wwPDB EM Validation Summary Report

Sep 14, 2026 – 02:45 PM JST

PDB ID	:	7WG5 / pdb_00007wg5
EMDB ID	:	EMD-32477
Title	:	Cyclic electron transport supercomplex NDH-PSI from Arabidopsis
Authors	:	Pan, X.W.; Li, M.
Deposited on	:	2021-12-28
Resolution	:	3.89 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 ⓘ 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 ⓘ) were used in the production of this report:

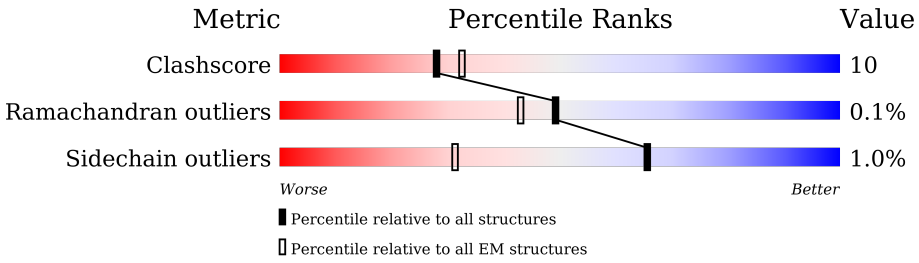
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

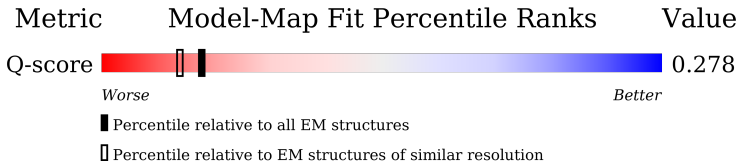
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.89 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	8712 (3.39 - 4.39)

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	AA	750	87% 11%
1	BA	750	7% 85% 13%
2	AB	734	85% 15%
2	BB	734	5% 85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	81	79% 20%
3	BC	81	70% 28%
4	AD	204	58% 11% 31%
4	BD	204	8% 54% 14% 30%
5	AE	143	41% 6% 53%
5	BE	143	8% 41% 8% 52%
6	AF	221	62% 7% 31%
6	BF	221	5% 61% 9% 30%
7	AG	160	49% 12% 38%
7	BG	160	16% 45% 12% 41%
8	AH	145	5% 54% 11% 34%
8	BH	145	13% 51% 14% 34%
9	AI	37	78% 11% 11%
9	BI	37	24% 59% 30% 11%
10	AJ	44	73% 23% 5%
10	BJ	44	7% 75% 23%
11	AK	130	6% 47% 50%
11	BK	130	11% 38% 10% 51%
12	AL	219	63% 9% 28%
12	BL	219	15% 58% 14% 27%
13	A1	241	71% 11% 19%
13	B1	241	6% 56% 15% 29%
14	A3	273	74% 7% 20%
14	B3	273	13% 69% 12% 19%
15	A4	251	70% 9% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	A6	270	69% 9% 21%
17	B2	257	11% 65% 16% 19%
18	B5	256	66% 14% 20%
19	A	360	15% 63% 21% 15%
20	B	512	73% 21% 5%
21	C	120	18% 55% 23% 22%
22	D	506	71% 27%
23	E	101	5% 56% 32% 12%
24	F	746	6% 68% 22% 9%
25	G	176	6% 65% 30% 5%
26	a	461	57% 17% 26%
27	b	348	5% 65% 24% 12%
28	c	204	5% 47% 15% 37%
29	d	161	38% 20% 42%
30	e	212	59% 12% 29%
31	f	238	47% 16% 36%
32	g	190	54% 7% 39%
33	h	220	53% 13% 34%
34	i	217	55% 12% 33%
35	j	255	54% 14% 32%
36	H	393	87% 67% 23% 9%
37	I	172	66% 68% 24% 7%
38	J	158	87% 73% 25%
39	K	225	59% 56% 17% 26%
40	L	191	13% 38% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	M	217	49% 40% 10% 49%
42	N	209	60% 53% 16% 30%
43	O	158	44% 35% 13% 53%
44	T	122	80% 94% 6%

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
45	CLA	BG	202	-	-	X	-
49	SF4	AC	102	-	-	X	-
49	SF4	BC	102	-	-	X	-
49	SF4	I	202	-	-	X	-
57	FES	c	301	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 112687 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	742	Total	C	N	O	S	0	0
			5839	3826	992	1003	18		
1	BA	742	Total	C	N	O	S	0	0
			5841	3828	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	734	Total	C	N	O	S	0	0
			5862	3847	999	1001	15		
2	BB	733	Total	C	N	O	S	0	0
			5854	3842	998	1000	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		
3	BC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		
4	BD	143	Total	C	N	O	S	0	0
			1127	723	195	205	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	67	Total	C	N	O	0	0
			530	341	94	95		
5	BE	69	Total	C	N	O	0	0
			546	352	97	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	153	Total	C	N	O	S	0	0
			1213	792	208	210	3		
6	BF	154	Total	C	N	O	S	0	0
			1220	797	209	211	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	99	Total	C	N	O	0	0
			771	501	126	144		
7	BG	94	Total	C	N	O	0	0
			733	474	121	138		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	95	Total	C	N	O	0	0
			730	476	119	135		
8	BH	95	Total	C	N	O	0	0
			730	476	119	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		
9	BI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	43	Total	C	N	O	S	0	0
			344	233	52	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	65	Total	C	N	O	S	0	0
			451	290	74	84	3		
11	BK	64	Total	C	N	O	S	0	0
			445	285	73	84	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	157	Total	C	N	O	S	0	0
			1173	775	187	209	2		
12	BL	159	Total	C	N	O	S	0	0
			1184	781	190	211	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	196	Total	C	N	O	S	0	0
			1511	984	251	271	5		
13	B1	172	Total	C	N	O	S	0	0
			1339	873	221	240	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A3	219	Total	C	N	O	S	0	0
			1675	1096	272	302	5		
14	B3	221	Total	C	N	O	S	0	0
			1696	1111	276	304	5		

- Molecule 15 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	212	Total	C	N	O	S	0	0
			1671	1088	272	299	12		

- Molecule 17 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B2	208	Total	C	N	O	S	0	0
			1607	1051	261	291	4		

- Molecule 18 is a protein called Photosystem I chlorophyll a/b-binding protein 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B5	206	Total	C	N	O	S	0	0
			1599	1045	263	285	6		

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	305	Total	C	N	O	S	0	0
			2372	1593	366	409	4		

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	486	Total	C	N	O	S	0	0
			3780	2495	577	679	29		

- Molecule 21 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	94	Total	C	N	O	S	0	0
			776	544	109	121	2		

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	497	Total	C	N	O	S	0	0
			3946	2656	599	666	25		

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	89	Total	C	N	O	S	0	0
			695	458	112	119	6		

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	677	Total	C	N	O	S	0	0
			5330	3558	829	915	28		

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G	167	Total	C	N	O	S	0	0
			1281	858	194	224	5		

- Molecule 26 is a protein called Photosynthetic NDH subunit of subcomplex B 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	341	Total	C	N	O	S	0	0
			2655	1692	450	500	13		

- Molecule 27 is a protein called Photosynthetic NDH subunit of subcomplex B 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	307	Total	C	N	O	S	0	0
			2367	1508	392	452	15		

- Molecule 28 is a protein called Photosynthetic NDH subunit of subcomplex B 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	128	Total	C	N	O	S	0	0
			1005	636	180	183	6		

- Molecule 29 is a protein called NDH dependent flow 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	93	Total	C	N	O	S	0	0
			762	497	119	138	8		

- Molecule 30 is a protein called Photosynthetic NDH subunit of subcomplex B 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	150	Total	C	N	O	S	0	0
			1206	780	183	236	7		

- Molecule 31 is a protein called Photosynthetic NDH subunit of lumenal location 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	153	Total	C	N	O	S	0	0
			1277	823	219	233	2		

- Molecule 32 is a protein called Photosynthetic NDH subunit of lumenal location 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	115	Total	C	N	O	S	0	0
			965	620	159	180	6		

- Molecule 33 is a protein called Photosynthetic NDH subunit of lumenal location 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	145	Total	C	N	O	S	0	0
			1170	753	191	221	5		

- Molecule 34 is a protein called Photosynthetic NDH subunit of lumenal location 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	145	Total	C	N	O	S	0	0
			1098	698	190	204	6		

- Molecule 35 is a protein called Isoform 2 of Photosynthetic NDH subunit of lumenal location 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	173	Total	C	N	O	S	0	0
			1331	840	236	248	7		

- Molecule 36 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	356	Total	C	N	O	S	0	0
			2812	1830	465	499	18		

- Molecule 37 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	160	Total	C	N	O	S	0	0
			1236	776	214	233	13		

- Molecule 38 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	J	155	Total	C	N	O	S	0	0
			1116	722	189	202	3		

- Molecule 39 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	K	167	Total	C	N	O	S	0	0
			1199	765	203	221	10		

- Molecule 40 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L	77	Total	C	N	O	S	0	0
			646	437	106	99	4		

- Molecule 41 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	M	110	Total	C	N	O	S	0	0
			771	494	132	143	2		

- Molecule 42 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N	146	Total	C	N	O	S	0	0
			908	584	156	166	2		

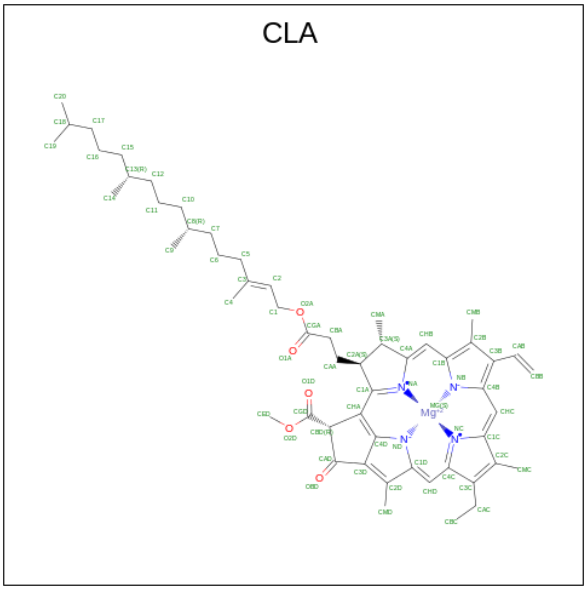
- Molecule 43 is a protein called NdhO.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	O	75	Total 520	C 334	N 90	O 96	0	0

- Molecule 44 is a protein called NdhT.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	T	122	Total 610	C 366	N 122	O 122	0	0

- Molecule 45 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 52	C 42	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
45	AA	1	Total 50	C 40	Mg 1	N 4	O 5	0
45	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			51	42	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	AB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AF	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	AF	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AF	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AG	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	AG	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AG	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AH	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AJ	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	AK	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
45	AK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AK	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	AL	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AL	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
45	A3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
45	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
45	A6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	A6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
45	A6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
45	BA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	BB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BF	1	Total	C	Mg	N	O	0
			55	46	1	4	4	
45	BF	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BF	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BG	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BG	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BH	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BJ	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BK	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
45	BK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BK	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	BL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	BL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BL	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
45	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
45	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

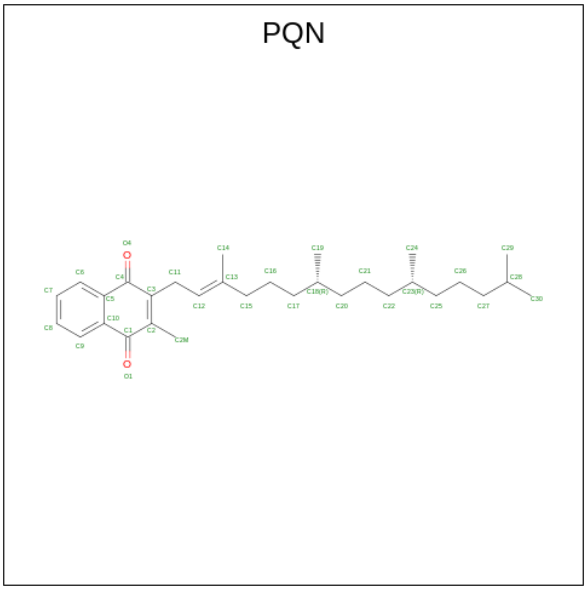
Mol	Chain	Residues	Atoms					AltConf
45	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
45	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

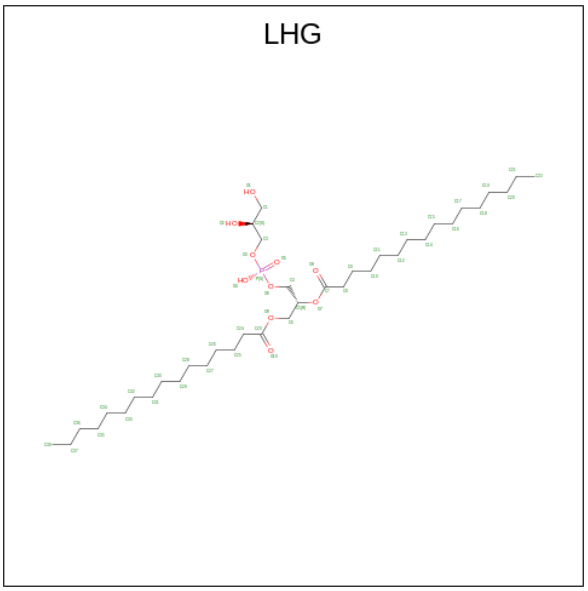
Mol	Chain	Residues	Atoms					AltConf
45	B5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



Mol	Chain	Residues	Atoms			AltConf
46	AA	1	Total	C	O	0
			33	31	2	
46	AB	1	Total	C	O	0
			33	31	2	
46	BA	1	Total	C	O	0
			33	31	2	
46	BB	1	Total	C	O	0
			33	31	2	

- Molecule 47 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



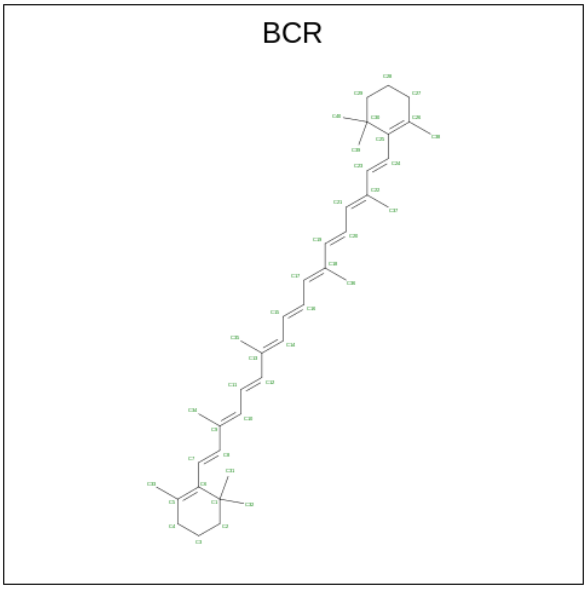
Mol	Chain	Residues	Atoms				AltConf
47	AA	1	Total	C	O	P	0
			49	38	10	1	
47	AJ	1	Total	C	O	P	0
			40	29	10	1	
47	A1	1	Total	C	O	P	0
			38	27	10	1	
47	A1	1	Total	C	O	P	0
			36	25	10	1	
47	A1	1	Total	C	O	P	0
			49	38	10	1	
47	A3	1	Total	C	O	P	0
			36	25	10	1	
47	A3	1	Total	C	O	P	0
			23	12	10	1	
47	A6	1	Total	C	O	P	0
			36	25	10	1	
47	BA	1	Total	C	O	P	0
			49	38	10	1	
47	BA	1	Total	C	O	P	0
			27	16	10	1	
47	BF	1	Total	C	O	P	0
			45	34	10	1	
47	B1	1	Total	C	O	P	0
			38	27	10	1	
47	B1	1	Total	C	O	P	0
			36	25	10	1	
47	B1	1	Total	C	O	P	0
			42	31	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
47	B2	1	Total	C	O	P	0
			35	24	10	1	
47	B3	1	Total	C	O	P	0
			23	12	10	1	
47	B5	1	Total	C	O	P	0
			30	19	10	1	
47	F	1	Total	C	O	P	0
			37	26	10	1	
47	a	1	Total	C	O	P	0
			29	18	10	1	

- Molecule 48 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AF	1	Total C 40 40	0
48	AF	1	Total C 40 40	0
48	AG	1	Total C 40 40	0
48	AI	1	Total C 40 40	0
48	AI	1	Total C 40 40	0
48	AJ	1	Total C 40 40	0
48	AJ	1	Total C 40 40	0
48	AK	1	Total C 40 40	0
48	AL	1	Total C 40 40	0
48	AL	1	Total C 40 40	0
48	A1	1	Total C 40 40	0
48	A3	1	Total C 40 40	0
48	A4	1	Total C 40 40	0
48	A6	1	Total C 40 40	0
48	BA	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

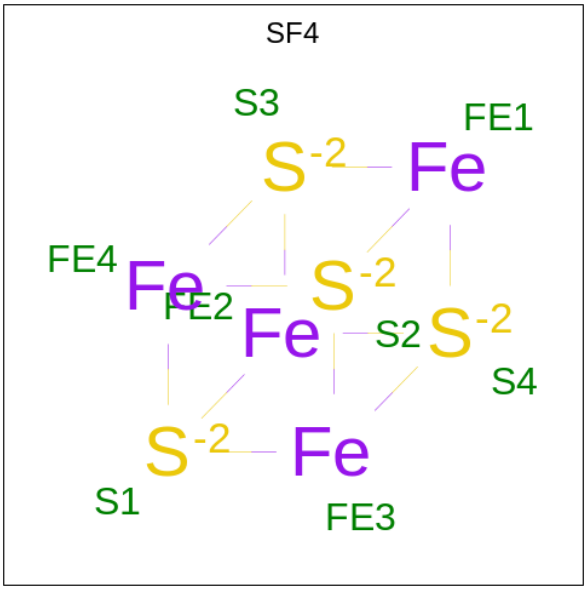
Mol	Chain	Residues	Atoms	AltConf
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BF	1	Total C 40 40	0
48	BG	1	Total C 40 40	0
48	BI	1	Total C 40 40	0
48	BJ	1	Total C 40 40	0
48	BJ	1	Total C 40 40	0
48	BK	1	Total C 40 40	0
48	BL	1	Total C 40 40	0
48	BL	1	Total C 40 40	0
48	BL	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
48	B2	1	Total C 40 40	0
48	B3	1	Total C 40 40	0
48	B5	1	Total C 40 40	0

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



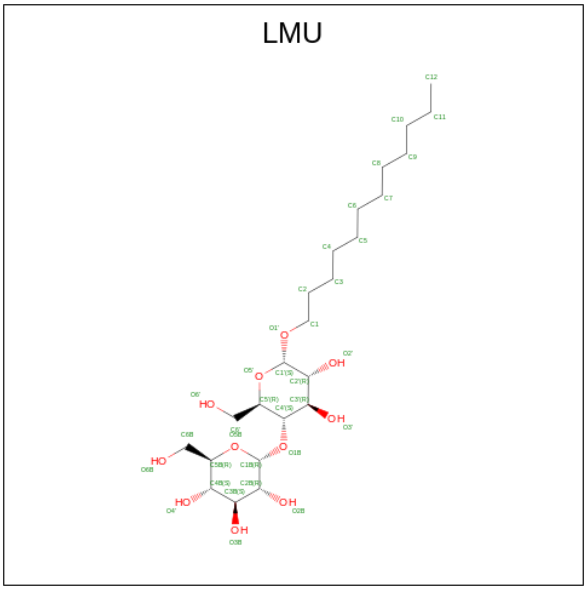
Mol	Chain	Residues	Atoms	AltConf
49	AA	1	Total Fe S 8 4 4	0
49	AC	1	Total Fe S 8 4 4	0
49	AC	1	Total Fe S 8 4 4	0
49	BA	1	Total Fe S 8 4 4	0
49	BC	1	Total Fe S 8 4 4	0
49	BC	1	Total Fe S 8 4 4	0
49	I	1	Total Fe S 8 4 4	0
49	I	1	Total Fe S 8 4 4	0

Continued on next page...

Continued from previous page...

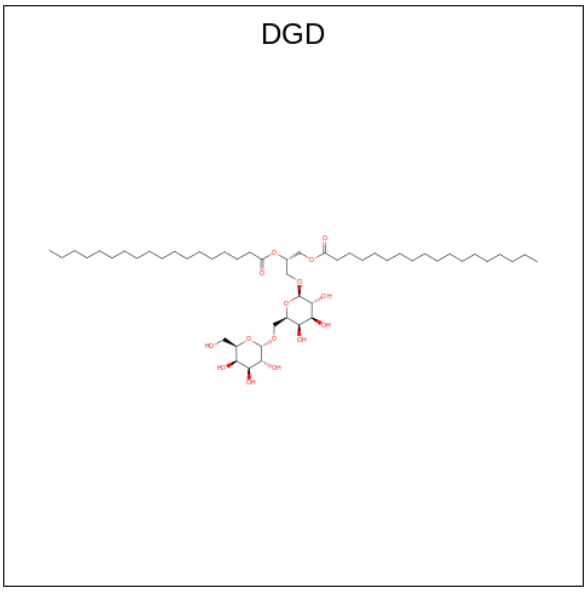
Mol	Chain	Residues	Atoms	AltConf
49	K	1	Total Fe S 8 4 4	0

- Molecule 50 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



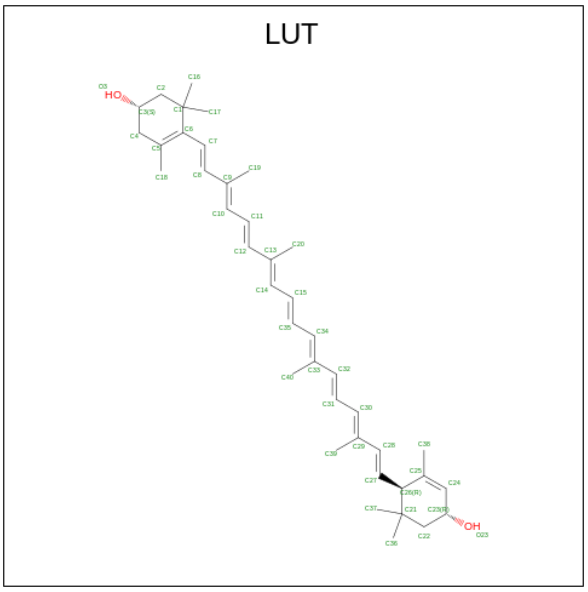
Mol	Chain	Residues	Atoms	AltConf
50	AA	1	Total C O 35 24 11	0
50	AB	1	Total C O 35 24 11	0
50	AB	1	Total C O 35 24 11	0
50	AB	1	Total C O 35 24 11	0
50	AL	1	Total C O 34 23 11	0
50	BA	1	Total C O 34 23 11	0
50	BA	1	Total C O 33 22 11	0
50	BB	1	Total C O 35 24 11	0

- Molecule 51 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
51	AB	1	Total	C	O	0
			66	51	15	
51	BB	1	Total	C	O	0
			66	51	15	

- Molecule 52 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



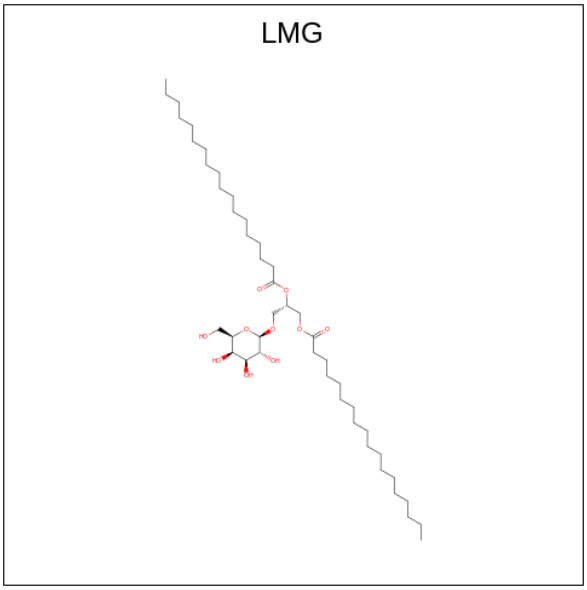
Mol	Chain	Residues	Atoms			AltConf
52	AF	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
52	A1	1	Total C O 42 40 2	0
52	A3	1	Total C O 42 40 2	0
52	A4	1	Total C O 42 40 2	0
52	A6	1	Total C O 42 40 2	0
52	B1	1	Total C O 42 40 2	0
52	B2	1	Total C O 42 40 2	0
52	B3	1	Total C O 42 40 2	0
52	B5	1	Total C O 42 40 2	0

- Molecule 53 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



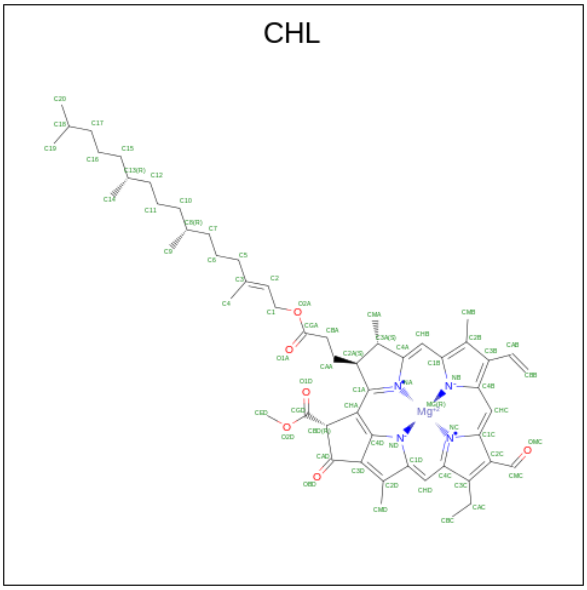
Mol	Chain	Residues	Atoms	AltConf
53	AG	1	Total C O 38 28 10	0
53	A1	1	Total C O 44 34 10	0
53	A4	1	Total C O 39 29 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
53	B5	1	Total 33	C 23	O 10	0

- Molecule 54 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



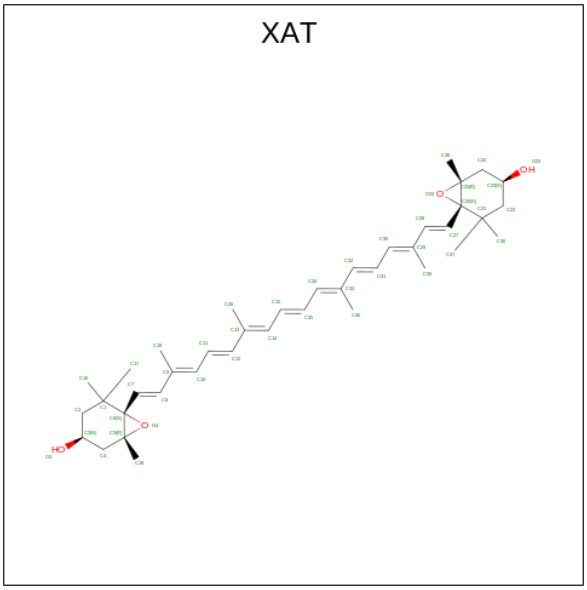
Mol	Chain	Residues	Atoms					AltConf
54	A1	1	Total 51	C 40	Mg 1	N 4	O 6	0
54	A1	1	Total 41	C 32	Mg 1	N 4	O 4	0
54	A3	1	Total 45	C 35	Mg 1	N 4	O 5	0
54	A4	1	Total 41	C 32	Mg 1	N 4	O 4	0
54	A4	1	Total 41	C 33	Mg 1	N 4	O 3	0
54	A4	1	Total 46	C 35	Mg 1	N 4	O 6	0
54	A4	1	Total 41	C 32	Mg 1	N 4	O 4	0
54	A6	1	Total 52	C 41	Mg 1	N 4	O 6	0
54	A6	1	Total 42	C 33	Mg 1	N 4	O 4	0
54	A6	1	Total 43	C 34	Mg 1	N 4	O 4	0

Continued on next page...

Continued from previous page...

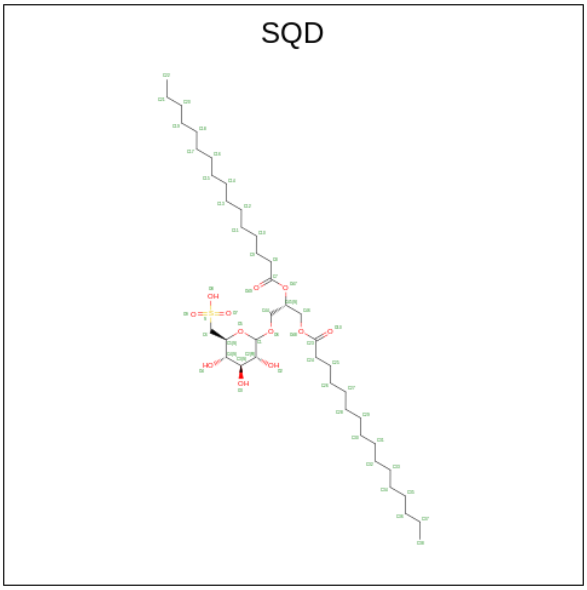
Mol	Chain	Residues	Atoms					AltConf
54	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
54	B1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	B1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	B5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
54	B5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 55 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



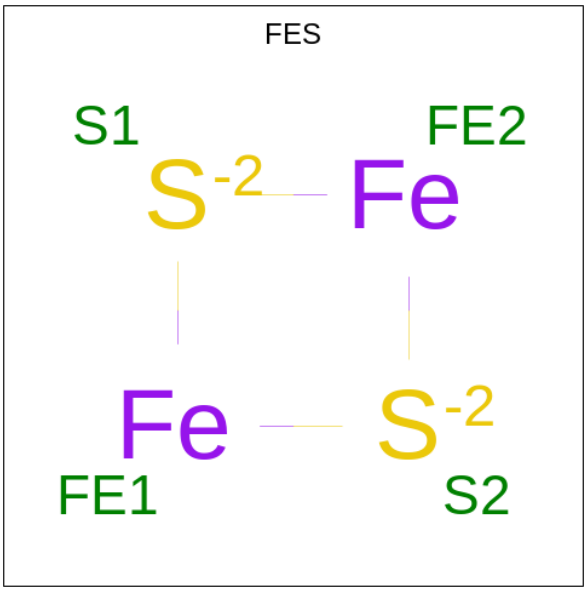
Mol	Chain	Residues	Atoms	AltConf
55	A1	1	Total C O 44 40 4	0
55	A3	1	Total C O 44 40 4	0
55	A4	1	Total C O 44 40 4	0
55	A6	1	Total C O 44 40 4	0
55	B1	1	Total C O 44 40 4	0
55	B2	1	Total C O 44 40 4	0
55	B3	1	Total C O 44 40 4	0
55	B5	1	Total C O 44 40 4	0

- Molecule 56 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	AltConf
56	BJ	1	Total C O S 47 34 12 1	0
56	e	1	Total C O S 34 21 12 1	0

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



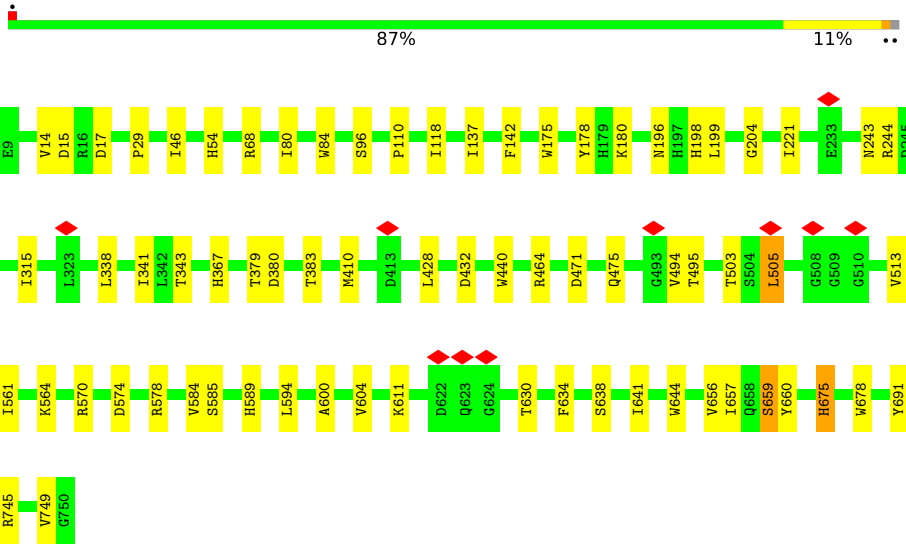
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
57	c	1	4	2	2	0

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.

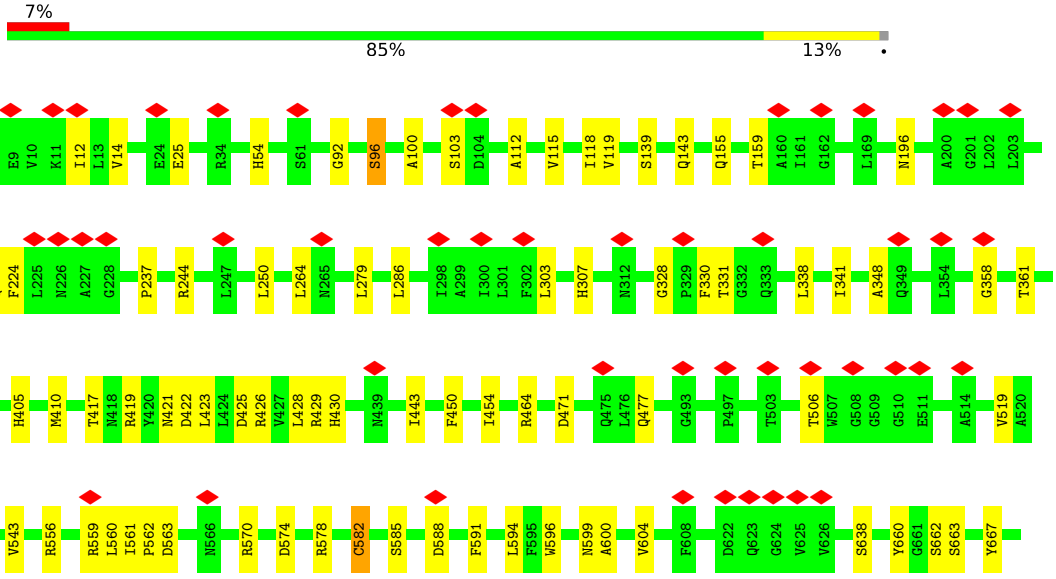
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain BA:

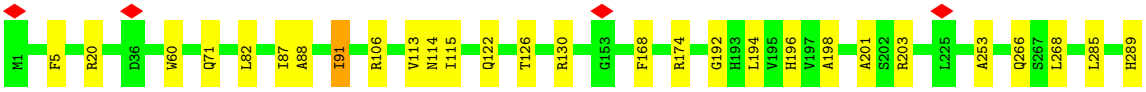


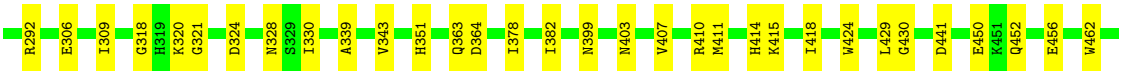


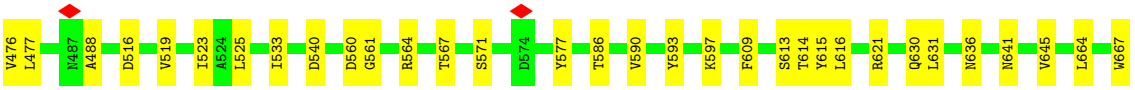
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain AB:







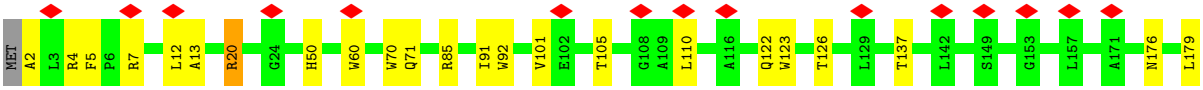


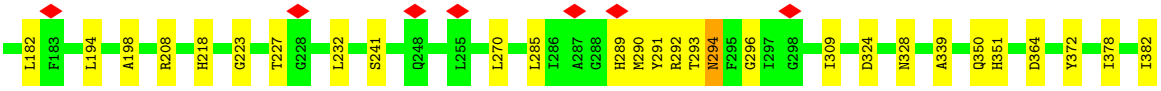


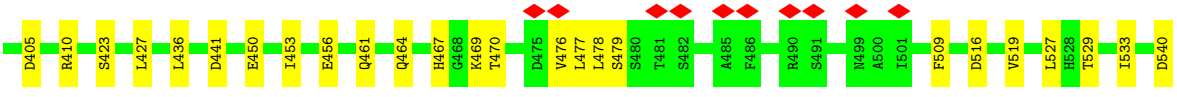
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain BB:

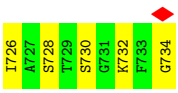








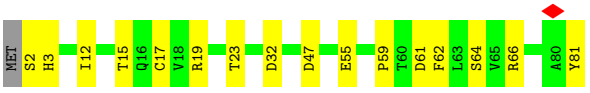




• Molecule 3: Photosystem I iron-sulfur center

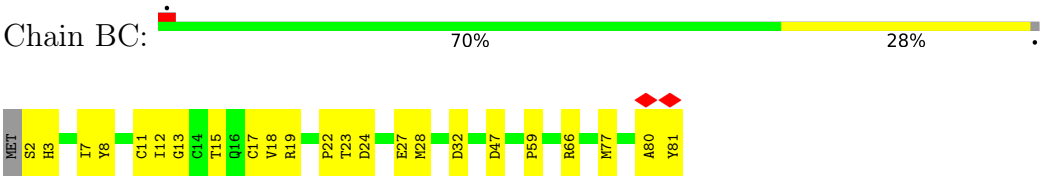
Chain AC:





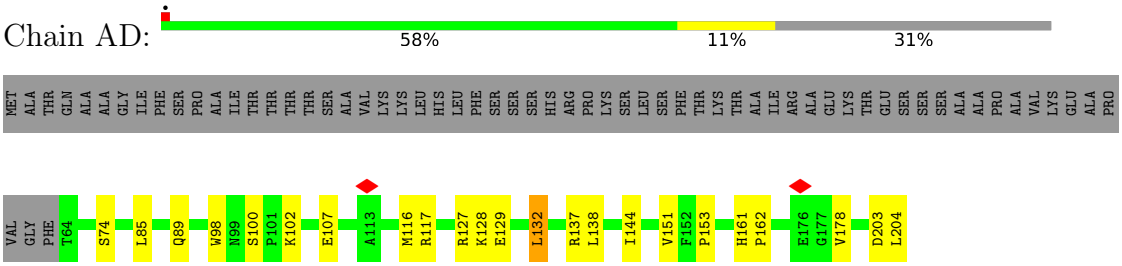
• Molecule 3: Photosystem I iron-sulfur center

Chain BC:



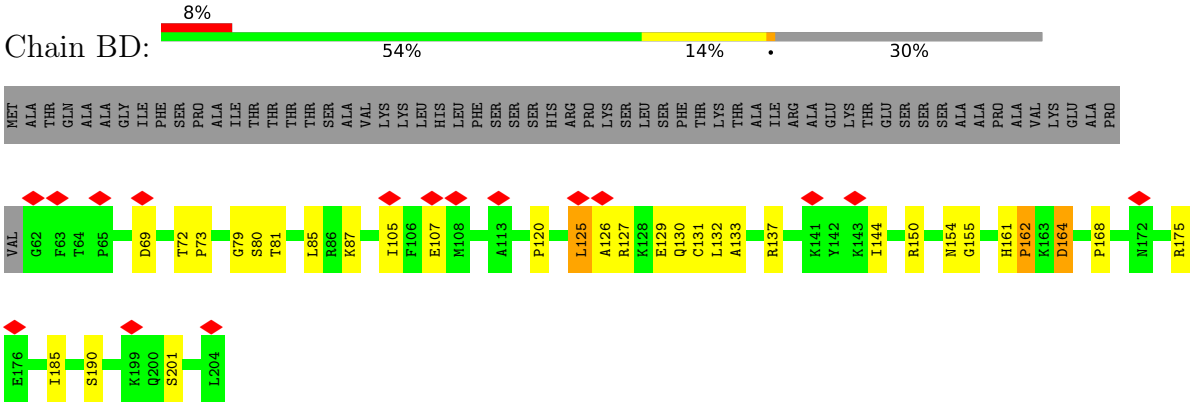
• Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain AD:



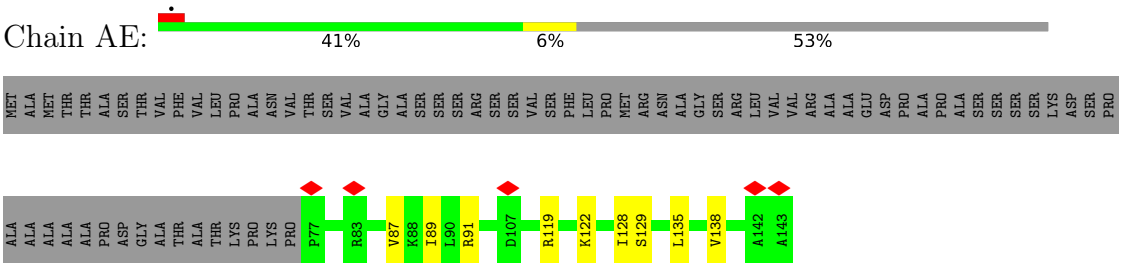
• Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain BD:



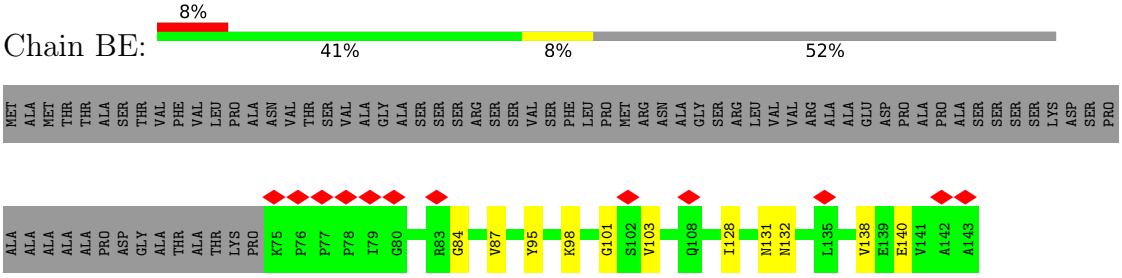
• Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain AE:



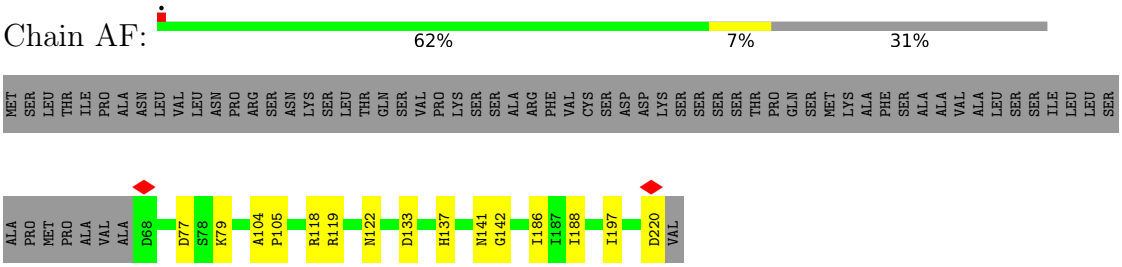
• Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain BE:



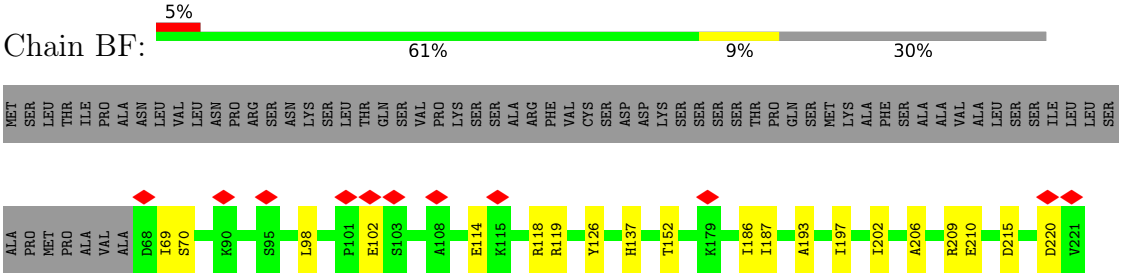
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain AF:



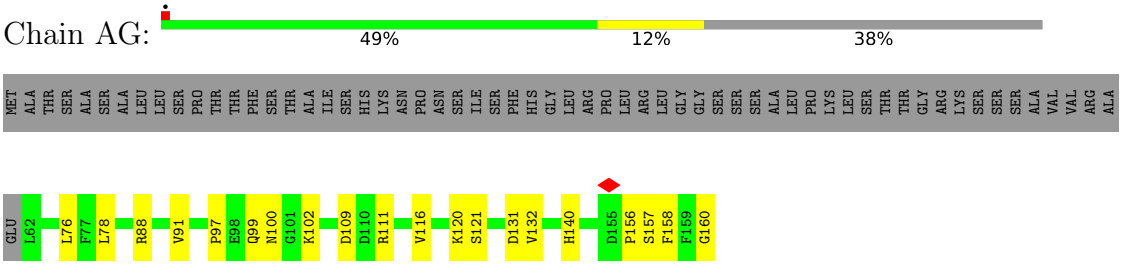
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain BF:



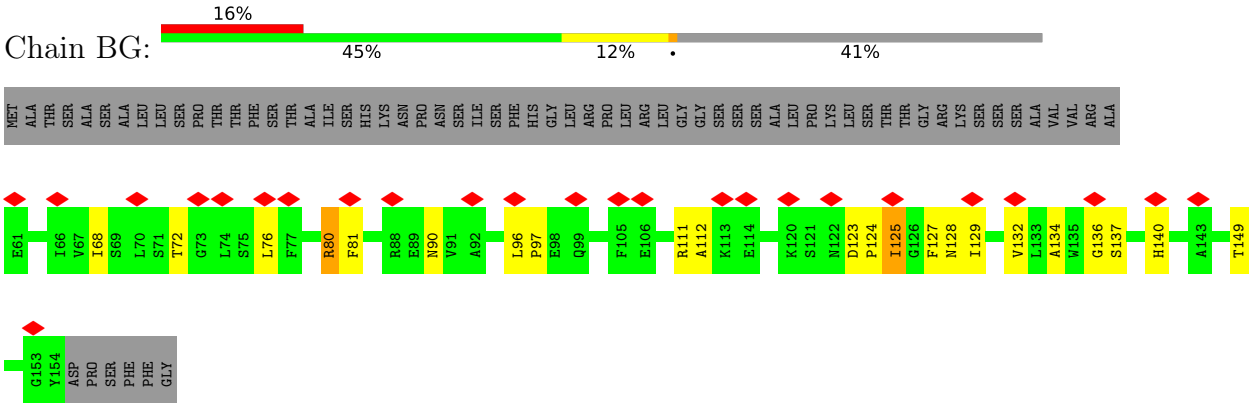
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain AG:



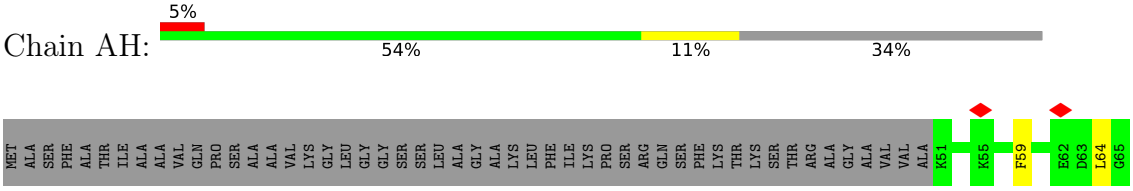
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

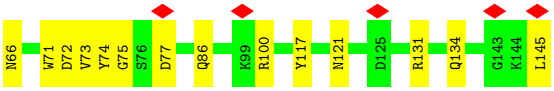
Chain BG:



• Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

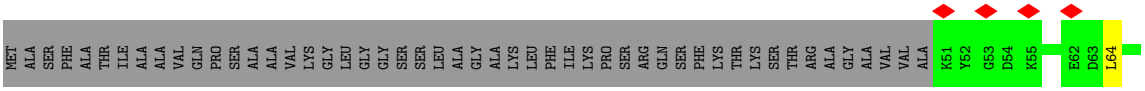
Chain AH:

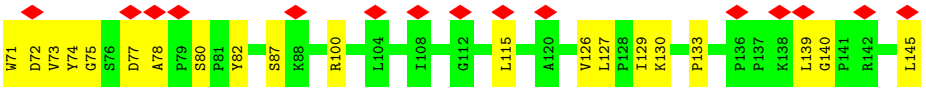




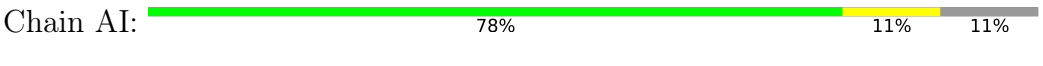
• Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic







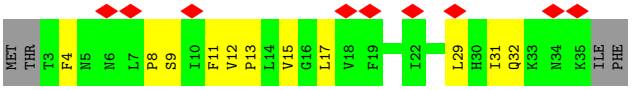
• Molecule 9: Photosystem I reaction center subunit VIII





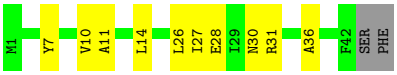
• Molecule 9: Photosystem I reaction center subunit VIII



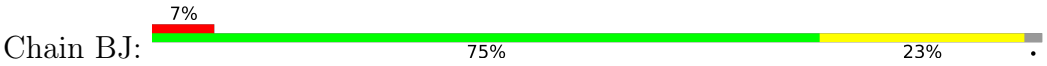


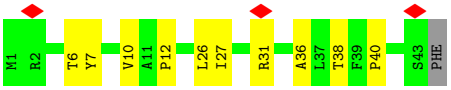
• Molecule 10: Photosystem I reaction center subunit IX





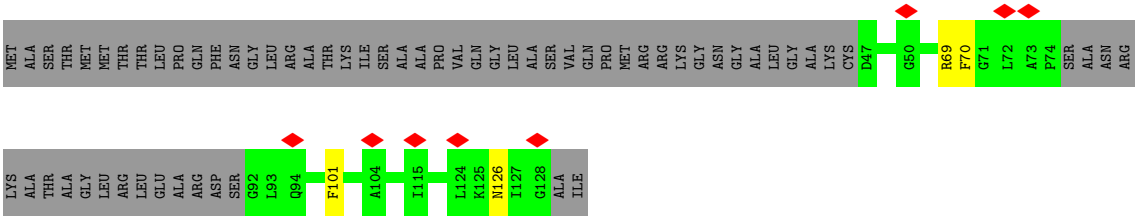
• Molecule 10: Photosystem I reaction center subunit IX





• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

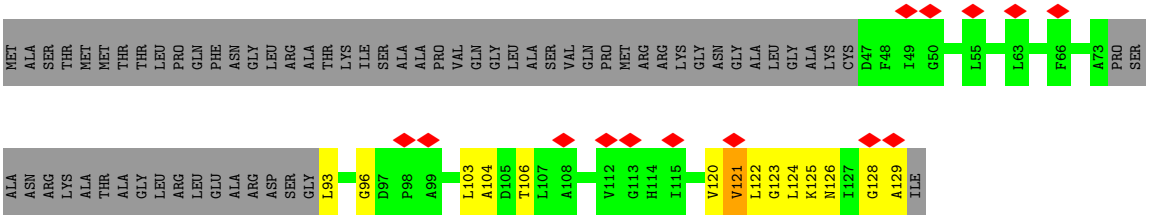




• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain BK:

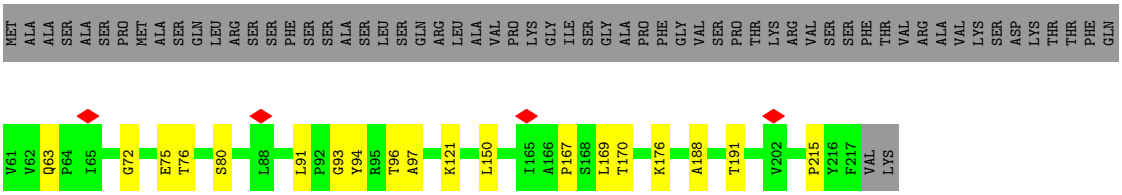




• Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain AL:

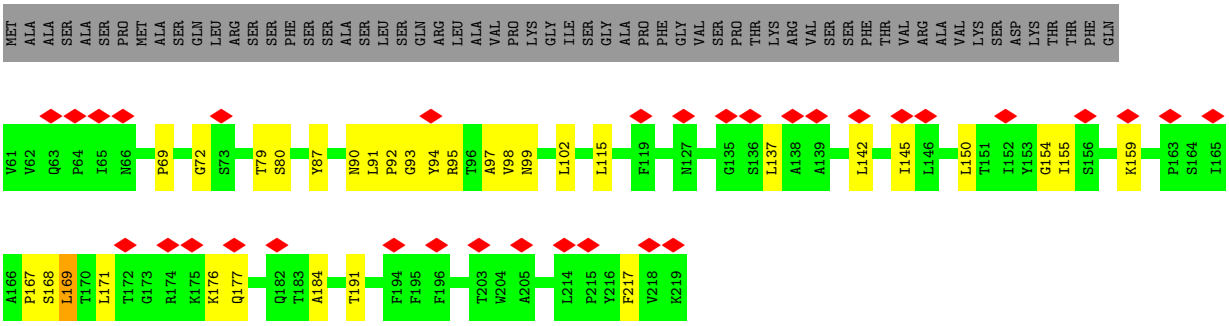




• Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain BL:

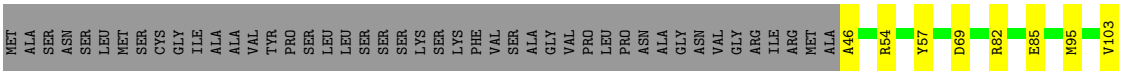




• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain A1:



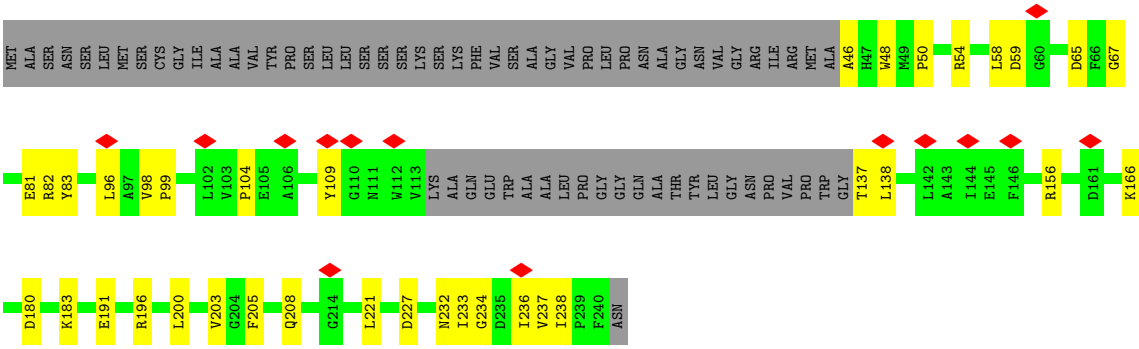




• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain B1:

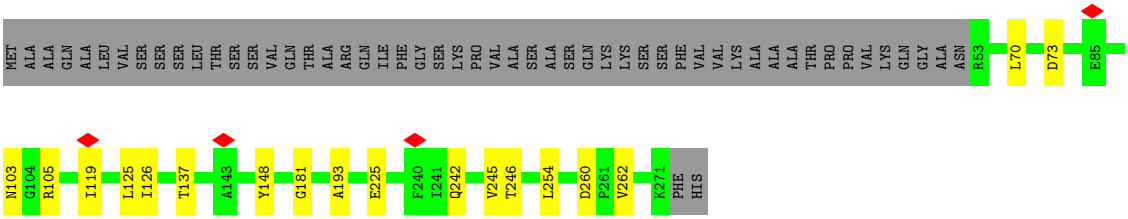




• Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain A3:

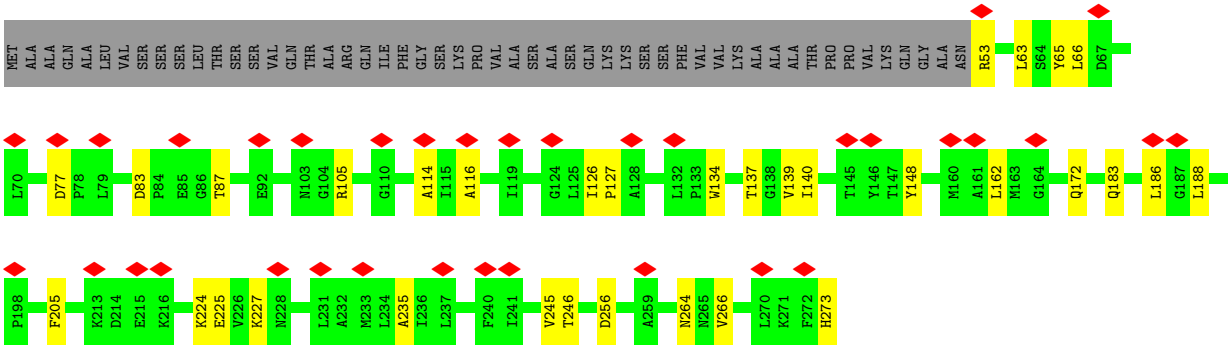




• Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain B3:

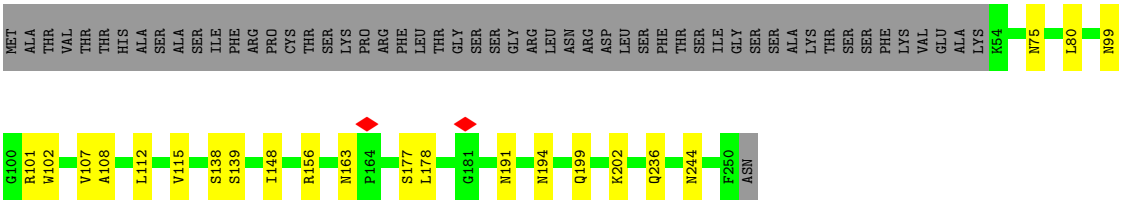




• Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic

Chain A4:

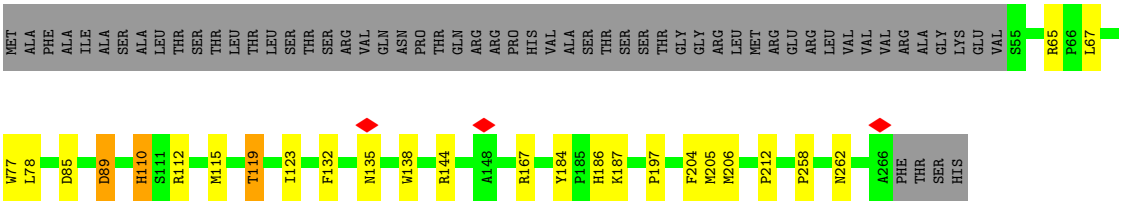




• Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic

Chain A6:

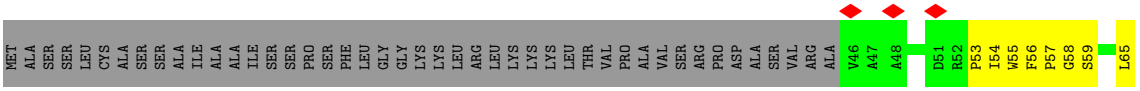


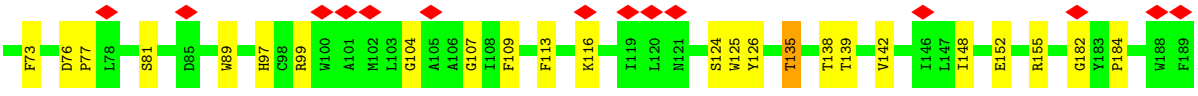


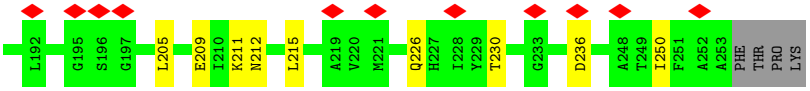
• Molecule 17: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

Chain B2:





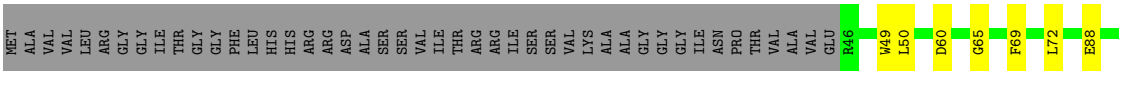


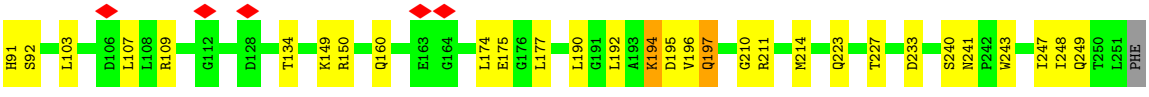


• Molecule 18: Photosystem I chlorophyll a/b-binding protein 5, chloroplastic

Chain B5:





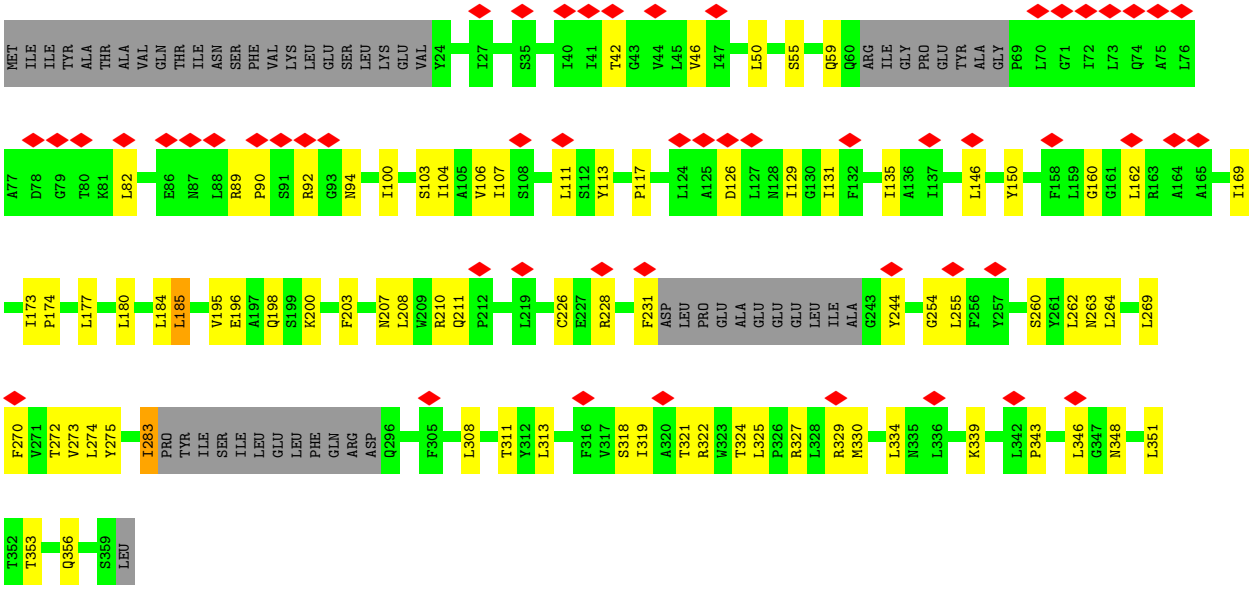




• Molecule 19: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

Chain A:

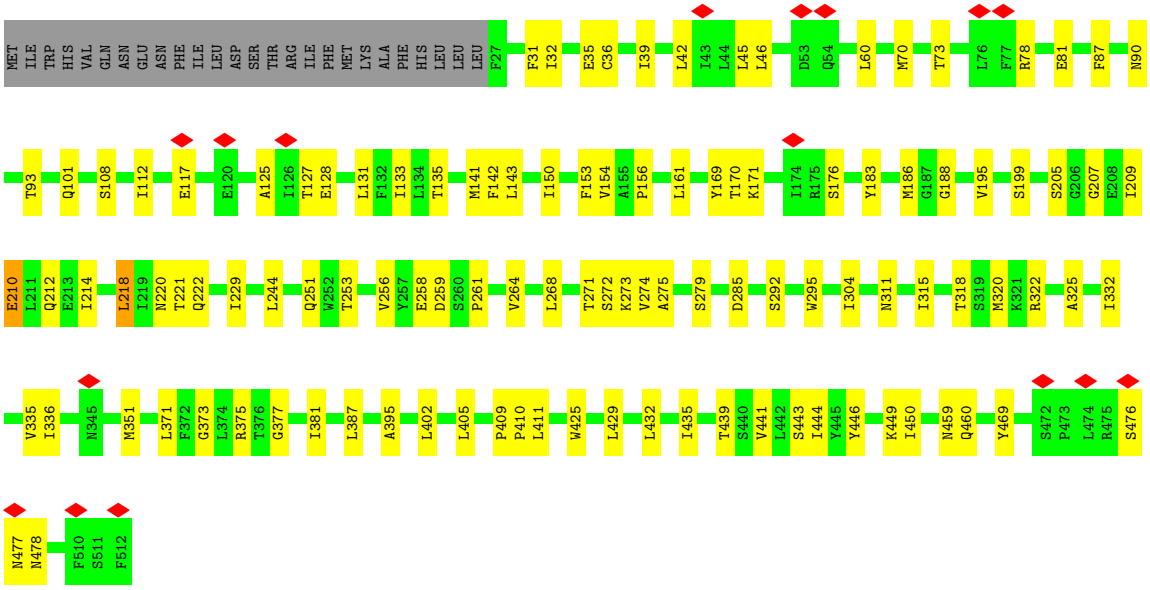




• Molecule 20: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

Chain B:

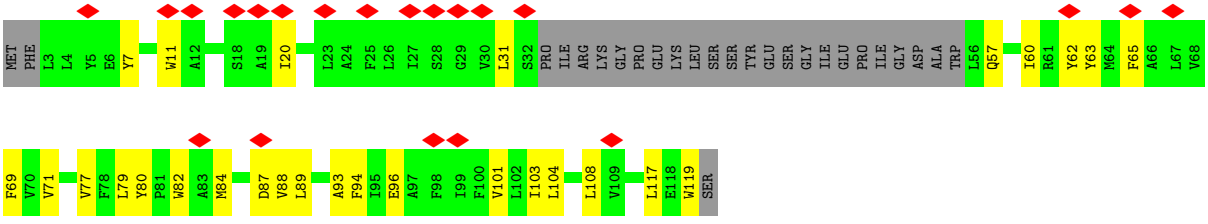




• Molecule 21: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic

Chain C:

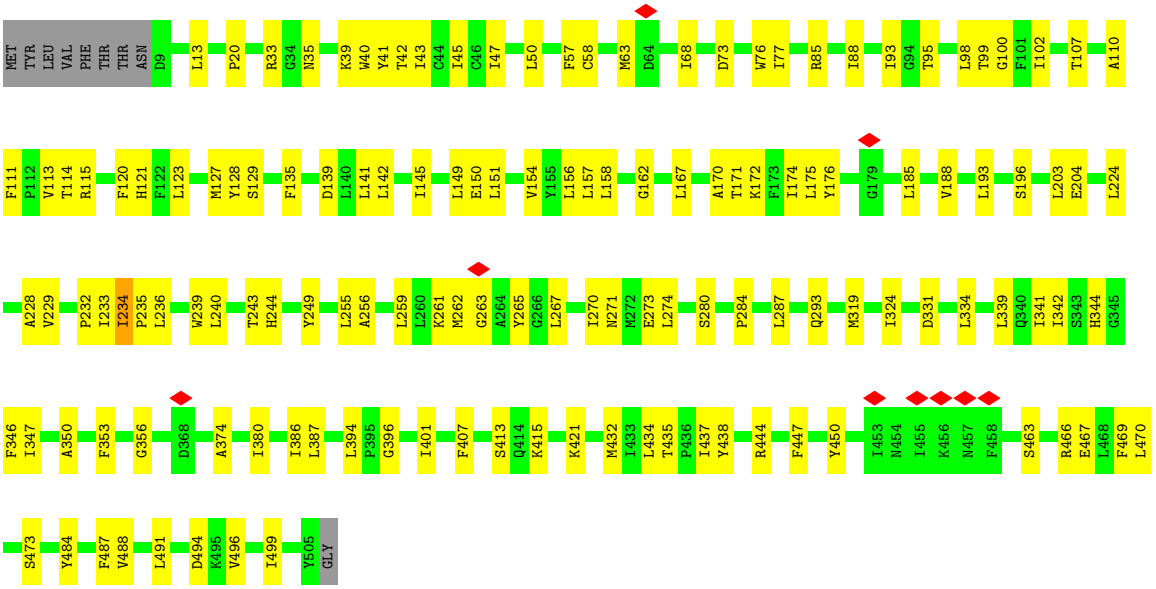




• Molecule 22: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

Chain D:

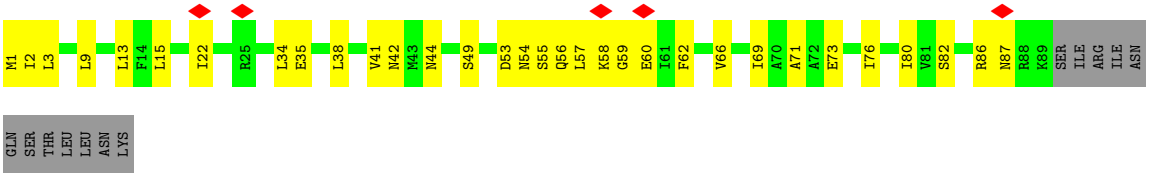




• Molecule 23: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

Chain E:

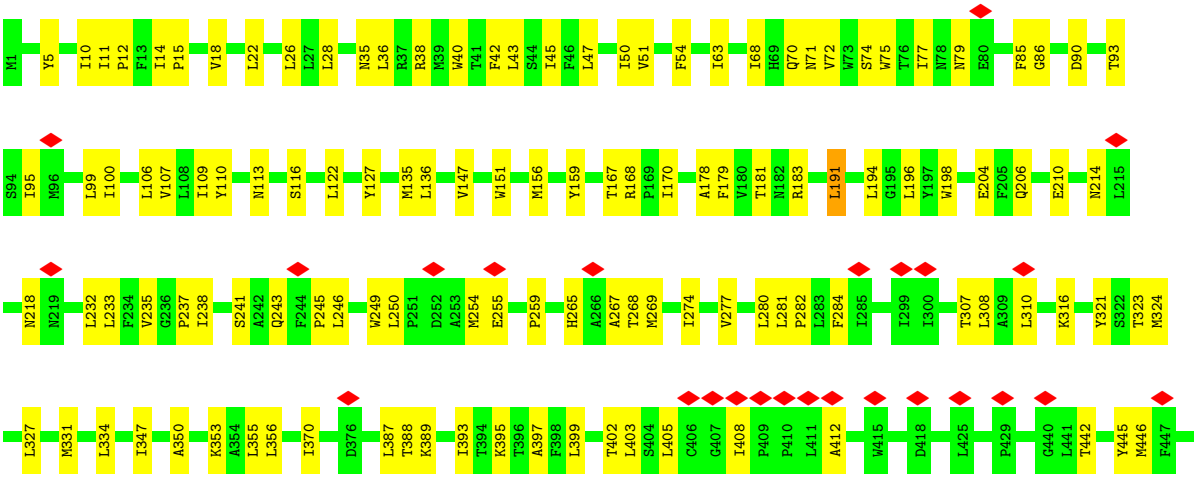


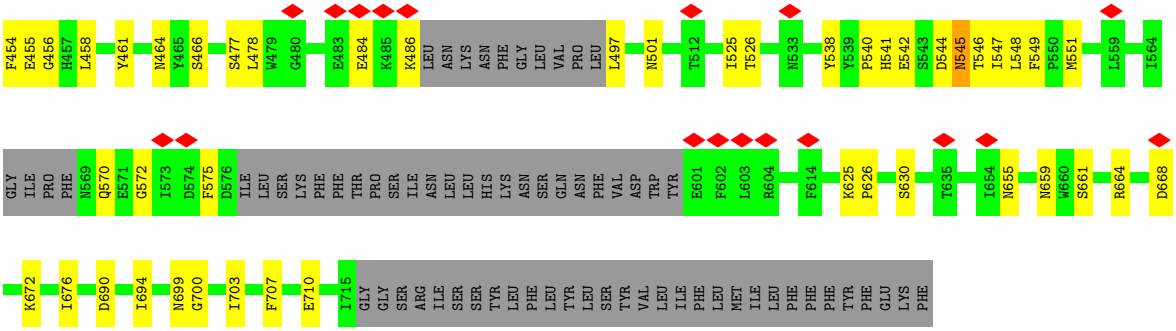


• Molecule 24: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic

Chain F:



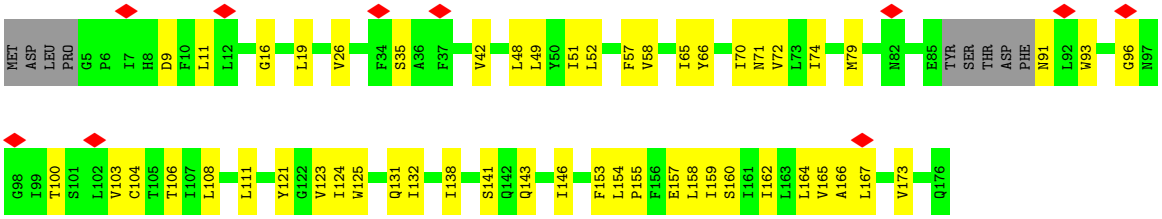




• Molecule 25: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

Chain G:

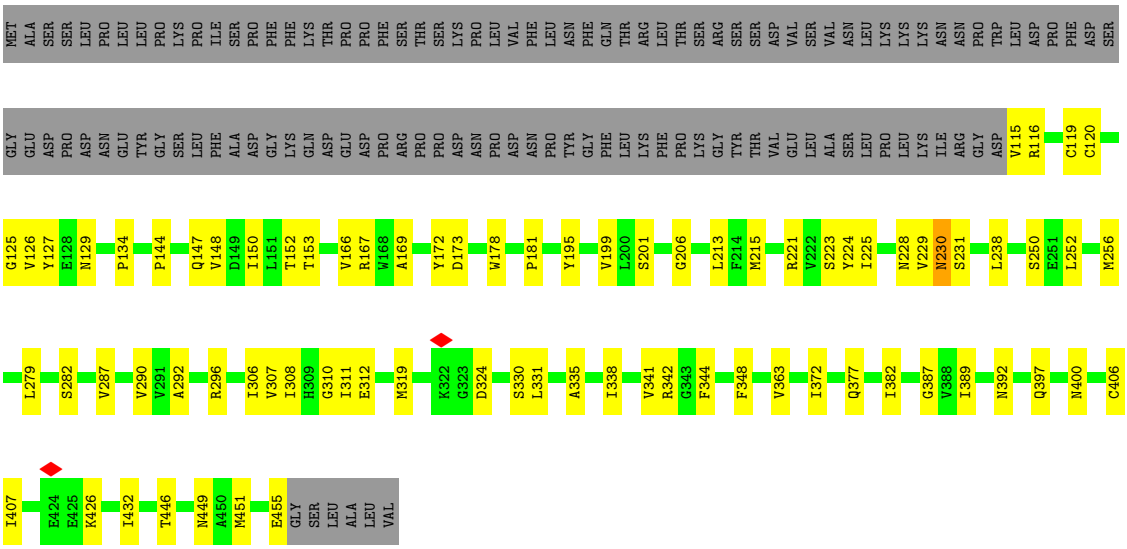




• Molecule 26: Photosynthetic NDH subunit of subcomplex B 1, chloroplastic

Chain a:

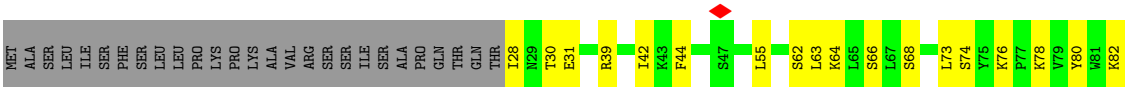


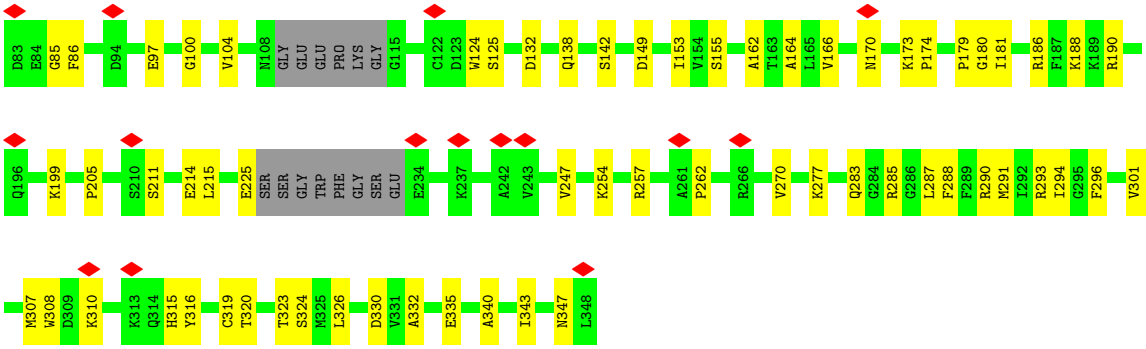


• Molecule 27: Photosynthetic NDH subunit of subcomplex B 2, chloroplastic

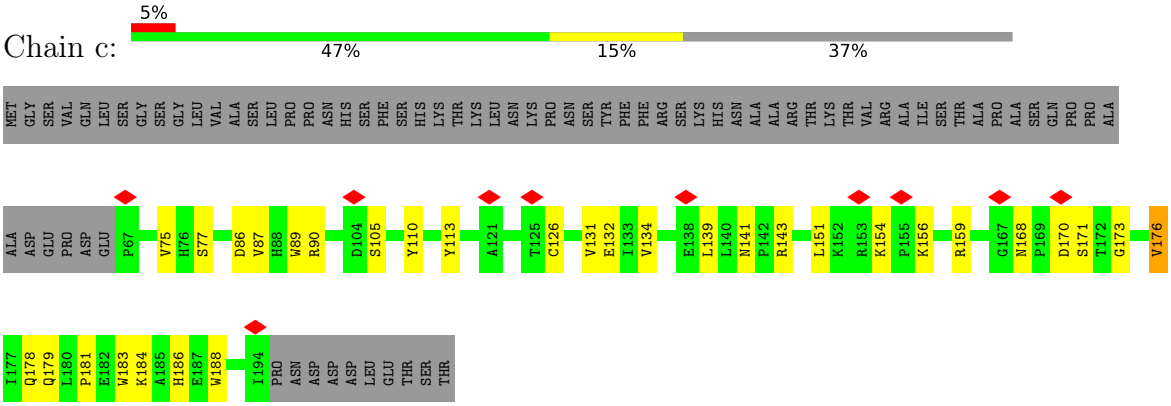
Chain b:



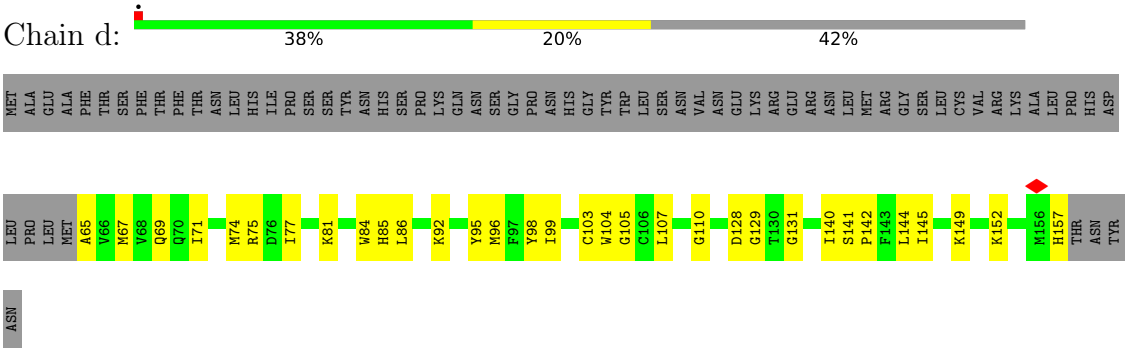




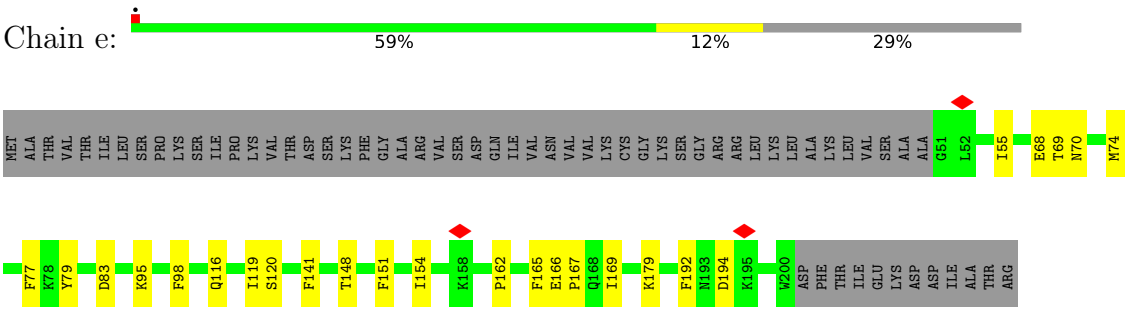
• Molecule 28: Photosynthetic NDH subunit of subcomplex B 3, chloroplastic



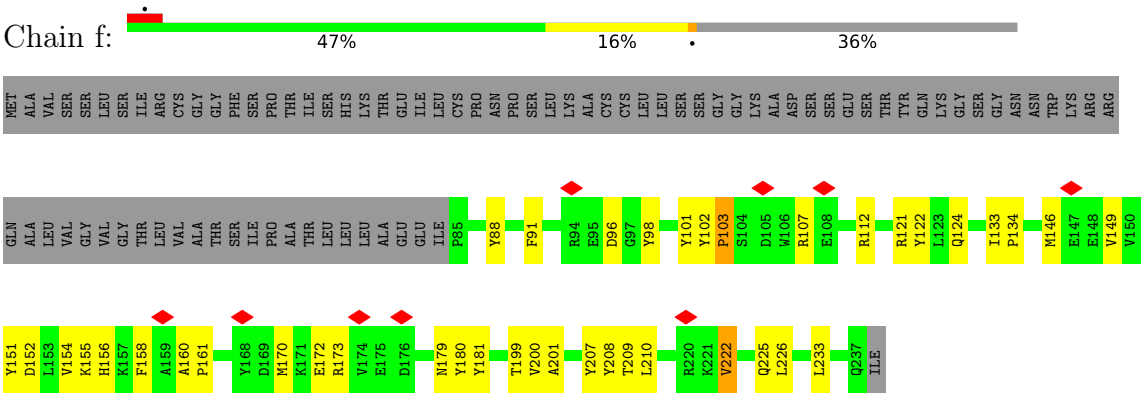
• Molecule 29: NDH dependent flow 6



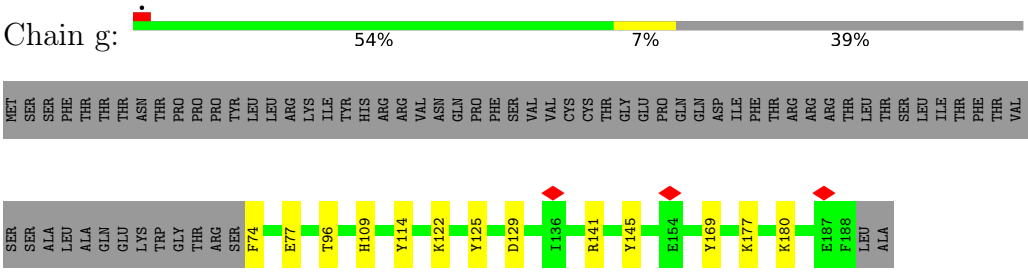
• Molecule 30: Photosynthetic NDH subunit of subcomplex B 5, chloroplastic



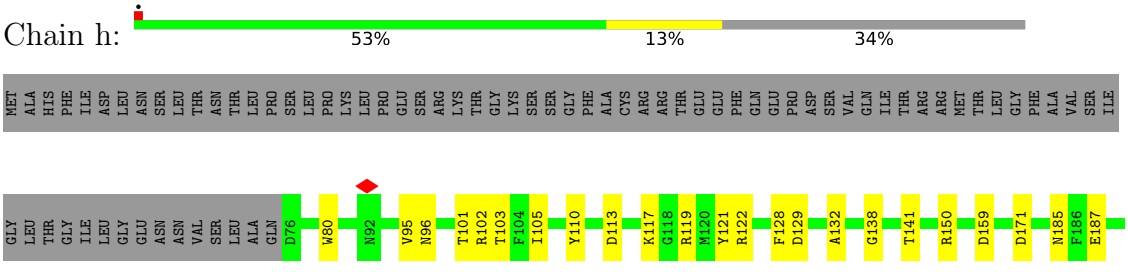
• Molecule 31: Photosynthetic NDH subunit of lumenal location 1, chloroplastic



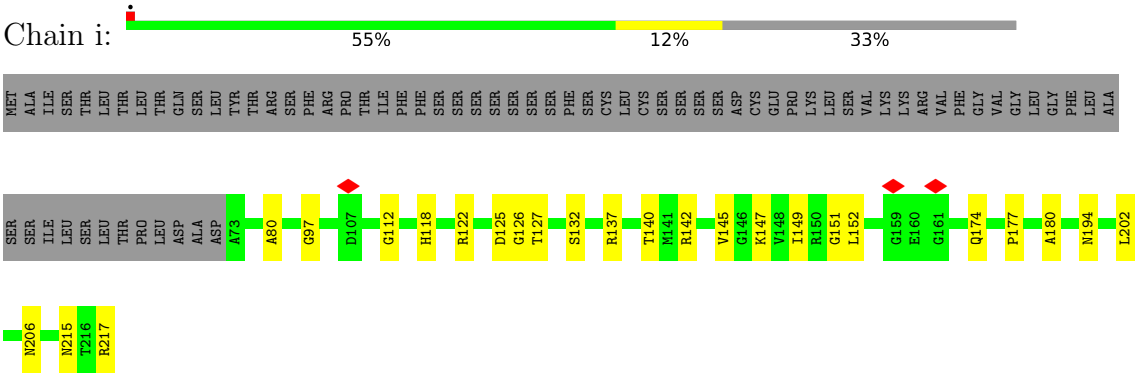
• Molecule 32: Photosynthetic NDH subunit of lumenal location 2, chloroplastic



• Molecule 33: Photosynthetic NDH subunit of lumenal location 3, chloroplastic

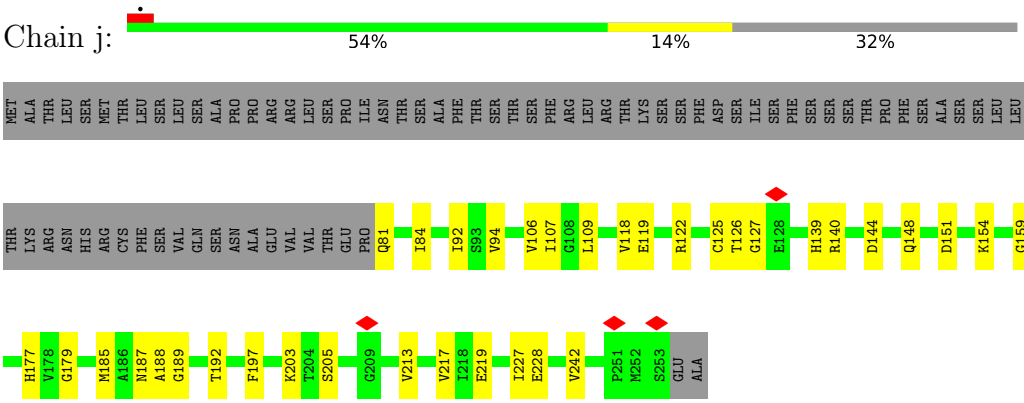


• Molecule 34: Photosynthetic NDH subunit of lumenal location 4, chloroplastic



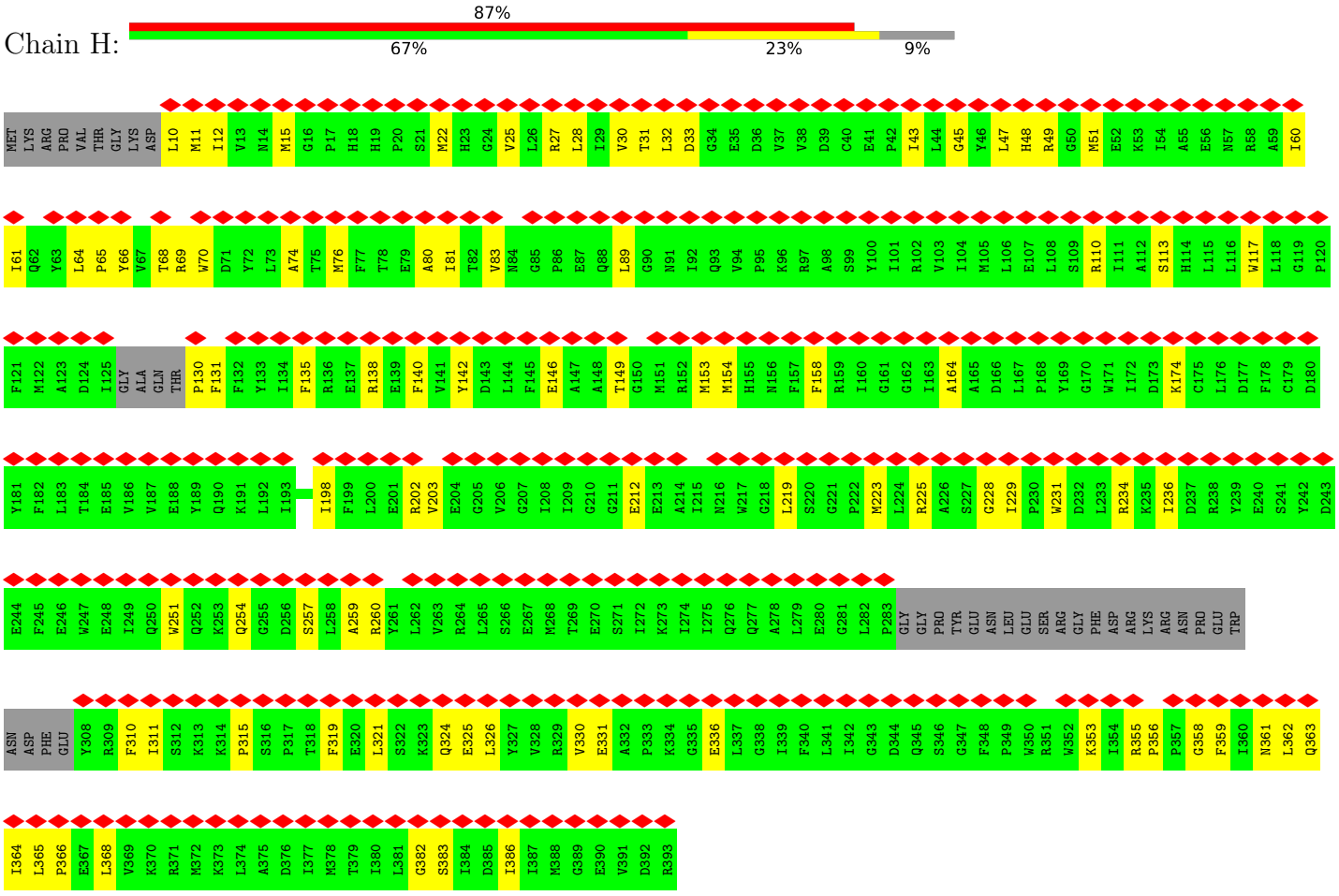
• Molecule 35: Isoform 2 of Photosynthetic NDH subunit of lumenal location 5, chloroplastic

Chain j:



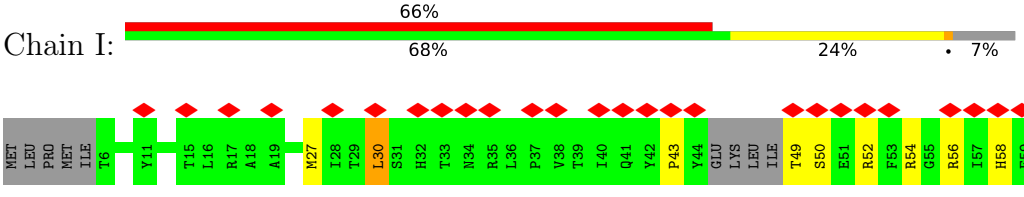
• Molecule 36: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

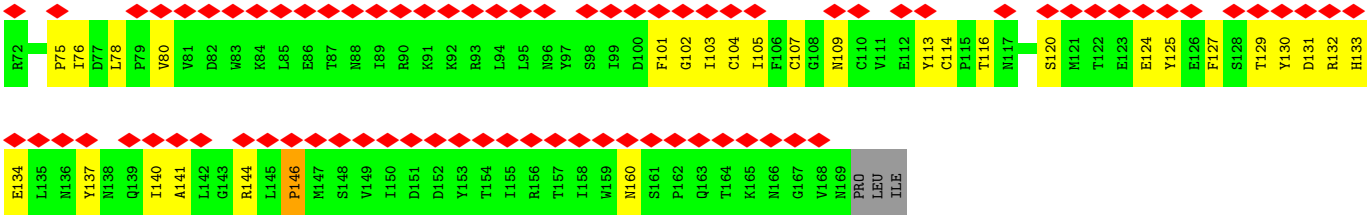
Chain H:



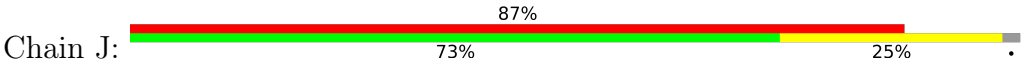
• Molecule 37: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

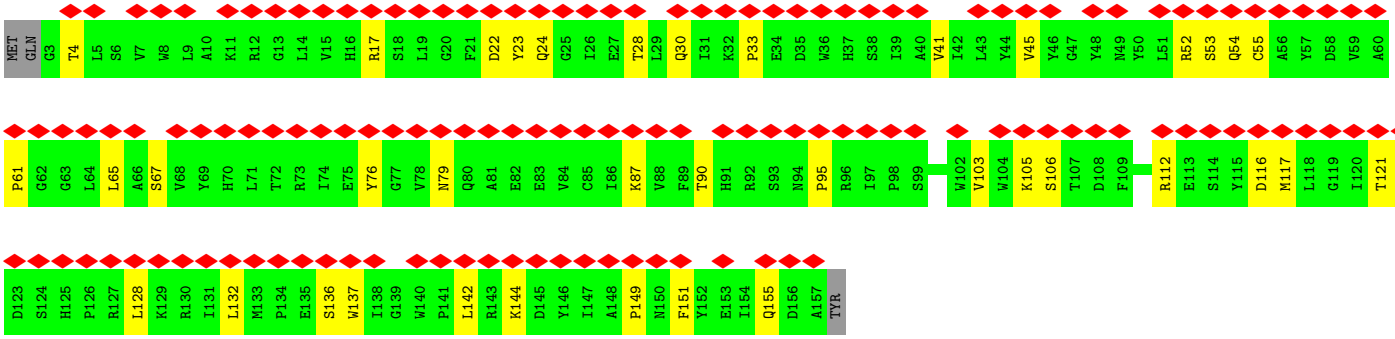
Chain I:





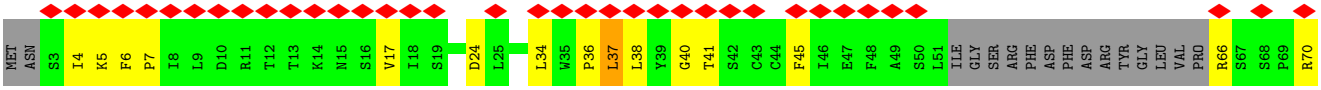
• Molecule 38: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic

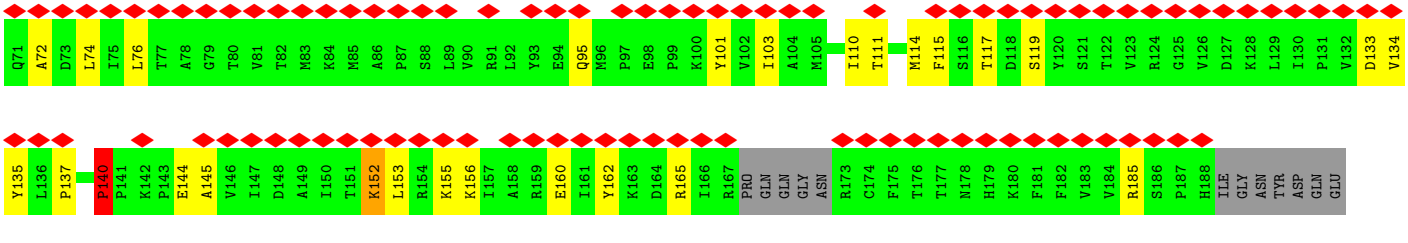




• Molecule 39: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic

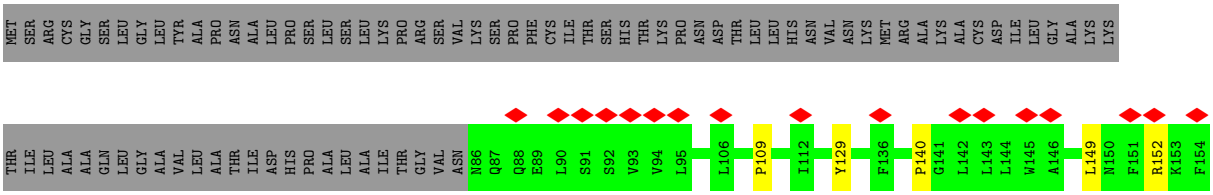


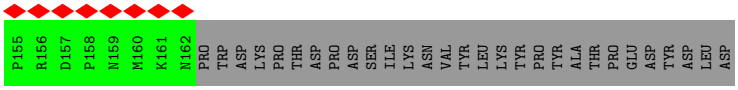




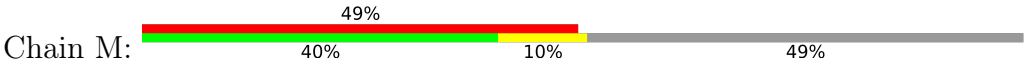
• Molecule 40: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic

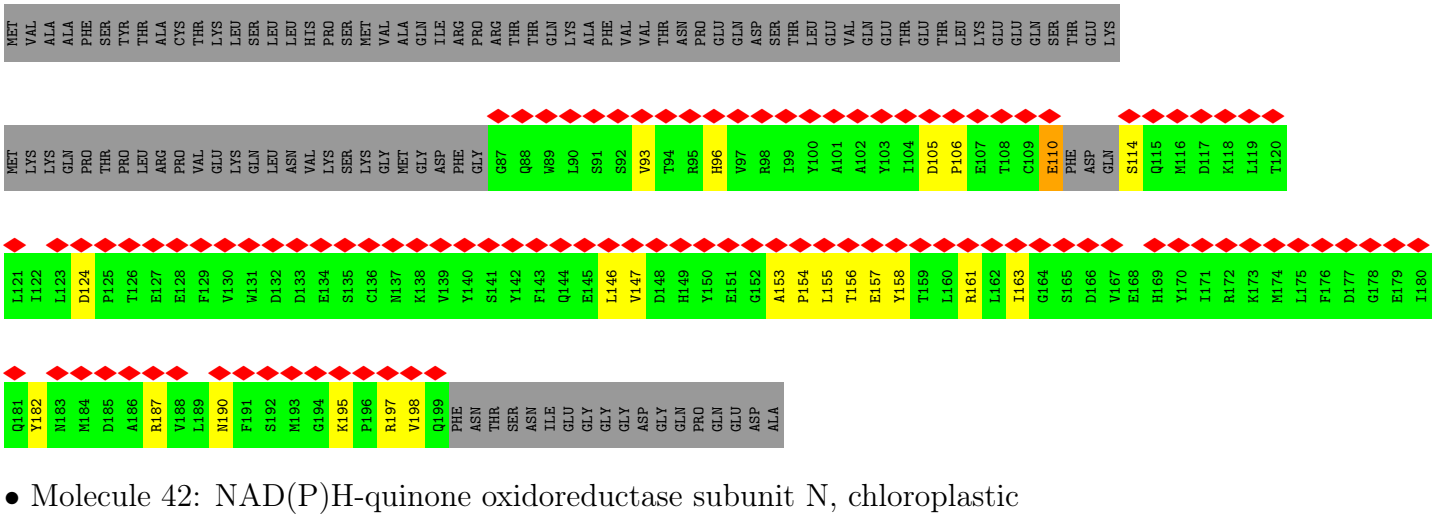






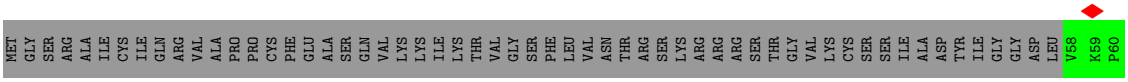
• Molecule 41: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic

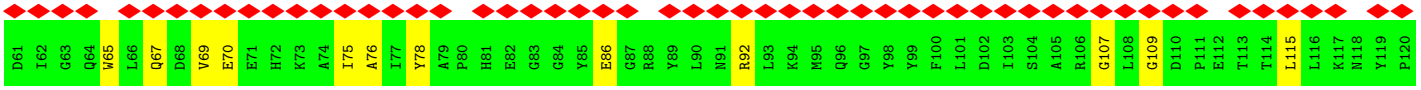




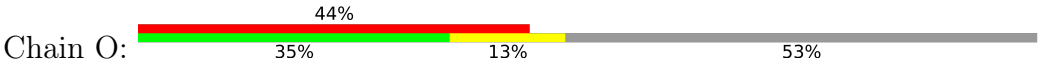
• Molecule 42: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic

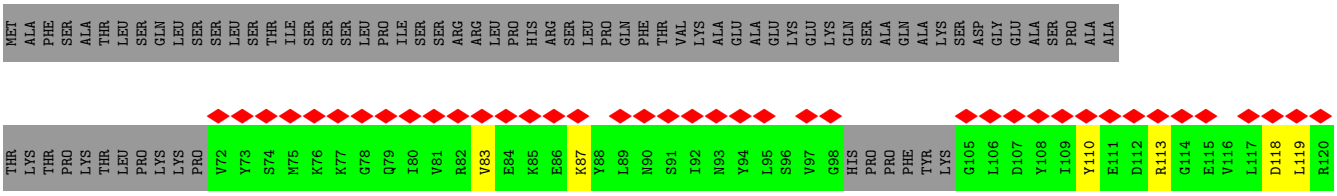


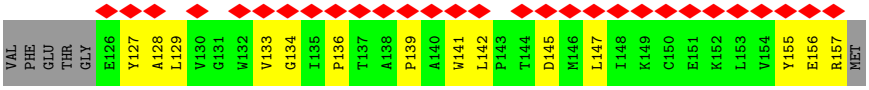




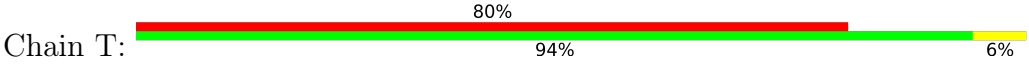
• Molecule 43: NdhO







• Molecule 44: NdhT





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, FES, LMG, LHG, DGD, CLA, CHL, SQD, LUT, LMU, PQN, BCR, SF4

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	AA	0.32	1/6037 (0.0%)	0.47	0/8236
1	BA	0.31	0/6039	0.48	1/8239 (0.0%)
2	AB	0.30	0/6073	0.44	0/8291
2	BB	0.31	0/6065	0.48	1/8281 (0.0%)
3	AC	0.37	0/628	0.57	0/852
3	BC	0.39	0/628	0.63	0/852
4	AD	0.22	0/1140	0.45	0/1542
4	BD	0.32	0/1156	0.55	0/1563
5	AE	0.20	0/542	0.36	0/736
5	BE	0.20	0/559	0.37	0/760
6	AF	0.23	0/1243	0.44	0/1677
6	BF	0.25	0/1250	0.46	0/1687
7	AG	0.41	1/791 (0.1%)	0.49	0/1072
7	BG	0.31	0/750	0.54	0/1016
8	AH	0.19	0/751	0.41	0/1018
8	BH	0.25	0/751	0.48	0/1018
9	AI	0.22	0/264	0.39	0/359
9	BI	0.39	0/264	0.84	2/359 (0.6%)
10	AJ	0.31	0/348	0.54	0/474
10	BJ	0.29	0/354	0.52	0/482
11	AK	0.28	0/456	0.45	0/617
11	BK	0.40	0/449	0.68	1/607 (0.2%)
12	AL	0.26	0/1208	0.47	1/1650 (0.1%)
12	BL	0.28	0/1218	0.50	0/1663
13	A1	0.32	1/1562 (0.1%)	0.47	0/2131
13	B1	0.22	0/1381	0.43	0/1879
14	A3	0.22	0/1726	0.41	0/2347
14	B3	0.21	0/1749	0.39	0/2378
15	A4	0.27	0/1611	0.45	0/2194
16	A6	0.28	0/1732	0.49	0/2363
17	B2	0.23	0/1663	0.47	0/2277
18	B5	0.25	0/1646	0.48	1/2239 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	A	0.26	0/2430	0.60	0/3312
20	B	0.31	0/3872	0.64	2/5263 (0.0%)
21	C	0.35	1/802 (0.1%)	0.59	0/1094
22	D	0.37	0/4058	0.63	1/5509 (0.0%)
23	E	0.28	0/705	0.56	0/952
24	F	0.30	0/5478	0.63	6/7446 (0.1%)
25	G	0.27	0/1307	0.63	2/1785 (0.1%)
26	a	0.33	0/2708	0.70	0/3668
27	b	0.22	0/2417	0.60	0/3265
28	c	0.33	0/1030	0.70	0/1401
29	d	0.38	0/784	0.68	0/1057
30	e	0.26	0/1241	0.62	0/1685
31	f	0.24	0/1312	0.60	0/1777
32	g	0.22	0/986	0.51	0/1329
33	h	0.25	0/1193	0.64	0/1610
34	i	0.24	0/1124	0.53	0/1523
35	j	0.26	0/1357	0.60	0/1823
36	H	0.25	0/2877	0.53	0/3894
37	I	0.37	0/1256	0.66	1/1701 (0.1%)
38	J	0.22	0/1142	0.48	0/1545
39	K	0.34	0/1222	0.69	2/1656 (0.1%)
40	L	0.28	0/669	0.61	1/911 (0.1%)
41	M	0.31	0/783	0.54	0/1062
42	N	0.43	0/921	0.60	0/1252
43	O	0.29	0/525	0.40	0/705
All	All	0.30	4/94233 (0.0%)	0.54	22/128084 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A1	103	VAL	CA-CB	8.58	1.58	1.54
7	AG	156	PRO	C-O	-6.81	1.15	1.24
21	C	20	ILE	C-N	5.55	1.40	1.34
1	AA	17	ASP	C-O	-5.00	1.21	1.23

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	K	140	PRO	N-CA-C	8.24	120.75	110.70
9	BI	9	SER	CA-C-N	-7.60	114.79	122.77
9	BI	9	SER	C-N-CA	-7.60	114.79	122.77
12	AL	215	PRO	N-CA-C	-6.45	106.29	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	K	37	LEU	N-CA-C	-6.34	105.91	113.21

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	AA	5839	0	5683	76	0
1	BA	5841	0	5690	110	0
2	AB	5862	0	5649	97	0
2	BB	5854	0	5637	114	0
3	AC	615	0	593	16	0
3	BC	615	0	595	38	0
4	AD	1112	0	1122	14	0
4	BD	1127	0	1134	52	0
5	AE	530	0	536	14	0
5	BE	546	0	555	13	0
6	AF	1213	0	1243	10	0
6	BF	1220	0	1252	14	0
7	AG	771	0	749	16	0
7	BG	733	0	718	82	0
8	AH	730	0	720	25	0
8	BH	730	0	720	71	0
9	AI	257	0	274	7	0
9	BI	257	0	274	34	0
10	AJ	338	0	351	14	0
10	BJ	344	0	356	13	0
11	AK	451	0	462	11	0
11	BK	445	0	453	36	0
12	AL	1173	0	1162	27	0
12	BL	1184	0	1179	73	0
13	A1	1511	0	1464	16	0
13	B1	1339	0	1316	39	0
14	A3	1675	0	1647	11	0
14	B3	1696	0	1663	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A4	1562	0	1516	22	0
16	A6	1671	0	1599	56	0
17	B2	1607	0	1555	56	0
18	B5	1599	0	1581	37	0
19	A	2372	0	2454	64	0
20	B	3780	0	3840	87	0
21	C	776	0	777	30	0
22	D	3946	0	4068	107	0
23	E	695	0	732	34	0
24	F	5330	0	5289	175	0
25	G	1281	0	1340	59	0
26	a	2655	0	2673	67	0
27	b	2367	0	2371	60	0
28	c	1005	0	1006	22	0
29	d	762	0	730	49	0
30	e	1206	0	1110	27	0
31	f	1277	0	1235	31	0
32	g	965	0	945	12	0
33	h	1170	0	1176	26	0
34	i	1098	0	1082	21	0
35	j	1331	0	1320	22	0
36	H	2812	0	2795	93	0
37	I	1236	0	1180	70	0
38	J	1116	0	938	65	0
39	K	1199	0	1106	82	0
40	L	646	0	630	12	0
41	M	771	0	652	43	0
42	N	908	0	717	59	0
43	O	520	0	438	20	0
44	T	610	0	133	12	0
45	A1	575	0	447	8	0
45	A3	575	0	420	2	0
45	A4	480	0	376	5	0
45	A6	485	0	399	14	0
45	AA	2411	0	2371	32	0
45	AB	2452	0	2461	37	0
45	AF	140	0	113	1	0
45	AG	131	0	94	5	0
45	AH	60	0	59	1	0
45	AJ	42	0	31	1	0
45	AK	126	0	88	12	0
45	AL	143	0	119	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B1	519	0	402	8	0
45	B2	442	0	366	15	0
45	B3	578	0	422	6	0
45	B5	476	0	368	4	0
45	BA	2446	0	2387	39	0
45	BB	2422	0	2404	50	0
45	BF	138	0	110	1	0
45	BG	87	0	64	48	0
45	BH	60	0	59	0	0
45	BJ	42	0	31	0	0
45	BK	127	0	88	7	0
45	BL	148	0	125	11	0
46	AA	33	0	46	3	0
46	AB	33	0	46	2	0
46	BA	33	0	46	3	0
46	BB	33	0	46	2	0
47	A1	123	0	162	0	0
47	A3	59	0	58	1	0
47	A6	36	0	42	0	0
47	AA	49	0	74	1	0
47	AJ	40	0	53	0	0
47	B1	116	0	145	1	0
47	B2	35	0	40	2	0
47	B3	23	0	16	1	0
47	B5	30	0	30	0	0
47	BA	76	0	98	3	0
47	BF	45	0	63	1	0
47	F	37	0	44	3	0
47	a	29	0	28	2	0
48	A1	40	0	56	3	0
48	A3	40	0	56	2	0
48	A4	40	0	56	0	0
48	A6	40	0	56	3	0
48	AA	240	0	336	6	0
48	AB	240	0	336	9	0
48	AF	80	0	112	6	0
48	AG	40	0	56	1	0
48	AI	80	0	112	3	0
48	AJ	80	0	112	5	0
48	AK	40	0	56	2	0
48	AL	80	0	112	1	0
48	B2	40	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	B3	40	0	56	4	0
48	B5	40	0	56	0	0
48	BA	280	0	392	13	0
48	BB	240	0	336	13	0
48	BF	40	0	56	1	0
48	BG	40	0	56	13	0
48	BI	40	0	56	1	0
48	BJ	80	0	112	9	0
48	BK	40	0	56	0	0
48	BL	120	0	167	6	0
49	AA	8	0	0	0	0
49	AC	16	0	0	4	0
49	BA	8	0	0	1	0
49	BC	16	0	0	7	0
49	I	16	0	0	4	0
49	K	8	0	0	1	0
50	AA	35	0	46	0	0
50	AB	105	0	138	0	0
50	AL	34	0	41	1	0
50	BA	67	0	80	0	0
50	BB	35	0	46	0	0
51	AB	66	0	96	0	0
51	BB	66	0	96	1	0
52	A1	42	0	56	1	0
52	A3	42	0	56	1	0
52	A4	42	0	56	4	0
52	A6	42	0	56	4	0
52	AF	42	0	56	2	0
52	B1	42	0	56	3	0
52	B2	42	0	56	0	0
52	B3	42	0	56	3	0
52	B5	42	0	56	0	0
53	A1	44	0	58	1	0
53	A4	39	0	48	4	0
53	AG	38	0	46	0	0
53	B5	33	0	36	0	0
54	A1	92	0	60	3	0
54	A3	45	0	30	0	0
54	A4	169	0	100	2	0
54	A6	187	0	127	2	0
54	B1	91	0	58	2	0
54	B2	227	0	154	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B3	45	0	30	1	0
54	B5	126	0	67	0	0
55	A1	44	0	56	1	0
55	A3	44	0	56	2	0
55	A4	44	0	56	2	0
55	A6	44	0	56	4	0
55	B1	44	0	56	0	0
55	B2	44	0	56	6	0
55	B3	44	0	56	1	0
55	B5	44	0	56	1	0
56	BJ	47	0	61	6	0
56	e	34	0	32	1	0
57	c	4	0	0	2	0
All	All	112687	0	110283	2142	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 10.

The worst 5 of 2142 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)
40:L:149:LEU:HD21	40:L:152:ARG:CD	1.39	1.52
18:B5:175:GLU:CB	26:a:229:VAL:HG12	1.46	1.45
8:BH:100:ARG:NH1	12:BL:155:ILE:HA	1.35	1.35
2:AB:87:ILE:HG23	2:AB:113:VAL:CG1	1.58	1.33
8:AH:71:TRP:CD1	12:AL:169:LEU:HD11	1.65	1.30

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	AA	740/750 (99%)	686 (93%)	53 (7%)	1 (0%)	48 80
1	BA	740/750 (99%)	692 (94%)	48 (6%)	0	100 100
2	AB	732/734 (100%)	695 (95%)	37 (5%)	0	100 100
2	BB	731/734 (100%)	696 (95%)	35 (5%)	0	100 100
3	AC	78/81 (96%)	72 (92%)	6 (8%)	0	100 100
3	BC	78/81 (96%)	73 (94%)	5 (6%)	0	100 100
4	AD	139/204 (68%)	126 (91%)	13 (9%)	0	100 100
4	BD	141/204 (69%)	121 (86%)	18 (13%)	2 (1%)	9 38
5	AE	65/143 (46%)	58 (89%)	7 (11%)	0	100 100
5	BE	67/143 (47%)	61 (91%)	6 (9%)	0	100 100
6	AF	151/221 (68%)	144 (95%)	7 (5%)	0	100 100
6	BF	152/221 (69%)	149 (98%)	3 (2%)	0	100 100
7	AG	97/160 (61%)	90 (93%)	7 (7%)	0	100 100
7	BG	92/160 (58%)	84 (91%)	8 (9%)	0	100 100
8	AH	93/145 (64%)	89 (96%)	4 (4%)	0	100 100
8	BH	93/145 (64%)	87 (94%)	6 (6%)	0	100 100
9	AI	31/37 (84%)	30 (97%)	1 (3%)	0	100 100
9	BI	31/37 (84%)	29 (94%)	2 (6%)	0	100 100
10	AJ	40/44 (91%)	38 (95%)	2 (5%)	0	100 100
10	BJ	41/44 (93%)	38 (93%)	3 (7%)	0	100 100
11	AK	61/130 (47%)	57 (93%)	4 (7%)	0	100 100
11	BK	60/130 (46%)	53 (88%)	7 (12%)	0	100 100
12	AL	155/219 (71%)	145 (94%)	10 (6%)	0	100 100
12	BL	157/219 (72%)	149 (95%)	8 (5%)	0	100 100
13	A1	194/241 (80%)	178 (92%)	16 (8%)	0	100 100
13	B1	168/241 (70%)	160 (95%)	8 (5%)	0	100 100
14	A3	217/273 (80%)	192 (88%)	25 (12%)	0	100 100
14	B3	219/273 (80%)	206 (94%)	13 (6%)	0	100 100
15	A4	195/251 (78%)	185 (95%)	10 (5%)	0	100 100
16	A6	210/270 (78%)	197 (94%)	13 (6%)	0	100 100
17	B2	206/257 (80%)	191 (93%)	15 (7%)	0	100 100
18	B5	204/256 (80%)	188 (92%)	15 (7%)	1 (0%)	24 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	A	297/360 (82%)	279 (94%)	18 (6%)	0	100	100
20	B	484/512 (94%)	443 (92%)	40 (8%)	1 (0%)	43	74
21	C	90/120 (75%)	87 (97%)	3 (3%)	0	100	100
22	D	495/506 (98%)	453 (92%)	42 (8%)	0	100	100
23	E	87/101 (86%)	79 (91%)	8 (9%)	0	100	100
24	F	669/746 (90%)	614 (92%)	55 (8%)	0	100	100
25	G	163/176 (93%)	151 (93%)	12 (7%)	0	100	100
26	a	339/461 (74%)	277 (82%)	61 (18%)	1 (0%)	36	69
27	b	301/348 (86%)	267 (89%)	34 (11%)	0	100	100
28	c	126/204 (62%)	109 (86%)	17 (14%)	0	100	100
29	d	91/161 (56%)	78 (86%)	13 (14%)	0	100	100
30	e	148/212 (70%)	122 (82%)	26 (18%)	0	100	100
31	f	151/238 (63%)	132 (87%)	18 (12%)	1 (1%)	18	53
32	g	113/190 (60%)	113 (100%)	0	0	100	100
33	h	143/220 (65%)	130 (91%)	13 (9%)	0	100	100
34	i	143/217 (66%)	125 (87%)	18 (13%)	0	100	100
35	j	171/255 (67%)	150 (88%)	21 (12%)	0	100	100
36	H	350/393 (89%)	315 (90%)	35 (10%)	0	100	100
37	I	156/172 (91%)	132 (85%)	22 (14%)	2 (1%)	9	40
38	J	153/158 (97%)	134 (88%)	19 (12%)	0	100	100
39	K	161/225 (72%)	137 (85%)	23 (14%)	1 (1%)	21	55
40	L	75/191 (39%)	67 (89%)	8 (11%)	0	100	100
41	M	106/217 (49%)	94 (89%)	12 (11%)	0	100	100
42	N	144/209 (69%)	128 (89%)	15 (10%)	1 (1%)	18	53
43	O	69/158 (44%)	62 (90%)	7 (10%)	0	100	100
All	All	11603/14548 (80%)	10637 (92%)	955 (8%)	11 (0%)	49	80

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	164	ASP
39	K	140	PRO
26	a	230	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	N	166	LYS
18	B5	49	TRP

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	AA	600/610 (98%)	590 (98%)	10 (2%)	53 68
1	BA	601/610 (98%)	593 (99%)	8 (1%)	61 71
2	AB	598/600 (100%)	594 (99%)	4 (1%)	76 78
2	BB	597/600 (100%)	590 (99%)	7 (1%)	63 72
3	AC	70/71 (99%)	70 (100%)	0	100 100
3	BC	70/71 (99%)	70 (100%)	0	100 100
4	AD	120/170 (71%)	118 (98%)	2 (2%)	53 68
4	BD	121/170 (71%)	119 (98%)	2 (2%)	53 68
5	AE	56/114 (49%)	56 (100%)	0	100 100
5	BE	58/114 (51%)	58 (100%)	0	100 100
6	AF	125/185 (68%)	124 (99%)	1 (1%)	73 77
6	BF	126/185 (68%)	123 (98%)	3 (2%)	43 63
7	AG	83/133 (62%)	80 (96%)	3 (4%)	31 54
7	BG	79/133 (59%)	76 (96%)	3 (4%)	29 52
8	AH	77/113 (68%)	76 (99%)	1 (1%)	61 71
8	BH	77/113 (68%)	75 (97%)	2 (3%)	40 60
9	AI	29/33 (88%)	29 (100%)	0	100 100
9	BI	29/33 (88%)	29 (100%)	0	100 100
10	AJ	37/39 (95%)	37 (100%)	0	100 100
10	BJ	38/39 (97%)	37 (97%)	1 (3%)	40 60
11	AK	47/95 (50%)	47 (100%)	0	100 100
11	BK	46/95 (48%)	45 (98%)	1 (2%)	45 64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	119/174 (68%)	119 (100%)	0	100	100
12	BL	120/174 (69%)	118 (98%)	2 (2%)	53	68
13	A1	151/190 (80%)	147 (97%)	4 (3%)	40	60
13	B1	138/190 (73%)	137 (99%)	1 (1%)	76	78
14	A3	168/211 (80%)	167 (99%)	1 (1%)	78	80
14	B3	170/211 (81%)	170 (100%)	0	100	100
15	A4	164/210 (78%)	163 (99%)	1 (1%)	78	80
16	A6	177/226 (78%)	172 (97%)	5 (3%)	38	59
17	B2	165/205 (80%)	164 (99%)	1 (1%)	78	80
18	B5	166/205 (81%)	162 (98%)	4 (2%)	43	63
19	A	258/312 (83%)	256 (99%)	2 (1%)	73	77
20	B	420/446 (94%)	419 (100%)	1 (0%)	87	87
21	C	78/103 (76%)	78 (100%)	0	100	100
22	D	430/439 (98%)	428 (100%)	2 (0%)	81	82
23	E	75/87 (86%)	75 (100%)	0	100	100
24	F	561/661 (85%)	559 (100%)	2 (0%)	84	83
25	G	145/154 (94%)	145 (100%)	0	100	100
26	a	288/397 (72%)	288 (100%)	0	100	100
27	b	263/297 (89%)	262 (100%)	1 (0%)	84	83
28	c	112/177 (63%)	111 (99%)	1 (1%)	70	75
29	d	81/143 (57%)	81 (100%)	0	100	100
30	e	125/178 (70%)	125 (100%)	0	100	100
31	f	134/207 (65%)	133 (99%)	1 (1%)	76	78
32	g	104/172 (60%)	104 (100%)	0	100	100
33	h	127/192 (66%)	126 (99%)	1 (1%)	73	77
34	i	114/180 (63%)	114 (100%)	0	100	100
35	j	143/219 (65%)	141 (99%)	2 (1%)	59	71
36	H	291/342 (85%)	290 (100%)	1 (0%)	86	85
37	I	132/159 (83%)	130 (98%)	2 (2%)	57	70
38	J	87/140 (62%)	84 (97%)	3 (3%)	32	55
39	K	114/205 (56%)	112 (98%)	2 (2%)	51	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	L	66/171 (39%)	66 (100%)	0	100 100
41	M	58/195 (30%)	56 (97%)	2 (3%)	32 55
42	N	49/174 (28%)	48 (98%)	1 (2%)	48 65
43	O	36/138 (26%)	36 (100%)	0	100 100
All	All	9513/12210 (78%)	9422 (99%)	91 (1%)	65 75

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	BJ	38	THR
22	D	470	LEU
12	BL	137	LEU
18	B5	174	LEU
28	c	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
20	B	465	HIS
25	G	56	HIS
35	j	249	GLN
22	D	248	HIS
24	F	62	GLN

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)

423 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	$\#\|Z\| > 2$
45	CLA	B1	313	13	49,53,73	1.47	7 (14%)	59,89,113	1.35	3 (5%)
45	CLA	BA	808	1	69,73,73	1.23	7 (10%)	83,113,113	1.15	6 (7%)
45	CLA	A3	305	-	44,49,73	1.54	8 (18%)	52,84,113	1.30	5 (9%)
45	CLA	BB	807	2	69,73,73	1.27	8 (11%)	83,113,113	1.21	7 (8%)
45	CLA	BA	840	1	69,73,73	1.22	7 (10%)	83,113,113	1.23	6 (7%)
56	SQD	BJ	104	-	46,47,54	1.28	5 (10%)	55,58,65	4.16	12 (21%)
48	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
45	CLA	A6	613	16	68,72,73	1.27	8 (11%)	81,111,113	1.12	5 (6%)
45	CLA	BL	302	12	49,53,73	1.48	7 (14%)	59,89,113	1.50	10 (16%)
45	CLA	AL	303	12	45,49,73	1.53	7 (15%)	54,84,113	1.29	7 (12%)
54	CHL	B5	606	-	44,48,74	2.36	17 (38%)	56,83,114	2.88	28 (50%)
48	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)
45	CLA	B3	304	-	44,49,73	1.55	7 (15%)	52,84,113	1.30	4 (7%)
45	CLA	BA	839	1	55,59,73	1.40	7 (12%)	66,96,113	1.33	8 (12%)
45	CLA	BA	803	1	69,73,73	1.21	8 (11%)	83,113,113	1.25	7 (8%)
45	CLA	A1	311	13	63,67,73	1.32	8 (12%)	76,106,113	1.12	5 (6%)
45	CLA	BG	201	-	46,50,73	1.48	7 (15%)	55,85,113	1.21	5 (9%)
45	CLA	BA	823	1	45,49,73	1.51	6 (13%)	54,84,113	1.33	7 (12%)
48	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)
45	CLA	AA	838	1	59,63,73	1.32	9 (15%)	71,101,113	1.22	10 (14%)
45	CLA	AB	810	2	69,73,73	1.25	10 (14%)	83,113,113	1.25	4 (4%)
45	CLA	A4	303	-	47,51,73	1.56	9 (19%)	60,87,113	1.39	8 (13%)
54	CHL	B2	606	-	47,51,74	2.38	19 (40%)	52,86,114	2.72	22 (42%)
47	LHG	A6	618	45	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
45	CLA	AB	833	2	69,73,73	1.24	7 (10%)	83,113,113	1.18	8 (9%)
47	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	BG	203	-	41,41,41	0.91	2 (4%)	56,56,56	6.99	26 (46%)
45	CLA	A3	313	14	43,48,73	1.55	8 (18%)	51,83,113	1.31	8 (15%)
45	CLA	AJ	102	10	46,50,73	1.49	6 (13%)	55,85,113	1.30	4 (7%)
45	CLA	BA	844	47	45,49,73	1.52	6 (13%)	54,84,113	1.25	7 (12%)
45	CLA	BB	813	2	58,62,73	1.41	9 (15%)	73,100,113	1.34	9 (12%)
49	SF4	BC	102	3	0,12,12	-	-	-		
45	CLA	AB	813	2	47,51,73	1.46	8 (17%)	56,86,113	1.28	6 (10%)
45	CLA	BA	825	-	69,73,73	1.25	9 (13%)	83,113,113	1.21	5 (6%)
52	LUT	B2	615	-	42,43,43	0.81	0	51,60,60	1.98	15 (29%)
45	CLA	BB	831	2	60,64,73	1.37	9 (15%)	72,102,113	1.22	3 (4%)
45	CLA	AB	826	-	66,70,73	1.27	8 (12%)	79,109,113	1.21	6 (7%)
45	CLA	BA	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.22	6 (7%)
48	BCR	BB	848	-	41,41,41	0.81	0	56,56,56	2.15	19 (33%)
48	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
53	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
45	CLA	BB	823	2	49,54,73	1.45	6 (12%)	58,90,113	1.17	5 (8%)
45	CLA	BB	840	2	51,55,73	1.42	7 (13%)	61,91,113	1.31	6 (9%)
47	LHG	F	801	-	36,36,48	0.73	1 (2%)	39,42,54	1.22	3 (7%)
48	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
45	CLA	AB	807	2	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
52	LUT	B1	316	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	10 (19%)
45	CLA	A3	314	-	41,44,73	1.58	9 (21%)	49,77,113	1.25	5 (10%)
45	CLA	B3	313	-	41,44,73	1.57	8 (19%)	49,77,113	1.22	5 (10%)
53	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
48	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.37	21 (37%)
45	CLA	BA	837	1	55,59,73	1.38	10 (18%)	66,96,113	1.31	5 (7%)
55	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
48	BCR	BA	850	-	41,41,41	0.78	0	56,56,56	2.09	11 (19%)
45	CLA	AA	812	1	58,62,73	1.37	9 (15%)	69,99,113	1.36	5 (7%)
45	CLA	B3	305	-	45,49,73	1.56	8 (17%)	57,84,113	1.49	8 (14%)
45	CLA	AA	841	1	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
49	SF4	AA	850	1,2	0,12,12	-	-	-		
45	CLA	AB	842	47	69,73,73	1.24	9 (13%)	83,113,113	1.30	9 (10%)
45	CLA	AB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.57	13 (15%)
55	XAT	B1	317	-	39,47,47	0.93	2 (5%)	54,74,74	2.43	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AA	820	1	49,53,73	1.47	9 (18%)	59,89,113	1.32	4 (6%)
45	CLA	BA	809	1	54,58,73	1.42	9 (16%)	65,95,113	1.34	8 (12%)
45	CLA	B5	612	18	61,65,73	1.33	8 (13%)	73,103,113	1.14	4 (5%)
48	BCR	BL	301	-	41,41,41	0.87	1 (2%)	56,56,56	2.36	14 (25%)
45	CLA	B3	307	14	49,53,73	1.47	7 (14%)	59,89,113	1.29	6 (10%)
49	SF4	AC	102	3	0,12,12	-	-	-		
48	BCR	BJ	101	-	41,41,41	0.89	0	56,56,56	1.70	14 (25%)
45	CLA	A1	314	13	67,72,73	1.26	7 (10%)	80,112,113	1.17	6 (7%)
54	CHL	A6	606	-	46,50,74	2.33	19 (41%)	52,85,114	2.83	25 (48%)
45	CLA	AA	817	1	64,68,73	1.29	7 (10%)	77,107,113	1.24	8 (10%)
48	BCR	B3	317	-	41,41,41	0.84	0	56,56,56	3.61	28 (50%)
45	CLA	BB	830	2	69,73,73	1.27	9 (13%)	83,113,113	1.17	9 (10%)
45	CLA	AB	806	2	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
45	CLA	B2	612	17	69,73,73	1.26	7 (10%)	83,113,113	1.14	6 (7%)
45	CLA	AA	837	1	55,59,73	1.38	8 (14%)	66,96,113	1.44	9 (13%)
45	CLA	B3	309	47	43,48,73	1.56	6 (13%)	51,83,113	1.20	4 (7%)
52	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)
45	CLA	BB	829	2	69,73,73	1.22	8 (11%)	83,113,113	1.22	5 (6%)
52	LUT	A6	615	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
45	CLA	BB	811	2	69,73,73	1.26	10 (14%)	83,113,113	1.22	8 (9%)
45	CLA	A4	311	15	59,64,73	1.35	7 (11%)	70,102,113	1.20	6 (8%)
47	LHG	B5	618	45	29,29,48	1.17	2 (6%)	32,35,54	1.20	3 (9%)
45	CLA	B2	603	17	47,52,73	1.51	7 (14%)	56,88,113	1.37	5 (8%)
45	CLA	AB	824	2	47,51,73	1.47	10 (21%)	56,86,113	1.46	7 (12%)
49	SF4	I	202	37	0,12,12	-	-	-		
45	CLA	B1	305	13	58,62,73	1.36	7 (12%)	69,99,113	1.41	8 (11%)
45	CLA	B1	312	47	41,46,73	1.63	7 (17%)	52,81,113	1.38	7 (13%)
45	CLA	BB	828	2	66,70,73	1.28	8 (12%)	79,109,113	1.34	9 (11%)
46	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
45	CLA	BA	820	1	49,53,73	1.45	9 (18%)	59,89,113	1.36	4 (6%)
48	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)
45	CLA	BA	818	1	60,64,73	1.34	8 (13%)	72,102,113	1.24	8 (11%)
45	CLA	AA	801	1	69,73,73	1.24	7 (10%)	83,113,113	1.20	6 (7%)
45	CLA	AB	821	2	54,58,73	1.41	9 (16%)	65,95,113	1.34	7 (10%)
45	CLA	AB	816	2	47,51,73	1.47	8 (17%)	56,86,113	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	LHG	A1	320	45	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
45	CLA	A6	601	15	50,54,73	1.44	10 (20%)	60,90,113	1.32	6 (10%)
45	CLA	BA	805	1	69,73,73	1.26	8 (11%)	83,113,113	1.25	6 (7%)
47	LHG	B1	302	-	35,35,48	1.09	2 (5%)	38,41,54	0.99	2 (5%)
53	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.20	4 (9%)
45	CLA	AA	806	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
45	CLA	BB	805	-	69,73,73	1.22	10 (14%)	83,113,113	1.45	10 (12%)
45	CLA	A3	310	47	40,45,73	1.58	7 (17%)	50,79,113	1.29	5 (10%)
45	CLA	A1	315	13	41,46,73	1.64	8 (19%)	52,81,113	1.47	11 (21%)
45	CLA	BA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.10	5 (6%)
45	CLA	B3	308	14	45,49,73	1.50	7 (15%)	54,84,113	1.29	4 (7%)
45	CLA	A6	603	16	69,73,73	1.25	9 (13%)	83,113,113	1.20	8 (9%)
45	CLA	BB	819	2	63,67,73	1.29	8 (12%)	75,105,113	1.29	8 (10%)
45	CLA	AA	836	1	49,53,73	1.50	8 (16%)	59,89,113	1.36	7 (11%)
47	LHG	a	501	-	28,28,48	0.89	1 (3%)	31,34,54	1.24	2 (6%)
55	XAT	B5	615	-	39,47,47	0.99	2 (5%)	54,74,74	2.41	18 (33%)
49	SF4	BC	101	3	0,12,12	-	-	-		
45	CLA	BA	828	1	69,73,73	1.22	7 (10%)	83,113,113	1.31	10 (12%)
56	SQD	e	301	-	33,34,54	1.20	6 (18%)	42,45,65	1.77	10 (23%)
48	BCR	B5	616	-	41,41,41	0.79	0	56,56,56	2.31	23 (41%)
45	CLA	AB	820	-	59,63,73	1.39	8 (13%)	71,101,113	1.20	6 (8%)
45	CLA	AL	305	-	46,50,73	1.50	8 (17%)	55,85,113	1.41	6 (10%)
45	CLA	AA	831	1	51,55,73	1.44	9 (17%)	61,91,113	1.30	5 (8%)
45	CLA	AB	809	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	9 (10%)
45	CLA	AB	827	2	66,70,73	1.27	10 (15%)	79,109,113	1.37	9 (11%)
45	CLA	AB	830	2	60,64,73	1.35	8 (13%)	72,102,113	1.24	4 (5%)
45	CLA	BA	826	-	57,61,73	1.36	8 (14%)	68,98,113	1.27	10 (14%)
45	CLA	AB	823	2	69,73,73	1.23	8 (11%)	83,113,113	1.21	7 (8%)
45	CLA	A6	614	16	47,51,73	1.52	7 (14%)	56,86,113	1.27	4 (7%)
45	CLA	B2	610	47	41,45,73	2.47	10 (24%)	47,76,113	1.42	9 (19%)
45	CLA	AK	201	11	39,43,73	1.72	8 (20%)	50,75,113	1.45	9 (18%)
45	CLA	BB	825	2	49,53,73	1.47	7 (14%)	59,89,113	1.29	7 (11%)
45	CLA	B5	604	-	47,51,73	1.58	9 (19%)	60,87,113	1.34	9 (15%)
45	CLA	AA	803	1	69,73,73	1.23	8 (11%)	83,113,113	1.27	8 (9%)
45	CLA	B1	309	-	47,52,73	1.51	8 (17%)	56,88,113	1.31	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
45	CLA	BB	814	2	47,51,73	1.47	8 (17%)	56,86,113	1.28	5 (8%)
45	CLA	AB	841	2	69,73,73	1.27	9 (13%)	83,113,113	1.15	5 (6%)
48	BCR	BA	856	-	41,41,41	0.93	1 (2%)	56,56,56	2.15	17 (30%)
45	CLA	B1	314	13	64,68,73	1.32	7 (10%)	77,107,113	1.11	7 (9%)
45	CLA	BA	814	1	49,53,73	1.49	9 (18%)	59,89,113	1.35	6 (10%)
45	CLA	A3	304	-	45,50,73	1.60	9 (20%)	57,86,113	1.34	7 (12%)
45	CLA	B1	306	-	45,49,73	1.51	5 (11%)	54,84,113	1.29	4 (7%)
48	BCR	BA	849	-	41,41,41	0.84	0	56,56,56	2.01	18 (32%)
45	CLA	AG	201	-	47,52,73	1.52	8 (17%)	56,88,113	1.29	4 (7%)
45	CLA	A4	301	15	64,68,73	1.28	8 (12%)	77,107,113	1.23	8 (10%)
45	CLA	B5	608	18	48,52,73	1.50	9 (18%)	58,88,113	1.31	6 (10%)
45	CLA	BB	842	2	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
45	CLA	B1	304	13	65,69,73	1.28	8 (12%)	78,108,113	1.28	5 (6%)
45	CLA	BB	839	2	69,73,73	1.23	8 (11%)	83,113,113	1.19	5 (6%)
55	XAT	B2	616	-	39,47,47	1.01	1 (2%)	54,74,74	2.30	20 (37%)
48	BCR	BB	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.19	18 (32%)
45	CLA	BA	813	1	69,73,73	1.25	8 (11%)	83,113,113	1.24	6 (7%)
54	CHL	A6	602	16	55,60,74	2.21	21 (38%)	61,97,114	2.59	31 (50%)
45	CLA	A1	313	13	49,53,73	1.48	9 (18%)	59,89,113	1.39	5 (8%)
45	CLA	A6	610	16	59,63,73	1.35	9 (15%)	71,101,113	1.22	9 (12%)
45	CLA	AK	202	-	49,53,73	1.49	8 (16%)	59,89,113	1.24	4 (6%)
54	CHL	B3	306	-	49,53,74	2.27	20 (40%)	59,89,114	2.66	26 (44%)
45	CLA	BA	816	-	49,53,73	1.48	6 (12%)	59,89,113	1.33	8 (13%)
45	CLA	BA	812	1	58,62,73	1.36	8 (13%)	69,99,113	1.29	6 (8%)
57	FES	c	301	28	0,4,4	-	-	-		
45	CLA	B3	311	14	57,62,73	1.38	8 (14%)	68,100,113	1.14	4 (5%)
45	CLA	A1	305	13	59,63,73	1.34	7 (11%)	71,101,113	1.50	8 (11%)
45	CLA	BB	815	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	10 (12%)
48	BCR	AI	102	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
49	SF4	BA	852	1,2	0,12,12	-	-	-		
54	CHL	A6	608	-	54,58,74	2.22	19 (35%)	65,95,114	2.61	26 (40%)
45	CLA	AB	822	2	51,55,73	1.44	7 (13%)	61,91,113	1.20	4 (6%)
45	CLA	A3	312	14	57,62,73	1.37	8 (14%)	68,100,113	1.28	6 (8%)
50	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	BA	811	1	69,73,73	1.23	8 (11%)	83,113,113	1.17	6 (7%)
45	CLA	B5	610	47	46,50,73	1.49	7 (15%)	55,85,113	1.30	6 (10%)
45	CLA	A3	315	14	43,48,73	1.53	7 (16%)	51,83,113	1.23	5 (9%)
50	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
45	CLA	A3	303	14	59,63,73	1.38	9 (15%)	71,101,113	1.37	9 (12%)
48	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
45	CLA	AA	808	1	69,73,73	1.25	8 (11%)	83,113,113	1.20	6 (7%)
48	BCR	BL	305	-	41,41,41	0.78	0	56,56,56	2.22	20 (35%)
45	CLA	A4	308	15	58,62,73	1.35	9 (15%)	69,99,113	1.17	6 (8%)
45	CLA	AF	803	-	46,50,73	1.52	8 (17%)	55,85,113	1.41	6 (10%)
45	CLA	AB	817	2	59,63,73	1.35	7 (11%)	71,101,113	1.21	5 (7%)
45	CLA	BL	303	12	64,68,73	1.32	7 (10%)	77,107,113	1.25	9 (11%)
55	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)
45	CLA	BA	831	1	51,55,73	1.45	9 (17%)	61,91,113	1.38	10 (16%)
45	CLA	AA	807	1	54,58,73	1.42	9 (16%)	65,95,113	1.27	4 (6%)
47	LHG	A3	319	45	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)
45	CLA	BK	201	11	41,44,73	1.63	8 (19%)	52,77,113	1.47	7 (13%)
45	CLA	AF	804	-	45,49,73	1.52	7 (15%)	54,84,113	1.43	6 (11%)
52	LUT	B3	315	-	42,43,43	0.97	1 (2%)	51,60,60	2.10	17 (33%)
45	CLA	AA	833	1	69,73,73	1.27	8 (11%)	83,113,113	1.31	9 (10%)
45	CLA	B2	608	17	49,53,73	1.47	7 (14%)	59,89,113	1.24	7 (11%)
47	LHG	B1	301	45	37,37,48	1.08	2 (5%)	40,43,54	1.01	3 (7%)
45	CLA	BB	810	2	69,73,73	1.23	9 (13%)	83,113,113	1.23	10 (12%)
48	BCR	AK	204	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
45	CLA	BA	806	1	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
47	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
45	CLA	BF	301	-	59,63,73	1.33	7 (11%)	69,100,113	1.17	5 (7%)
45	CLA	BF	302	-	46,50,73	1.51	8 (17%)	55,85,113	1.41	5 (9%)
48	BCR	BA	848	-	41,41,41	0.80	0	56,56,56	2.03	17 (30%)
54	CHL	A4	306	-	50,54,74	2.30	20 (40%)	56,90,114	2.78	26 (46%)
48	BCR	BA	847	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	11 (19%)
45	CLA	BB	824	2	69,73,73	1.23	8 (11%)	83,113,113	1.22	8 (9%)
45	CLA	BB	822	2	45,49,73	1.49	8 (17%)	54,84,113	1.41	4 (7%)
45	CLA	BJ	102	10	46,50,73	1.50	7 (15%)	55,85,113	1.29	4 (7%)
45	CLA	BB	838	2	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	BF	304	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	19 (33%)
45	CLA	BA	822	1	46,50,73	1.49	6 (13%)	55,85,113	1.33	5 (9%)
45	CLA	AA	815	1	44,49,73	1.42	6 (13%)	51,83,113	1.45	7 (13%)
45	CLA	AB	814	2	69,73,73	1.26	11 (15%)	83,113,113	1.23	6 (7%)
45	CLA	AB	818	2	63,67,73	1.30	8 (12%)	75,105,113	1.24	9 (12%)
45	CLA	AB	840	-	69,73,73	1.27	9 (13%)	83,113,113	1.14	6 (7%)
45	CLA	BB	801	2	69,73,73	1.24	9 (13%)	83,113,113	1.37	11 (13%)
45	CLA	AB	801	2	69,73,73	1.24	8 (11%)	83,113,113	1.49	12 (14%)
54	CHL	B5	607	-	49,53,74	2.34	21 (42%)	56,89,114	2.76	24 (42%)
45	CLA	AB	836	-	46,50,73	1.51	7 (15%)	55,85,113	1.36	6 (10%)
45	CLA	AA	839	1	56,60,73	1.38	8 (14%)	67,97,113	1.29	6 (8%)
47	LHG	BA	845	-	48,48,48	0.88	2 (4%)	51,54,54	0.97	3 (5%)
45	CLA	AB	831	2	47,51,73	1.49	10 (21%)	56,86,113	1.23	7 (12%)
51	DGD	BB	850	-	67,67,67	0.81	2 (2%)	81,81,81	0.98	4 (4%)
45	CLA	AL	304	12	64,68,73	1.32	8 (12%)	77,107,113	1.28	9 (11%)
45	CLA	BA	827	1	69,73,73	1.24	7 (10%)	83,113,113	1.14	5 (6%)
45	CLA	A4	302	15	48,52,73	1.56	9 (18%)	61,88,113	1.46	8 (13%)
47	LHG	B3	318	45	22,22,48	1.49	2 (9%)	25,28,54	1.38	2 (8%)
45	CLA	A4	313	15	54,58,73	1.42	8 (14%)	65,95,113	1.35	7 (10%)
48	BCR	BB	847	-	41,41,41	0.87	1 (2%)	56,56,56	1.93	11 (19%)
45	CLA	BB	809	2	56,60,73	1.39	8 (14%)	67,97,113	1.25	7 (10%)
45	CLA	AB	832	2	69,73,73	1.24	8 (11%)	83,113,113	1.22	7 (8%)
45	CLA	B5	602	18	64,68,73	1.34	10 (15%)	77,107,113	1.22	5 (6%)
49	SF4	AC	101	3	0,12,12	-	-	-		
48	BCR	BB	849	-	41,41,41	0.90	1 (2%)	56,56,56	1.86	16 (28%)
45	CLA	A3	302	14	64,68,73	1.30	8 (12%)	77,107,113	1.16	8 (10%)
45	CLA	B3	302	14	59,63,73	1.35	8 (13%)	71,101,113	1.27	7 (9%)
45	CLA	BB	826	-	69,73,73	1.27	11 (15%)	83,113,113	1.17	5 (6%)
45	CLA	AA	821	-	69,73,73	1.25	10 (14%)	83,113,113	1.24	10 (12%)
50	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
45	CLA	BA	824	1	59,63,73	1.36	8 (13%)	71,101,113	1.27	6 (8%)
45	CLA	A1	309	-	47,52,73	1.52	8 (17%)	56,88,113	1.27	8 (14%)
45	CLA	BL	304	-	47,51,73	1.46	6 (12%)	56,86,113	1.32	7 (12%)
45	CLA	BB	841	-	69,73,73	1.24	9 (13%)	83,113,113	1.20	8 (9%)
45	CLA	A6	605	-	47,51,73	1.49	8 (17%)	55,86,113	1.23	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AB	835	2	64,68,73	1.28	7 (10%)	77,107,113	1.24	7 (9%)
54	CHL	B1	303	13	53,58,74	2.21	21 (39%)	59,95,114	2.61	27 (45%)
45	CLA	AB	837	2	54,58,73	1.43	11 (20%)	65,95,113	1.35	7 (10%)
45	CLA	B3	314	14	43,48,73	1.53	7 (16%)	51,83,113	1.24	6 (11%)
45	CLA	BA	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	10 (12%)
45	CLA	A3	308	14	49,53,73	1.48	8 (16%)	59,89,113	1.27	6 (10%)
45	CLA	BB	820	2	64,68,73	1.28	8 (12%)	77,107,113	1.48	9 (11%)
45	CLA	AB	808	2	55,59,73	1.39	8 (14%)	65,95,113	1.33	7 (10%)
45	CLA	AA	829	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	11 (13%)
54	CHL	A6	607	-	47,51,74	2.32	19 (40%)	52,86,114	2.78	24 (46%)
49	SF4	I	201	37	0,12,12	-	-	-		
50	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
45	CLA	B2	602	17	69,73,73	1.25	9 (13%)	83,113,113	1.20	10 (12%)
45	CLA	AG	203	7	46,50,73	1.50	8 (17%)	55,85,113	1.29	5 (9%)
48	BCR	AA	852	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
45	CLA	A4	310	15	44,49,73	1.53	9 (20%)	52,84,113	1.33	7 (13%)
48	BCR	BB	803	-	41,41,41	0.85	0	56,56,56	1.99	19 (33%)
46	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
45	CLA	A1	307	-	43,48,73	1.54	8 (18%)	52,82,113	1.59	9 (17%)
45	CLA	AB	803	2	69,73,73	1.24	9 (13%)	83,113,113	1.14	6 (7%)
50	LMU	BA	854	-	34,34,36	1.18	2 (5%)	45,45,47	0.91	2 (4%)
55	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
45	CLA	B5	611	18	44,49,73	1.52	8 (18%)	52,84,113	1.31	4 (7%)
45	CLA	B3	303	-	45,50,73	1.60	8 (17%)	57,86,113	1.35	7 (12%)
45	CLA	BK	202	-	49,53,73	1.47	6 (12%)	59,89,113	1.34	6 (10%)
45	CLA	A6	609	16	49,53,73	1.48	8 (16%)	59,89,113	1.25	7 (11%)
55	XAT	B3	316	-	39,47,47	0.97	1 (2%)	54,74,74	2.48	21 (38%)
45	CLA	BB	812	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	8 (9%)
45	CLA	BB	808	2	69,73,73	1.25	9 (13%)	83,113,113	1.24	5 (6%)
48	BCR	BI	101	-	41,41,41	0.92	2 (4%)	56,56,56	2.15	21 (37%)
54	CHL	B5	605	-	44,49,74	2.38	20 (45%)	49,84,114	2.72	23 (46%)
54	CHL	B2	614	17	47,51,74	2.31	19 (40%)	52,86,114	2.80	24 (46%)
45	CLA	BA	815	1	46,50,73	1.47	7 (15%)	55,85,113	1.40	5 (9%)
45	CLA	AA	828	1	69,73,73	1.25	8 (11%)	83,113,113	1.35	8 (9%)
45	CLA	BB	818	2	59,63,73	1.33	6 (10%)	71,101,113	1.25	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	BK	204	-	41,41,41	0.88	1 (2%)	56,56,56	2.14	21 (37%)
45	CLA	AA	834	1	69,73,73	1.24	8 (11%)	83,113,113	1.38	12 (14%)
48	BCR	B2	617	-	41,41,41	0.89	1 (2%)	56,56,56	2.47	23 (41%)
48	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
45	CLA	AA	830	1	69,73,73	1.28	8 (11%)	83,113,113	1.18	5 (6%)
48	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
45	CLA	BA	841	1	69,73,73	1.23	9 (13%)	83,113,113	1.40	10 (12%)
45	CLA	B2	611	17	48,52,73	1.51	7 (14%)	58,88,113	1.27	6 (10%)
48	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
45	CLA	A3	306	14	45,49,73	1.57	9 (20%)	57,84,113	1.45	8 (14%)
45	CLA	B3	312	14	43,48,73	1.55	7 (16%)	51,83,113	1.25	7 (13%)
45	CLA	AA	823	1	45,49,73	1.56	8 (17%)	54,84,113	1.31	8 (14%)
45	CLA	AB	838	2	69,73,73	1.22	10 (14%)	83,113,113	1.23	7 (8%)
47	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
54	CHL	B1	308	-	44,49,74	2.51	22 (50%)	48,84,114	2.71	22 (45%)
45	CLA	BA	802	-	69,73,73	1.27	9 (13%)	83,113,113	1.19	6 (7%)
55	XAT	A6	616	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
45	CLA	BB	817	2	45,50,73	1.48	7 (15%)	53,85,113	1.28	4 (7%)
54	CHL	B2	605	-	46,50,74	2.35	20 (43%)	52,85,114	2.80	24 (46%)
45	CLA	AA	802	-	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
45	CLA	BB	832	2	47,51,73	1.49	8 (17%)	56,86,113	1.23	6 (10%)
47	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)
45	CLA	BB	833	2	47,51,73	1.47	8 (17%)	56,86,113	1.43	7 (12%)
45	CLA	BB	802	-	69,73,73	1.28	10 (14%)	83,113,113	1.34	8 (9%)
45	CLA	AA	805	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	9 (10%)
45	CLA	BG	202	7	49,53,73	1.50	7 (14%)	59,89,113	1.45	7 (11%)
45	CLA	AB	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.49	12 (15%)
50	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
45	CLA	BB	843	47	69,73,73	1.27	10 (14%)	83,113,113	1.19	6 (7%)
45	CLA	B3	310	14	47,51,73	1.48	5 (10%)	56,86,113	1.27	5 (8%)
51	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)
54	CHL	B2	607	-	50,54,74	2.31	20 (40%)	56,90,114	2.77	25 (44%)
45	CLA	AA	827	1	69,73,73	1.25	8 (11%)	83,113,113	1.23	6 (7%)
54	CHL	A4	304	-	44,49,74	2.40	21 (47%)	49,84,114	2.73	24 (48%)
54	CHL	A3	307	-	49,53,74	2.27	19 (38%)	59,89,114	2.64	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
48	BCR	BL	306	-	41,41,41	0.88	1 (2%)	56,56,56	11.27	26 (46%)
52	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)
48	BCR	BB	846	-	41,41,41	0.85	1 (2%)	56,56,56	2.14	19 (33%)
48	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
45	CLA	B1	310	13	42,47,73	1.62	8 (19%)	53,82,113	1.34	8 (15%)
45	CLA	BA	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.39	10 (12%)
45	CLA	BA	836	1	49,53,73	1.47	6 (12%)	59,89,113	1.40	7 (11%)
45	CLA	AA	813	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
45	CLA	A6	612	16	48,52,73	1.50	8 (16%)	58,88,113	1.24	4 (6%)
45	CLA	AG	204	7	49,53,73	1.50	8 (16%)	59,89,113	1.33	5 (8%)
45	CLA	B5	613	18	49,53,73	1.48	8 (16%)	59,89,113	1.24	7 (11%)
52	LUT	B5	614	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	15 (29%)
45	CLA	AB	812	2	58,62,73	1.41	9 (15%)	73,100,113	1.37	10 (13%)
45	CLA	A4	307	15	49,53,73	1.50	8 (16%)	59,89,113	1.24	6 (10%)
45	CLA	AA	822	1	46,50,73	1.50	7 (15%)	55,85,113	1.31	5 (9%)
48	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
45	CLA	AB	825	-	69,73,73	1.27	11 (15%)	83,113,113	1.24	7 (8%)
45	CLA	BA	835	1	49,53,73	1.48	6 (12%)	59,89,113	1.26	3 (5%)
45	CLA	A1	306	-	53,57,73	1.41	8 (15%)	62,93,113	1.28	5 (8%)
45	CLA	AB	815	2	69,73,73	1.22	10 (14%)	83,113,113	1.27	10 (12%)
52	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
45	CLA	A4	312	15	49,53,73	1.48	8 (16%)	59,89,113	1.27	6 (10%)
45	CLA	B2	613	17	47,51,73	1.47	7 (14%)	56,86,113	1.27	8 (14%)
45	CLA	B2	604	-	47,51,73	1.50	8 (17%)	55,86,113	1.23	7 (12%)
45	CLA	AA	825	-	69,73,73	1.27	9 (13%)	83,113,113	1.18	5 (6%)
45	CLA	AA	810	1	69,72,73	1.29	9 (13%)	78,111,113	1.19	5 (6%)
45	CLA	BB	816	2	68,72,73	1.25	9 (13%)	82,112,113	1.23	9 (10%)
47	LHG	B1	318	45	41,41,48	1.01	2 (4%)	44,47,54	0.95	2 (4%)
45	CLA	AA	819	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
49	SF4	K	301	39	0,12,12	-	-	-		
45	CLA	A1	304	13	64,68,73	1.28	8 (12%)	76,106,113	1.21	6 (7%)
45	CLA	BB	821	-	59,63,73	1.36	9 (15%)	71,101,113	1.10	6 (8%)
45	CLA	BB	806	2	45,49,73	1.48	8 (17%)	54,84,113	1.35	6 (11%)
45	CLA	BB	836	2	64,68,73	1.29	7 (10%)	77,107,113	1.28	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	A6	604	16	45,50,73	1.55	8 (17%)	53,85,113	1.44	5 (9%)
45	CLA	A3	311	14	47,51,73	1.49	6 (12%)	56,86,113	1.31	4 (7%)
45	CLA	A4	309	-	46,50,73	1.46	6 (13%)	55,85,113	1.33	4 (7%)
45	CLA	AA	826	-	63,67,73	1.32	10 (15%)	75,105,113	1.16	6 (8%)
45	CLA	B1	311	13	63,67,73	1.30	7 (11%)	76,106,113	1.12	6 (7%)
45	CLA	AA	842	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	9 (10%)
45	CLA	B5	603	18	48,52,73	1.57	8 (16%)	61,88,113	1.41	6 (9%)
48	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
45	CLA	A6	611	47	41,45,73	2.52	9 (21%)	47,76,113	1.49	9 (19%)
45	CLA	AA	809	1	54,58,73	1.45	9 (16%)	65,95,113	1.35	10 (15%)
47	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.09	3 (6%)
45	CLA	B1	315	13	41,46,73	1.65	9 (21%)	52,81,113	1.41	10 (19%)
45	CLA	AF	802	-	61,65,73	1.33	10 (16%)	73,103,113	1.30	7 (9%)
45	CLA	A3	309	14	45,49,73	1.53	8 (17%)	54,84,113	1.33	9 (16%)
45	CLA	BB	835	2	69,73,73	1.25	8 (11%)	83,113,113	1.10	5 (6%)
45	CLA	BB	837	-	46,50,73	1.51	6 (13%)	55,85,113	1.32	5 (9%)
45	CLA	BA	801	1	69,73,73	1.25	7 (10%)	83,113,113	1.15	5 (6%)
48	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
45	CLA	AB	839	2	51,55,73	1.43	7 (13%)	61,91,113	1.42	6 (9%)
45	CLA	BA	838	1	59,62,73	1.40	8 (13%)	66,99,113	1.35	10 (15%)
54	CHL	B2	601	17	57,61,74	2.19	21 (36%)	64,98,114	2.64	30 (46%)
45	CLA	A1	316	13	47,51,73	1.59	8 (17%)	60,87,113	1.44	7 (11%)
45	CLA	AB	802	-	68,72,73	1.35	9 (13%)	85,112,113	1.26	9 (10%)
45	CLA	BA	832	1	60,64,73	1.33	7 (11%)	72,102,113	1.20	6 (8%)
45	CLA	B5	609	18	58,62,73	1.36	9 (15%)	69,99,113	1.17	7 (10%)
45	CLA	BA	807	1	54,58,73	1.42	8 (14%)	65,95,113	1.18	4 (6%)
45	CLA	AA	814	1	49,53,73	1.48	9 (18%)	59,89,113	1.35	7 (11%)
45	CLA	AA	818	1	63,67,73	1.31	9 (14%)	75,105,113	1.26	8 (10%)
45	CLA	BA	810	1	69,73,73	1.24	8 (11%)	83,113,113	1.14	5 (6%)
45	CLA	AB	805	2	45,49,73	1.50	7 (15%)	54,84,113	1.31	6 (11%)
45	CLA	AA	840	1	69,73,73	1.25	9 (13%)	83,113,113	1.25	9 (10%)
45	CLA	B5	601	18	50,54,73	1.44	8 (16%)	60,90,113	1.26	6 (10%)
50	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.89	0
54	CHL	A4	305	-	45,49,74	2.32	17 (37%)	57,84,114	2.85	28 (49%)
45	CLA	AA	804	1	56,60,73	1.37	9 (16%)	67,97,113	1.37	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	B1	307	-	43,48,73	1.57	6 (13%)	52,82,113	1.37	6 (11%)
47	LHG	BA	846	45	26,26,48	1.06	2 (7%)	29,32,54	1.00	1 (3%)
52	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
48	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
54	CHL	A1	308	13	44,49,74	2.46	21 (47%)	48,84,114	2.80	23 (47%)
45	CLA	BH	201	-	64,68,73	1.31	7 (10%)	77,107,113	1.22	7 (9%)
48	BCR	AL	302	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
45	CLA	BA	829	1	69,73,73	1.27	10 (14%)	83,113,113	1.24	9 (10%)
50	LMU	BA	853	-	35,35,36	1.15	2 (5%)	46,46,47	0.93	0
48	BCR	A6	617	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
45	CLA	AA	816	-	49,53,73	1.49	8 (16%)	59,89,113	1.39	6 (10%)
45	CLA	AH	201	8	64,68,73	1.30	7 (10%)	77,107,113	1.26	8 (10%)
48	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
45	CLA	AA	824	1	57,62,73	1.38	8 (14%)	68,100,113	1.36	9 (13%)
45	CLA	AB	828	2	69,73,73	1.23	9 (13%)	83,113,113	1.29	6 (7%)
48	BCR	BA	851	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	20 (35%)
46	PQN	BA	843	-	34,34,34	3.47	12 (35%)	42,45,45	1.62	5 (11%)
45	CLA	AA	832	1	60,64,73	1.33	6 (10%)	72,102,113	1.26	8 (11%)
45	CLA	AB	834	2	69,73,73	1.23	8 (11%)	83,113,113	1.12	6 (7%)
54	CHL	A4	314	15	44,49,74	2.32	18 (40%)	51,84,114	2.88	25 (49%)
45	CLA	AB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.23	11 (13%)
45	CLA	AB	811	2	69,73,73	1.26	9 (13%)	83,113,113	1.37	8 (9%)
48	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
45	CLA	BF	303	-	45,49,73	1.51	5 (11%)	54,84,113	1.30	5 (9%)
46	PQN	BB	844	-	34,34,34	3.42	10 (29%)	42,45,45	1.66	8 (19%)
45	CLA	AA	811	1	69,73,73	1.24	7 (10%)	83,113,113	1.20	5 (6%)
45	CLA	BK	203	-	50,54,73	1.43	6 (12%)	60,90,113	1.35	6 (10%)
47	LHG	A1	301	45	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)
45	CLA	BA	817	1	64,68,73	1.27	6 (9%)	77,107,113	1.25	8 (10%)
48	BCR	BA	855	-	41,41,41	0.77	0	56,56,56	2.19	24 (42%)
45	CLA	AK	203	11	50,54,73	1.45	7 (14%)	60,90,113	1.34	4 (6%)
45	CLA	A1	310	13	44,48,73	1.59	7 (15%)	56,83,113	1.46	9 (16%)
45	CLA	B3	301	14	64,68,73	1.30	9 (14%)	77,107,113	1.12	6 (7%)
54	CHL	A1	303	13	54,59,74	2.23	19 (35%)	60,96,114	2.66	29 (48%)
45	CLA	BA	833	1	69,73,73	1.27	8 (11%)	83,113,113	1.24	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AA	835	1	47,52,73	1.51	7 (14%)	56,88,113	1.30	5 (8%)
45	CLA	BB	804	2	69,73,73	1.24	8 (11%)	83,113,113	1.20	6 (7%)
45	CLA	B2	609	17	59,63,73	1.35	8 (13%)	71,101,113	1.22	9 (12%)
45	CLA	BA	842	-	69,73,73	1.26	8 (11%)	83,113,113	1.21	7 (8%)
45	CLA	BA	804	1	56,60,73	1.38	9 (16%)	67,97,113	1.41	10 (14%)
45	CLA	A1	312	47	41,46,73	1.65	9 (21%)	52,81,113	1.30	9 (17%)
45	CLA	BB	834	2	69,73,73	1.24	7 (10%)	83,113,113	1.28	9 (10%)
45	CLA	BB	827	-	66,70,73	1.27	7 (10%)	79,109,113	1.17	6 (7%)
47	LHG	B2	618	45	34,34,48	1.04	2 (5%)	37,40,54	0.96	2 (5%)
48	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
53	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
48	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)

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
45	CLA	B1	313	13	-	5/15/91/115	-
45	CLA	BA	808	1	-	12/39/115/115	-
45	CLA	A3	305	-	-	6/10/86/115	-
45	CLA	BB	807	2	-	13/39/115/115	-
45	CLA	BA	840	1	-	13/39/115/115	-
56	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
48	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
45	CLA	A6	613	16	-	7/37/113/115	-
45	CLA	BL	302	12	-	6/15/91/115	-
45	CLA	AL	303	12	-	7/10/86/115	-
54	CHL	B5	606	-	-	2/8/84/117	-
48	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
45	CLA	B3	304	-	-	6/10/86/115	-
45	CLA	BA	839	1	-	7/23/99/115	-
45	CLA	BA	803	1	-	19/39/115/115	-
45	CLA	A1	311	13	-	3/31/107/115	-
45	CLA	BG	201	-	-	7/12/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BA	823	1	-	6/10/86/115	-
48	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	AA	838	1	-	8/27/103/115	-
45	CLA	AB	810	2	-	17/39/115/115	-
45	CLA	A4	303	-	-	4/11/87/115	-
54	CHL	B2	606	-	-	2/14/90/117	-
47	LHG	A6	618	45	-	17/40/40/53	-
45	CLA	AB	833	2	-	10/39/115/115	-
47	LHG	A1	302	-	-	15/40/40/53	-
48	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
45	CLA	A3	313	14	-	3/8/84/115	-
45	CLA	AJ	102	10	-	5/12/88/115	-
45	CLA	BA	844	47	-	4/10/86/115	-
45	CLA	BB	813	2	-	4/25/101/115	-
49	SF4	BC	102	3	-	-	0/6/5/5
45	CLA	AB	813	2	-	5/13/89/115	-
45	CLA	BA	825	-	-	15/39/115/115	-
52	LUT	B2	615	-	-	0/29/67/67	0/2/2/2
45	CLA	BB	831	2	-	8/29/105/115	-
45	CLA	AB	826	-	-	6/36/112/115	-
45	CLA	BA	819	1	-	13/39/115/115	-
48	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
48	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
53	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
45	CLA	BB	823	2	-	4/16/92/115	-
45	CLA	BB	840	2	-	4/18/94/115	-
47	LHG	F	801	-	-	21/41/41/53	-
48	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
45	CLA	AB	807	2	-	11/39/115/115	-
52	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
45	CLA	A3	314	-	-	2/2/74/115	-
45	CLA	B3	313	-	-	2/2/74/115	-
53	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
48	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	837	1	-	3/23/99/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
48	BCR	BA	850	-	-	3/29/63/63	0/2/2/2
45	CLA	AA	812	1	-	9/26/102/115	-
45	CLA	B3	305	-	-	2/10/86/115	-
45	CLA	AA	841	1	-	12/39/115/115	-
49	SF4	AA	850	1,2	-	-	0/6/5/5
45	CLA	AB	842	47	-	20/39/115/115	-
45	CLA	AB	804	-	-	16/39/115/115	-
55	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
45	CLA	AA	820	1	-	5/15/91/115	-
45	CLA	BA	809	1	-	11/21/97/115	-
45	CLA	B5	612	18	-	8/30/106/115	-
48	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
45	CLA	B3	307	14	-	3/15/91/115	-
49	SF4	AC	102	3	-	-	0/6/5/5
48	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
45	CLA	A1	314	13	-	14/37/113/115	-
54	CHL	A6	606	-	-	2/12/88/117	-
45	CLA	AA	817	1	-	6/33/109/115	-
48	BCR	B3	317	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	830	2	-	11/39/115/115	-
45	CLA	AB	806	2	-	15/39/115/115	-
45	CLA	B2	612	17	-	13/39/115/115	-
45	CLA	AA	837	1	-	6/23/99/115	-
45	CLA	B3	309	47	-	2/8/84/115	-
52	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
45	CLA	BB	829	2	-	17/39/115/115	-
52	LUT	A6	615	-	-	0/29/67/67	0/2/2/2
45	CLA	BB	811	2	-	15/39/115/115	-
45	CLA	A4	311	15	-	8/28/104/115	-
47	LHG	B5	618	45	-	13/34/34/53	-
45	CLA	B2	603	17	-	4/13/89/115	-
45	CLA	AB	824	2	-	5/13/89/115	-
49	SF4	I	202	37	-	-	0/6/5/5
45	CLA	B1	305	13	-	6/25/101/115	-
45	CLA	B1	312	47	-	0/4/80/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BB	828	2	-	9/36/112/115	-
46	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
45	CLA	BA	820	1	-	6/15/91/115	-
48	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
45	CLA	BA	818	1	-	8/29/105/115	-
45	CLA	AA	801	1	-	13/39/115/115	-
45	CLA	AB	821	2	-	9/21/97/115	-
45	CLA	AB	816	2	-	4/13/89/115	-
47	LHG	A1	320	45	-	16/53/53/53	-
45	CLA	A6	601	15	-	2/17/93/115	-
45	CLA	BA	805	1	-	22/39/115/115	-
47	LHG	B1	302	-	-	14/40/40/53	-
53	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
45	CLA	AA	806	1	-	13/39/115/115	-
45	CLA	BB	805	-	-	14/39/115/115	-
45	CLA	A3	310	47	-	2/2/78/115	-
45	CLA	A1	315	13	-	0/4/80/115	-
45	CLA	BA	830	1	-	13/39/115/115	-
45	CLA	B3	308	14	-	5/10/86/115	-
45	CLA	A6	603	16	-	11/39/115/115	-
45	CLA	BB	819	2	-	14/32/108/115	-
45	CLA	AA	836	1	-	9/15/91/115	-
47	LHG	a	501	-	-	17/33/33/53	-
55	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
49	SF4	BC	101	3	-	-	0/6/5/5
45	CLA	BA	828	1	-	14/39/115/115	-
56	SQD	e	301	-	-	10/29/49/69	0/1/1/1
48	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
45	CLA	AB	820	-	-	10/27/103/115	-
45	CLA	AL	305	-	-	5/12/88/115	-
45	CLA	AA	831	1	-	9/18/94/115	-
45	CLA	AB	809	2	-	16/39/115/115	-
45	CLA	AB	827	2	-	14/36/112/115	-
45	CLA	AB	830	2	-	10/29/105/115	-
45	CLA	BA	826	-	-	6/25/101/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AB	823	2	-	19/39/115/115	-
45	CLA	A6	614	16	-	4/13/89/115	-
45	CLA	B2	610	47	-	7/10/70/115	-
45	CLA	AK	201	11	-	0/2/74/115	-
45	CLA	BB	825	2	-	8/15/91/115	-
45	CLA	B5	604	-	-	3/11/87/115	-
45	CLA	AA	803	1	-	15/39/115/115	-
45	CLA	B1	309	-	-	4/13/89/115	-
48	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
45	CLA	BB	814	2	-	1/13/89/115	-
45	CLA	AB	841	2	-	9/39/115/115	-
48	BCR	BA	856	-	-	5/29/63/63	0/2/2/2
45	CLA	B1	314	13	-	9/33/109/115	-
45	CLA	BA	814	1	-	8/15/91/115	-
45	CLA	A3	304	-	-	0/9/85/115	-
45	CLA	B1	306	-	-	3/10/86/115	-
48	BCR	BA	849	-	-	4/29/63/63	0/2/2/2
45	CLA	AG	201	-	-	5/13/89/115	-
45	CLA	A4	301	15	-	10/33/109/115	-
45	CLA	B5	608	18	-	5/13/89/115	-
45	CLA	BB	842	2	-	11/39/115/115	-
45	CLA	B1	304	13	-	7/35/111/115	-
45	CLA	BB	839	2	-	8/39/115/115	-
55	XAT	B2	616	-	-	0/31/93/93	0/4/4/4
48	BCR	BB	845	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	813	1	-	17/39/115/115	-
54	CHL	A6	602	16	-	6/24/100/117	-
45	CLA	A1	313	13	-	4/15/91/115	-
45	CLA	A6	610	16	-	6/27/103/115	-
45	CLA	AK	202	-	-	7/15/91/115	-
54	CHL	B3	306	-	-	5/15/91/117	-
45	CLA	BA	816	-	-	4/15/91/115	-
45	CLA	BA	812	1	-	5/26/102/115	-
57	FES	c	301	28	-	-	0/1/1/1
45	CLA	B3	311	14	-	8/25/101/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A1	305	13	-	8/27/103/115	-
45	CLA	BB	815	2	-	21/39/115/115	-
48	BCR	AI	102	-	-	3/29/63/63	0/2/2/2
49	SF4	BA	852	1,2	-	-	0/6/5/5
54	CHL	A6	608	-	-	8/21/97/117	-
45	CLA	AB	822	2	-	7/18/94/115	-
45	CLA	A3	312	14	-	13/25/101/115	-
50	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
45	CLA	BA	811	1	-	16/39/115/115	-
45	CLA	B5	610	47	-	6/12/88/115	-
45	CLA	A3	315	14	-	0/8/84/115	-
50	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
45	CLA	A3	303	14	-	10/27/103/115	-
48	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	808	1	-	10/39/115/115	-
48	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
45	CLA	A4	308	15	-	6/26/102/115	-
45	CLA	AF	803	-	-	3/12/88/115	-
45	CLA	AB	817	2	-	8/27/103/115	-
45	CLA	BL	303	12	-	9/33/109/115	-
55	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	831	1	-	9/18/94/115	-
45	CLA	AA	807	1	-	4/21/97/115	-
47	LHG	A3	319	45	-	14/26/26/53	-
45	CLA	BK	201	11	-	0/2/74/115	-
45	CLA	AF	804	-	-	4/10/86/115	-
52	LUT	B3	315	-	-	4/29/67/67	0/2/2/2
45	CLA	AA	833	1	-	21/39/115/115	-
45	CLA	B2	608	17	-	4/15/91/115	-
47	LHG	B1	301	45	-	7/42/42/53	-
45	CLA	BB	810	2	-	15/39/115/115	-
48	BCR	AK	204	-	-	6/29/63/63	0/2/2/2
45	CLA	BA	806	1	-	18/39/115/115	-
47	LHG	AA	844	-	-	18/53/53/53	-
45	CLA	BF	301	-	-	8/26/102/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BF	302	-	-	3/12/88/115	-
48	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
54	CHL	A4	306	-	-	2/17/93/117	-
48	BCR	BA	847	-	-	5/29/63/63	0/2/2/2
45	CLA	BB	824	2	-	18/39/115/115	-
45	CLA	BB	822	2	-	2/10/86/115	-
45	CLA	BJ	102	10	-	4/12/88/115	-
45	CLA	BB	838	2	-	5/21/97/115	-
48	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
45	CLA	BA	822	1	-	8/12/88/115	-
45	CLA	AA	815	1	-	3/12/88/115	-
45	CLA	AB	814	2	-	16/39/115/115	-
45	CLA	AB	818	2	-	12/32/108/115	-
45	CLA	AB	840	-	-	7/39/115/115	-
45	CLA	BB	801	2	-	17/39/115/115	-
45	CLA	AB	801	2	-	17/39/115/115	-
54	CHL	B5	607	-	-	5/15/91/117	-
45	CLA	AB	836	-	-	3/12/88/115	-
45	CLA	AA	839	1	-	6/24/100/115	-
47	LHG	BA	845	-	-	29/53/53/53	-
45	CLA	AB	831	2	-	5/13/89/115	-
51	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
45	CLA	AL	304	12	-	9/33/109/115	-
45	CLA	BA	827	1	-	14/39/115/115	-
45	CLA	A4	302	15	-	5/13/89/115	-
47	LHG	B3	318	45	-	11/26/26/53	-
45	CLA	A4	313	15	-	11/21/97/115	-
48	BCR	BB	847	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	809	2	-	6/24/100/115	-
45	CLA	AB	832	2	-	9/39/115/115	-
45	CLA	B5	602	18	-	11/33/109/115	-
49	SF4	AC	101	3	-	-	0/6/5/5
48	BCR	BB	849	-	-	2/29/63/63	0/2/2/2
45	CLA	A3	302	14	-	8/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	B3	302	14	-	6/27/103/115	-
45	CLA	BB	826	-	-	10/39/115/115	-
45	CLA	AA	821	-	-	15/39/115/115	-
50	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
45	CLA	BA	824	1	-	10/27/103/115	-
45	CLA	A1	309	-	-	7/13/89/115	-
45	CLA	BL	304	-	-	5/13/89/115	-
45	CLA	BB	841	-	-	7/39/115/115	-
45	CLA	A6	605	-	-	3/11/88/115	-
45	CLA	AB	835	2	-	7/33/109/115	-
54	CHL	B1	303	13	-	3/21/97/117	-
45	CLA	AB	837	2	-	7/21/97/115	-
45	CLA	B3	314	14	-	0/8/84/115	-
45	CLA	BA	821	-	-	12/39/115/115	-
45	CLA	A3	308	14	-	7/15/91/115	-
45	CLA	BB	820	2	-	12/33/109/115	-
45	CLA	AB	808	2	-	6/22/98/115	-
45	CLA	AA	829	1	-	18/39/115/115	-
54	CHL	A6	607	-	-	2/14/90/117	-
49	SF4	I	201	37	-	-	0/6/5/5
50	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
45	CLA	B2	602	17	-	11/39/115/115	-
45	CLA	AG	203	7	-	4/12/88/115	-
48	BCR	AA	852	-	-	5/29/63/63	0/2/2/2
45	CLA	A4	310	15	-	7/10/86/115	-
48	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
46	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
45	CLA	A1	307	-	-	6/10/82/115	-
45	CLA	AB	803	2	-	19/39/115/115	-
50	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
55	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
45	CLA	B5	611	18	-	4/10/86/115	-
45	CLA	B3	303	-	-	2/9/85/115	-
45	CLA	BK	202	-	-	8/15/91/115	-
45	CLA	A6	609	16	-	3/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	XAT	B3	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BB	812	2	-	13/39/115/115	-
45	CLA	BB	808	2	-	10/39/115/115	-
48	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
54	CHL	B5	605	-	-	2/10/86/117	-
54	CHL	B2	614	17	-	0/14/90/117	-
45	CLA	BA	815	1	-	4/12/88/115	-
45	CLA	AA	828	1	-	15/39/115/115	-
45	CLA	BB	818	2	-	9/27/103/115	-
48	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
45	CLA	AA	834	1	-	17/39/115/115	-
48	BCR	B2	617	-	-	0/29/63/63	0/2/2/2
48	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
45	CLA	AA	830	1	-	14/39/115/115	-
48	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	841	1	-	17/39/115/115	-
45	CLA	B2	611	17	-	7/13/89/115	-
48	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
45	CLA	A3	306	14	-	0/10/86/115	-
45	CLA	B3	312	14	-	2/8/84/115	-
45	CLA	AA	823	1	-	6/10/86/115	-
45	CLA	AB	838	2	-	7/39/115/115	-
47	LHG	A3	301	-	-	11/40/40/53	-
54	CHL	B1	308	-	-	0/10/86/117	-
45	CLA	BA	802	-	-	4/39/115/115	-
55	XAT	A6	616	-	-	0/31/93/93	0/4/4/4
45	CLA	BB	817	2	-	4/11/87/115	-
54	CHL	B2	605	-	-	3/12/88/117	-
45	CLA	AA	802	-	-	8/39/115/115	-
45	CLA	BB	832	2	-	6/13/89/115	-
47	LHG	AJ	104	-	-	16/44/44/53	-
45	CLA	BB	833	2	-	4/13/89/115	-
45	CLA	BB	802	-	-	16/39/115/115	-
45	CLA	AA	805	1	-	17/39/115/115	-
45	CLA	BG	202	7	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AB	819	2	-	14/33/109/115	-
50	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
45	CLA	BB	843	47	-	13/39/115/115	-
45	CLA	B3	310	14	-	2/13/89/115	-
51	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
54	CHL	B2	607	-	-	4/17/93/117	-
45	CLA	AA	827	1	-	18/39/115/115	-
54	CHL	A4	304	-	-	1/10/86/117	-
54	CHL	A3	307	-	-	4/15/91/117	-
48	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
48	BCR	BL	306	-	-	15/29/63/63	0/2/2/2
52	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
48	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
48	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	B1	310	13	-	3/6/82/115	-
45	CLA	BA	834	1	-	13/39/115/115	-
45	CLA	BA	836	1	-	8/15/91/115	-
45	CLA	AA	813	1	-	19/39/115/115	-
45	CLA	A6	612	16	-	8/13/89/115	-
45	CLA	AG	204	7	-	6/15/91/115	-
45	CLA	B5	613	18	-	7/15/91/115	-
52	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
45	CLA	AB	812	2	-	8/25/101/115	-
45	CLA	A4	307	15	-	3/15/91/115	-
45	CLA	AA	822	1	-	5/12/88/115	-
48	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	825	-	-	14/39/115/115	-
45	CLA	BA	835	1	-	6/15/91/115	-
45	CLA	A1	306	-	-	9/20/96/115	-
45	CLA	AB	815	2	-	17/39/115/115	-
52	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
45	CLA	A4	312	15	-	6/15/91/115	-
45	CLA	B2	613	17	-	1/13/89/115	-
45	CLA	B2	604	-	-	4/11/88/115	-
45	CLA	AA	825	-	-	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	810	1	-	10/39/111/115	-
45	CLA	BB	816	2	-	15/37/113/115	-
47	LHG	B1	318	45	-	12/46/46/53	-
45	CLA	AA	819	1	-	14/39/115/115	-
49	SF4	K	301	39	-	-	0/6/5/5
45	CLA	A1	304	13	-	11/33/109/115	-
45	CLA	BB	821	-	-	8/27/103/115	-
45	CLA	BB	806	2	-	2/10/86/115	-
45	CLA	BB	836	2	-	11/33/109/115	-
45	CLA	A6	604	16	-	2/11/87/115	-
45	CLA	A3	311	14	-	1/13/89/115	-
45	CLA	A4	309	-	-	5/12/88/115	-
45	CLA	AA	826	-	-	12/32/108/115	-
45	CLA	B1	311	13	-	3/31/107/115	-
45	CLA	AA	842	-	-	20/39/115/115	-
45	CLA	B5	603	18	-	4/13/89/115	-
48	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
45	CLA	A6	611	47	-	6/10/70/115	-
45	CLA	AA	809	1	-	7/21/97/115	-
47	LHG	BF	305	-	-	18/49/49/53	-
45	CLA	B1	315	13	-	0/4/80/115	-
45	CLA	AF	802	-	-	10/30/106/115	-
45	CLA	A3	309	14	-	5/10/86/115	-
45	CLA	BB	835	2	-	18/39/115/115	-
45	CLA	BB	837	-	-	6/12/88/115	-
45	CLA	BA	801	1	-	9/39/115/115	-
48	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
45	CLA	AB	839	2	-	3/18/94/115	-
45	CLA	BA	838	1	-	11/27/99/115	-
54	CHL	B2	601	17	-	9/26/102/117	-
45	CLA	A1	316	13	-	9/11/87/115	-
45	CLA	AB	802	-	-	16/37/113/115	-
45	CLA	BA	832	1	-	7/29/105/115	-
45	CLA	B5	609	18	-	5/26/102/115	-
45	CLA	BA	807	1	-	4/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	814	1	-	5/15/91/115	-
45	CLA	AA	818	1	-	9/32/108/115	-
45	CLA	BA	810	1	-	12/39/115/115	-
45	CLA	AB	805	2	-	2/10/86/115	-
45	CLA	AA	840	1	-	16/39/115/115	-
45	CLA	B5	601	18	-	10/17/93/115	-
50	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
54	CHL	A4	305	-	-	0/10/86/117	-
45	CLA	AA	804	1	-	7/24/100/115	-
45	CLA	B1	307	-	-	4/10/82/115	-
47	LHG	BA	846	45	-	7/30/30/53	-
52	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
48	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
54	CHL	A1	308	13	-	2/10/86/117	-
45	CLA	BH	201	-	-	13/33/109/115	-
48	BCR	AL	302	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	829	1	-	11/39/115/115	-
50	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
48	BCR	A6	617	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	816	-	-	8/15/91/115	-
45	CLA	AH	201	8	-	12/33/109/115	-
48	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
45	CLA	AA	824	1	-	9/25/101/115	-
45	CLA	AB	828	2	-	13/39/115/115	-
48	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
46	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
45	CLA	AA	832	1	-	7/29/105/115	-
45	CLA	AB	834	2	-	18/39/115/115	-
54	CHL	A4	314	15	-	0/10/86/117	-
45	CLA	AB	829	2	-	15/39/115/115	-
45	CLA	AB	811	2	-	15/39/115/115	-
48	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	BF	303	-	-	2/10/86/115	-
46	PQN	BB	844	-	-	9/23/43/43	0/2/2/2
45	CLA	AA	811	1	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BK	203	-	-	5/17/93/115	-
47	LHG	A1	301	45	-	11/42/42/53	-
45	CLA	BA	817	1	-	9/33/109/115	-
48	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
45	CLA	AK	203	11	-	9/17/93/115	-
45	CLA	A1	310	13	-	2/8/84/115	-
45	CLA	B3	301	14	-	7/33/109/115	-
54	CHL	A1	303	13	-	4/23/99/117	-
45	CLA	BA	833	1	-	17/39/115/115	-
45	CLA	AA	835	1	-	2/13/89/115	-
45	CLA	BB	804	2	-	16/39/115/115	-
45	CLA	B2	609	17	-	8/27/103/115	-
45	CLA	BA	842	-	-	15/39/115/115	-
45	CLA	BA	804	1	-	5/24/100/115	-
45	CLA	A1	312	47	-	0/4/80/115	-
45	CLA	BB	834	2	-	11/39/115/115	-
45	CLA	BB	827	-	-	8/36/112/115	-
47	LHG	B2	618	45	-	22/39/39/53	-
48	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
53	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
48	BCR	AB	849	-	-	5/29/63/63	0/2/2/2

The worst 5 of 2908 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	611	CLA	C1A-NA	12.32	1.40	1.29
45	B2	610	CLA	C1A-NA	11.85	1.40	1.29
46	BB	844	PQN	C12-C13	9.75	1.56	1.33
46	AA	843	PQN	C12-C13	9.56	1.55	1.33
46	BA	843	PQN	C12-C13	9.52	1.55	1.33

The worst 5 of 3852 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BL	306	BCR	C37-C22-C21	-32.50	77.40	122.92
48	BL	306	BCR	C35-C13-C14	-31.52	78.78	122.92
48	BL	306	BCR	C34-C9-C10	-29.92	81.01	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BG	203	BCR	C35-C13-C14	-29.72	81.29	122.92
48	BL	306	BCR	C37-C22-C23	-27.87	74.16	118.08

There are no chirality outliers.

5 of 3232 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	AA	801	CLA	CBD-CGD-O2D-CED
45	AA	802	CLA	CBD-CGD-O2D-CED
45	AA	804	CLA	C1A-C2A-CAA-CBA
45	AA	804	CLA	C3A-C2A-CAA-CBA
45	AA	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

224 monomers are involved in 480 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	808	CLA	4	0
45	BA	840	CLA	4	0
56	BJ	104	SQD	6	0
48	A1	319	BCR	3	0
45	A6	613	CLA	1	0
45	BL	302	CLA	8	0
48	AF	801	BCR	4	0
45	BA	803	CLA	3	0
45	A1	311	CLA	2	0
45	BG	201	CLA	9	0
48	AJ	103	BCR	1	0
45	AA	838	CLA	1	0
45	AB	810	CLA	2	0
54	B2	606	CHL	1	0
45	AB	833	CLA	2	0
48	BG	203	BCR	13	0
45	AJ	102	CLA	1	0
45	BB	813	CLA	1	0
49	BC	102	SF4	7	0
48	BB	848	BCR	2	0
48	AB	845	BCR	1	0
45	BB	823	CLA	2	0
45	BB	840	CLA	1	0
47	F	801	LHG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	AJ	101	BCR	4	0
52	B1	316	LUT	3	0
45	B3	313	CLA	3	0
53	A4	318	LMG	4	0
48	BJ	103	BCR	3	0
55	A4	316	XAT	2	0
45	AA	841	CLA	1	0
45	AB	842	CLA	1	0
45	AA	820	CLA	1	0
45	B5	612	CLA	1	0
48	BL	301	BCR	3	0
49	AC	102	SF4	3	0
48	BJ	101	BCR	6	0
45	A1	314	CLA	2	0
45	AA	817	CLA	1	0
48	B3	317	BCR	4	0
45	BB	830	CLA	1	0
45	B2	612	CLA	3	0
52	A4	315	LUT	4	0
45	BB	829	CLA	1	0
52	A6	615	LUT	4	0
45	A4	311	CLA	1	0
45	B2	603	CLA	4	0
45	AB	824	CLA	1	0
49	I	202	SF4	3	0
45	B1	305	CLA	1	0
45	BB	828	CLA	2	0
46	AB	843	PQN	2	0
45	BA	820	CLA	1	0
45	AA	801	CLA	11	0
45	A6	601	CLA	1	0
45	BA	805	CLA	1	0
45	AA	806	CLA	1	0
45	BB	805	CLA	2	0
45	BA	830	CLA	4	0
45	BB	819	CLA	1	0
47	a	501	LHG	2	0
55	B5	615	XAT	1	0
56	e	301	SQD	1	0
45	AB	809	CLA	2	0
45	AB	827	CLA	4	0
45	B2	610	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	AK	201	CLA	7	0
45	AA	803	CLA	1	0
45	B1	309	CLA	1	0
48	BA	856	BCR	1	0
45	B1	314	CLA	1	0
45	A3	304	CLA	1	0
45	B1	306	CLA	2	0
48	BA	849	BCR	2	0
45	A4	301	CLA	1	0
45	B5	608	CLA	1	0
45	B1	304	CLA	2	0
55	B2	616	XAT	6	0
48	BB	845	BCR	2	0
45	A6	610	CLA	10	0
45	AK	202	CLA	4	0
54	B3	306	CHL	1	0
45	BA	812	CLA	1	0
57	c	301	FES	2	0
45	B3	311	CLA	1	0
45	A1	305	CLA	1	0
45	BB	815	CLA	7	0
48	AI	102	BCR	3	0
49	BA	852	SF4	1	0
54	A6	608	CHL	2	0
45	AB	822	CLA	1	0
45	BA	811	CLA	1	0
48	BL	305	BCR	2	0
45	AF	803	CLA	1	0
45	BL	303	CLA	1	0
55	A1	318	XAT	1	0
45	BK	201	CLA	3	0
52	B3	315	LUT	3	0
45	AA	833	CLA	1	0
47	B1	301	LHG	1	0
45	BB	810	CLA	1	0
48	AK	204	BCR	2	0
45	BA	806	CLA	2	0
47	AA	844	LHG	1	0
45	BF	302	CLA	1	0
48	BA	848	BCR	1	0
54	A4	306	CHL	2	0
48	BA	847	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BB	838	CLA	1	0
48	BF	304	BCR	1	0
45	AA	815	CLA	1	0
45	AB	814	CLA	1	0
45	AB	818	CLA	2	0
45	AB	840	CLA	1	0
45	BB	801	CLA	3	0
45	AB	801	CLA	1	0
47	BA	845	LHG	2	0
45	AB	831	CLA	1	0
51	BB	850	DGD	1	0
45	AL	304	CLA	1	0
47	B3	318	LHG	1	0
45	A4	313	CLA	1	0
48	BB	847	BCR	1	0
45	BB	809	CLA	6	0
45	B5	602	CLA	1	0
49	AC	101	SF4	1	0
48	BB	849	BCR	2	0
45	BL	304	CLA	2	0
45	BB	841	CLA	5	0
54	B1	303	CHL	2	0
45	A3	308	CLA	1	0
45	BB	820	CLA	1	0
45	AB	808	CLA	4	0
49	I	201	SF4	1	0
45	B2	602	CLA	5	0
45	AG	203	CLA	1	0
48	BB	803	BCR	5	0
46	AA	843	PQN	3	0
45	AB	803	CLA	3	0
55	A3	317	XAT	2	0
45	B3	303	CLA	1	0
45	BK	202	CLA	4	0
55	B3	316	XAT	1	0
45	BB	812	CLA	5	0
48	BI	101	BCR	1	0
45	AA	828	CLA	1	0
45	AA	834	CLA	1	0
48	B2	617	BCR	2	0
48	AA	847	BCR	1	0
45	AA	830	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	A3	318	BCR	2	0
45	BA	841	CLA	1	0
45	B2	611	CLA	1	0
48	AA	848	BCR	2	0
45	AB	838	CLA	1	0
47	A3	301	LHG	1	0
45	BA	802	CLA	3	0
55	A6	616	XAT	4	0
45	AA	802	CLA	1	0
45	BB	802	CLA	4	0
45	BG	202	CLA	39	0
50	AL	301	LMU	1	0
45	B3	310	CLA	1	0
54	B2	607	CHL	3	0
45	AA	827	CLA	4	0
48	AA	849	BCR	2	0
48	BL	306	BCR	1	0
52	A3	316	LUT	1	0
48	BB	846	BCR	1	0
48	AB	846	BCR	1	0
45	BA	834	CLA	1	0
45	AG	204	CLA	4	0
45	B5	613	CLA	1	0
45	AB	812	CLA	1	0
45	A4	307	CLA	1	0
48	AA	846	BCR	1	0
45	AB	825	CLA	1	0
45	A1	306	CLA	2	0
52	AF	806	LUT	2	0
45	AA	825	CLA	2	0
45	AA	810	CLA	1	0
45	BB	816	CLA	1	0
49	K	301	SF4	1	0
45	BB	821	CLA	1	0
45	A6	604	CLA	2	0
45	A4	309	CLA	1	0
45	B1	311	CLA	1	0
47	BF	305	LHG	1	0
45	BA	801	CLA	14	0
48	AB	844	BCR	2	0
45	AB	839	CLA	2	0
54	B2	601	CHL	12	0

Continued on next page...

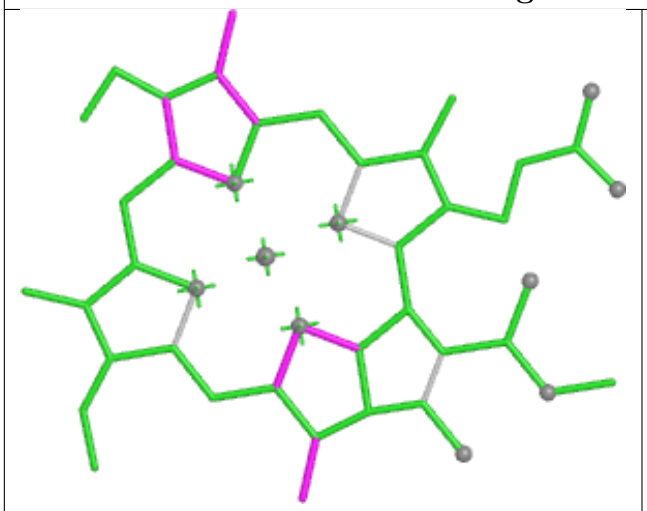
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A1	316	CLA	1	0
45	AB	802	CLA	4	0
45	BA	832	CLA	1	0
45	AA	818	CLA	2	0
45	BA	810	CLA	1	0
47	BA	846	LHG	1	0
52	A1	317	LUT	1	0
48	AF	805	BCR	2	0
54	A1	308	CHL	1	0
48	AL	302	BCR	1	0
45	BA	829	CLA	1	0
48	A6	617	BCR	3	0
45	AH	201	CLA	1	0
48	AB	847	BCR	3	0
45	AB	828	CLA	1	0
48	BA	851	BCR	6	0
46	BA	843	PQN	3	0
45	AB	834	CLA	3	0
48	AB	848	BCR	2	0
46	BB	844	PQN	2	0
45	AA	811	CLA	1	0
48	BA	855	BCR	2	0
45	AK	203	CLA	1	0
54	A1	303	CHL	2	0
45	BB	804	CLA	2	0
45	B2	609	CLA	2	0
45	BA	842	CLA	1	0
45	BB	834	CLA	2	0
45	BB	827	CLA	1	0
47	B2	618	LHG	2	0
48	AG	205	BCR	1	0
53	A1	321	LMG	1	0

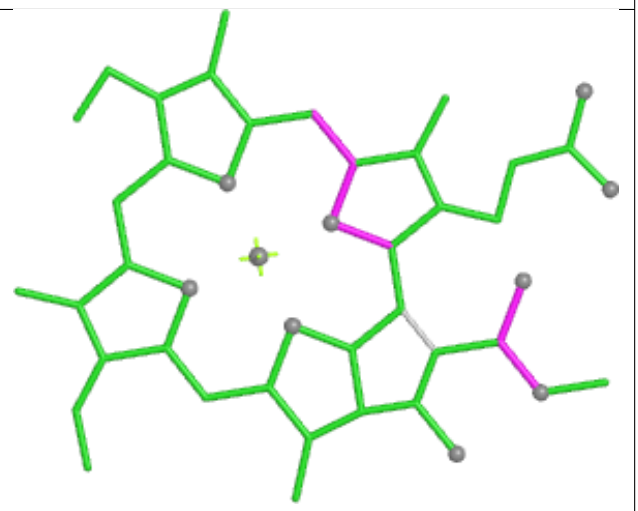
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

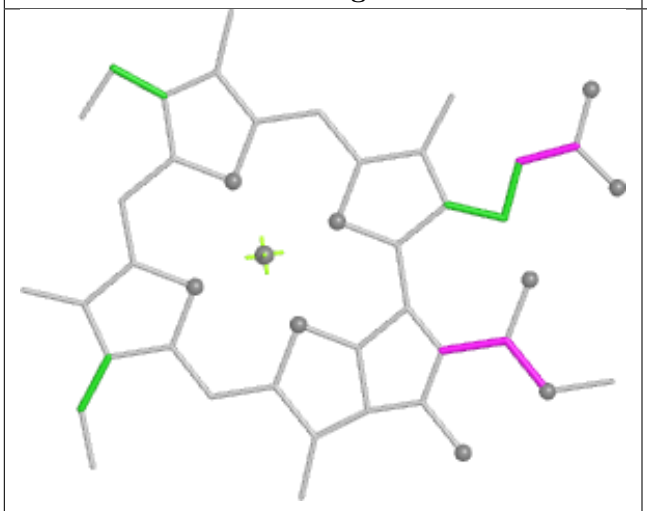
Ligand CLA B1 313



Bond lengths



Bond angles

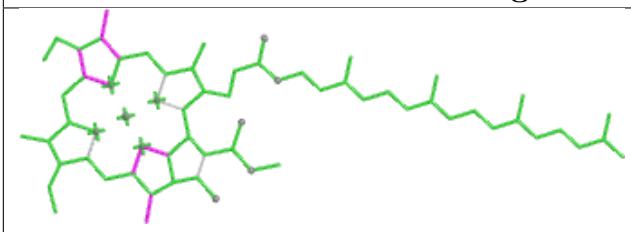


Torsions

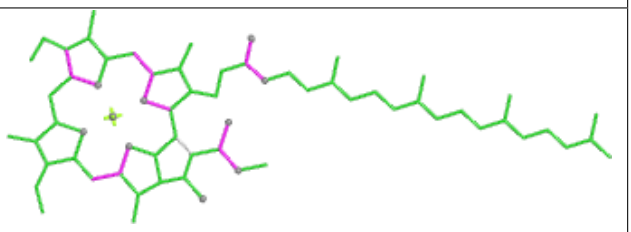


Rings

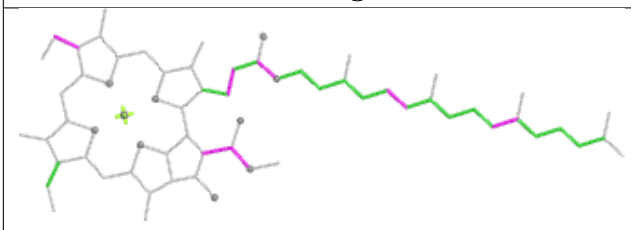
Ligand CLA BA 808



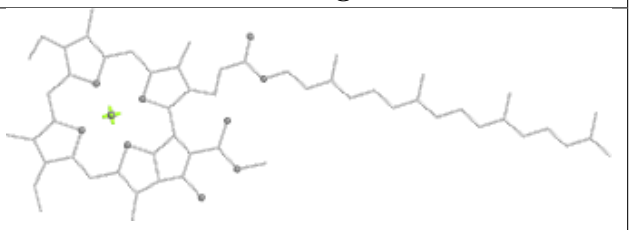
Bond lengths



Bond angles

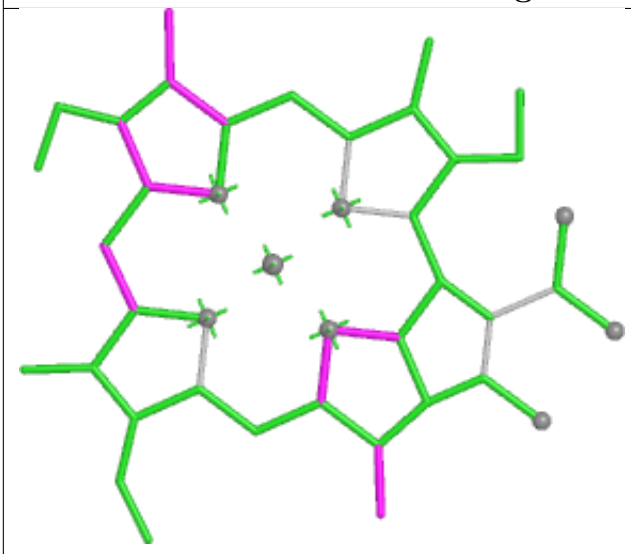


Torsions

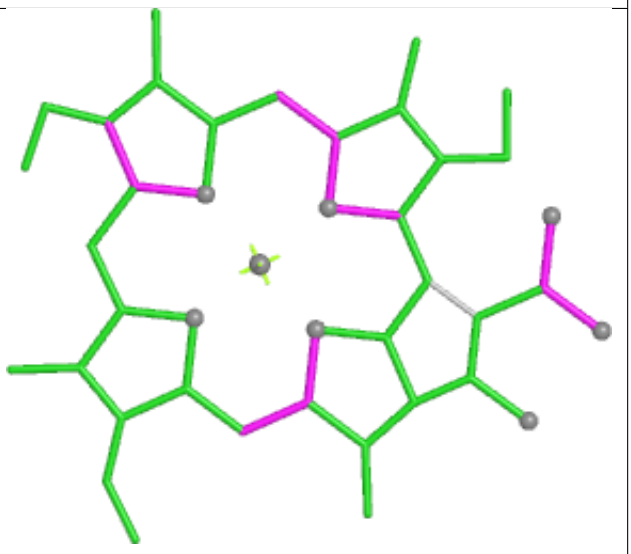


Rings

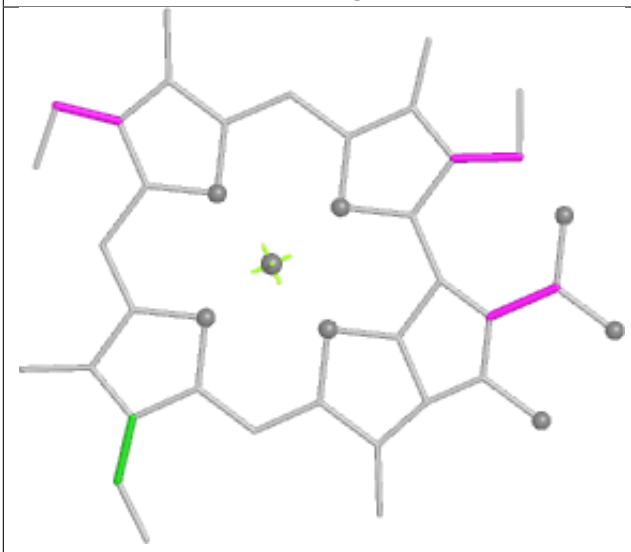
Ligand CLA A3 305



Bond lengths



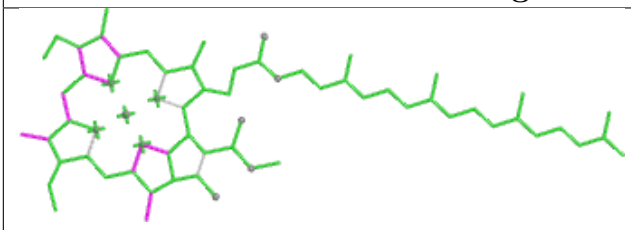
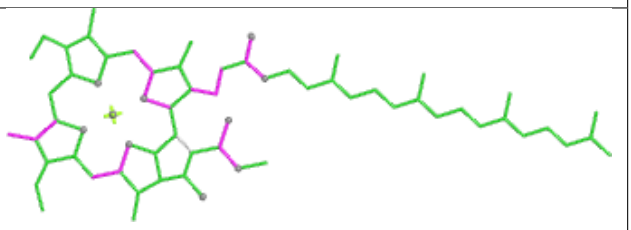
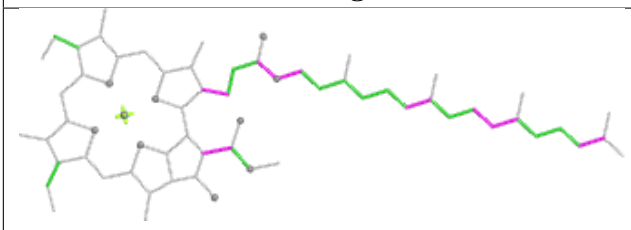
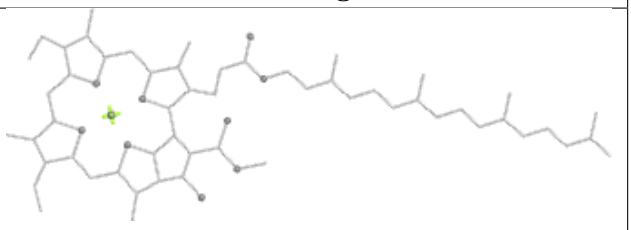
Bond angles

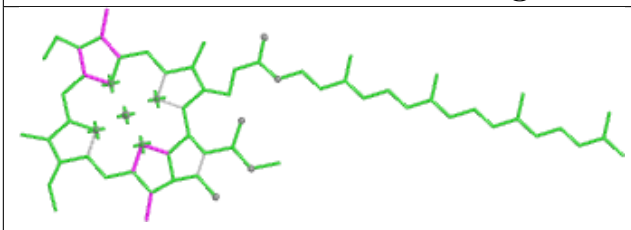
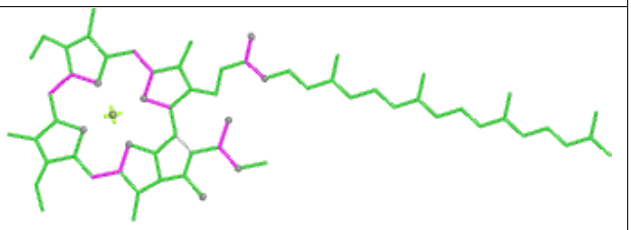
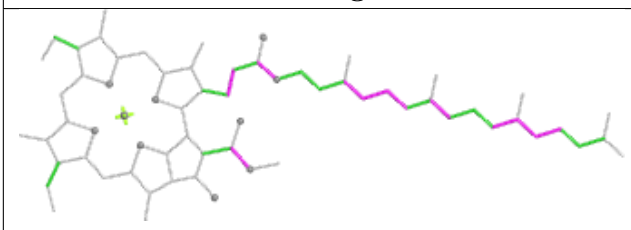
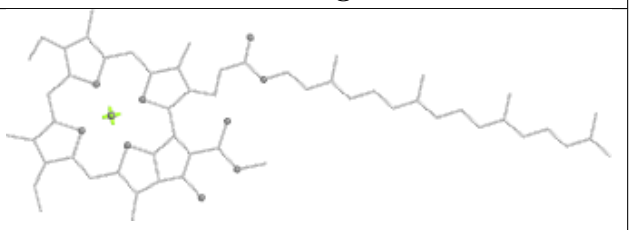


Torsions

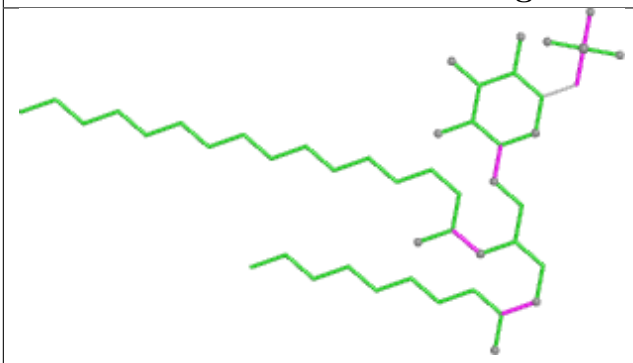


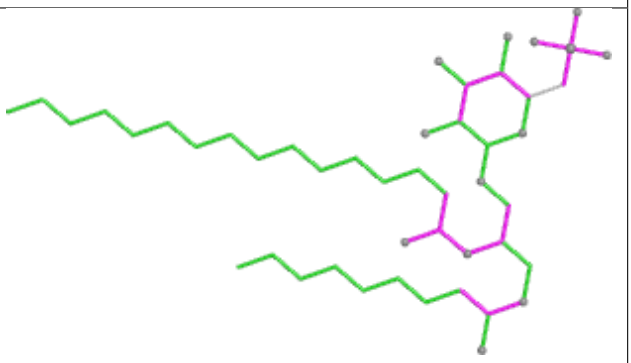
Rings

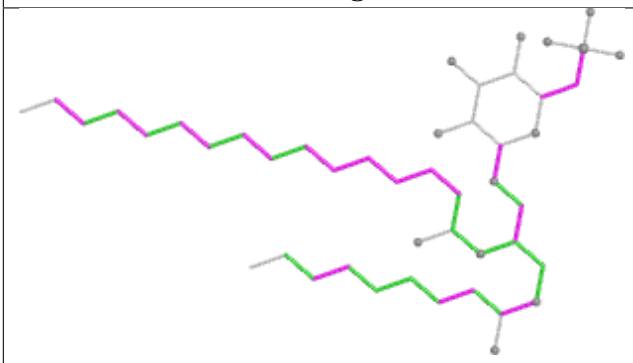
Ligand CLA BB 807	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

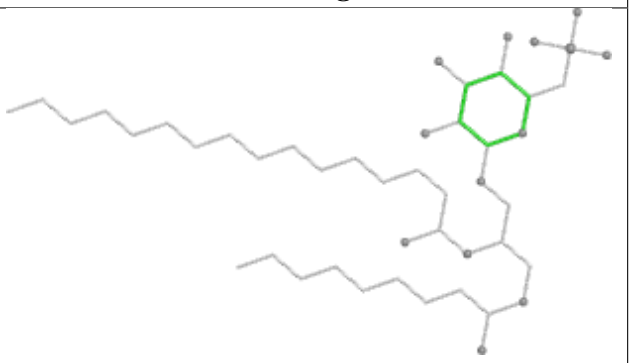
Ligand CLA BA 840	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SQD BJ 104

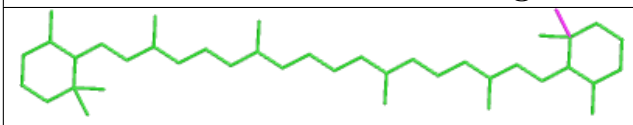

Bond lengths

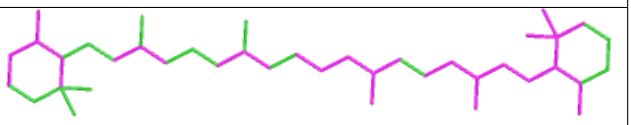

Bond angles

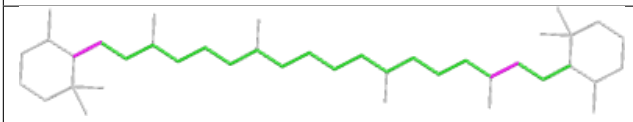

Torsions

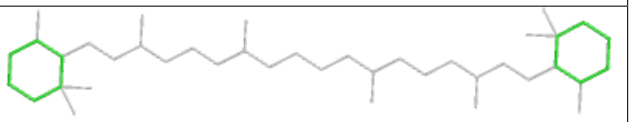

Rings

Ligand BCR A1 319

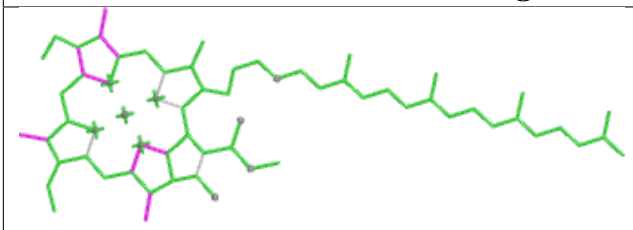

Bond lengths

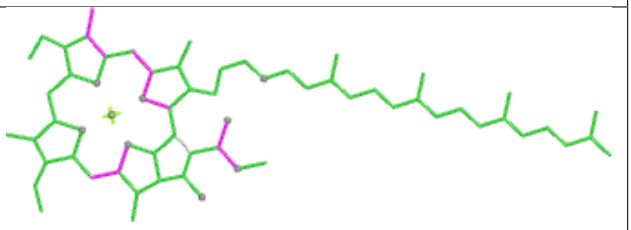

Bond angles

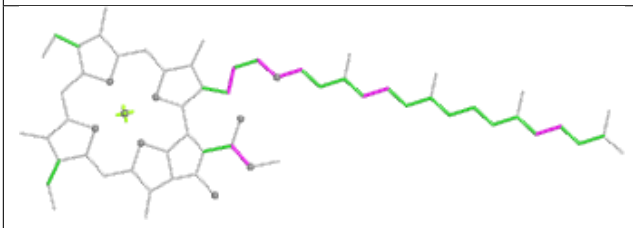

Torsions

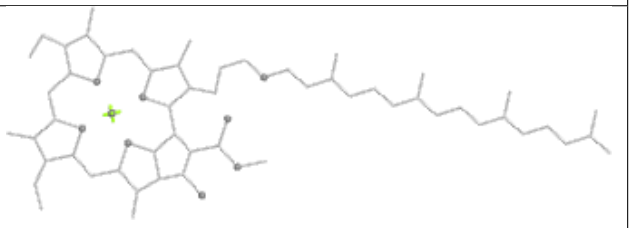

Rings

Ligand CLA A6 613

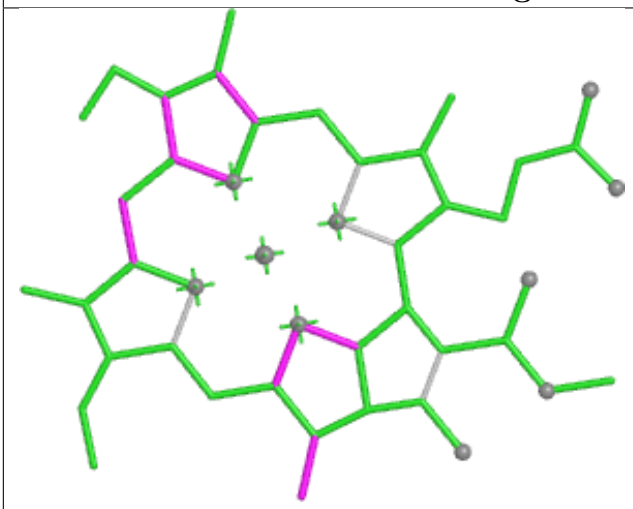

Bond lengths


Bond angles

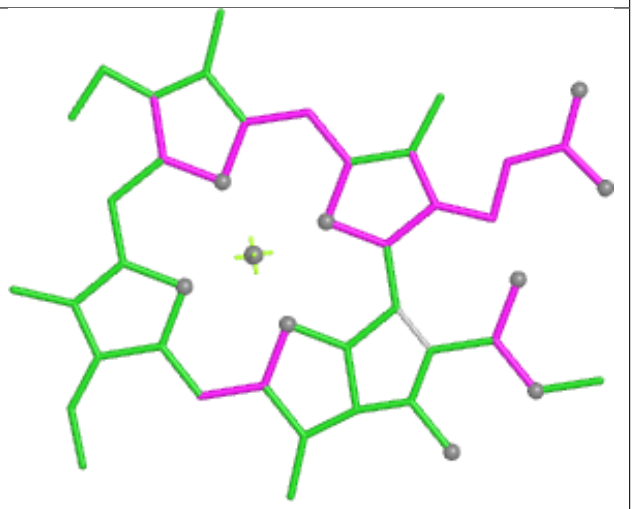

Torsions


Rings

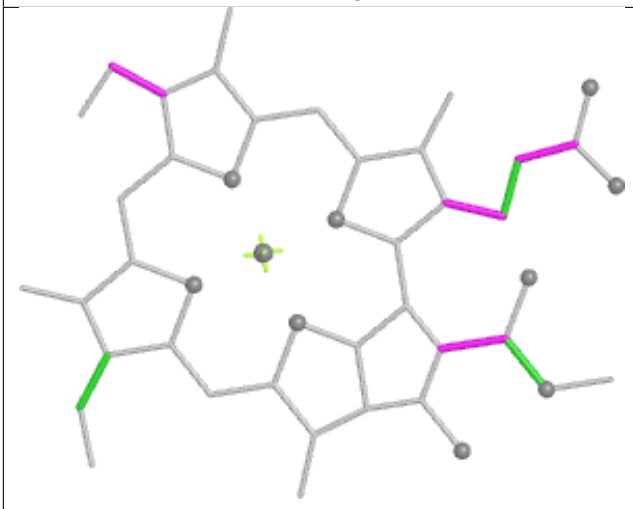
Ligand CLA BL 302



Bond lengths



Bond angles

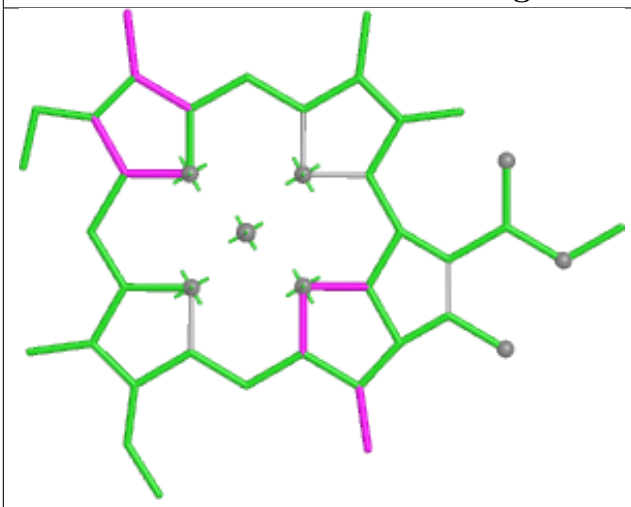


Torsions

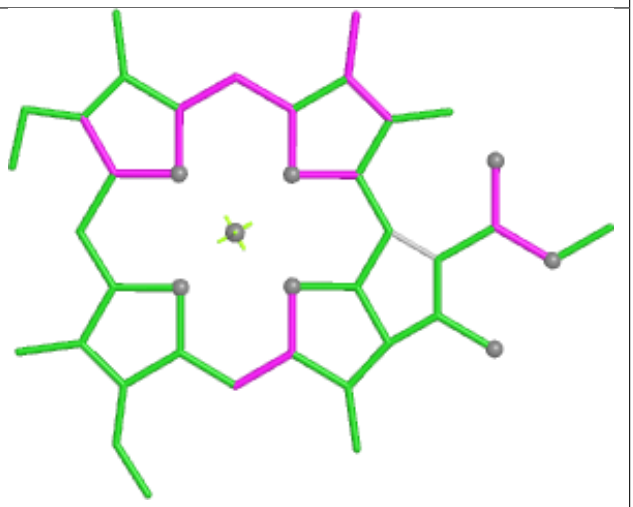


Rings

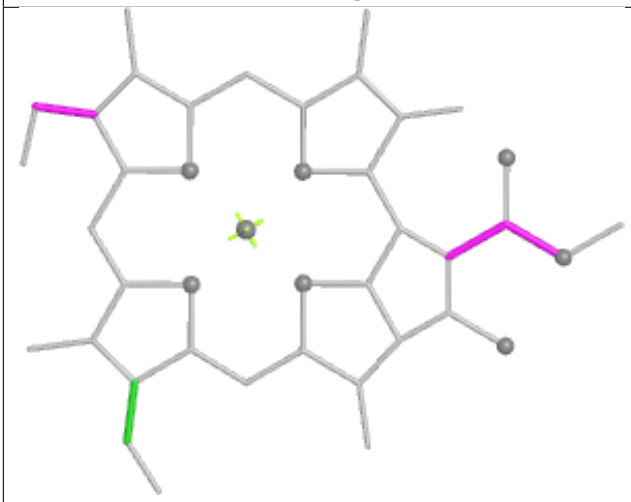
Ligand CLA AL 303



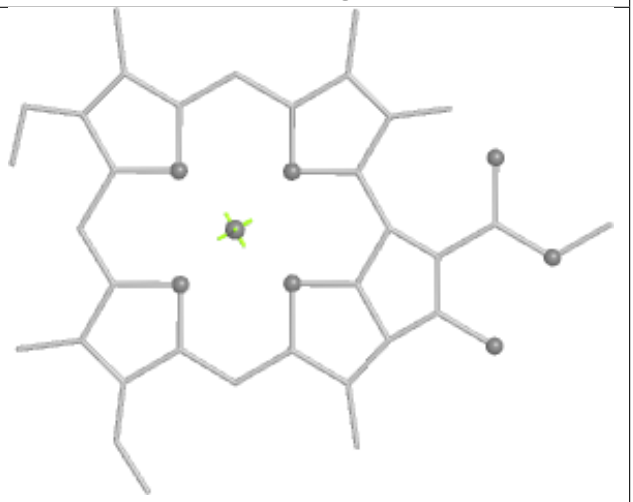
Bond lengths



Bond angles

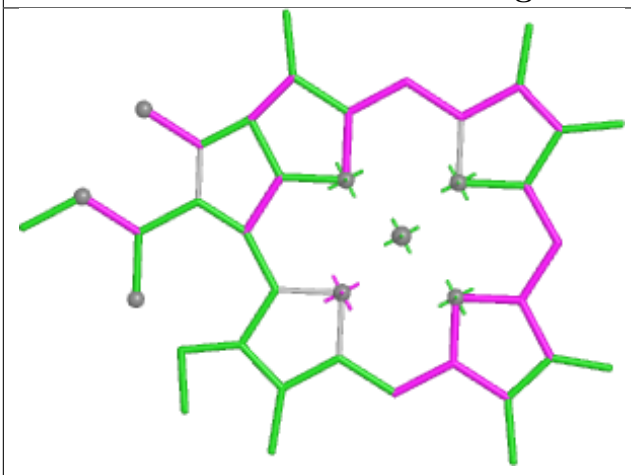


Torsions

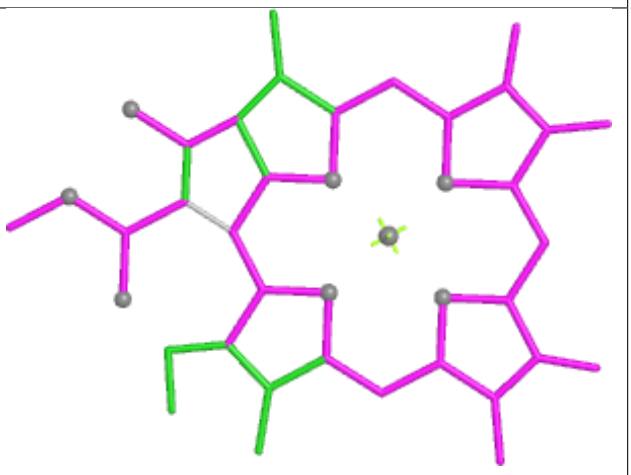


Rings

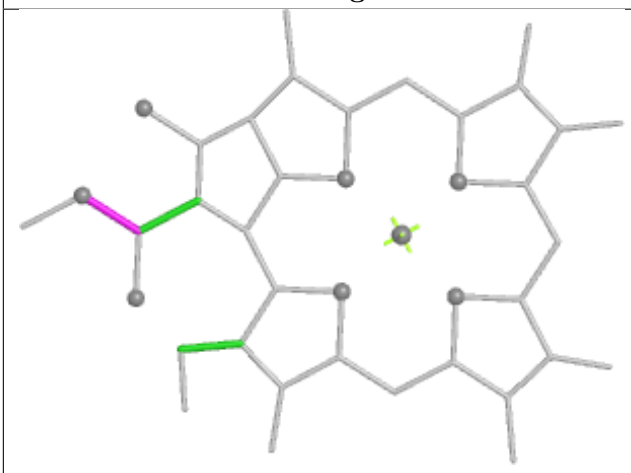
Ligand CHL B5 606



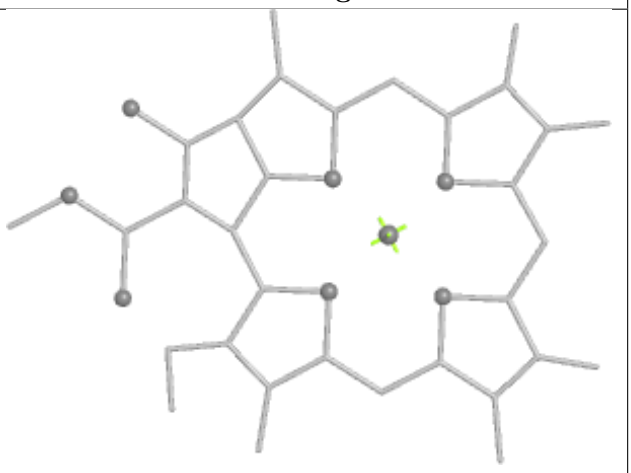
Bond lengths



Bond angles

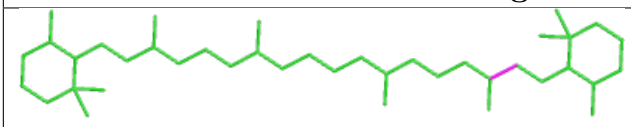


Torsions

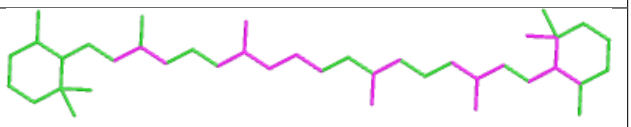


Rings

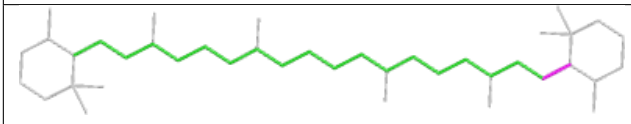
Ligand BCR AF 801



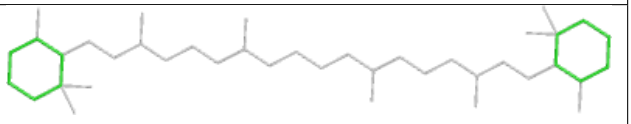
Bond lengths



Bond angles

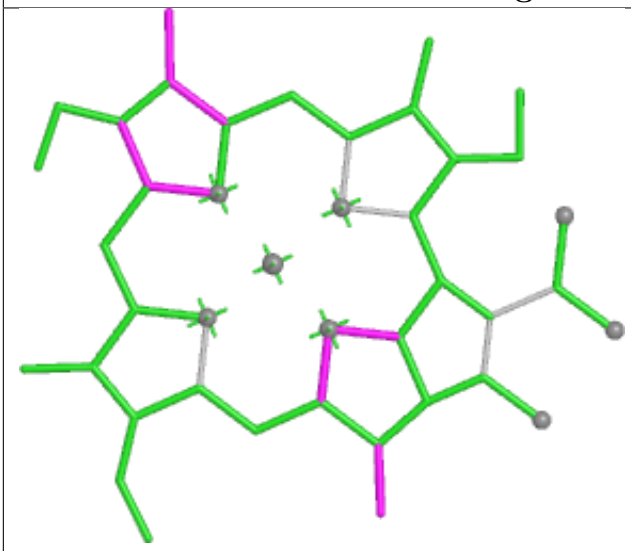


Torsions

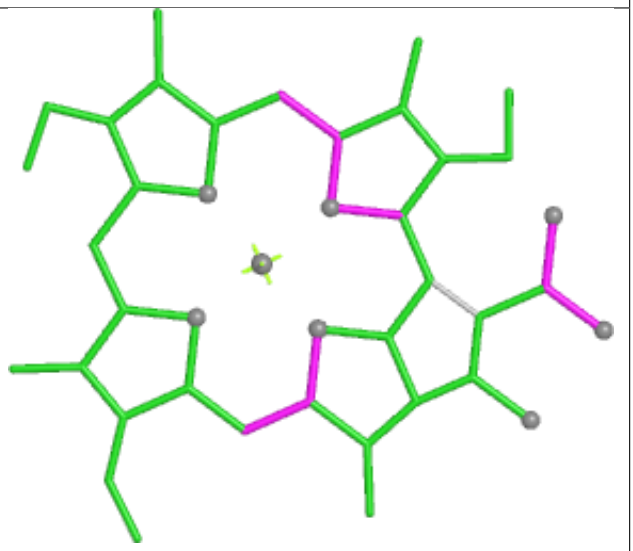


Rings

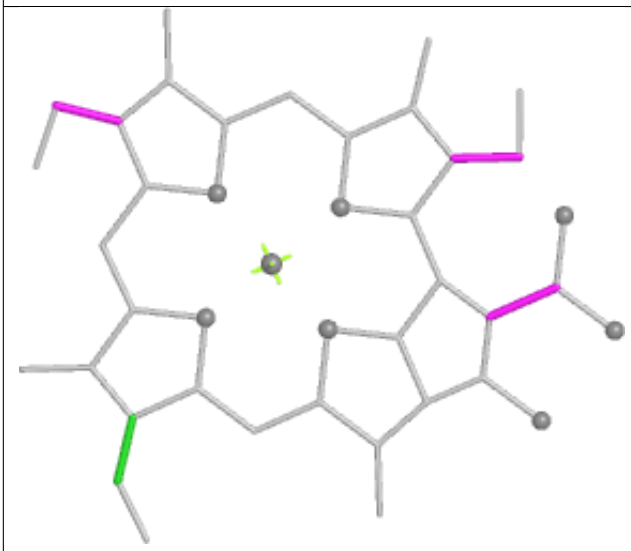
Ligand CLA B3 304



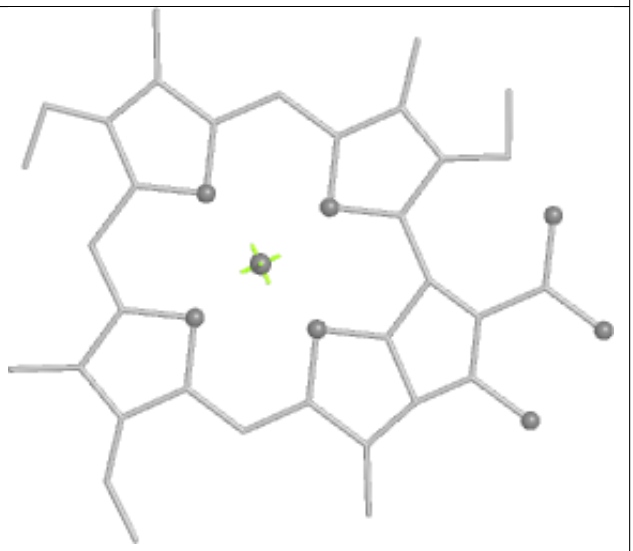
Bond lengths



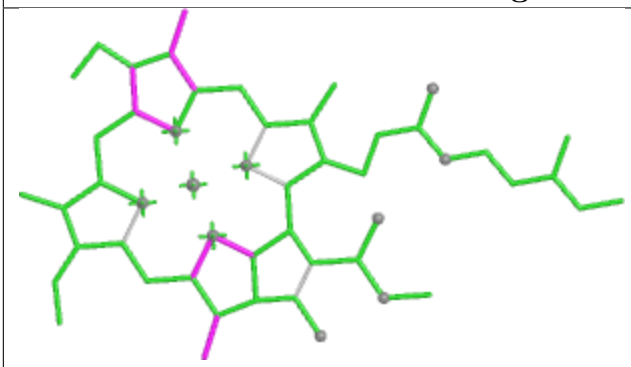
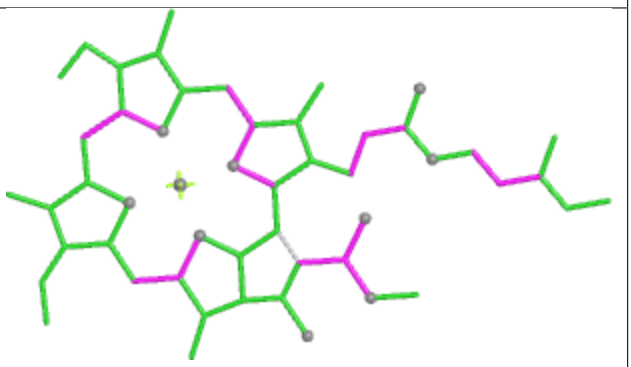
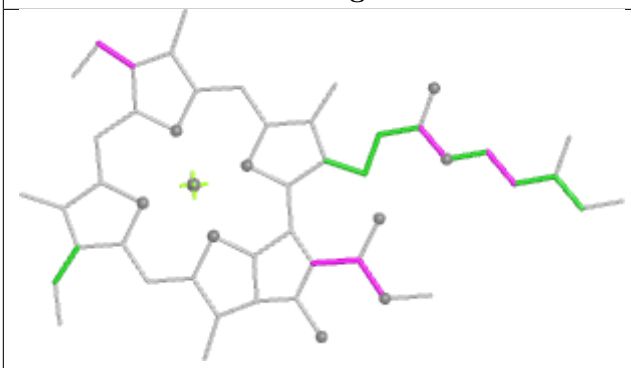
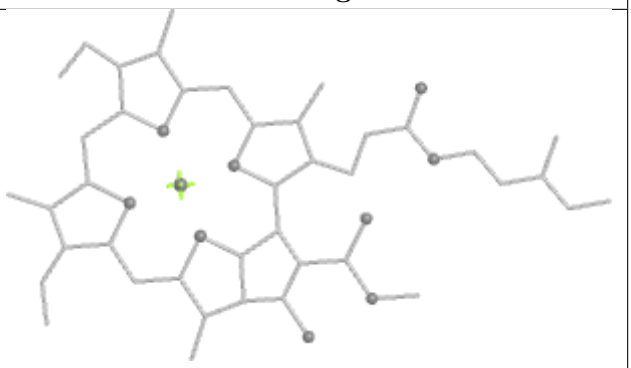
Bond angles

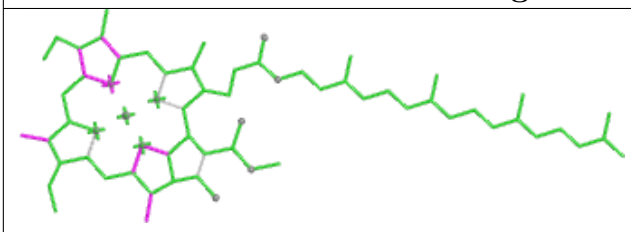
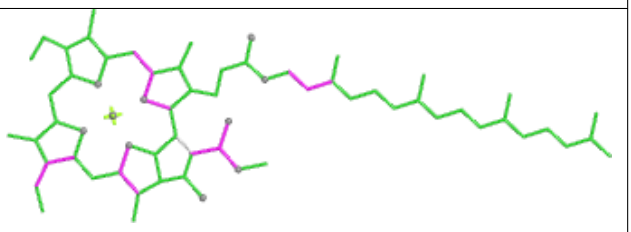
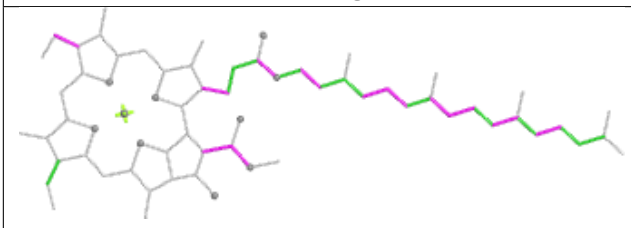
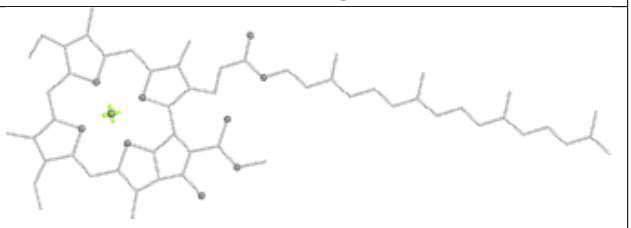


Torsions

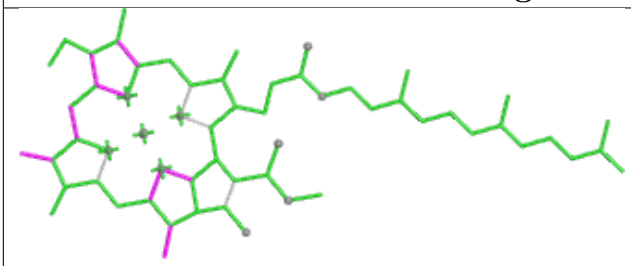


Rings

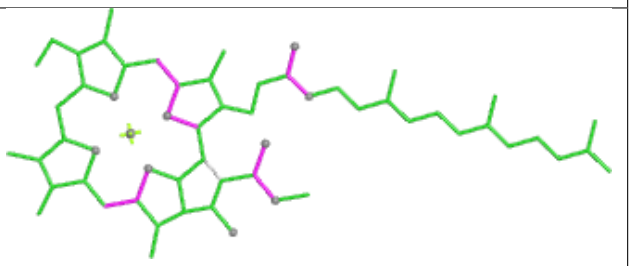
Ligand CLA BA 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BA 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

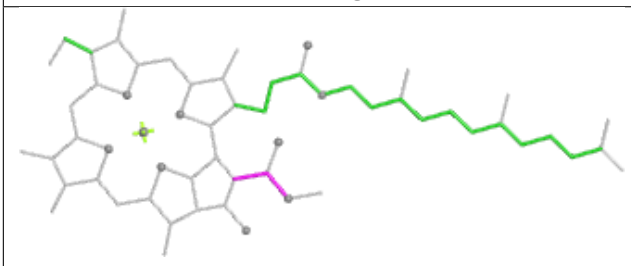
Ligand CLA A1 311



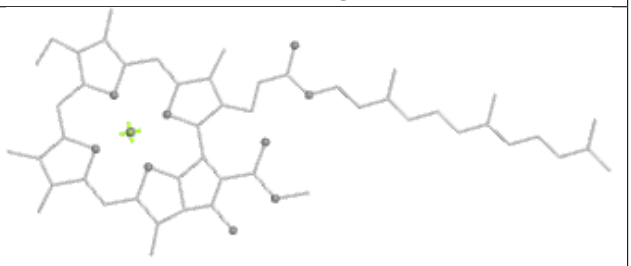
Bond lengths



Bond angles

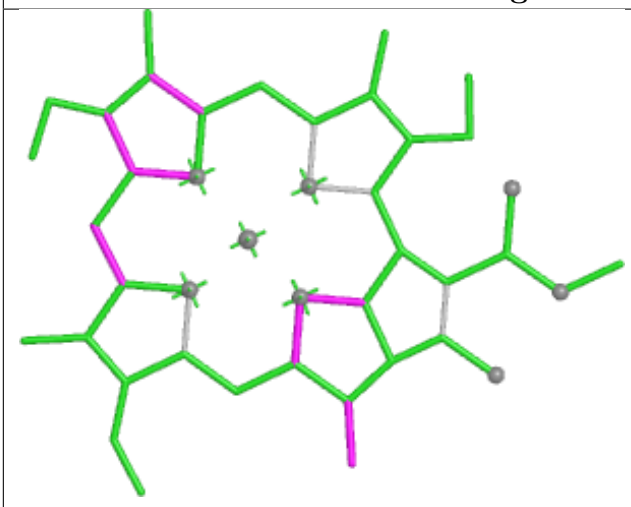


Torsions

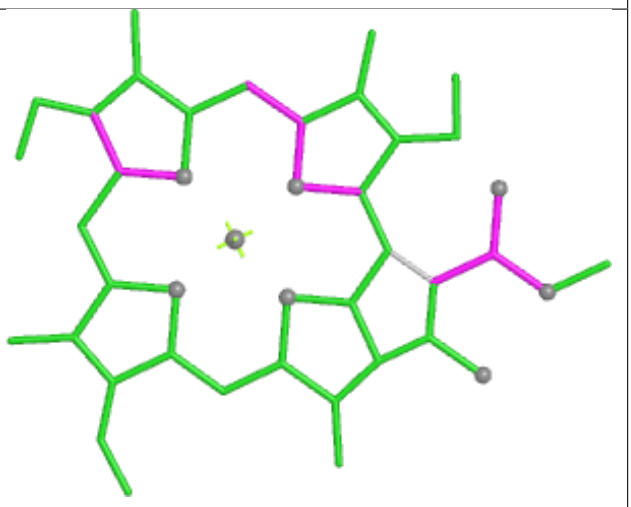


Rings

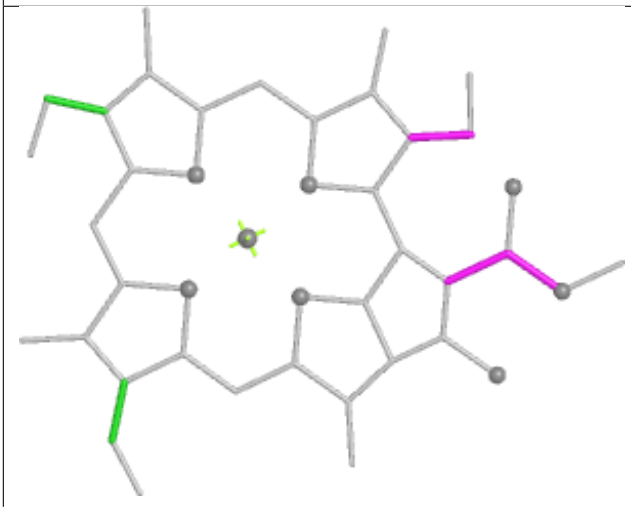
Ligand CLA BG 201



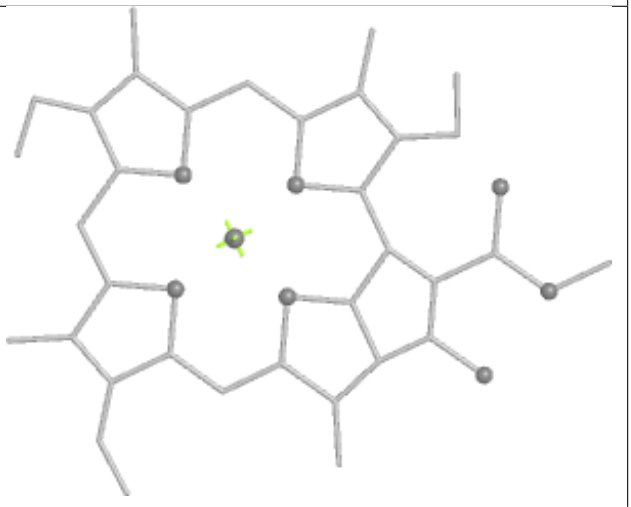
Bond lengths



Bond angles

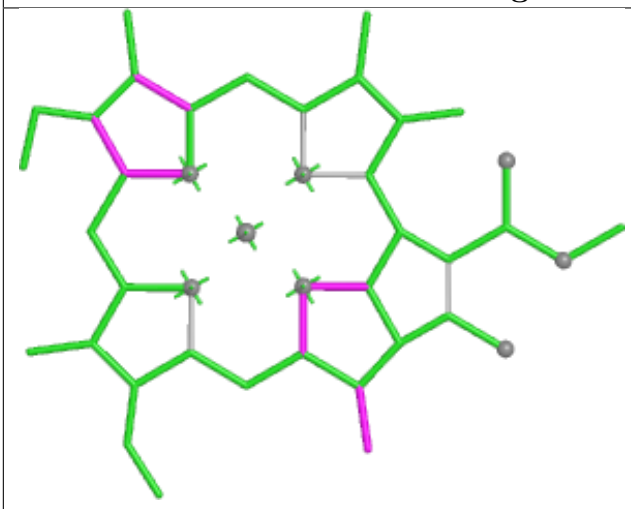


Torsions

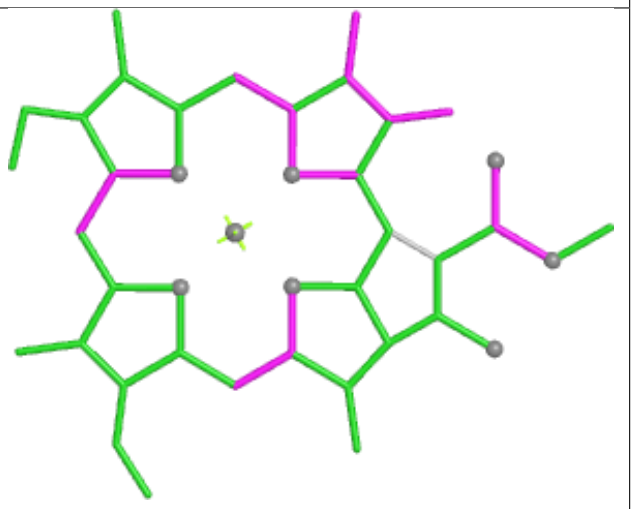


Rings

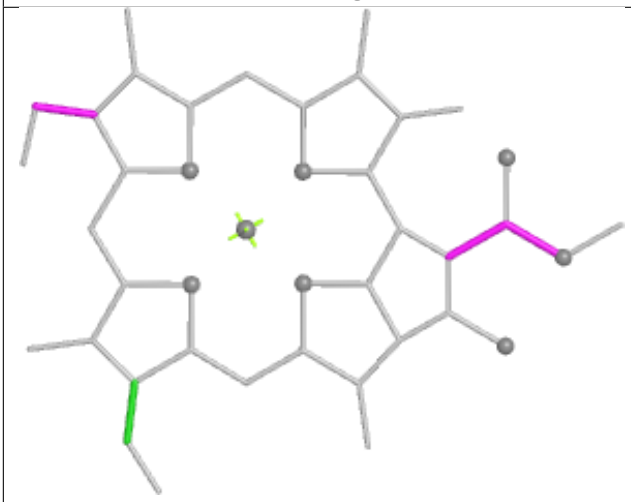
Ligand CLA BA 823



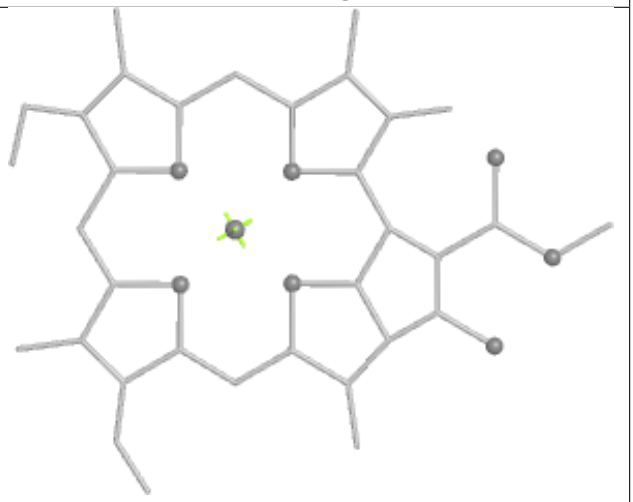
Bond lengths



Bond angles



Torsions

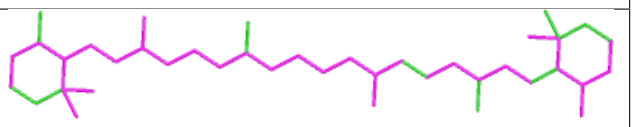


Rings

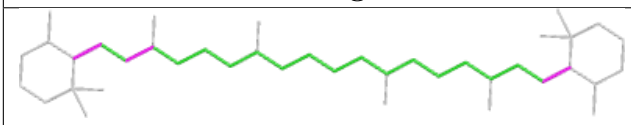
Ligand BCR AJ 103



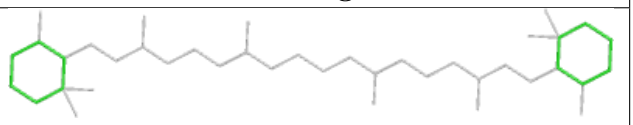
Bond lengths



Bond angles

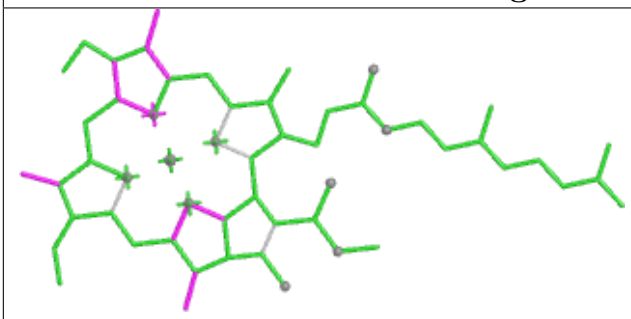


Torsions

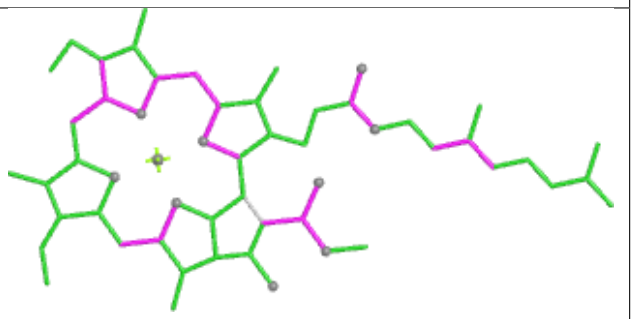


Rings

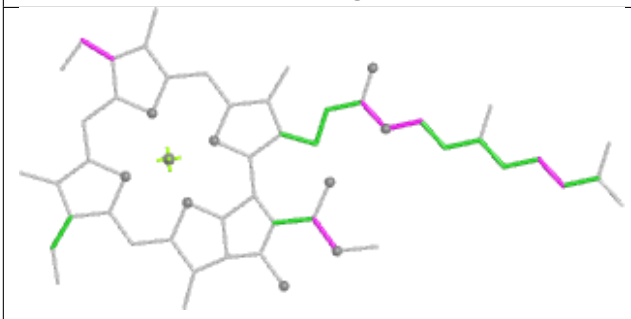
Ligand CLA AA 838



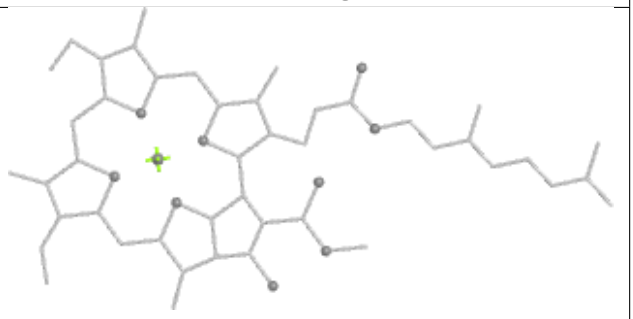
Bond lengths



Bond angles

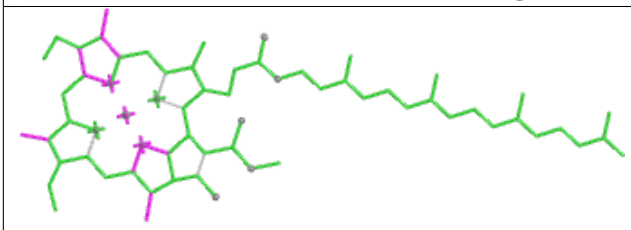


Torsions

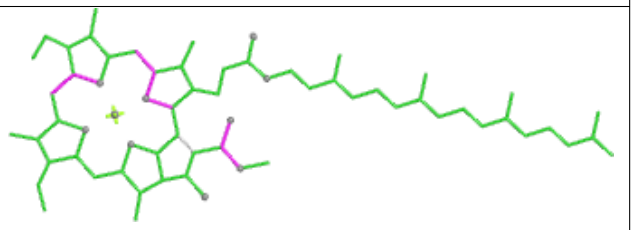


Rings

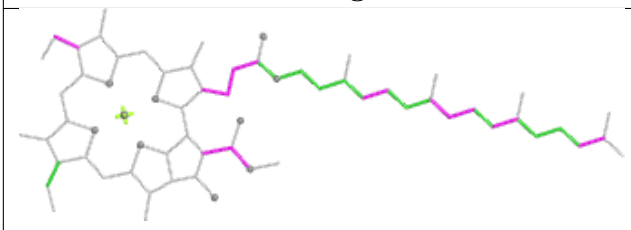
Ligand CLA AB 810



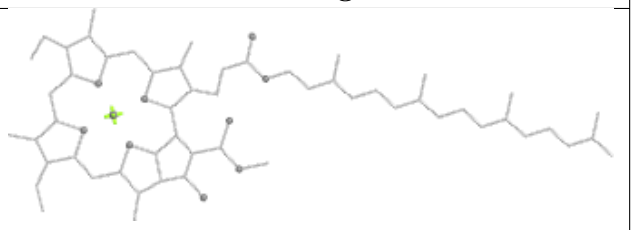
Bond lengths



Bond angles

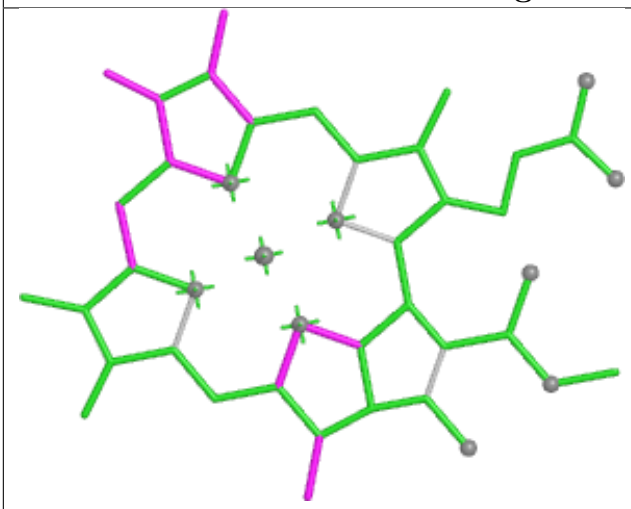


Torsions

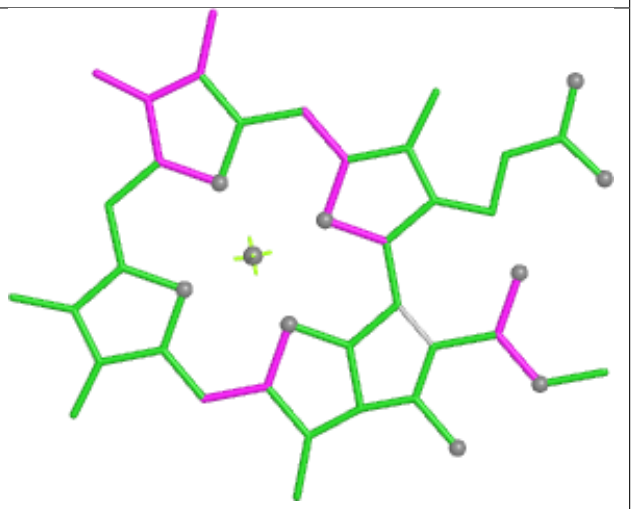


Rings

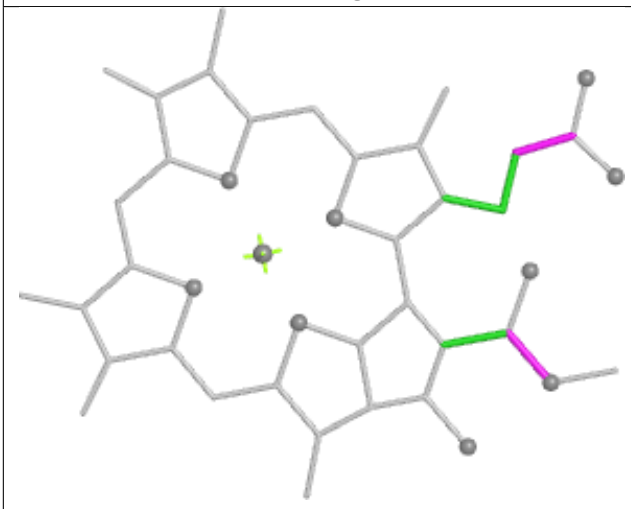
Ligand CLA A4 303



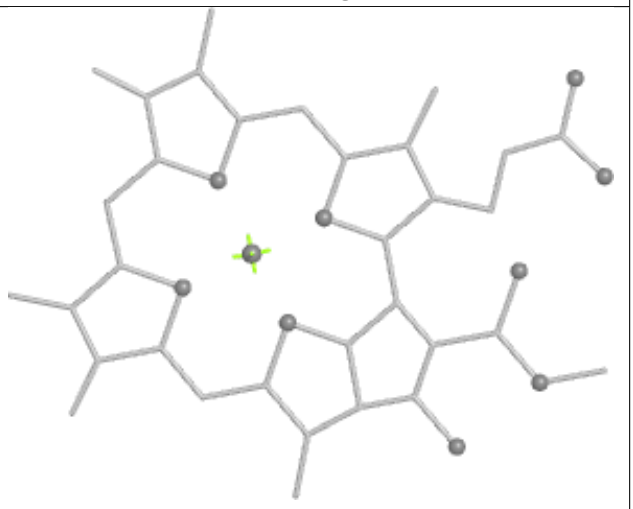
Bond lengths



Bond angles

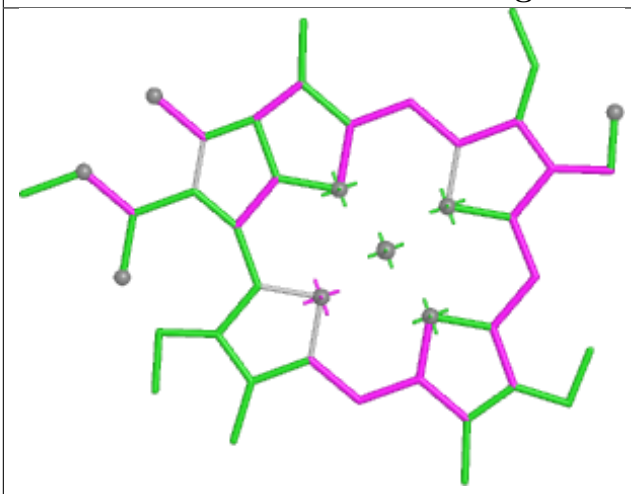


Torsions

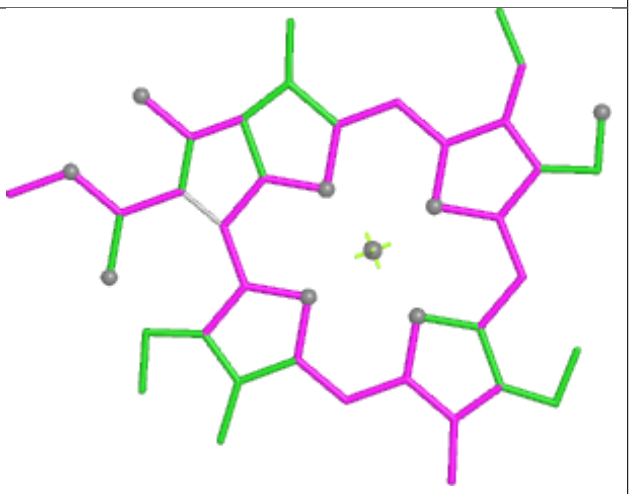


Rings

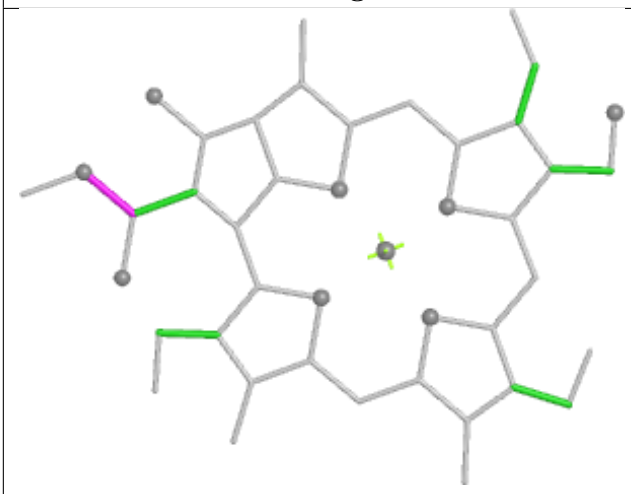
Ligand CHL B2 606



Bond lengths



Bond angles

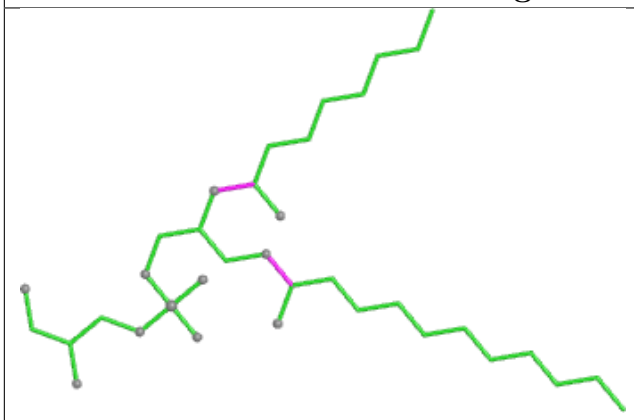


Torsions

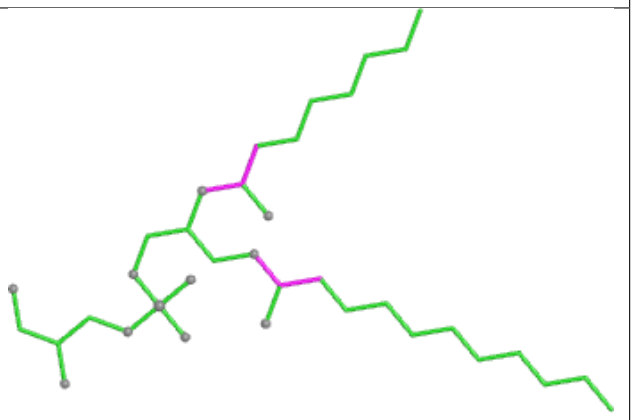


Rings

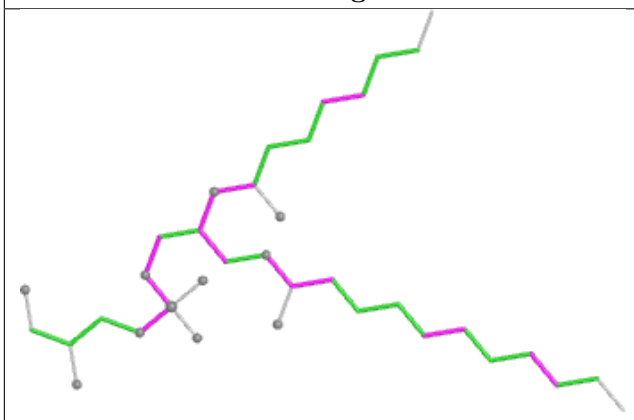
Ligand LHG A6 618



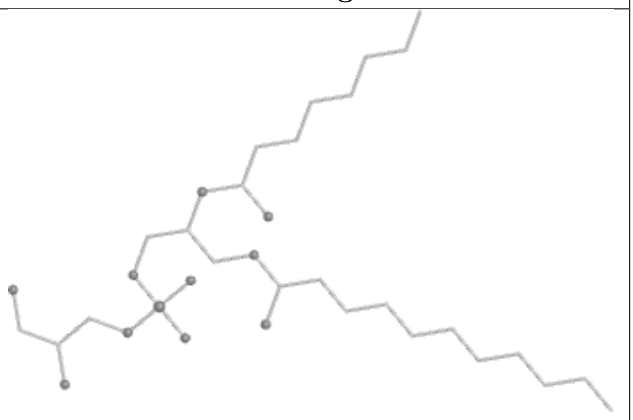
Bond lengths



Bond angles

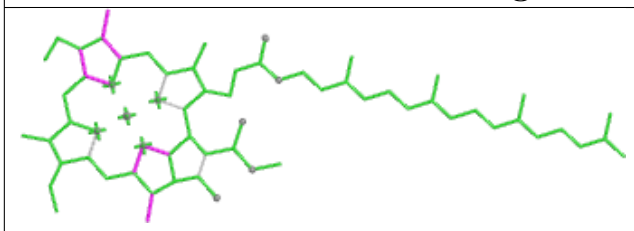


Torsions

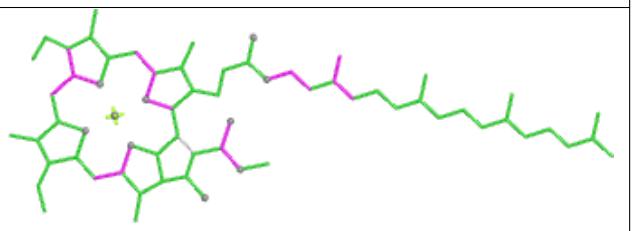


Rings

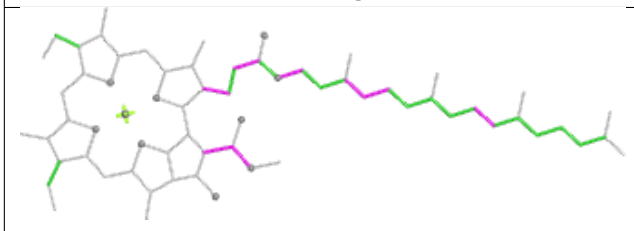
Ligand CLA AB 833



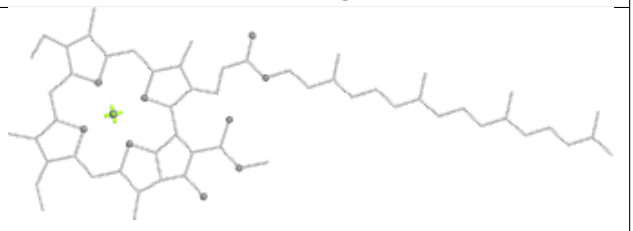
Bond lengths



Bond angles

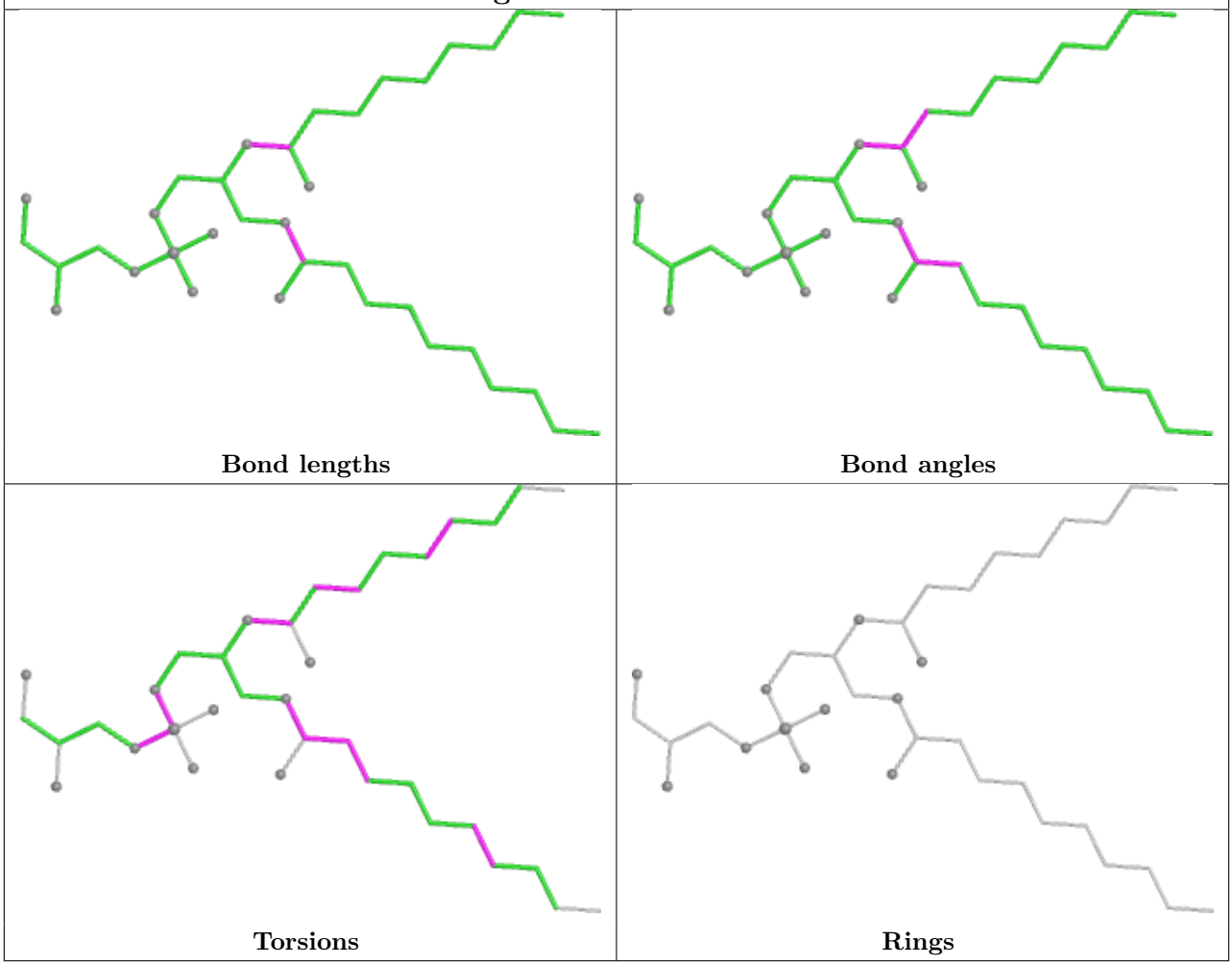


Torsions

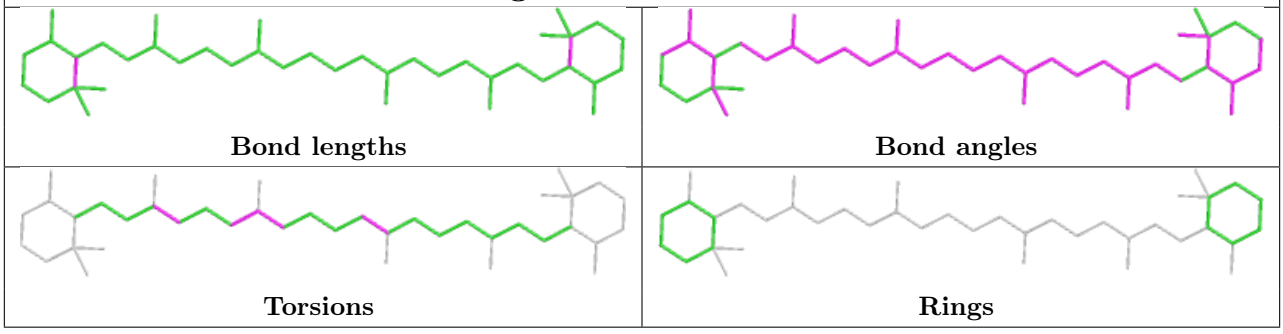


Rings

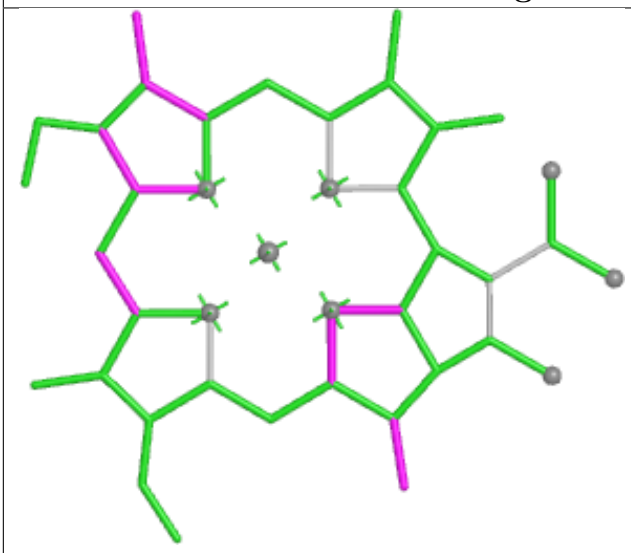
Ligand LHG A1 302



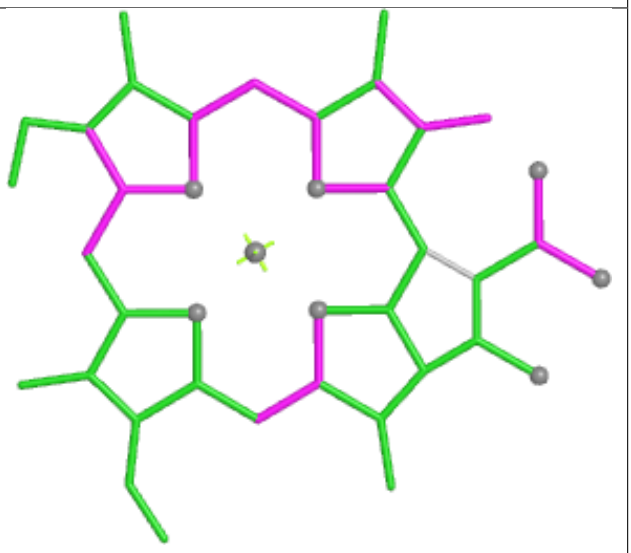
Ligand BCR BG 203



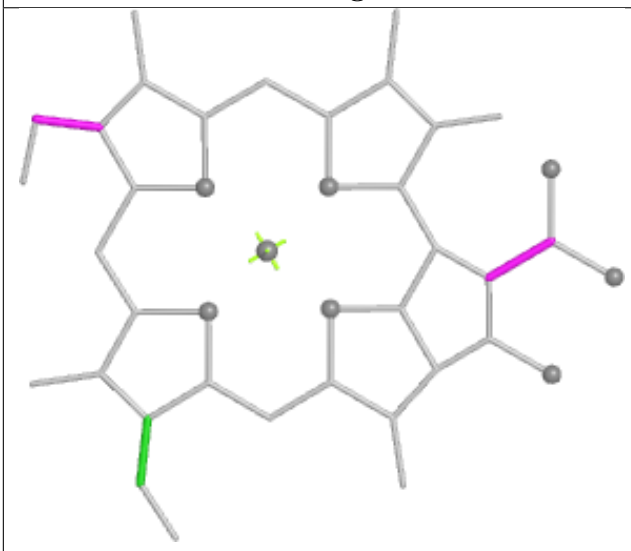
Ligand CLA A3 313



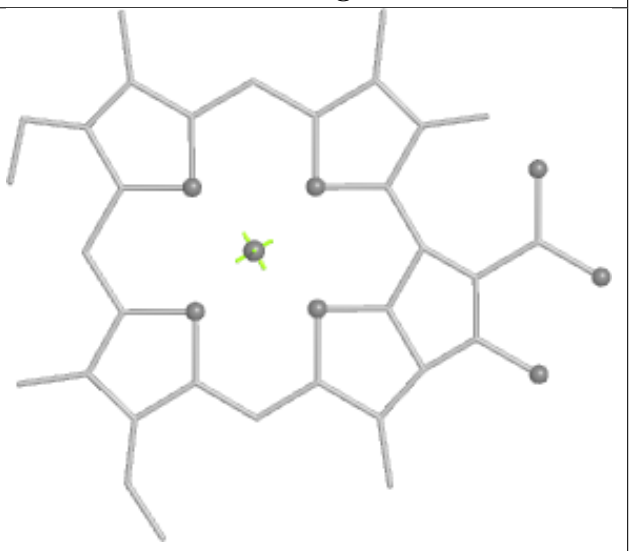
Bond lengths



Bond angles

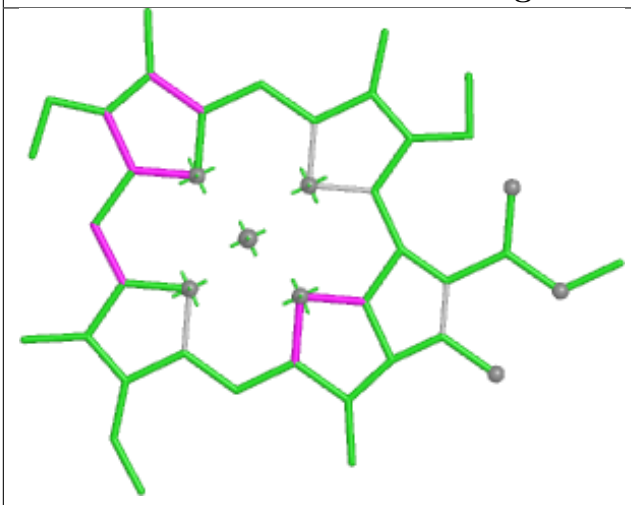


Torsions

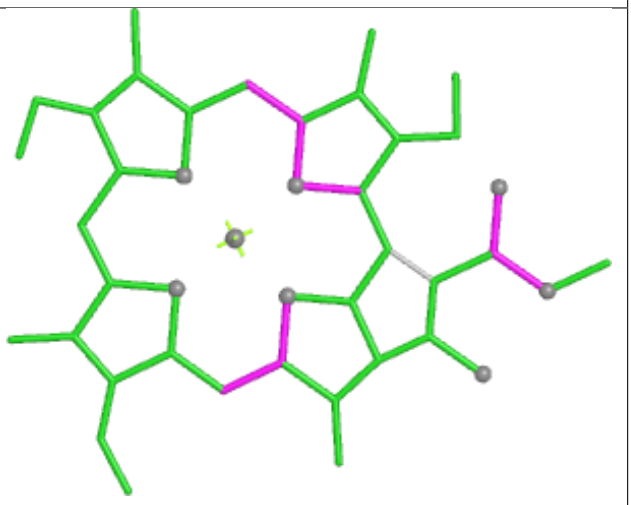


Rings

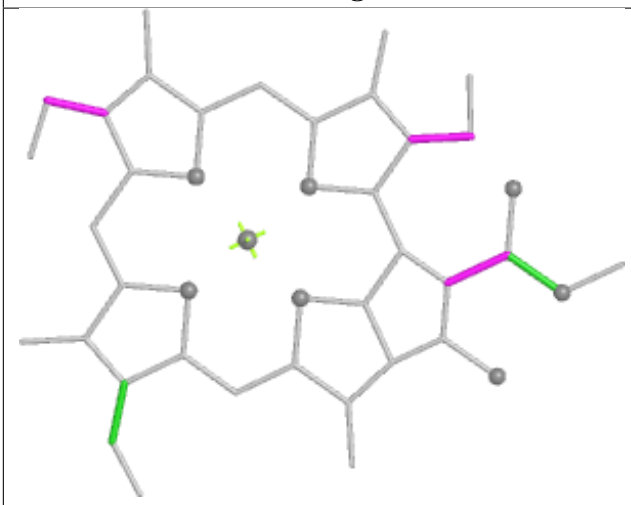
Ligand CLA AJ 102



Bond lengths



Bond angles

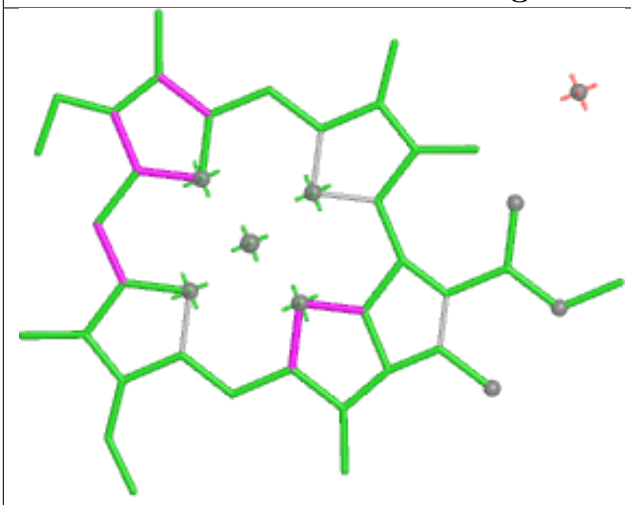


Torsions

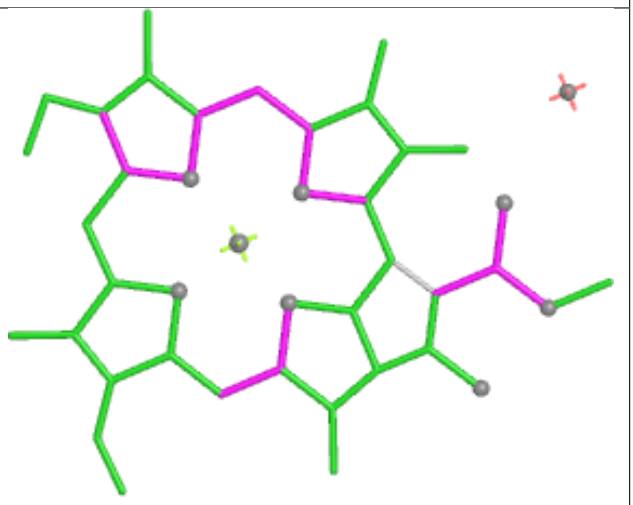


Rings

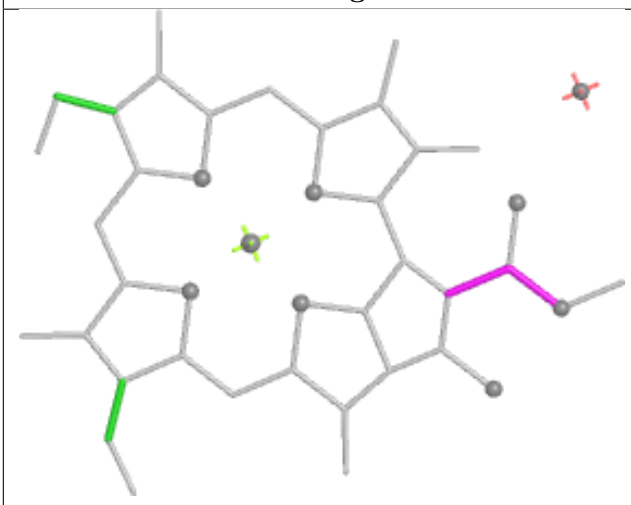
Ligand CLA BA 844



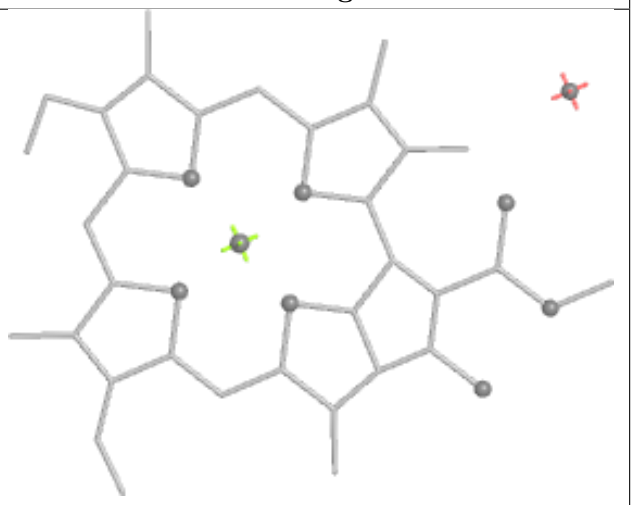
Bond lengths



Bond angles

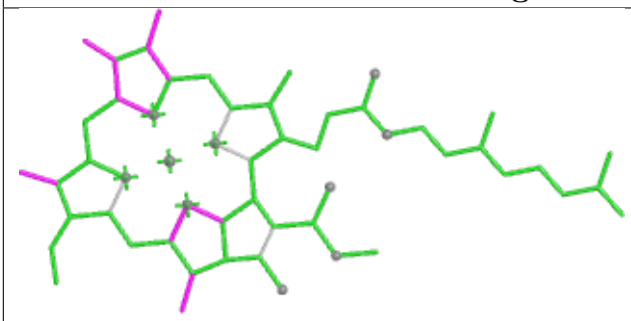


Torsions

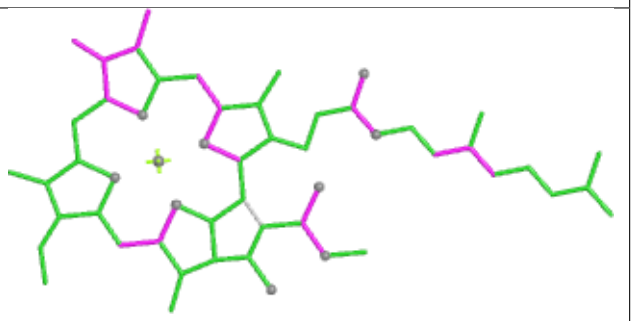


Rings

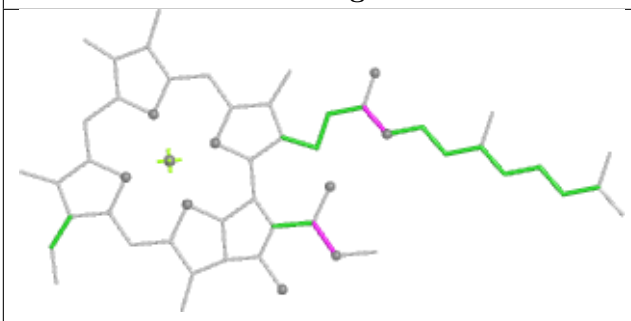
Ligand CLA BB 813



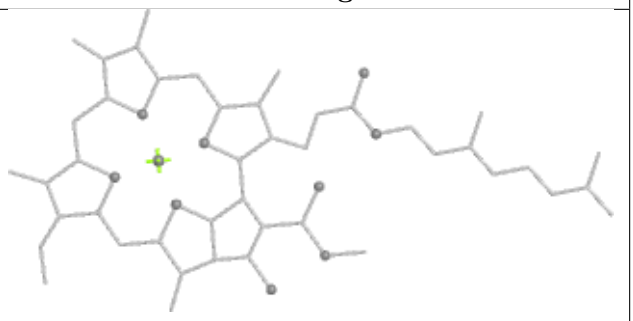
Bond lengths



Bond angles

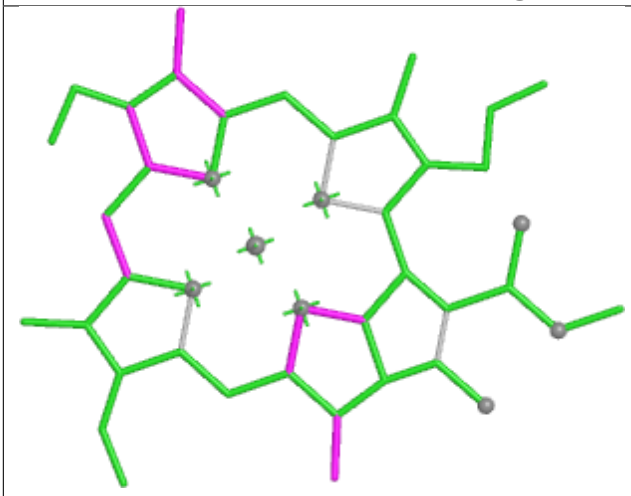


Torsions

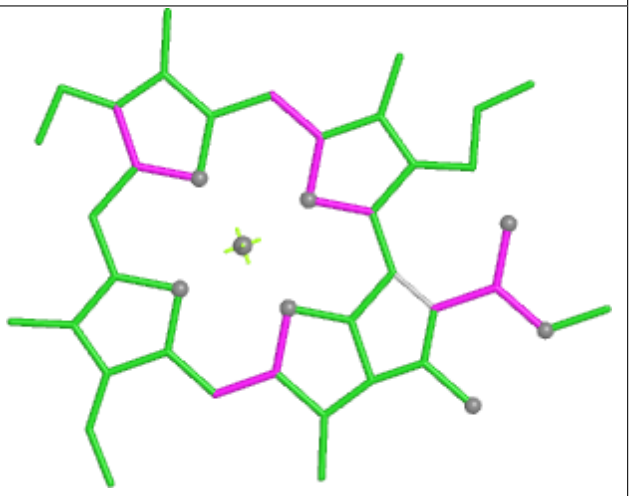


Rings

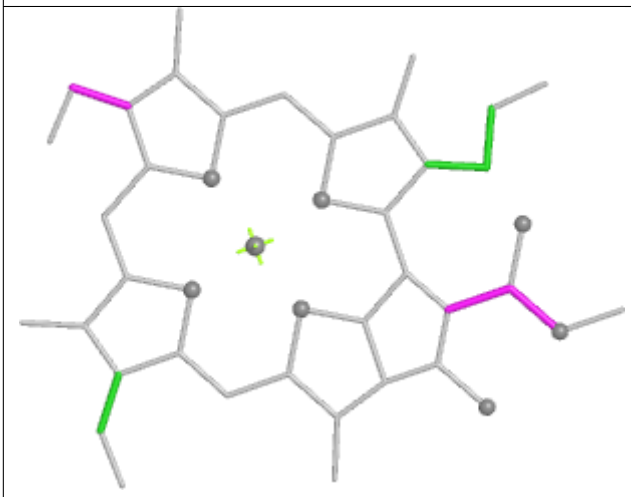
Ligand CLA AB 813



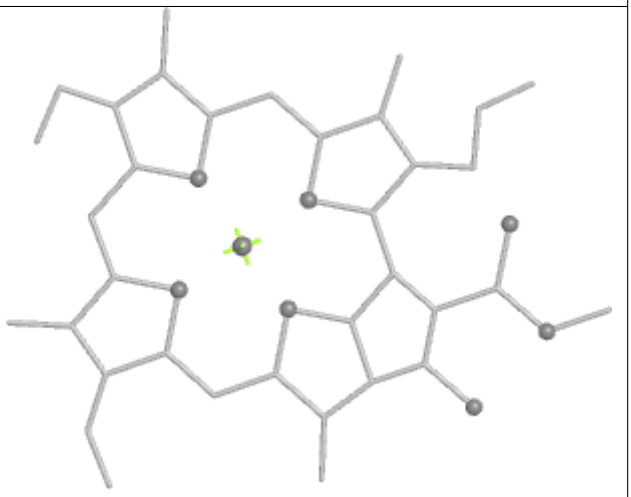
Bond lengths



Bond angles

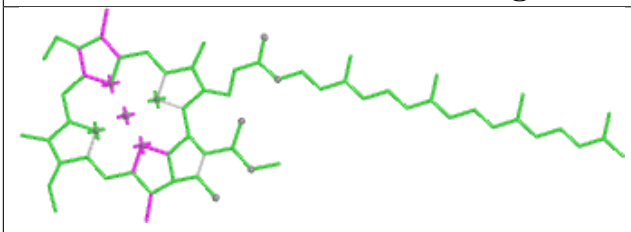


Torsions

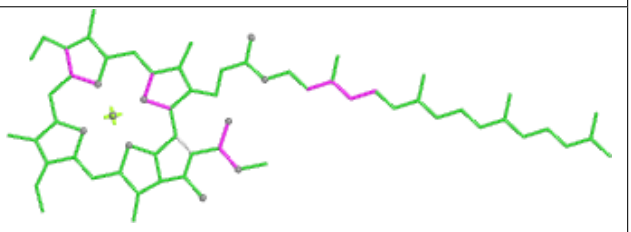


Rings

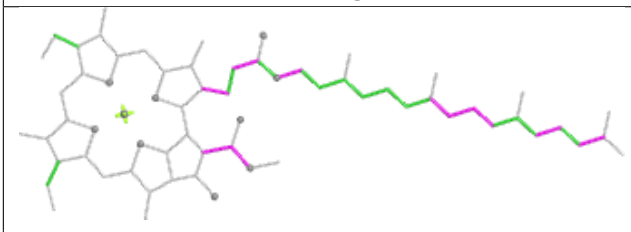
Ligand CLA BA 825



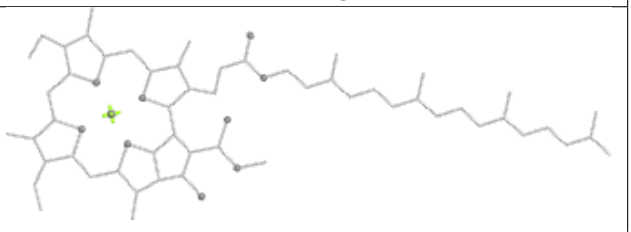
Bond lengths



Bond angles

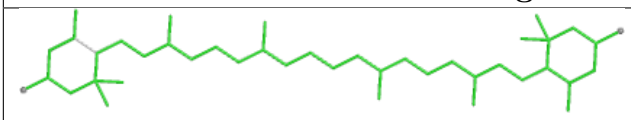


Torsions

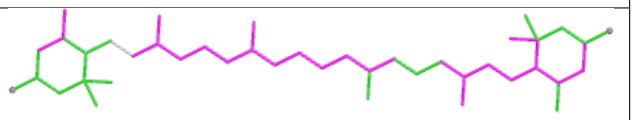


Rings

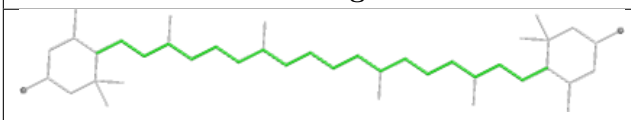
Ligand LUT B2 615



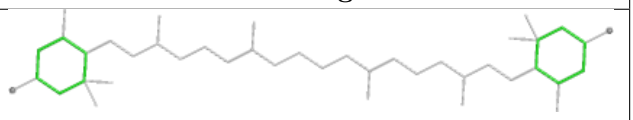
Bond lengths



Bond angles

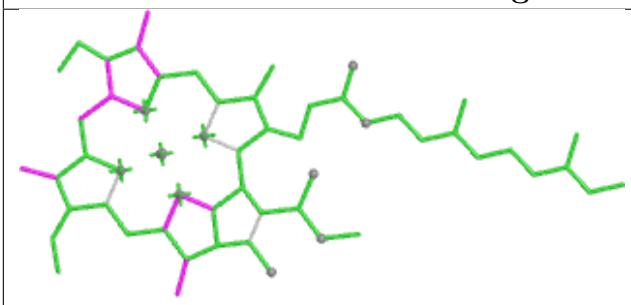


Torsions

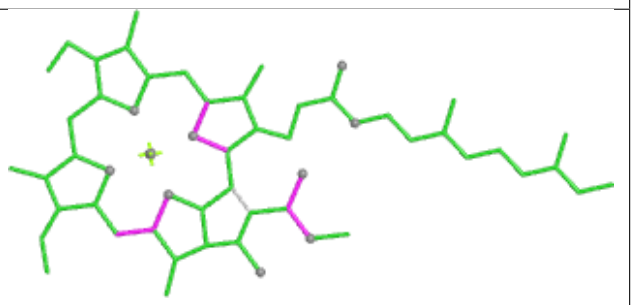


Rings

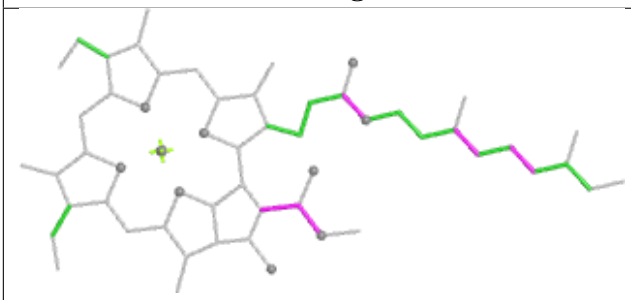
Ligand CLA BB 831



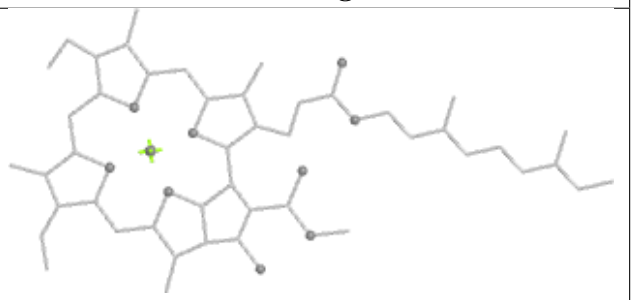
Bond lengths



Bond angles

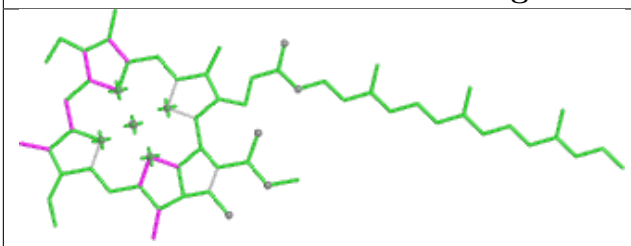


Torsions

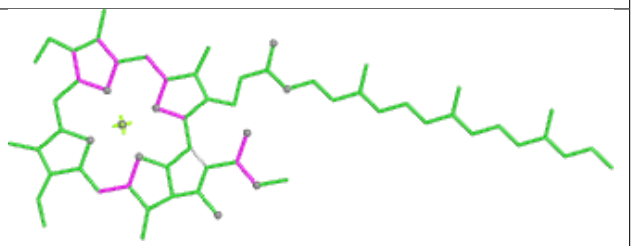


Rings

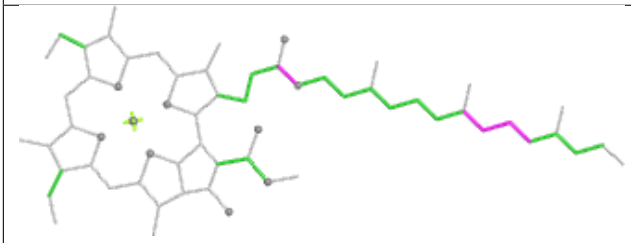
Ligand CLA AB 826



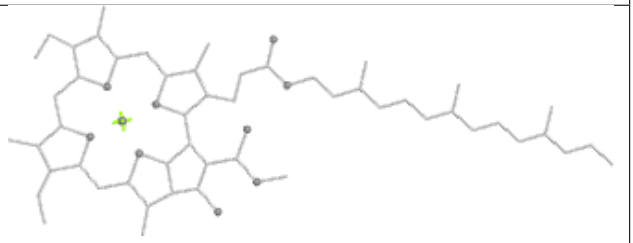
Bond lengths



Bond angles

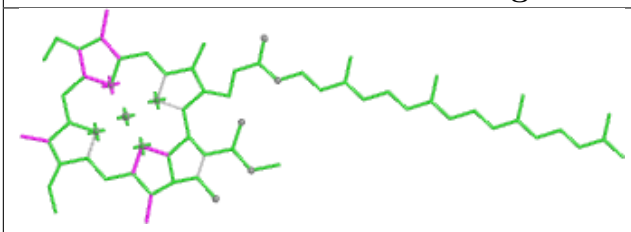


Torsions

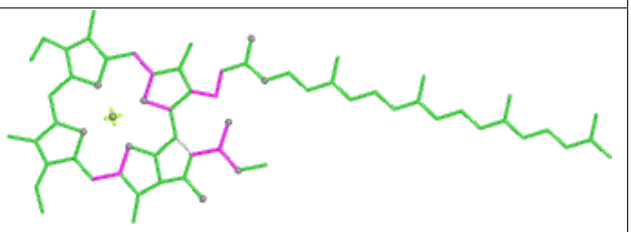


Rings

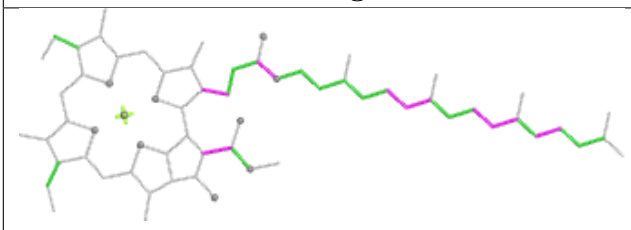
Ligand CLA BA 819



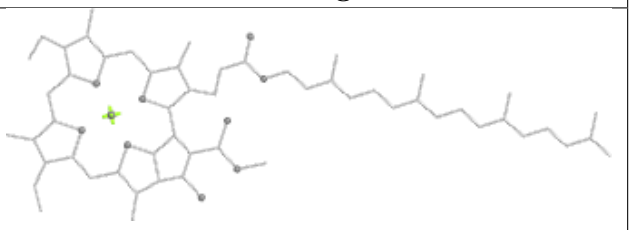
Bond lengths



Bond angles



Torsions

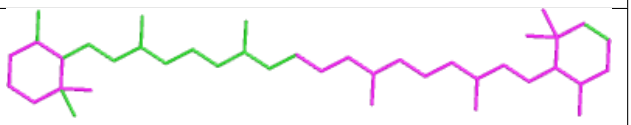


Rings

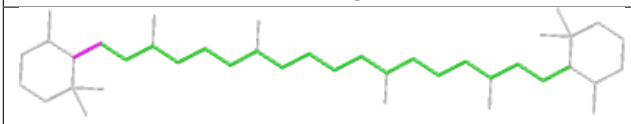
Ligand BCR BB 848



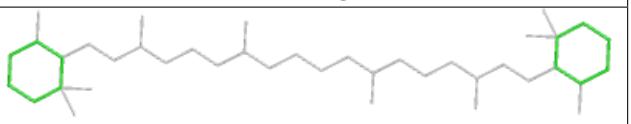
Bond lengths



Bond angles

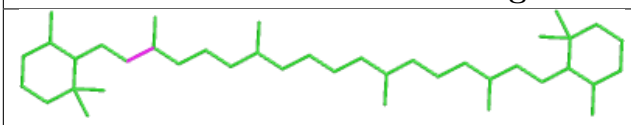


Torsions

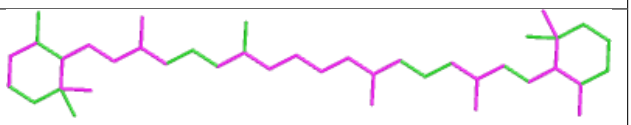


Rings

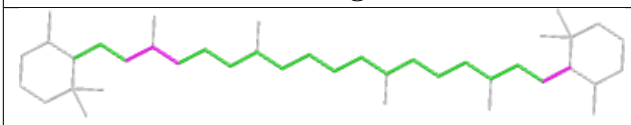
Ligand BCR AB 845



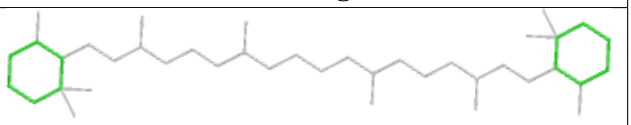
Bond lengths



Bond angles

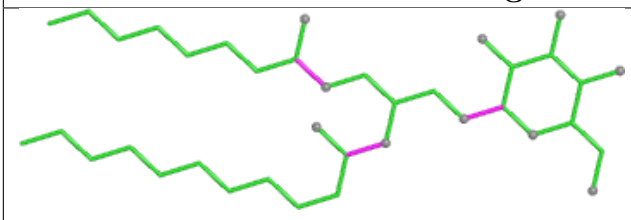


Torsions

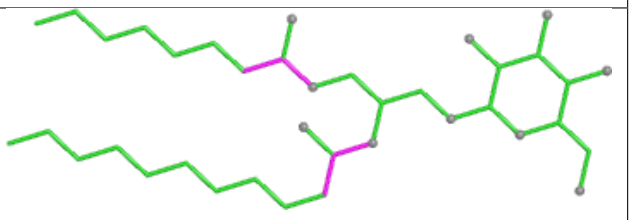


Rings

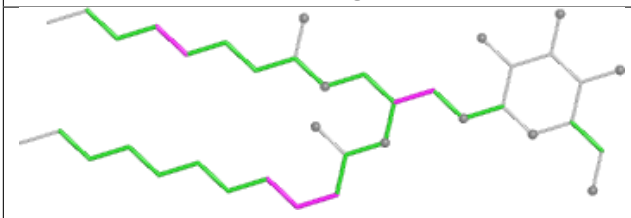
Ligand LMG AG 202



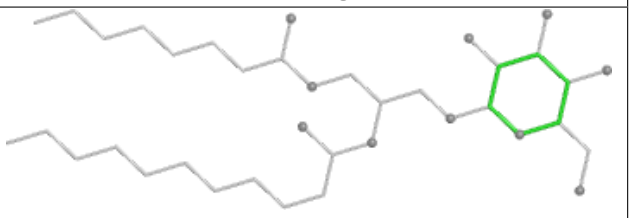
Bond lengths



Bond angles

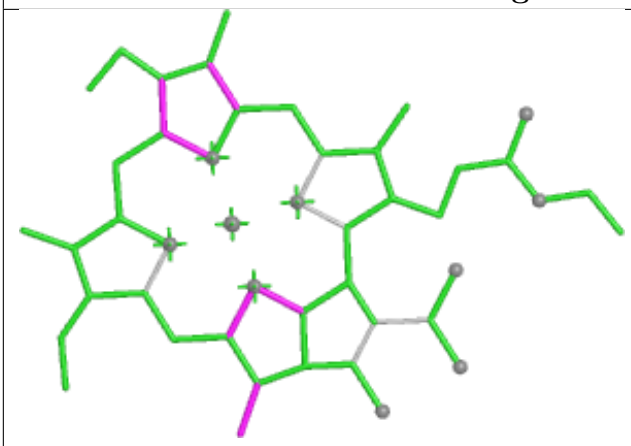


Torsions

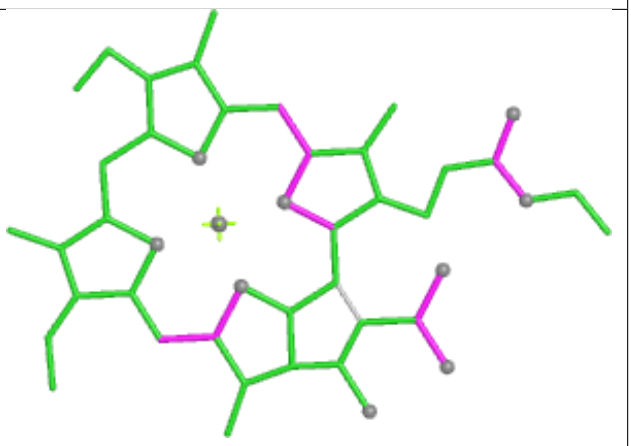


Rings

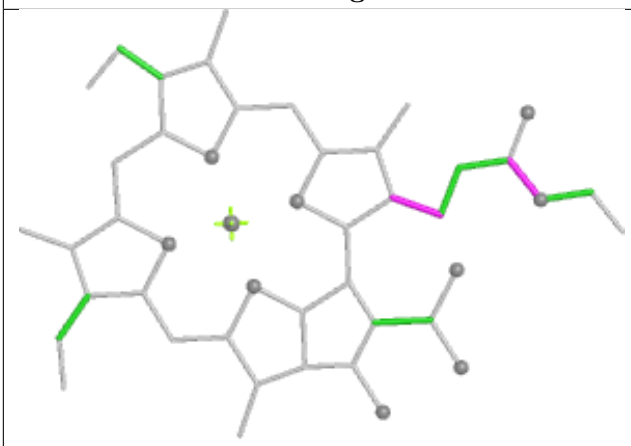
Ligand CLA BB 823



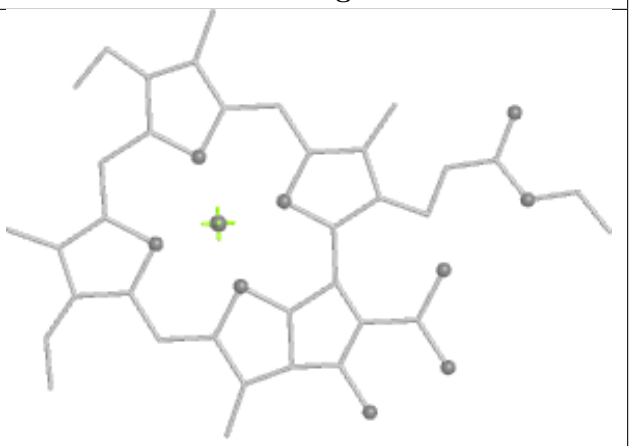
Bond lengths



Bond angles

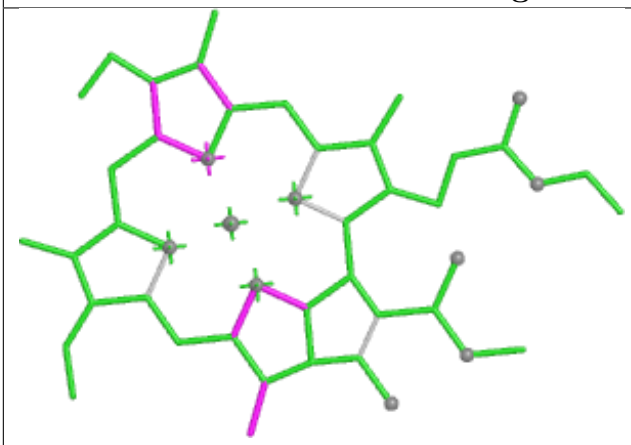


Torsions

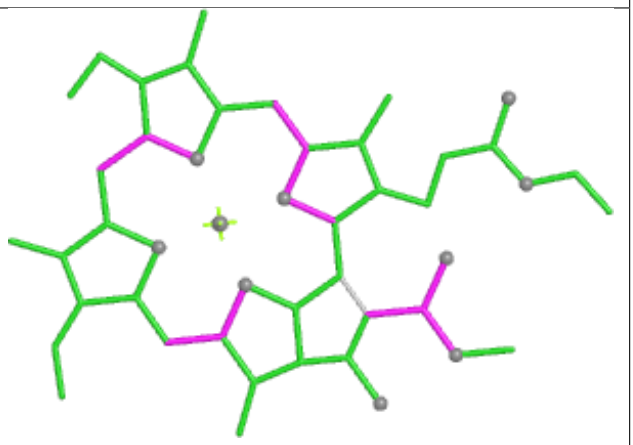


Rings

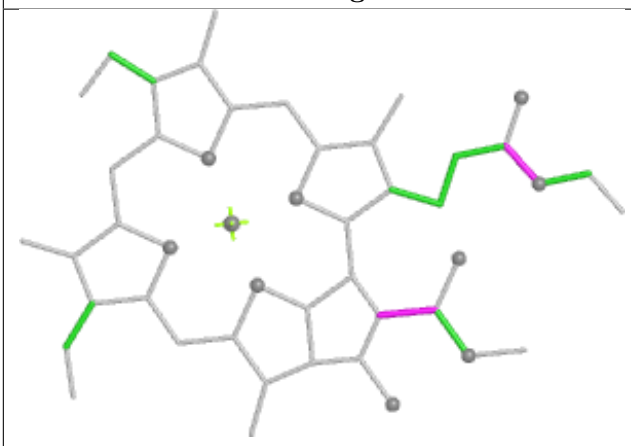
Ligand CLA BB 840



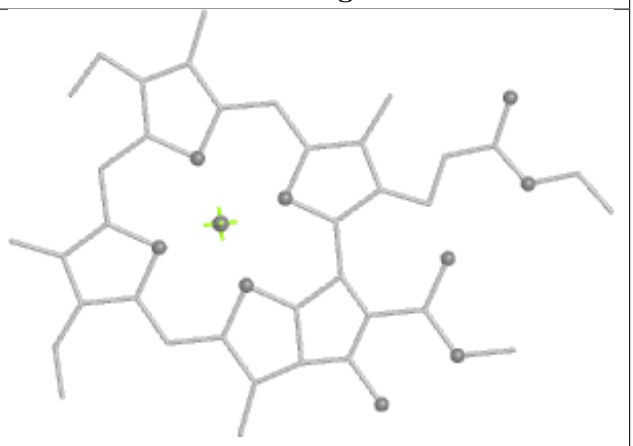
Bond lengths



Bond angles

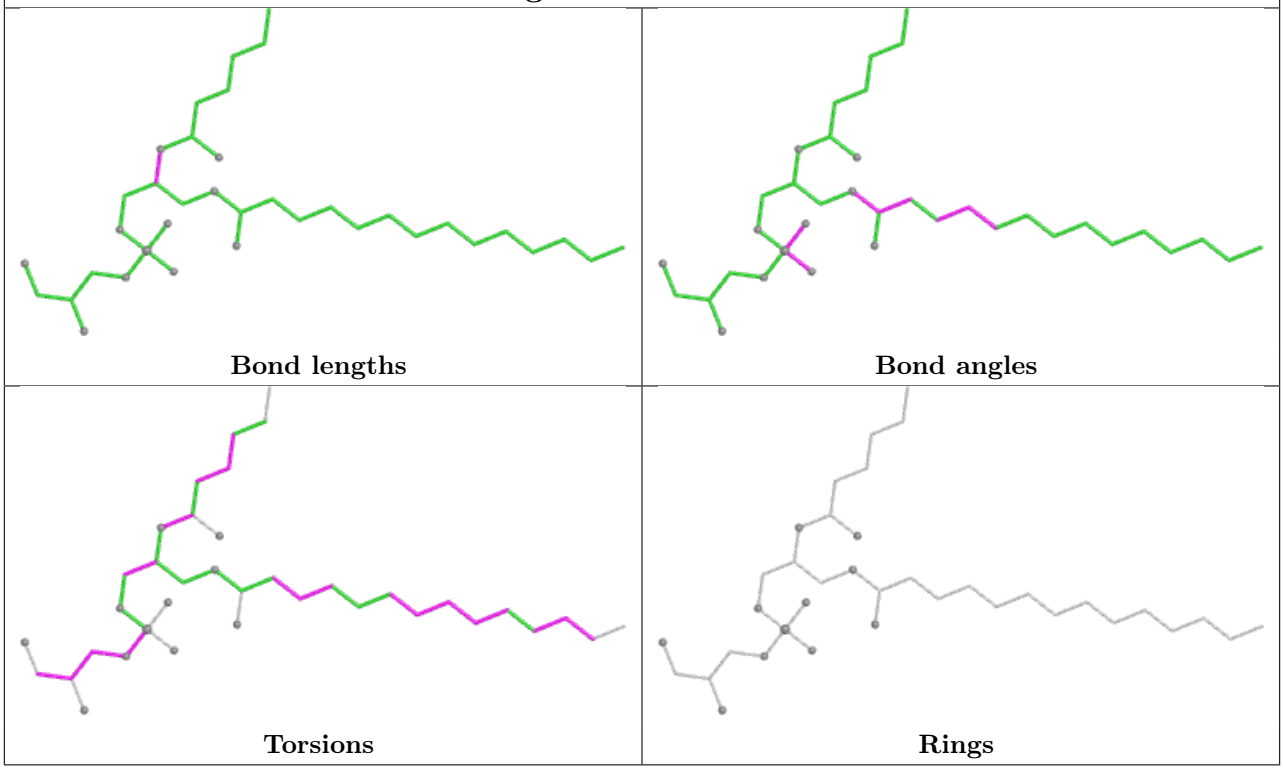


Torsions

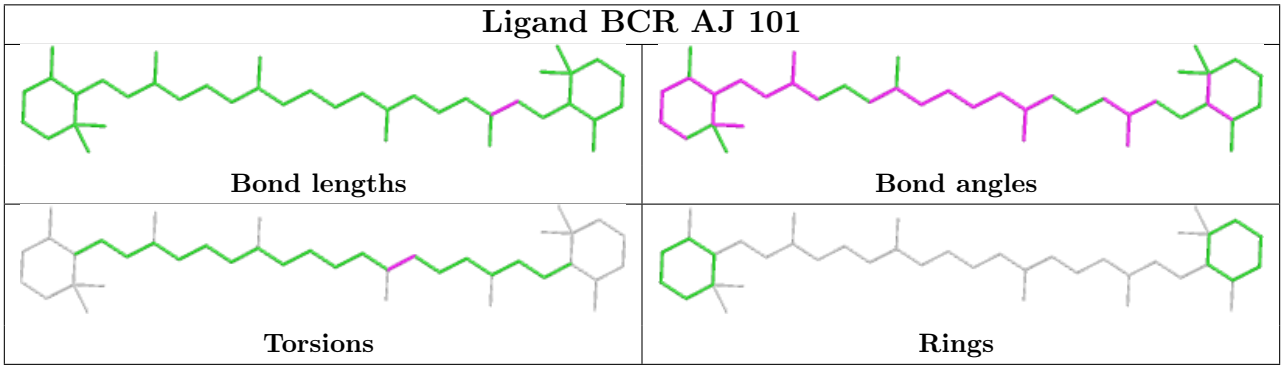


Rings

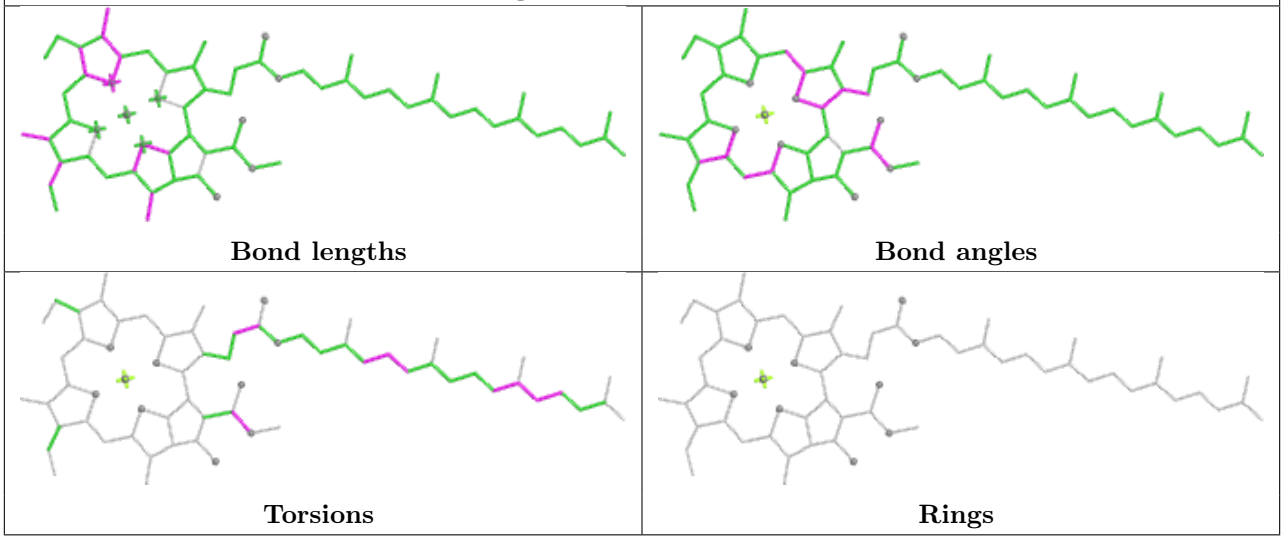
Ligand LHG F 801



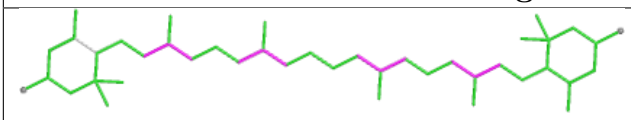
Ligand BCR AJ 101



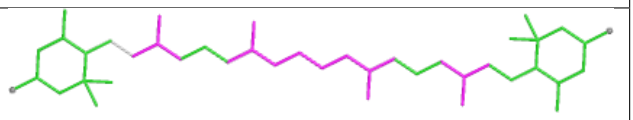
Ligand CLA AB 807



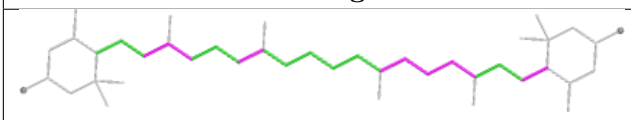
Ligand LUT B1 316



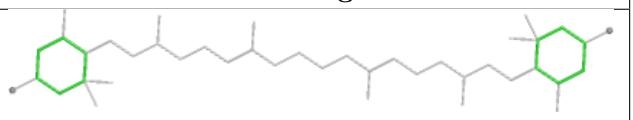
Bond lengths



Bond angles



Torsions

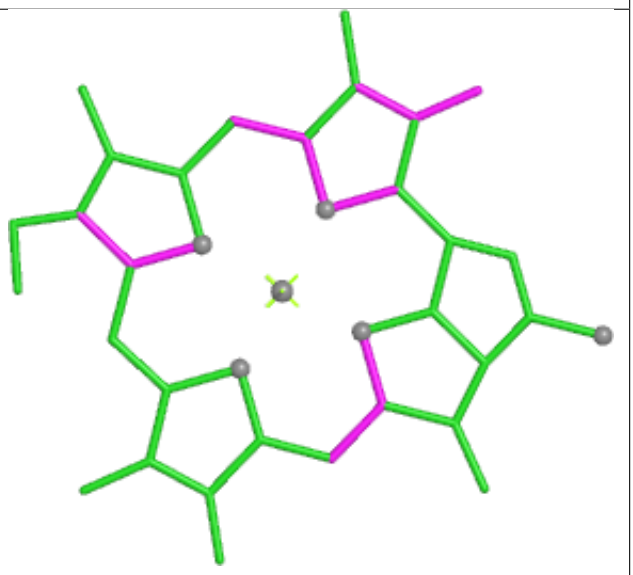


Rings

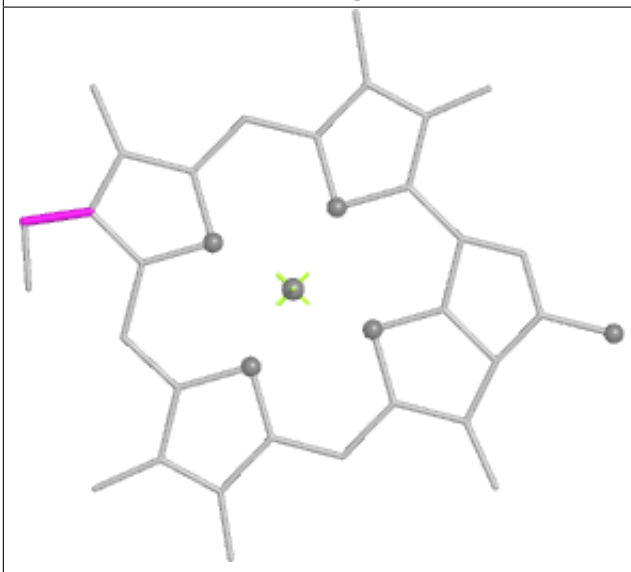
Ligand CLA A3 314



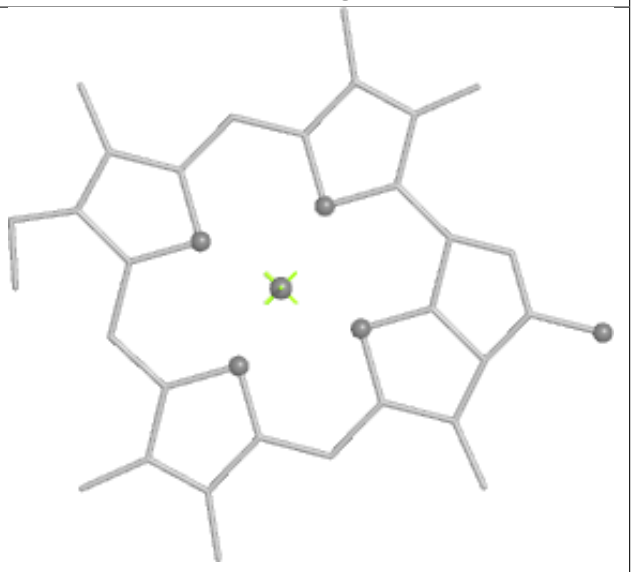
Bond lengths



Bond angles

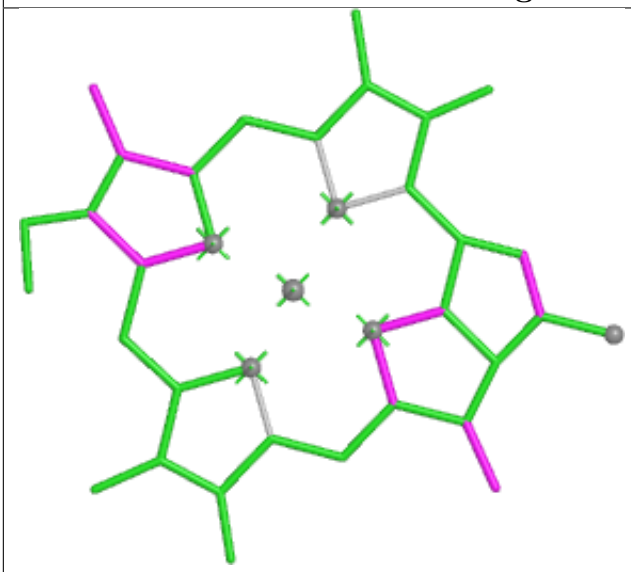


Torsions



Rings

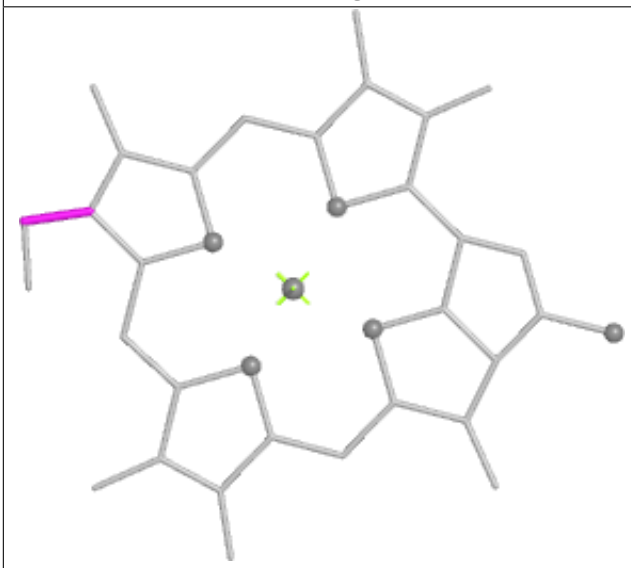
Ligand CLA B3 313



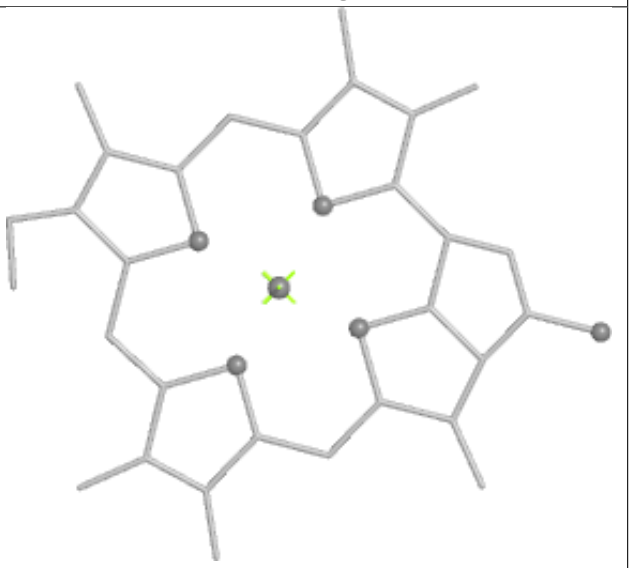
Bond lengths



Bond angles

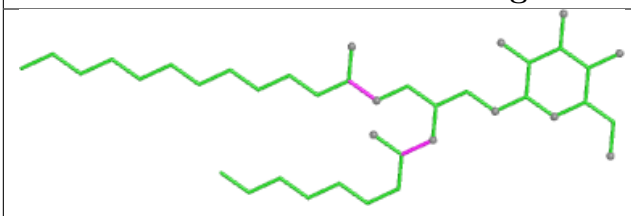


Torsions

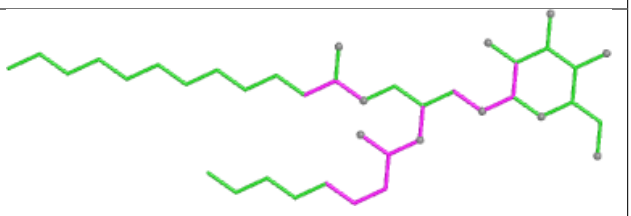


Rings

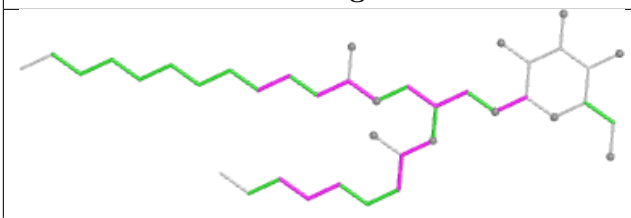
Ligand LMG A4 318



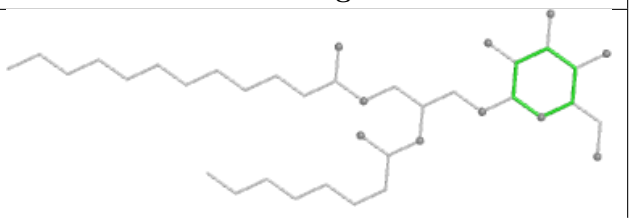
Bond lengths



Bond angles

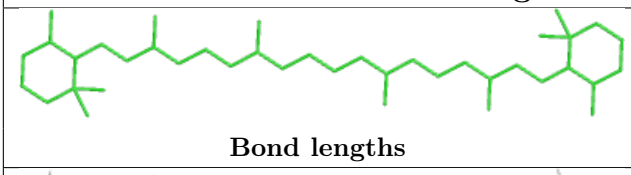


Torsions

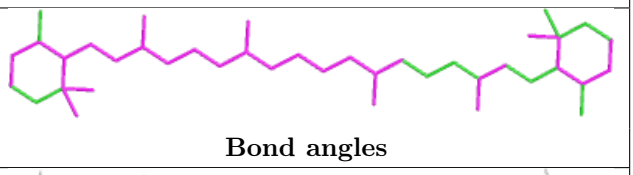


Rings

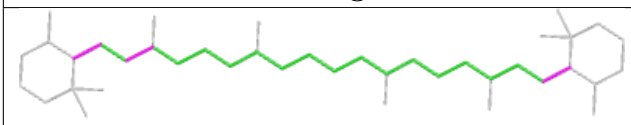
Ligand BCR BJ 103



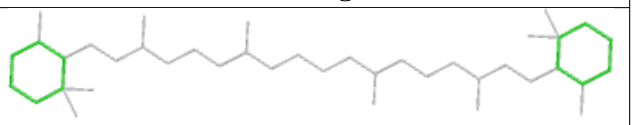
Bond lengths



Bond angles

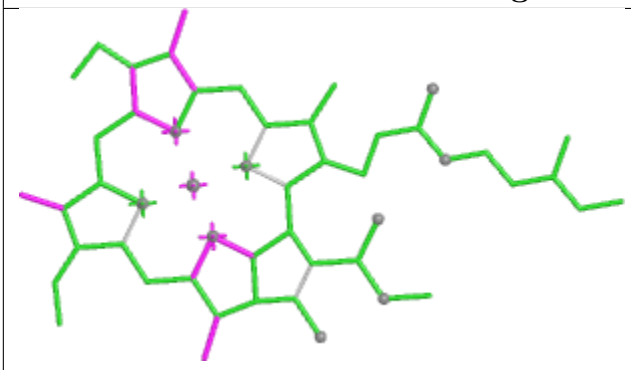


Torsions

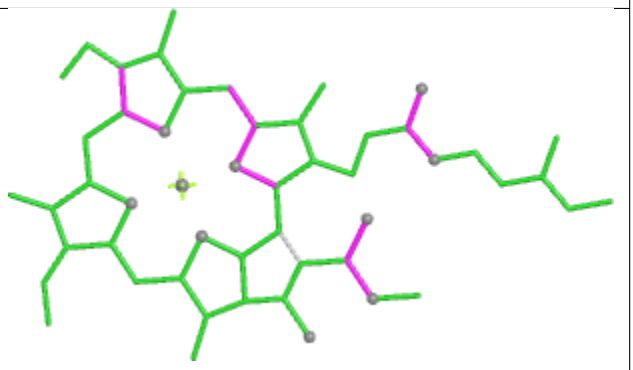


Rings

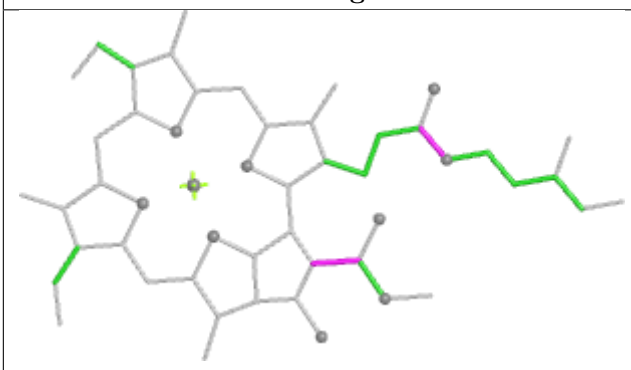
Ligand CLA BA 837



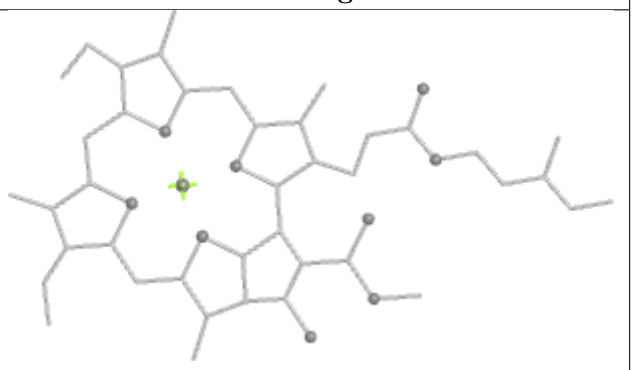
Bond lengths



Bond angles

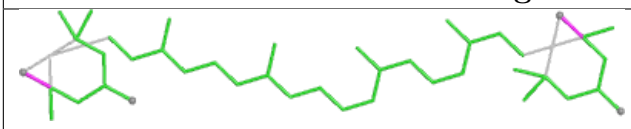


Torsions

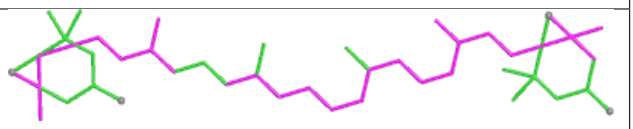


Rings

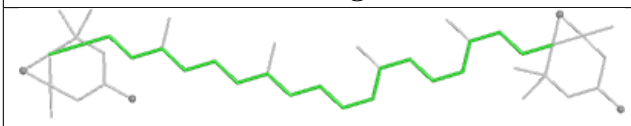
Ligand XAT A4 316



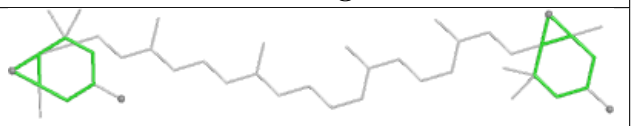
Bond lengths



Bond angles

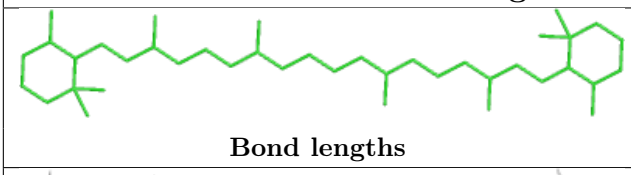


Torsions

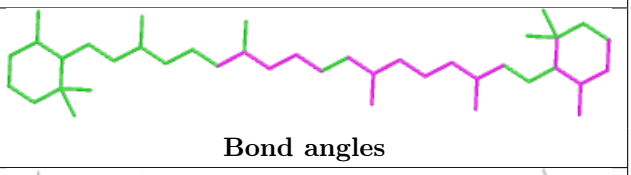


Rings

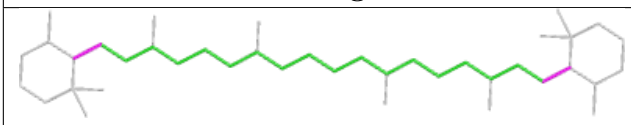
Ligand BCR BA 850



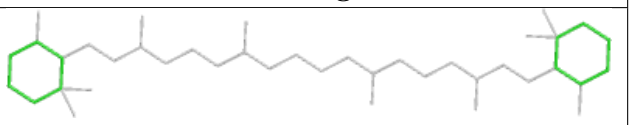
Bond lengths



Bond angles

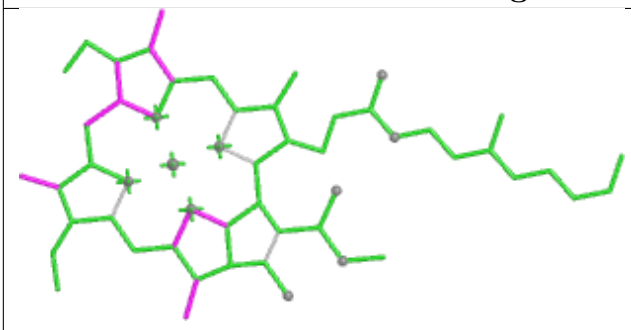


Torsions

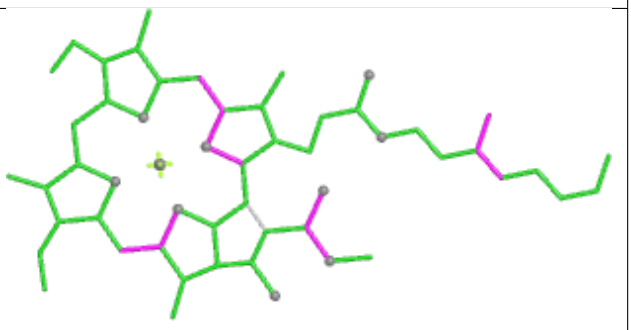


Rings

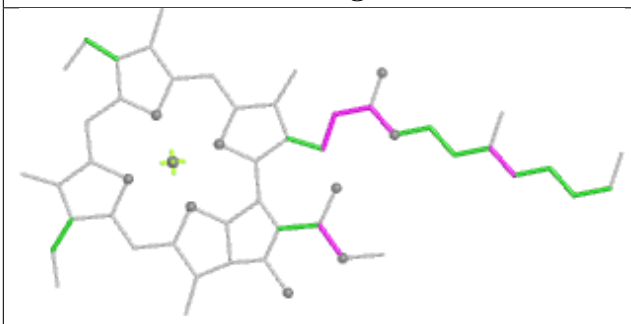
Ligand CLA AA 812



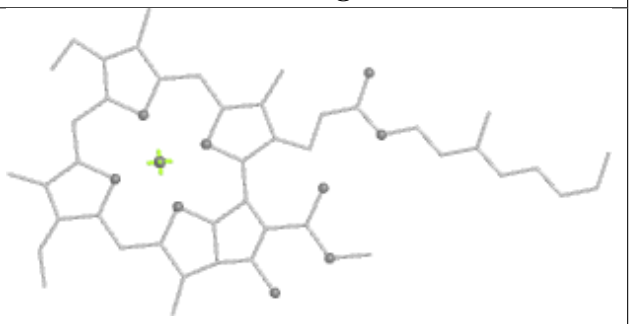
Bond lengths



Bond angles

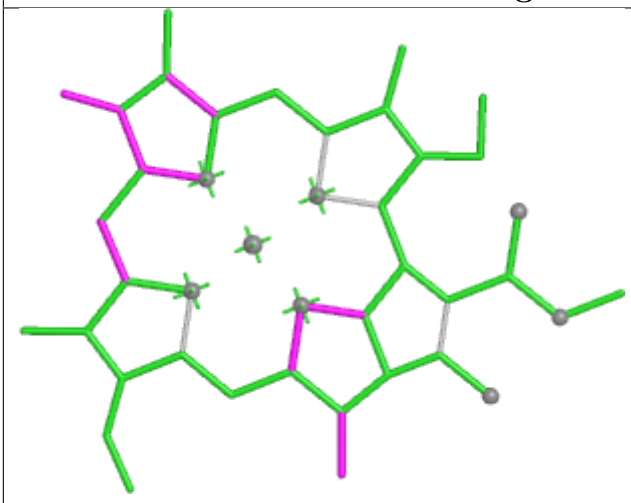


Torsions

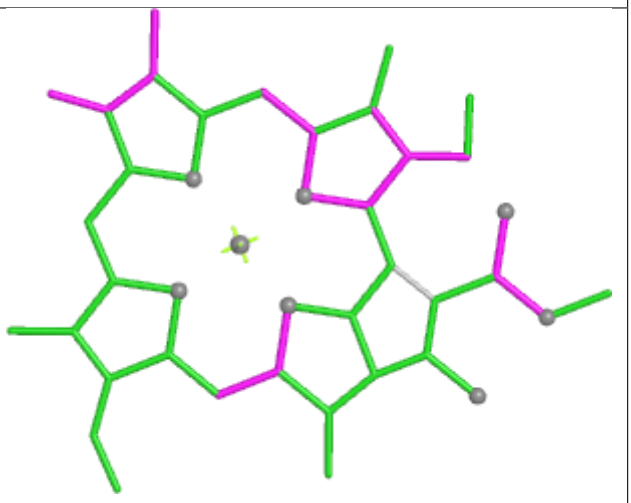


Rings

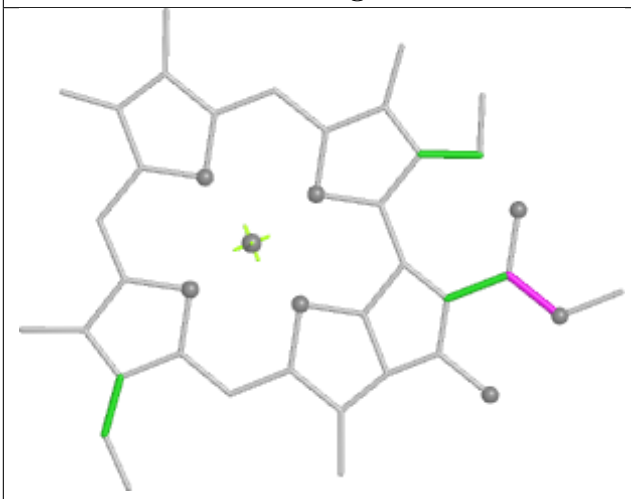
Ligand CLA B3 305



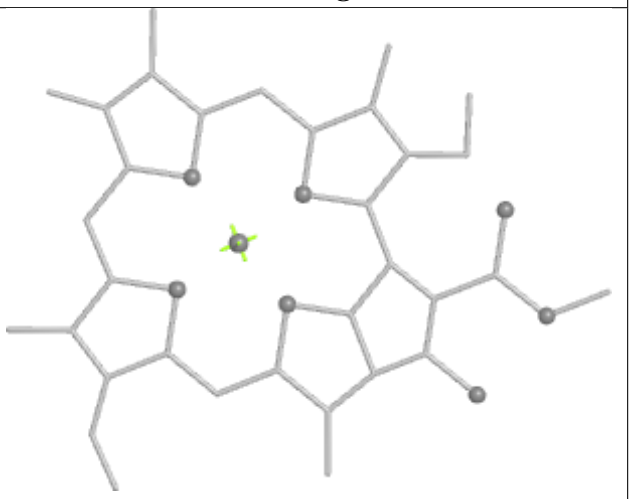
Bond lengths



Bond angles

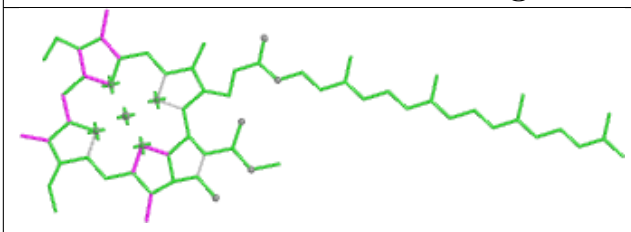


Torsions

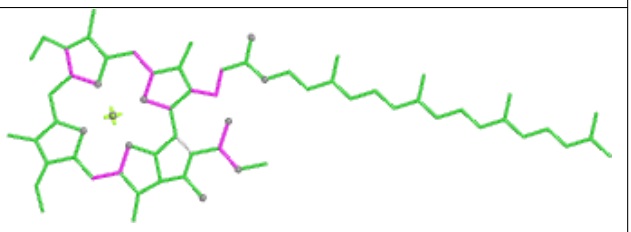


Rings

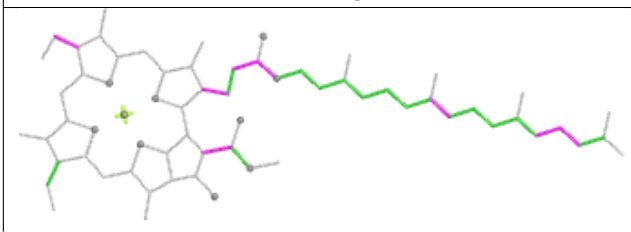
Ligand CLA AA 841



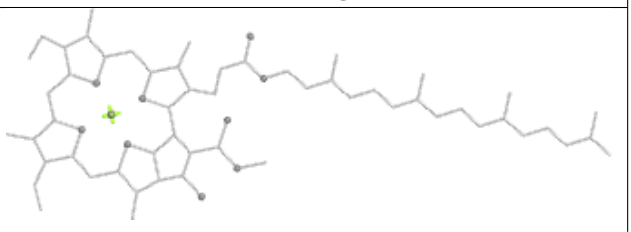
Bond lengths



Bond angles

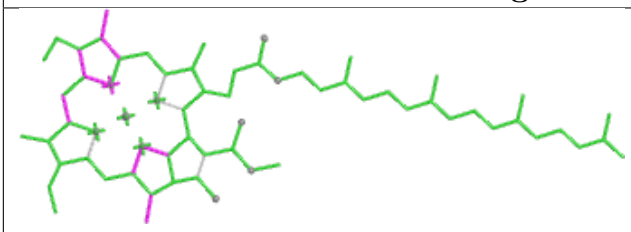


Torsions

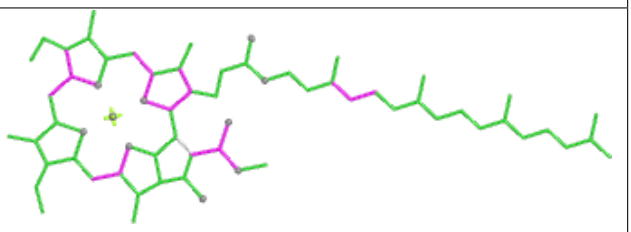


Rings

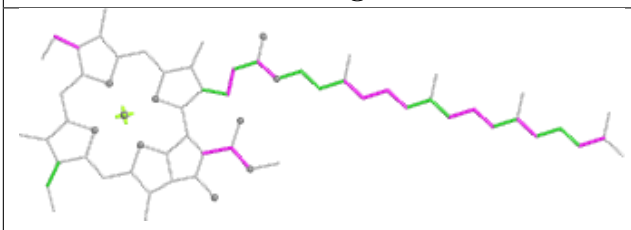
Ligand CLA AB 842



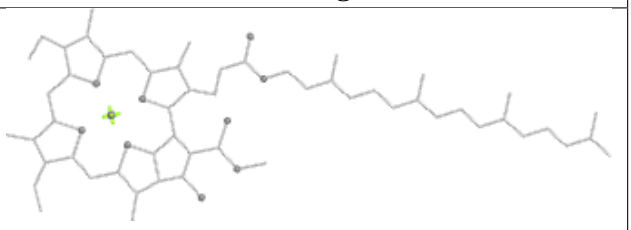
Bond lengths



Bond angles

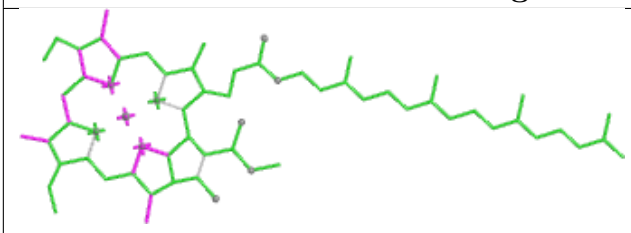


Torsions

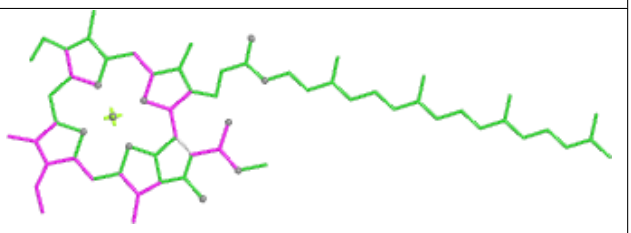


Rings

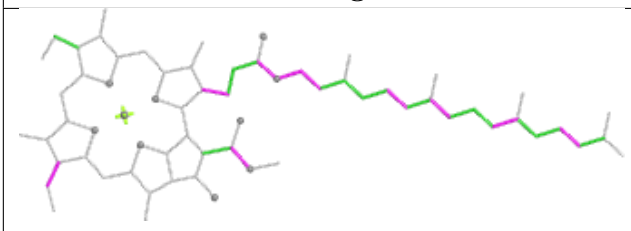
Ligand CLA AB 804



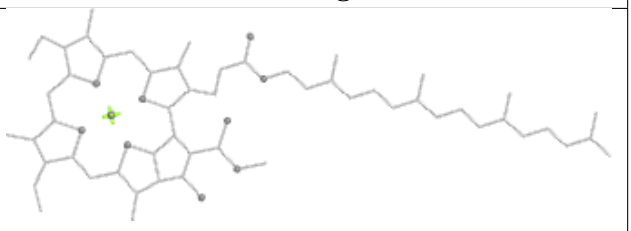
Bond lengths



Bond angles

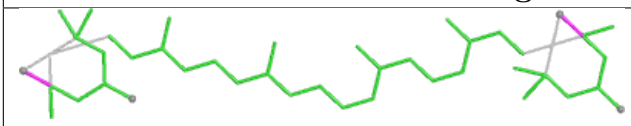


Torsions

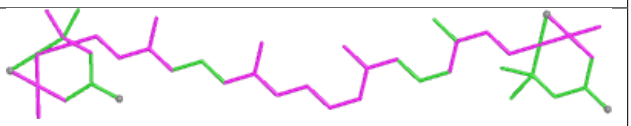


Rings

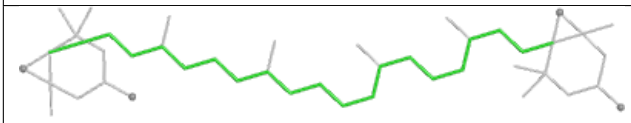
Ligand XAT B1 317



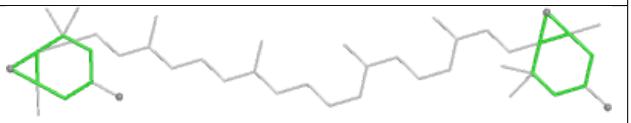
Bond lengths



Bond angles

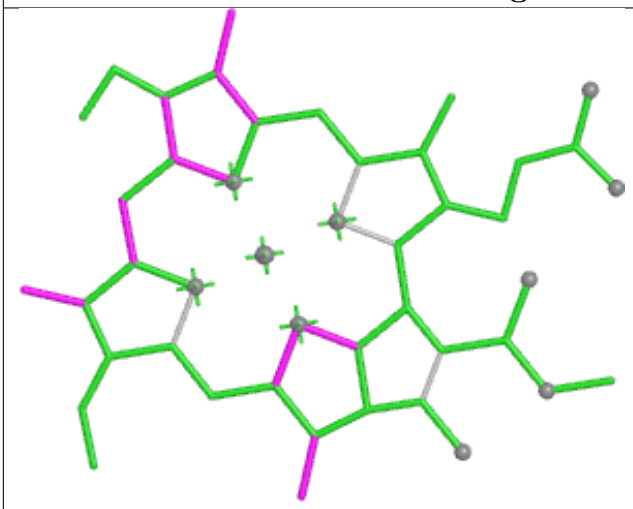


Torsions

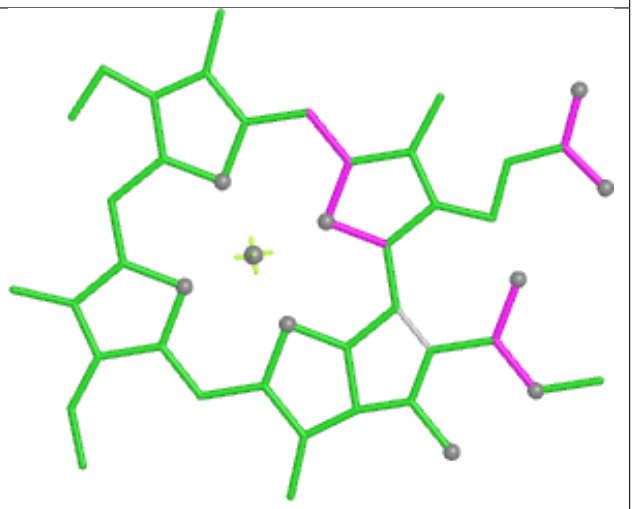


Rings

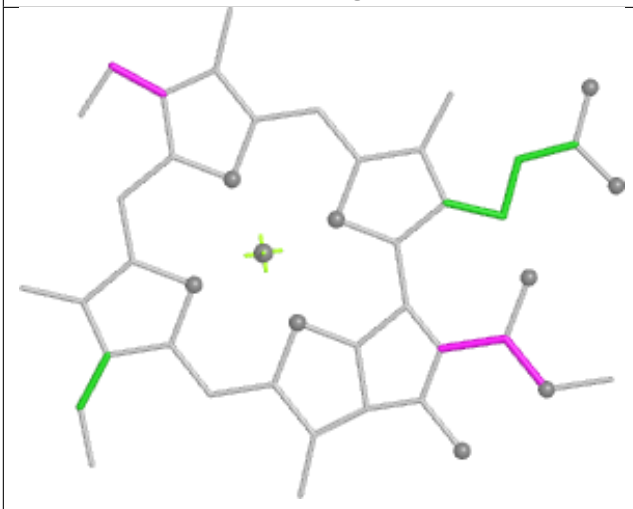
Ligand CLA AA 820



Bond lengths



Bond angles

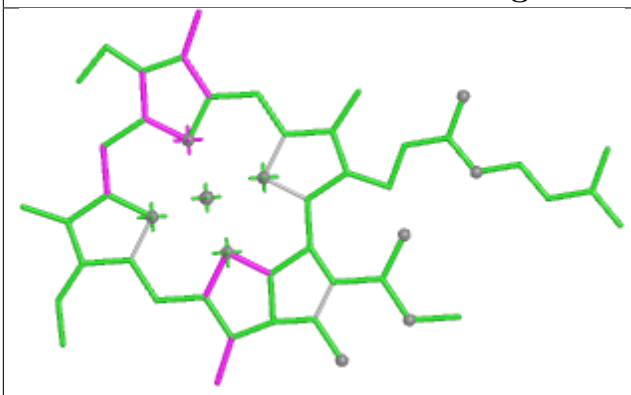


Torsions

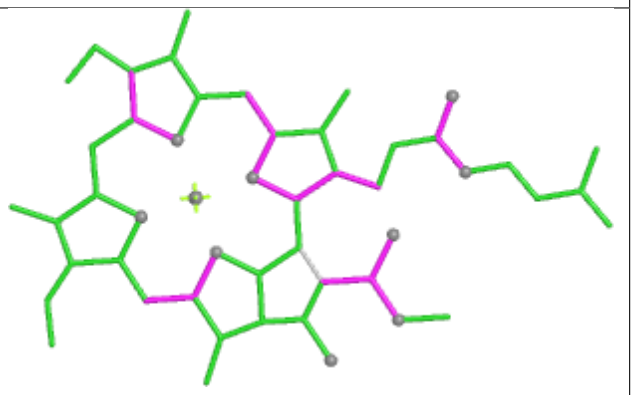


Rings

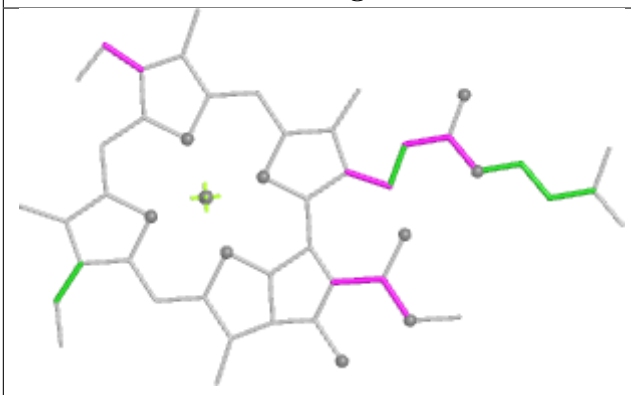
Ligand CLA BA 809



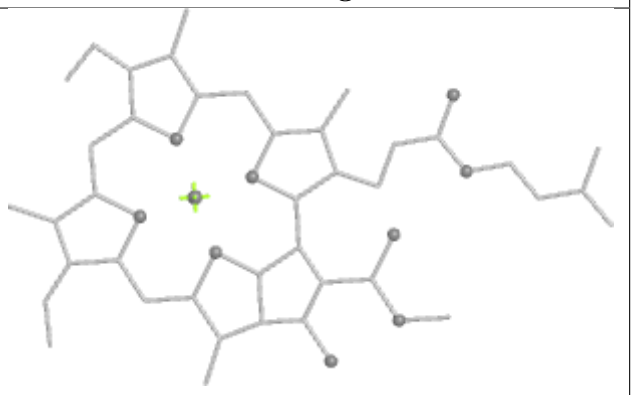
Bond lengths



Bond angles

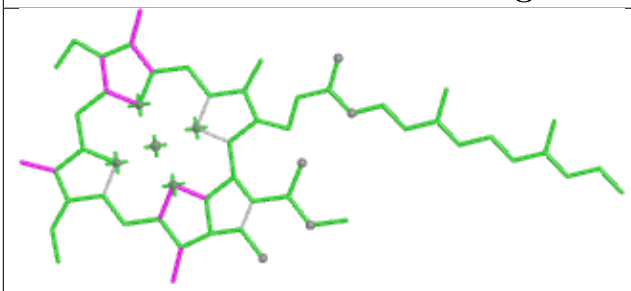


Torsions

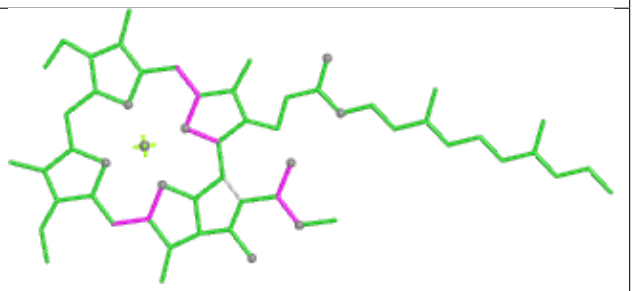


Rings

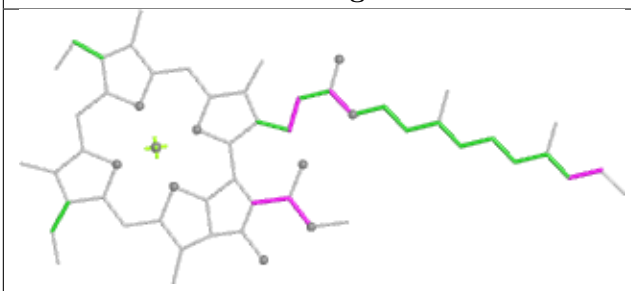
Ligand CLA B5 612



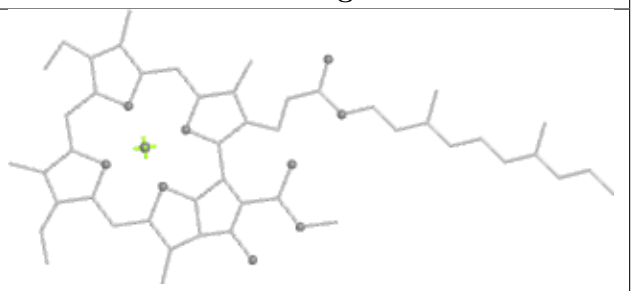
Bond lengths



Bond angles

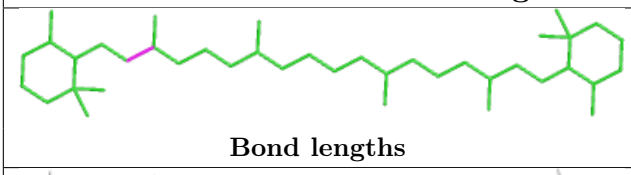


Torsions

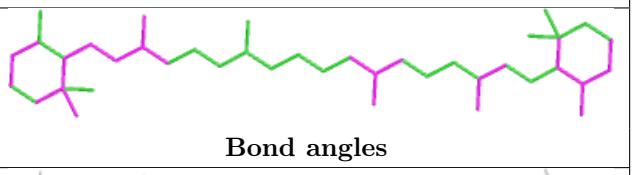


Rings

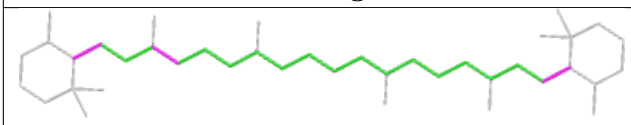
Ligand BCR BL 301



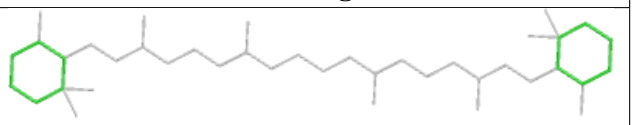
Bond lengths



Bond angles

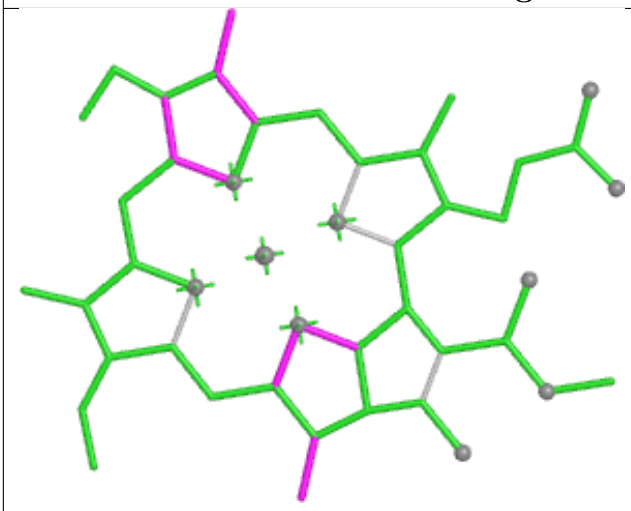


Torsions

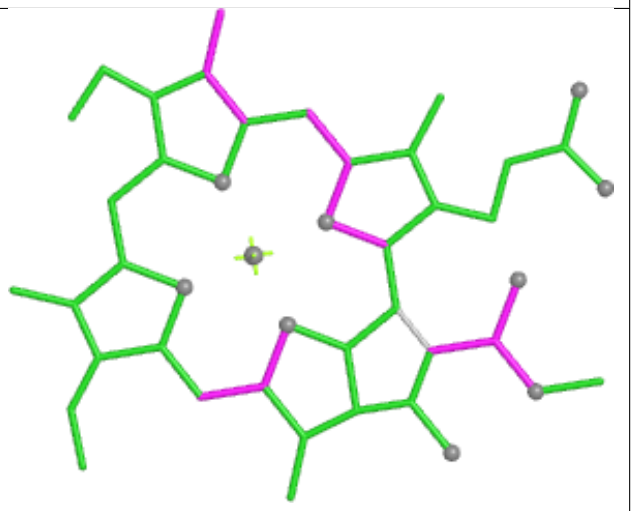


Rings

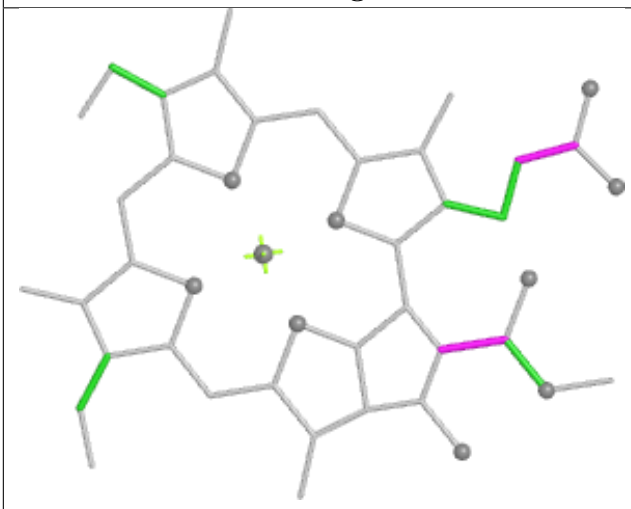
Ligand CLA B3 307



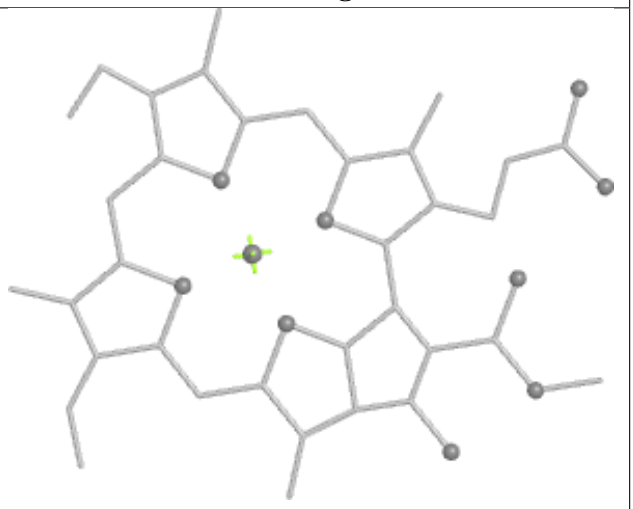
Bond lengths



Bond angles

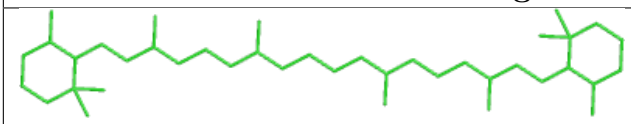


Torsions

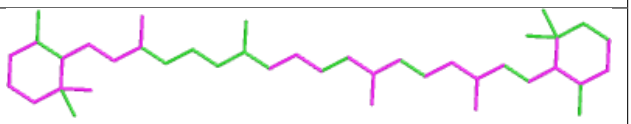


Rings

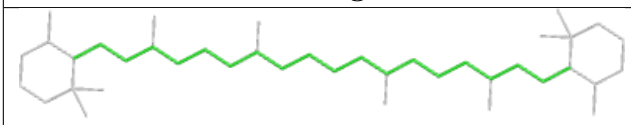
Ligand BCR BJ 101



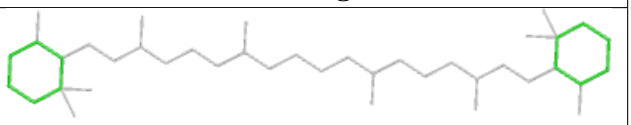
Bond lengths



Bond angles

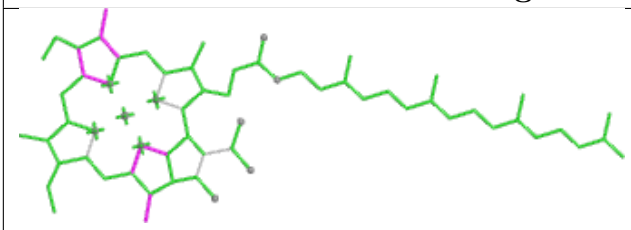


Torsions

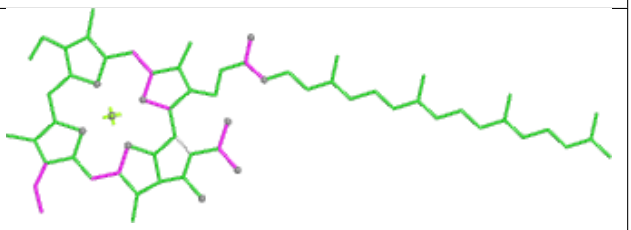


Rings

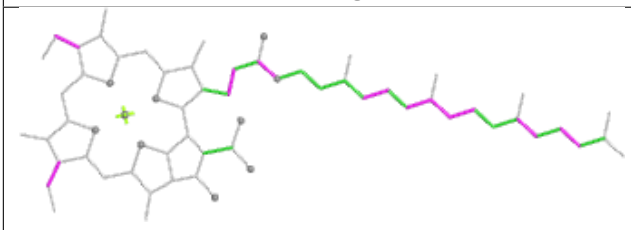
Ligand CLA A1 314



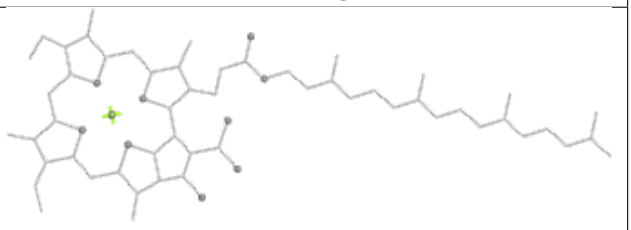
Bond lengths



Bond angles

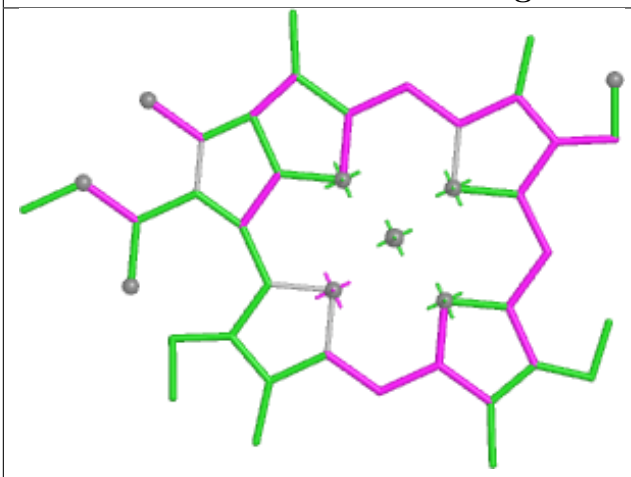


Torsions

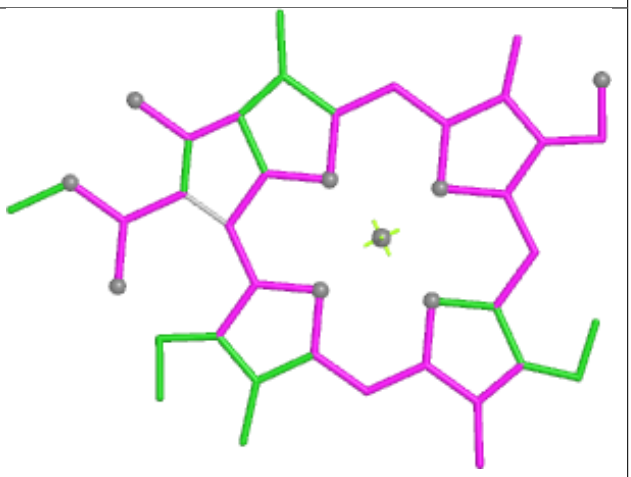


Rings

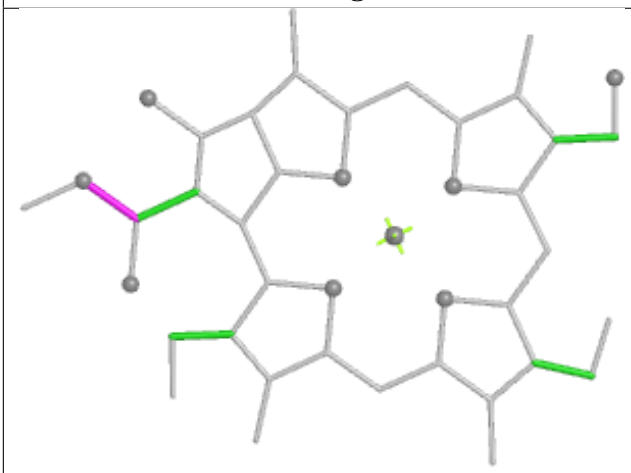
Ligand CHL A6 606



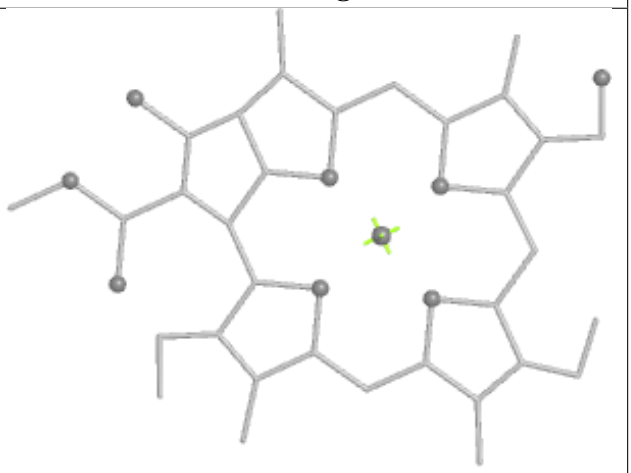
Bond lengths



Bond angles

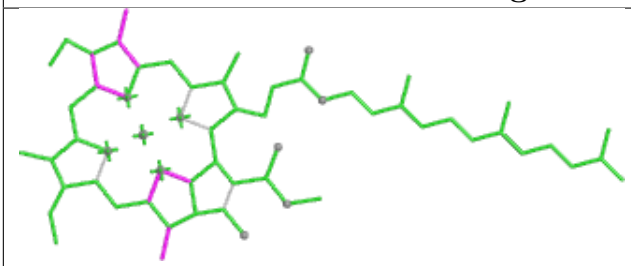


Torsions

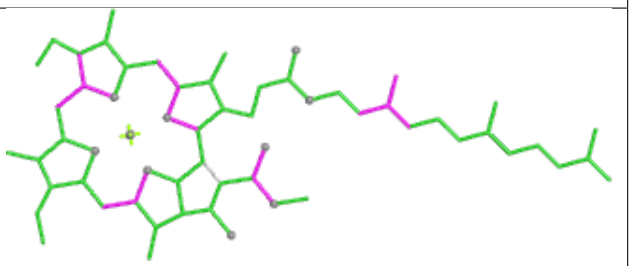


Rings

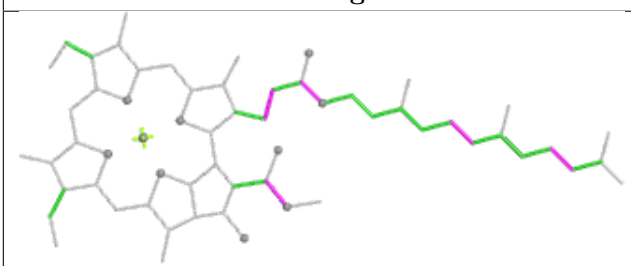
Ligand CLA AA 817



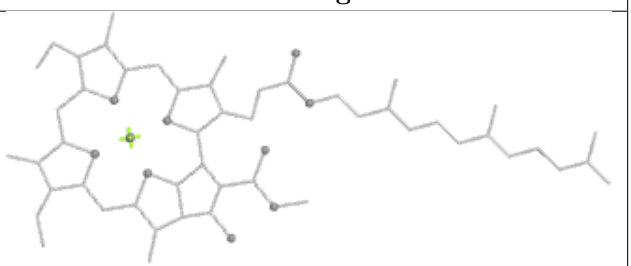
Bond lengths



Bond angles

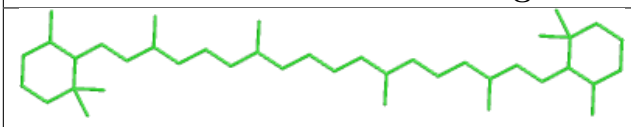


Torsions

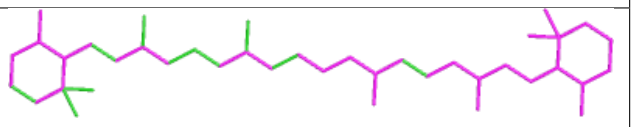


Rings

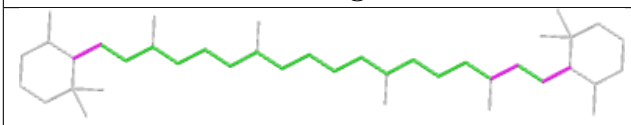
Ligand BCR B3 317



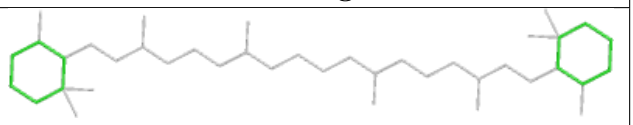
Bond lengths



Bond angles

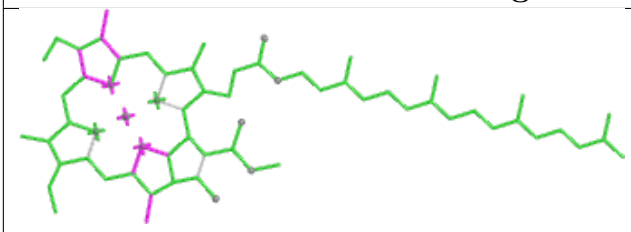


Torsions

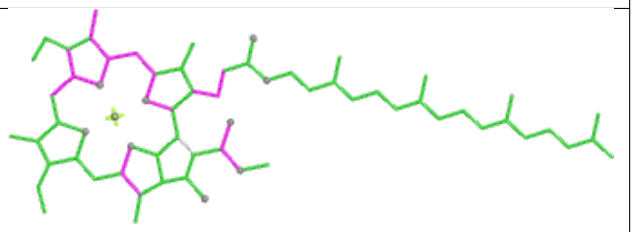


Rings

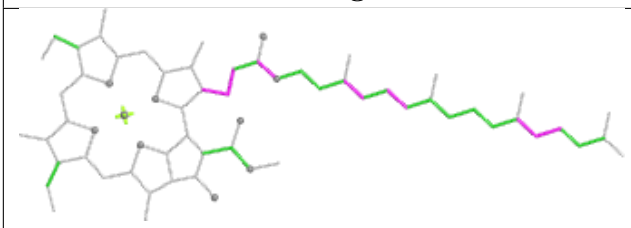
Ligand CLA BB 830



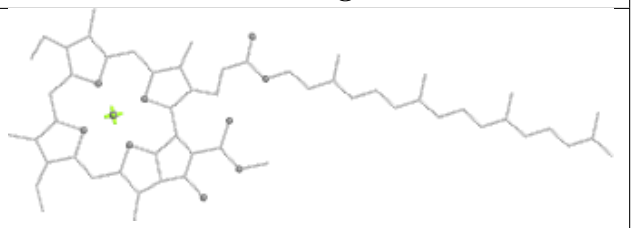
Bond lengths



Bond angles

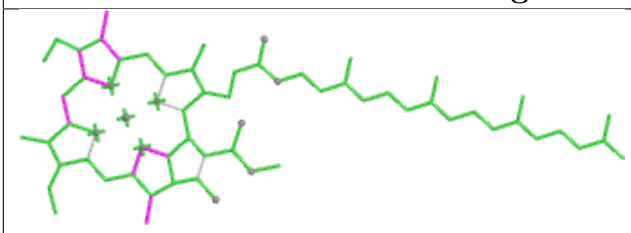


Torsions

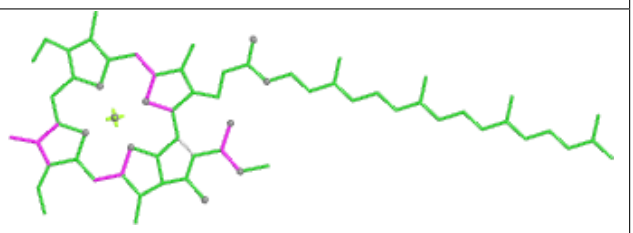


Rings

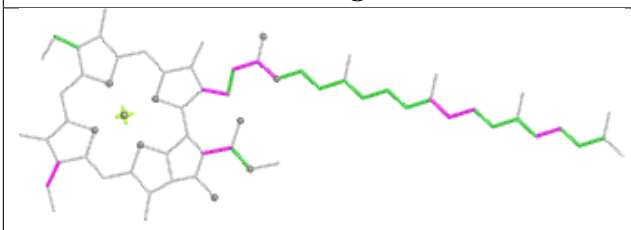
Ligand CLA AB 806



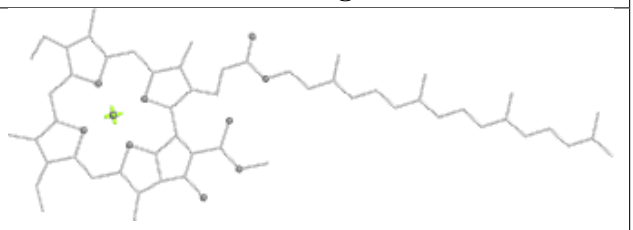
Bond lengths



Bond angles

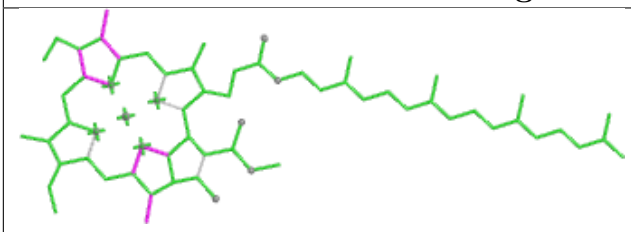


Torsions

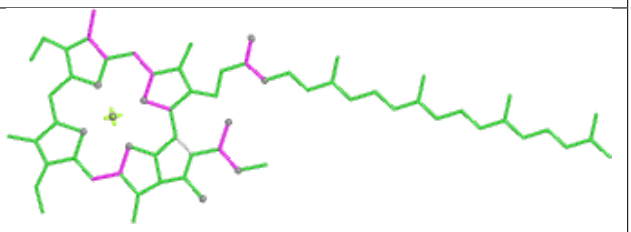


Rings

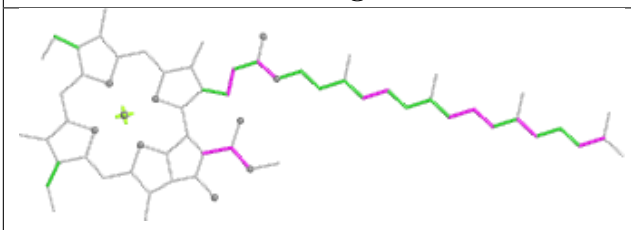
Ligand CLA B2 612



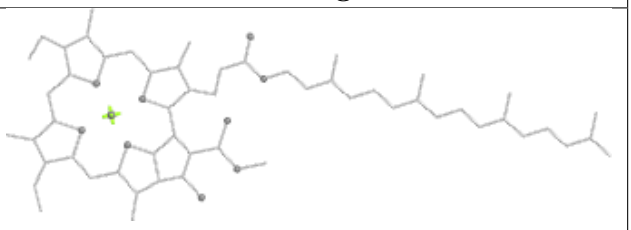
Bond lengths



Bond angles

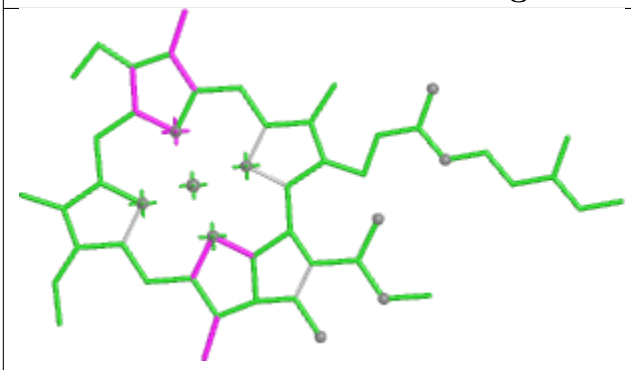


Torsions

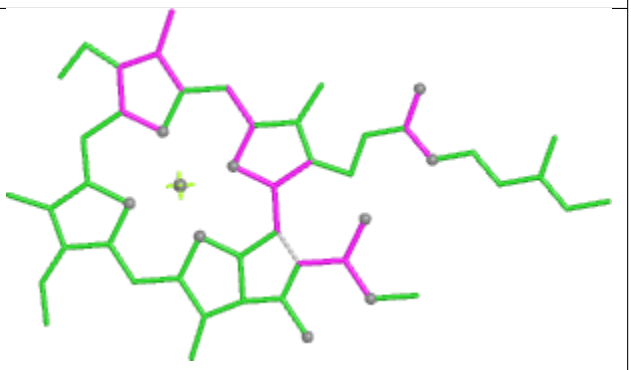


Rings

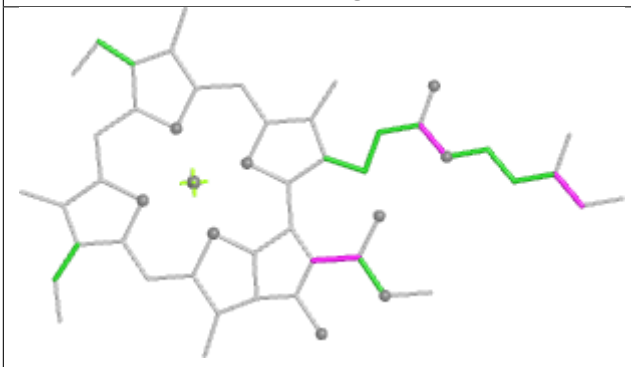
Ligand CLA AA 837



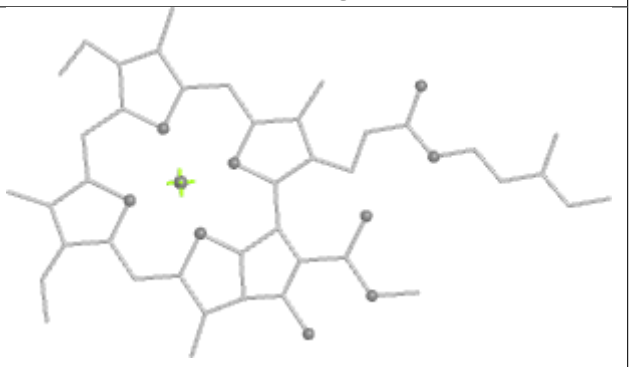
Bond lengths



Bond angles

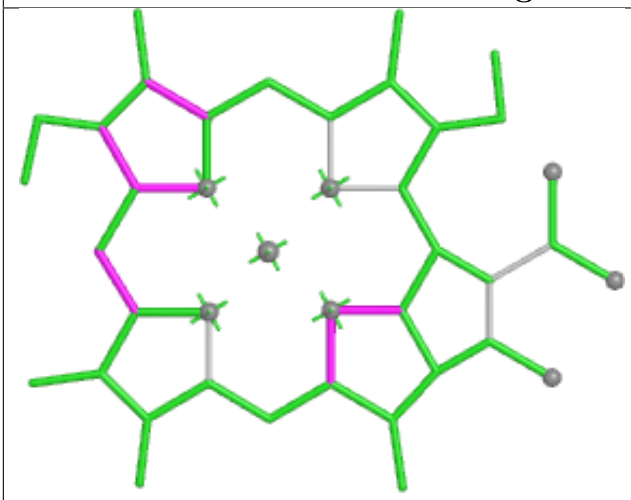


Torsions

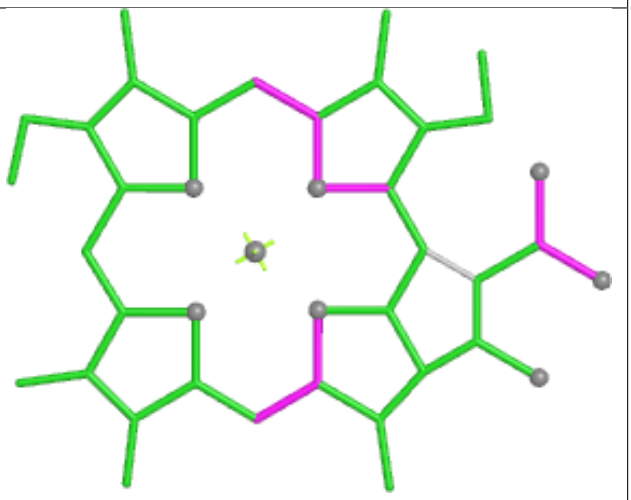


Rings

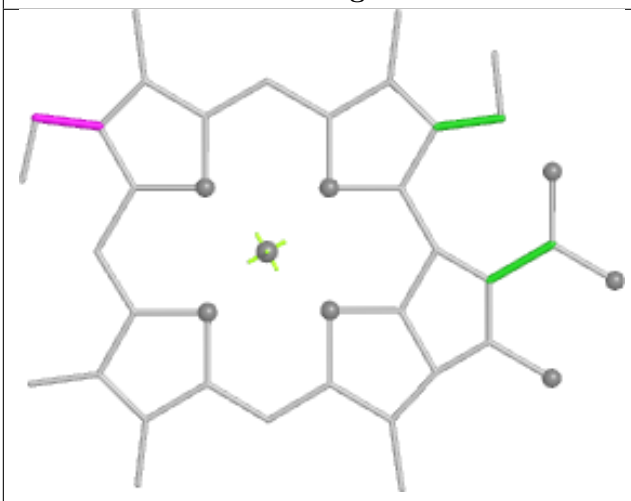
Ligand CLA B3 309



Bond lengths



Bond angles

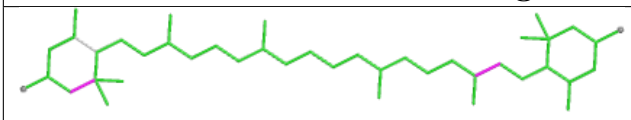


Torsions

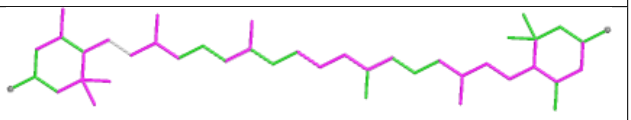


Rings

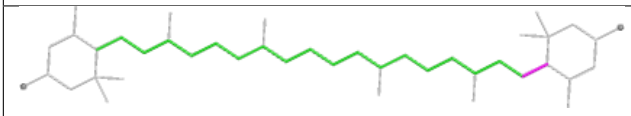
Ligand LUT A4 315



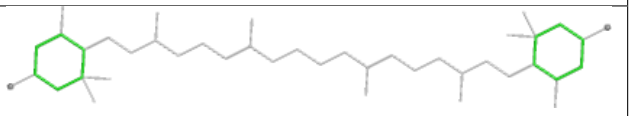
Bond lengths



Bond angles

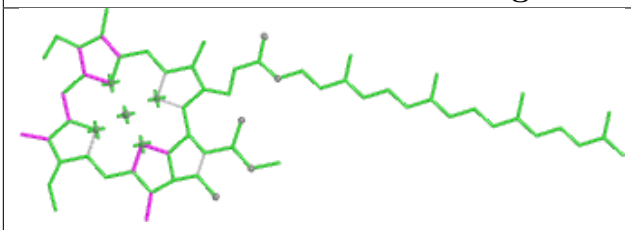


Torsions

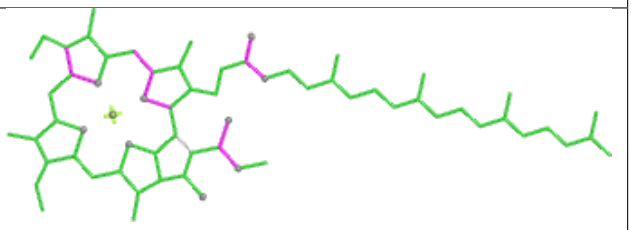


Rings

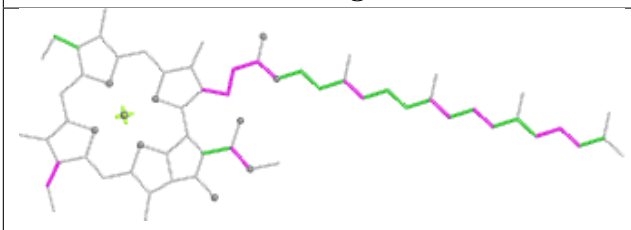
Ligand CLA BB 829



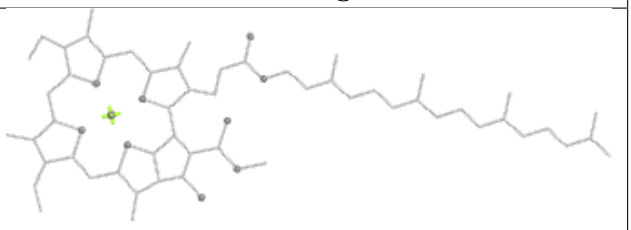
Bond lengths



Bond angles

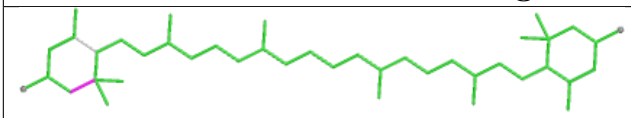


Torsions

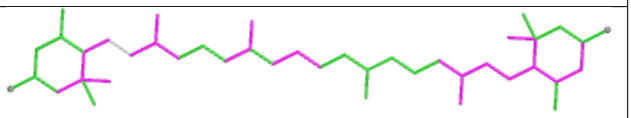


Rings

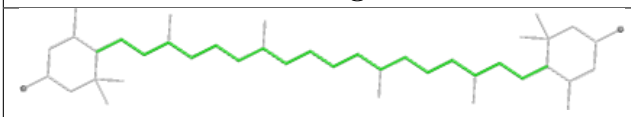
Ligand LUT A6 615



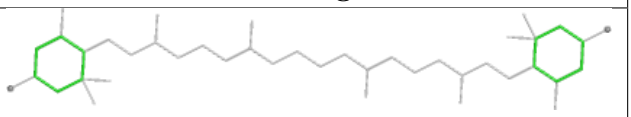
Bond lengths



Bond angles

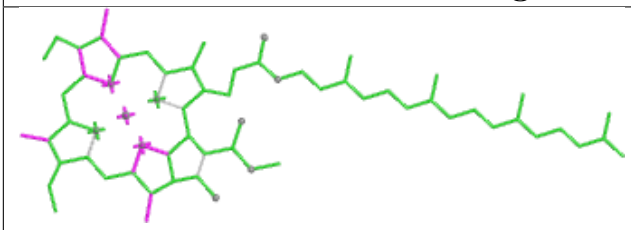


Torsions

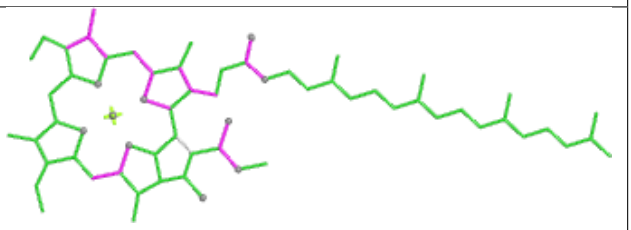


Rings

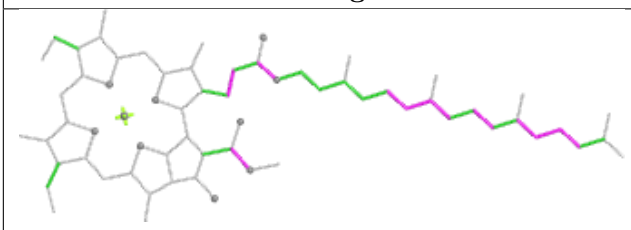
Ligand CLA BB 811



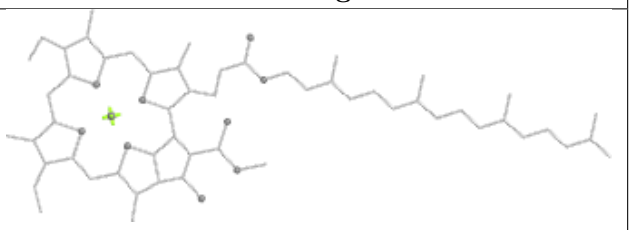
Bond lengths



Bond angles

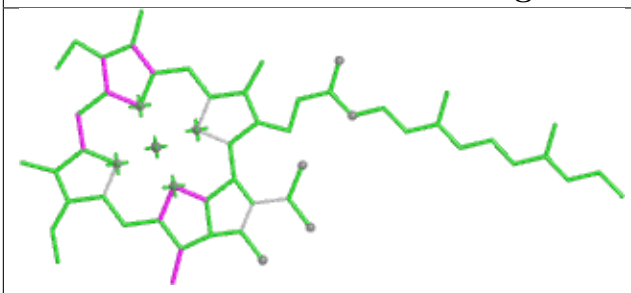


Torsions

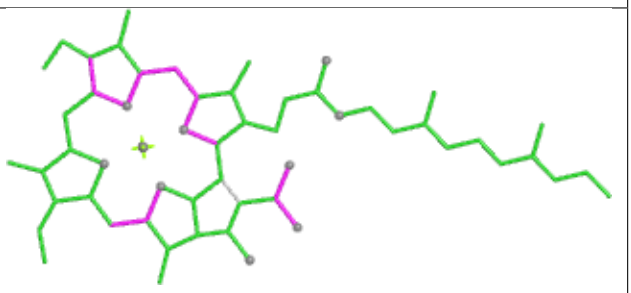


Rings

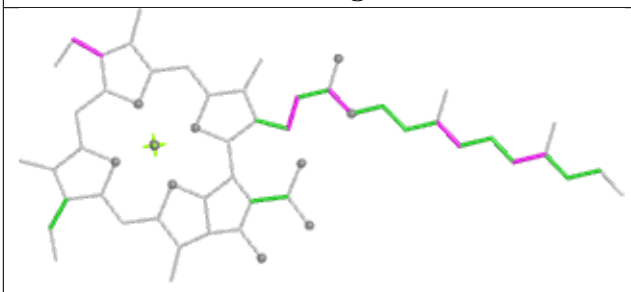
Ligand CLA A4 311



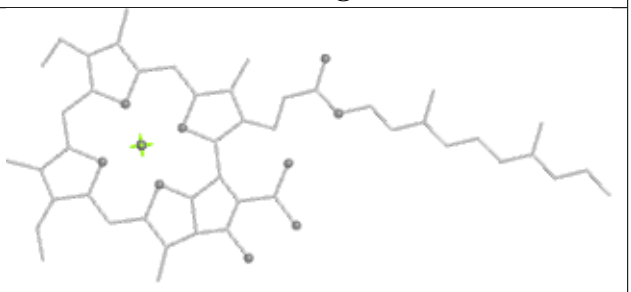
Bond lengths



Bond angles

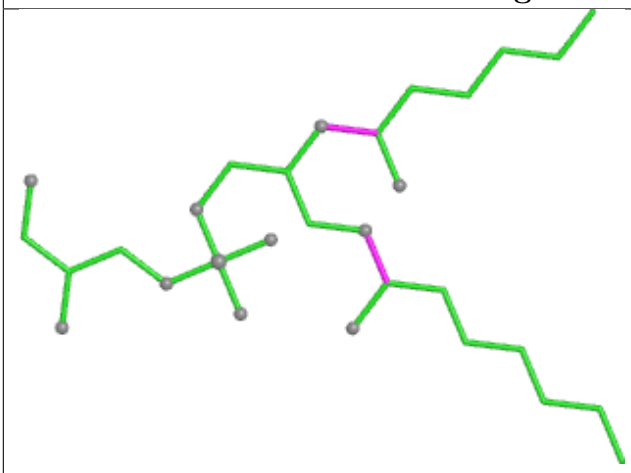


Torsions

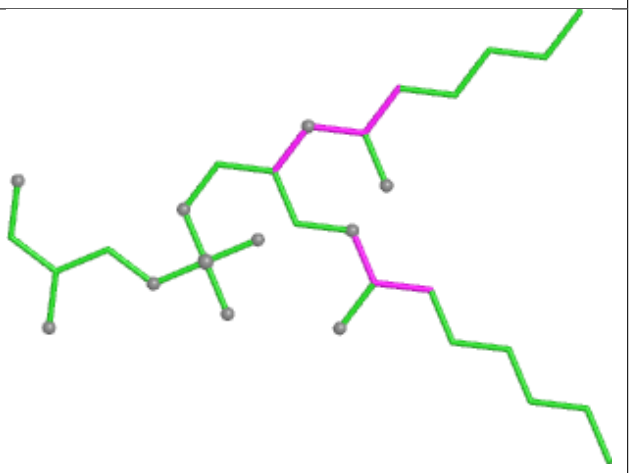


Rings

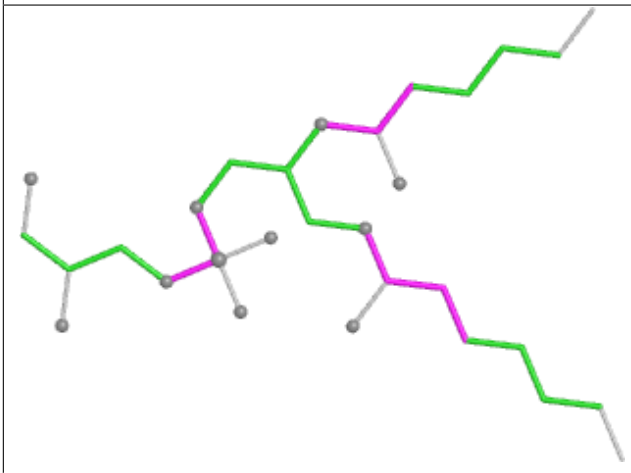
Ligand LHG B5 618



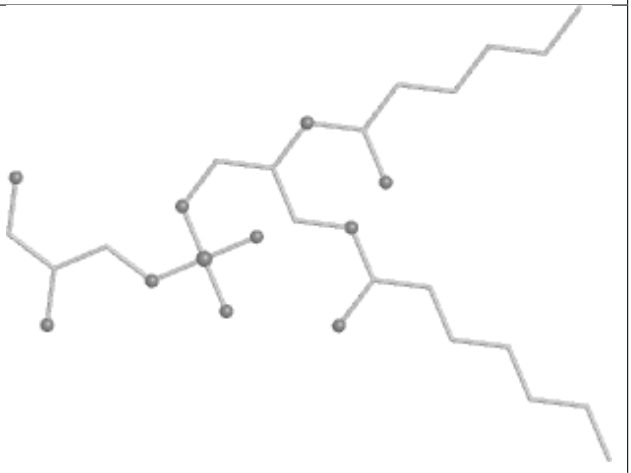
Bond lengths



Bond angles

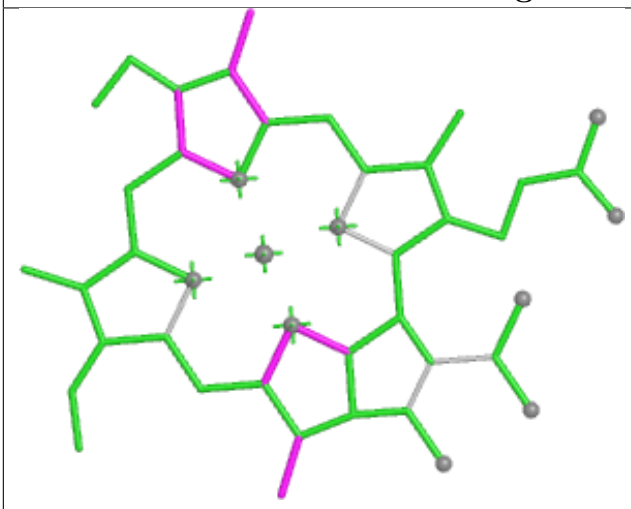


Torsions

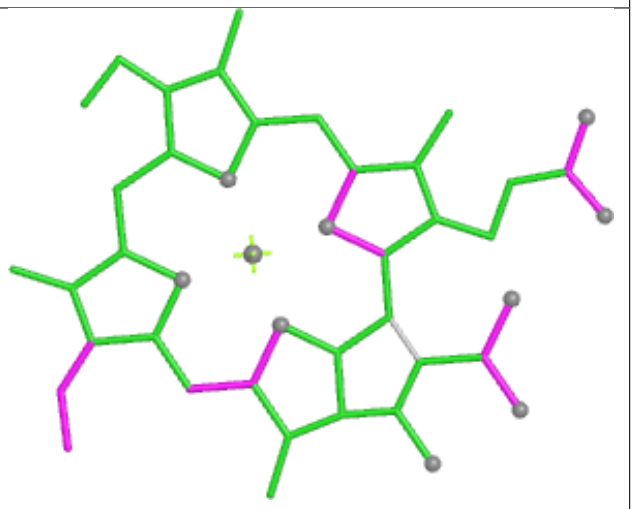


Rings

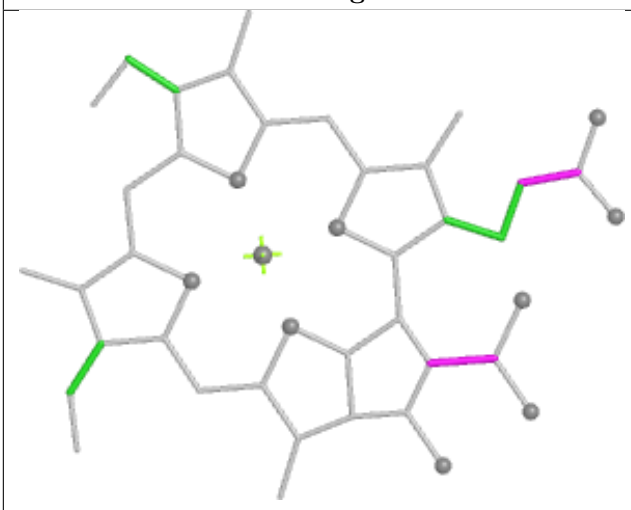
Ligand CLA B2 603



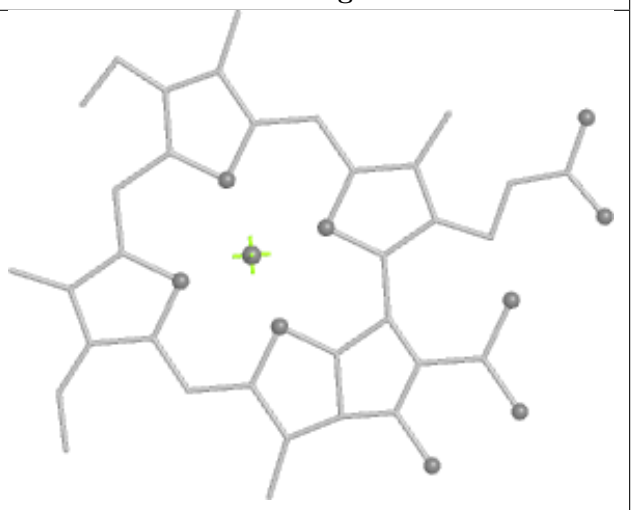
Bond lengths



Bond angles

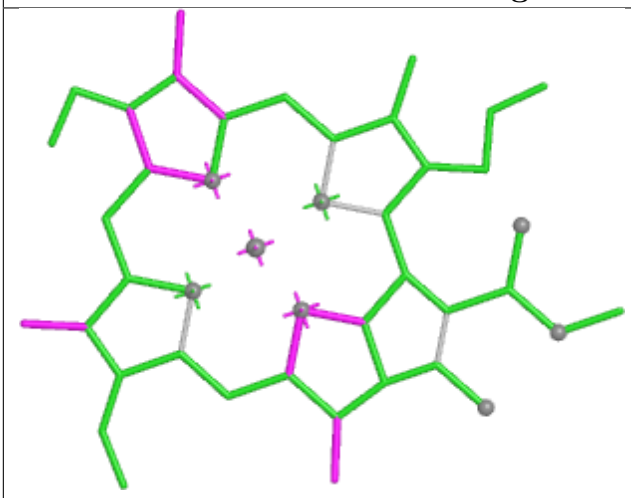


Torsions

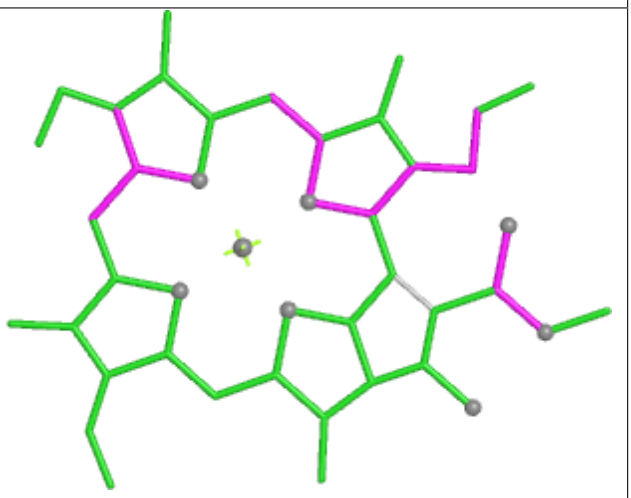


Rings

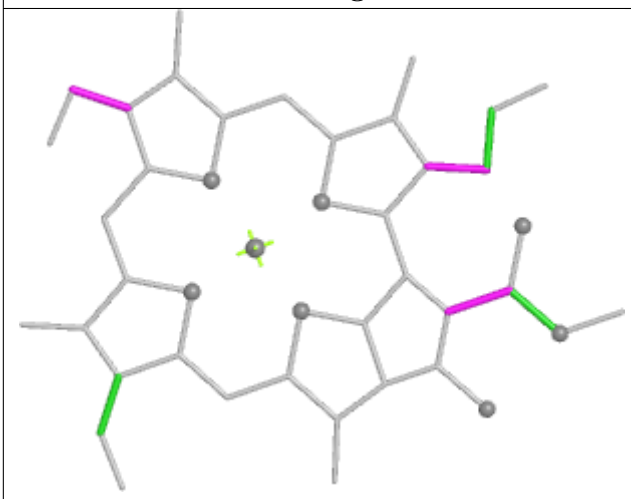
Ligand CLA AB 824



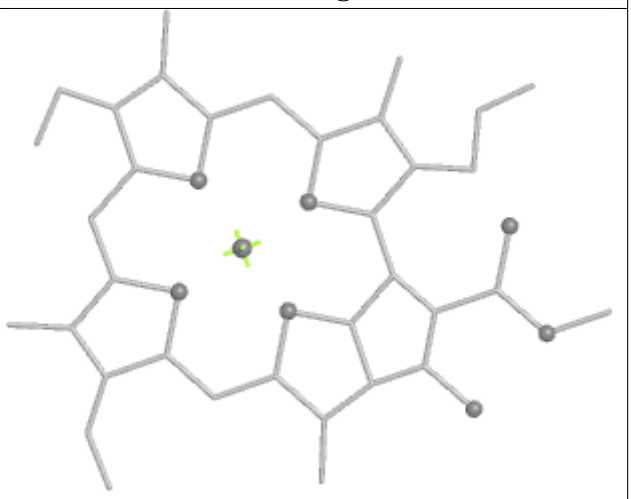
Bond lengths



Bond angles

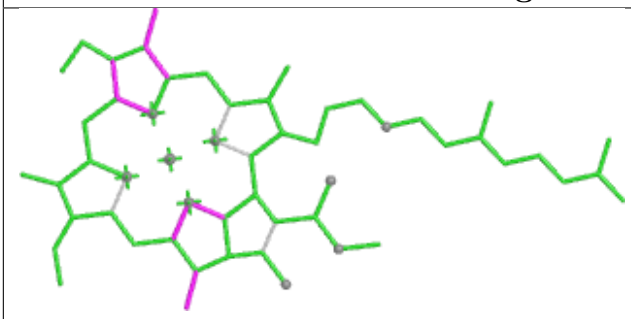


Torsions

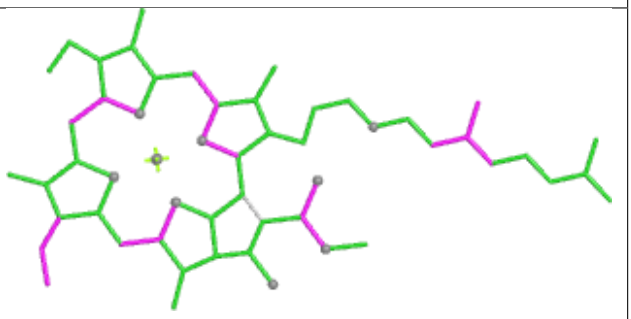


Rings

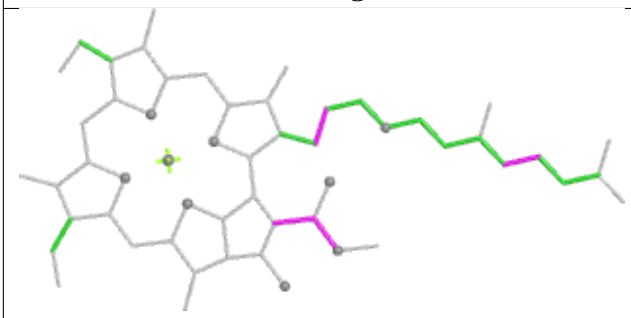
Ligand CLA B1 305



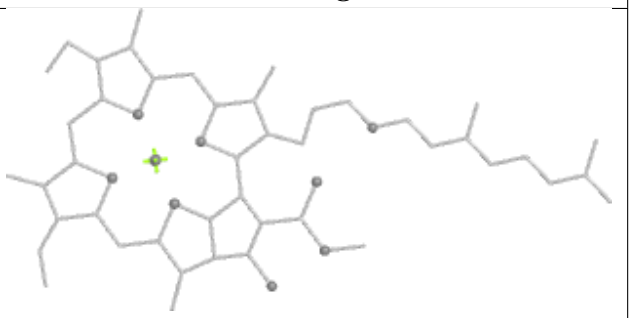
Bond lengths



Bond angles

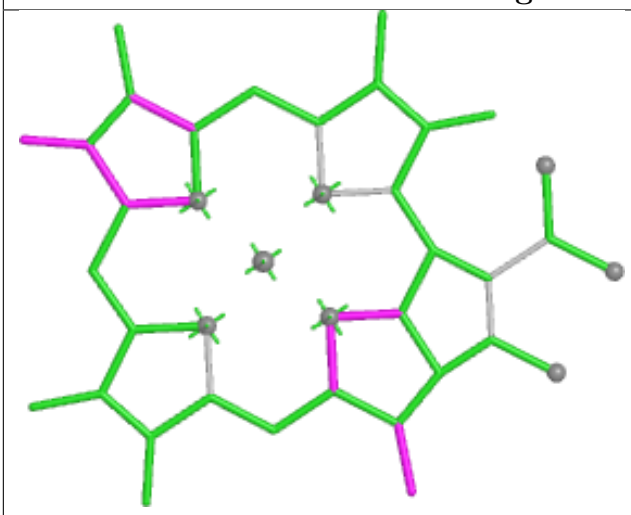


Torsions

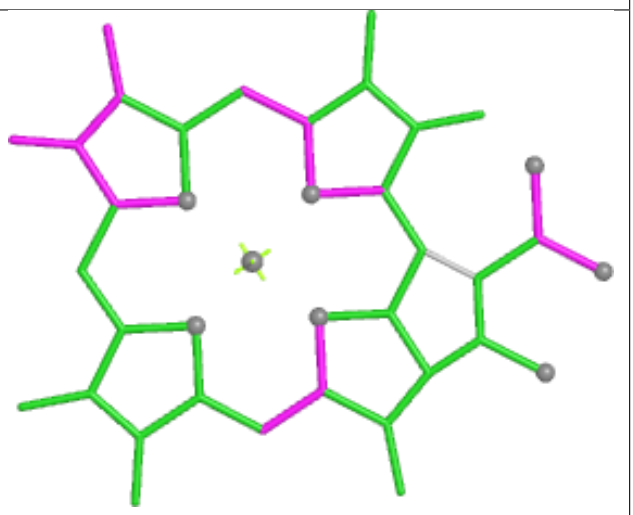


Rings

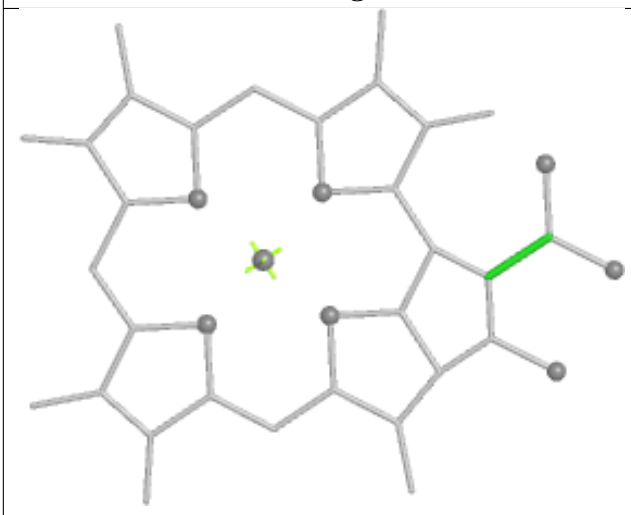
Ligand CLA B1 312



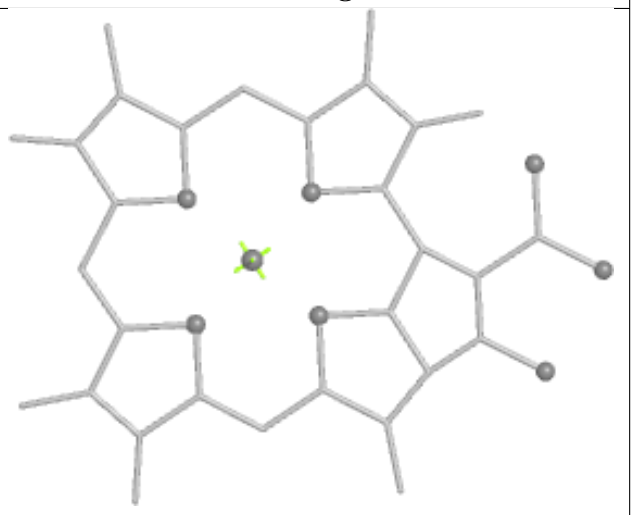
Bond lengths



Bond angles

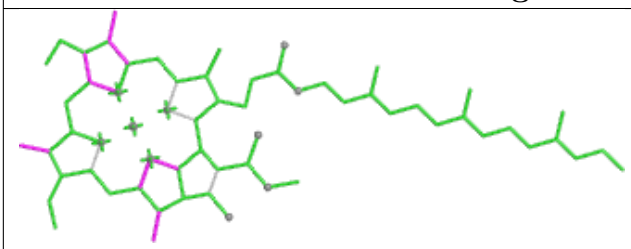


Torsions

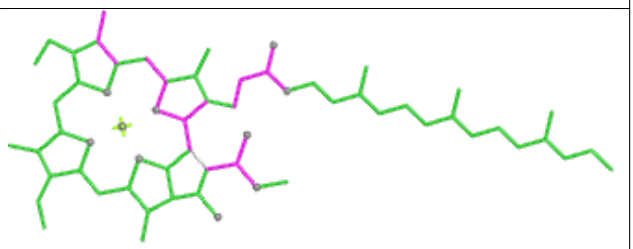


Rings

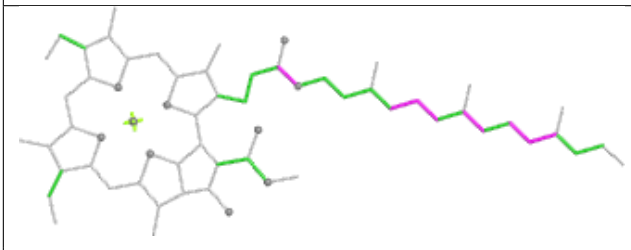
Ligand CLA BB 828



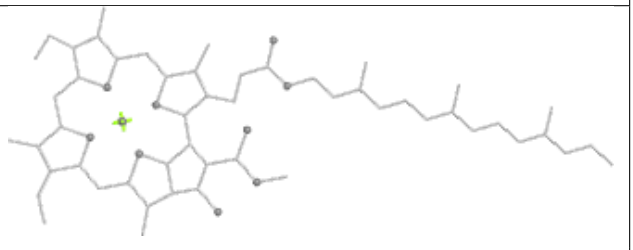
Bond lengths



Bond angles

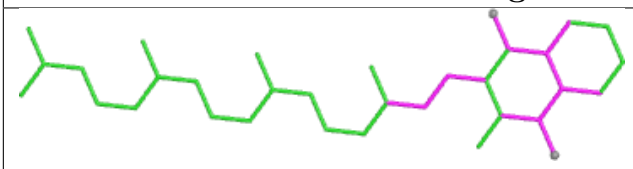


Torsions

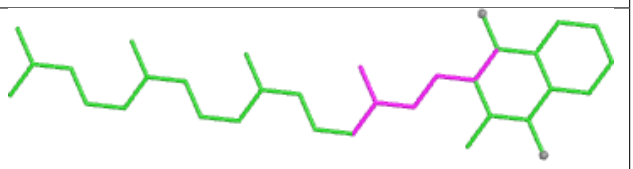


Rings

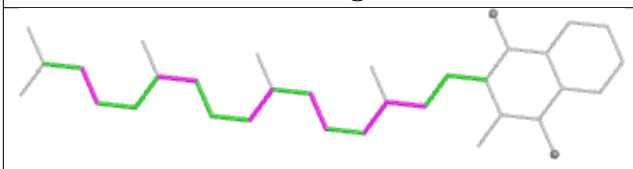
Ligand PQN AB 843



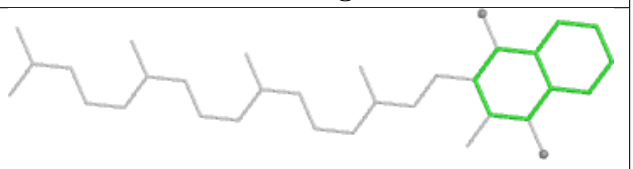
Bond lengths



Bond angles

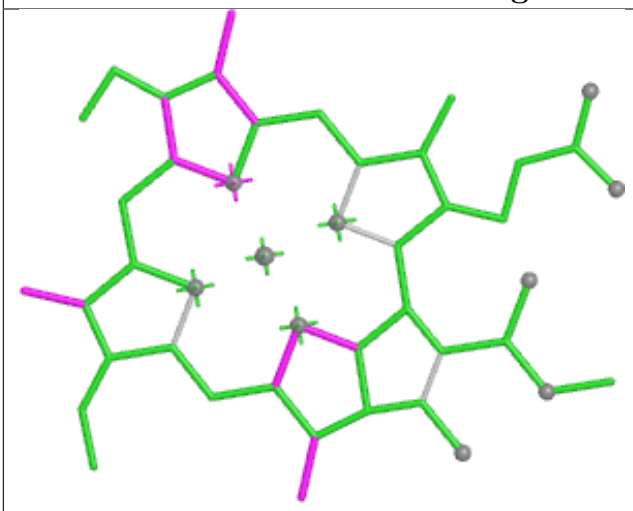


Torsions

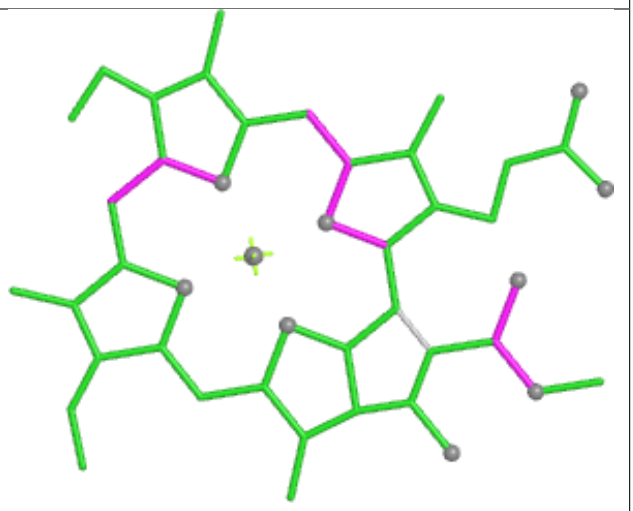


Rings

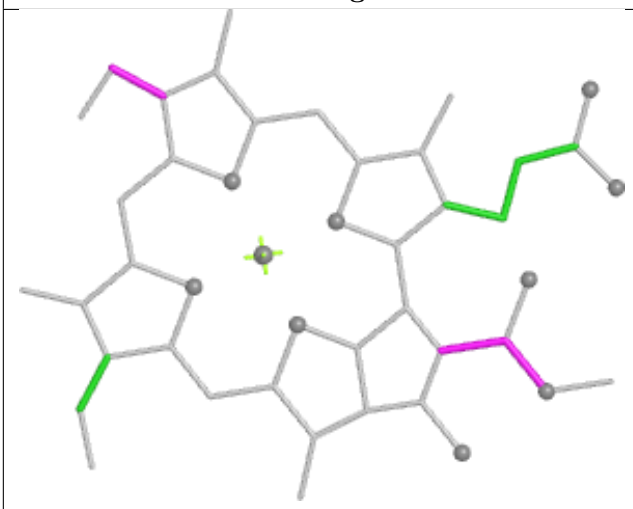
Ligand CLA BA 820



Bond lengths



Bond angles

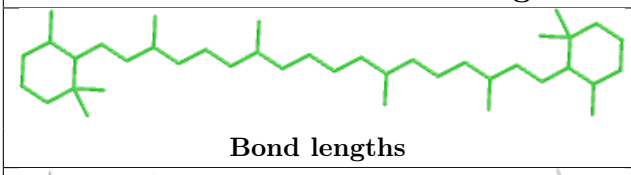


Torsions

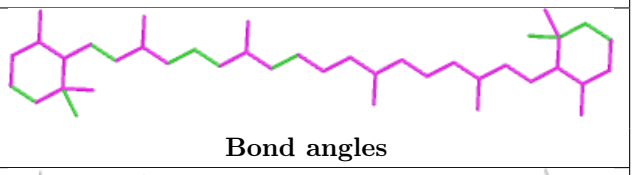


Rings

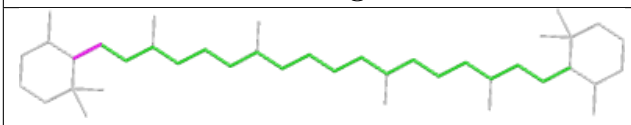
Ligand BCR A4 317



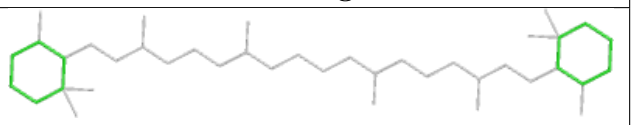
Bond lengths



Bond angles

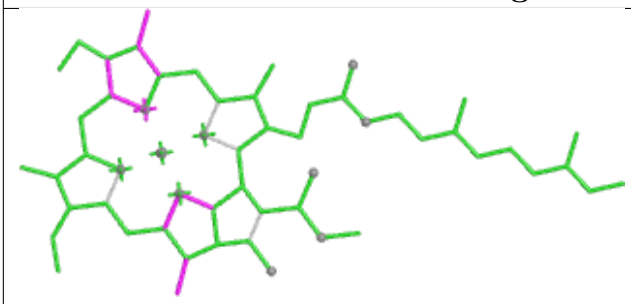


Torsions

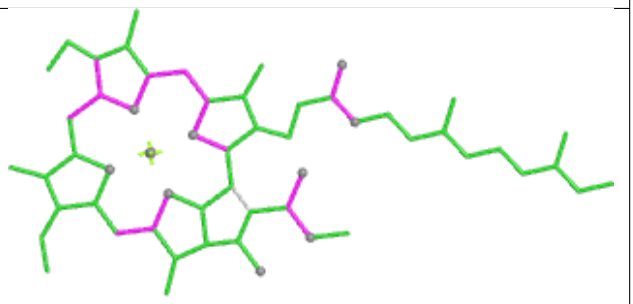


Rings

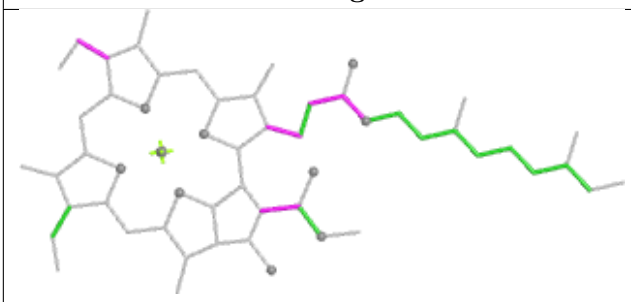
Ligand CLA BA 818



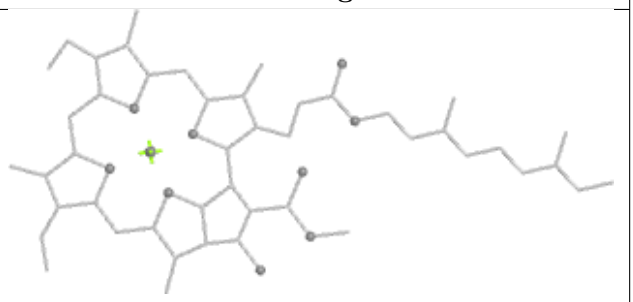
Bond lengths



Bond angles

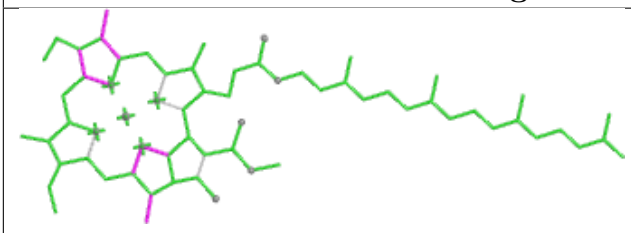


Torsions

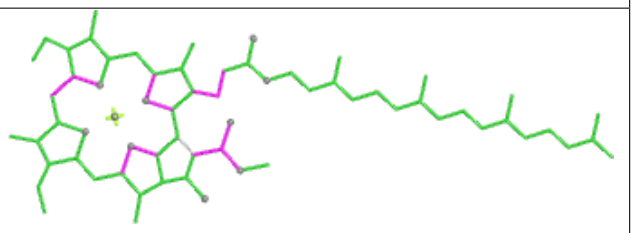


Rings

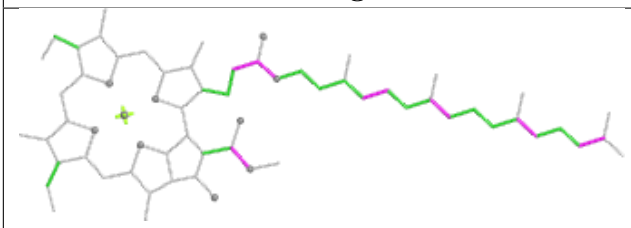
Ligand CLA AA 801



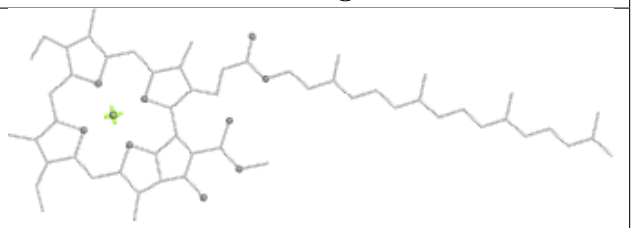
Bond lengths



Bond angles

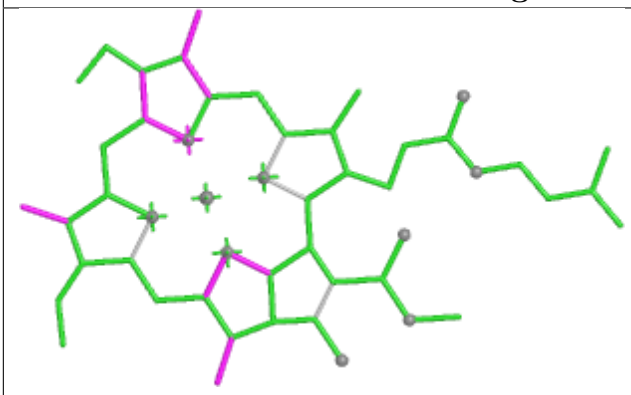


Torsions

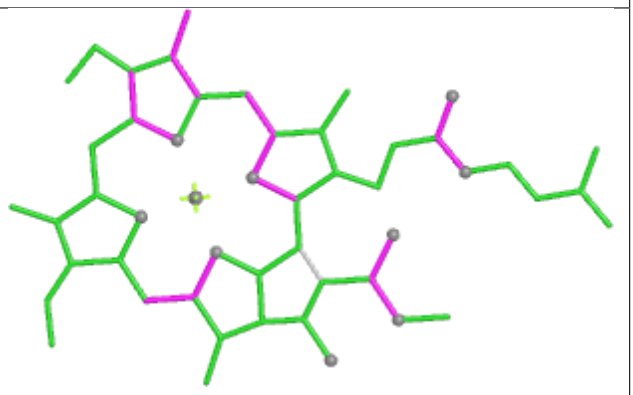


Rings

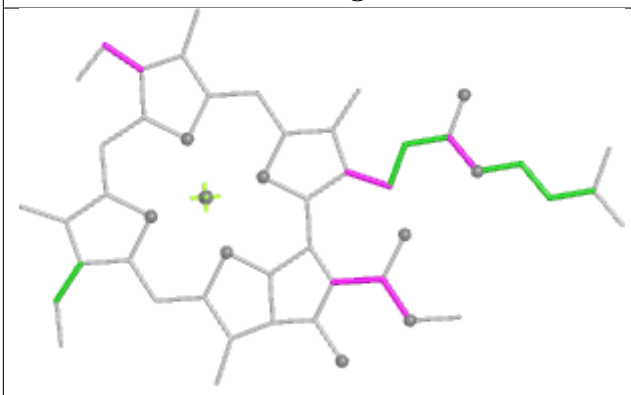
Ligand CLA AB 821



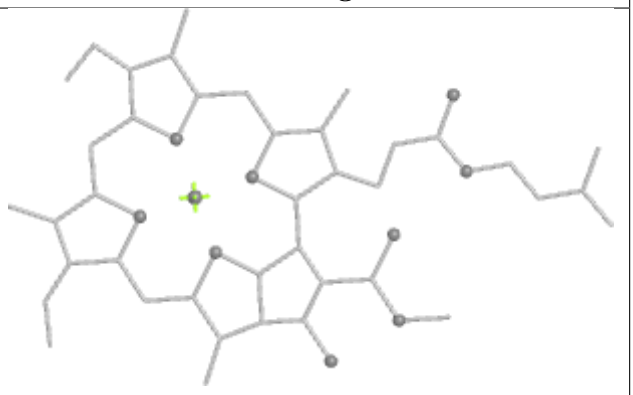
Bond lengths



Bond angles

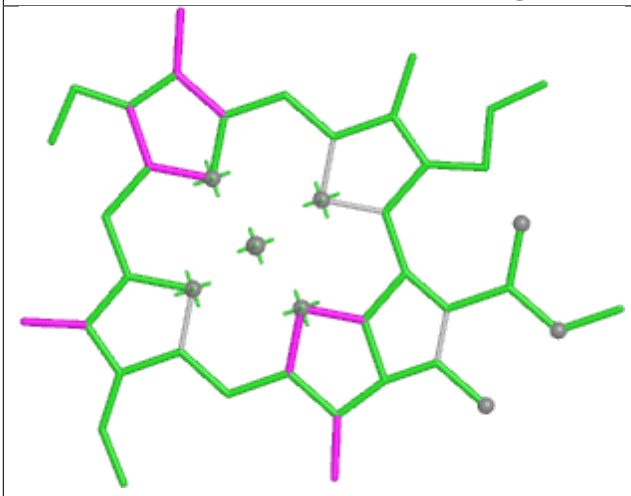


Torsions

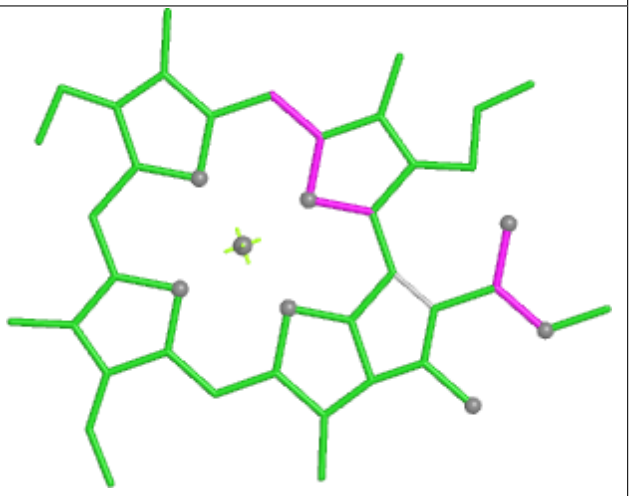


Rings

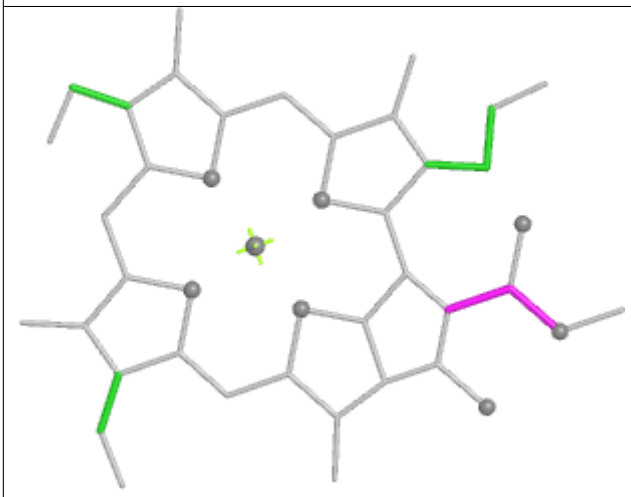
Ligand CLA AB 816



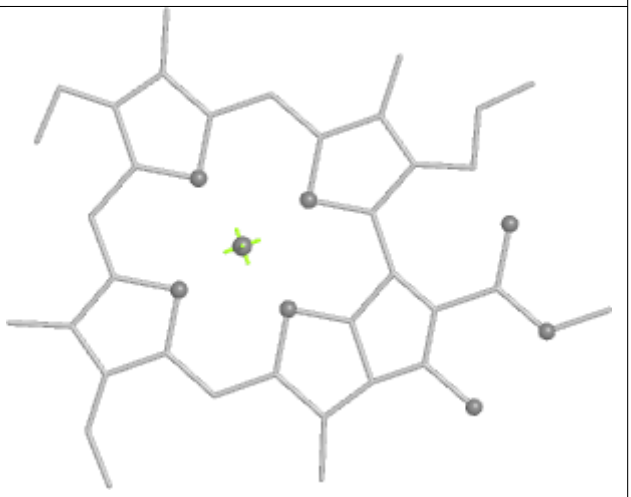
Bond lengths



Bond angles

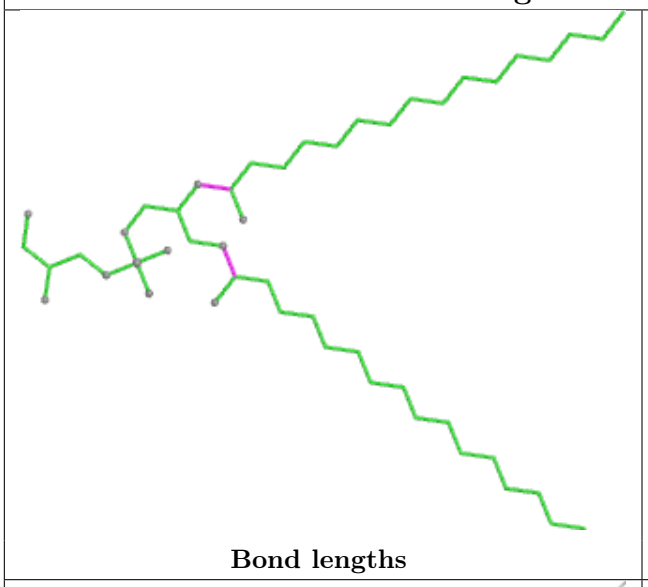


Torsions

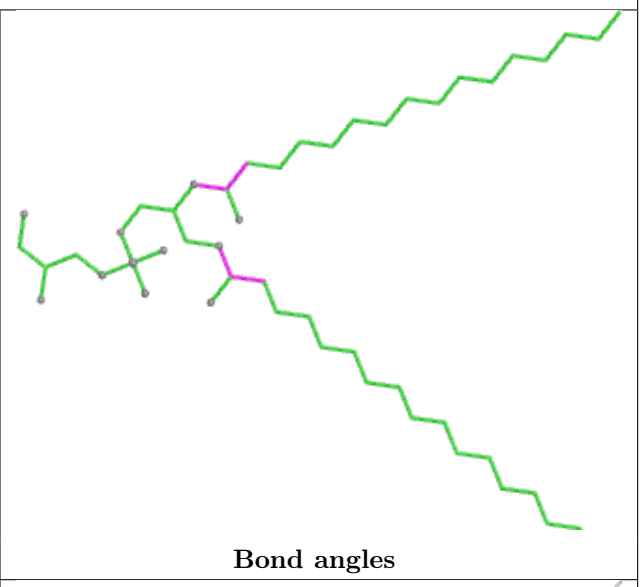


Rings

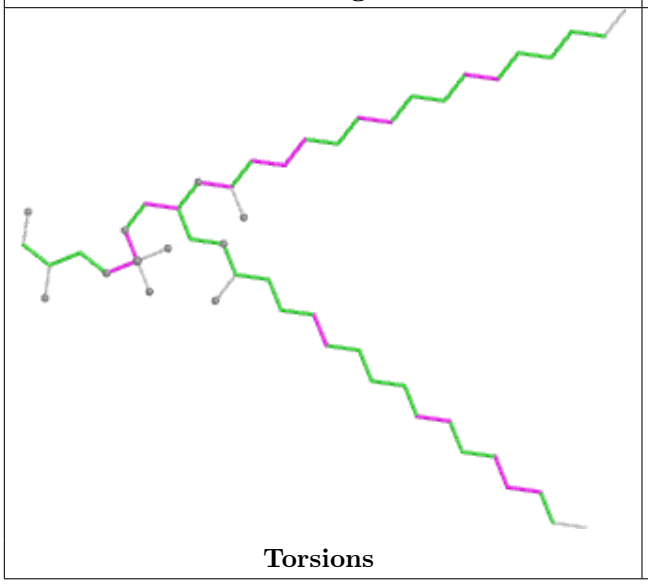
Ligand LHG A1 320



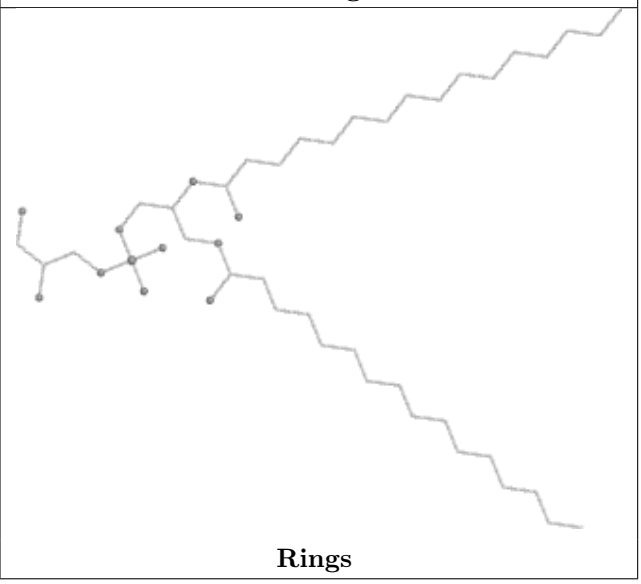
Bond lengths



Bond angles

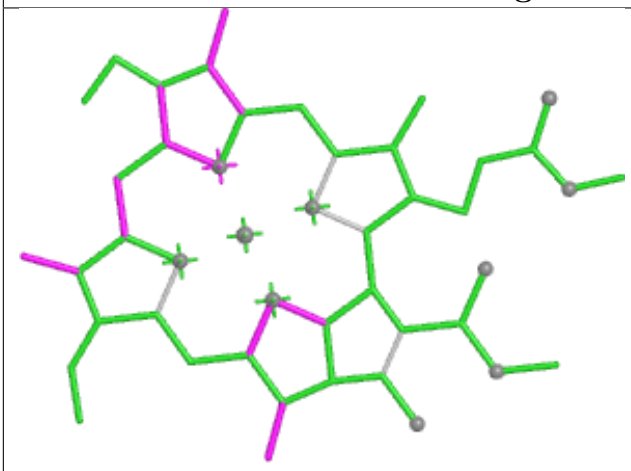


Torsions

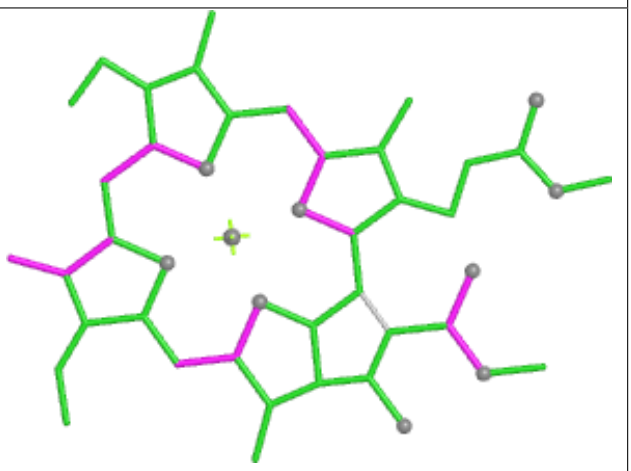


Rings

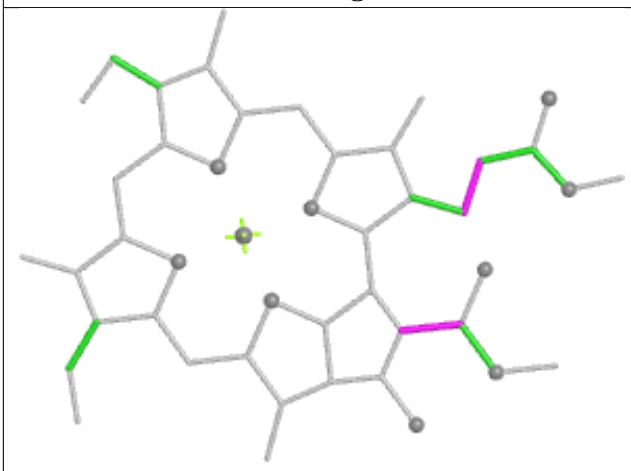
Ligand CLA A6 601



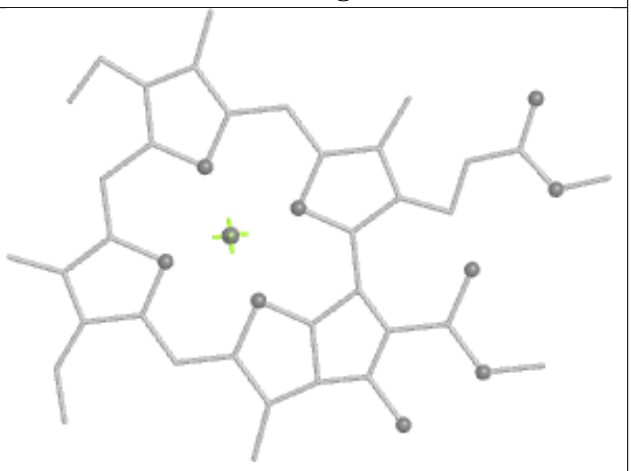
Bond lengths



Bond angles

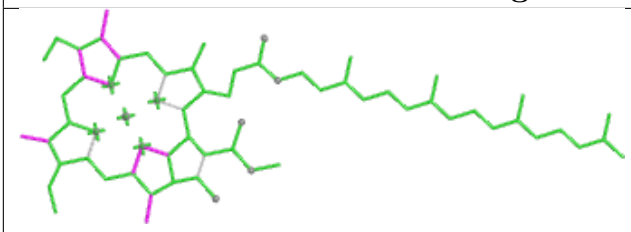


Torsions

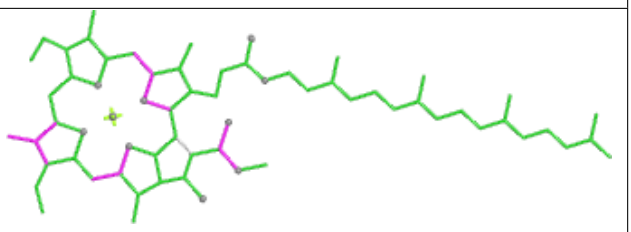


Rings

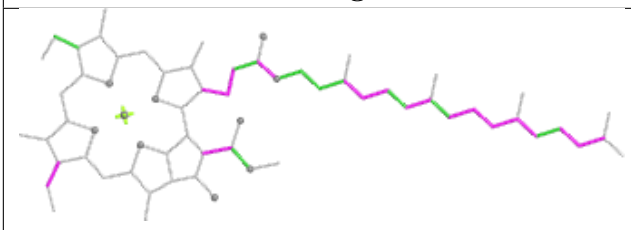
Ligand CLA BA 805



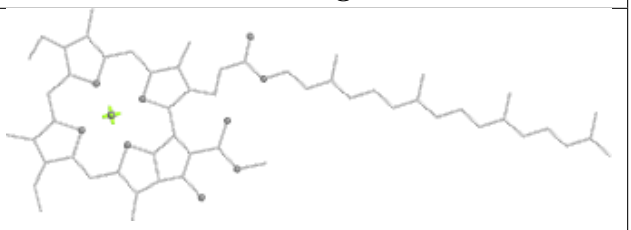
Bond lengths



Bond angles

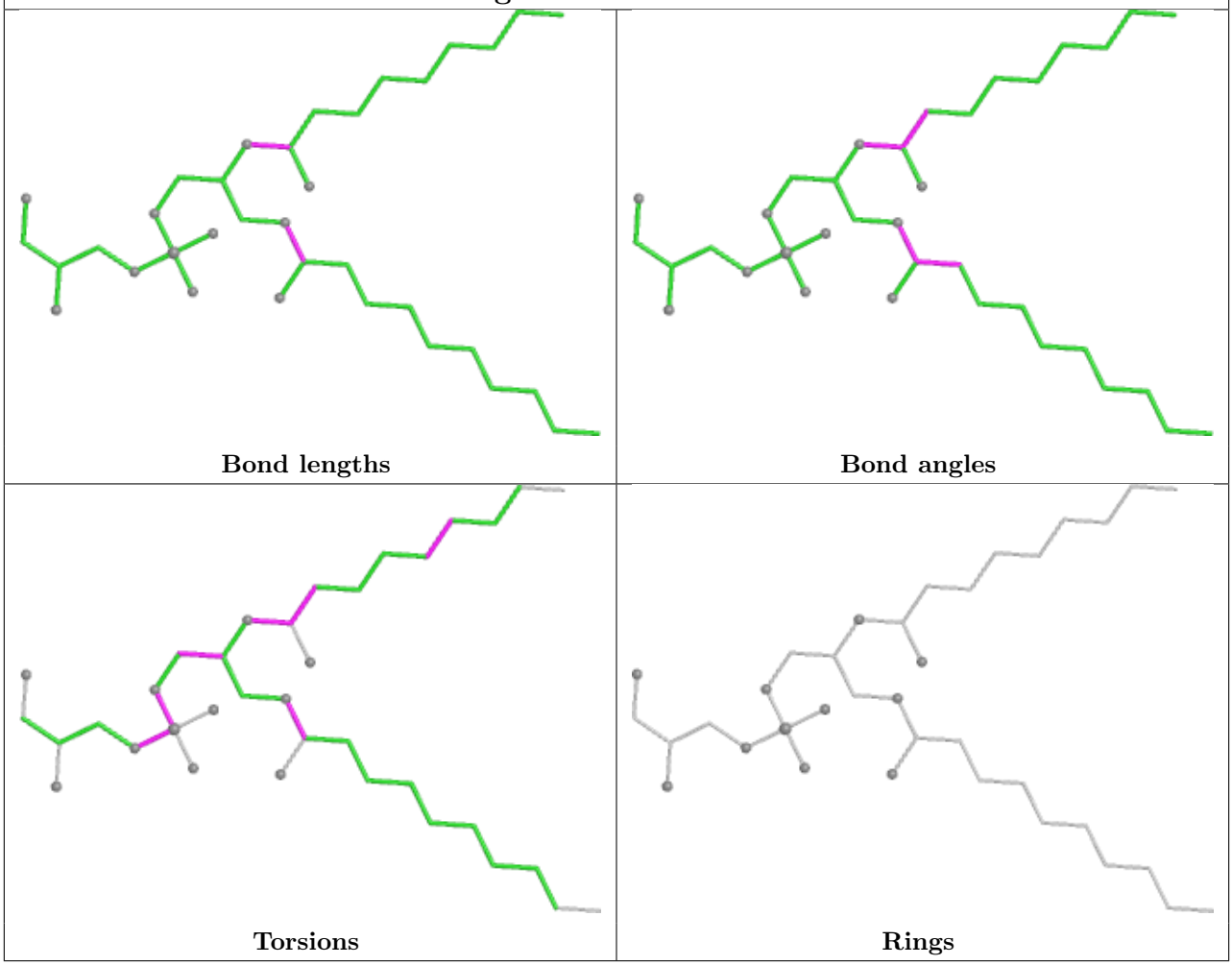


Torsions

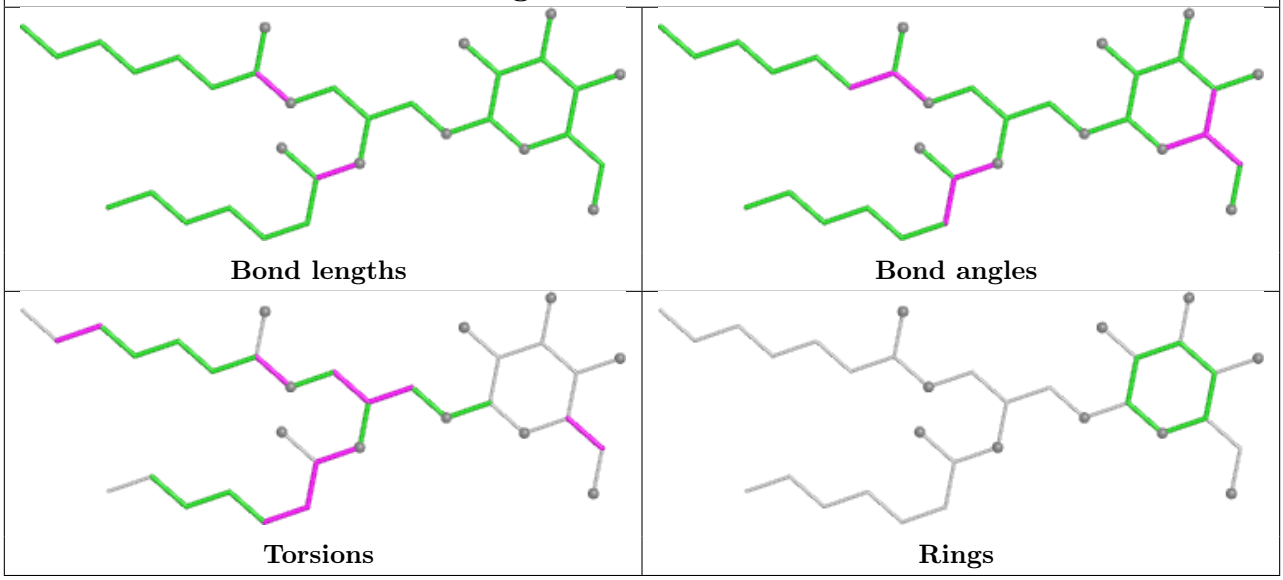


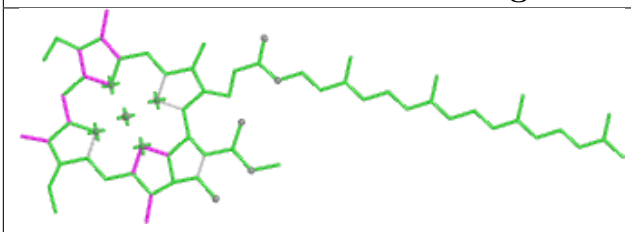
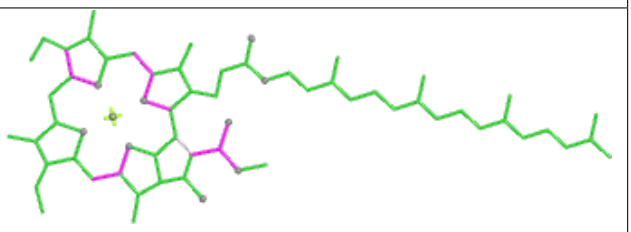
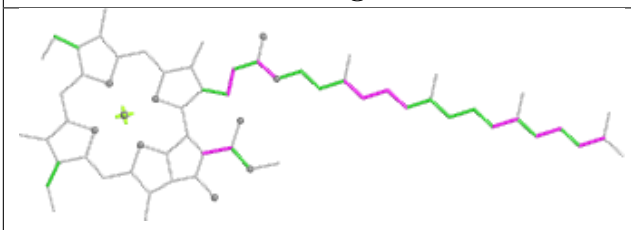
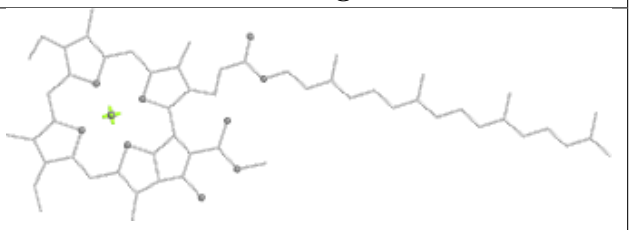
Rings

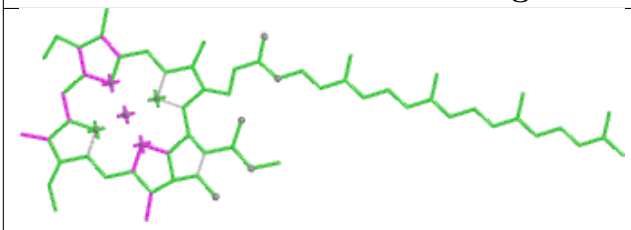
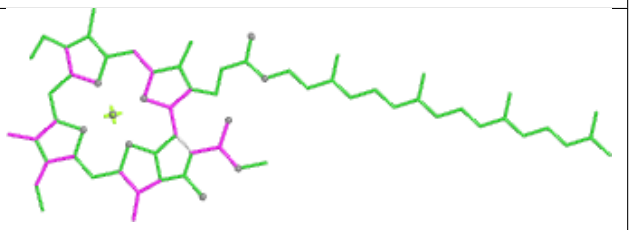
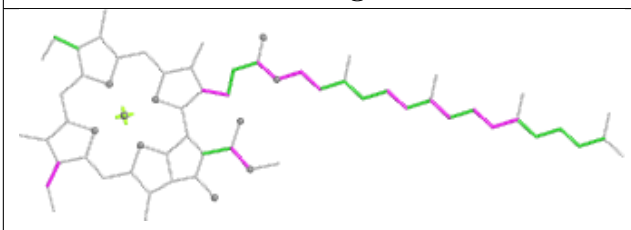
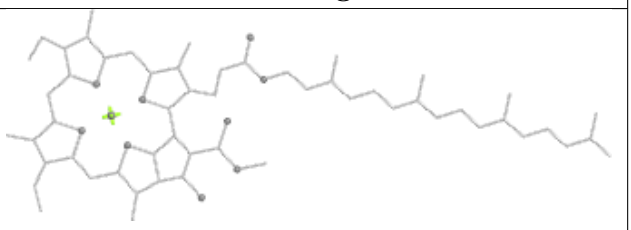
Ligand LHG B1 302



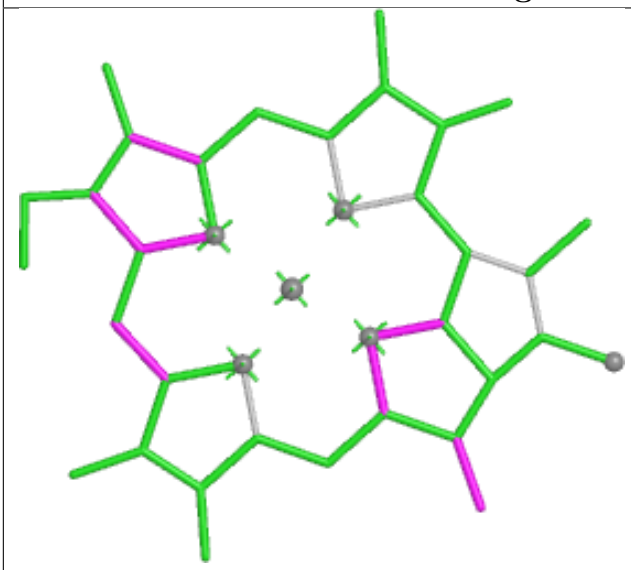
Ligand LMG B5 617



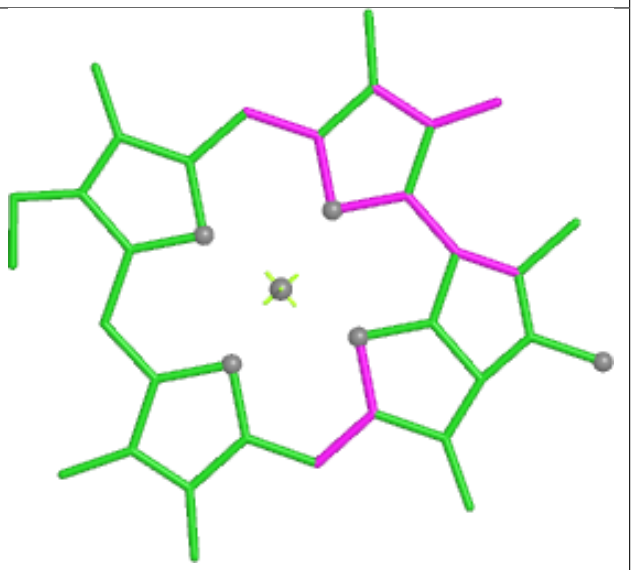
Ligand CLA AA 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BB 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

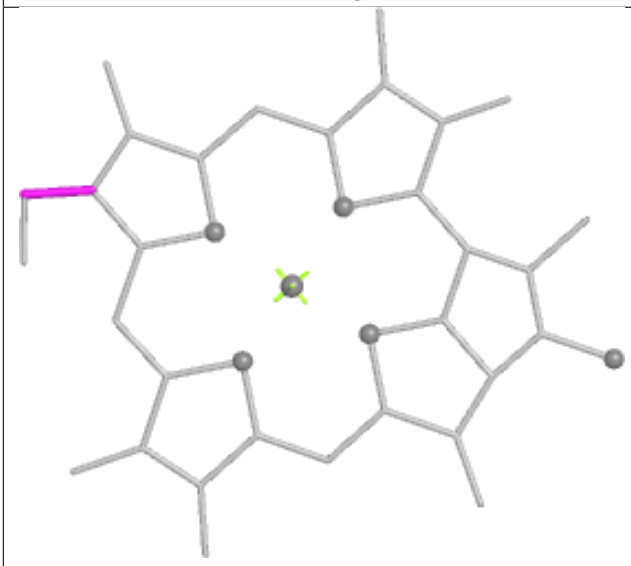
Ligand CLA A3 310



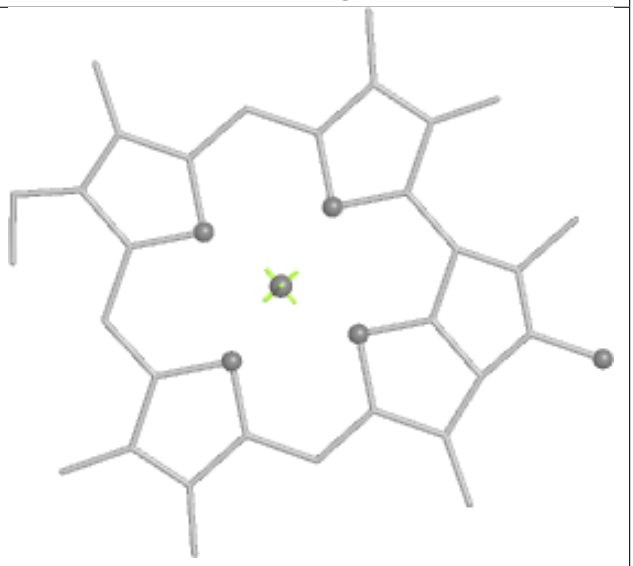
Bond lengths



Bond angles

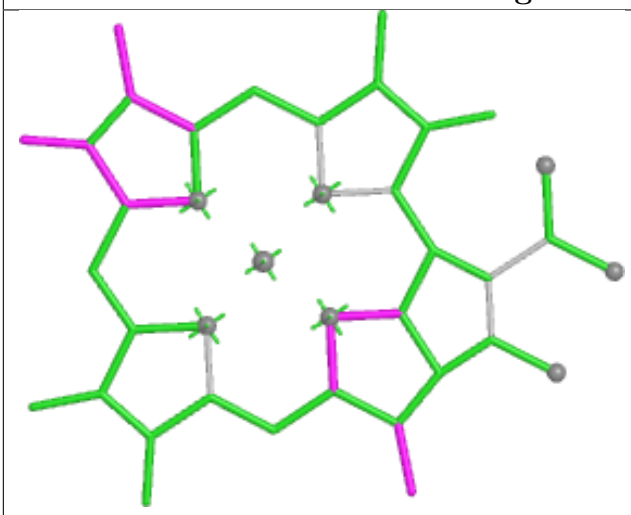


Torsions

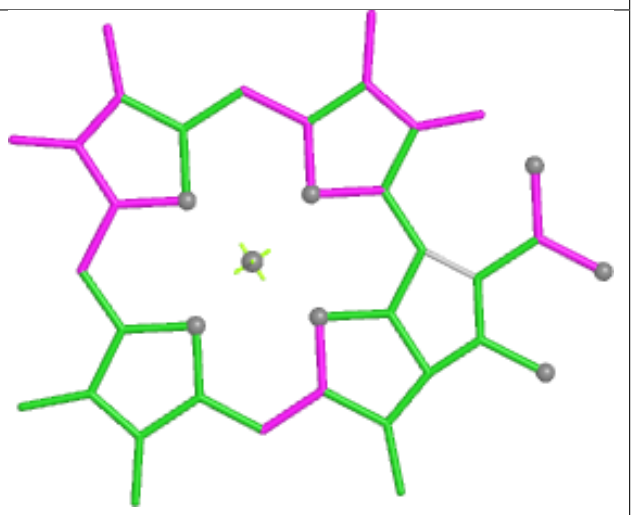


Rings

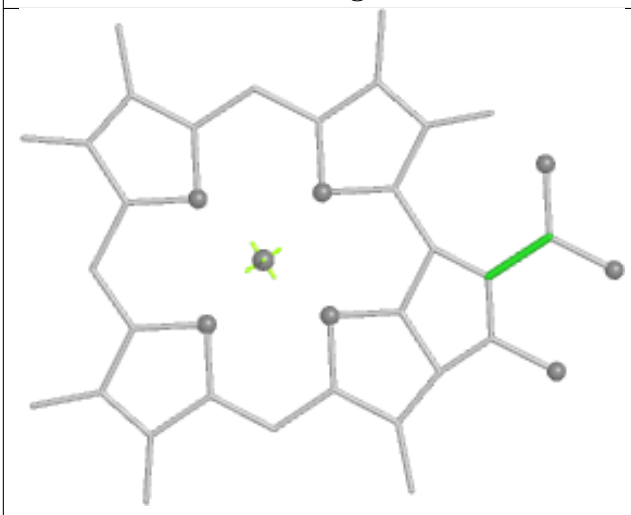
Ligand CLA A1 315



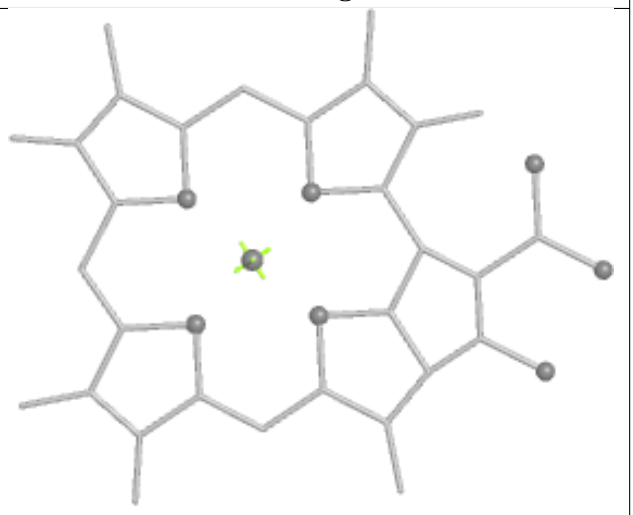
Bond lengths



Bond angles

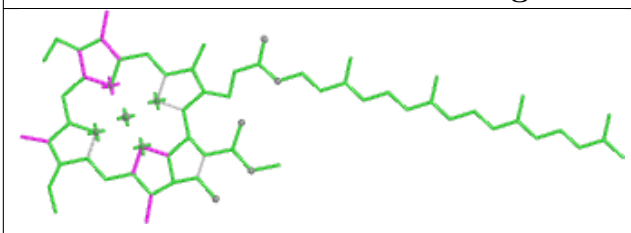


Torsions

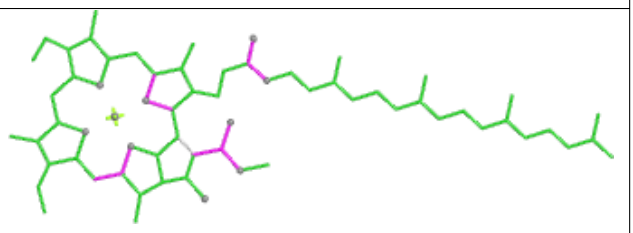


Rings

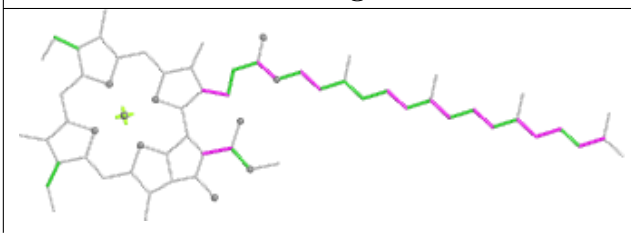
Ligand CLA BA 830



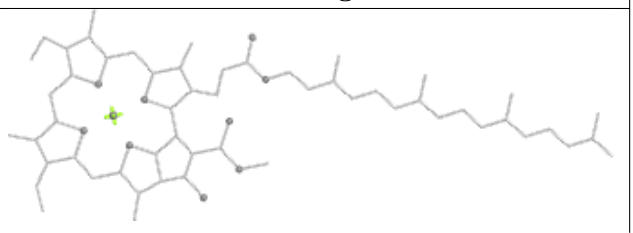
Bond lengths



Bond angles

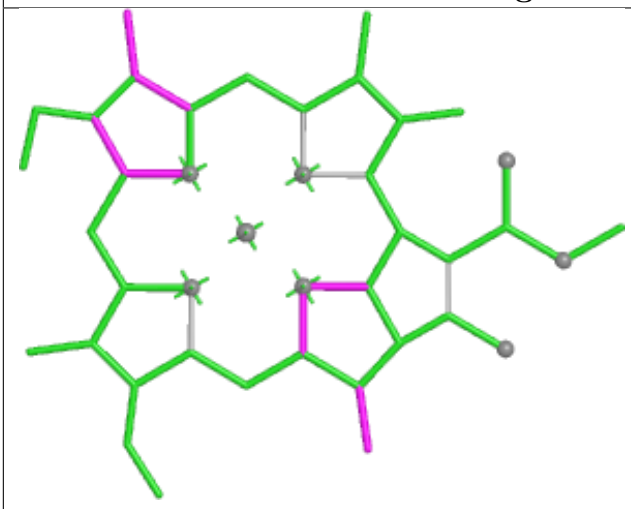


Torsions

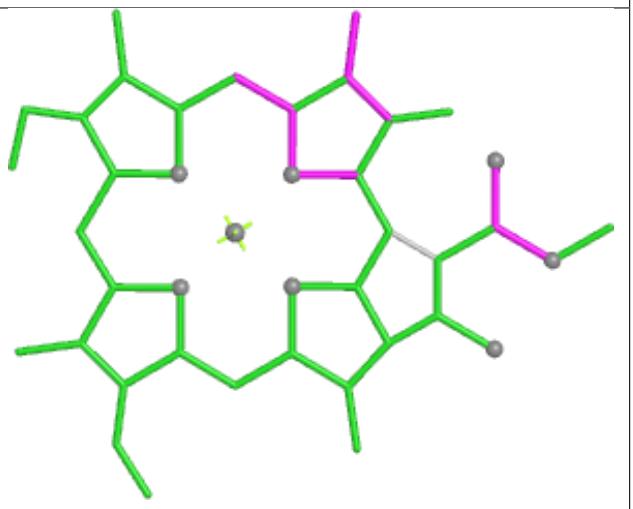


Rings

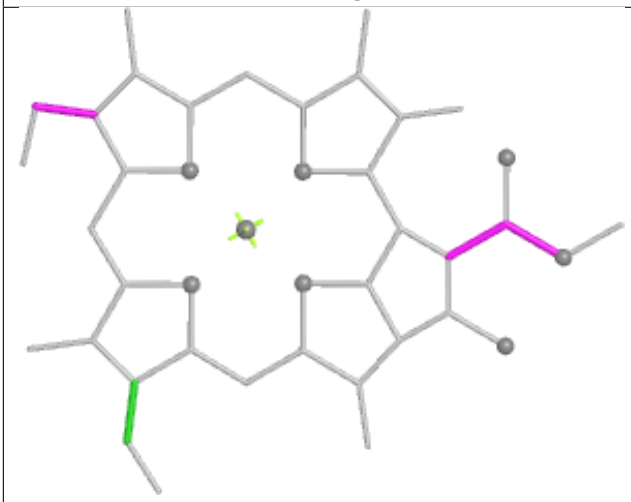
Ligand CLA B3 308



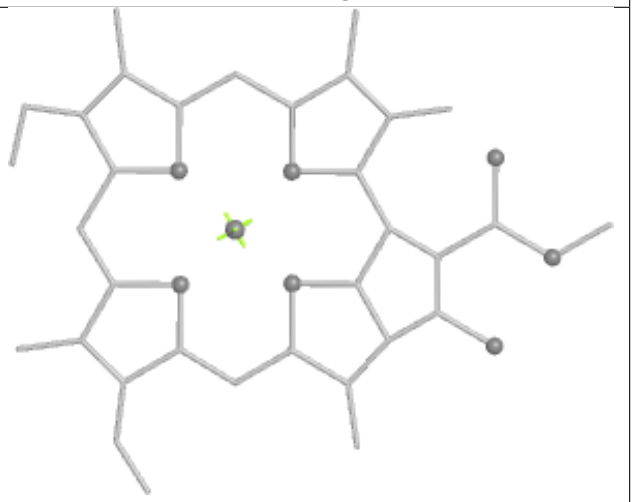
Bond lengths



Bond angles

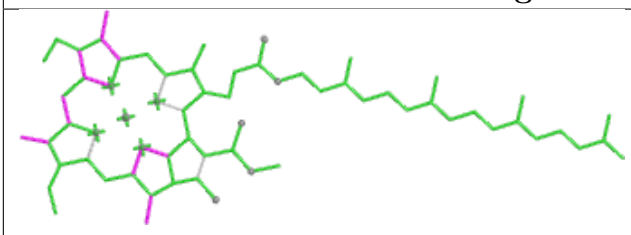


Torsions

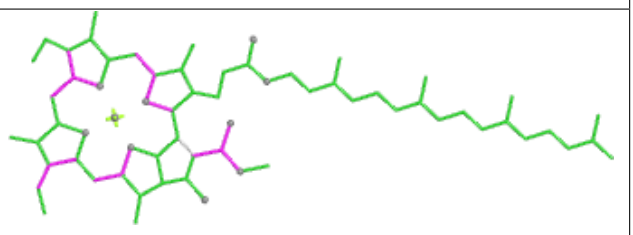


Rings

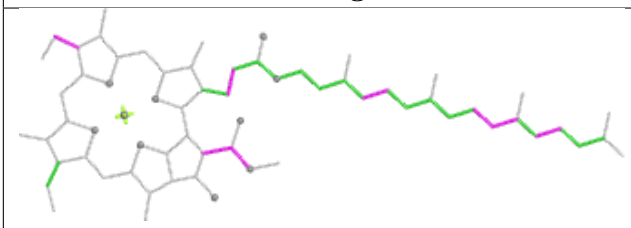
Ligand CLA A6 603



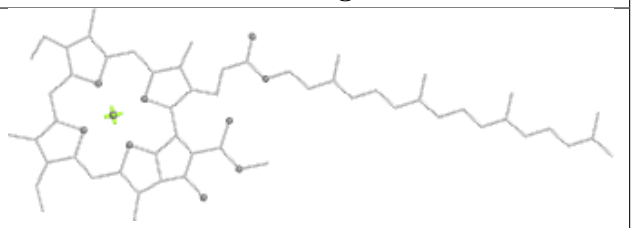
Bond lengths



Bond angles

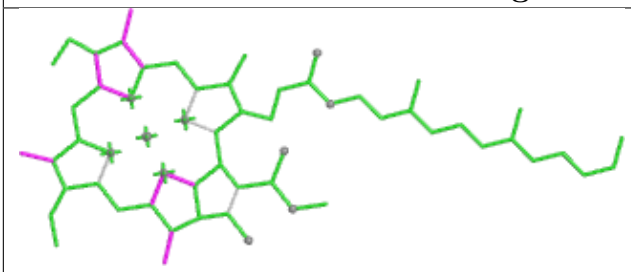


Torsions

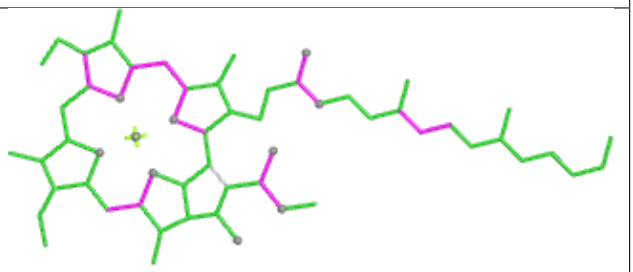


Rings

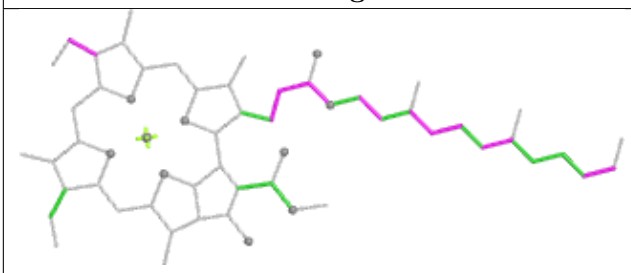
Ligand CLA BB 819



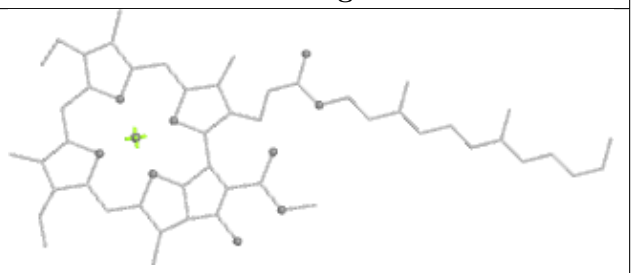
Bond lengths



Bond angles

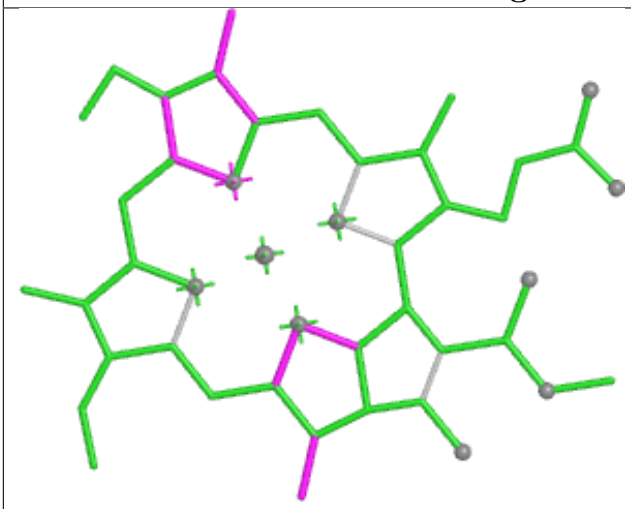


Torsions

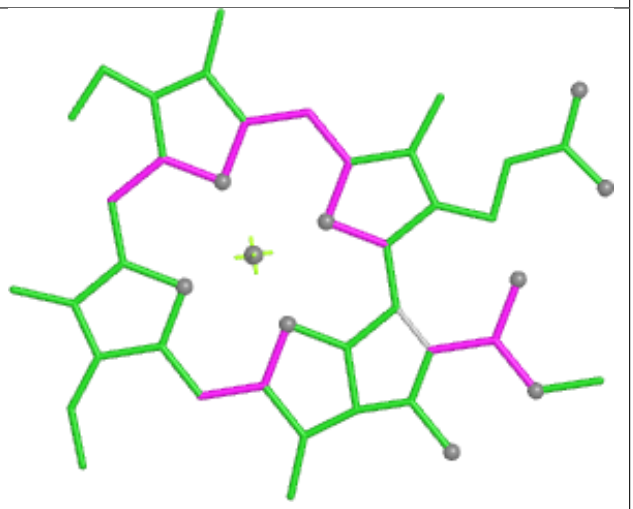


Rings

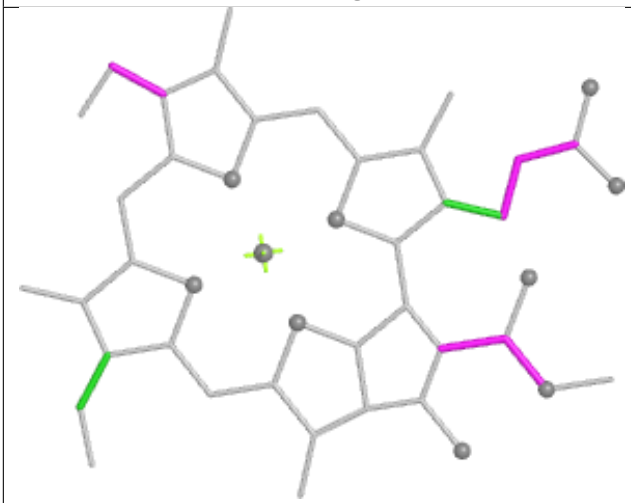
Ligand CLA AA 836



Bond lengths



Bond angles

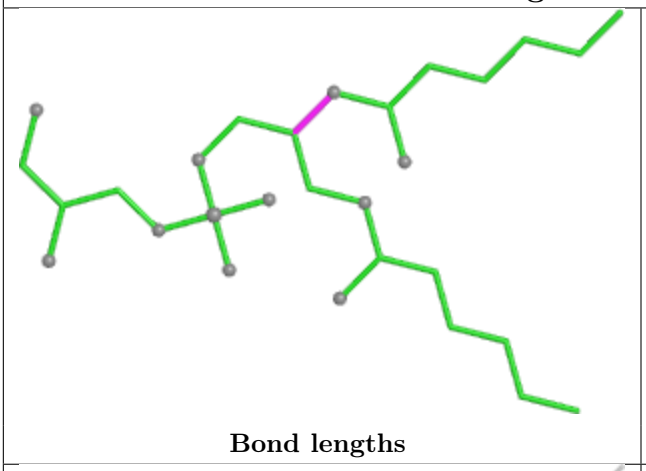


Torsions

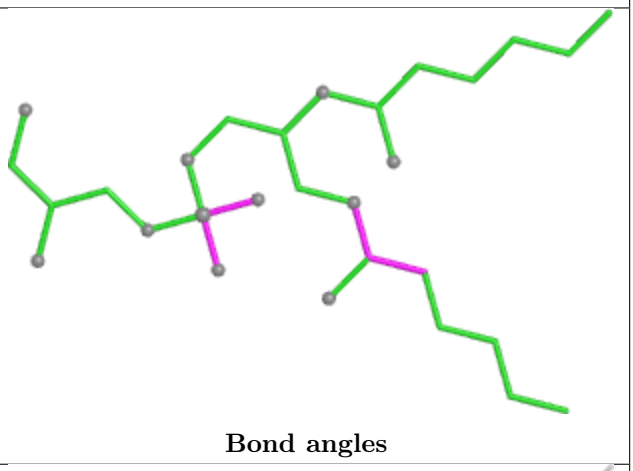


Rings

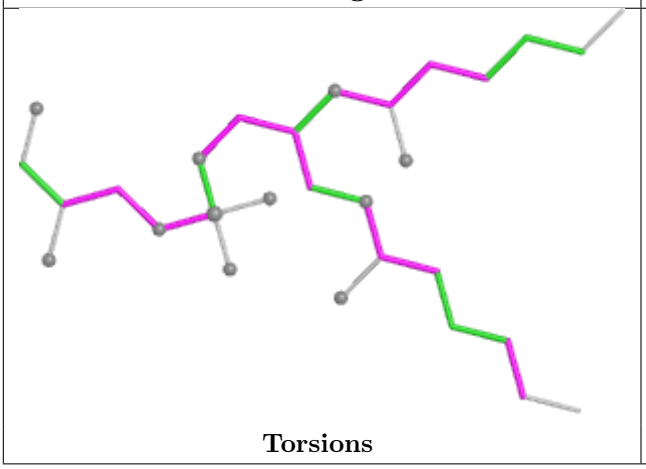
Ligand LHG a 501



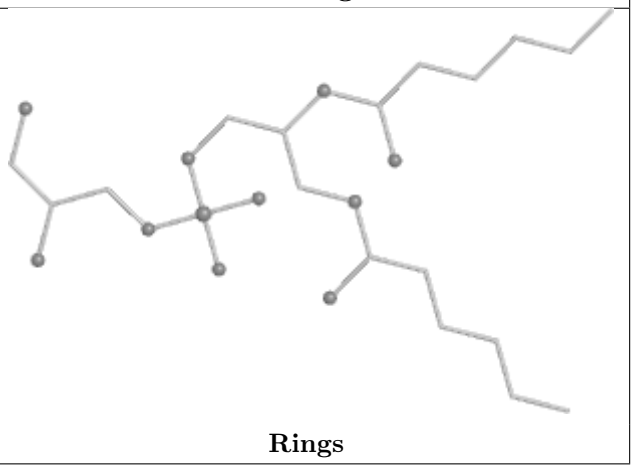
Bond lengths



Bond angles



Torsions

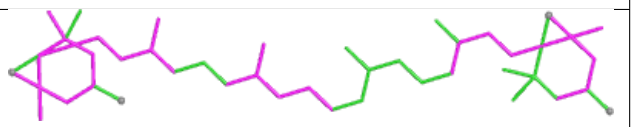


Rings

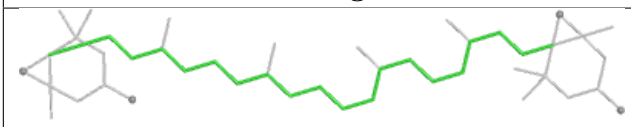
Ligand XAT B5 615



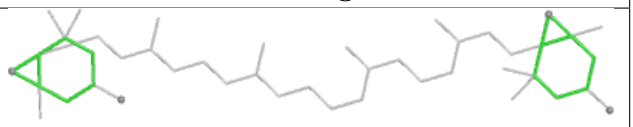
Bond lengths



Bond angles

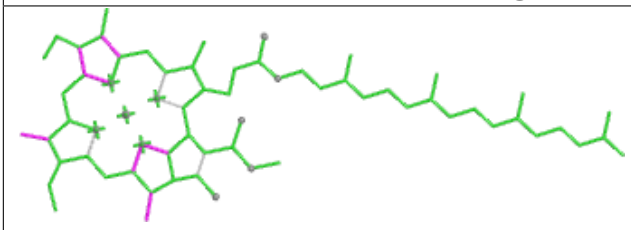


Torsions

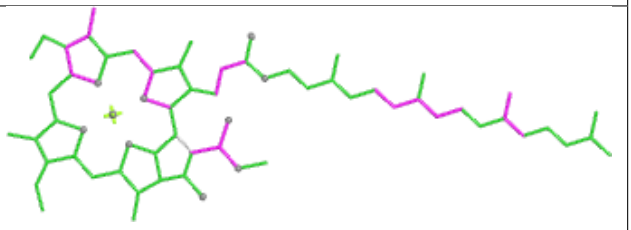


Rings

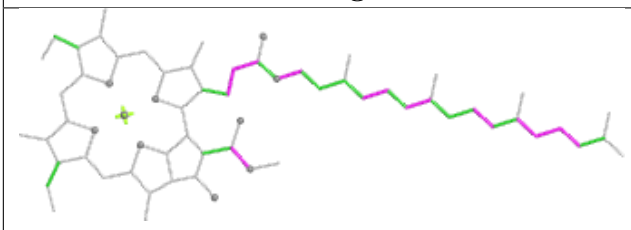
Ligand CLA BA 828



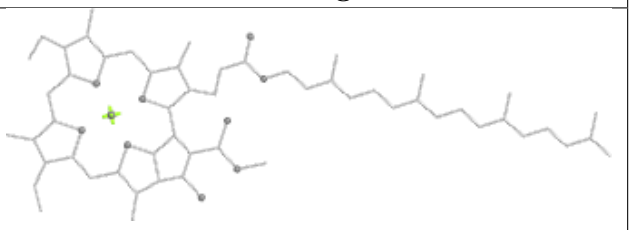
Bond lengths



Bond angles

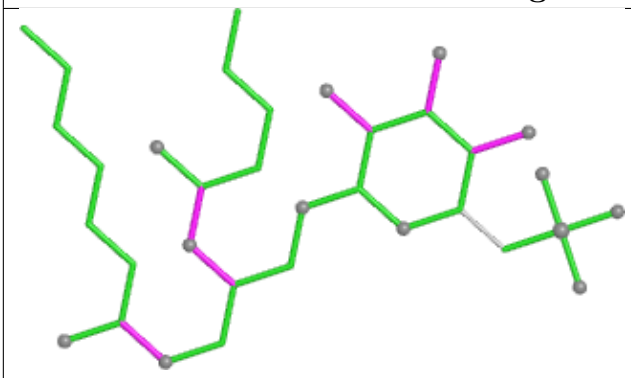


Torsions

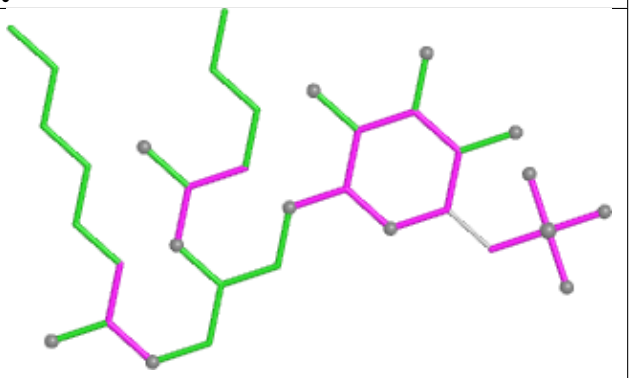


Rings

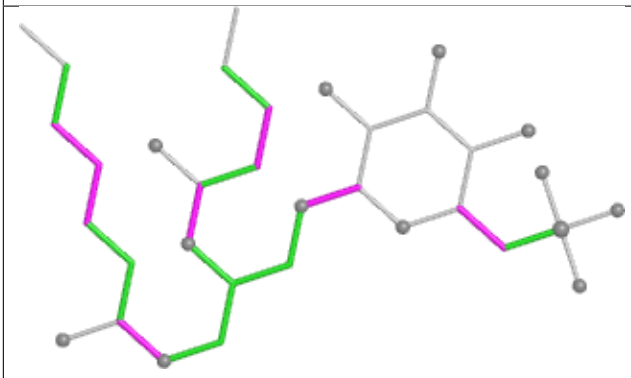
Ligand SQD e 301



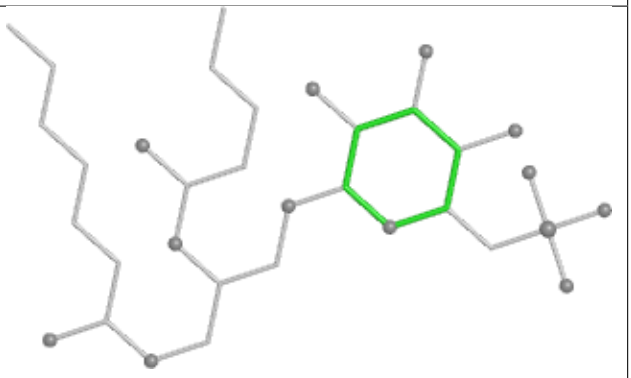
Bond lengths



Bond angles

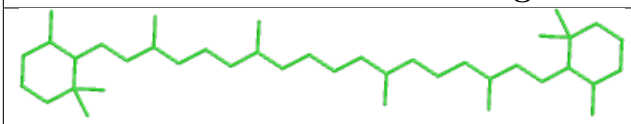


Torsions

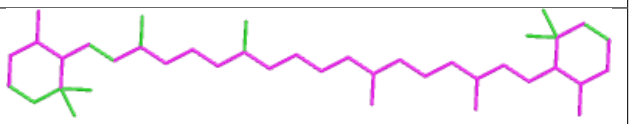


Rings

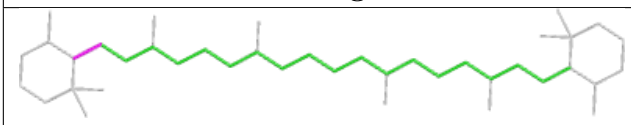
Ligand BCR B5 616



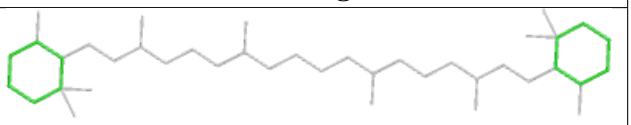
Bond lengths



Bond angles

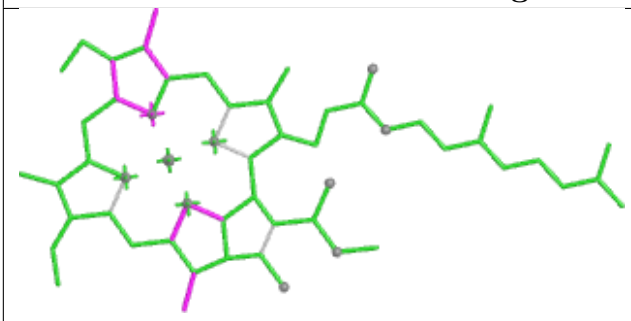


Torsions

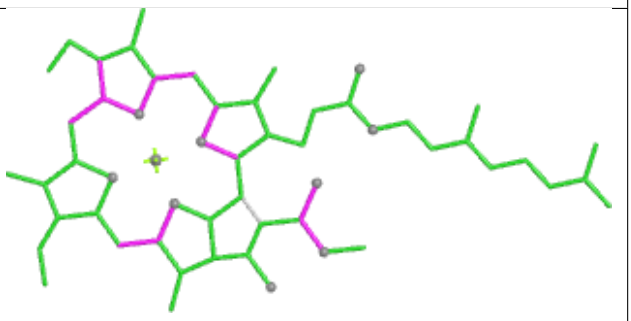


Rings

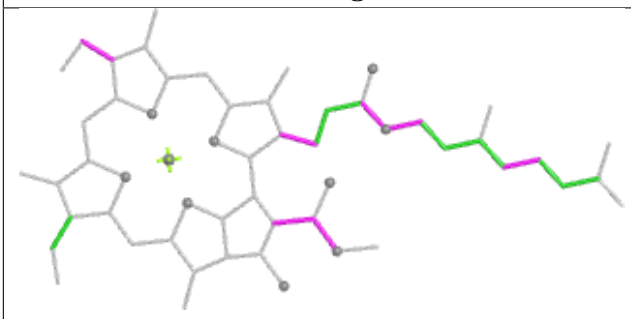
Ligand CLA AB 820



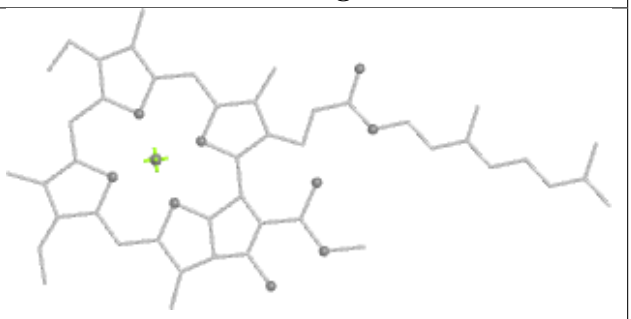
Bond lengths



Bond angles

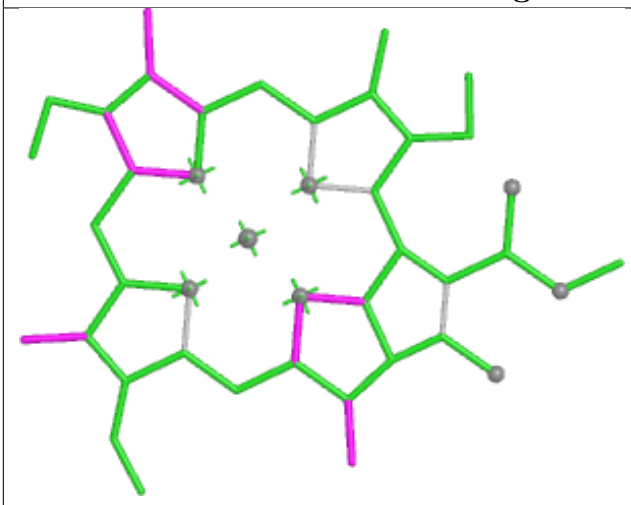


Torsions

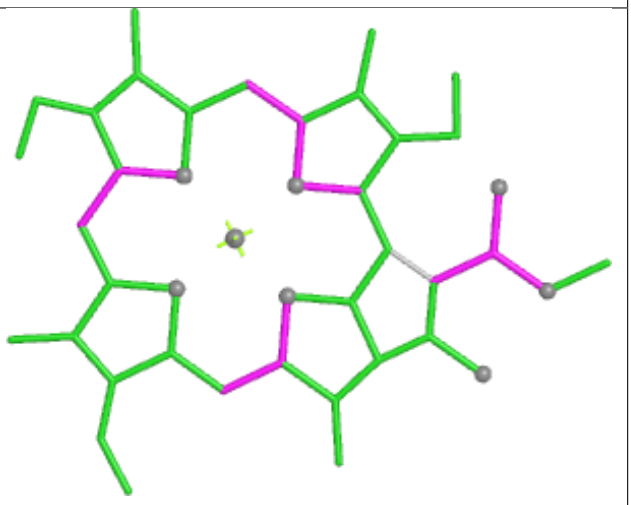


Rings

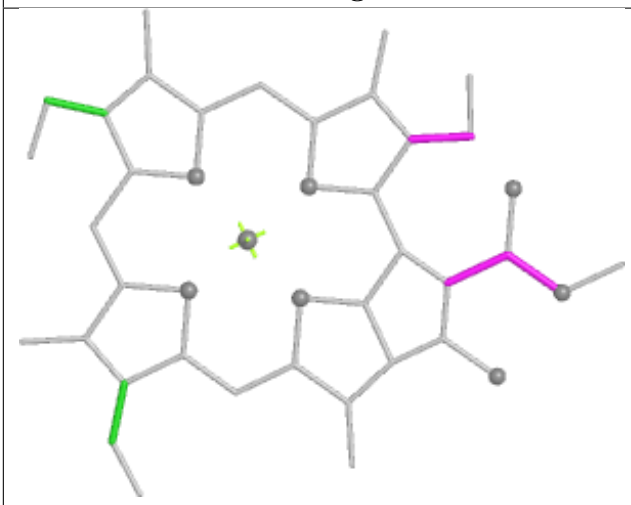
Ligand CLA AL 305



Bond lengths



Bond angles

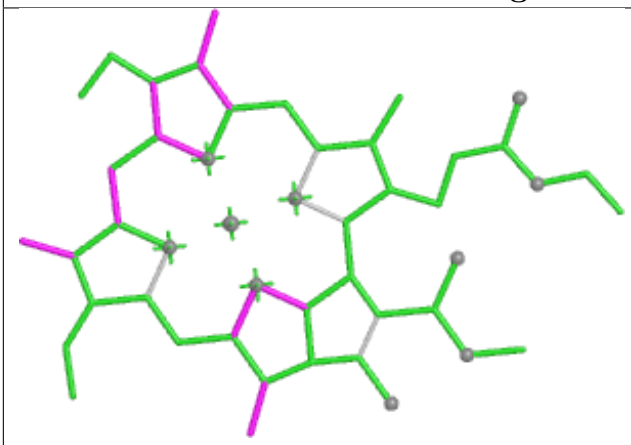


Torsions

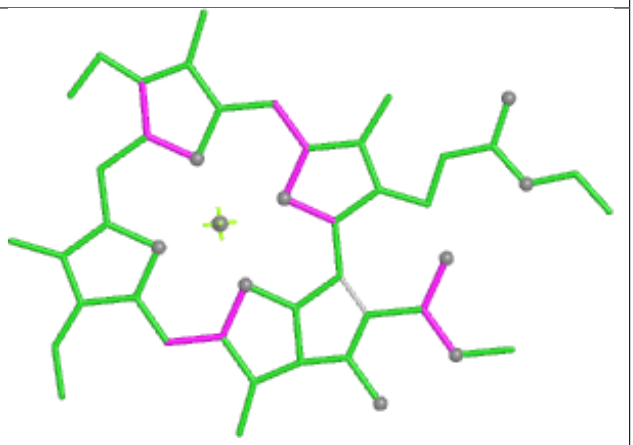


Rings

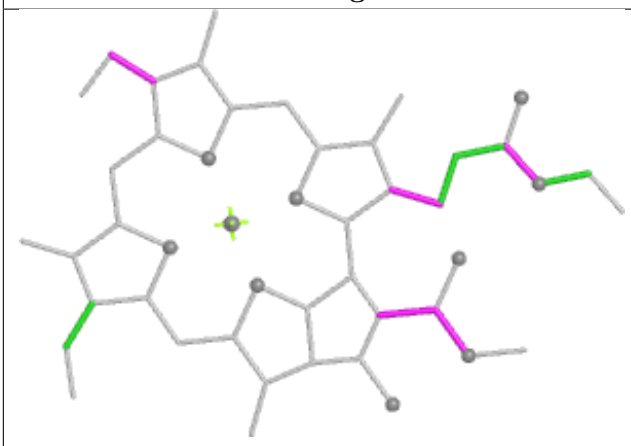
Ligand CLA AA 831



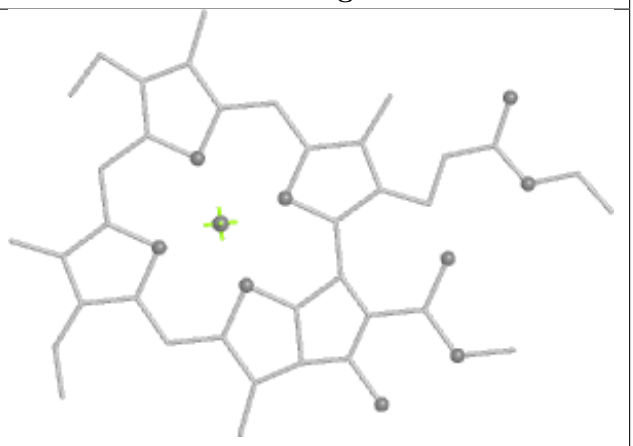
Bond lengths



Bond angles

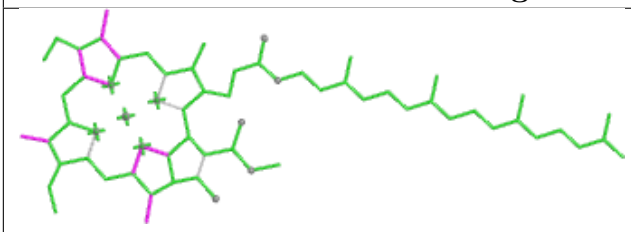


Torsions

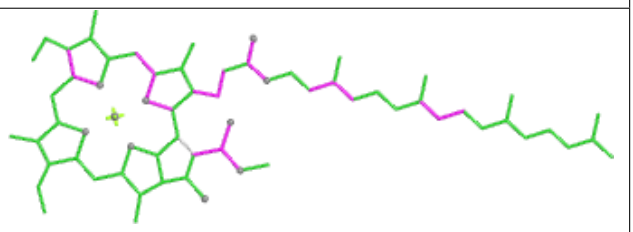


Rings

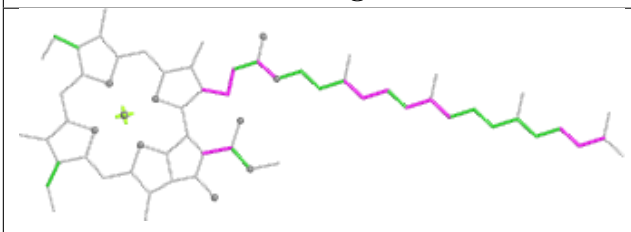
Ligand CLA AB 809



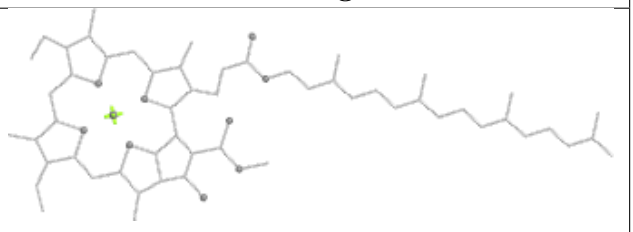
Bond lengths



Bond angles

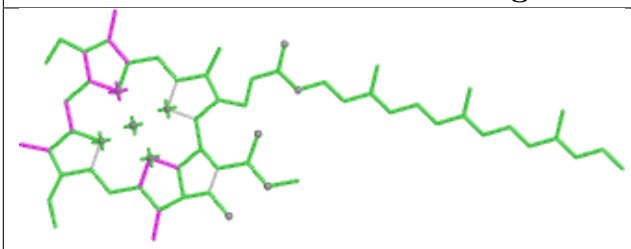


Torsions

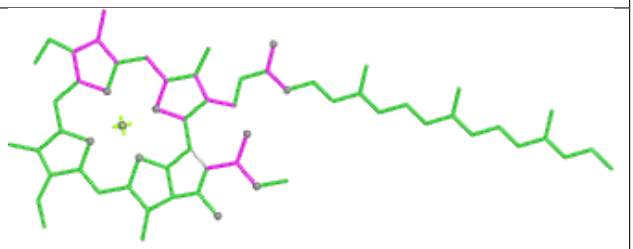


Rings

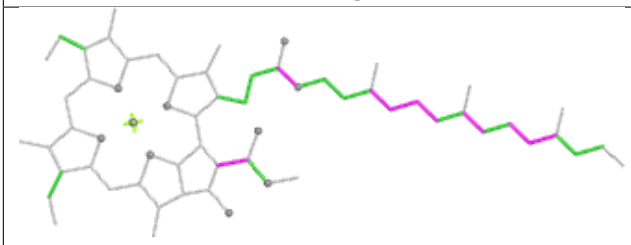
Ligand CLA AB 827



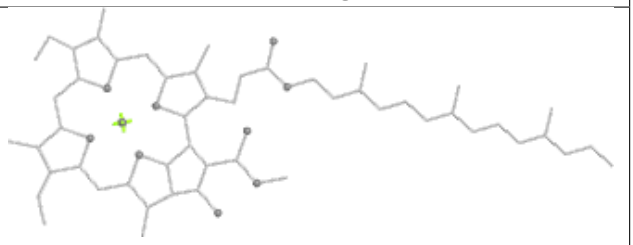
Bond lengths



Bond angles

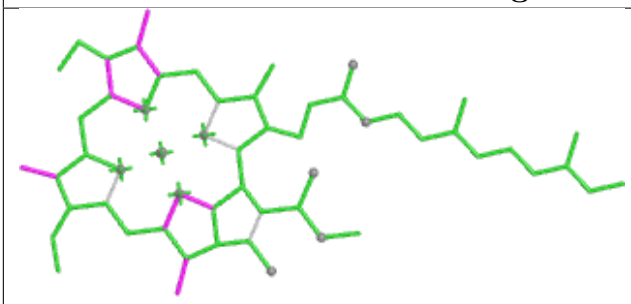


Torsions

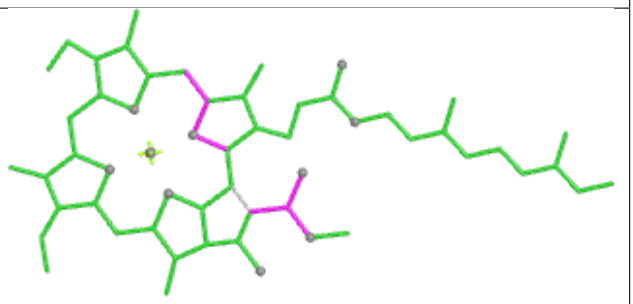


Rings

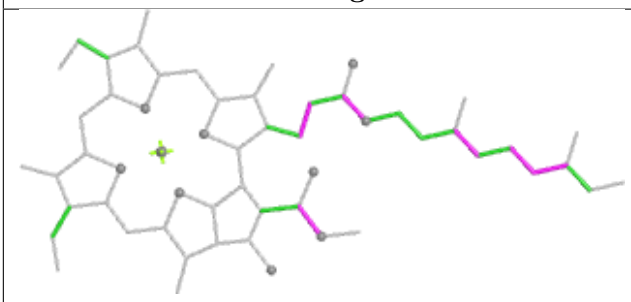
Ligand CLA AB 830



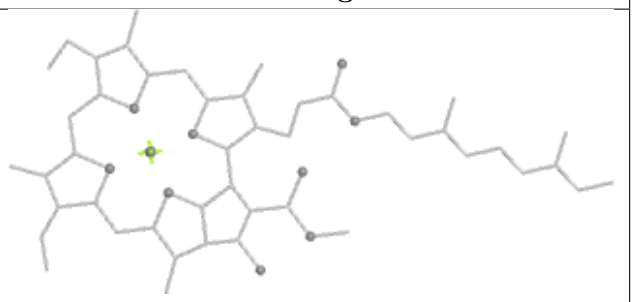
Bond lengths



Bond angles

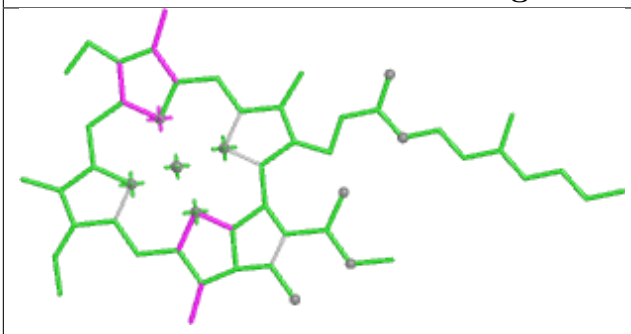


Torsions

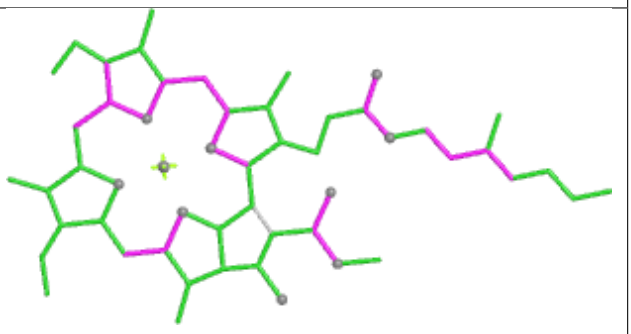


Rings

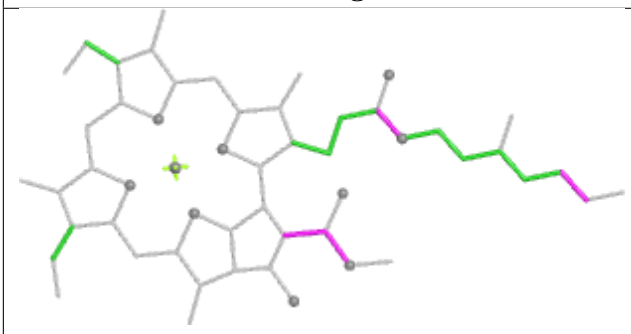
Ligand CLA BA 826



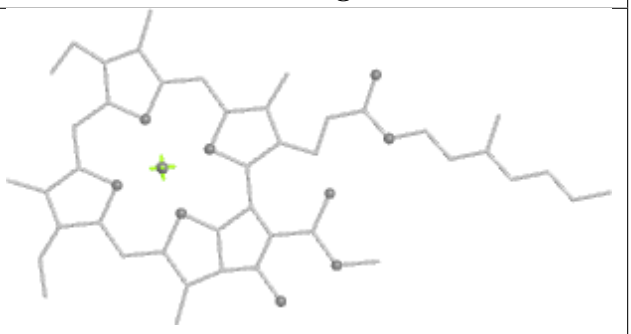
Bond lengths



Bond angles

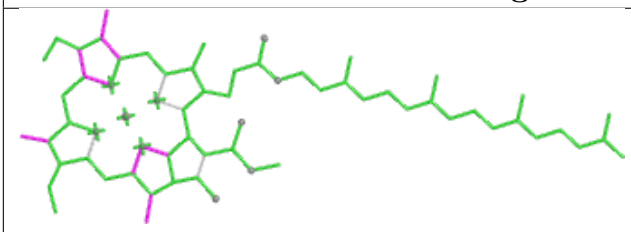


Torsions

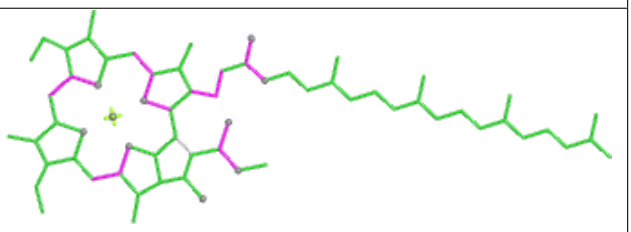


Rings

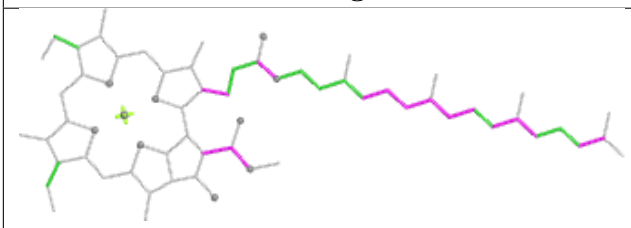
Ligand CLA AB 823



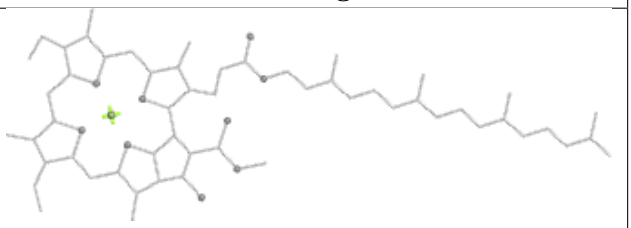
Bond lengths



Bond angles

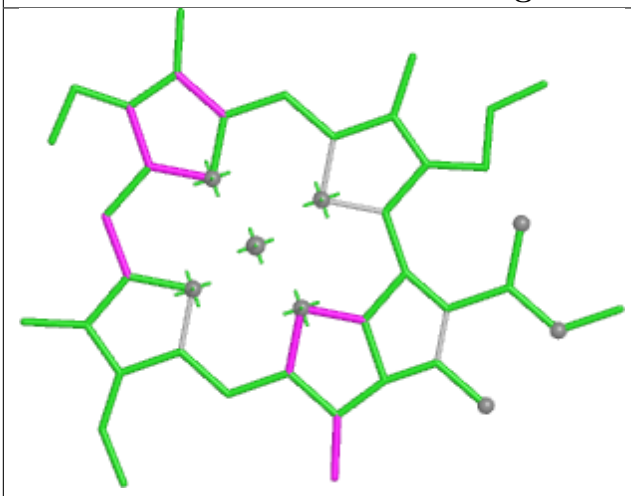


Torsions

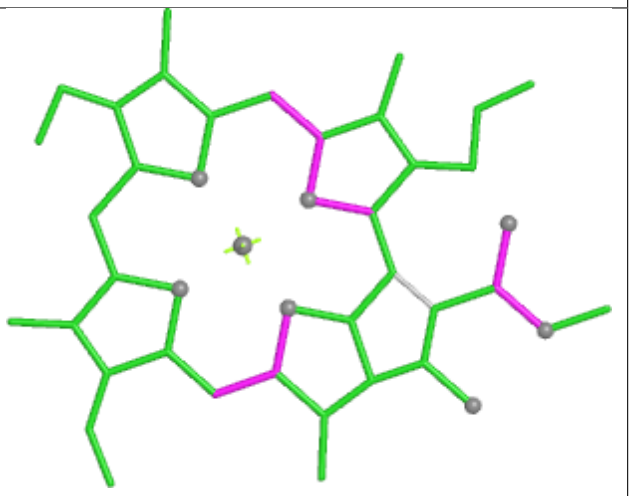


Rings

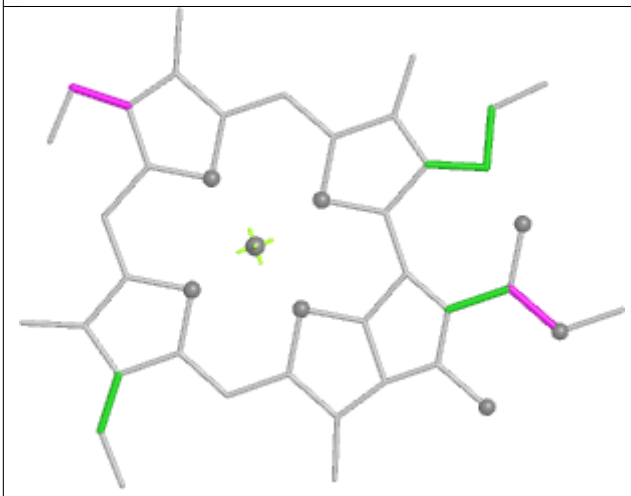
Ligand CLA A6 614



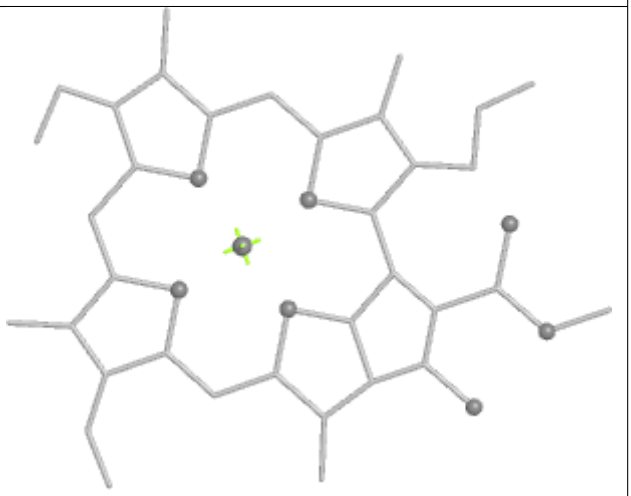
Bond lengths



Bond angles

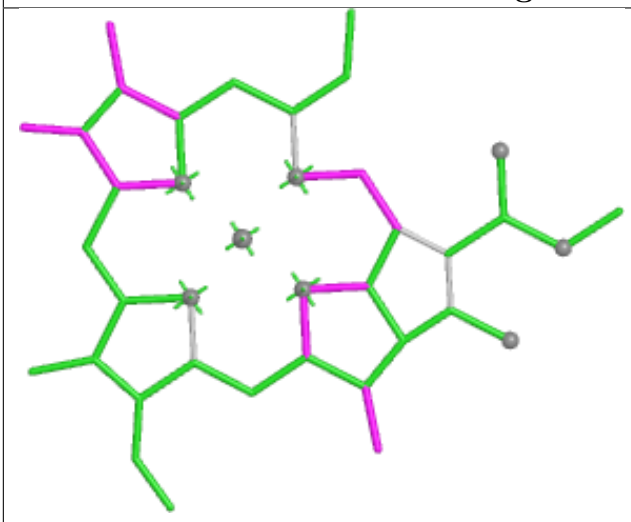


Torsions

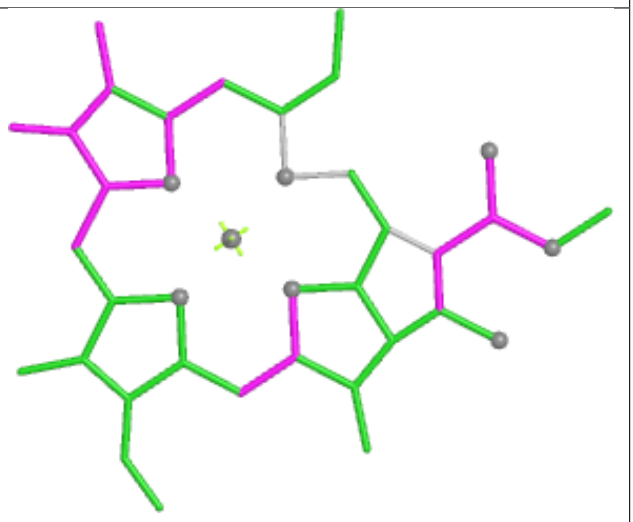


Rings

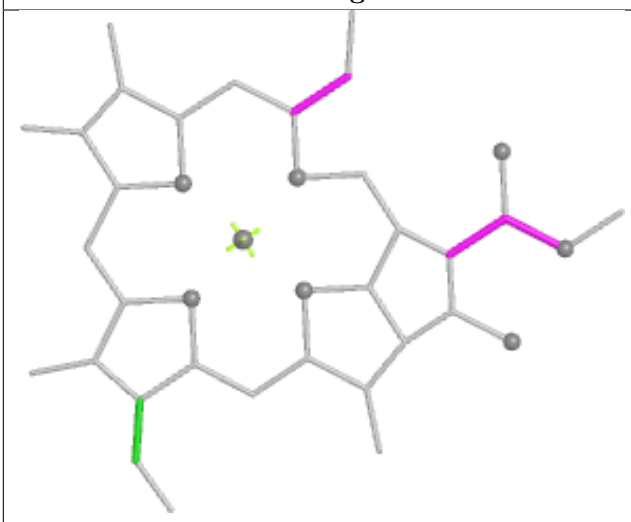
Ligand CLA B2 610



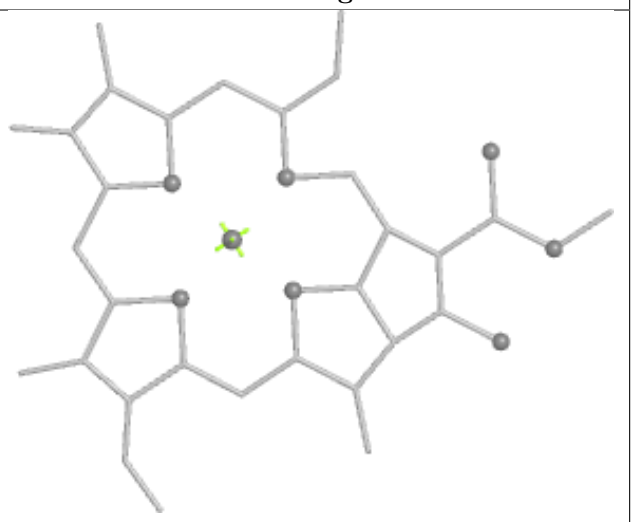
Bond lengths



Bond angles

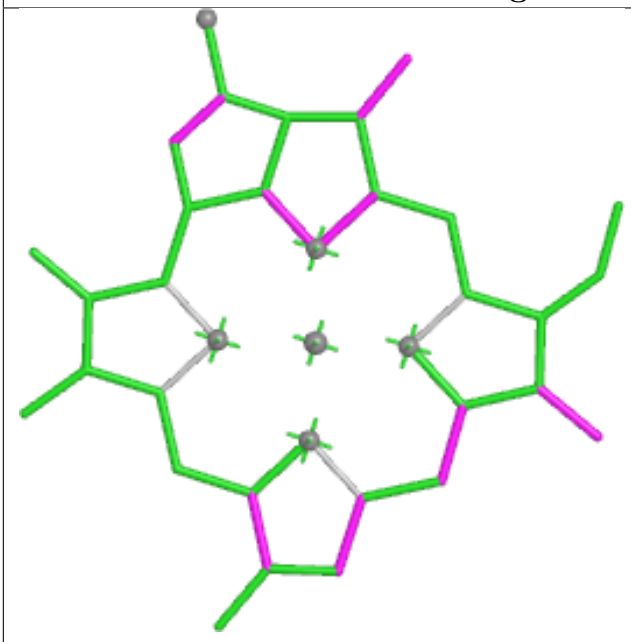


Torsions

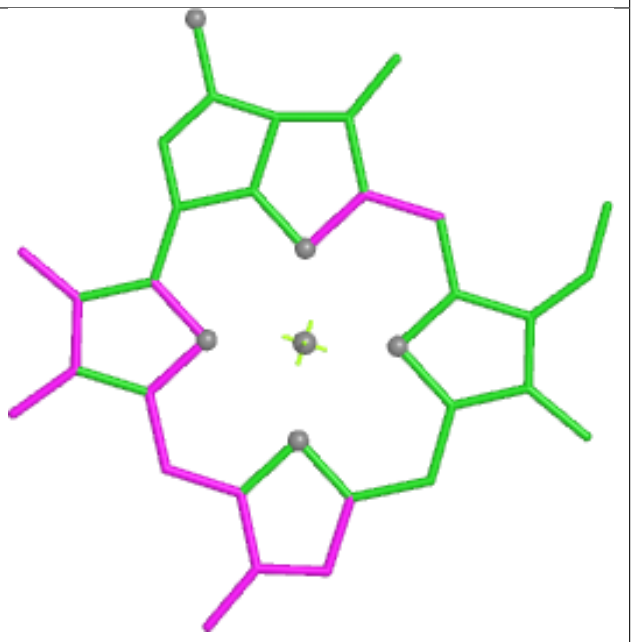


Rings

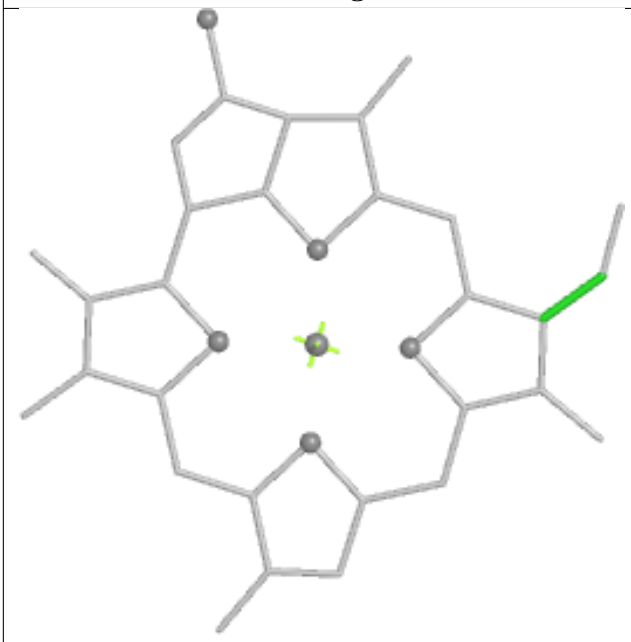
Ligand CLA AK 201



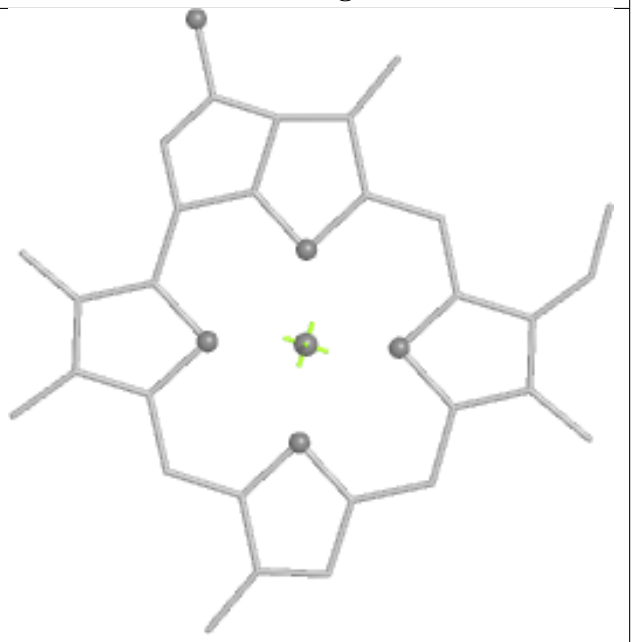
Bond lengths



Bond angles

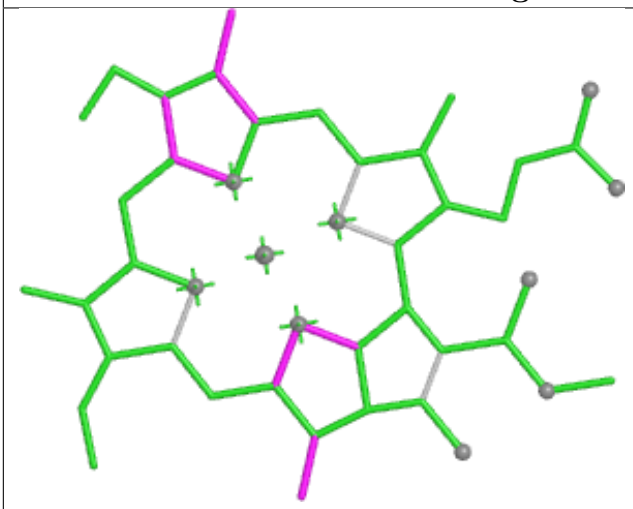


Torsions

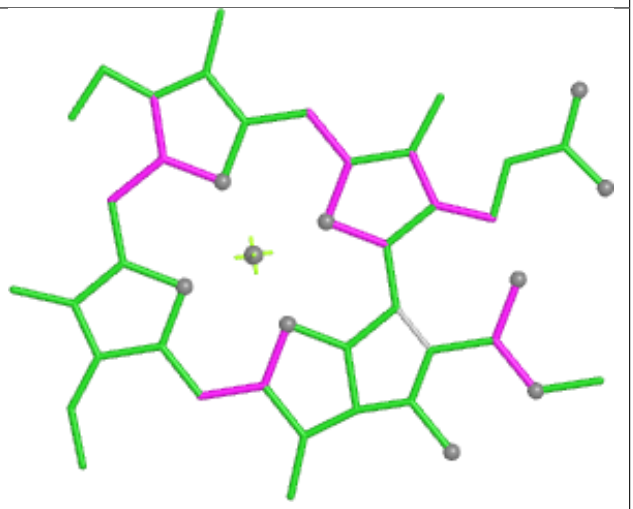


Rings

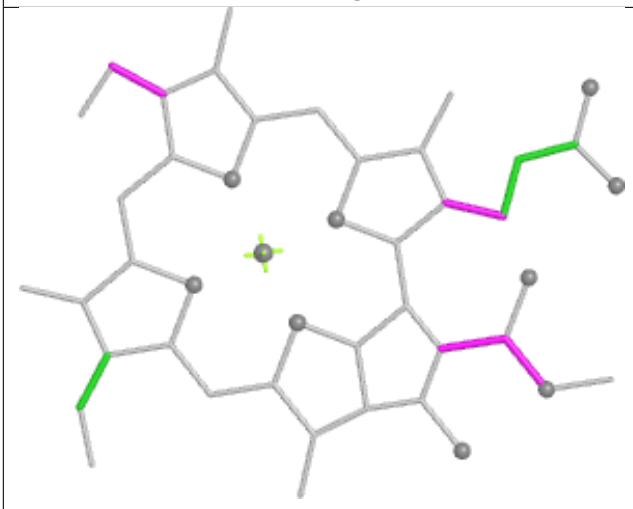
Ligand CLA BB 825



Bond lengths



Bond angles

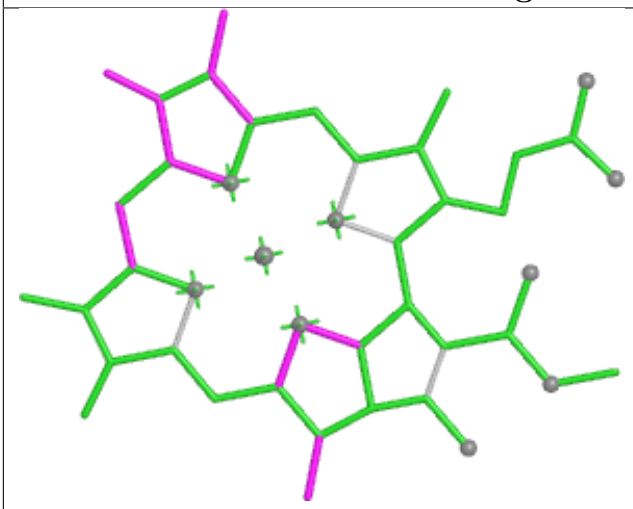


Torsions

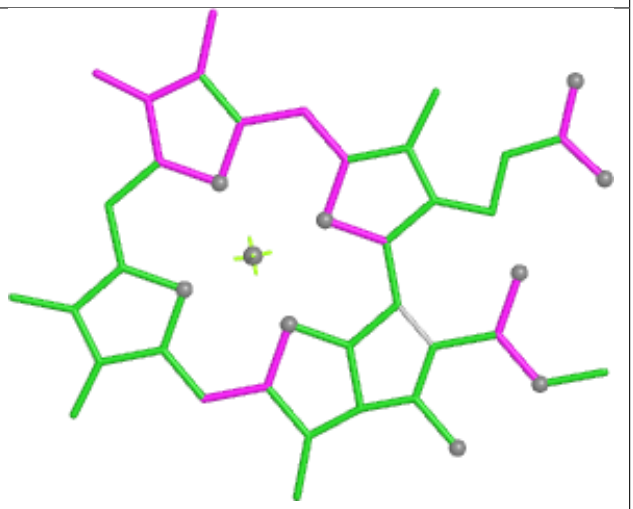


Rings

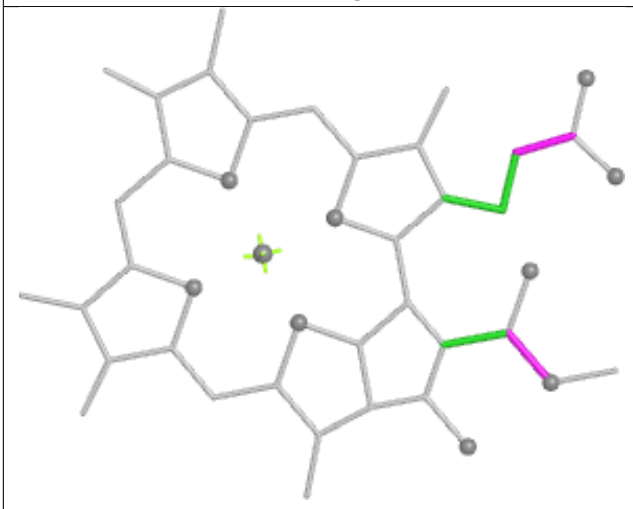
Ligand CLA B5 604



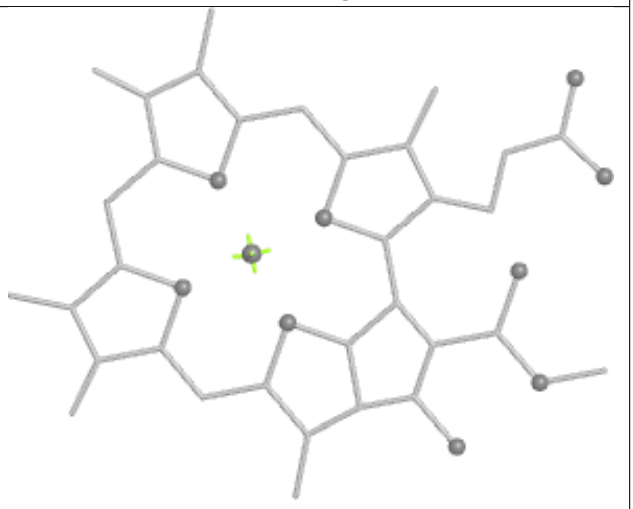
Bond lengths



Bond angles

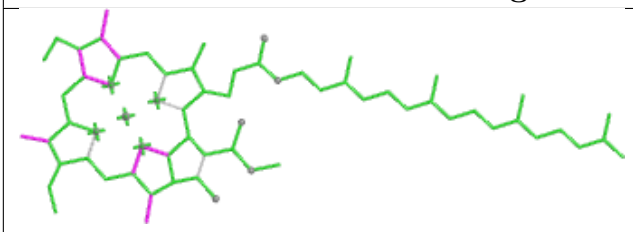


Torsions

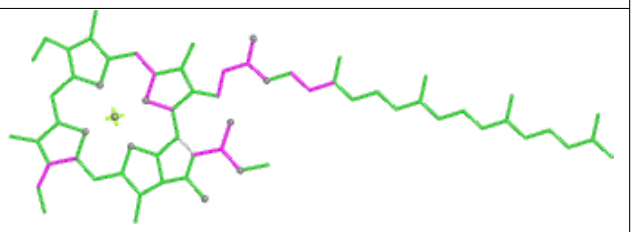


Rings

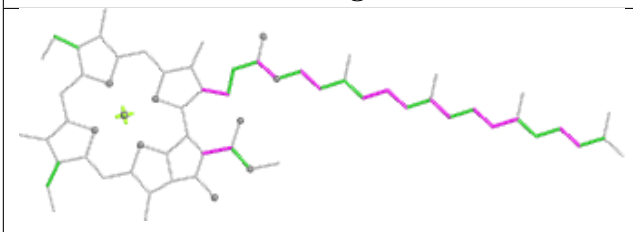
Ligand CLA AA 803



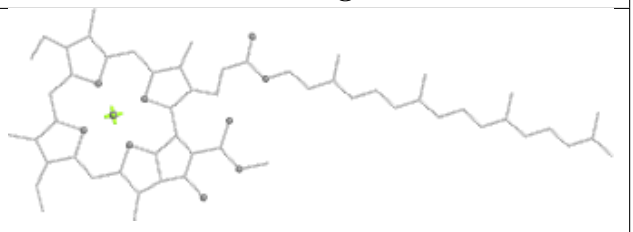
Bond lengths



Bond angles

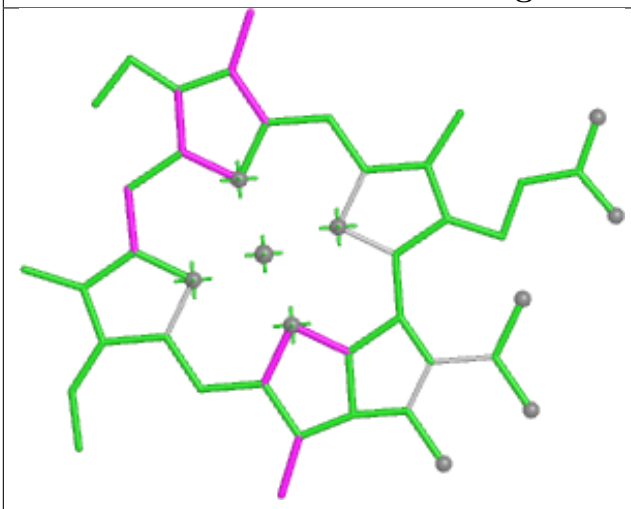


Torsions

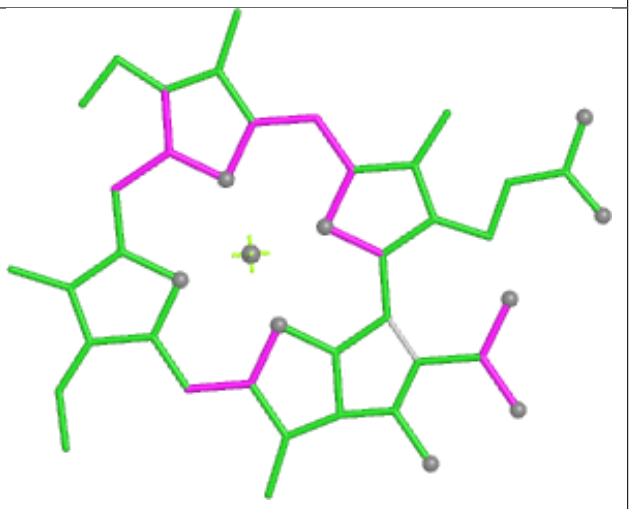


Rings

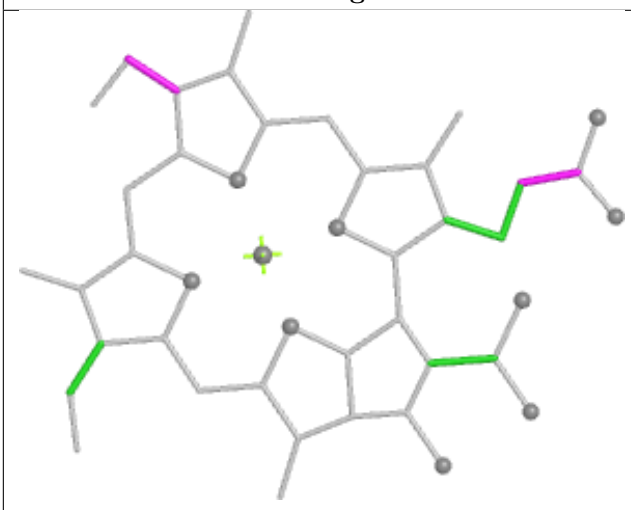
Ligand CLA B1 309



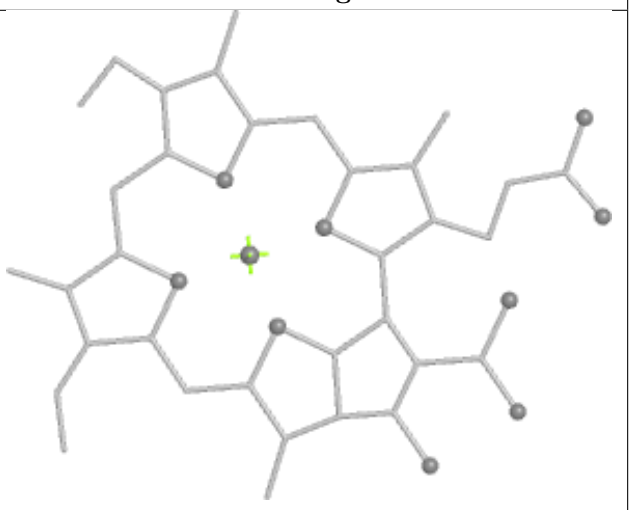
Bond lengths



Bond angles

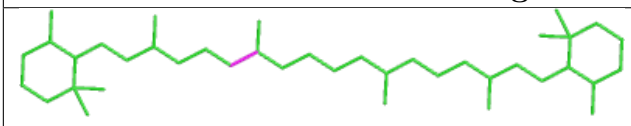


Torsions

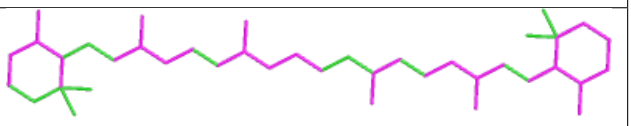


Rings

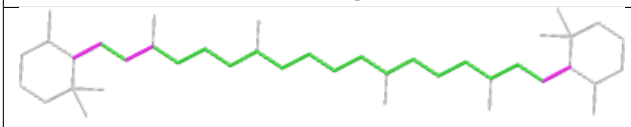
Ligand BCR AL 306



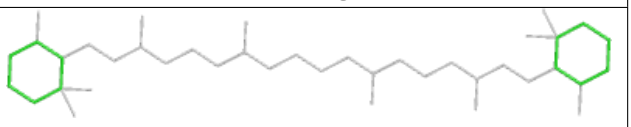
Bond lengths



Bond angles

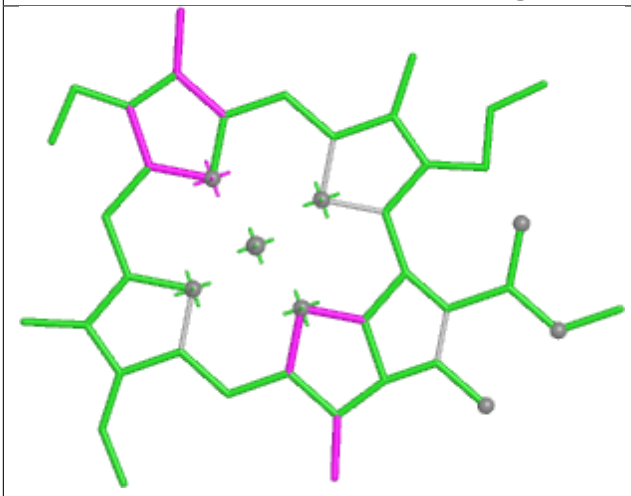


Torsions

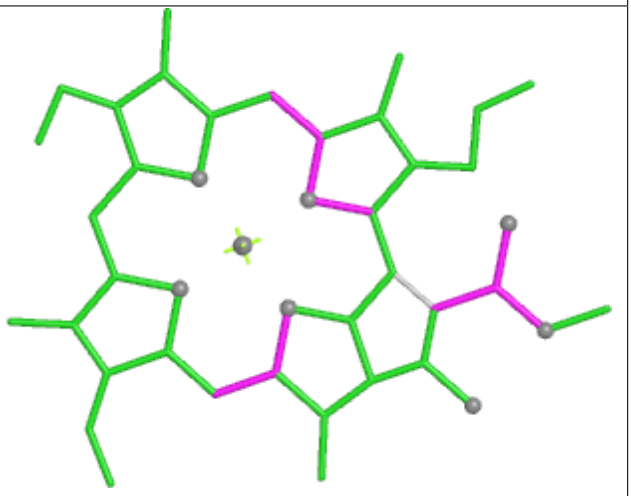


Rings

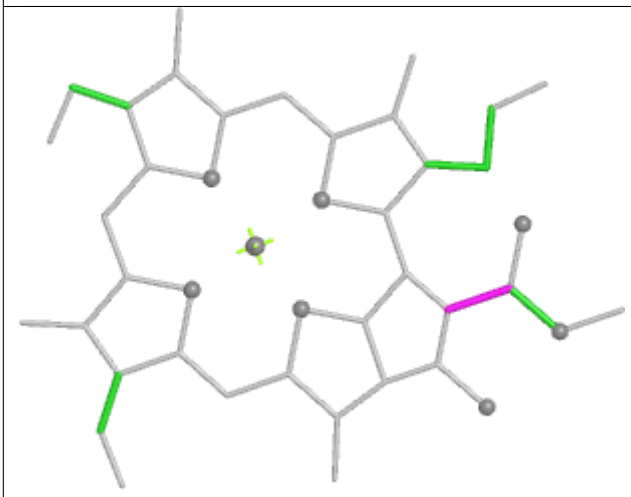
Ligand CLA BB 814



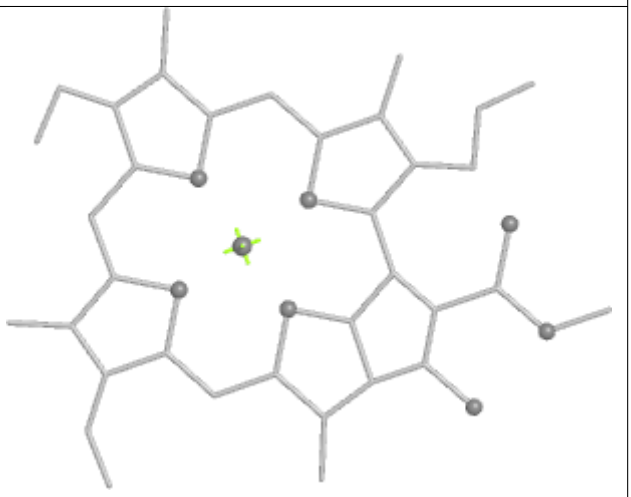
Bond lengths



Bond angles

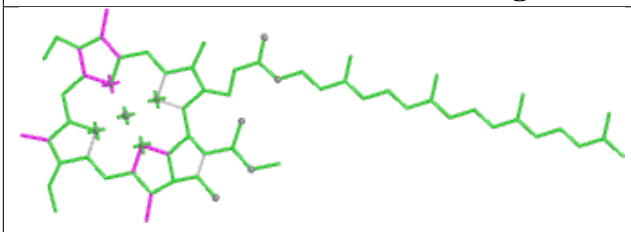


Torsions

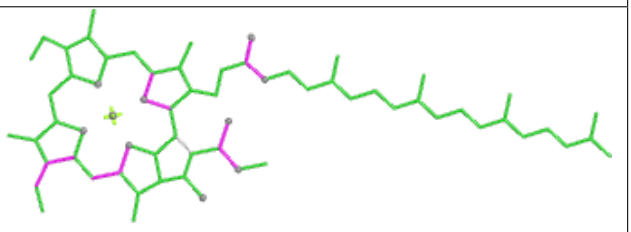


Rings

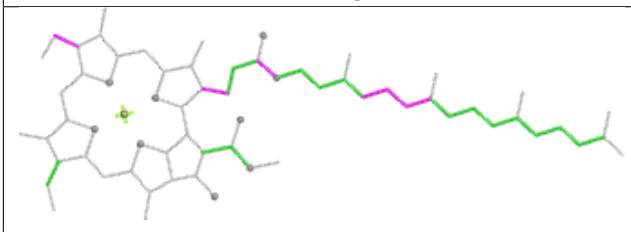
Ligand CLA AB 841



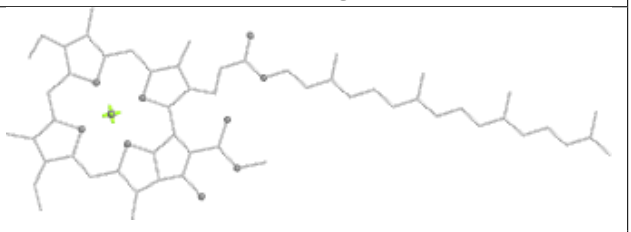
Bond lengths



Bond angles

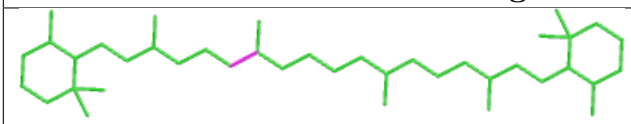


Torsions

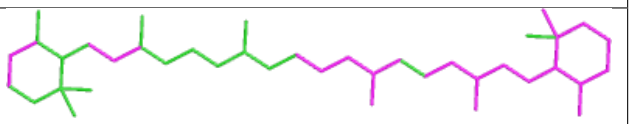


Rings

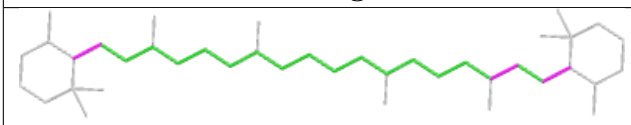
Ligand BCR BA 856



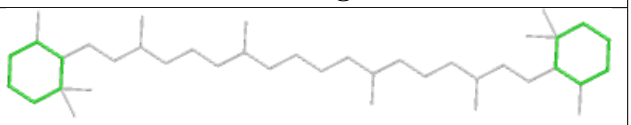
Bond lengths



Bond angles

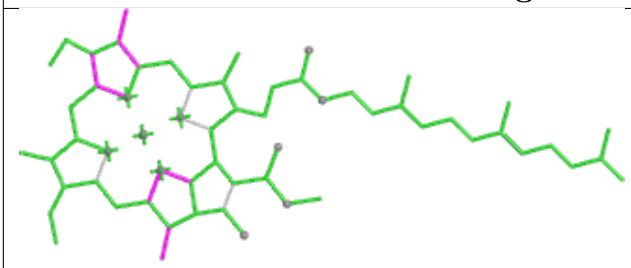


Torsions

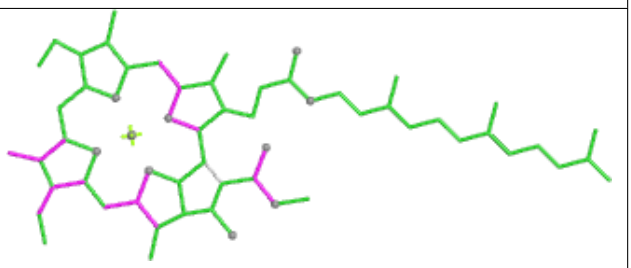


Rings

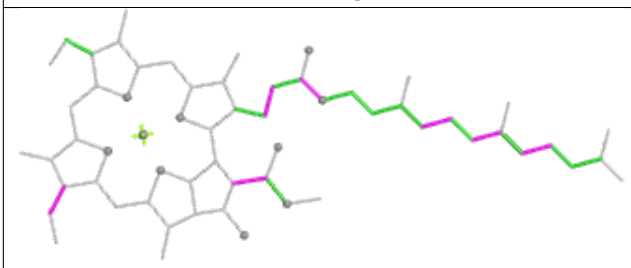
Ligand CLA B1 314



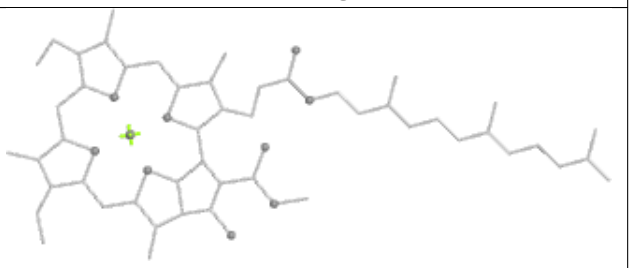
Bond lengths



Bond angles

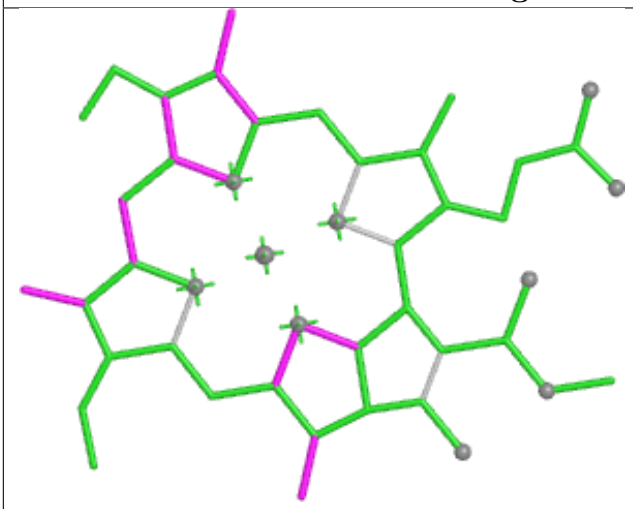


Torsions

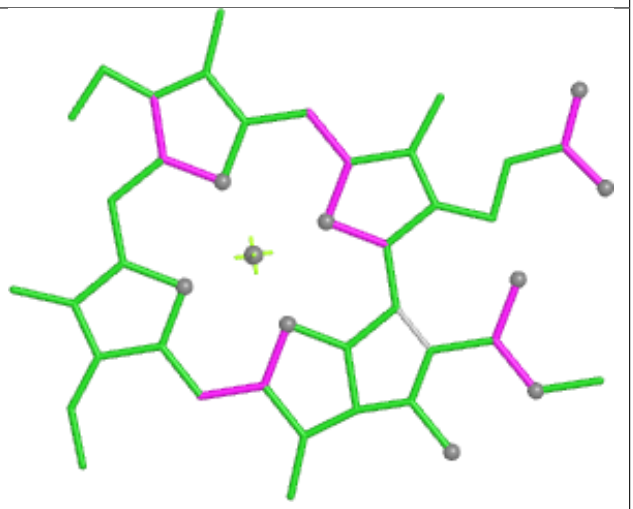


Rings

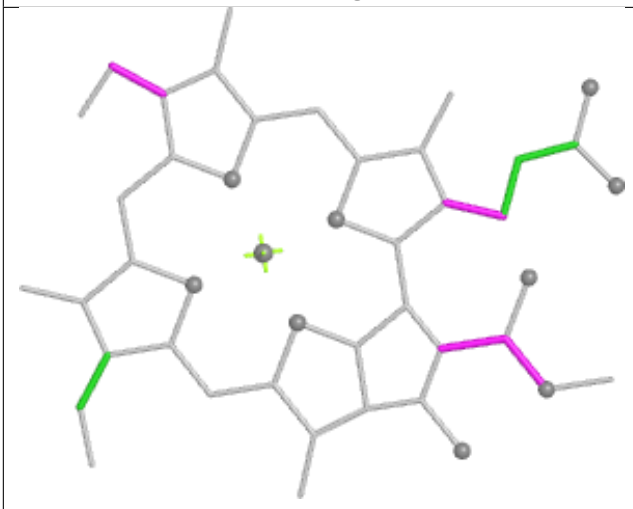
Ligand CLA BA 814



Bond lengths



Bond angles

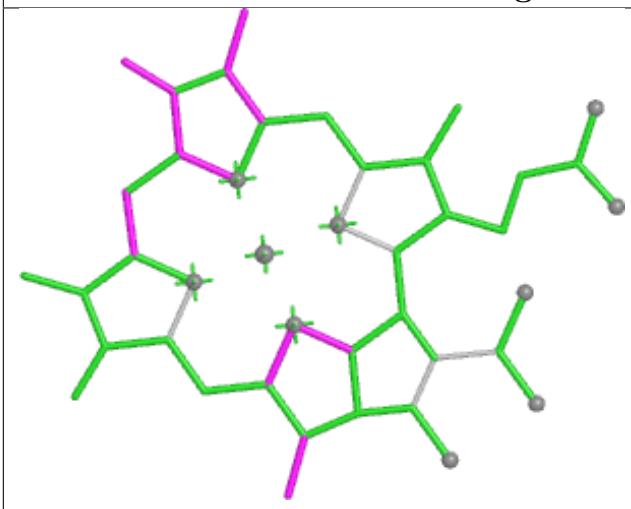


Torsions

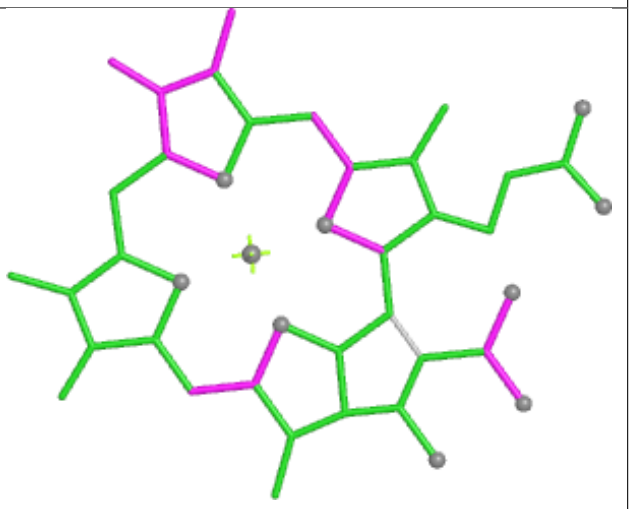


Rings

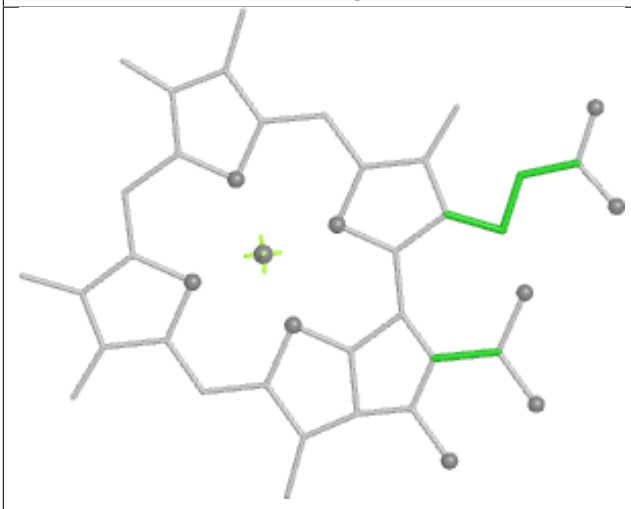
Ligand CLA A3 304



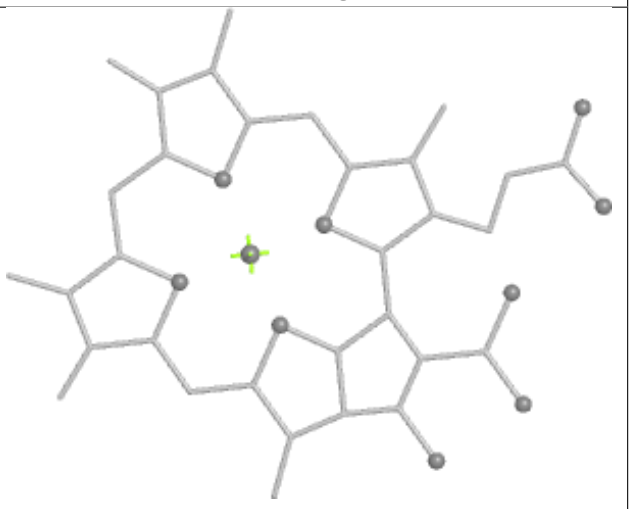
Bond lengths



Bond angles

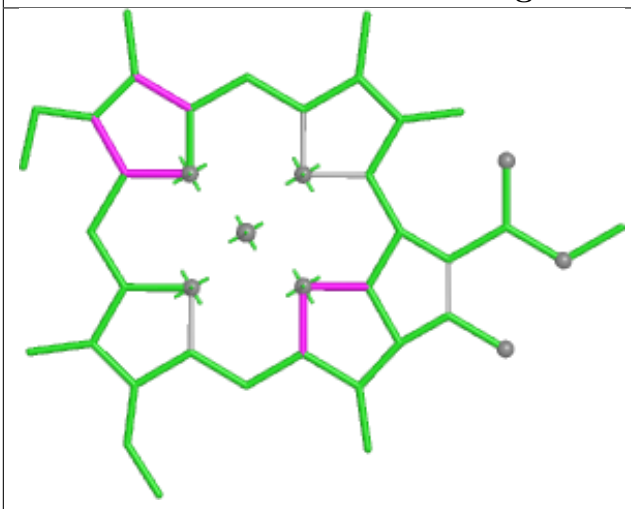


Torsions

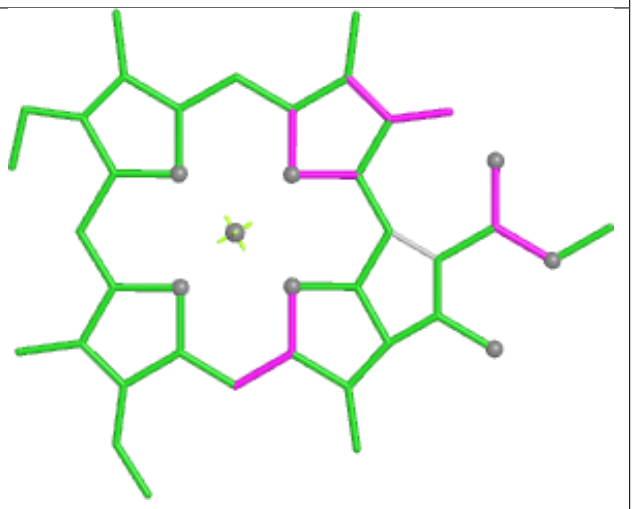


Rings

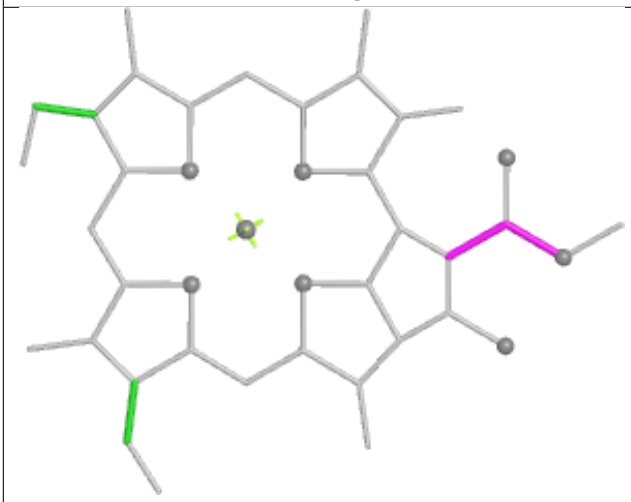
Ligand CLA B1 306



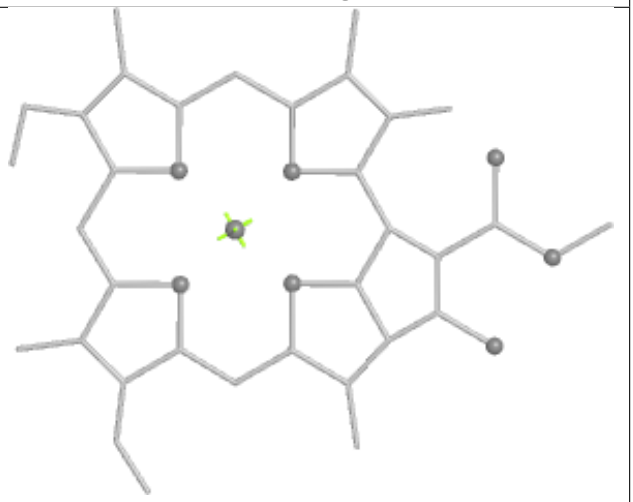
Bond lengths



Bond angles



Torsions

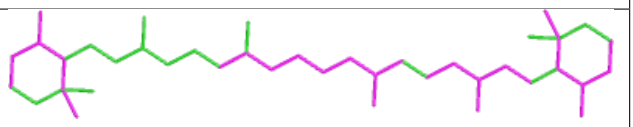


Rings

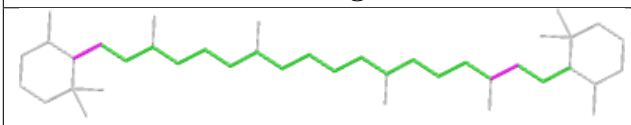
Ligand BCR BA 849



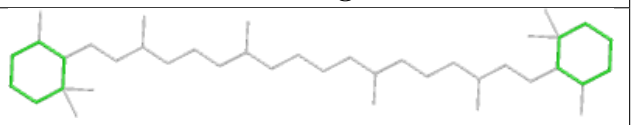
Bond lengths



Bond angles

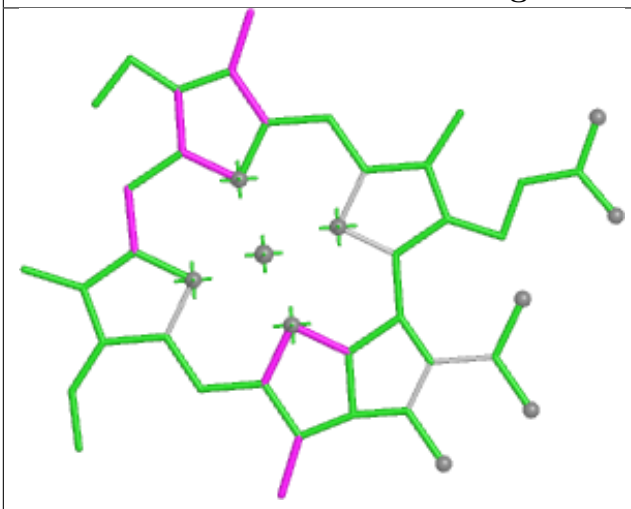


Torsions

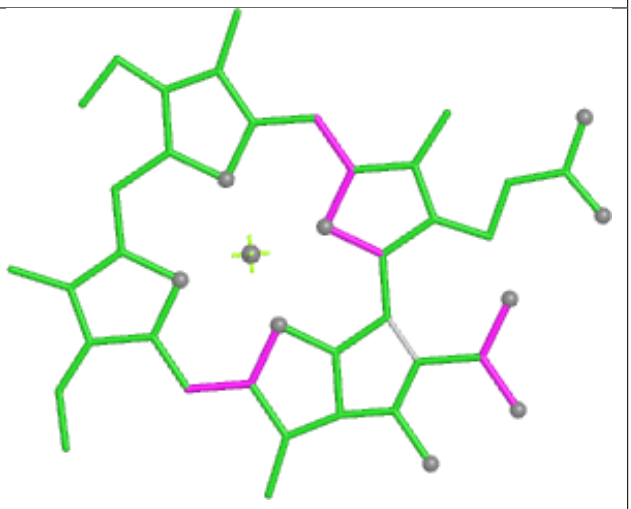


Rings

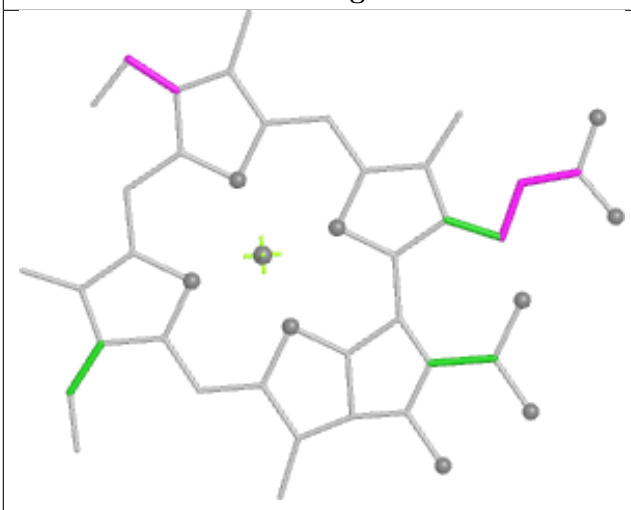
Ligand CLA AG 201



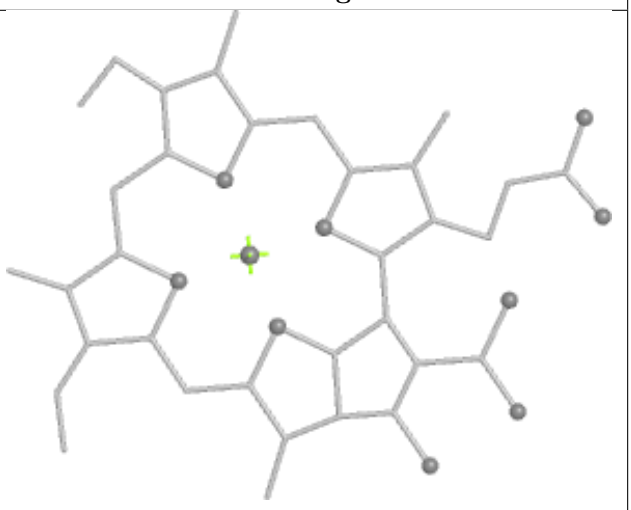
Bond lengths



Bond angles

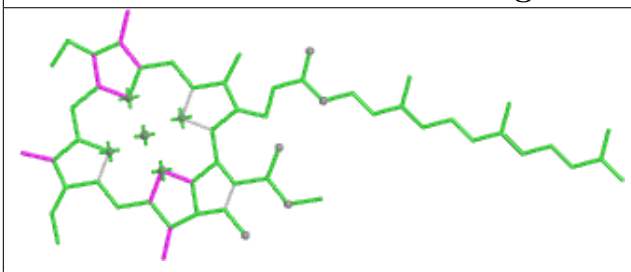


Torsions

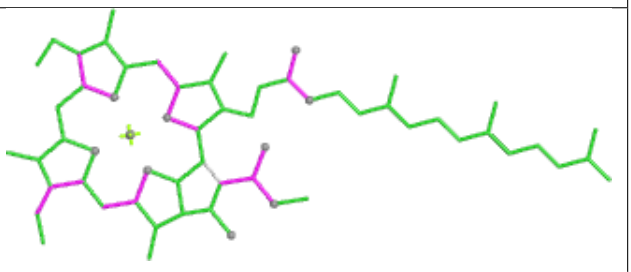


Rings

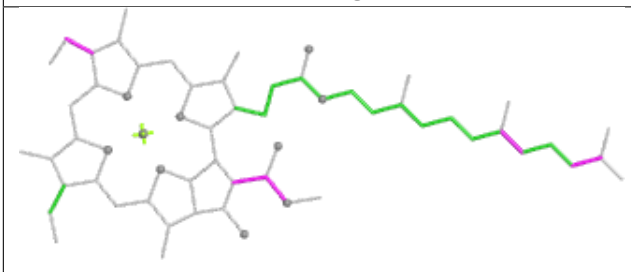
Ligand CLA A4 301



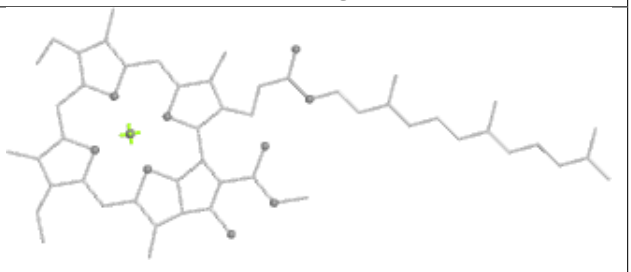
Bond lengths



Bond angles

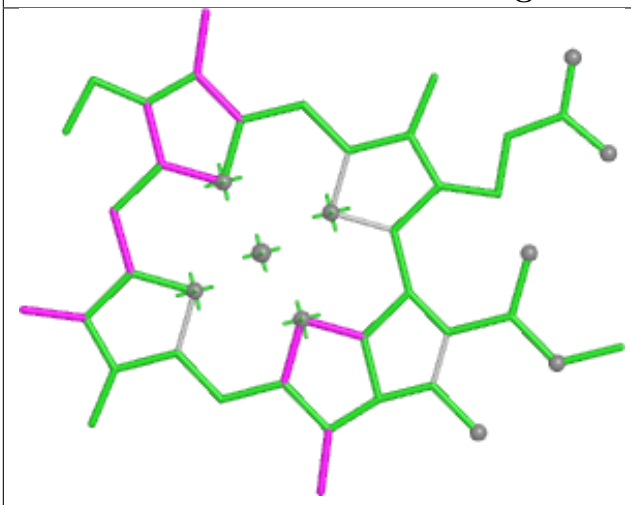


Torsions

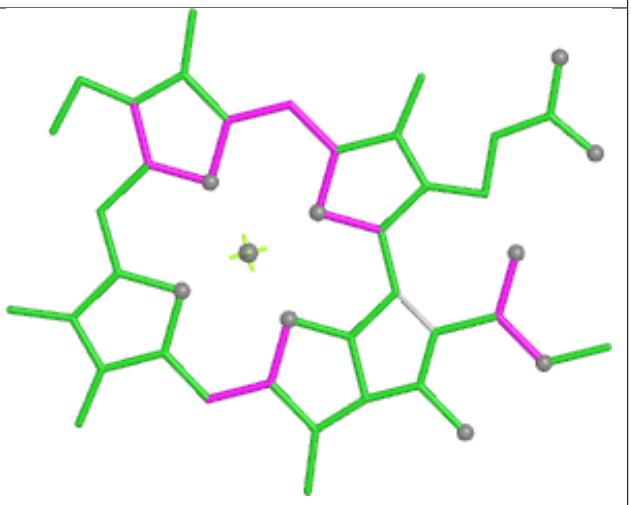


Rings

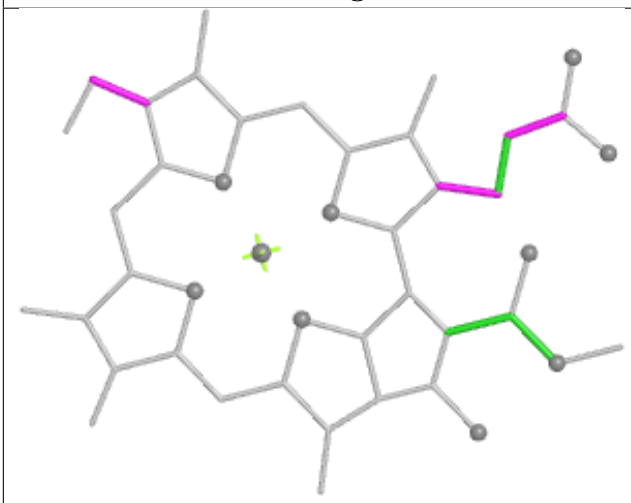
Ligand CLA B5 608



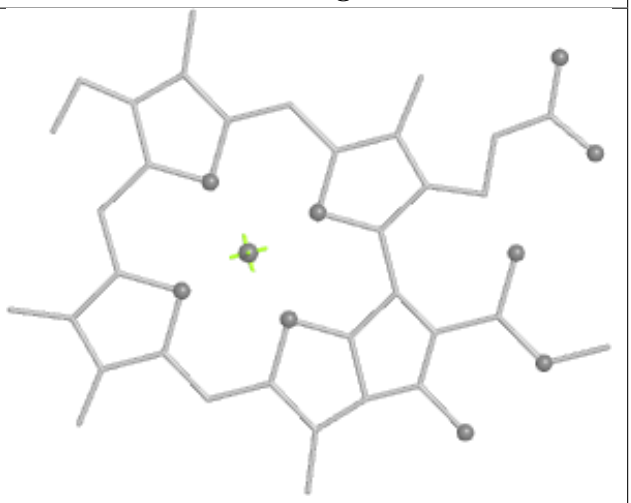
Bond lengths



Bond angles

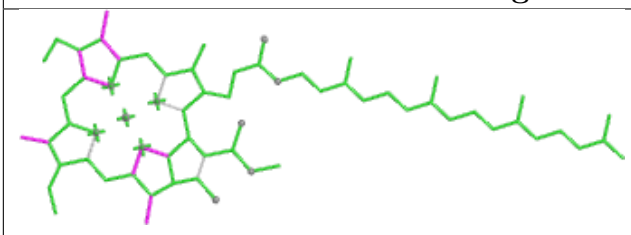


Torsions

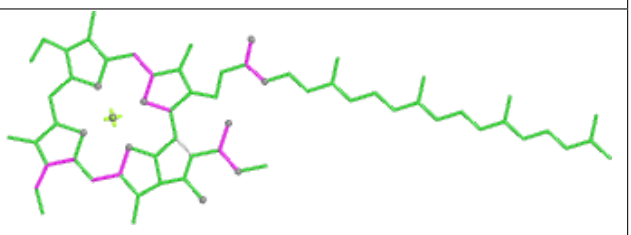


Rings

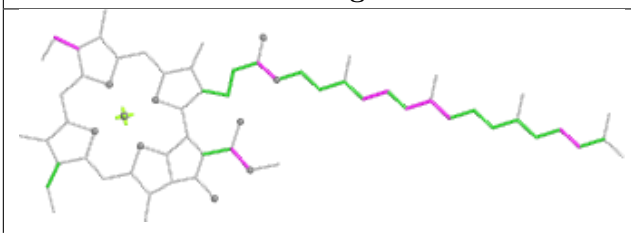
Ligand CLA BB 842



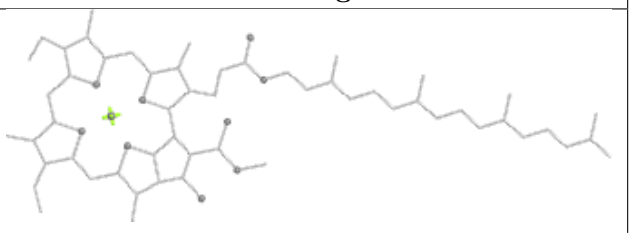
Bond lengths



Bond angles

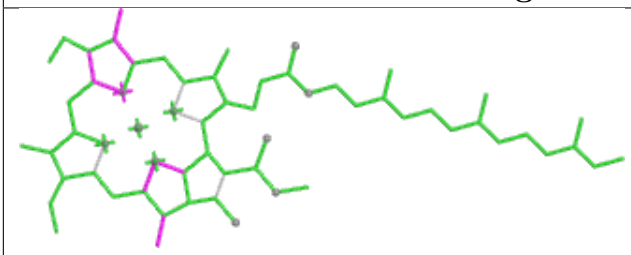


Torsions

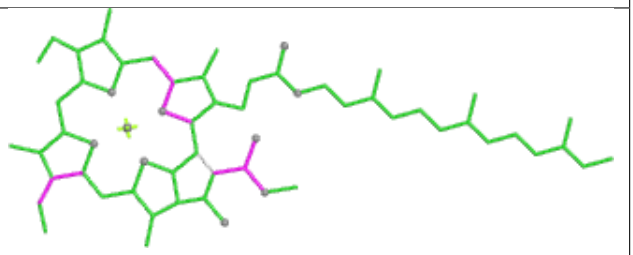


Rings

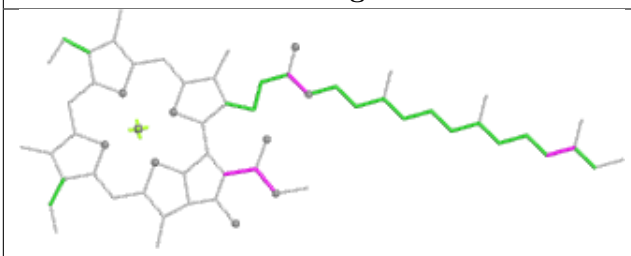
Ligand CLA B1 304



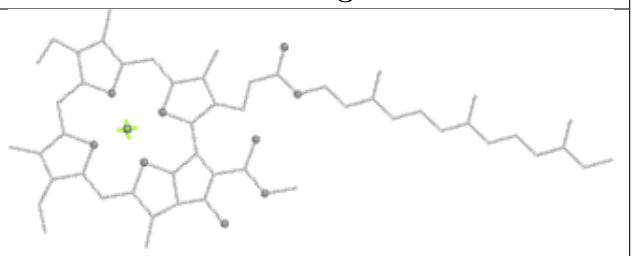
Bond lengths



Bond angles

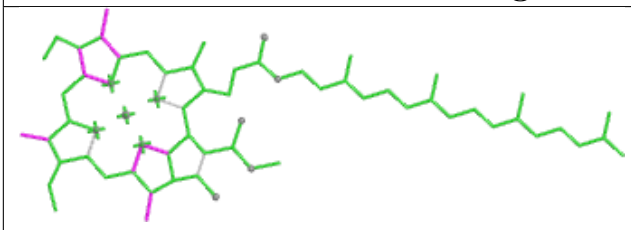


Torsions

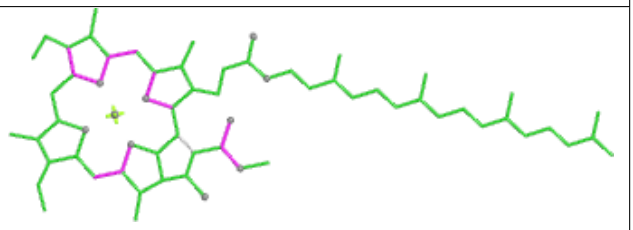


Rings

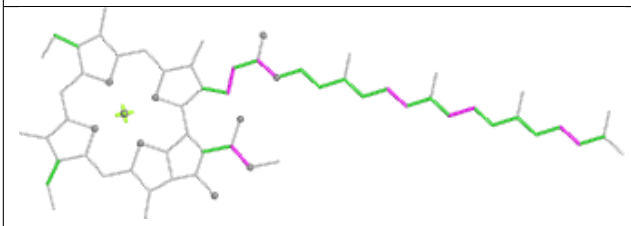
Ligand CLA BB 839



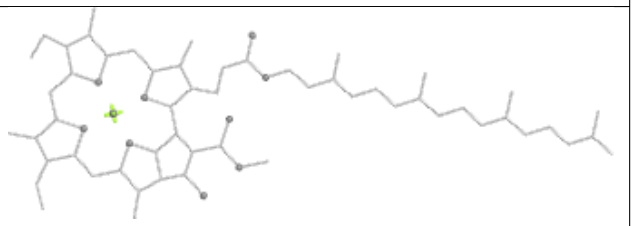
Bond lengths



Bond angles

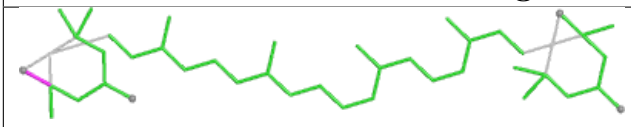


Torsions

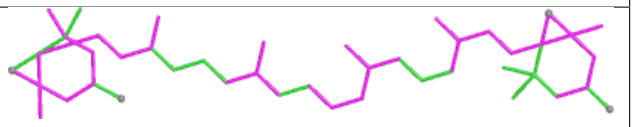


Rings

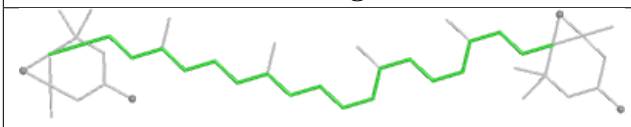
Ligand XAT B2 616



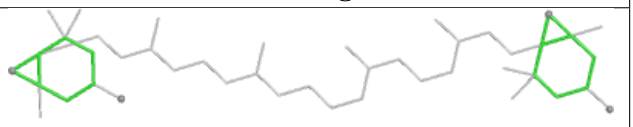
Bond lengths



Bond angles

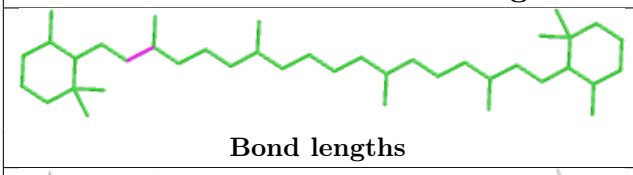


Torsions

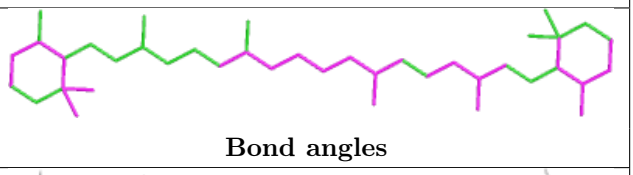


Rings

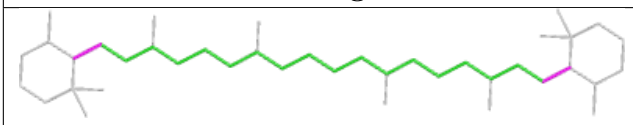
Ligand BCR BB 845



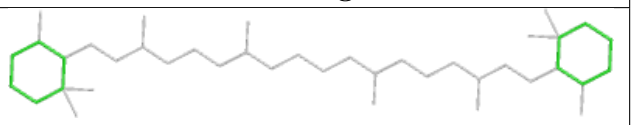
Bond lengths



Bond angles

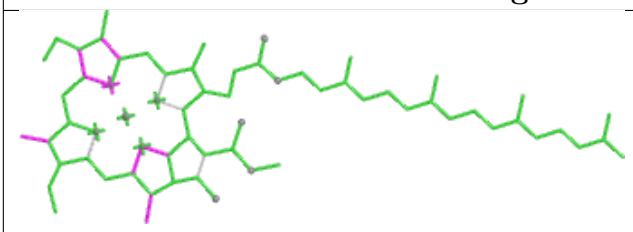


Torsions

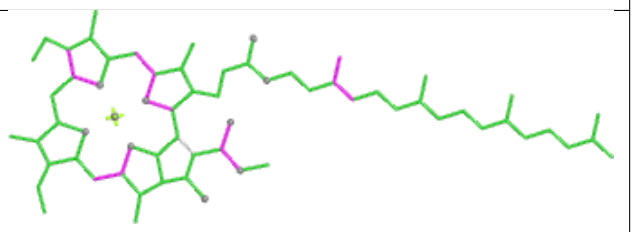


Rings

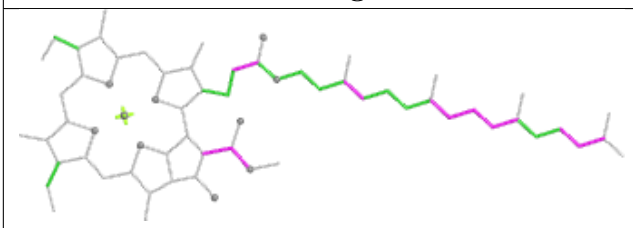
Ligand CLA BA 813



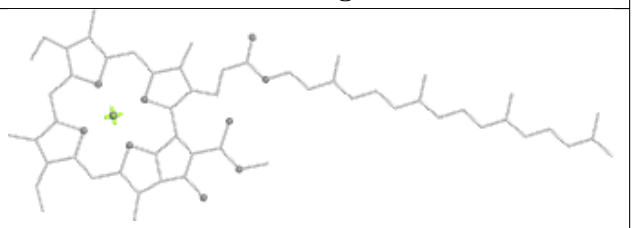
Bond lengths



Bond angles

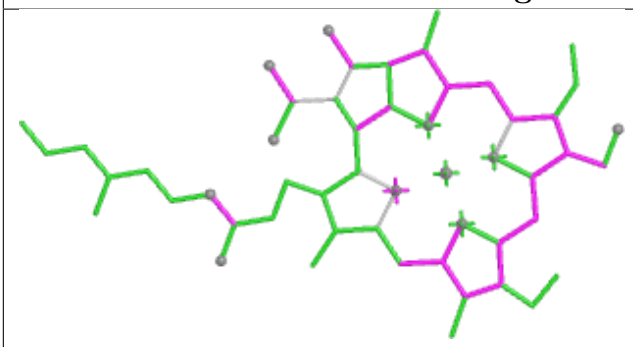


Torsions

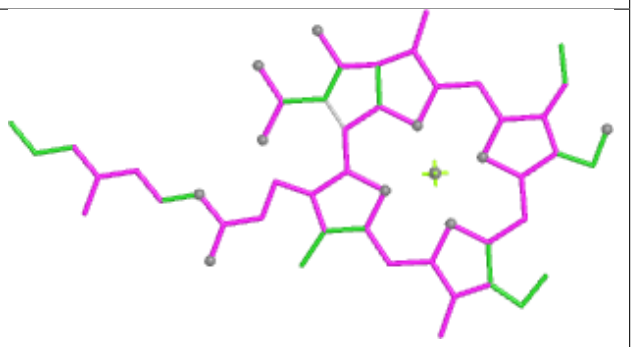


Rings

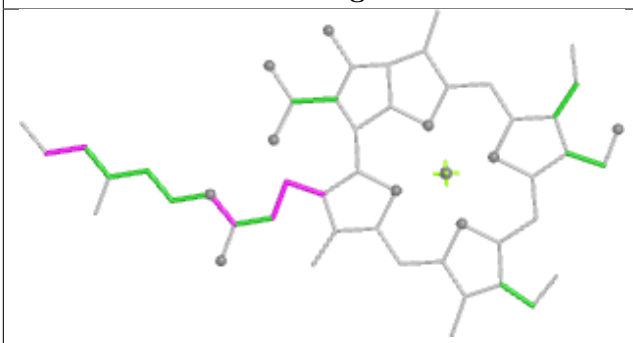
Ligand CHL A6 602



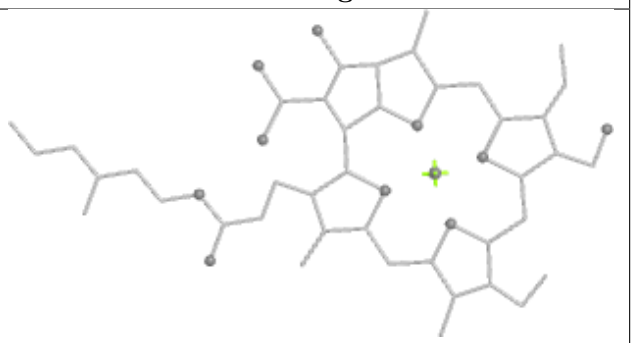
Bond lengths



Bond angles

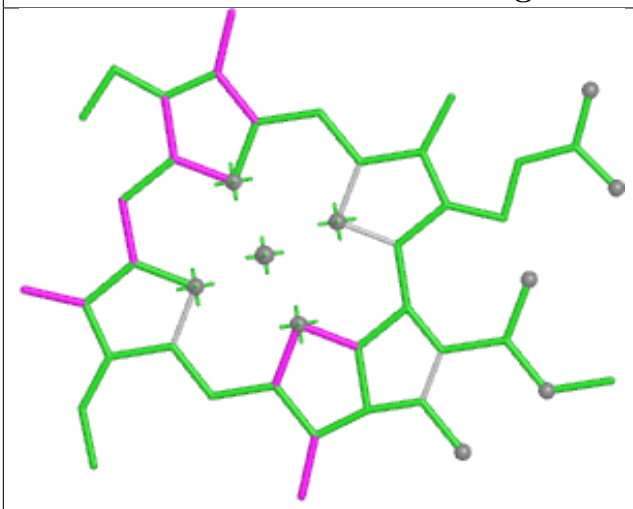


Torsions

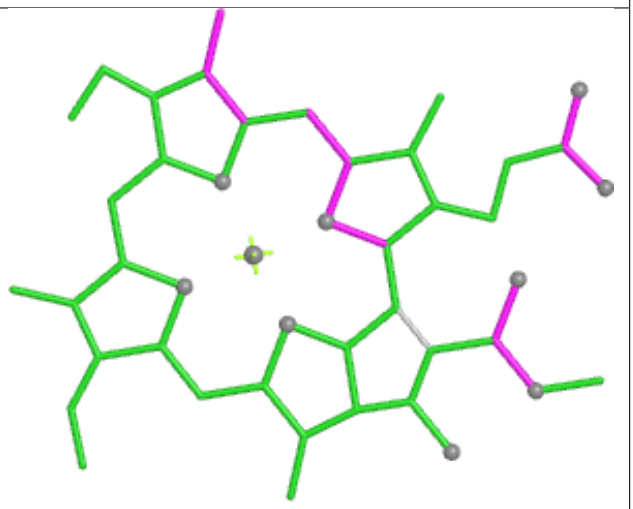


Rings

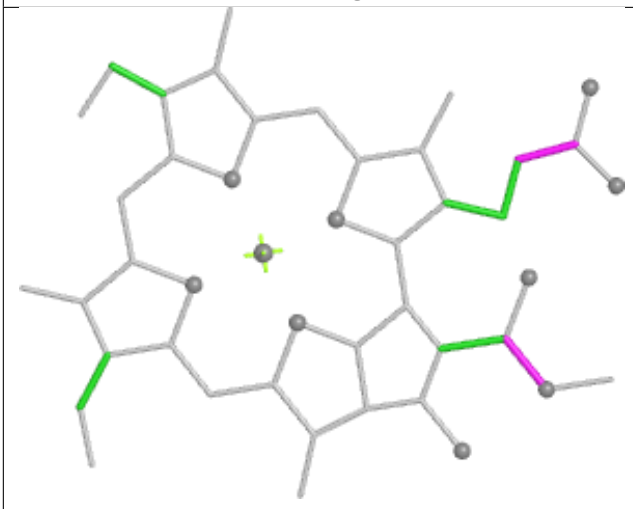
Ligand CLA A1 313



Bond lengths



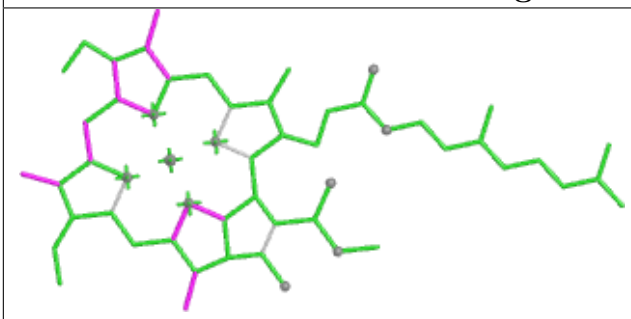
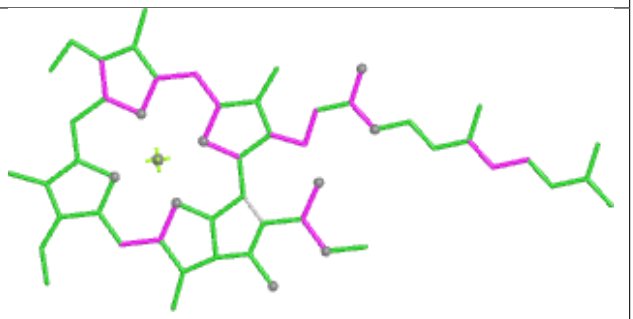
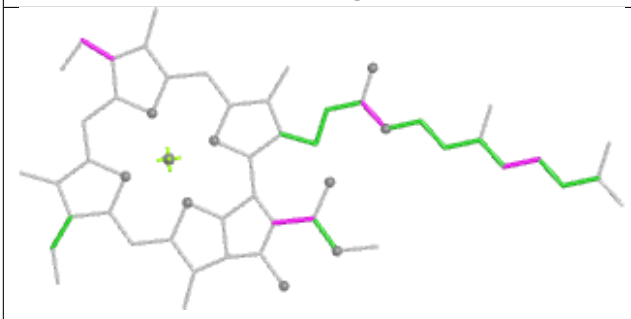
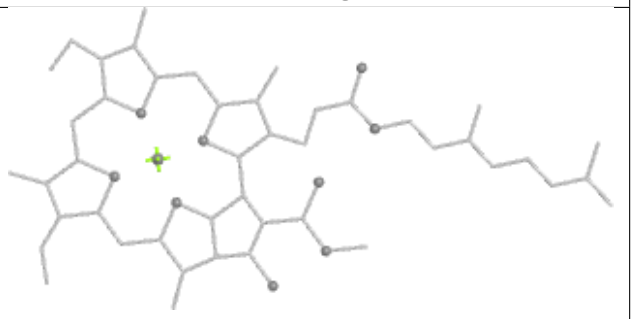
Bond angles



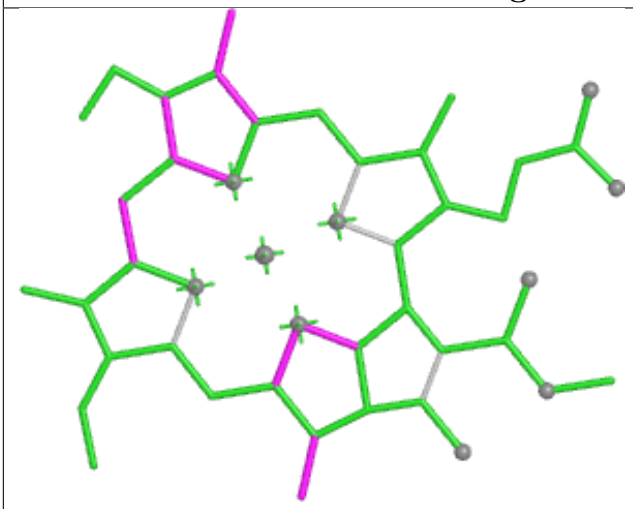
Torsions



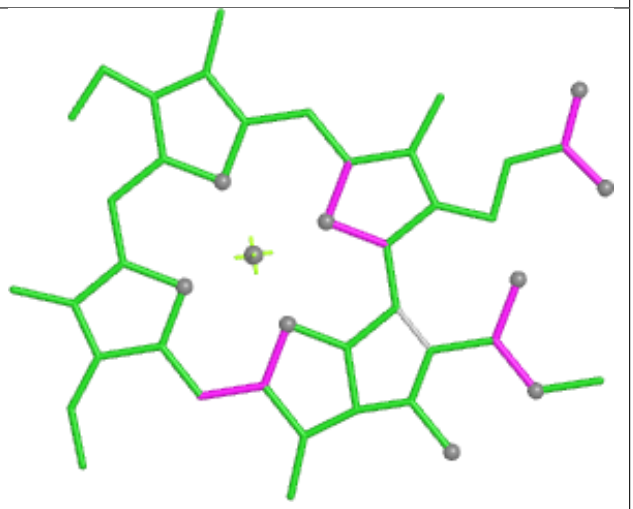
Rings

Ligand CLA A6 610	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

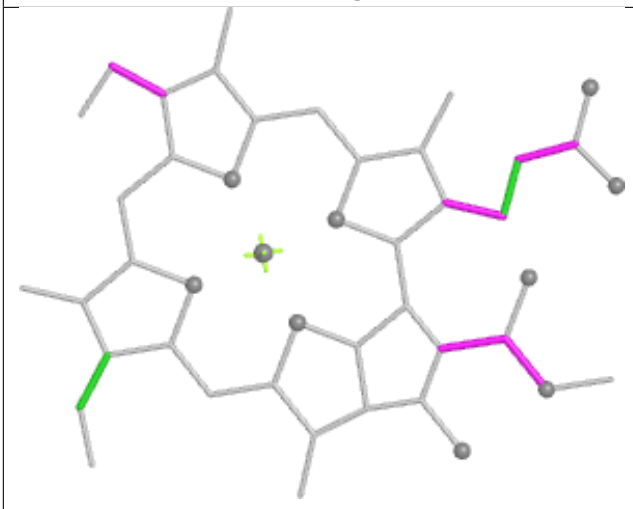
Ligand CLA AK 202



Bond lengths



Bond angles

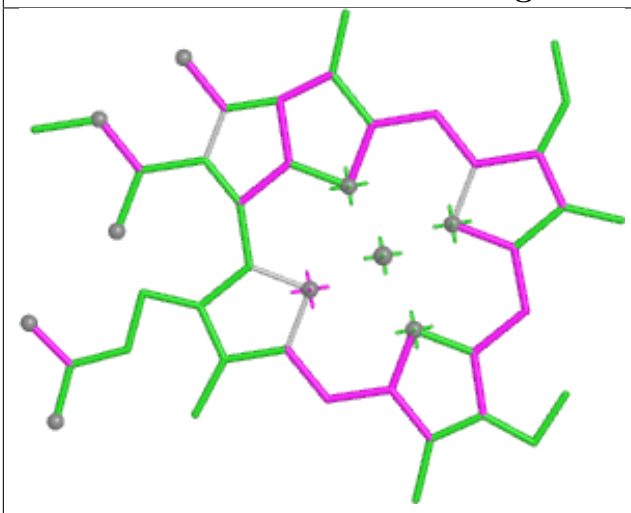


Torsions

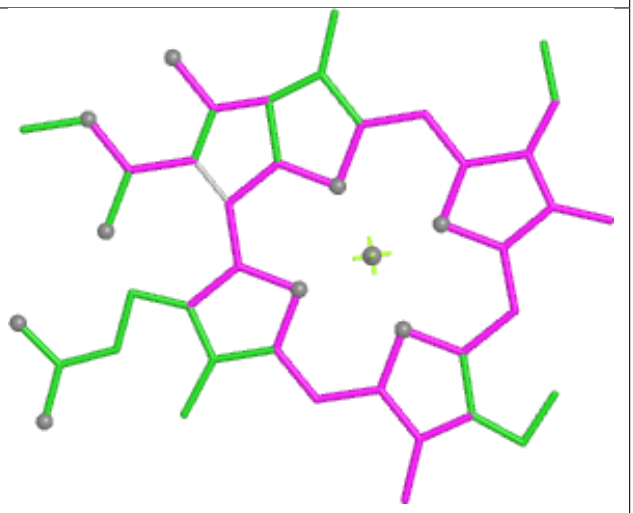


Rings

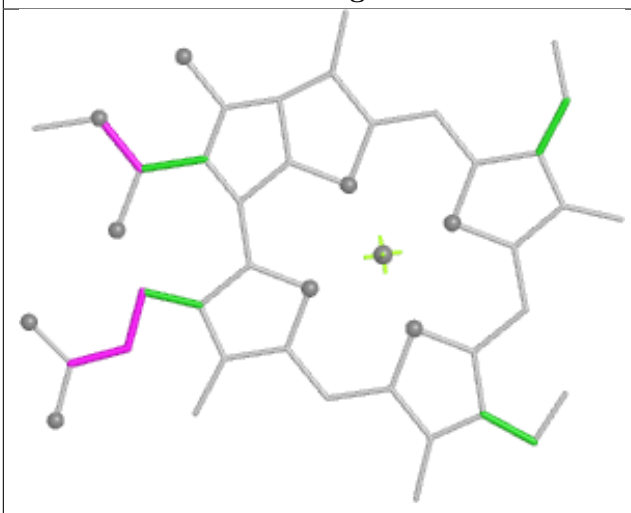
Ligand CHL B3 306



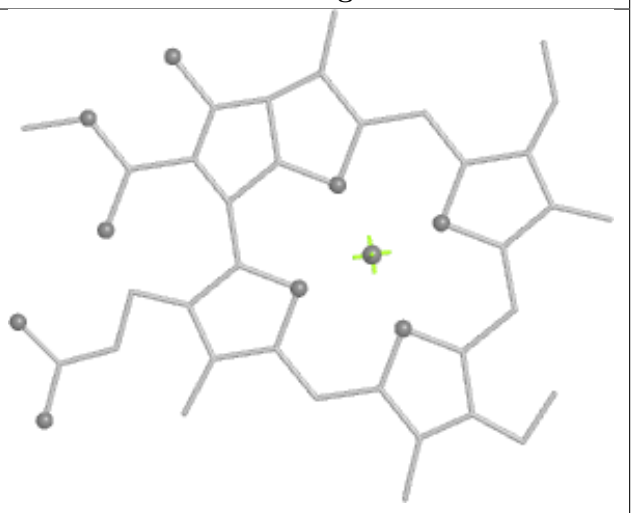
Bond lengths



Bond angles

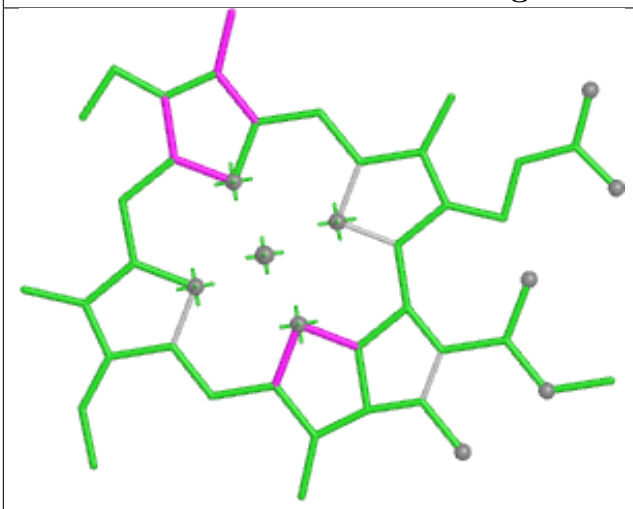


Torsions

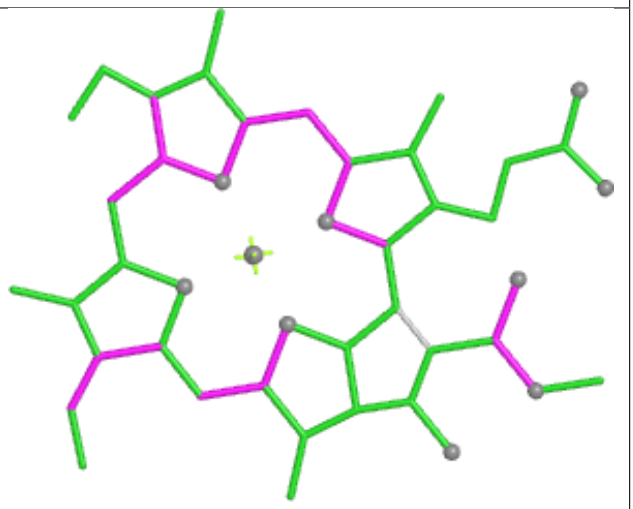


Rings

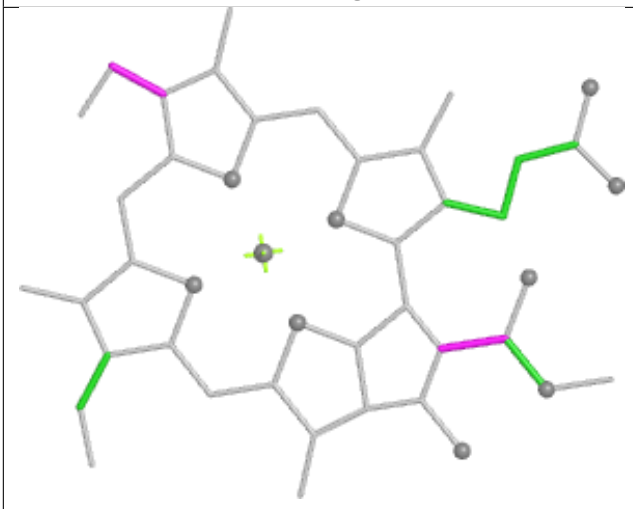
Ligand CLA BA 816



Bond lengths



Bond angles

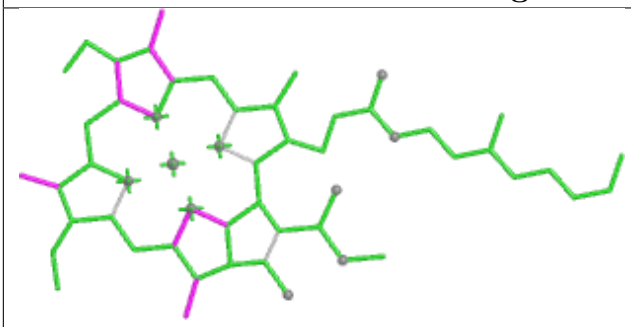


Torsions

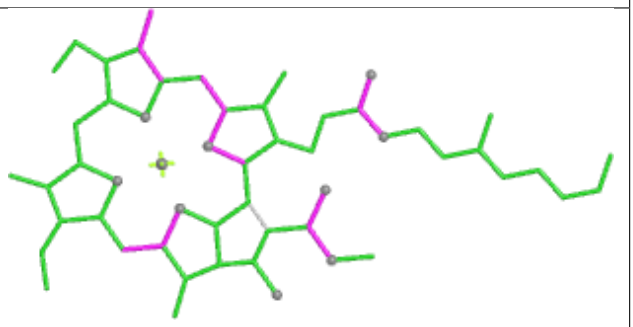


Rings

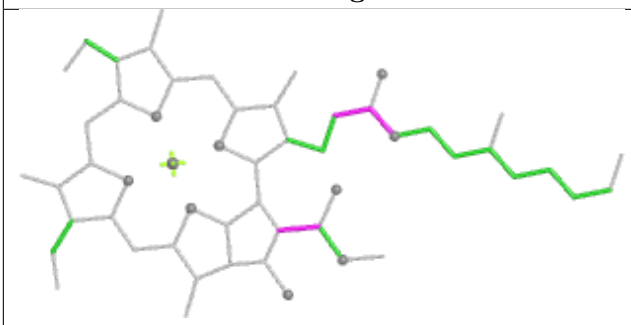
Ligand CLA BA 812



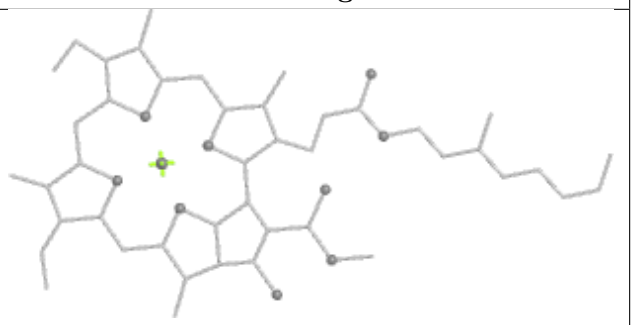
Bond lengths



Bond angles

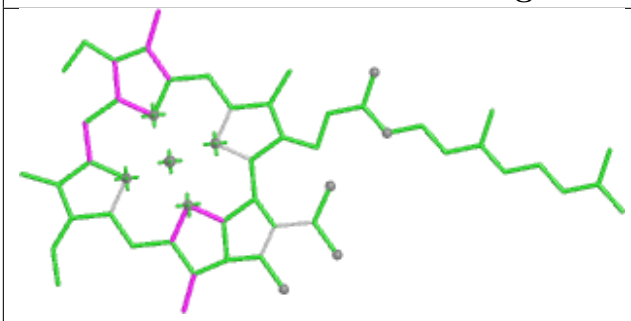


Torsions

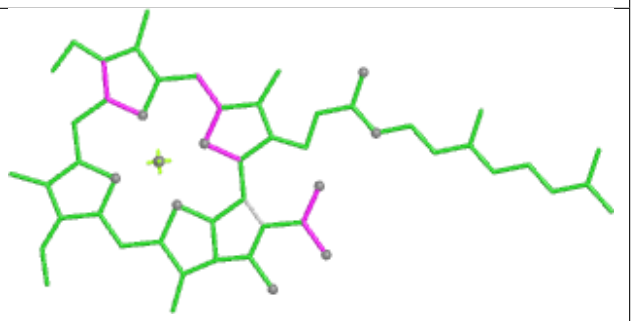


Rings

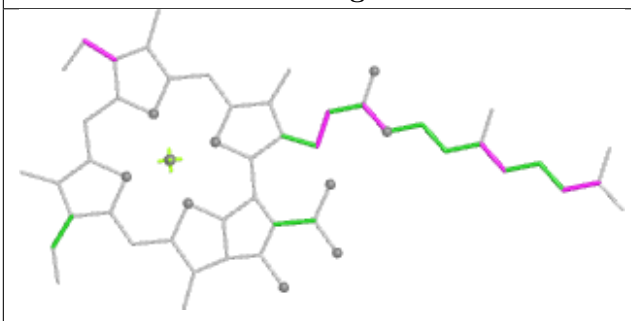
Ligand CLA B3 311



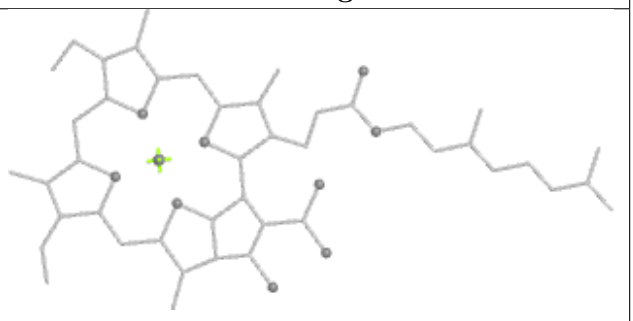
Bond lengths



Bond angles

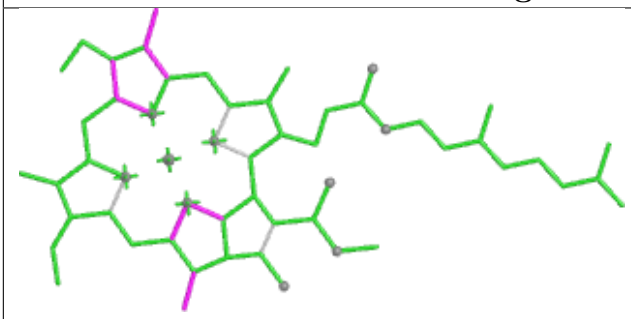


Torsions

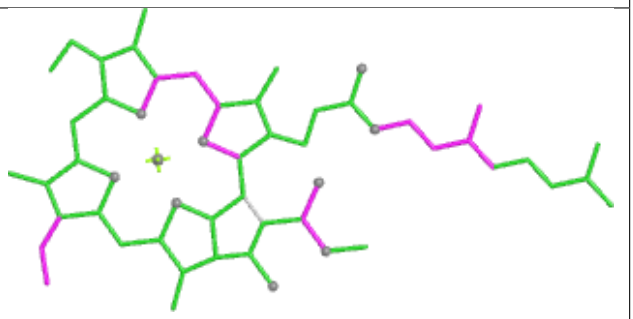


Rings

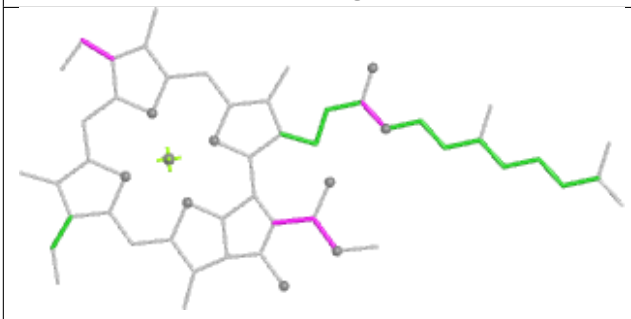
Ligand CLA A1 305



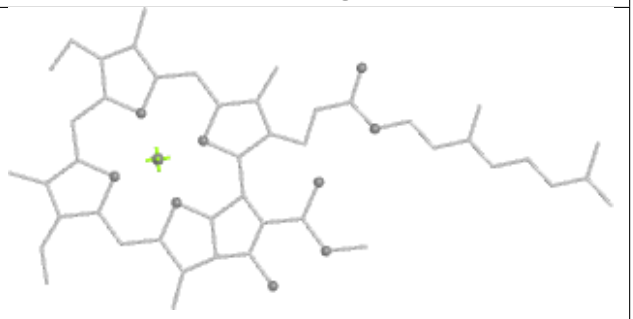
Bond lengths



Bond angles

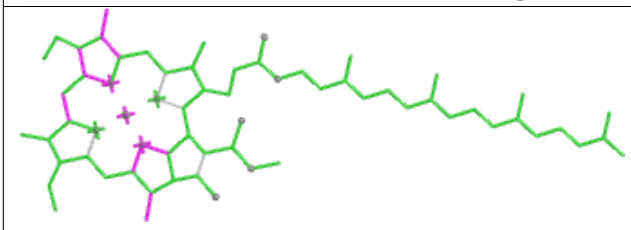


Torsions

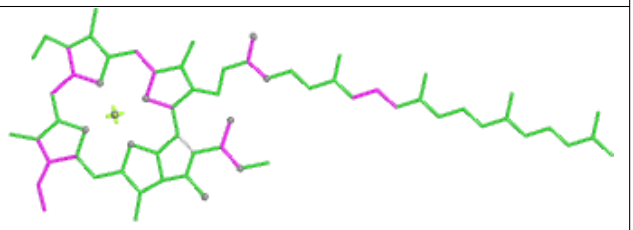


Rings

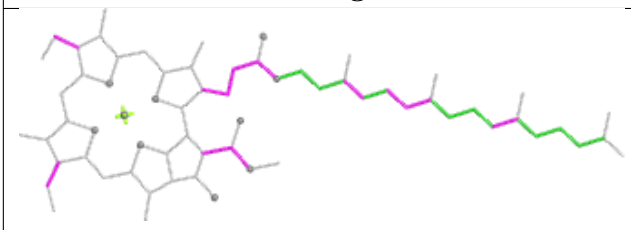
Ligand CLA BB 815



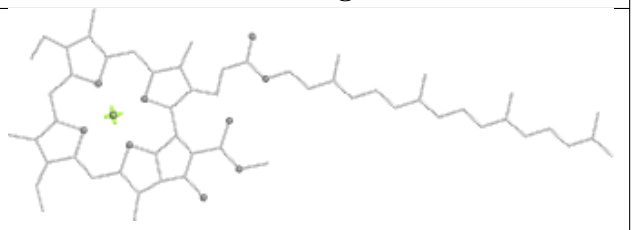
Bond lengths



Bond angles

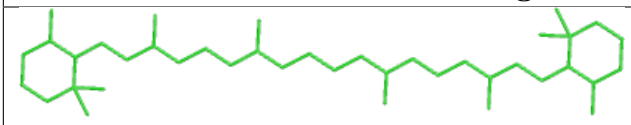


Torsions

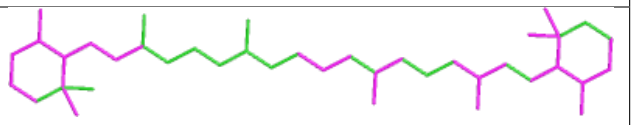


Rings

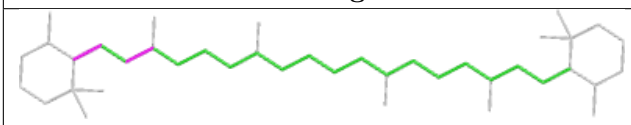
Ligand BCR AI 102



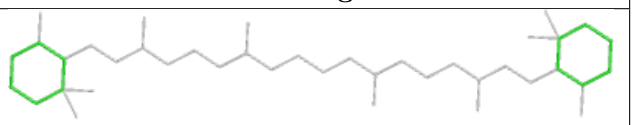
Bond lengths



Bond angles

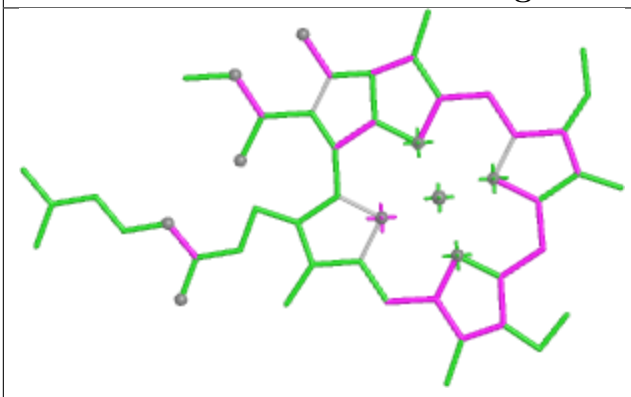


Torsions

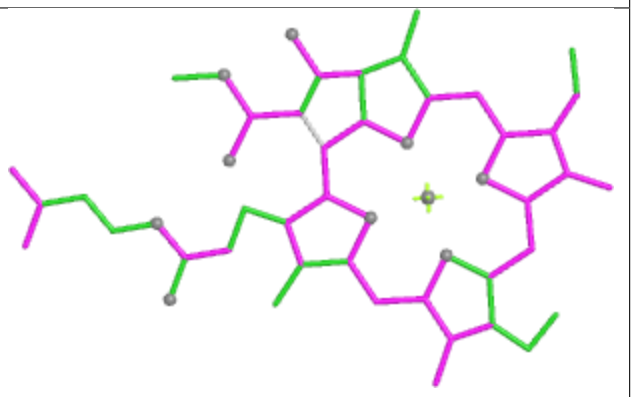


Rings

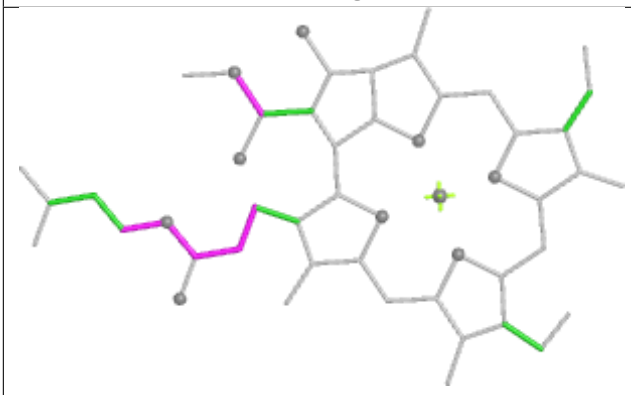
Ligand CHL A6 608



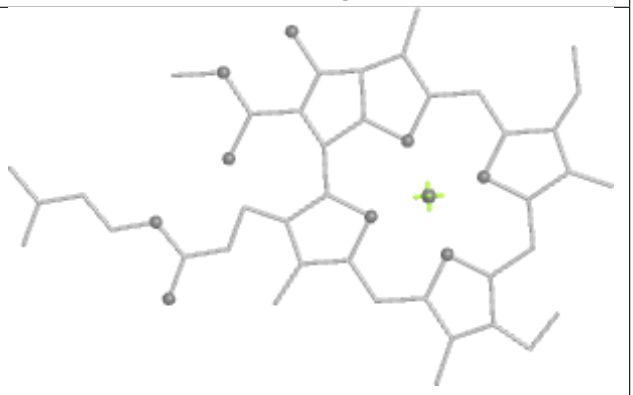
Bond lengths



Bond angles

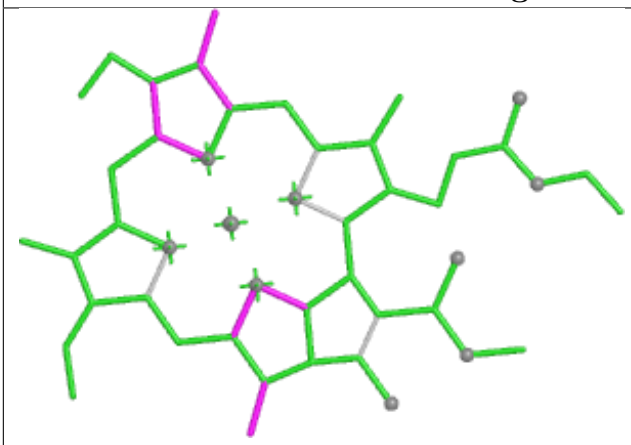


Torsions

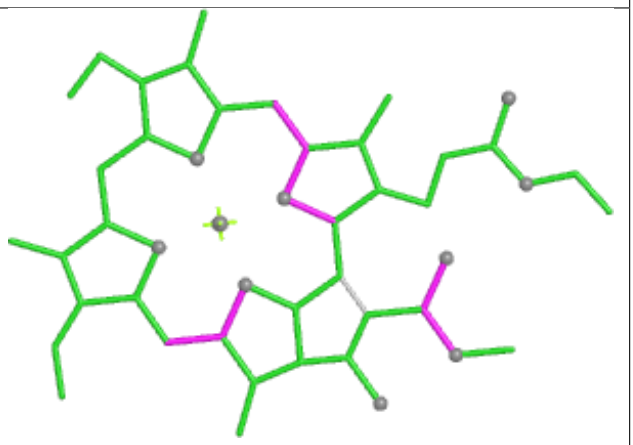


Rings

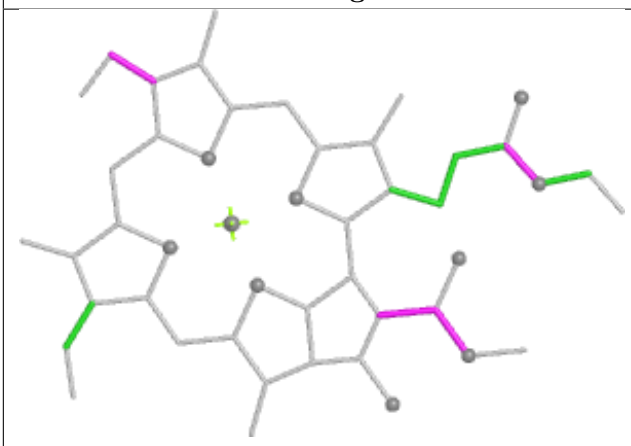
Ligand CLA AB 822



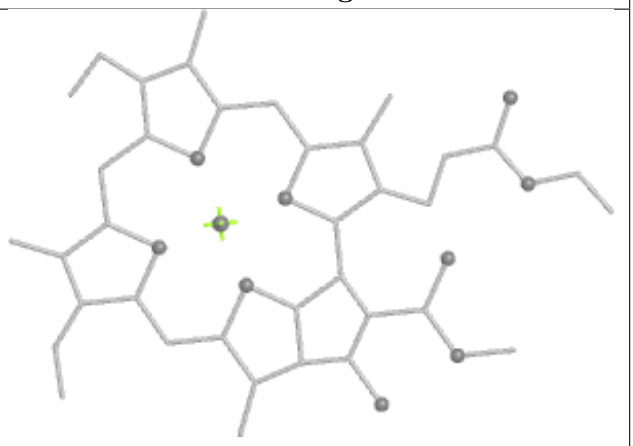
Bond lengths



Bond angles

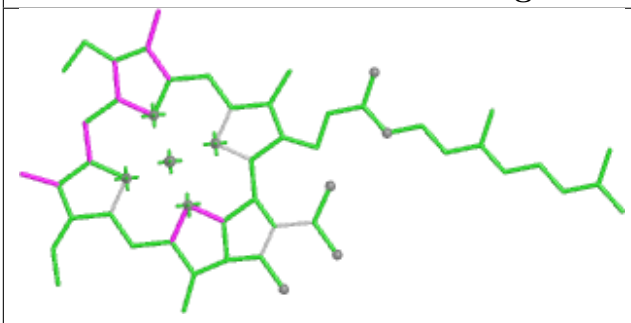


Torsions

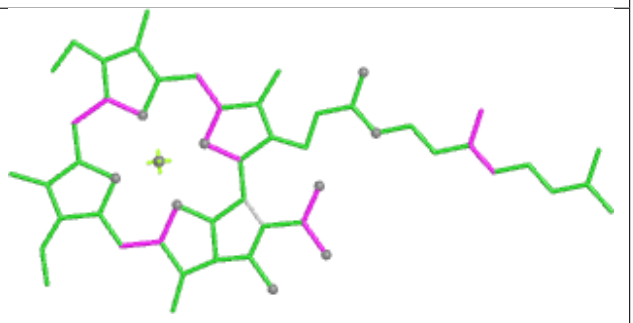


Rings

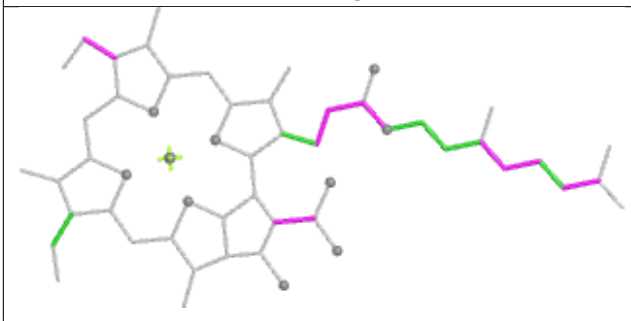
Ligand CLA A3 312



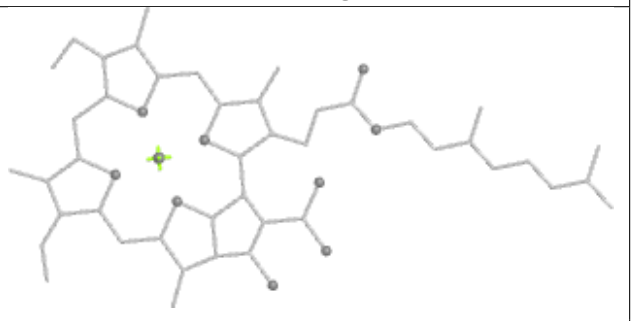
Bond lengths



Bond angles

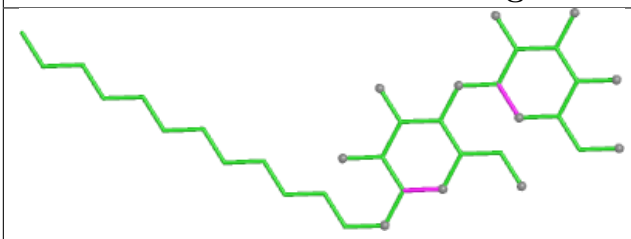


Torsions

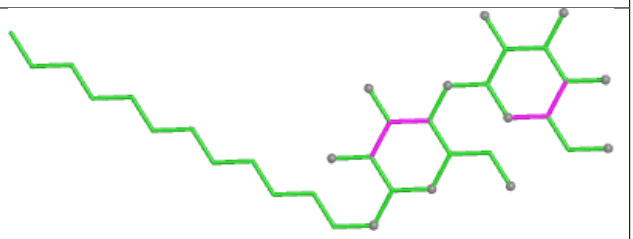


Rings

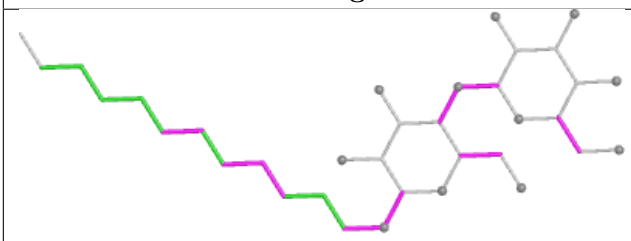
Ligand LMU AB 853



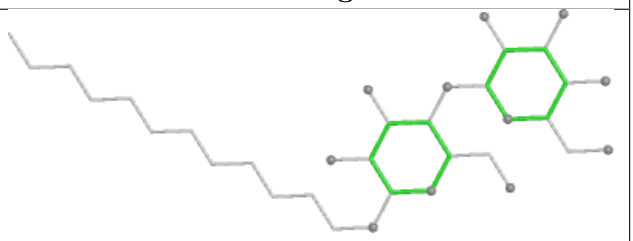
Bond lengths



Bond angles

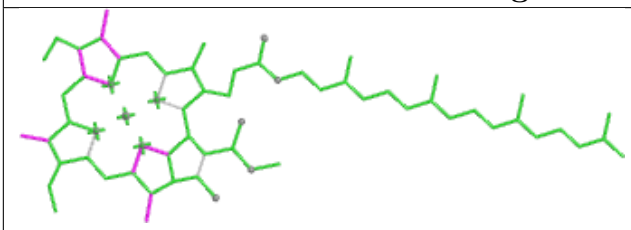


Torsions

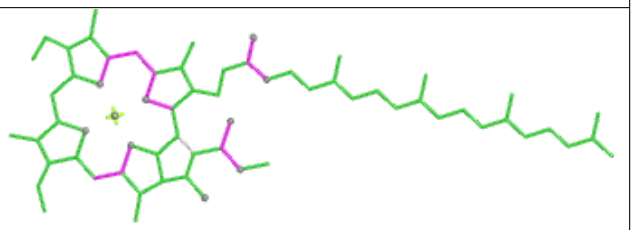


Rings

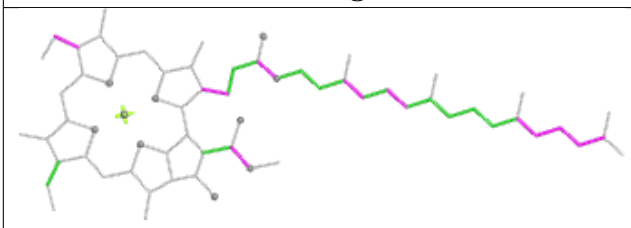
Ligand CLA BA 811



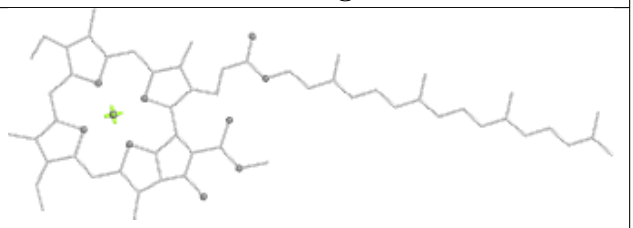
Bond lengths



Bond angles

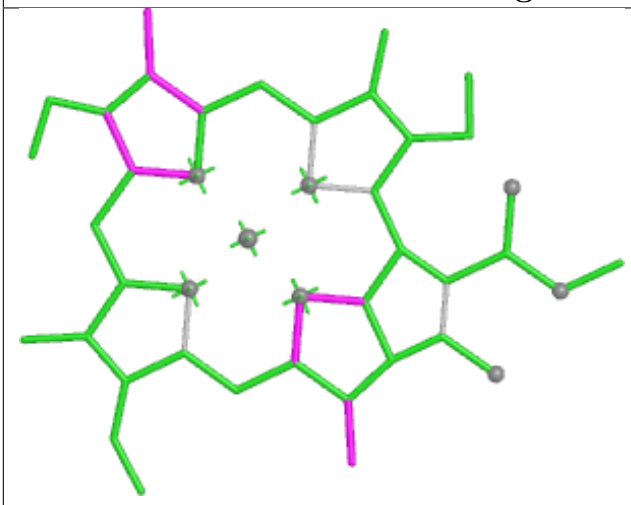


Torsions

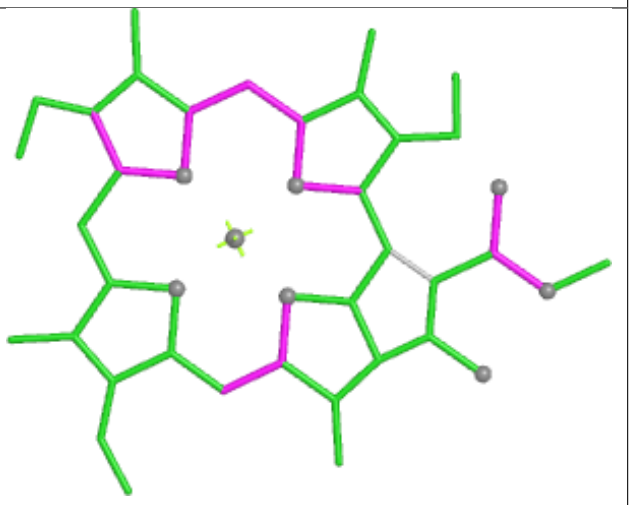


Rings

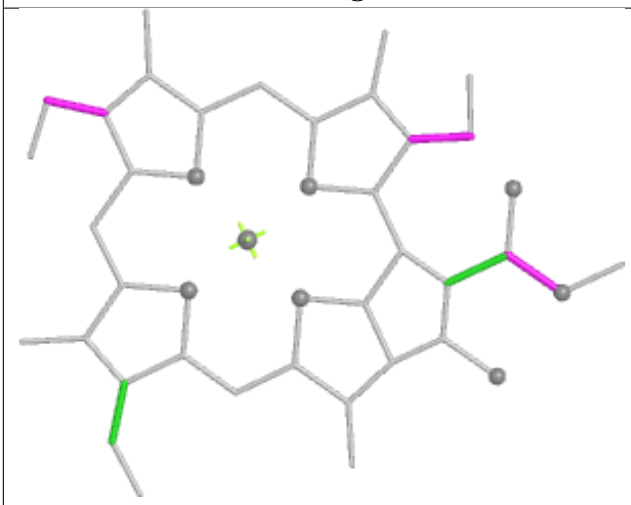
Ligand CLA B5 610



Bond lengths



Bond angles

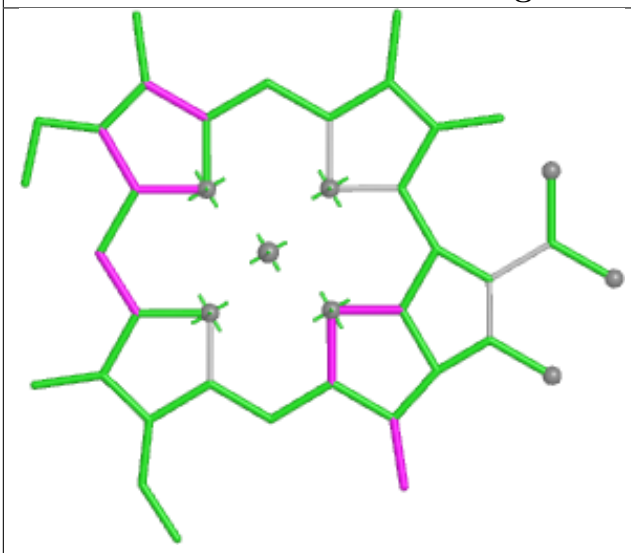


Torsions

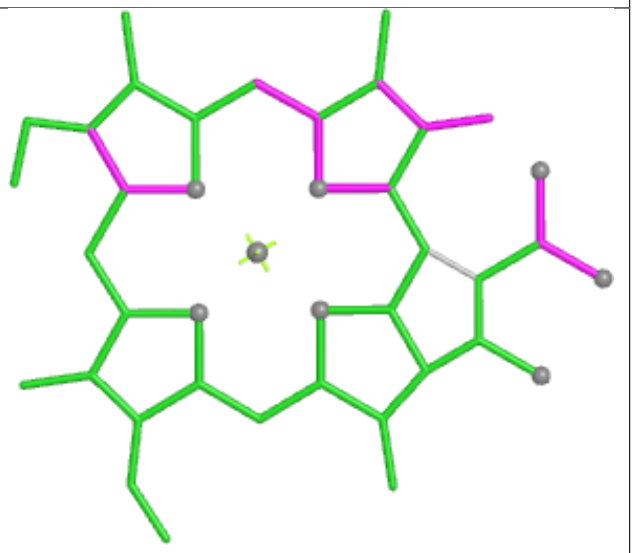


Rings

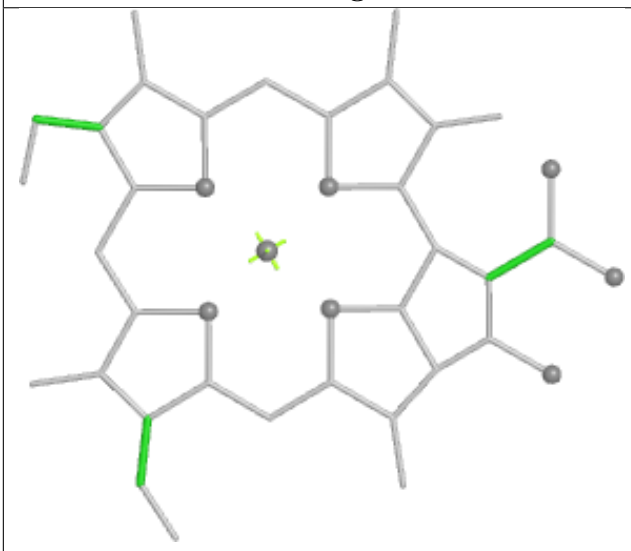
Ligand CLA A3 315



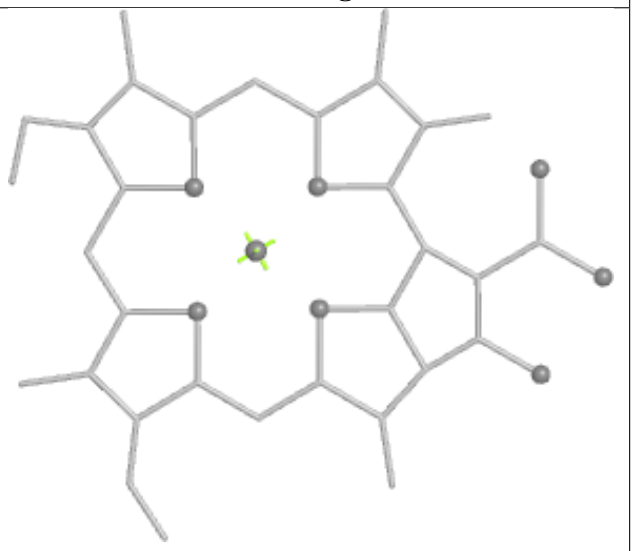
Bond lengths



Bond angles

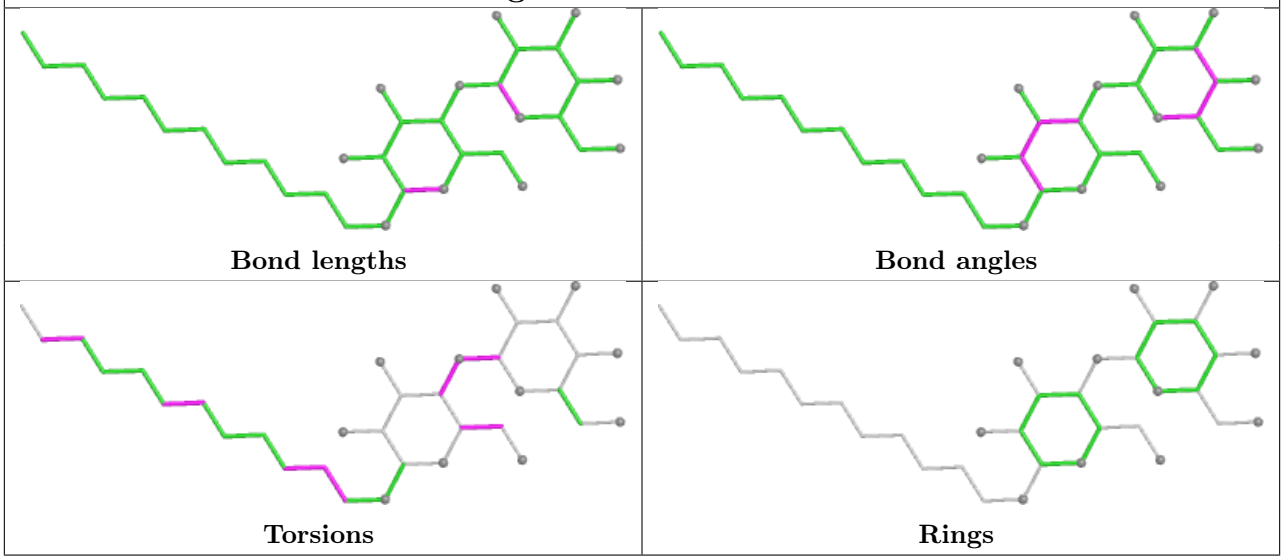


Torsions

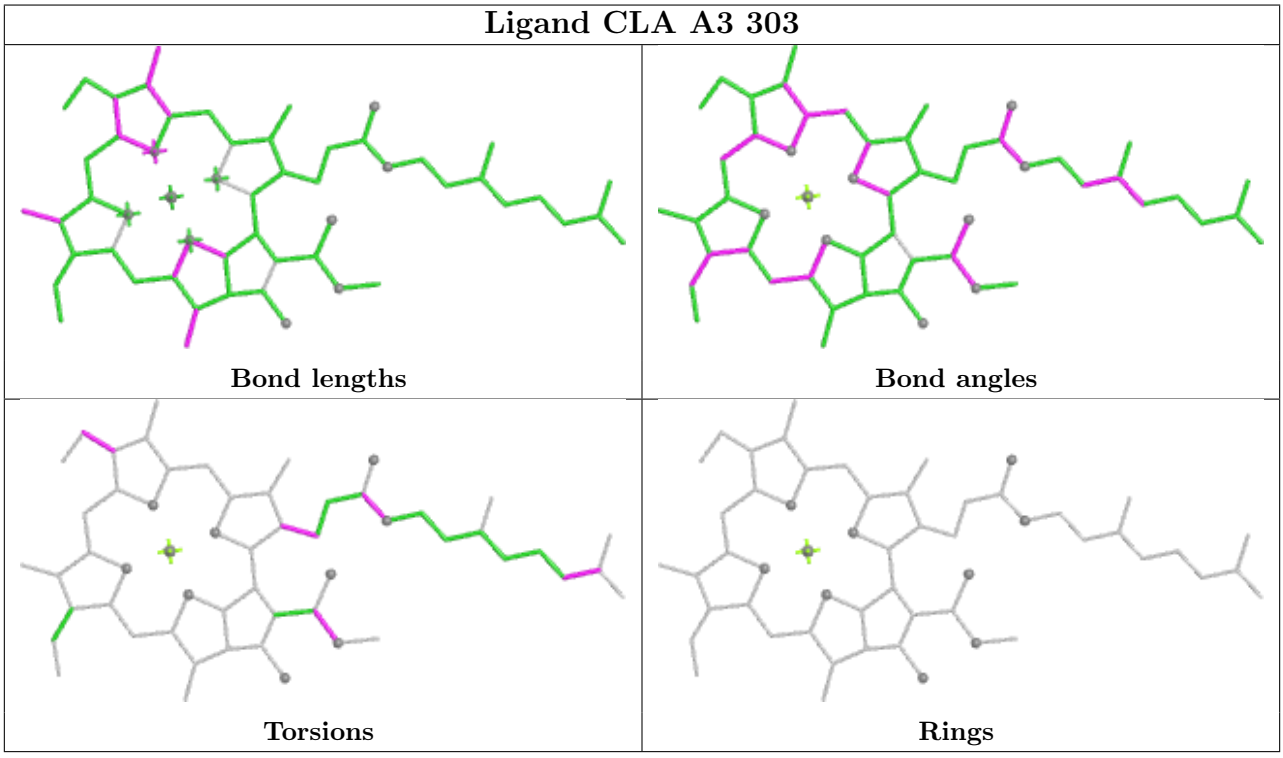


Rings

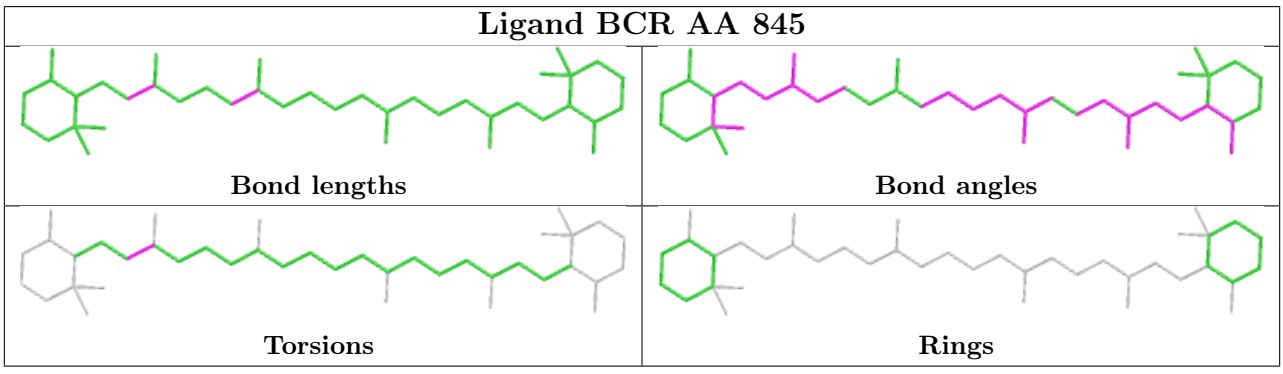
Ligand LMU AB 850



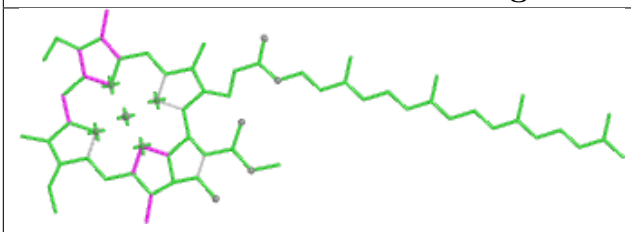
Ligand CLA A3 303



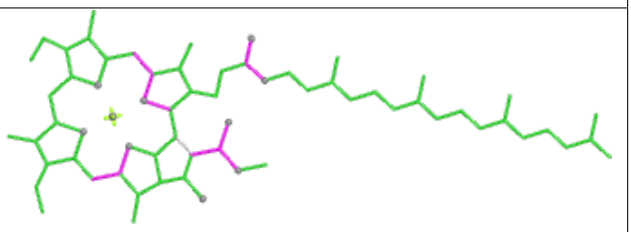
Ligand BCR AA 845



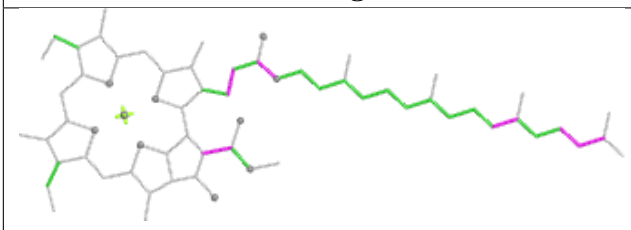
Ligand CLA AA 808



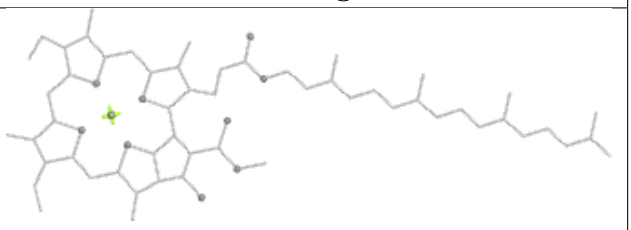
Bond lengths



Bond angles



Torsions



Rings

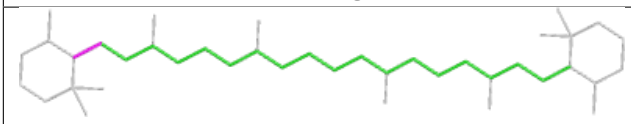
Ligand BCR BL 305



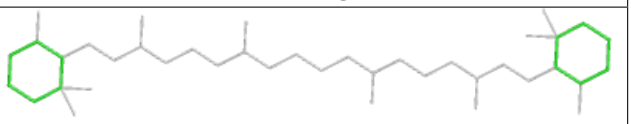
Bond lengths



Bond angles

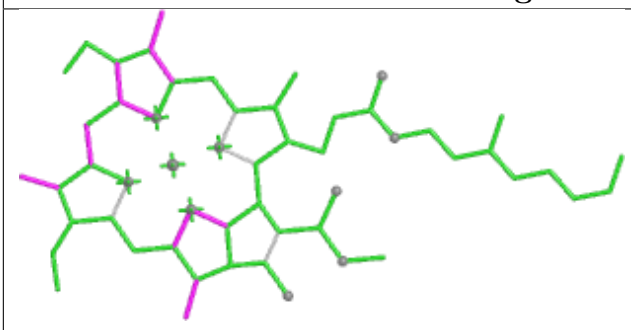


Torsions

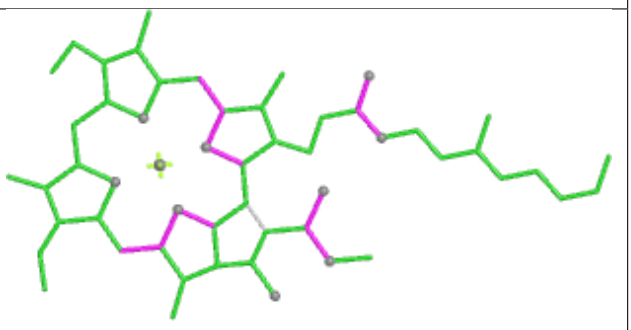


Rings

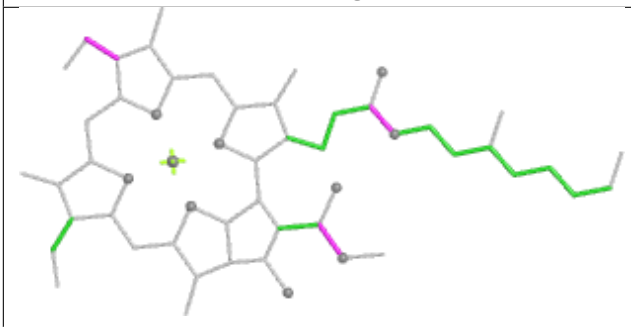
Ligand CLA A4 308



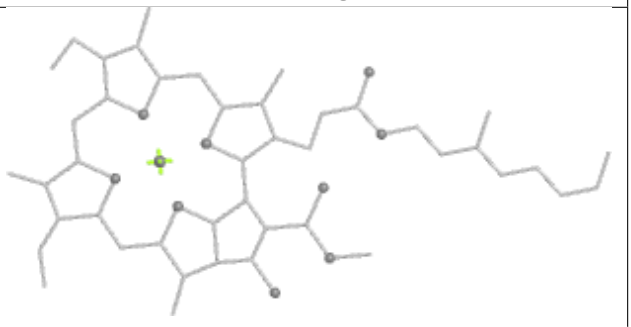
Bond lengths



Bond angles

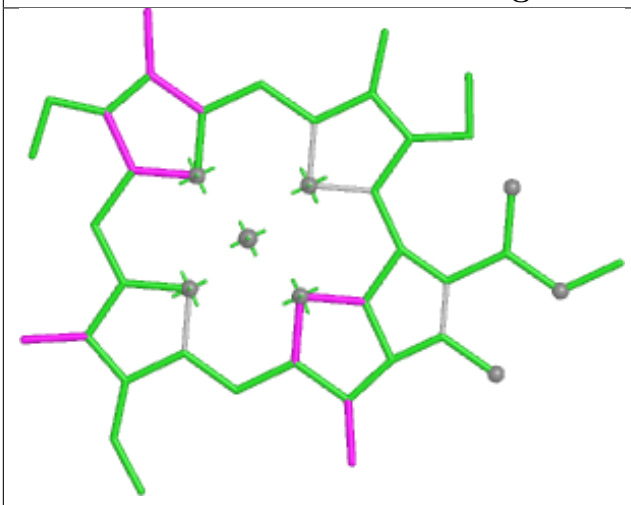


Torsions

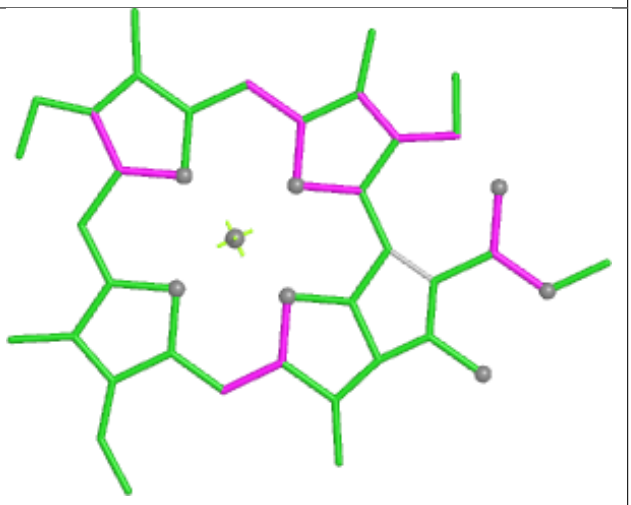


Rings

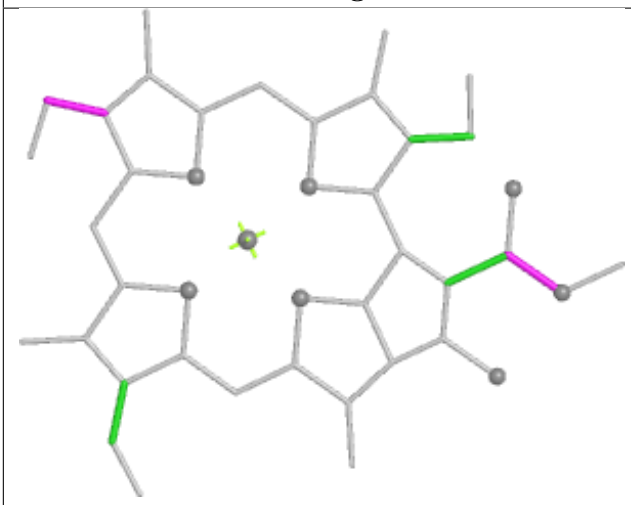
Ligand CLA AF 803



Bond lengths



Bond angles

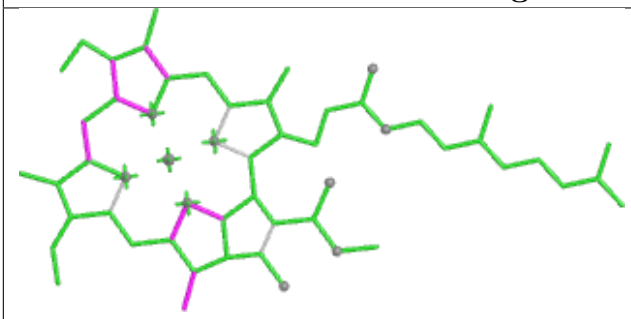


Torsions

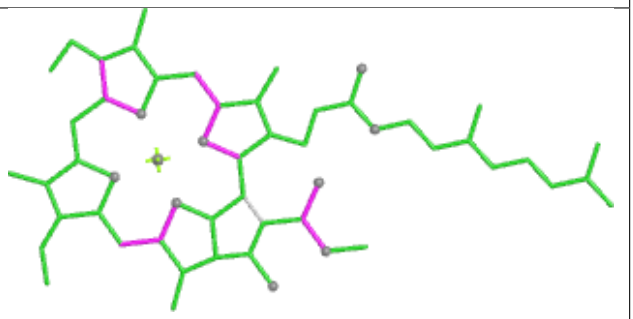


Rings

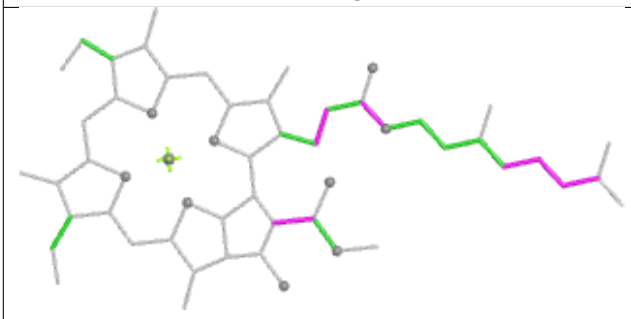
Ligand CLA AB 817



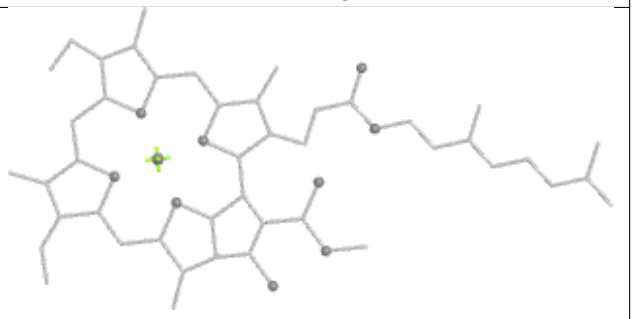
Bond lengths



Bond angles

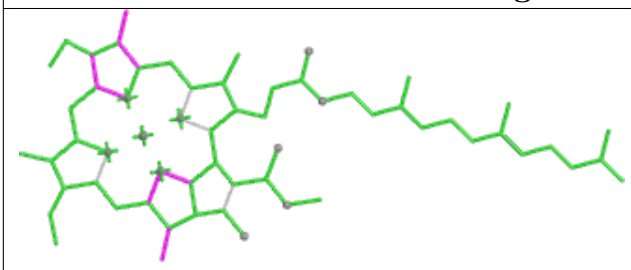


Torsions

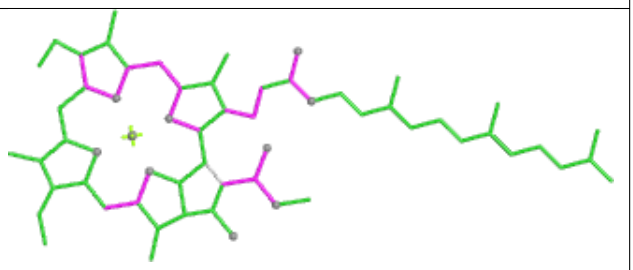


Rings

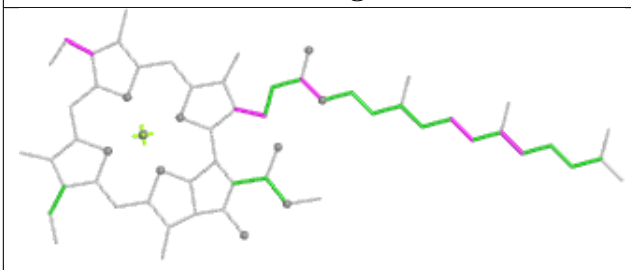
Ligand CLA BL 303



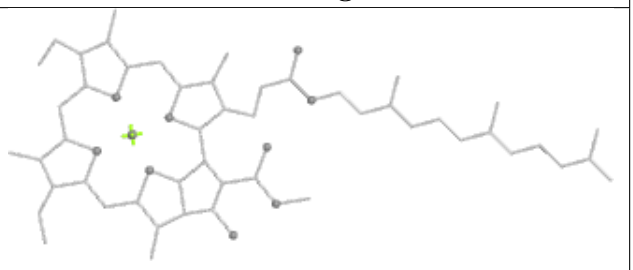
Bond lengths



Bond angles



Torsions

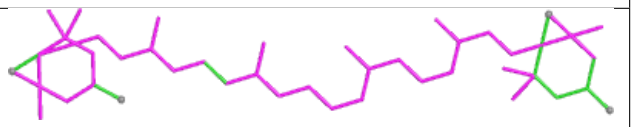


Rings

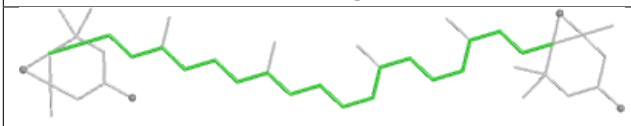
Ligand XAT A1 318



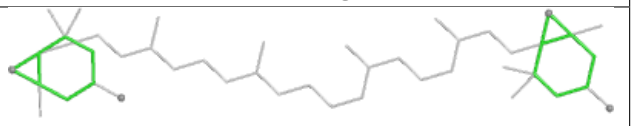
Bond lengths



Bond angles

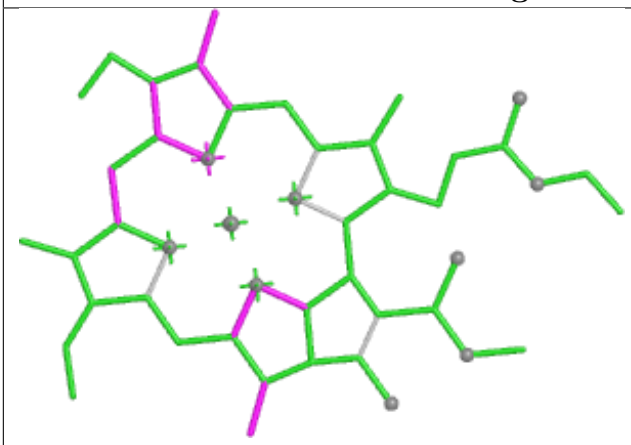


Torsions

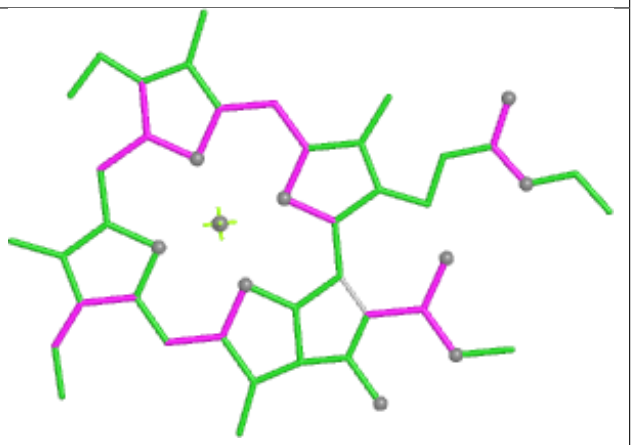


Rings

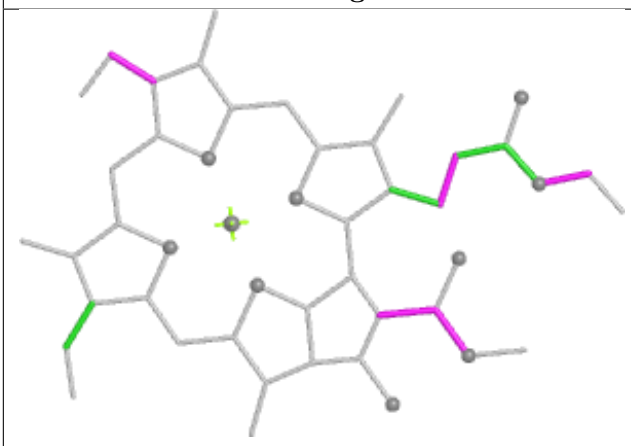
Ligand CLA BA 831



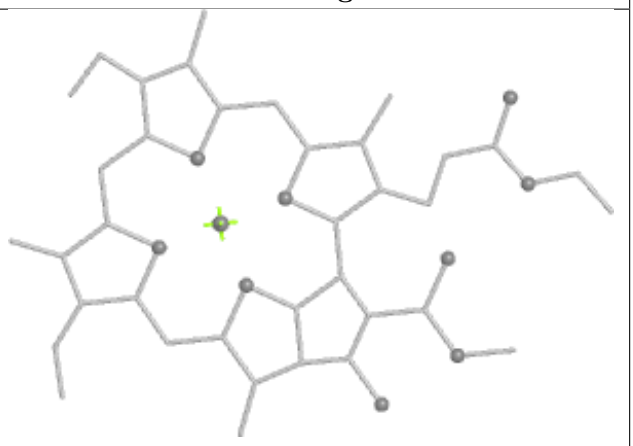
Bond lengths



Bond angles

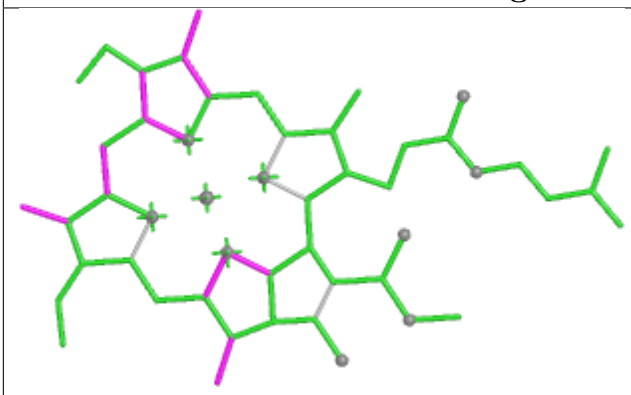


Torsions

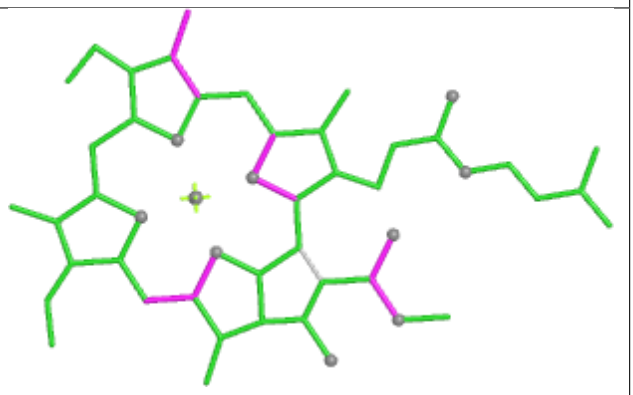


Rings

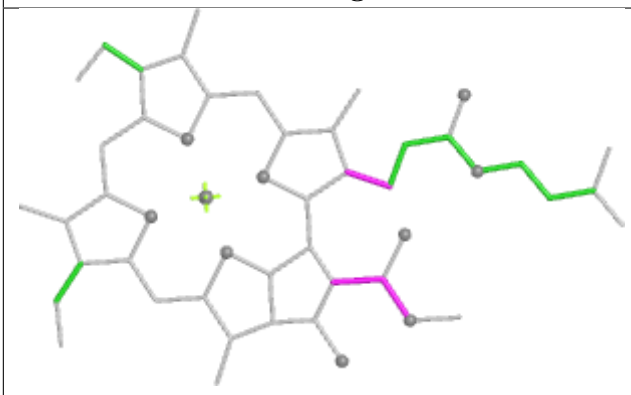
Ligand CLA AA 807



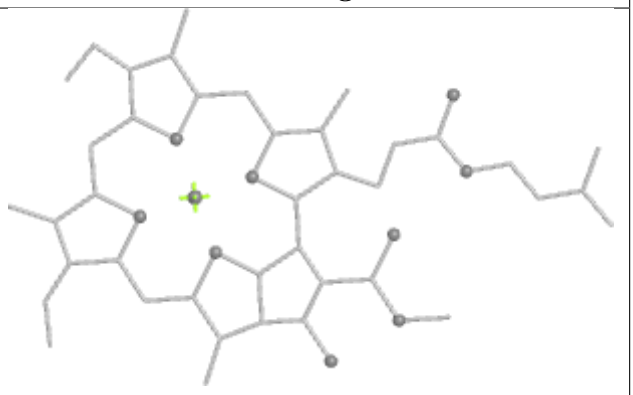
Bond lengths



Bond angles

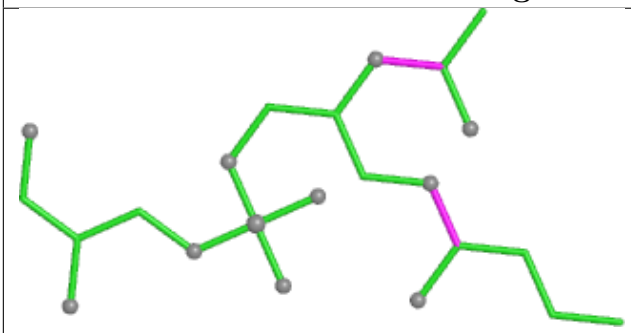


Torsions

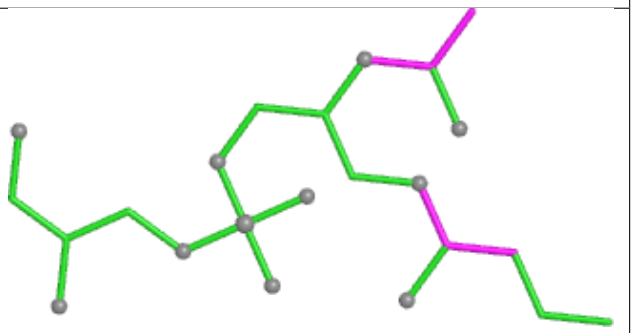


Rings

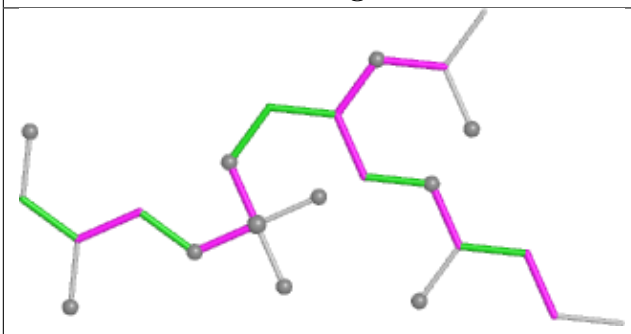
Ligand LHG A3 319



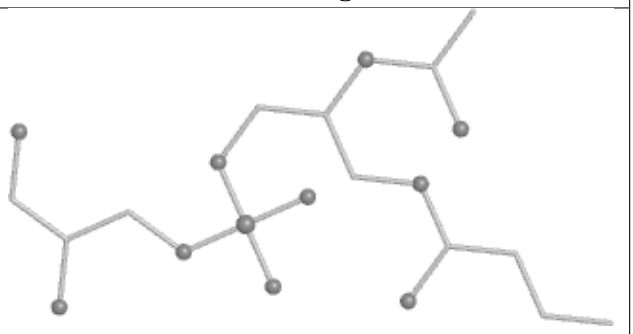
Bond lengths



Bond angles

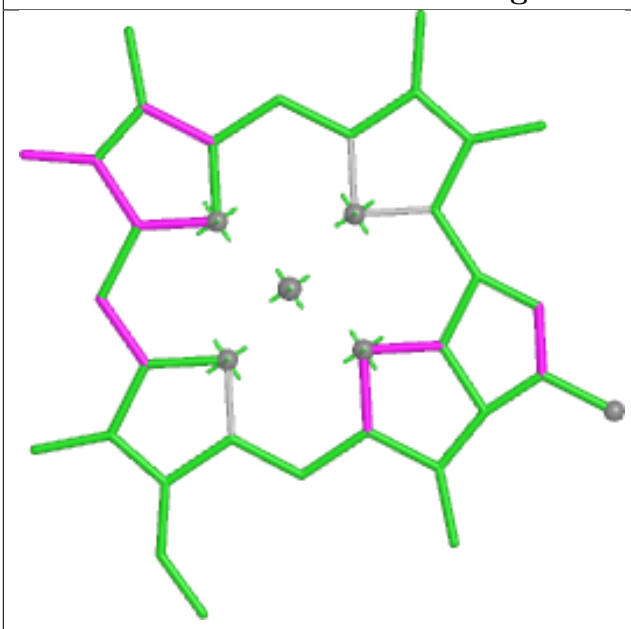


Torsions

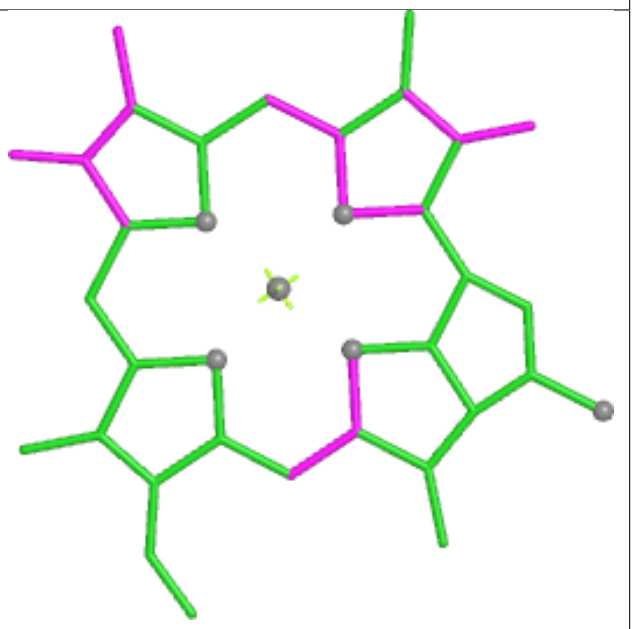


Rings

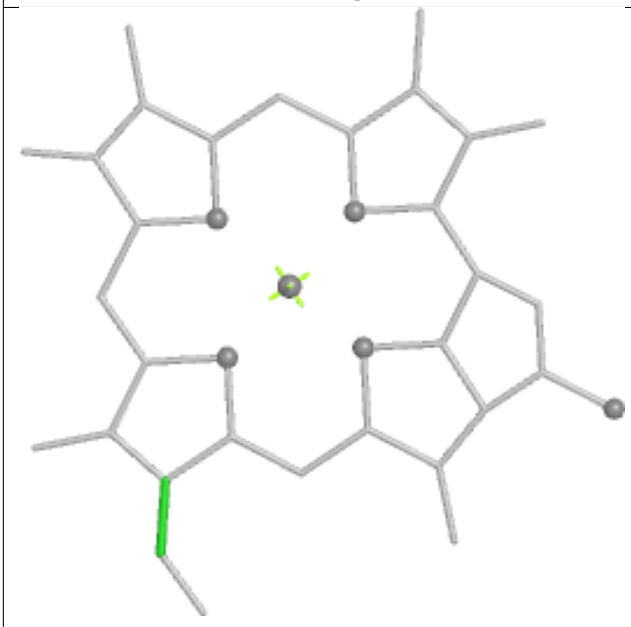
Ligand CLA BK 201



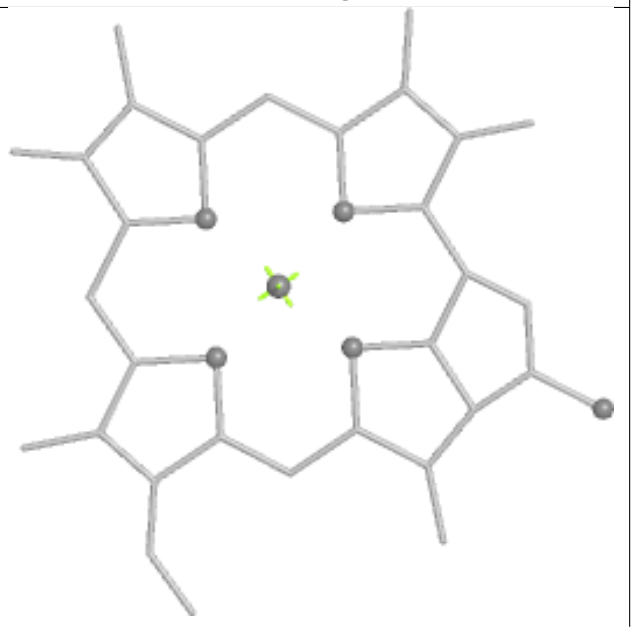
Bond lengths



Bond angles

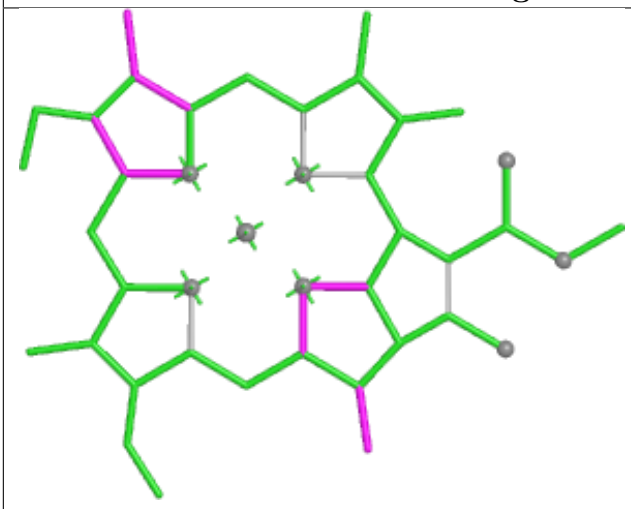


Torsions

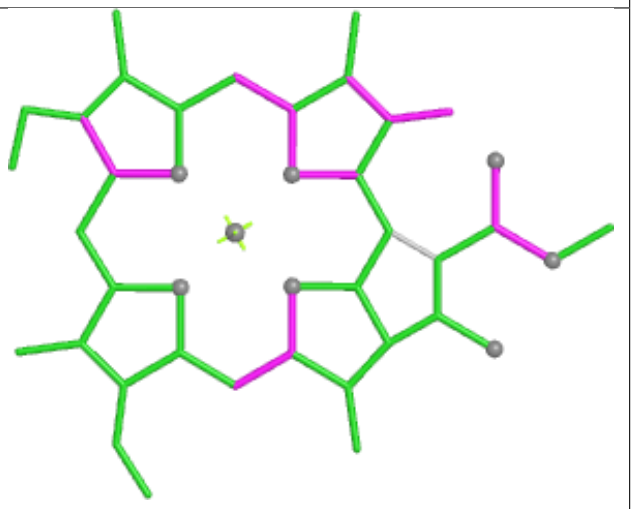


Rings

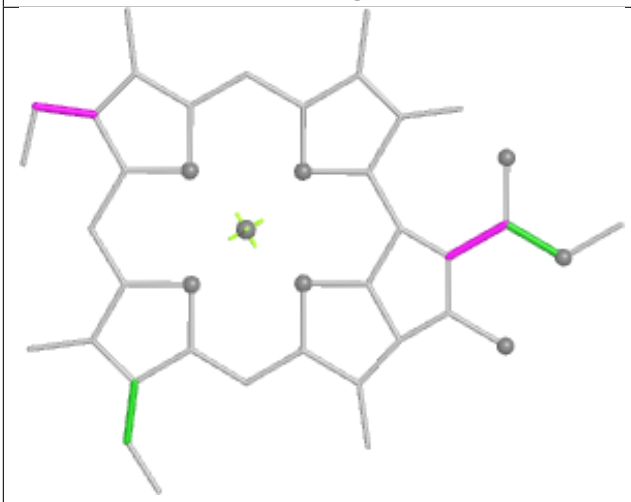
Ligand CLA AF 804



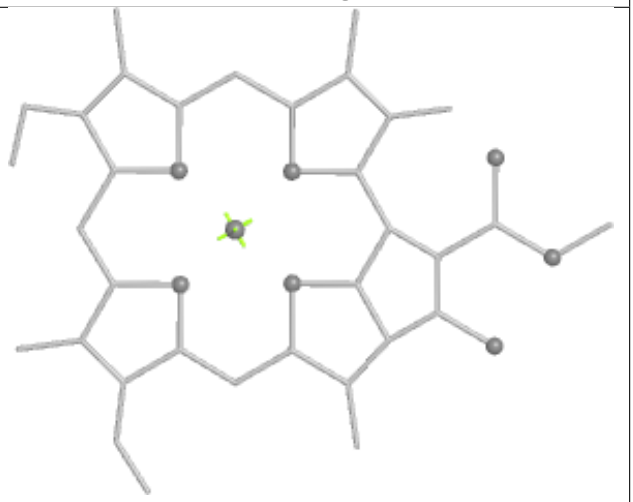
Bond lengths



Bond angles

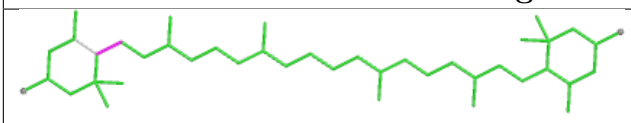


Torsions

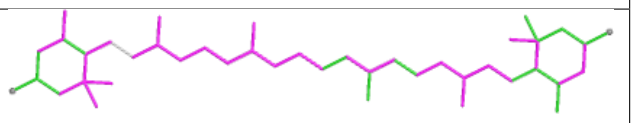


Rings

Ligand LUT B3 315



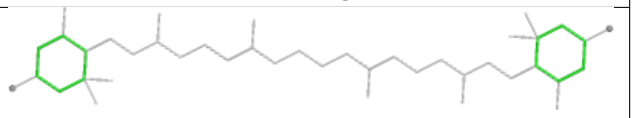
Bond lengths



Bond angles

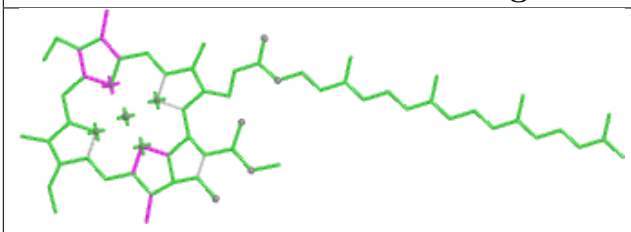


Torsions

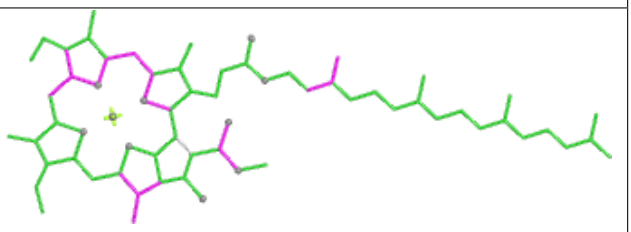


Rings

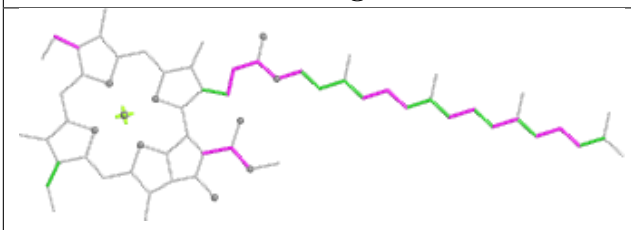
Ligand CLA AA 833



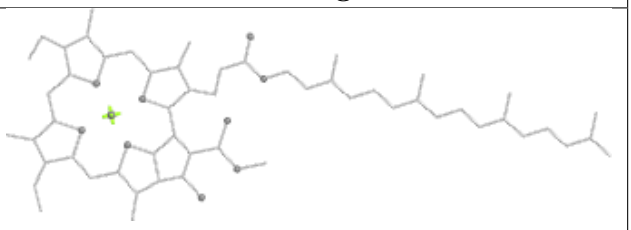
Bond lengths



Bond angles

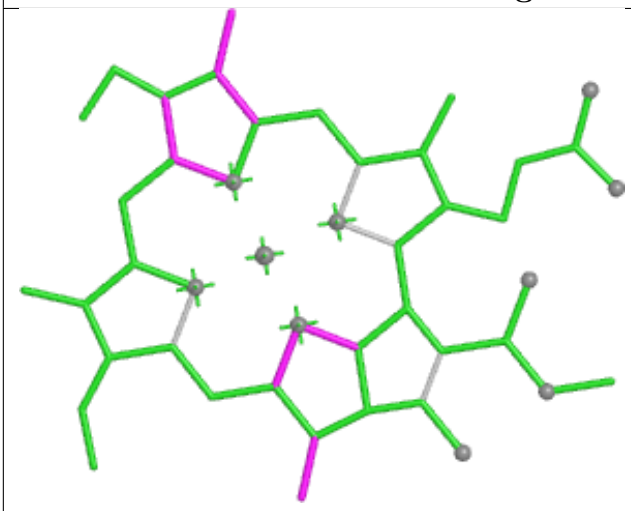


Torsions

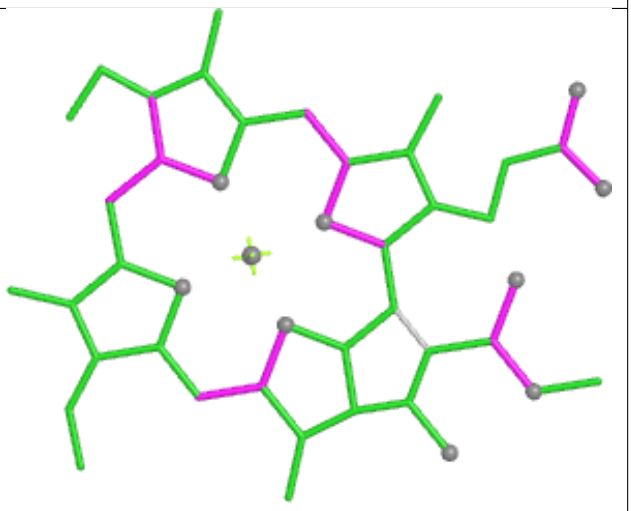


Rings

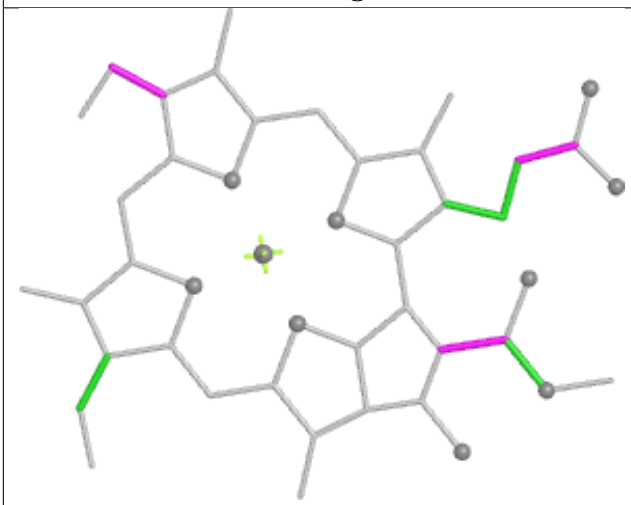
Ligand CLA B2 608



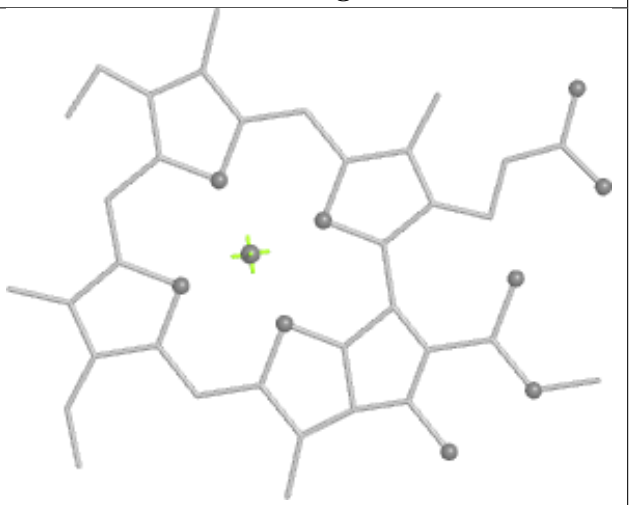
Bond lengths



Bond angles

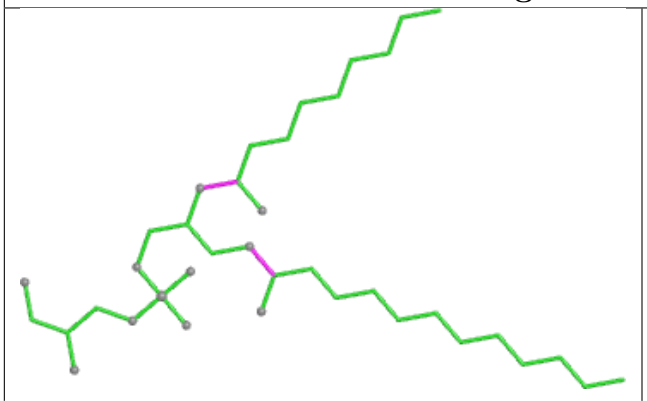


Torsions

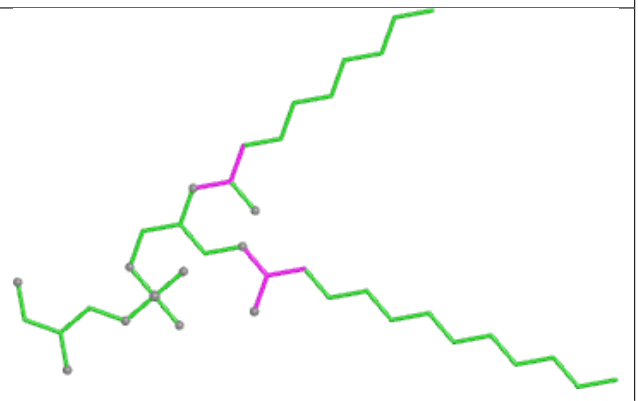


Rings

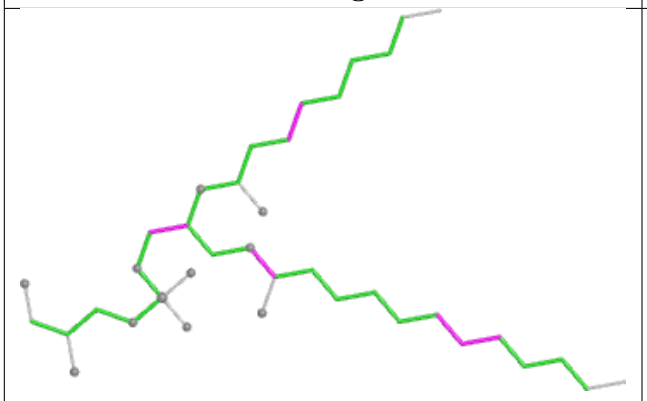
Ligand LHG B1 301



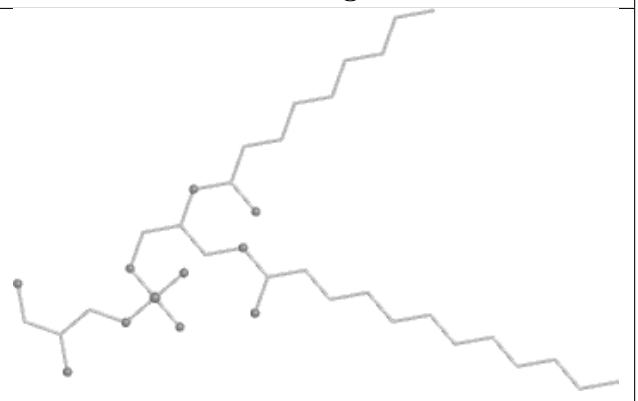
Bond lengths



Bond angles

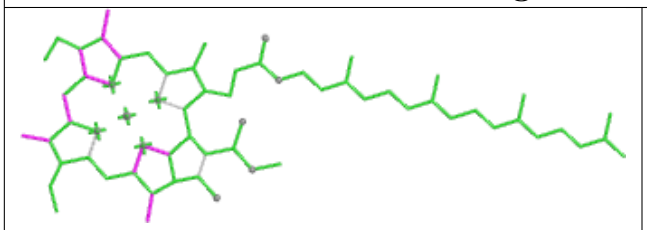


Torsions

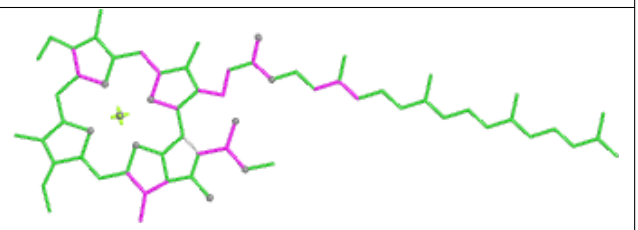


Rings

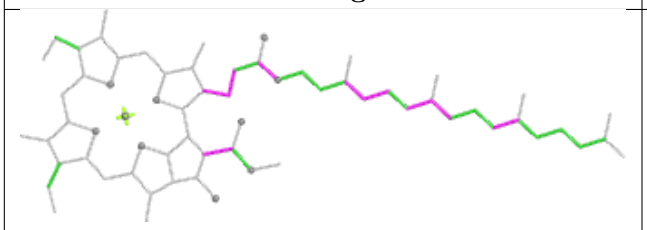
Ligand CLA BB 810



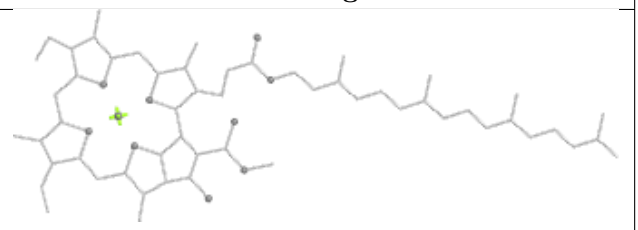
Bond lengths



Bond angles

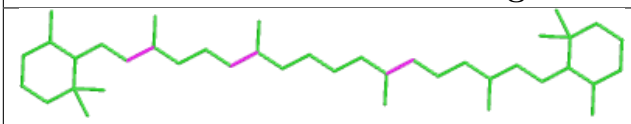


Torsions

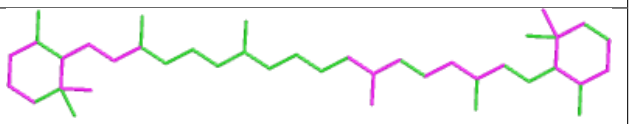


Rings

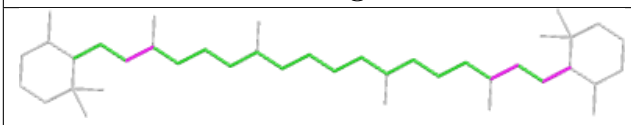
Ligand BCR AK 204



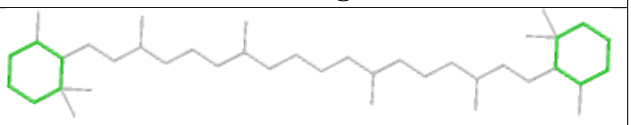
Bond lengths



Bond angles

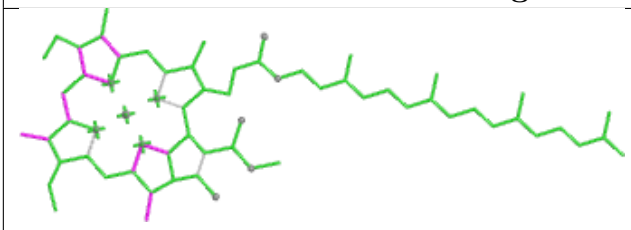


Torsions

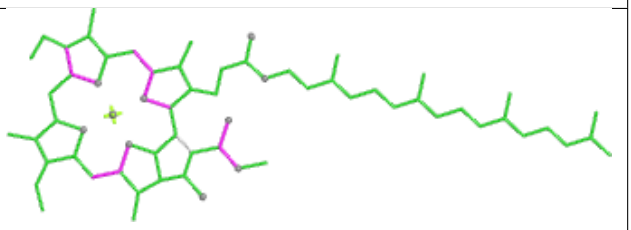


Rings

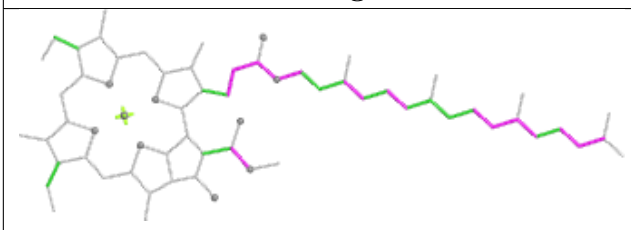
Ligand CLA BA 806



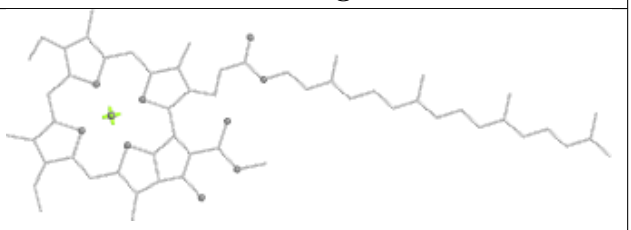
Bond lengths



Bond angles

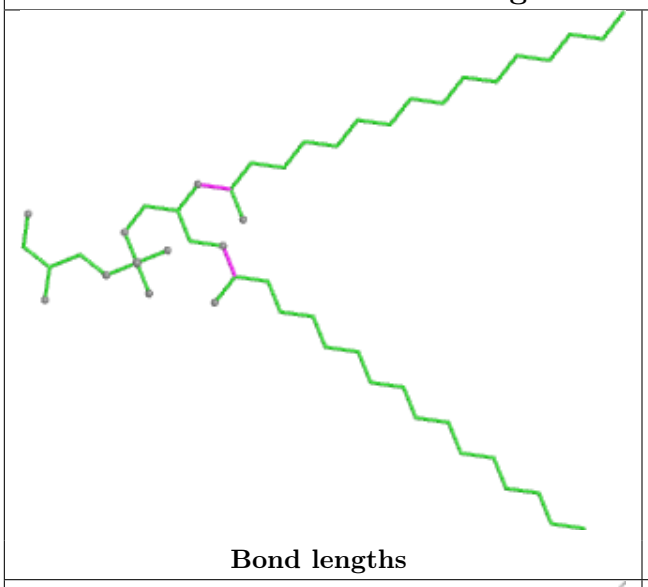


Torsions

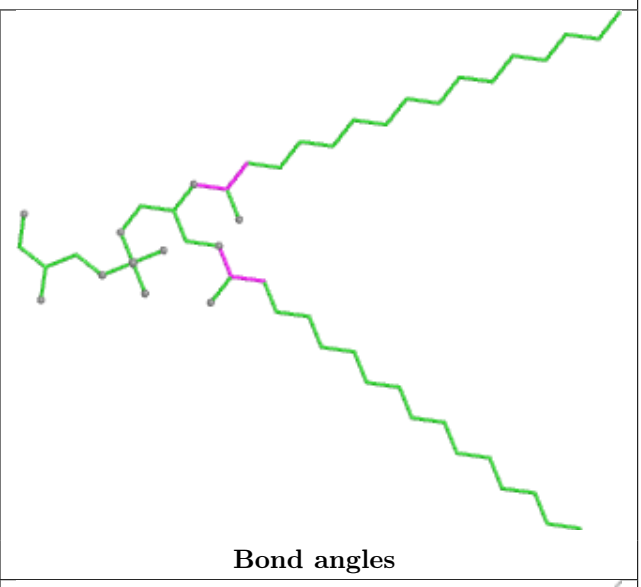


Rings

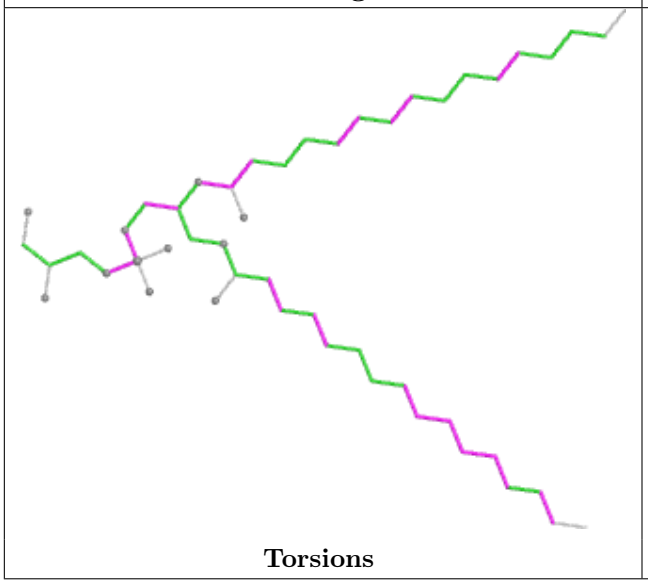
Ligand LHG AA 844



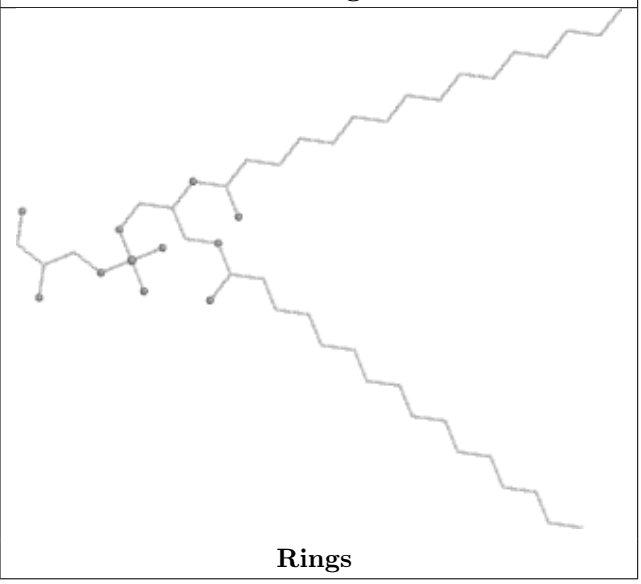
Bond lengths



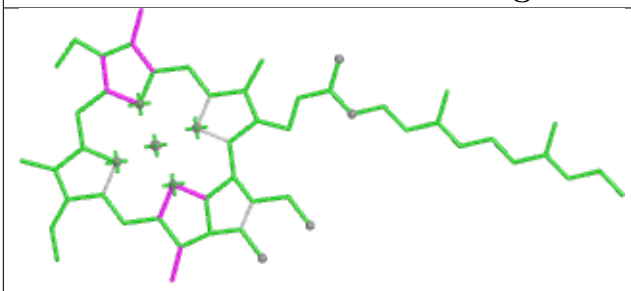
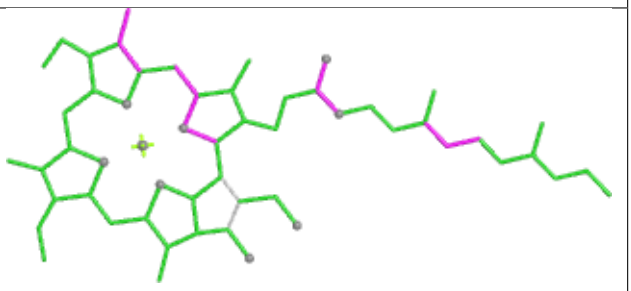
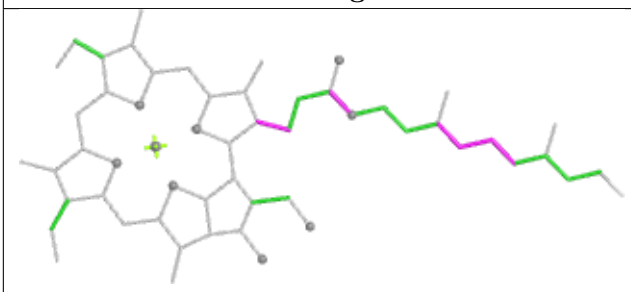
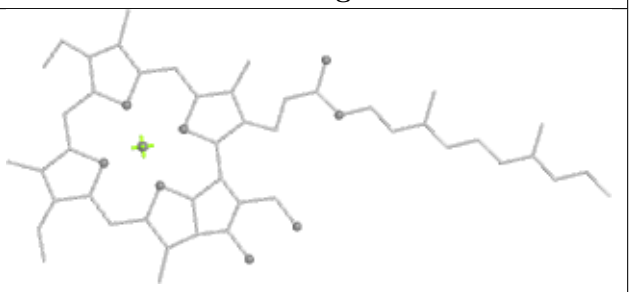
Bond angles



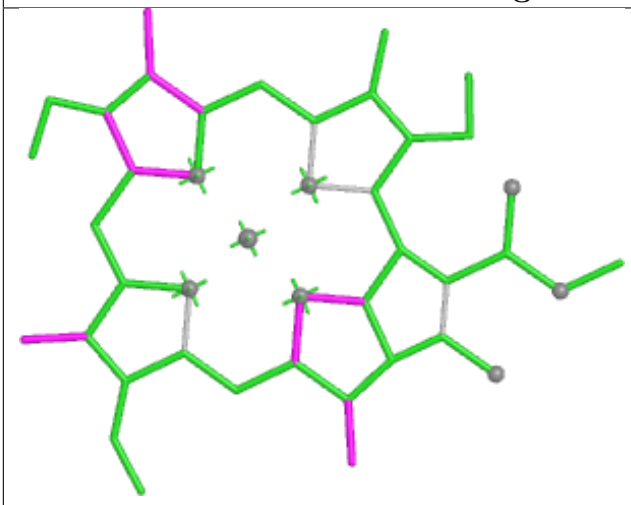
Torsions



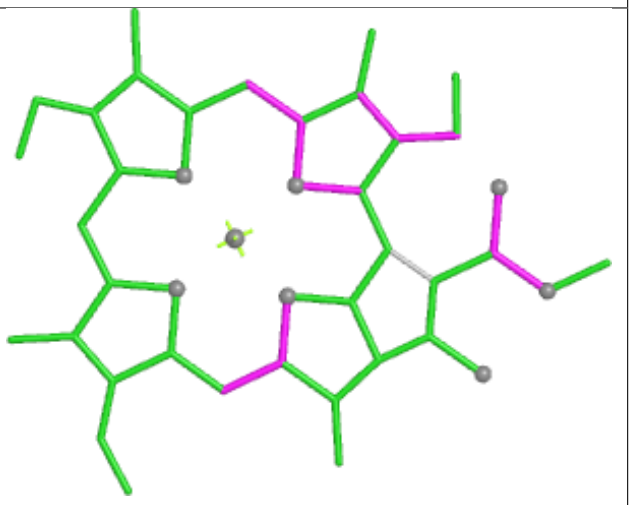
Rings

Ligand CLA BF 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

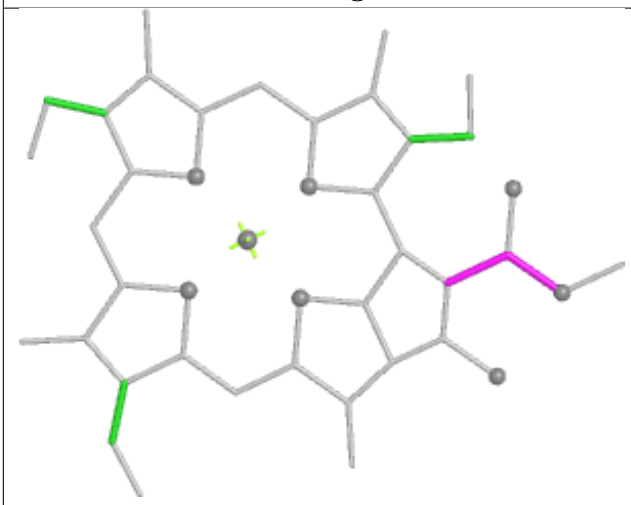
Ligand CLA BF 302



Bond lengths



Bond angles



Torsions

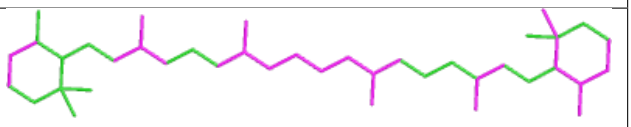


Rings

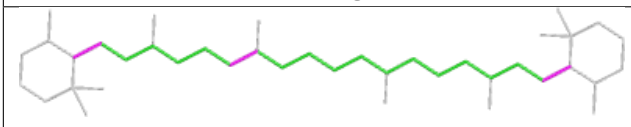
Ligand BCR BA 848



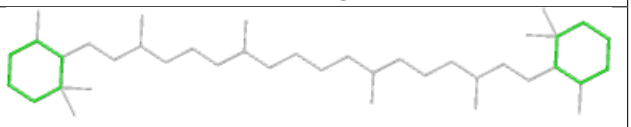
Bond lengths



Bond angles

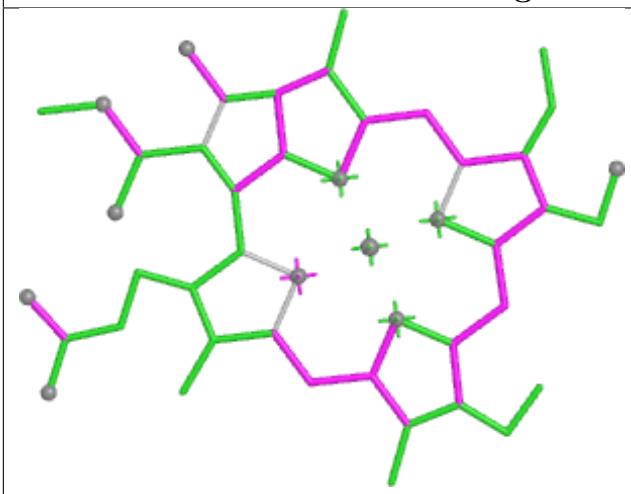


Torsions

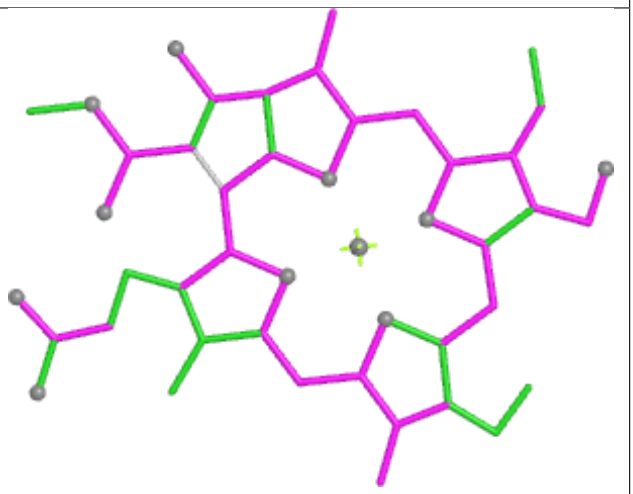


Rings

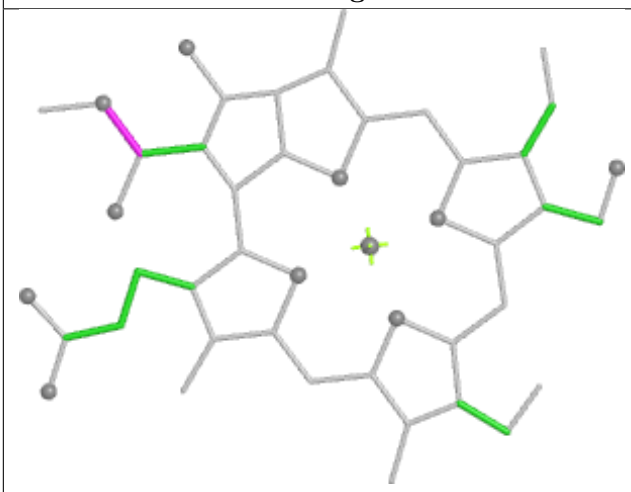
Ligand CHL A4 306



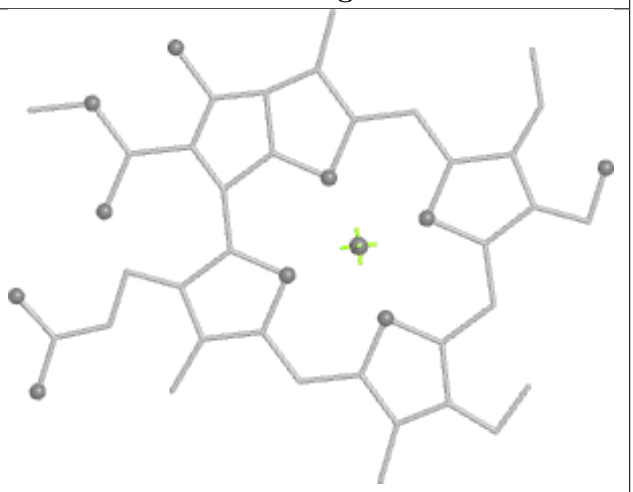
Bond lengths



Bond angles



Torsions

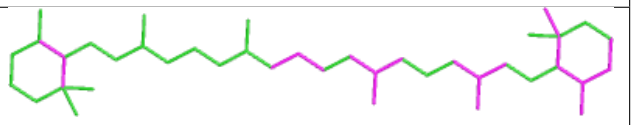


Rings

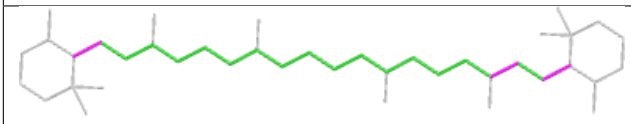
Ligand BCR BA 847



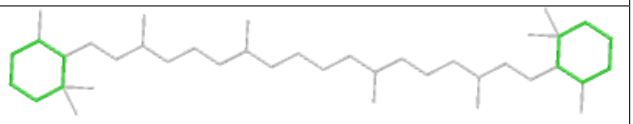
Bond lengths



Bond angles

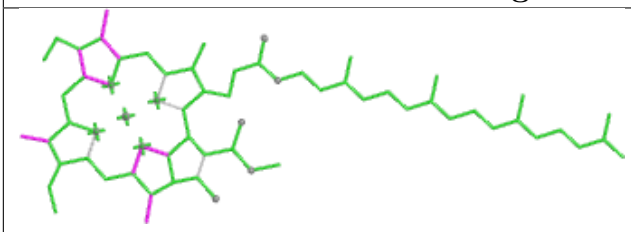


Torsions

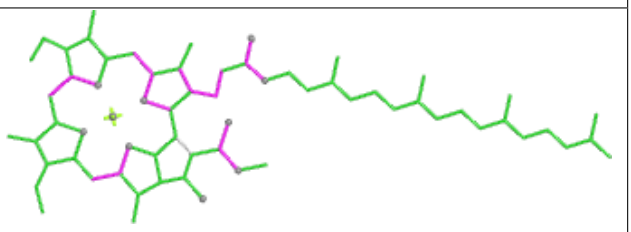


Rings

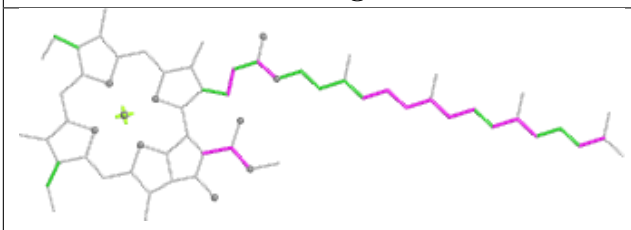
Ligand CLA BB 824



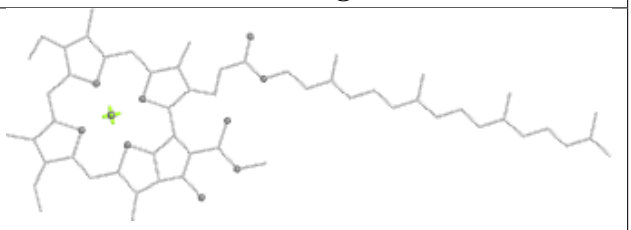
Bond lengths



Bond angles

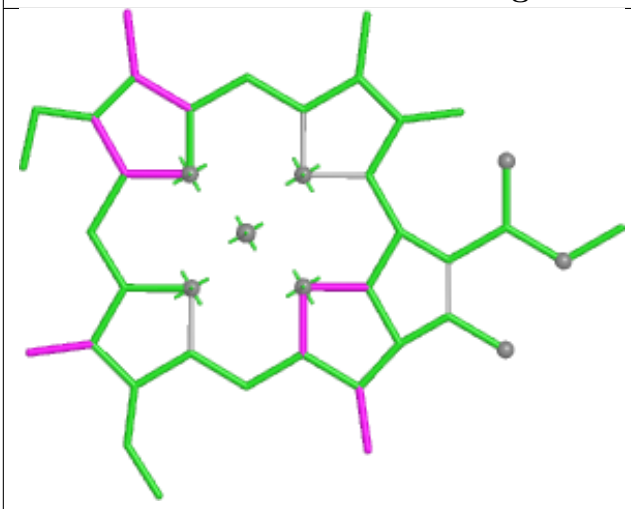


Torsions

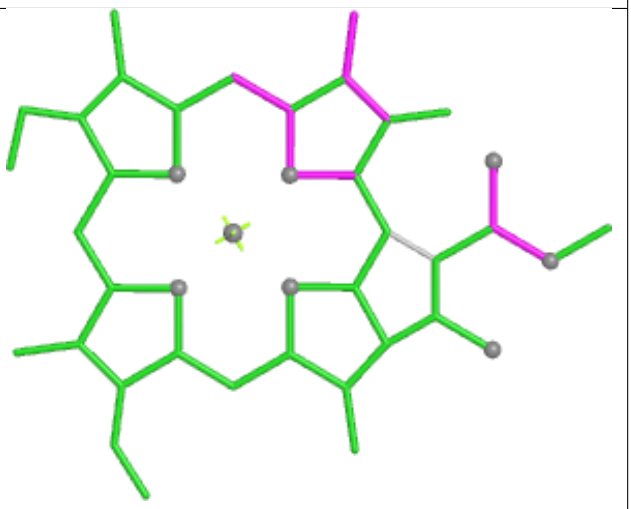


Rings

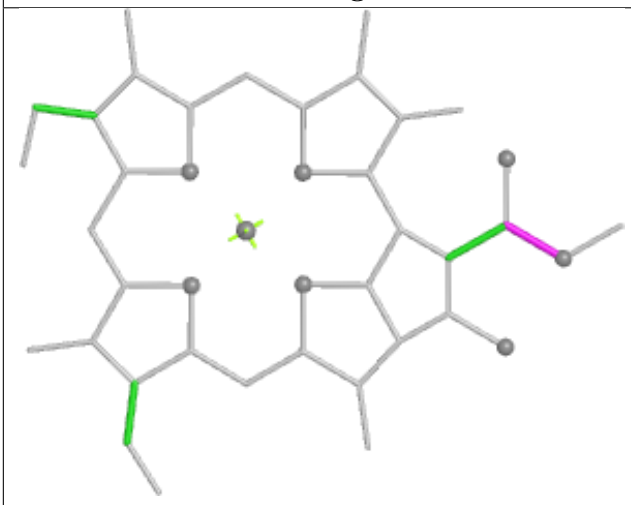
Ligand CLA BB 822



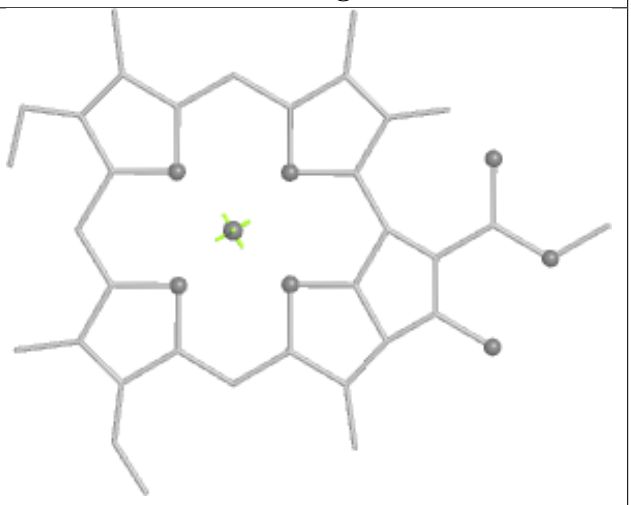
Bond lengths



Bond angles

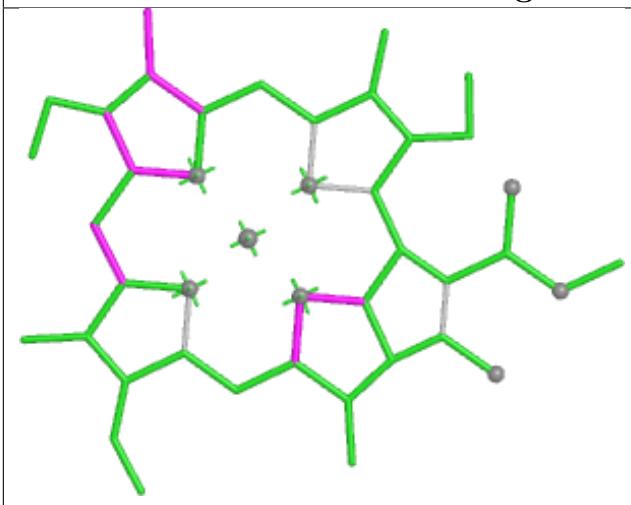


Torsions

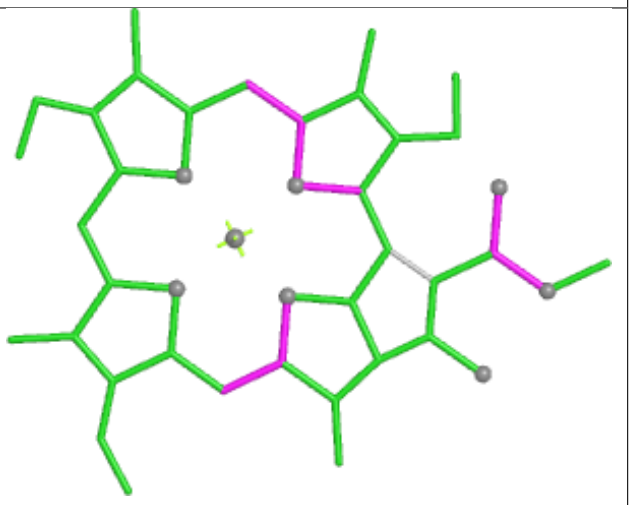


Rings

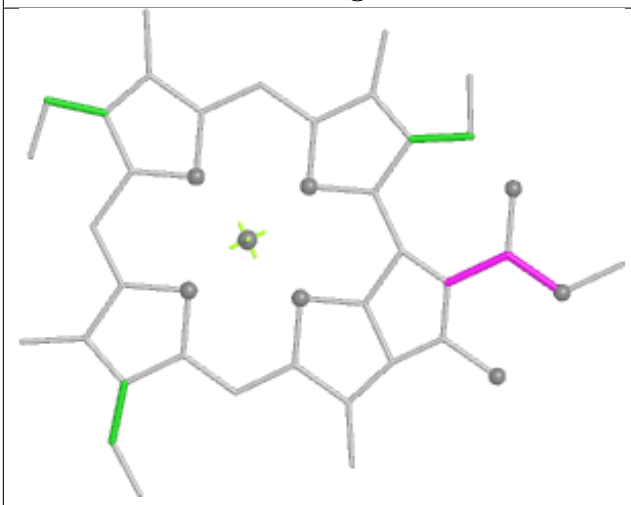
Ligand CLA BJ 102



Bond lengths



Bond angles

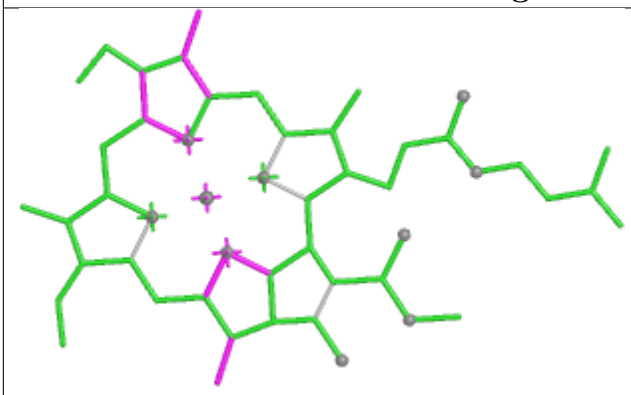


Torsions

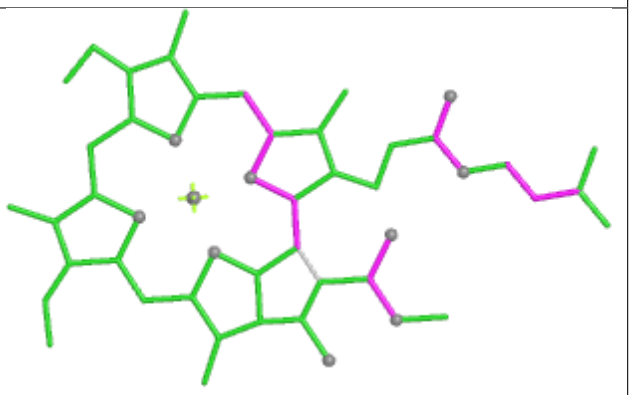


Rings

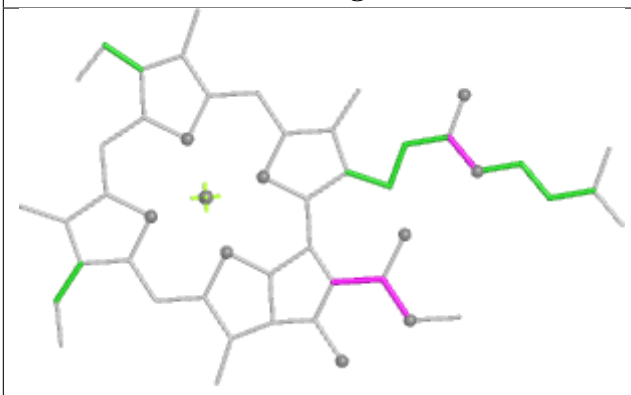
Ligand CLA BB 838



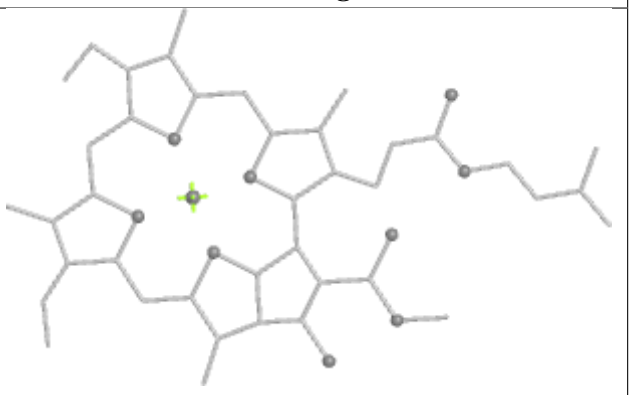
Bond lengths



Bond angles



Torsions

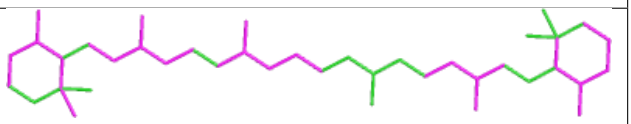


Rings

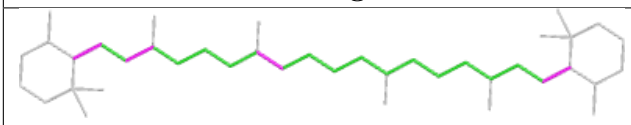
Ligand BCR BF 304



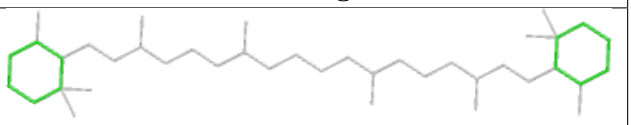
Bond lengths



Bond angles

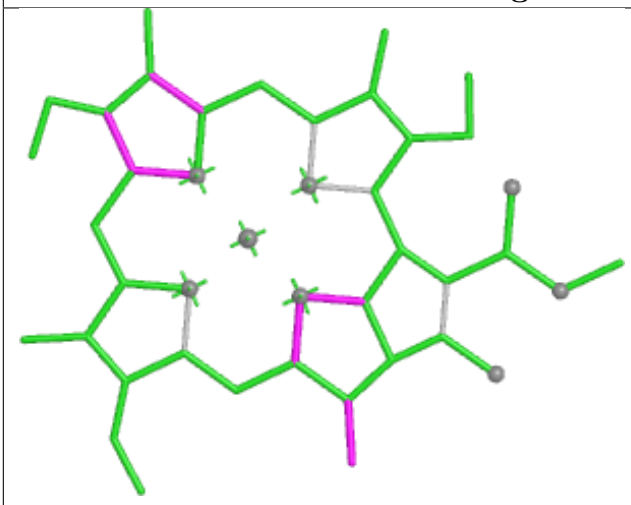


Torsions

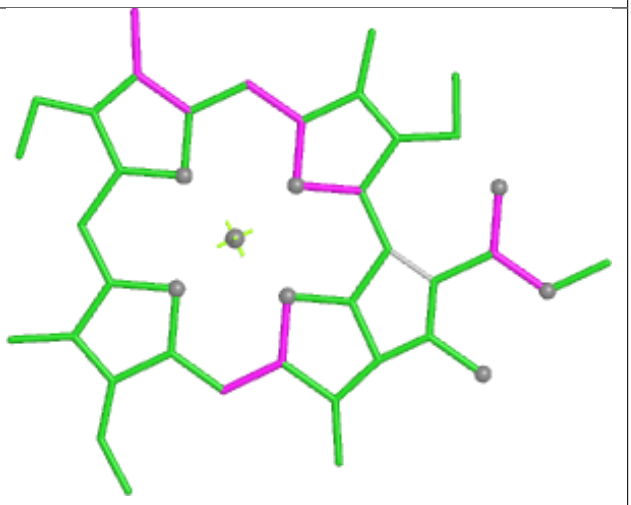


Rings

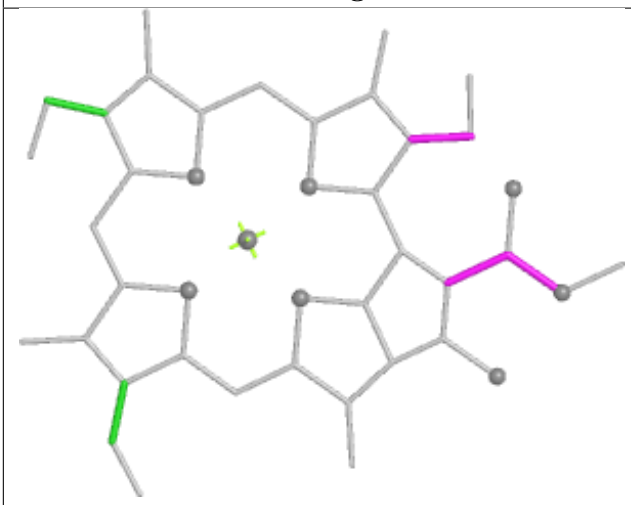
Ligand CLA BA 822



Bond lengths



Bond angles

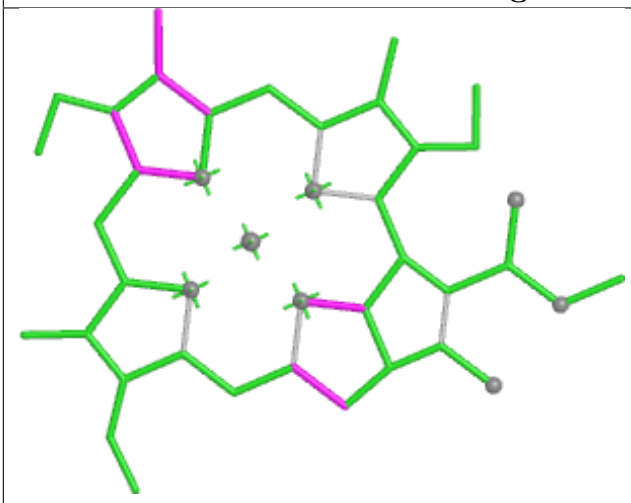


Torsions

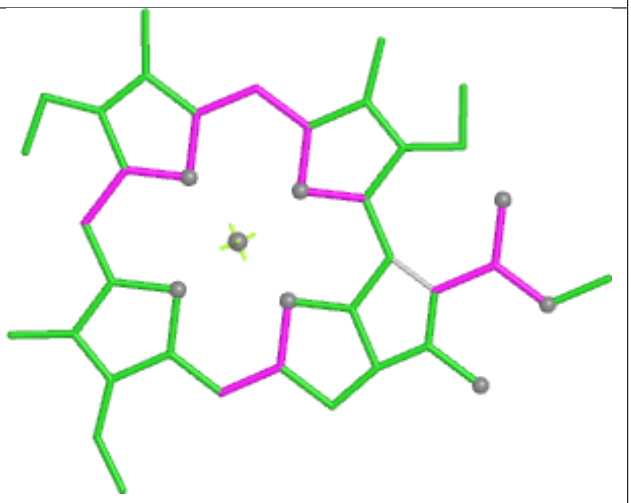


Rings

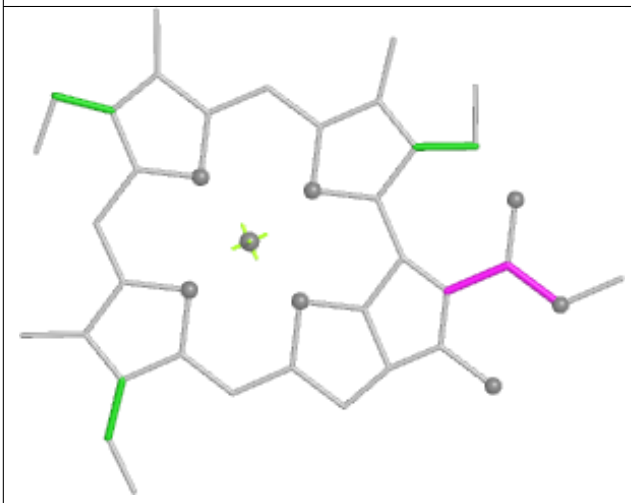
Ligand CLA AA 815



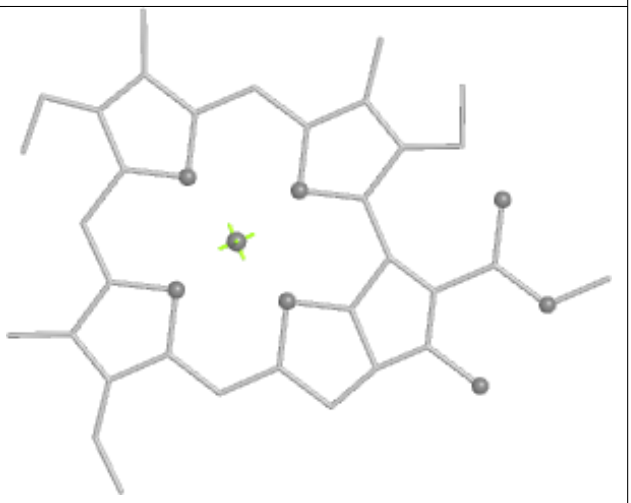
Bond lengths



Bond angles

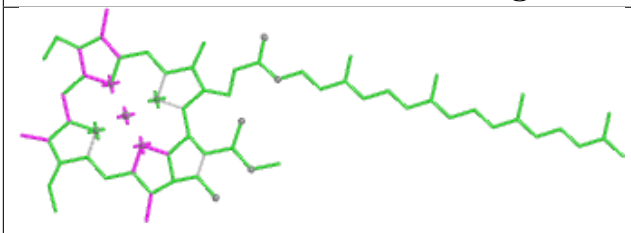


Torsions

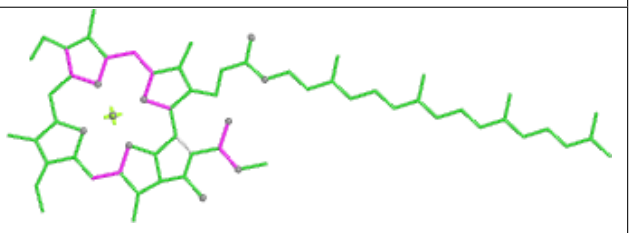


Rings

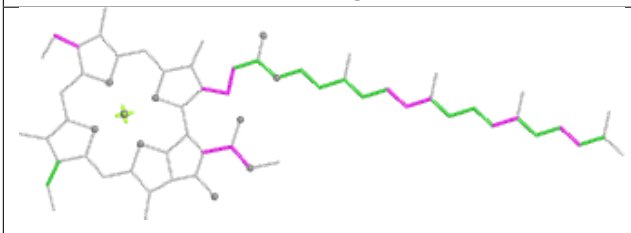
Ligand CLA AB 814



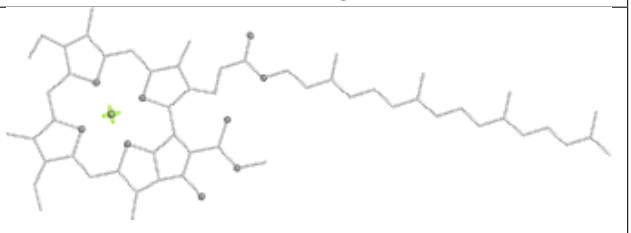
Bond lengths



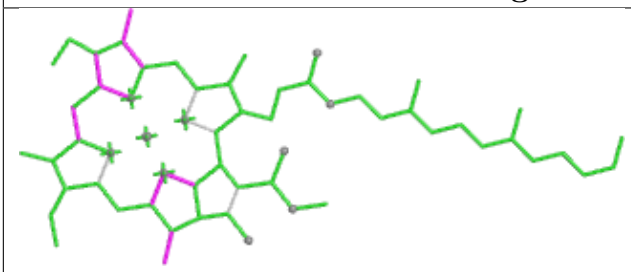
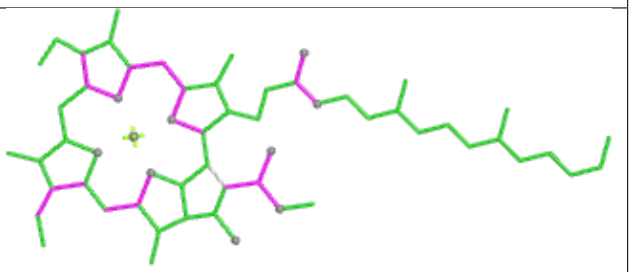
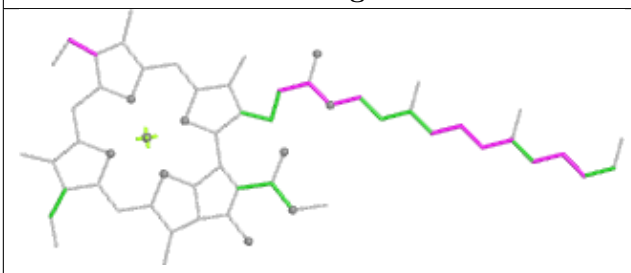
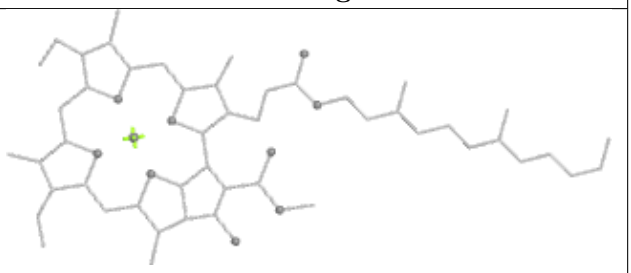
Bond angles

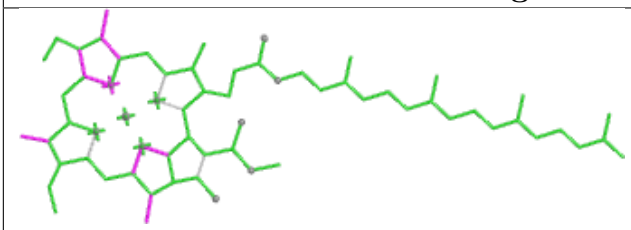
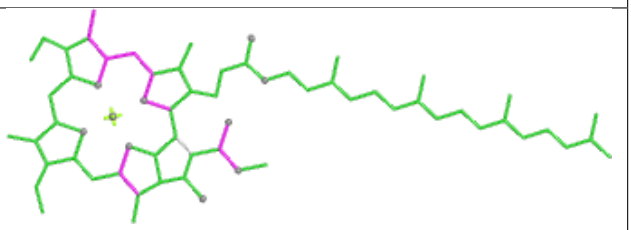
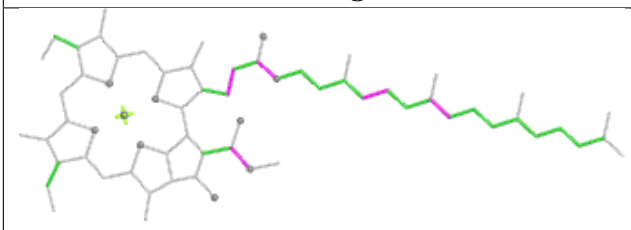
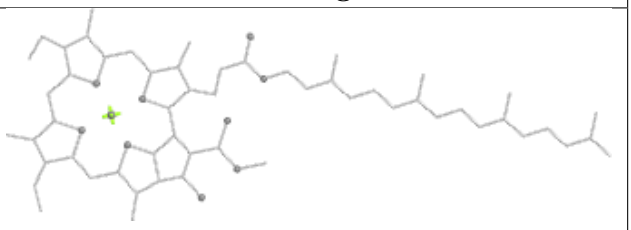


Torsions

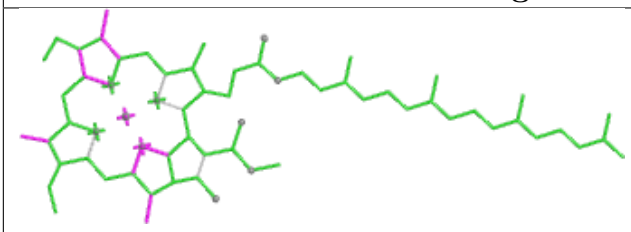


Rings

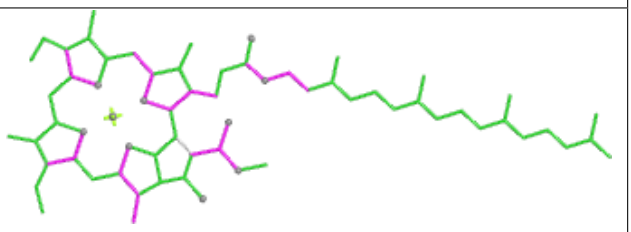
Ligand CLA AB 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AB 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

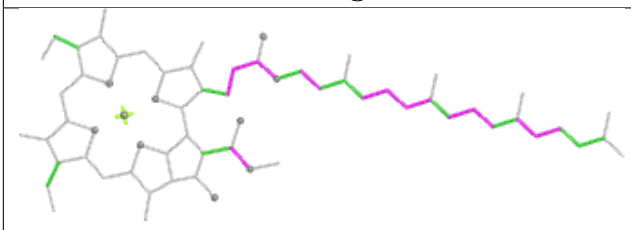
Ligand CLA BB 801



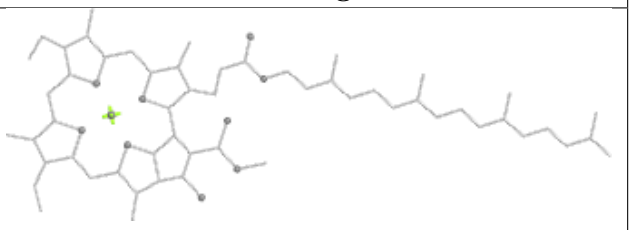
Bond lengths



Bond angles

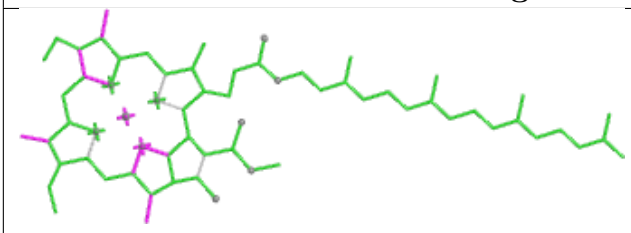


Torsions

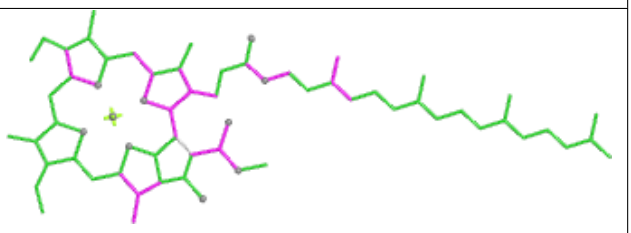


Rings

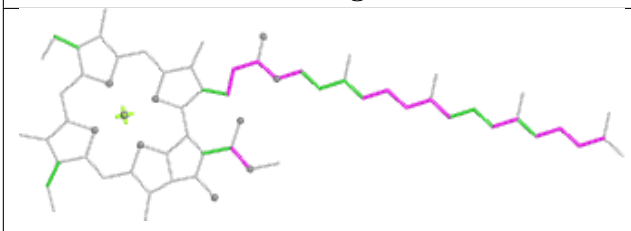
Ligand CLA AB 801



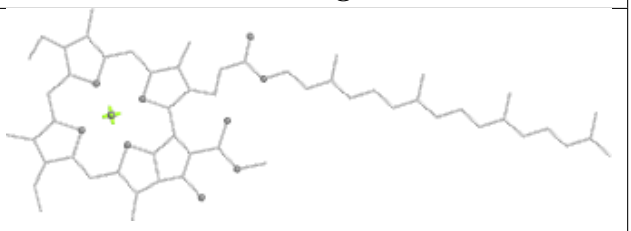
Bond lengths



Bond angles

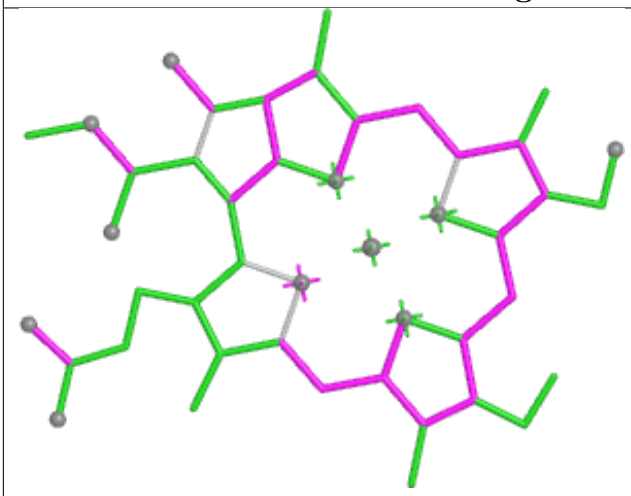


Torsions

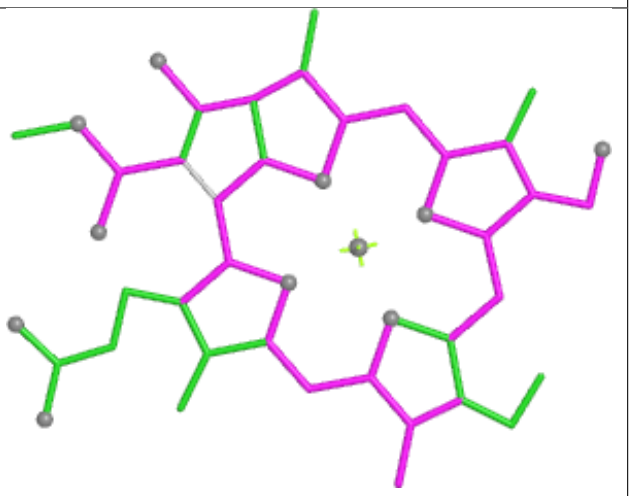


Rings

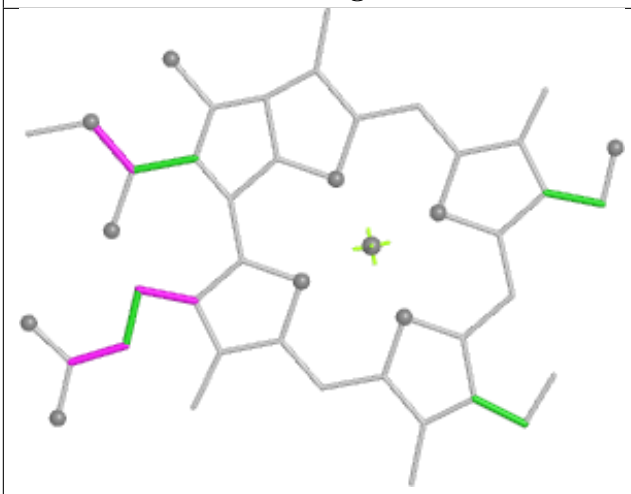
Ligand CHL B5 607



Bond lengths



Bond angles

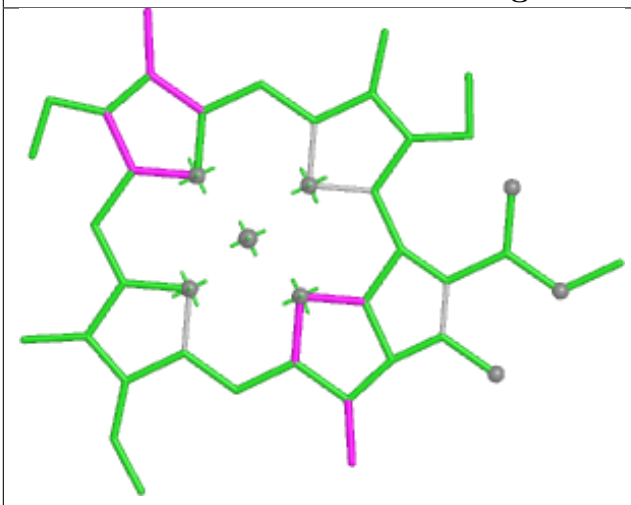


Torsions

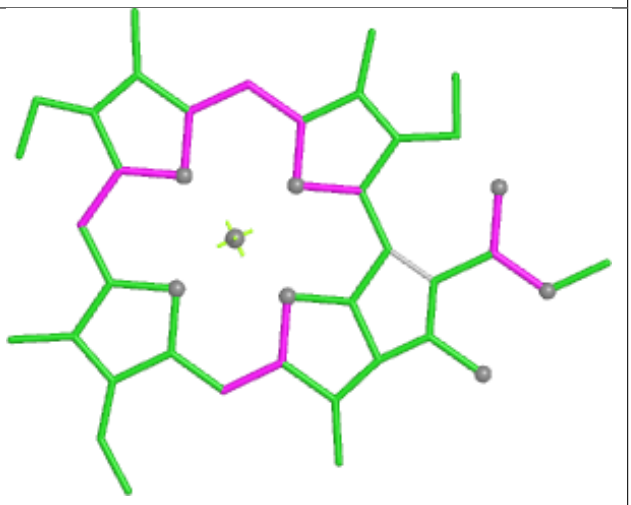


Rings

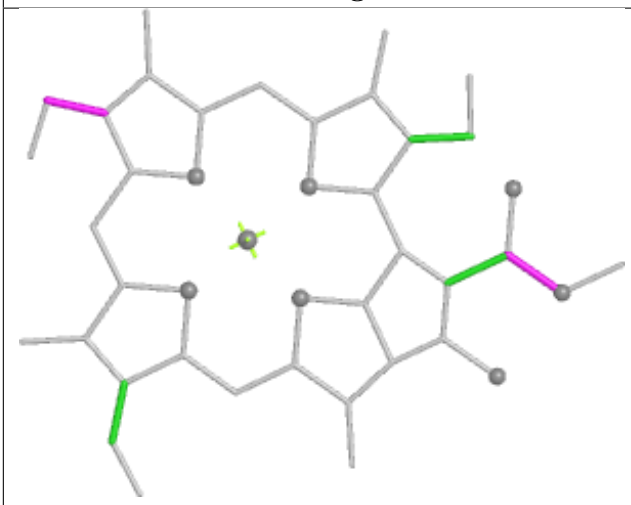
Ligand CLA AB 836



Bond lengths



Bond angles

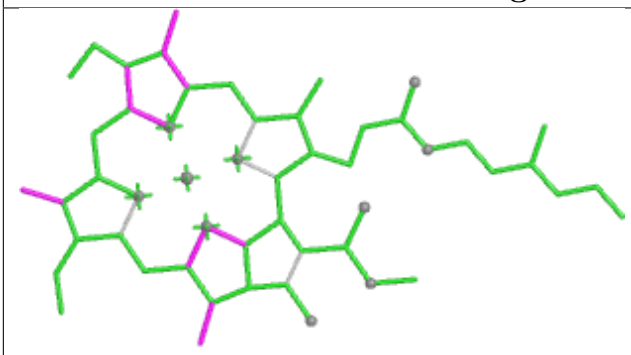


Torsions

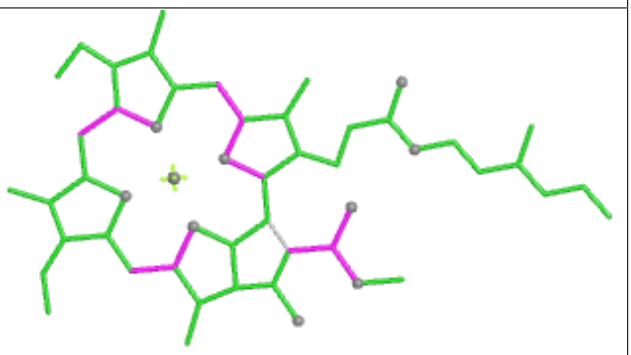


Rings

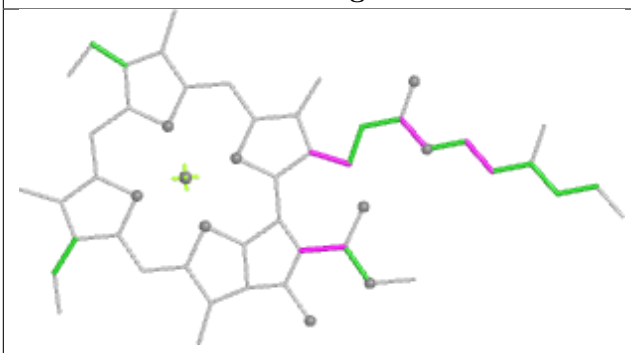
Ligand CLA AA 839



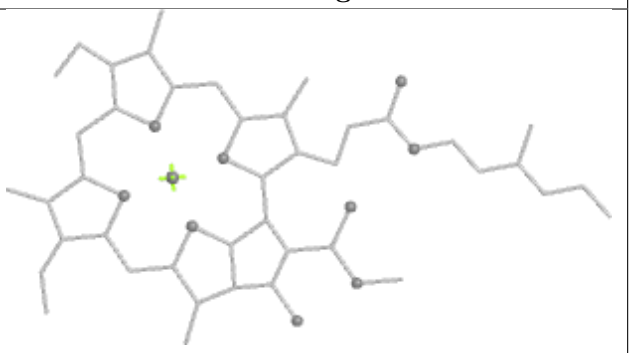
Bond lengths



Bond angles

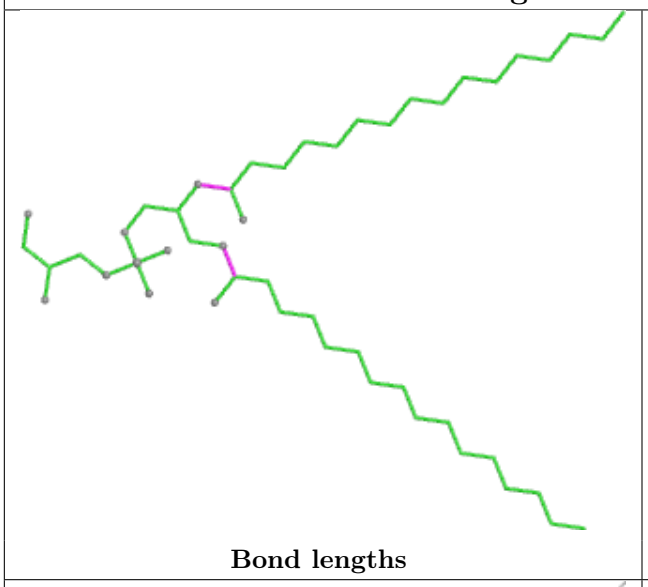


Torsions

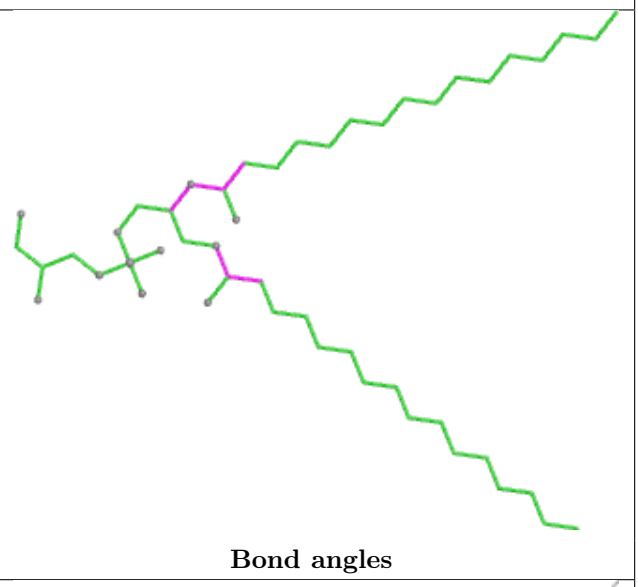


Rings

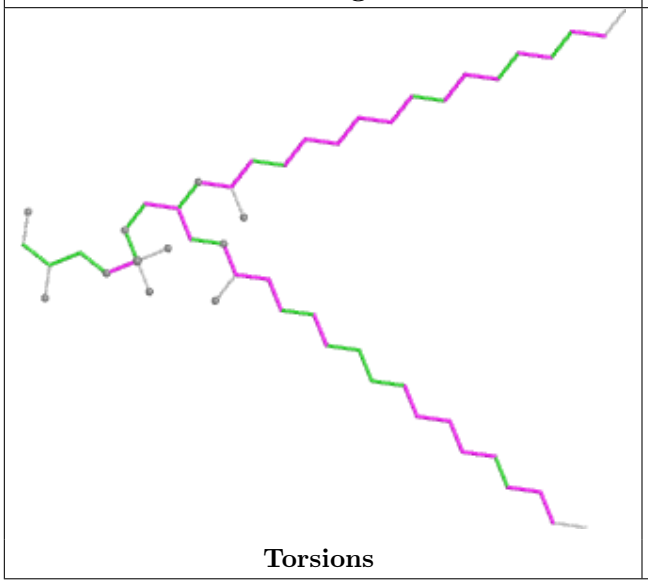
Ligand LHG BA 845



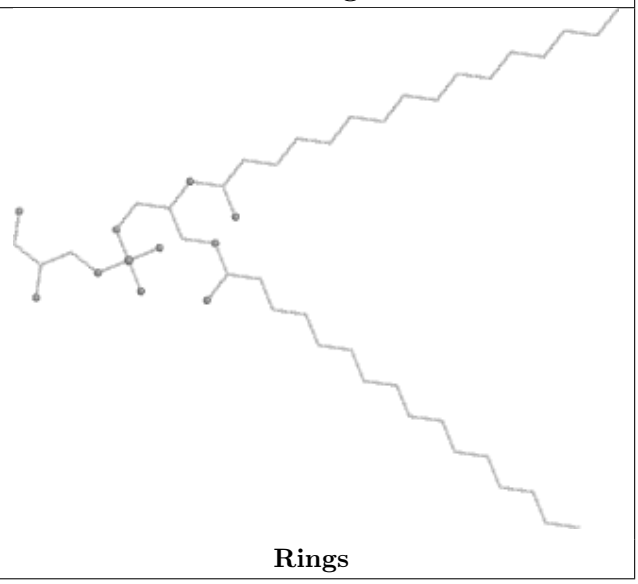
Bond lengths



Bond angles

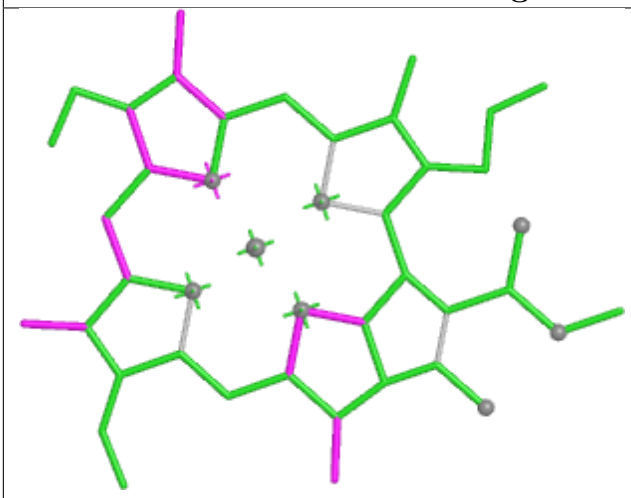


Torsions

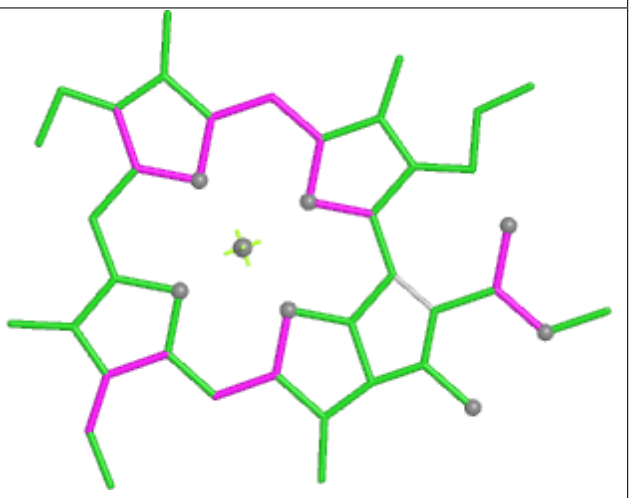


Rings

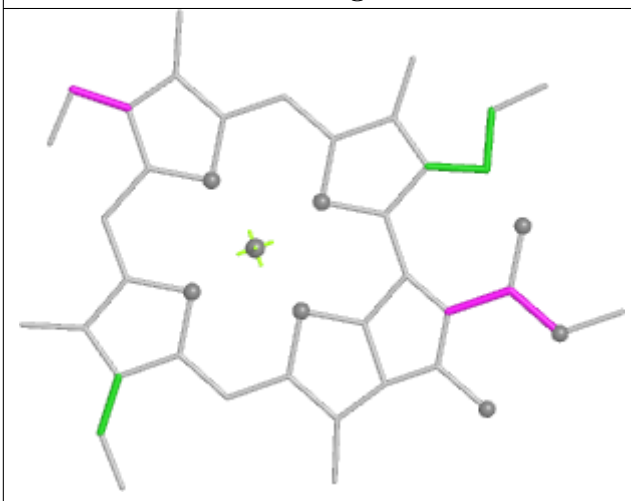
Ligand CLA AB 831



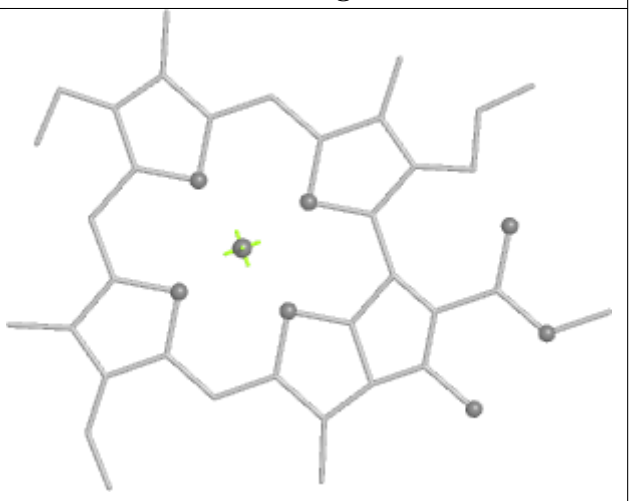
Bond lengths



Bond angles

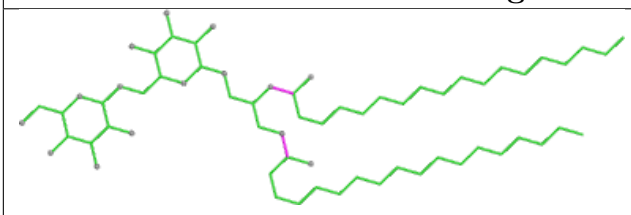


Torsions

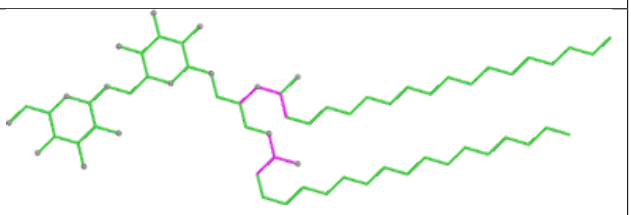


Rings

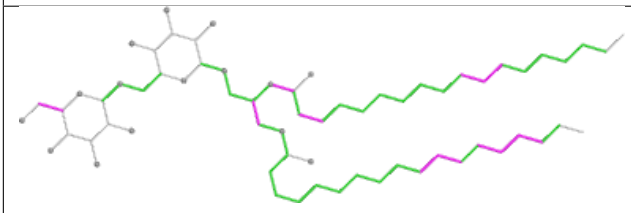
Ligand DGD BB 850



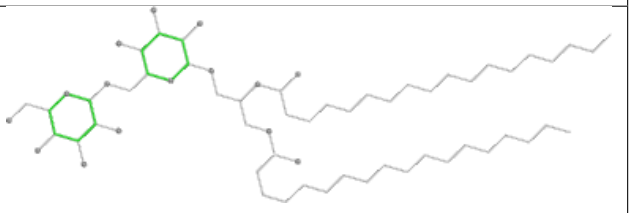
Bond lengths



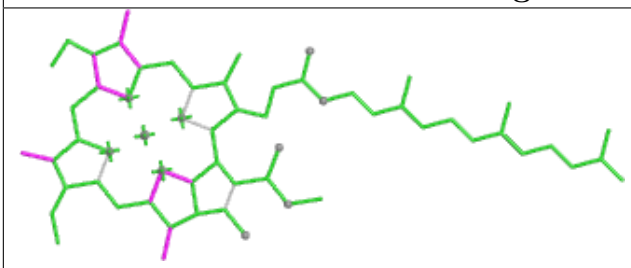
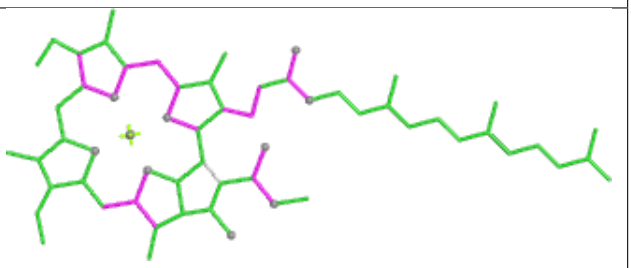
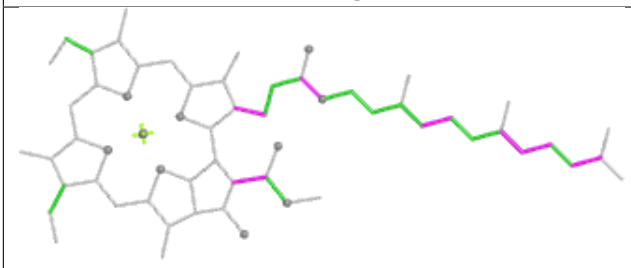
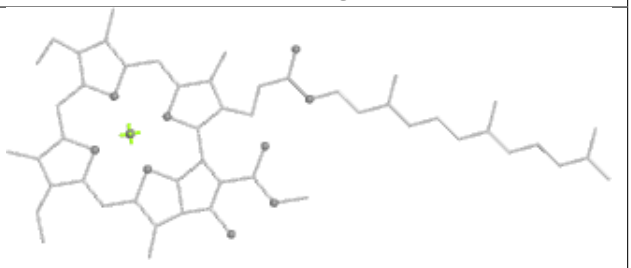
Bond angles

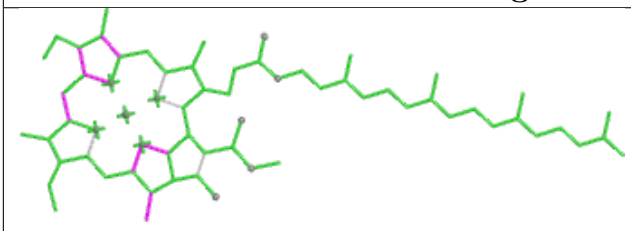
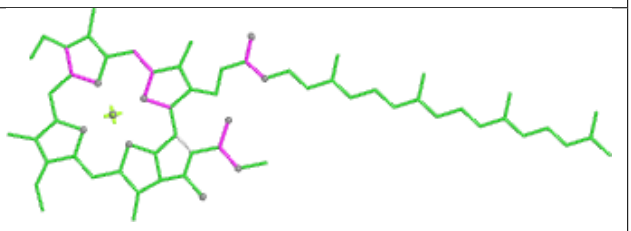
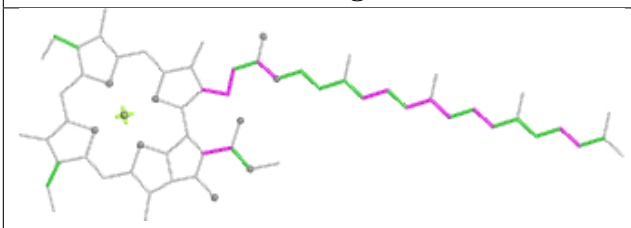
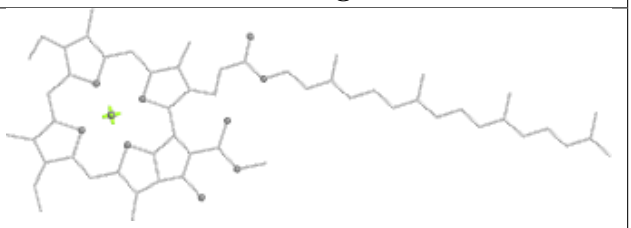


Torsions

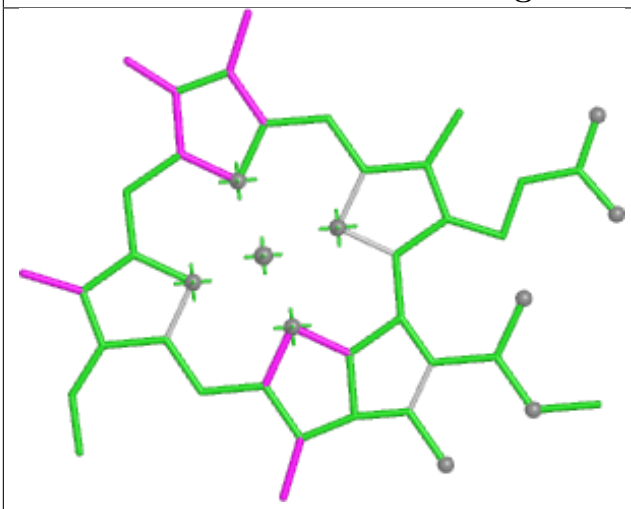


Rings

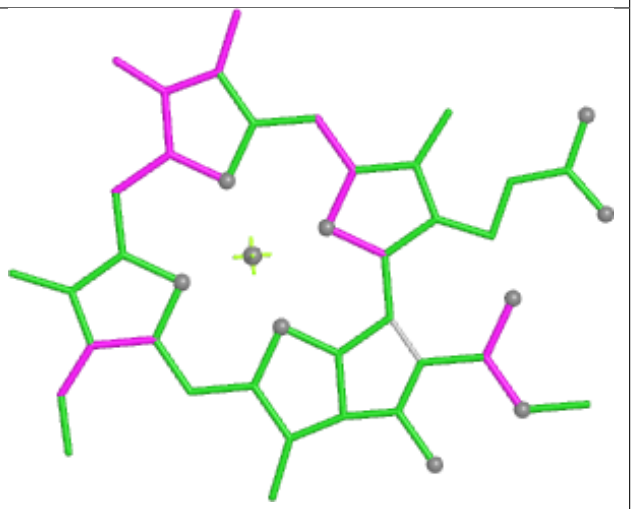
Ligand CLA AL 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA BA 827	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

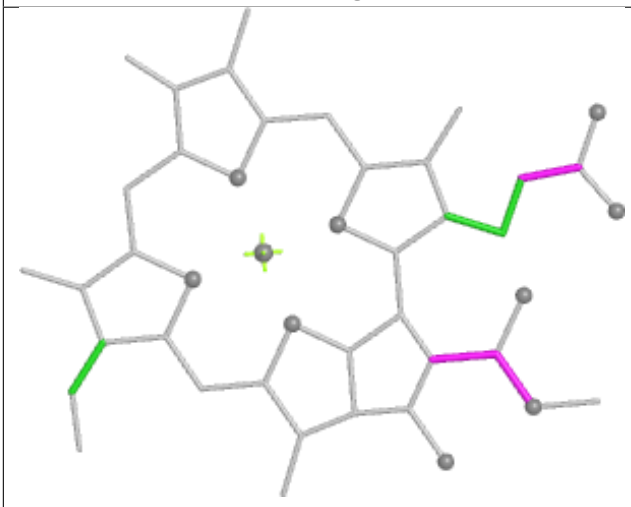
Ligand CLA A4 302



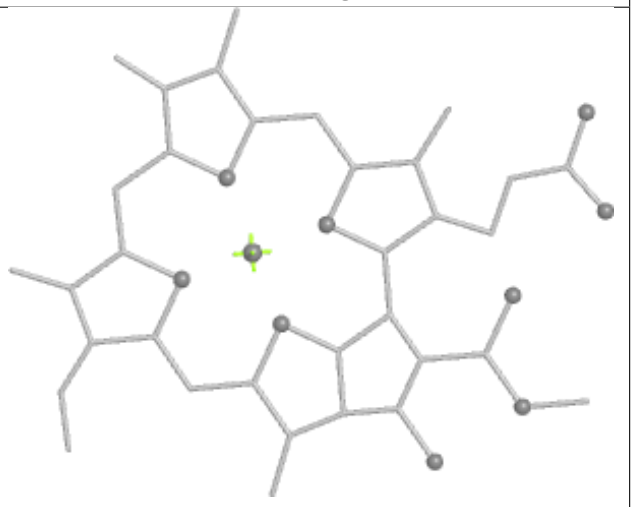
Bond lengths



Bond angles

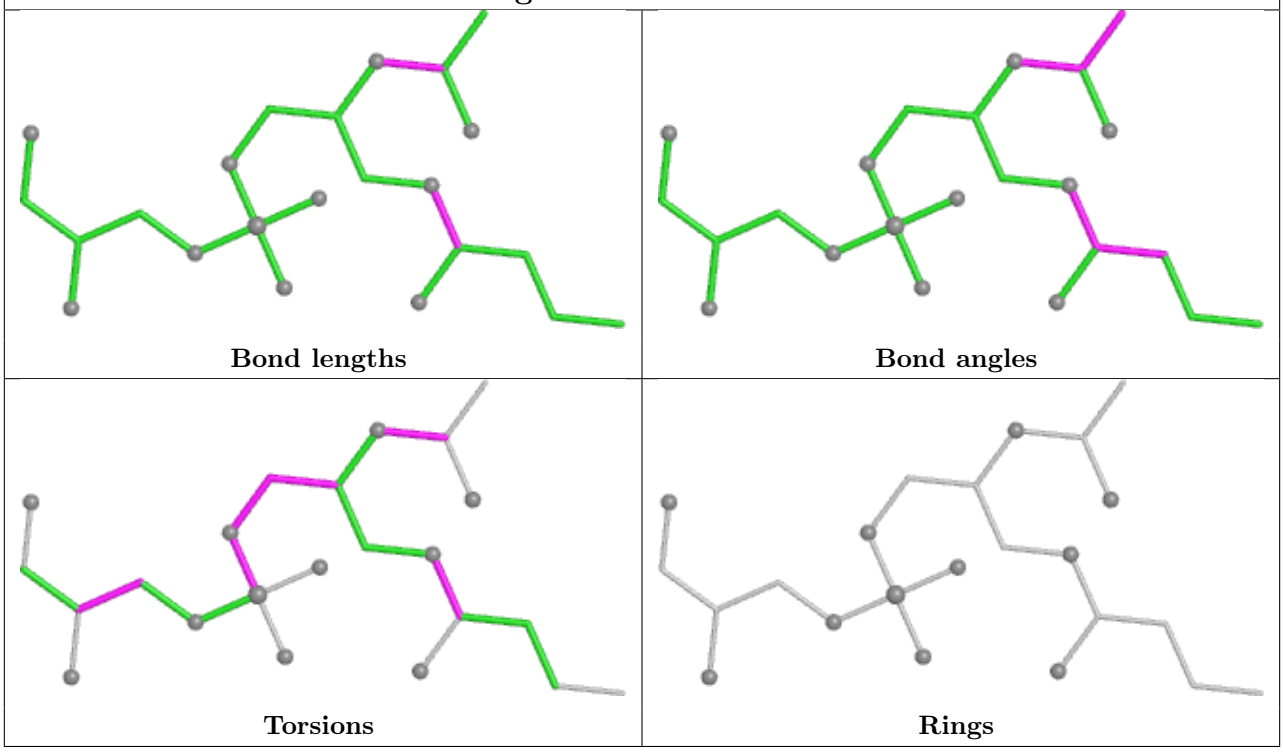


Torsions

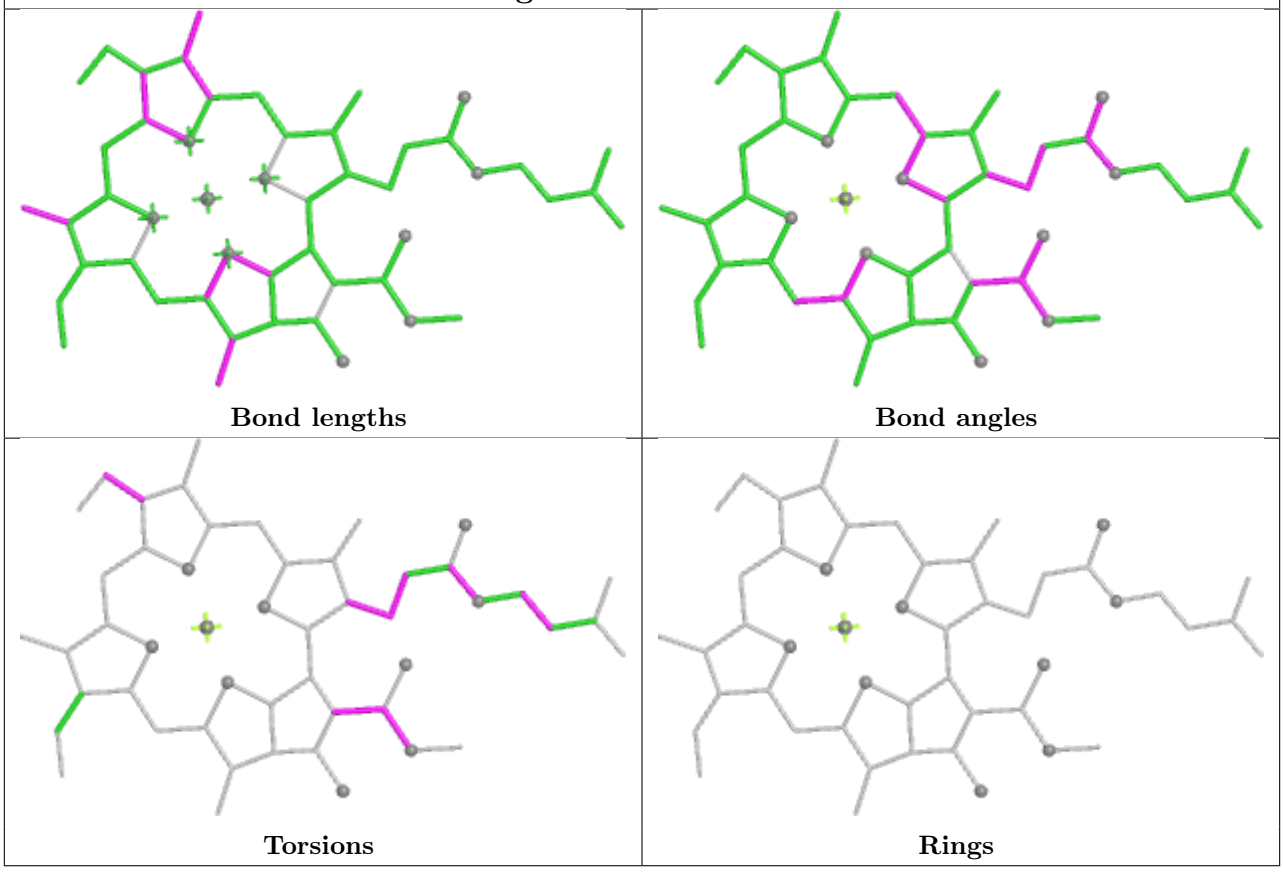


Rings

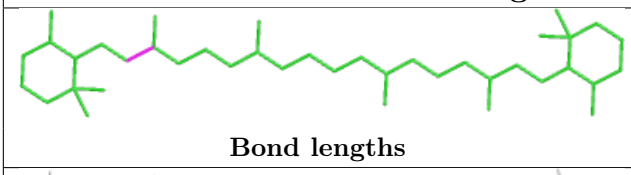
Ligand LHG B3 318



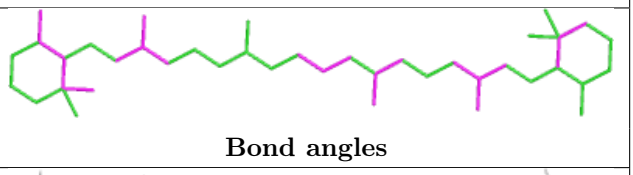
Ligand CLA A4 313



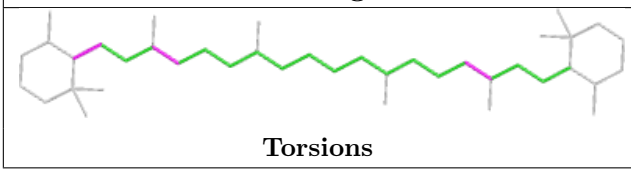
Ligand BCR BB 847



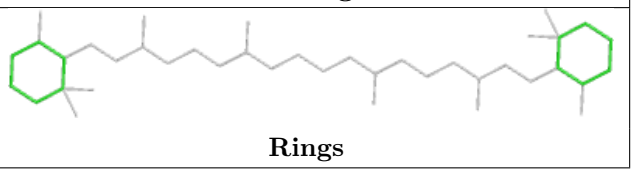
Bond lengths



Bond angles

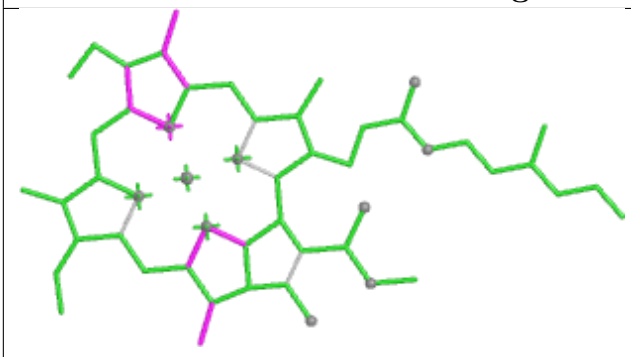


Torsions

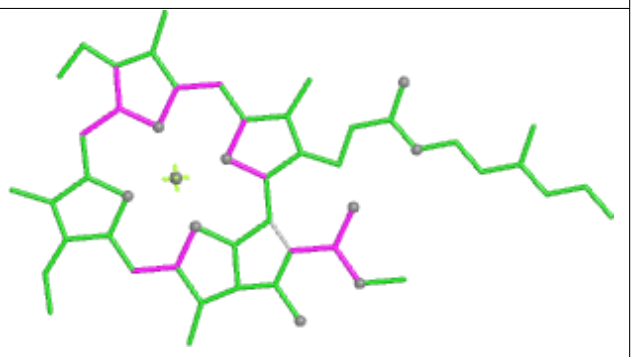


Rings

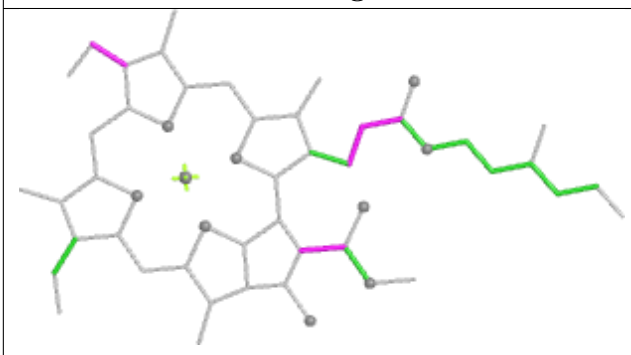
Ligand CLA BB 809



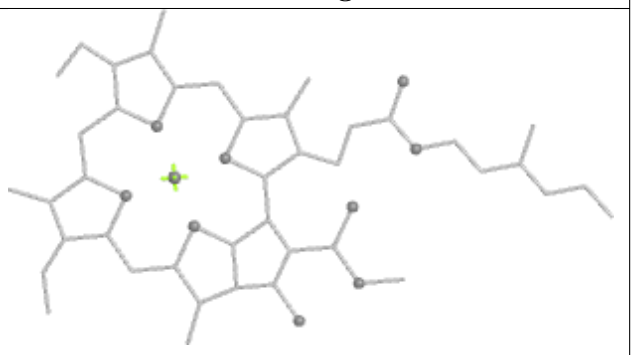
Bond lengths



Bond angles

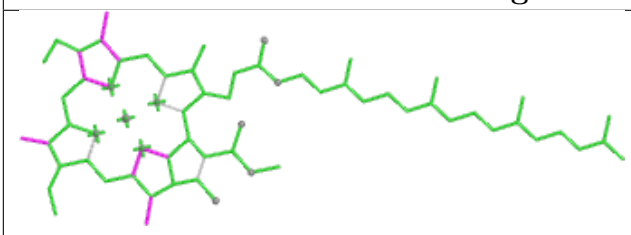


Torsions

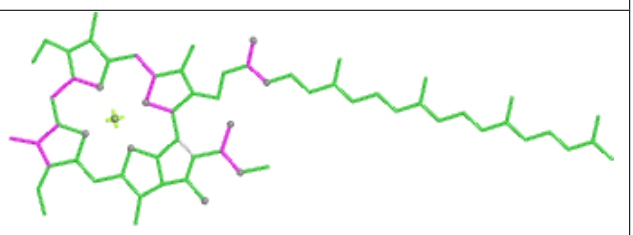


Rings

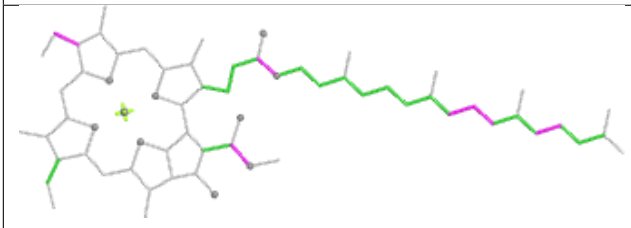
Ligand CLA AB 832



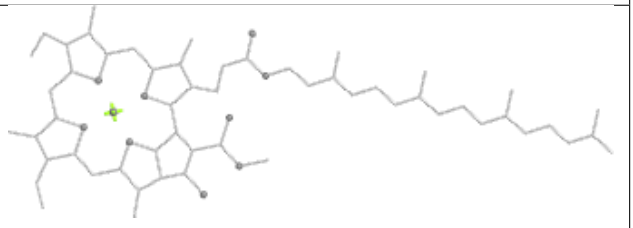
Bond lengths



Bond angles

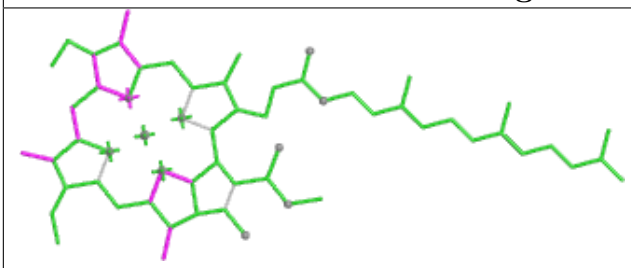


Torsions

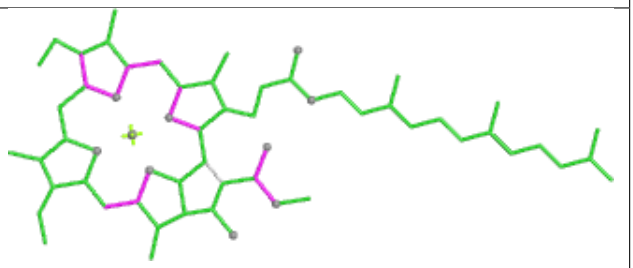


Rings

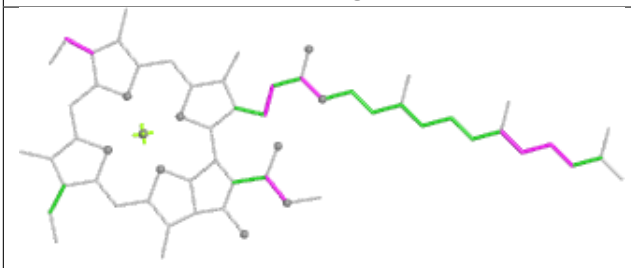
Ligand CLA B5 602



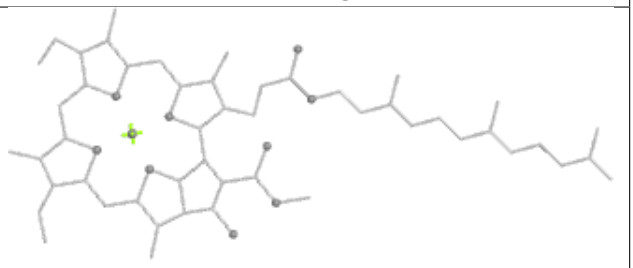
Bond lengths



Bond angles

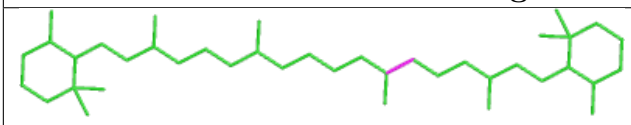


Torsions

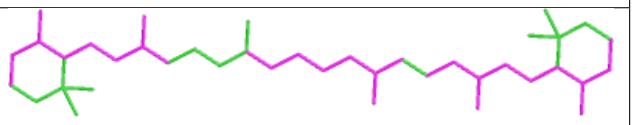


Rings

Ligand BCR BB 849



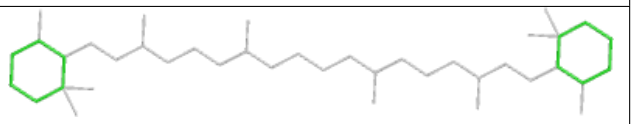
Bond lengths



Bond angles

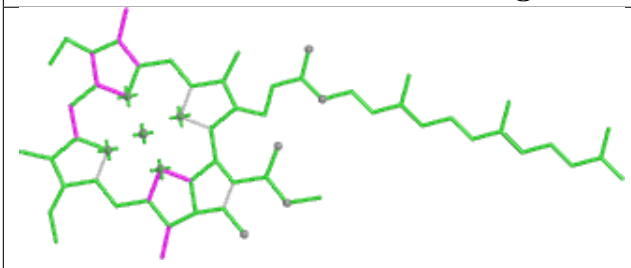


Torsions

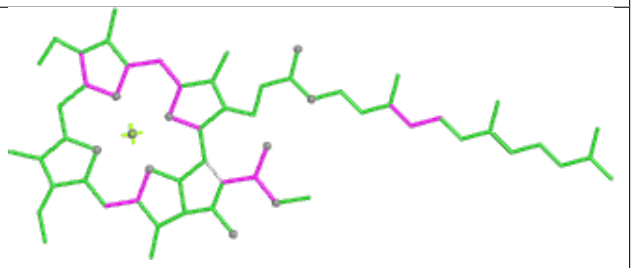


Rings

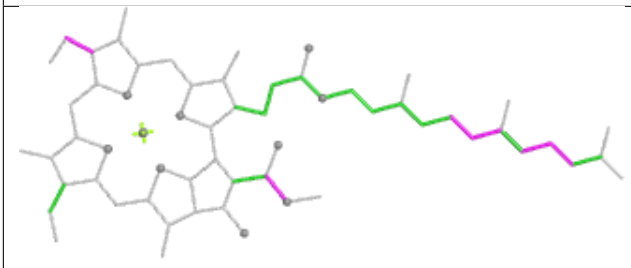
Ligand CLA A3 302



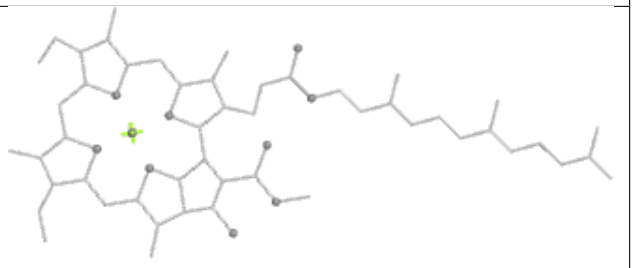
Bond lengths



Bond angles

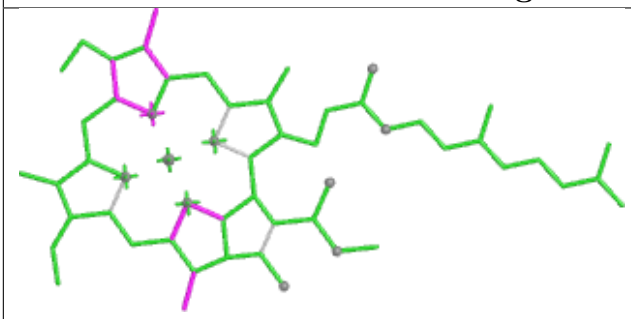


Torsions

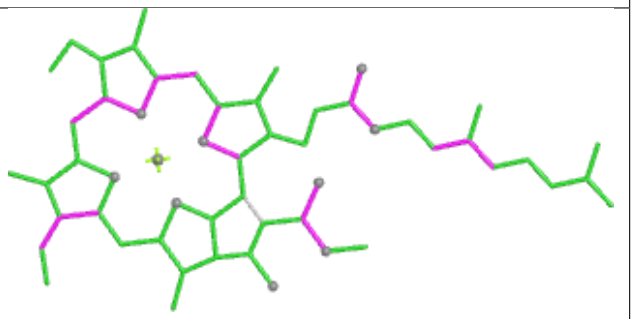


Rings

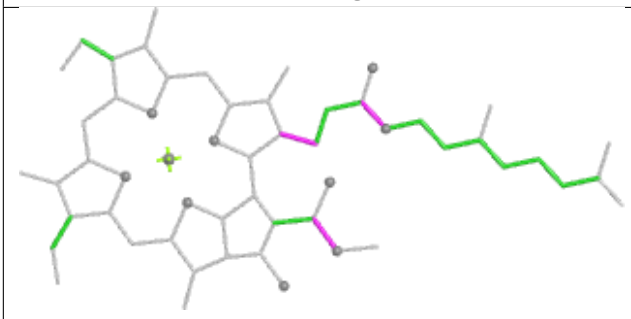
Ligand CLA B3 302



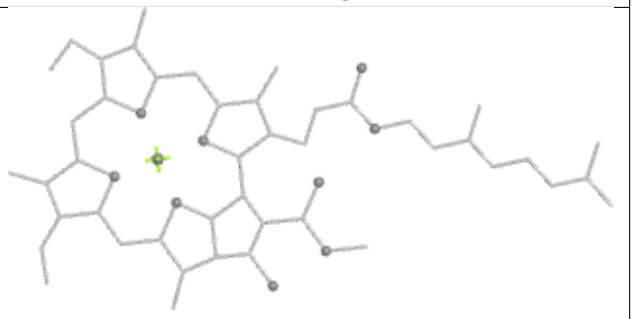
Bond lengths



Bond angles

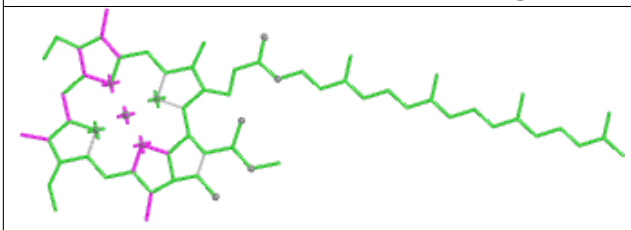


Torsions

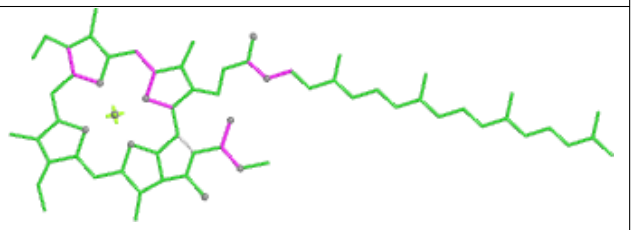


Rings

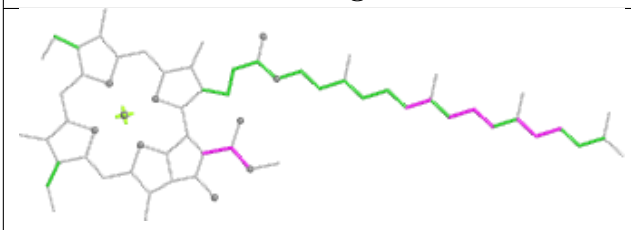
Ligand CLA BB 826



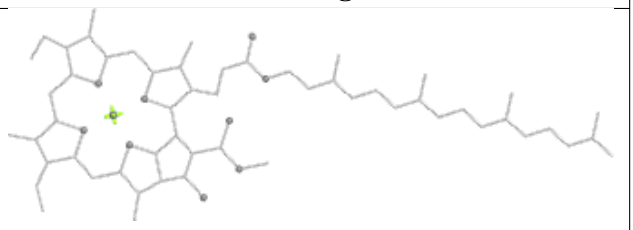
Bond lengths



Bond angles

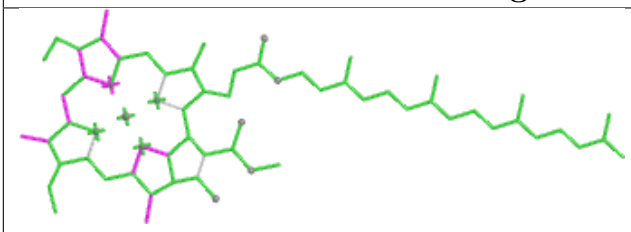


Torsions

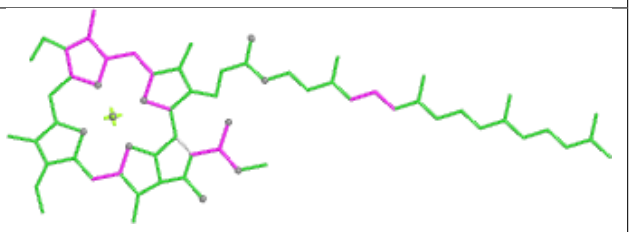


Rings

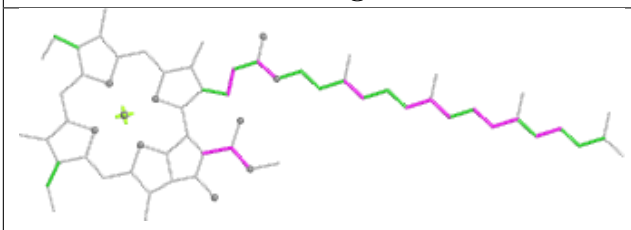
Ligand CLA AA 821



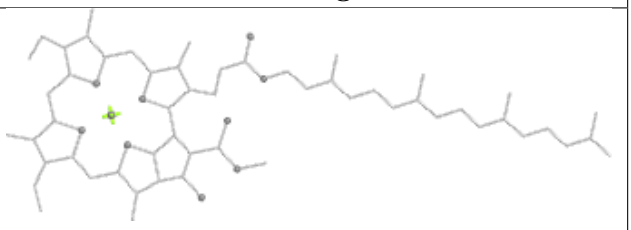
Bond lengths



Bond angles

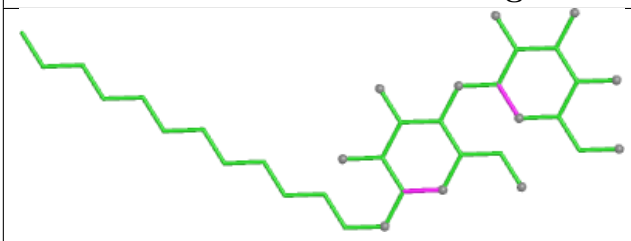


Torsions

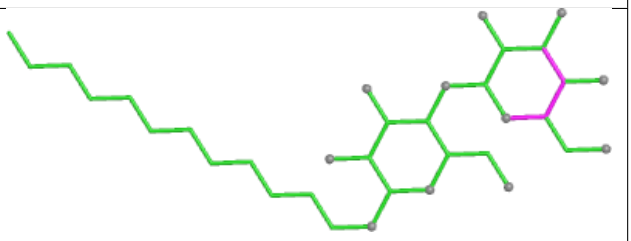


Rings

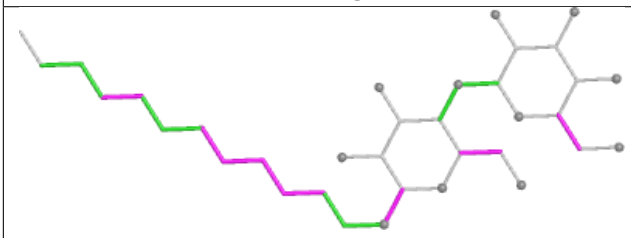
Ligand LMU AA 851



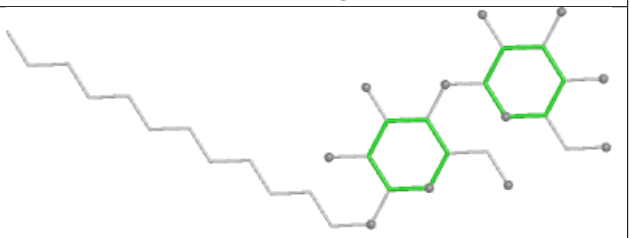
Bond lengths



Bond angles

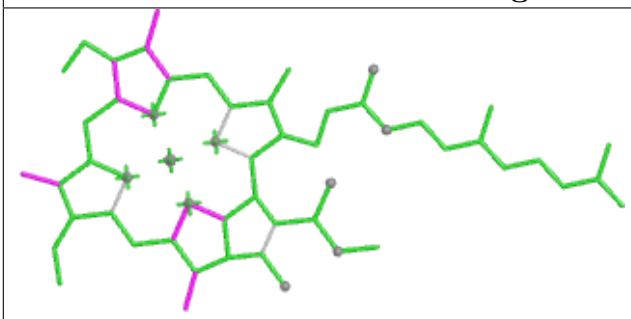


Torsions

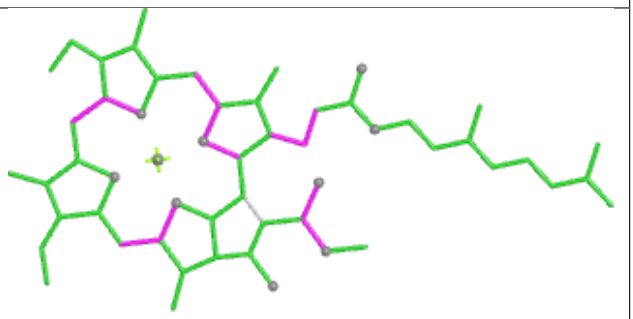


Rings

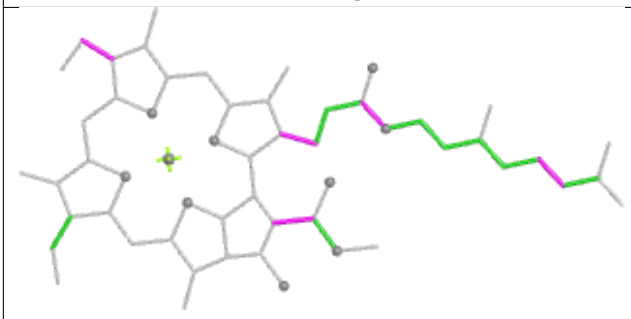
Ligand CLA BA 824



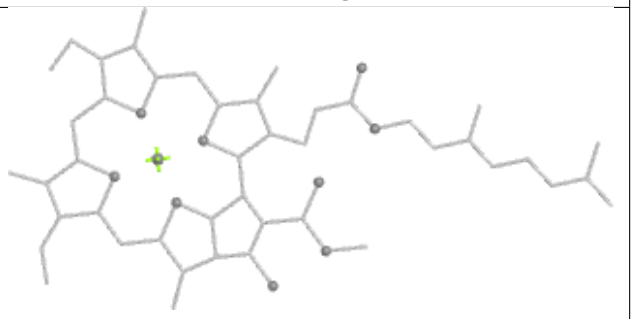
Bond lengths



Bond angles

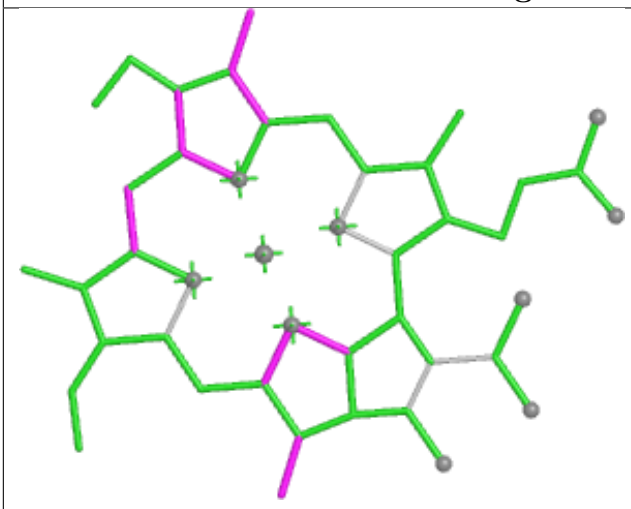


Torsions

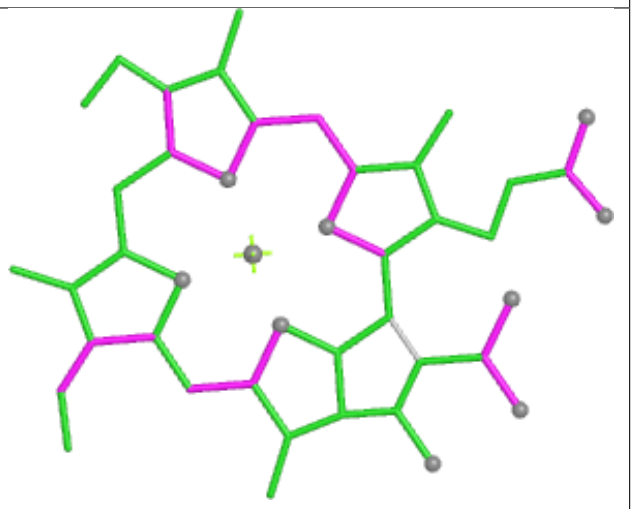


Rings

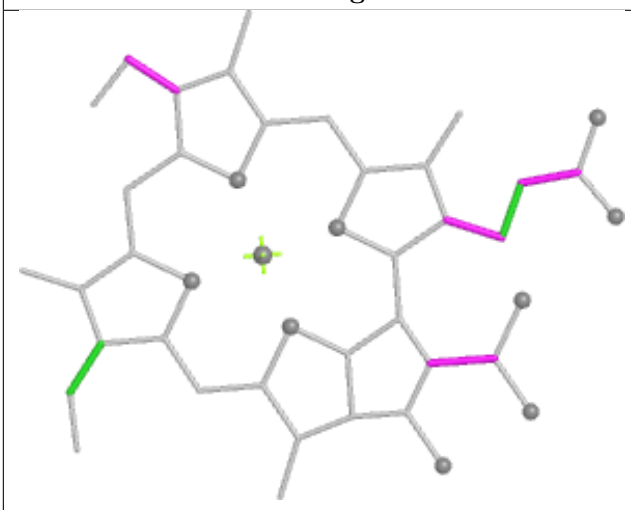
Ligand CLA A1 309



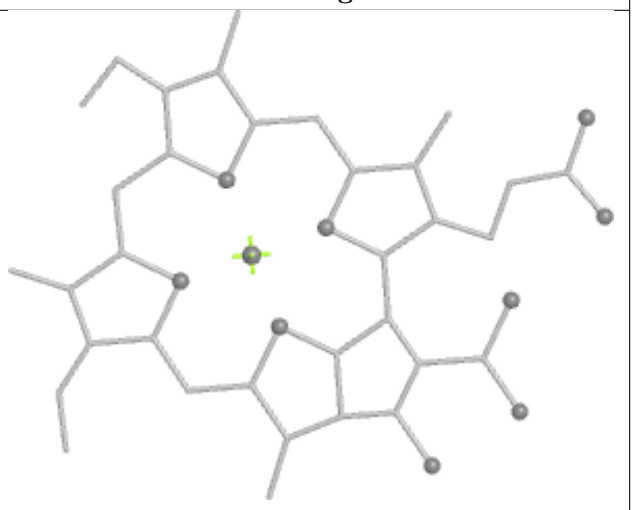
Bond lengths



Bond angles

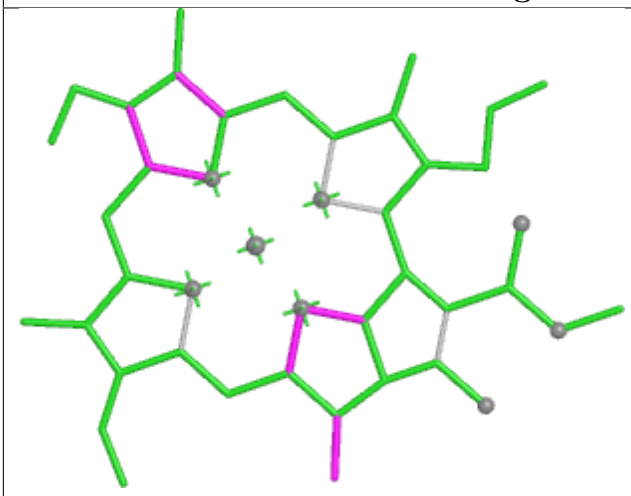


Torsions

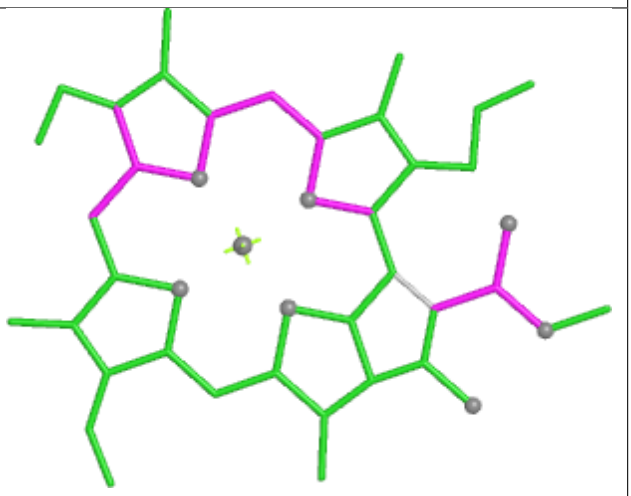


Rings

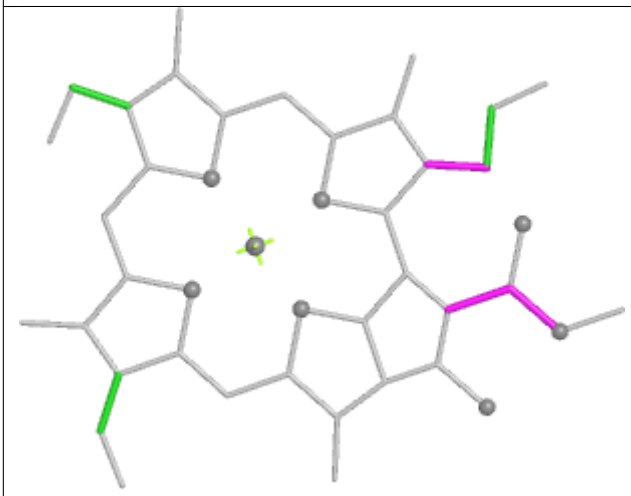
Ligand CLA BL 304



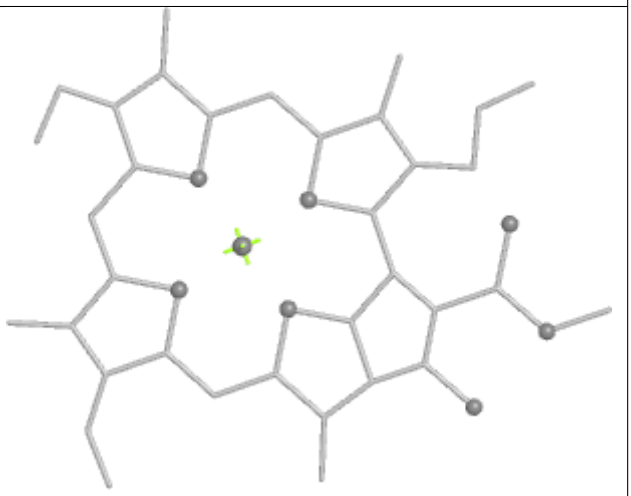
Bond lengths



Bond angles

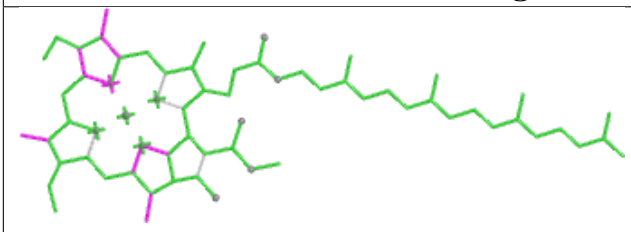


Torsions

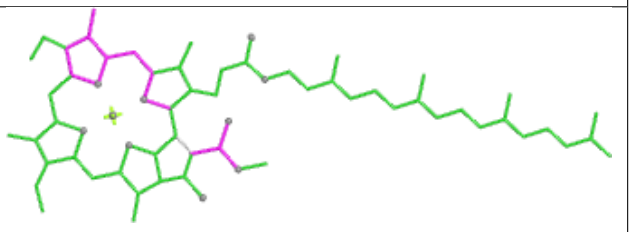


Rings

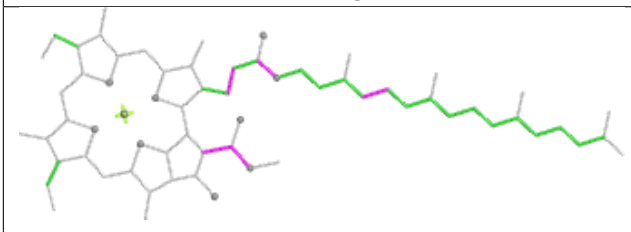
Ligand CLA BB 841



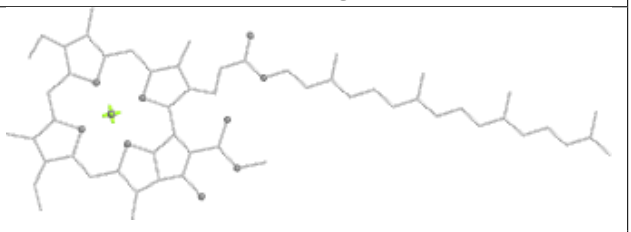
Bond lengths



Bond angles

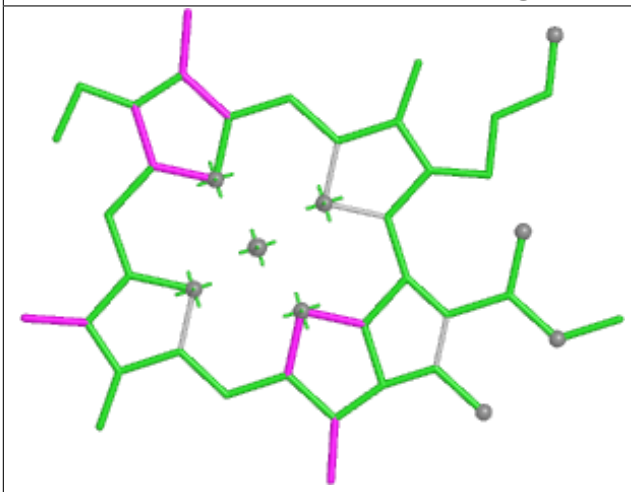


Torsions

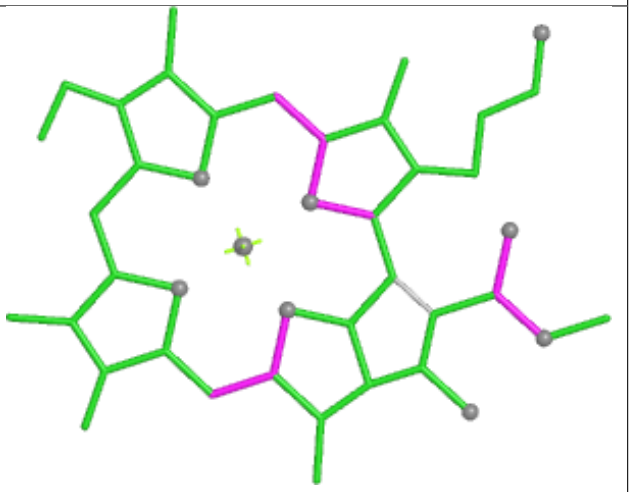


Rings

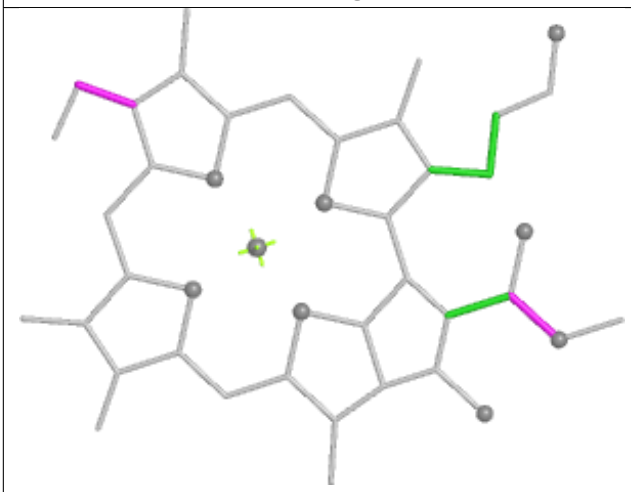
Ligand CLA A6 605



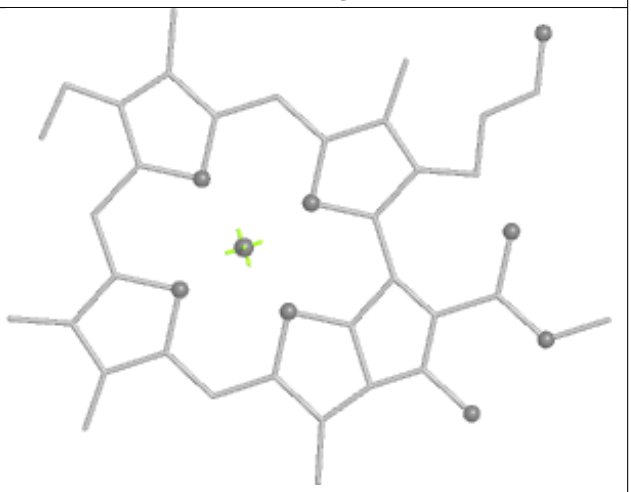
Bond lengths



Bond angles

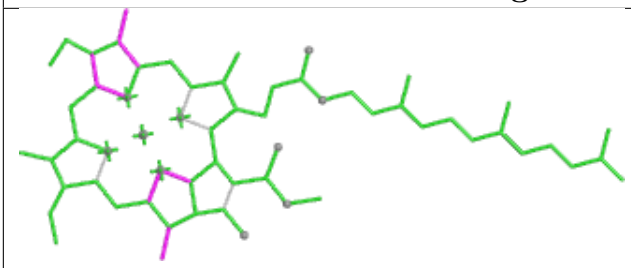


Torsions

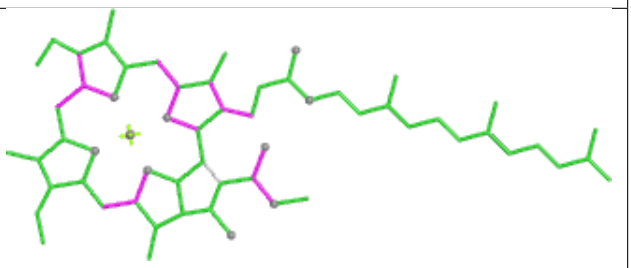


Rings

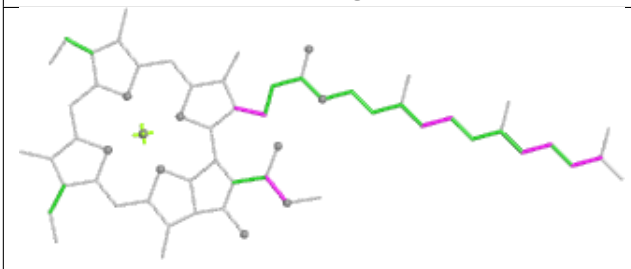
Ligand CLA AB 835



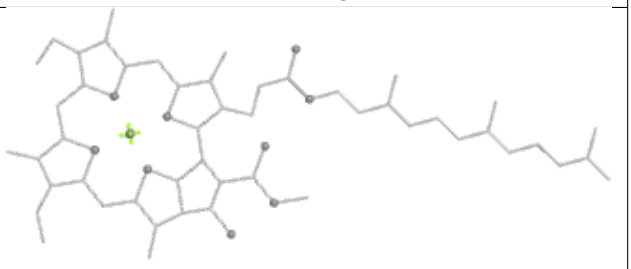
Bond lengths



Bond angles

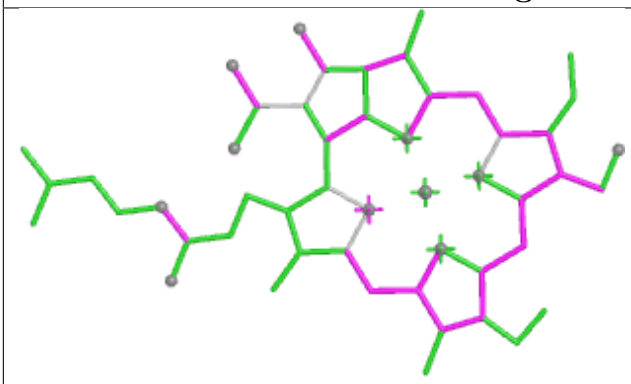


Torsions

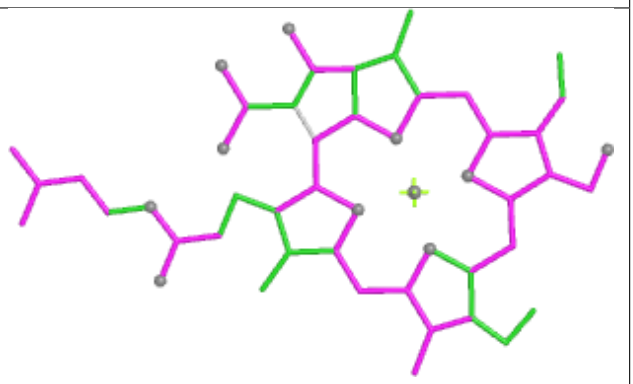


Rings

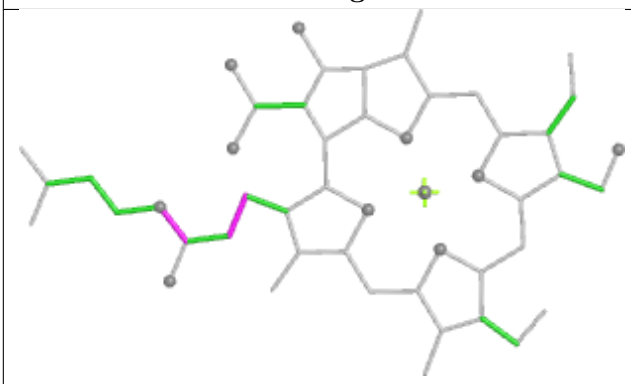
Ligand CHL B1 303



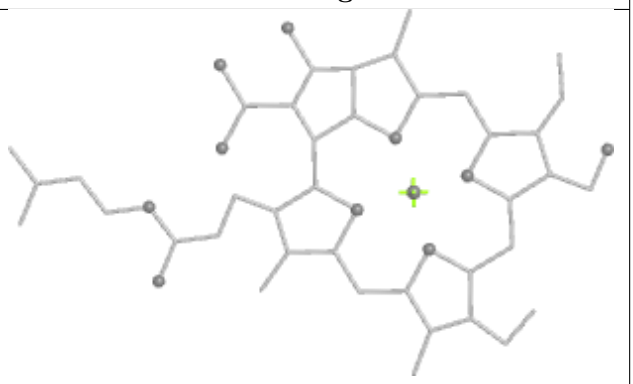
Bond lengths



Bond angles

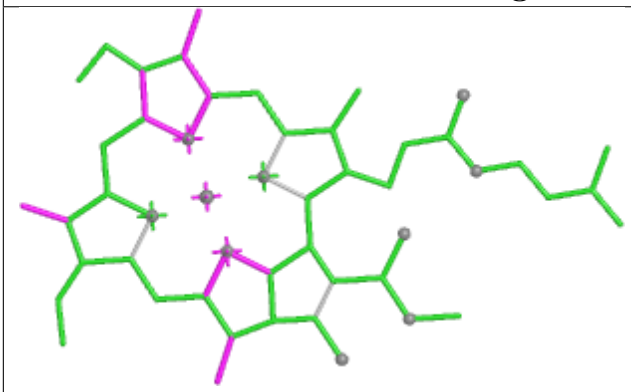


Torsions

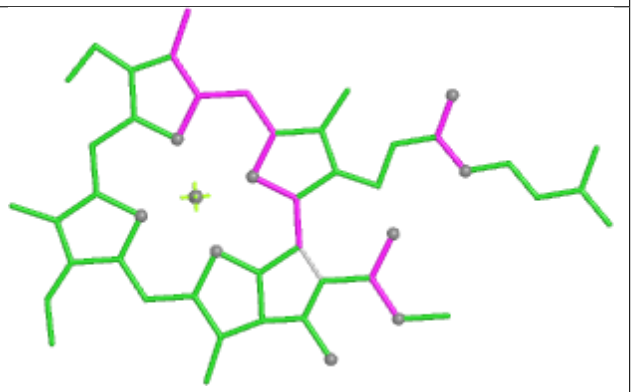


Rings

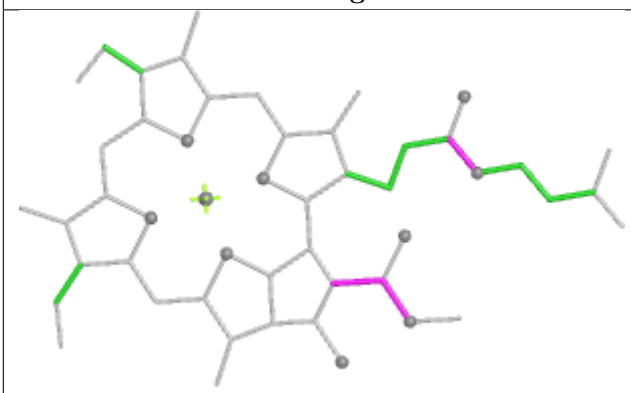
Ligand CLA AB 837



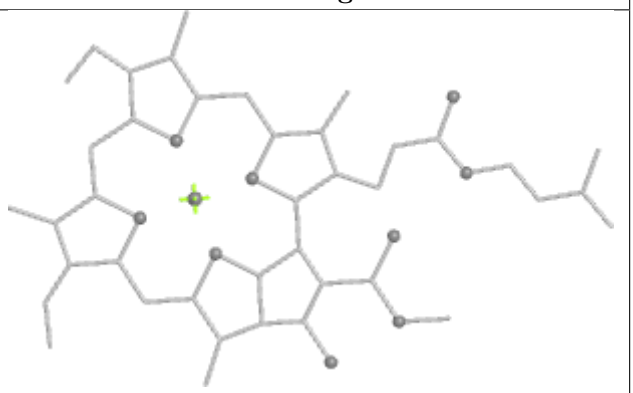
Bond lengths



Bond angles

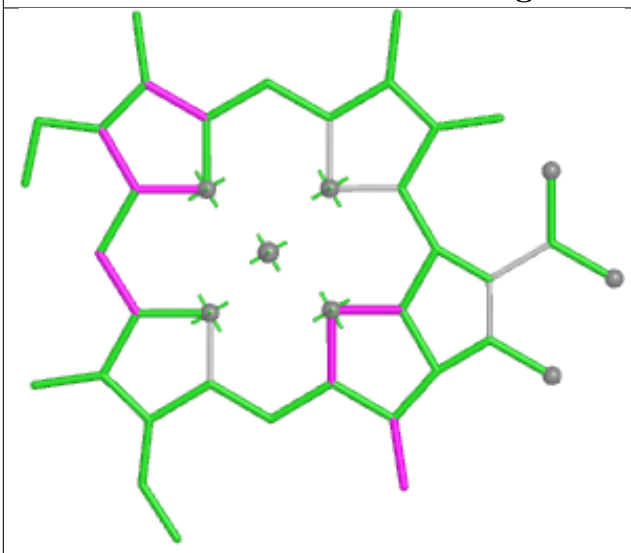


Torsions

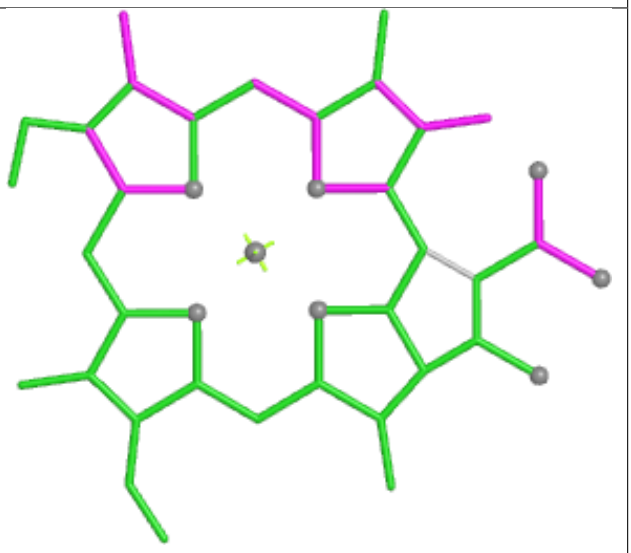


Rings

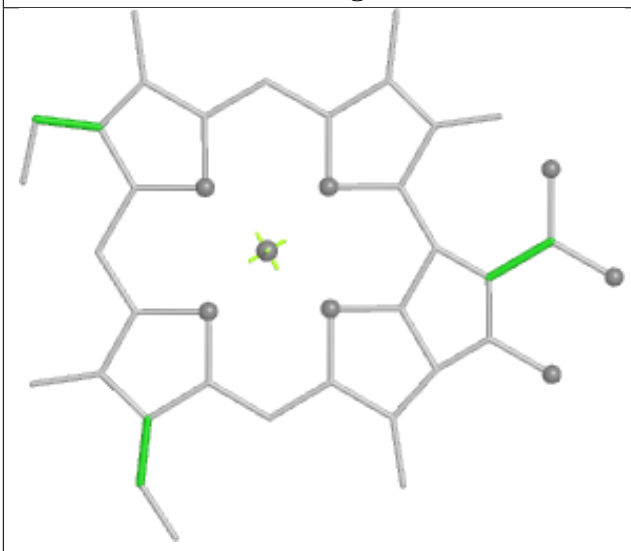
Ligand CLA B3 314



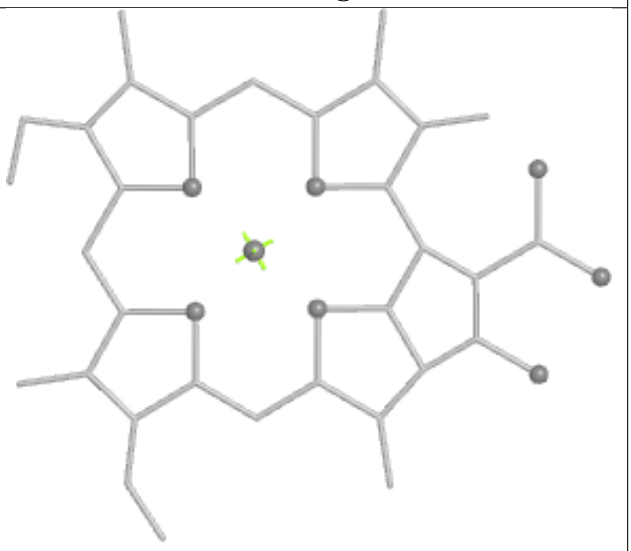
Bond lengths



Bond angles

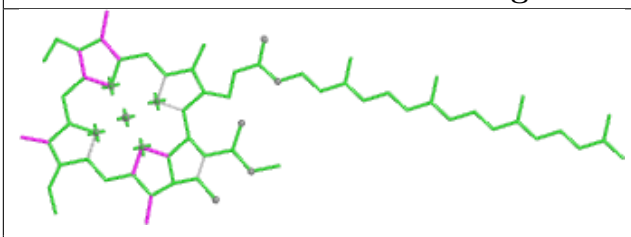


Torsions

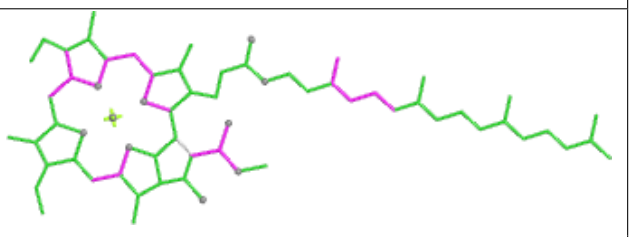


Rings

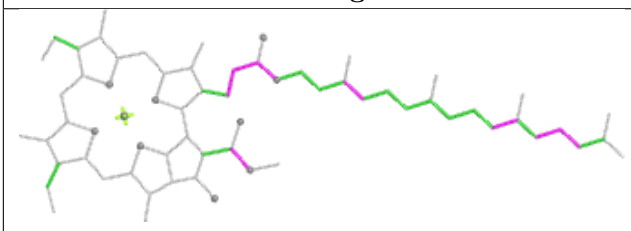
Ligand CLA BA 821



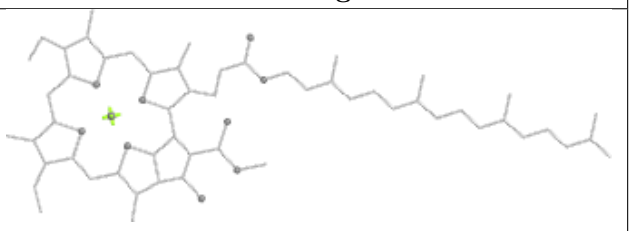
Bond lengths



Bond angles

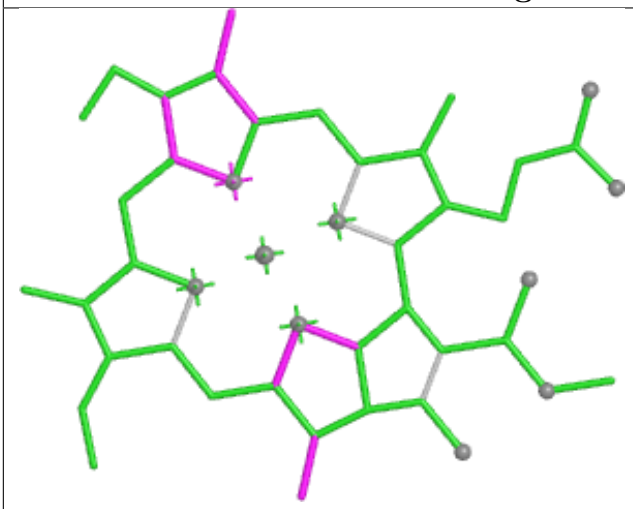


Torsions

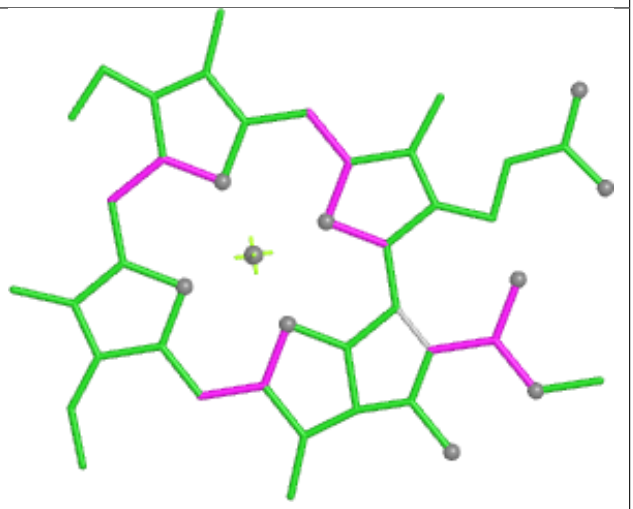


Rings

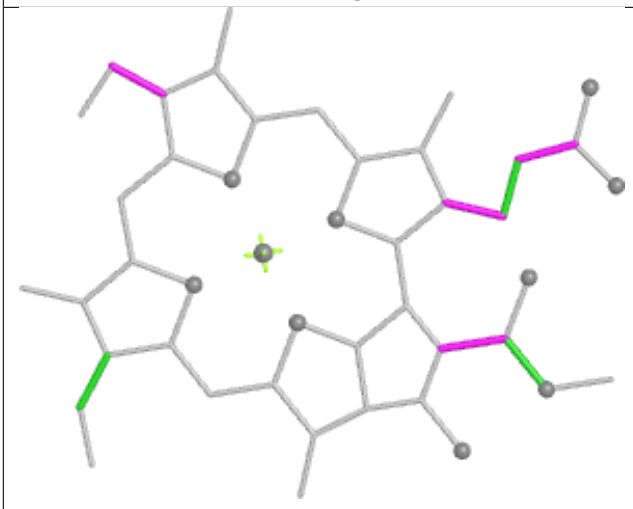
Ligand CLA A3 308



Bond lengths



Bond angles

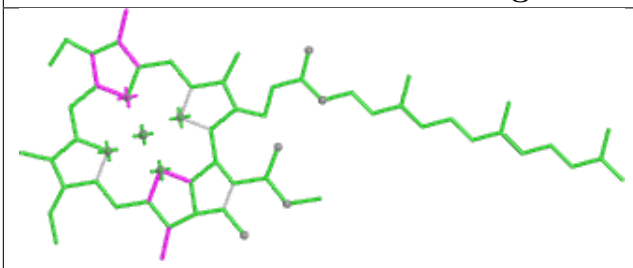


Torsions

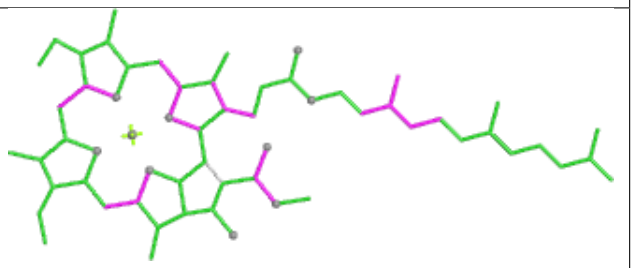


Rings

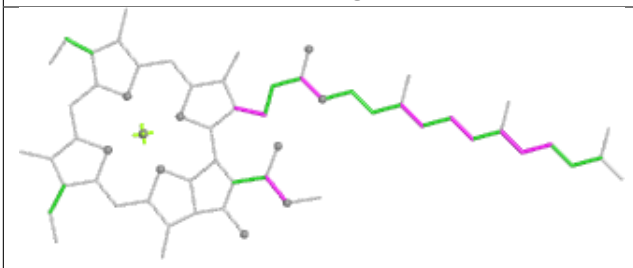
Ligand CLA BB 820



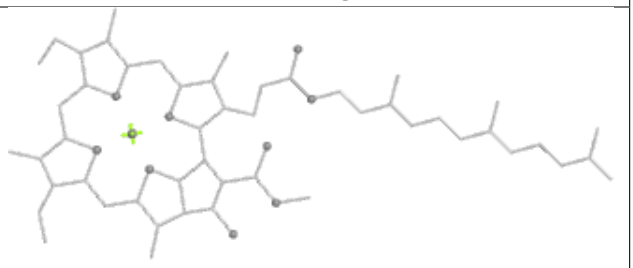
Bond lengths



Bond angles

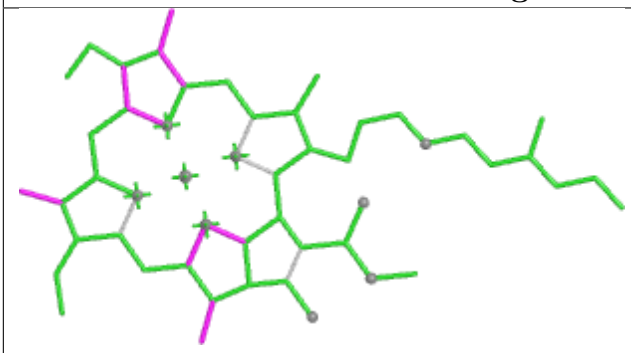


Torsions

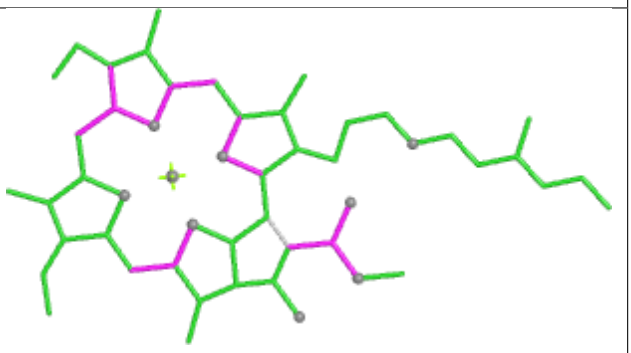


Rings

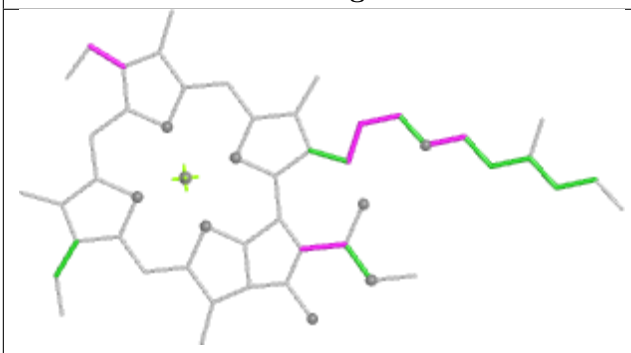
Ligand CLA AB 808



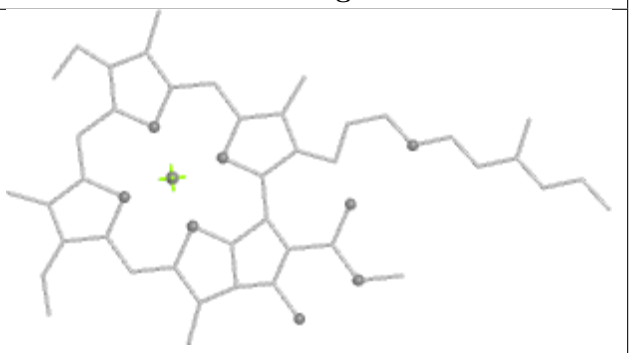
Bond lengths



Bond angles

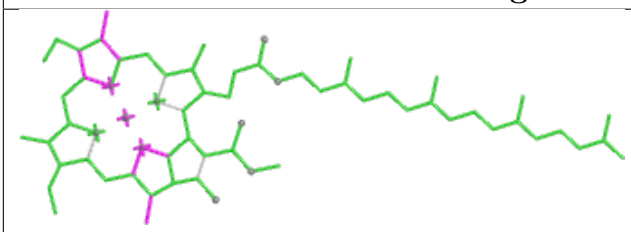


Torsions

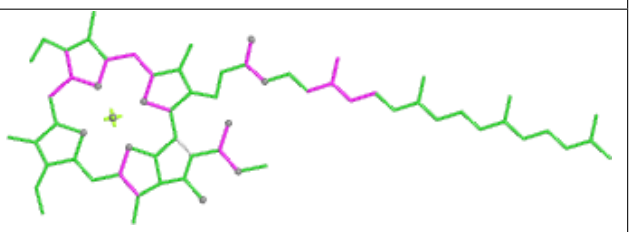


Rings

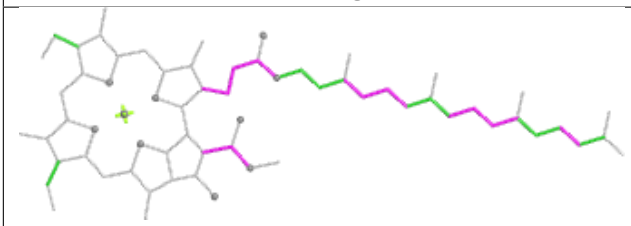
Ligand CLA AA 829



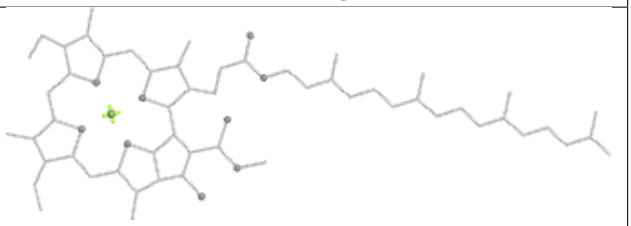
Bond lengths



Bond angles

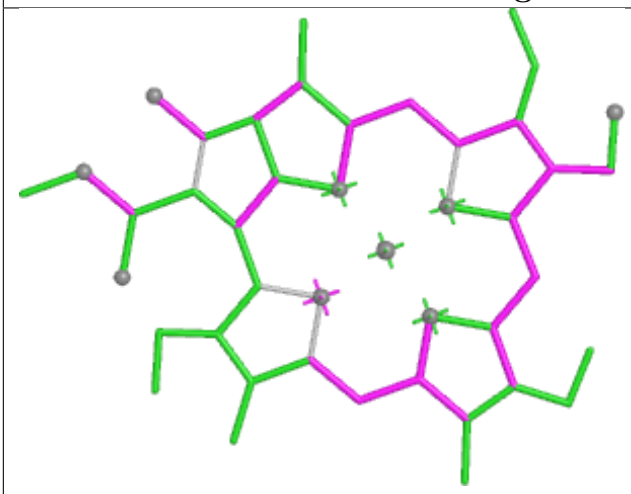


Torsions

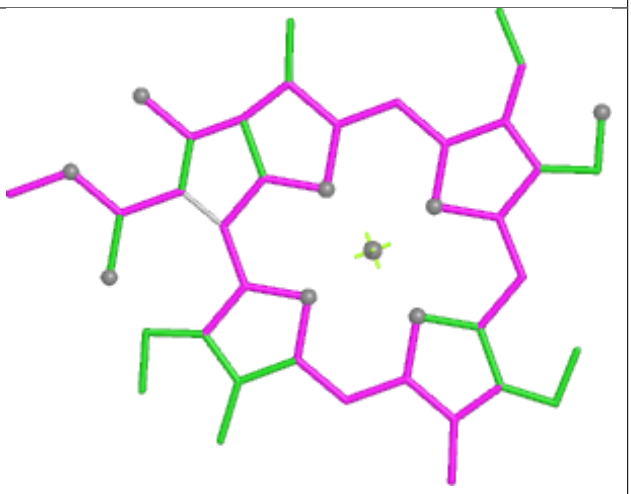


Rings

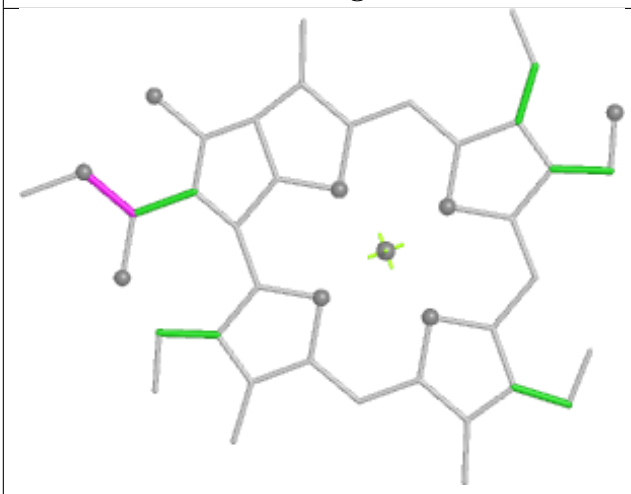
Ligand CHL A6 607



Bond lengths



Bond angles

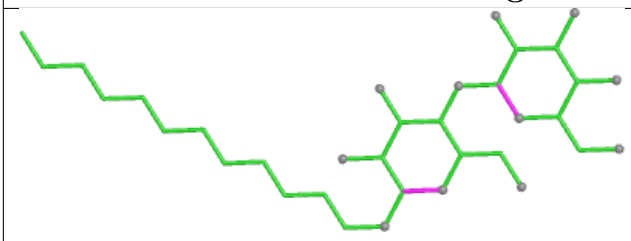


Torsions

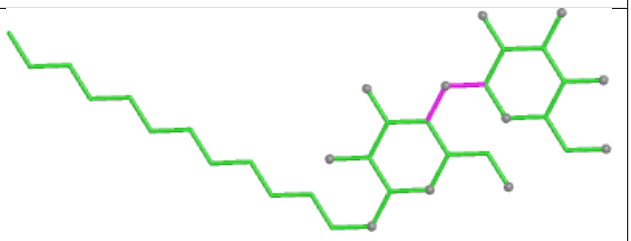


Rings

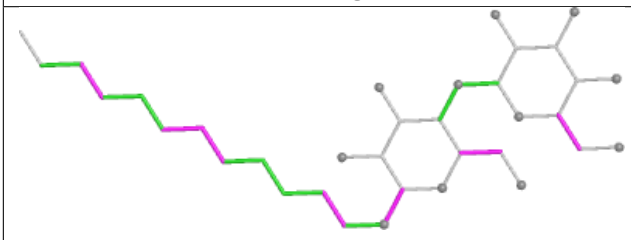
Ligand LMU AB 852



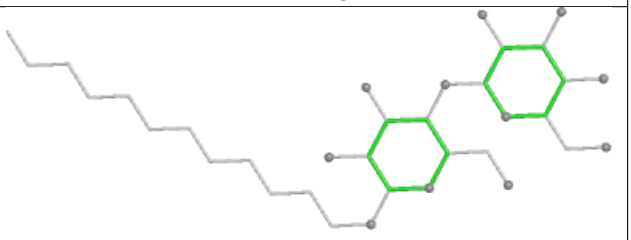
Bond lengths



Bond angles

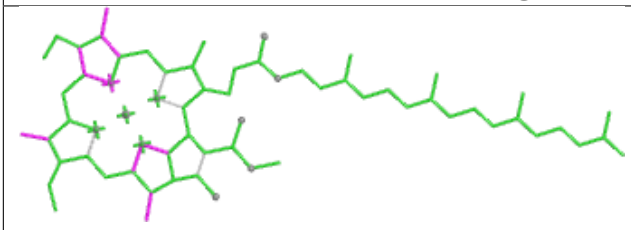


Torsions

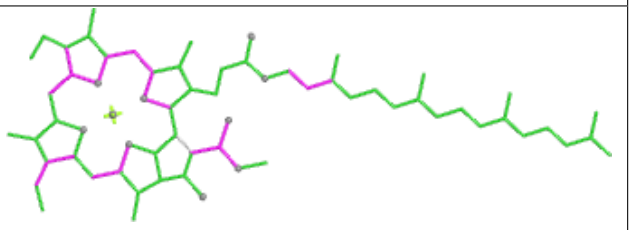


Rings

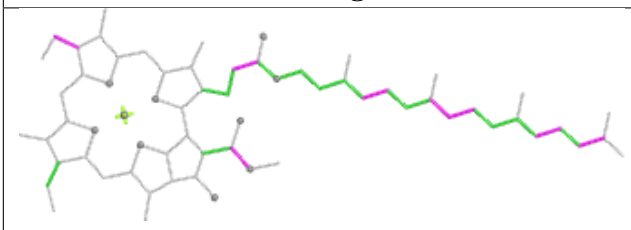
Ligand CLA B2 602



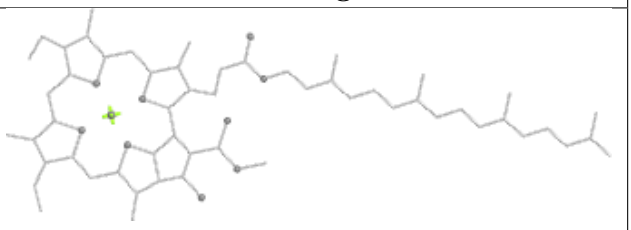
Bond lengths



Bond angles

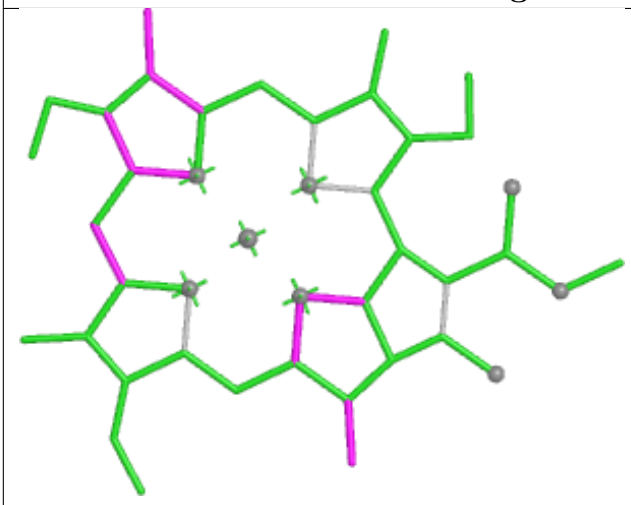


Torsions

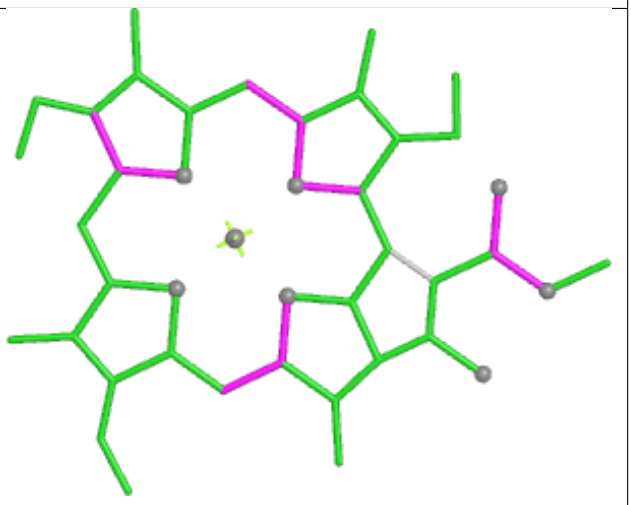


Rings

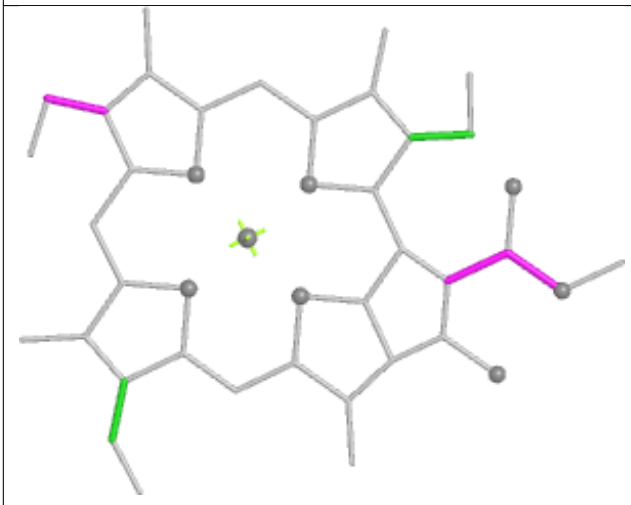
Ligand CLA AG 203



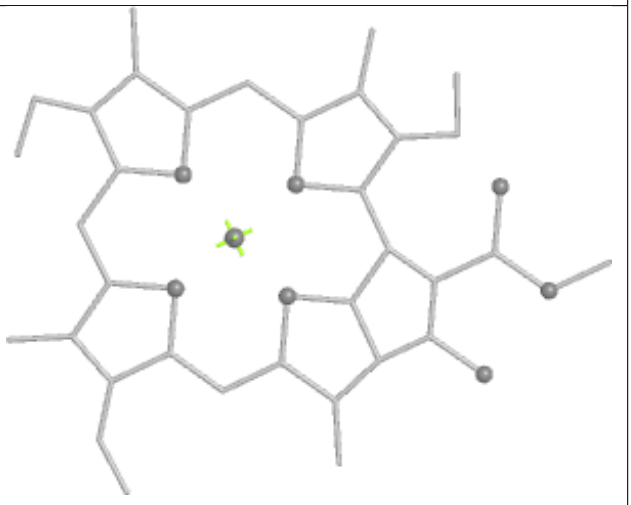
Bond lengths



Bond angles

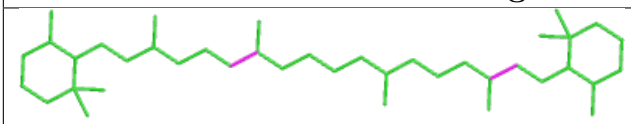


Torsions

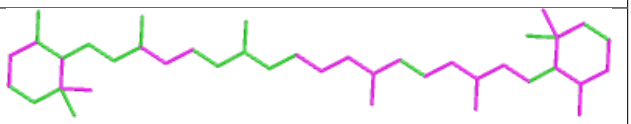


Rings

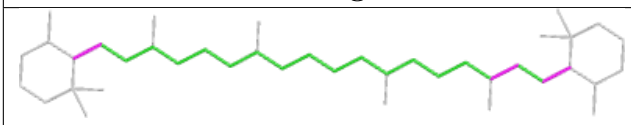
Ligand BCR AA 852



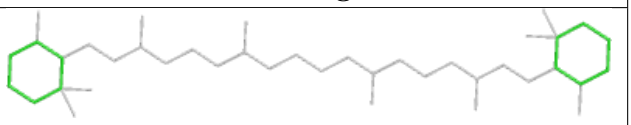
Bond lengths



Bond angles

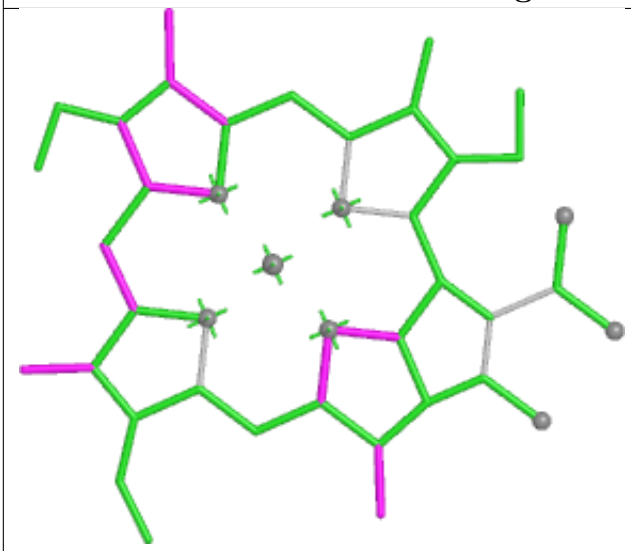


Torsions



Rings

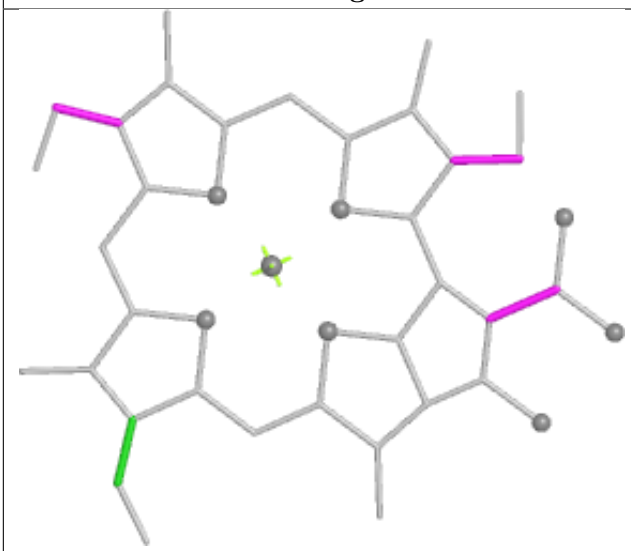
Ligand CLA A4 310



Bond lengths



Bond angles

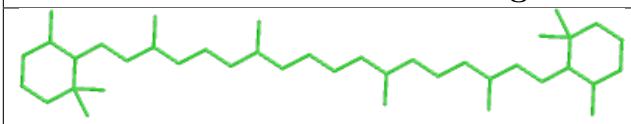


Torsions

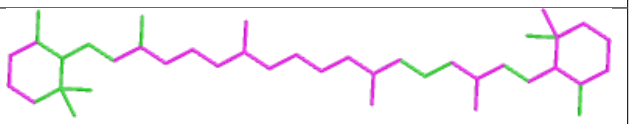


Rings

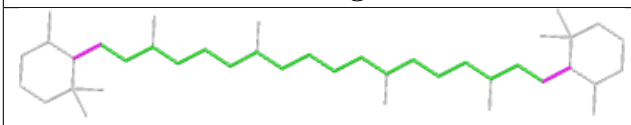
Ligand BCR BB 803



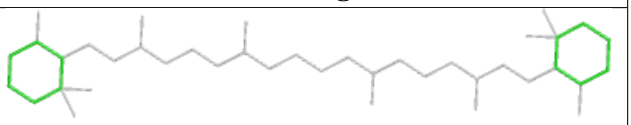
Bond lengths



Bond angles

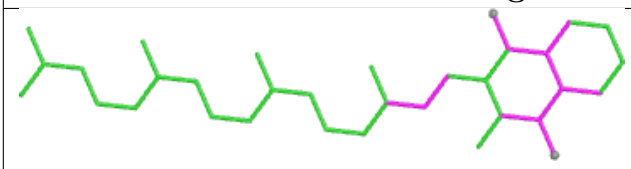


Torsions

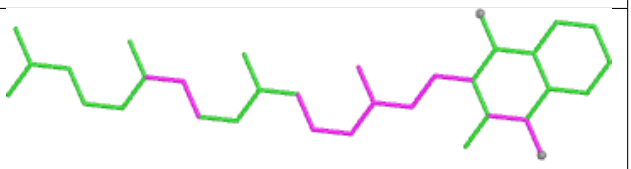


Rings

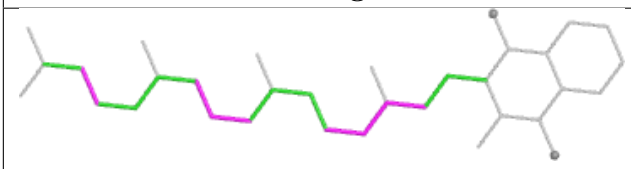
Ligand PQN AA 843



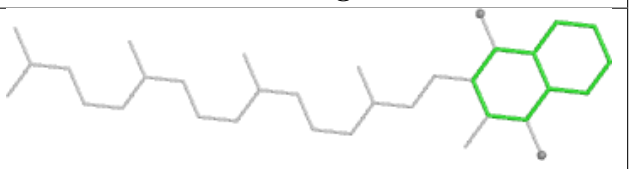
Bond lengths



Bond angles

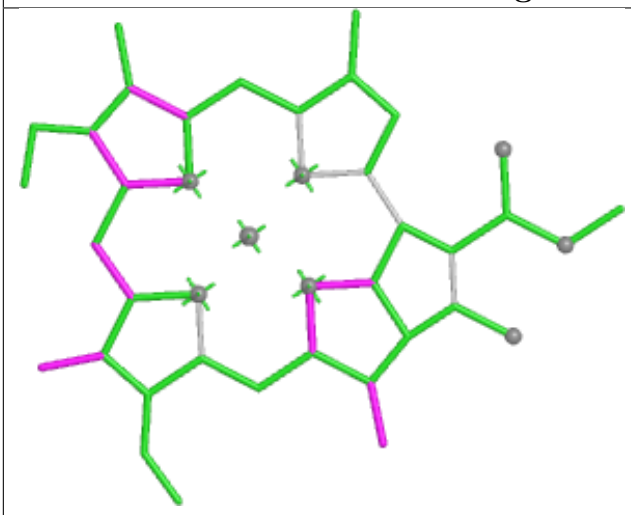


Torsions

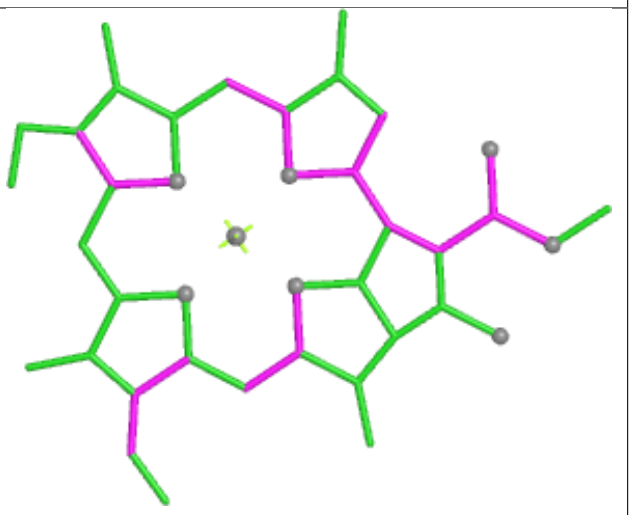


Rings

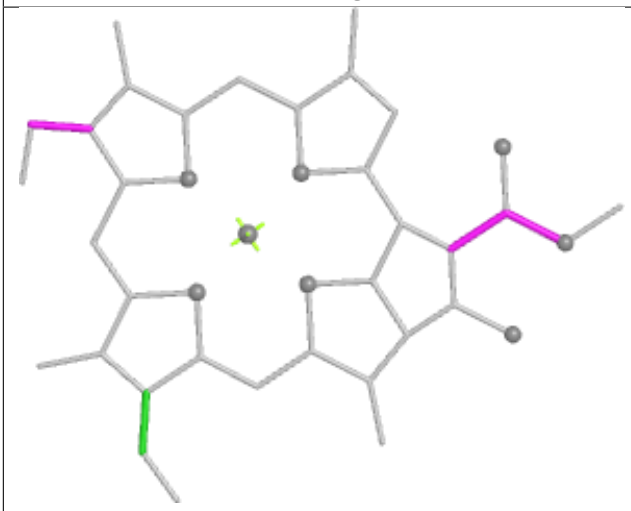
Ligand CLA A1 307



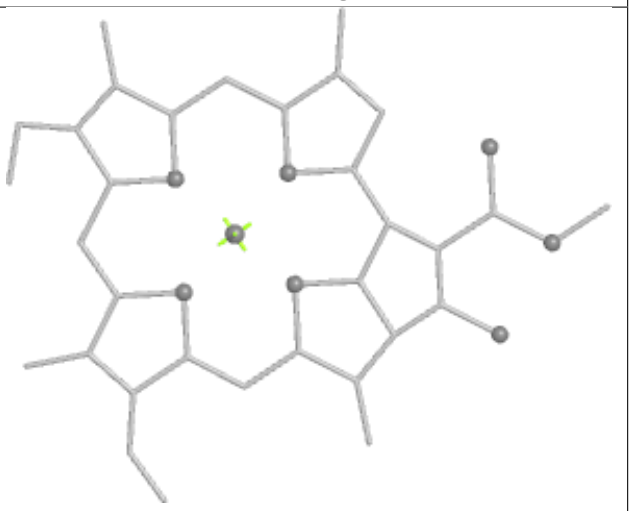
Bond lengths



Bond angles

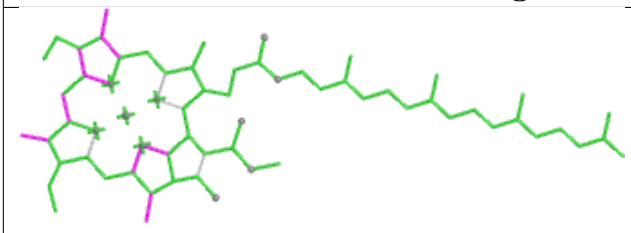


Torsions

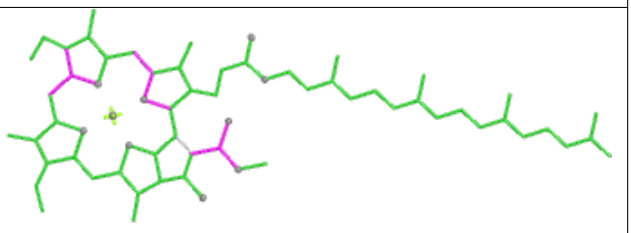


Rings

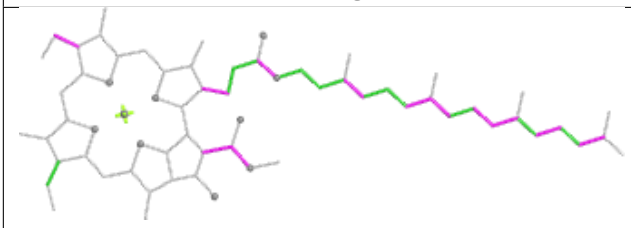
Ligand CLA AB 803



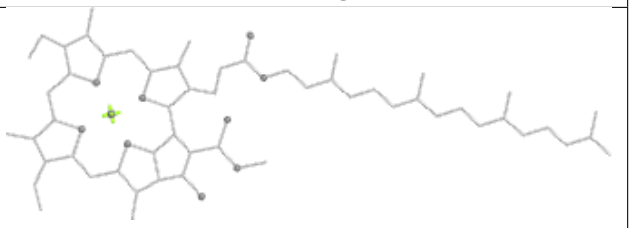
Bond lengths



Bond angles

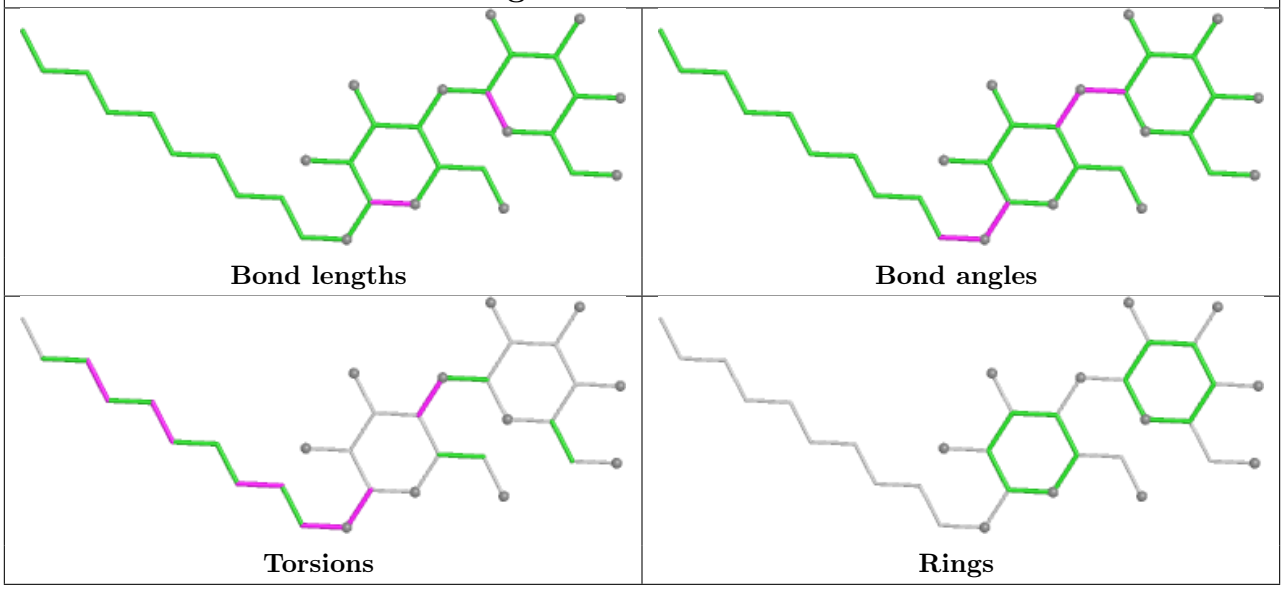


Torsions

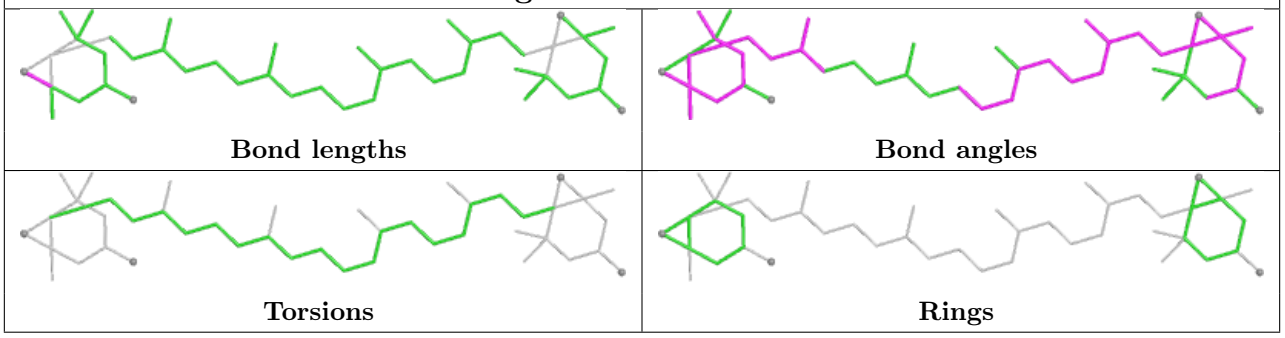


Rings

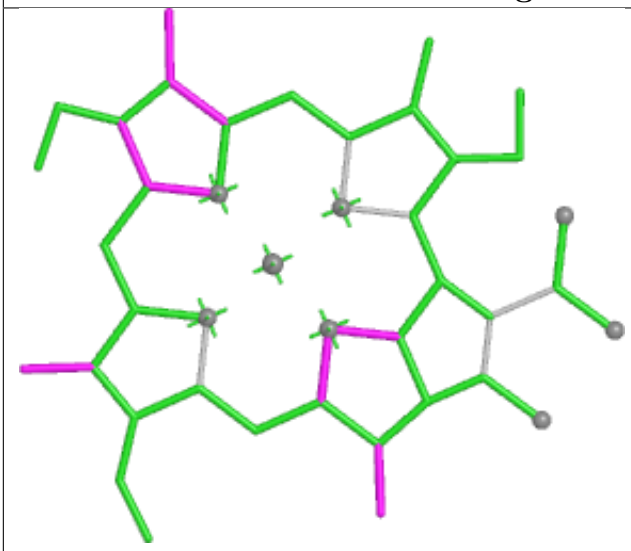
Ligand LMU BA 854



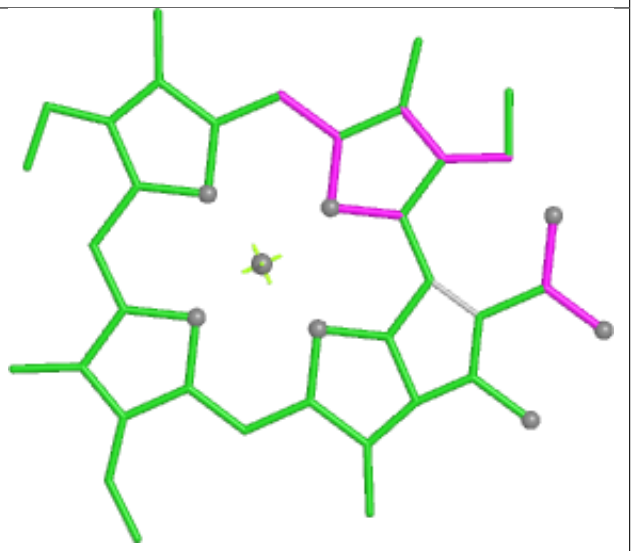
Ligand XAT A3 317



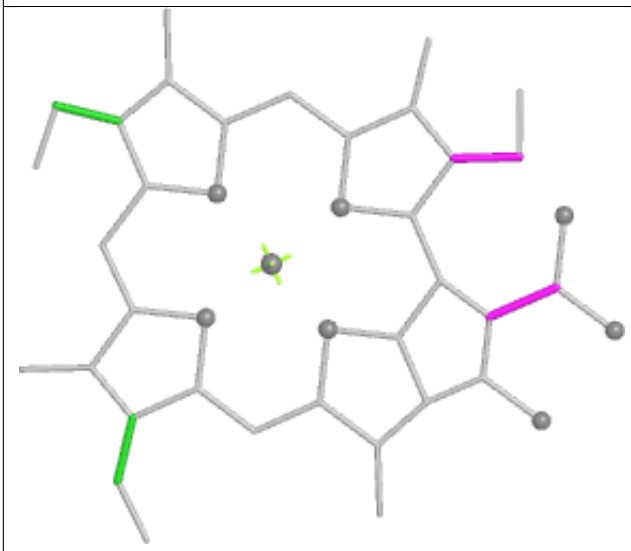
Ligand CLA B5 611



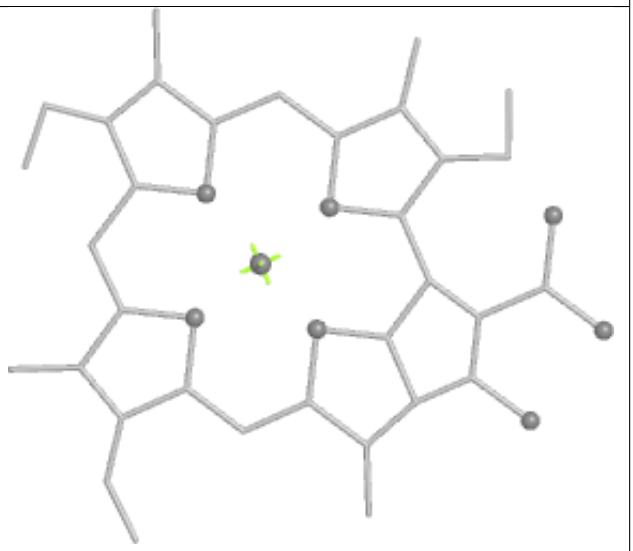
Bond lengths



Bond angles

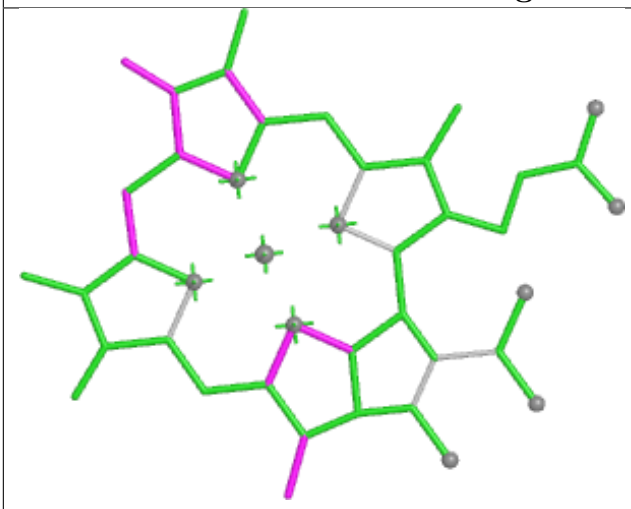


Torsions

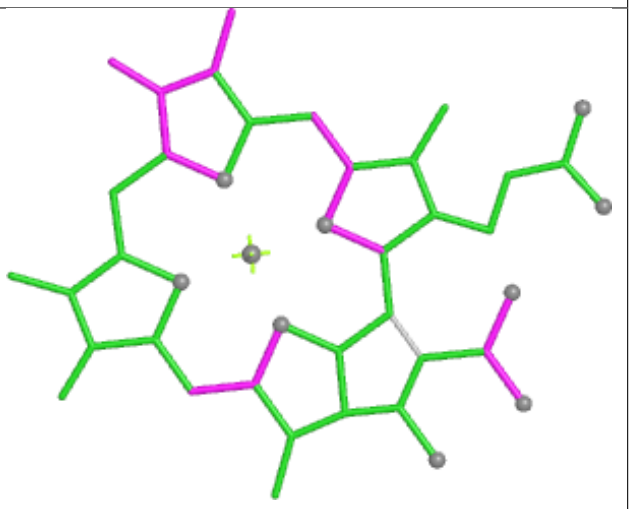


Rings

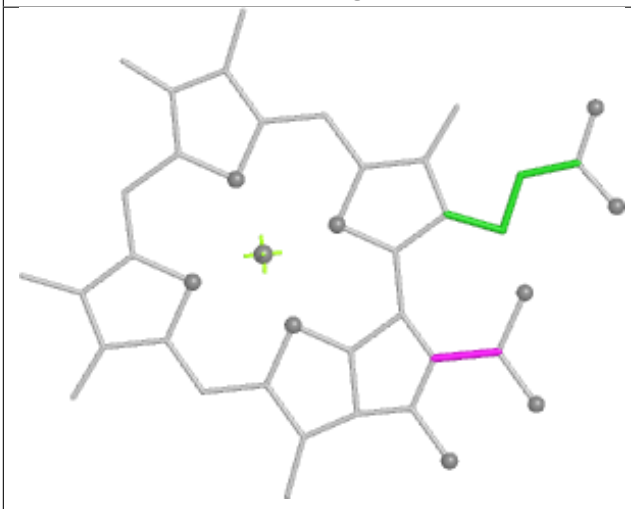
Ligand CLA B3 303



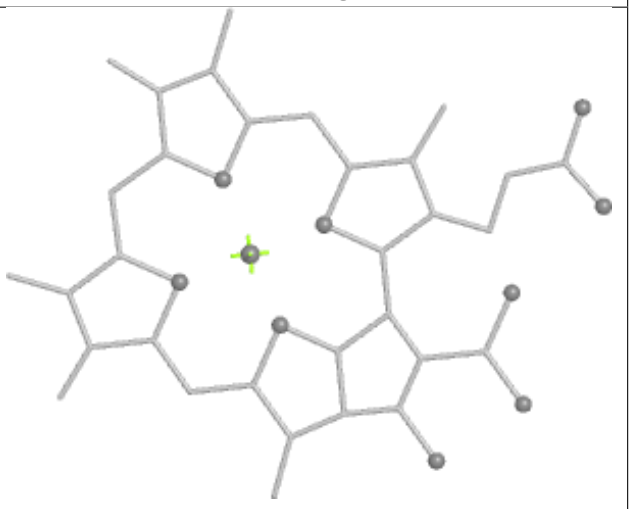
Bond lengths



Bond angles

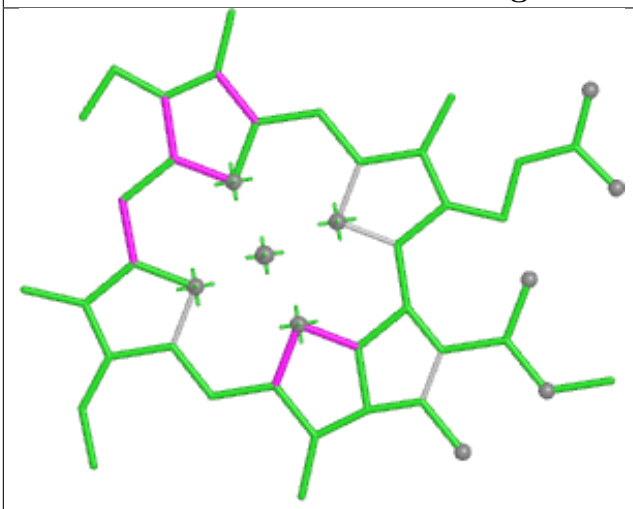


Torsions

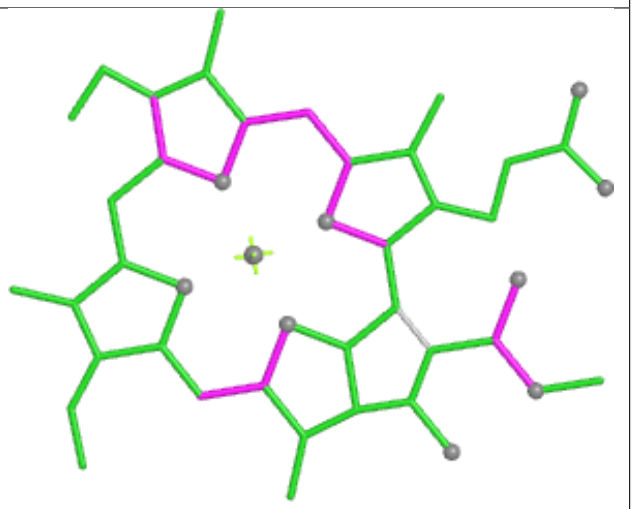


Rings

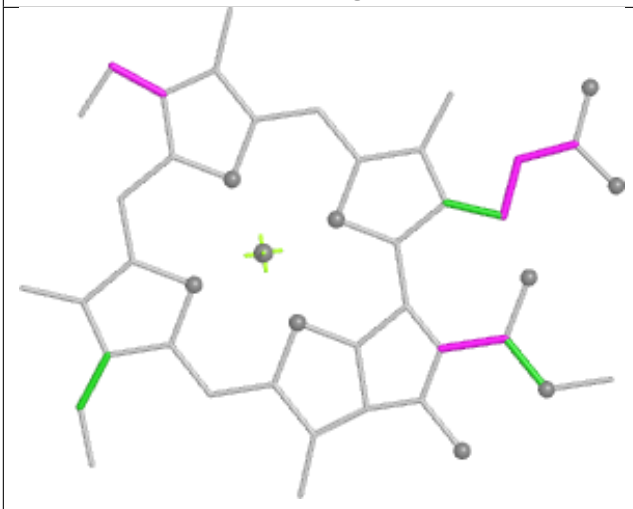
Ligand CLA BK 202



Bond lengths



Bond angles

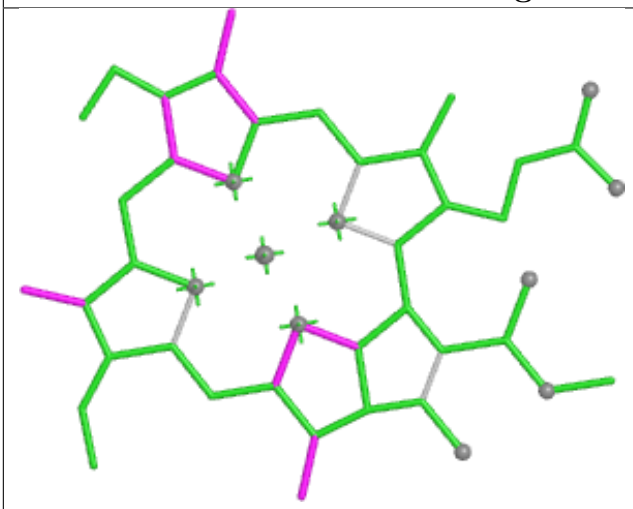


Torsions

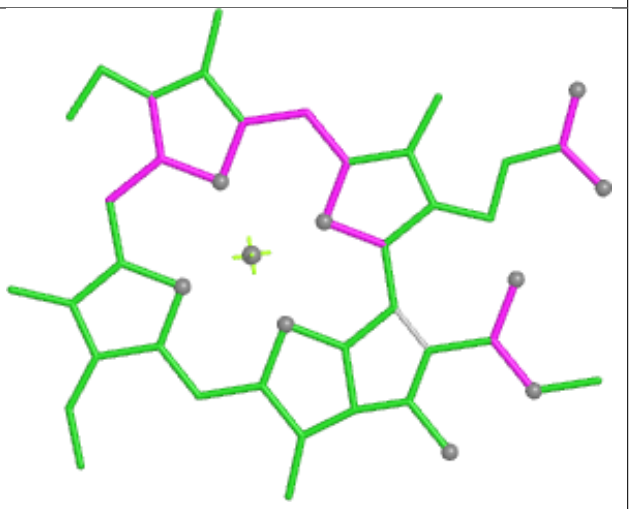


Rings

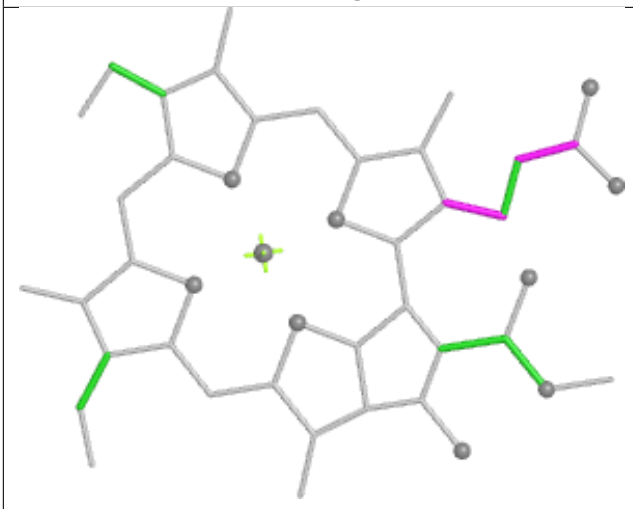
Ligand CLA A6 609



Bond lengths



Bond angles

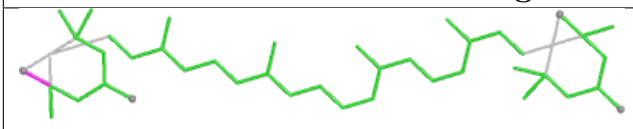


Torsions

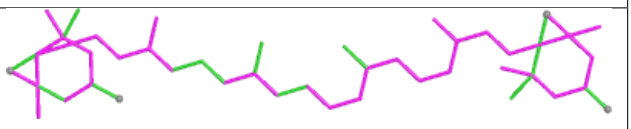


Rings

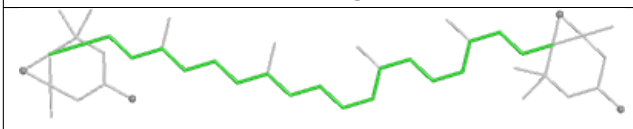
Ligand XAT B3 316



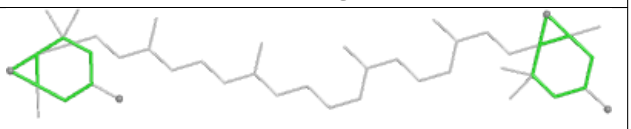
Bond lengths



Bond angles

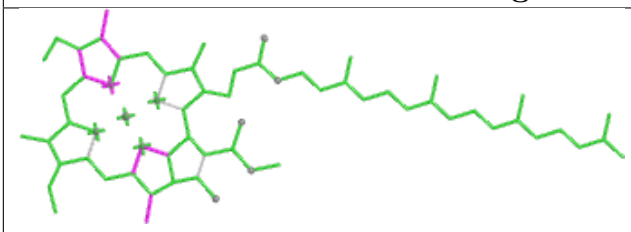


Torsions

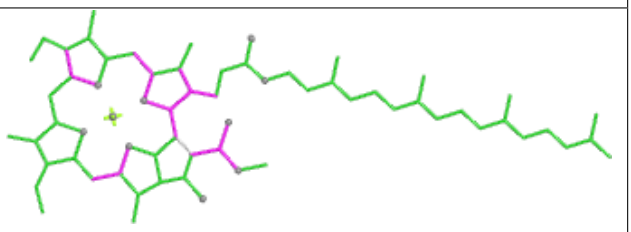


Rings

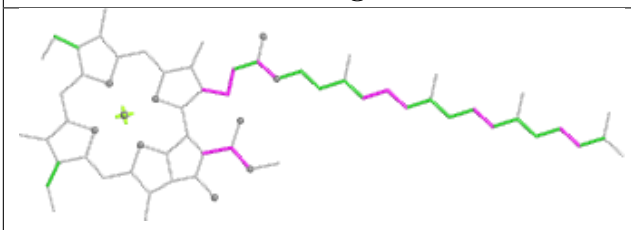
Ligand CLA BB 812



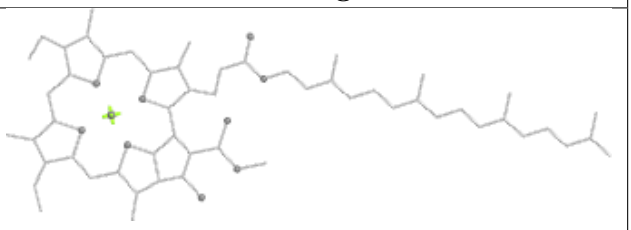
Bond lengths



Bond angles

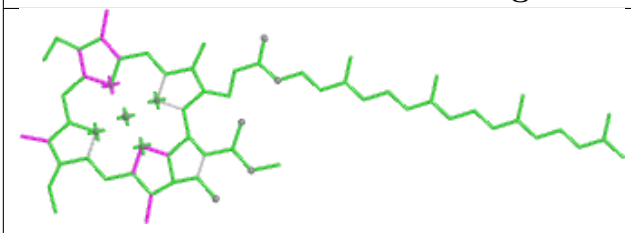


Torsions

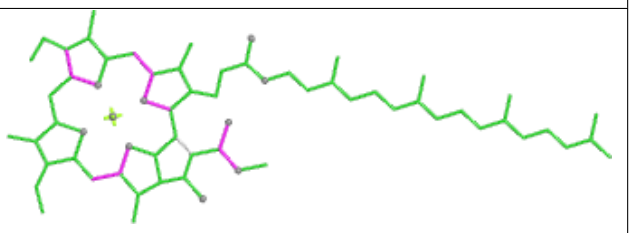


Rings

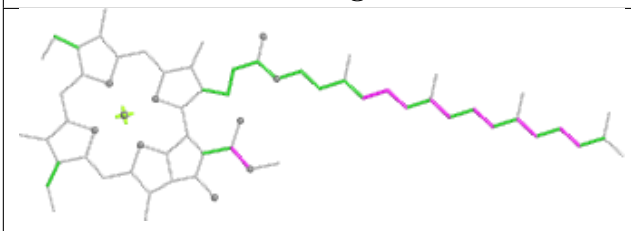
Ligand CLA BB 808



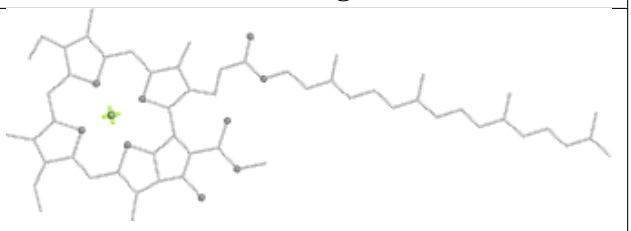
Bond lengths



Bond angles

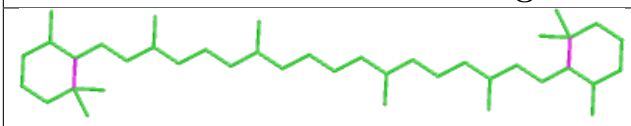


Torsions

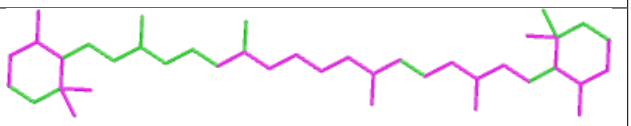


Rings

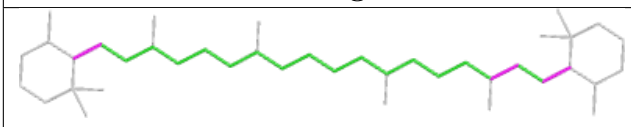
Ligand BCR BI 101



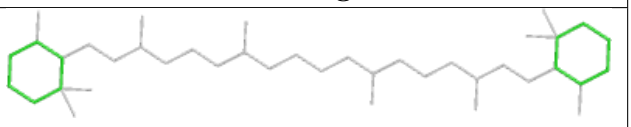
Bond lengths



Bond angles

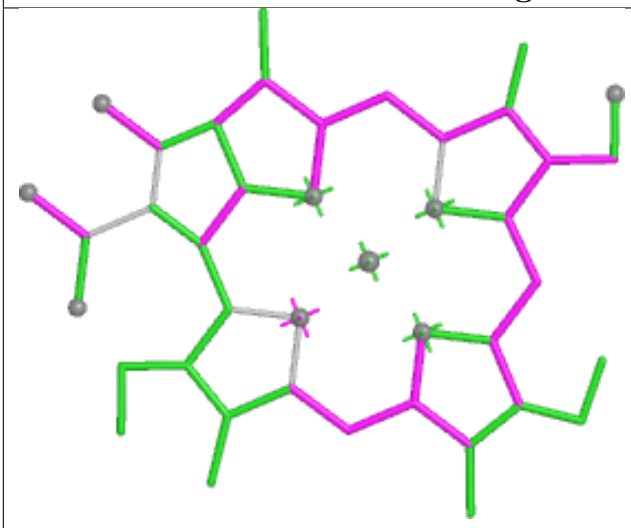


Torsions

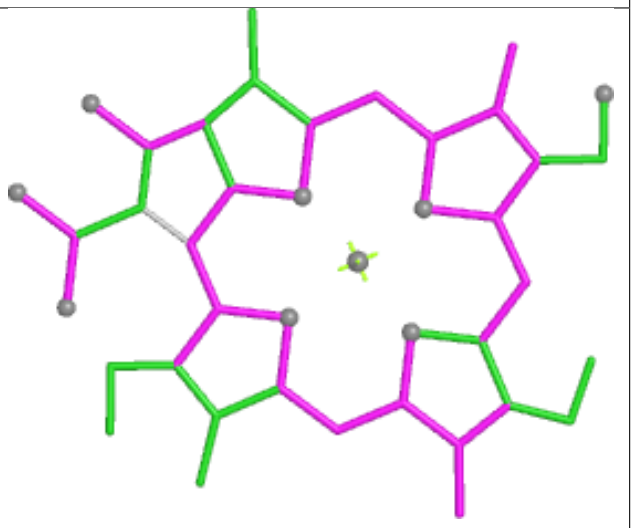


Rings

Ligand CHL B5 605



Bond lengths



Bond angles

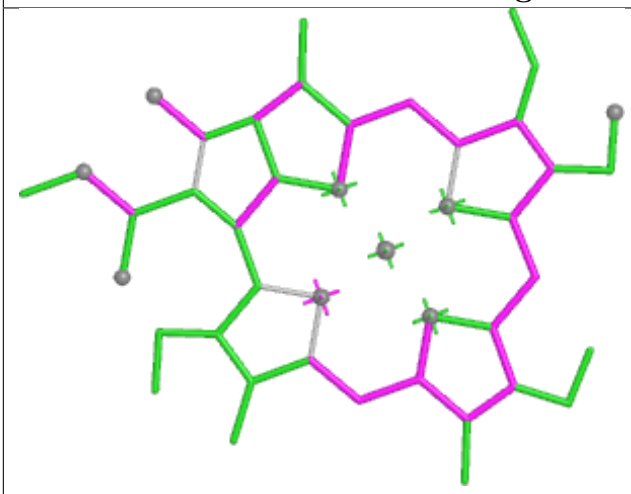


Torsions

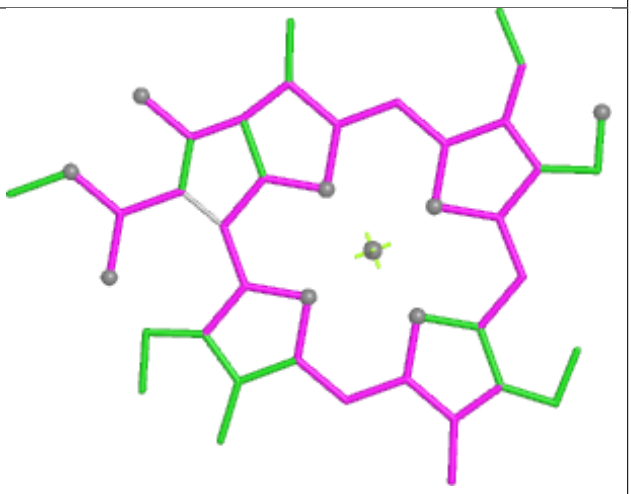


Rings

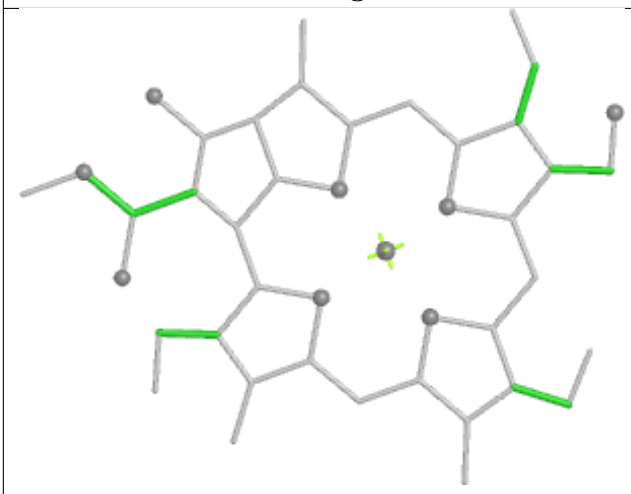
Ligand CHL B2 614



Bond lengths



Bond angles

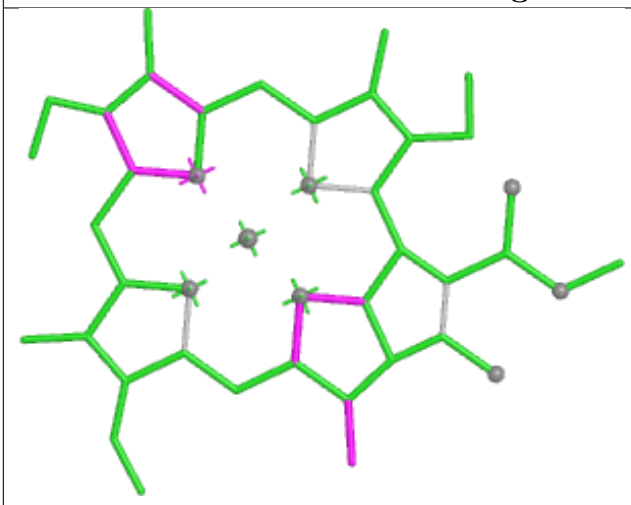


Torsions

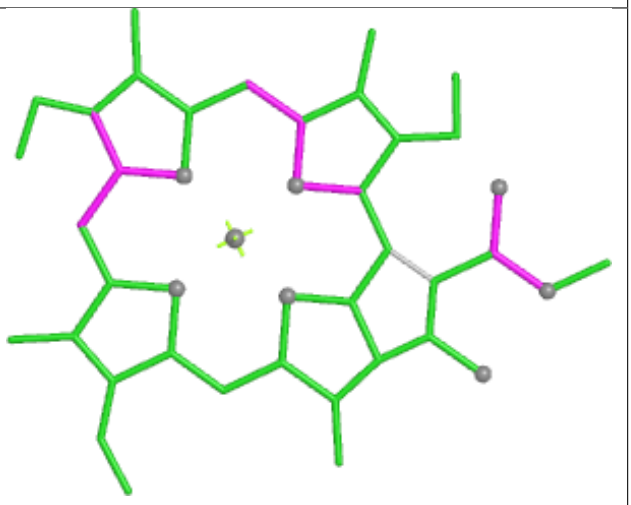


Rings

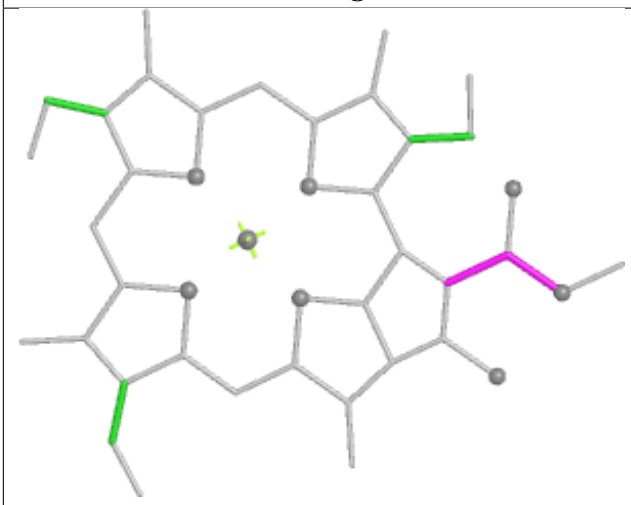
Ligand CLA BA 815



Bond lengths



Bond angles

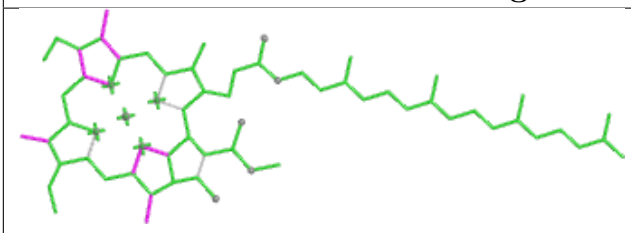


Torsions

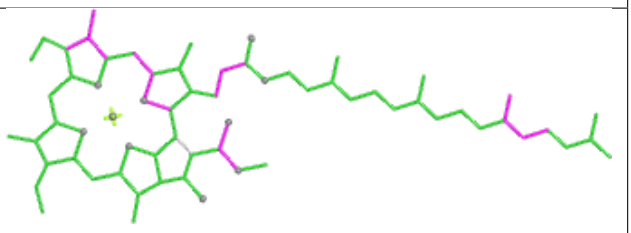


Rings

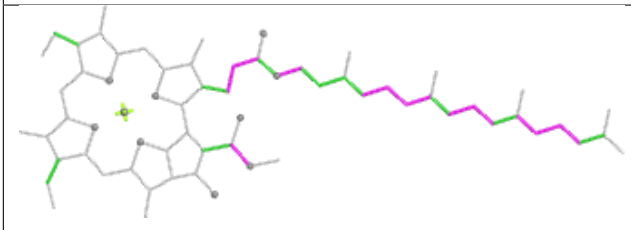
Ligand CLA AA 828



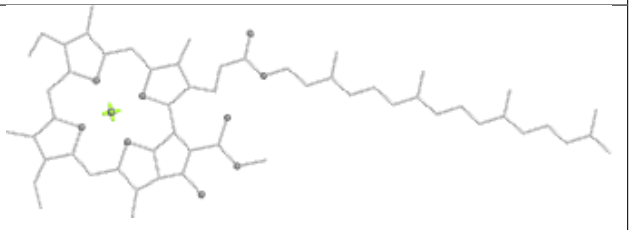
Bond lengths



Bond angles

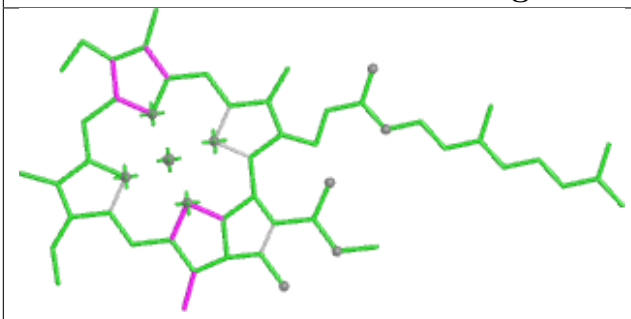


Torsions

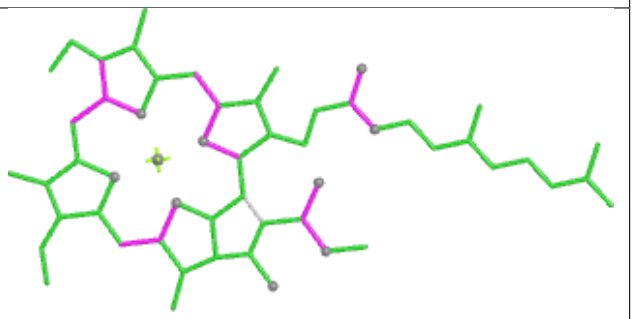


Rings

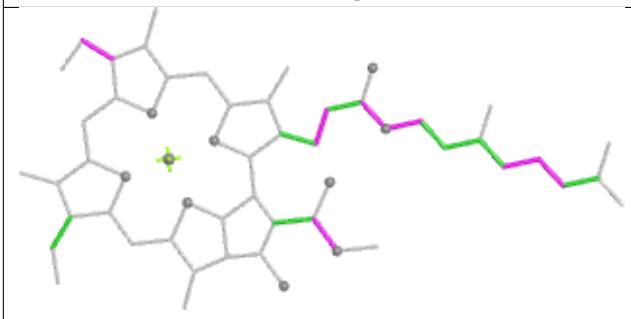
Ligand CLA BB 818



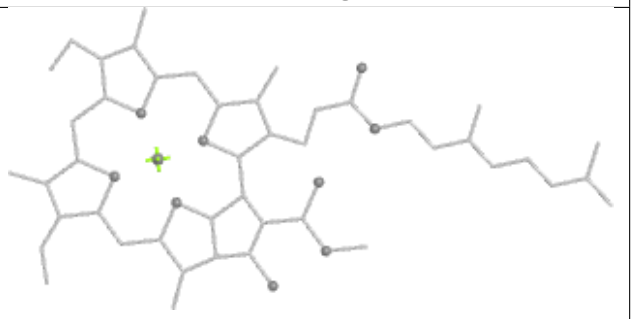
Bond lengths



Bond angles

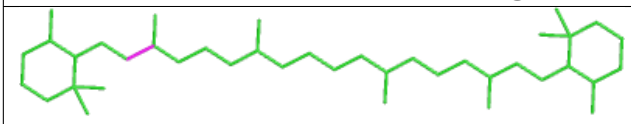


Torsions

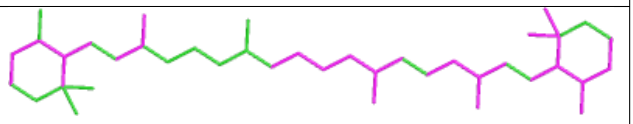


Rings

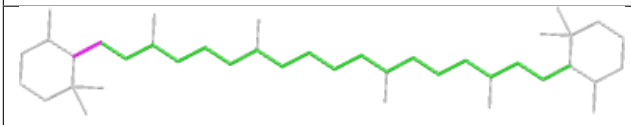
Ligand BCR BK 204



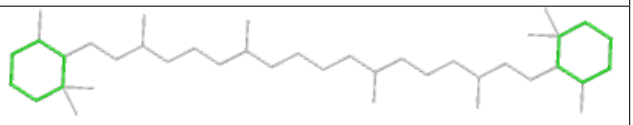
Bond lengths



Bond angles

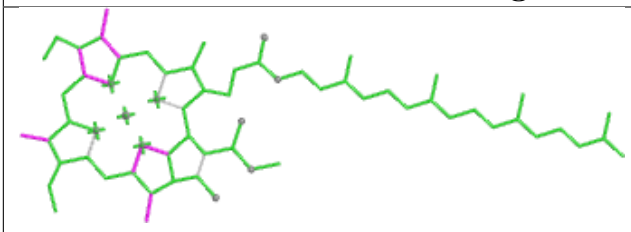


Torsions

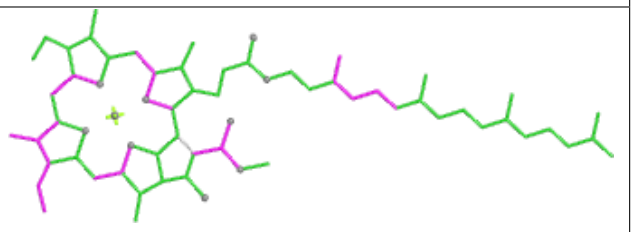


Rings

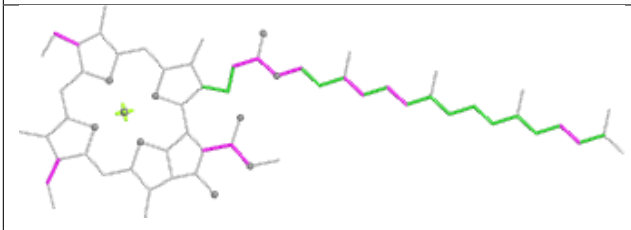
Ligand CLA AA 834



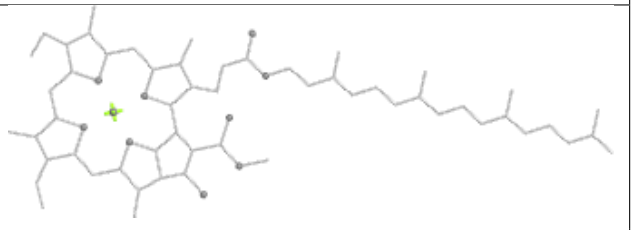
Bond lengths



Bond angles

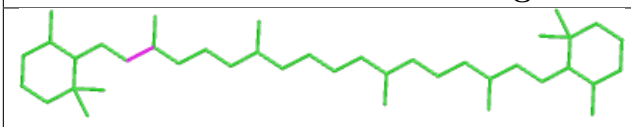


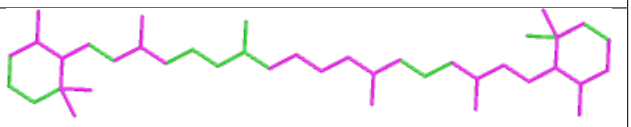
Torsions

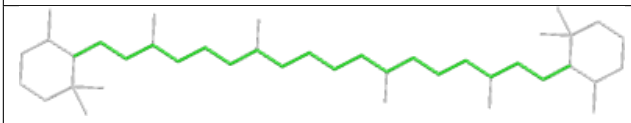


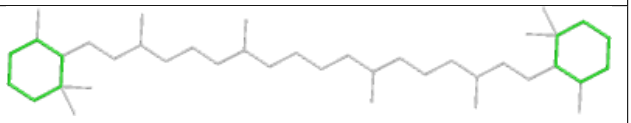
Rings

Ligand BCR B2 617


Bond lengths


Bond angles

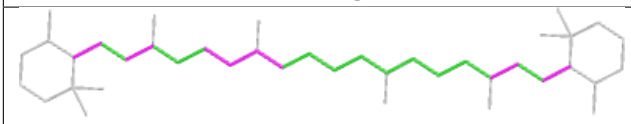

Torsions

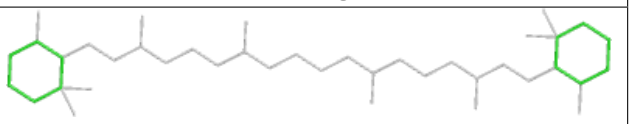

Rings

Ligand BCR AA 847

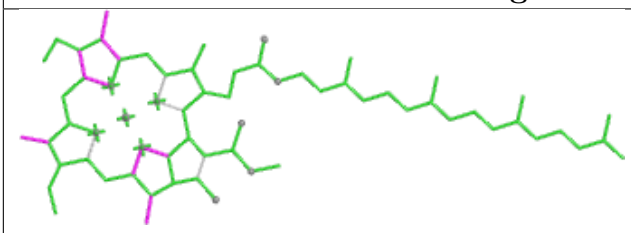

Bond lengths

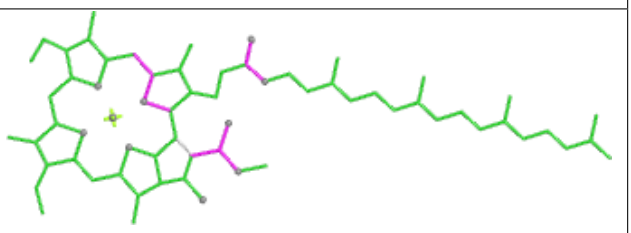

Bond angles

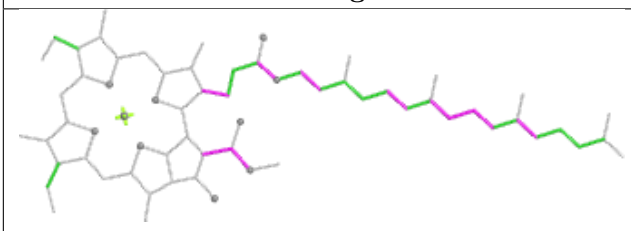

Torsions

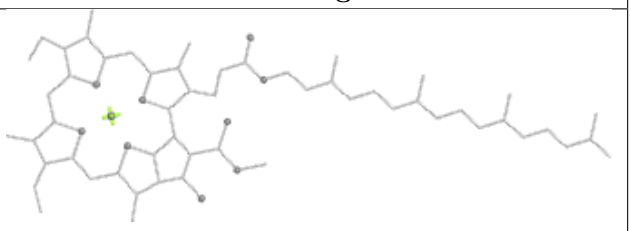

Rings

Ligand CLA AA 830


Bond lengths

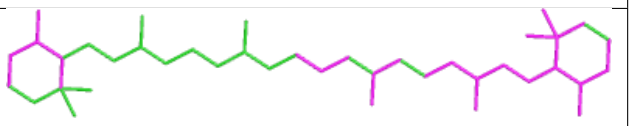

Bond angles

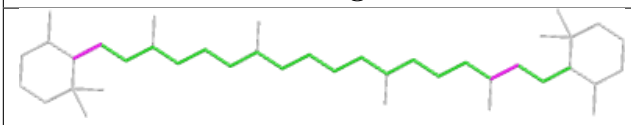

Torsions

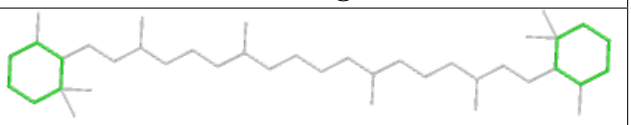

Rings

Ligand BCR A3 318

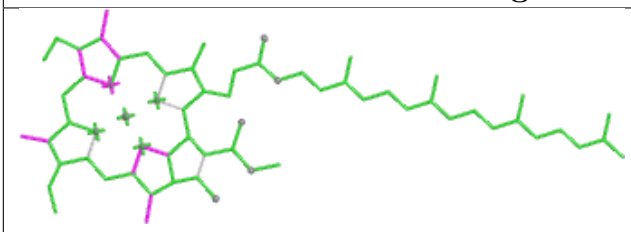

Bond lengths


Bond angles

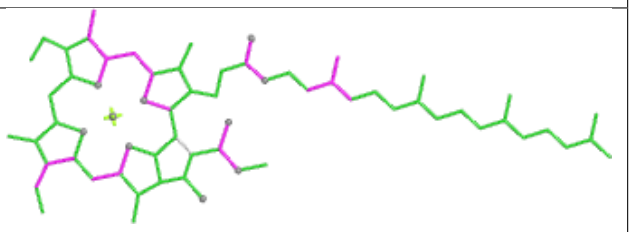

Torsions


Rings

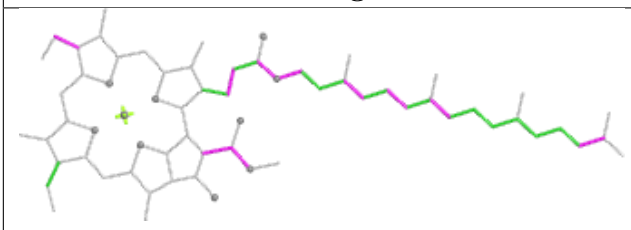
Ligand CLA BA 841



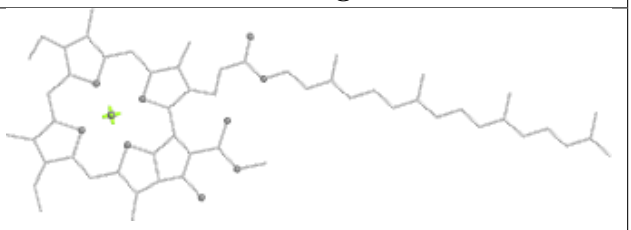
Bond lengths



Bond angles

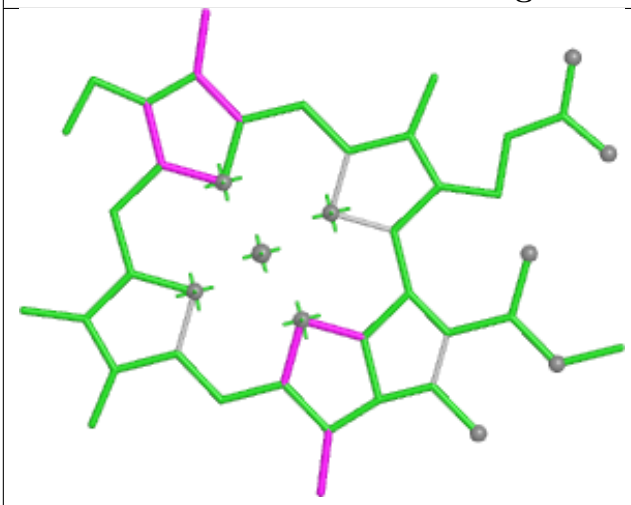


Torsions

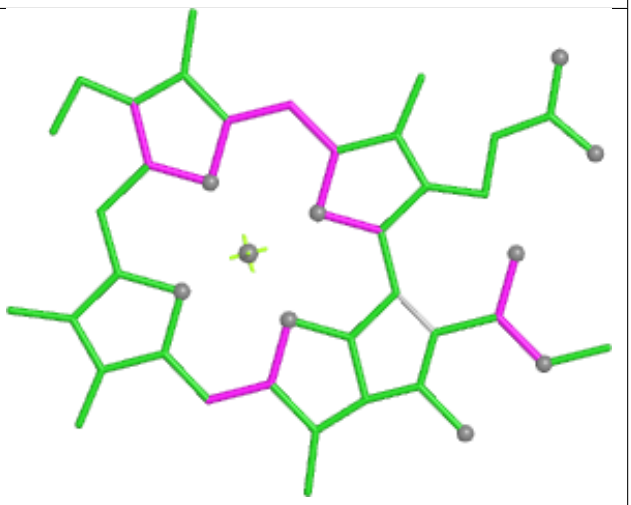


Rings

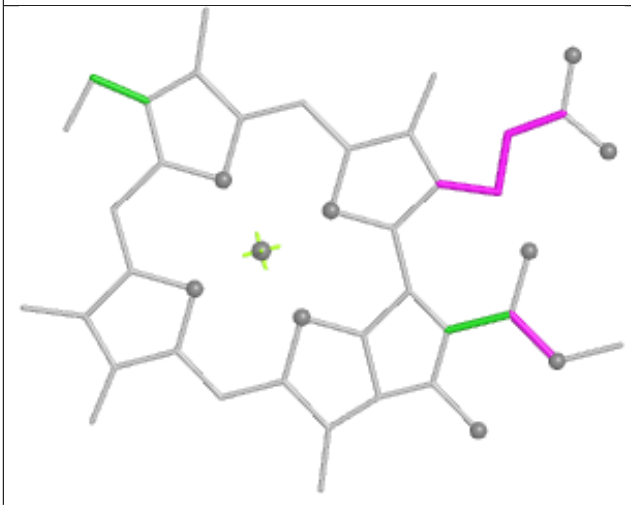
Ligand CLA B2 611



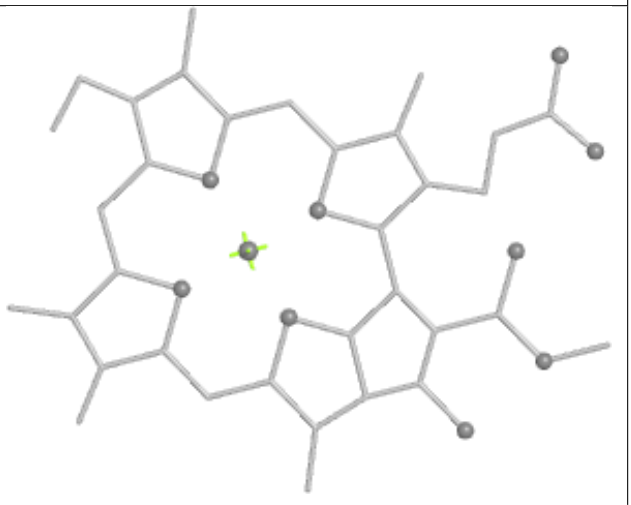
Bond lengths



Bond angles

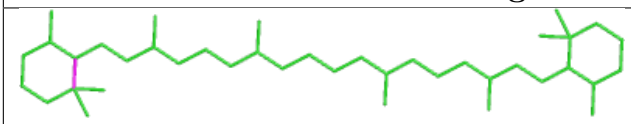


Torsions

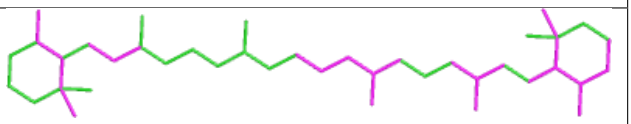


Rings

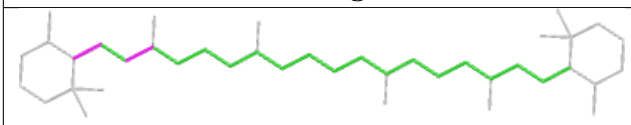
Ligand BCR AA 848



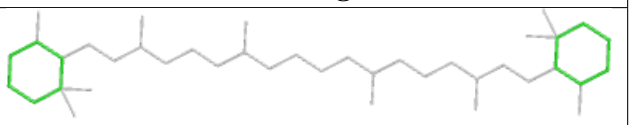
Bond lengths



Bond angles

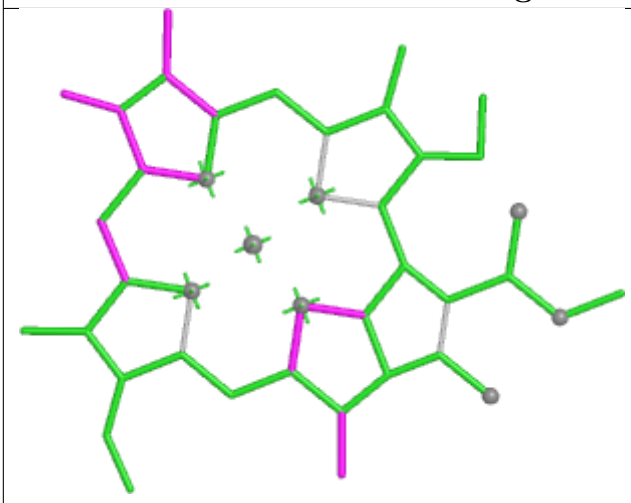


Torsions

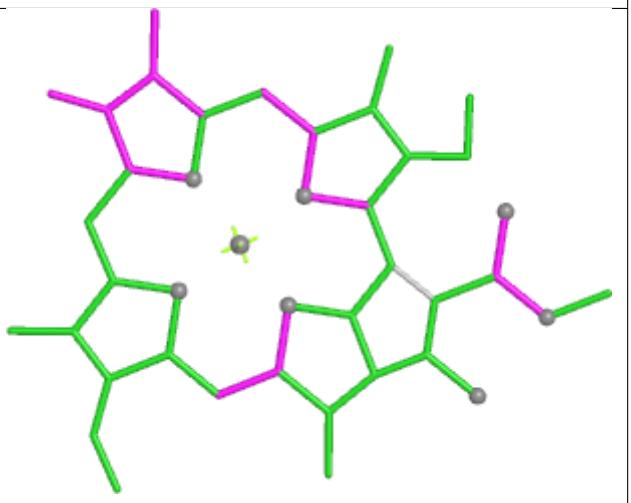


Rings

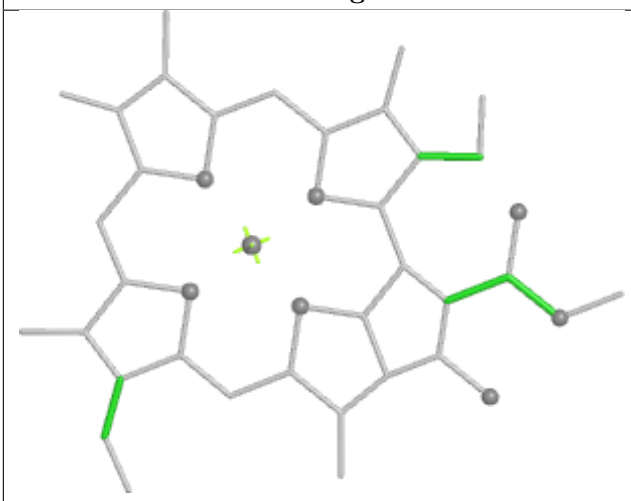
Ligand CLA A3 306



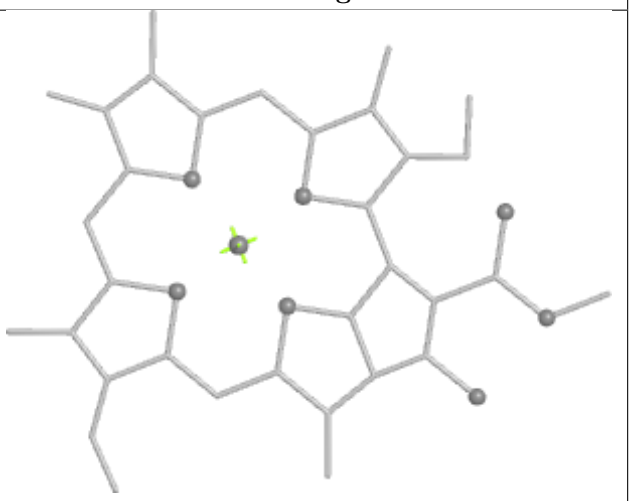
Bond lengths



Bond angles

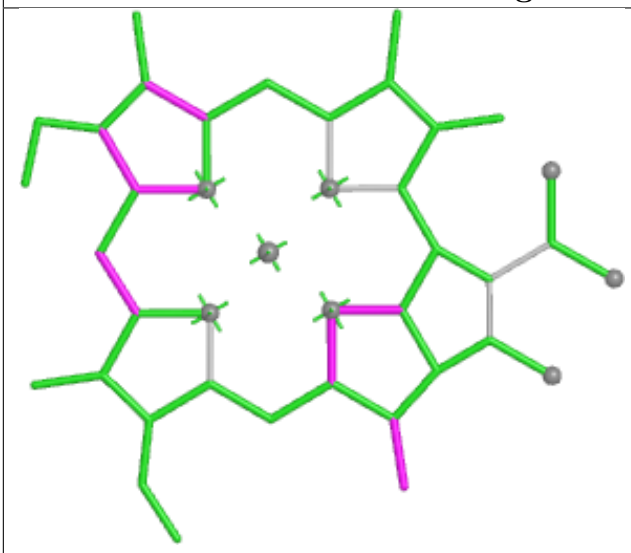


Torsions

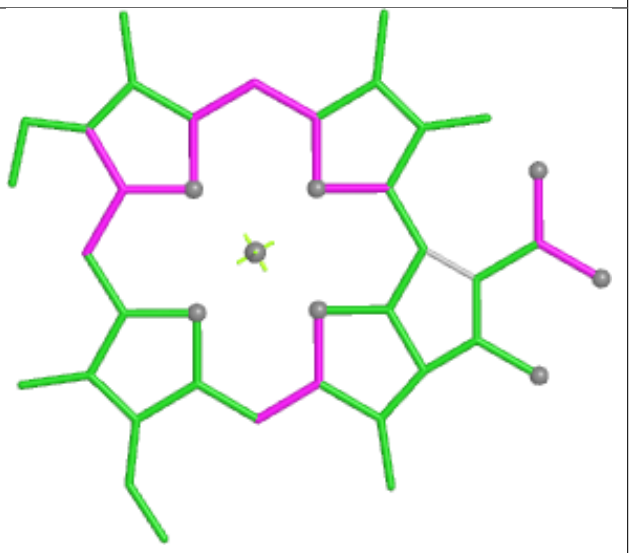


Rings

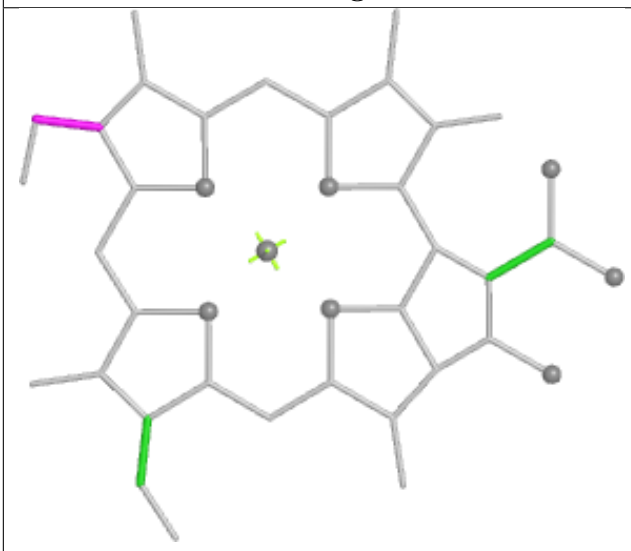
Ligand CLA B3 312



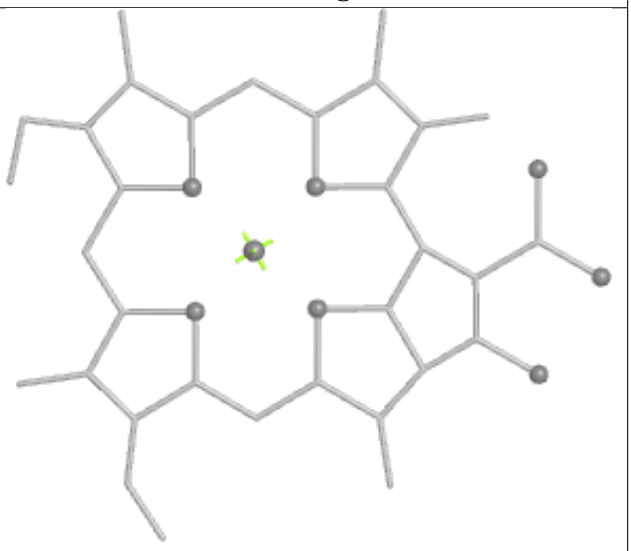
Bond lengths



Bond angles

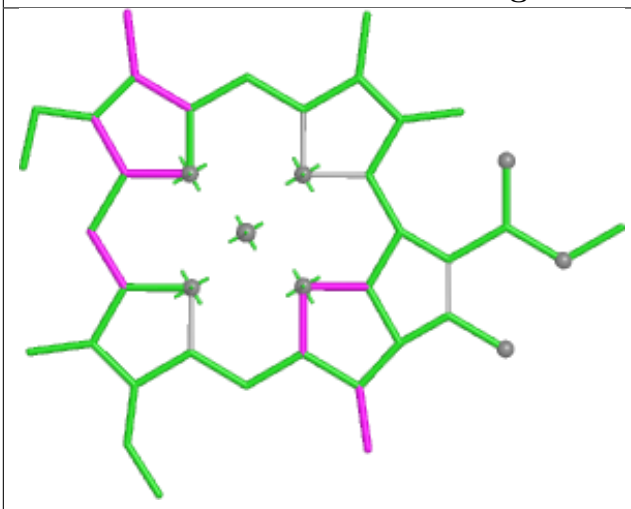


Torsions

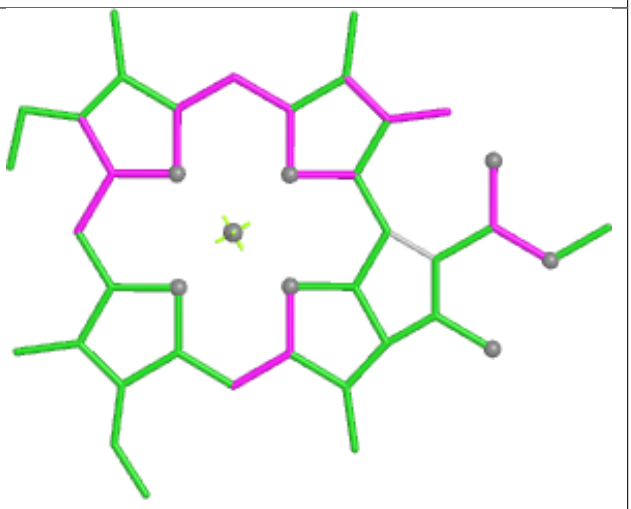


Rings

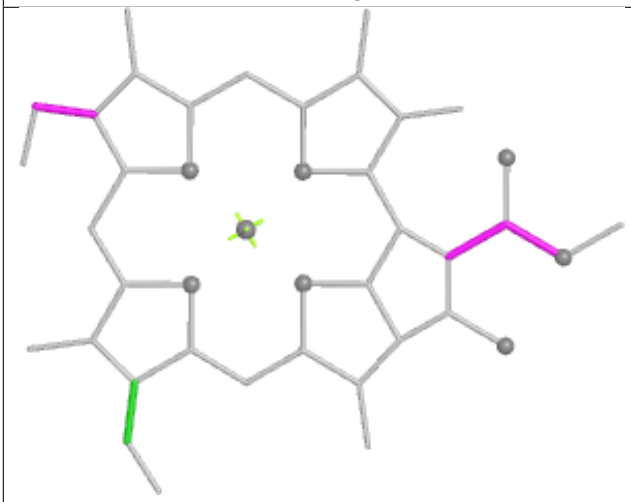
Ligand CLA AA 823



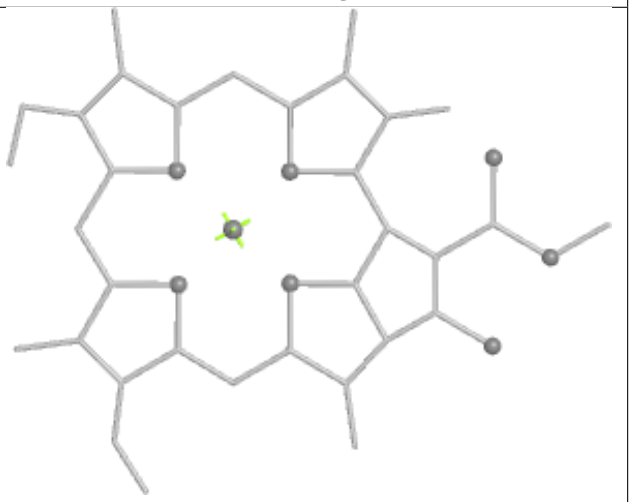
Bond lengths



Bond angles

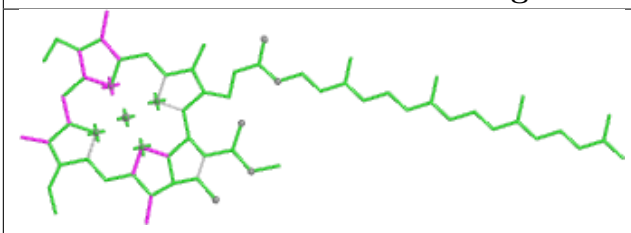


Torsions

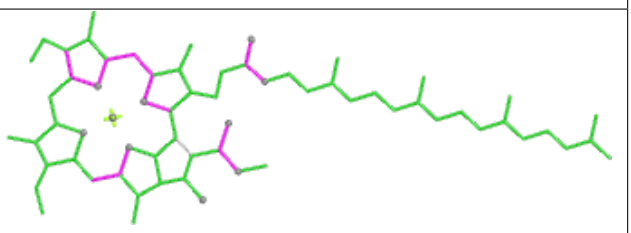


Rings

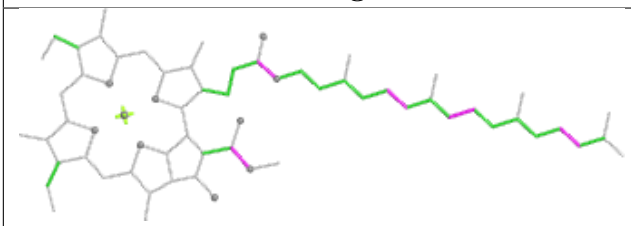
Ligand CLA AB 838



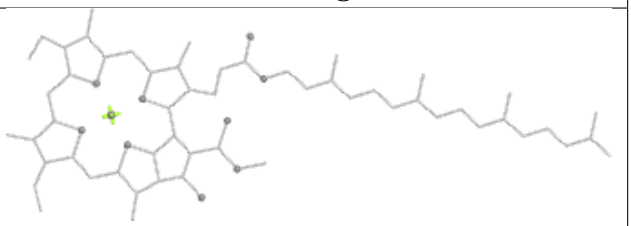
Bond lengths



Bond angles

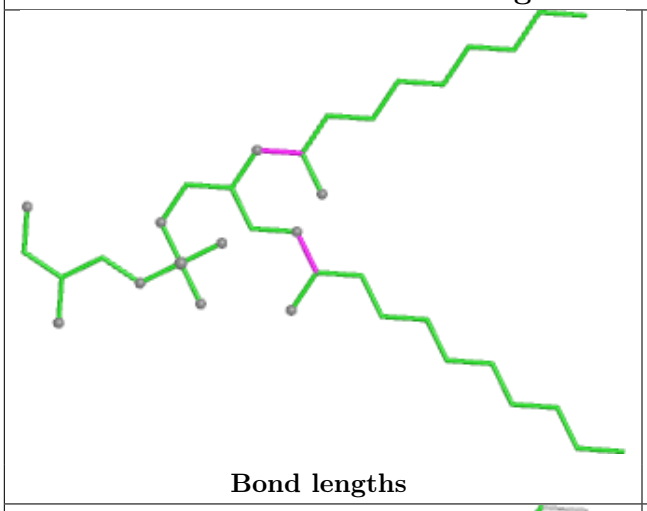


Torsions

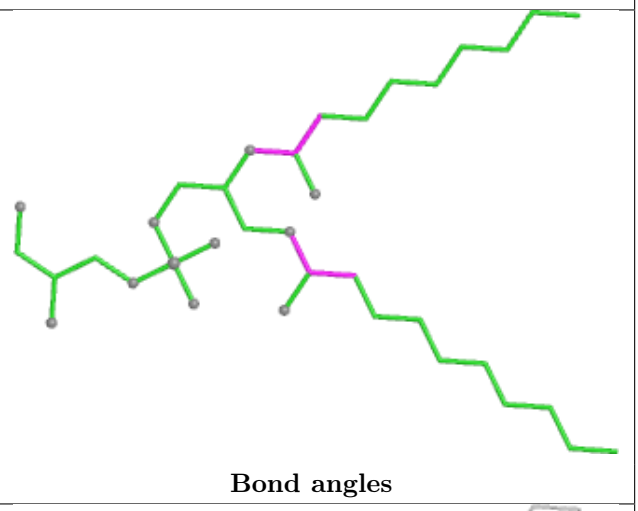


Rings

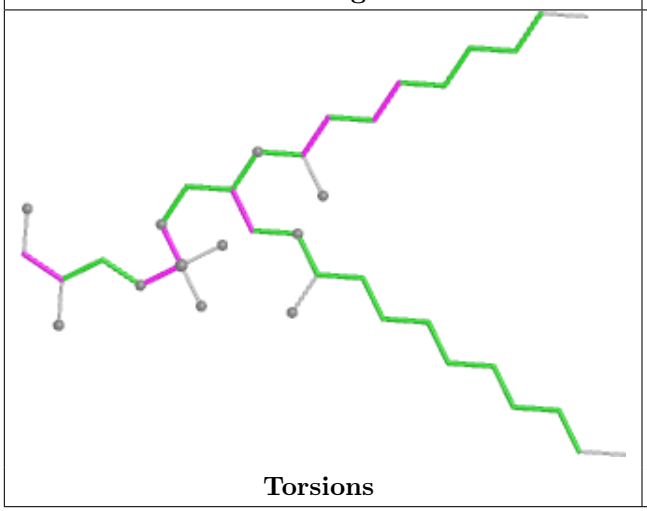
Ligand LHG A3 301



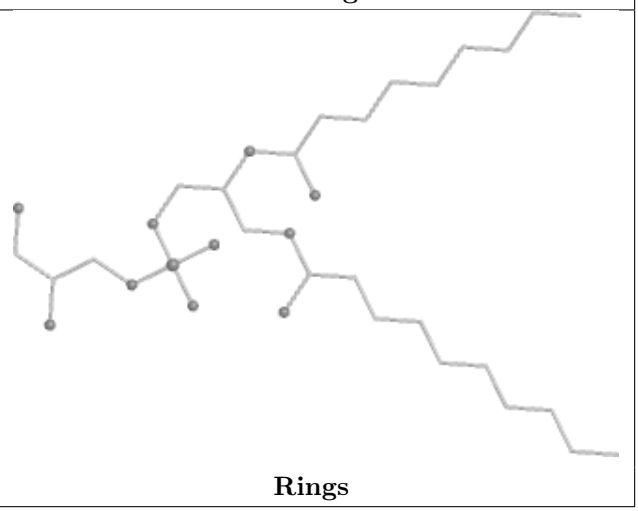
Bond lengths



Bond angles

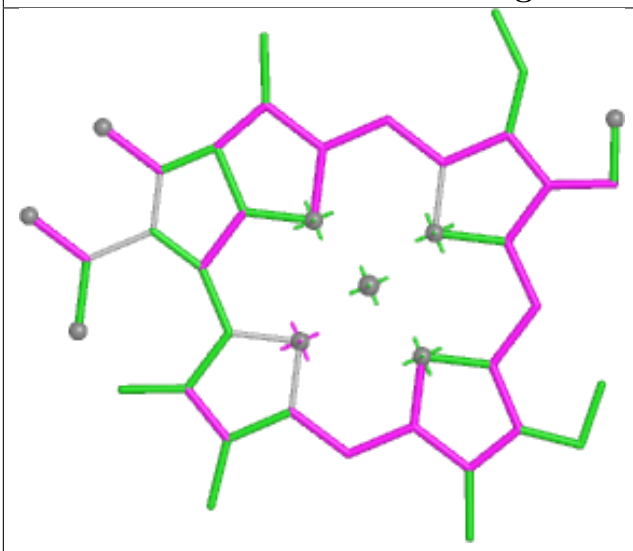


Torsions

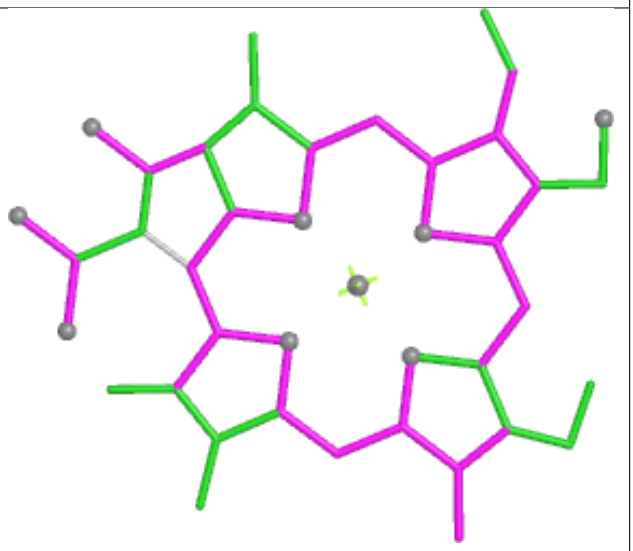


Rings

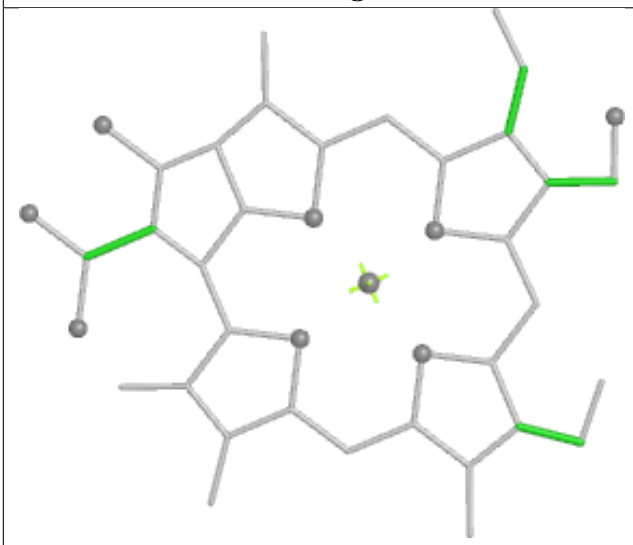
Ligand CHL B1 308



Bond lengths



Bond angles

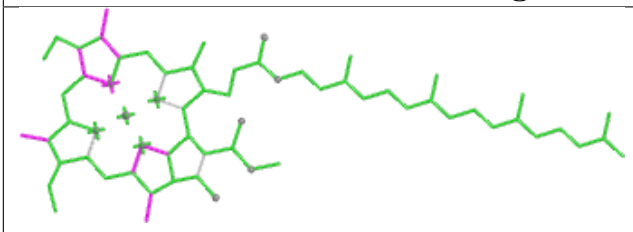


Torsions

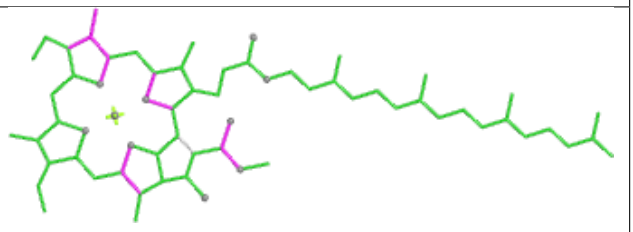


Rings

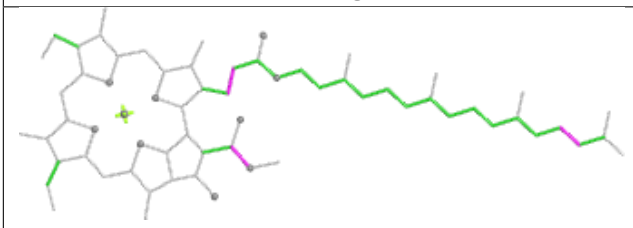
Ligand CLA BA 802



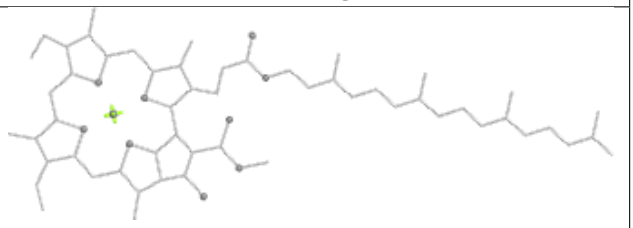
Bond lengths



Bond angles

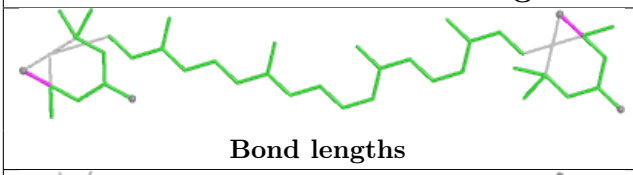


Torsions

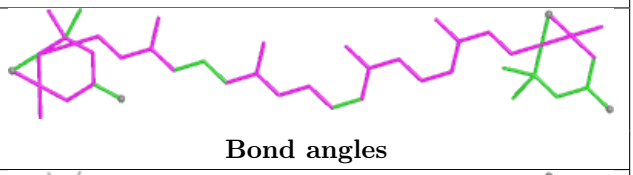


Rings

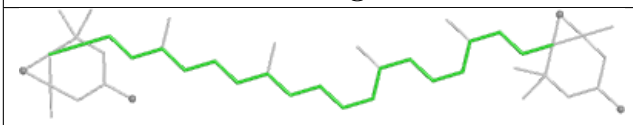
Ligand XAT A6 616



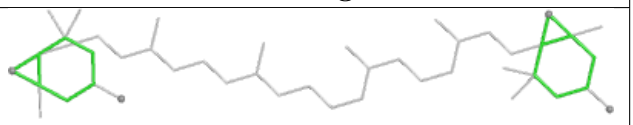
Bond lengths



Bond angles

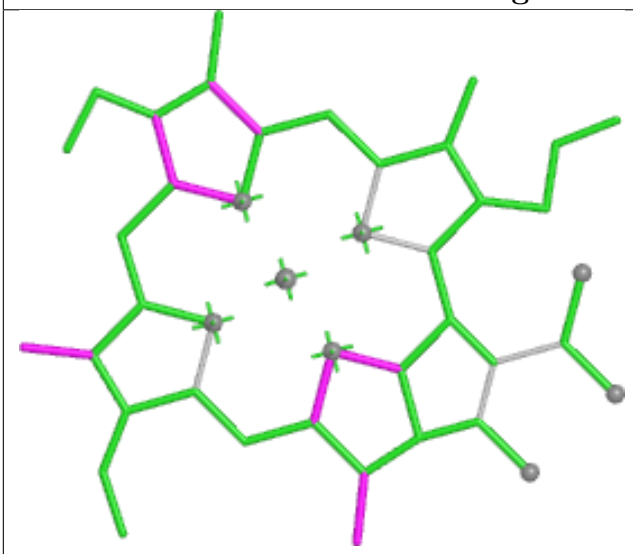


Torsions

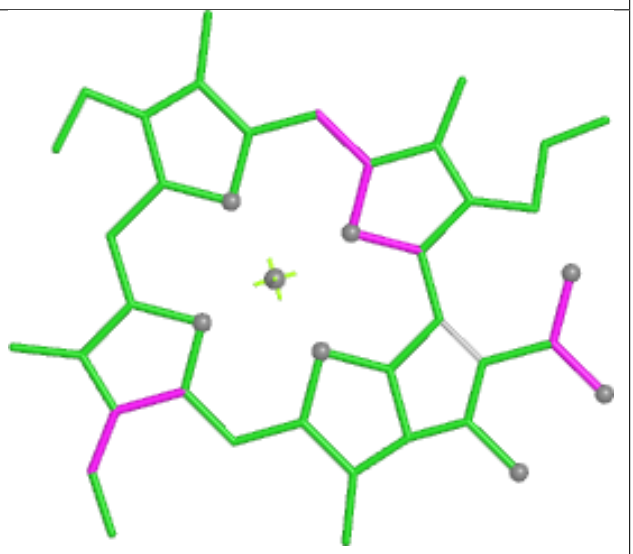


Rings

Ligand CLA BB 817



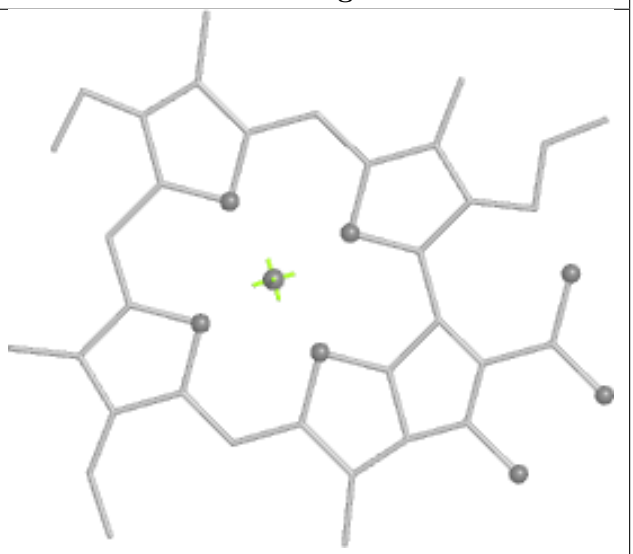
Bond lengths



Bond angles

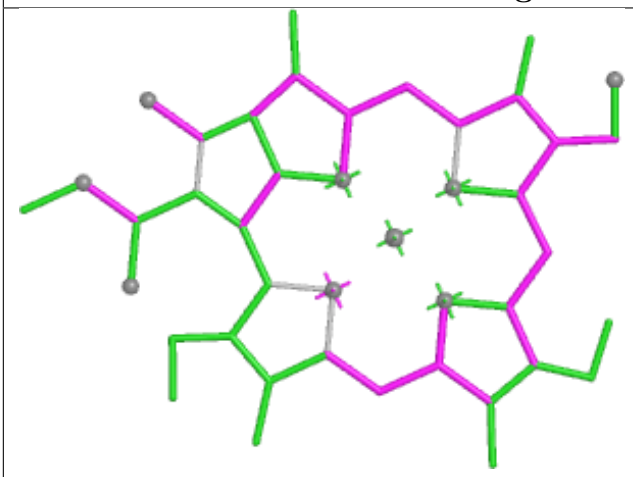


Torsions

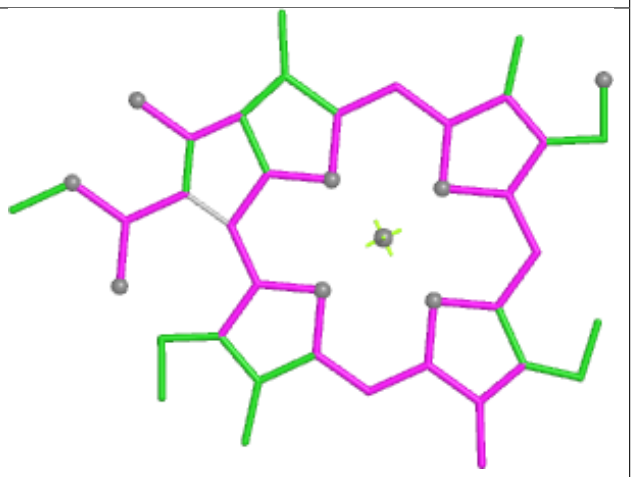


Rings

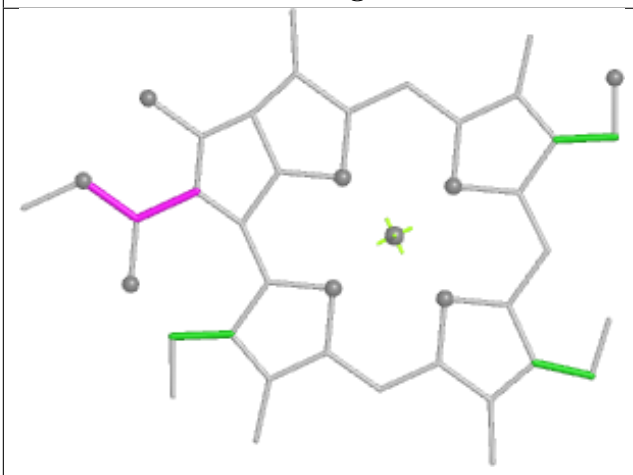
Ligand CHL B2 605



Bond lengths



Bond angles

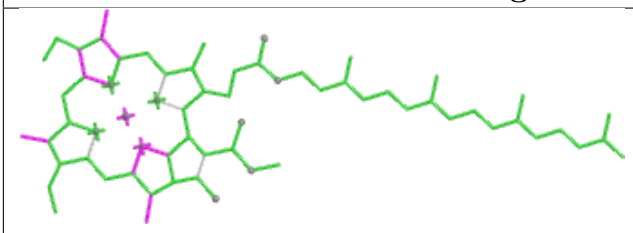


Torsions

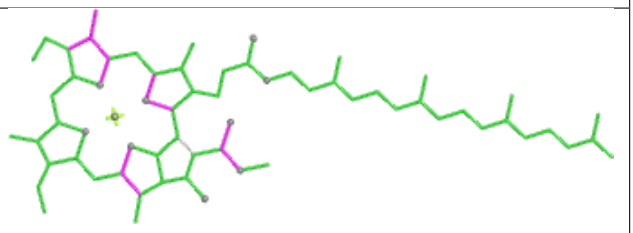


Rings

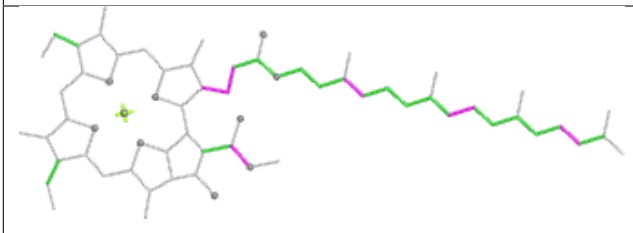
Ligand CLA AA 802



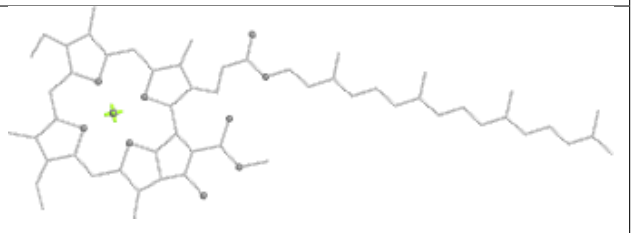
Bond lengths



Bond angles

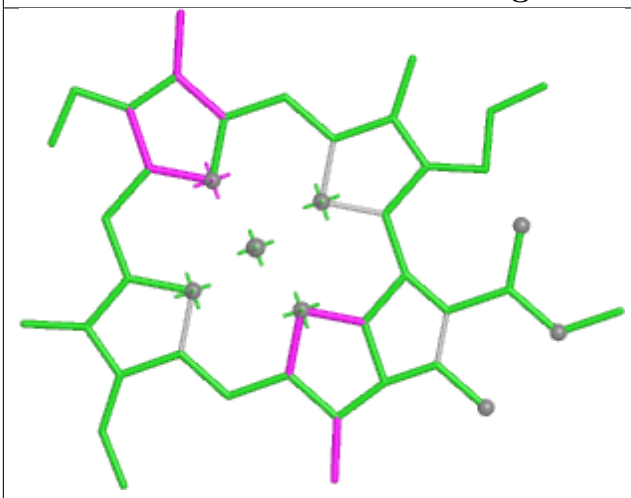


Torsions

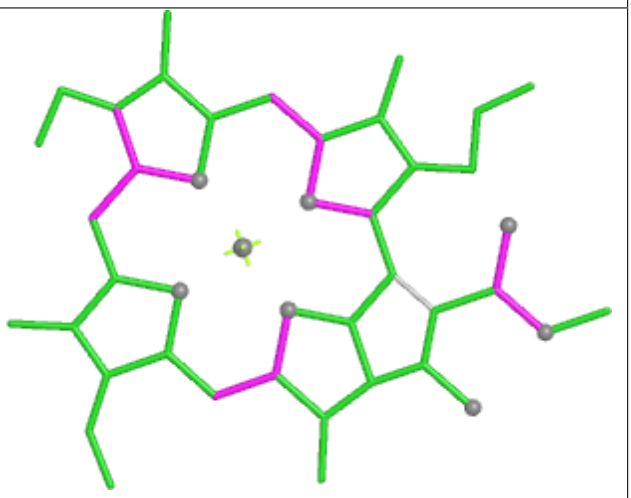


Rings

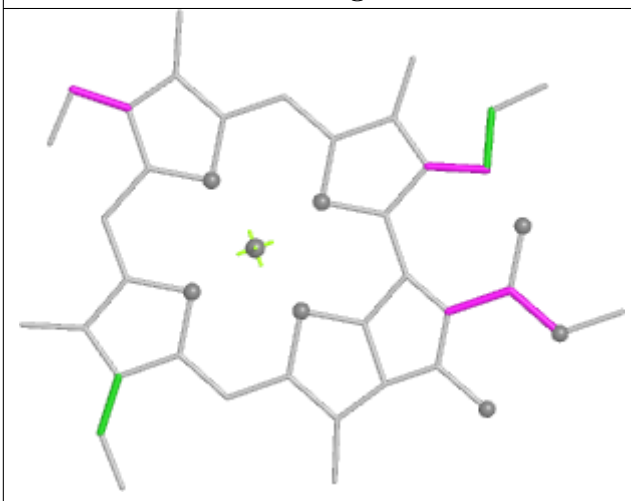
Ligand CLA BB 832



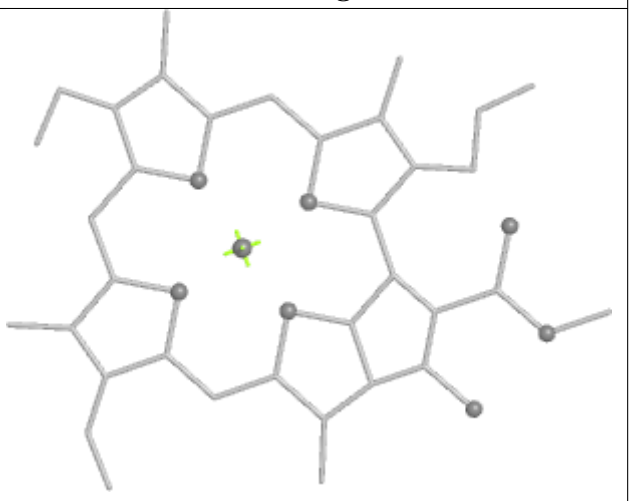
Bond lengths



Bond angles

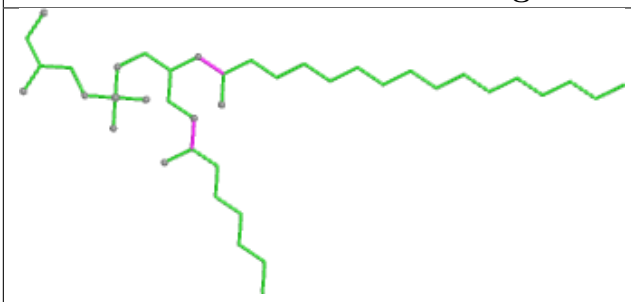


Torsions

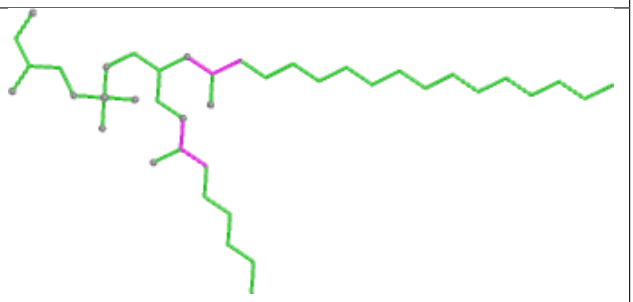


Rings

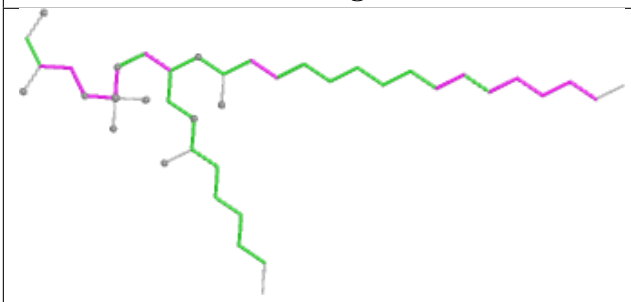
Ligand LHG AJ 104



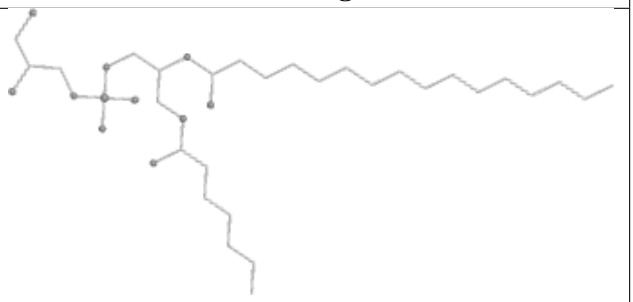
Bond lengths



Bond angles

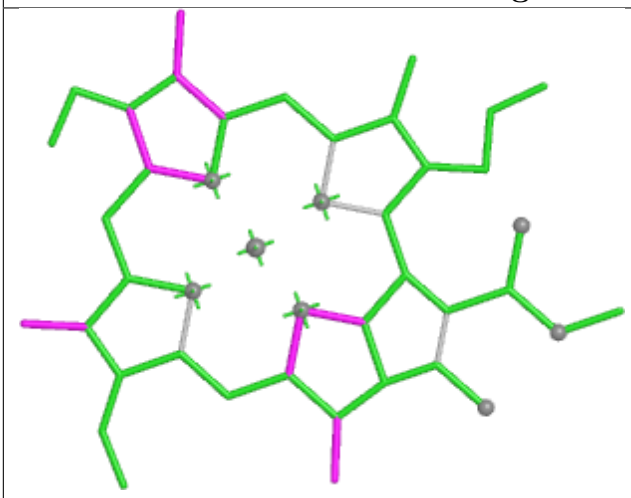


Torsions

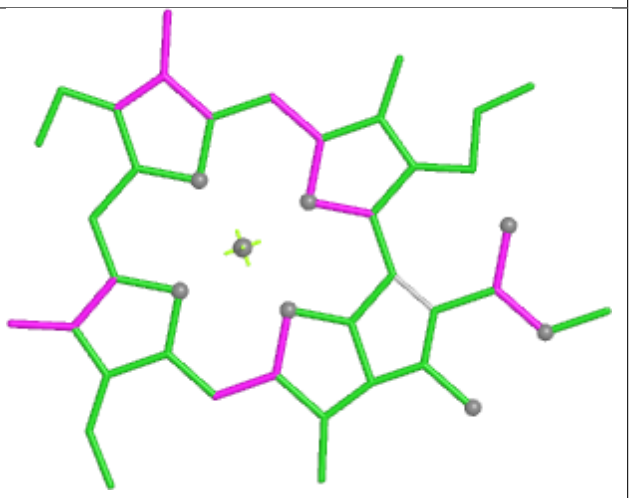


Rings

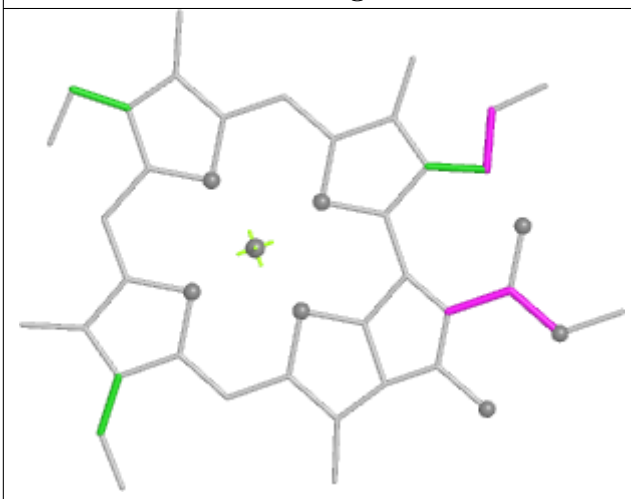
Ligand CLA BB 833



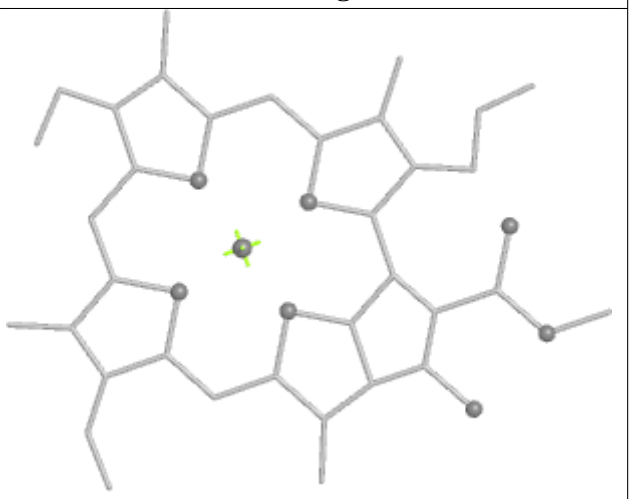
Bond lengths



Bond angles

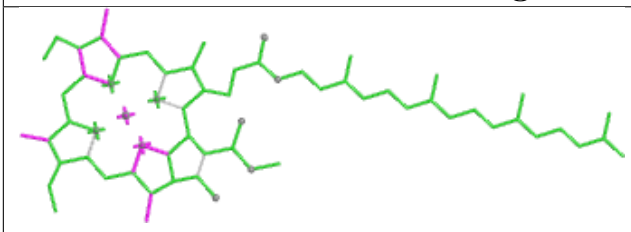


Torsions

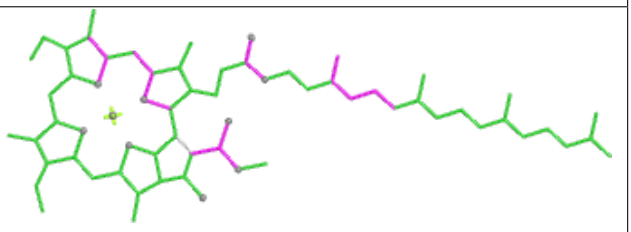


Rings

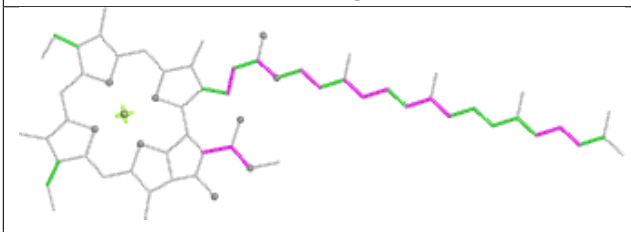
Ligand CLA BB 802



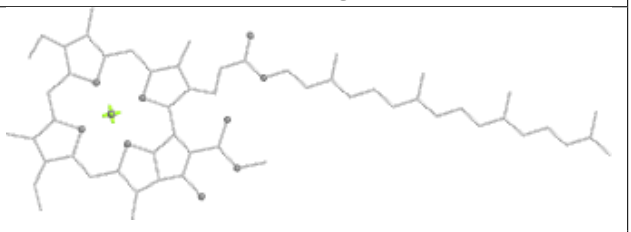
Bond lengths



Bond angles

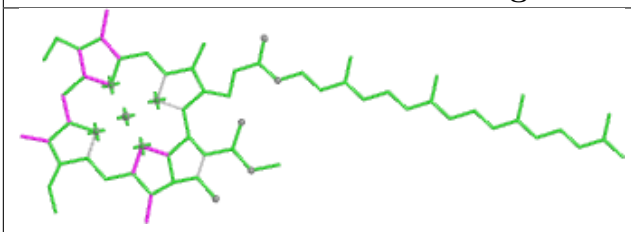


Torsions

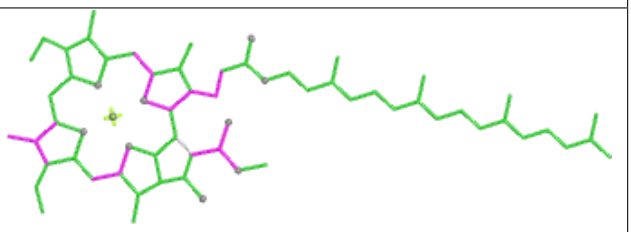


Rings

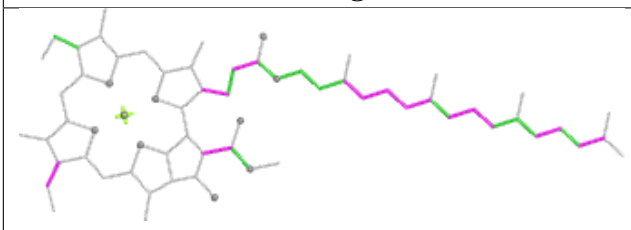
Ligand CLA AA 805



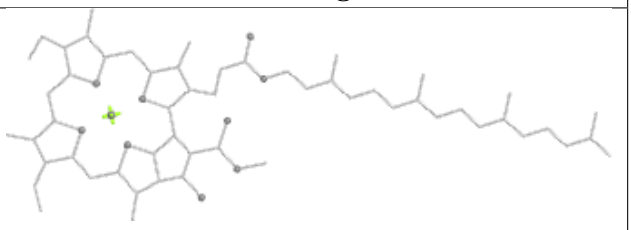
Bond lengths



Bond angles

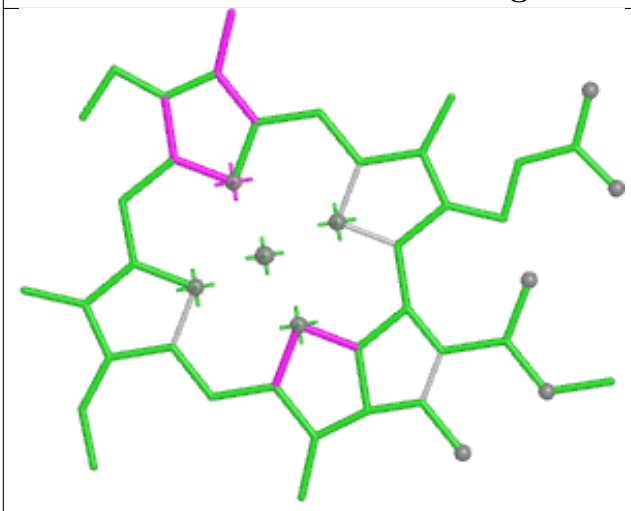


Torsions

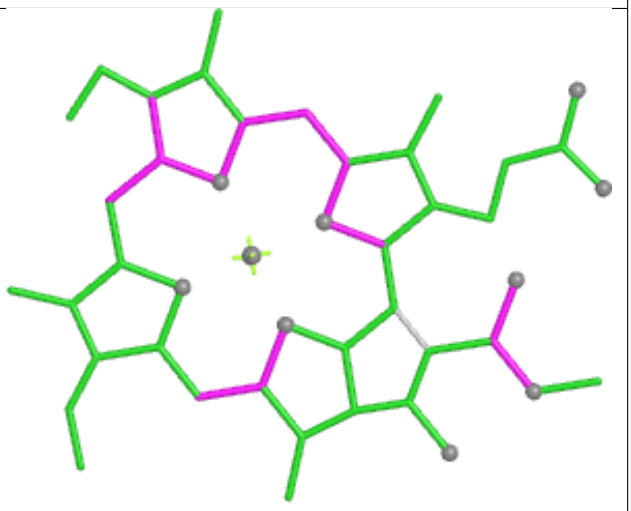


Rings

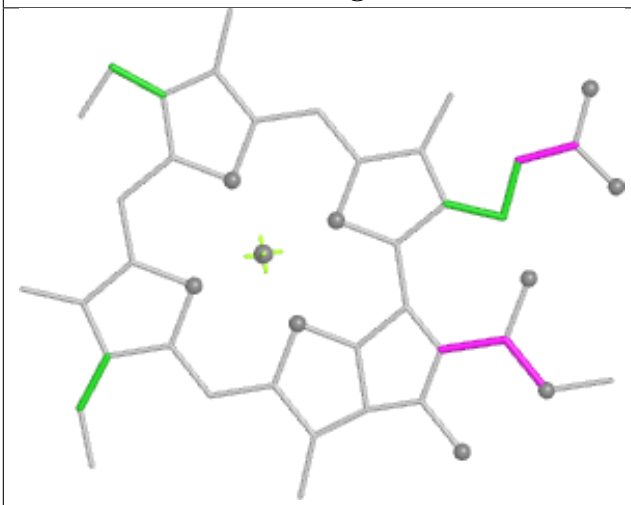
Ligand CLA BG 202



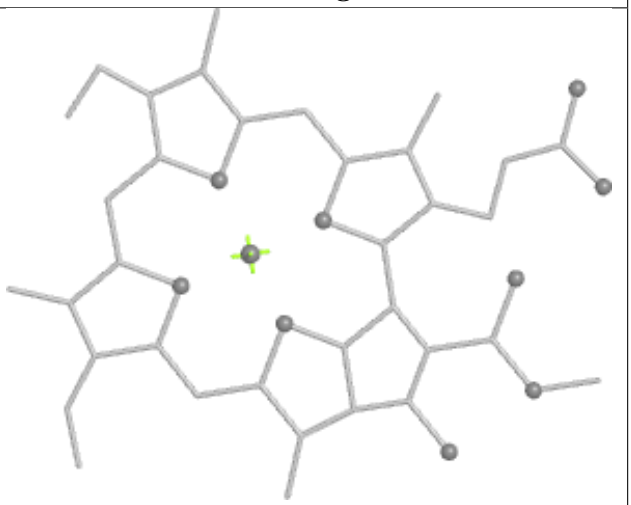
Bond lengths



Bond angles

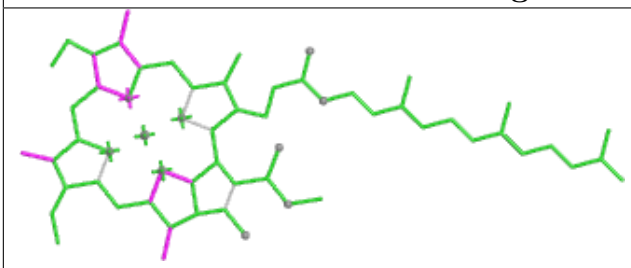


Torsions

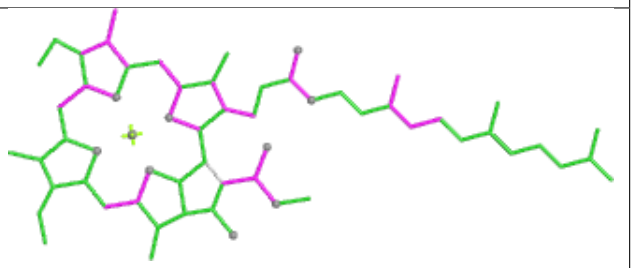


Rings

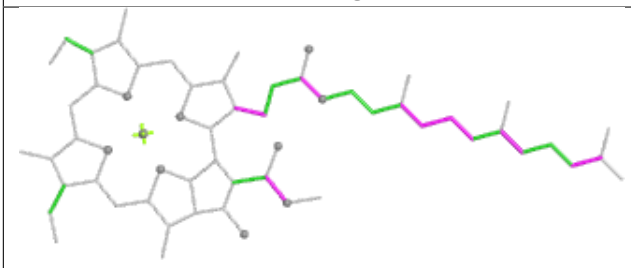
Ligand CLA AB 819



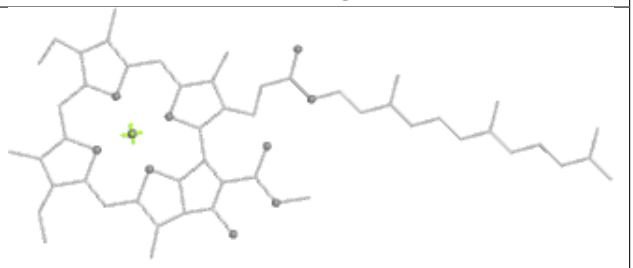
Bond lengths



Bond angles

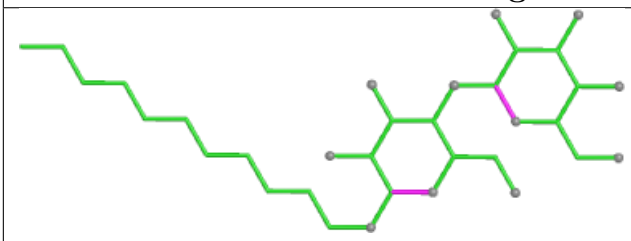


Torsions

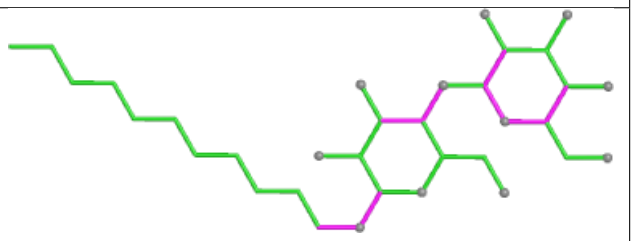


Rings

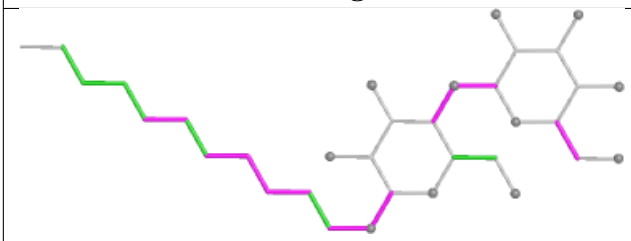
Ligand LMU AL 301



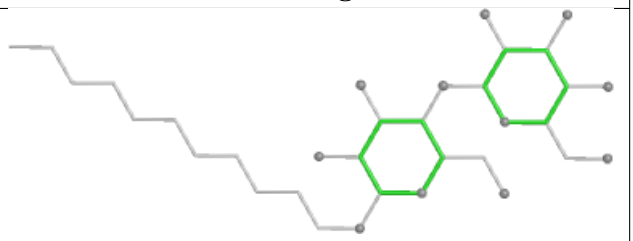
Bond lengths



Bond angles

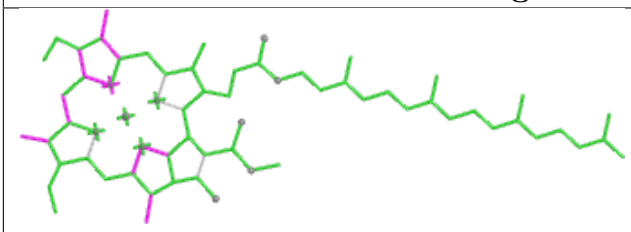


Torsions

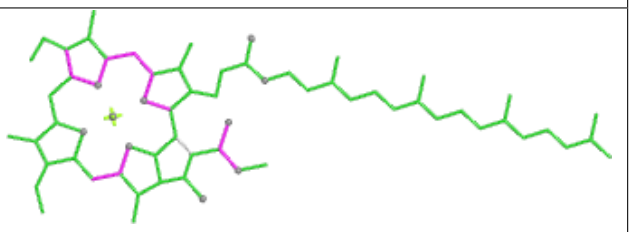


Rings

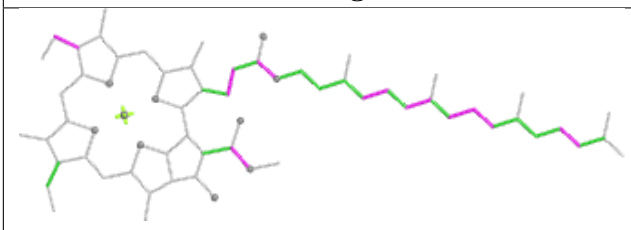
Ligand CLA BB 843



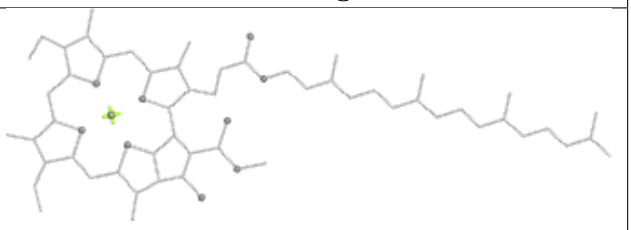
Bond lengths



Bond angles

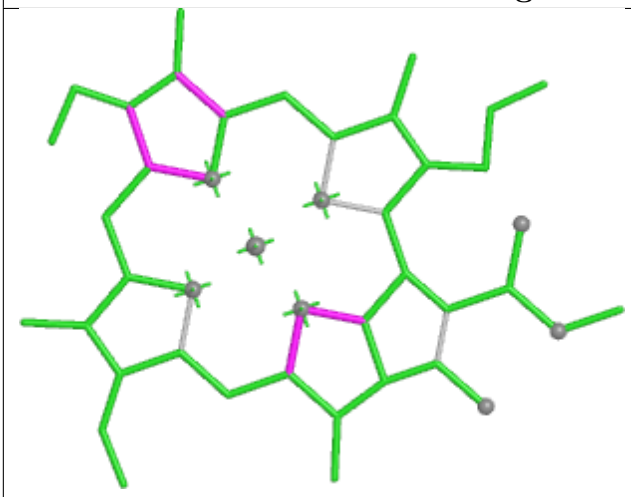


Torsions

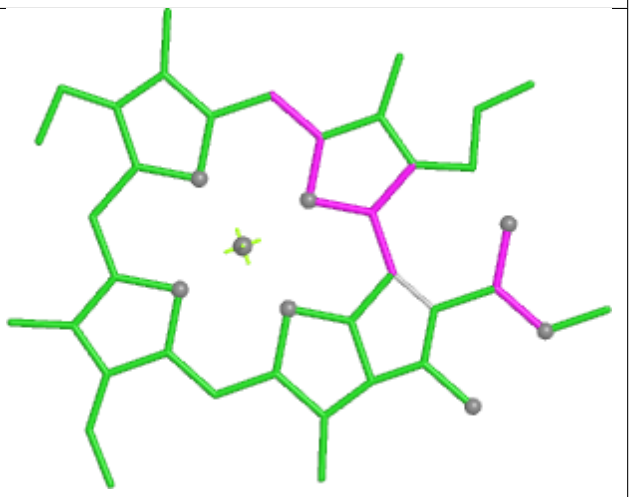


Rings

Ligand CLA B3 310



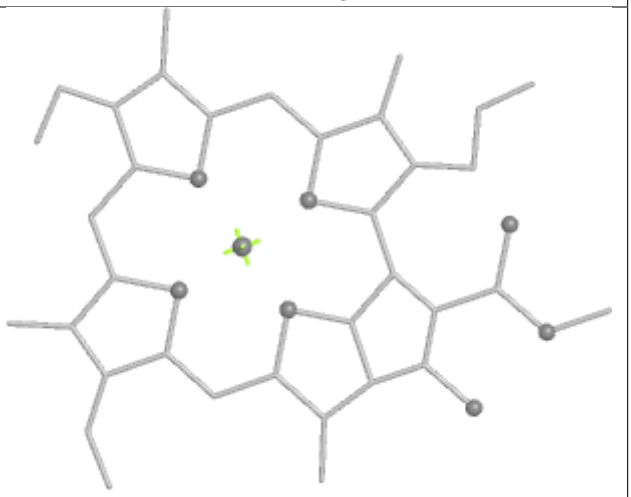
Bond lengths



Bond angles

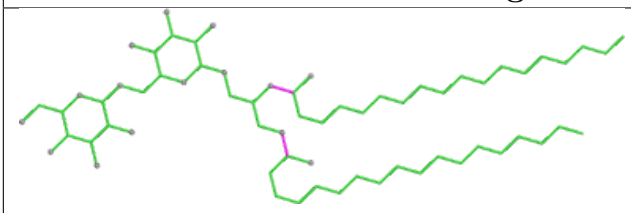


Torsions

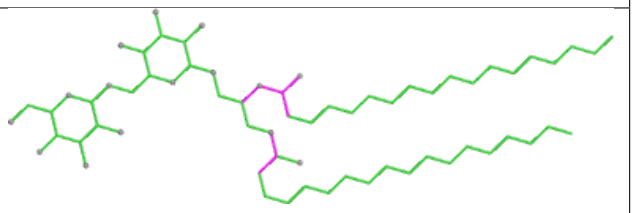


Rings

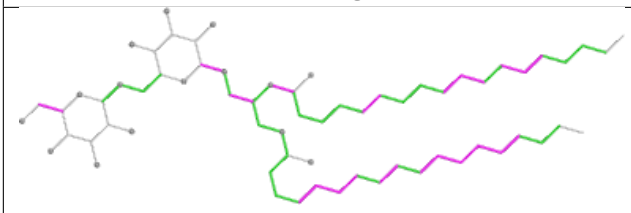
Ligand DGD AB 851



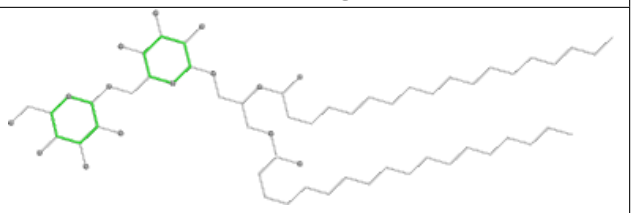
Bond lengths



Bond angles

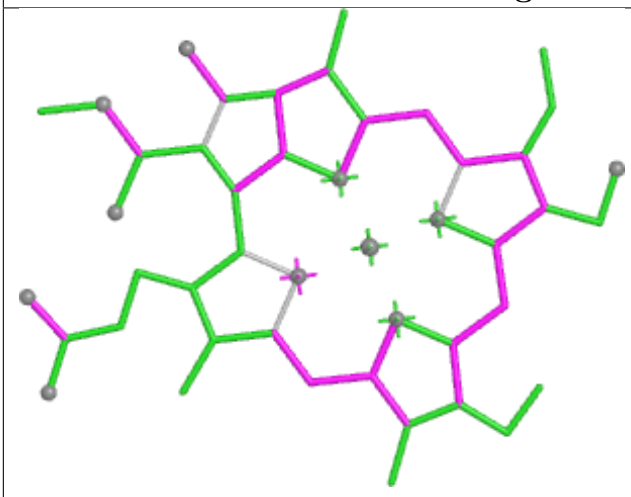


Torsions

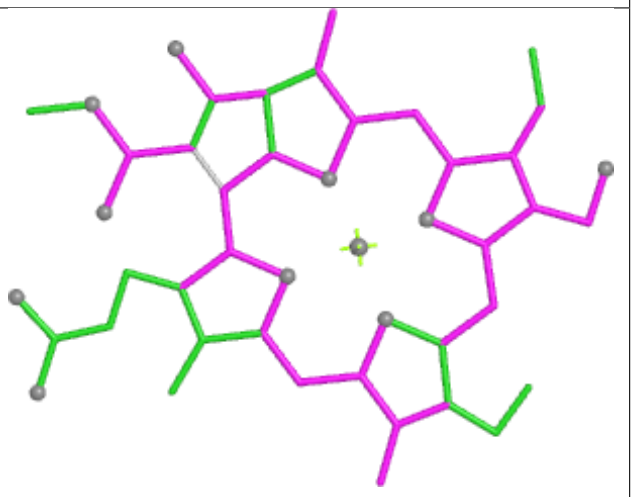


Rings

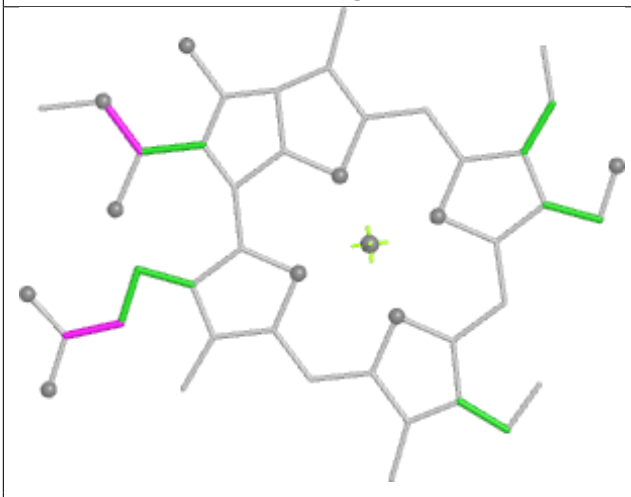
Ligand CHL B2 607



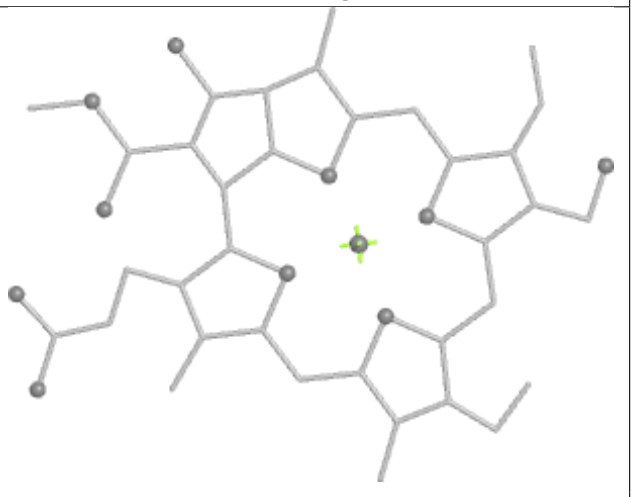
Bond lengths



Bond angles

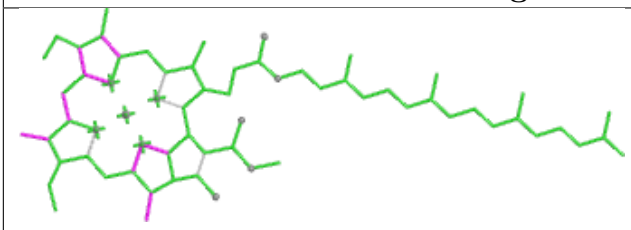


Torsions

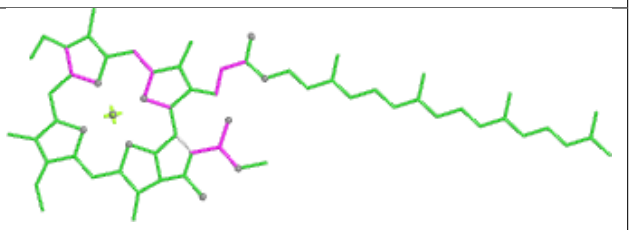


Rings

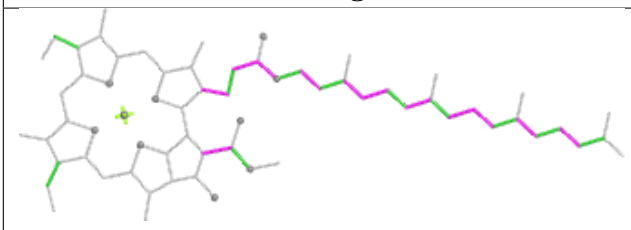
Ligand CLA AA 827



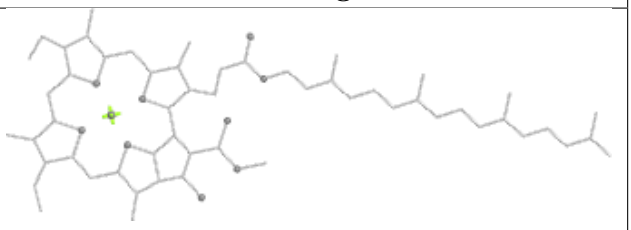
Bond lengths



Bond angles

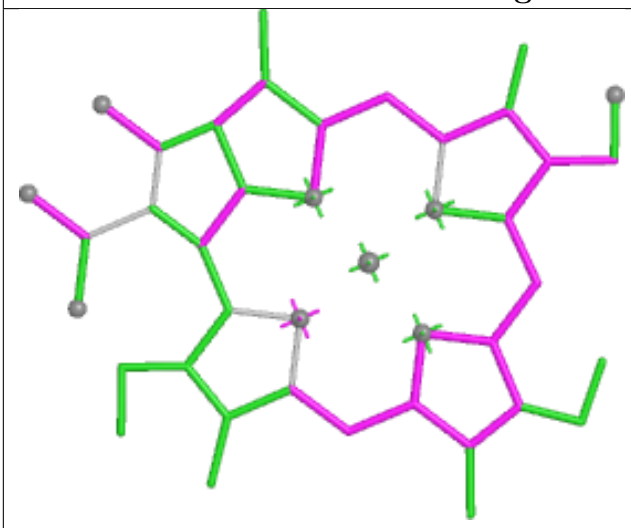


Torsions

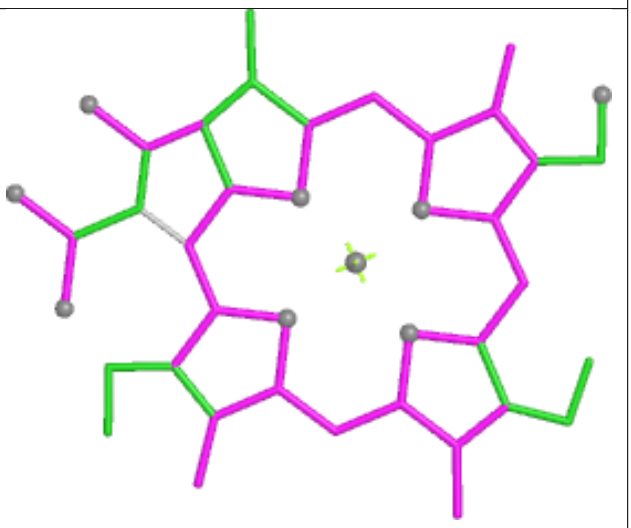


Rings

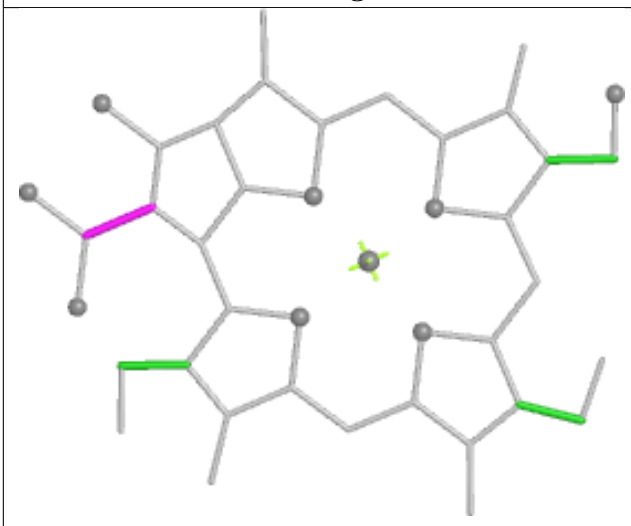
Ligand CHL A4 304



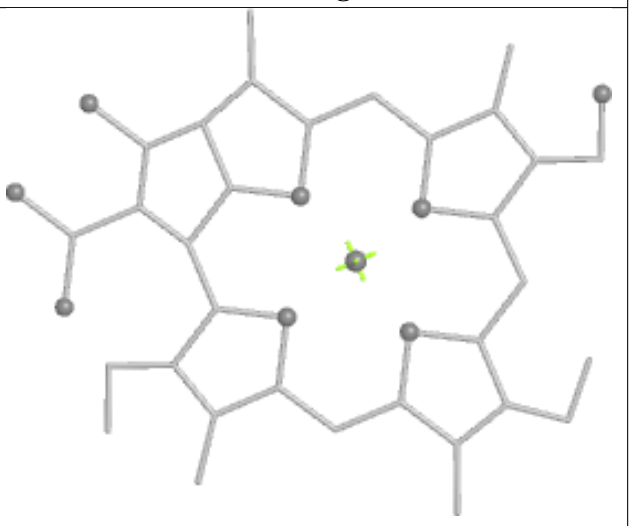
Bond lengths



Bond angles

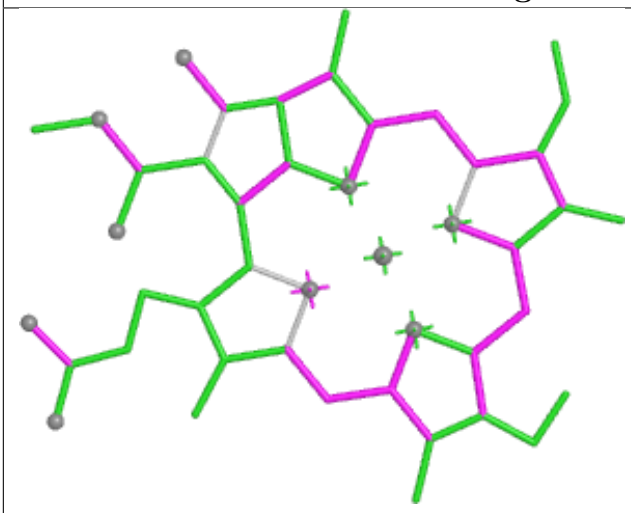


Torsions

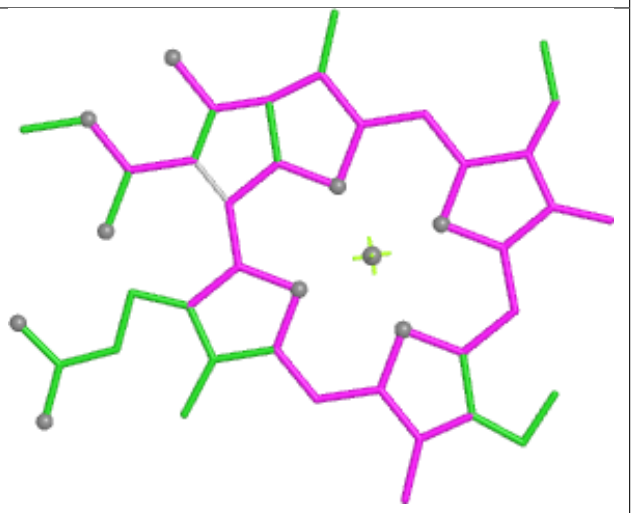


Rings

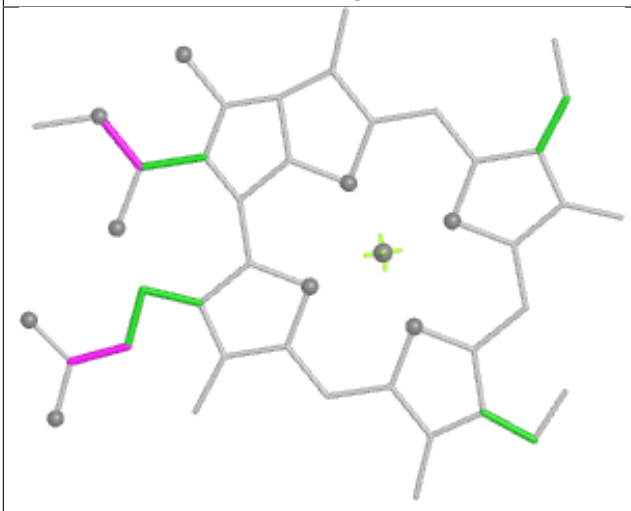
Ligand CHL A3 307



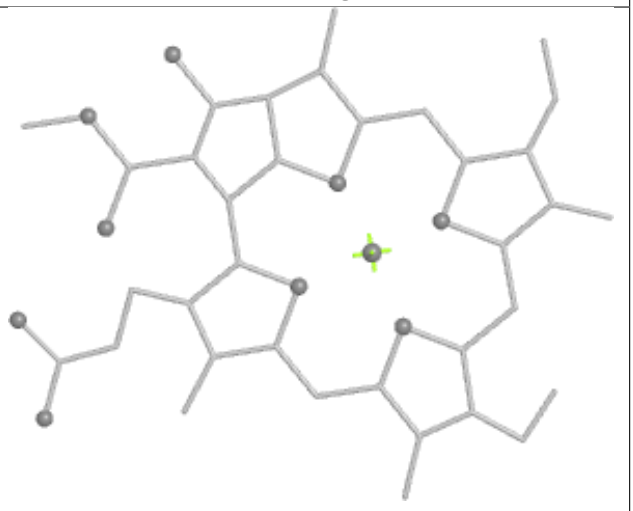
Bond lengths



Bond angles

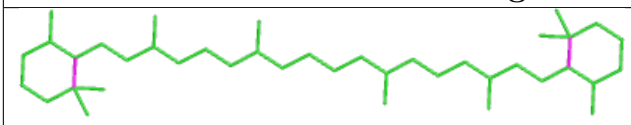


Torsions

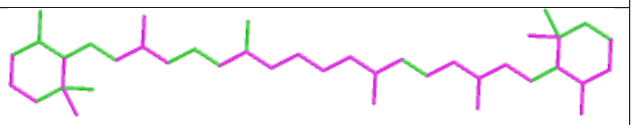


Rings

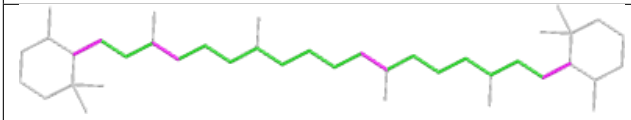
Ligand BCR AA 849



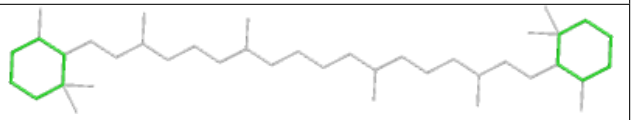
Bond lengths



Bond angles

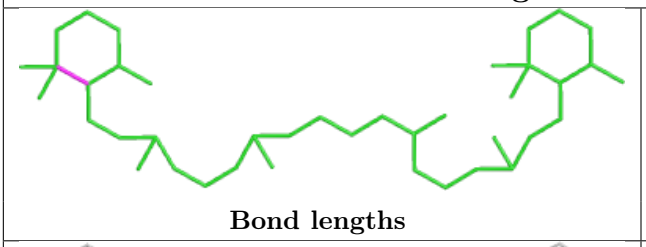


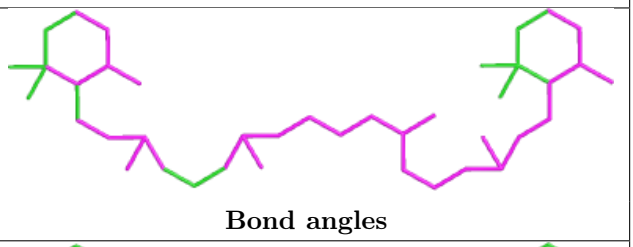
Torsions

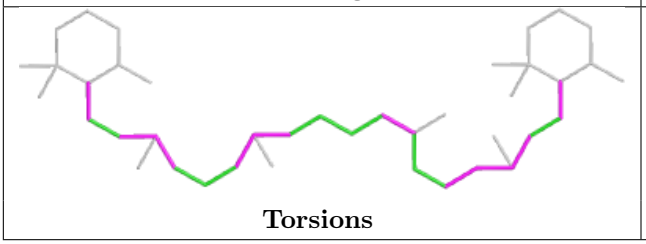


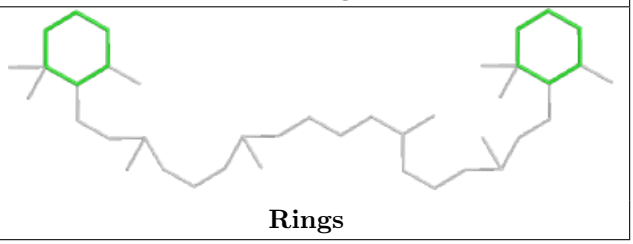
Rings

Ligand BCR BL 306


Bond lengths

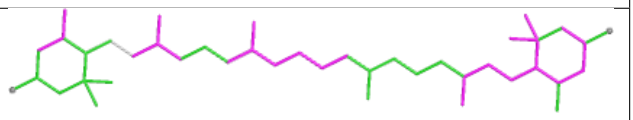

Bond angles

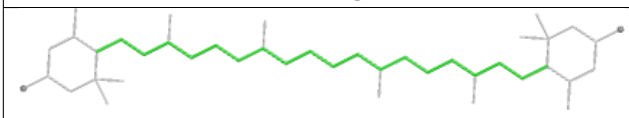

Torsions

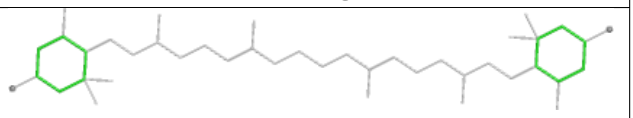

Rings

Ligand LUT A3 316

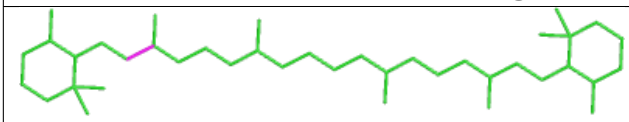

Bond lengths

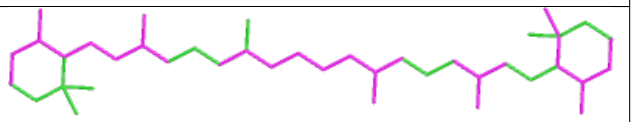

Bond angles

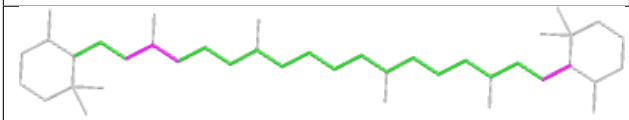

Torsions

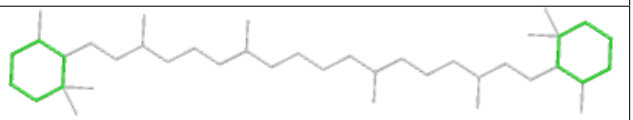

Rings

Ligand BCR BB 846

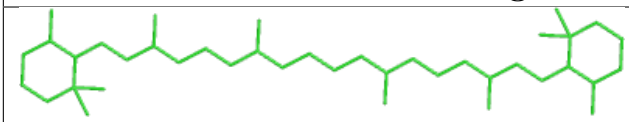

Bond lengths

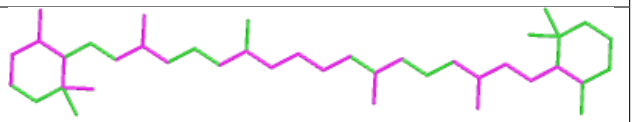

Bond angles

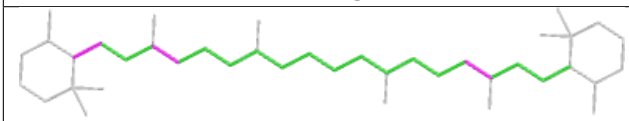

Torsions

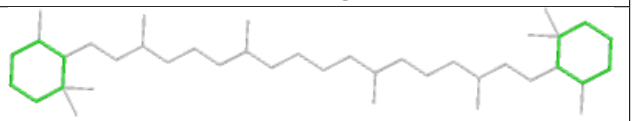

Rings

Ligand BCR AB 846

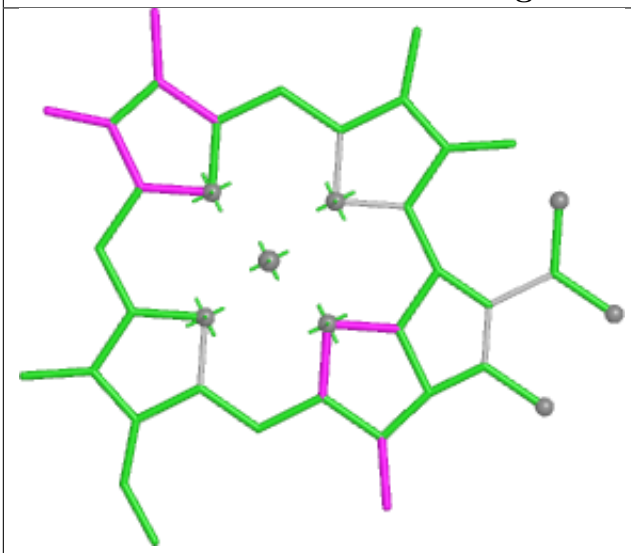

Bond lengths


Bond angles

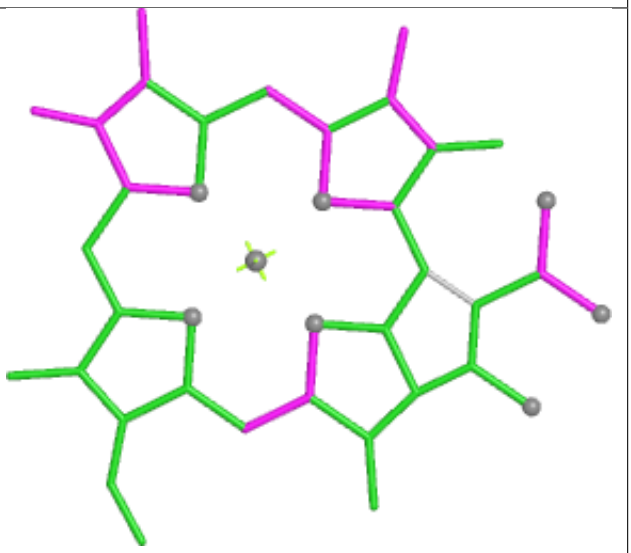

Torsions


Rings

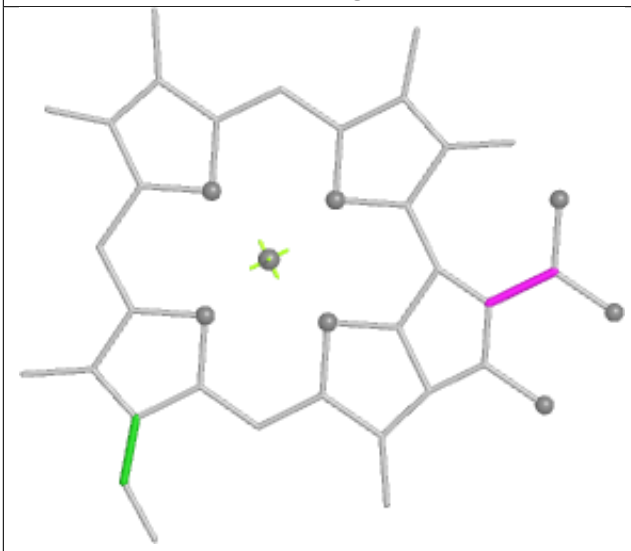
Ligand CLA B1 310



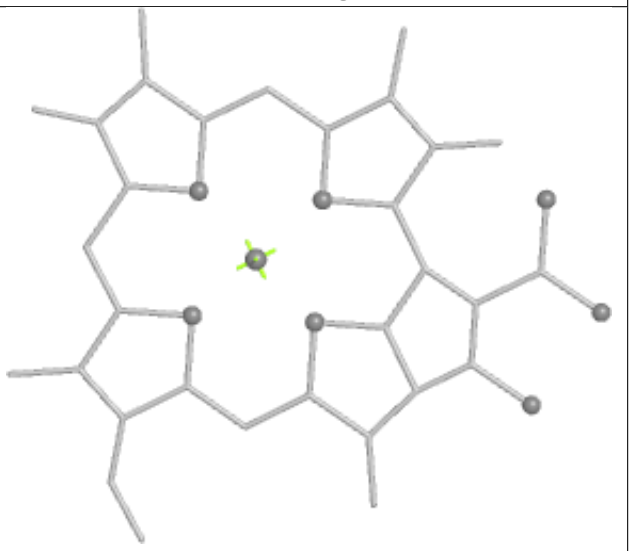
Bond lengths



Bond angles

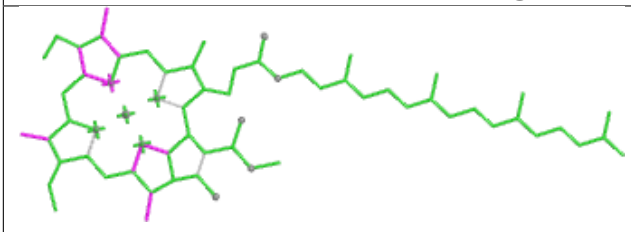


Torsions

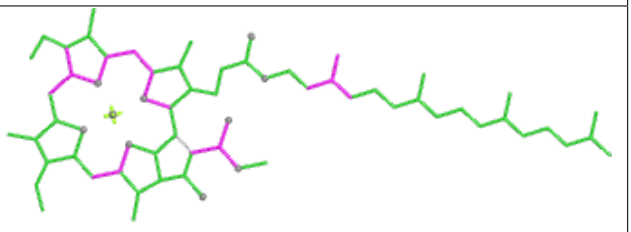


Rings

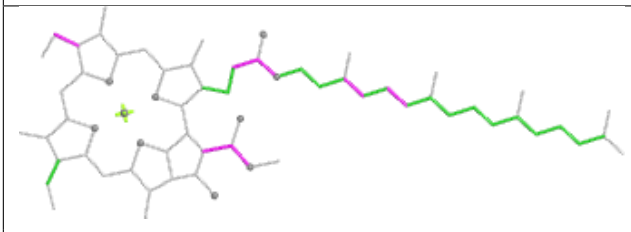
Ligand CLA BA 834



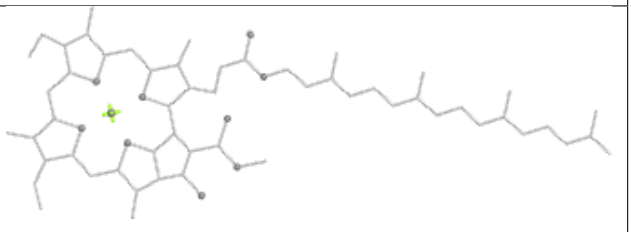
Bond lengths



Bond angles

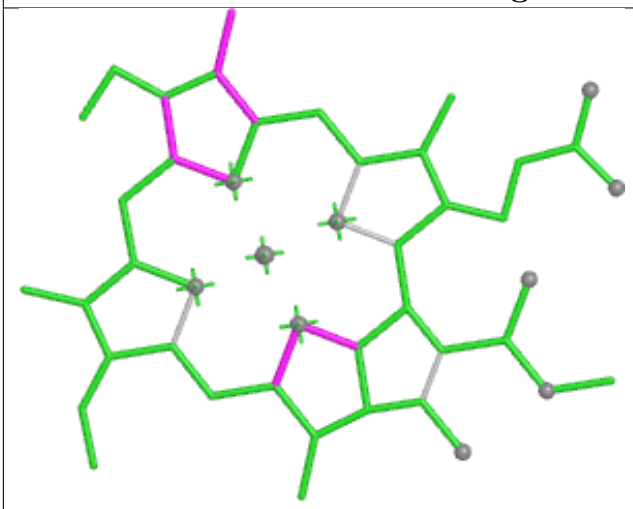


Torsions

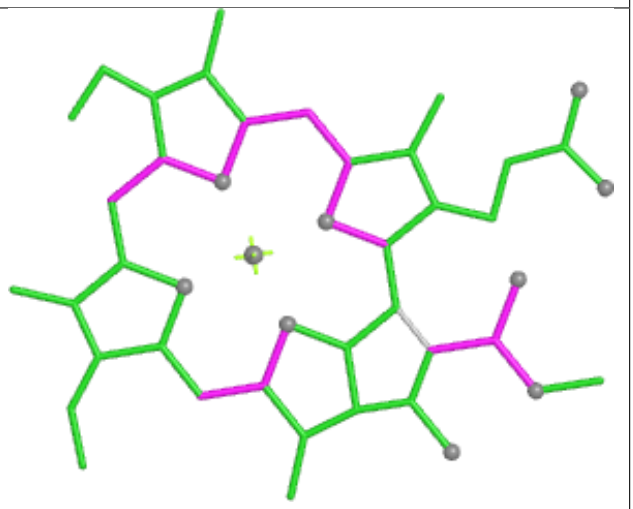


Rings

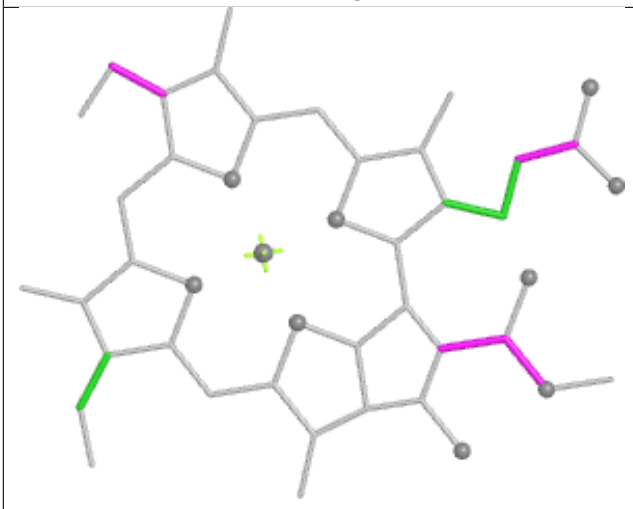
Ligand CLA BA 836



Bond lengths



Bond angles

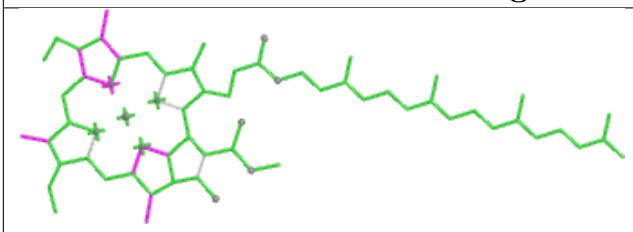


Torsions

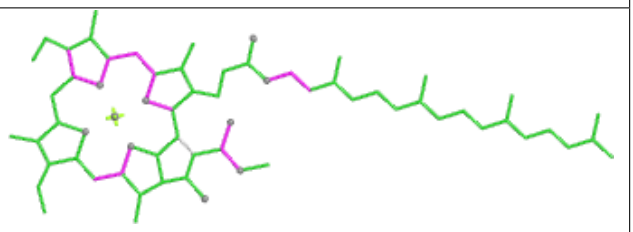


Rings

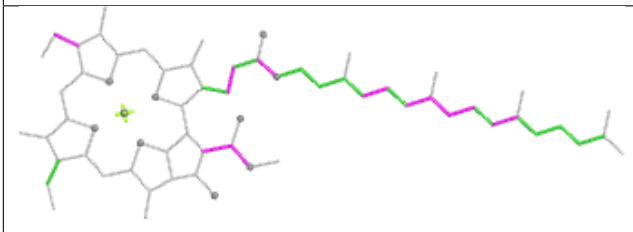
Ligand CLA AA 813



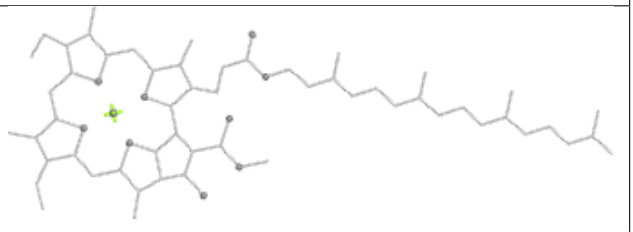
Bond lengths



Bond angles

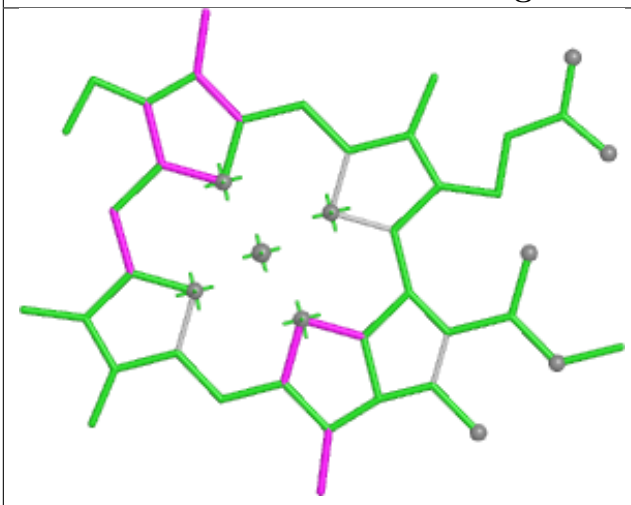


Torsions

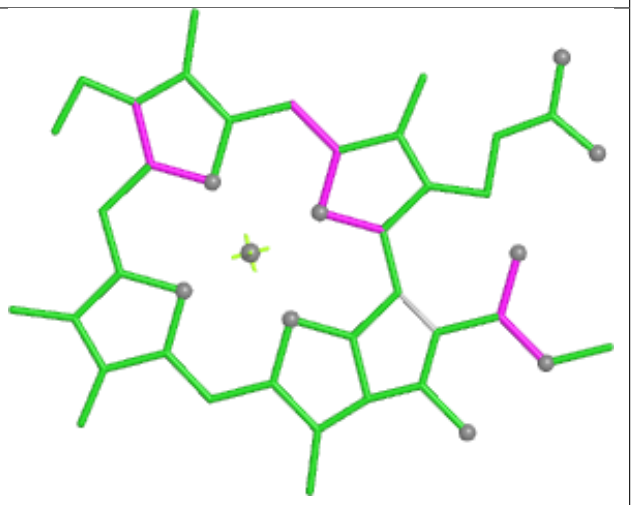


Rings

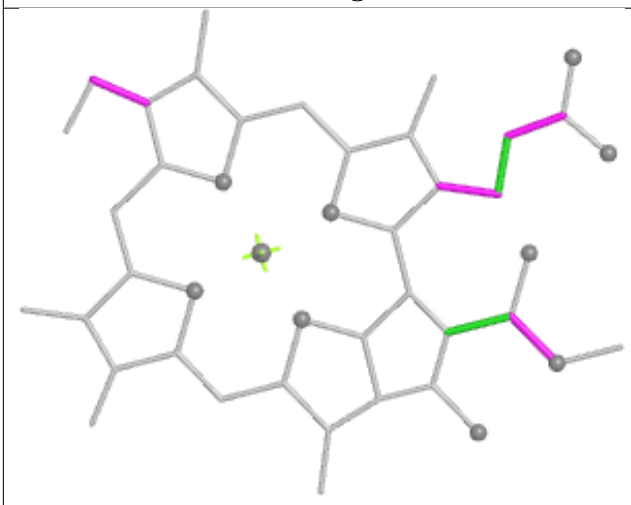
Ligand CLA A6 612



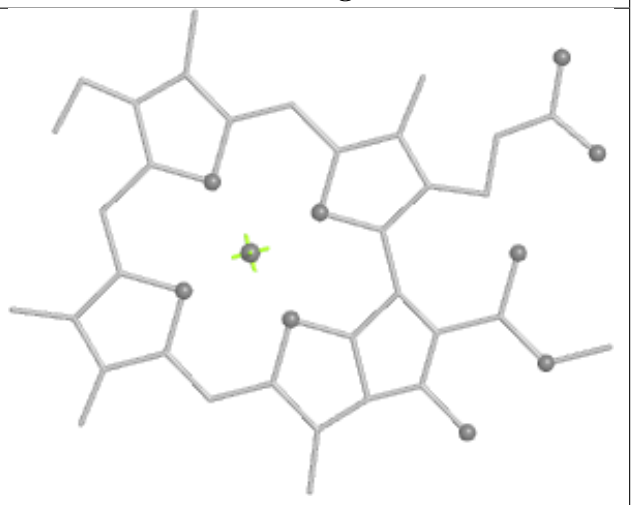
Bond lengths



Bond angles

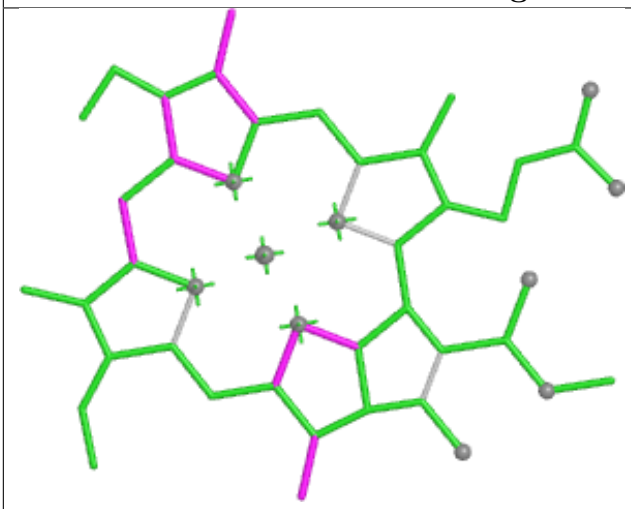


Torsions

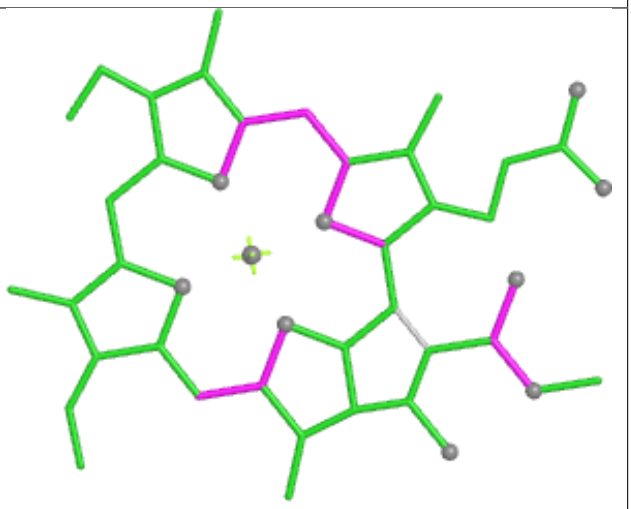


Rings

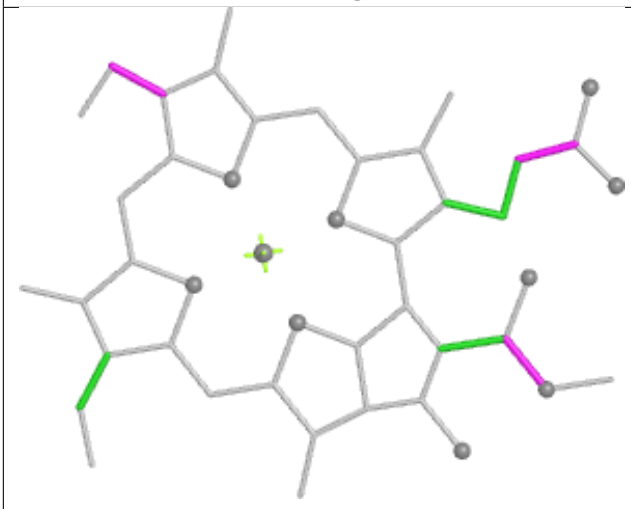
Ligand CLA AG 204



Bond lengths



Bond angles

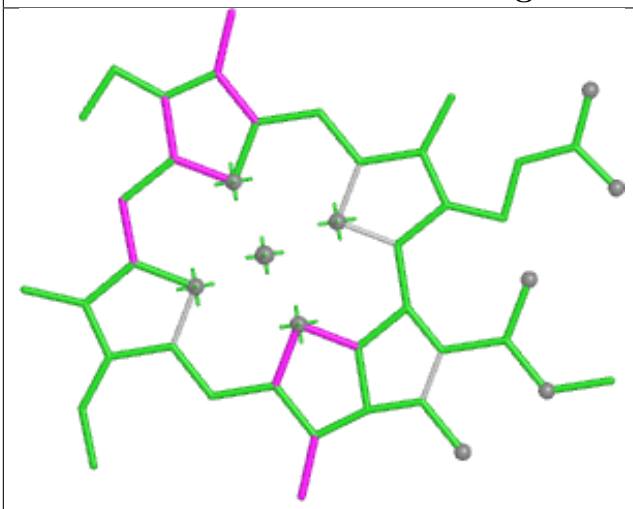


Torsions

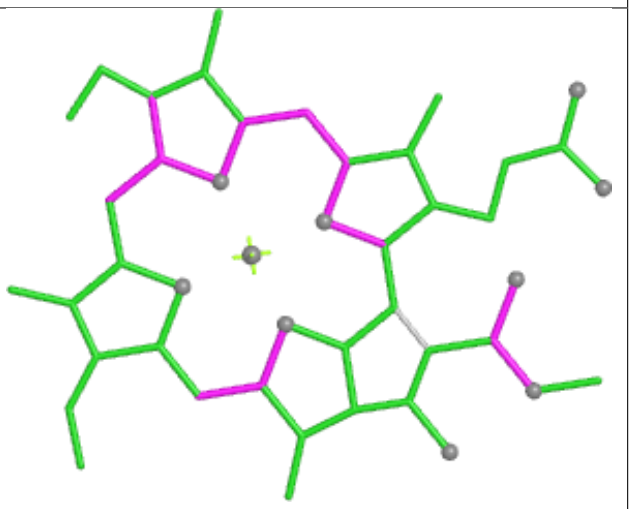


Rings

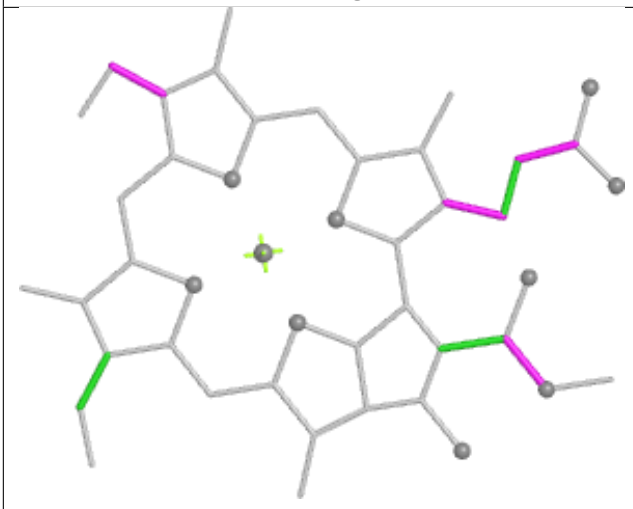
Ligand CLA B5 613



Bond lengths



Bond angles

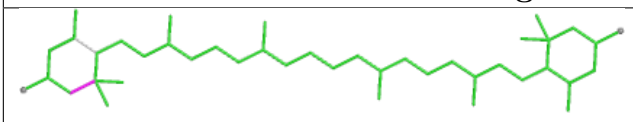


Torsions

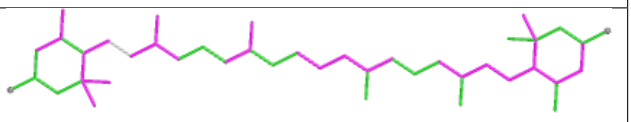


Rings

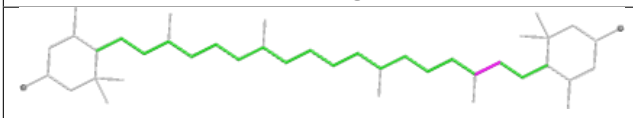
Ligand LUT B5 614



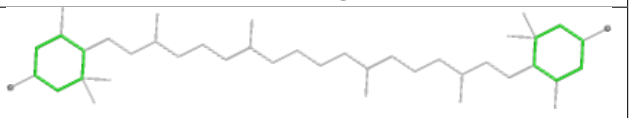
Bond lengths



Bond angles

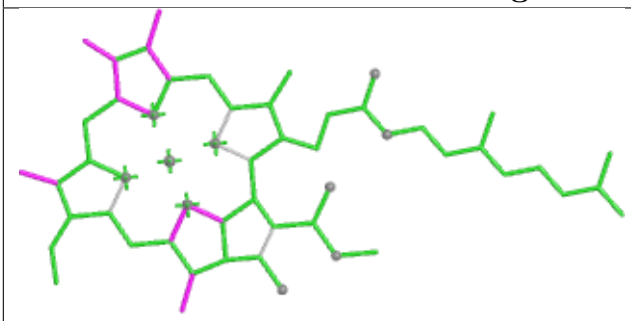


Torsions

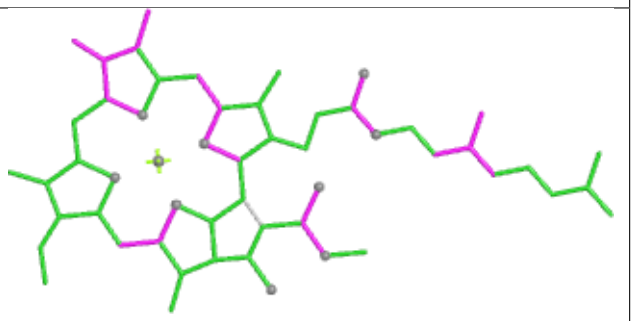


Rings

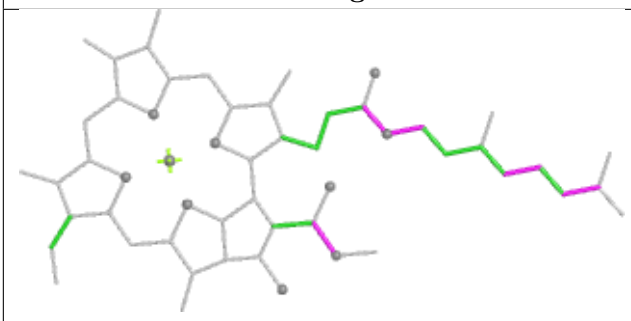
Ligand CLA AB 812



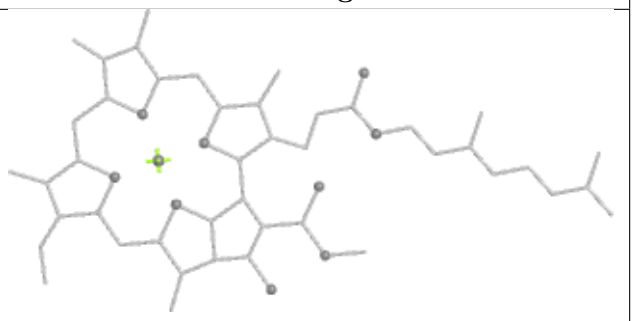
Bond lengths



Bond angles

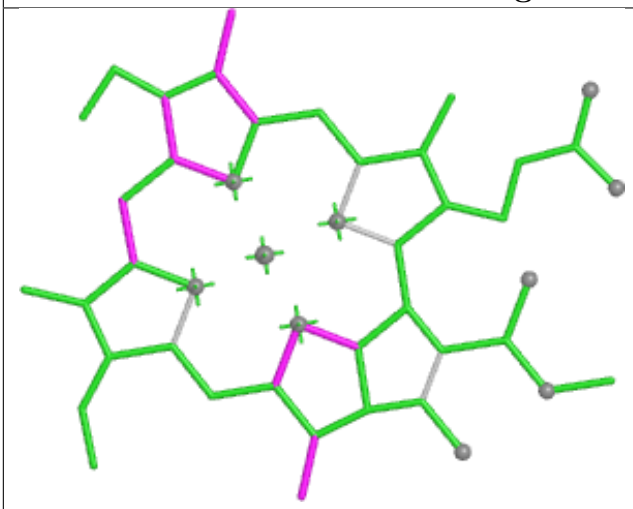


Torsions

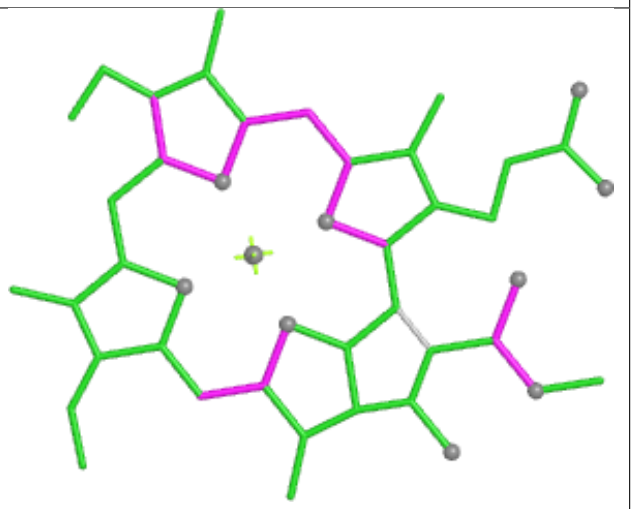


Rings

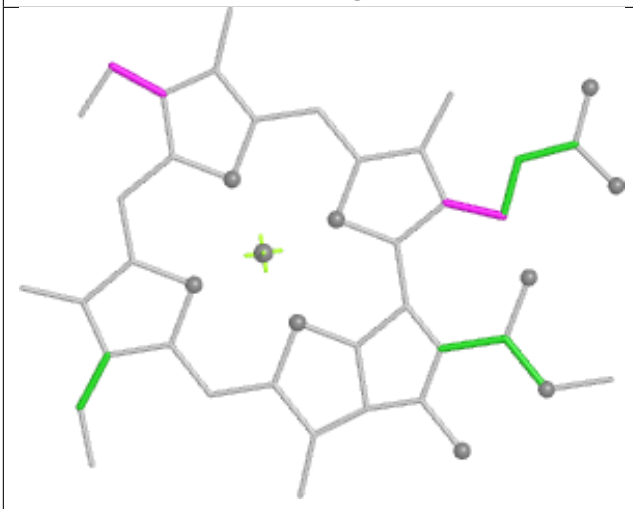
Ligand CLA A4 307



Bond lengths



Bond angles

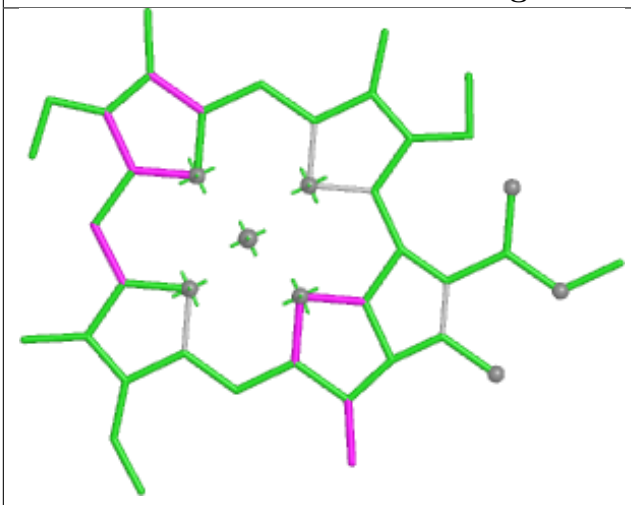


Torsions

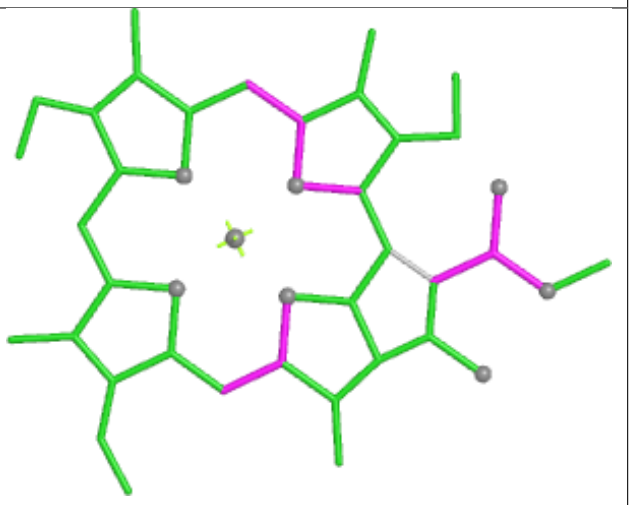


Rings

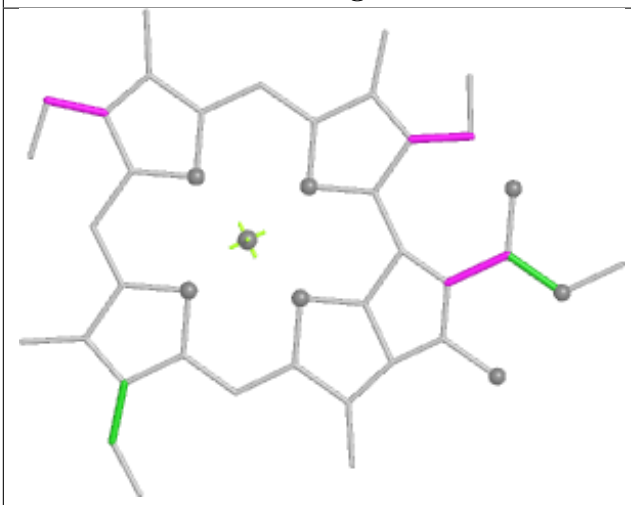
Ligand CLA AA 822



Bond lengths



Bond angles



Torsions

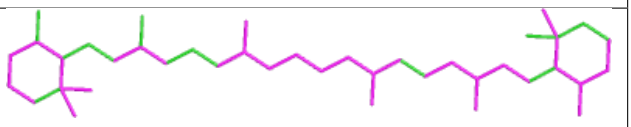


Rings

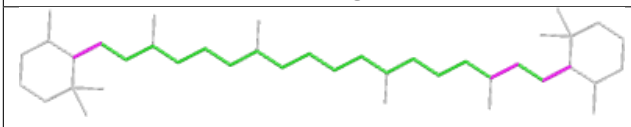
Ligand BCR AA 846



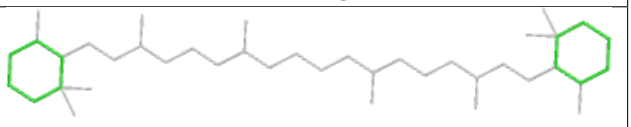
Bond lengths



Bond angles

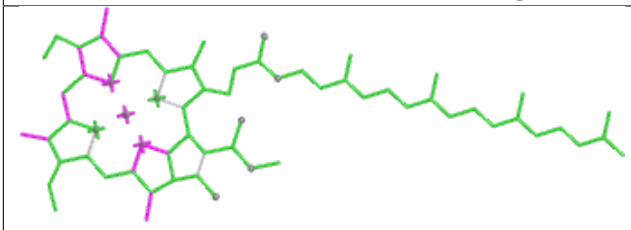


Torsions

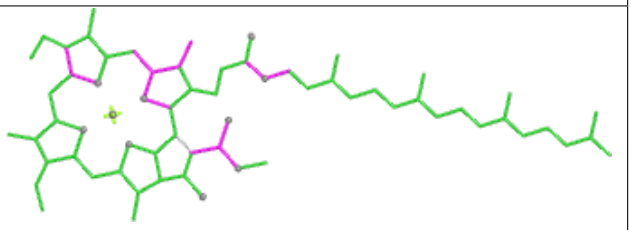


Rings

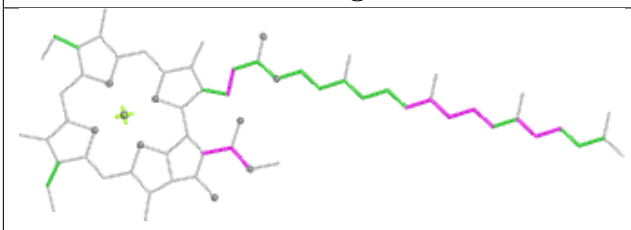
Ligand CLA AB 825



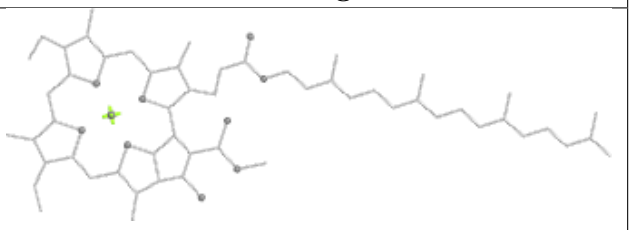
Bond lengths



Bond angles

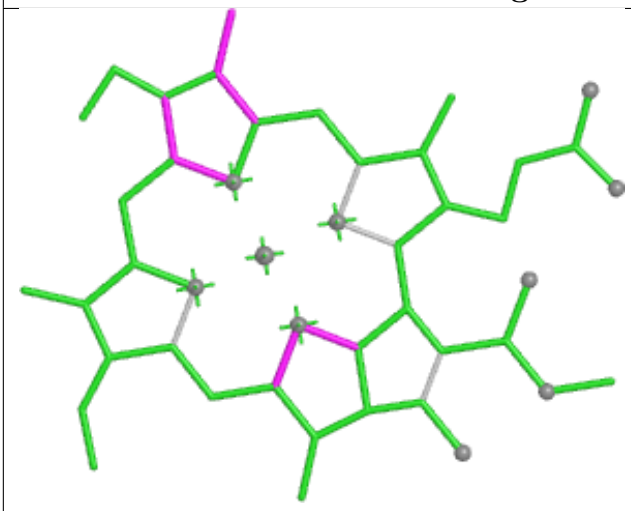


Torsions

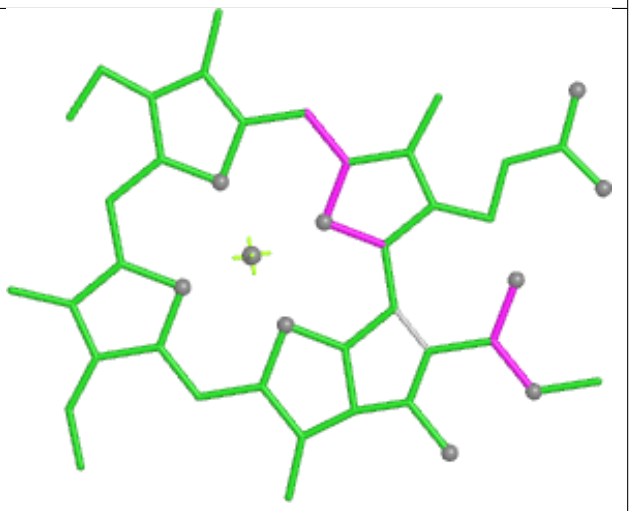


Rings

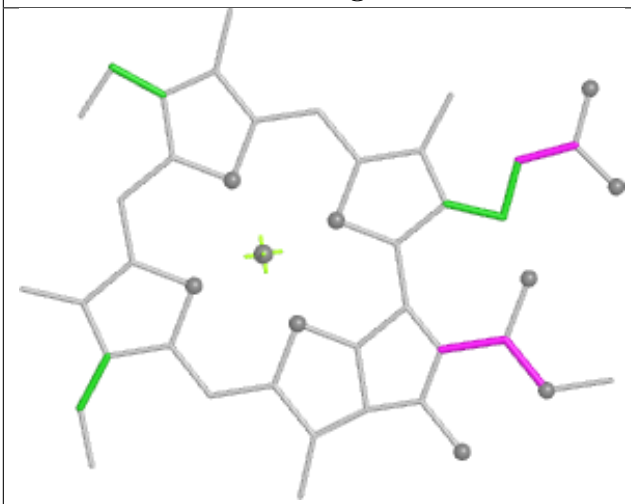
Ligand CLA BA 835



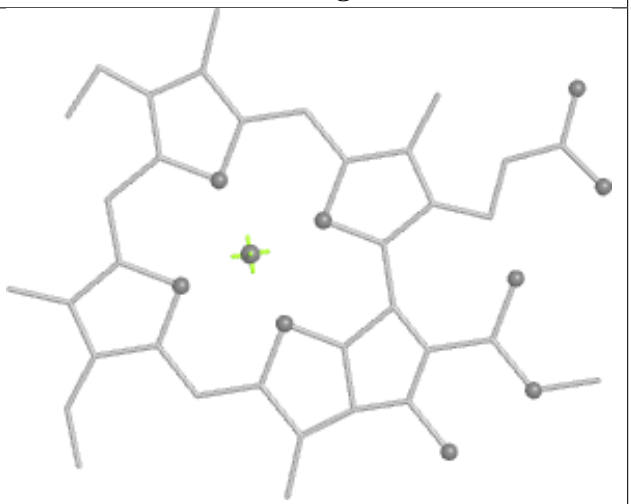
Bond lengths



Bond angles

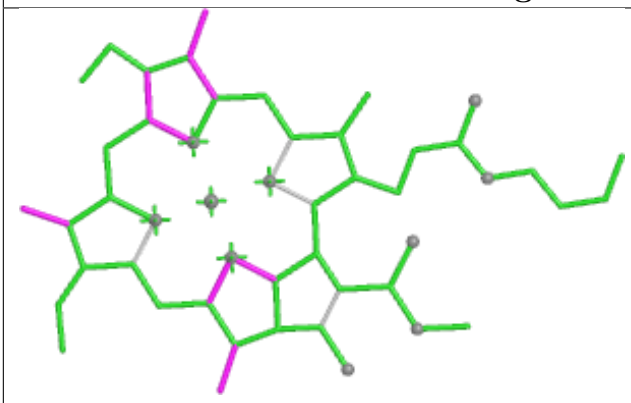


Torsions

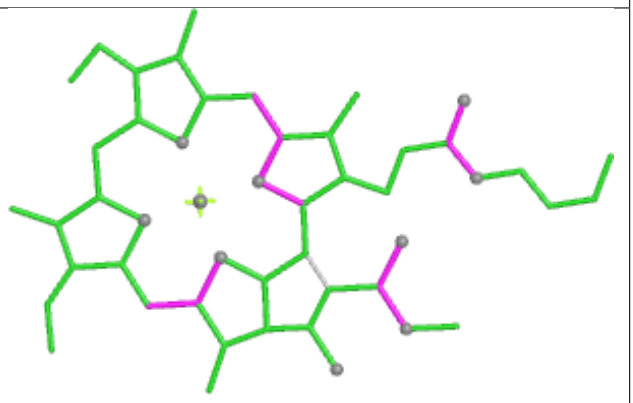


Rings

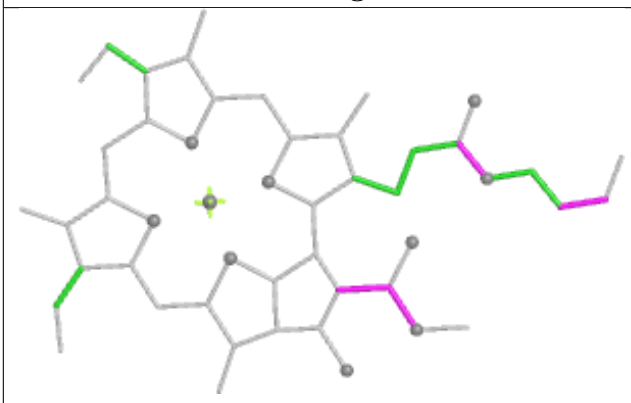
Ligand CLA A1 306



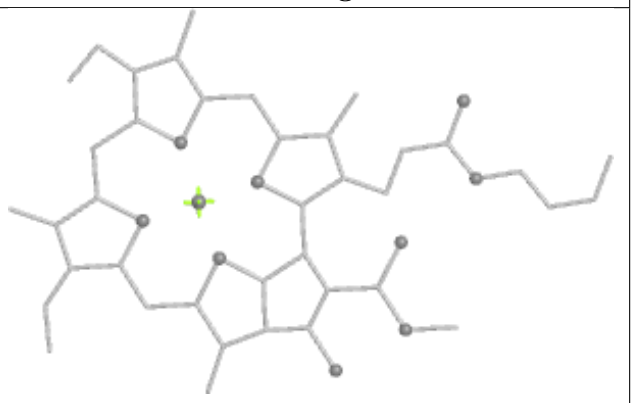
Bond lengths



Bond angles

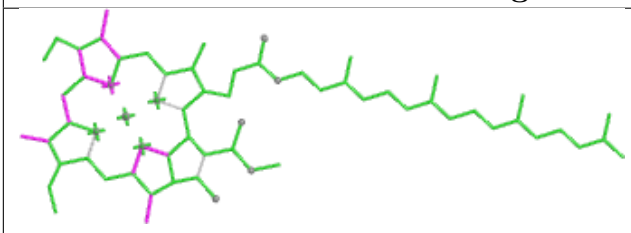


Torsions

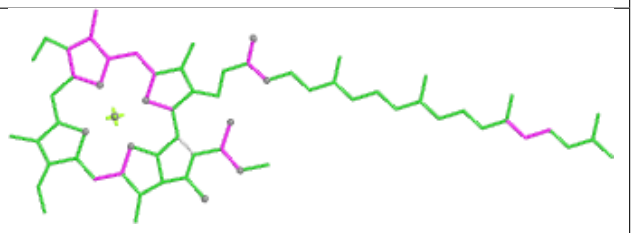


Rings

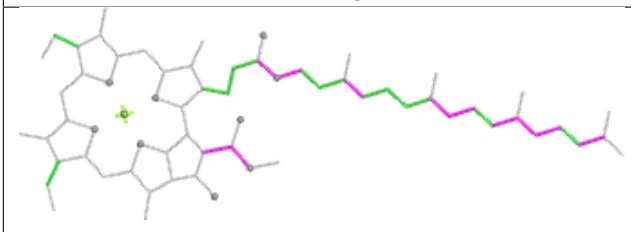
Ligand CLA AB 815



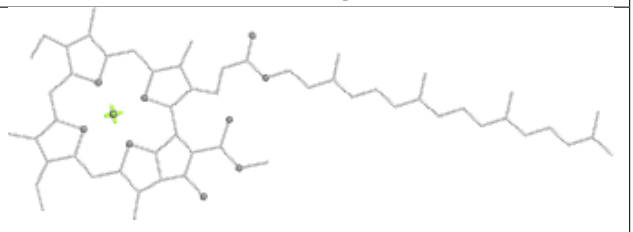
Bond lengths



Bond angles

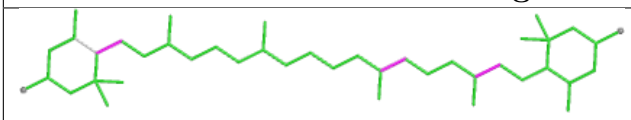


Torsions

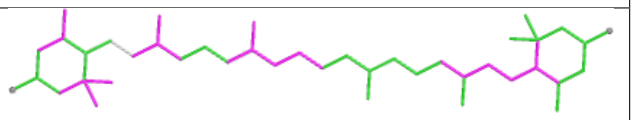


Rings

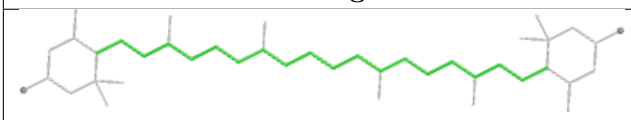
Ligand LUT AF 806



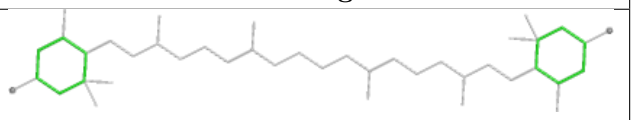
Bond lengths



Bond angles

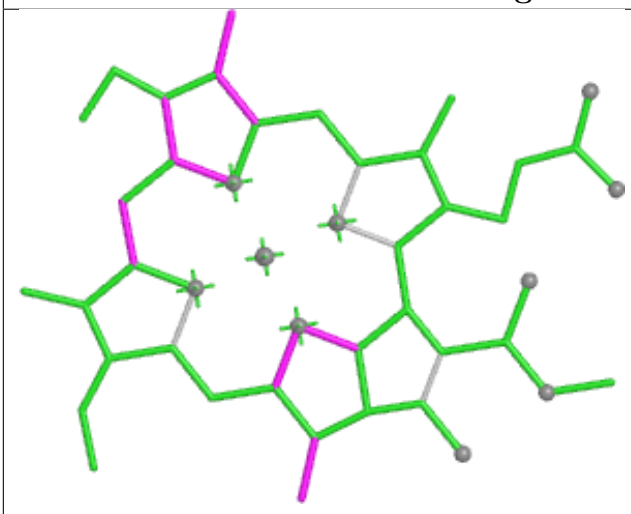


Torsions

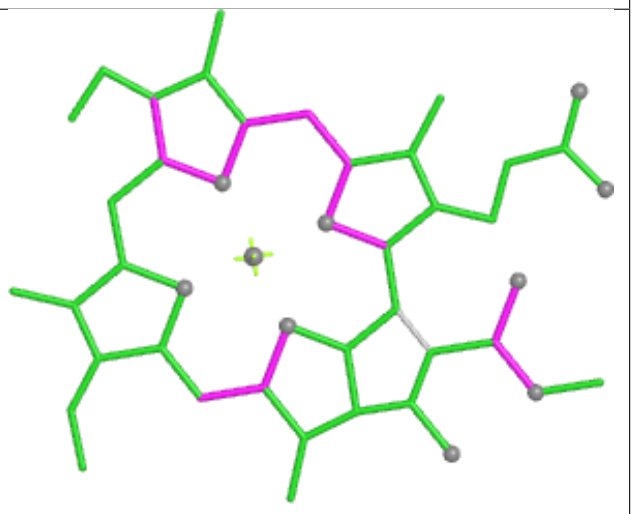


Rings

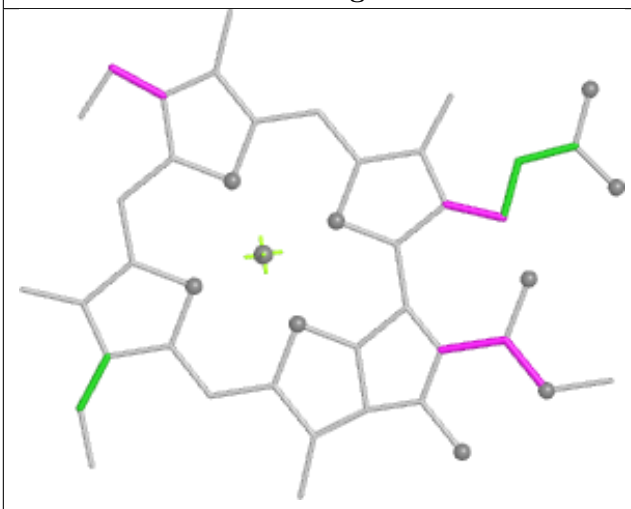
Ligand CLA A4 312



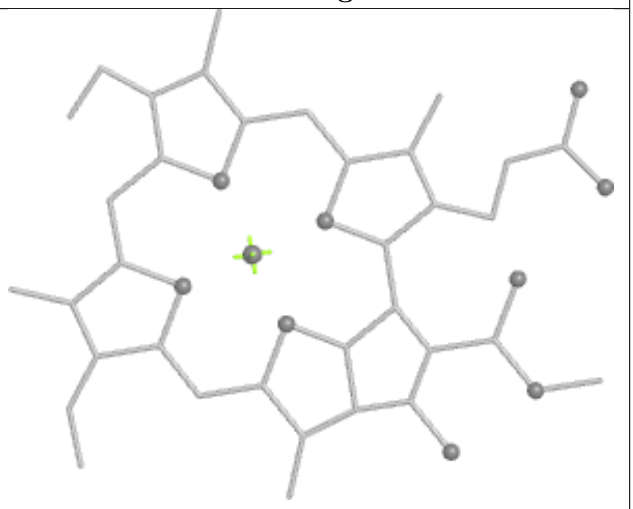
Bond lengths



Bond angles

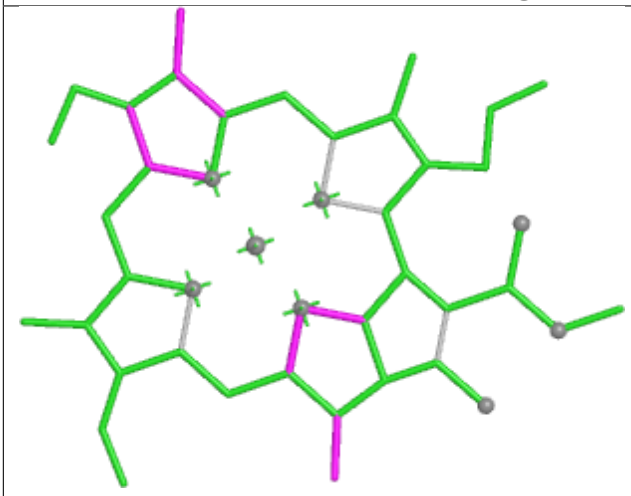


Torsions

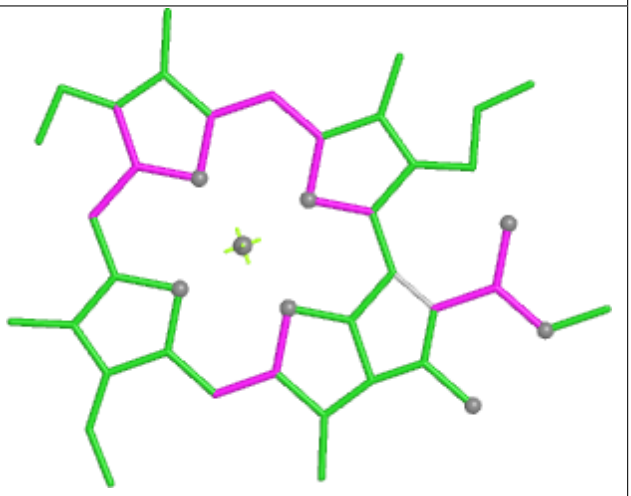


Rings

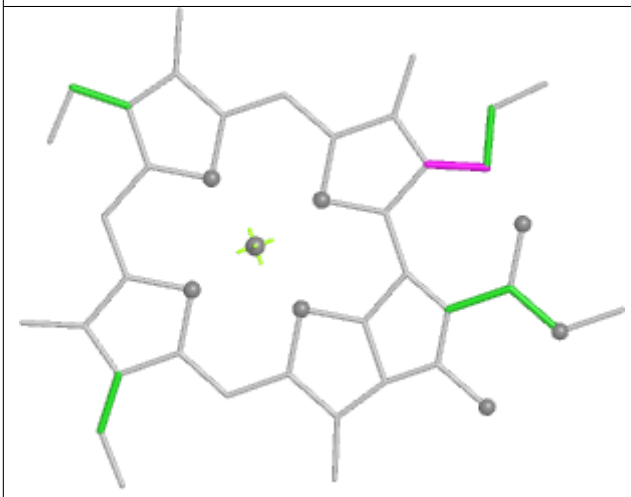
Ligand CLA B2 613



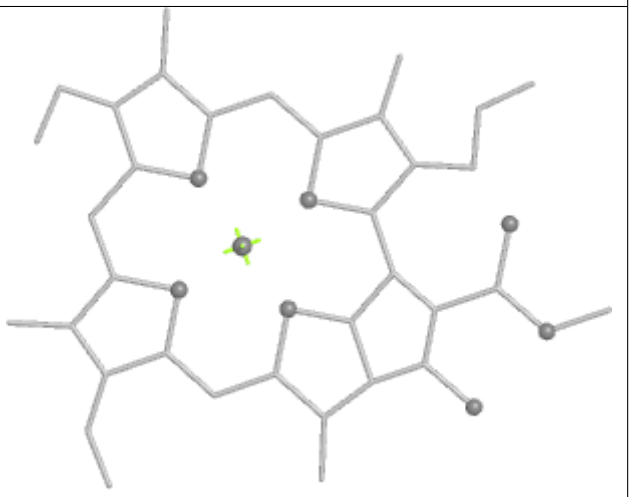
Bond lengths



Bond angles

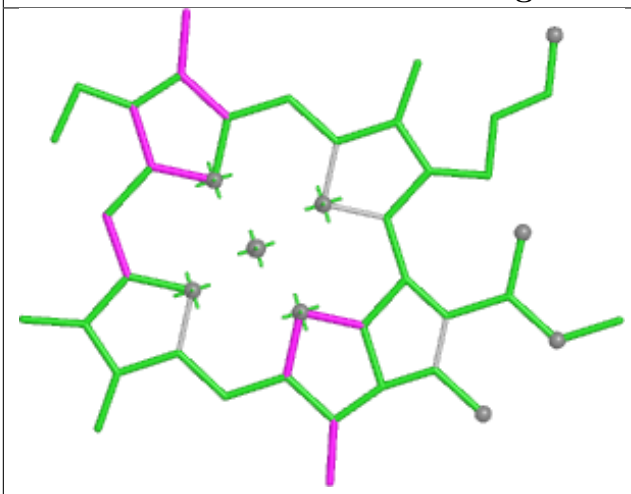


Torsions

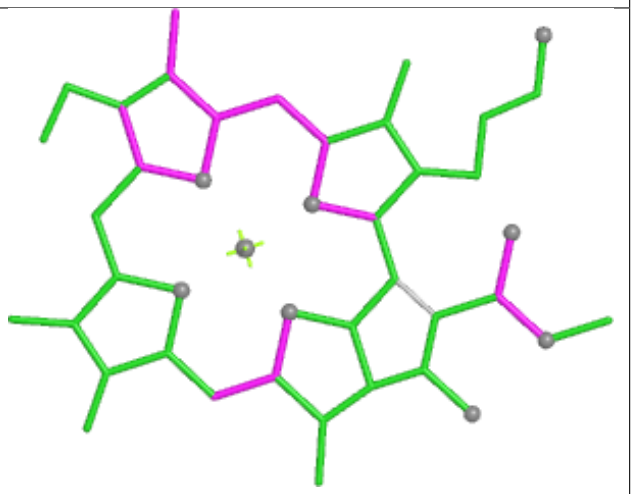


Rings

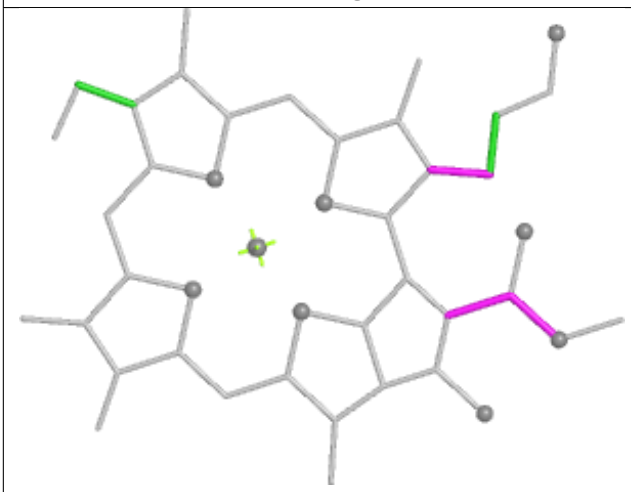
Ligand CLA B2 604



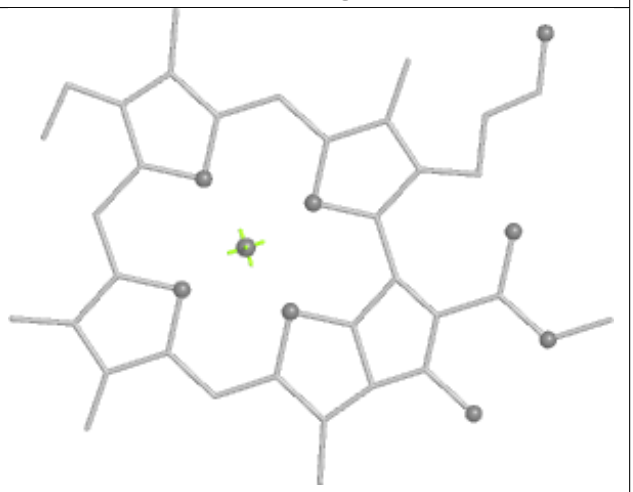
Bond lengths



Bond angles

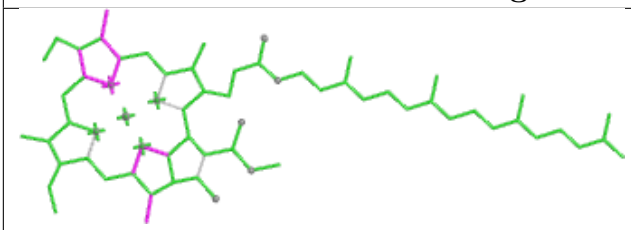


Torsions

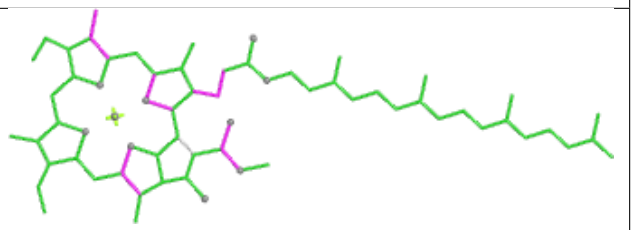


Rings

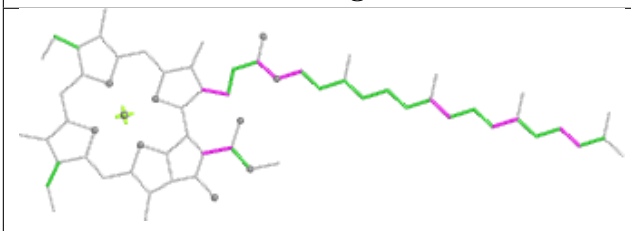
Ligand CLA AA 825



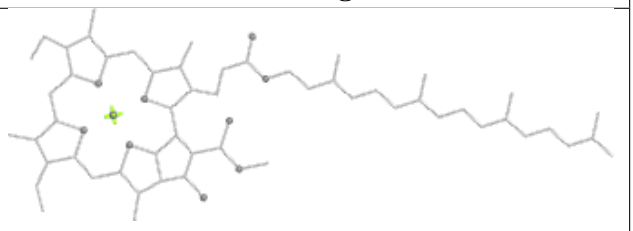
Bond lengths



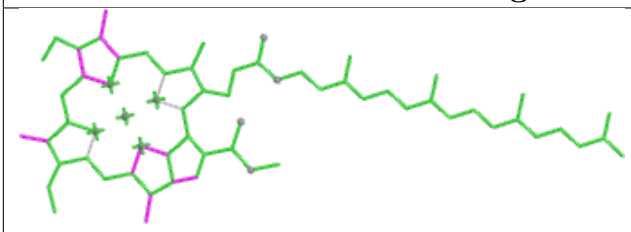
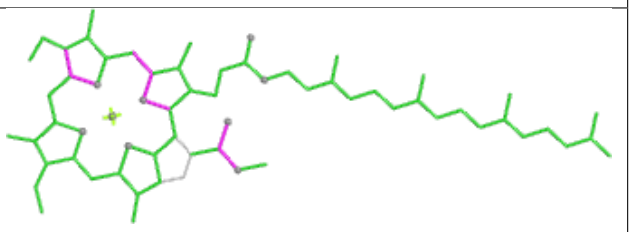
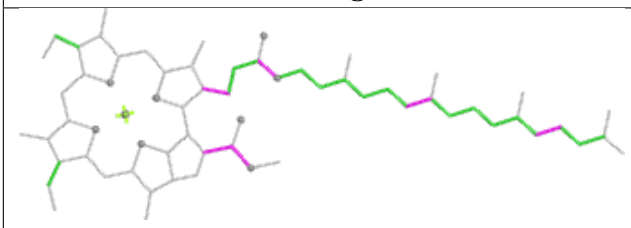
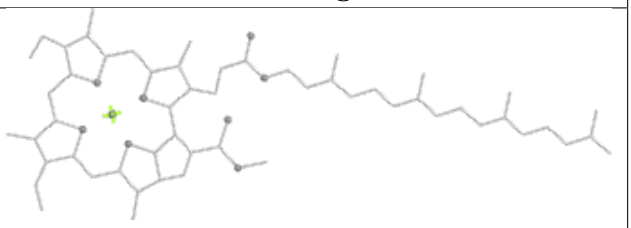
Bond angles

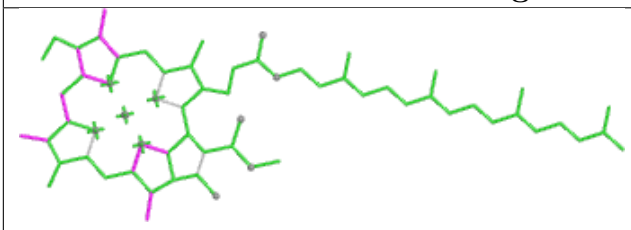
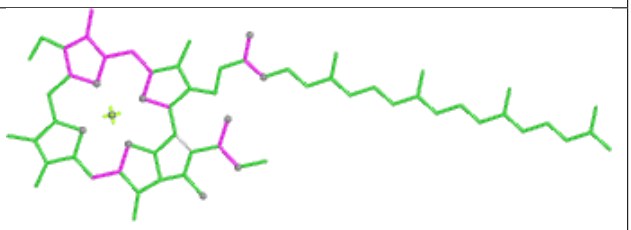
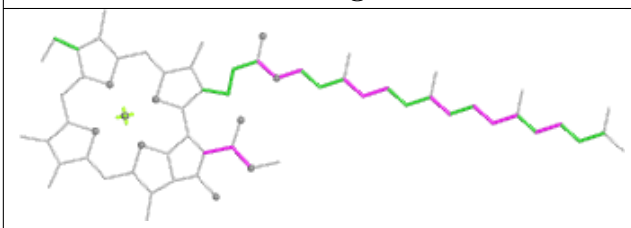
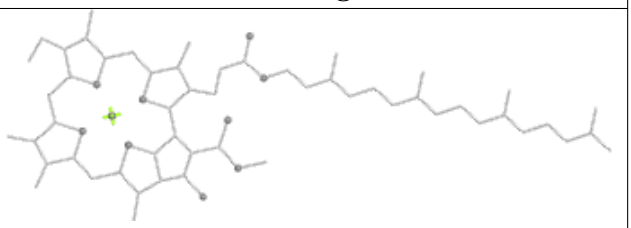


Torsions

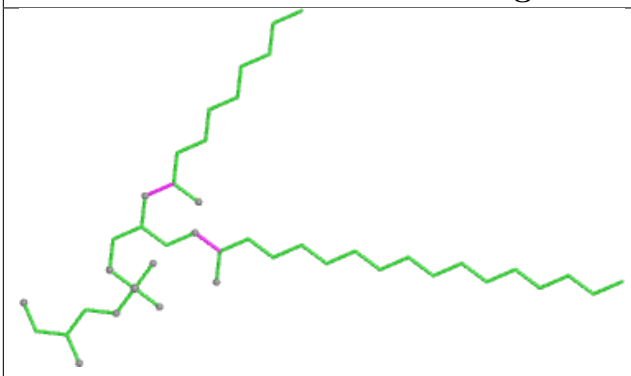


Rings

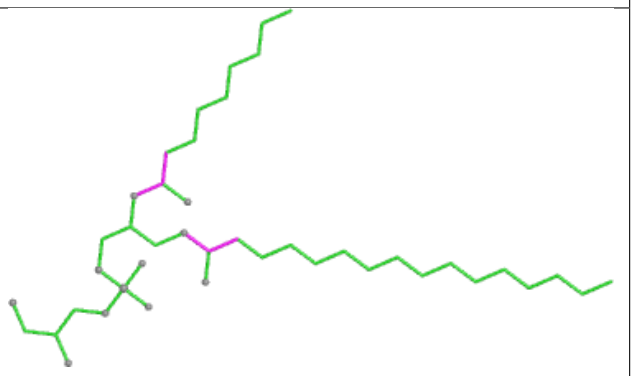
Ligand CLA AA 810	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA BB 816	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

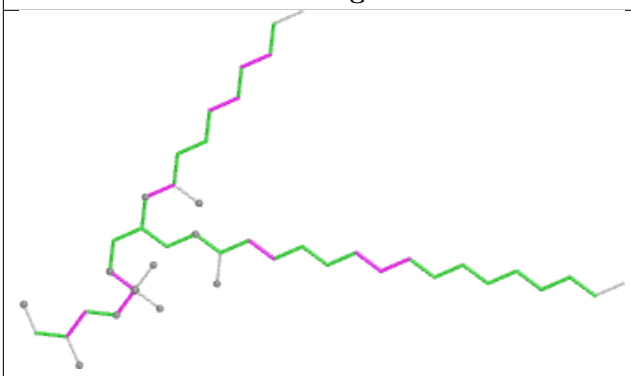
Ligand LHG B1 318



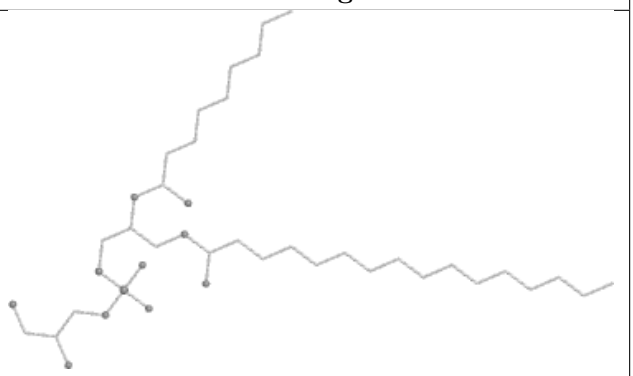
Bond lengths



Bond angles

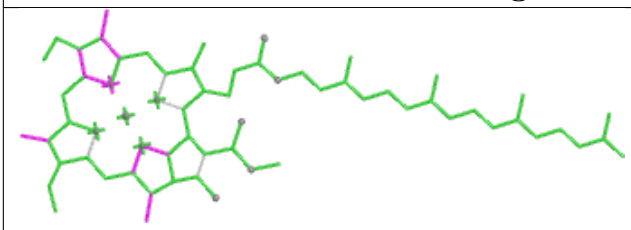


Torsions

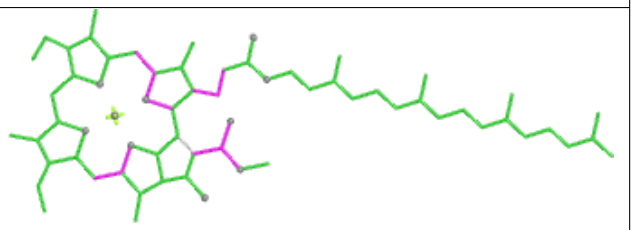


Rings

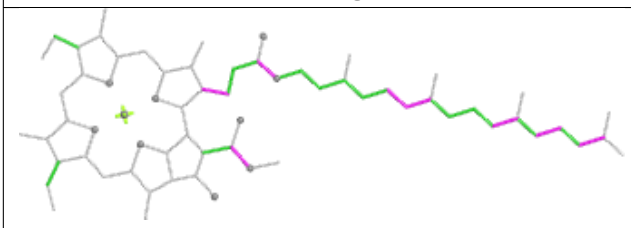
Ligand CLA AA 819



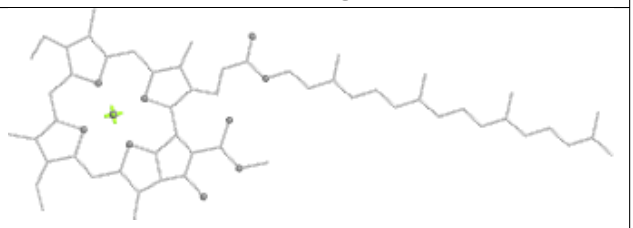
Bond lengths



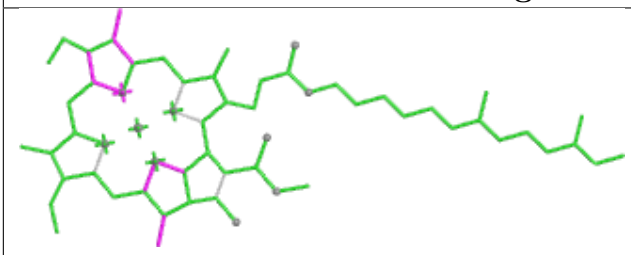
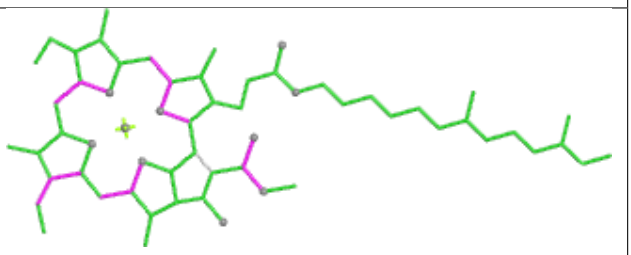
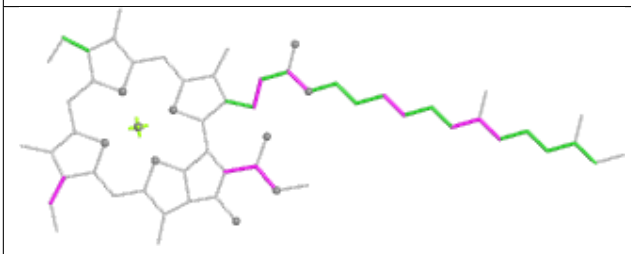
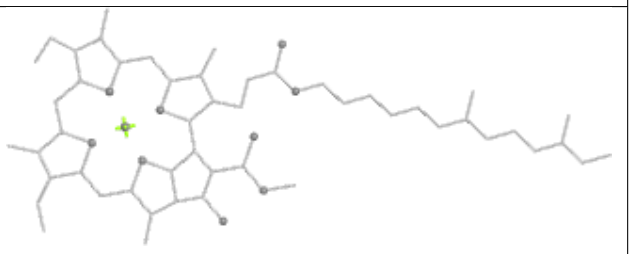
Bond angles

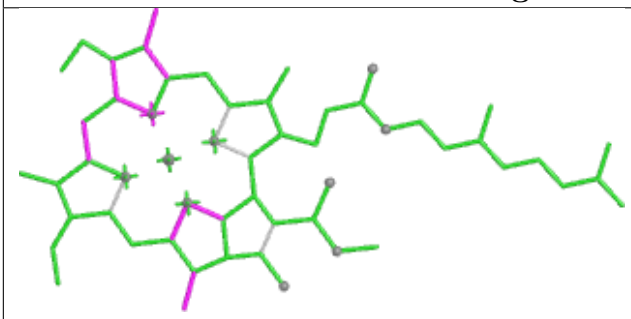
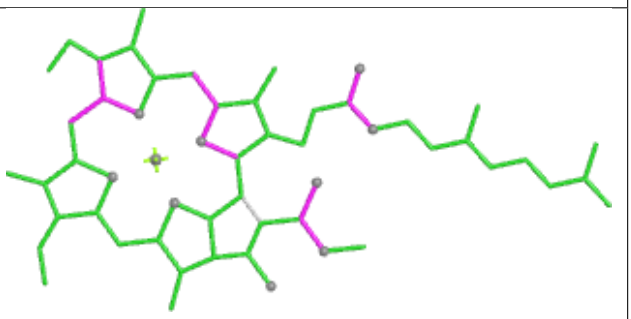
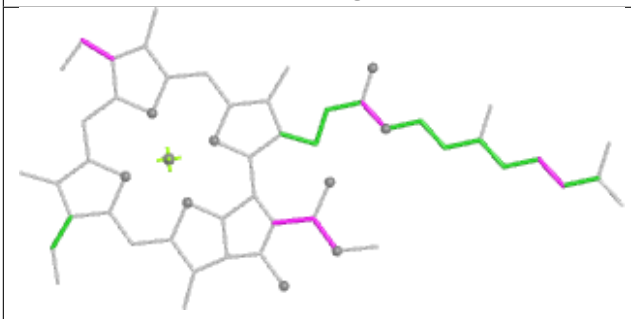
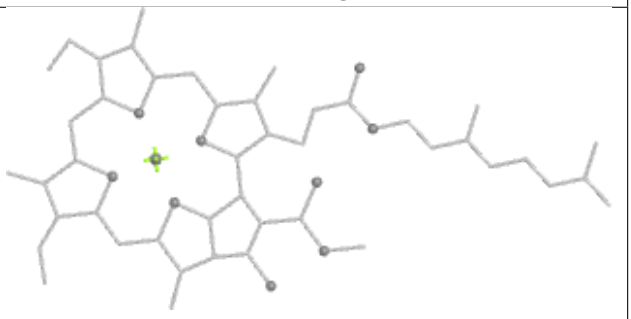


Torsions

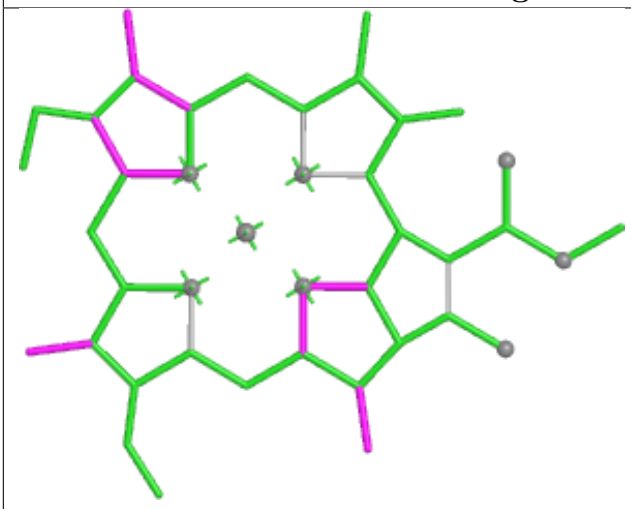


Rings

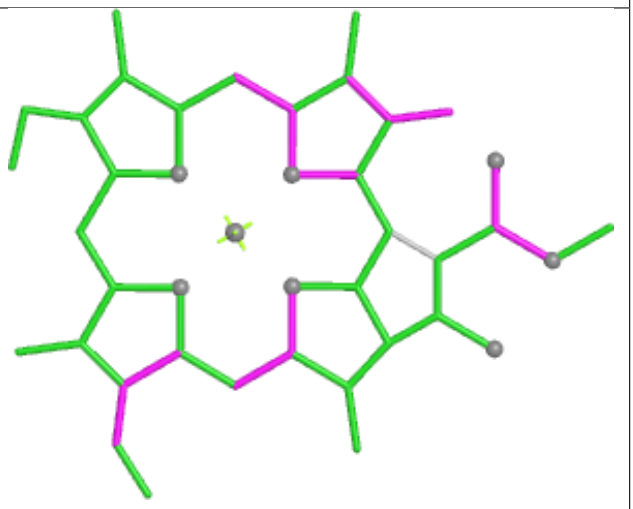
Ligand CLA A1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

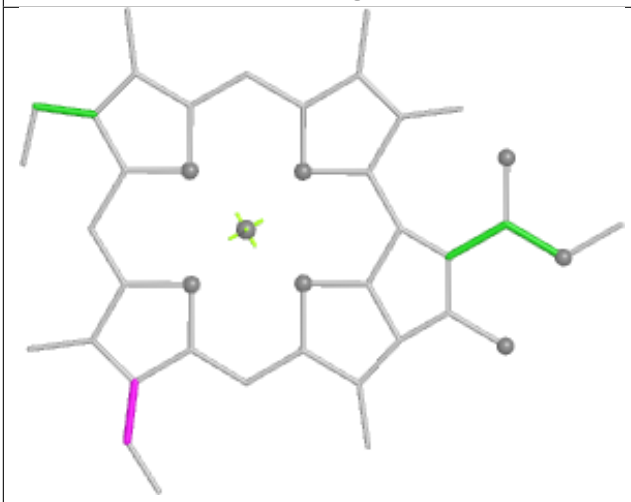
Ligand CLA BB 806



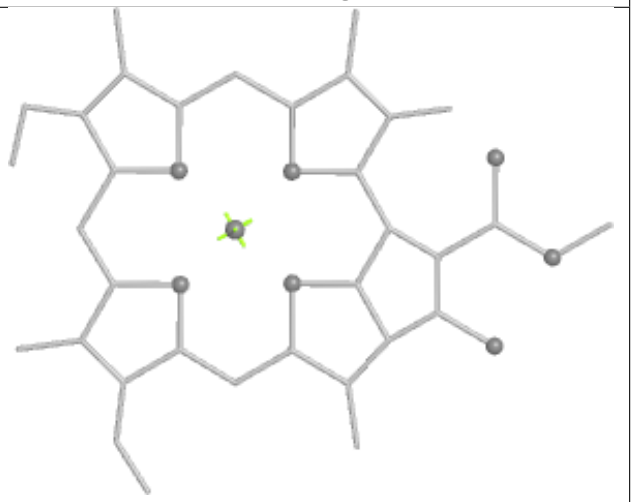
Bond lengths



Bond angles

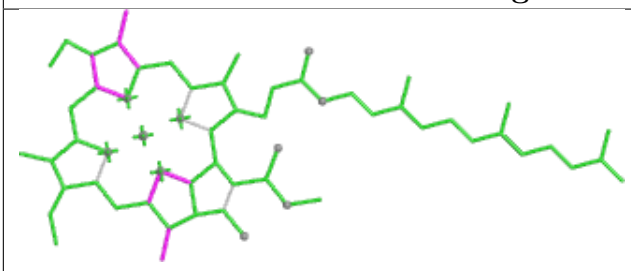


Torsions

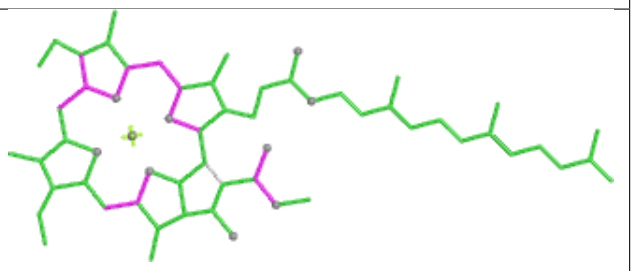


Rings

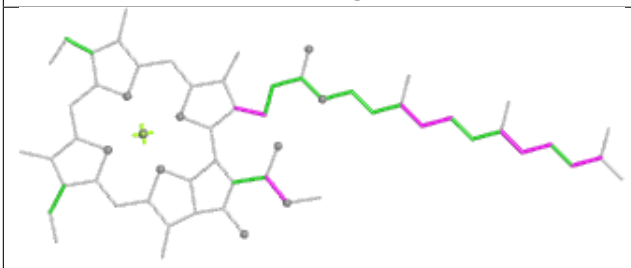
Ligand CLA BB 836



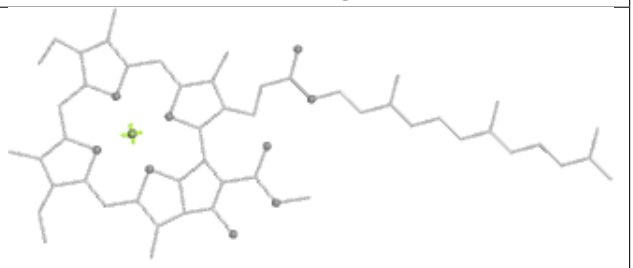
Bond lengths



Bond angles

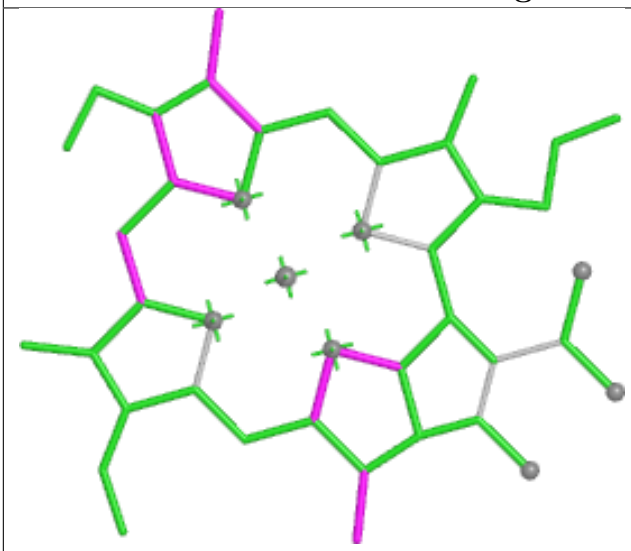


Torsions

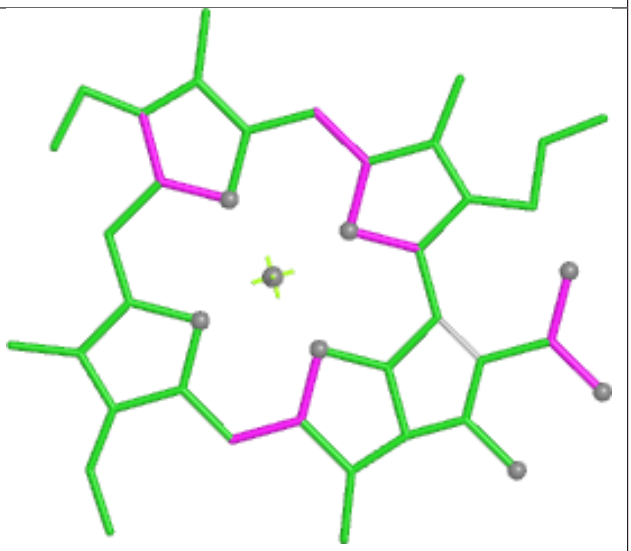


Rings

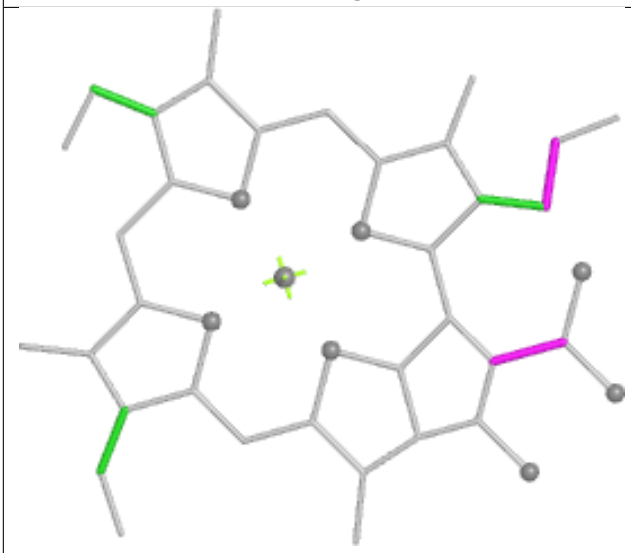
Ligand CLA A6 604



Bond lengths



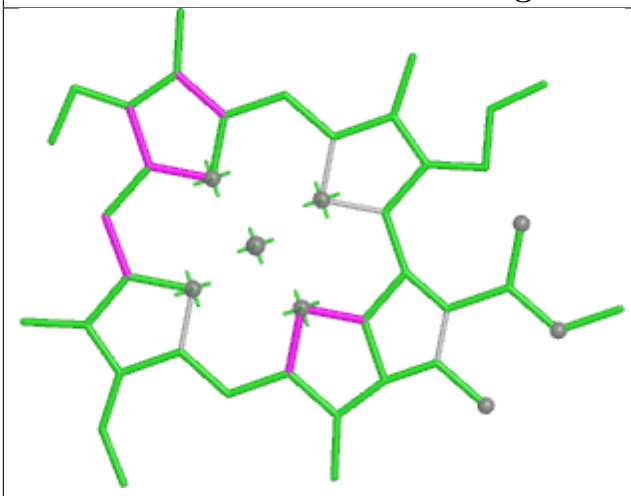
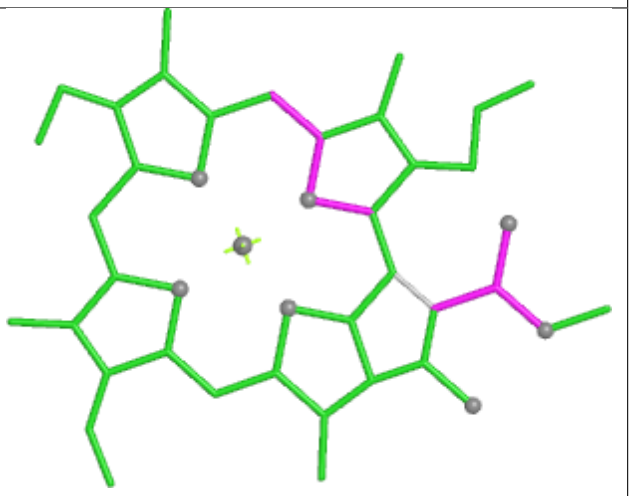
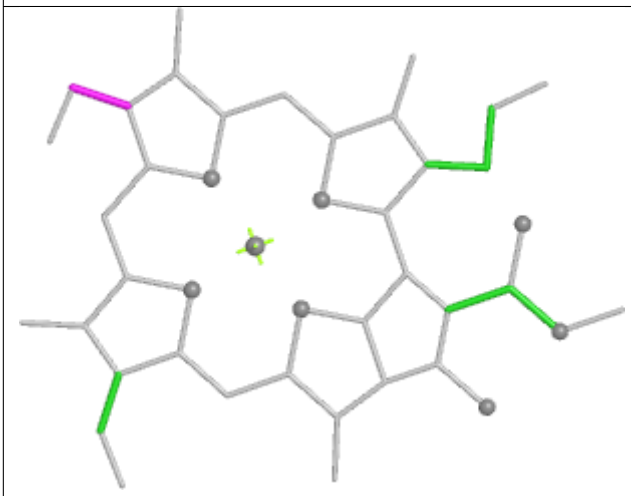
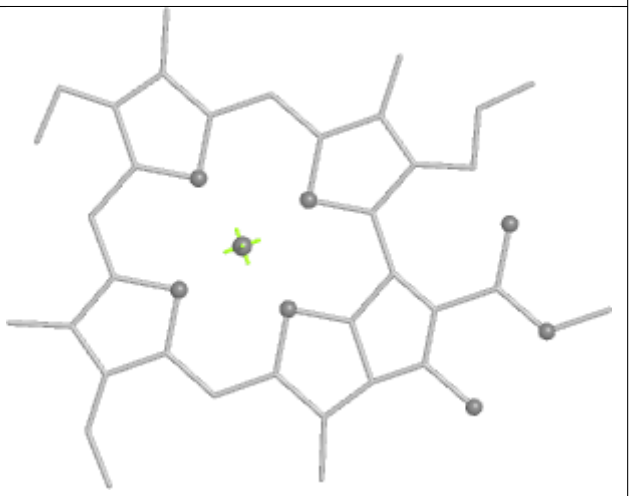
Bond angles



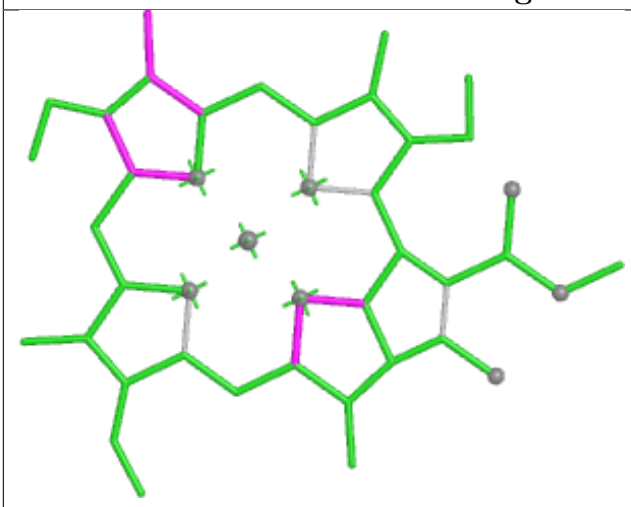
Torsions



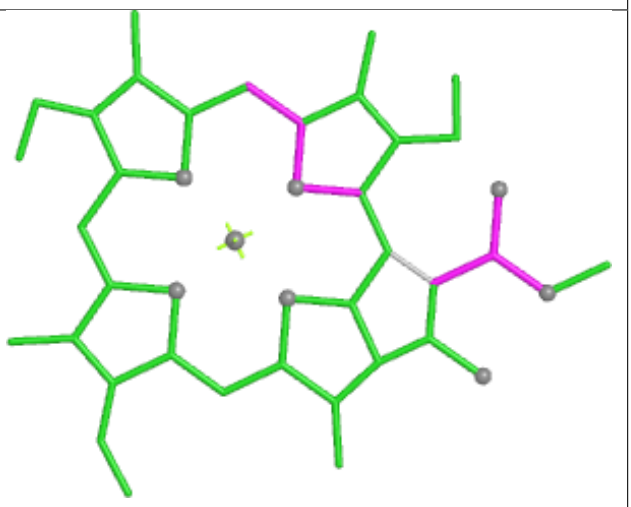
Rings

Ligand CLA A3 311	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

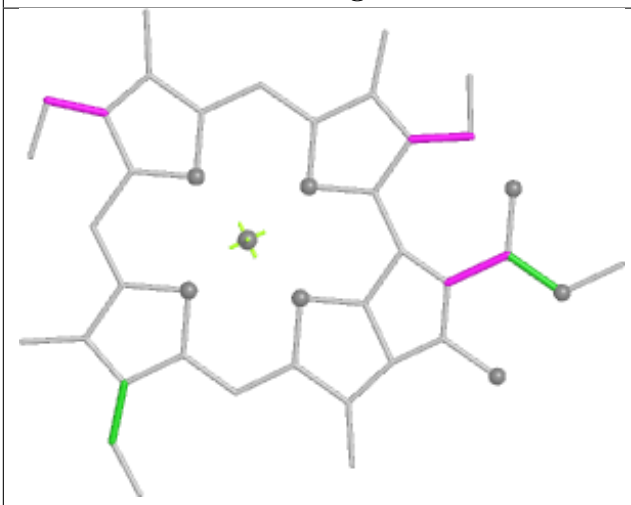
Ligand CLA A4 309



Bond lengths



Bond angles

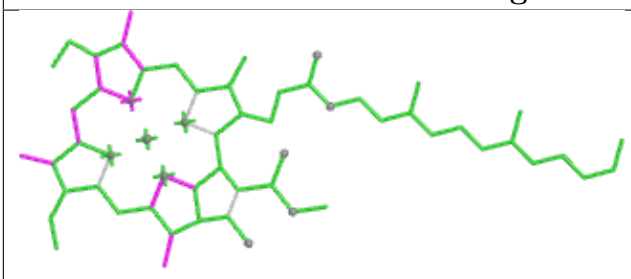


Torsions

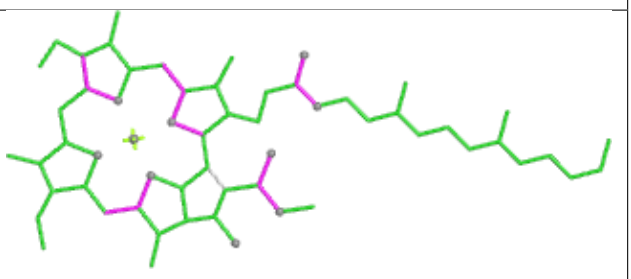


Rings

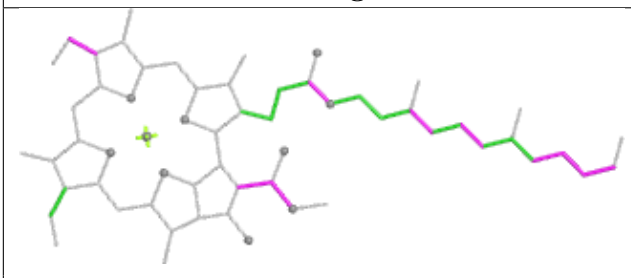
Ligand CLA AA 826



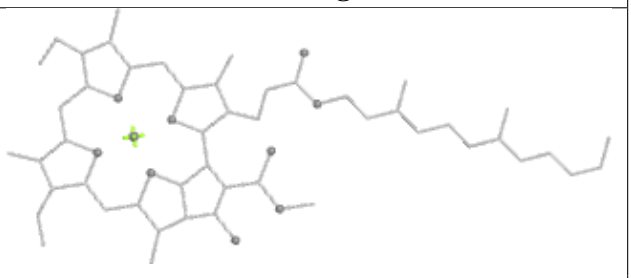
Bond lengths



Bond angles

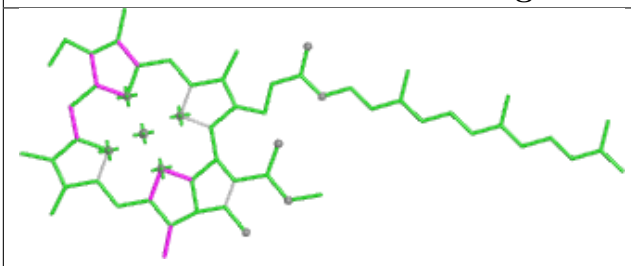


Torsions

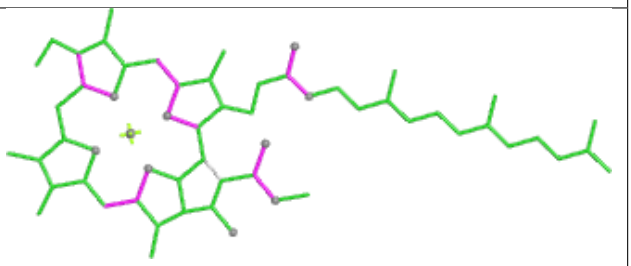


Rings

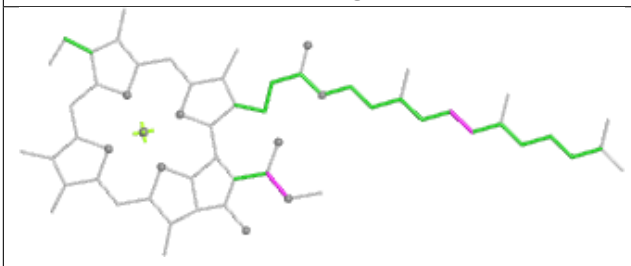
Ligand CLA B1 311



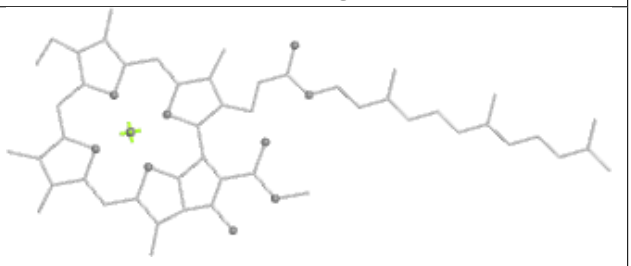
Bond lengths



Bond angles

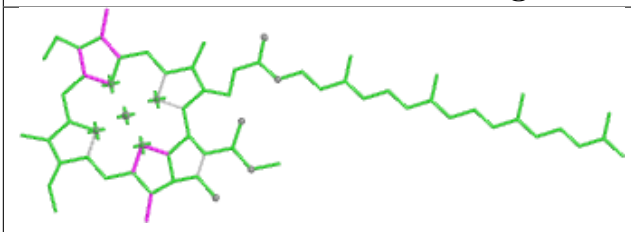


Torsions

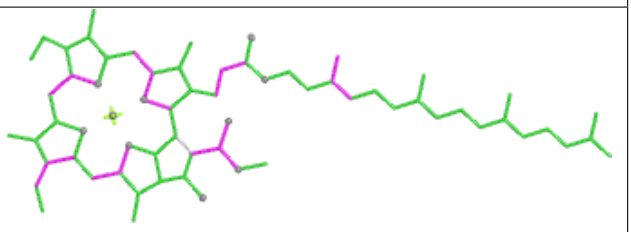


Rings

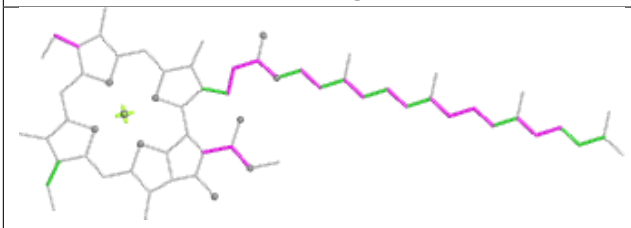
Ligand CLA AA 842



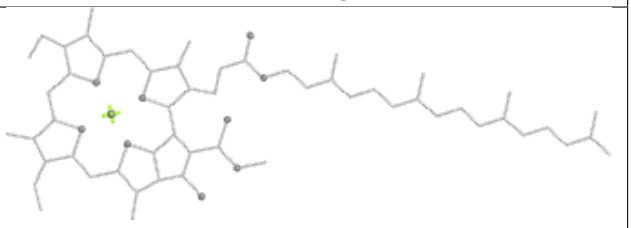
Bond lengths



Bond angles

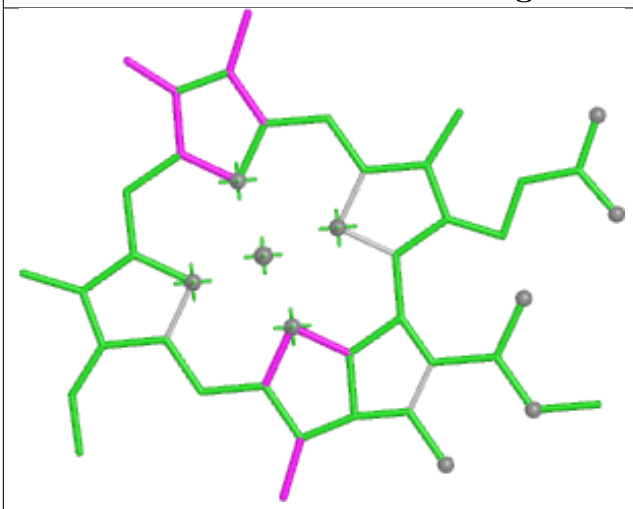


Torsions

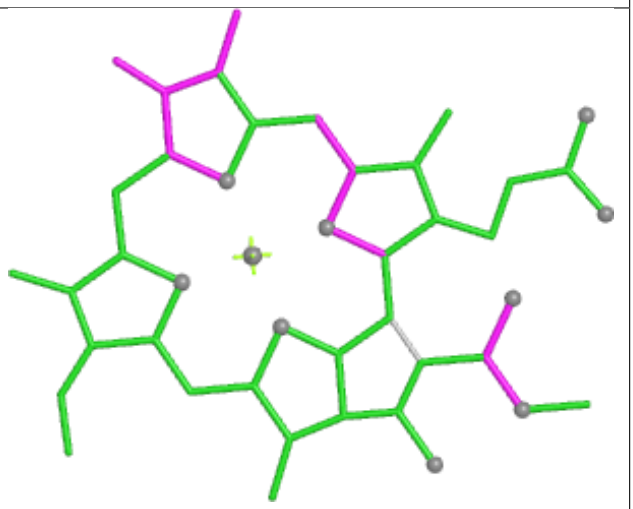


Rings

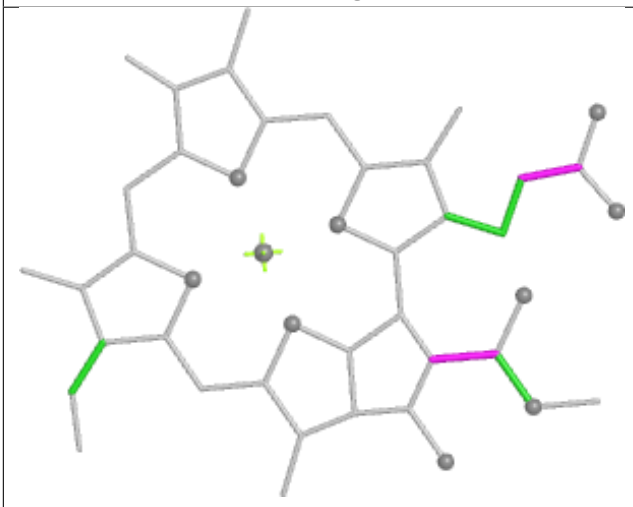
Ligand CLA B5 603



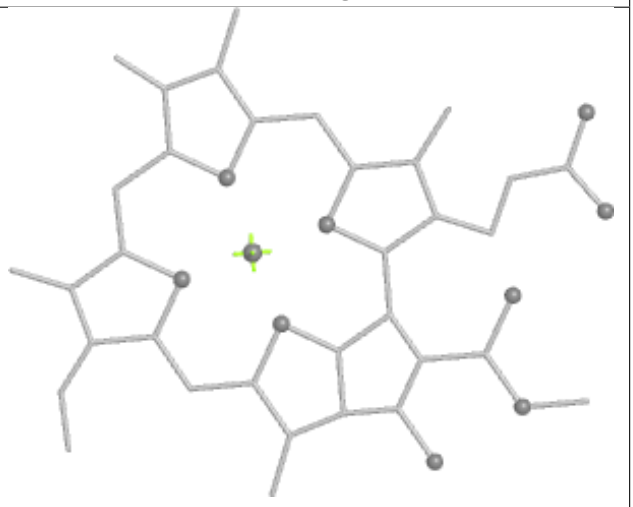
Bond lengths



Bond angles

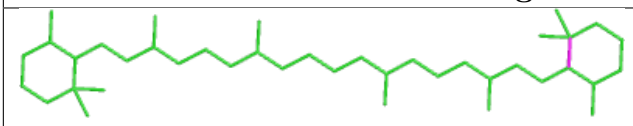


Torsions

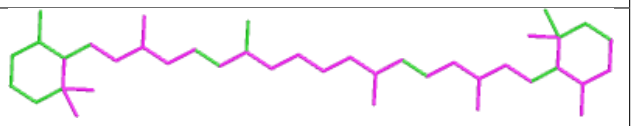


Rings

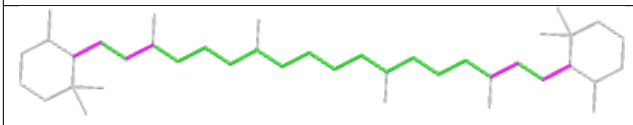
Ligand BCR AI 101



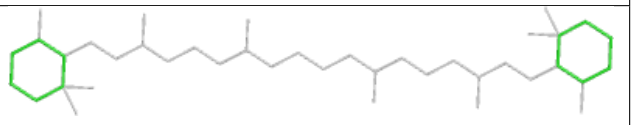
Bond lengths



Bond angles

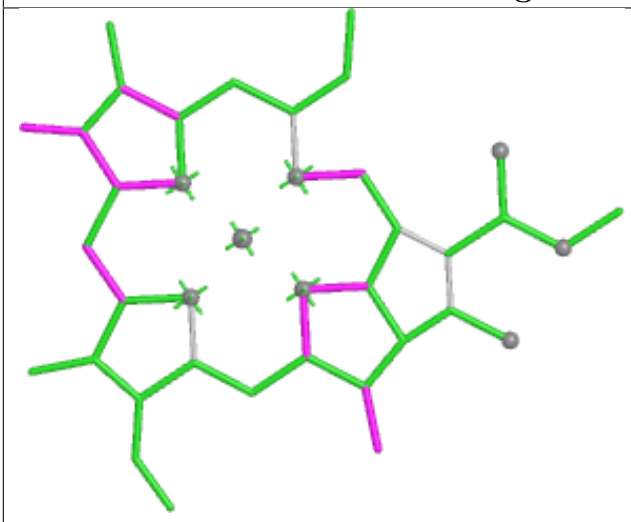


Torsions

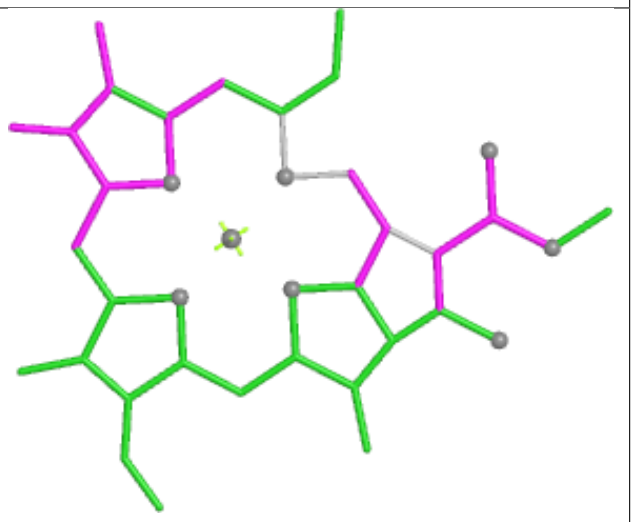


Rings

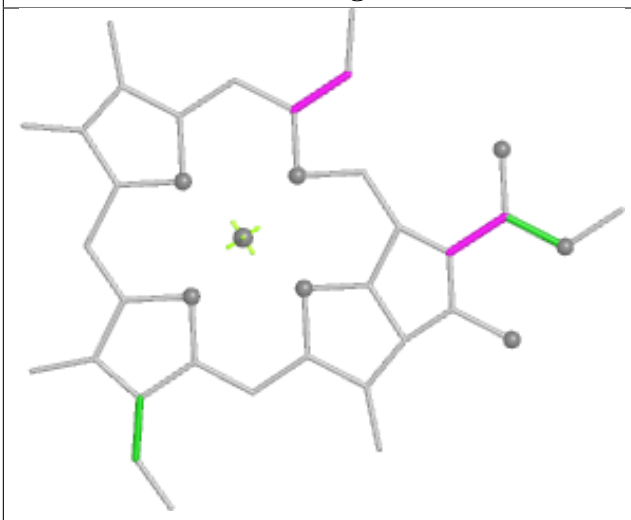
Ligand CLA A6 611



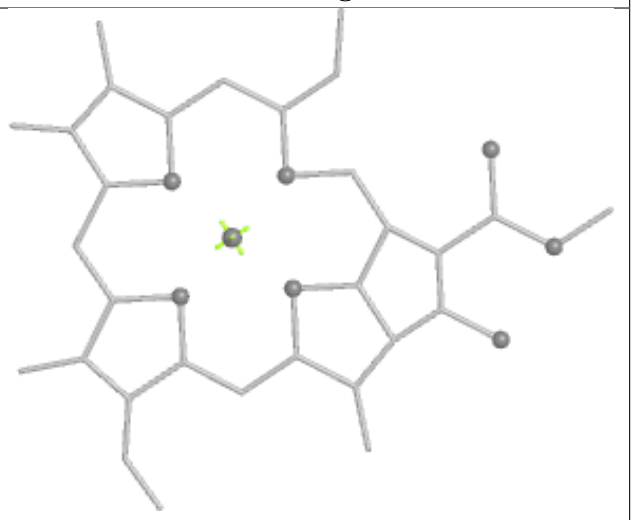
Bond lengths



Bond angles

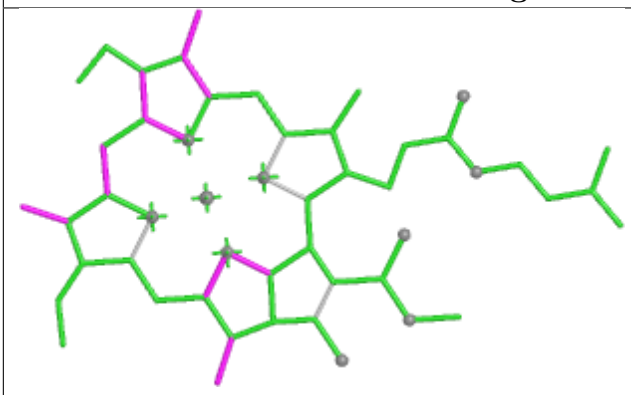


Torsions

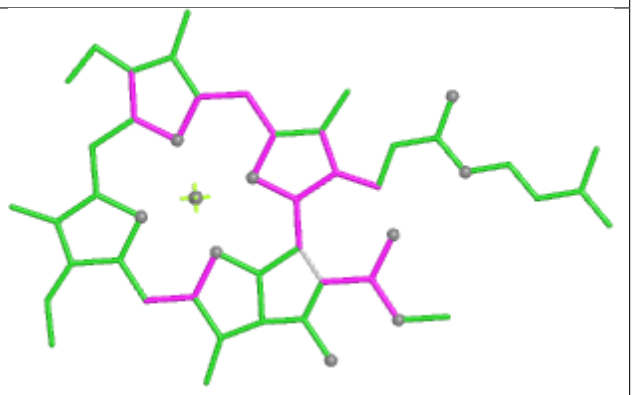


Rings

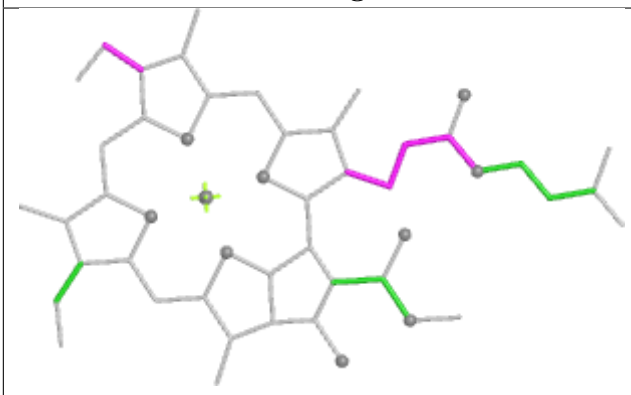
Ligand CLA AA 809



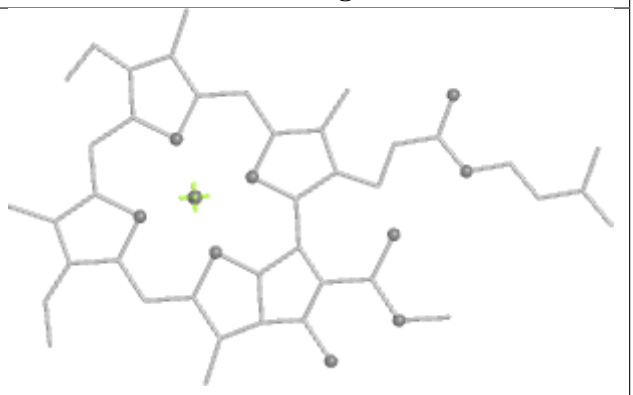
Bond lengths



Bond angles

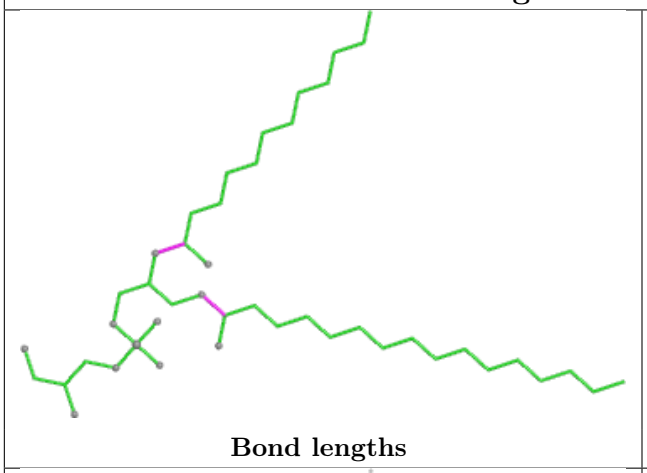


Torsions

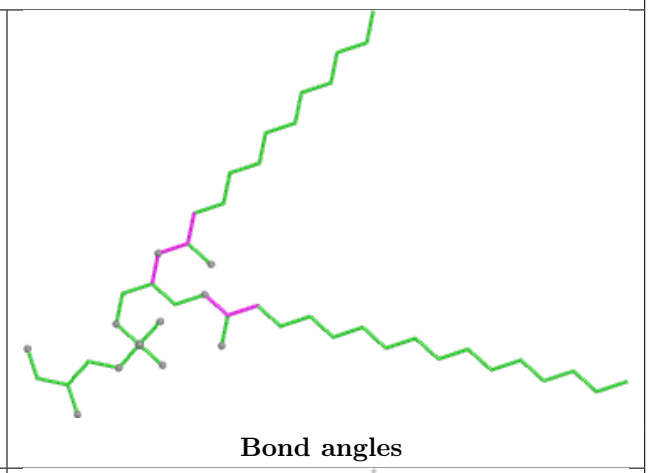


Rings

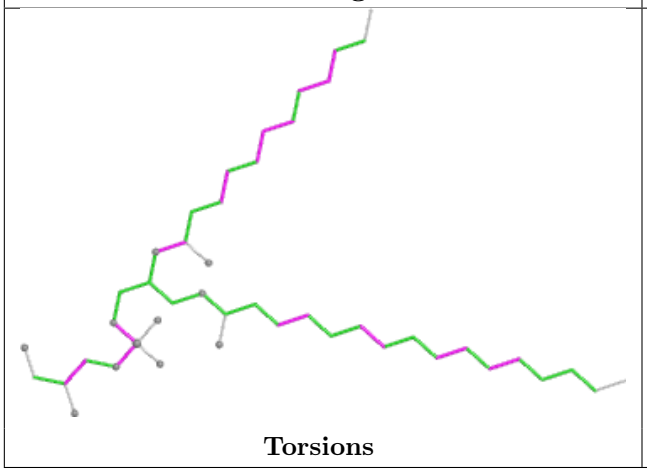
Ligand LHG BF 305



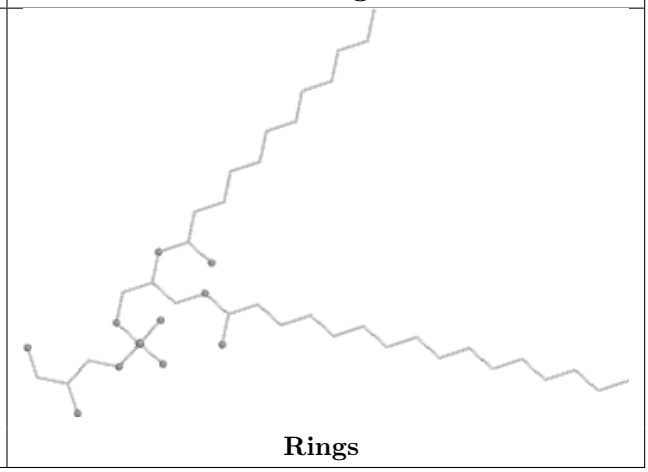
Bond lengths



Bond angles

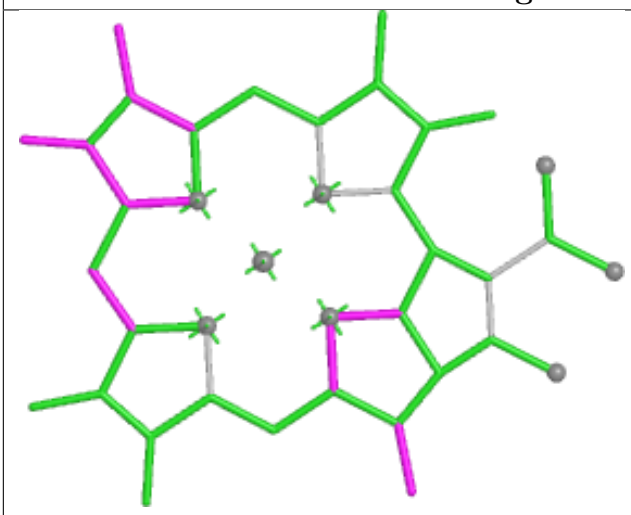


Torsions

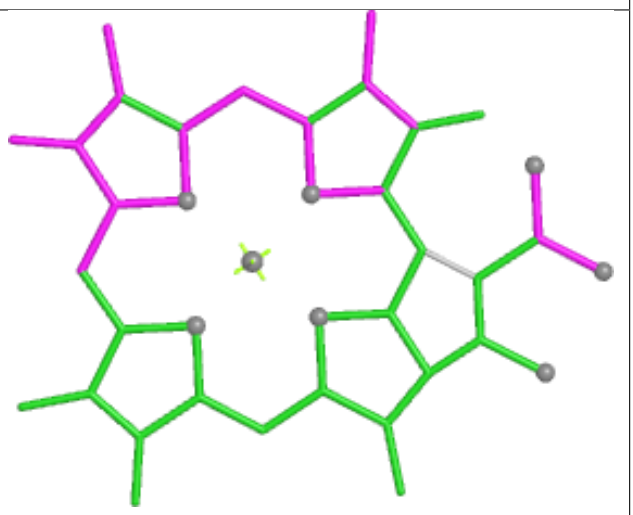


Rings

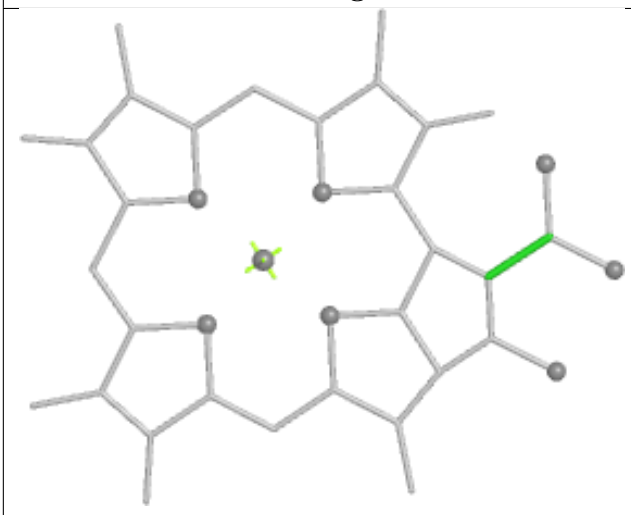
Ligand CLA B1 315



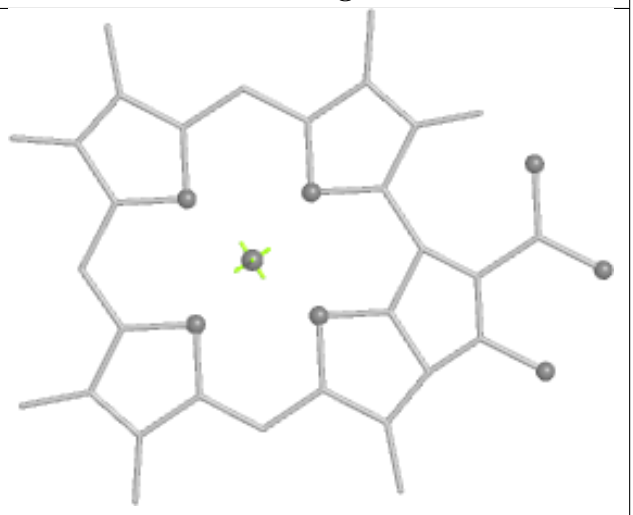
Bond lengths



Bond angles

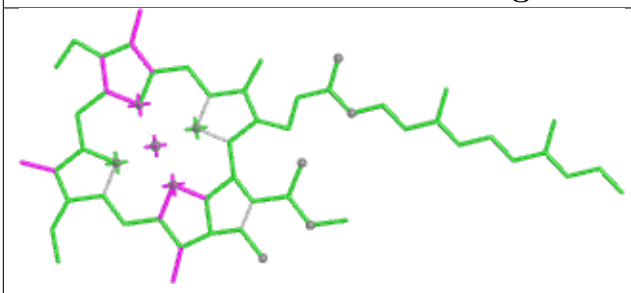


Torsions

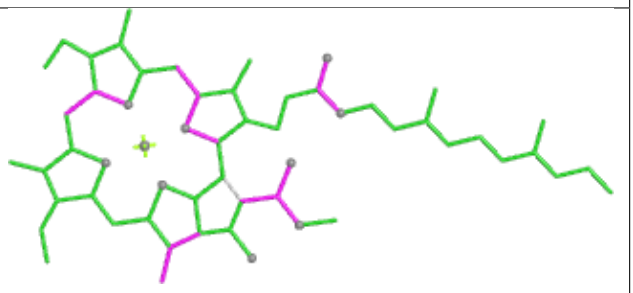


Rings

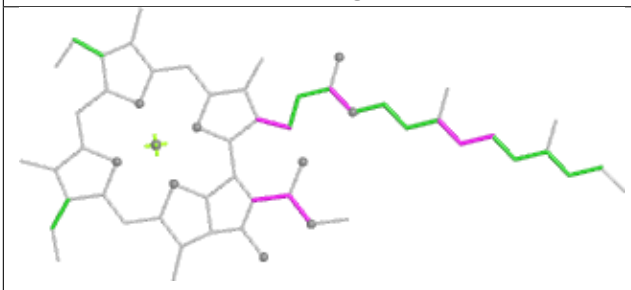
Ligand CLA AF 802



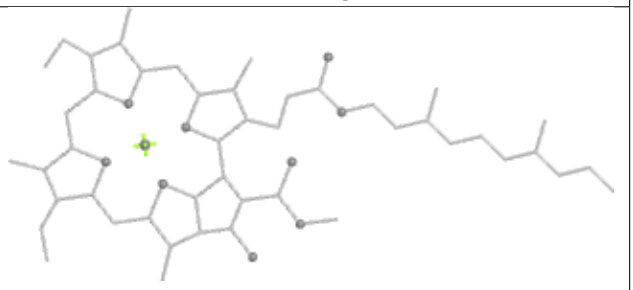
Bond lengths



Bond angles

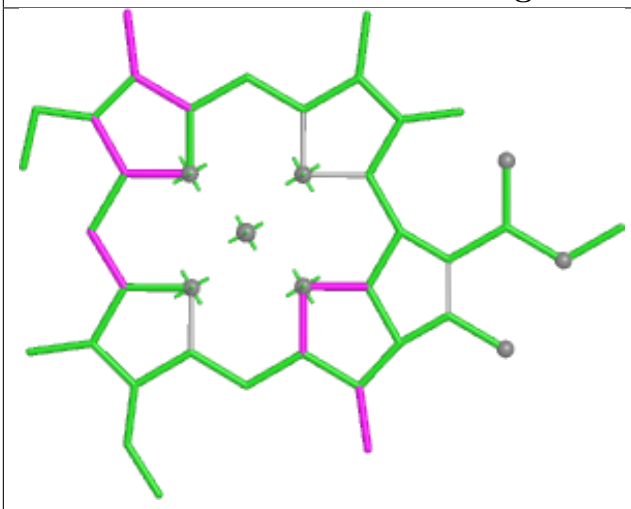


Torsions

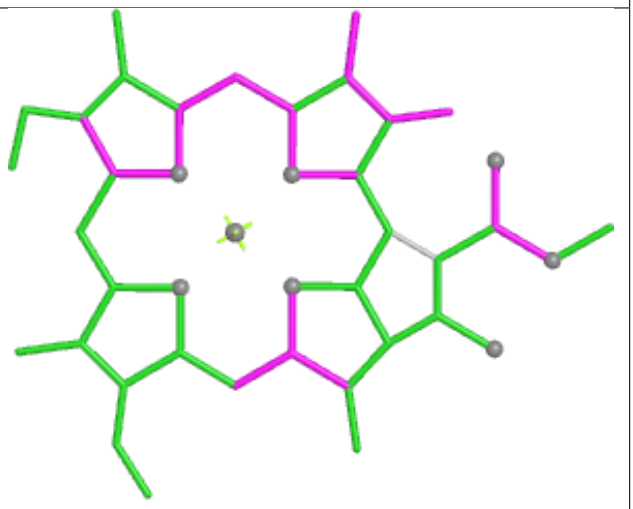


Rings

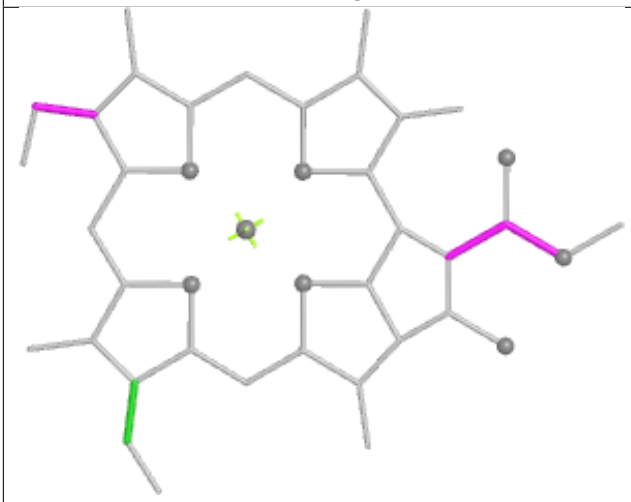
Ligand CLA A3 309



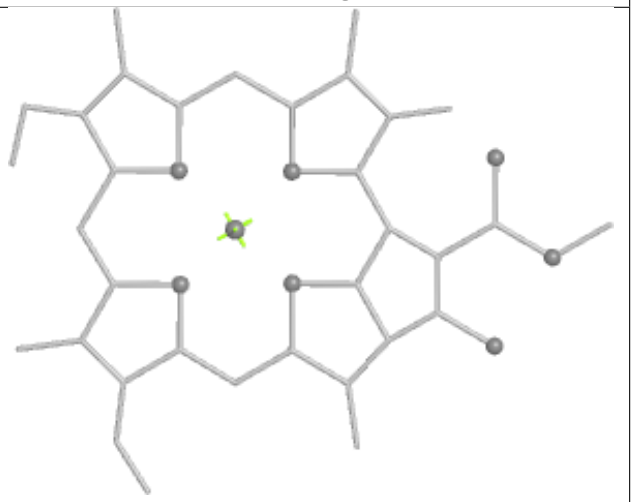
Bond lengths



Bond angles

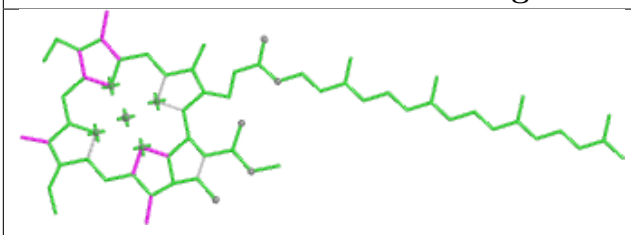


Torsions

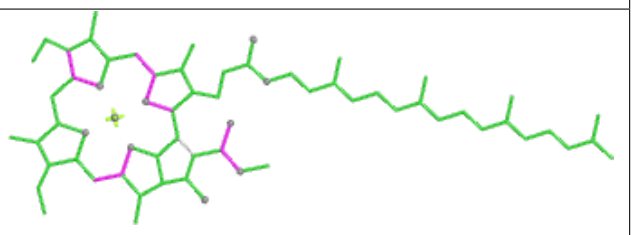


Rings

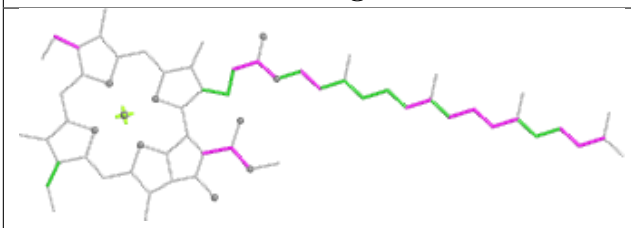
Ligand CLA BB 835



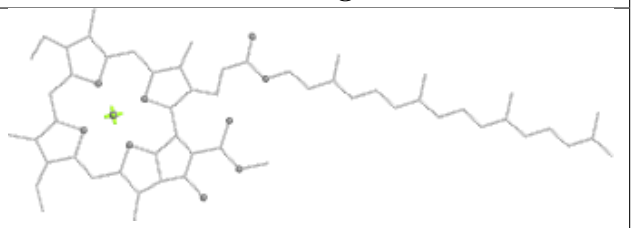
Bond lengths



Bond angles

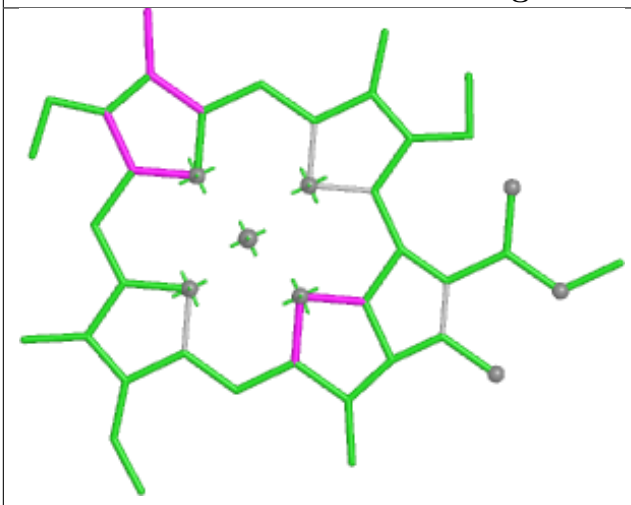


Torsions

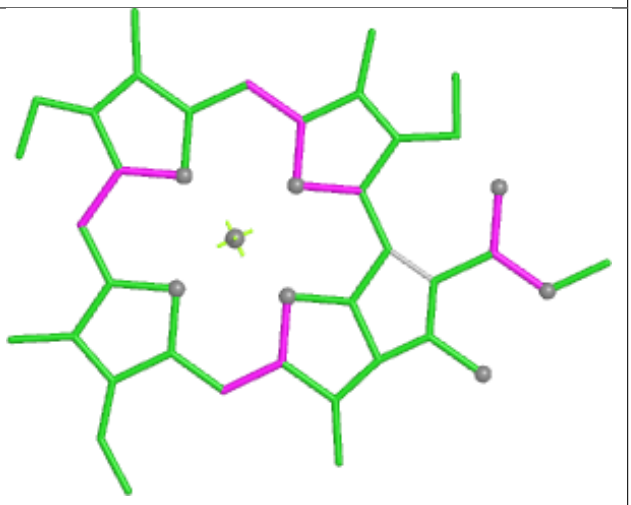


Rings

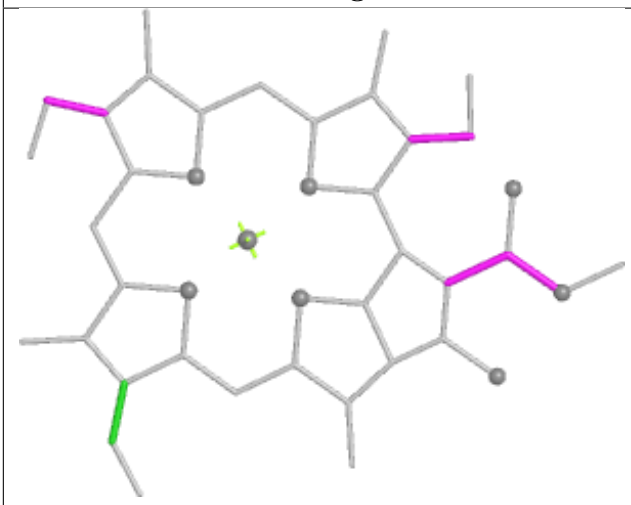
Ligand CLA BB 837



Bond lengths



Bond angles

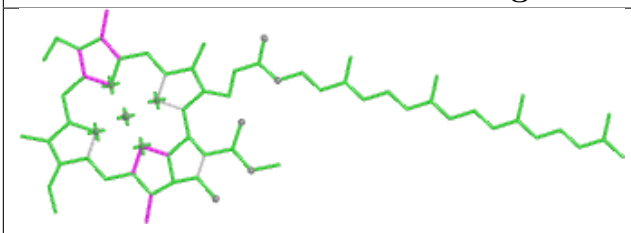


Torsions

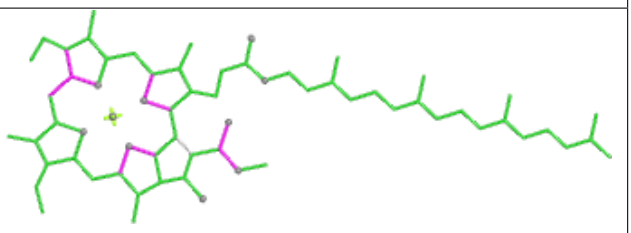


Rings

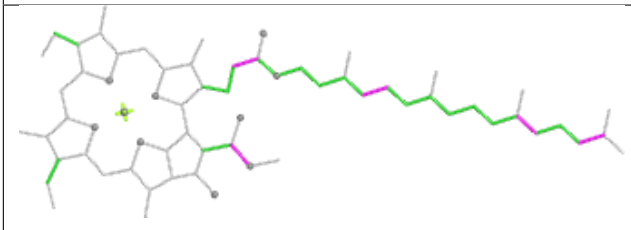
Ligand CLA BA 801



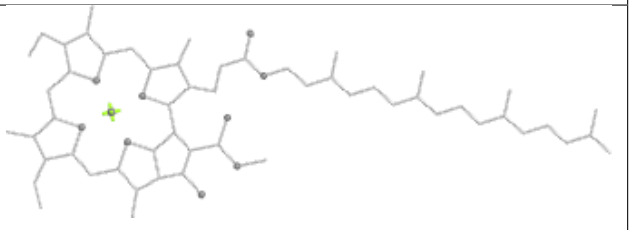
Bond lengths



Bond angles

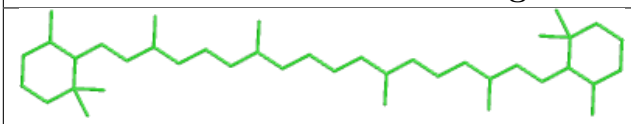


Torsions

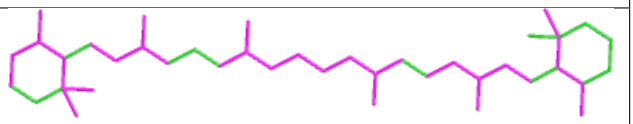


Rings

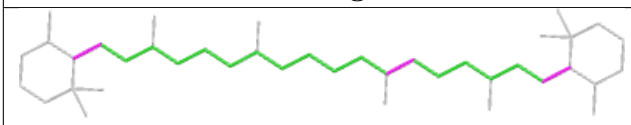
Ligand BCR AB 844



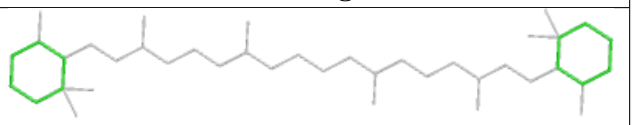
Bond lengths



Bond angles

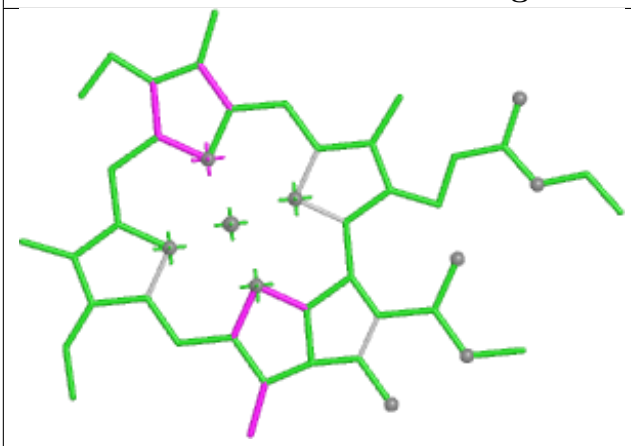


Torsions

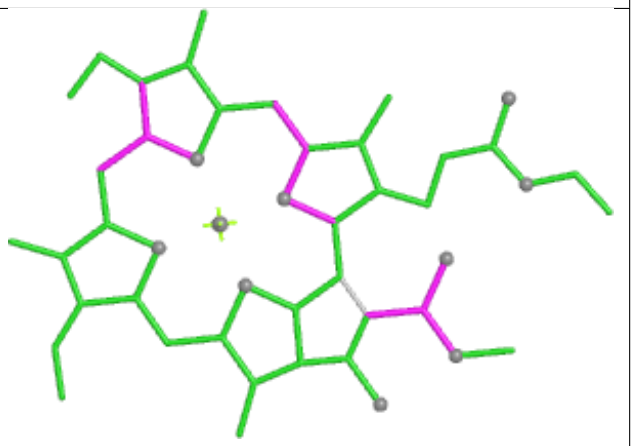


Rings

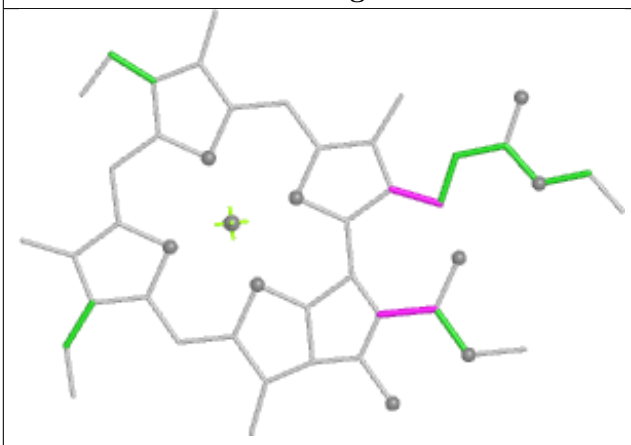
Ligand CLA AB 839



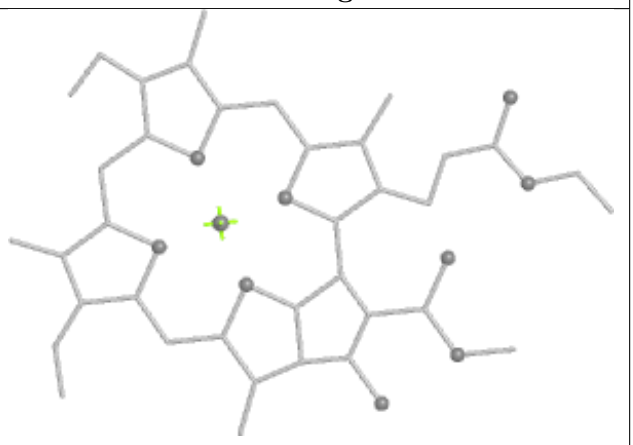
Bond lengths



Bond angles

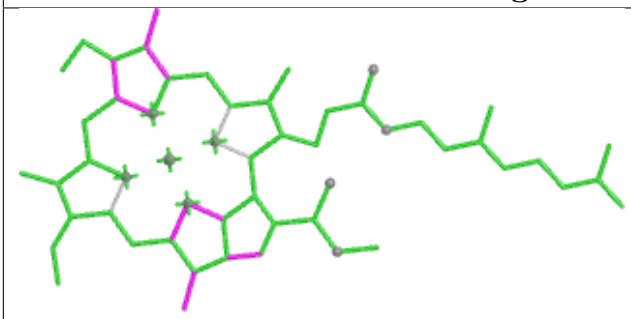


Torsions

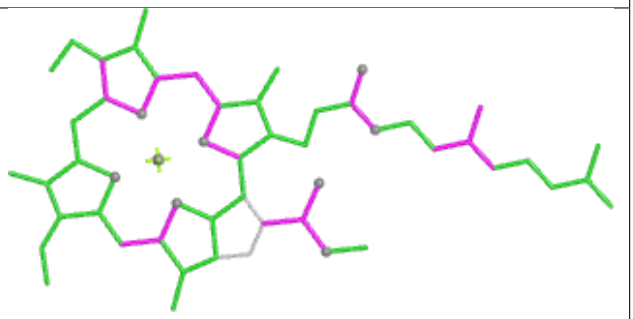


Rings

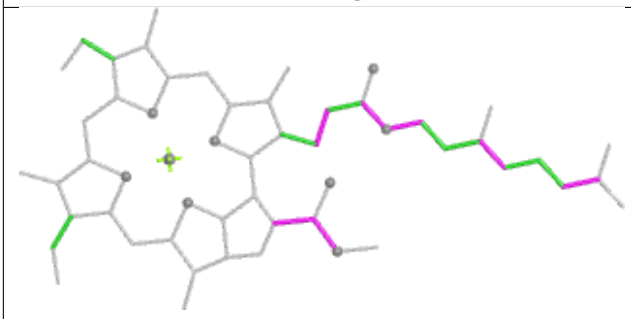
Ligand CLA BA 838



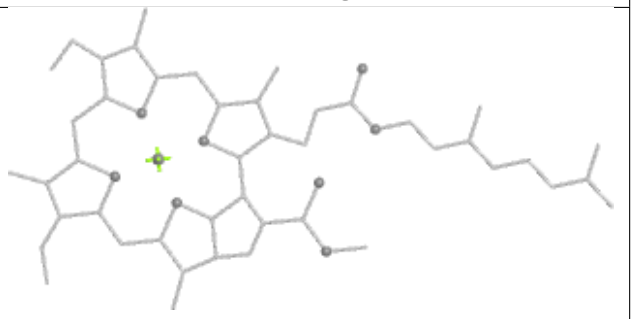
Bond lengths



Bond angles

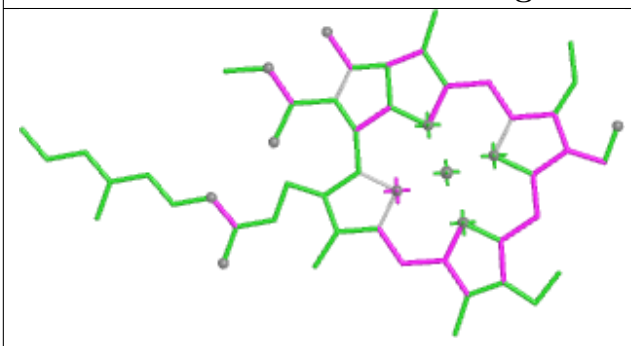


Torsions

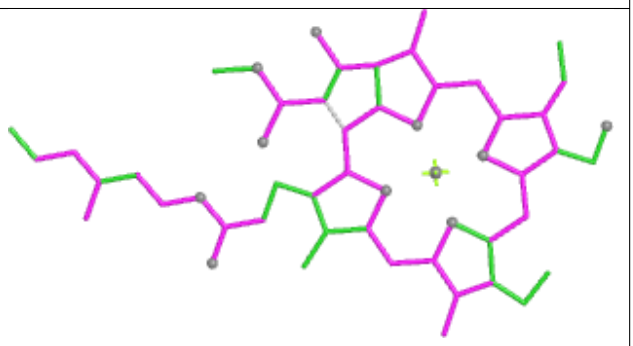


Rings

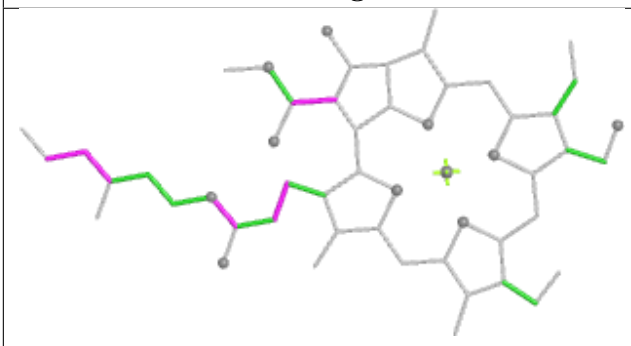
Ligand CHL B2 601



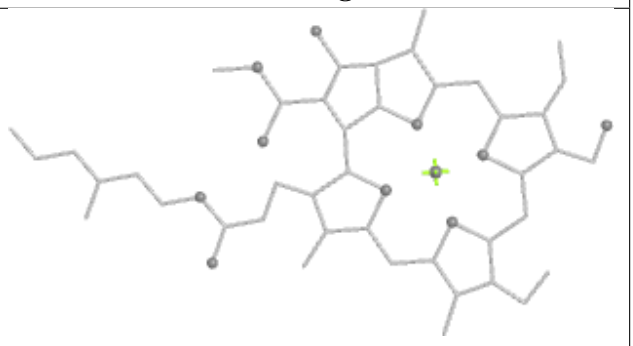
Bond lengths



Bond angles

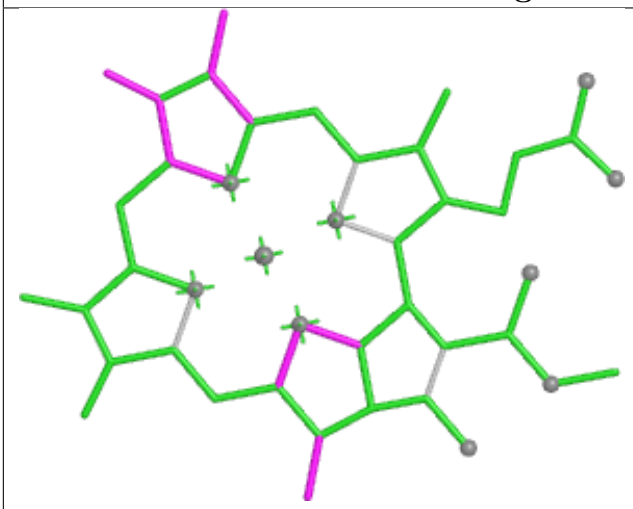


Torsions

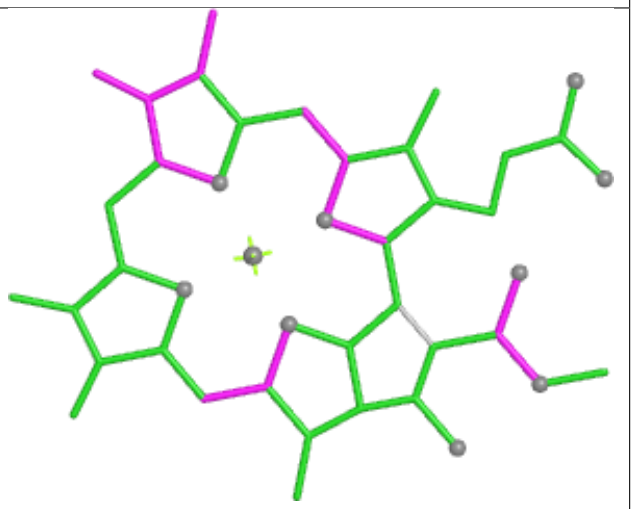


Rings

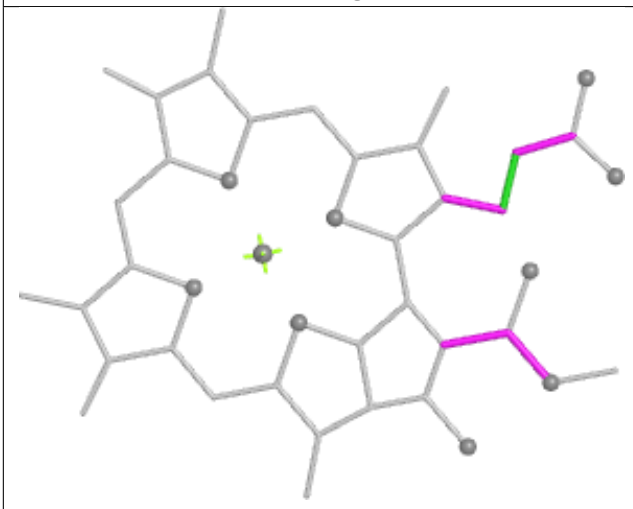
Ligand CLA A1 316



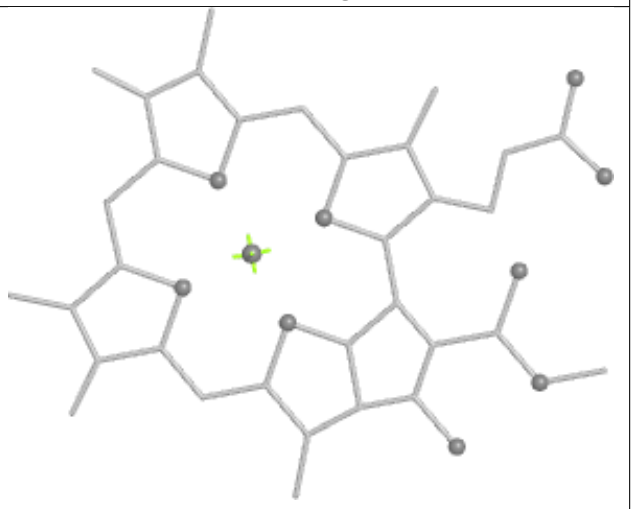
Bond lengths



Bond angles

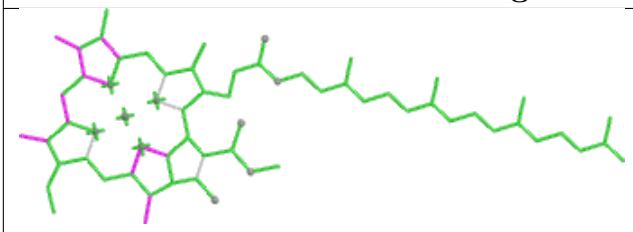


Torsions

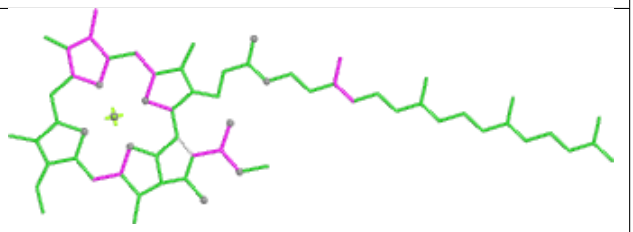


Rings

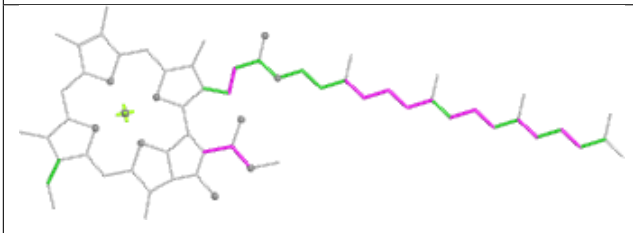
Ligand CLA AB 802



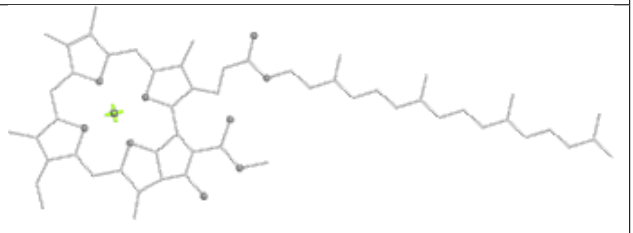
Bond lengths



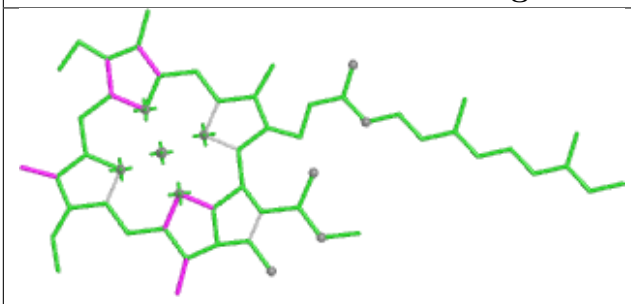
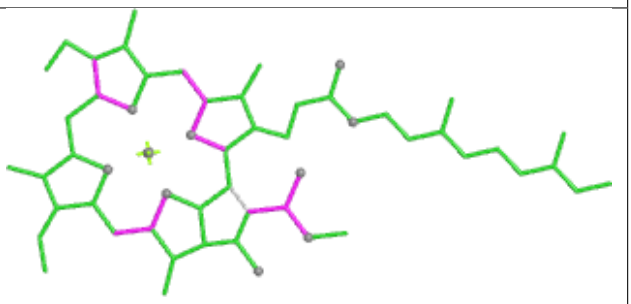
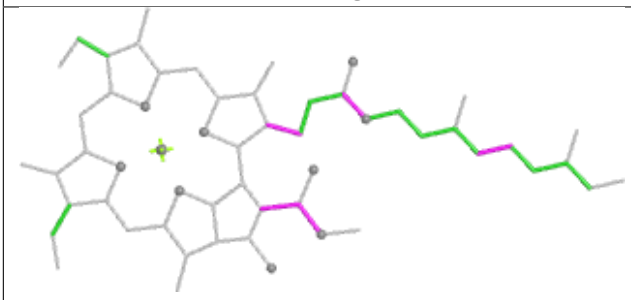
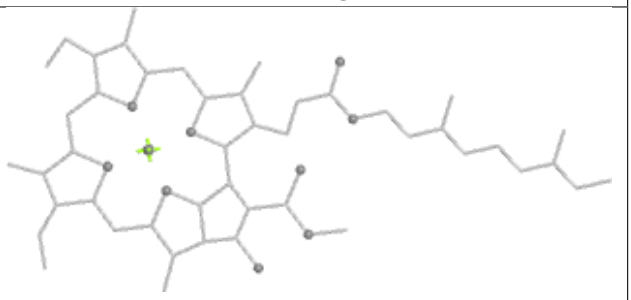
Bond angles

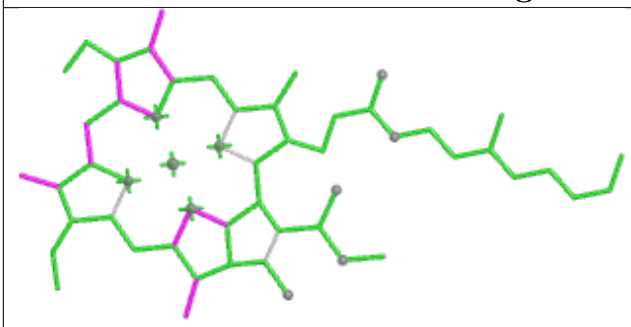
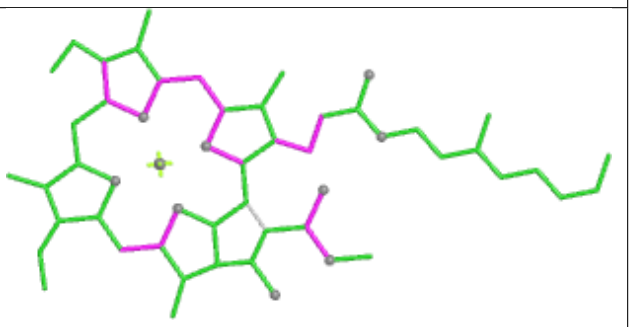
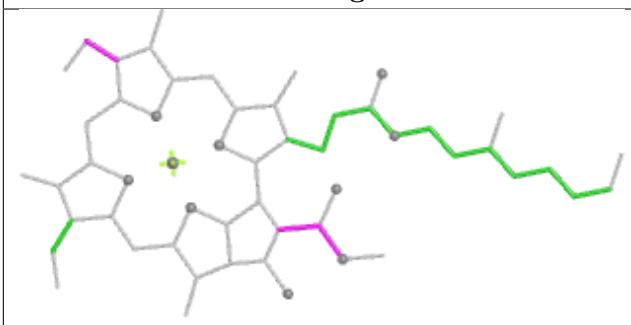
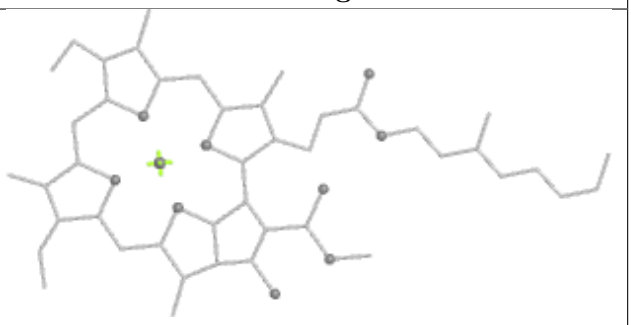


Torsions

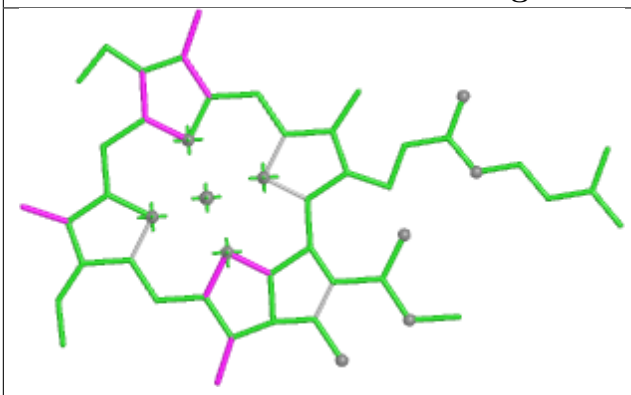


Rings

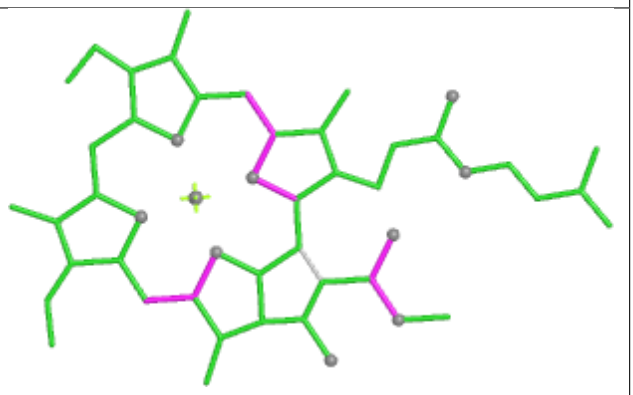
Ligand CLA BA 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B5 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

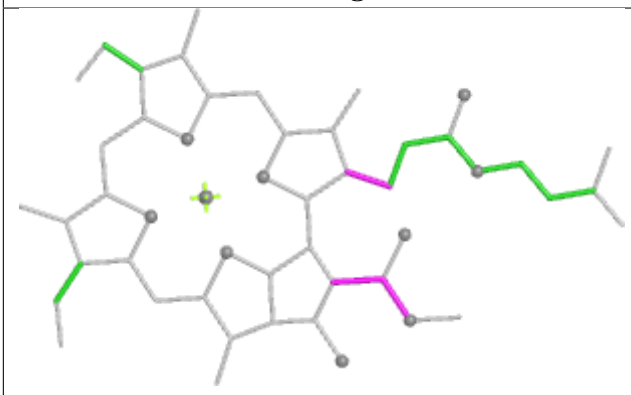
Ligand CLA BA 807



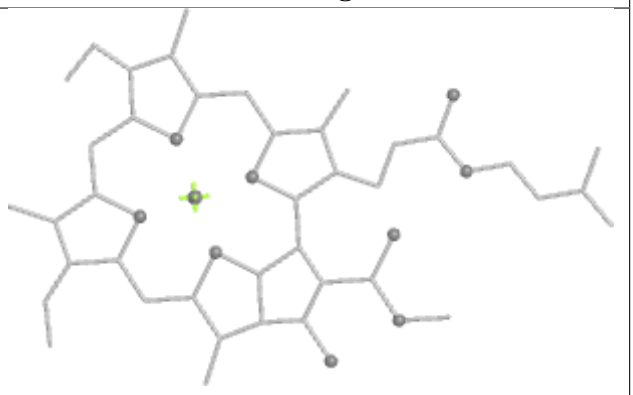
Bond lengths



Bond angles

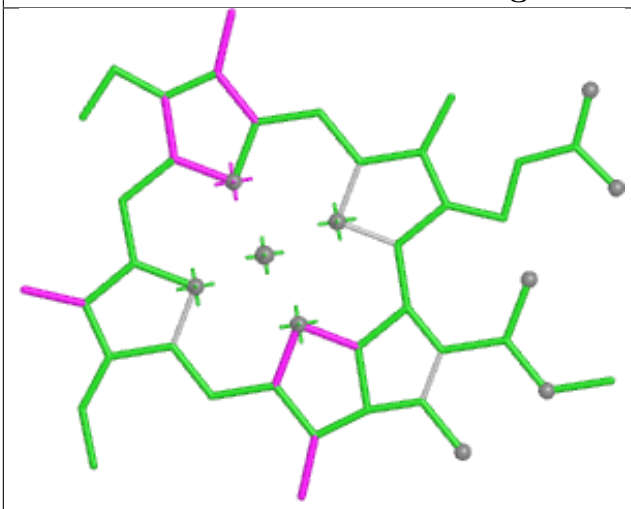


Torsions

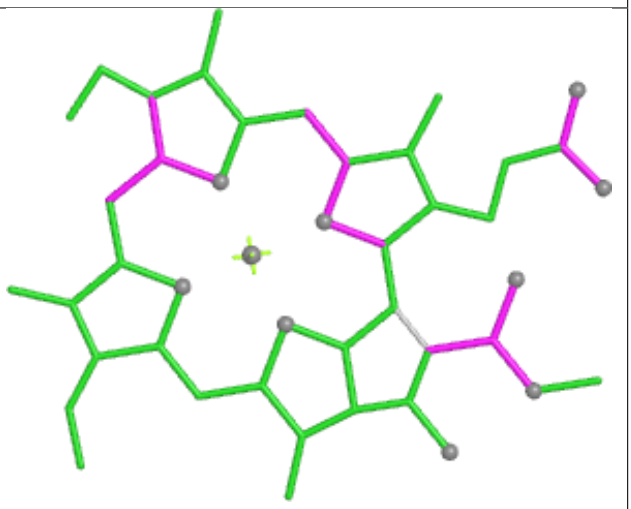


Rings

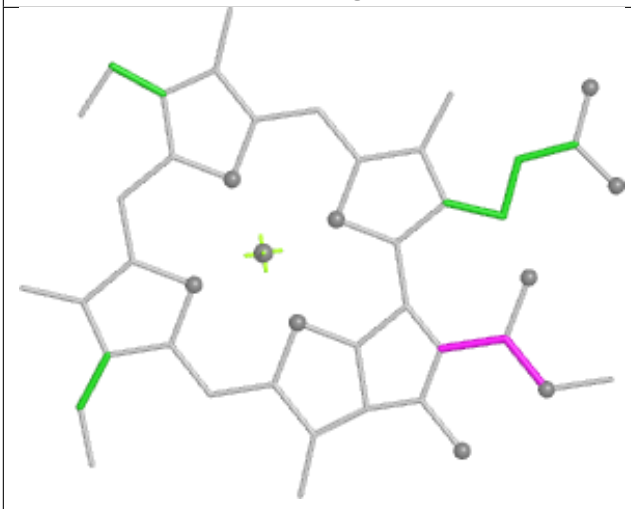
Ligand CLA AA 814



Bond lengths



Bond angles

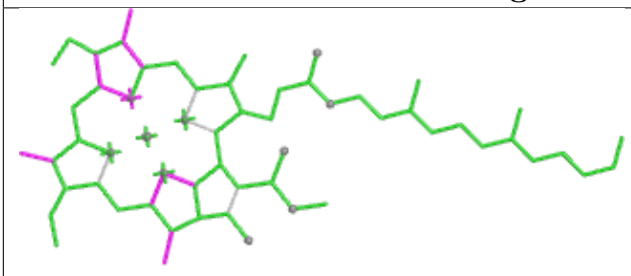


Torsions

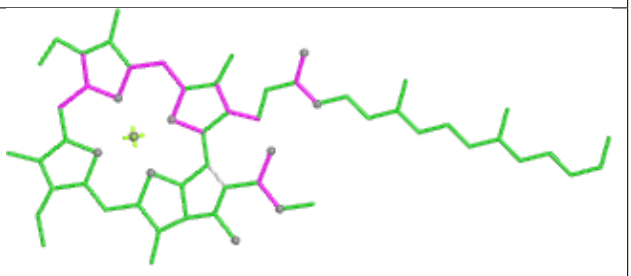


Rings

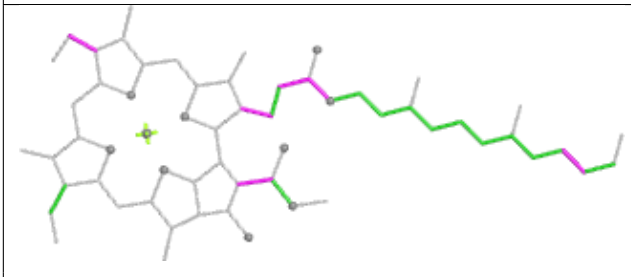
Ligand CLA AA 818



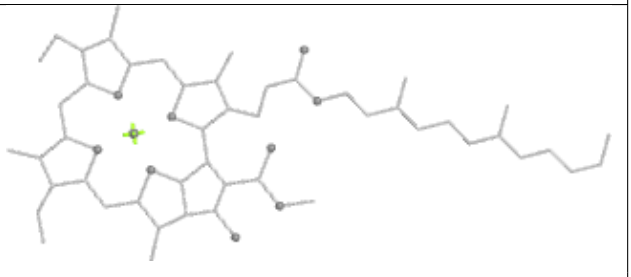
Bond lengths



Bond angles

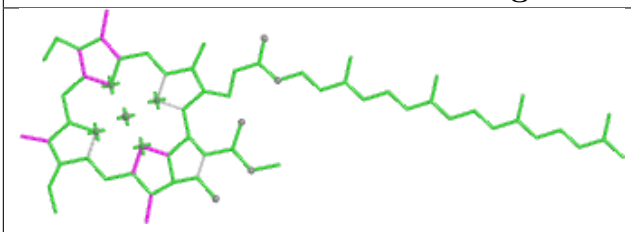


Torsions

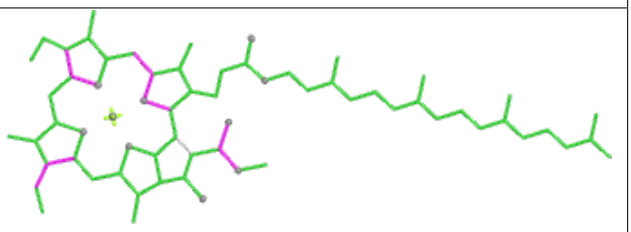


Rings

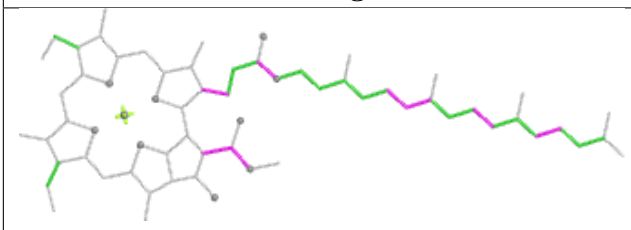
Ligand CLA BA 810



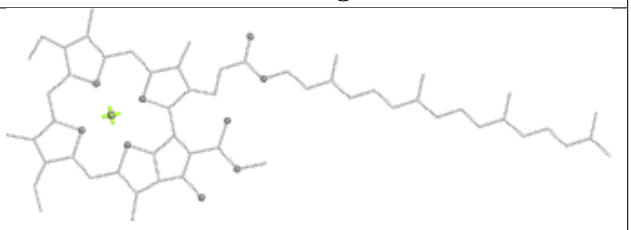
Bond lengths



Bond angles

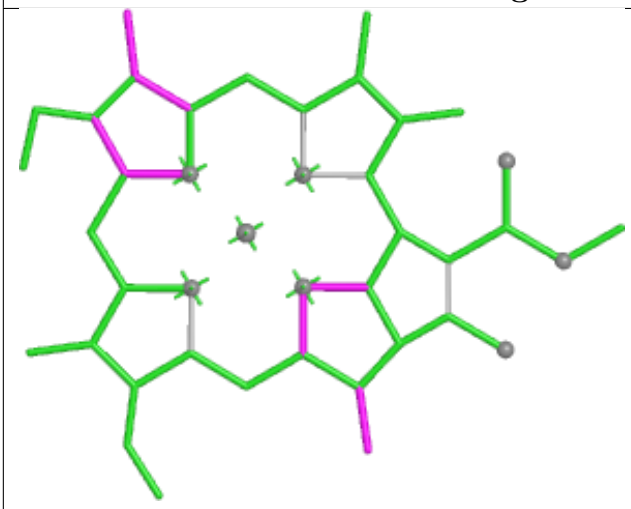


Torsions

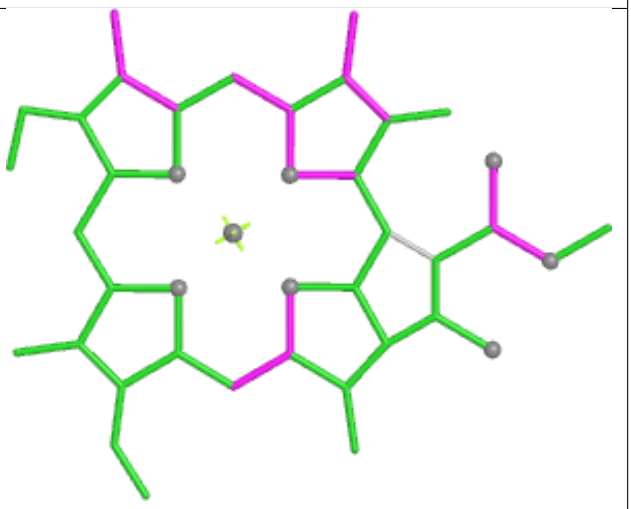


Rings

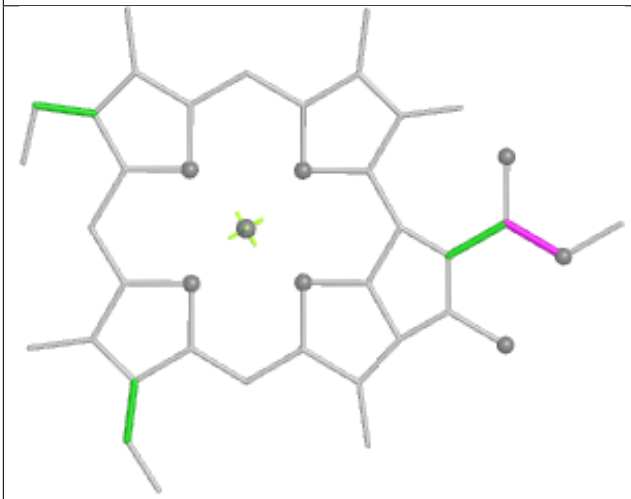
Ligand CLA AB 805



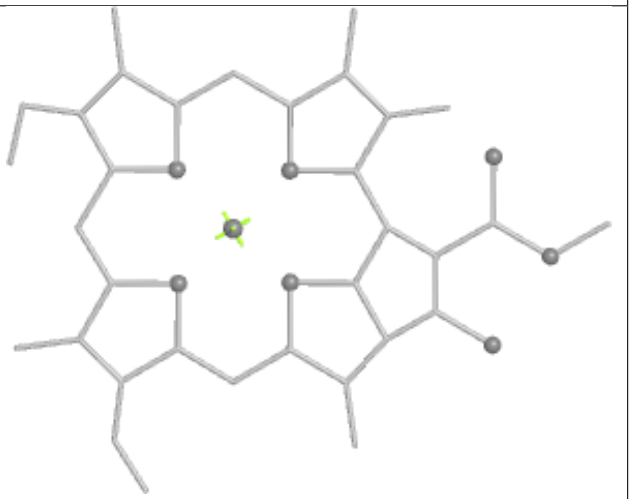
Bond lengths



Bond angles

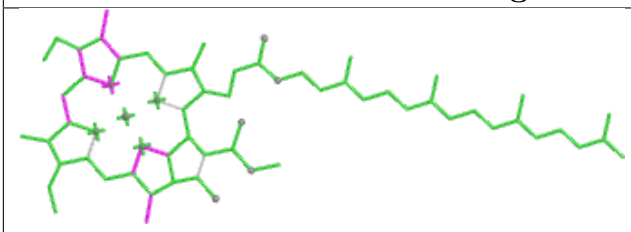


Torsions

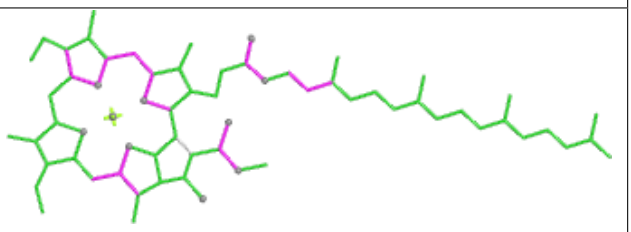


Rings

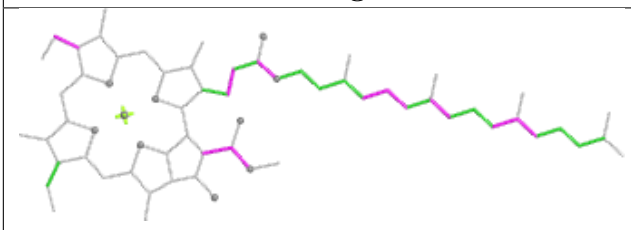
Ligand CLA AA 840



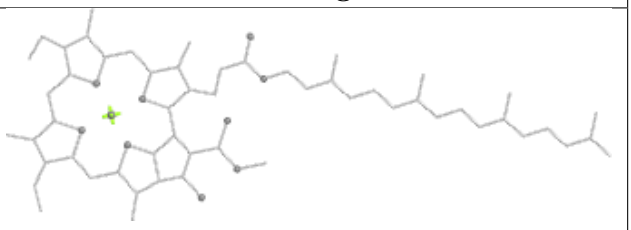
Bond lengths



Bond angles

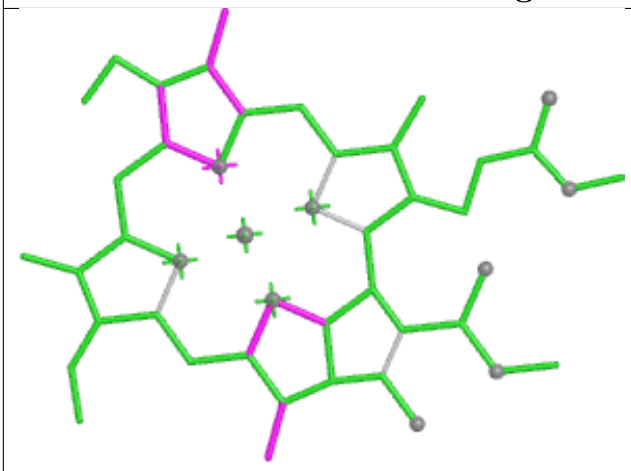


Torsions

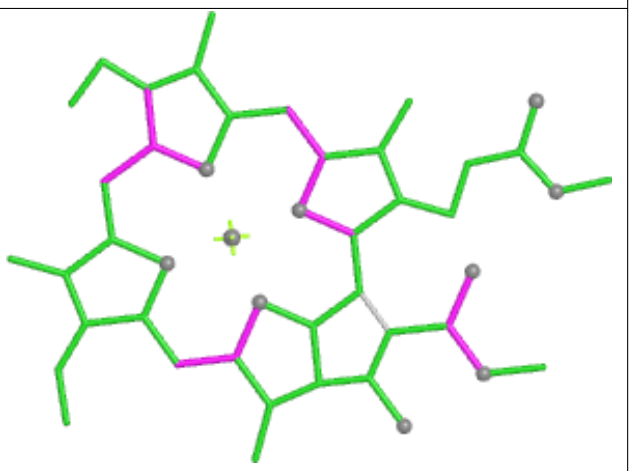


Rings

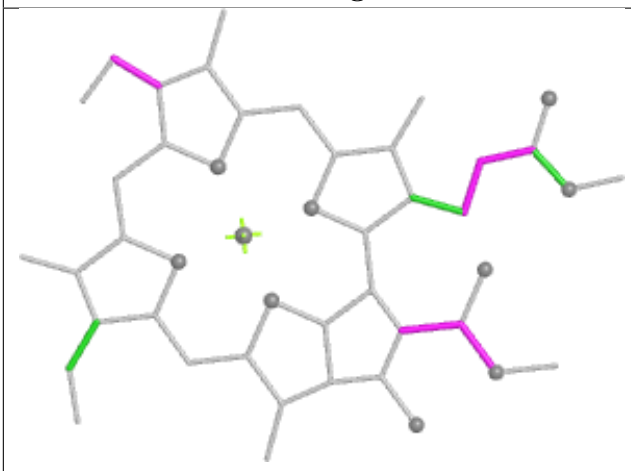
Ligand CLA B5 601



Bond lengths



Bond angles

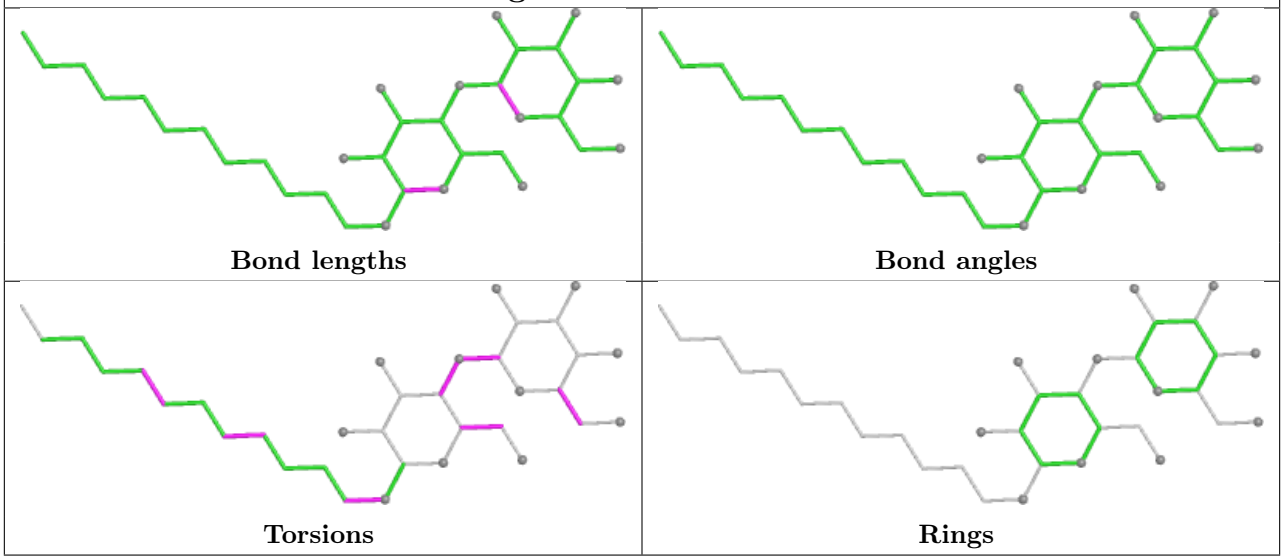


Torsions

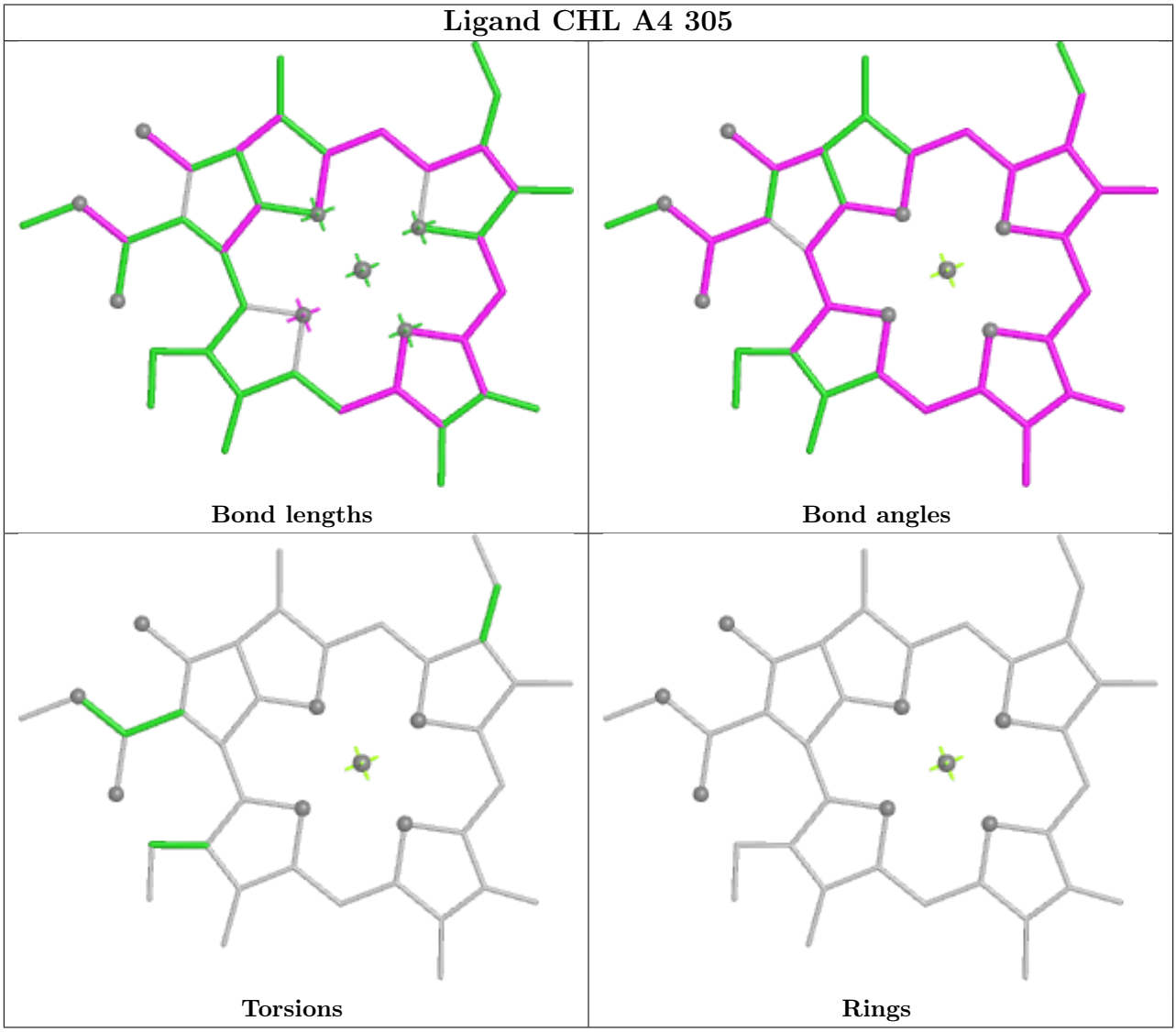


Rings

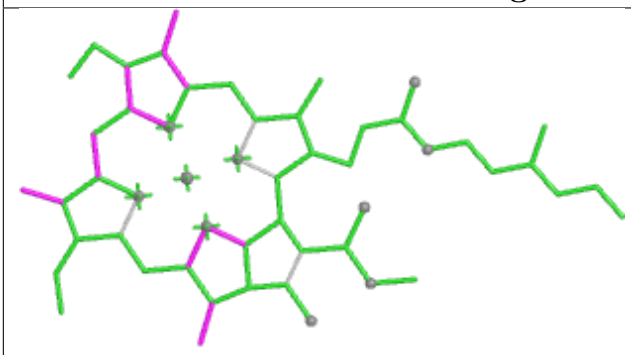
Ligand LMU BB 851



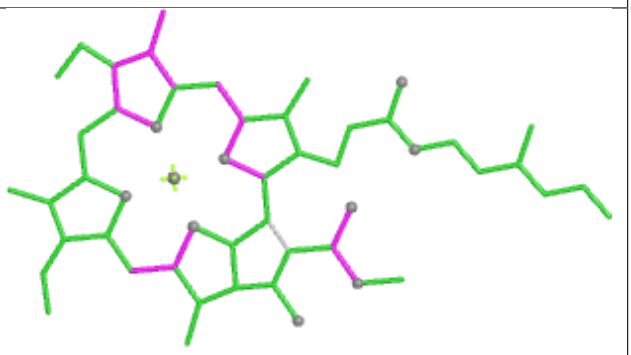
Ligand CHL A4 305



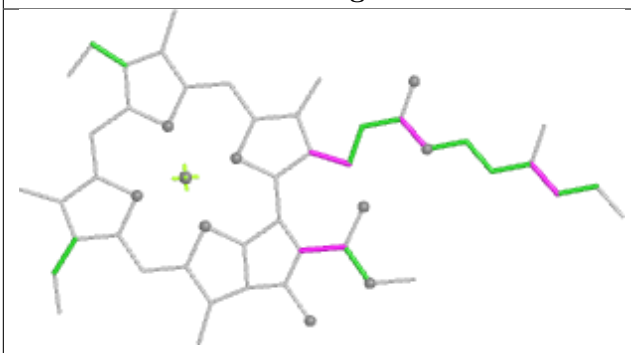
Ligand CLA AA 804



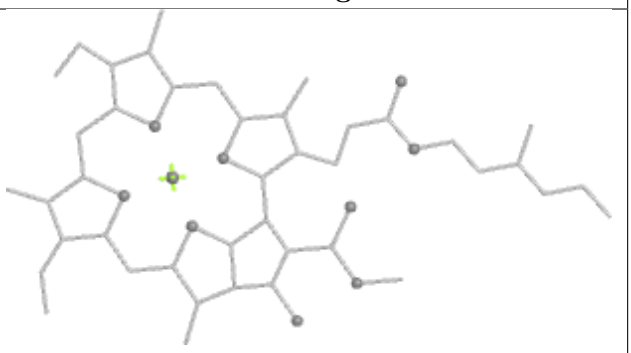
Bond lengths



Bond angles

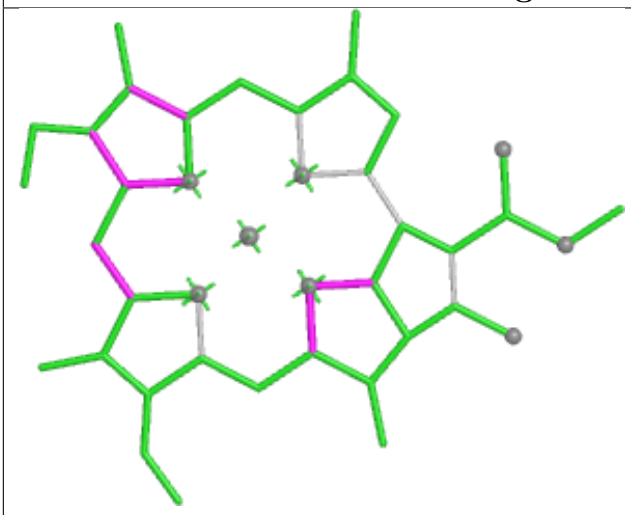


Torsions

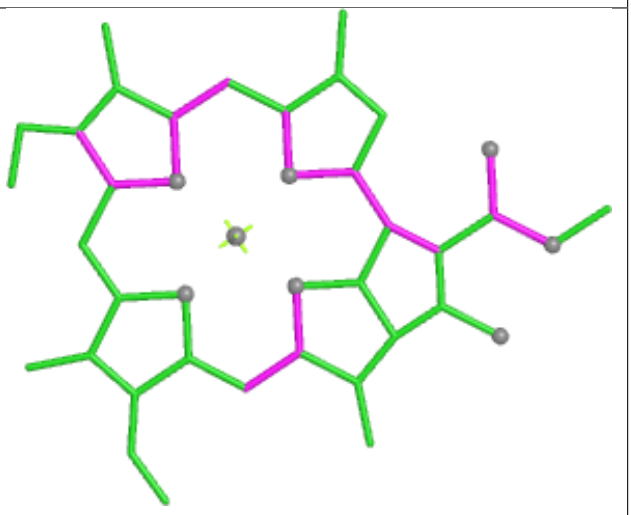


Rings

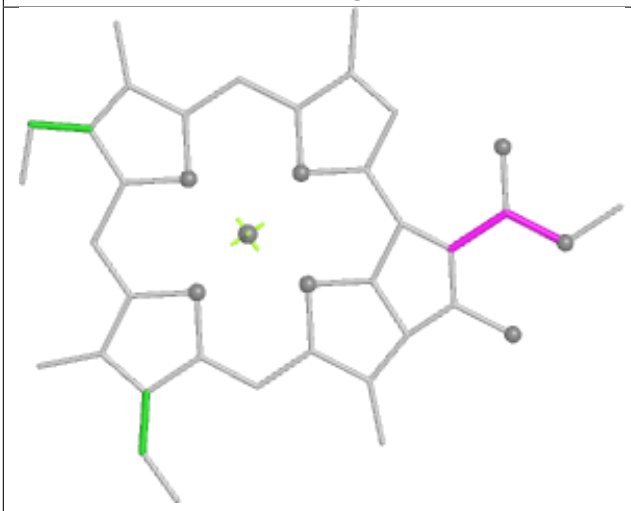
Ligand CLA B1 307



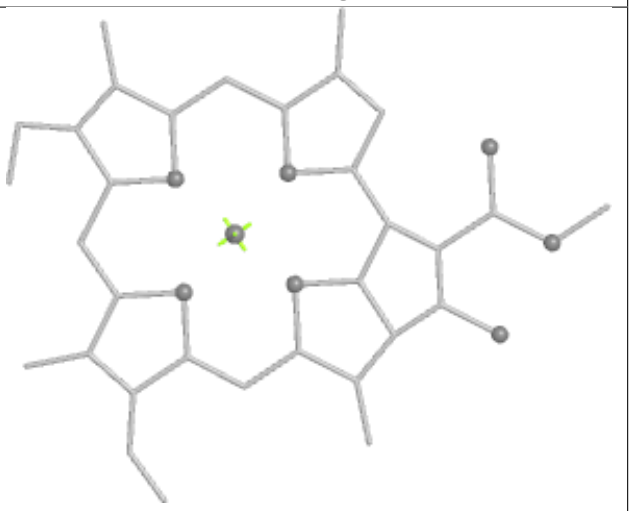
Bond lengths



Bond angles

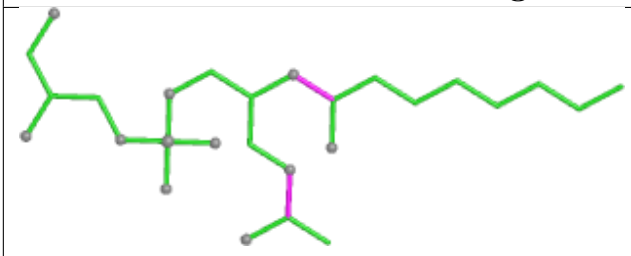


Torsions

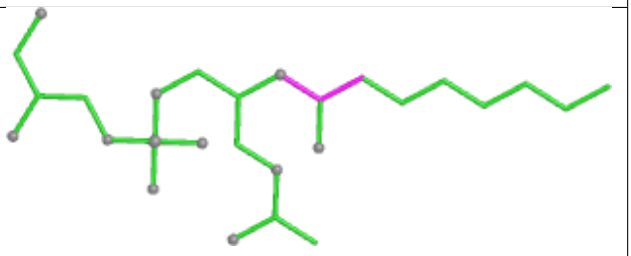


Rings

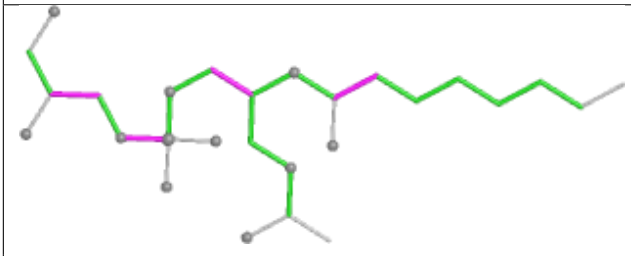
Ligand LHG BA 846



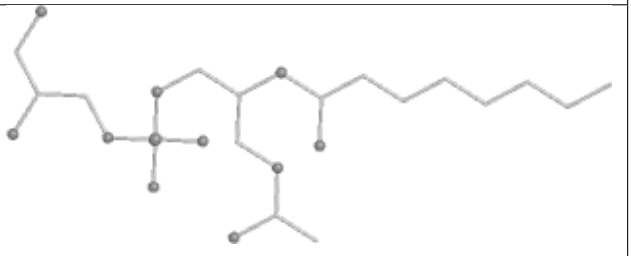
Bond lengths



Bond angles

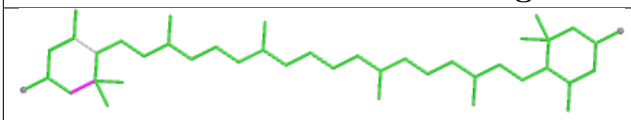


Torsions

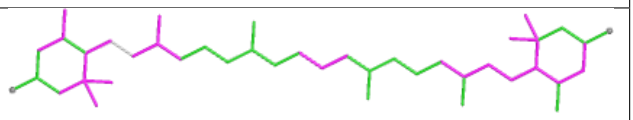


Rings

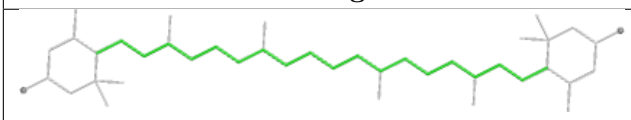
Ligand LUT A1 317



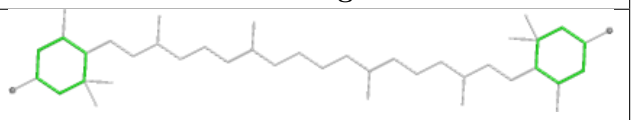
Bond lengths



Bond angles



Torsions

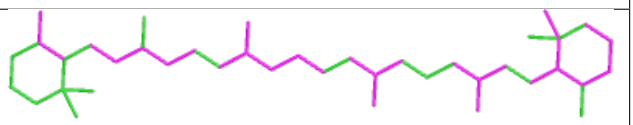


Rings

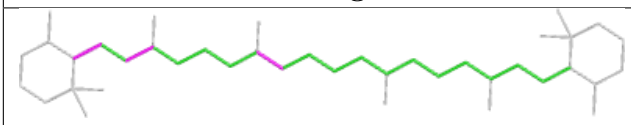
Ligand BCR AF 805



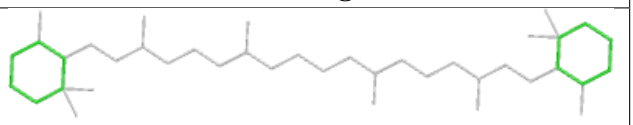
Bond lengths



Bond angles

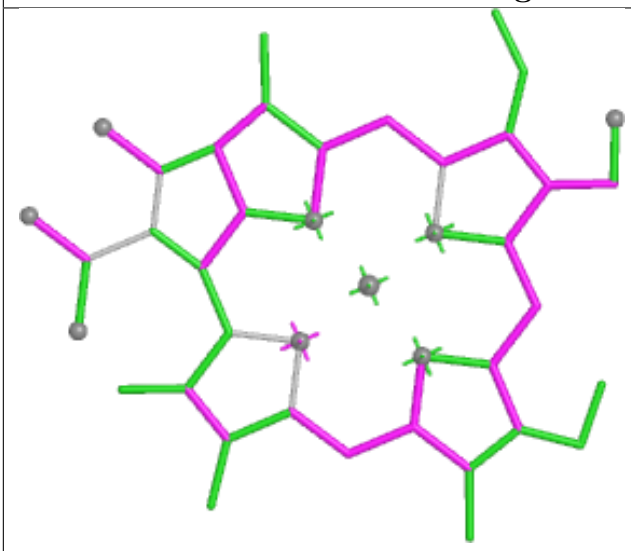


Torsions

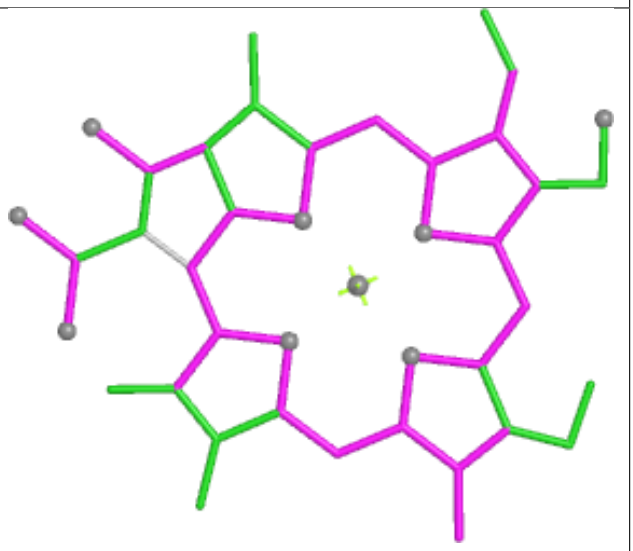


Rings

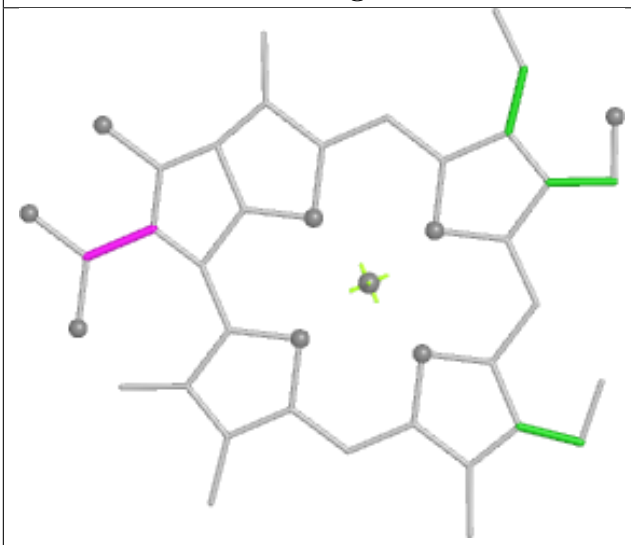
Ligand CHL A1 308



Bond lengths



Bond angles

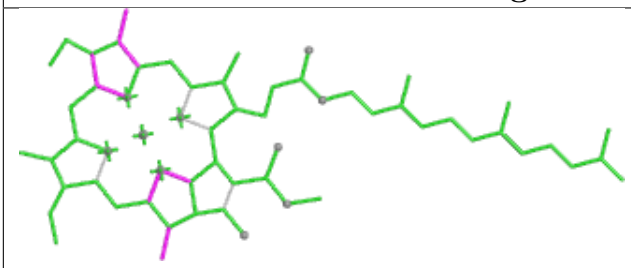


Torsions

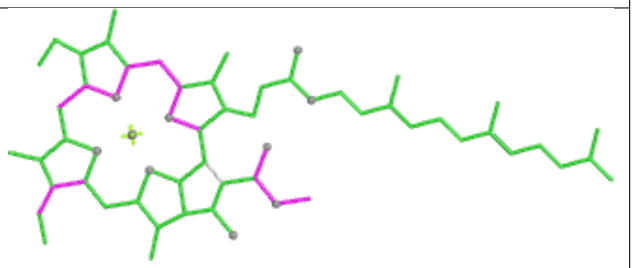


Rings

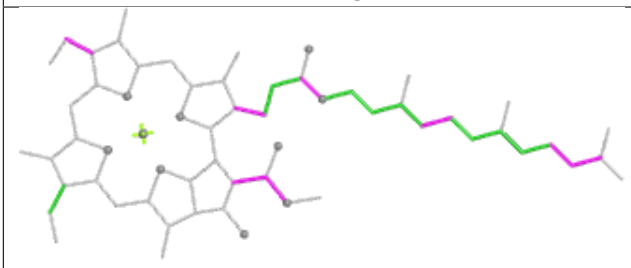
Ligand CLA BH 201



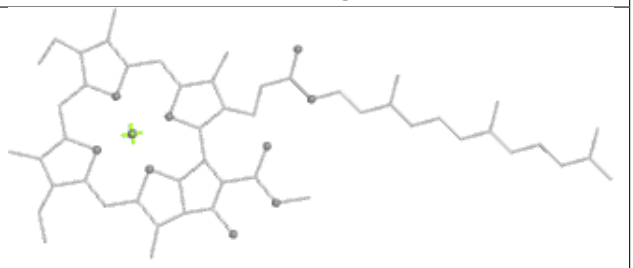
Bond lengths



Bond angles

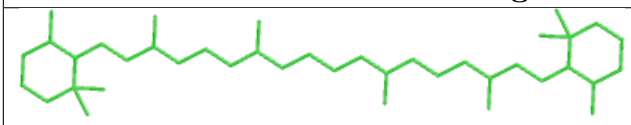


Torsions

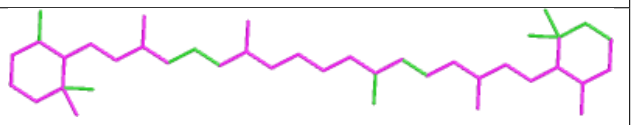


Rings

Ligand BCR AL 302



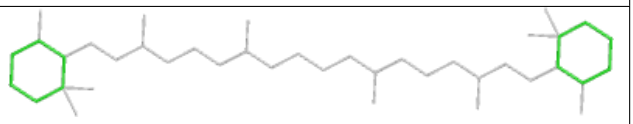
Bond lengths



Bond angles

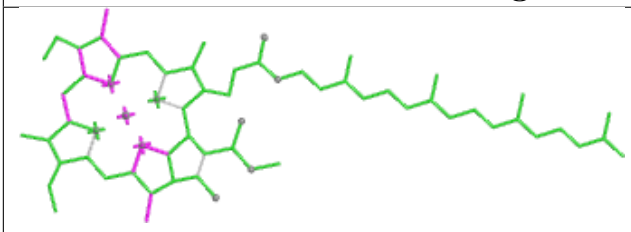


Torsions

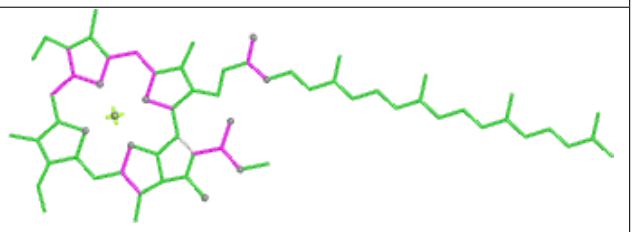


Rings

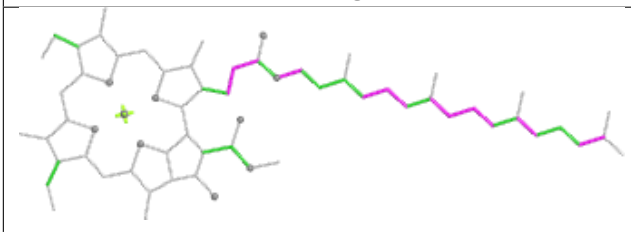
Ligand CLA BA 829



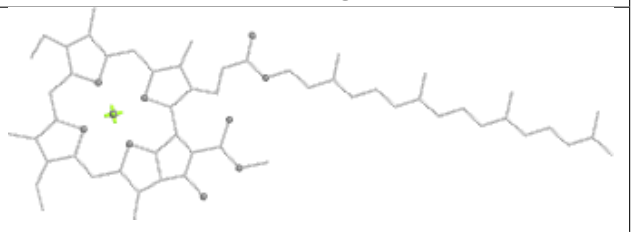
Bond lengths



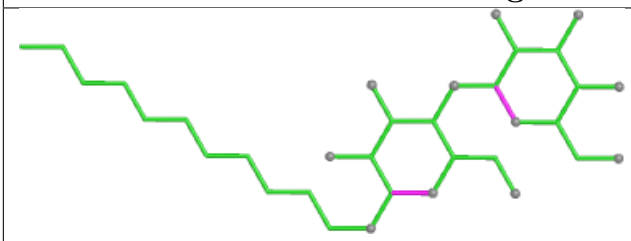
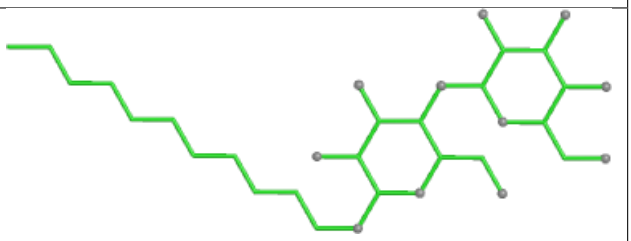
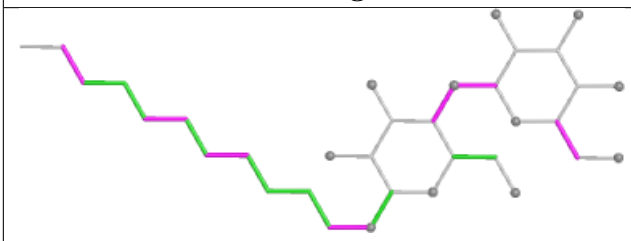
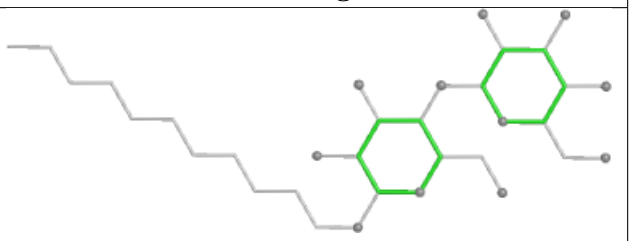
Bond angles

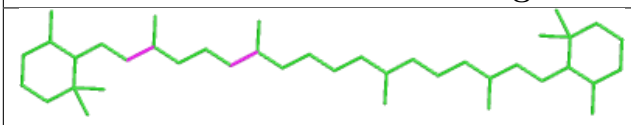
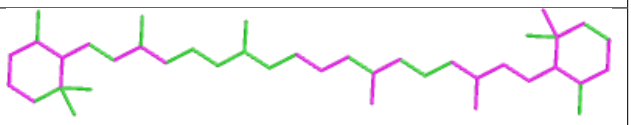
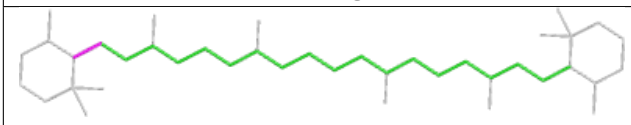
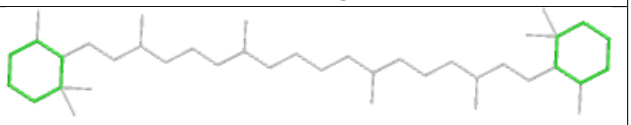


Torsions

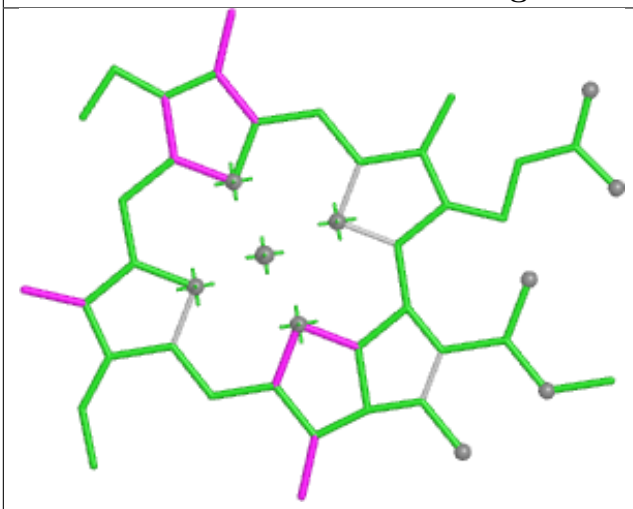


Rings

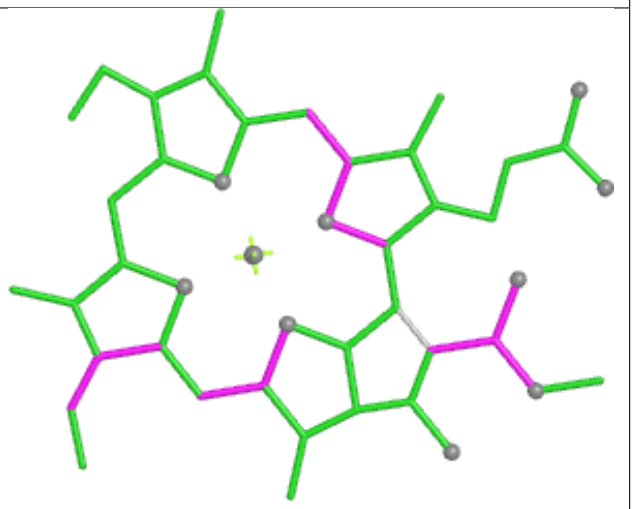
Ligand LMU BA 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A6 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

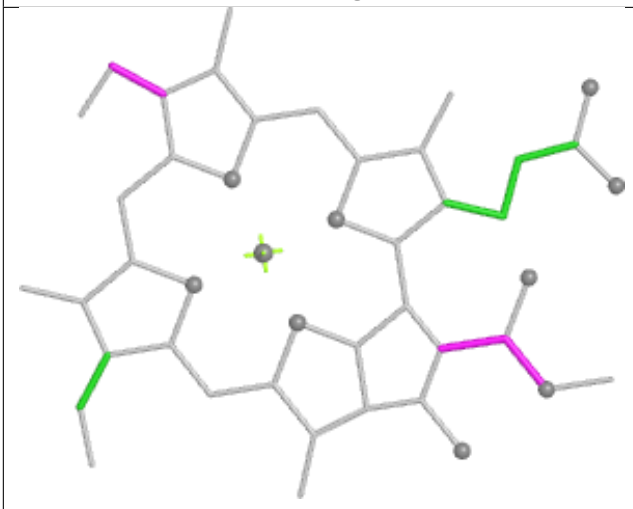
Ligand CLA AA 816



Bond lengths



Bond angles

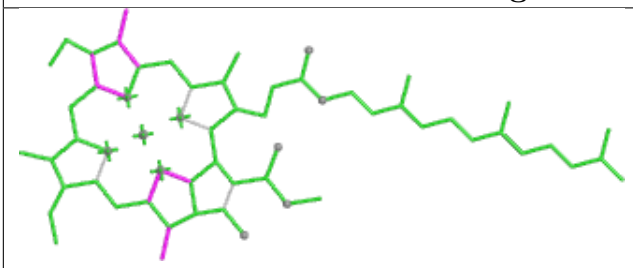


Torsions

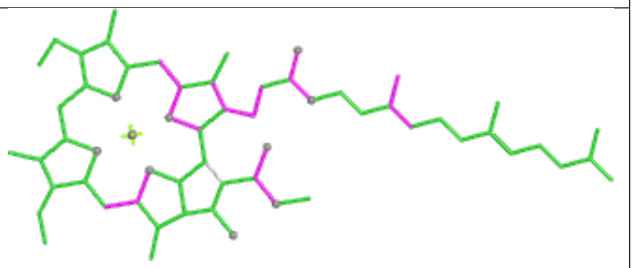


Rings

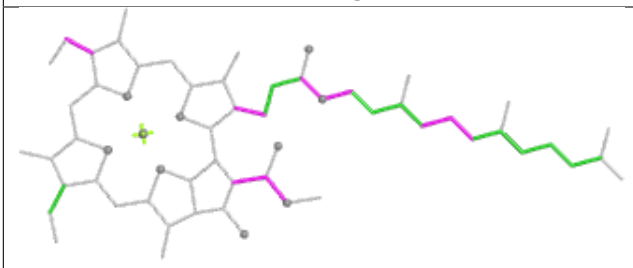
Ligand CLA AH 201



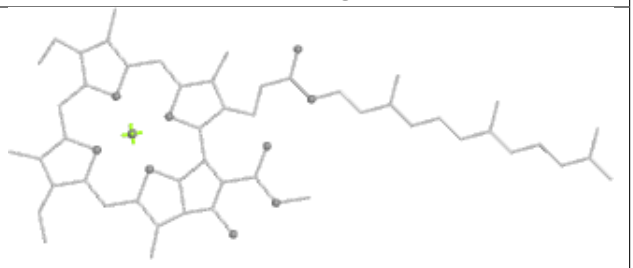
Bond lengths



Bond angles

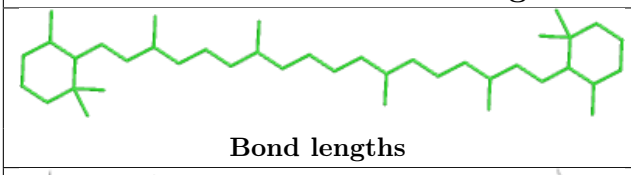


Torsions

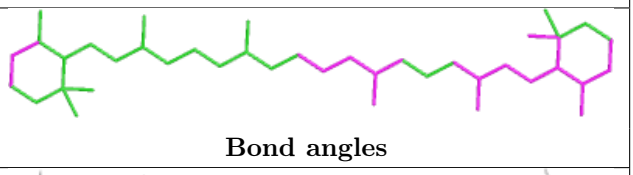


Rings

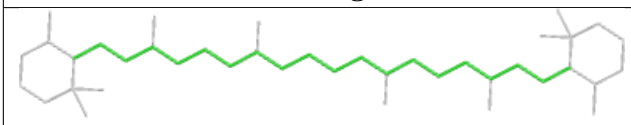
Ligand BCR AB 847



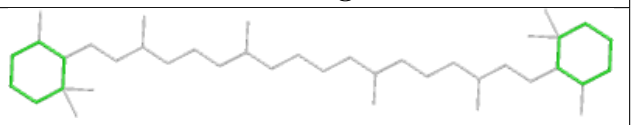
Bond lengths



Bond angles

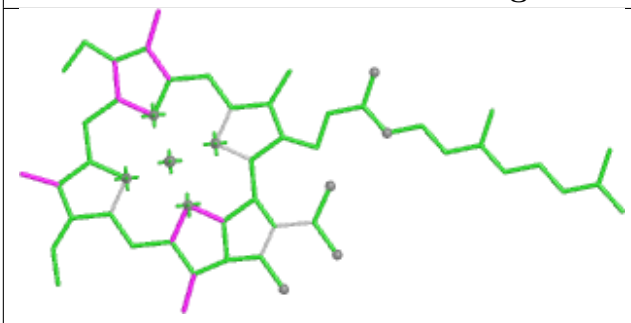


Torsions

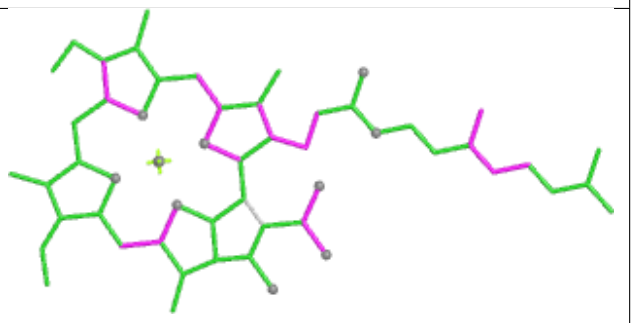


Rings

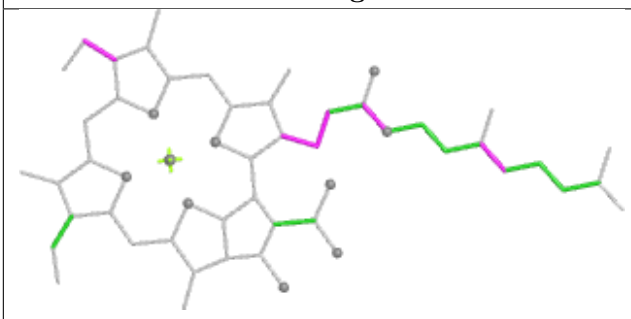
Ligand CLA AA 824



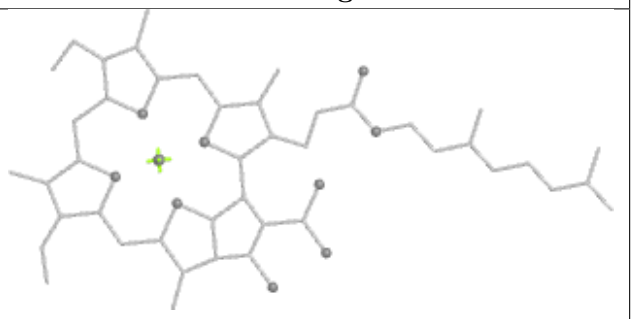
Bond lengths



Bond angles

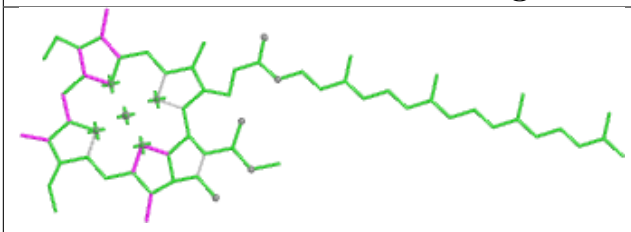


Torsions

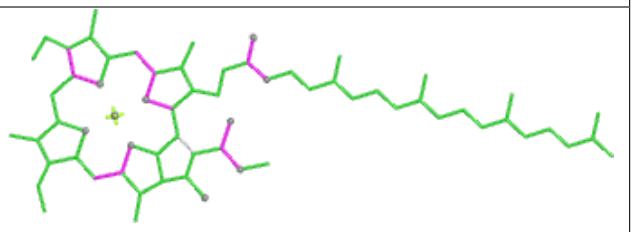


Rings

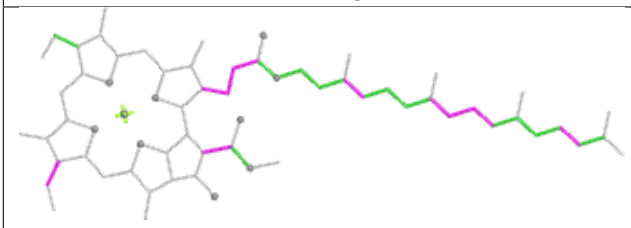
Ligand CLA AB 828



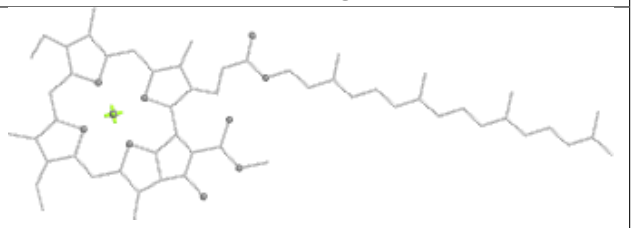
Bond lengths



Bond angles

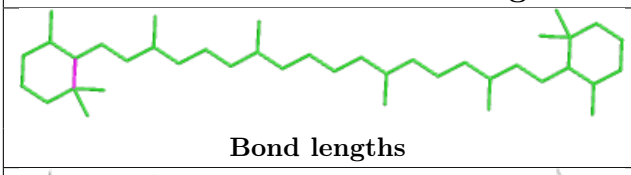


Torsions

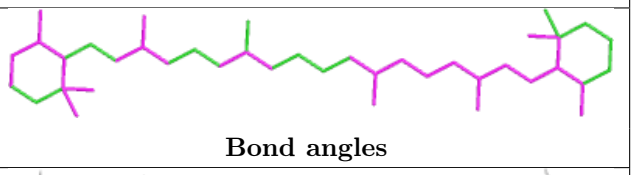


Rings

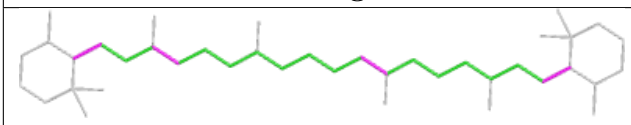
Ligand BCR BA 851



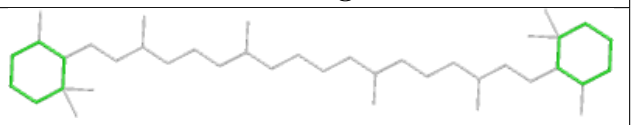
Bond lengths



Bond angles

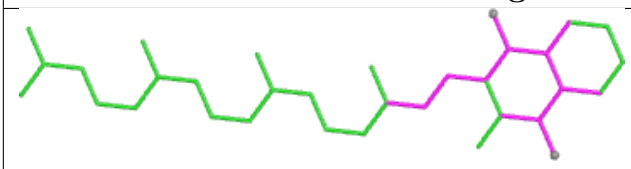


Torsions

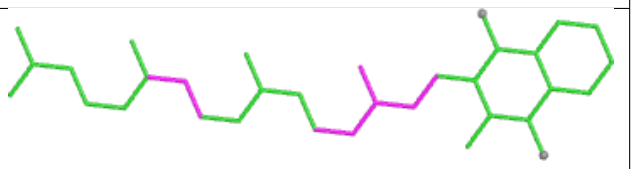


Rings

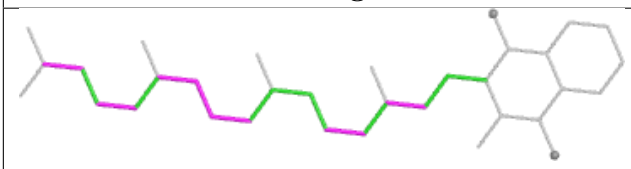
Ligand PQN BA 843



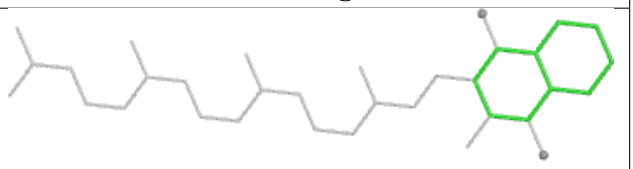
Bond lengths



Bond angles

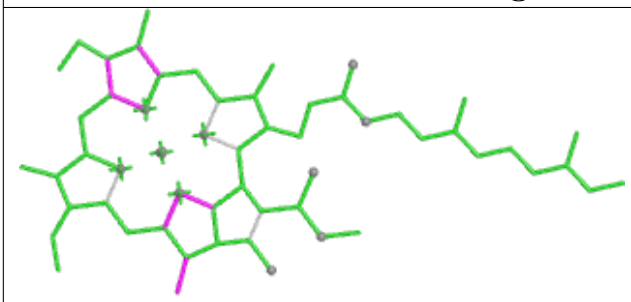


Torsions

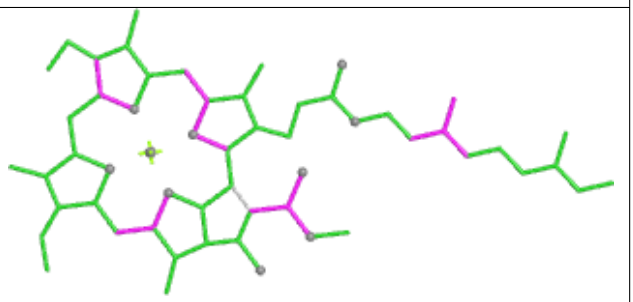


Rings

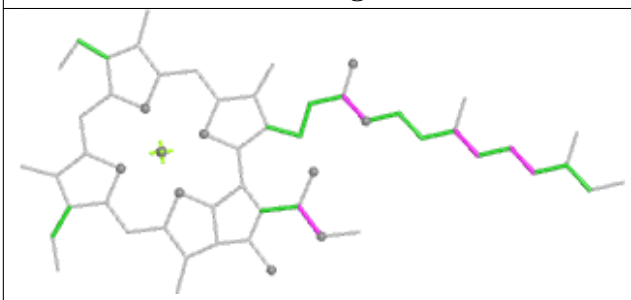
Ligand CLA AA 832



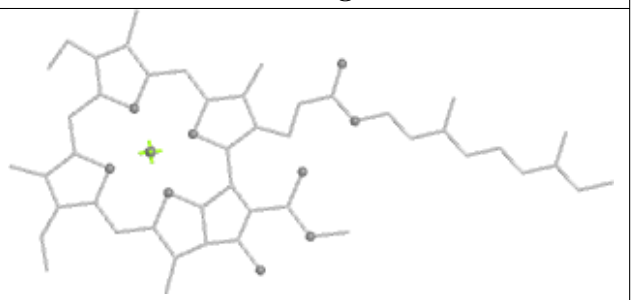
Bond lengths



Bond angles

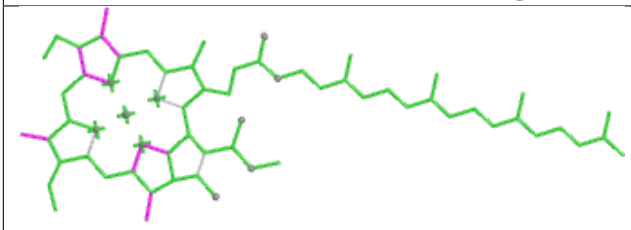


Torsions

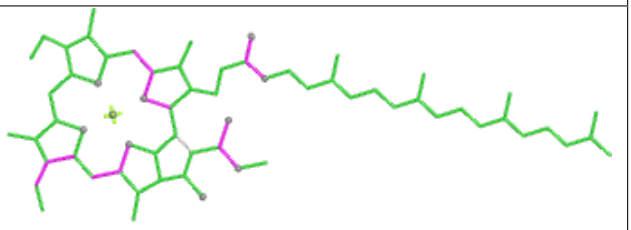


Rings

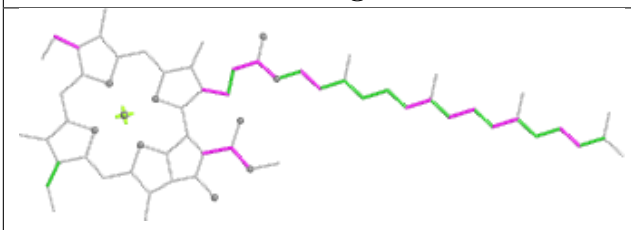
Ligand CLA AB 834



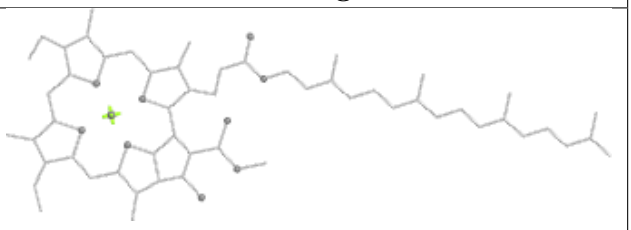
Bond lengths



Bond angles

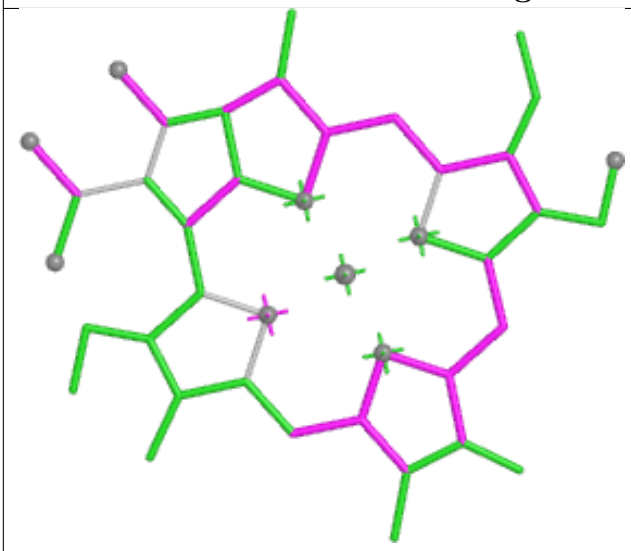


Torsions

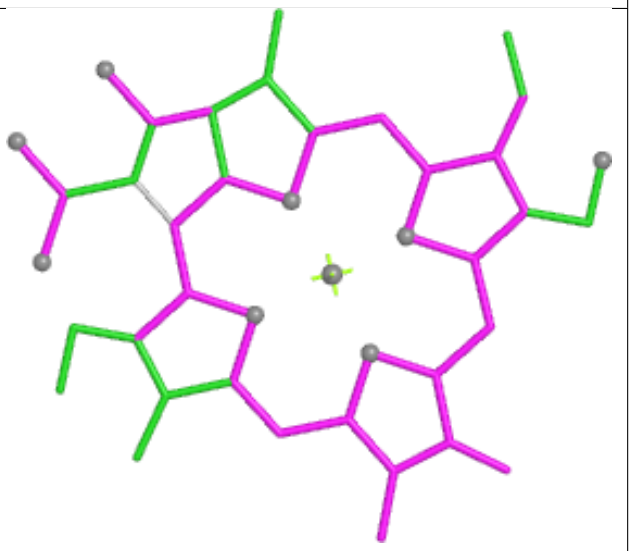


Rings

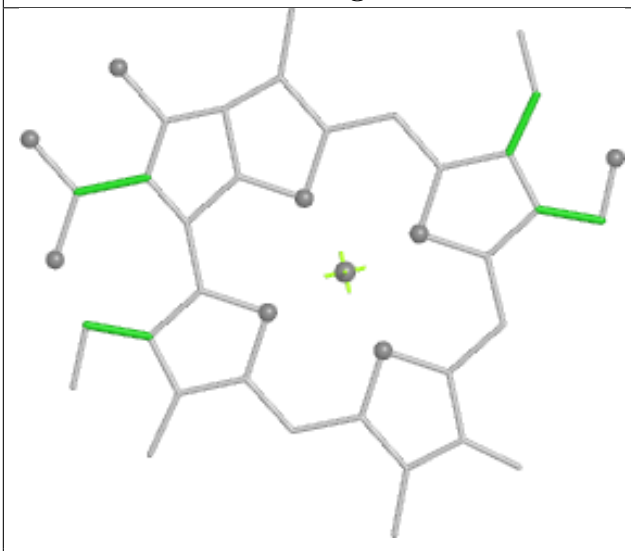
Ligand CHL A4 314



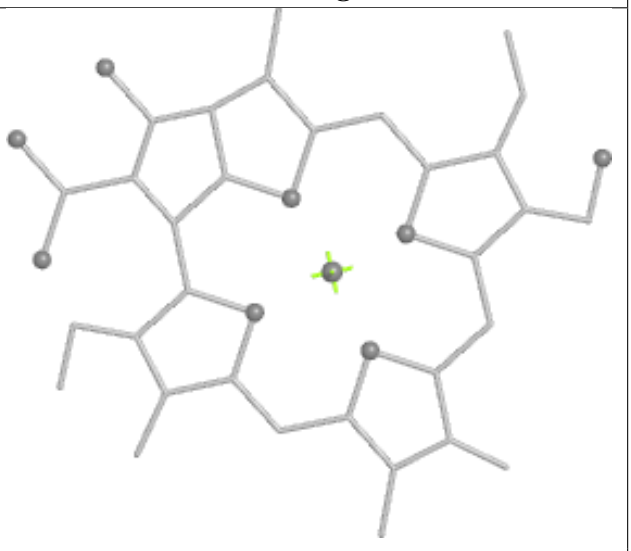
Bond lengths



Bond angles

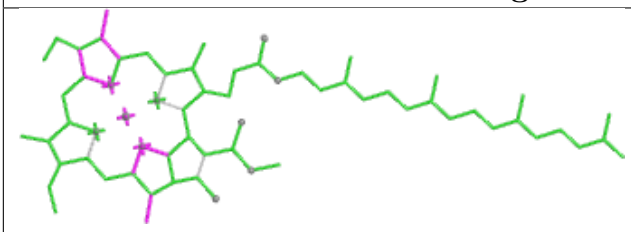


Torsions

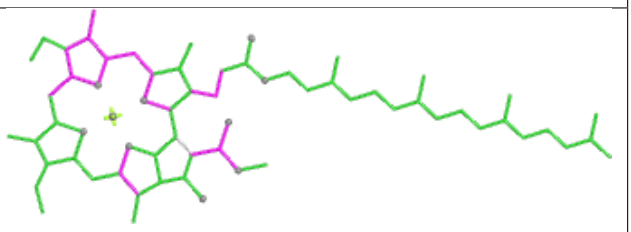


Rings

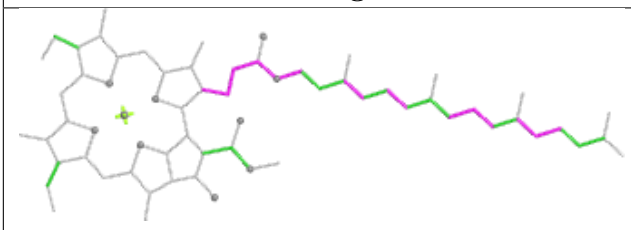
Ligand CLA AB 829



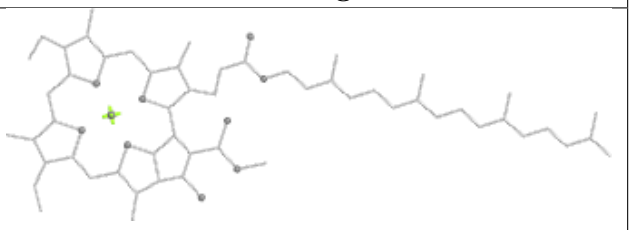
Bond lengths



Bond angles

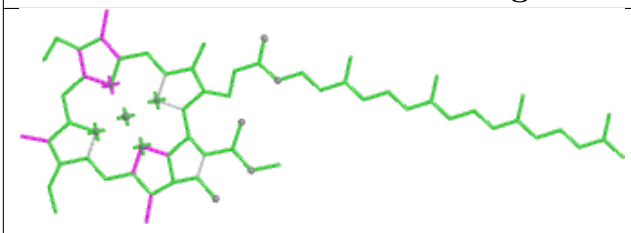


Torsions

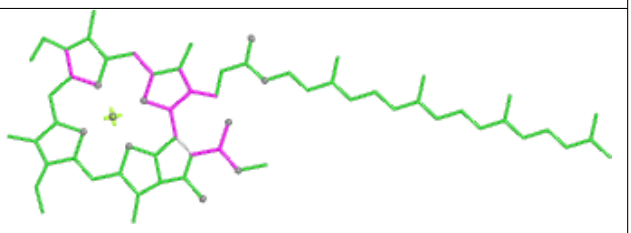


Rings

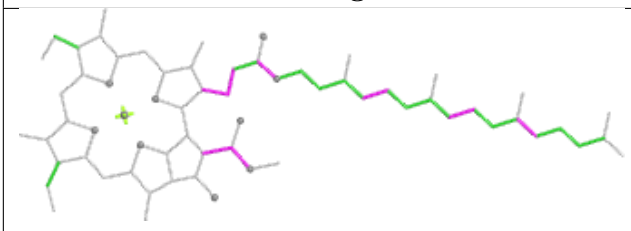
Ligand CLA AB 811



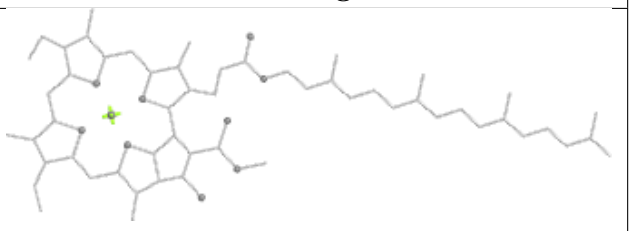
Bond lengths



Bond angles

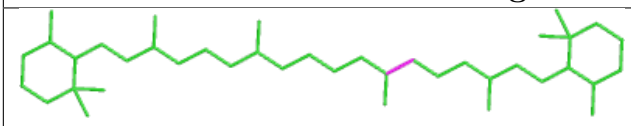


Torsions

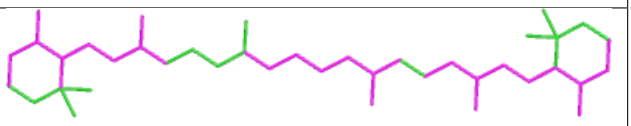


Rings

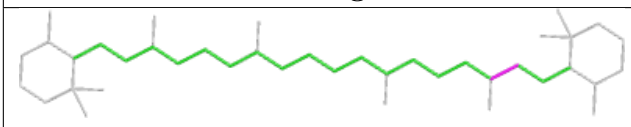
Ligand BCR AB 848



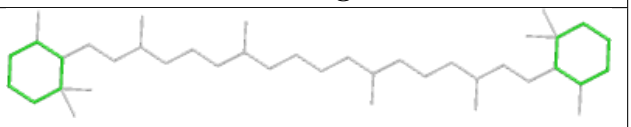
Bond lengths



Bond angles

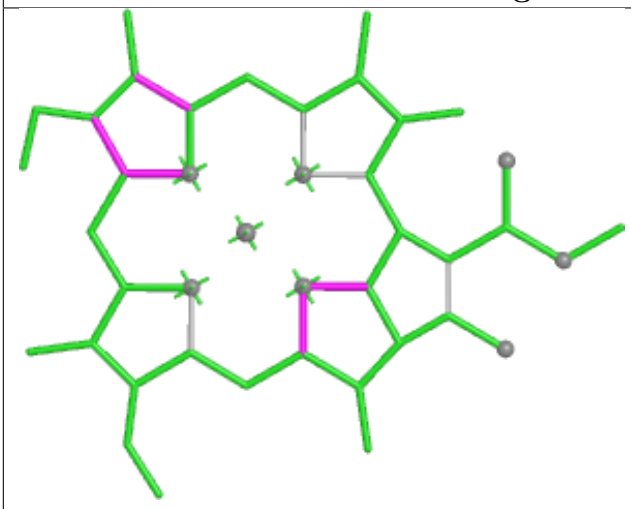


Torsions

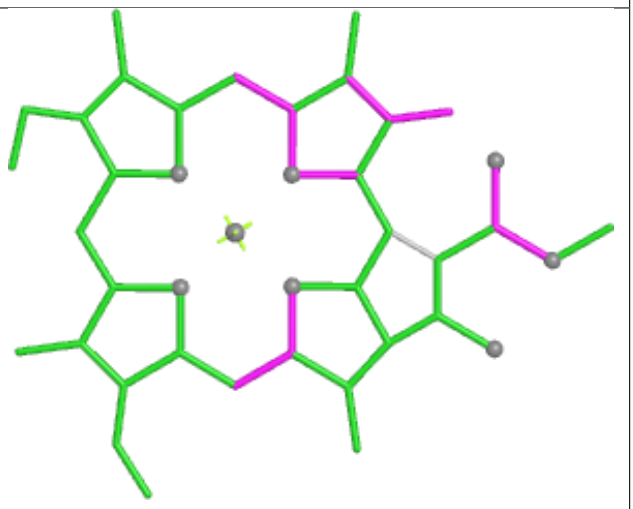


Rings

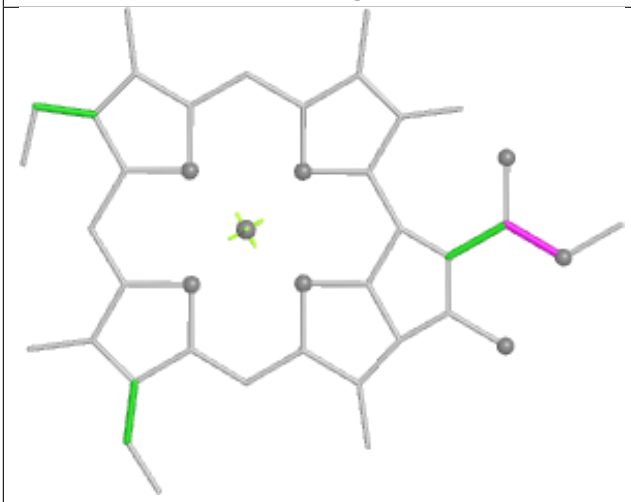
Ligand CLA BF 303



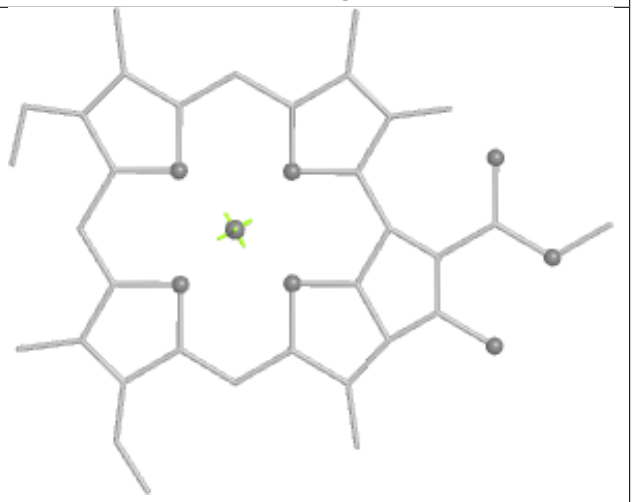
Bond lengths



Bond angles

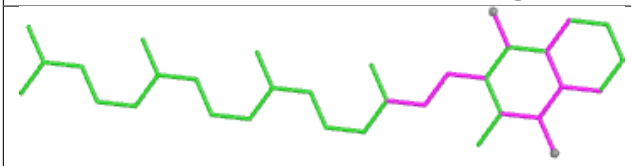


Torsions

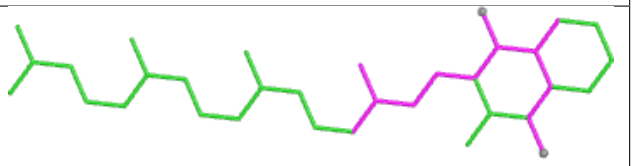


Rings

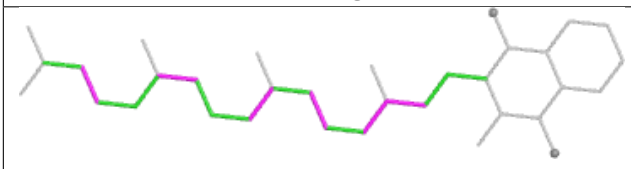
Ligand PQN BB 844



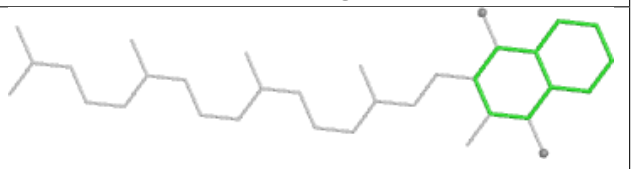
Bond lengths



Bond angles

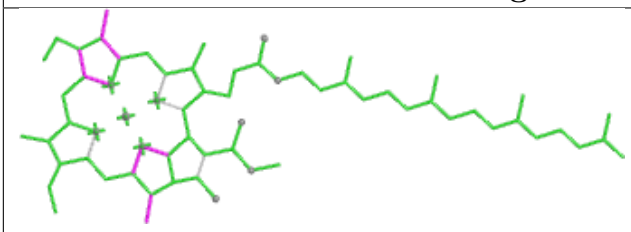


Torsions

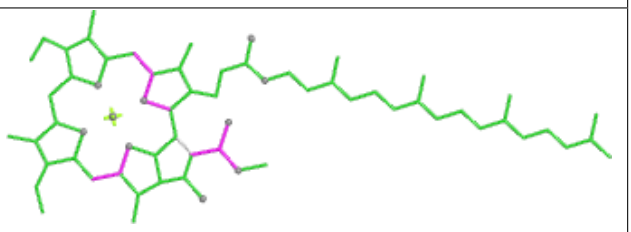


Rings

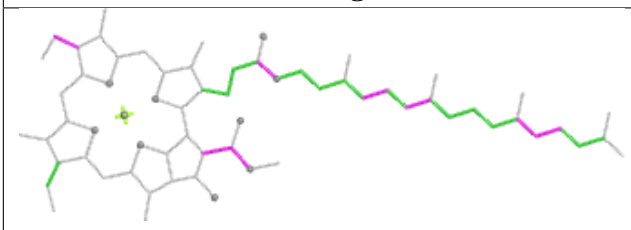
Ligand CLA AA 811



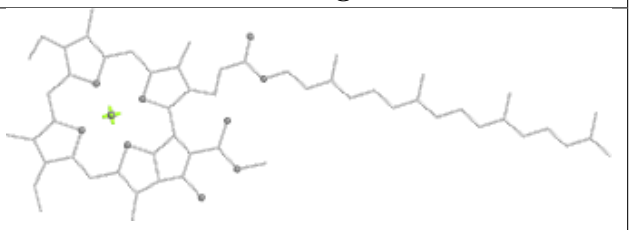
Bond lengths



Bond angles

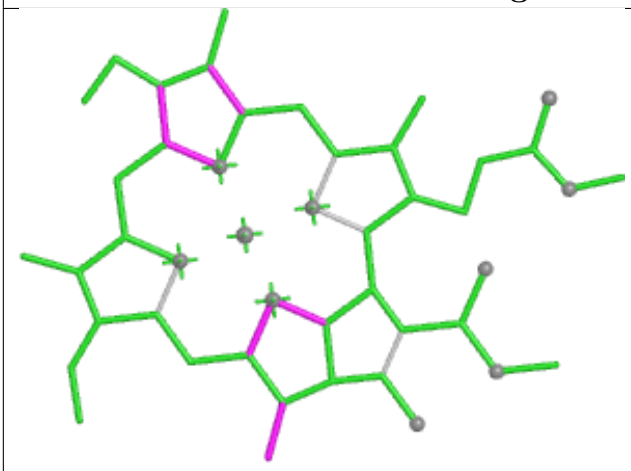


Torsions

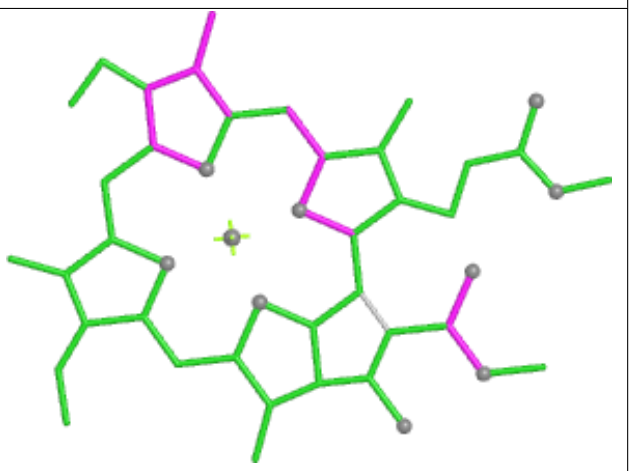


Rings

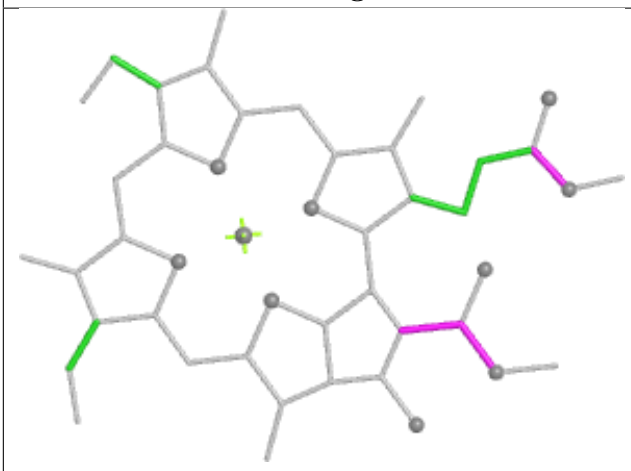
Ligand CLA BK 203



Bond lengths



Bond angles

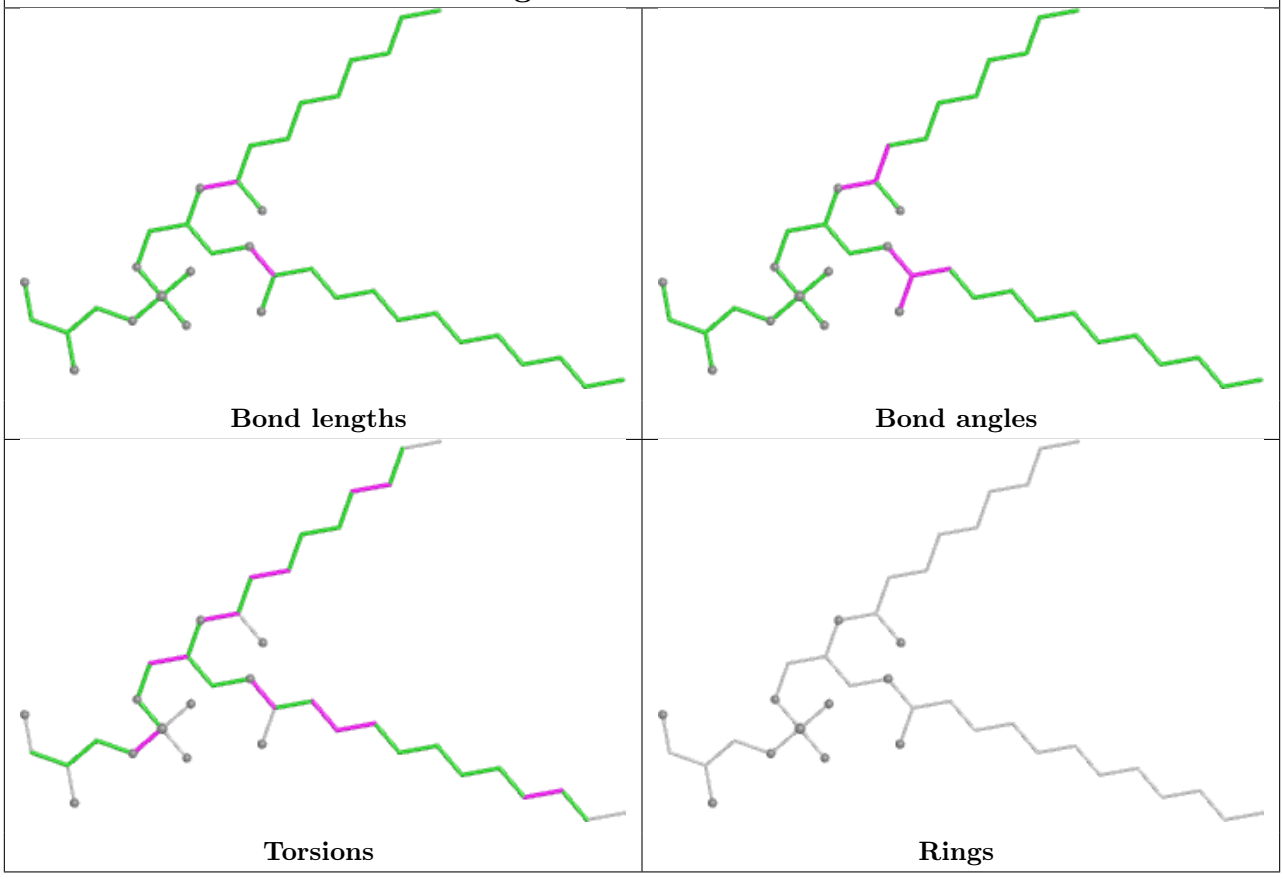


Torsions

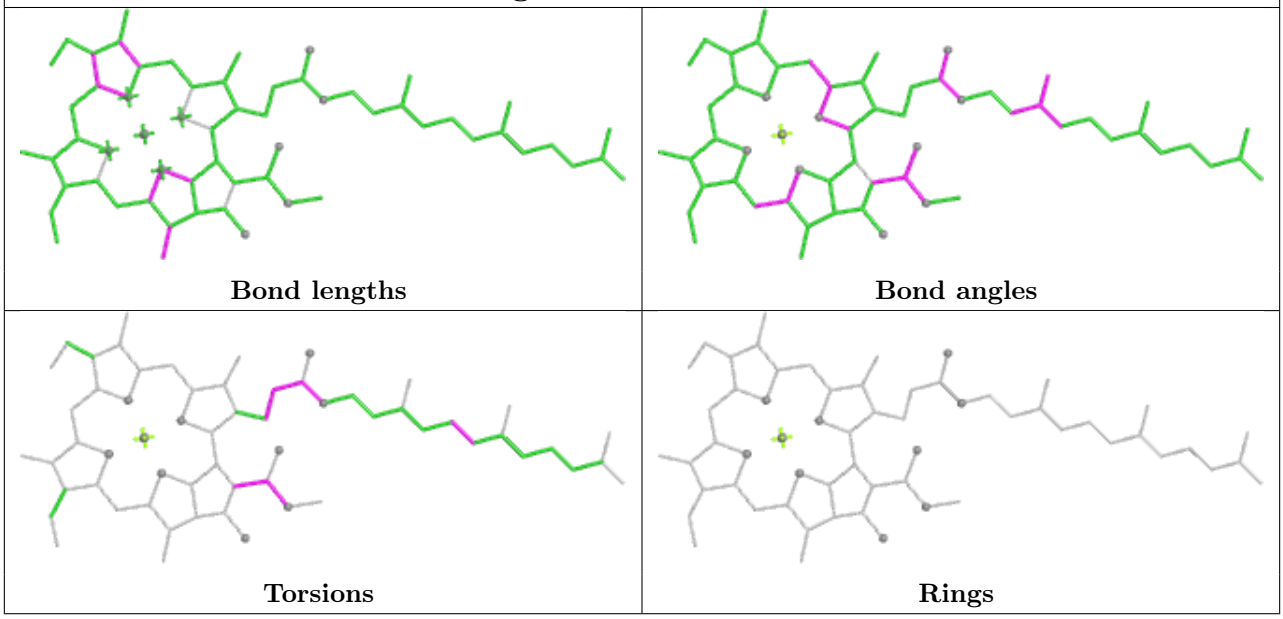


Rings

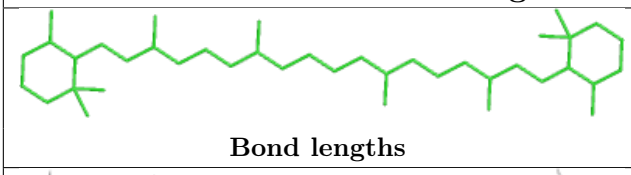
Ligand LHG A1 301



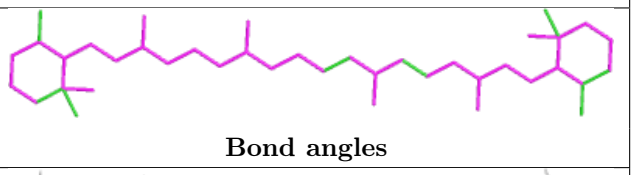
Ligand CLA BA 817



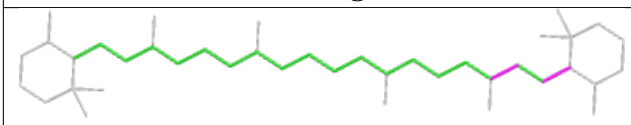
Ligand BCR BA 855



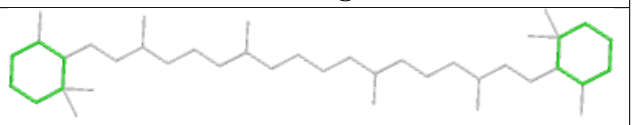
Bond lengths



Bond angles

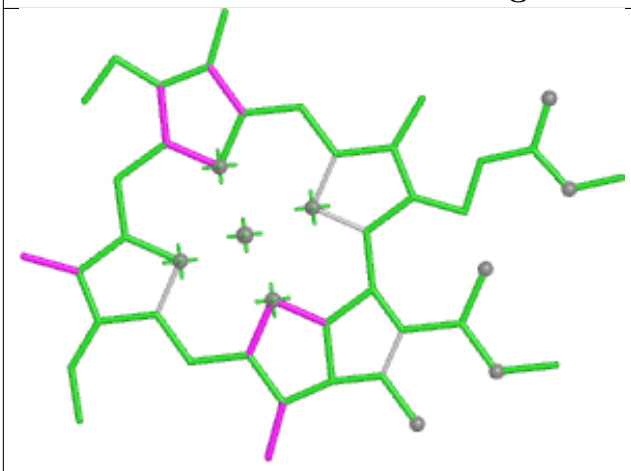


Torsions

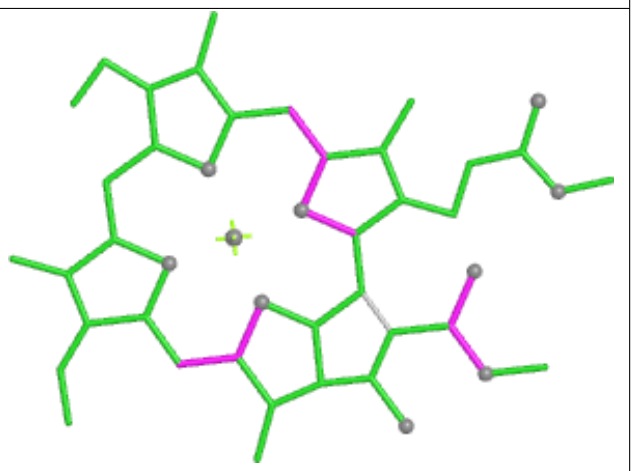


Rings

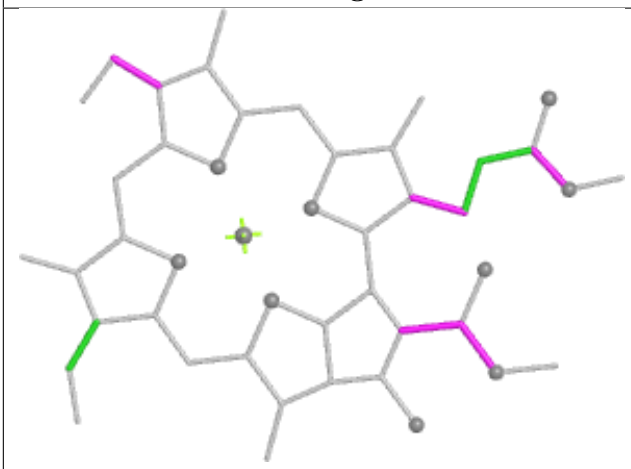
Ligand CLA AK 203



Bond lengths



Bond angles

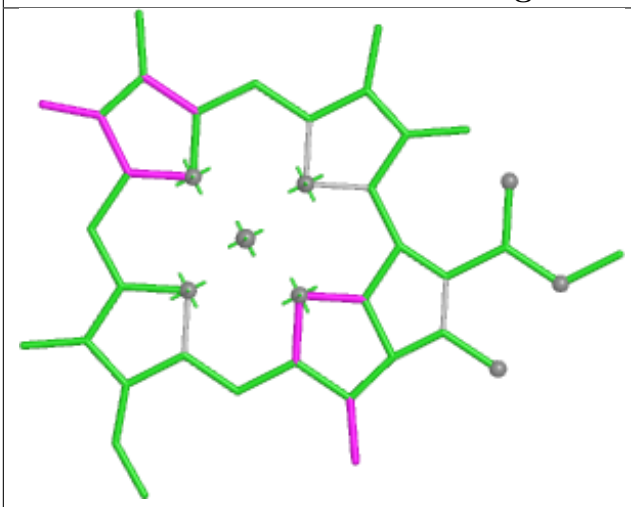


Torsions

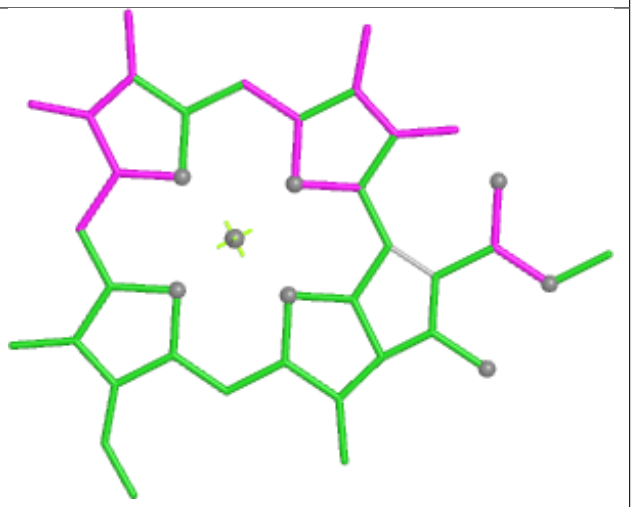


Rings

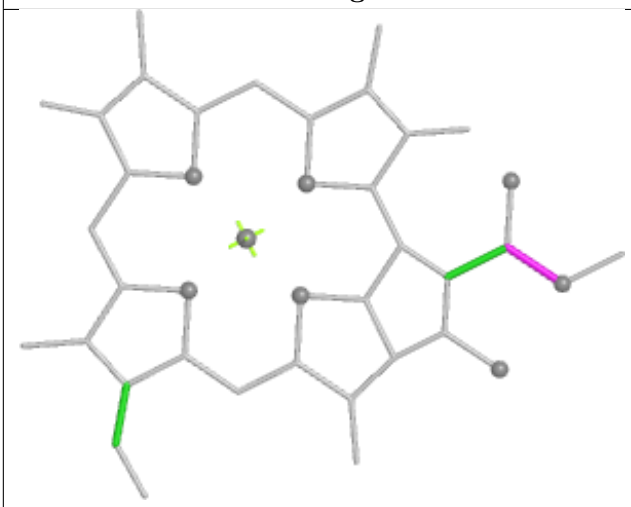
Ligand CLA A1 310



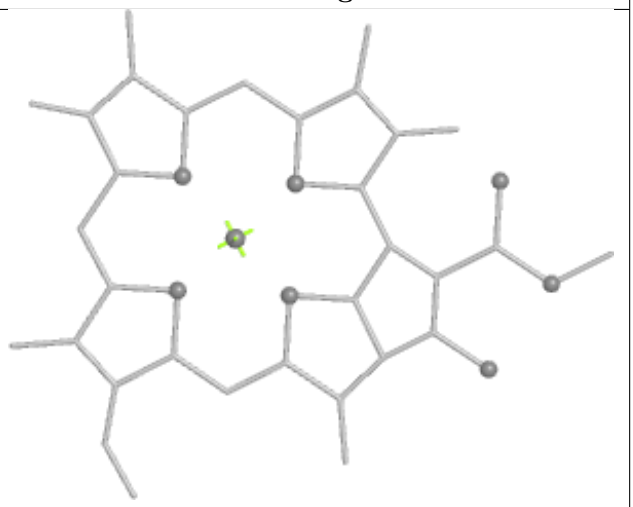
Bond lengths



Bond angles

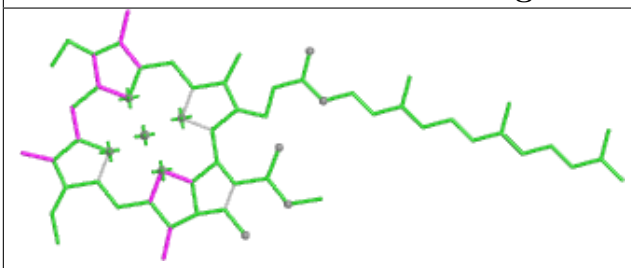


Torsions

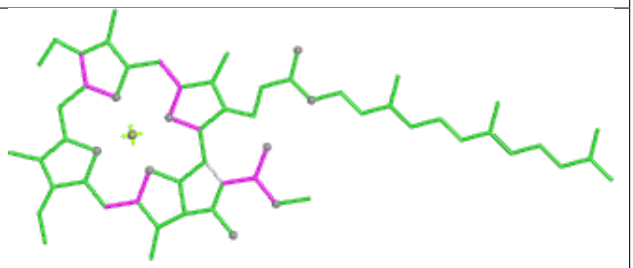


Rings

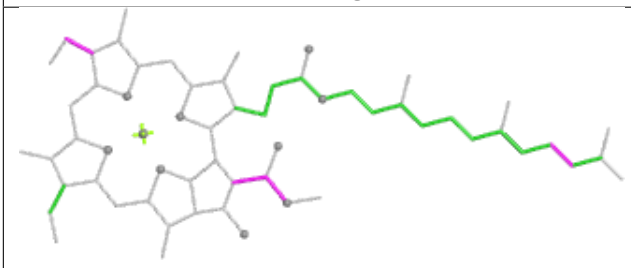
Ligand CLA B3 301



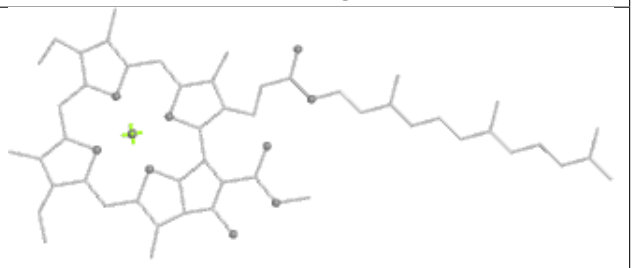
Bond lengths



Bond angles

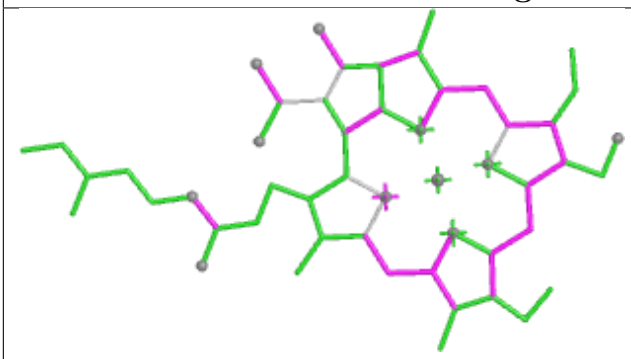


Torsions

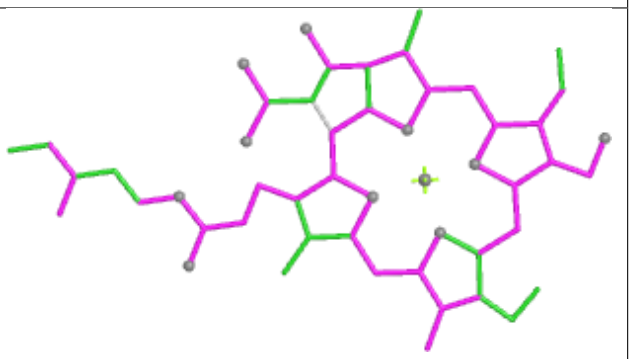


Rings

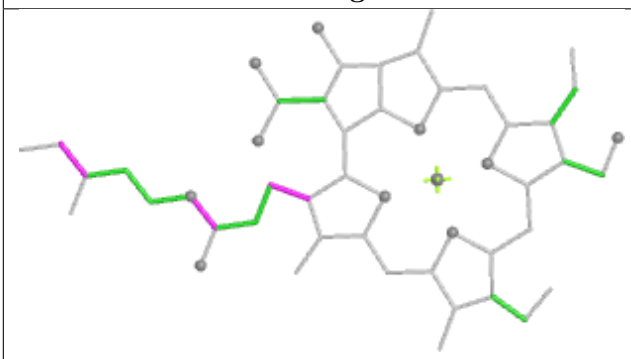
Ligand CHL A1 303



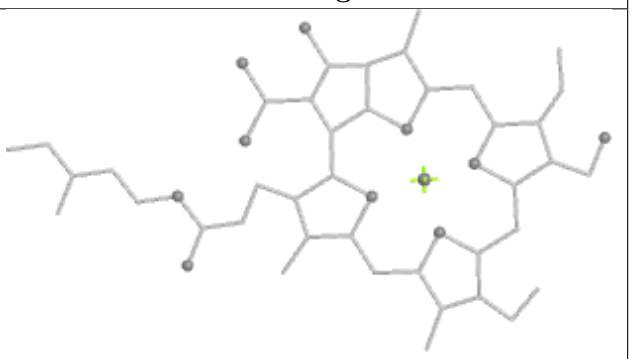
Bond lengths



Bond angles

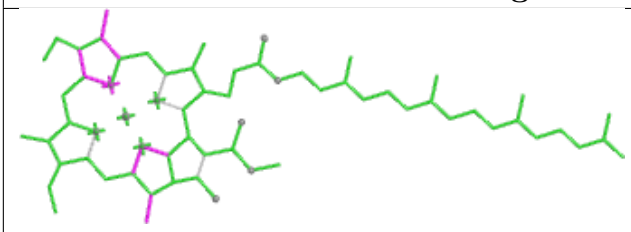


Torsions

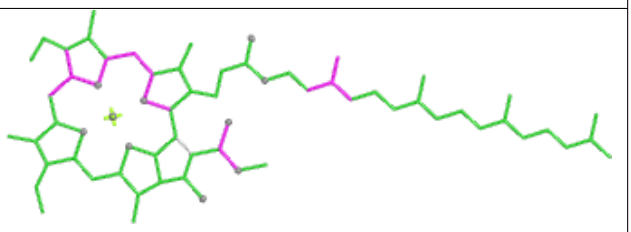


Rings

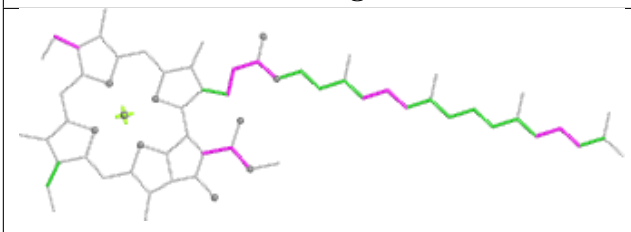
Ligand CLA BA 833



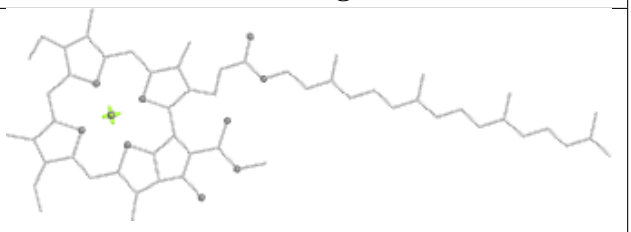
Bond lengths



Bond angles

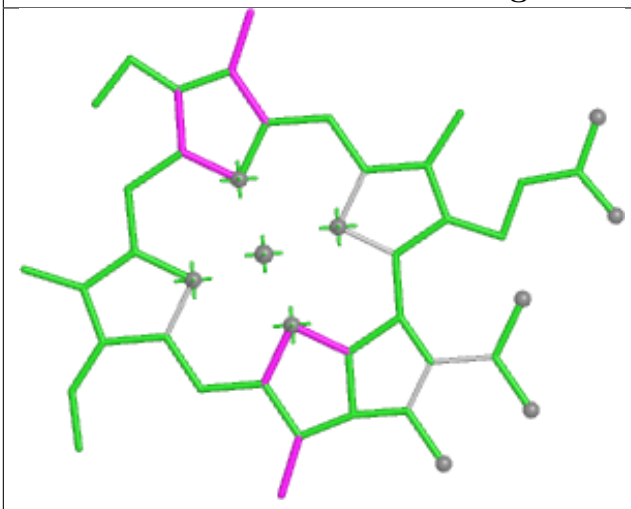


Torsions

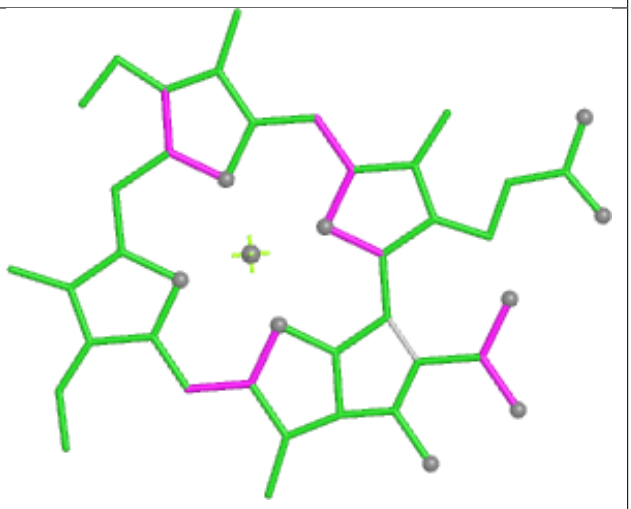


Rings

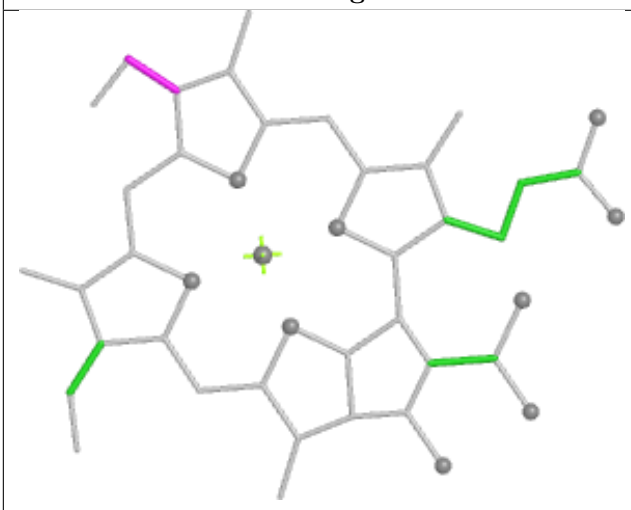
Ligand CLA AA 835



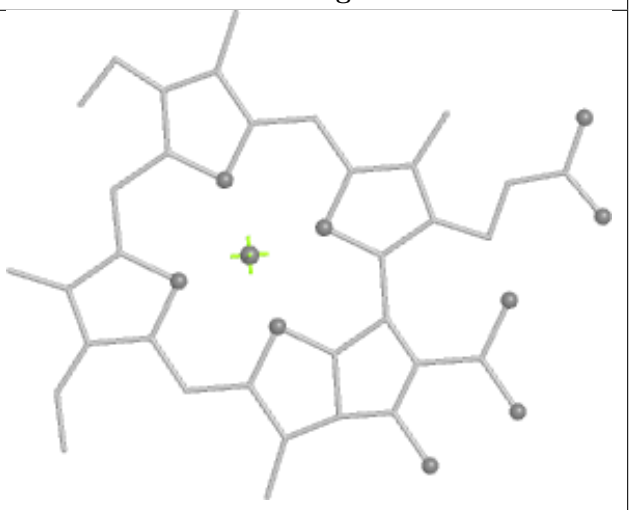
Bond lengths



Bond angles

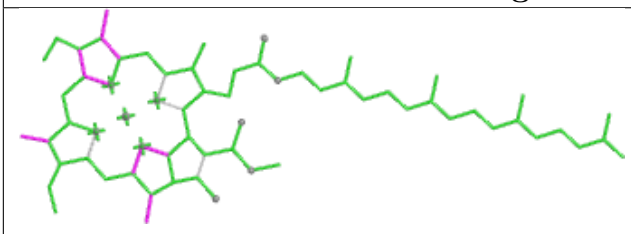


Torsions

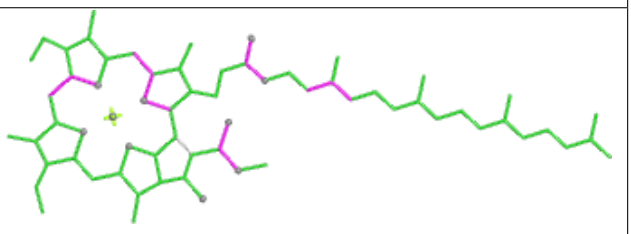


Rings

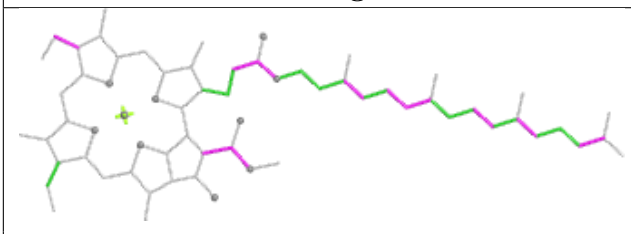
Ligand CLA BB 804



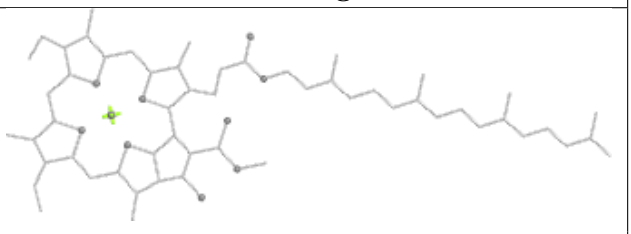
Bond lengths



Bond angles

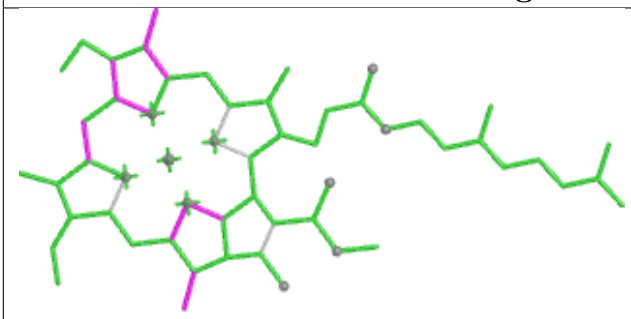


Torsions

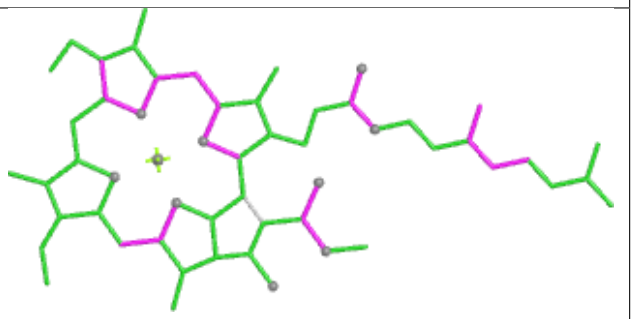


Rings

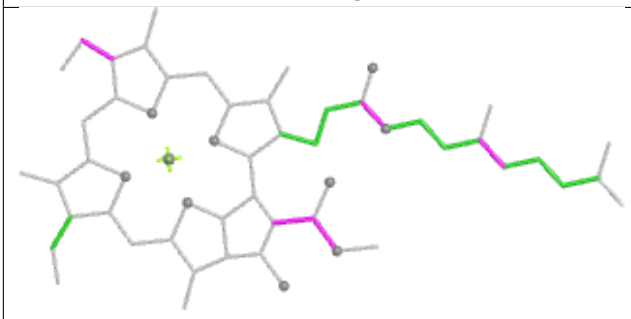
Ligand CLA B2 609



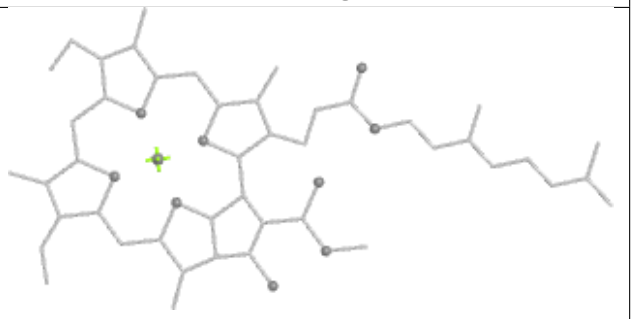
Bond lengths



Bond angles

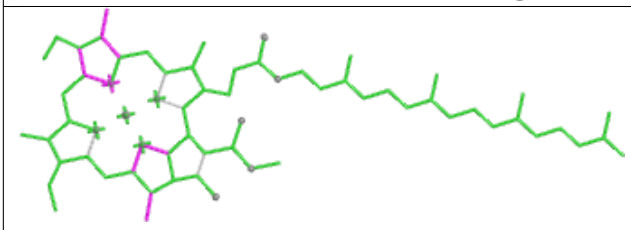


Torsions

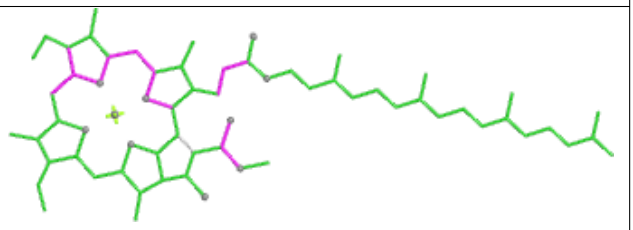


Rings

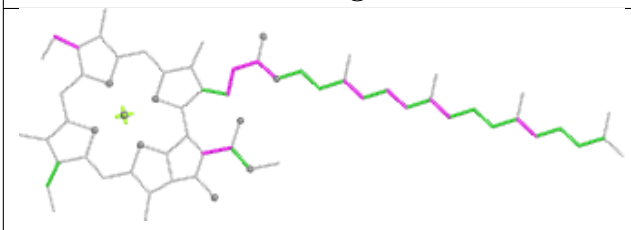
Ligand CLA BA 842



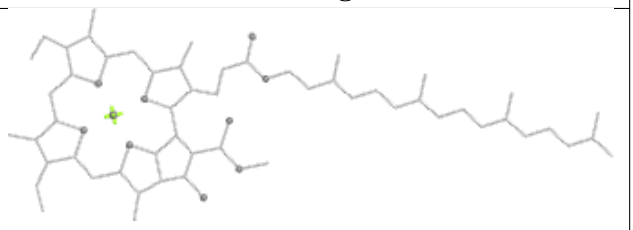
Bond lengths



Bond angles

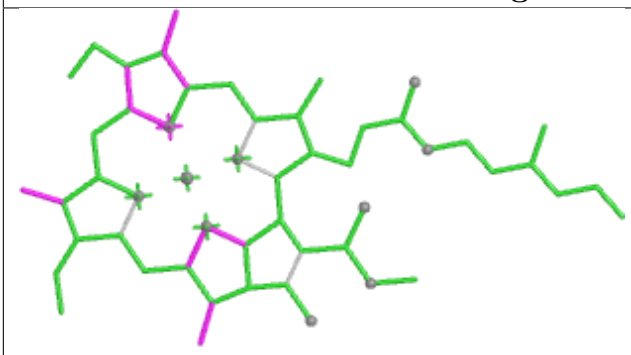


Torsions

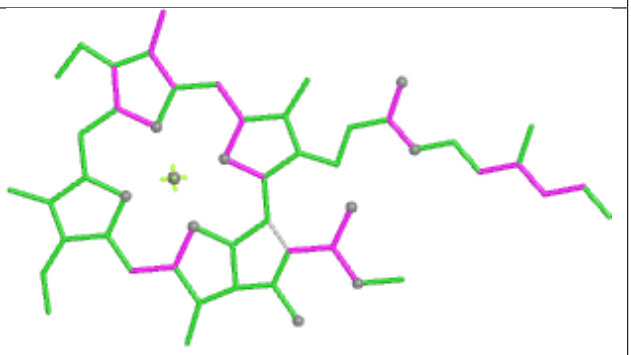


Rings

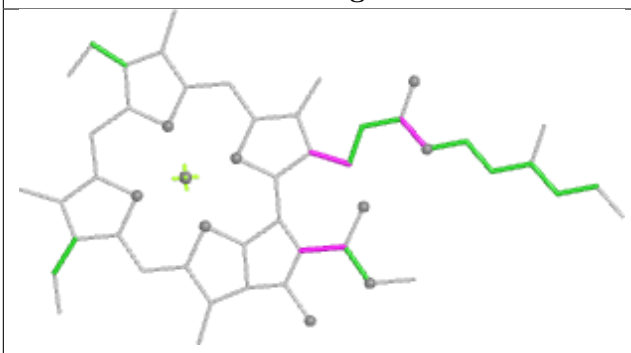
Ligand CLA BA 804



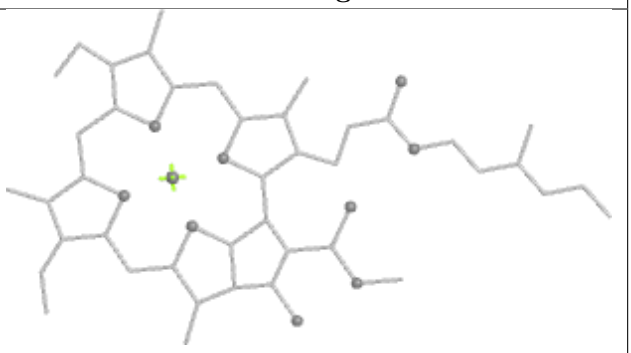
Bond lengths



Bond angles

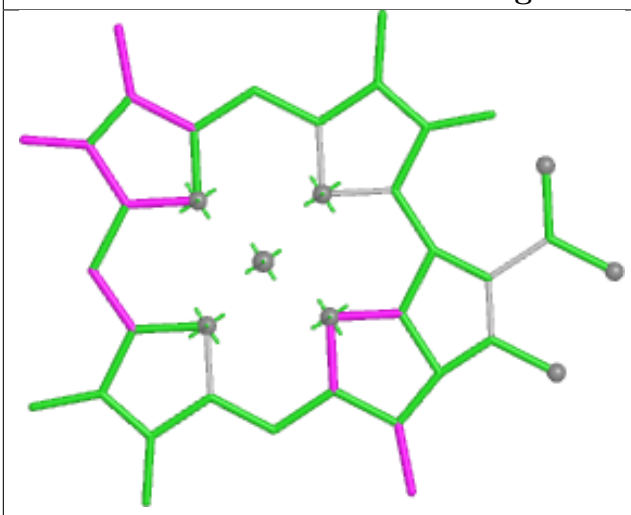


Torsions

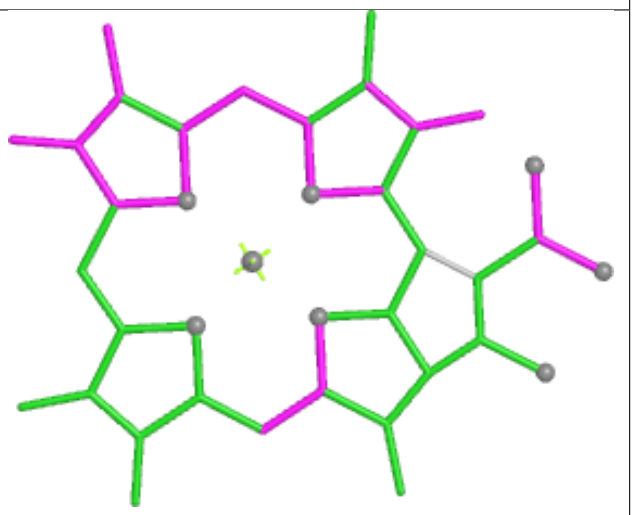


Rings

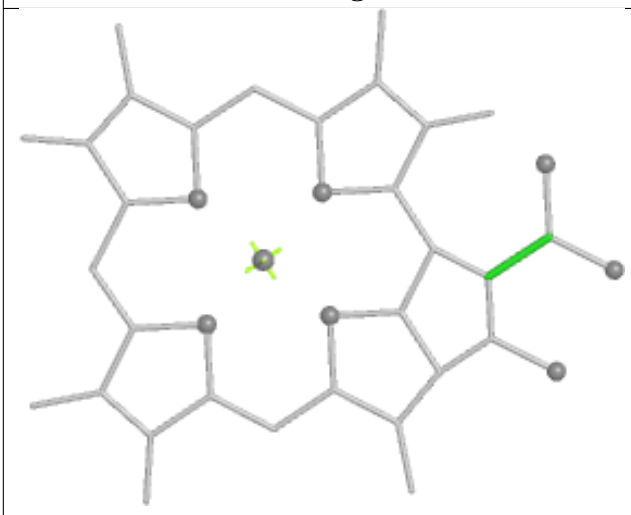
Ligand CLA A1 312



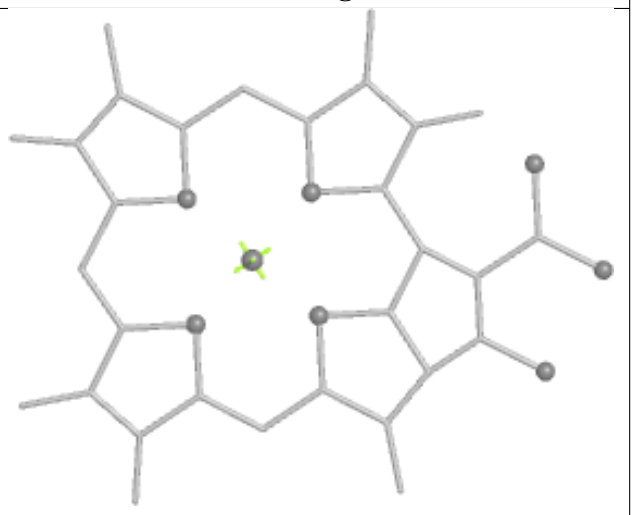
Bond lengths



Bond angles

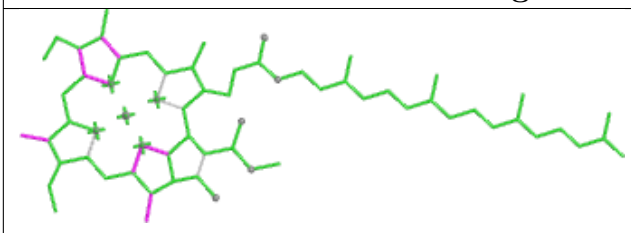


Torsions

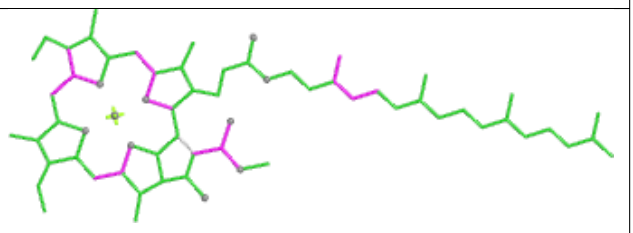


Rings

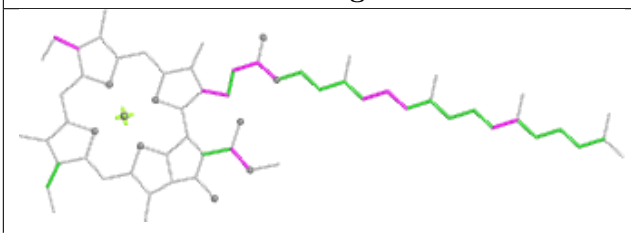
Ligand CLA BB 834



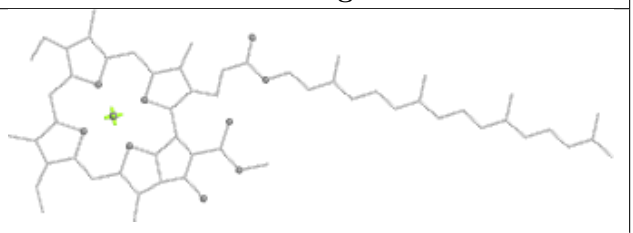
Bond lengths



Bond angles

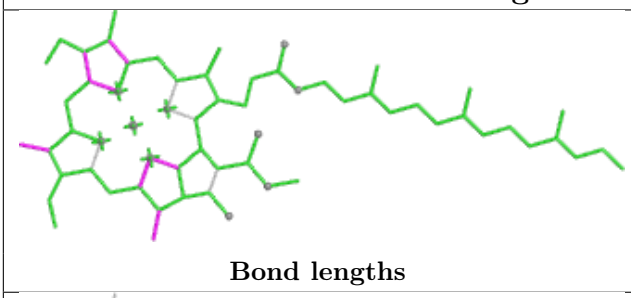


Torsions

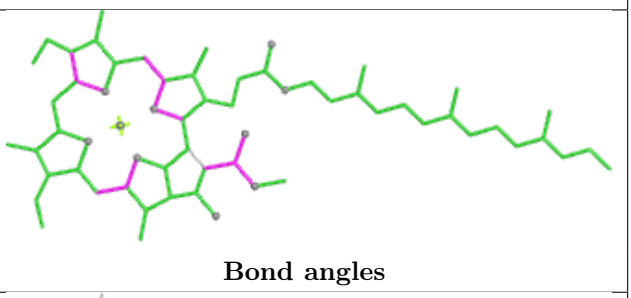


Rings

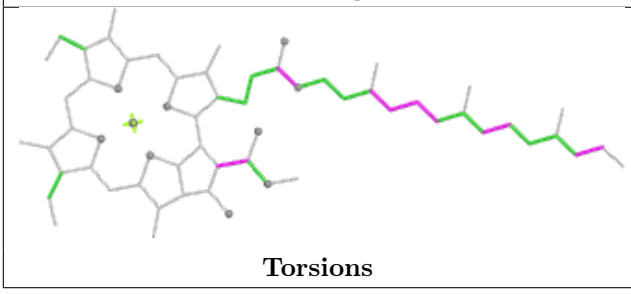
Ligand CLA BB 827



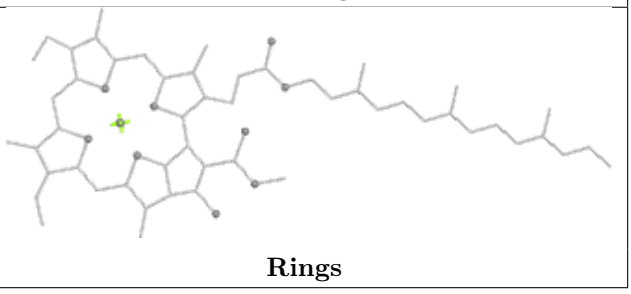
Bond lengths



Bond angles

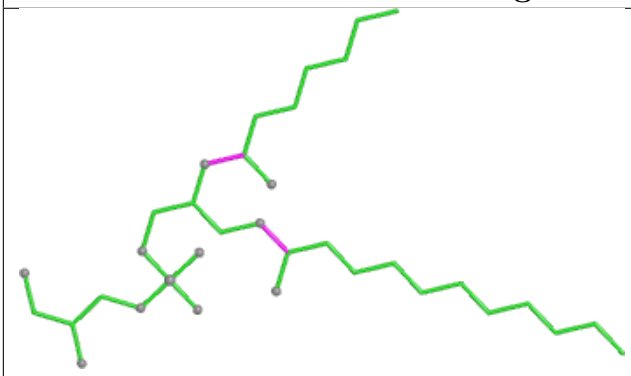


Torsions

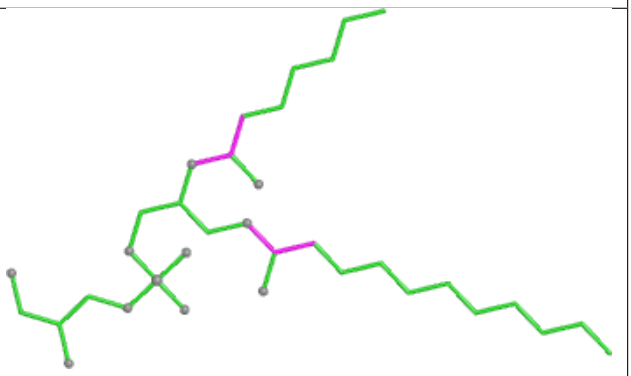


Rings

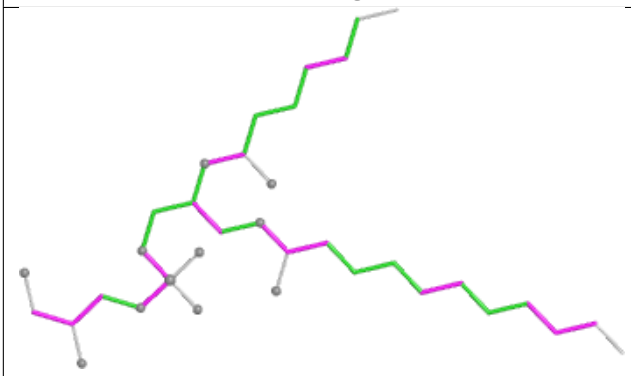
Ligand LHG B2 618



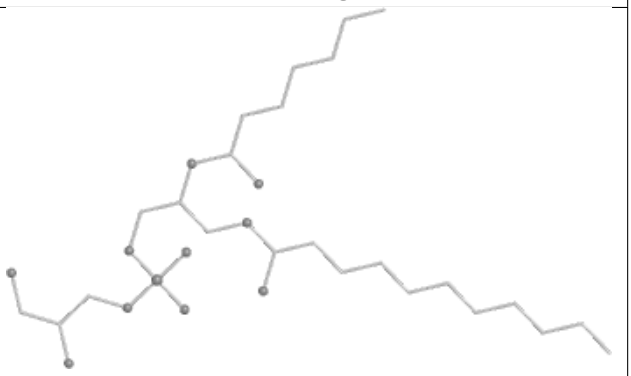
Bond lengths



Bond angles

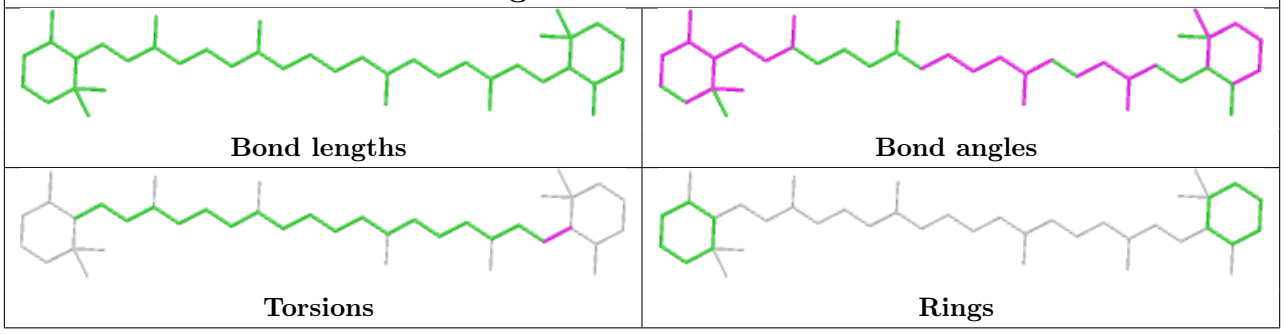


Torsions

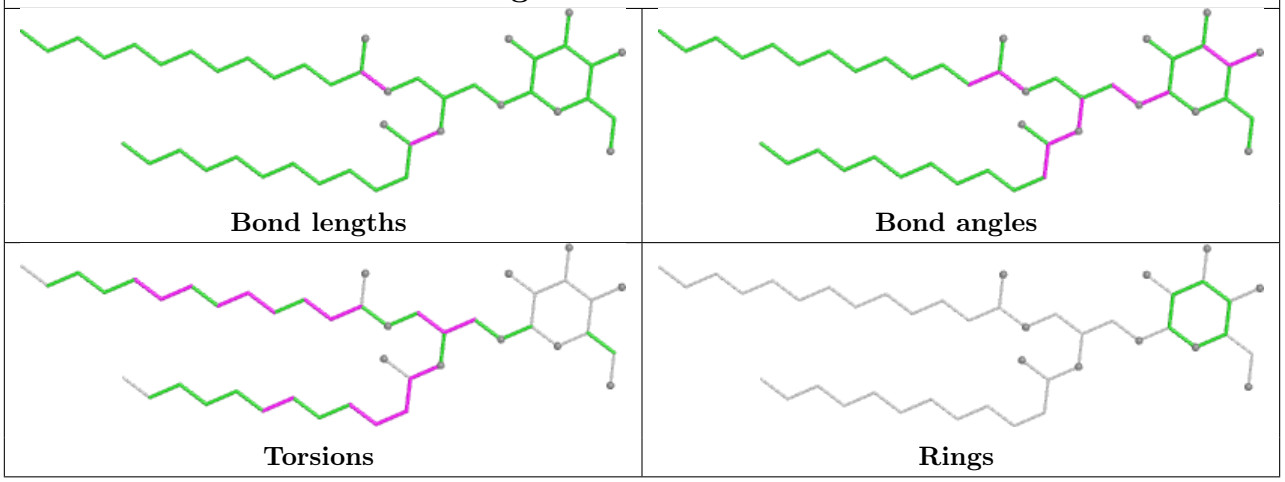


Rings

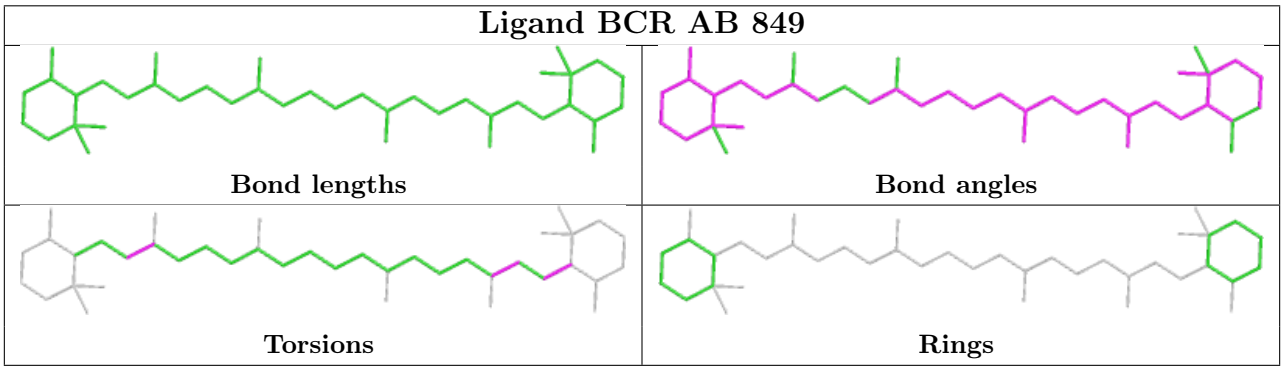
Ligand BCR AG 205



Ligand LMG A1 321



Ligand BCR AB 849



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

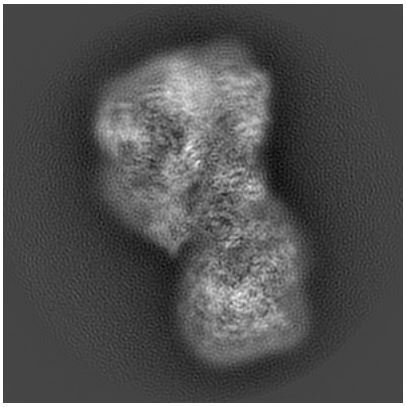
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32477. These allow visual inspection of the internal detail of the map and identification of artifacts.

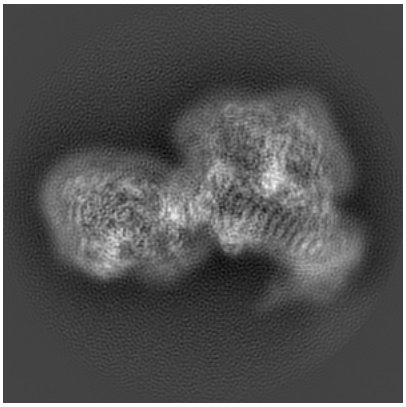
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

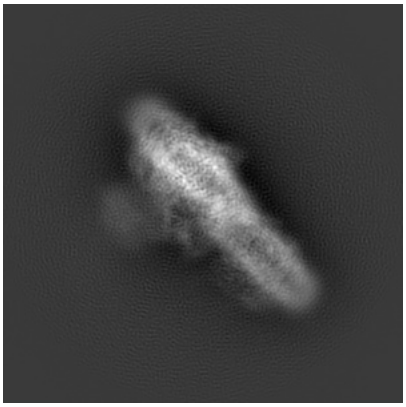
6.1.1 Primary map



X



Y

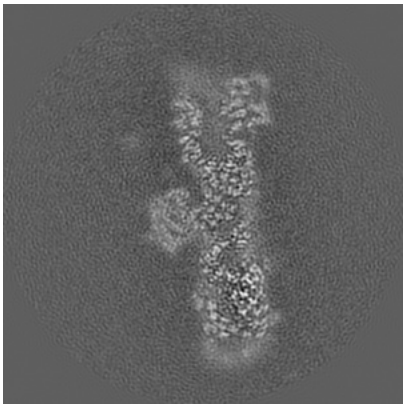


Z

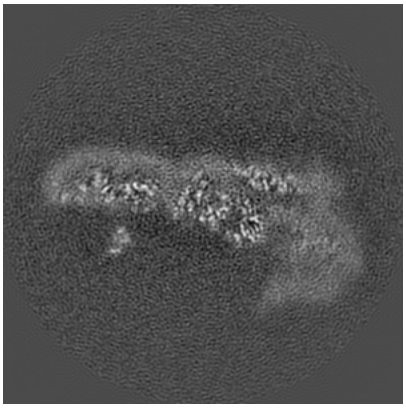
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 200



Y Index: 200

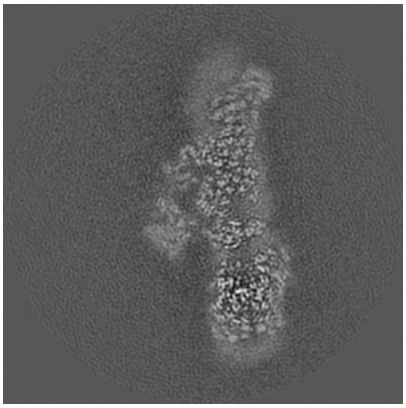


Z Index: 200

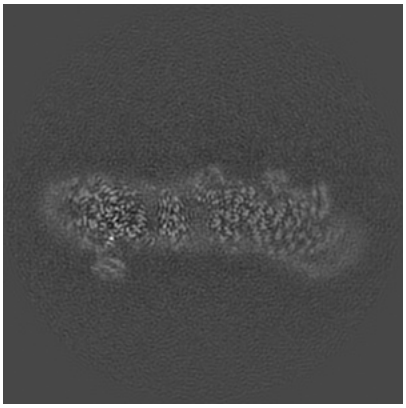
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

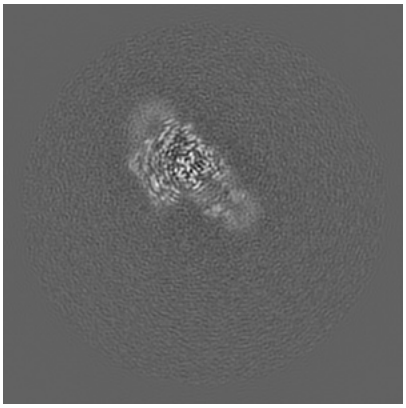
6.3.1 Primary map



X Index: 185



Y Index: 235

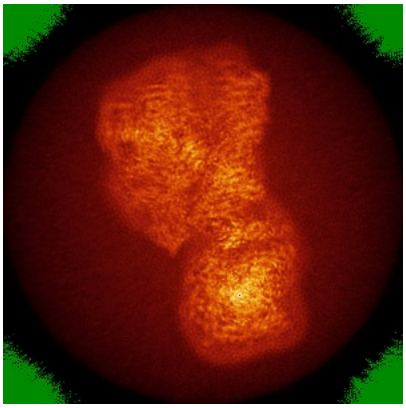


Z Index: 112

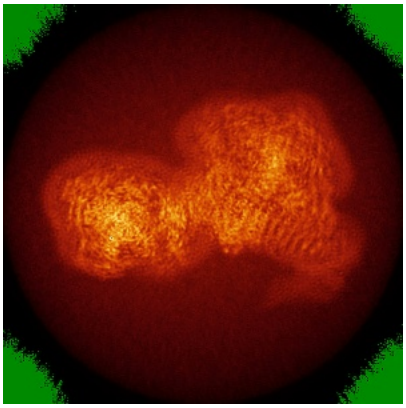
The images above show the largest variance slices of the map in three orthogonal directions.

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

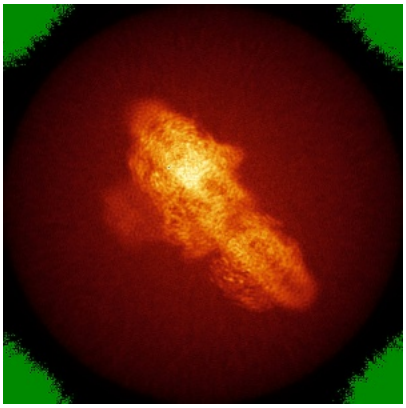
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

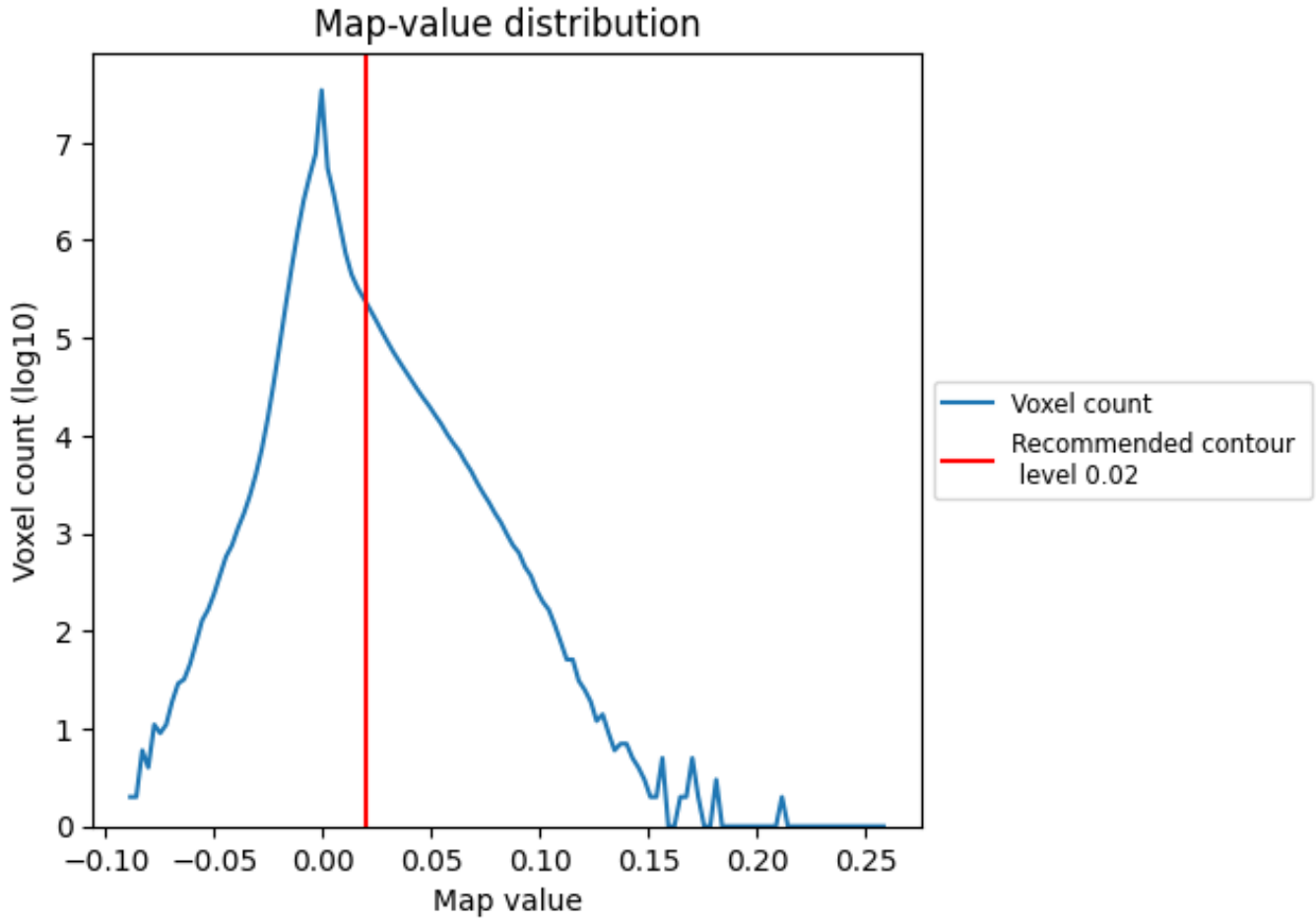
6.6 Mask visualisation (i)

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

7 Map analysis

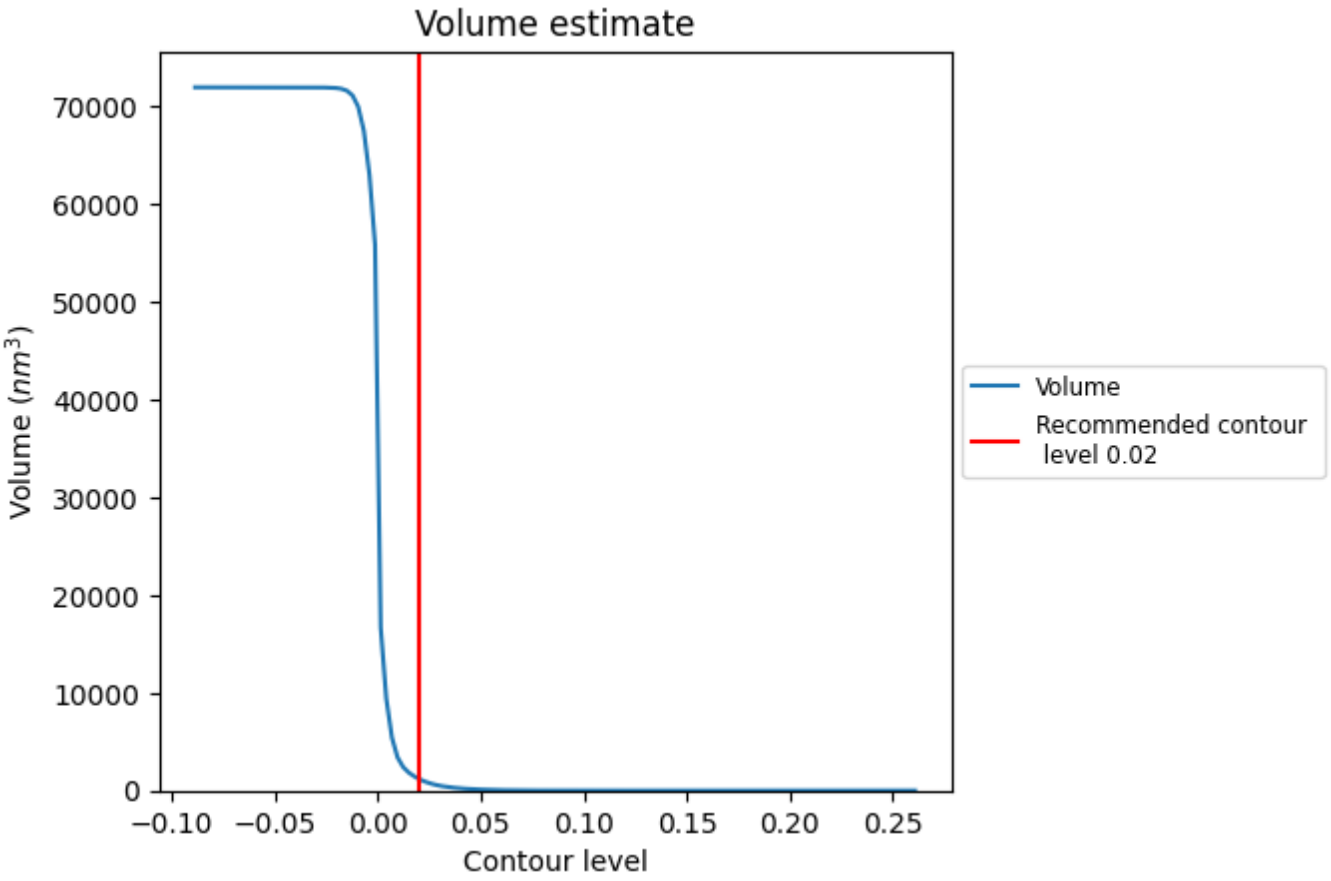
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

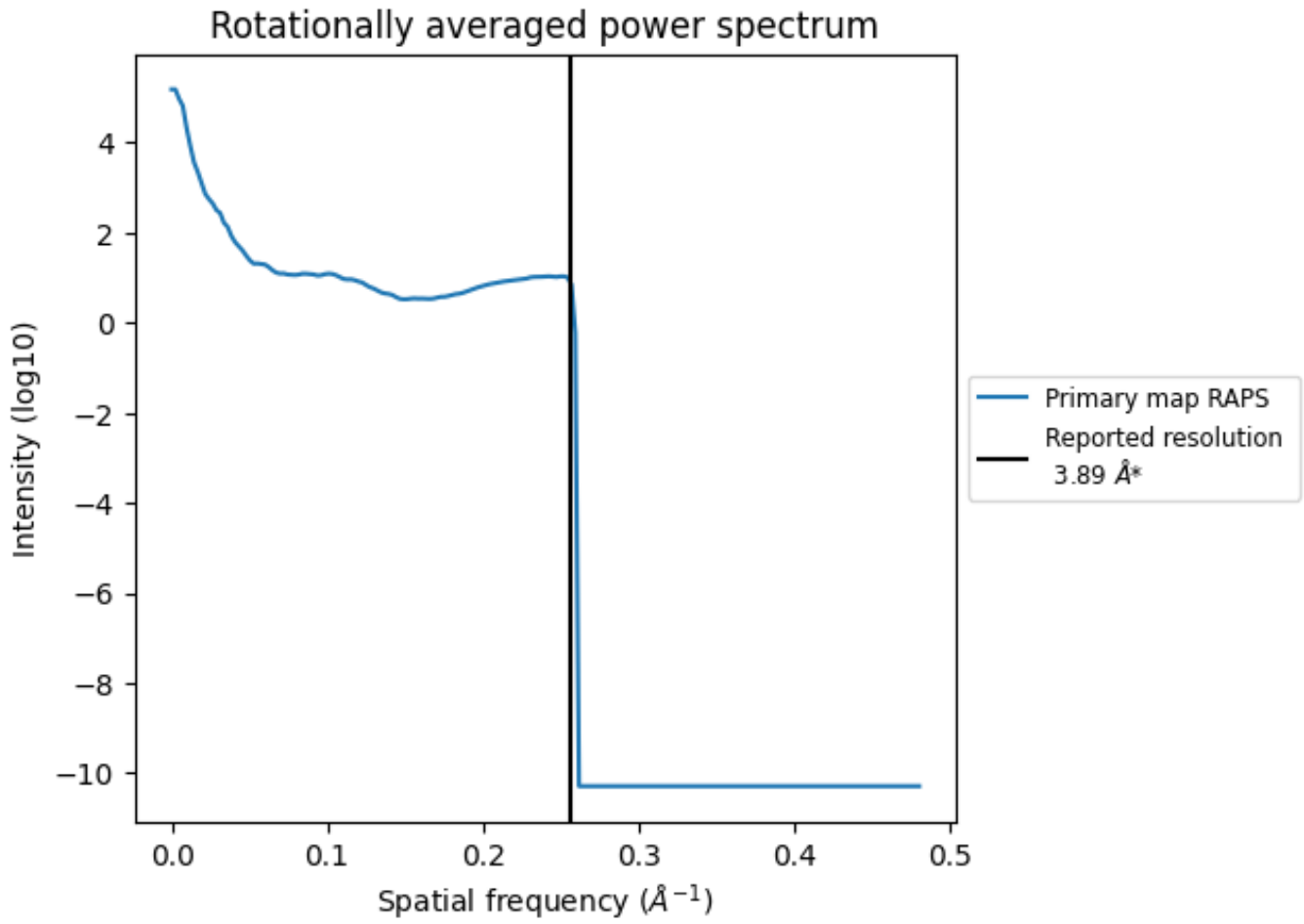
7.2 Volume estimate (i)



The volume at the recommended contour level is 1193 nm^3; this corresponds to an approximate mass of 1078 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 0.257 Å^{-1}

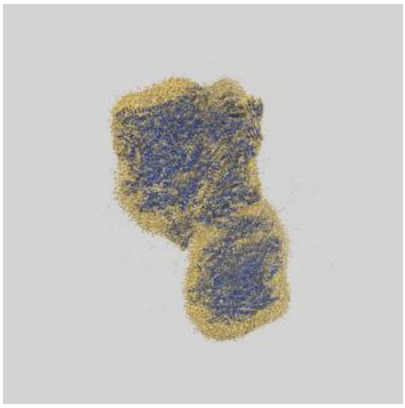
8 Fourier-Shell correlation (i)

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

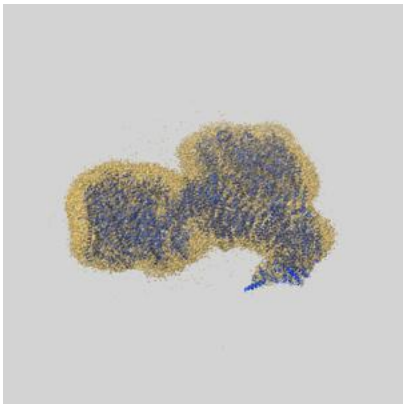
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32477 and PDB model 7WG5. Per-residue inclusion information can be found in section 3 on page 40.

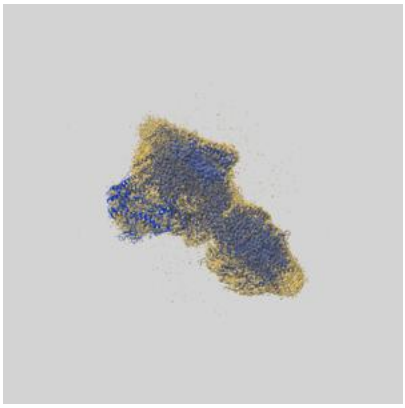
9.1 Map-model overlay



X



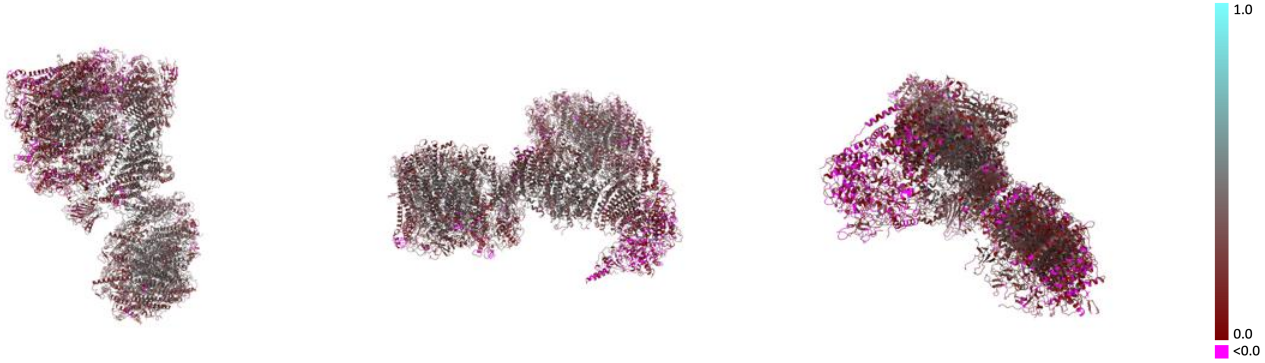
Y



Z

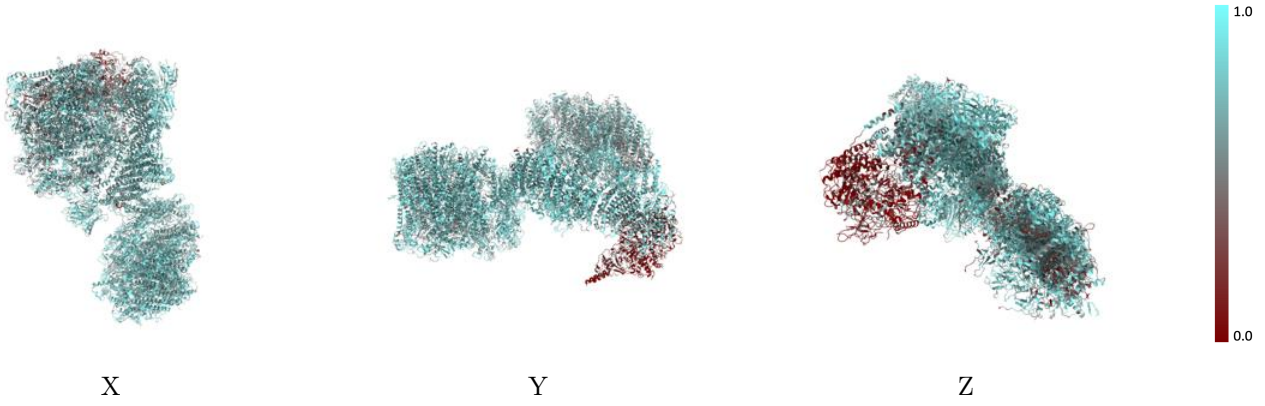
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



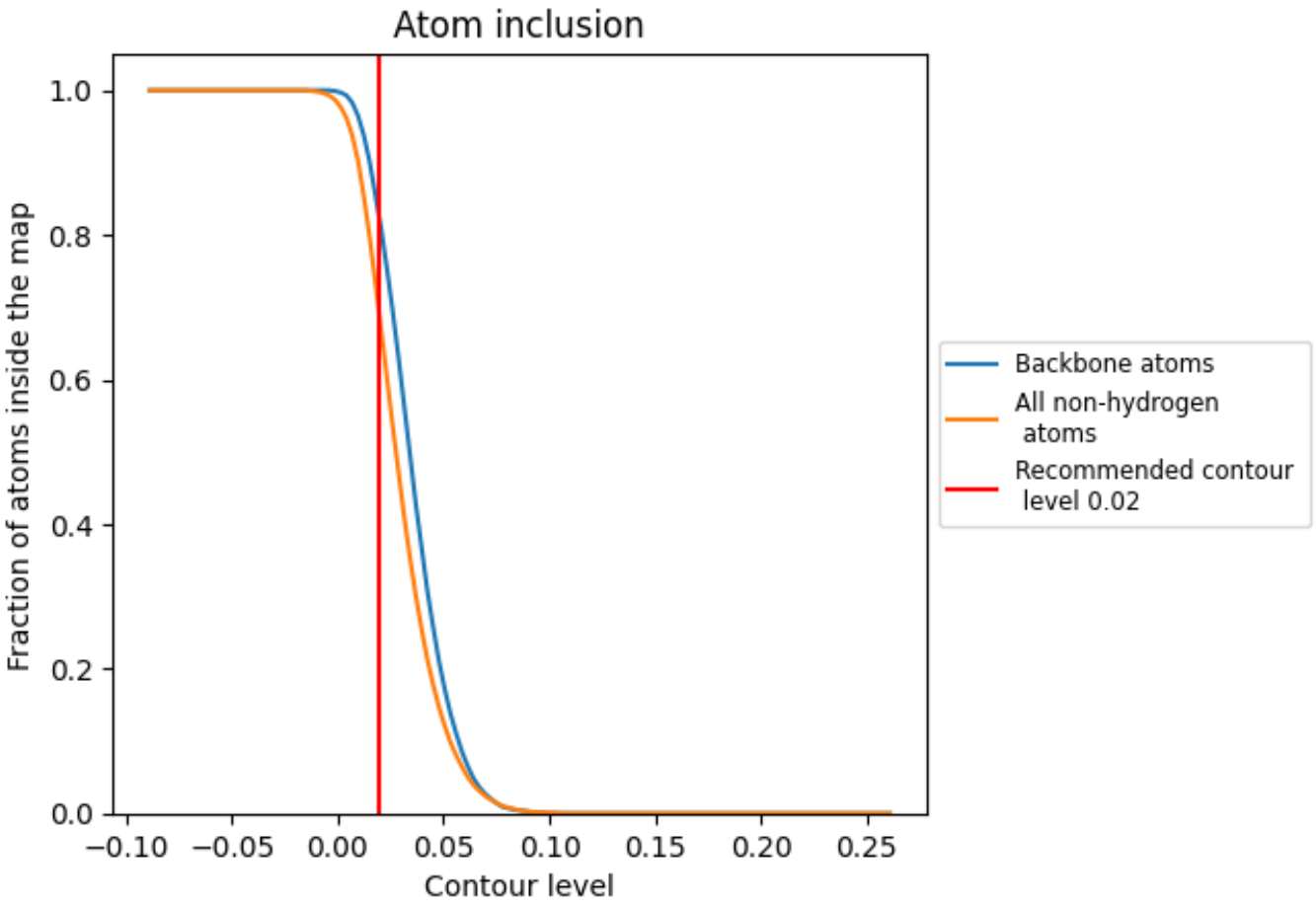
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.2780
A	0.6080	0.1850
A1	0.7370	0.2670
A3	0.7700	0.2850
A4	0.7720	0.3150
A6	0.7980	0.3780
AA	0.7720	0.3600
AB	0.7770	0.3740
AC	0.8600	0.3480
AD	0.7990	0.3020
AE	0.7820	0.3420
AF	0.8030	0.3850
AG	0.7630	0.2510
AH	0.7180	0.1970
AI	0.6970	0.2870
AJ	0.7650	0.3900
AK	0.6720	0.1590
AL	0.7300	0.2350
B	0.7500	0.3510
B1	0.6830	0.2740
B2	0.6620	0.1940
B3	0.6670	0.1720
B5	0.7600	0.3430
BA	0.6660	0.2590
BB	0.6890	0.2790
BC	0.7820	0.2570
BD	0.6810	0.1900
BE	0.6530	0.2750
BF	0.7310	0.3310
BG	0.5700	0.1030
BH	0.6430	0.1250
BI	0.5080	0.1090
BJ	0.6880	0.3150
BK	0.5580	0.0830
BL	0.5590	0.1090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
C	0.5990	0.2350
D	0.7970	0.4030
E	0.7000	0.3040
F	0.7410	0.3140
G	0.6920	0.2930
H	0.0960	0.0450
I	0.2630	0.0770
J	0.1660	0.0950
K	0.2170	0.1070
L	0.5280	0.1300
M	0.1140	0.0580
N	0.1750	0.1100
O	0.1100	0.1230
T	0.2430	0.0880
a	0.7990	0.3570
b	0.7730	0.2460
c	0.7430	0.3020
d	0.8280	0.3790
e	0.7900	0.3720
f	0.7530	0.2040
g	0.7560	0.2360
h	0.8010	0.3240
i	0.7870	0.3360
j	0.7610	0.3130