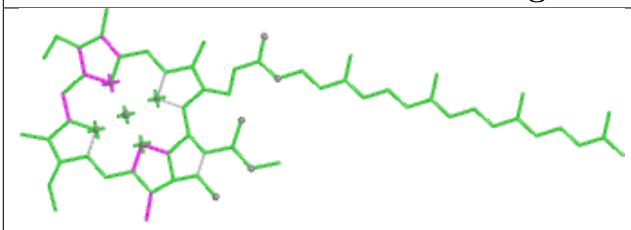


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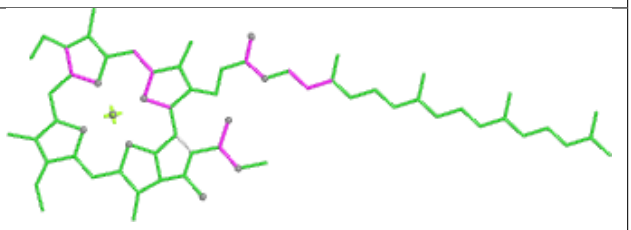


Rings

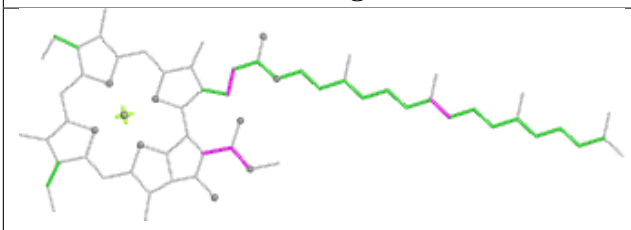
Ligand CLA a 838



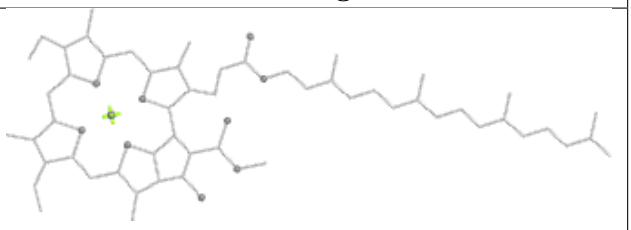
Bond lengths



Bond angles

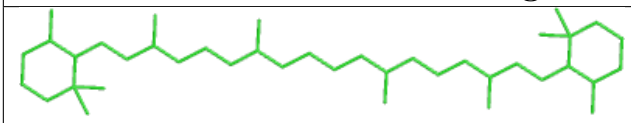


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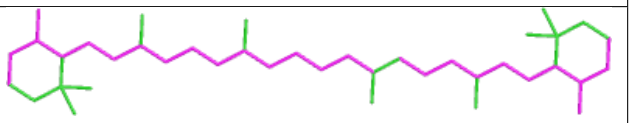


Rings

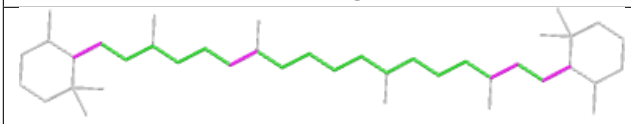
Ligand BCR A 856



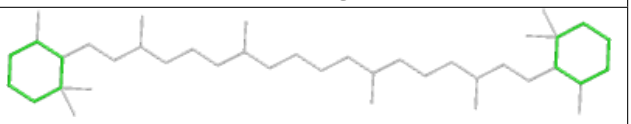
Bond lengths



Bond angles

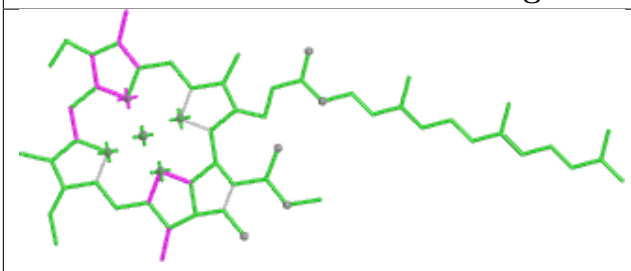


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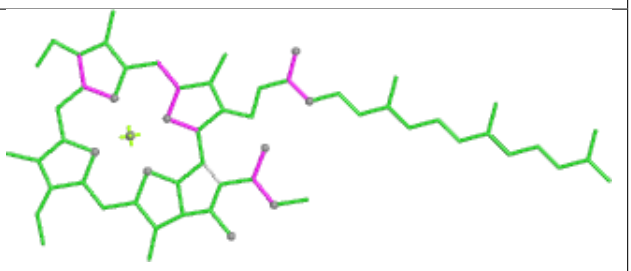


Rings

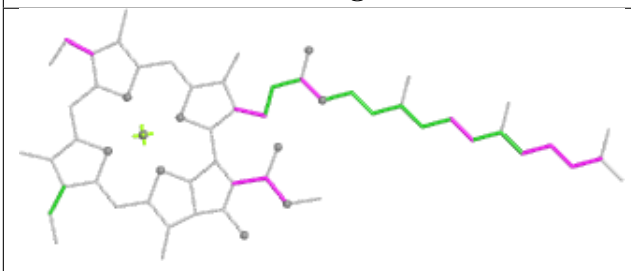
Ligand CLA N 838



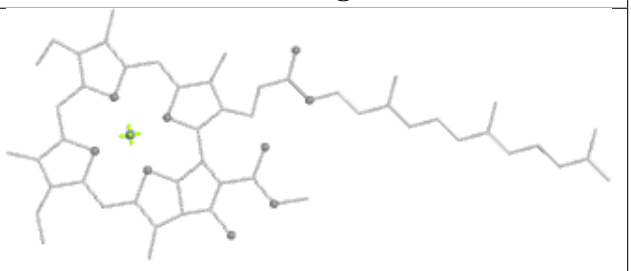
Bond lengths



Bond angles

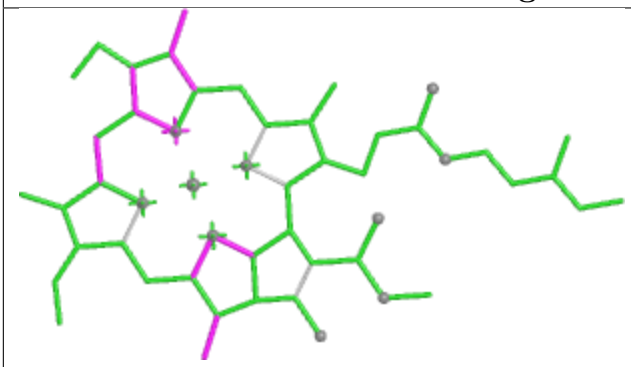


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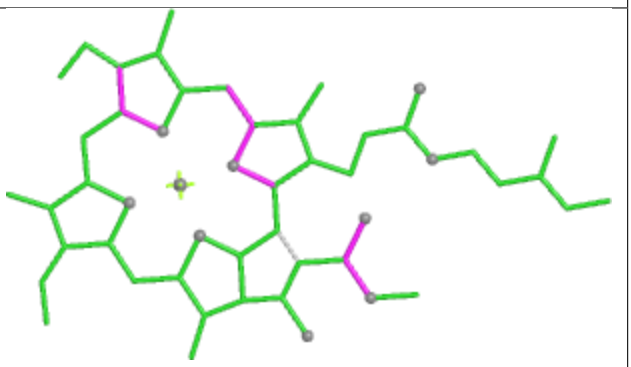


Rings

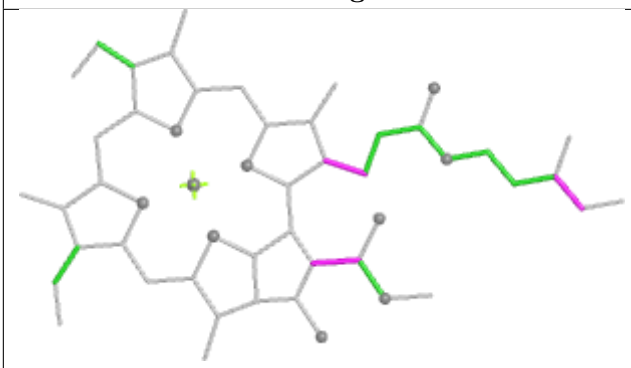
Ligand CLA W 202



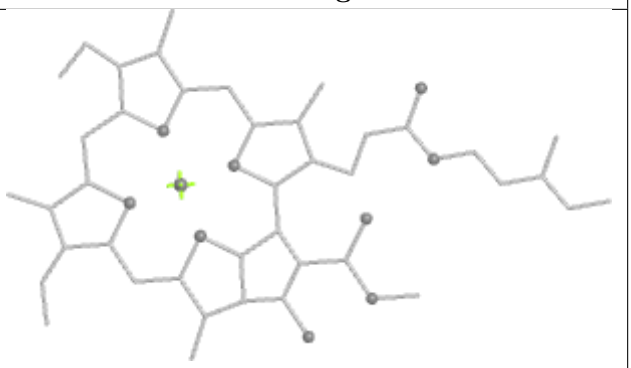
Bond lengths



Bond angles

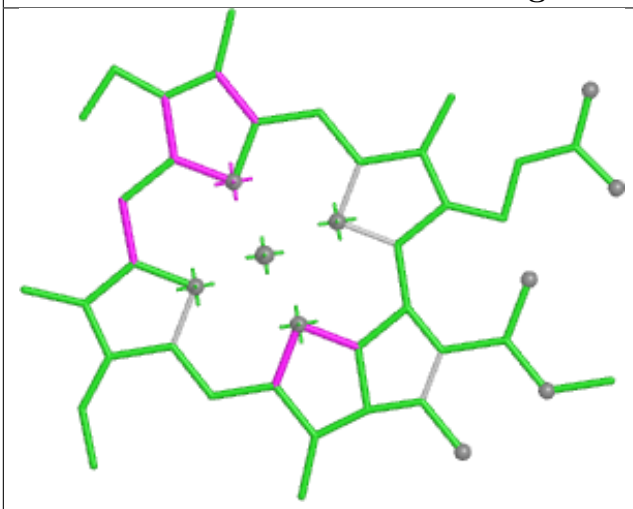


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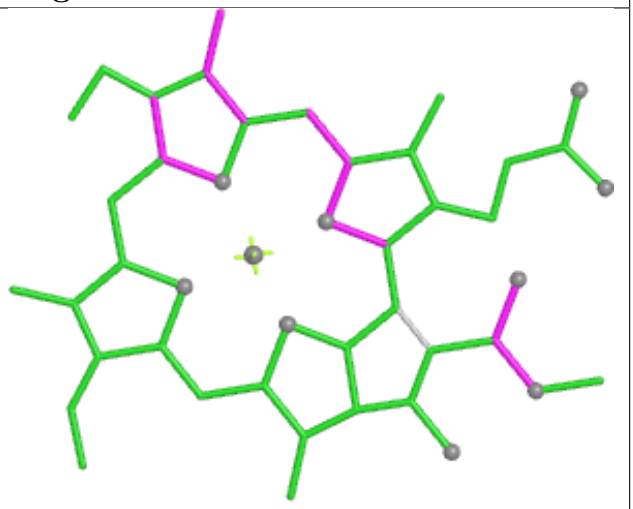


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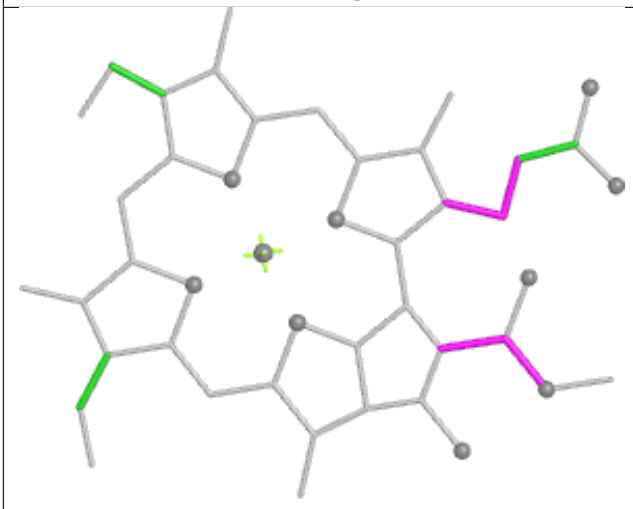
Ligand CLA g 834



Bond lengths



Bond angles

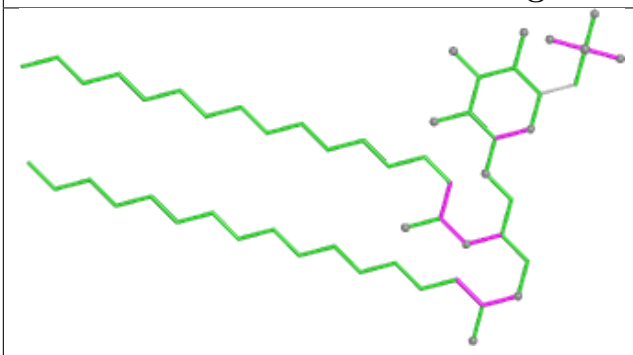


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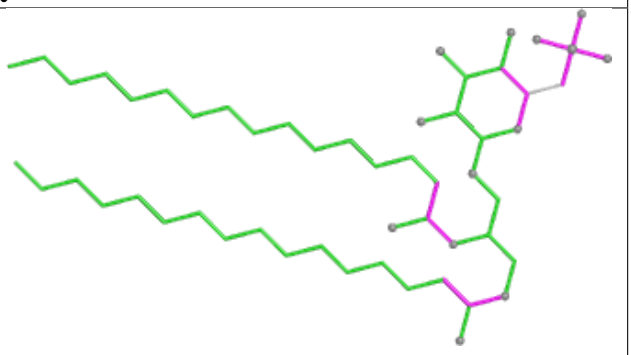


Rings

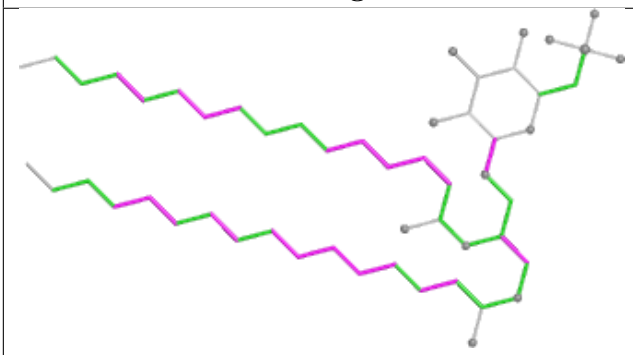
Ligand SQD b 801



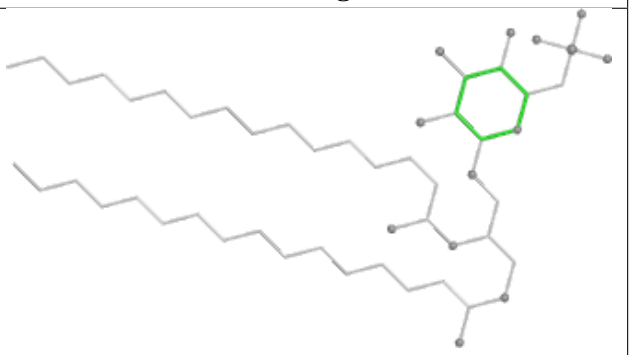
Bond lengths



Bond angles

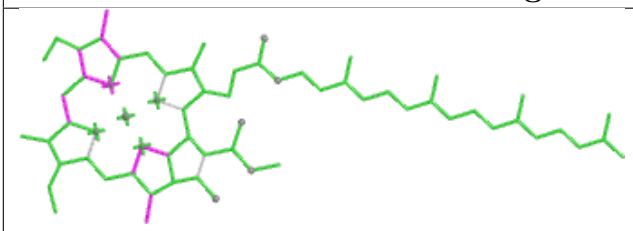


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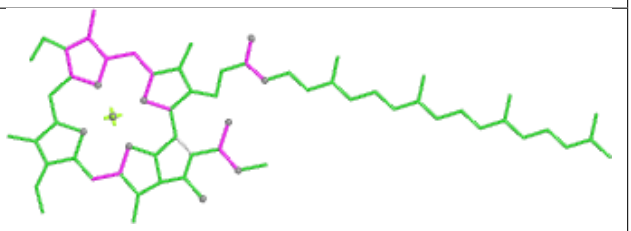


Rings

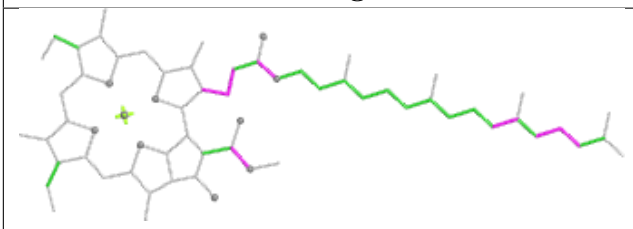
Ligand CLA B 829



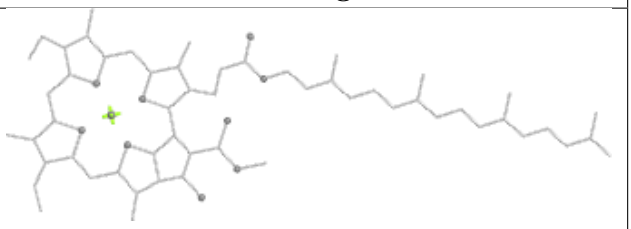
Bond lengths



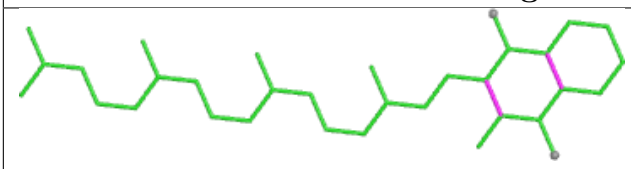
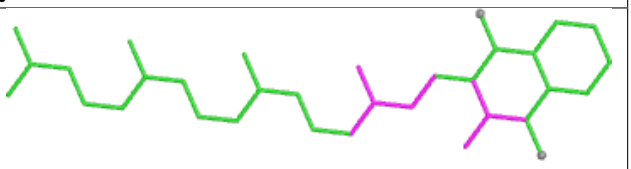
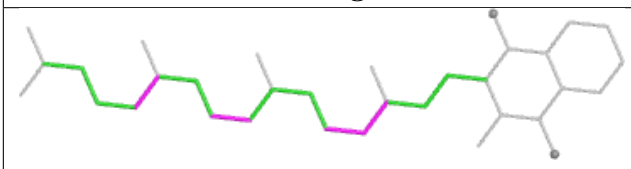
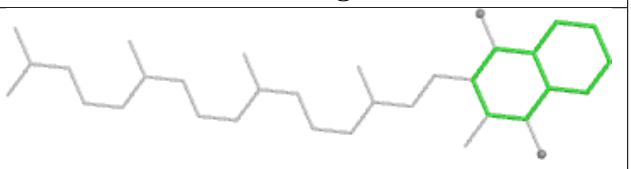
Bond angles

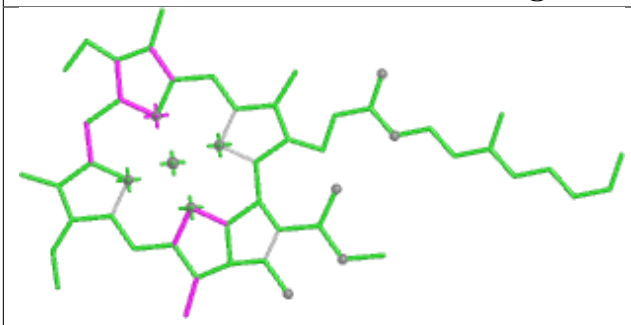
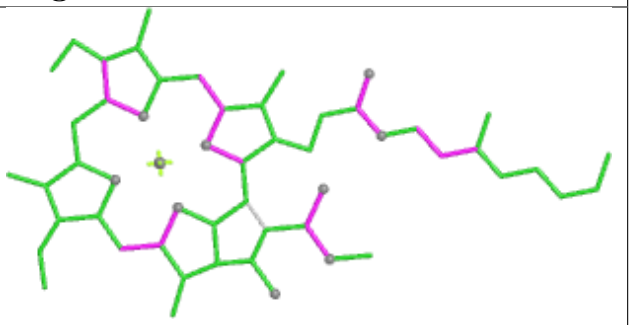
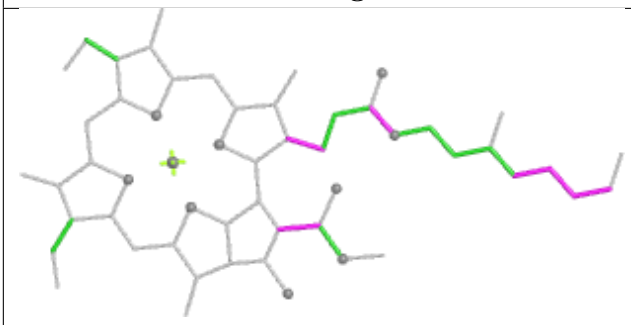
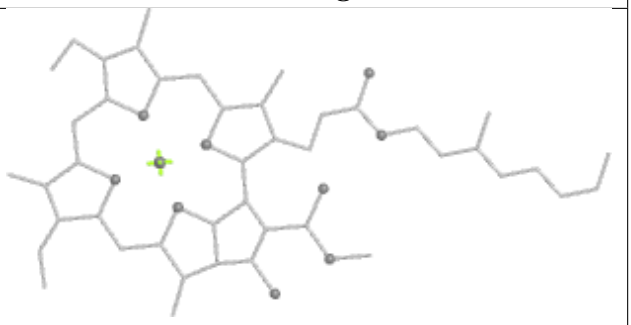


Torsions

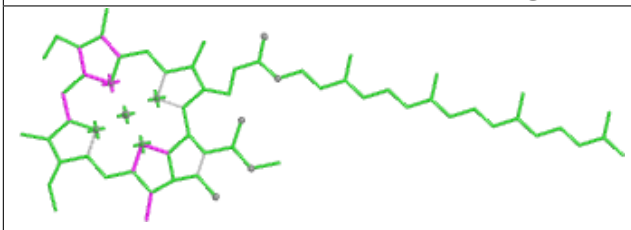


Rings

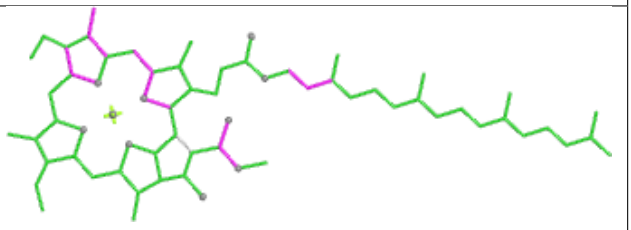
Ligand PQN G 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

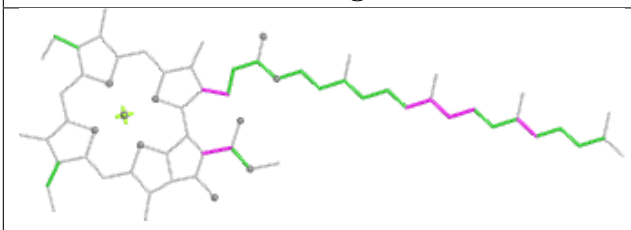
Ligand CLA B 827



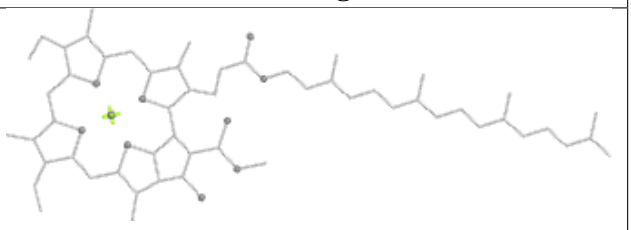
Bond lengths



Bond angles

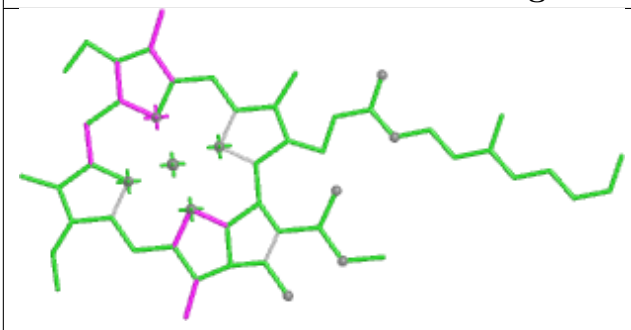


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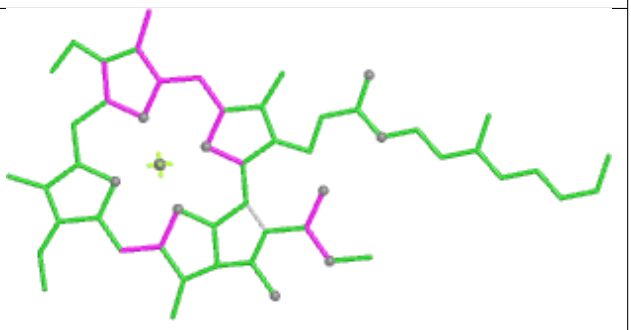


Rings

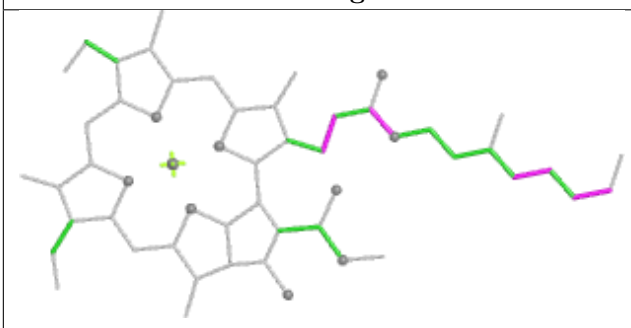
Ligand CLA a 829



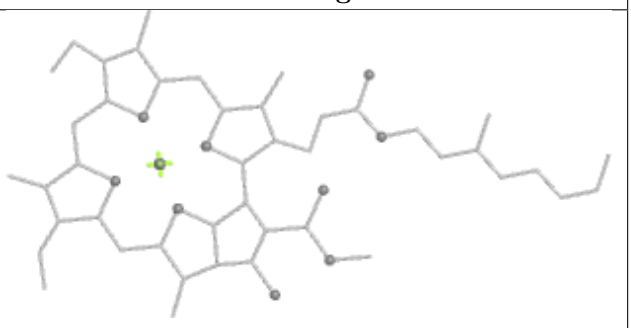
Bond lengths



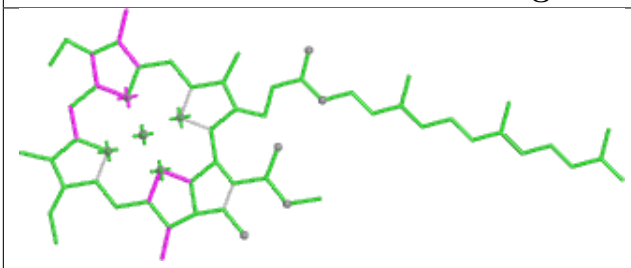
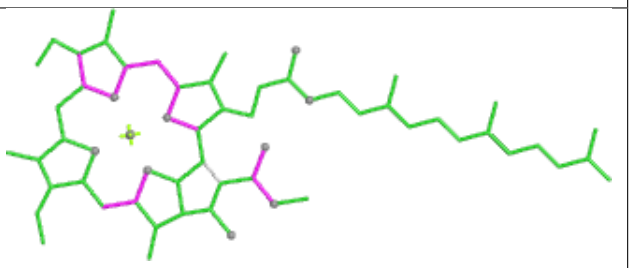
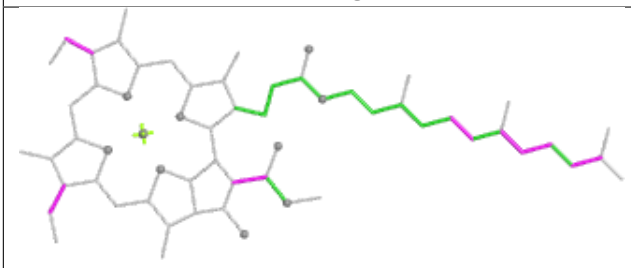
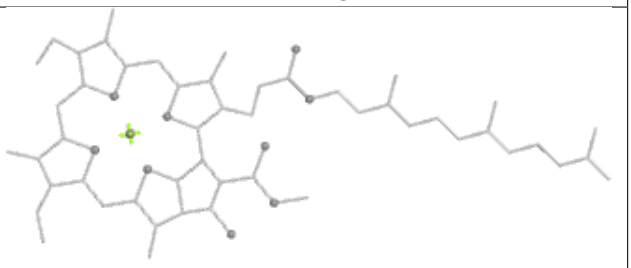
Bond angles

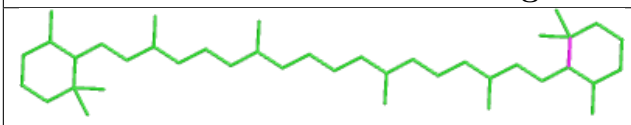
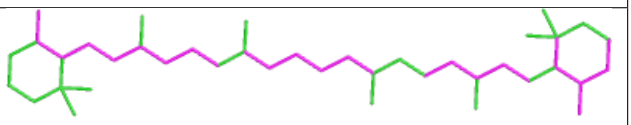
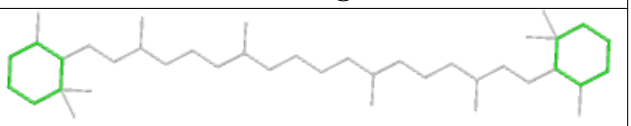


Torsions

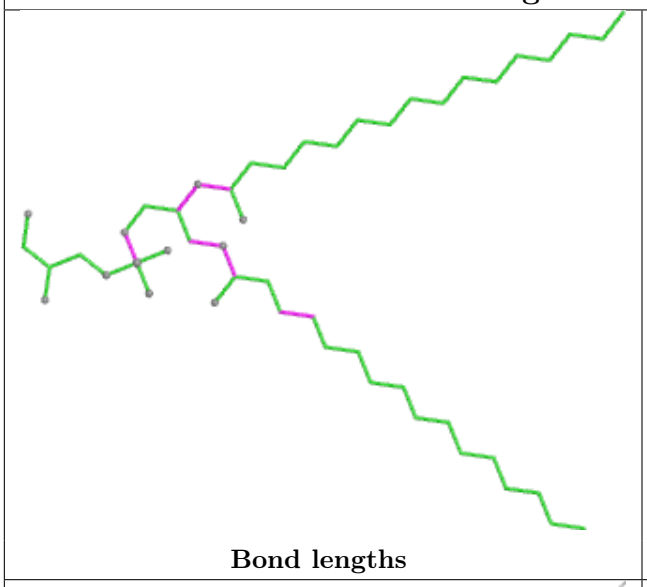


Rings

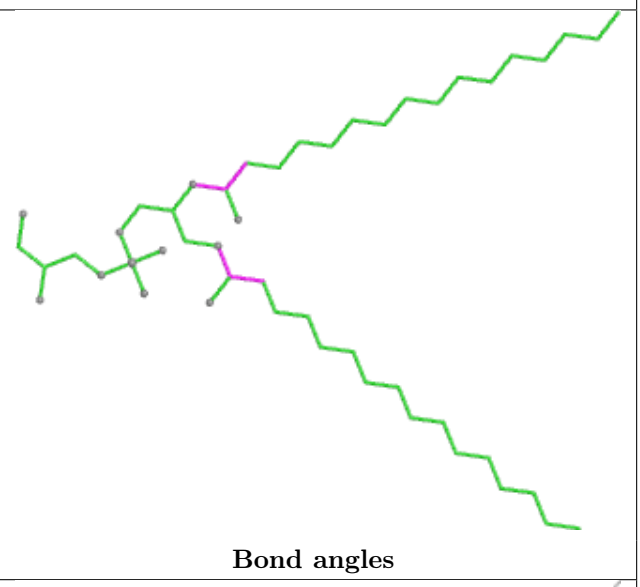
Ligand CLA l 203	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCR G 847	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

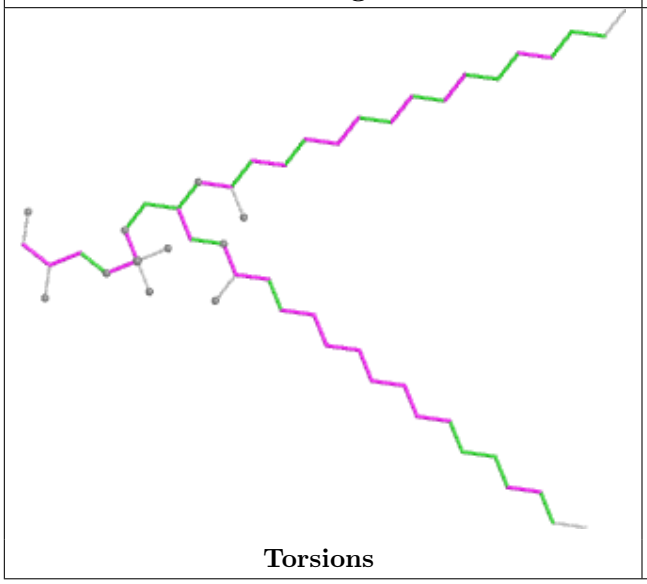
Ligand LHG G 850



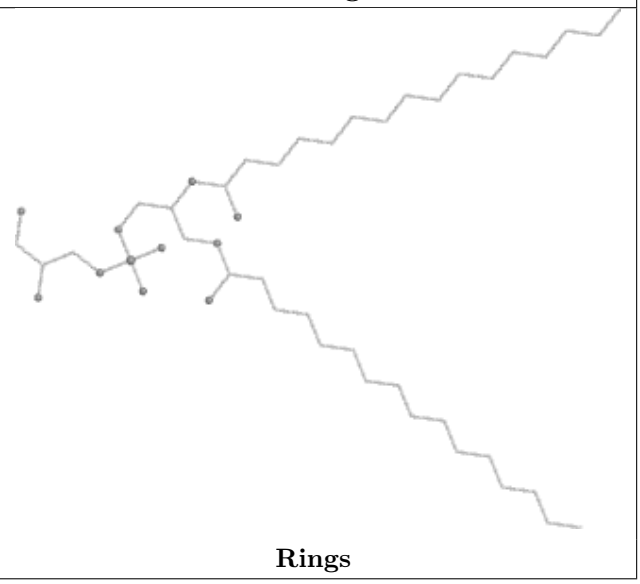
Bond lengths



Bond angles



Torsions

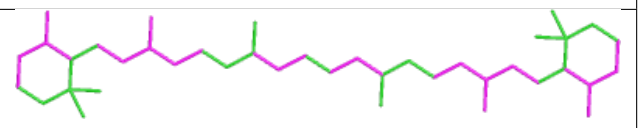


Rings

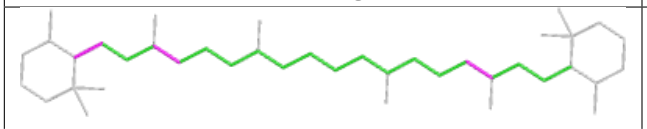
Ligand BCR b 844



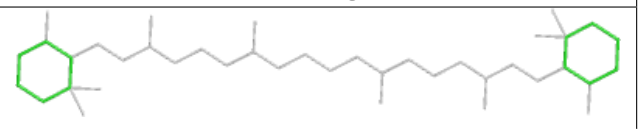
Bond lengths



Bond angles

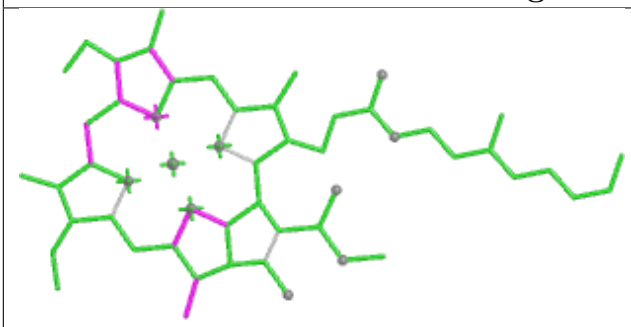


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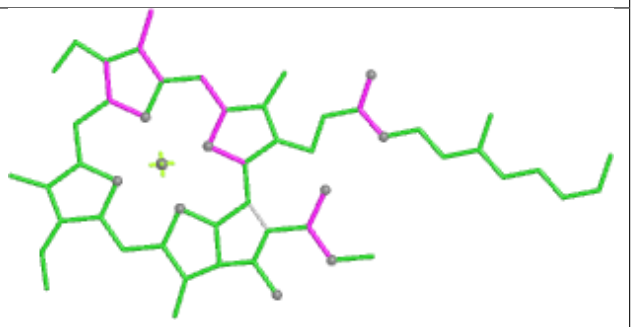


Rings

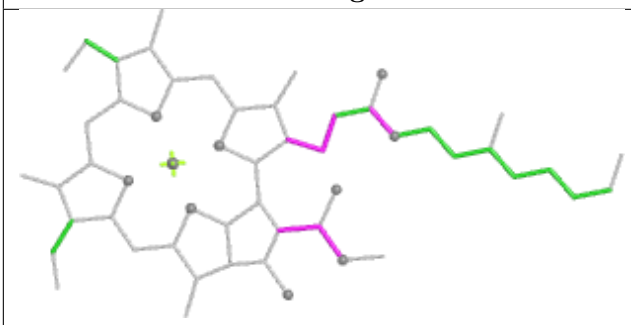
Ligand CLA b 812



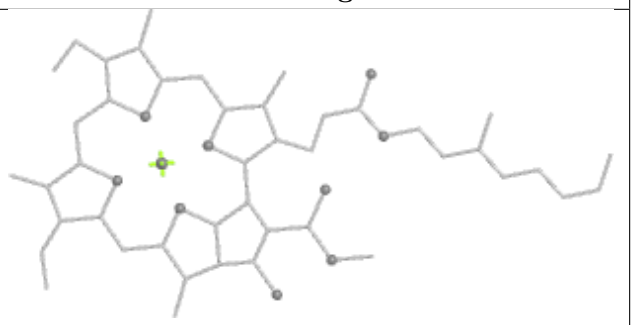
Bond lengths



Bond angles

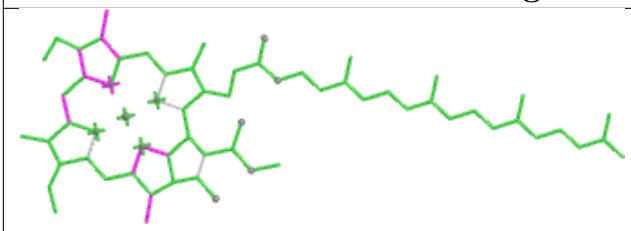


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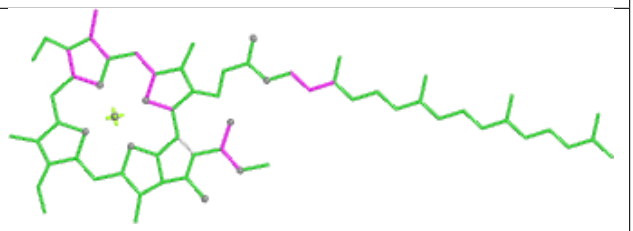


Rings

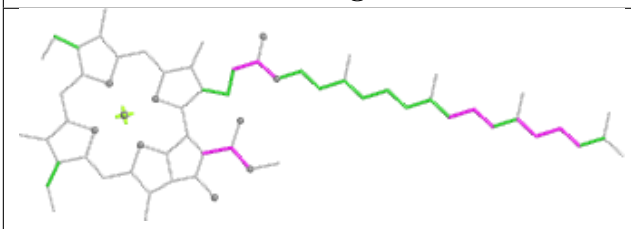
Ligand CLA G 824



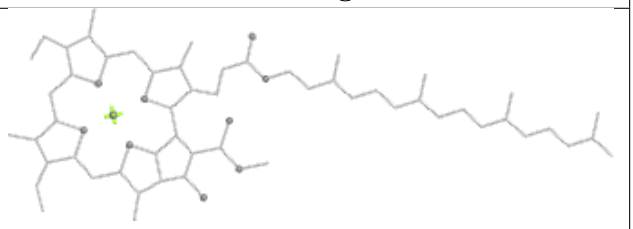
Bond lengths



Bond angles

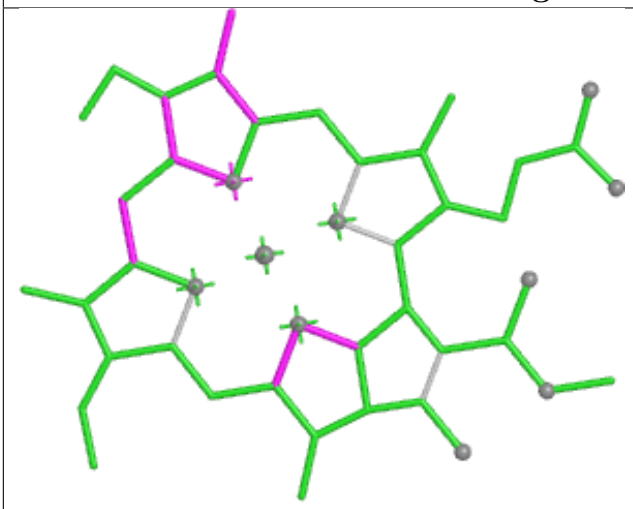


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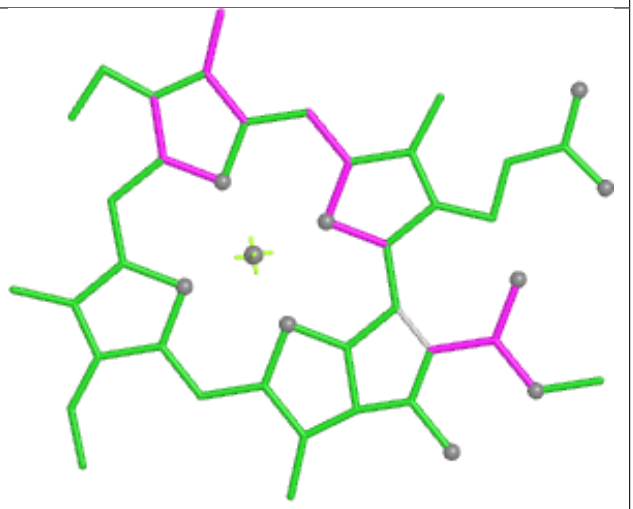


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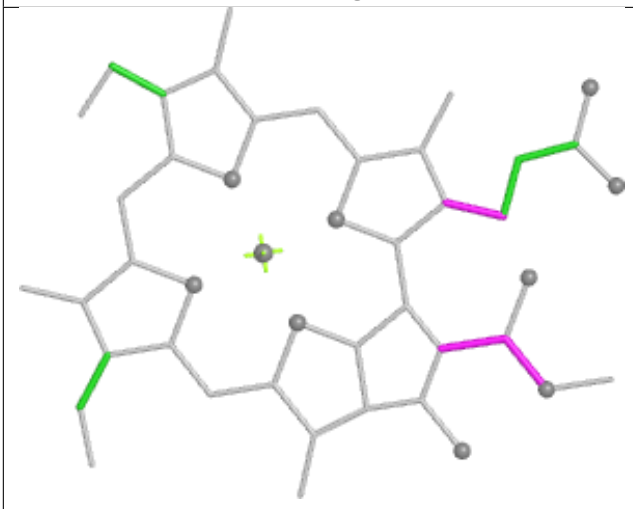
Ligand CLA l 202



Bond lengths



Bond angles

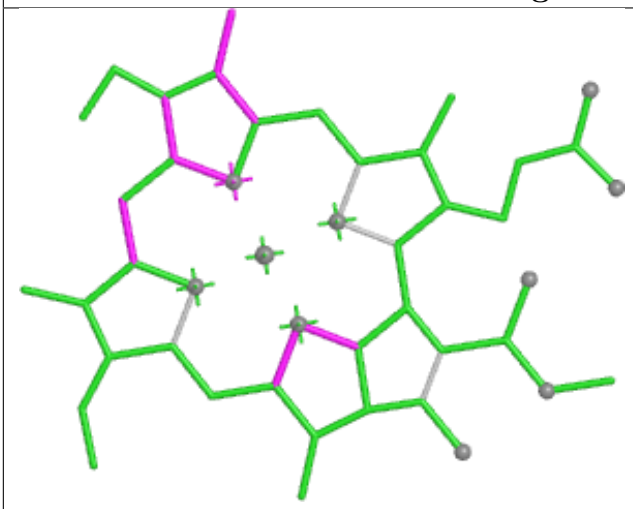


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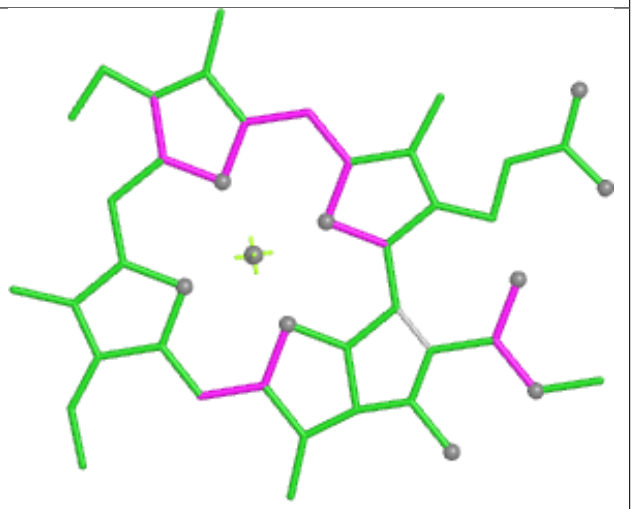


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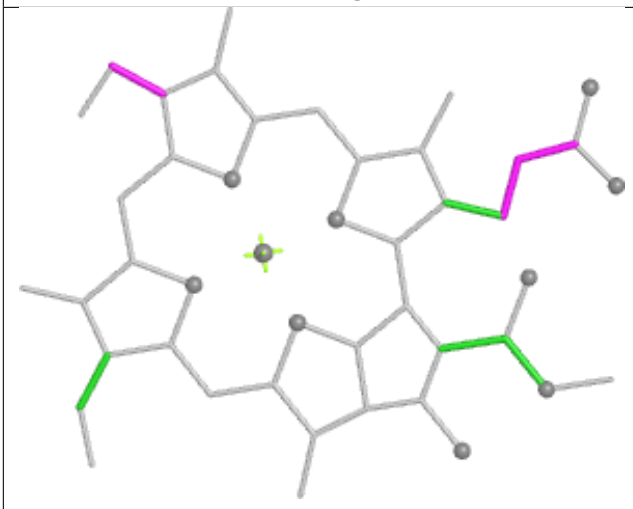
Ligand CLA f 202



Bond lengths



Bond angles

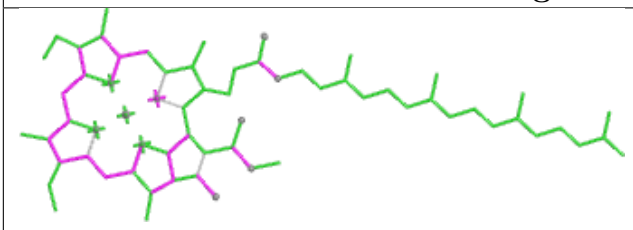


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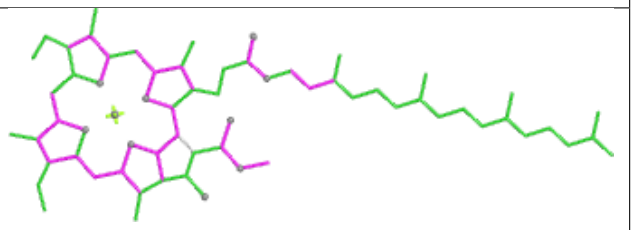


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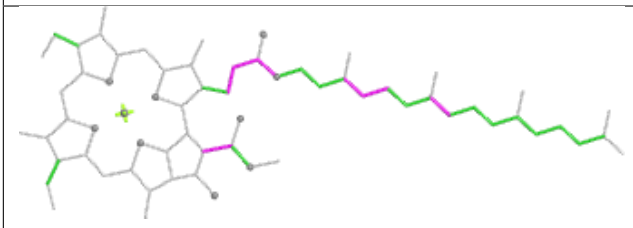
Ligand CL0 a 851



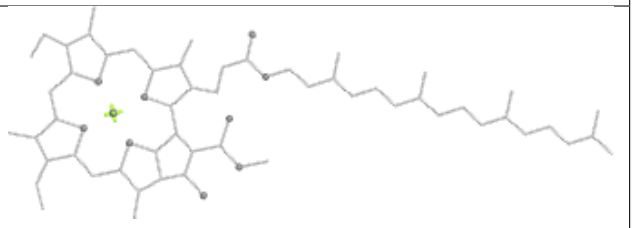
Bond lengths



Bond angles

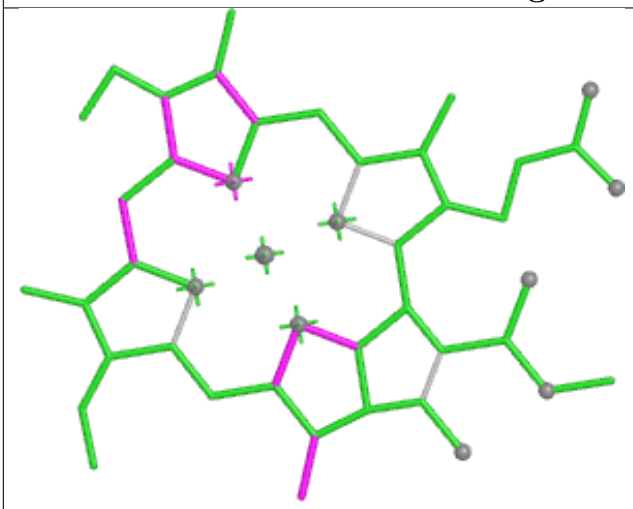


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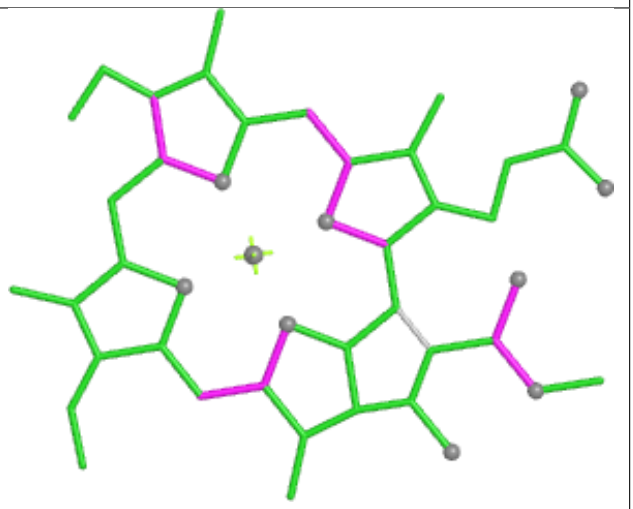


Rings

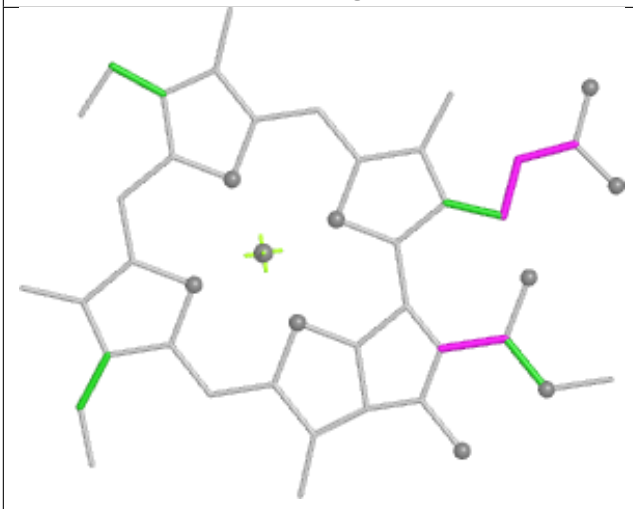
Ligand CLA a 814



Bond lengths



Bond angles

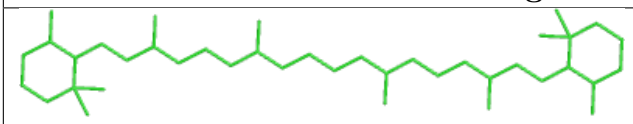


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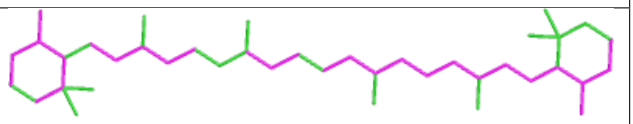


Rings

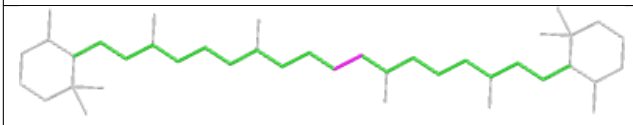
Ligand BCR b 851



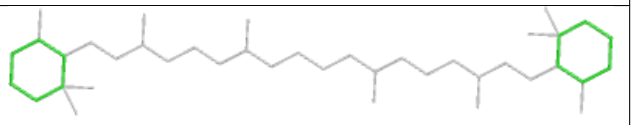
Bond lengths



Bond angles

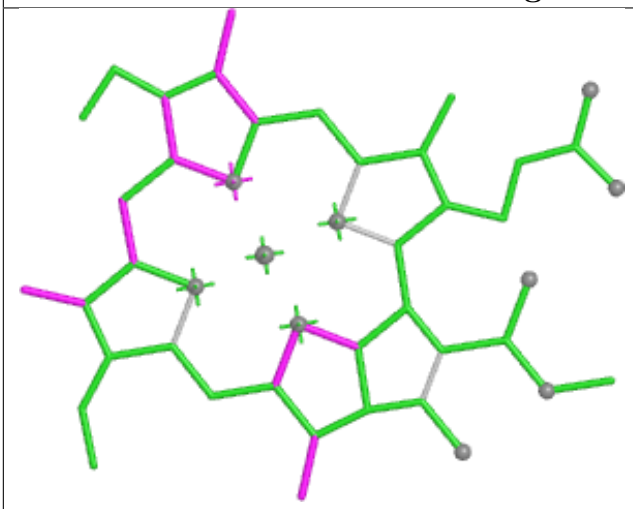


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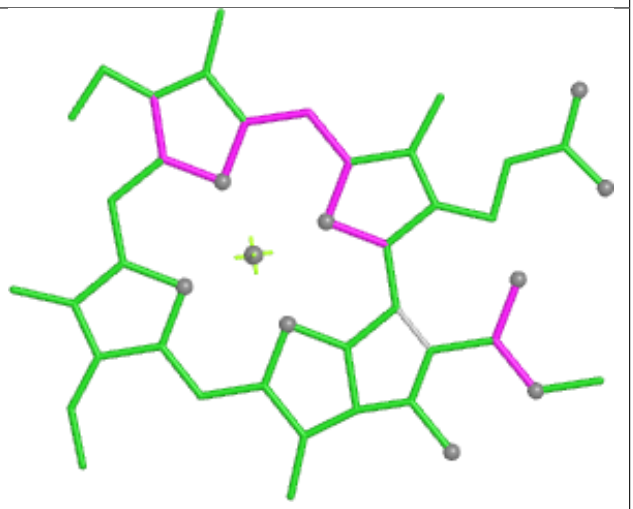


Rings

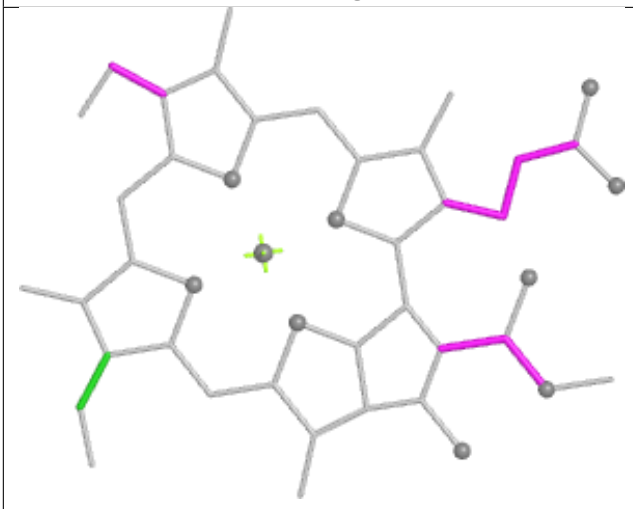
Ligand CLA B 817



Bond lengths



Bond angles

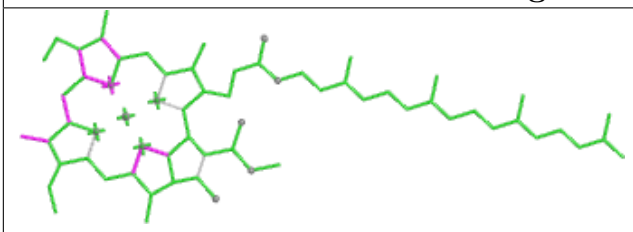


Torsions

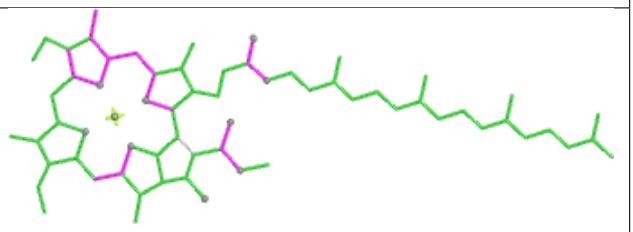


Rings

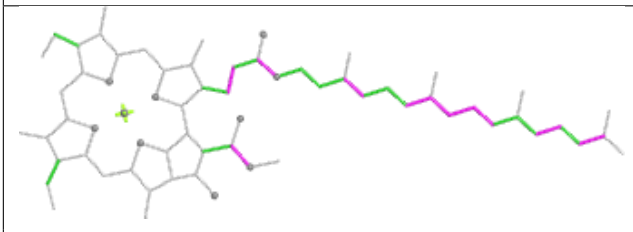
Ligand CLA a 819



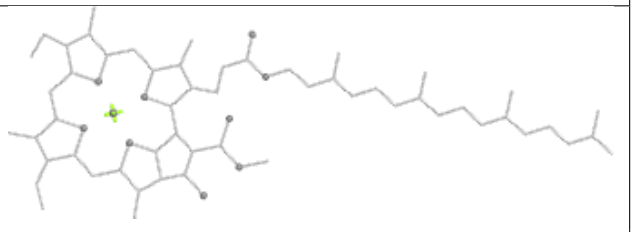
Bond lengths



Bond angles

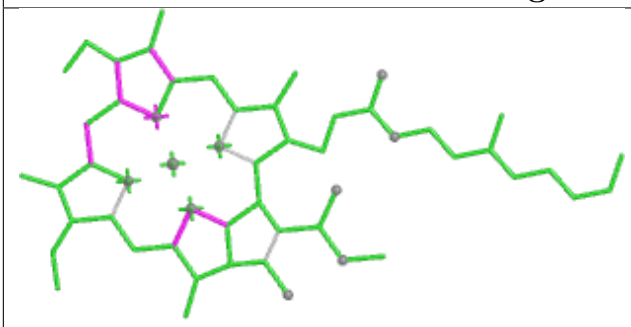


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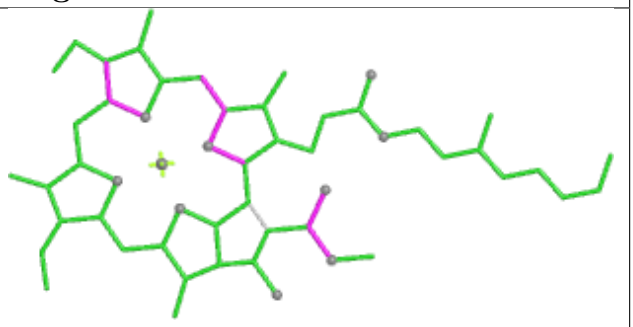


Rings

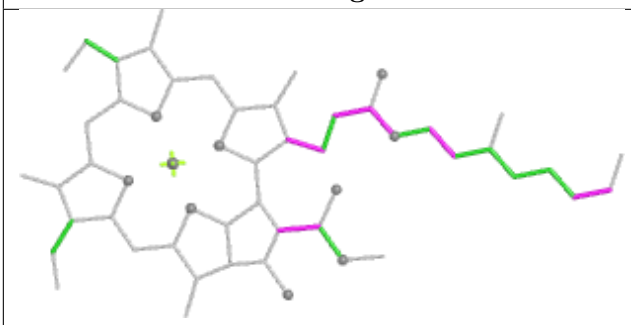
Ligand CLA g 818



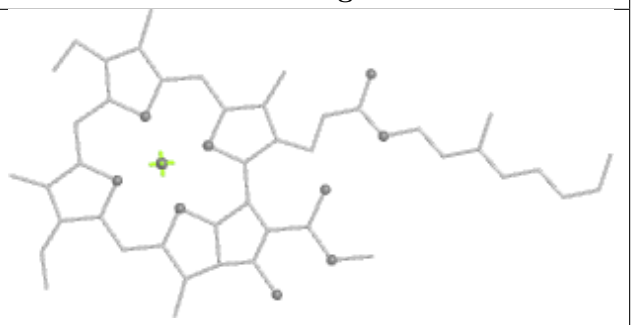
Bond lengths



Bond angles

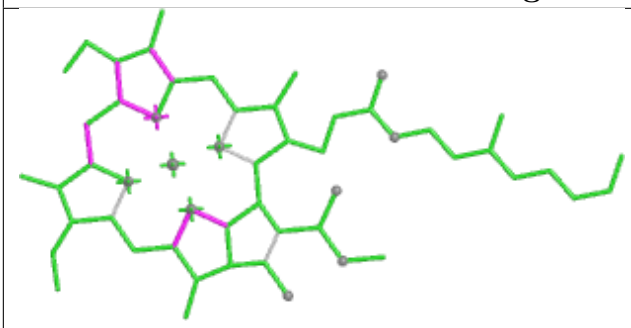


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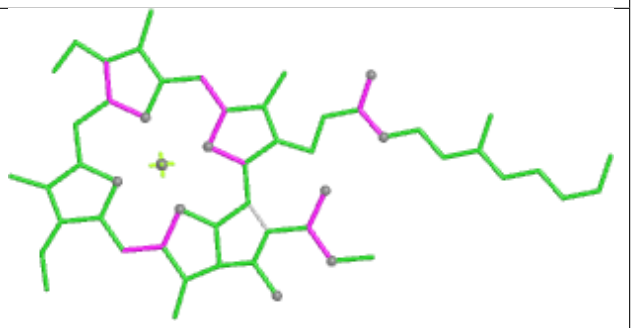


Rings

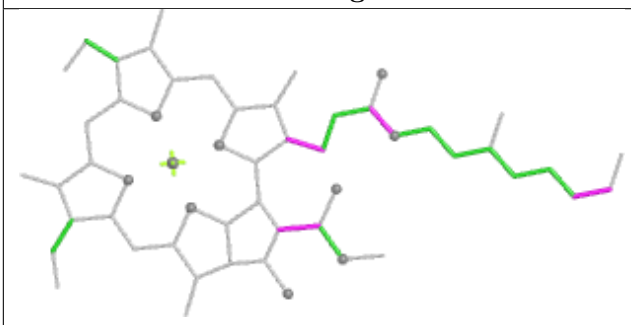
Ligand CLA G 813



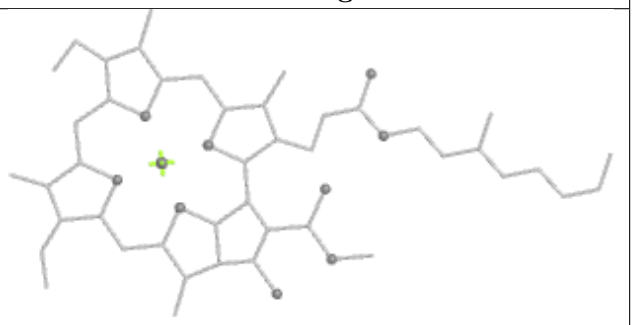
Bond lengths



Bond angles

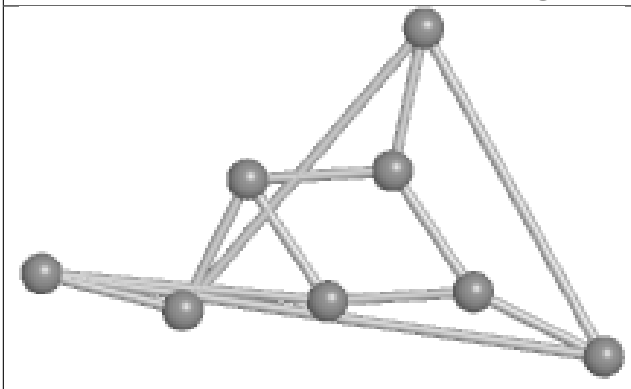


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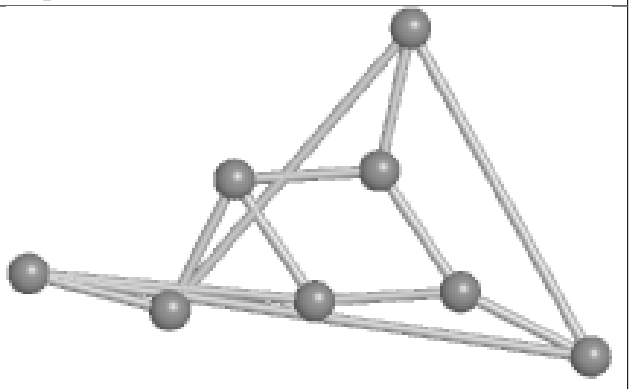


Rings

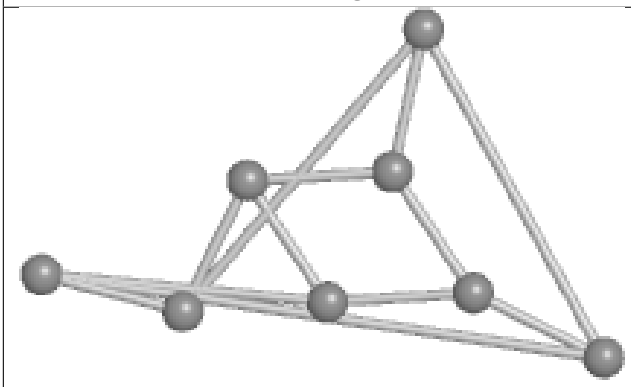
Ligand SF4 p 102



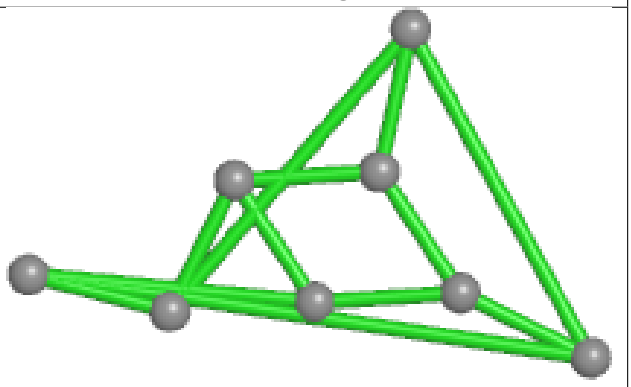
Bond lengths



Bond angles

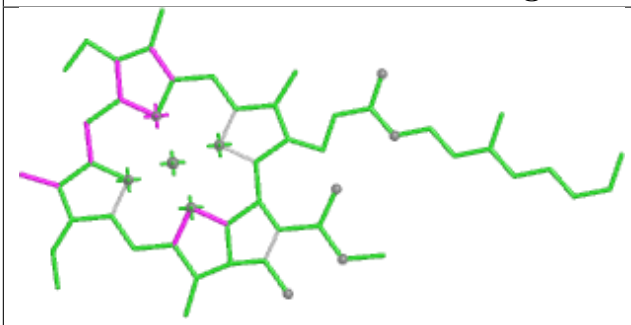


Torsions

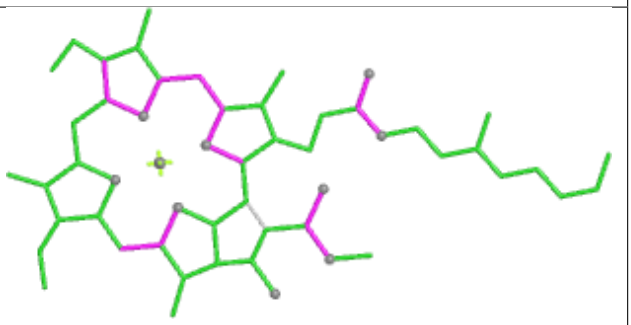


Rings

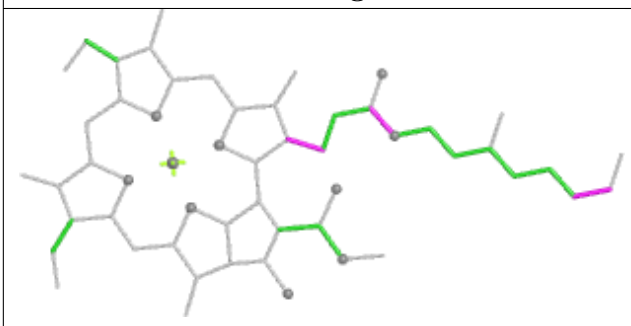
Ligand CLA G 803



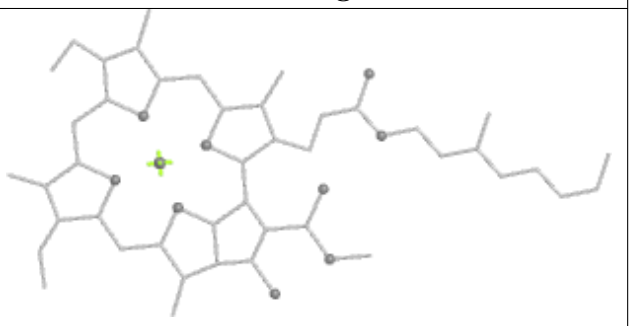
Bond lengths



Bond angles

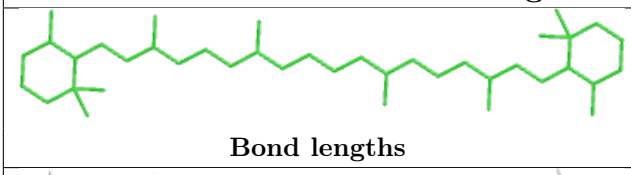


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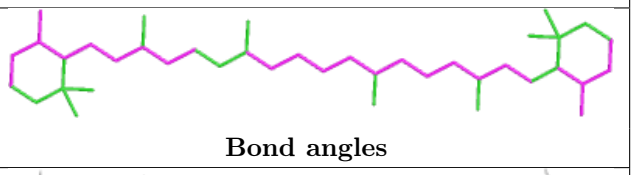


Rings

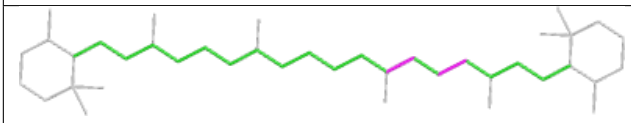
Ligand BCR n 849



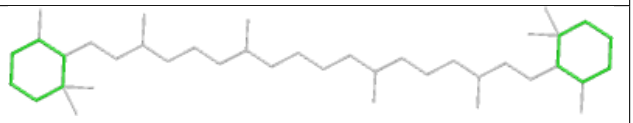
Bond lengths



Bond angles



Torsions

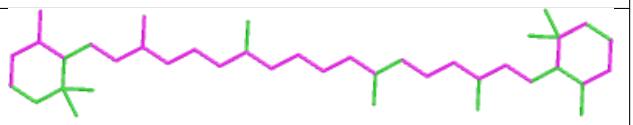


Rings

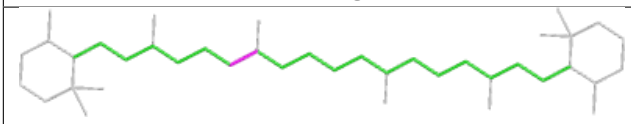
Ligand BCR A 844



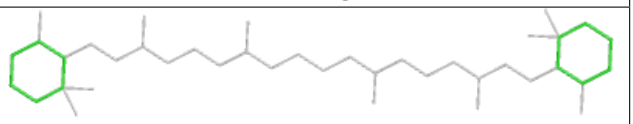
Bond lengths



Bond angles

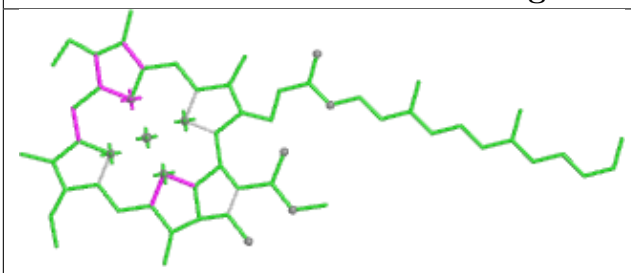


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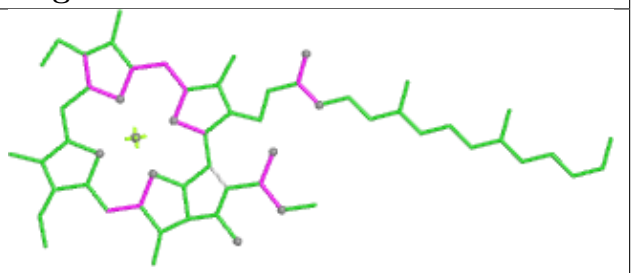


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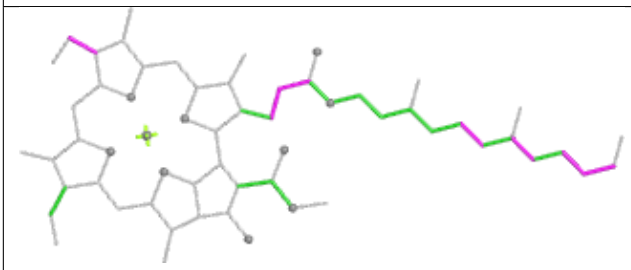
Ligand CLA g 815



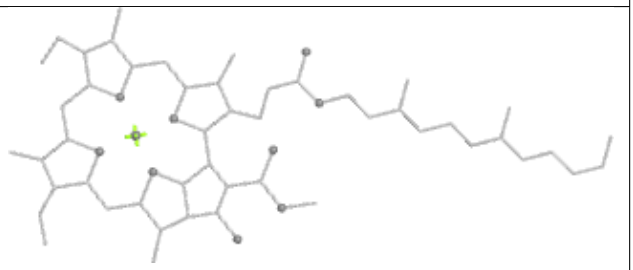
Bond lengths



Bond angles

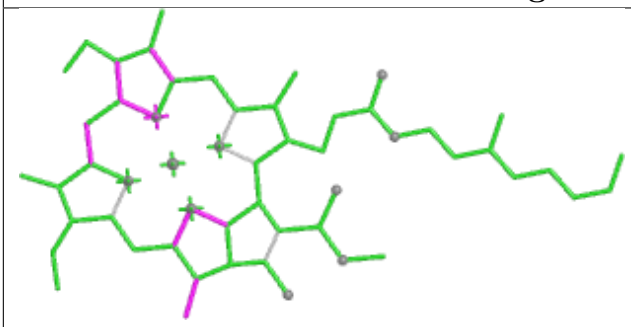


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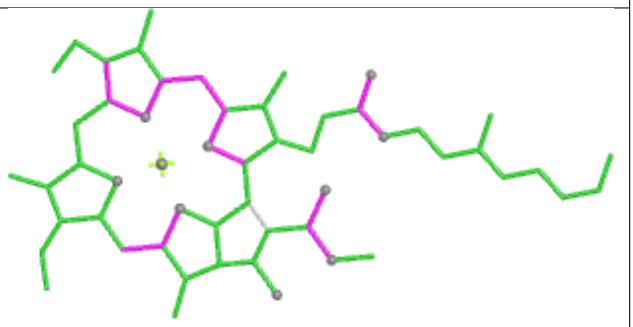


Rings

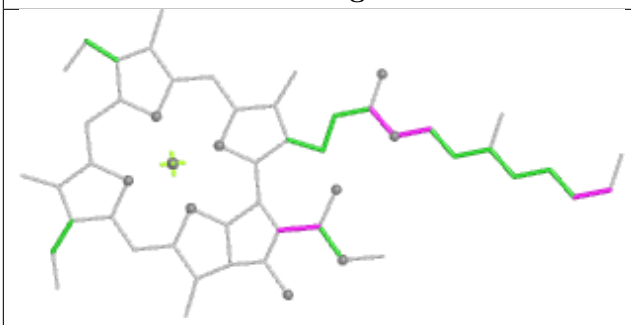
Ligand CLA a 802



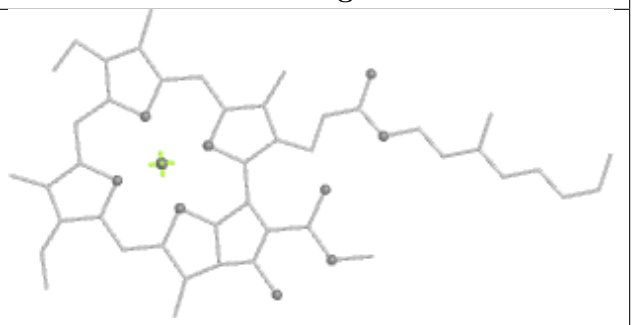
Bond lengths



Bond angles

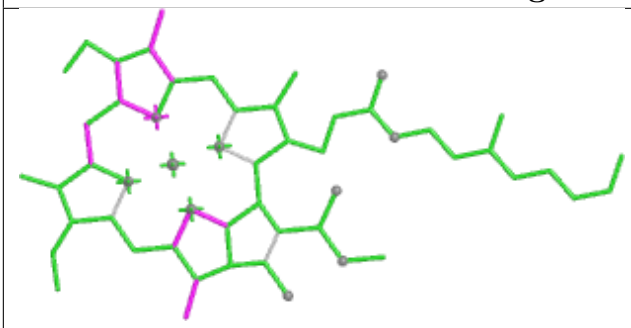


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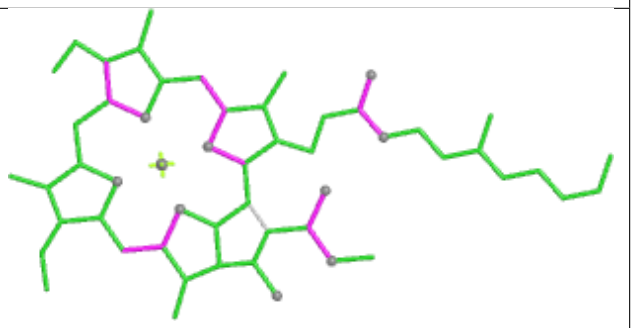


Rings

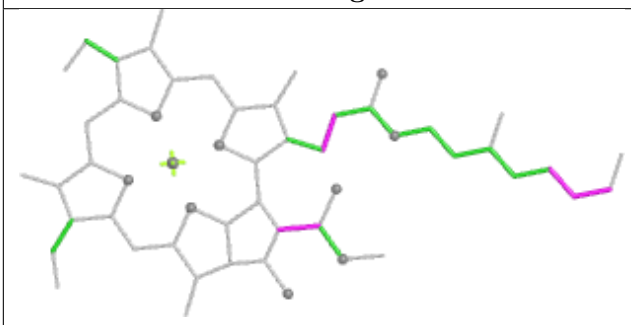
Ligand CLA a 833



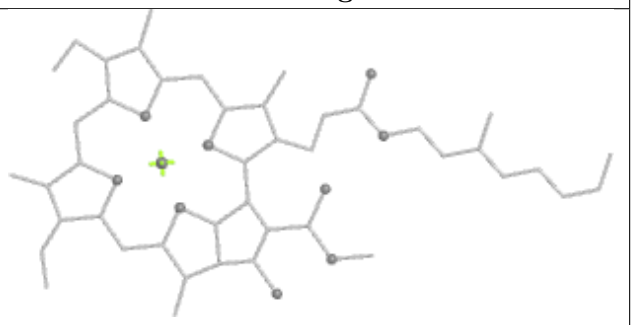
Bond lengths



Bond angles

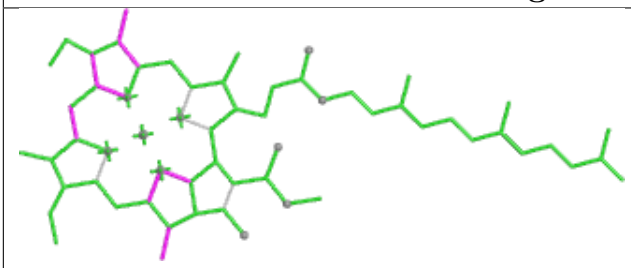


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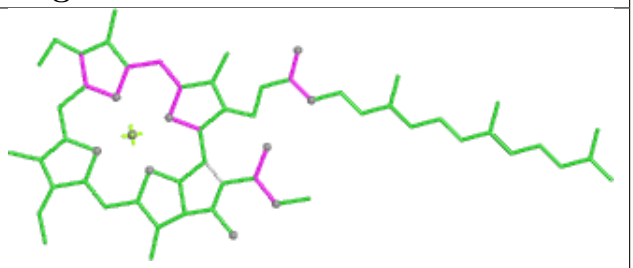


Rings

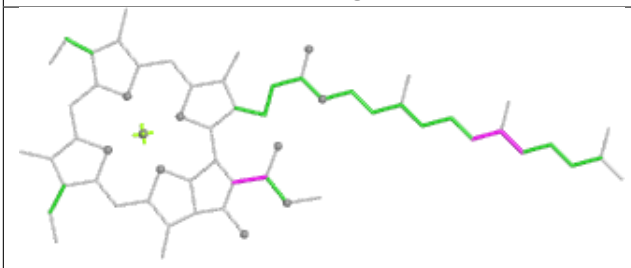
Ligand CLA g 805



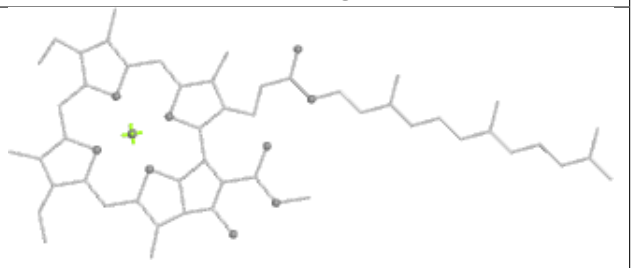
Bond lengths



Bond angles

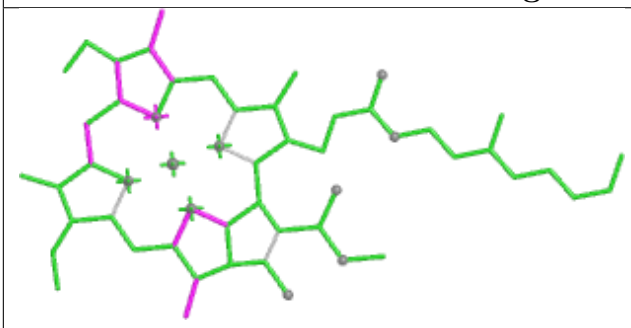


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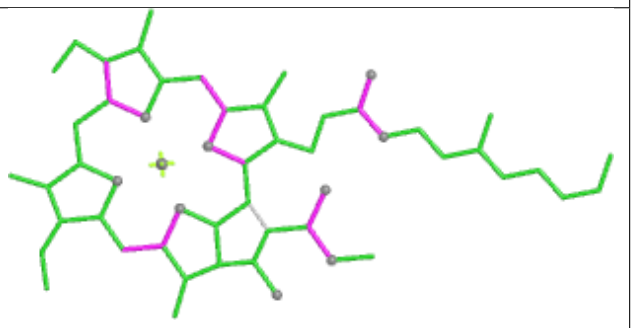


Rings

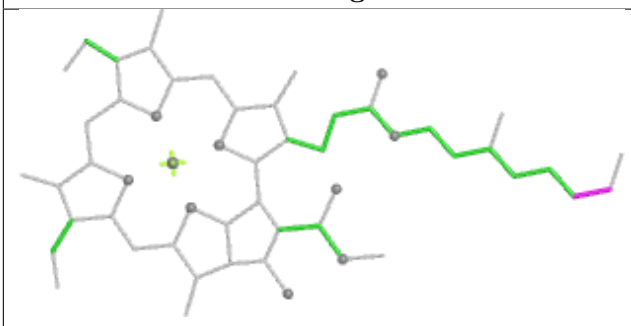
Ligand CLA G 834



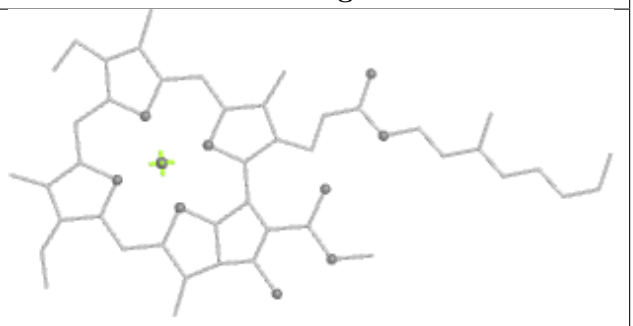
Bond lengths



Bond angles



Torsions

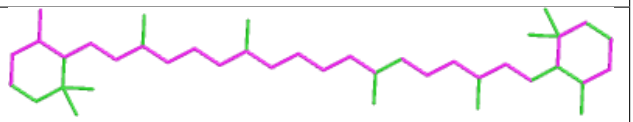


Rings

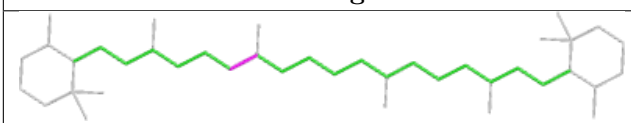
Ligand BCR a 843



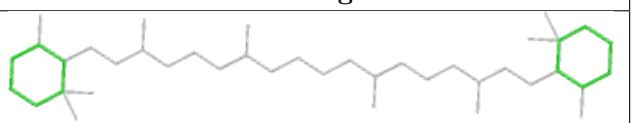
Bond lengths



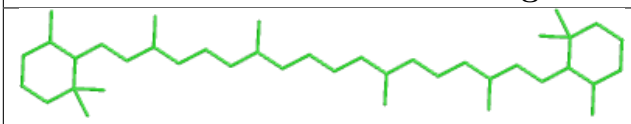
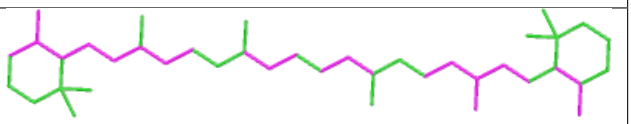
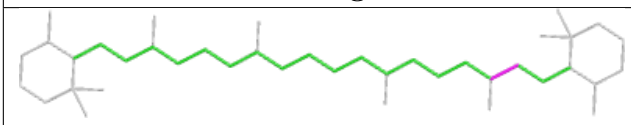
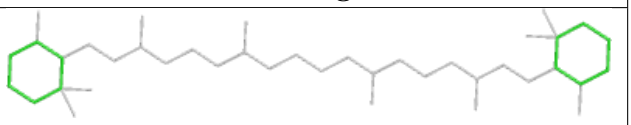
Bond angles

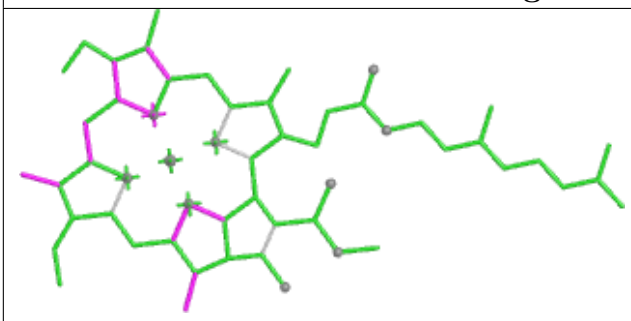
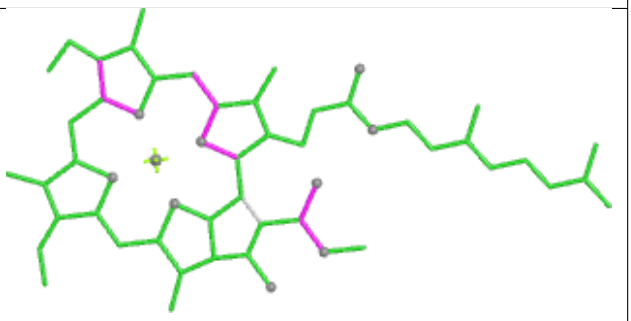
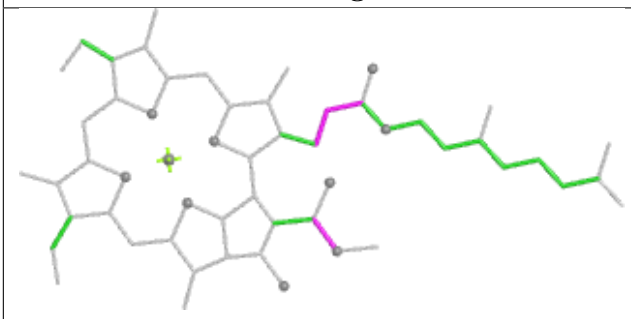
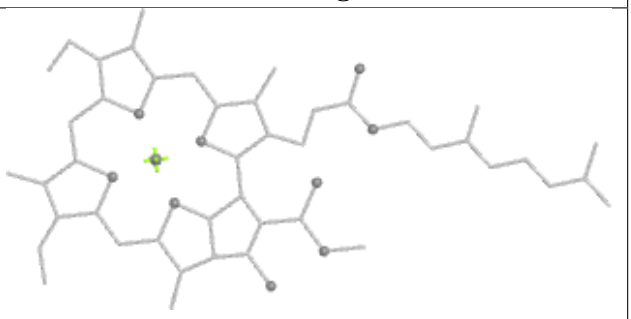


Torsions

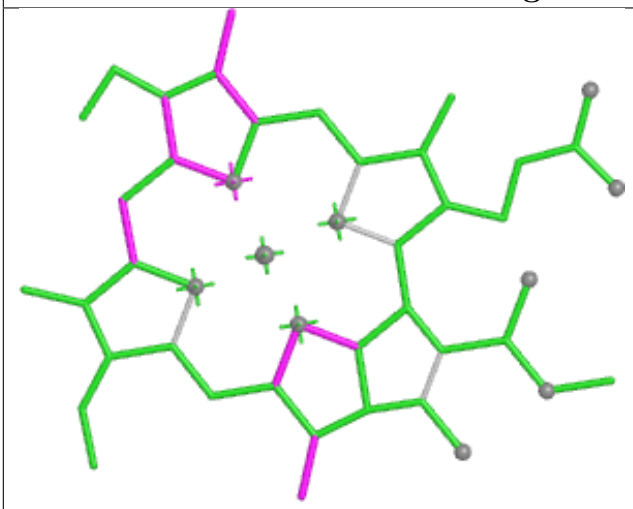


Rings

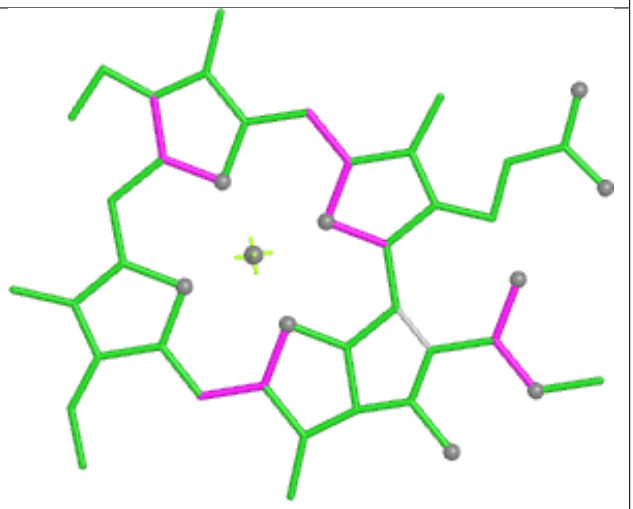
Ligand BCR N 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

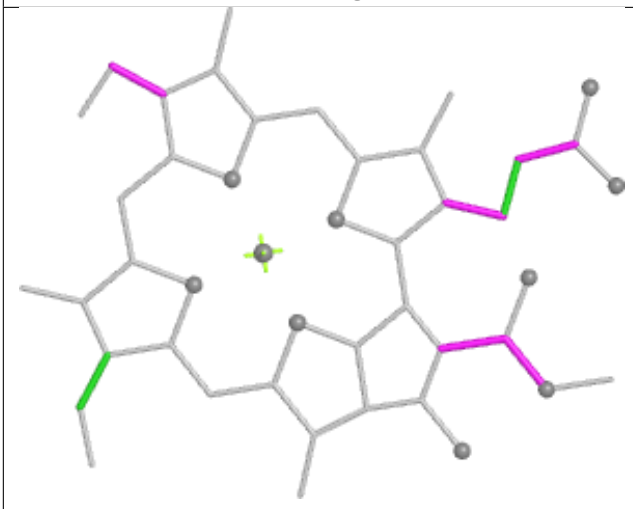
Ligand CLA G 823



Bond lengths



Bond angles

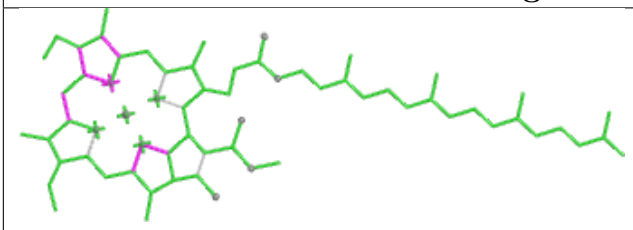


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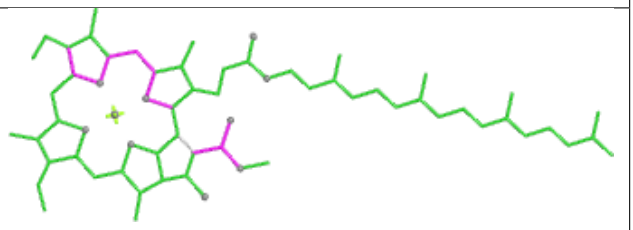


Rings

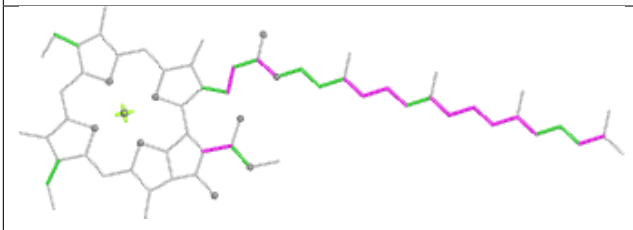
Ligand CLA G 837



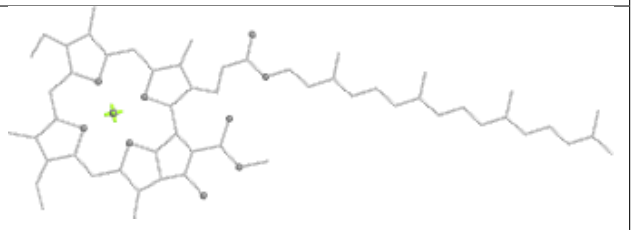
Bond lengths



Bond angles

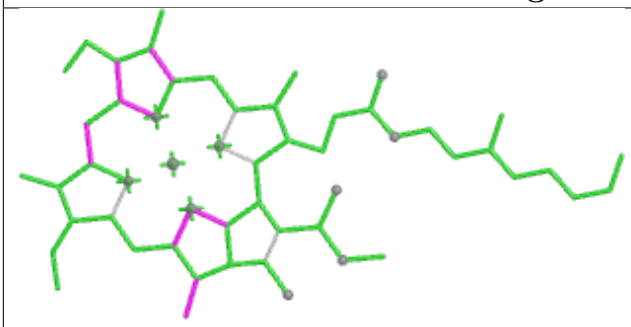


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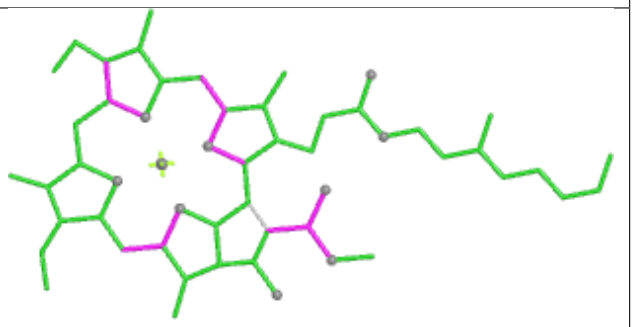


Rings

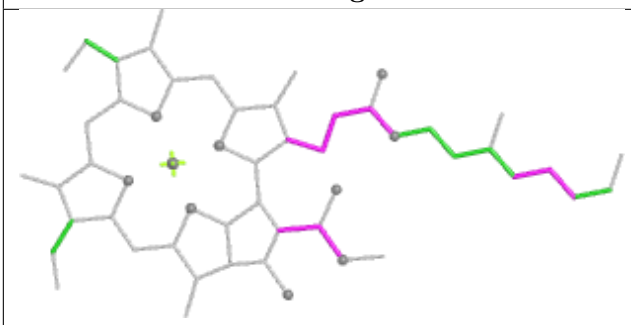
Ligand CLA n 833



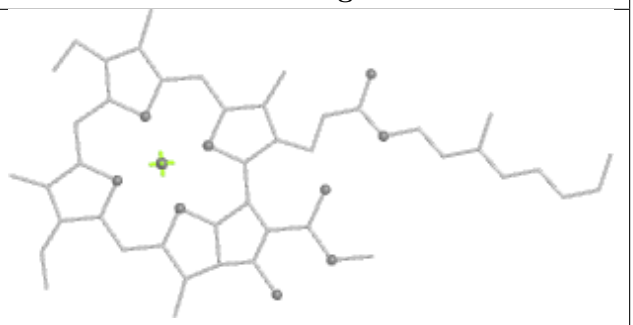
Bond lengths



Bond angles

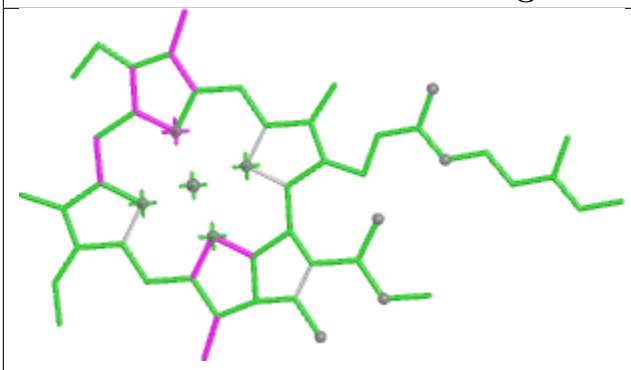


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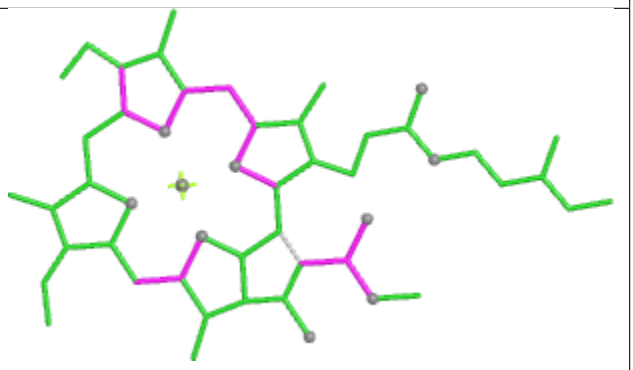


Rings

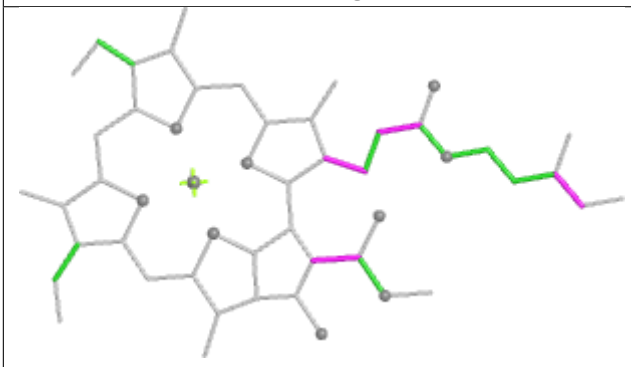
Ligand CLA L 1501



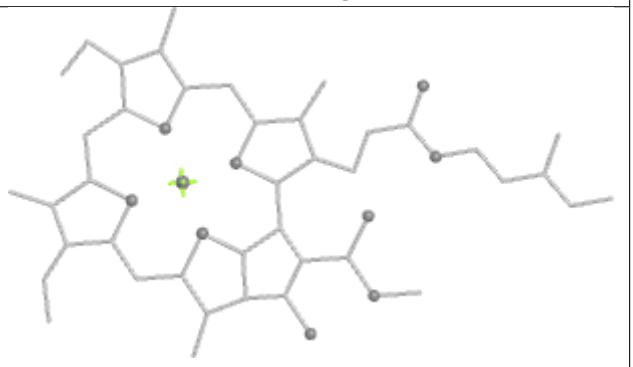
Bond lengths



Bond angles

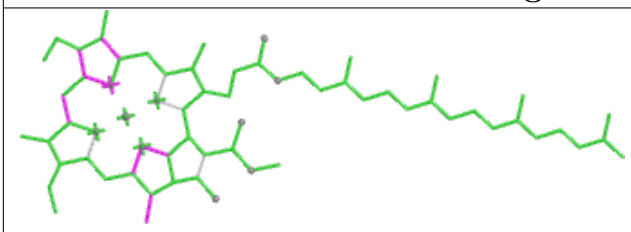


Torsions

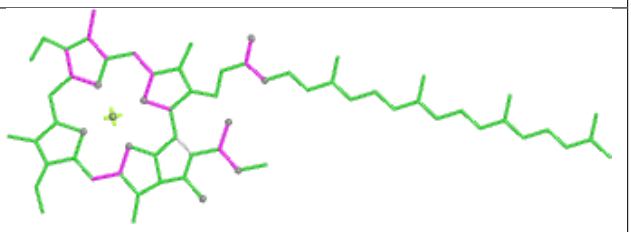


Rings

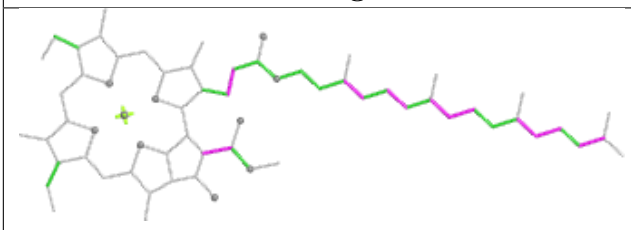
Ligand CLA B 808



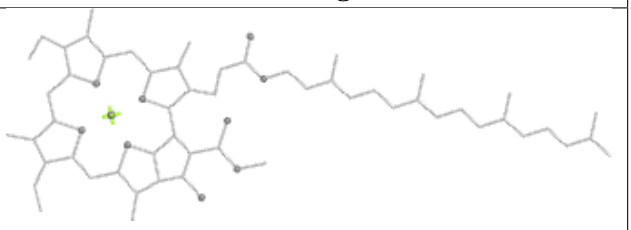
Bond lengths



Bond angles

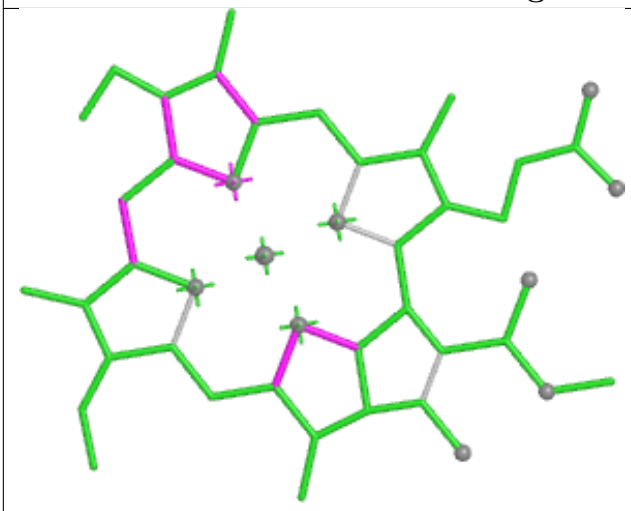


Torsions

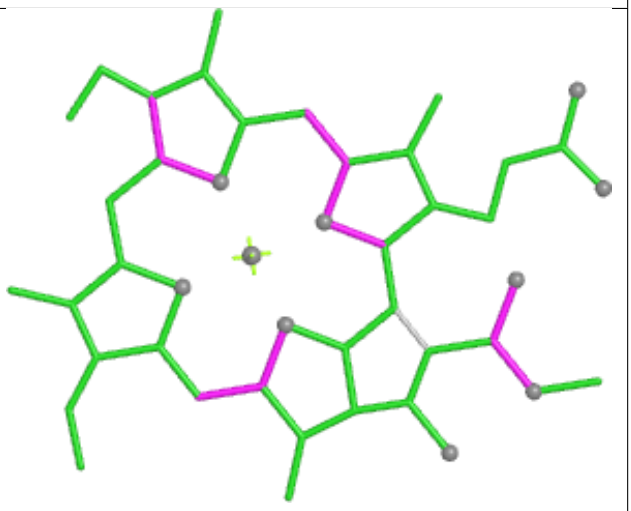


Rings

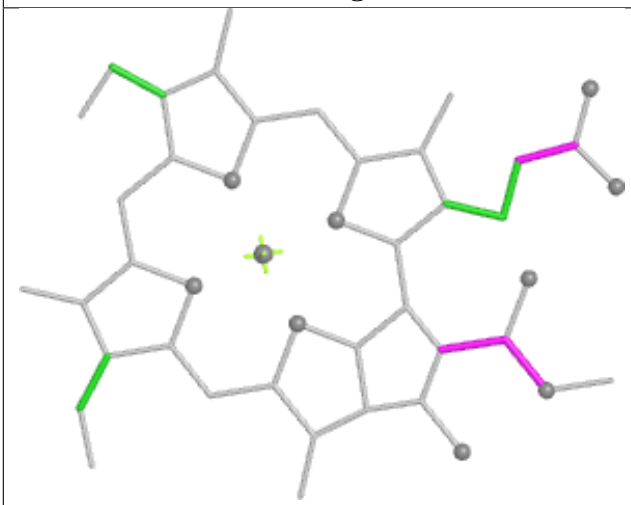
Ligand CLA b 835



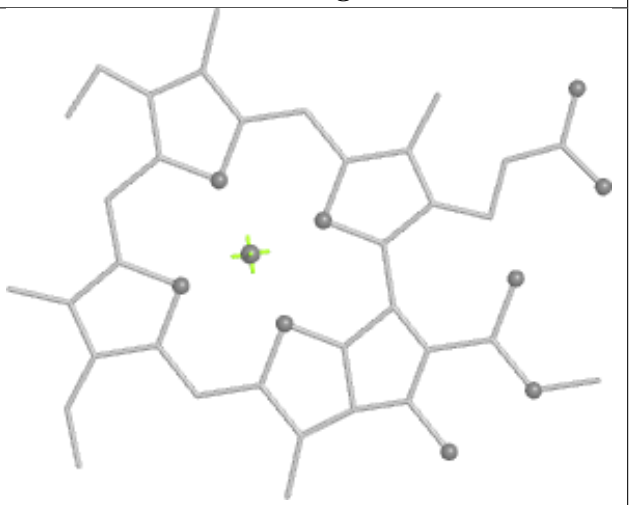
Bond lengths



Bond angles

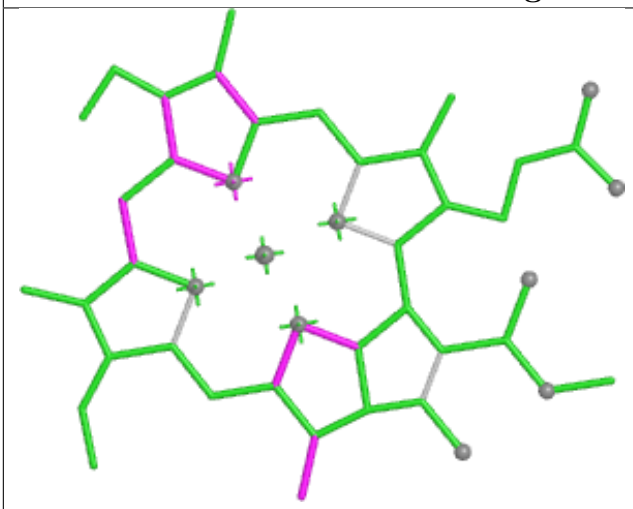


Torsions

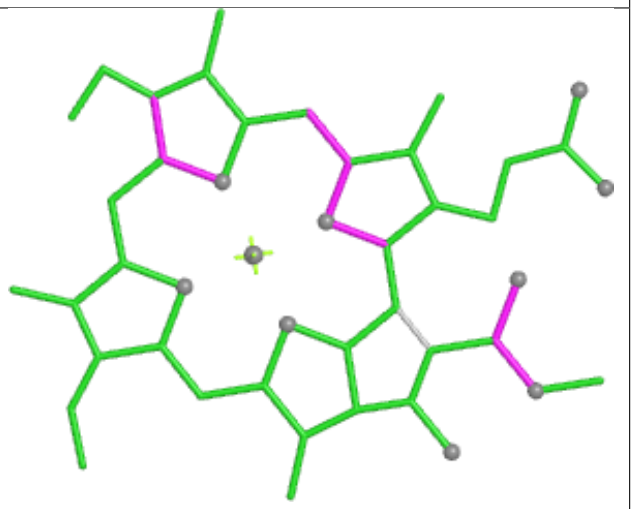


Rings

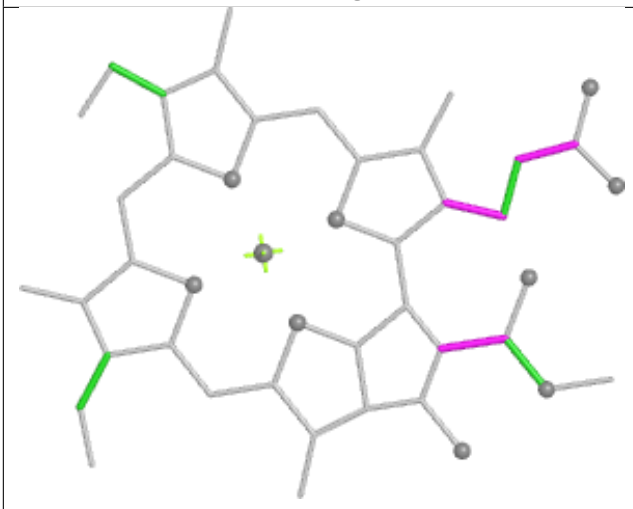
Ligand CLA B 822



Bond lengths



Bond angles

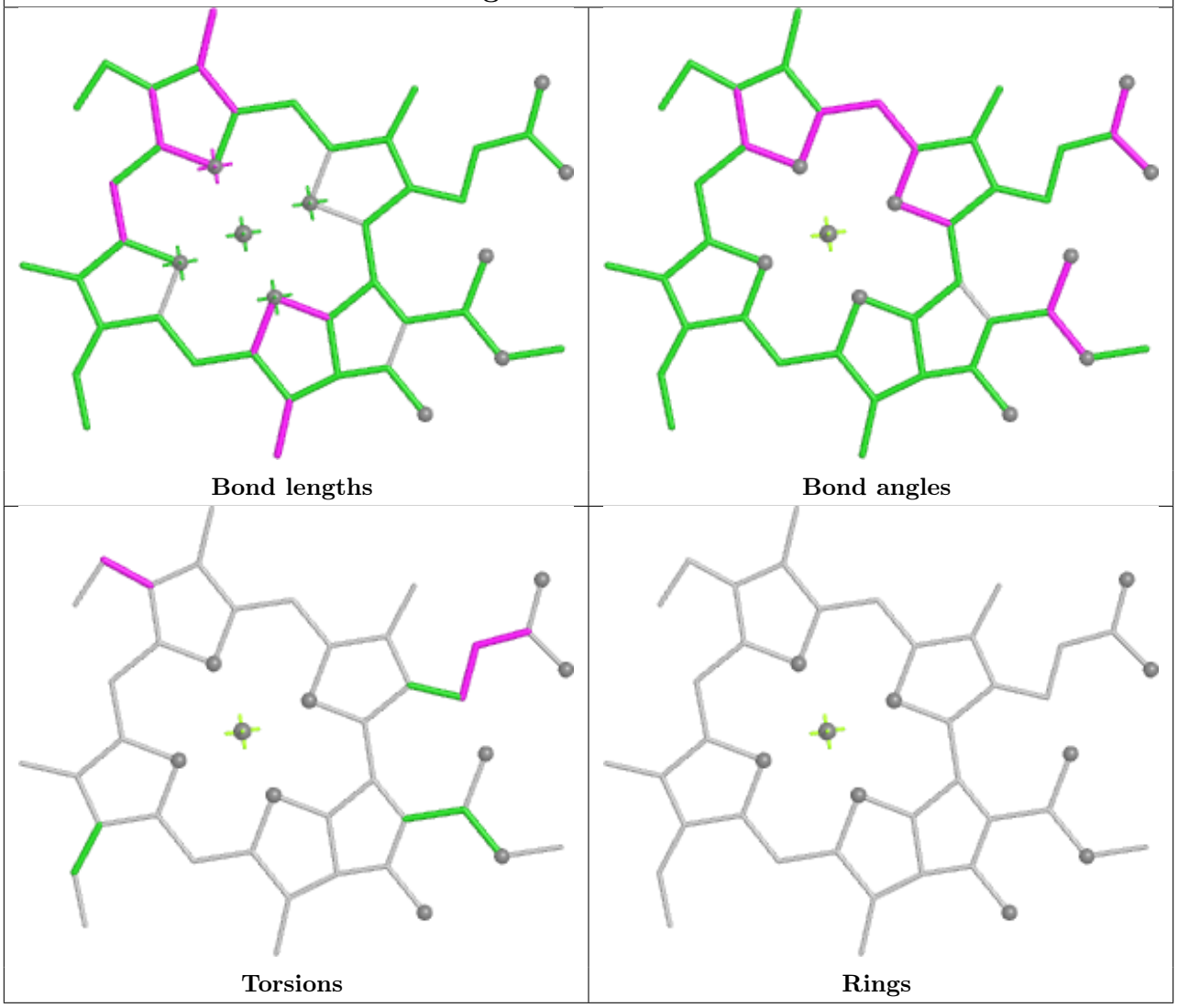


Torsions

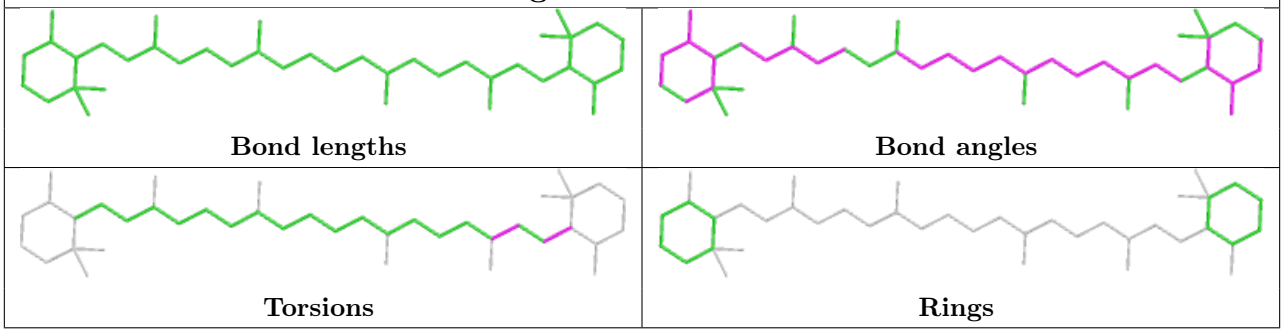


Rings

Ligand CLA F 202



Ligand BCR I 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

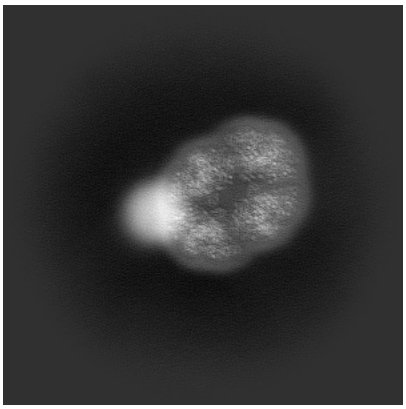
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65883. These allow visual inspection of the internal detail of the map and identification of artifacts.

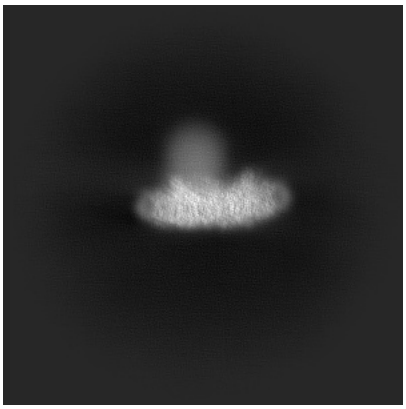
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

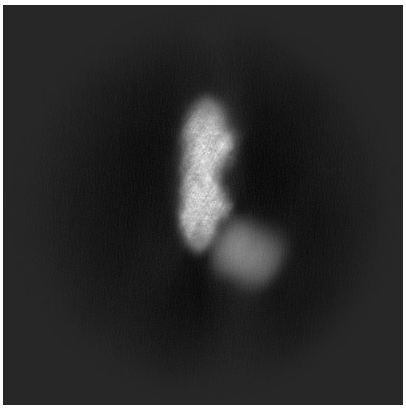
6.1.1 Primary map



X

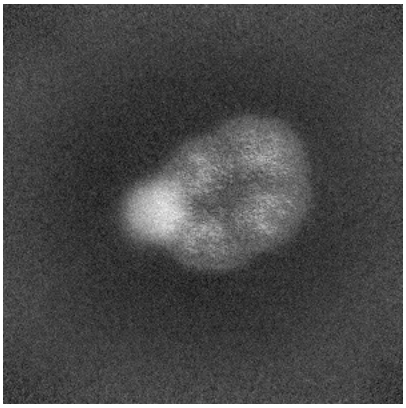


Y

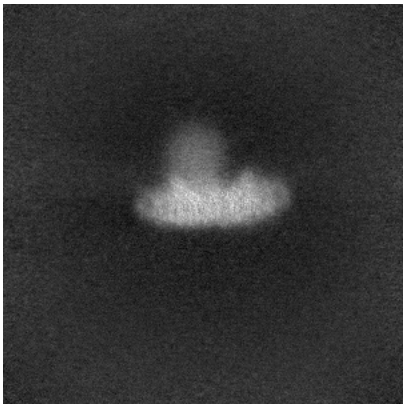


Z

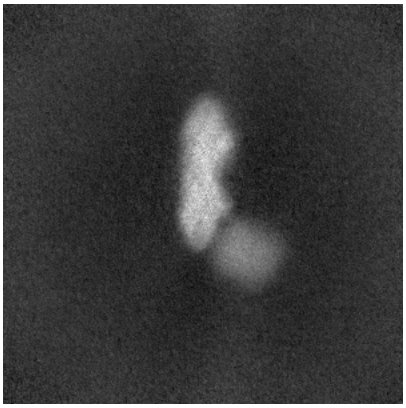
6.1.2 Raw map



X



Y

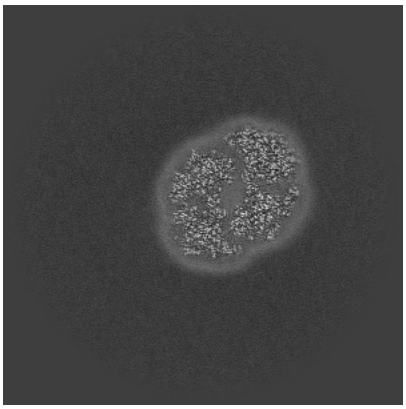


Z

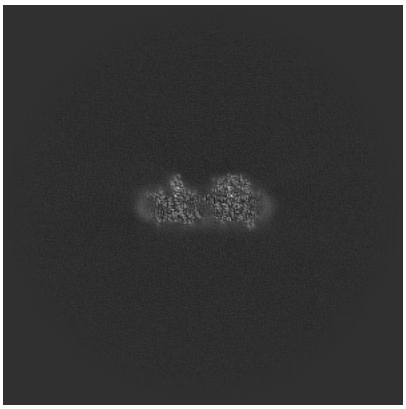
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

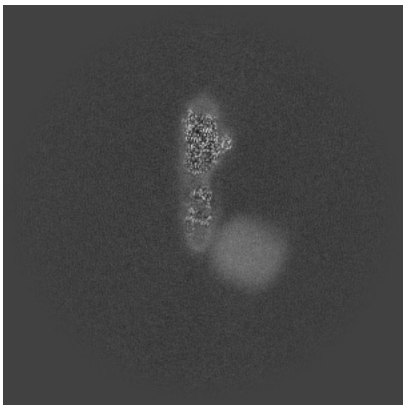
6.2.1 Primary map



X Index: 330

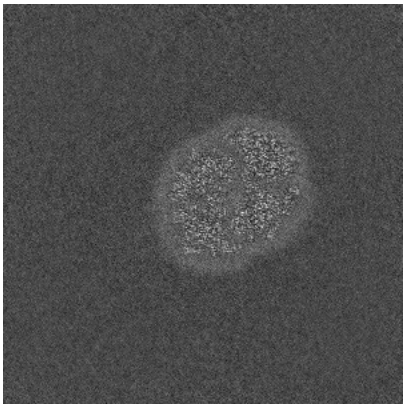


Y Index: 330

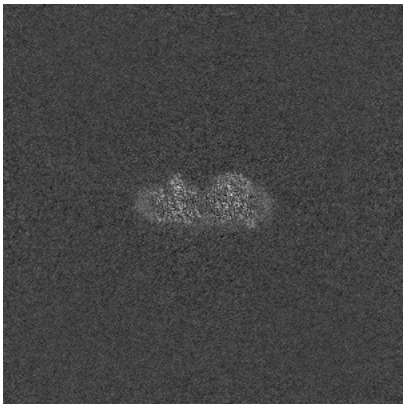


Z Index: 330

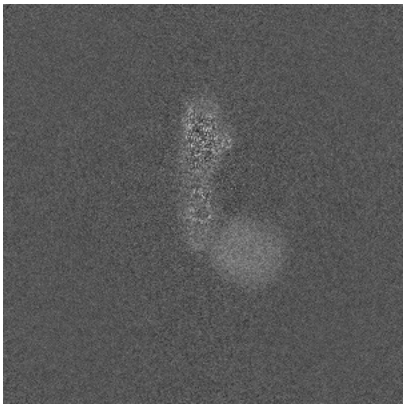
6.2.2 Raw map



X Index: 330



Y Index: 330

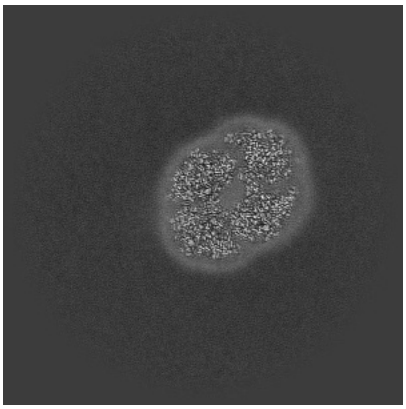


Z Index: 330

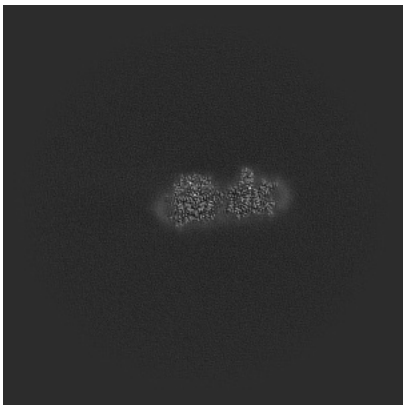
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

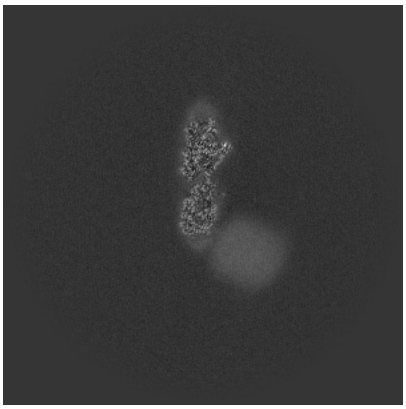
6.3.1 Primary map



X Index: 335

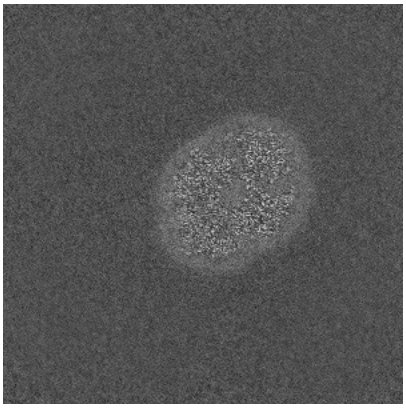


Y Index: 427

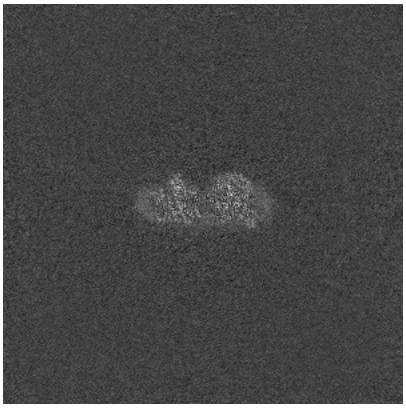


Z Index: 309

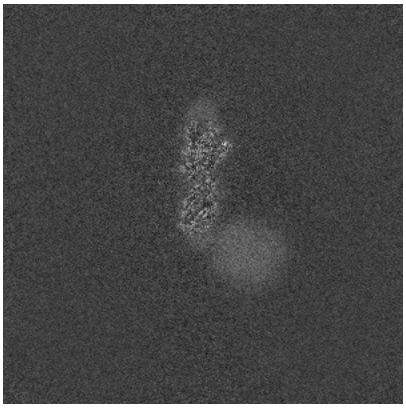
6.3.2 Raw map



X Index: 334



Y Index: 330

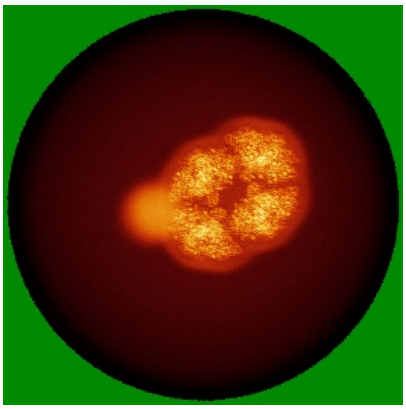


Z Index: 308

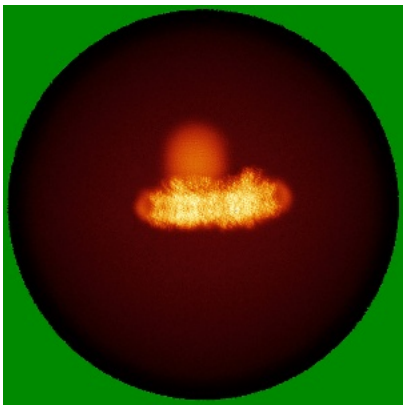
The images above show the largest variance slices of the map in three orthogonal directions.

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

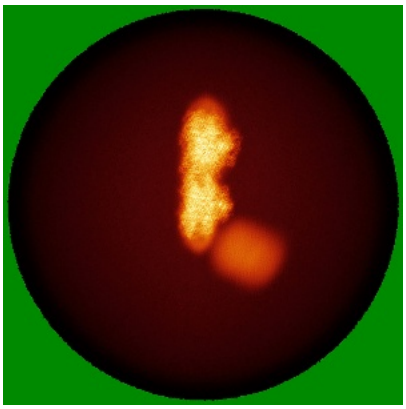
6.4.1 Primary map



X

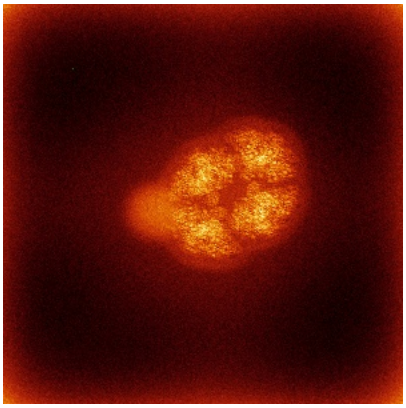


Y

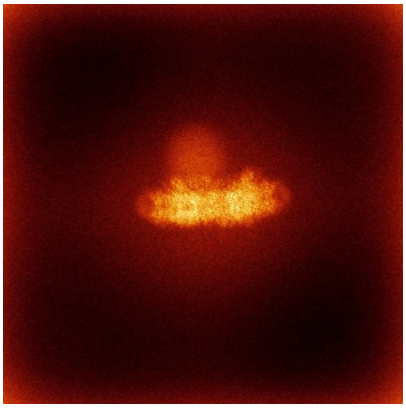


Z

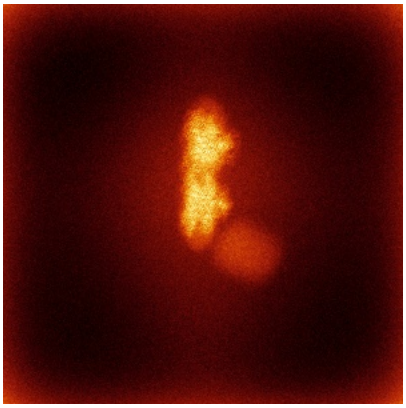
6.4.2 Raw map



X



Y

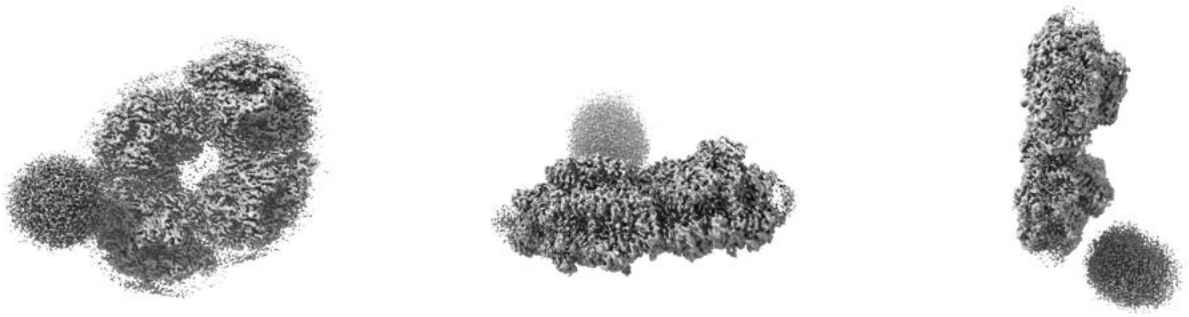


Z

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 0.185. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

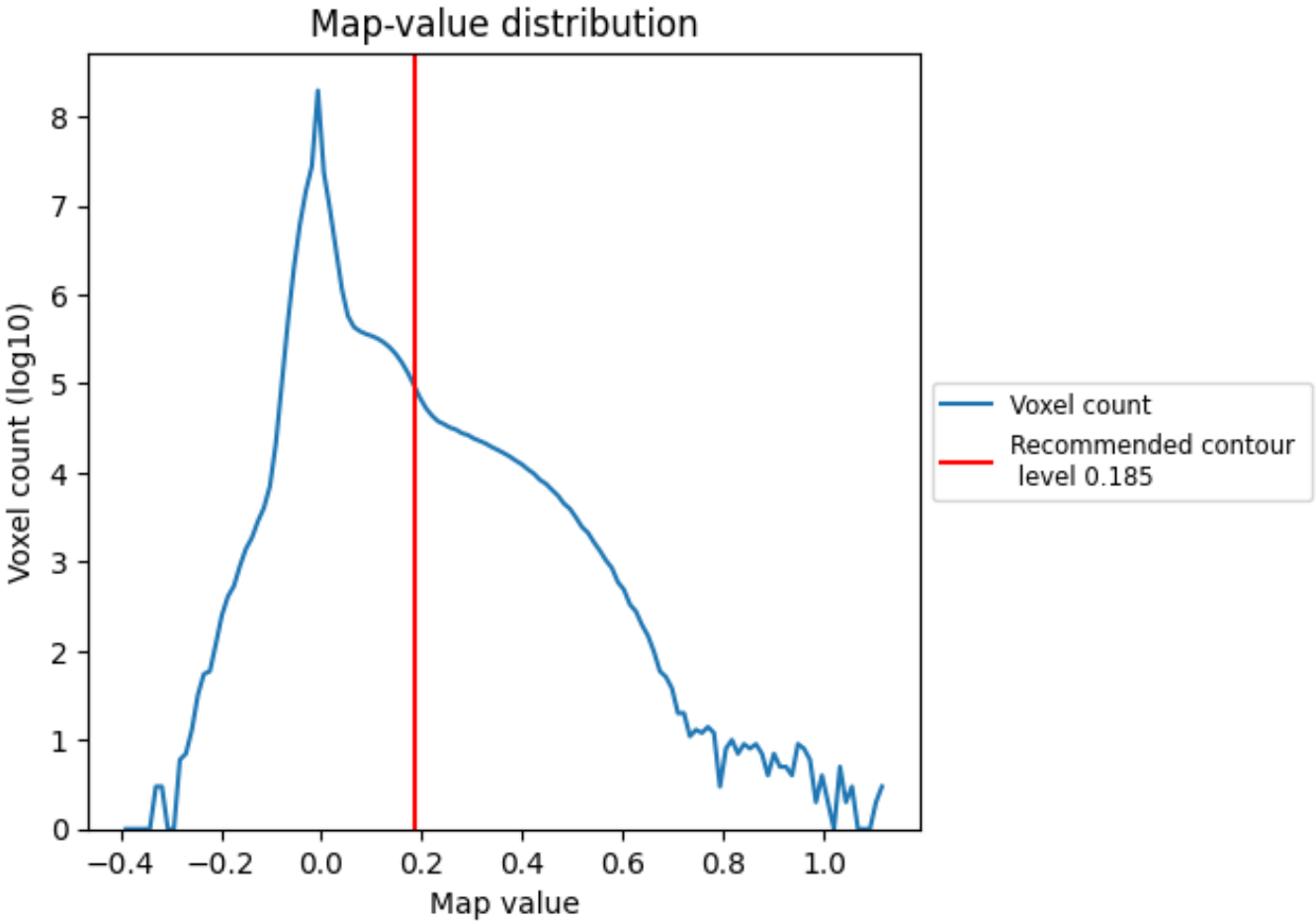
6.6 Mask visualisation (i)

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

7 Map analysis

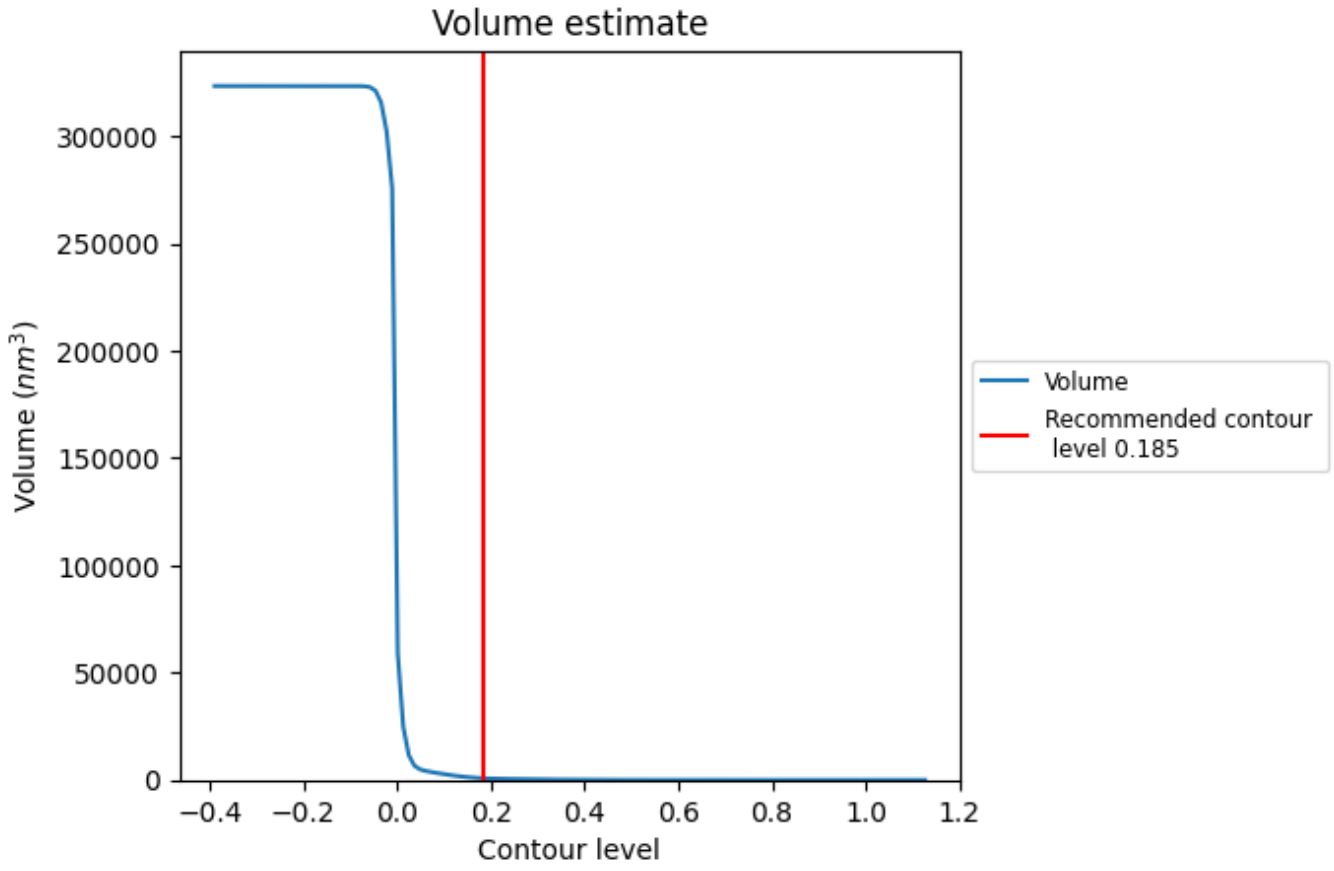
This section contains the results of statistical analysis of the map.

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.

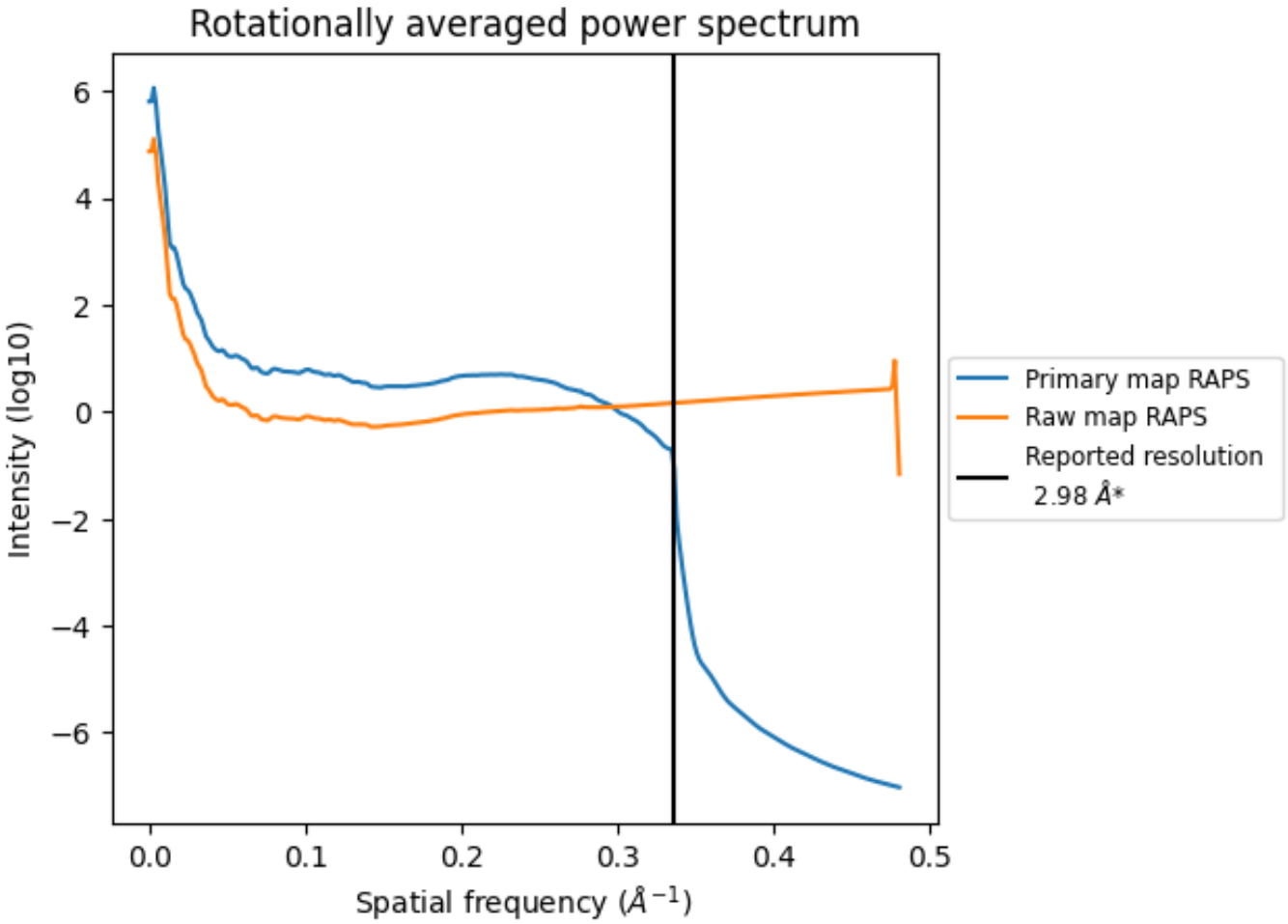
7.2 Volume estimate (i)



The volume at the recommended contour level is 767 nm^3; this corresponds to an approximate mass of 693 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)

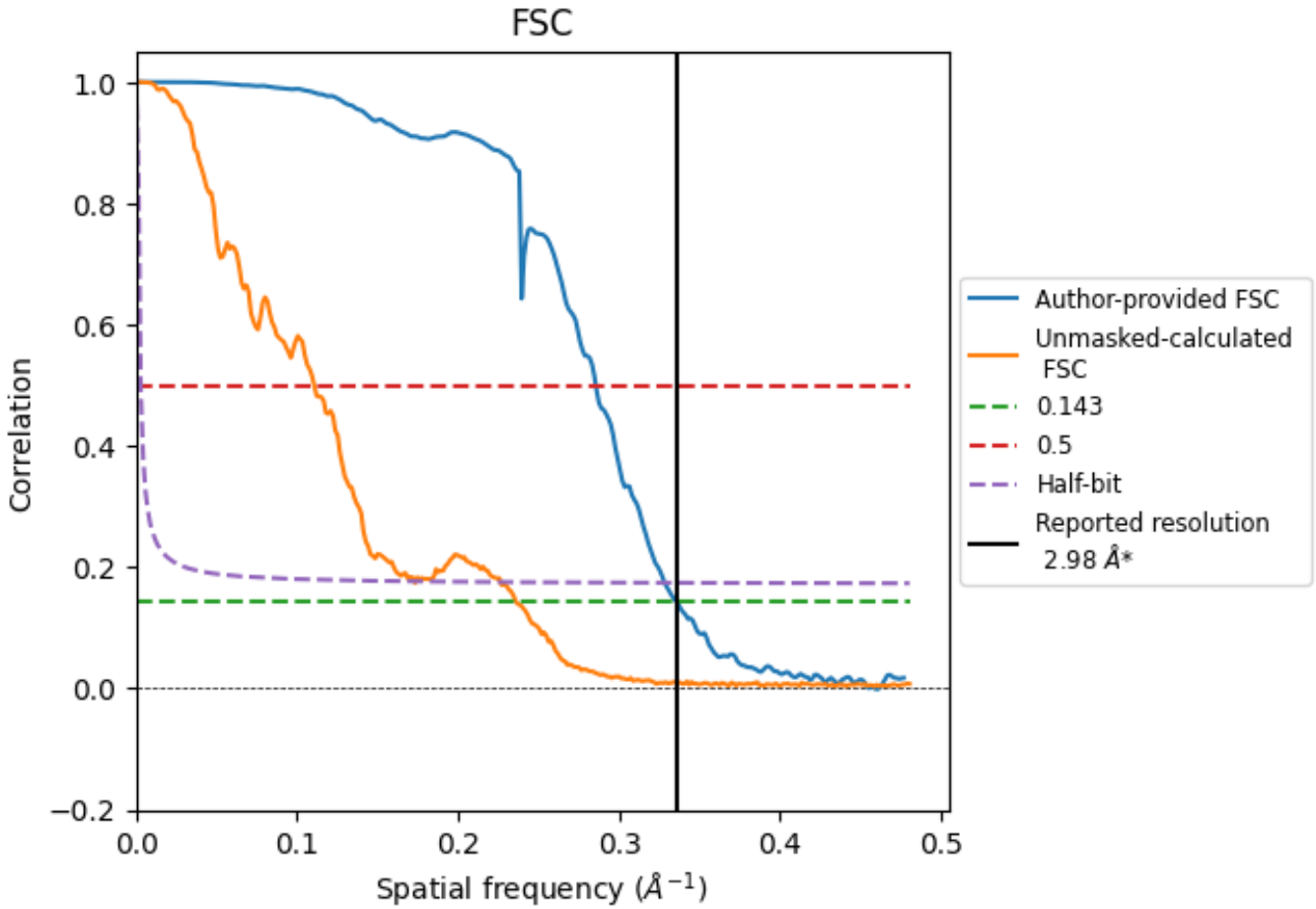


*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

8.2 Resolution estimates (i)

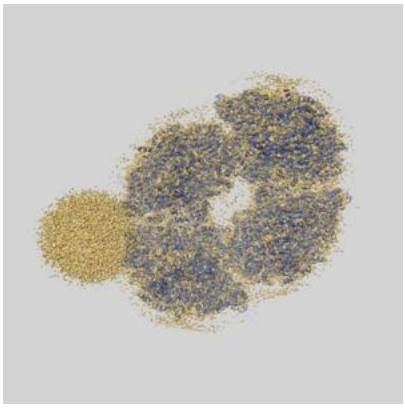
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.50	3.04
Unmasked-calculated*	4.24	9.04	5.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 2.98 by more than 10 %

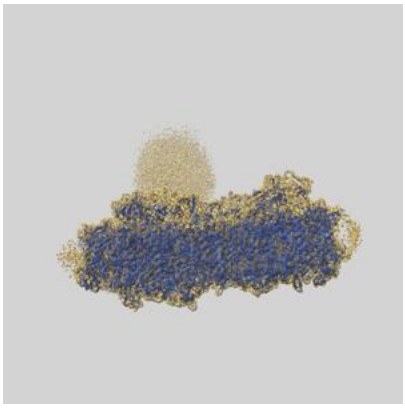
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65883 and PDB model 9WD5. Per-residue inclusion information can be found in section 3 on page 38.

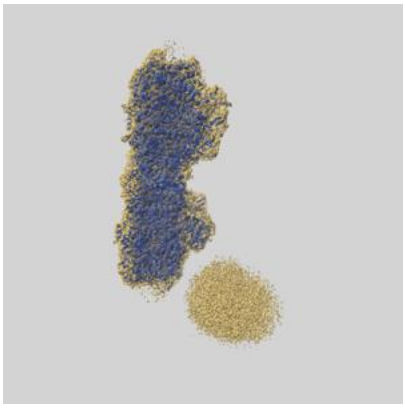
9.1 Map-model overlay



X



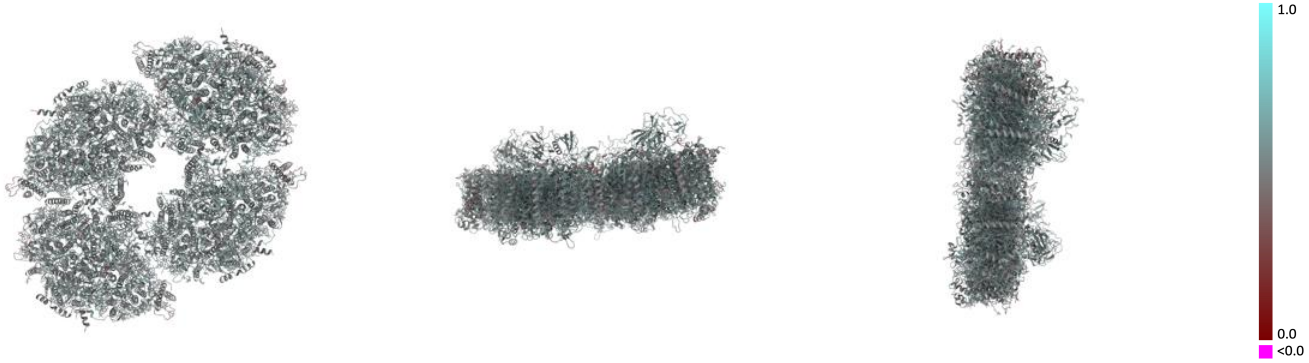
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.185 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.

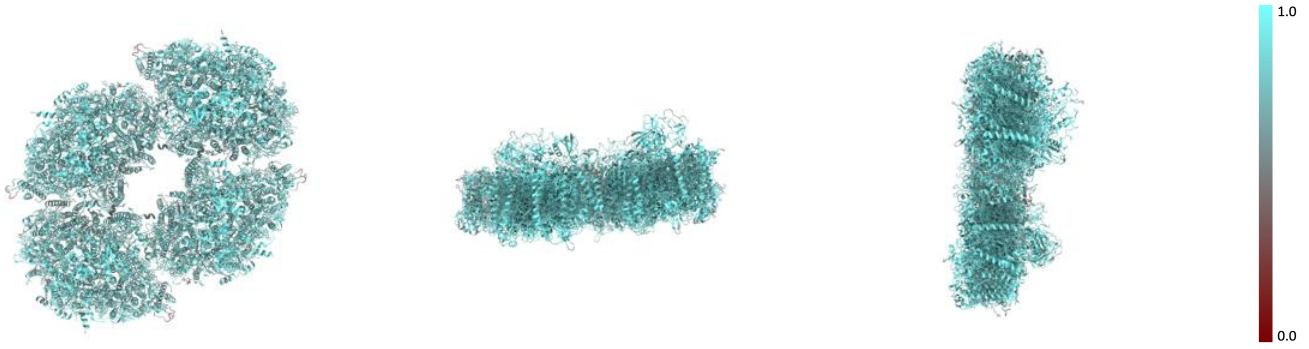
9.2 Q-score mapped to coordinate model



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.

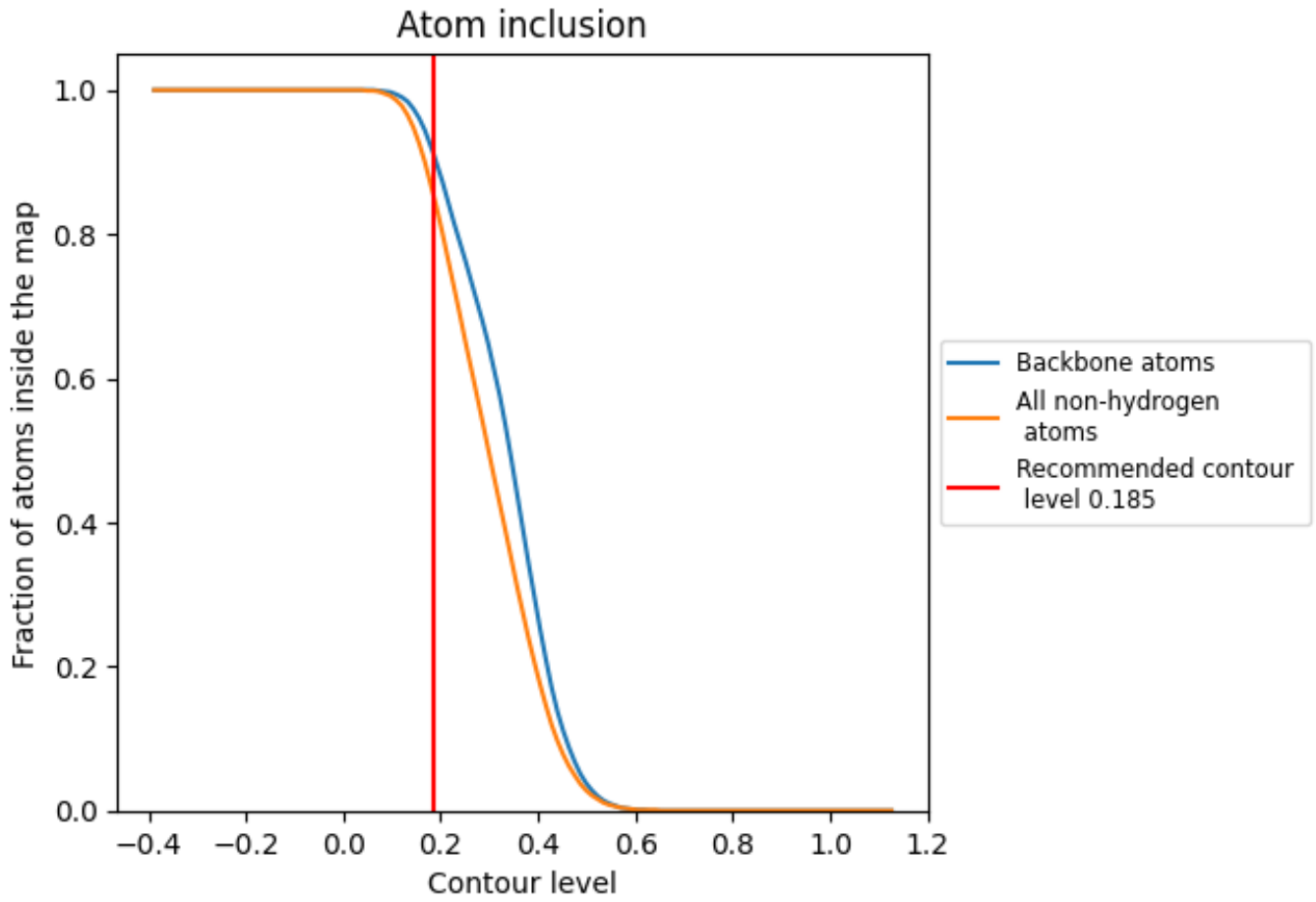
9.3 Atom inclusion mapped to coordinate model



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 (0.185).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.185) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8550	0.5300
1	0.7220	0.4730
A	0.8720	0.5330
B	0.8600	0.5380
C	0.9270	0.5160
D	0.8760	0.5210
E	0.8260	0.5260
F	0.8440	0.5160
G	0.8790	0.5400
H	0.7940	0.5160
I	0.7620	0.5260
J	0.8230	0.5080
K	0.7070	0.4420
L	0.7900	0.5260
M	0.7830	0.5170
N	0.8720	0.5430
P	0.9270	0.5110
Q	0.8720	0.5280
R	0.8540	0.5240
S	0.8300	0.5190
T	0.8530	0.5110
U	0.7150	0.4570
V	0.8490	0.5360
W	0.8430	0.5280
X	0.7990	0.5050
Y	0.7640	0.5170
a	0.8590	0.5340
b	0.8620	0.5290
c	0.9420	0.5120
d	0.8680	0.5170
e	0.8430	0.5180
f	0.8060	0.4940
g	0.8720	0.5430
h	0.7300	0.4690
i	0.7920	0.5160



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Chain	Atom inclusion	Q-score
j	0.8350	0.4920
k	0.6840	0.4650
l	0.8230	0.5290
m	0.7300	0.5130
n	0.8690	0.5390
p	0.9400	0.5290
q	0.8910	0.5330
r	0.8190	0.5270
s	0.8040	0.4900
t	0.8170	0.4980
u	0.6530	0.4800
v	0.7910	0.5220
w	0.8350	0.5360
x	0.7630	0.4950
y	0.7970	0.5220