wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 01:03 AM JST

PDB ID	:	5ZGB / pdb_00005zgb
EMDB ID	:	EMD-6929
Title	:	Cryo-EM structure of the red algal PSI-LHCR
Authors	:	Pi, X.
Deposited on	:	2018-03-08
Resolution	:	3.63 Å(reported)

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

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

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

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

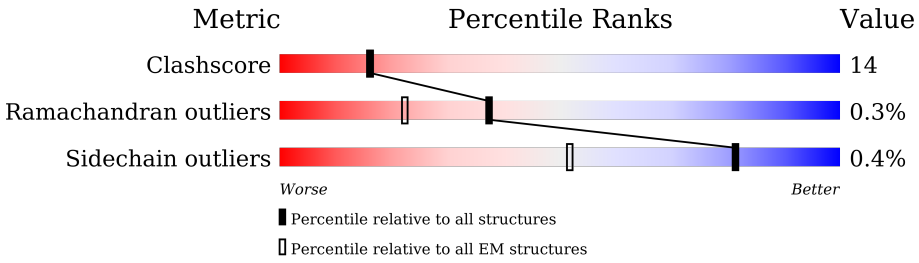
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

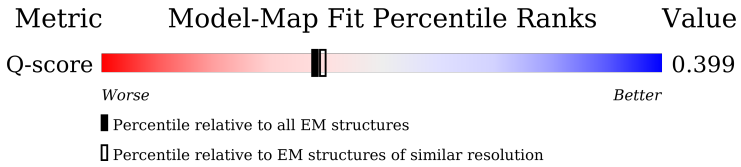
1 Overall quality at a glance

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

The reported resolution of this entry is 3.63 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	11696 (3.13 - 4.13)

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

Mol	Chain	Length	Quality of chain
1	A	748	70% 29%
2	B	732	75% 24%
3	C	81	68% 31%
4	D	139	58% 24% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	94	5% 54% 11% 35%
6	F	185	74% 9% 17%
7	I	32	66% 31%
8	J	38	71% 29%
9	K	60	5% 80% 18%
10	L	140	66% 19% 15%
11	M	29	14% 72% 21% 7%
12	O	155	5% 43% 11% 46%
13	1	175	8% 75% 22%
13	4	175	74% 74% 23%
14	2	199	10% 61% 26% 12%
14	5	199	71% 61% 26% 12%
15	3	188	7% 62% 29% 10%

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
16	CL0	A	801	-	-	X	-
25	ZEX	1	615	-	X	-	-
25	ZEX	1	616	-	X	-	-
25	ZEX	2	614	-	X	-	-
25	ZEX	3	216	-	X	-	-
25	ZEX	3	218	-	X	-	-
25	ZEX	4	612	-	X	-	-
25	ZEX	5	614	-	X	-	-
25	ZEX	5	615	-	X	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 35011 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5798	3792	996	983	27		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5819	3827	982	991	19		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			597	367	104	114	12		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			950	600	167	179	4		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			493	322	79	92		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	154	Total	C	N	O	S	0	0
			1263	811	214	234	4		

- Molecule 7 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	31	Total	C	N	O	S	0	0
			230	158	32	39	1		

- Molecule 8 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	38	Total	C	N	O	S	0	0
			312	214	46	51	1		

- Molecule 9 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	59	Total	C	N	O	S	0	0
			428	279	70	74	5		

- Molecule 10 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	119	Total	C	N	O	S	0	0
			900	591	148	159	2		

- Molecule 11 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	27	Total	C	N	O	S	0	0
			204	136	32	34	2		

- Molecule 12 is a protein called PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	83	Total	C	N	O	0	0
			641	439	97	105		

- Molecule 13 is a protein called Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	169	Total	C	N	O	S	0	0
			1351	887	227	229	8		
13	4	170	Total	C	N	O	S	0	0
			1358	892	228	230	8		

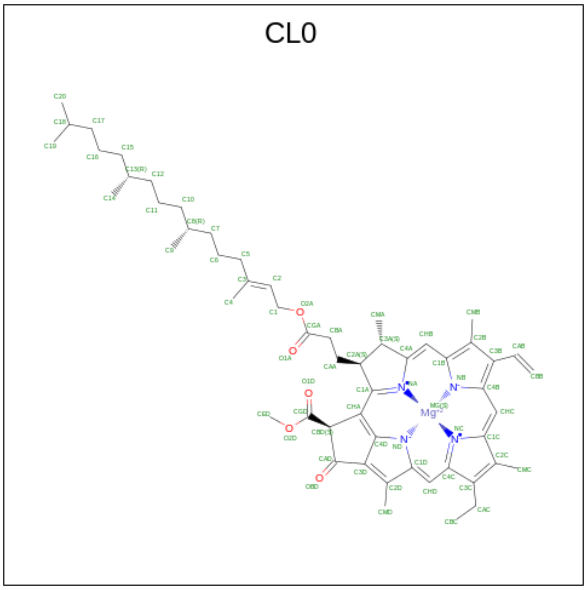
- Molecule 14 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		
14	5	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		

- Molecule 15 is a protein called Lhcr3.

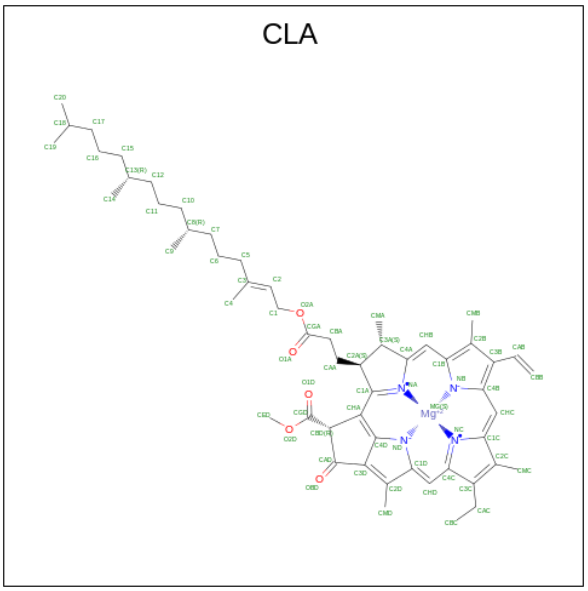
Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	170	Total	C	N	O	S	0	0
			1303	845	219	232	7		

- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 62	C 52	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	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
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	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
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	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
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	J	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

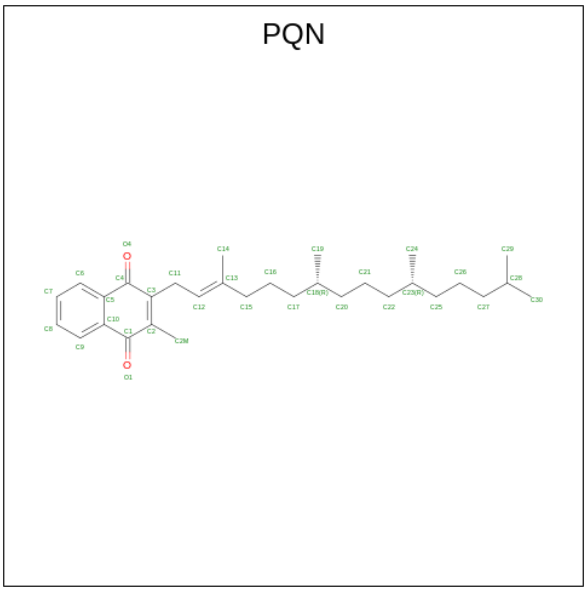
Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

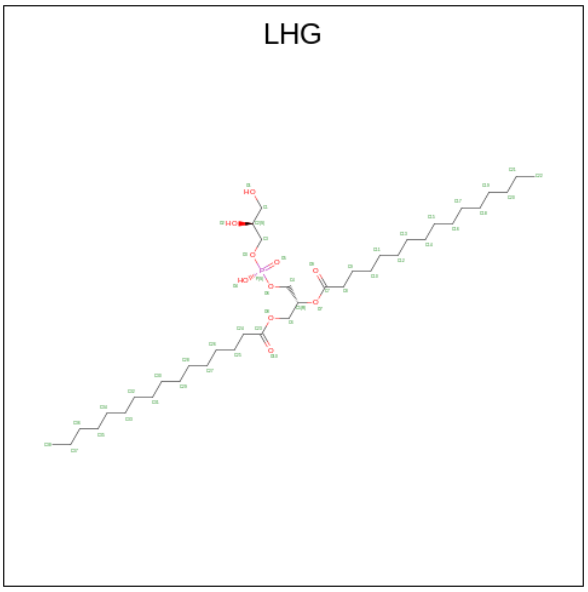
Mol	Chain	Residues	Atoms					AltConf
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			44	36	1	4	3	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			33	31	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



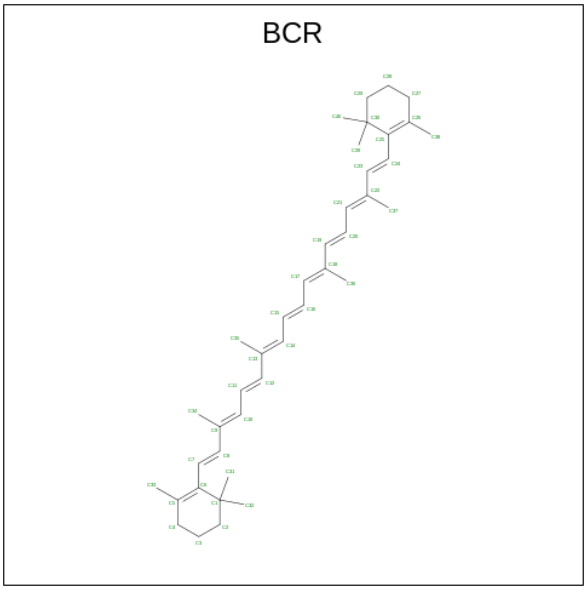
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



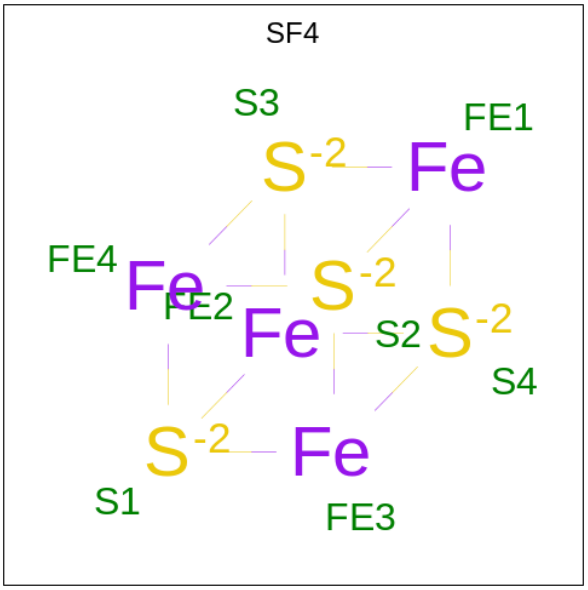
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

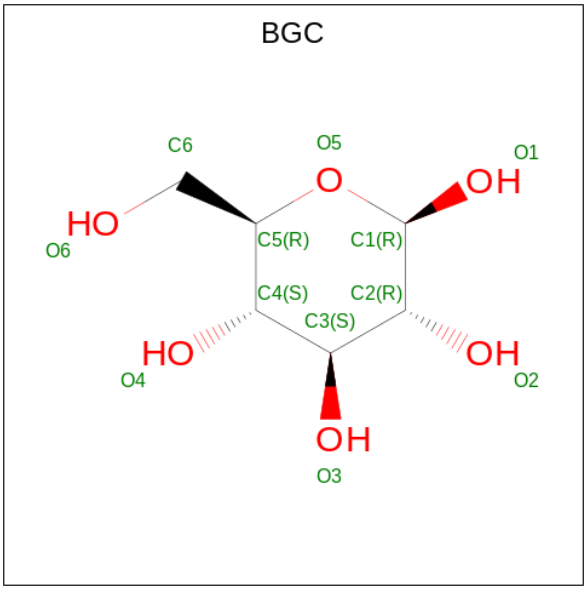
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	O	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



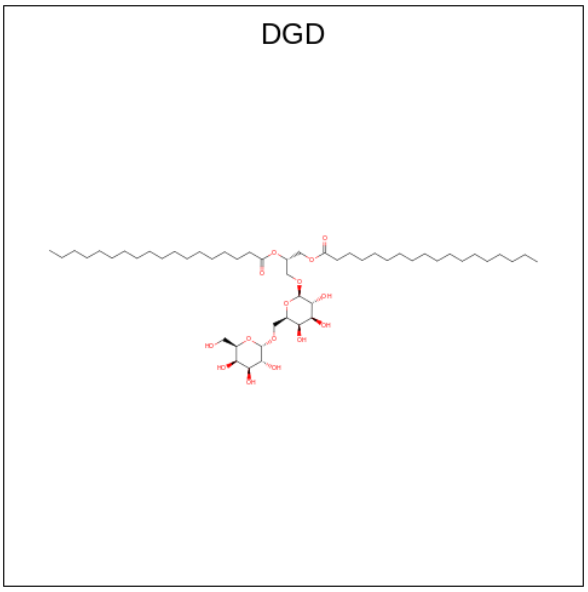
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0

- Molecule 22 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



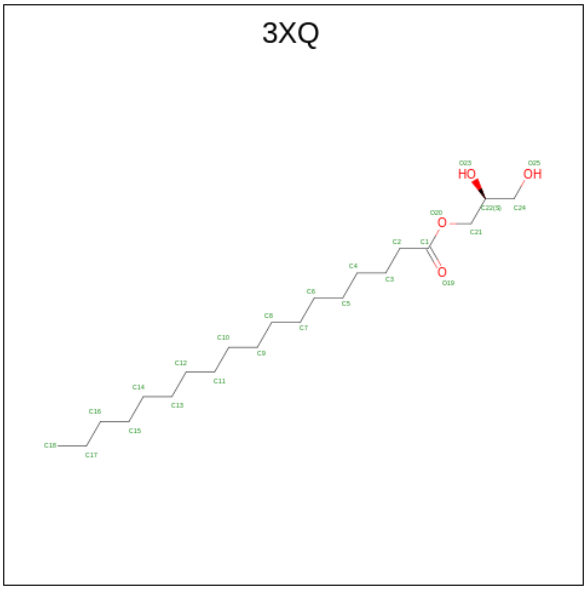
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O 11 6 5	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



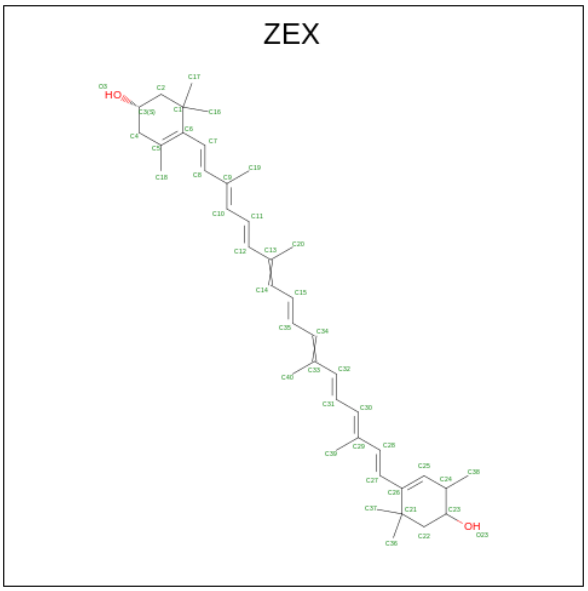
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			66	51	15	

- Molecule 24 is (2S)-2,3-dihydroxypropyl octadecanoate (CCD ID: 3XQ) (formula: $C_{21}H_{42}O_4$).



Mol	Chain	Residues	Atoms			AltConf
24	J	1	Total	C	O	0
			25	21	4	

- Molecule 25 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



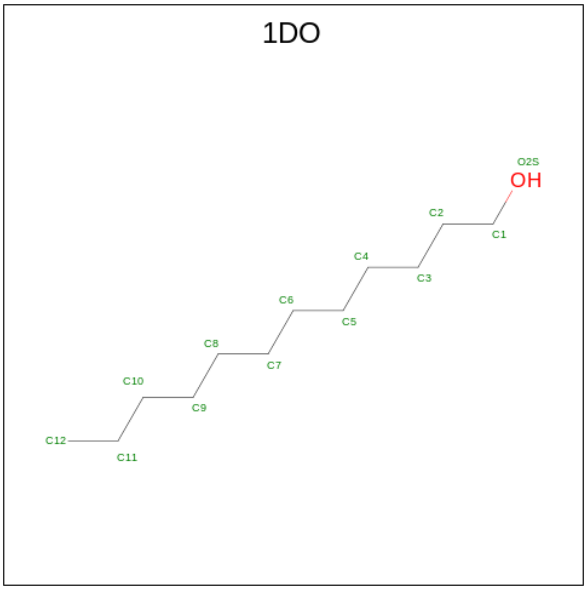
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0

- Molecule 26 is 1-DODECANOL (CCD ID: 1DO) (formula: $C_{12}H_{26}O$).



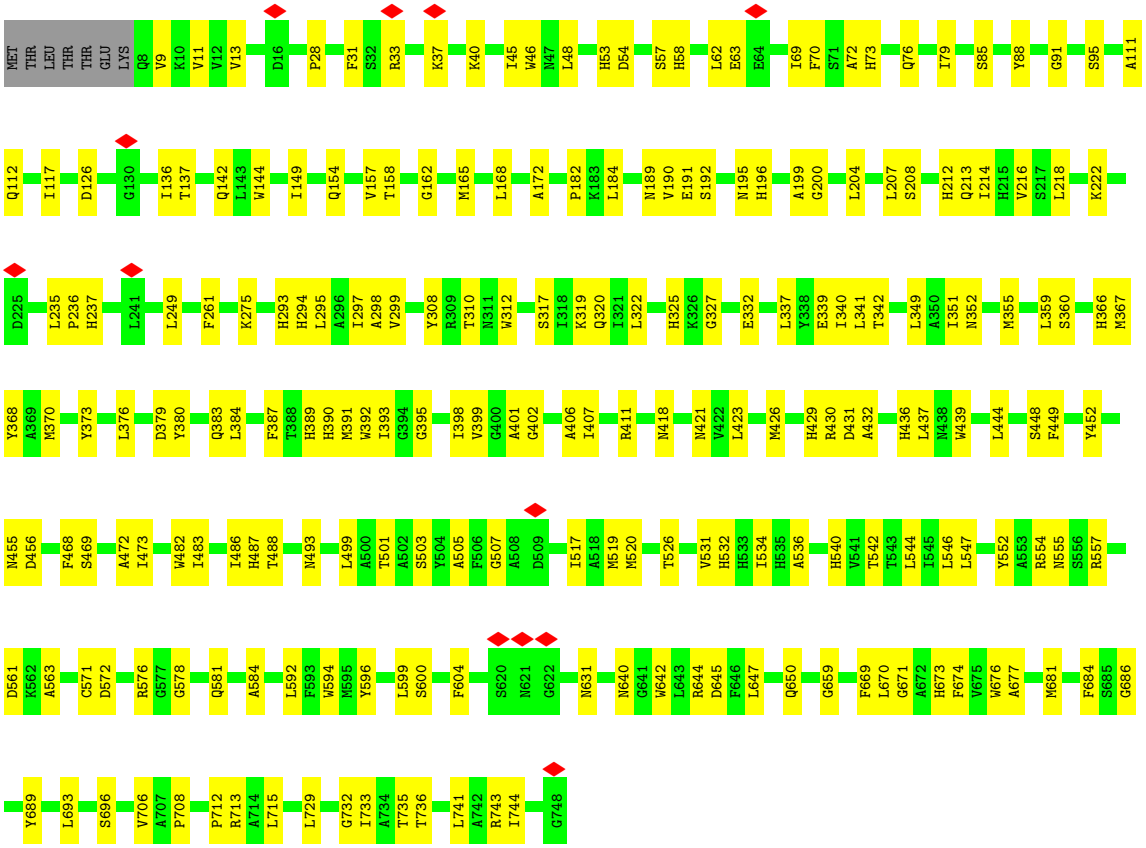
Mol	Chain	Residues	Atoms			AltConf
26	3	1	Total	C	O	0
			13	12	1	

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.

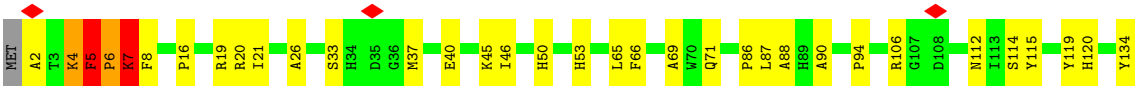
• Molecule 1: PsaA

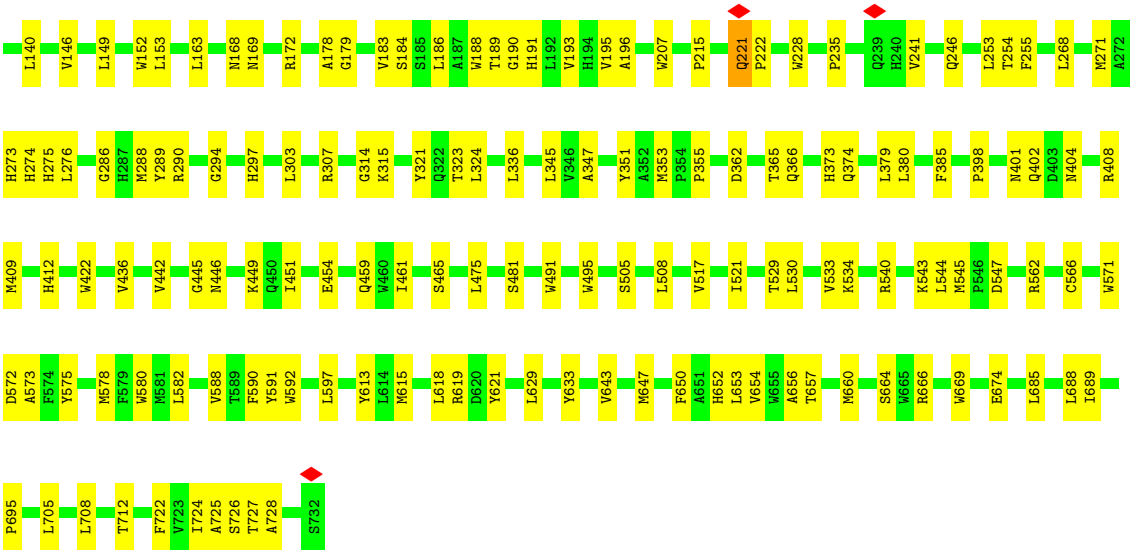
Chain A:



• Molecule 2: PsaB

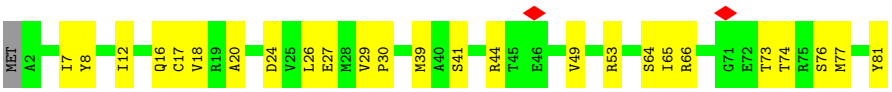
Chain B:





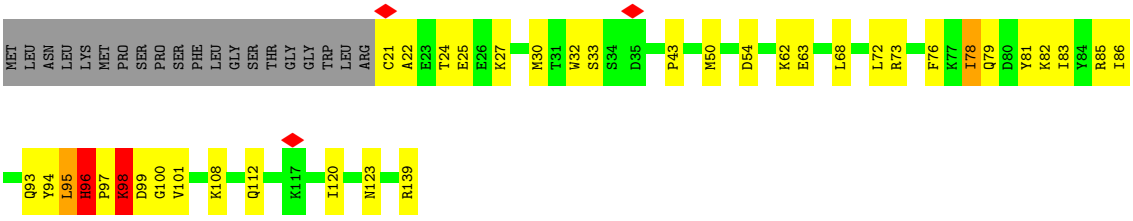
• Molecule 3: PsaC

Chain C:



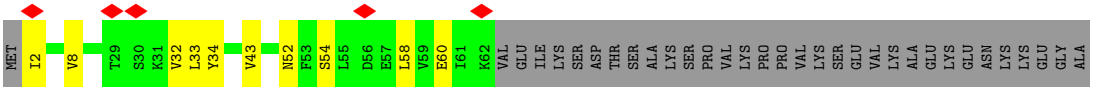
• Molecule 4: PsaD

Chain D:



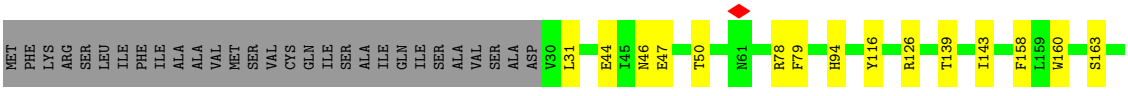
• Molecule 5: PsaE

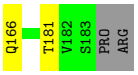
Chain E:



• Molecule 6: PsaF

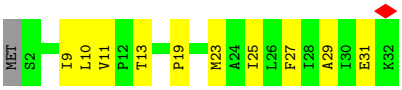
Chain F:





• Molecule 7: PsaI

Chain I:

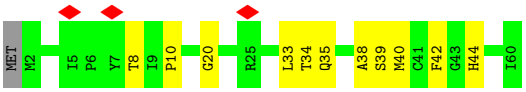


• Molecule 8: PsaJ

Chain J:

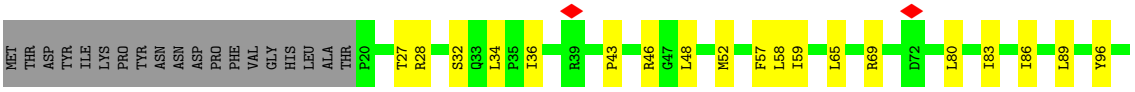
• Molecule 9: PsaK

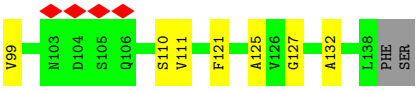
Chain K:



• Molecule 10: PsaL

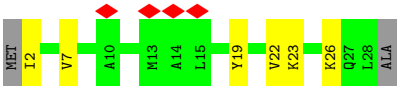
Chain L:





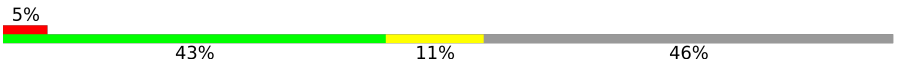
• Molecule 11: PsaM

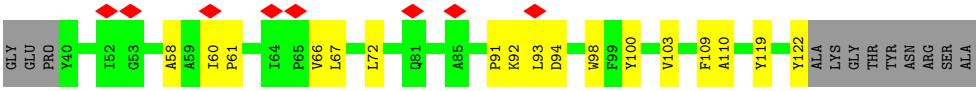
Chain M:



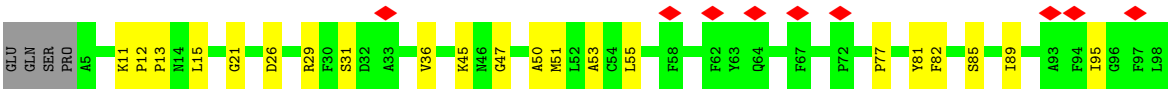
• Molecule 12: PsaO

Chain O:

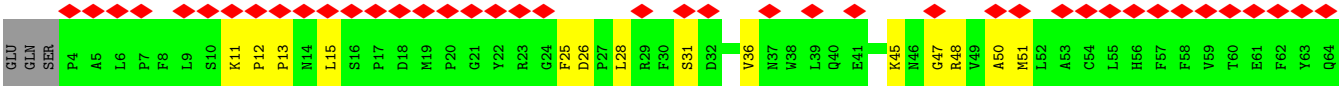


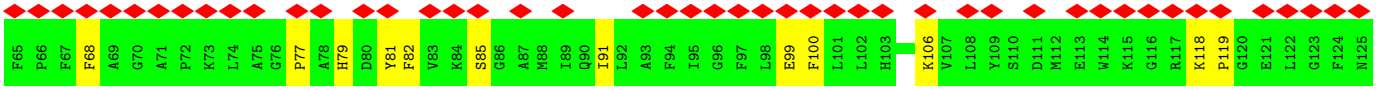


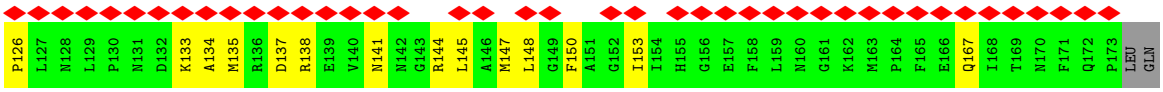
• Molecule 13: Lhcr1



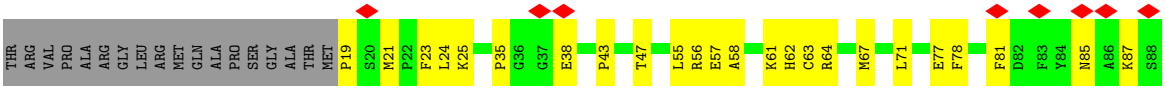
• Molecule 13: Lhcr1

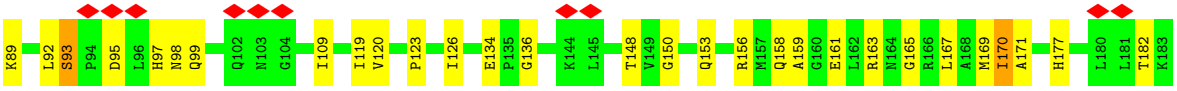


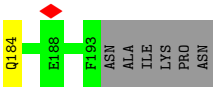




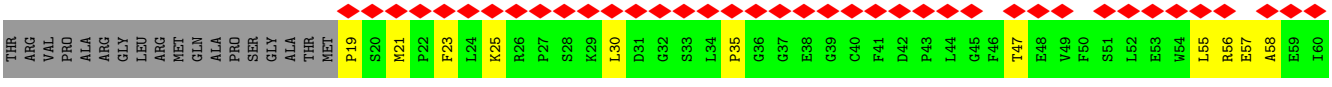
• Molecule 14: Lhcr2





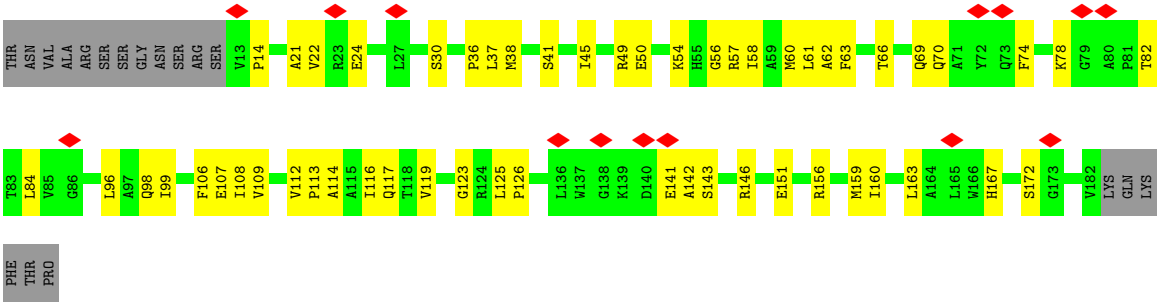


• Molecule 14: Lhcr2



• Molecule 15: Lhcr3

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.653	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0562	Depositor
Map size (Å)	294.0, 294.0, 294.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, SF4, ZEX, DGD, CL0, 3XQ, BGC, BCR, LHG, 1DO, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.52	0/5985	0.64	3/8158 (0.0%)
2	B	0.50	0/6028	0.65	9/8236 (0.1%)
3	C	0.44	0/607	0.56	0/822
4	D	0.33	0/969	0.64	2/1307 (0.2%)
5	E	0.36	0/502	0.55	0/680
6	F	0.35	0/1296	0.64	0/1760
7	I	0.34	0/235	0.76	0/321
8	J	0.42	0/321	0.52	0/437
9	K	0.33	0/433	0.69	0/588
10	L	0.28	0/919	0.54	0/1247
11	M	0.21	0/205	0.53	0/277
12	O	0.29	0/664	0.66	0/913
13	1	0.30	0/1395	0.71	0/1884
13	4	0.30	0/1403	0.72	0/1895
14	2	0.30	0/1407	0.71	1/1898 (0.1%)
14	5	0.30	0/1407	0.70	1/1898 (0.1%)
15	3	0.33	0/1337	0.72	0/1817
All	All	0.42	0/25113	0.66	16/34138 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	2	0	2
14	5	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	96	HIS	CA-C-N	6.55	128.03	119.84
4	D	96	HIS	C-N-CA	6.55	128.03	119.84
14	5	93	SER	N-CA-C	6.20	123.51	109.81
14	2	93	SER	N-CA-C	6.19	123.49	109.81
2	B	7	LYS	CA-C-N	-5.63	113.39	122.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	2	136	GLY	Peptide
14	2	98	ASN	Peptide
14	5	136	GLY	Peptide
14	5	98	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5798	0	5727	207	0
2	B	5819	0	5648	164	0
3	C	597	0	584	22	0
4	D	950	0	943	95	0
5	E	493	0	509	6	0
6	F	1263	0	1236	14	0
7	I	230	0	253	9	0
8	J	312	0	327	15	0
9	K	428	0	464	10	0
10	L	900	0	931	22	0
11	M	204	0	226	5	0
12	O	641	0	650	11	0
13	1	1351	0	1322	28	0
13	4	1358	0	1330	31	0
14	2	1371	0	1362	41	0
14	5	1371	0	1362	40	0
15	3	1303	0	1305	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	65	0	71	53	0
17	1	565	0	443	14	0
17	2	600	0	466	21	0
17	3	565	0	440	24	0
17	4	505	0	384	19	0
17	5	600	0	463	19	0
17	A	2310	0	2337	129	0
17	B	2469	0	2499	140	0
17	F	147	0	123	4	0
17	J	165	0	158	11	0
17	K	87	0	64	1	0
17	L	172	0	164	5	0
17	O	188	0	144	3	0
18	A	33	0	46	4	0
18	B	33	0	46	2	0
19	A	89	0	127	5	0
20	A	160	0	224	14	0
20	B	280	0	392	23	0
20	F	40	0	56	2	0
20	I	40	0	56	3	0
20	J	80	0	112	6	0
20	K	80	0	112	10	0
20	L	120	0	168	11	0
20	O	40	0	56	5	0
21	A	8	0	0	0	0
21	C	16	0	0	2	0
22	A	11	0	9	0	0
23	B	66	0	96	5	0
24	J	25	0	0	0	0
25	1	210	0	280	16	0
25	2	168	0	224	10	0
25	3	252	0	336	19	0
25	4	252	0	336	16	0
25	5	168	0	224	14	0
26	3	13	0	25	1	0
All	All	35011	0	34860	997	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 997 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:TRP:CD2	16:A:801:CL0:H56	1.25	1.63
4:D:82:LYS:HE3	4:D:95:LEU:CA	1.36	1.50
4:D:82:LYS:CE	4:D:95:LEU:C	1.87	1.48
1:A:642:TRP:CE2	16:A:801:CL0:H56	1.50	1.45
4:D:82:LYS:NZ	4:D:95:LEU:HB2	1.26	1.44

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	739/748 (99%)	681 (92%)	57 (8%)	1 (0%)	48 78
2	B	729/732 (100%)	654 (90%)	72 (10%)	3 (0%)	30 59
3	C	78/81 (96%)	68 (87%)	10 (13%)	0	100 100
4	D	117/139 (84%)	102 (87%)	12 (10%)	3 (3%)	4 23
5	E	59/94 (63%)	52 (88%)	7 (12%)	0	100 100
6	F	152/185 (82%)	134 (88%)	18 (12%)	0	100 100
7	I	29/32 (91%)	26 (90%)	3 (10%)	0	100 100
8	J	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
9	K	57/60 (95%)	51 (90%)	6 (10%)	0	100 100
10	L	117/140 (84%)	106 (91%)	11 (9%)	0	100 100
11	M	25/29 (86%)	23 (92%)	2 (8%)	0	100 100
12	O	81/155 (52%)	67 (83%)	14 (17%)	0	100 100
13	1	167/175 (95%)	130 (78%)	36 (22%)	1 (1%)	21 51
13	4	168/175 (96%)	131 (78%)	36 (21%)	1 (1%)	21 51
14	2	173/199 (87%)	130 (75%)	43 (25%)	0	100 100
14	5	173/199 (87%)	130 (75%)	43 (25%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	3	168/188 (89%)	143 (85%)	25 (15%)	0	100 100
All	All	3068/3369 (91%)	2663 (87%)	396 (13%)	9 (0%)	37 64

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	PHE
2	B	7	LYS
4	D	96	HIS
4	D	100	GLY
2	B	6	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	598/605 (99%)	597 (100%)	1 (0%)	87 84
2	B	598/599 (100%)	596 (100%)	2 (0%)	86 81
3	C	66/67 (98%)	65 (98%)	1 (2%)	57 66
4	D	101/118 (86%)	98 (97%)	3 (3%)	36 55
5	E	58/87 (67%)	58 (100%)	0	100 100
6	F	136/162 (84%)	136 (100%)	0	100 100
7	I	26/27 (96%)	26 (100%)	0	100 100
8	J	34/34 (100%)	34 (100%)	0	100 100
9	K	48/49 (98%)	48 (100%)	0	100 100
10	L	94/113 (83%)	94 (100%)	0	100 100
11	M	22/23 (96%)	22 (100%)	0	100 100
12	O	64/121 (53%)	64 (100%)	0	100 100
13	1	139/145 (96%)	139 (100%)	0	100 100
13	4	140/145 (97%)	140 (100%)	0	100 100
14	2	142/160 (89%)	140 (99%)	2 (1%)	59 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	5	142/160 (89%)	140 (99%)	2 (1%)	59 68
15	3	132/148 (89%)	132 (100%)	0	100 100
All	All	2540/2763 (92%)	2529 (100%)	11 (0%)	81 79

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	2	85	ASN
14	2	170	ILE
14	5	170	ILE
14	5	85	ASN
4	D	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
14	5	76	GLN
14	5	85	ASN
2	B	702	GLN
2	B	634	ASN
14	5	98	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

215 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	$\#\|Z\| > 2$
17	CLA	B	803	-	69,73,73	1.25	10 (14%)	83,113,113	1.54	10 (12%)
17	CLA	B	816	-	69,73,73	1.28	10 (14%)	83,113,113	1.45	13 (15%)
17	CLA	2	605	-	49,53,73	1.50	10 (20%)	59,89,113	1.69	9 (15%)
17	CLA	1	604	-	49,53,73	1.48	12 (24%)	59,89,113	1.55	10 (16%)
17	CLA	A	827	-	69,73,73	1.38	11 (15%)	83,113,113	1.54	14 (16%)
25	ZEX	5	617	-	42,43,43	4.98	19 (45%)	55,60,60	5.31	26 (47%)
17	CLA	A	810	-	58,62,73	1.37	11 (18%)	69,99,113	1.43	6 (8%)
17	CLA	A	805	-	69,73,73	1.26	10 (14%)	83,113,113	1.60	15 (18%)
17	CLA	J	102	-	62,66,73	1.33	11 (17%)	74,104,113	1.52	7 (9%)
20	BCR	B	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.34	8 (14%)
17	CLA	5	609	-	45,49,73	1.59	8 (17%)	54,84,113	1.93	14 (25%)
17	CLA	L	203	-	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
17	CLA	B	829	-	69,73,73	1.28	11 (15%)	83,113,113	1.45	11 (13%)
17	CLA	B	839	2	69,73,73	1.32	11 (15%)	83,113,113	1.46	8 (9%)
17	CLA	5	605	-	49,53,73	1.47	8 (16%)	59,89,113	1.54	6 (10%)
17	CLA	O	204	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	9 (13%)
20	BCR	B	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
17	CLA	5	607	-	49,53,73	1.57	10 (20%)	59,89,113	1.75	12 (20%)
17	CLA	B	802	-	69,73,73	1.42	10 (14%)	83,113,113	1.76	24 (28%)
17	CLA	B	808	-	69,73,73	1.26	11 (15%)	83,113,113	1.56	16 (19%)
17	CLA	1	603	-	49,53,73	1.52	10 (20%)	59,89,113	1.58	8 (13%)
17	CLA	B	836	-	69,73,73	1.29	10 (14%)	83,113,113	1.45	10 (12%)
20	BCR	L	201	-	41,41,41	1.30	3 (7%)	56,56,56	1.35	9 (16%)
17	CLA	B	809	2	69,73,73	1.32	10 (14%)	83,113,113	1.48	9 (10%)
17	CLA	3	211	-	46,50,73	1.50	11 (23%)	55,85,113	1.59	8 (14%)
25	ZEX	3	201	-	42,43,43	5.19	19 (45%)	55,60,60	5.28	30 (54%)
17	CLA	2	603	-	49,53,73	1.47	11 (22%)	59,89,113	1.62	9 (15%)
20	BCR	A	846	-	41,41,41	1.33	2 (4%)	56,56,56	1.39	9 (16%)
17	CLA	O	203	-	45,49,73	1.53	8 (17%)	54,84,113	1.63	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	J	104	-	41,41,41	1.28	3 (7%)	56,56,56	1.42	9 (16%)
25	ZEX	5	614	-	42,43,43	5.17	20 (47%)	55,60,60	5.13	32 (58%)
17	CLA	A	834	-	49,53,73	1.49	10 (20%)	59,89,113	1.59	8 (13%)
16	CL0	A	801	1	69,73,73	2.99	22 (31%)	83,113,113	3.10	41 (49%)
17	CLA	A	833	-	69,73,73	1.25	11 (15%)	83,113,113	1.47	10 (12%)
17	CLA	A	821	-	55,59,73	1.41	11 (20%)	66,96,113	1.48	7 (10%)
17	CLA	B	830	-	69,73,73	1.28	9 (13%)	83,113,113	1.46	11 (13%)
17	CLA	2	606	-	49,53,73	1.46	11 (22%)	59,89,113	1.58	9 (15%)
26	1DO	3	219	22	12,12,12	0.26	0	11,11,11	0.85	0
25	ZEX	2	617	-	42,43,43	4.80	19 (45%)	55,60,60	5.29	29 (52%)
25	ZEX	4	616	-	42,43,43	5.04	19 (45%)	55,60,60	5.19	32 (58%)
17	CLA	A	832	-	69,73,73	1.25	10 (14%)	83,113,113	1.64	12 (14%)
25	ZEX	4	613	-	42,43,43	5.05	20 (47%)	55,60,60	5.08	31 (56%)
17	CLA	2	601	-	49,53,73	1.46	8 (16%)	59,89,113	1.68	7 (11%)
17	CLA	A	822	-	59,63,73	1.38	11 (18%)	71,101,113	1.55	8 (11%)
18	PQN	B	844	-	34,34,34	2.78	9 (26%)	42,45,45	2.32	7 (16%)
17	CLA	A	819	-	69,73,73	1.33	11 (15%)	83,113,113	1.57	10 (12%)
17	CLA	A	838	1	69,73,73	1.25	10 (14%)	83,113,113	1.47	9 (10%)
17	CLA	L	204	-	54,58,73	1.39	10 (18%)	65,95,113	1.56	9 (13%)
24	3XQ	J	106	-	24,24,24	0.60	1 (4%)	25,25,25	1.13	0
25	ZEX	3	216	-	42,43,43	5.09	19 (45%)	55,60,60	5.10	31 (56%)
17	CLA	5	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.62	7 (11%)
17	CLA	B	813	-	69,73,73	1.30	11 (15%)	83,113,113	1.38	11 (13%)
17	CLA	5	610	-	49,53,73	1.47	8 (16%)	59,89,113	1.55	7 (11%)
17	CLA	1	601	-	52,56,73	1.45	10 (19%)	62,92,113	2.06	15 (24%)
17	CLA	A	812	-	49,53,73	1.46	11 (22%)	59,89,113	1.65	11 (18%)
17	CLA	B	840	-	51,55,73	1.44	10 (19%)	61,91,113	1.64	10 (16%)
17	CLA	4	609	-	45,49,73	1.53	7 (15%)	54,84,113	1.63	7 (12%)
20	BCR	A	843	-	41,41,41	1.23	3 (7%)	56,56,56	1.35	7 (12%)
17	CLA	B	828	-	69,73,73	1.32	10 (14%)	83,113,113	1.52	11 (13%)
25	ZEX	4	617	-	42,43,43	5.16	19 (45%)	55,60,60	5.04	30 (54%)
17	CLA	1	611	-	49,53,73	1.47	11 (22%)	59,89,113	1.99	9 (15%)
17	CLA	A	823	-	69,73,73	1.29	11 (15%)	83,113,113	1.46	14 (16%)
17	CLA	4	608	-	49,53,73	1.50	9 (18%)	59,89,113	1.65	10 (16%)
17	CLA	B	822	-	69,73,73	1.29	10 (14%)	83,113,113	1.48	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	2	610	-	46,50,73	1.49	10 (21%)	55,85,113	1.70	6 (10%)
17	CLA	B	815	-	59,63,73	1.35	11 (18%)	71,101,113	1.43	6 (8%)
17	CLA	K	102	-	49,53,73	1.46	11 (22%)	59,89,113	1.58	8 (13%)
21	SF4	C	102	-	0,12,12	-	-	-		
25	ZEX	3	215	-	42,43,43	4.97	19 (45%)	55,60,60	5.27	33 (60%)
25	ZEX	5	616	-	42,43,43	5.23	20 (47%)	55,60,60	5.04	28 (50%)
20	BCR	K	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.35	7 (12%)
17	CLA	4	605	-	45,50,73	1.54	7 (15%)	53,85,113	1.54	7 (13%)
17	CLA	5	612	-	49,53,73	1.47	8 (16%)	59,89,113	1.70	7 (11%)
25	ZEX	2	616	-	42,43,43	5.27	20 (47%)	55,60,60	4.77	29 (52%)
17	CLA	A	816	1	69,73,73	1.32	10 (14%)	83,113,113	1.52	10 (12%)
17	CLA	J	103	-	46,50,73	1.46	11 (23%)	55,85,113	1.63	6 (10%)
17	CLA	4	611	-	49,53,73	1.52	9 (18%)	59,89,113	1.53	7 (11%)
17	CLA	A	814	-	49,53,73	1.48	8 (16%)	59,89,113	1.67	11 (18%)
20	BCR	B	845	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
17	CLA	A	835	1	55,59,73	1.40	9 (16%)	66,96,113	1.64	11 (16%)
17	CLA	A	836	-	69,73,73	1.28	10 (14%)	83,113,113	1.55	13 (15%)
20	BCR	B	849	-	41,41,41	1.27	3 (7%)	56,56,56	1.57	10 (17%)
17	CLA	3	212	-	50,54,73	1.43	9 (18%)	60,90,113	1.51	5 (8%)
17	CLA	A	815	-	66,70,73	1.28	11 (16%)	79,109,113	1.46	9 (11%)
17	CLA	5	606	-	49,53,73	1.62	10 (20%)	59,89,113	2.27	23 (38%)
22	BGC	A	849	26	11,11,12	1.66	3 (27%)	15,15,17	1.04	0
25	ZEX	3	214	-	42,43,43	5.06	19 (45%)	55,60,60	5.27	30 (54%)
17	CLA	2	612	-	49,53,73	1.48	10 (20%)	59,89,113	1.60	6 (10%)
17	CLA	B	807	-	49,53,73	1.46	11 (22%)	59,89,113	1.64	9 (15%)
17	CLA	A	820	-	53,57,73	1.42	12 (22%)	62,93,113	1.66	9 (14%)
17	CLA	B	834	-	47,51,73	1.52	10 (21%)	56,86,113	1.63	11 (19%)
17	CLA	4	607	-	49,53,73	1.45	8 (16%)	59,89,113	1.66	8 (13%)
23	DGD	B	851	-	67,67,67	1.03	3 (4%)	81,81,81	1.47	11 (13%)
20	BCR	A	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	10 (17%)
17	CLA	5	601	-	49,53,73	1.48	7 (14%)	59,89,113	1.57	8 (13%)
19	LHG	A	841	-	48,48,48	0.69	1 (2%)	51,54,54	1.27	6 (11%)
17	CLA	5	602	-	49,53,73	1.49	8 (16%)	59,89,113	1.69	11 (18%)
17	CLA	1	610	-	49,53,73	1.50	12 (24%)	59,89,113	1.59	11 (18%)
20	BCR	L	206	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	ZEX	1	613	-	42,43,43	4.99	18 (42%)	55,60,60	5.22	32 (58%)
17	CLA	2	608	-	54,58,73	1.47	11 (20%)	65,95,113	1.70	12 (18%)
25	ZEX	4	615	-	42,43,43	5.16	19 (45%)	55,60,60	4.81	28 (50%)
17	CLA	A	813	1	46,50,73	1.52	11 (23%)	55,85,113	1.72	8 (14%)
17	CLA	B	821	-	64,68,73	1.32	12 (18%)	77,107,113	1.57	12 (15%)
17	CLA	B	835	-	69,73,73	1.30	10 (14%)	83,113,113	1.50	8 (9%)
17	CLA	5	611	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	9 (15%)
17	CLA	A	818	-	49,53,73	1.49	10 (20%)	59,89,113	1.84	13 (22%)
17	CLA	5	613	-	47,52,73	1.48	7 (14%)	58,87,113	1.51	9 (15%)
17	CLA	A	817	1	69,73,73	1.33	11 (15%)	83,113,113	1.52	13 (15%)
17	CLA	B	819	-	59,63,73	1.32	11 (18%)	71,101,113	1.51	8 (11%)
17	CLA	1	608	-	64,68,73	1.30	11 (17%)	77,107,113	1.46	8 (10%)
17	CLA	B	806	-	69,73,73	1.34	9 (13%)	83,113,113	1.92	17 (20%)
17	CLA	3	206	-	49,53,73	1.54	9 (18%)	59,89,113	1.70	13 (22%)
17	CLA	A	804	-	69,73,73	1.29	11 (15%)	83,113,113	1.54	10 (12%)
17	CLA	1	606	13	49,53,73	1.48	11 (22%)	59,89,113	1.61	9 (15%)
17	CLA	F	301	-	65,69,73	1.30	11 (16%)	78,108,113	1.44	8 (10%)
17	CLA	B	825	-	47,51,73	1.52	11 (23%)	56,86,113	1.60	10 (17%)
17	CLA	O	205	-	49,53,73	1.49	10 (20%)	59,89,113	1.50	7 (11%)
17	CLA	B	832	-	69,73,73	1.37	11 (15%)	83,113,113	1.75	14 (16%)
17	CLA	4	604	-	49,53,73	1.50	10 (20%)	59,89,113	1.49	7 (11%)
17	CLA	2	609	-	45,49,73	1.51	10 (22%)	54,84,113	1.67	8 (14%)
17	CLA	F	302	-	49,53,73	1.49	10 (20%)	59,89,113	1.61	8 (13%)
17	CLA	2	611	-	49,53,73	1.46	10 (20%)	59,89,113	1.76	9 (15%)
20	BCR	B	846	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	6 (10%)
20	BCR	B	850	-	41,41,41	1.26	3 (7%)	56,56,56	1.53	9 (16%)
20	BCR	F	304	-	41,41,41	1.18	2 (4%)	56,56,56	1.39	10 (17%)
17	CLA	B	837	-	49,53,73	1.49	11 (22%)	59,89,113	1.58	6 (10%)
17	CLA	B	814	-	58,62,73	1.50	10 (17%)	73,100,113	1.84	14 (19%)
17	CLA	B	801	-	69,73,73	1.30	10 (14%)	83,113,113	1.86	17 (20%)
25	ZEX	1	615	-	42,43,43	4.86	19 (45%)	55,60,60	5.26	33 (60%)
17	CLA	A	825	1	69,73,73	1.33	11 (15%)	83,113,113	1.50	11 (13%)
17	CLA	B	812	-	69,73,73	1.32	12 (17%)	83,113,113	1.49	14 (16%)
25	ZEX	1	616	-	42,43,43	5.05	19 (45%)	55,60,60	5.10	32 (58%)
17	CLA	4	601	-	52,56,73	1.43	7 (13%)	62,92,113	1.68	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	802	-	59,63,73	1.35	11 (18%)	71,101,113	1.71	11 (15%)
17	CLA	2	607	-	49,53,73	1.49	11 (22%)	59,89,113	1.63	8 (13%)
17	CLA	3	203	-	67,71,73	1.28	10 (14%)	80,110,113	1.59	10 (12%)
17	CLA	A	808	-	59,63,73	1.35	11 (18%)	71,101,113	1.48	8 (11%)
17	CLA	B	804	-	69,73,73	1.36	11 (15%)	83,113,113	1.65	18 (21%)
17	CLA	3	204	-	49,53,73	1.50	11 (22%)	59,89,113	1.57	8 (13%)
17	CLA	F	303	-	45,49,73	1.47	9 (20%)	54,84,113	1.66	6 (11%)
17	CLA	3	208	-	49,53,73	1.52	11 (22%)	59,89,113	1.55	7 (11%)
17	CLA	4	606	-	49,53,73	1.47	10 (20%)	59,89,113	1.64	6 (10%)
17	CLA	K	103	-	46,50,73	1.54	11 (23%)	55,85,113	1.66	7 (12%)
17	CLA	3	213	-	55,59,73	1.38	9 (16%)	66,96,113	1.51	7 (10%)
17	CLA	B	843	-	69,73,73	1.26	9 (13%)	83,113,113	1.38	10 (12%)
17	CLA	4	610	-	49,53,73	1.49	8 (16%)	59,89,113	1.58	6 (10%)
25	ZEX	2	615	-	42,43,43	4.79	18 (42%)	55,60,60	5.10	31 (56%)
17	CLA	A	824	-	59,63,73	1.37	11 (18%)	71,101,113	1.66	11 (15%)
17	CLA	B	833	-	49,53,73	1.53	10 (20%)	59,89,113	1.60	10 (16%)
17	CLA	B	827	-	69,73,73	1.32	10 (14%)	83,113,113	1.52	14 (16%)
17	CLA	4	602	-	63,67,73	1.31	11 (17%)	75,105,113	1.57	11 (14%)
17	CLA	5	603	-	69,73,73	1.26	9 (13%)	83,113,113	1.51	11 (13%)
17	CLA	3	210	-	45,49,73	1.50	9 (20%)	54,84,113	1.71	9 (16%)
17	CLA	B	810	-	69,73,73	1.23	11 (15%)	83,113,113	1.42	8 (9%)
17	CLA	A	807	1	69,73,73	1.33	11 (15%)	83,113,113	1.60	17 (20%)
17	CLA	5	608	-	49,53,73	1.49	10 (20%)	59,89,113	1.71	12 (20%)
17	CLA	B	826	-	59,63,73	1.38	12 (20%)	71,101,113	1.45	8 (11%)
25	ZEX	4	614	-	42,43,43	5.17	19 (45%)	55,60,60	4.78	29 (52%)
17	CLA	B	820	-	63,67,73	1.35	10 (15%)	75,105,113	1.54	12 (16%)
20	BCR	A	845	-	41,41,41	1.34	3 (7%)	56,56,56	1.43	9 (16%)
17	CLA	A	826	-	69,73,73	1.30	10 (14%)	83,113,113	1.61	10 (12%)
25	ZEX	1	617	-	42,43,43	4.91	18 (42%)	55,60,60	5.13	29 (52%)
17	CLA	2	613	-	49,53,73	1.47	9 (18%)	59,89,113	1.55	8 (13%)
20	BCR	B	805	-	41,41,41	1.27	3 (7%)	56,56,56	1.48	10 (17%)
17	CLA	1	609	-	45,49,73	1.48	9 (20%)	54,84,113	1.70	7 (12%)
25	ZEX	3	218	-	42,43,43	5.43	20 (47%)	55,60,60	4.52	33 (60%)
17	CLA	2	604	-	46,50,73	1.49	11 (23%)	55,85,113	1.70	8 (14%)
17	CLA	2	602	-	69,73,73	1.29	11 (15%)	83,113,113	1.45	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	1	605	-	45,50,73	1.51	8 (17%)	53,85,113	1.54	8 (15%)
17	CLA	B	838	2	64,68,73	1.39	10 (15%)	77,107,113	1.61	12 (15%)
25	ZEX	3	217	-	42,43,43	5.10	20 (47%)	55,60,60	4.94	27 (49%)
17	CLA	B	823	-	49,53,73	1.49	11 (22%)	59,89,113	1.58	8 (13%)
17	CLA	J	101	-	69,73,73	1.29	11 (15%)	83,113,113	1.54	10 (12%)
17	CLA	B	842	-	69,73,73	1.28	11 (15%)	83,113,113	1.49	9 (10%)
17	CLA	1	607	-	49,53,73	1.47	9 (18%)	59,89,113	1.82	9 (15%)
17	CLA	A	839	-	69,73,73	1.28	12 (17%)	83,113,113	1.52	9 (10%)
17	CLA	B	824	-	50,54,73	1.45	11 (22%)	60,90,113	1.57	7 (11%)
20	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.40	8 (14%)
20	BCR	K	101	-	41,41,41	1.23	3 (7%)	56,56,56	1.36	9 (16%)
17	CLA	1	602	-	63,67,73	1.31	12 (19%)	75,105,113	1.52	7 (9%)
21	SF4	A	847	-	0,12,12	-	-	-		
17	CLA	3	202	-	49,53,73	1.46	9 (18%)	59,89,113	1.55	7 (11%)
17	CLA	L	202	10	61,65,73	1.34	10 (16%)	73,103,113	1.40	5 (6%)
17	CLA	A	831	1	69,73,73	1.27	11 (15%)	83,113,113	1.51	11 (13%)
25	ZEX	1	614	-	42,43,43	5.03	19 (45%)	55,60,60	5.77	30 (54%)
17	CLA	A	828	-	69,73,73	1.44	11 (15%)	83,113,113	1.77	21 (25%)
25	ZEX	5	615	-	42,43,43	5.32	20 (47%)	55,60,60	4.94	31 (56%)
17	CLA	A	803	-	69,73,73	1.31	11 (15%)	83,113,113	1.65	15 (18%)
17	CLA	1	612	-	49,53,73	1.51	11 (22%)	59,89,113	1.57	9 (15%)
17	CLA	A	848	-	69,73,73	1.32	10 (14%)	83,113,113	1.95	19 (22%)
17	CLA	B	811	-	69,73,73	1.25	12 (17%)	83,113,113	1.74	13 (15%)
17	CLA	4	603	-	49,53,73	1.46	10 (20%)	59,89,113	1.60	10 (16%)
20	BCR	J	105	-	41,41,41	1.32	3 (7%)	56,56,56	1.33	7 (12%)
18	PQN	A	840	-	34,34,34	2.77	10 (29%)	42,45,45	2.16	5 (11%)
17	CLA	A	811	-	69,73,73	1.30	10 (14%)	83,113,113	1.45	8 (9%)
17	CLA	B	818	-	46,50,73	1.53	11 (23%)	55,85,113	1.67	8 (14%)
17	CLA	A	806	1	69,73,73	1.25	11 (15%)	83,113,113	1.46	8 (9%)
17	CLA	A	837	-	69,73,73	1.27	11 (15%)	83,113,113	1.43	11 (13%)
17	CLA	O	201	-	56,60,73	1.39	12 (21%)	67,97,113	1.53	10 (14%)
17	CLA	A	829	-	54,58,73	1.46	11 (20%)	65,95,113	1.51	10 (15%)
17	CLA	B	841	-	69,73,73	1.27	11 (15%)	83,113,113	1.48	9 (10%)
19	LHG	A	842	-	39,39,48	0.76	1 (2%)	42,45,54	1.32	6 (14%)
17	CLA	A	830	-	60,64,73	1.33	10 (16%)	72,102,113	1.46	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	3	205	-	49,53,73	1.52	11 (22%)	59,89,113	1.65	9 (15%)
20	BCR	O	202	-	41,41,41	1.34	3 (7%)	56,56,56	1.53	11 (19%)
25	ZEX	4	612	-	42,43,43	5.10	19 (45%)	55,60,60	5.09	31 (56%)
17	CLA	B	817	-	49,53,73	1.46	10 (20%)	59,89,113	1.60	8 (13%)
21	SF4	C	101	3	0,12,12	-	-	-		
25	ZEX	2	614	-	42,43,43	4.94	19 (45%)	55,60,60	5.25	33 (60%)
17	CLA	3	207	-	49,53,73	1.45	9 (18%)	59,89,113	1.67	9 (15%)
20	BCR	L	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.56	9 (16%)
17	CLA	3	209	-	56,60,73	1.37	11 (19%)	67,97,113	1.52	10 (14%)
17	CLA	B	831	-	69,73,73	1.37	10 (14%)	83,113,113	1.50	12 (14%)
17	CLA	A	809	-	69,73,73	1.24	12 (17%)	83,113,113	1.50	11 (13%)

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
17	CLA	B	803	-	-	24/39/115/115	-
17	CLA	B	816	-	-	19/39/115/115	-
17	CLA	2	605	-	-	9/15/91/115	-
17	CLA	1	604	-	-	7/15/91/115	-
17	CLA	A	827	-	-	20/39/115/115	-
25	ZEX	5	617	-	-	18/29/67/67	0/2/2/2
17	CLA	A	810	-	-	10/26/102/115	-
17	CLA	A	805	-	-	18/39/115/115	-
17	CLA	J	102	-	-	10/31/107/115	-
20	BCR	B	847	-	-	23/29/63/63	0/2/2/2
17	CLA	5	609	-	-	7/10/86/115	-
17	CLA	L	203	-	-	16/39/115/115	-
17	CLA	B	829	-	-	19/39/115/115	-
17	CLA	B	839	2	-	12/39/115/115	-
17	CLA	5	605	-	-	10/15/91/115	-
17	CLA	O	204	-	-	8/21/97/115	-
20	BCR	B	848	-	-	19/29/63/63	0/2/2/2
17	CLA	5	607	-	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	802	-	-	14/39/115/115	-
17	CLA	B	808	-	-	18/39/115/115	-
17	CLA	1	603	-	-	9/15/91/115	-
17	CLA	B	836	-	-	18/39/115/115	-
20	BCR	L	201	-	-	18/29/63/63	0/2/2/2
17	CLA	B	809	2	-	17/39/115/115	-
17	CLA	3	211	-	-	3/12/88/115	-
25	ZEX	3	201	-	-	16/29/67/67	0/2/2/2
17	CLA	2	603	-	-	2/15/91/115	-
20	BCR	A	846	-	-	18/29/63/63	0/2/2/2
17	CLA	O	203	-	-	5/10/86/115	-
20	BCR	J	104	-	-	16/29/63/63	0/2/2/2
25	ZEX	5	614	-	-	18/29/67/67	0/2/2/2
17	CLA	A	834	-	-	8/15/91/115	-
16	CL0	A	801	1	-	10/39/115/115	-
17	CLA	A	833	-	-	18/39/115/115	-
17	CLA	A	821	-	-	14/23/99/115	-
17	CLA	B	830	-	-	23/39/115/115	-
17	CLA	2	606	-	-	9/15/91/115	-
26	1DO	3	219	22	-	3/10/10/10	-
25	ZEX	2	617	-	-	19/29/67/67	0/2/2/2
25	ZEX	4	616	-	-	17/29/67/67	0/2/2/2
17	CLA	A	832	-	-	20/39/115/115	-
25	ZEX	4	613	-	-	16/29/67/67	0/2/2/2
17	CLA	2	601	-	-	8/15/91/115	-
17	CLA	A	822	-	-	9/27/103/115	-
18	PQN	B	844	-	-	7/23/43/43	0/2/2/2
17	CLA	A	819	-	-	13/39/115/115	-
17	CLA	A	838	1	-	13/39/115/115	-
17	CLA	L	204	-	-	8/21/97/115	-
24	3XQ	J	106	-	-	17/24/24/24	-
25	ZEX	3	216	-	-	19/29/67/67	0/2/2/2
17	CLA	5	604	-	-	8/15/91/115	-
17	CLA	B	813	-	-	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	5	610	-	-	8/15/91/115	-
17	CLA	1	601	-	-	8/19/95/115	-
17	CLA	A	812	-	-	6/15/91/115	-
17	CLA	B	840	-	-	4/18/94/115	-
17	CLA	4	609	-	-	7/10/86/115	-
20	BCR	A	843	-	-	16/29/63/63	0/2/2/2
17	CLA	B	828	-	-	6/39/115/115	-
25	ZEX	4	617	-	-	18/29/67/67	0/2/2/2
17	CLA	1	611	-	-	12/15/91/115	-
17	CLA	A	823	-	-	18/39/115/115	-
17	CLA	4	608	-	-	8/15/91/115	-
17	CLA	B	822	-	-	19/39/115/115	-
17	CLA	2	610	-	-	7/12/88/115	-
17	CLA	B	815	-	-	8/27/103/115	-
17	CLA	K	102	-	-	7/15/91/115	-
25	ZEX	3	215	-	-	16/29/67/67	0/2/2/2
21	SF4	C	102	-	-	-	0/6/5/5
25	ZEX	5	616	-	-	16/29/67/67	0/2/2/2
20	BCR	K	104	-	-	19/29/63/63	0/2/2/2
17	CLA	4	605	-	-	2/11/87/115	-
17	CLA	5	612	-	-	7/15/91/115	-
25	ZEX	2	616	-	-	19/29/67/67	0/2/2/2
17	CLA	A	816	1	-	13/39/115/115	-
17	CLA	J	103	-	-	8/12/88/115	-
17	CLA	4	611	-	-	10/15/91/115	-
17	CLA	A	814	-	-	6/15/91/115	-
20	BCR	B	845	-	-	16/29/63/63	0/2/2/2
17	CLA	A	835	1	-	10/23/99/115	-
17	CLA	A	836	-	-	15/39/115/115	-
20	BCR	B	849	-	-	23/29/63/63	0/2/2/2
17	CLA	3	212	-	-	10/17/93/115	-
17	CLA	A	815	-	-	15/36/112/115	-
17	CLA	5	606	-	-	5/15/91/115	-
22	BGC	A	849	26	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	ZEX	3	214	-	-	14/29/67/67	0/2/2/2
17	CLA	2	612	-	-	5/15/91/115	-
17	CLA	B	807	-	-	7/15/91/115	-
17	CLA	A	820	-	-	7/20/96/115	-
17	CLA	B	834	-	-	5/13/89/115	-
17	CLA	4	607	-	-	9/15/91/115	-
23	DGD	B	851	-	-	30/55/95/95	0/2/2/2
20	BCR	A	844	-	-	17/29/63/63	0/2/2/2
17	CLA	5	601	-	-	8/15/91/115	-
19	LHG	A	841	-	-	27/53/53/53	-
17	CLA	5	602	-	-	9/15/91/115	-
17	CLA	1	610	-	-	6/15/91/115	-
20	BCR	L	206	-	-	15/29/63/63	0/2/2/2
25	ZEX	1	613	-	-	16/29/67/67	0/2/2/2
17	CLA	2	608	-	-	8/21/97/115	-
25	ZEX	4	615	-	-	16/29/67/67	0/2/2/2
17	CLA	A	813	1	-	5/12/88/115	-
17	CLA	B	821	-	-	16/33/109/115	-
17	CLA	B	835	-	-	17/39/115/115	-
17	CLA	5	611	-	-	7/15/91/115	-
17	CLA	A	818	-	-	9/15/91/115	-
17	CLA	5	613	-	-	6/12/88/115	-
17	CLA	A	817	1	-	17/39/115/115	-
17	CLA	B	819	-	-	13/27/103/115	-
17	CLA	1	608	-	-	11/33/109/115	-
17	CLA	B	806	-	-	18/39/115/115	-
17	CLA	3	206	-	-	6/15/91/115	-
17	CLA	A	804	-	-	14/39/115/115	-
17	CLA	1	606	13	-	8/15/91/115	-
17	CLA	F	301	-	-	16/35/111/115	-
17	CLA	B	825	-	-	7/13/89/115	-
17	CLA	O	205	-	-	8/15/91/115	-
17	CLA	B	832	-	-	10/39/115/115	-
17	CLA	4	604	-	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	609	-	-	5/10/86/115	-
17	CLA	F	302	-	-	4/15/91/115	-
17	CLA	2	611	-	-	7/15/91/115	-
20	BCR	B	846	-	-	11/29/63/63	0/2/2/2
20	BCR	B	850	-	-	15/29/63/63	0/2/2/2
20	BCR	F	304	-	-	18/29/63/63	0/2/2/2
17	CLA	B	837	-	-	8/15/91/115	-
17	CLA	B	814	-	-	10/25/101/115	-
17	CLA	B	801	-	-	15/39/115/115	-
25	ZEX	1	615	-	-	20/29/67/67	0/2/2/2
17	CLA	A	825	1	-	11/39/115/115	-
17	CLA	B	812	-	-	20/39/115/115	-
25	ZEX	1	616	-	-	20/29/67/67	0/2/2/2
17	CLA	4	601	-	-	8/19/95/115	-
17	CLA	A	802	-	-	7/27/103/115	-
17	CLA	2	607	-	-	5/15/91/115	-
17	CLA	3	203	-	-	20/37/113/115	-
17	CLA	A	808	-	-	10/27/103/115	-
17	CLA	B	804	-	-	19/39/115/115	-
17	CLA	3	204	-	-	8/15/91/115	-
17	CLA	F	303	-	-	5/10/86/115	-
17	CLA	3	208	-	-	10/15/91/115	-
17	CLA	4	606	-	-	6/15/91/115	-
17	CLA	K	103	-	-	7/12/88/115	-
17	CLA	3	213	-	-	10/23/99/115	-
17	CLA	B	843	-	-	18/39/115/115	-
17	CLA	4	610	-	-	6/15/91/115	-
25	ZEX	2	615	-	-	16/29/67/67	0/2/2/2
17	CLA	A	824	-	-	7/27/103/115	-
17	CLA	B	833	-	-	7/15/91/115	-
17	CLA	B	827	-	-	11/39/115/115	-
17	CLA	4	602	-	-	14/32/108/115	-
17	CLA	5	603	-	-	22/39/115/115	-
17	CLA	3	210	-	-	7/10/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	810	-	-	19/39/115/115	-
17	CLA	A	807	1	-	21/39/115/115	-
17	CLA	5	608	-	-	7/15/91/115	-
17	CLA	B	826	-	-	9/27/103/115	-
25	ZEX	4	614	-	-	17/29/67/67	0/2/2/2
17	CLA	B	820	-	-	18/32/108/115	-
20	BCR	A	845	-	-	18/29/63/63	0/2/2/2
17	CLA	A	826	-	-	14/39/115/115	-
25	ZEX	1	617	-	-	18/29/67/67	0/2/2/2
17	CLA	2	613	-	-	7/15/91/115	-
20	BCR	B	805	-	-	15/29/63/63	0/2/2/2
17	CLA	1	609	-	-	2/10/86/115	-
25	ZEX	3	218	-	-	17/29/67/67	0/2/2/2
17	CLA	2	604	-	-	5/12/88/115	-
17	CLA	2	602	-	-	14/39/115/115	-
17	CLA	1	605	-	-	5/11/87/115	-
17	CLA	B	838	2	-	20/33/109/115	-
25	ZEX	3	217	-	-	15/29/67/67	0/2/2/2
17	CLA	B	823	-	-	4/15/91/115	-
17	CLA	J	101	-	-	20/39/115/115	-
17	CLA	B	842	-	-	16/39/115/115	-
17	CLA	1	607	-	-	9/15/91/115	-
17	CLA	A	839	-	-	19/39/115/115	-
17	CLA	B	824	-	-	8/17/93/115	-
20	BCR	I	101	-	-	18/29/63/63	0/2/2/2
20	BCR	K	101	-	-	11/29/63/63	0/2/2/2
17	CLA	1	602	-	-	10/32/108/115	-
21	SF4	A	847	-	-	-	0/6/5/5
17	CLA	3	202	-	-	7/15/91/115	-
17	CLA	L	202	10	-	16/30/106/115	-
17	CLA	A	831	1	-	20/39/115/115	-
25	ZEX	1	614	-	-	16/29/67/67	0/2/2/2
17	CLA	A	828	-	-	12/39/115/115	-
25	ZEX	5	615	-	-	19/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	803	-	-	4/39/115/115	-
17	CLA	1	612	-	-	9/15/91/115	-
17	CLA	A	848	-	-	9/39/115/115	-
17	CLA	B	811	-	-	8/39/115/115	-
17	CLA	4	603	-	-	10/15/91/115	-
20	BCR	J	105	-	-	14/29/63/63	0/2/2/2
18	PQN	A	840	-	-	11/23/43/43	0/2/2/2
17	CLA	A	811	-	-	15/39/115/115	-
17	CLA	B	818	-	-	6/12/88/115	-
17	CLA	A	806	1	-	18/39/115/115	-
17	CLA	A	837	-	-	12/39/115/115	-
17	CLA	O	201	-	-	7/24/100/115	-
17	CLA	A	829	-	-	6/21/97/115	-
17	CLA	B	841	-	-	16/39/115/115	-
19	LHG	A	842	-	-	19/44/44/53	-
17	CLA	A	830	-	-	6/29/105/115	-
17	CLA	3	205	-	-	9/15/91/115	-
20	BCR	O	202	-	-	14/29/63/63	0/2/2/2
25	ZEX	4	612	-	-	19/29/67/67	0/2/2/2
17	CLA	B	817	-	-	3/15/91/115	-
21	SF4	C	101	3	-	-	0/6/5/5
25	ZEX	2	614	-	-	18/29/67/67	0/2/2/2
17	CLA	3	207	-	-	7/15/91/115	-
20	BCR	L	205	-	-	15/29/63/63	0/2/2/2
17	CLA	3	209	-	-	7/24/100/115	-
17	CLA	B	831	-	-	14/39/115/115	-
17	CLA	A	809	-	-	15/39/115/115	-

The worst 5 of 2178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	218	ZEX	C14-C13	15.85	1.56	1.35
25	2	616	ZEX	C14-C13	14.96	1.55	1.35
25	1	616	ZEX	C14-C13	14.67	1.55	1.35
25	3	201	ZEX	C14-C13	14.51	1.55	1.35
25	3	216	ZEX	C14-C13	14.50	1.55	1.35

The worst 5 of 2567 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	614	ZEX	C31-C30-C29	-16.44	103.84	127.31
25	1	614	ZEX	C39-C29-C28	-14.08	95.90	118.08
25	5	617	ZEX	C15-C14-C13	-13.48	108.07	127.31
25	3	201	ZEX	C31-C30-C29	-13.33	108.28	127.31
16	A	801	CL0	C4A-NA-C1A	13.29	112.68	106.71

There are no chirality outliers.

5 of 2588 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	C4B-C3B-CAB-CBB
17	A	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

188 monomers are involved in 514 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	803	CLA	2	0
17	B	816	CLA	5	0
17	2	605	CLA	2	0
17	1	604	CLA	1	0
17	A	827	CLA	5	0
25	5	617	ZEX	7	0
17	A	810	CLA	2	0
17	A	805	CLA	4	0
17	J	102	CLA	5	0
20	B	847	BCR	5	0
17	5	609	CLA	1	0
17	L	203	CLA	3	0
17	B	829	CLA	6	0
17	B	839	CLA	5	0
17	5	605	CLA	1	0
17	O	204	CLA	2	0
20	B	848	BCR	4	0
17	5	607	CLA	3	0
17	B	802	CLA	6	0
17	B	808	CLA	4	0
17	1	603	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	836	CLA	4	0
20	L	201	BCR	3	0
17	B	809	CLA	5	0
25	3	201	ZEX	4	0
17	2	603	CLA	1	0
20	A	846	BCR	6	0
20	J	104	BCR	4	0
25	5	614	ZEX	4	0
17	A	834	CLA	5	0
16	A	801	CL0	53	0
17	A	833	CLA	4	0
17	A	821	CLA	1	0
17	B	830	CLA	6	0
17	2	606	CLA	1	0
26	3	219	1DO	1	0
25	2	617	ZEX	2	0
25	4	616	ZEX	2	0
17	A	832	CLA	4	0
25	4	613	ZEX	4	0
17	2	601	CLA	3	0
17	A	822	CLA	1	0
18	B	844	PQN	2	0
17	A	819	CLA	4	0
17	A	838	CLA	9	0
17	L	204	CLA	1	0
25	3	216	ZEX	1	0
17	5	604	CLA	1	0
17	B	813	CLA	3	0
17	1	601	CLA	1	0
17	A	812	CLA	1	0
17	B	840	CLA	1	0
17	4	609	CLA	3	0
20	A	843	BCR	5	0
17	B	828	CLA	4	0
25	4	617	ZEX	1	0
17	1	611	CLA	1	0
17	A	823	CLA	6	0
17	4	608	CLA	4	0
17	B	822	CLA	2	0
17	2	610	CLA	1	0
21	C	102	SF4	1	0
25	3	215	ZEX	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	616	ZEX	2	0
20	K	104	BCR	5	0
17	5	612	CLA	2	0
25	2	616	ZEX	1	0
17	A	816	CLA	3	0
17	J	103	CLA	1	0
17	4	611	CLA	4	0
17	A	814	CLA	1	0
17	A	835	CLA	1	0
17	A	836	CLA	4	0
20	B	849	BCR	3	0
17	3	212	CLA	3	0
17	A	815	CLA	4	0
17	5	606	CLA	2	0
25	3	214	ZEX	3	0
17	2	612	CLA	1	0
17	A	820	CLA	1	0
17	B	834	CLA	1	0
17	4	607	CLA	1	0
23	B	851	DGD	5	0
17	5	601	CLA	1	0
19	A	841	LHG	2	0
17	5	602	CLA	2	0
20	L	206	BCR	2	0
25	1	613	ZEX	2	0
17	2	608	CLA	1	0
25	4	615	ZEX	2	0
17	A	813	CLA	1	0
17	B	821	CLA	4	0
17	B	835	CLA	7	0
17	A	818	CLA	4	0
17	A	817	CLA	8	0
17	B	819	CLA	3	0
17	B	806	CLA	9	0
17	3	206	CLA	4	0
17	A	804	CLA	4	0
17	1	606	CLA	3	0
17	F	301	CLA	1	0
17	B	825	CLA	1	0
17	O	205	CLA	1	0
17	B	832	CLA	4	0
17	4	604	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	609	CLA	2	0
17	F	302	CLA	3	0
20	B	846	BCR	2	0
20	B	850	BCR	4	0
20	F	304	BCR	2	0
17	B	837	CLA	1	0
17	B	814	CLA	2	0
17	B	801	CLA	11	0
25	1	615	ZEX	1	0
17	A	825	CLA	5	0
17	B	812	CLA	8	0
25	1	616	ZEX	2	0
17	4	601	CLA	2	0
17	2	607	CLA	1	0
17	3	203	CLA	8	0
17	A	808	CLA	2	0
17	B	804	CLA	5	0
17	3	204	CLA	2	0
17	3	208	CLA	2	0
17	4	606	CLA	2	0
17	K	103	CLA	1	0
17	B	843	CLA	4	0
25	2	615	ZEX	4	0
17	A	824	CLA	3	0
17	B	833	CLA	1	0
17	B	827	CLA	7	0
17	4	602	CLA	2	0
17	5	603	CLA	5	0
17	3	210	CLA	1	0
17	B	810	CLA	5	0
17	A	807	CLA	2	0
17	5	608	CLA	2	0
17	B	826	CLA	1	0
25	4	614	ZEX	4	0
17	B	820	CLA	4	0
20	A	845	BCR	3	0
17	A	826	CLA	7	0
25	1	617	ZEX	2	0
17	2	613	CLA	1	0
20	B	805	BCR	6	0
17	1	609	CLA	1	0
25	3	218	ZEX	5	0

Continued on next page...

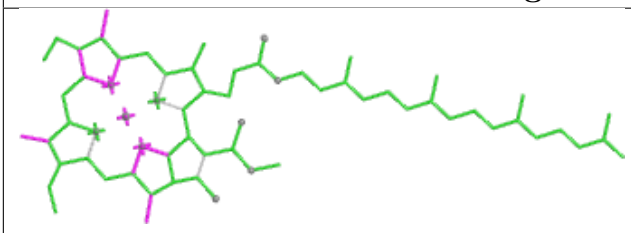
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	604	CLA	2	0
17	2	602	CLA	6	0
17	B	838	CLA	3	0
25	3	217	ZEX	1	0
17	J	101	CLA	5	0
17	B	842	CLA	13	0
17	1	607	CLA	1	0
17	A	839	CLA	3	0
20	I	101	BCR	3	0
20	K	101	BCR	6	0
17	1	602	CLA	2	0
17	L	202	CLA	1	0
17	A	831	CLA	9	0
25	1	614	ZEX	9	0
17	A	828	CLA	4	0
25	5	615	ZEX	1	0
17	A	803	CLA	7	0
17	1	612	CLA	1	0
17	A	848	CLA	8	0
17	B	811	CLA	6	0
20	J	105	BCR	2	0
18	A	840	PQN	4	0
17	A	811	CLA	4	0
17	B	818	CLA	1	0
17	A	806	CLA	7	0
17	A	837	CLA	3	0
17	A	829	CLA	1	0
17	B	841	CLA	9	0
19	A	842	LHG	3	0
17	A	830	CLA	3	0
17	3	205	CLA	2	0
20	O	202	BCR	5	0
25	4	612	ZEX	3	0
17	B	817	CLA	2	0
21	C	101	SF4	1	0
25	2	614	ZEX	3	0
17	3	207	CLA	2	0
20	L	205	BCR	6	0
17	3	209	CLA	2	0
17	B	831	CLA	7	0
17	A	809	CLA	1	0

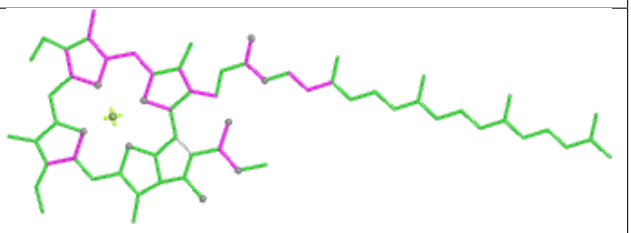
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

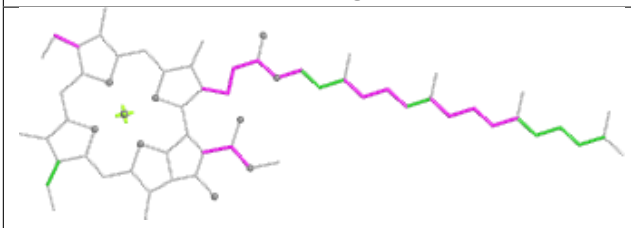
Ligand CLA B 803



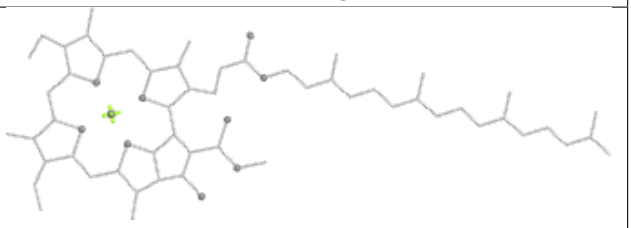
Bond lengths



Bond angles

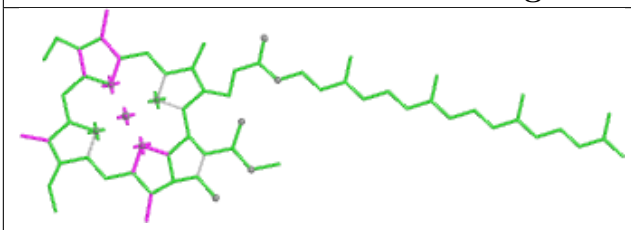


Torsions

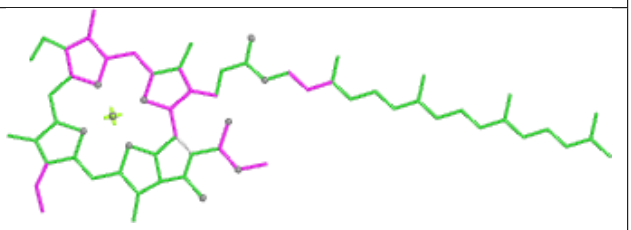


Rings

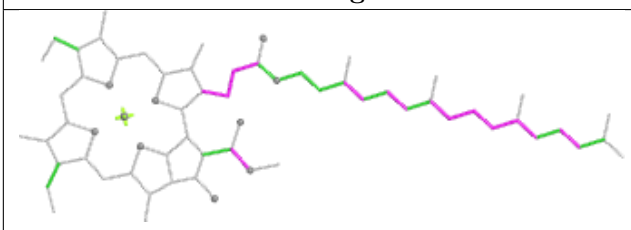
Ligand CLA B 816



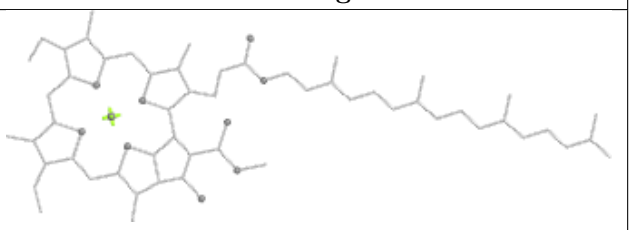
Bond lengths



Bond angles

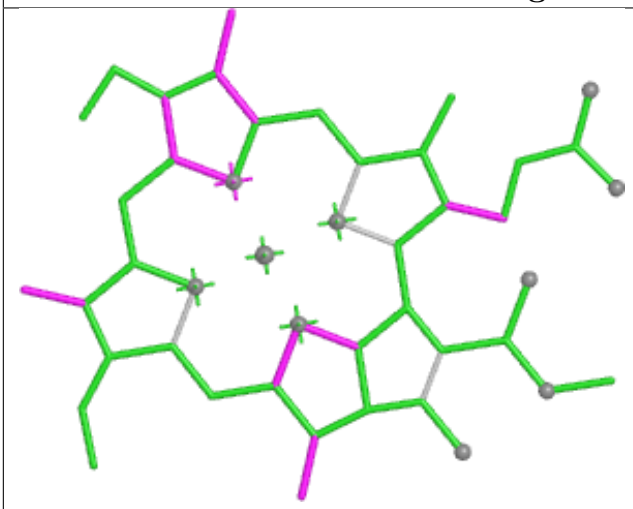


Torsions

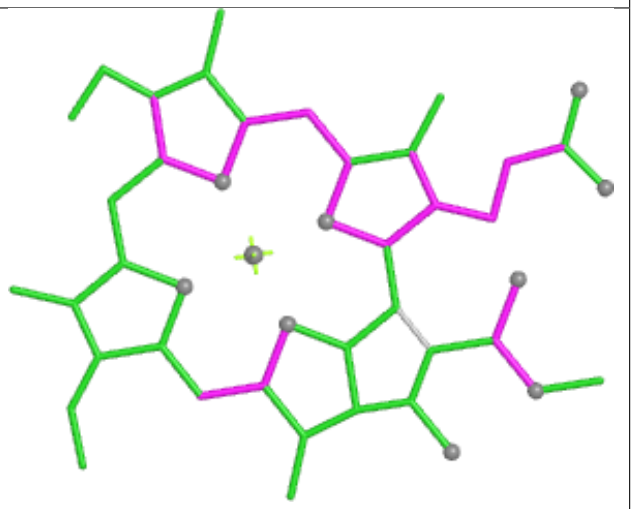


Rings

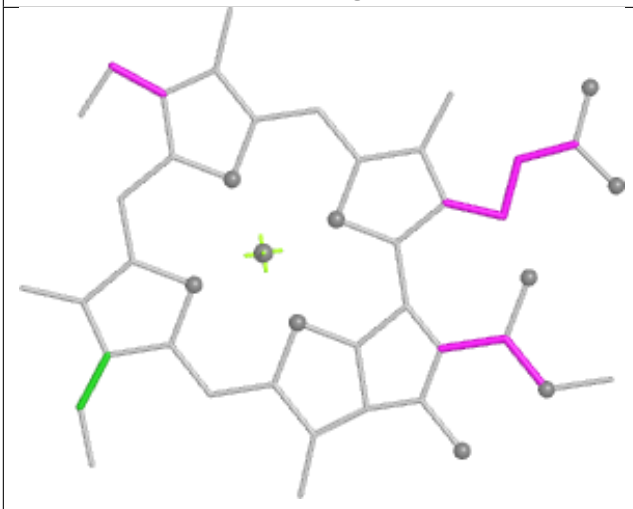
Ligand CLA 2 605



Bond lengths



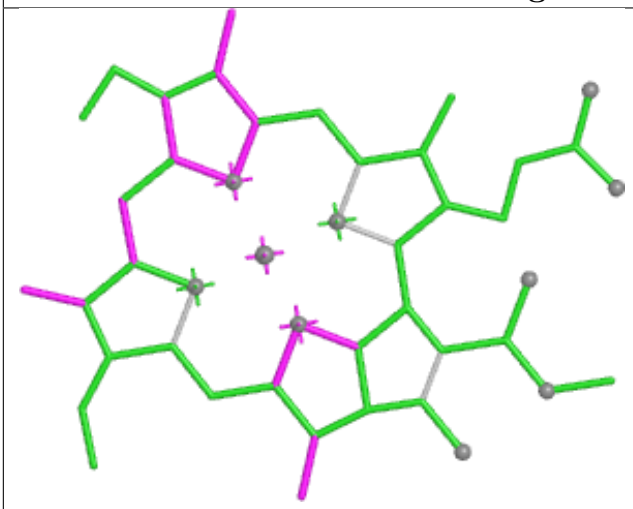
Bond angles



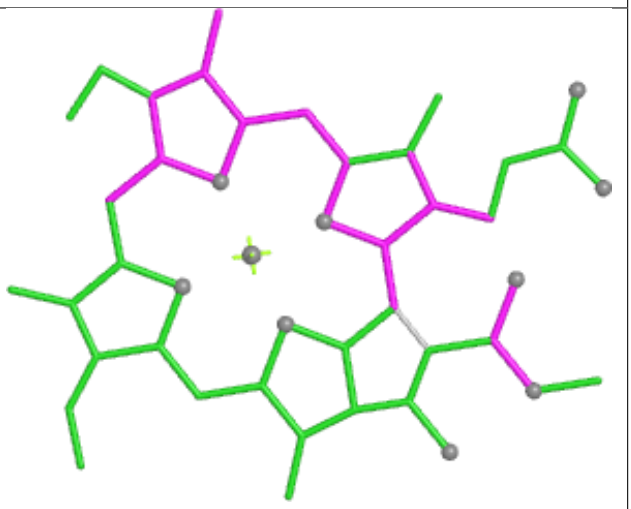
Torsions

Rings

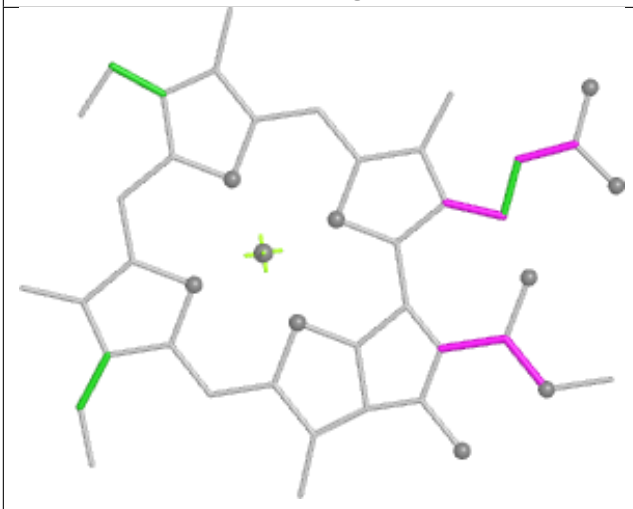
Ligand CLA 1 604



Bond lengths



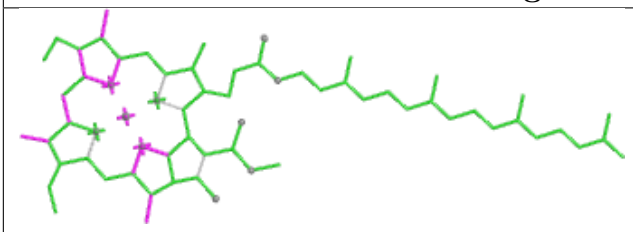
Bond angles



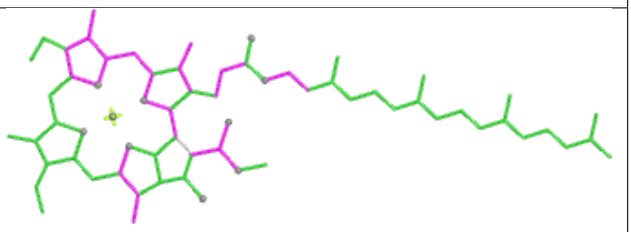
Torsions

Rings

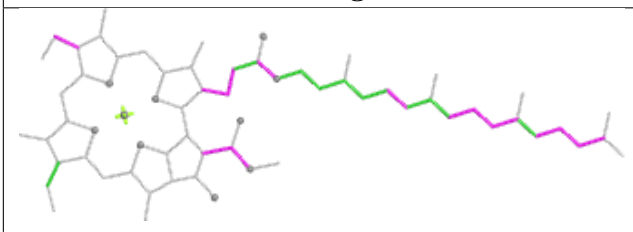
Ligand CLA A 827



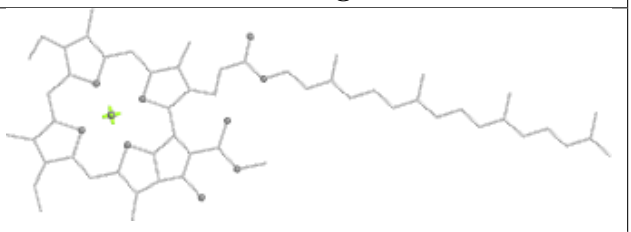
Bond lengths



Bond angles

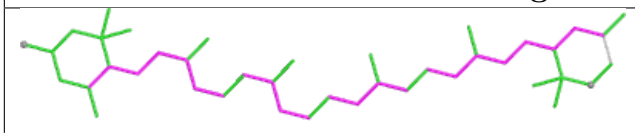


Torsions

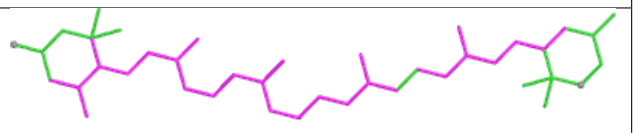


Rings

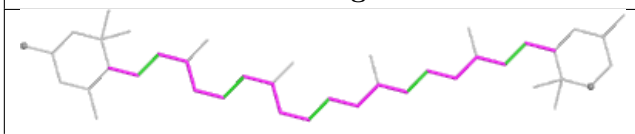
Ligand ZEX 5 617



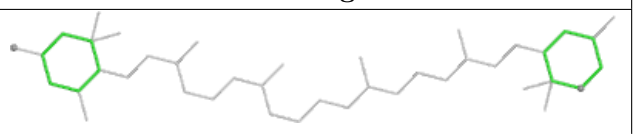
Bond lengths



Bond angles

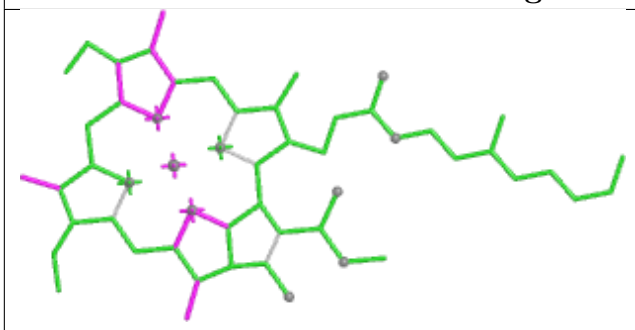


Torsions

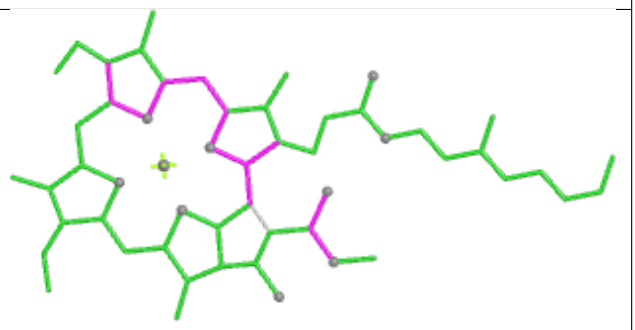


Rings

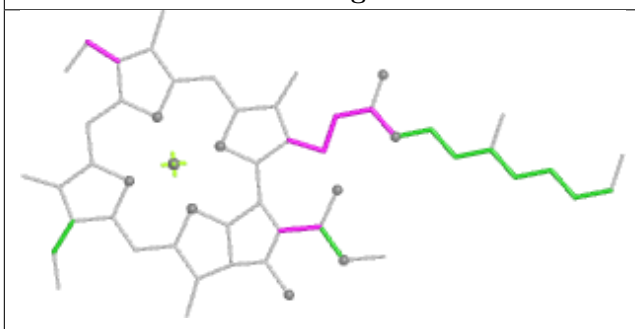
Ligand CLA A 810



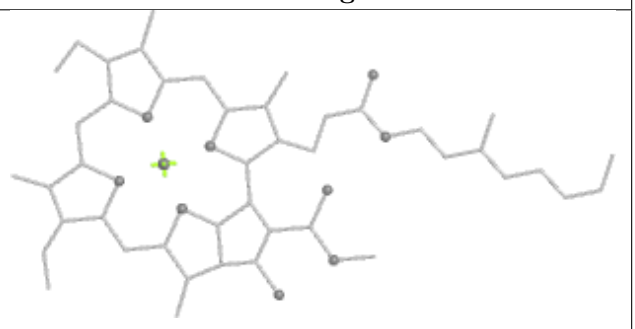
Bond lengths



Bond angles

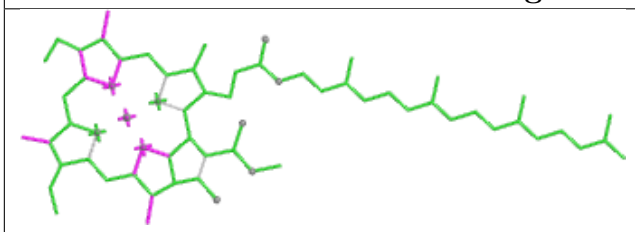


Torsions

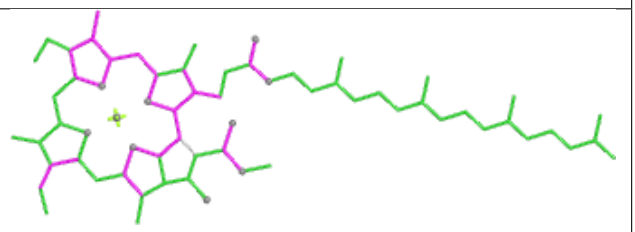


Rings

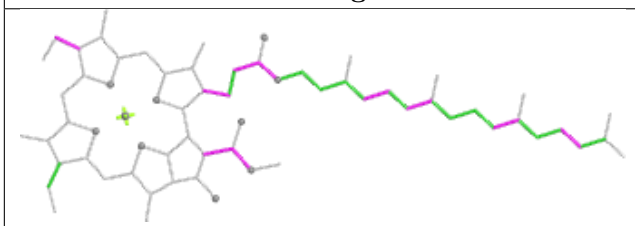
Ligand CLA A 805



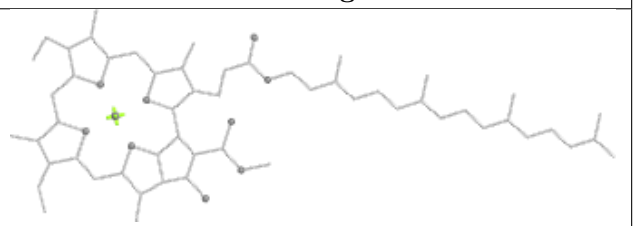
Bond lengths



Bond angles

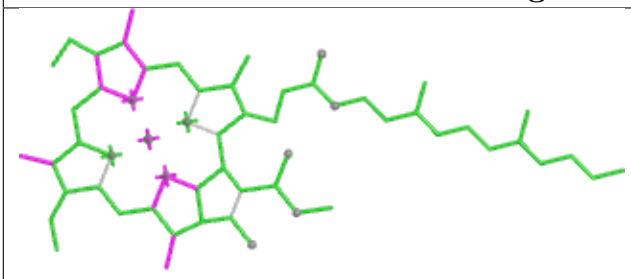


Torsions

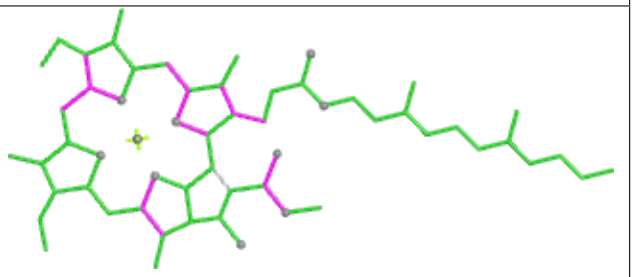


Rings

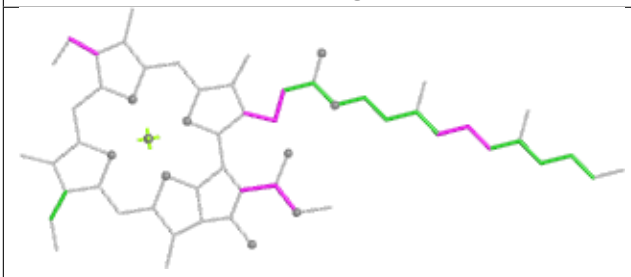
Ligand CLA J 102



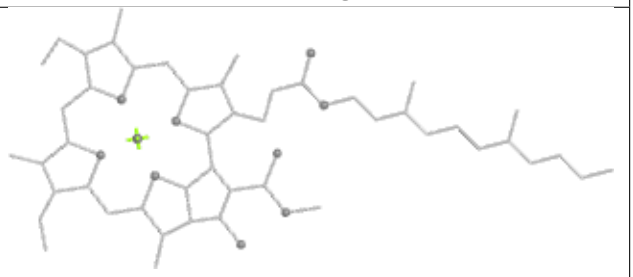
Bond lengths



Bond angles



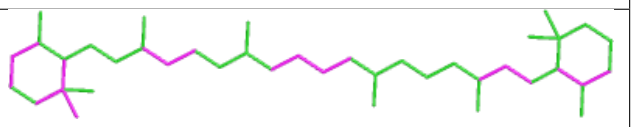
Torsions



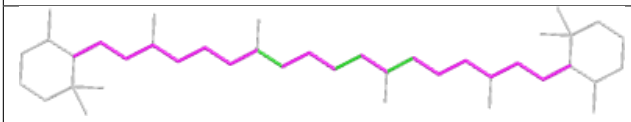
Rings

Ligand BCR B 847

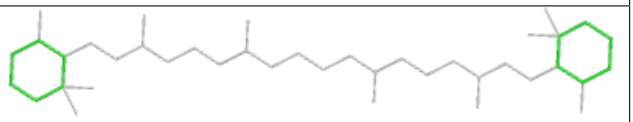
Bond lengths



Bond angles

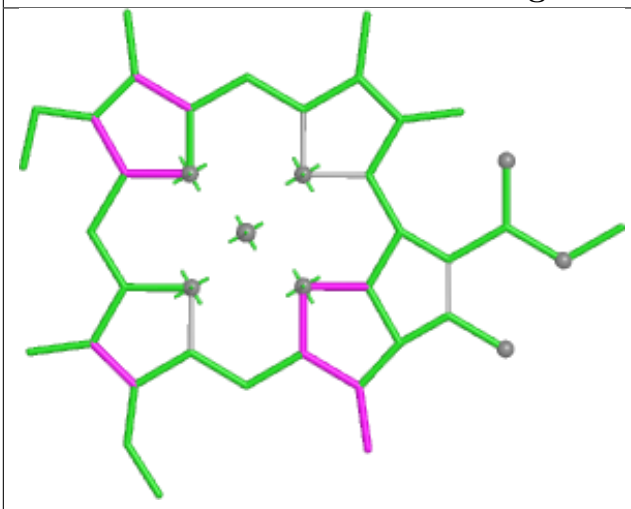


Torsions

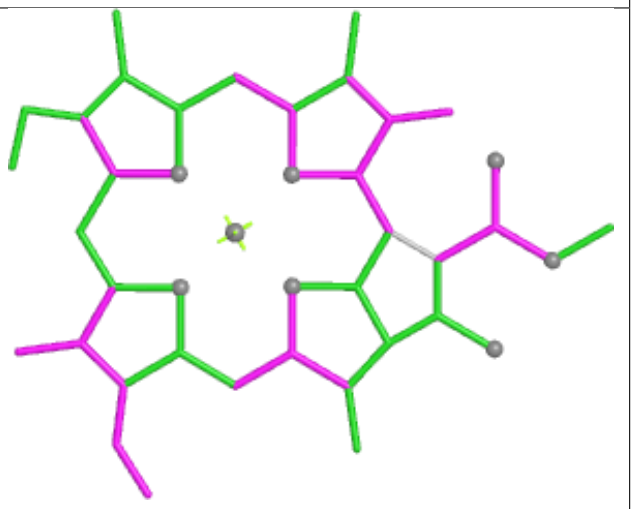


Rings

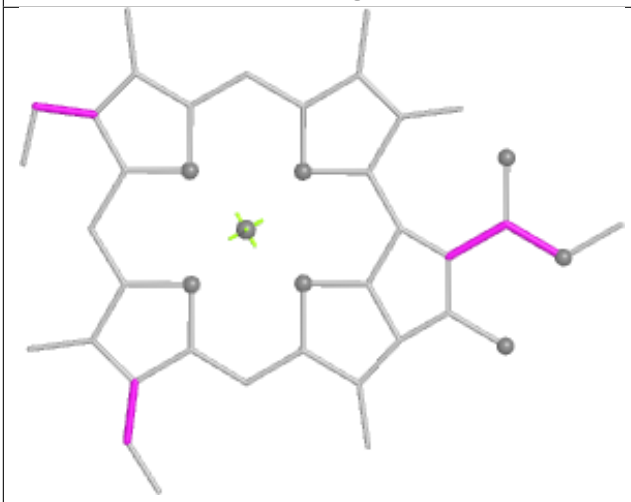
Ligand CLA 5 609



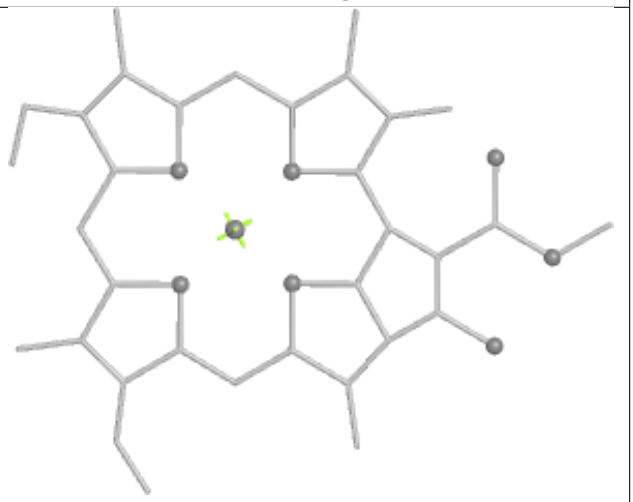
Bond lengths



Bond angles

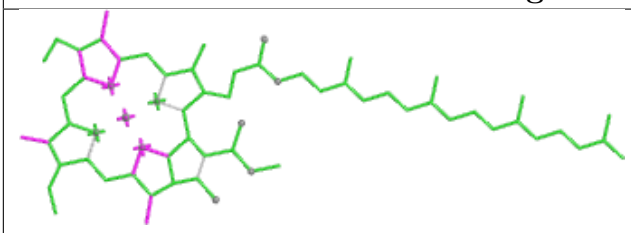


Torsions

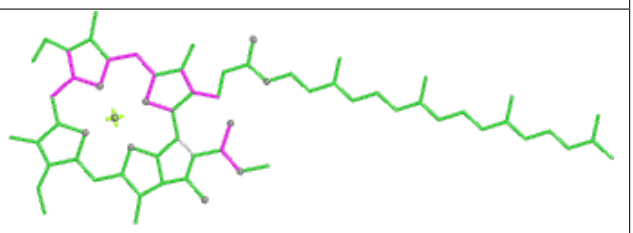


Rings

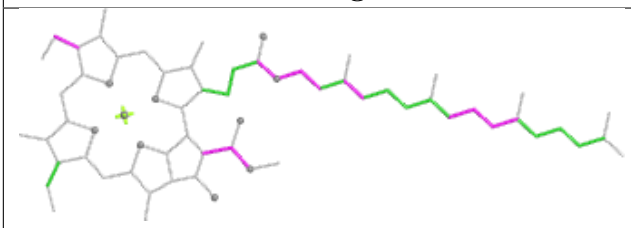
Ligand CLA L 203



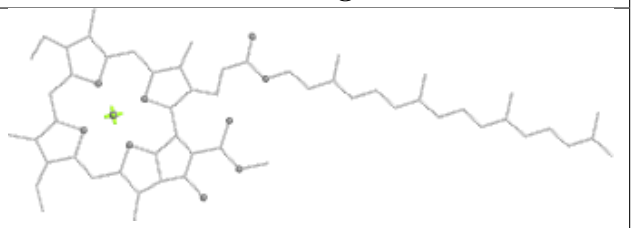
Bond lengths



Bond angles

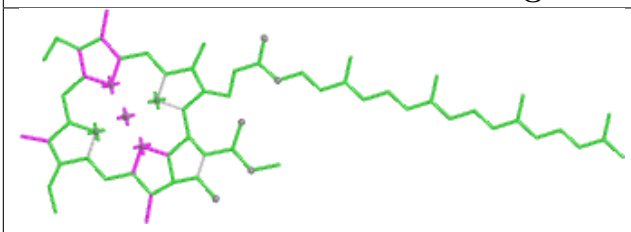


Torsions

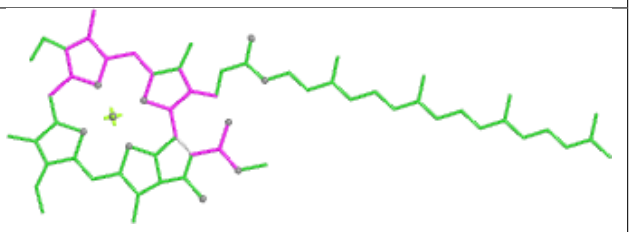


Rings

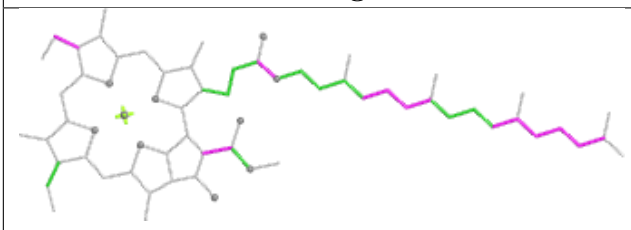
Ligand CLA B 829



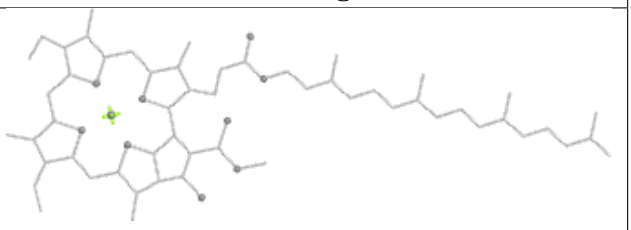
Bond lengths



Bond angles

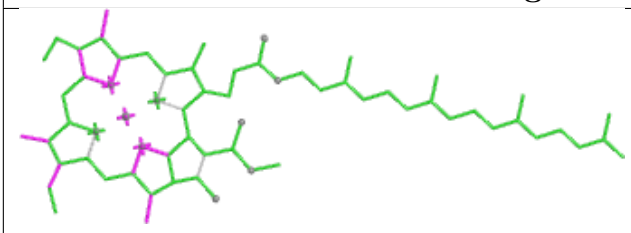


Torsions

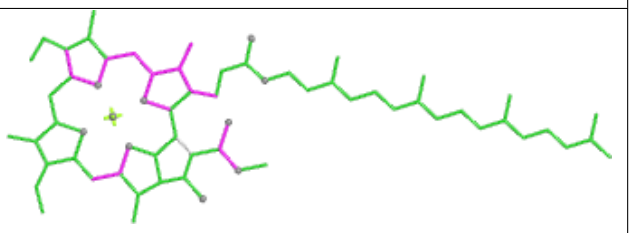


Rings

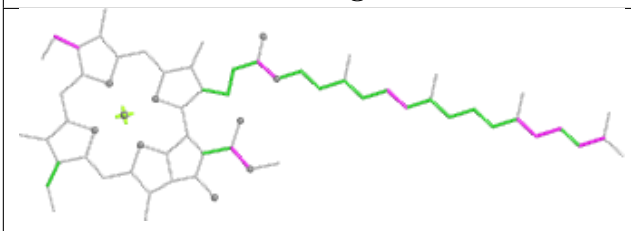
Ligand CLA B 839



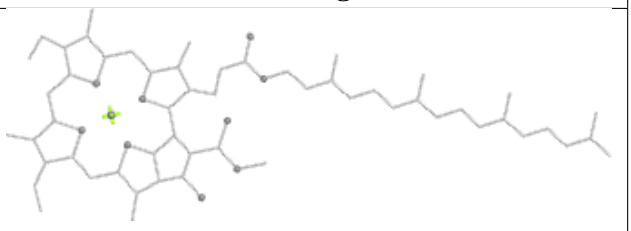
Bond lengths



Bond angles

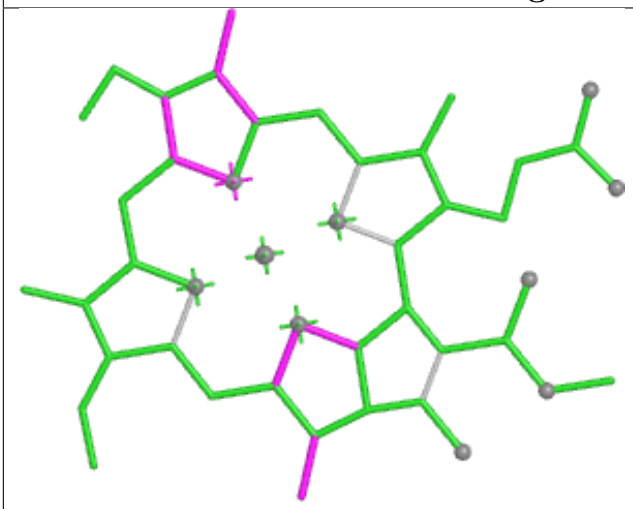


Torsions

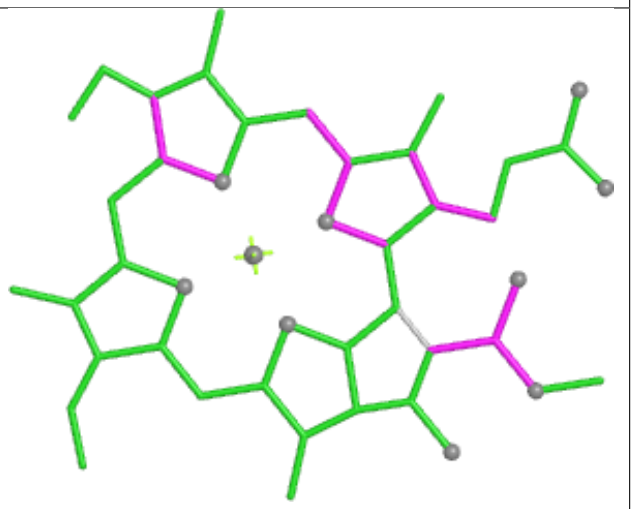


Rings

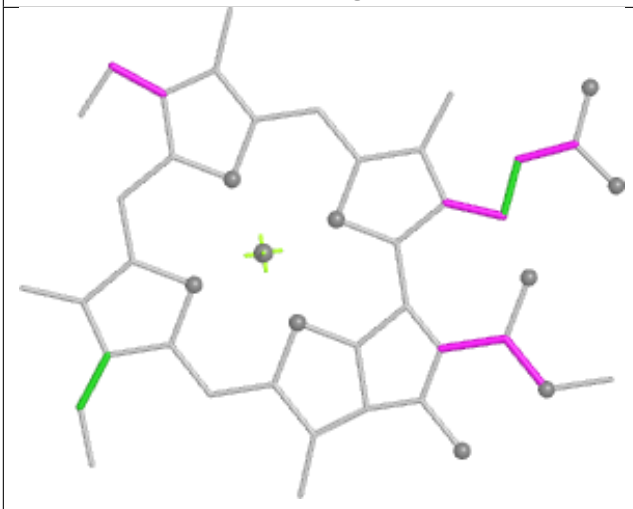
Ligand CLA 5 605



Bond lengths



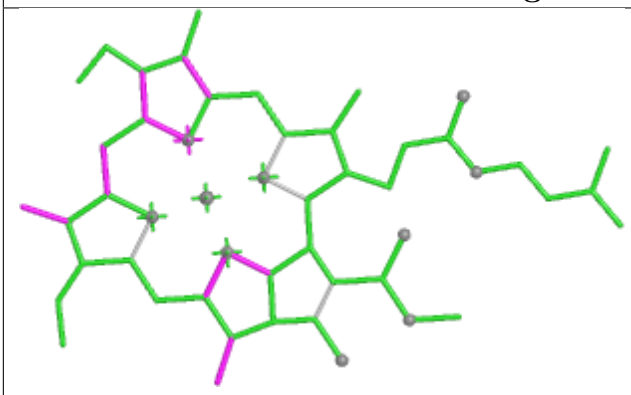
Bond angles



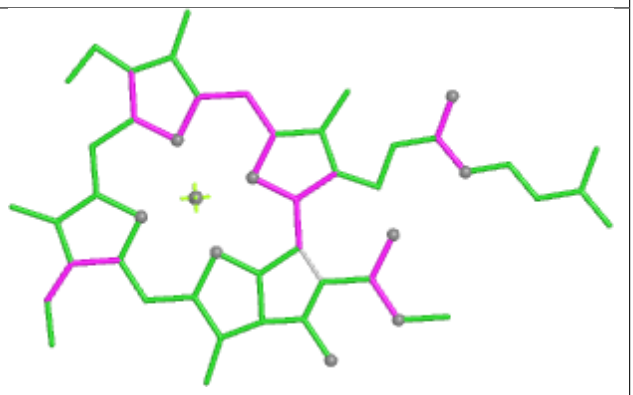
Torsions

Rings

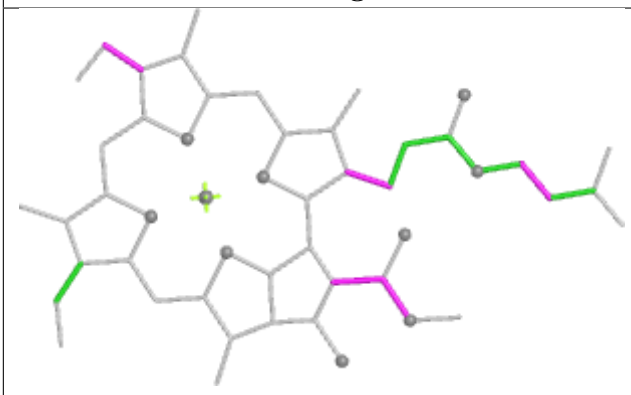
Ligand CLA O 204



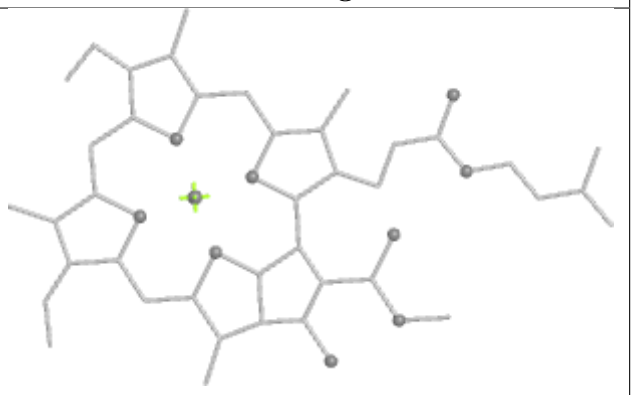
Bond lengths



Bond angles



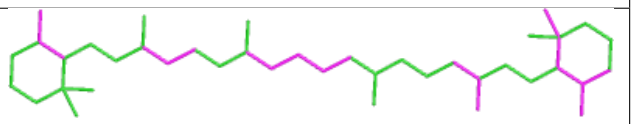
Torsions



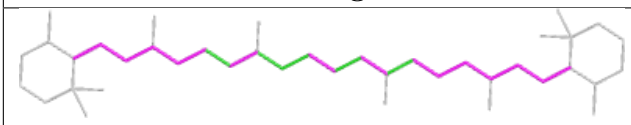
Rings

Ligand BCR B 848

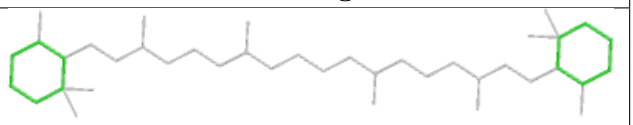
Bond lengths



Bond angles

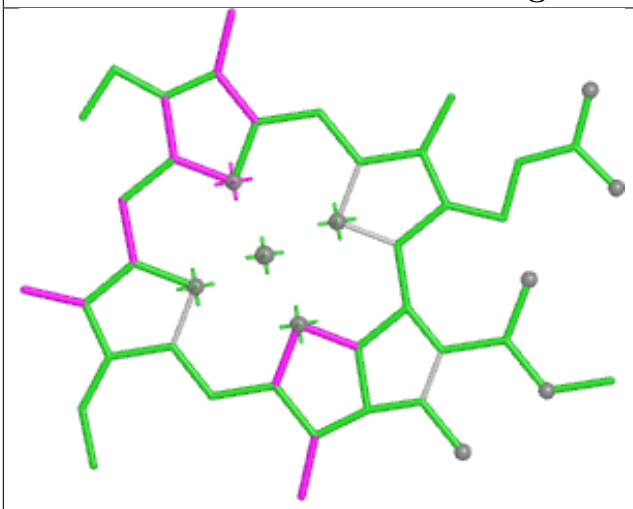


Torsions

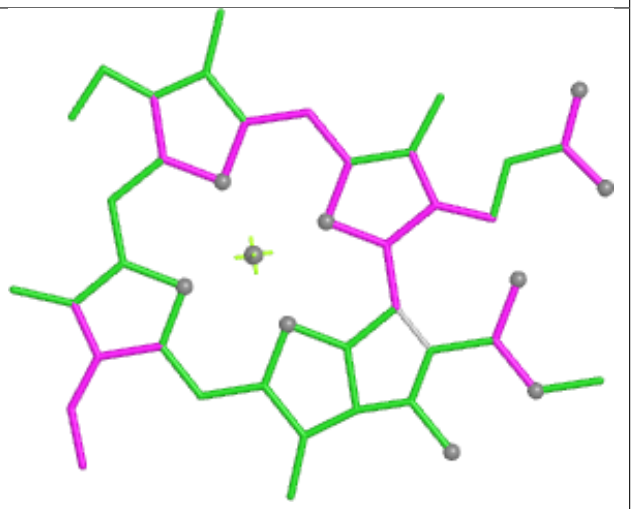


Rings

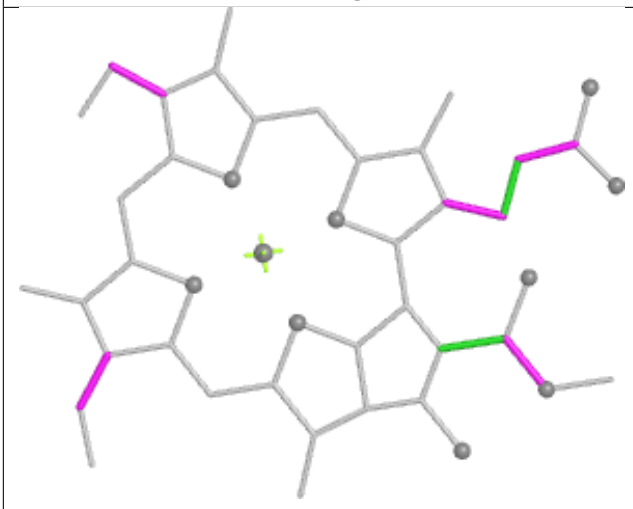
Ligand CLA 5 607



Bond lengths



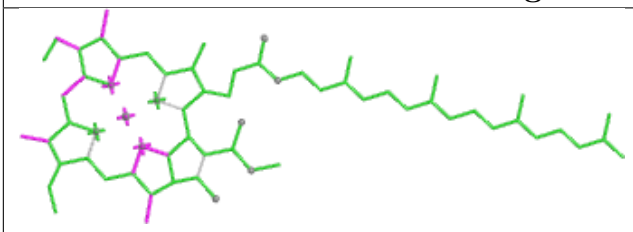
Bond angles



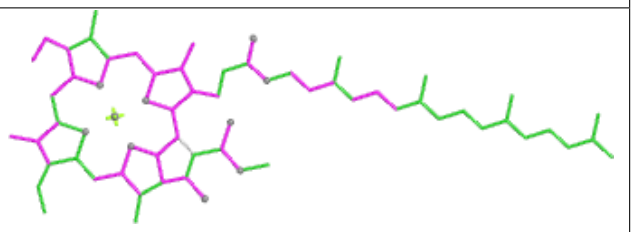
Torsions

Rings

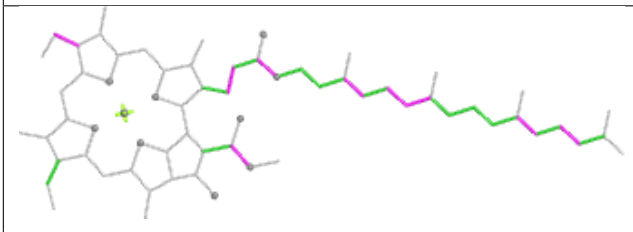
Ligand CLA B 802



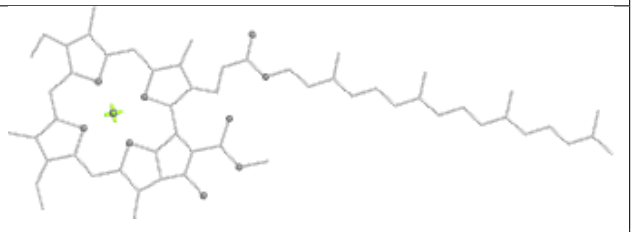
Bond lengths



Bond angles

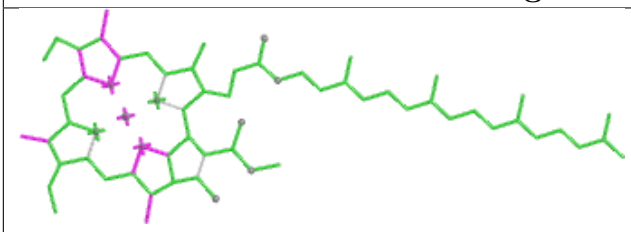


Torsions

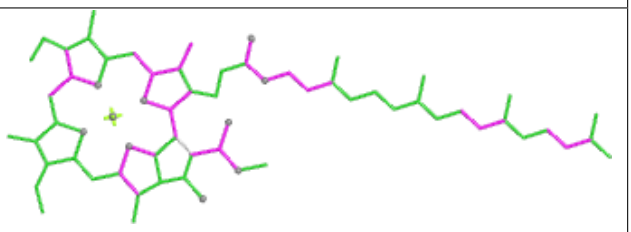


Rings

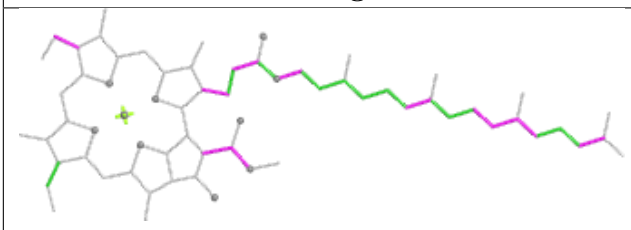
Ligand CLA B 808



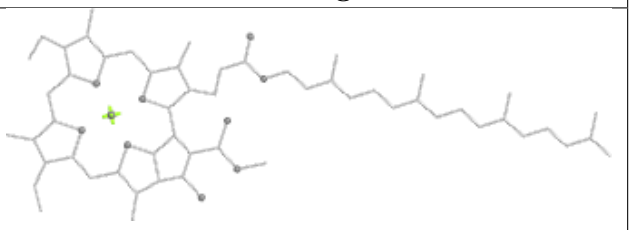
Bond lengths



Bond angles

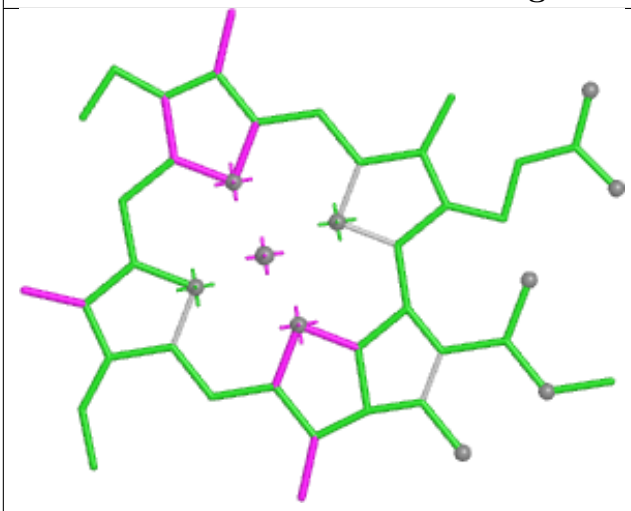


Torsions

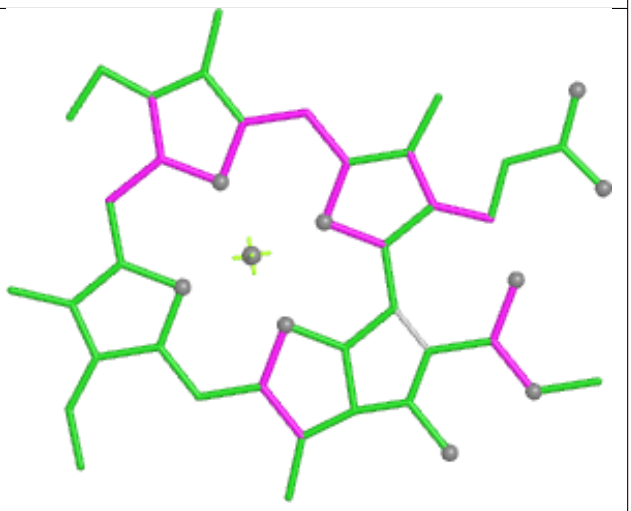


Rings

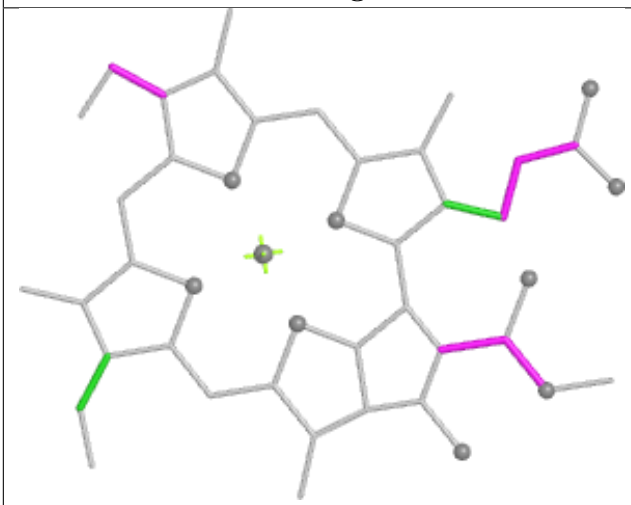
Ligand CLA 1 603



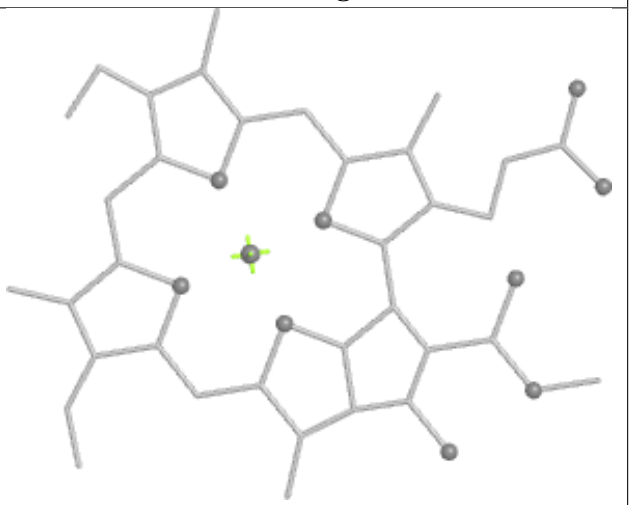
Bond lengths



Bond angles

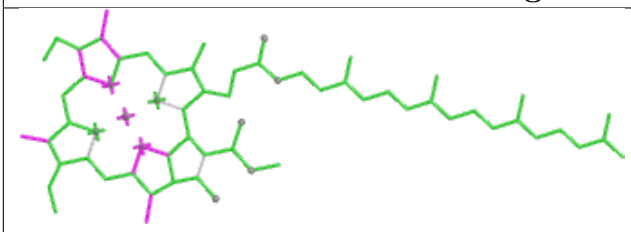


Torsions

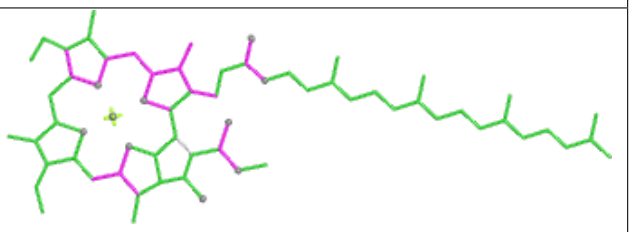


Rings

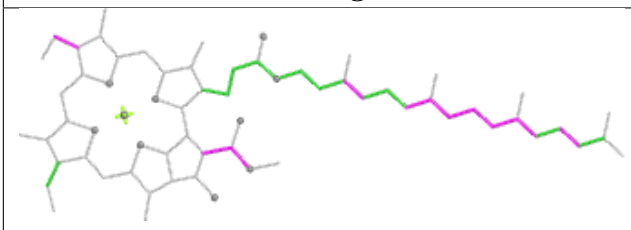
Ligand CLA B 836



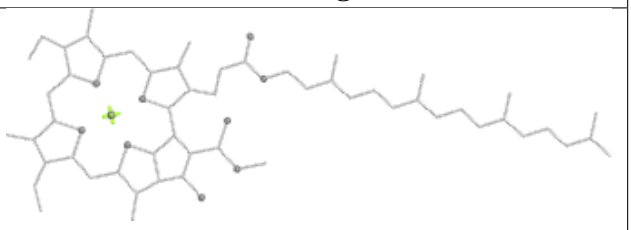
Bond lengths



Bond angles



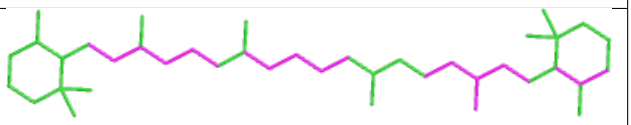
Torsions



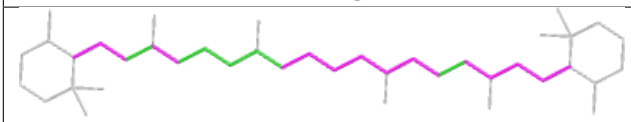
Rings

Ligand BCR L 201

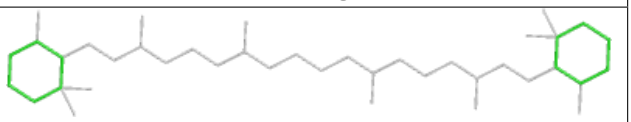
Bond lengths



Bond angles

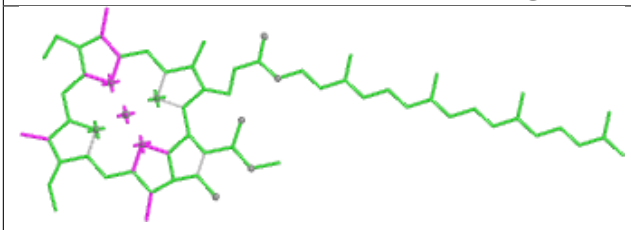


Torsions

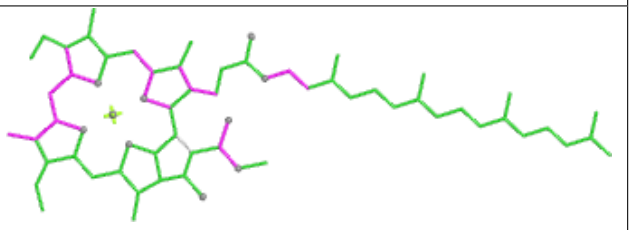


Rings

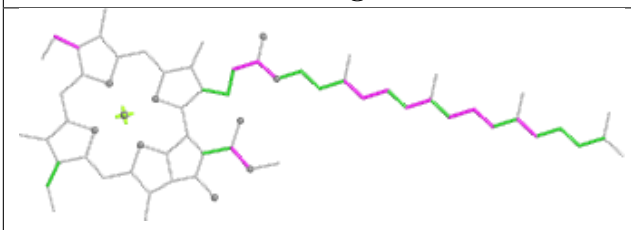
Ligand CLA B 809



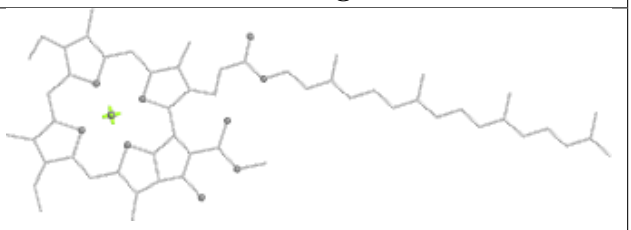
Bond lengths



Bond angles

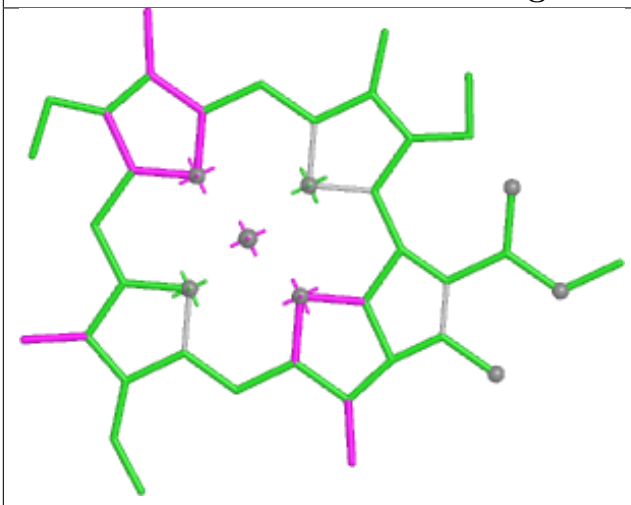


Torsions

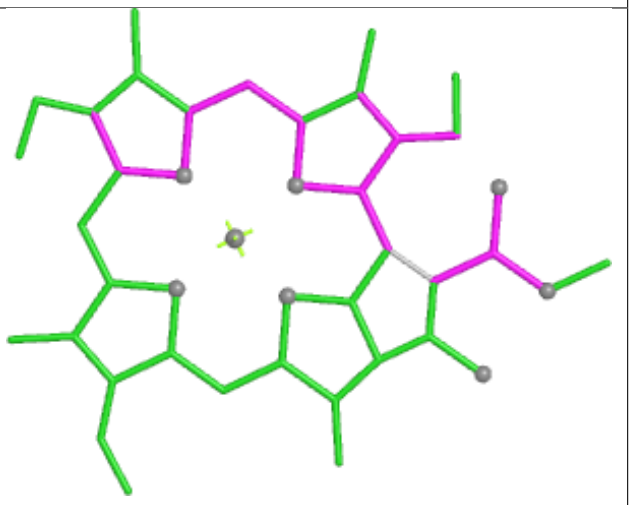


Rings

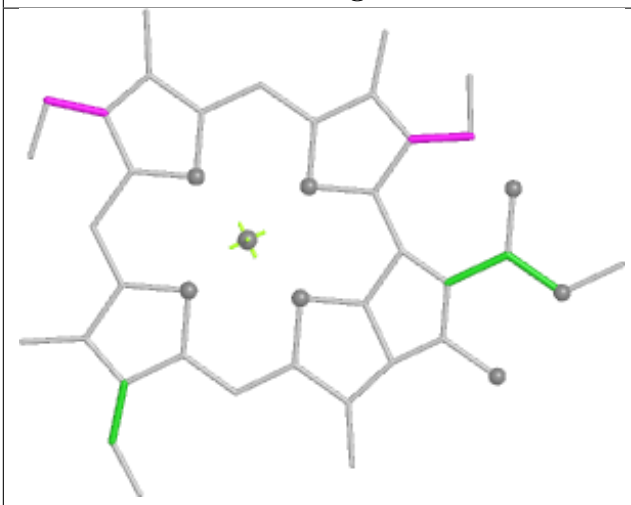
Ligand CLA 3 211



Bond lengths



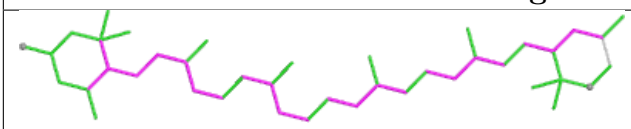
Bond angles



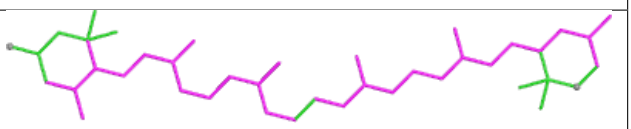
Torsions

Rings

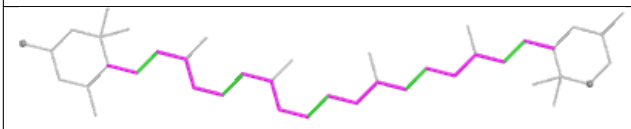
Ligand ZEX 3 201



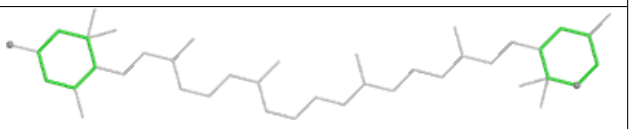
Bond lengths



Bond angles

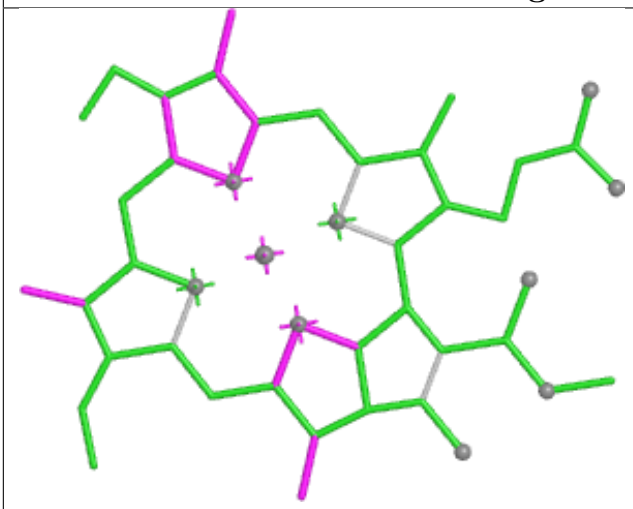


Torsions

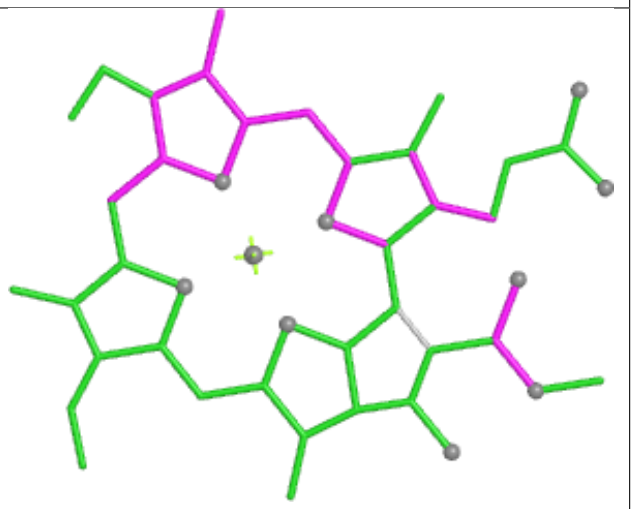


Rings

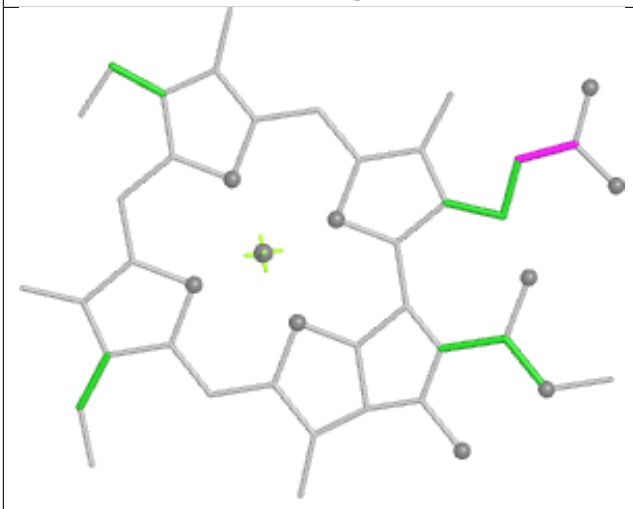
Ligand CLA 2 603



Bond lengths



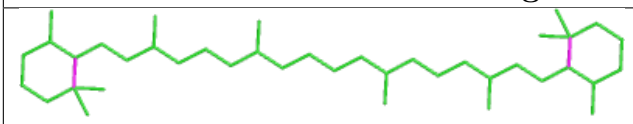
Bond angles



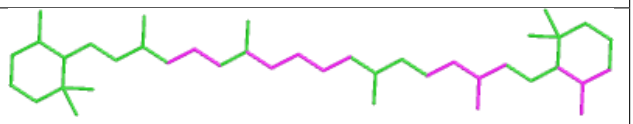
Torsions

Rings

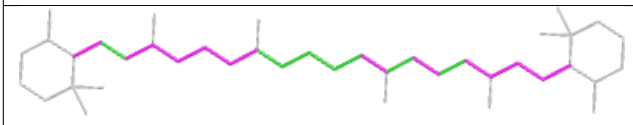
Ligand BCR A 846



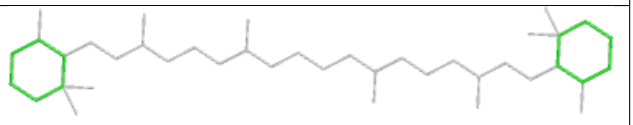
Bond lengths



Bond angles

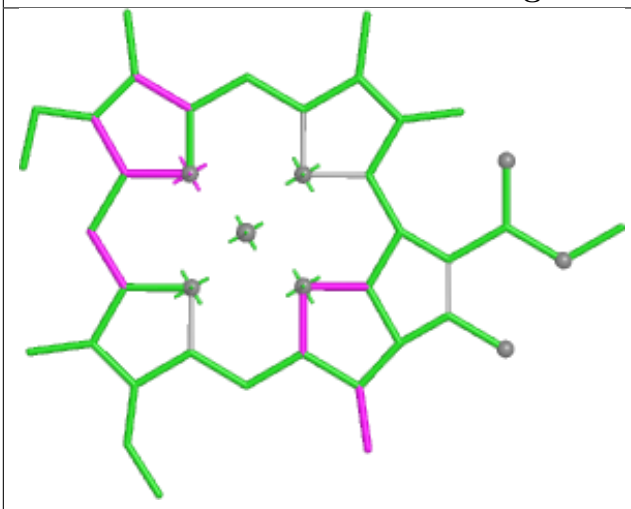


Torsions

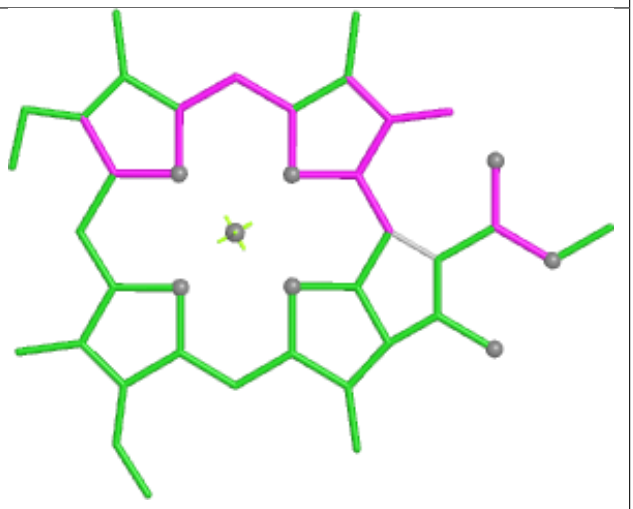


Rings

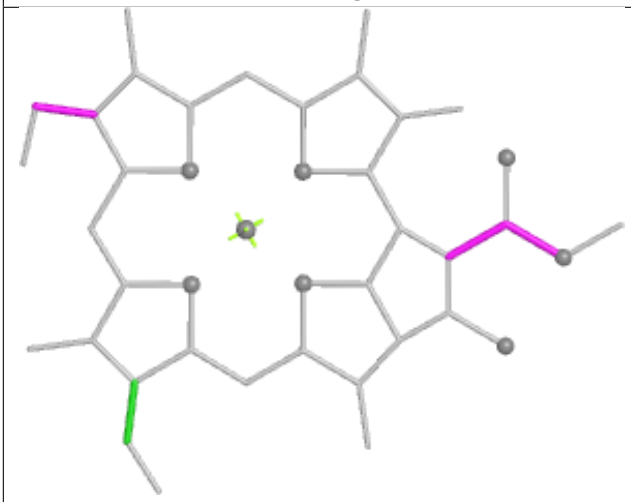
Ligand CLA O 203



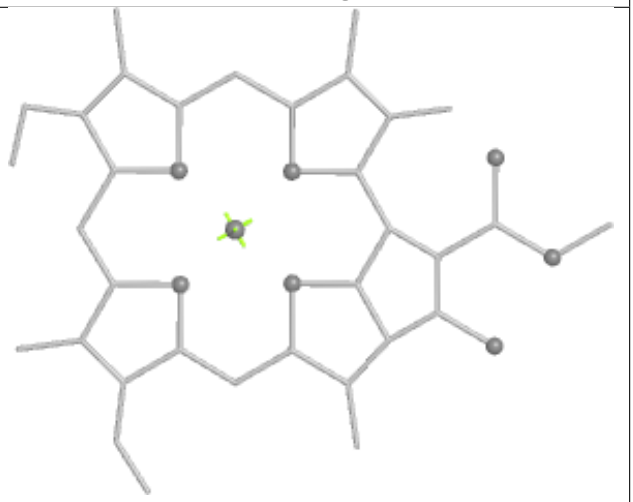
Bond lengths



Bond angles



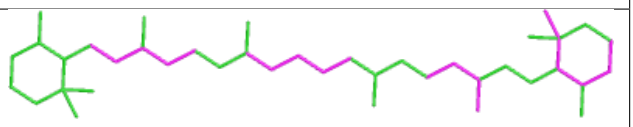
Torsions



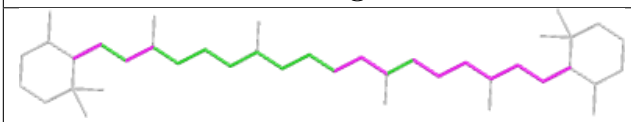
Rings

Ligand BCR J 104

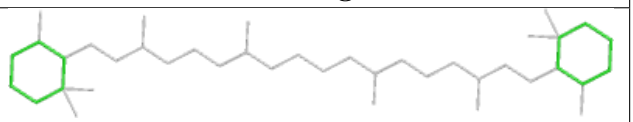
Bond lengths



Bond angles

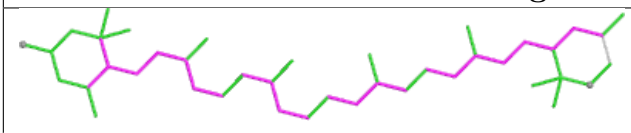


Torsions

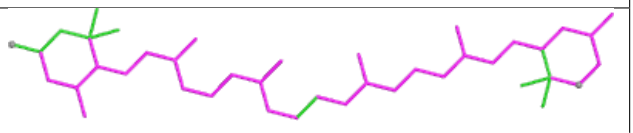


Rings

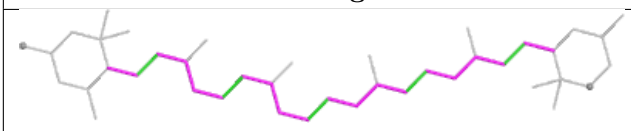
Ligand ZEX 5 614



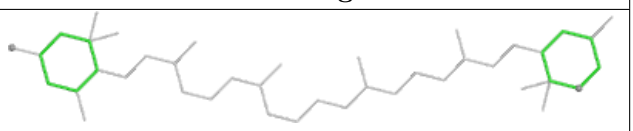
Bond lengths



Bond angles

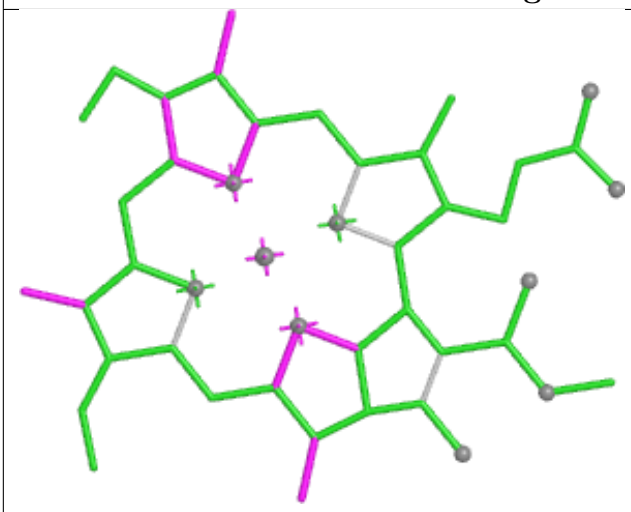


Torsions

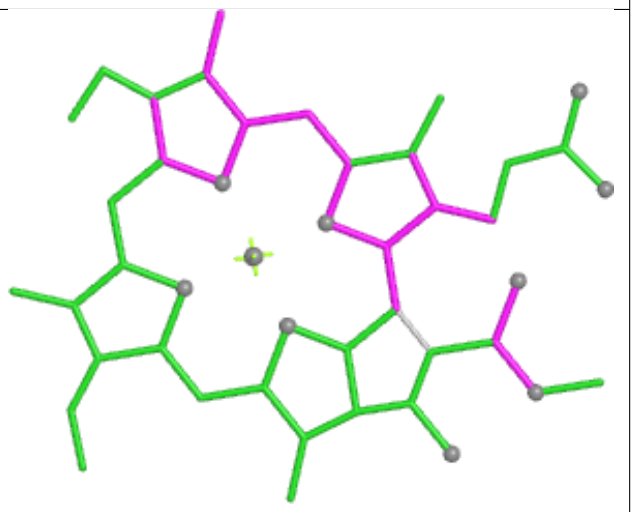


Rings

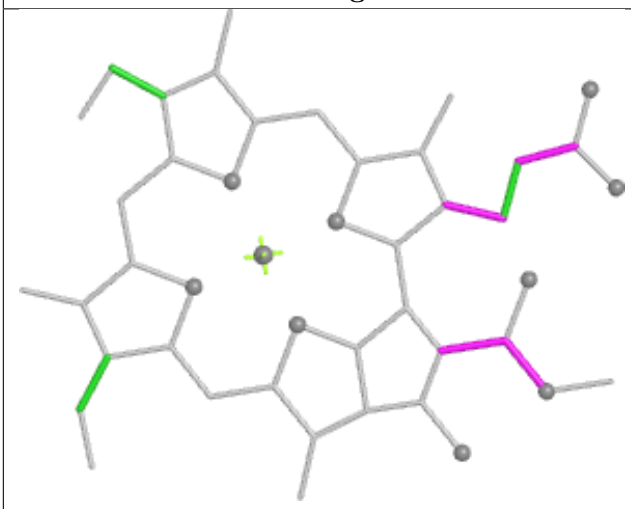
Ligand CLA A 834



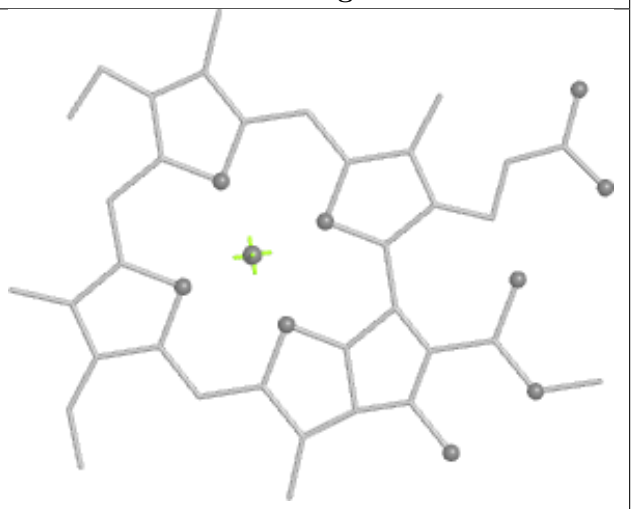
Bond lengths



Bond angles

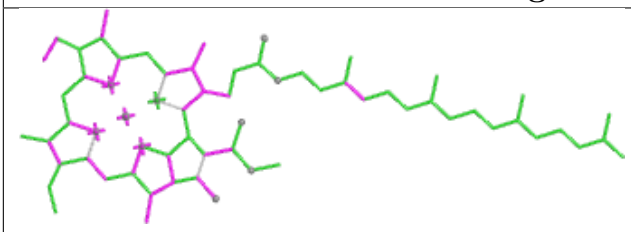


Torsions

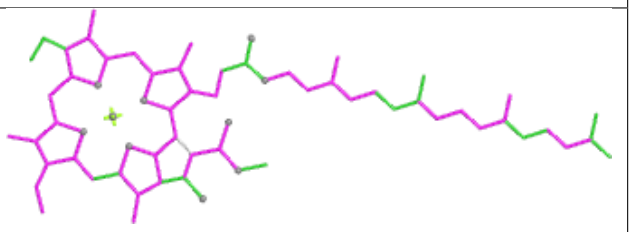


Rings

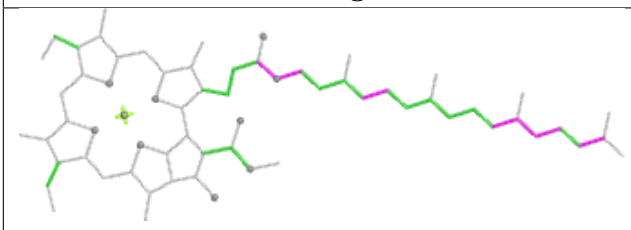
Ligand CL0 A 801



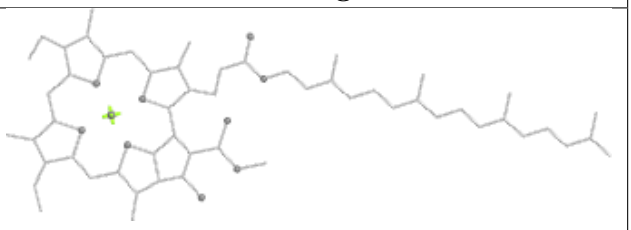
Bond lengths



Bond angles

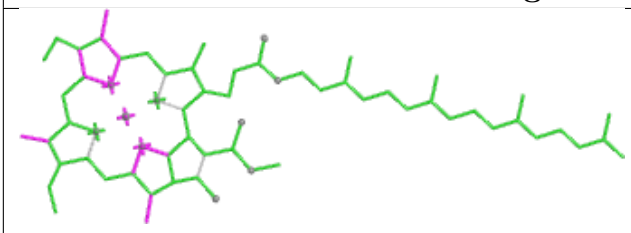


Torsions

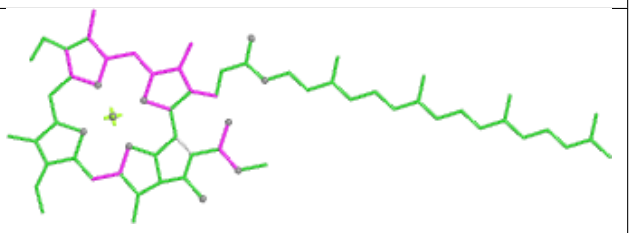


Rings

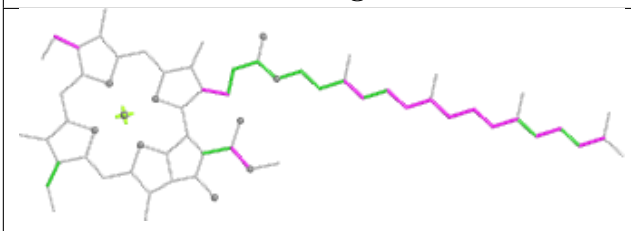
Ligand CLA A 833



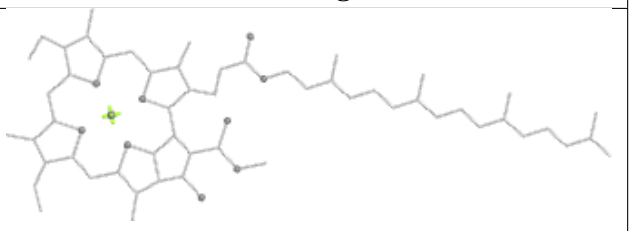
Bond lengths



Bond angles

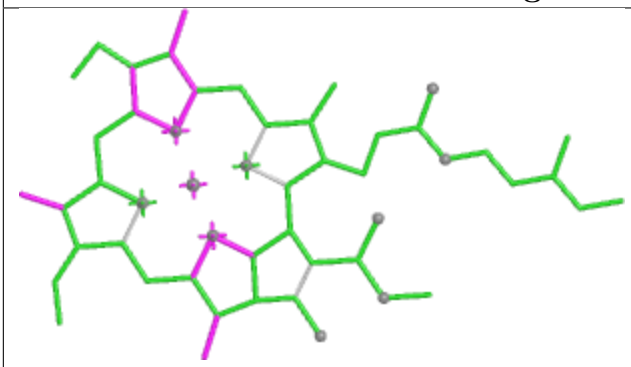


Torsions

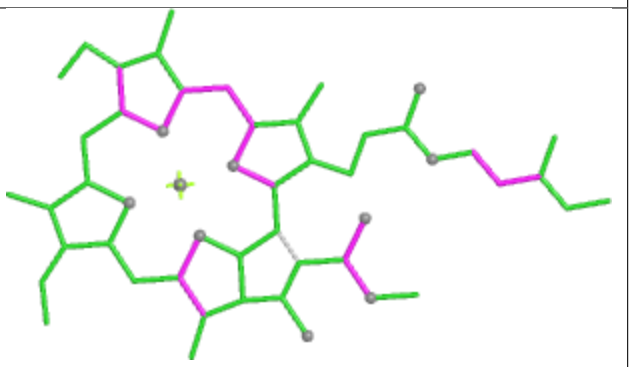


Rings

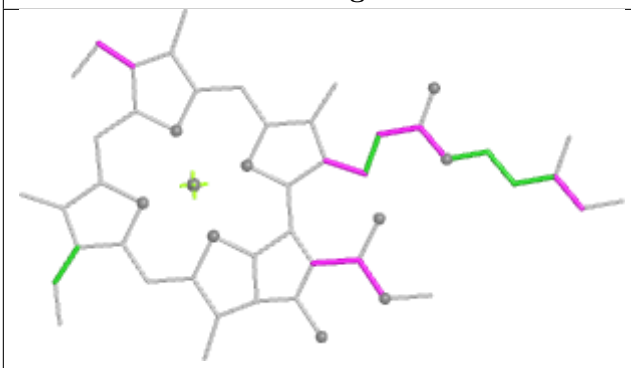
Ligand CLA A 821



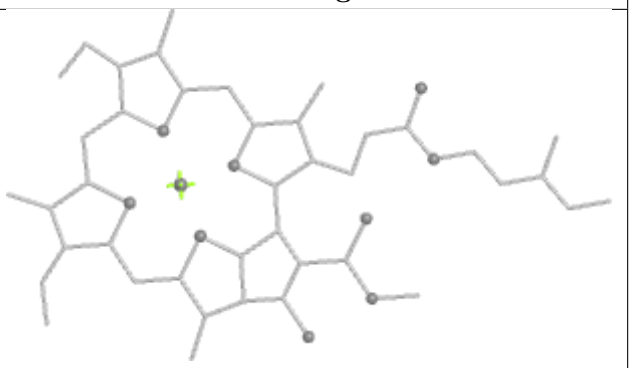
Bond lengths



Bond angles

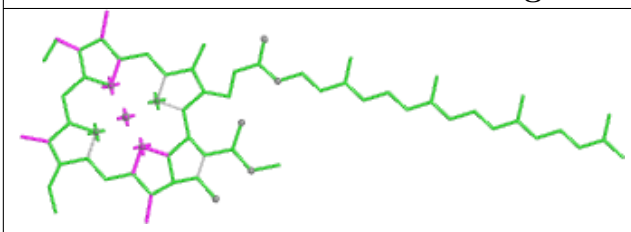


Torsions

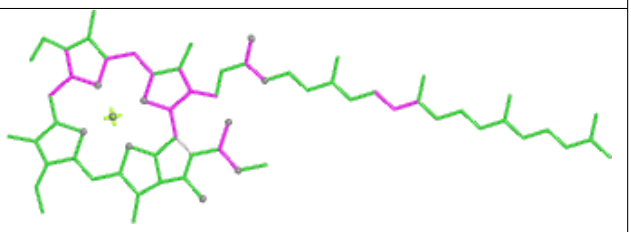


Rings

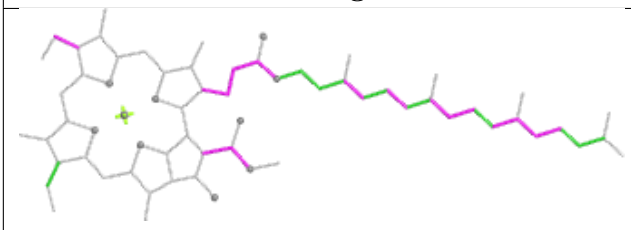
Ligand CLA B 830



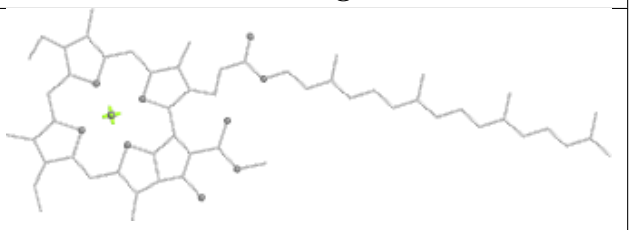
Bond lengths



Bond angles

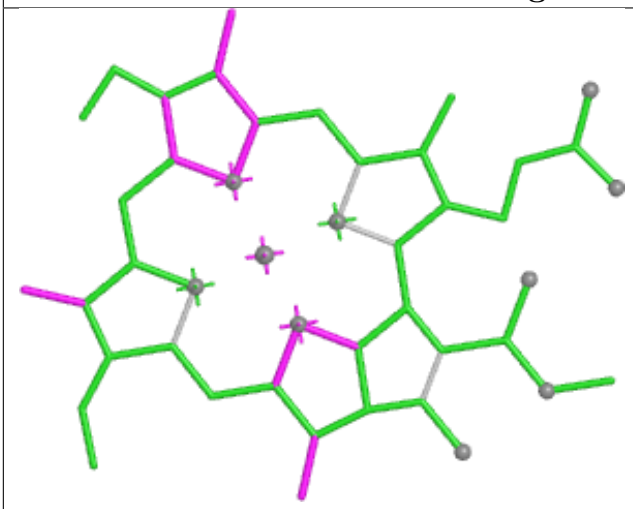


Torsions

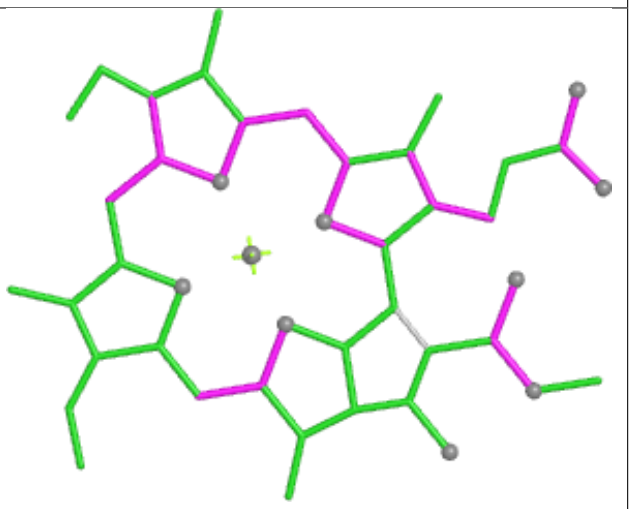


Rings

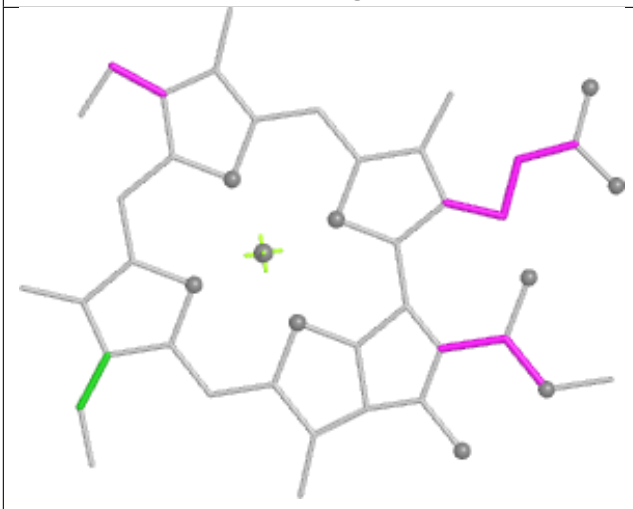
Ligand CLA 2 606



Bond lengths



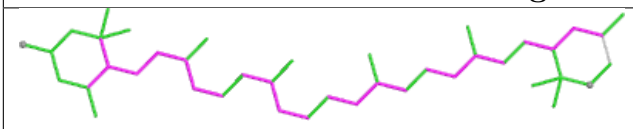
Bond angles



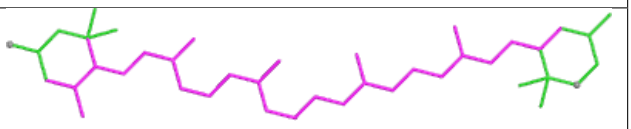
Torsions

Rings

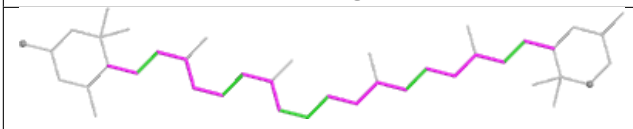
Ligand ZEX 2 617



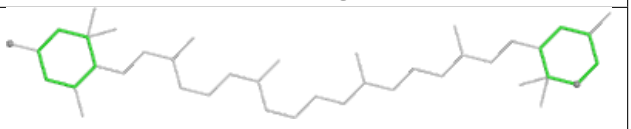
Bond lengths



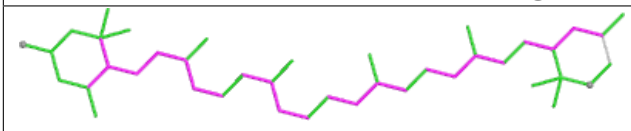
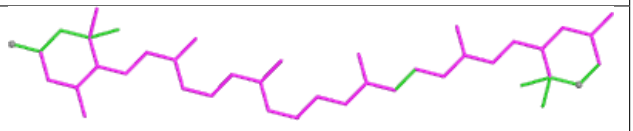
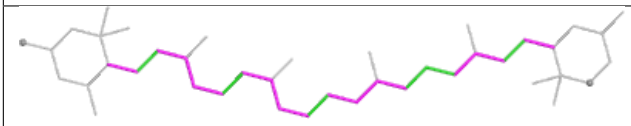
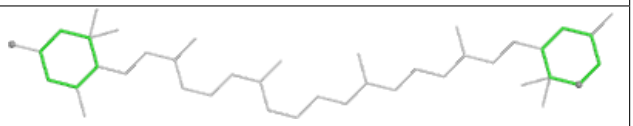
Bond angles

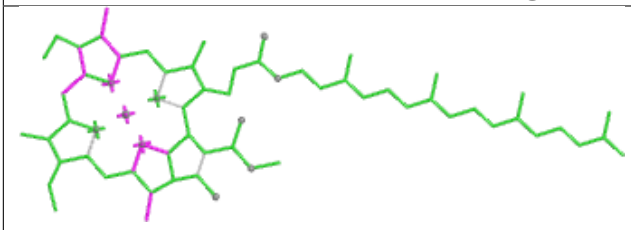
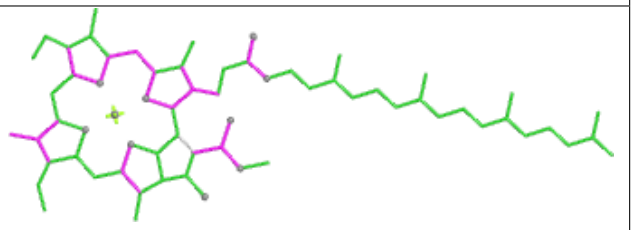
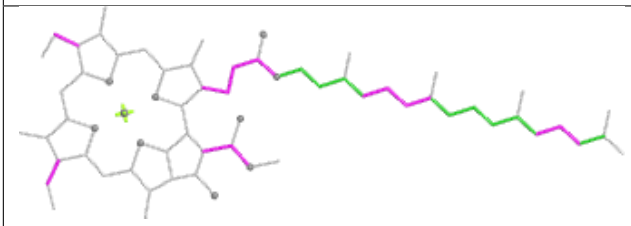
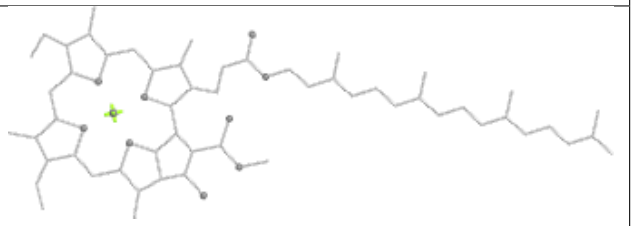


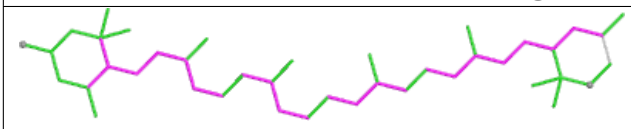
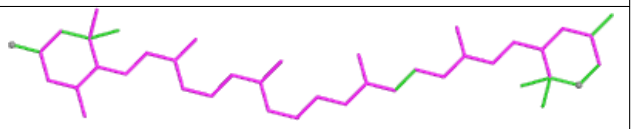
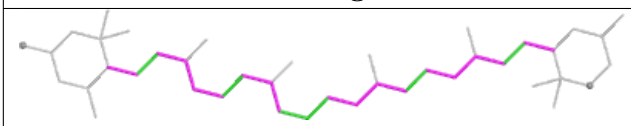
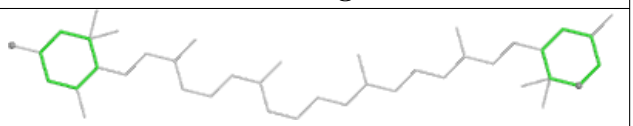
Torsions



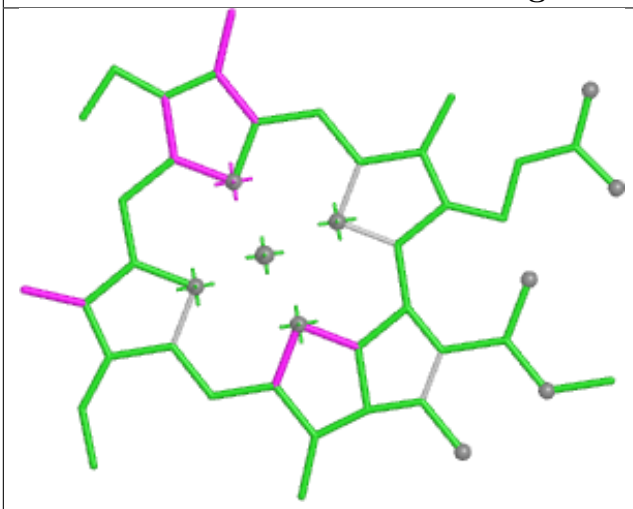
Rings

Ligand ZEX 4 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

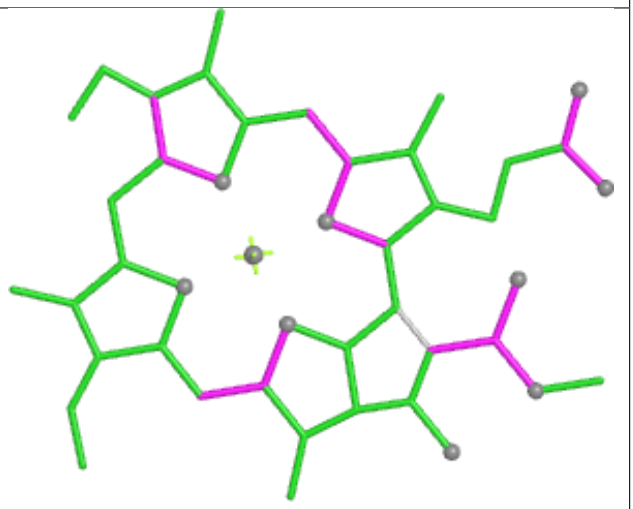
Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZEX 4 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

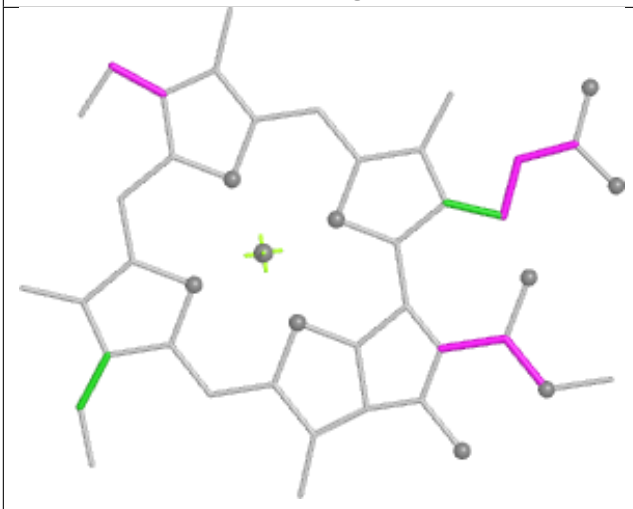
Ligand CLA 2 601



Bond lengths



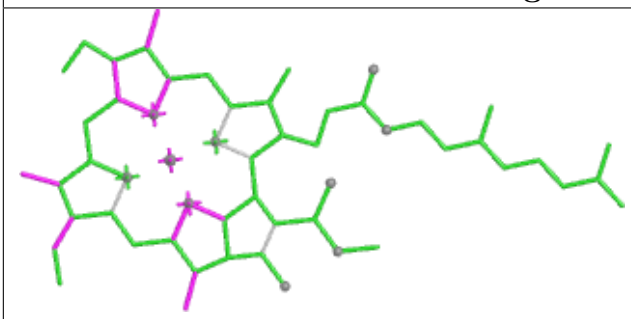
Bond angles



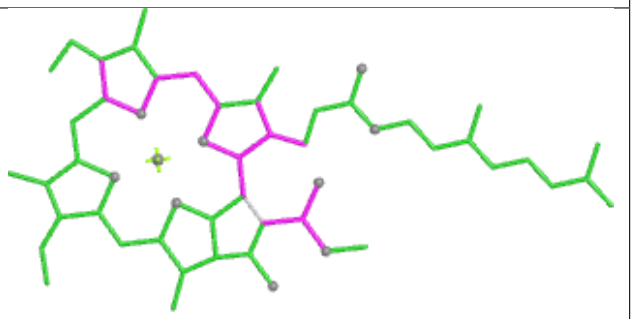
Torsions

Rings

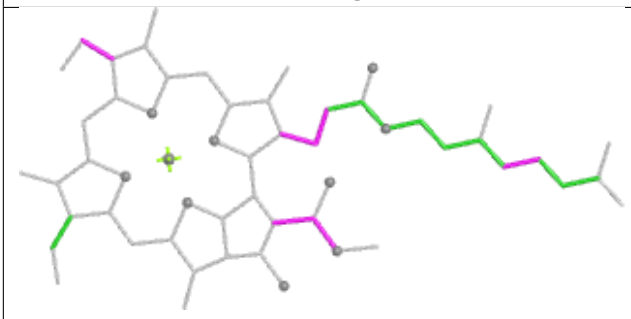
Ligand CLA A 822



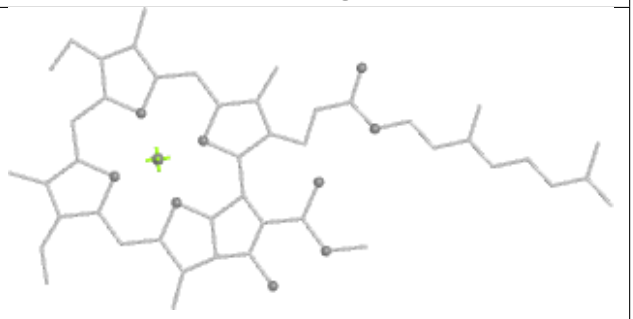
Bond lengths



Bond angles

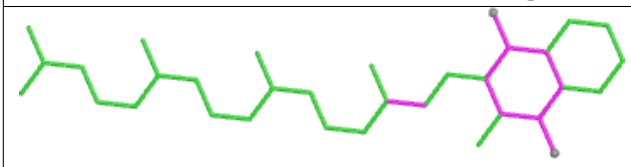


Torsions

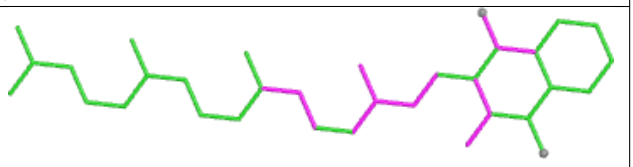


Rings

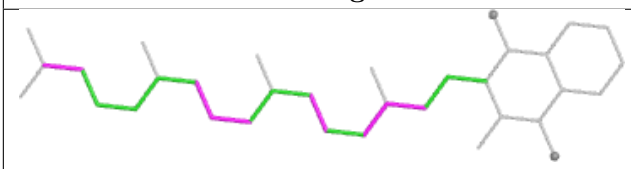
Ligand PQN B 844



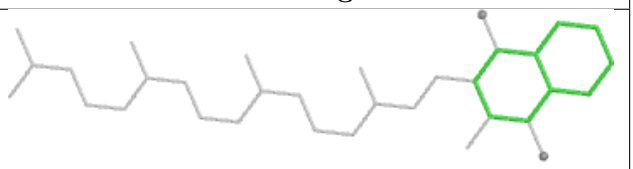
Bond lengths



Bond angles

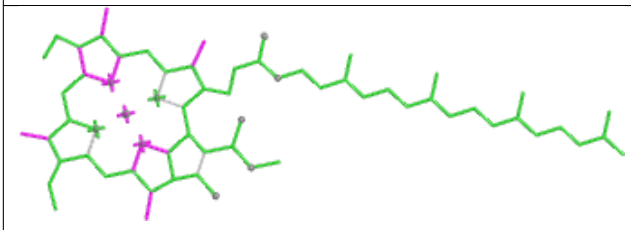


Torsions

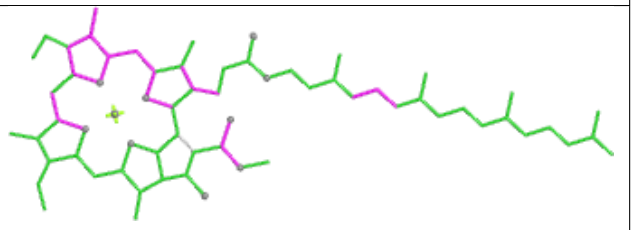


Rings

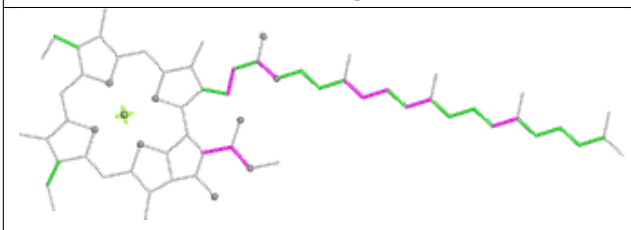
Ligand CLA A 819



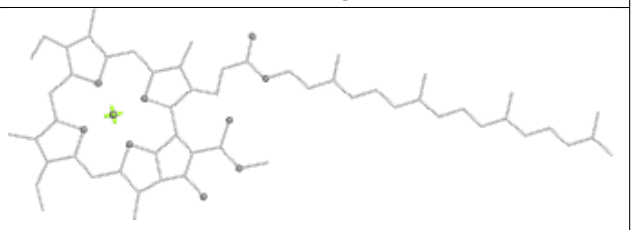
Bond lengths



Bond angles

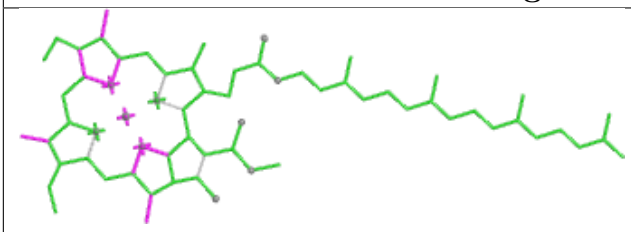


Torsions

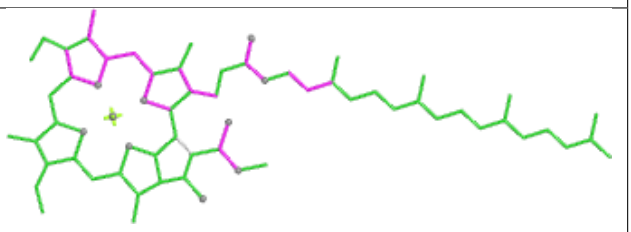


Rings

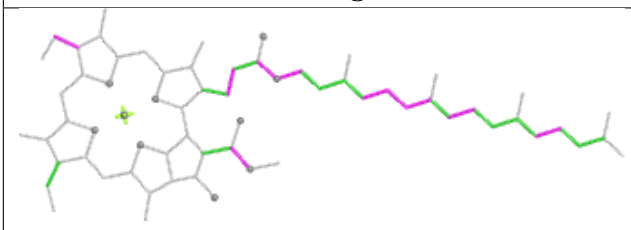
Ligand CLA A 838



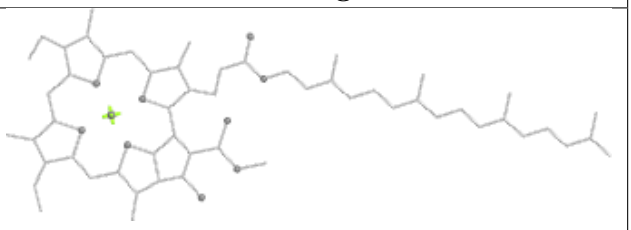
Bond lengths



Bond angles

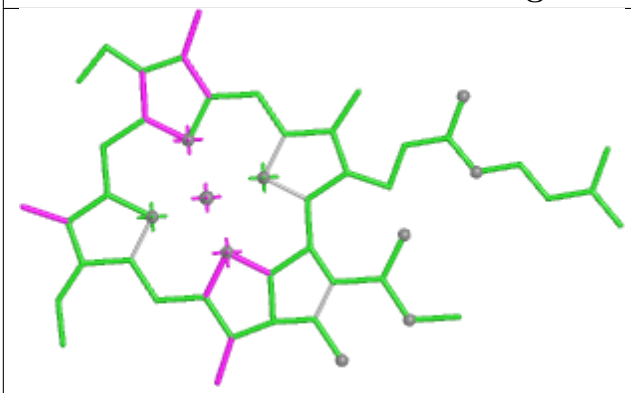


Torsions

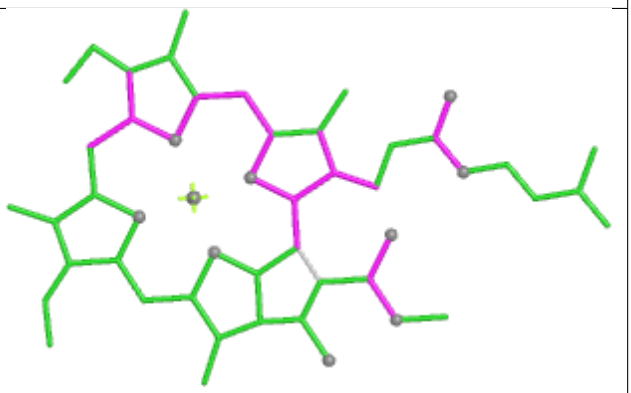


Rings

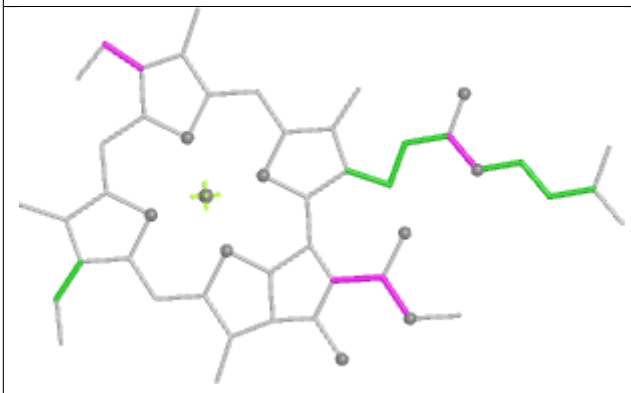
Ligand CLA L 204



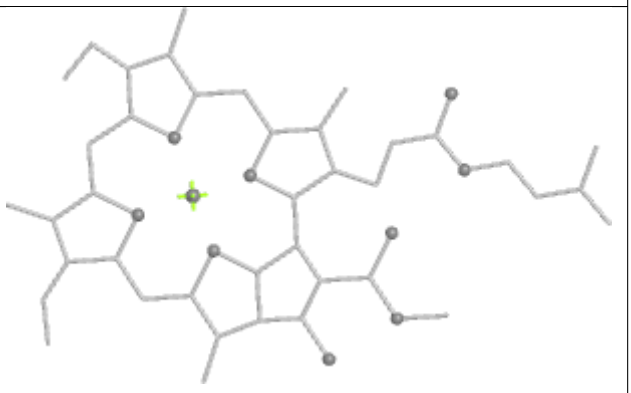
Bond lengths



Bond angles

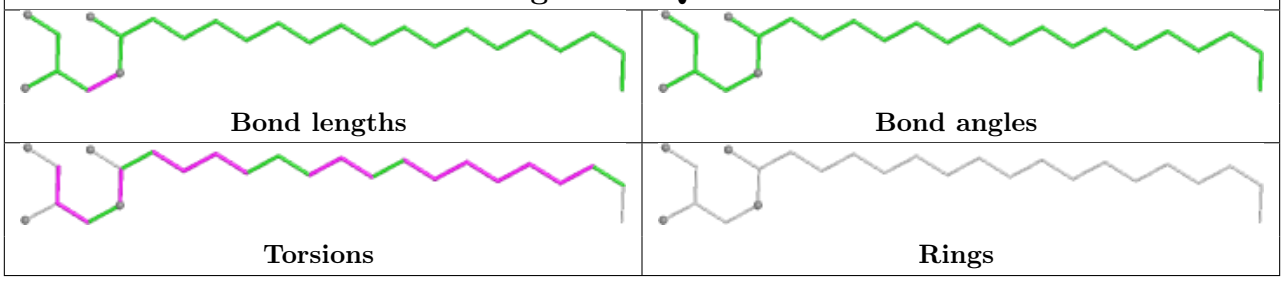


Torsions

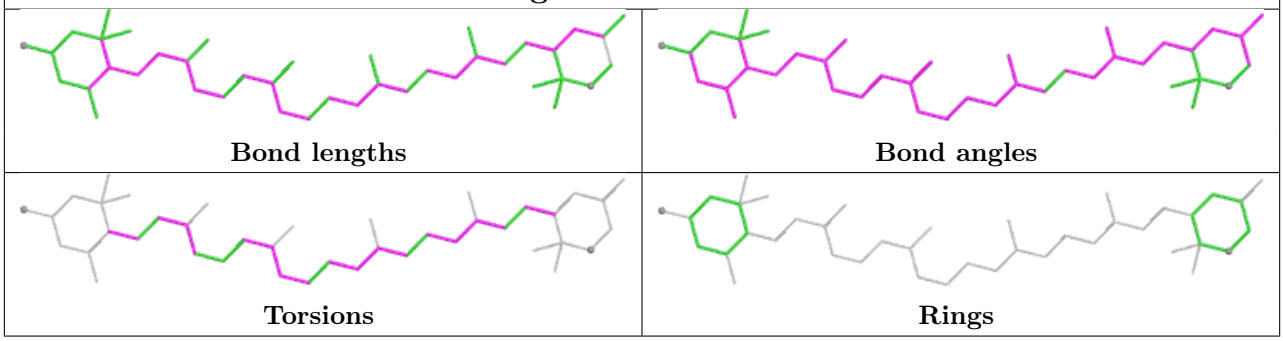


Rings

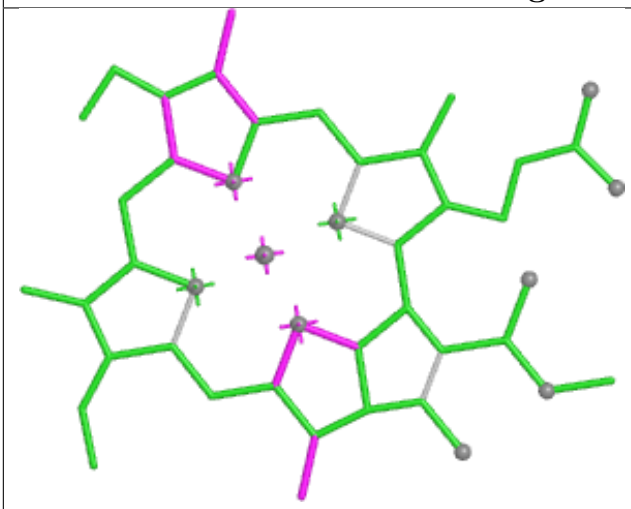
Ligand 3XQ J 106



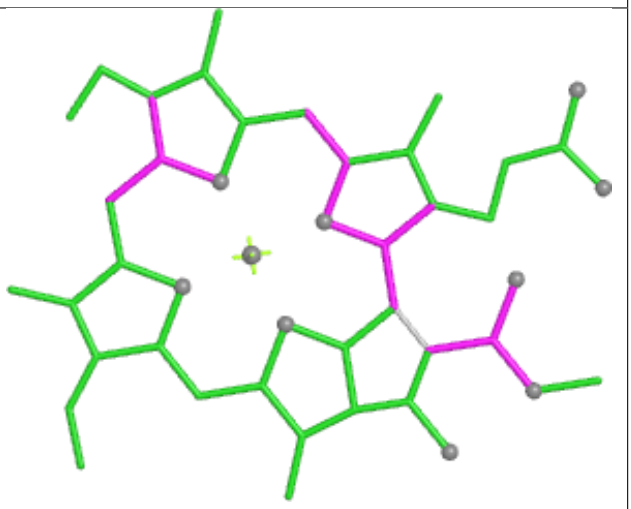
Ligand ZEX 3 216



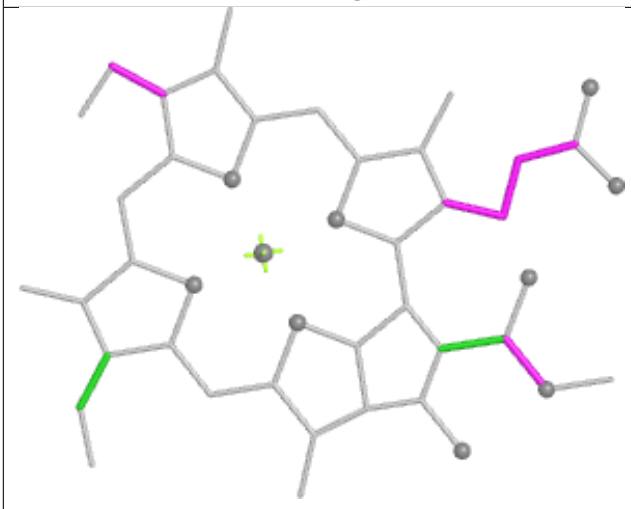
Ligand CLA 5 604



Bond lengths



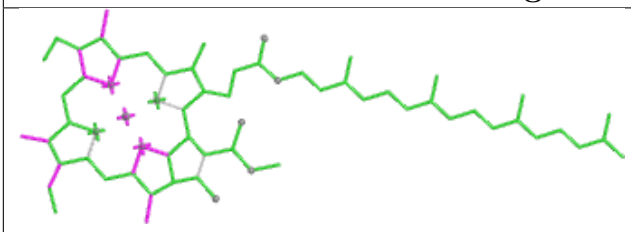
Bond angles



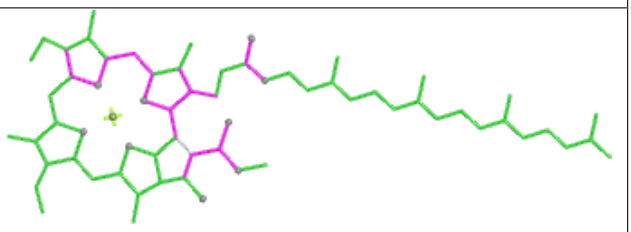
Torsions

Rings

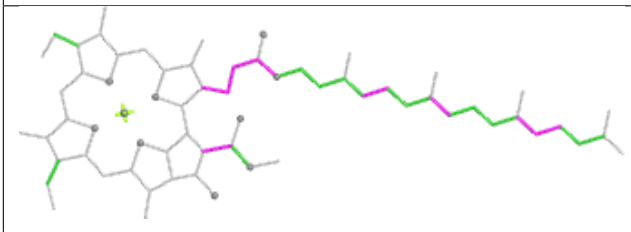
Ligand CLA B 813



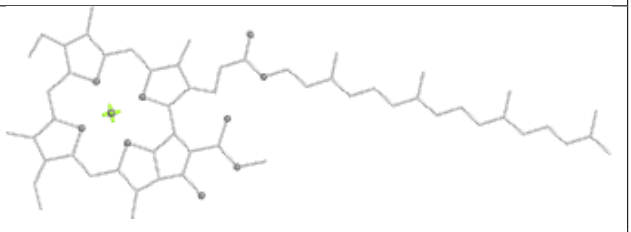
Bond lengths



Bond angles

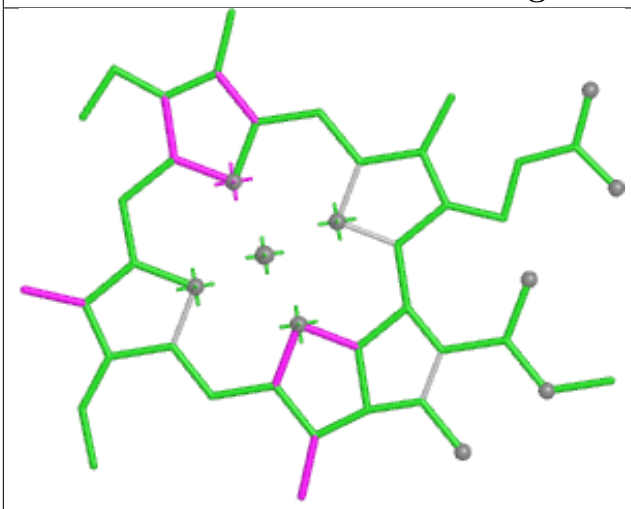


Torsions

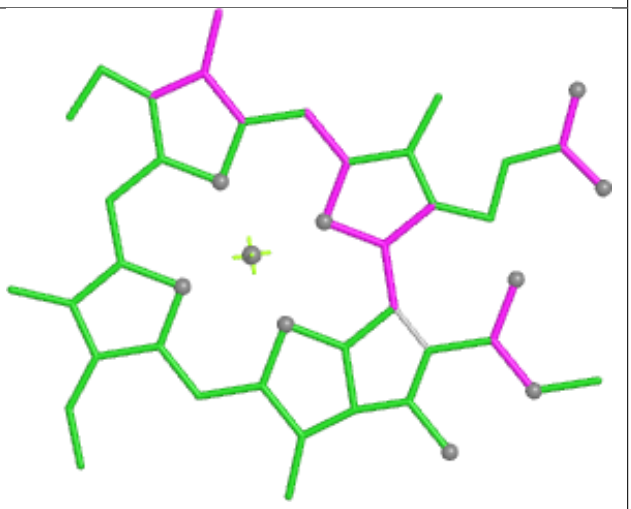


Rings

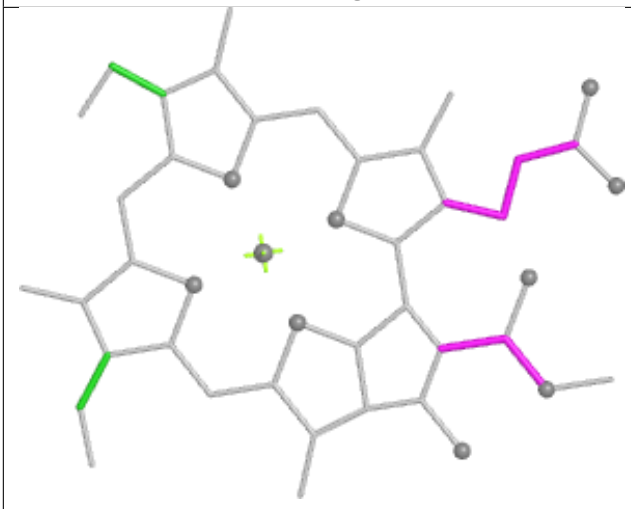
Ligand CLA 5 610



Bond lengths



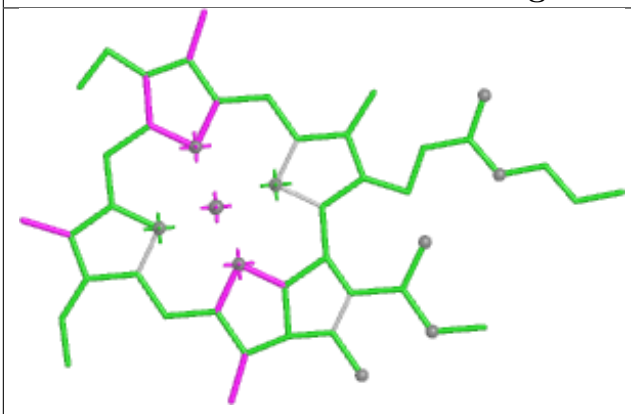
Bond angles



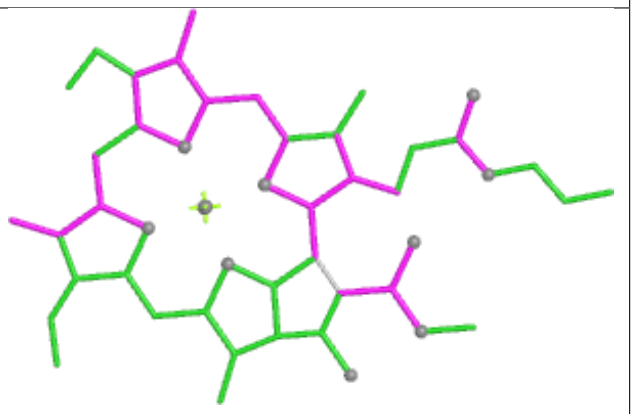
Torsions

Rings

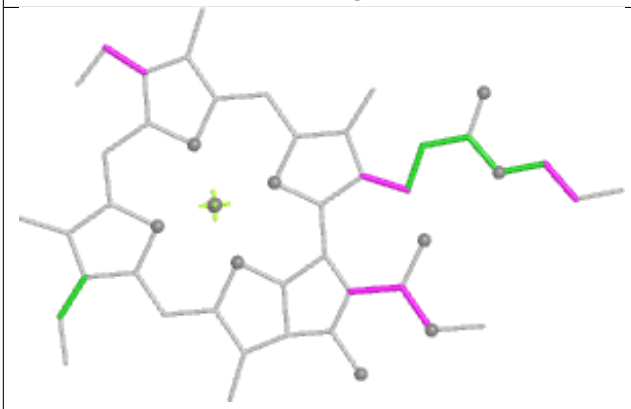
Ligand CLA 1 601



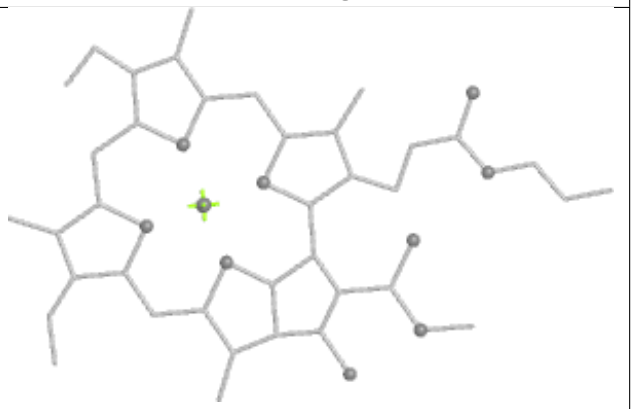
Bond lengths



Bond angles

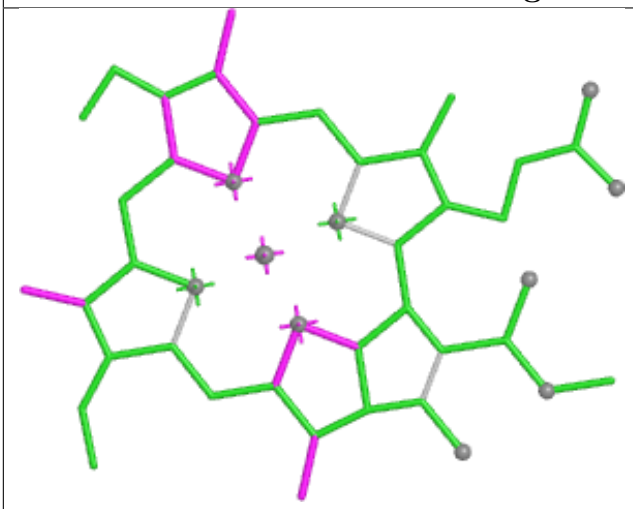


Torsions

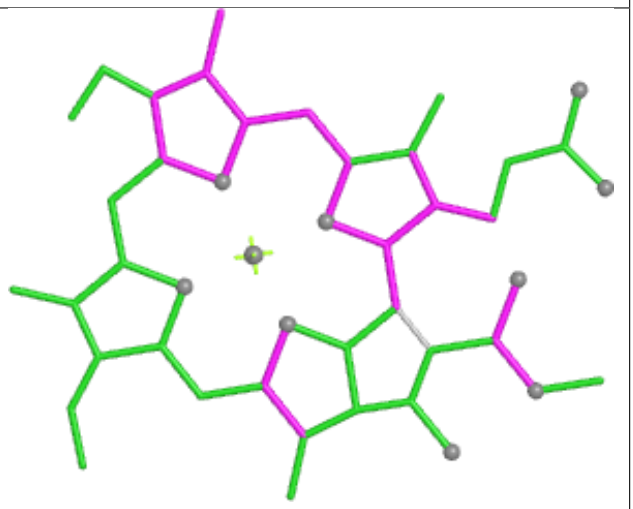


Rings

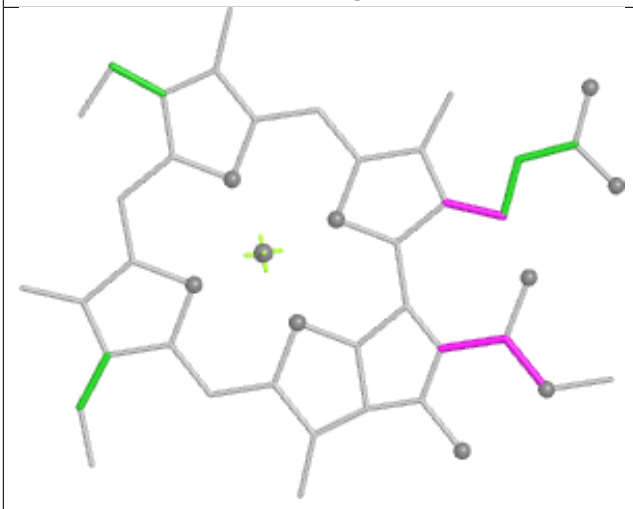
Ligand CLA A 812



Bond lengths



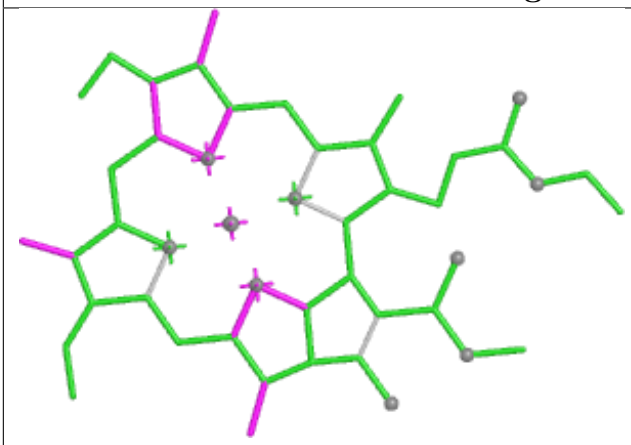
Bond angles



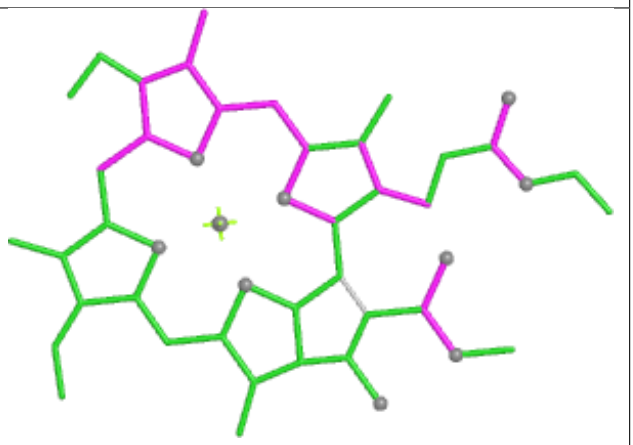
Torsions

Rings

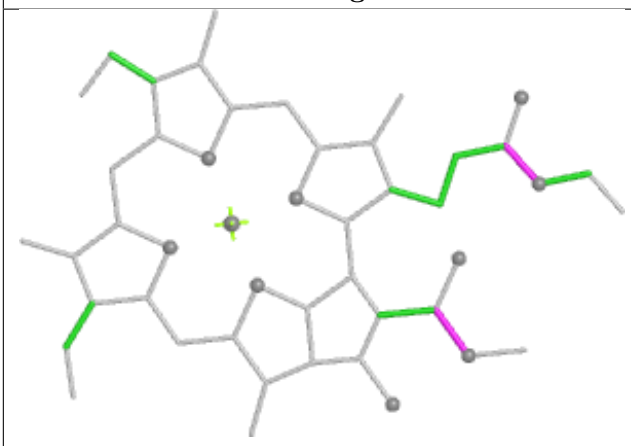
Ligand CLA B 840



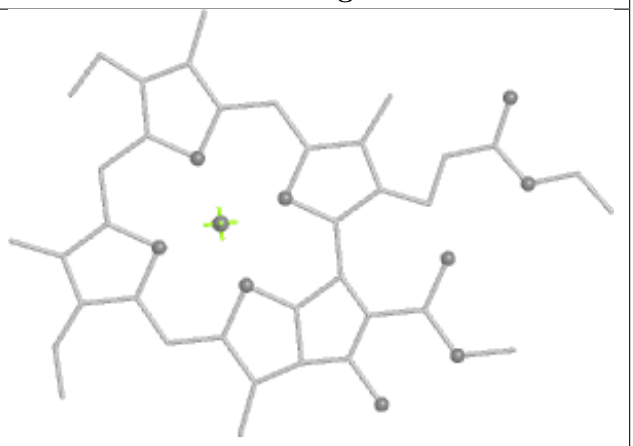
Bond lengths



Bond angles

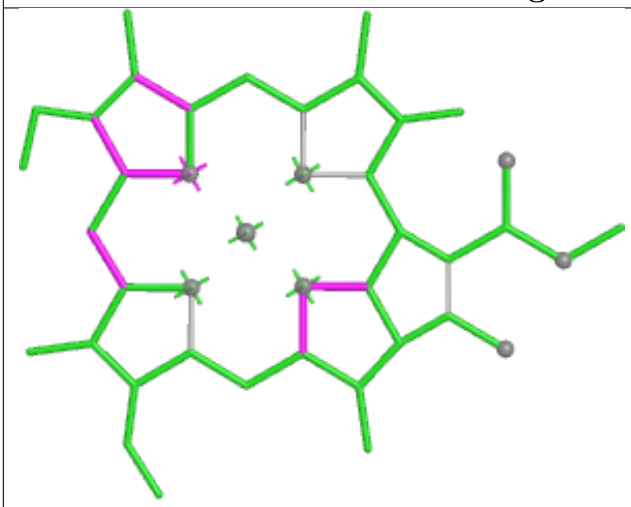


Torsions

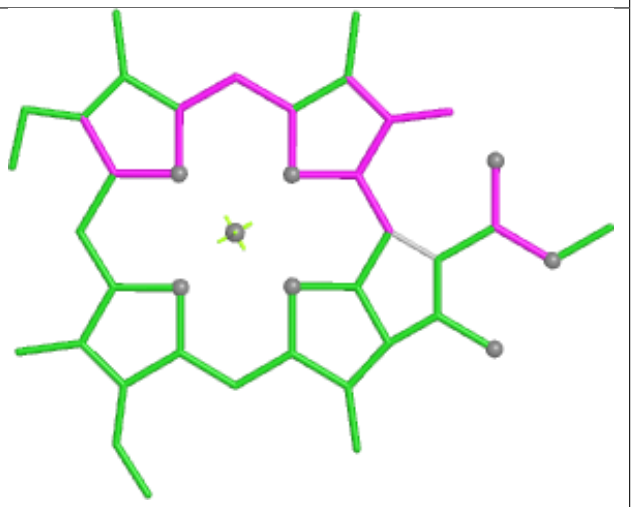


Rings

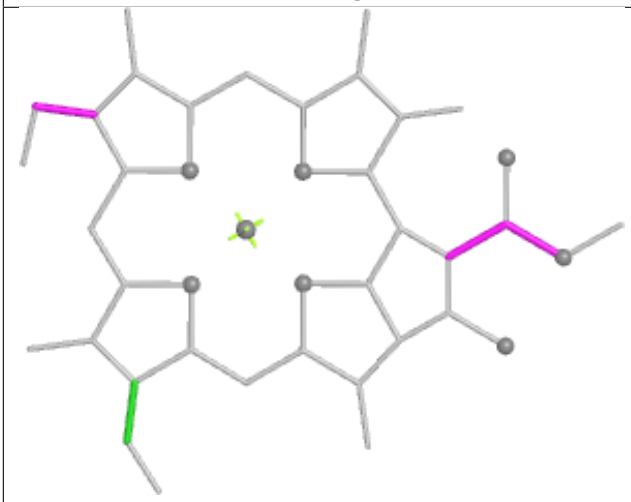
Ligand CLA 4 609



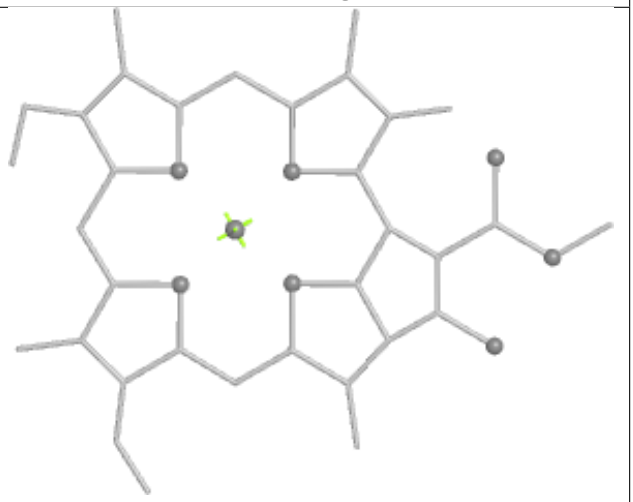
Bond lengths



Bond angles



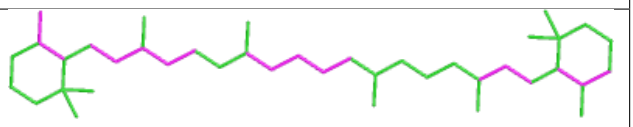
Torsions



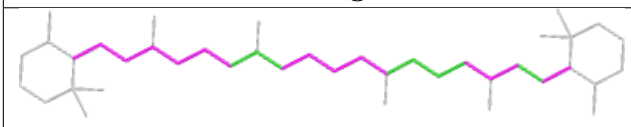
Rings

Ligand BCR A 843

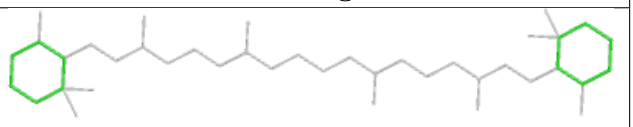
Bond lengths



Bond angles

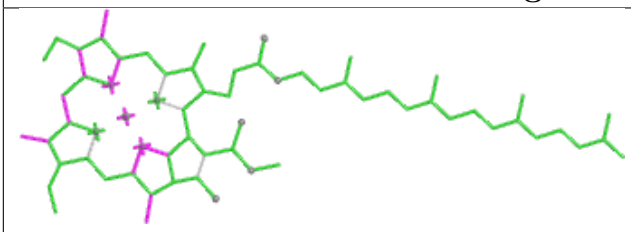


Torsions

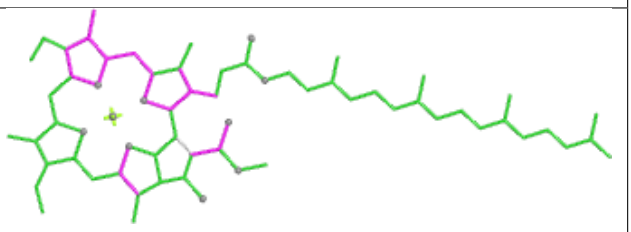


Rings

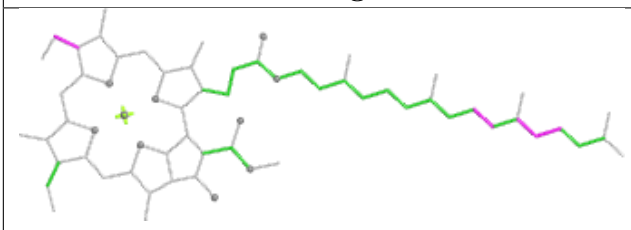
Ligand CLA B 828



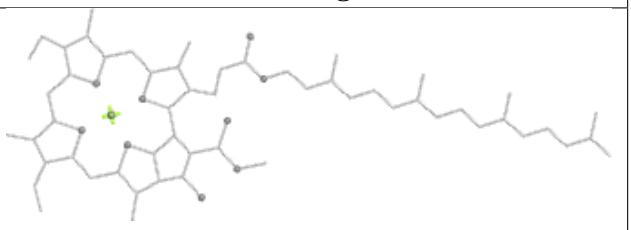
Bond lengths



Bond angles

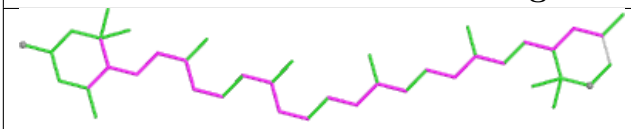


Torsions

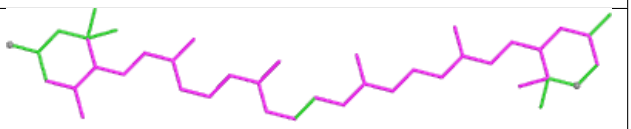


Rings

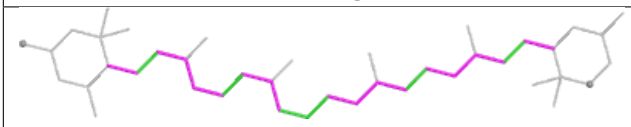
Ligand ZEX 4 617



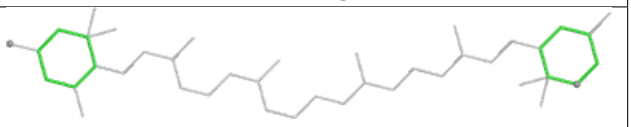
Bond lengths



Bond angles

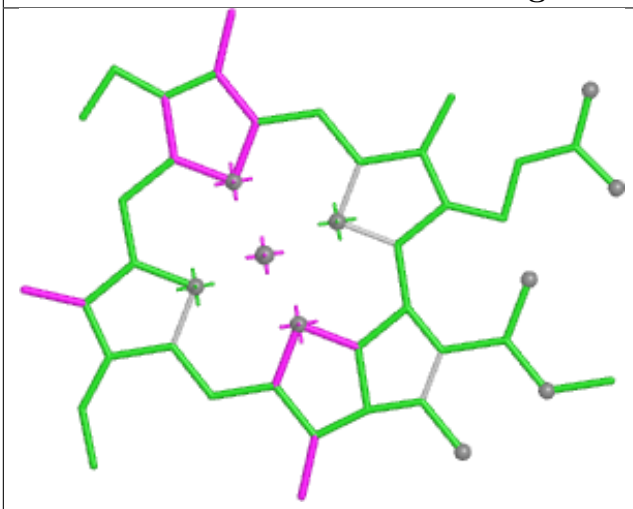


Torsions

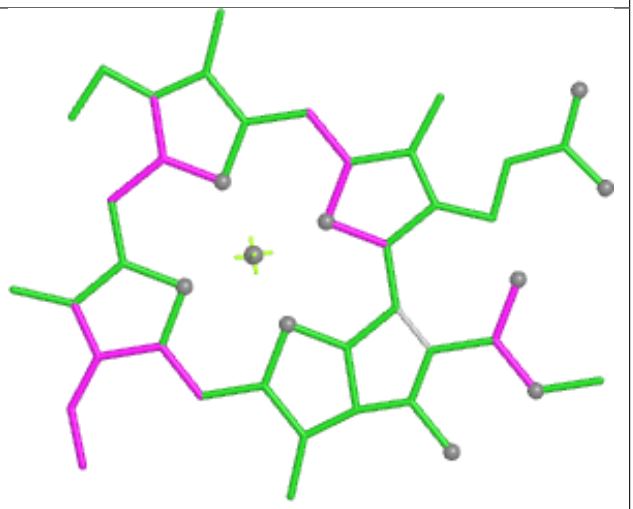


Rings

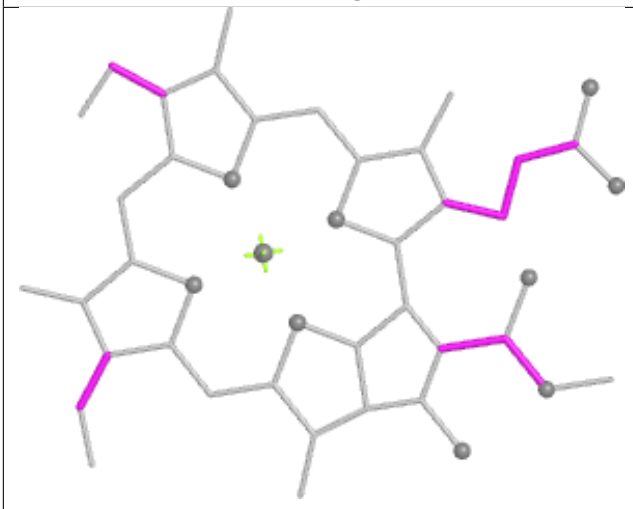
Ligand CLA 1 611



Bond lengths



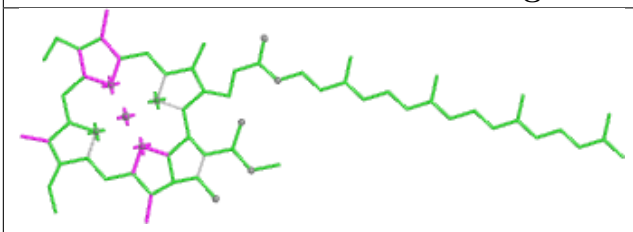
Bond angles



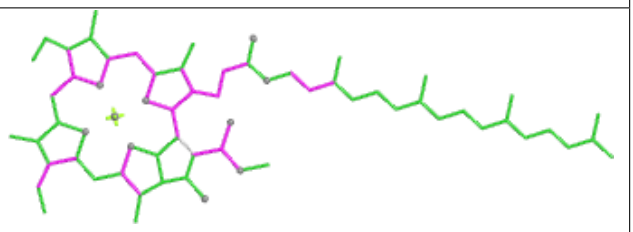
Torsions

Rings

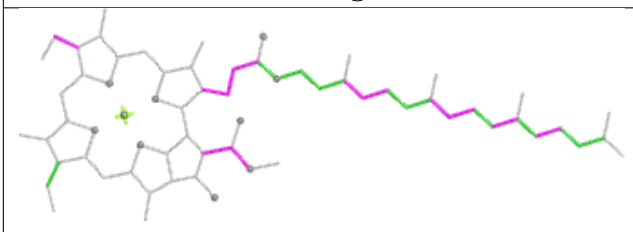
Ligand CLA A 823



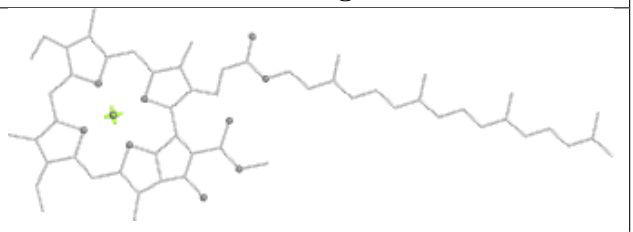
Bond lengths



Bond angles

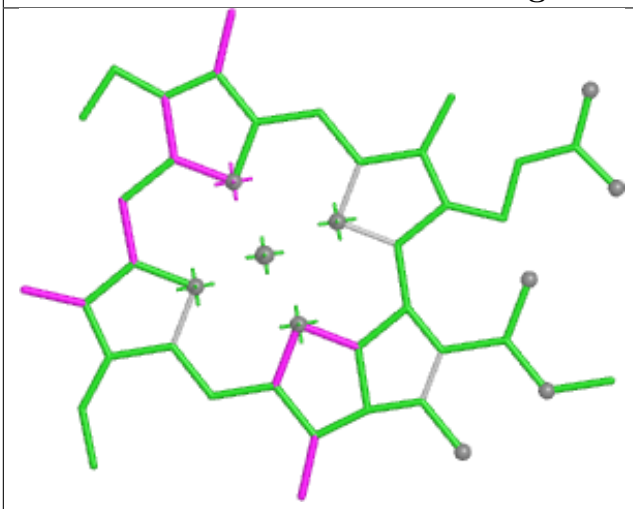


Torsions

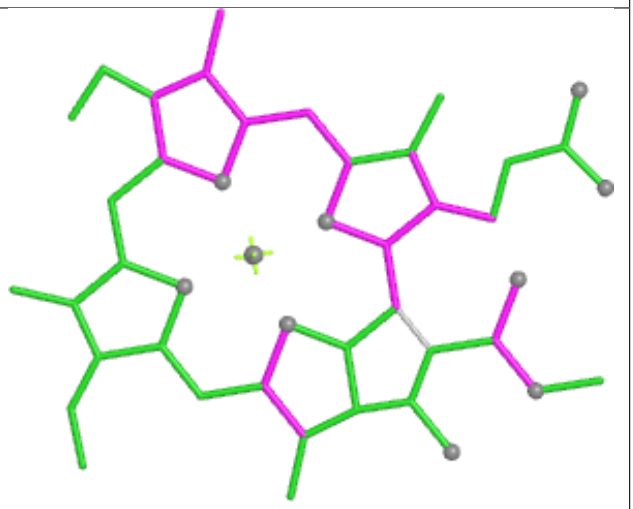


Rings

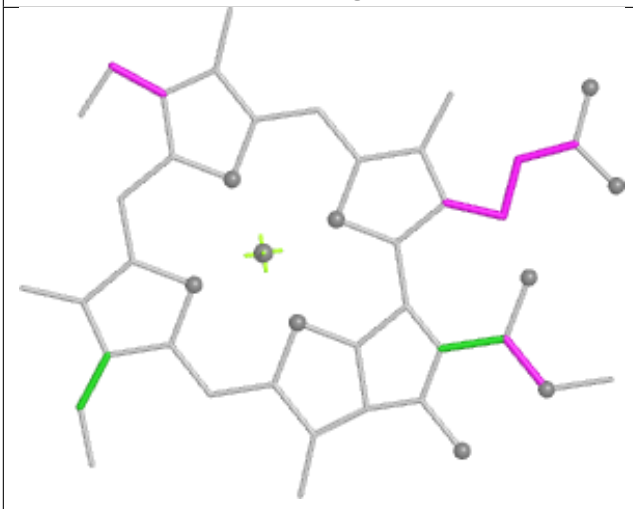
Ligand CLA 4 608



Bond lengths



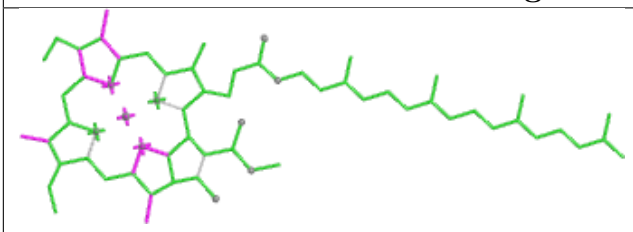
Bond angles



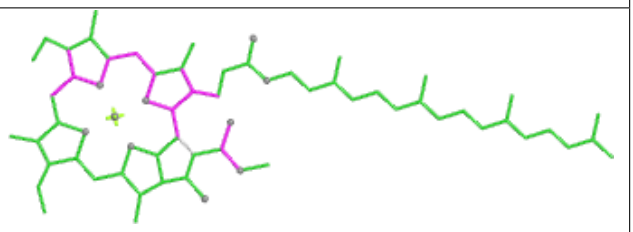
Torsions

Rings

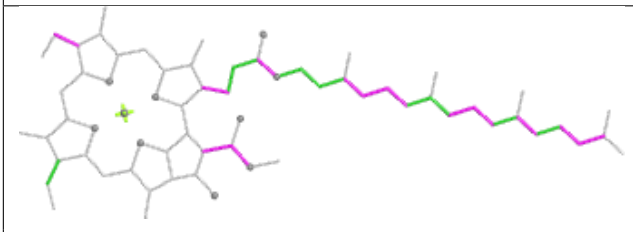
Ligand CLA B 822



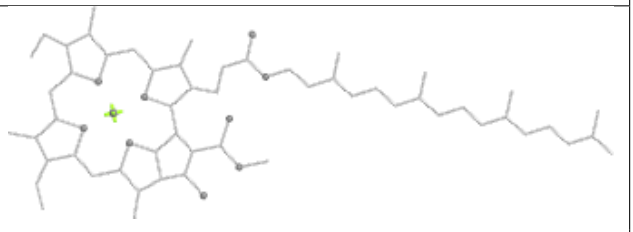
Bond lengths



Bond angles

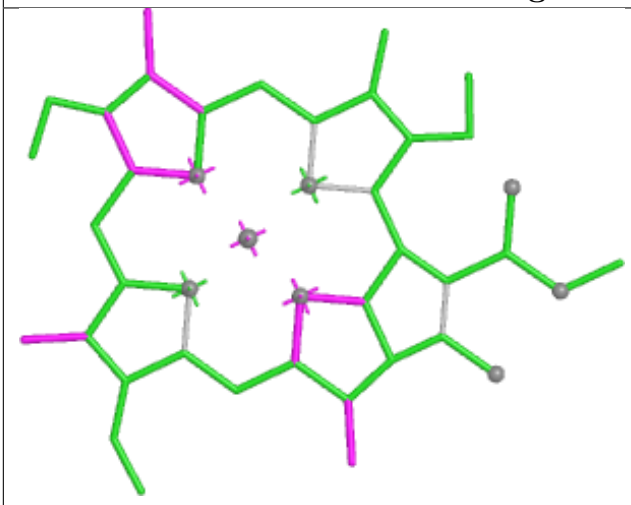


Torsions

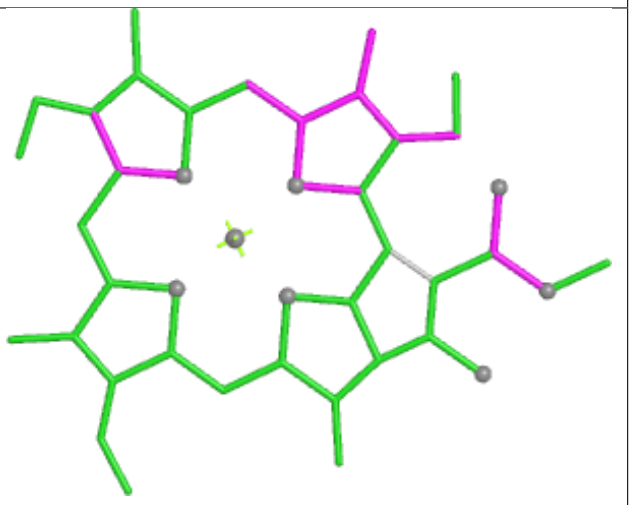


Rings

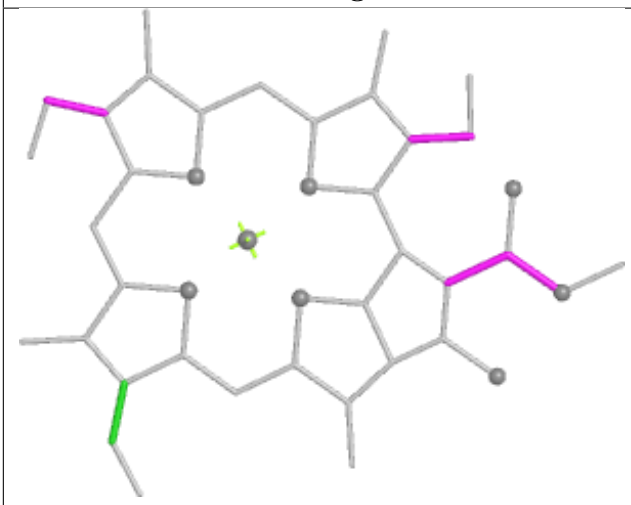
Ligand CLA 2 610



Bond lengths

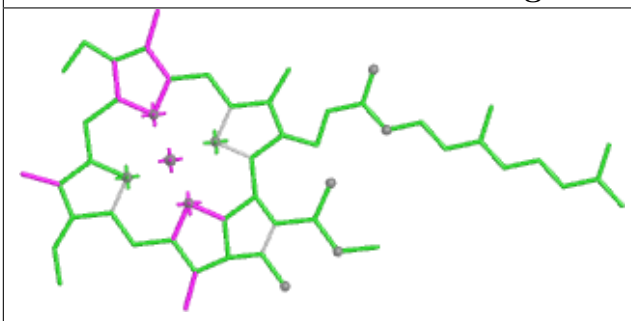
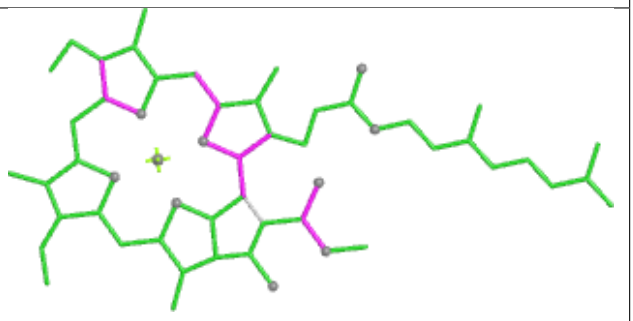
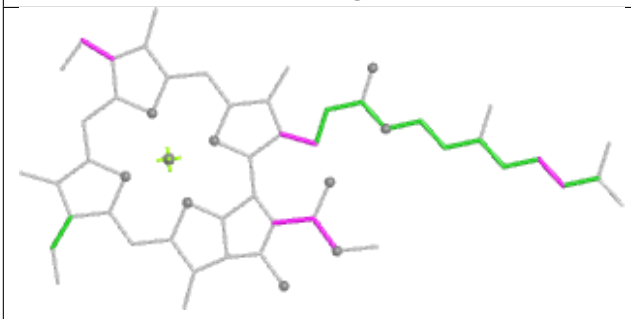
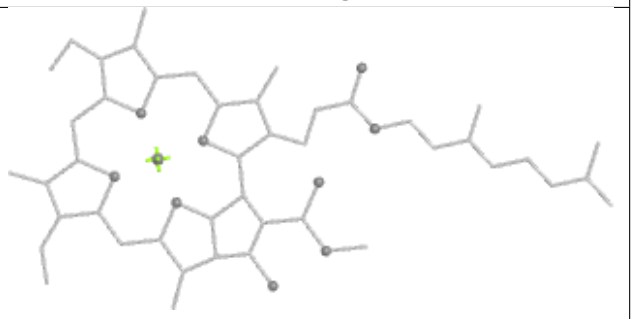


Bond angles

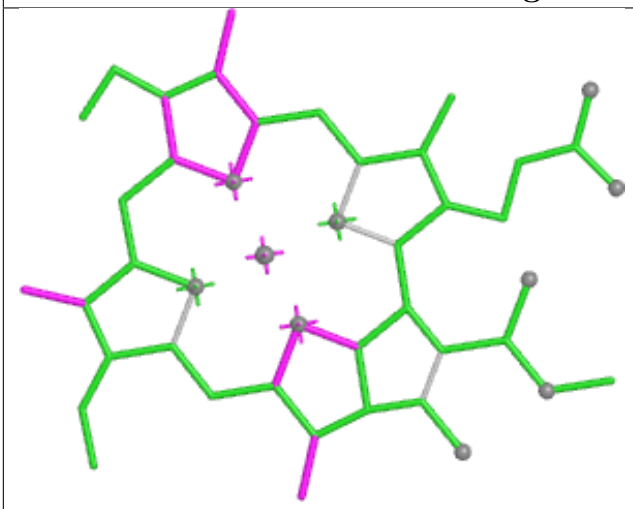


Torsions

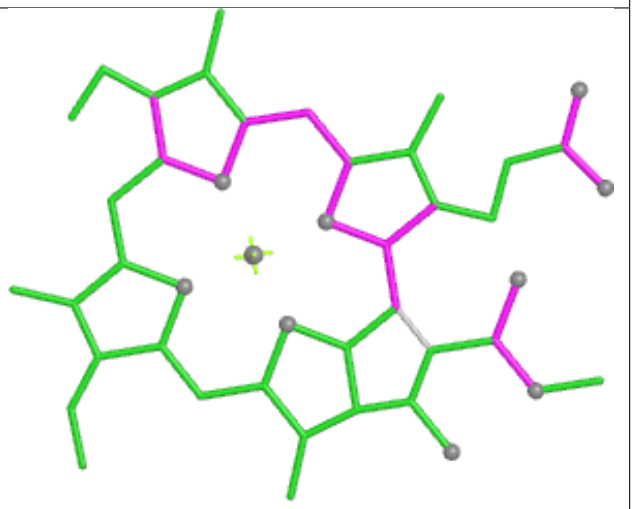
Rings

Ligand CLA B 815	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

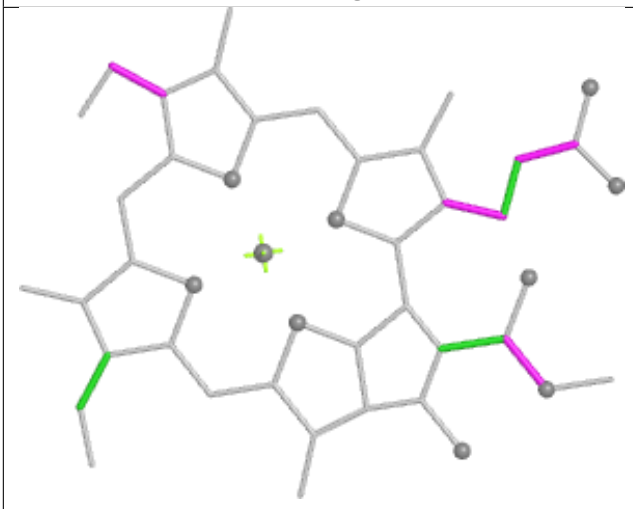
Ligand CLA K 102



Bond lengths



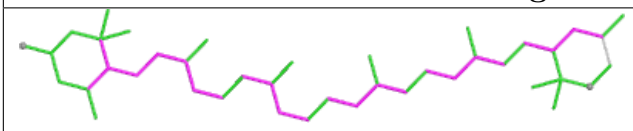
Bond angles



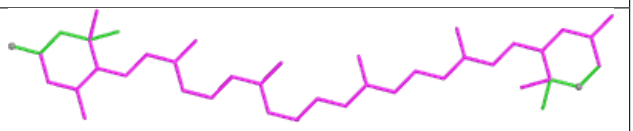
Torsions

Rings

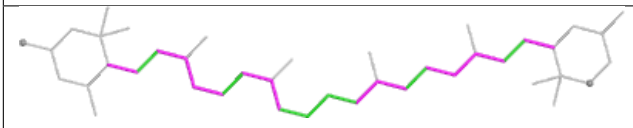
Ligand ZEX 3 215



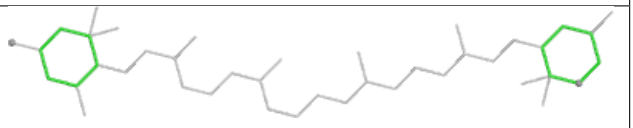
Bond lengths



Bond angles

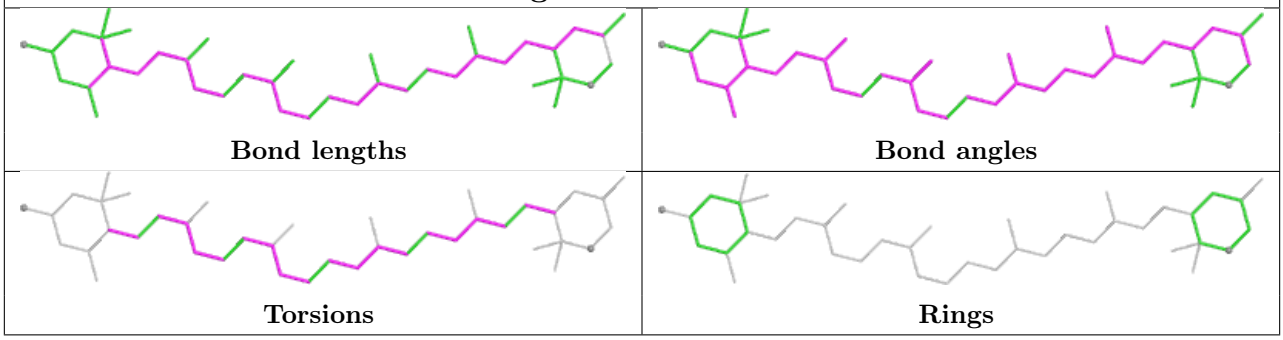


Torsions

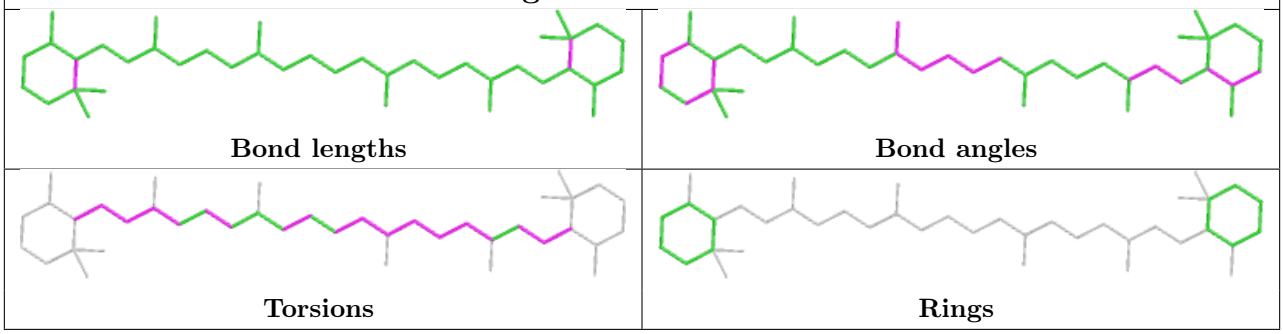


Rings

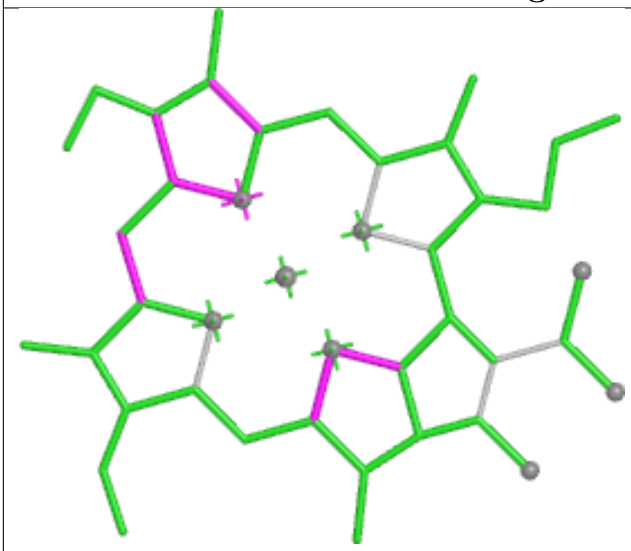
Ligand ZEX 5 616



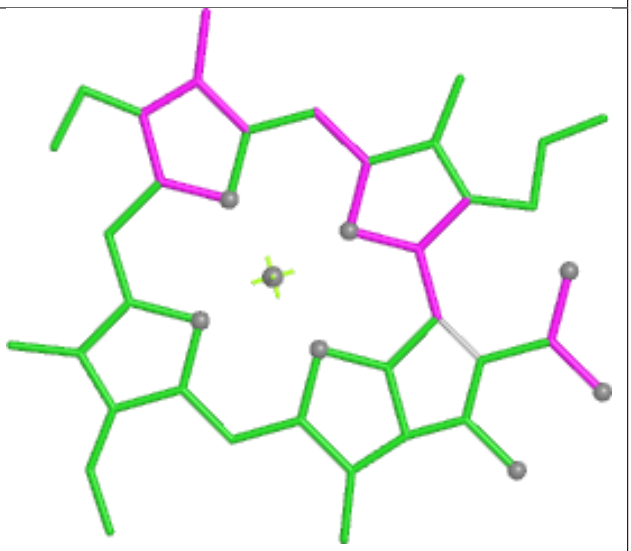
Ligand BCR K 104



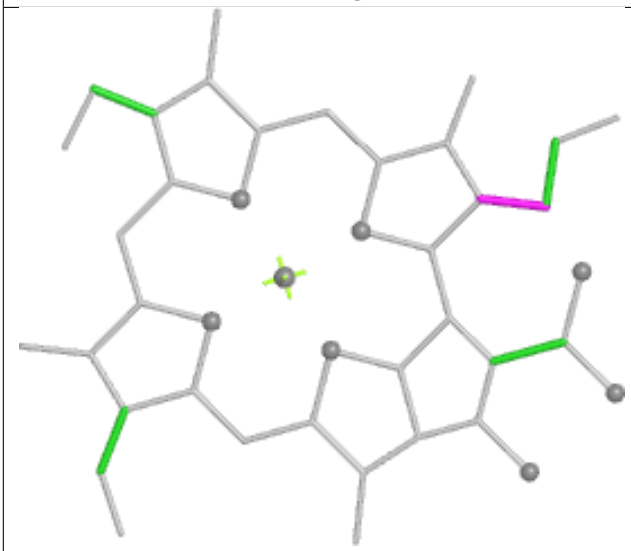
Ligand CLA 4 605



Bond lengths



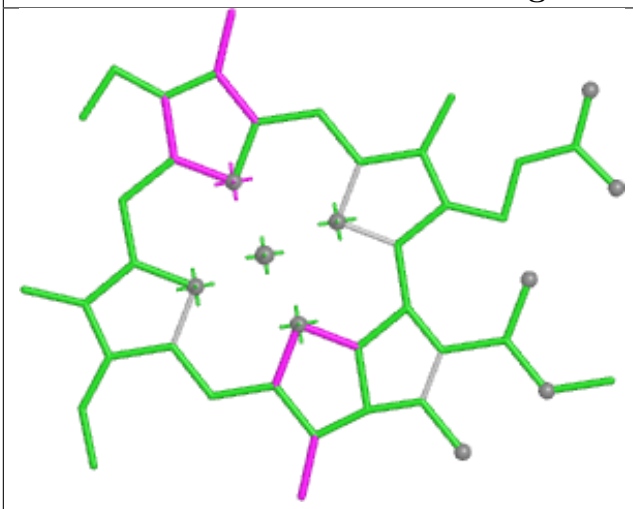
Bond angles



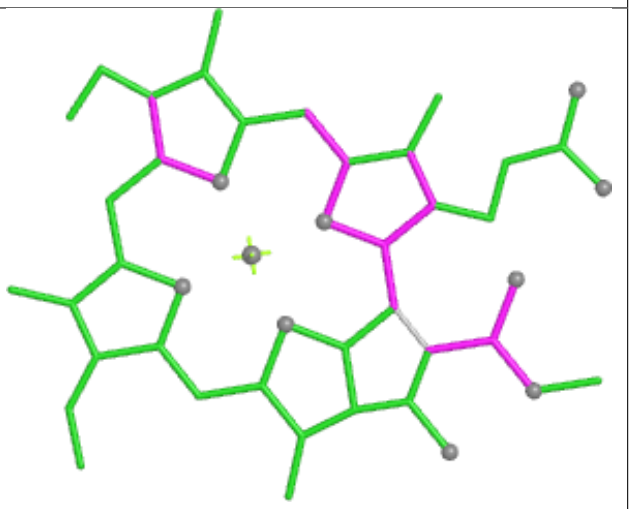
Torsions

Rings

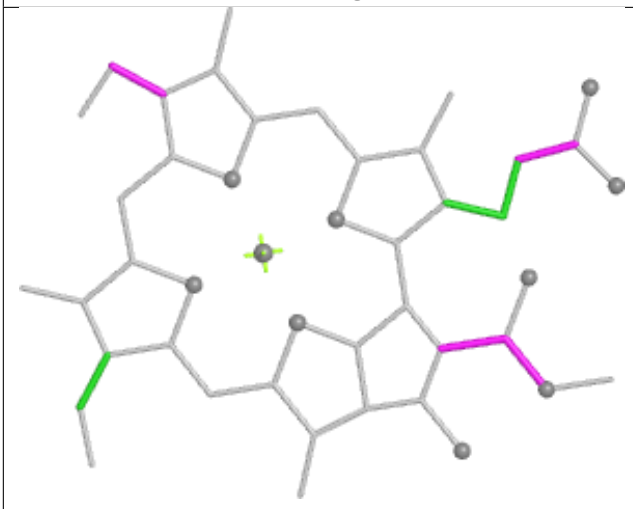
Ligand CLA 5 612



Bond lengths



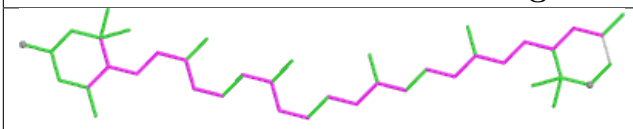
Bond angles



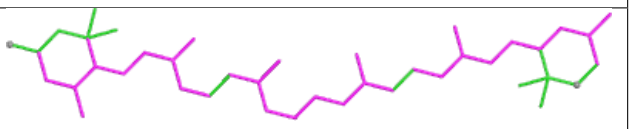
Torsions

Rings

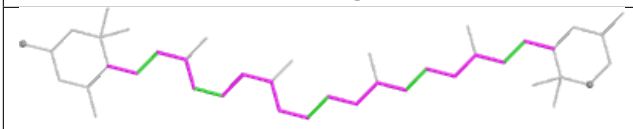
Ligand ZEX 2 616



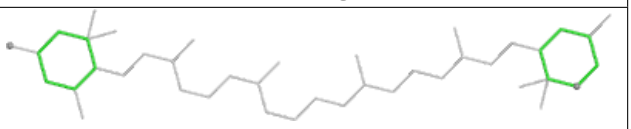
Bond lengths



Bond angles

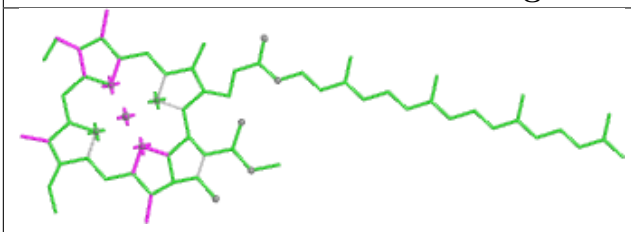


Torsions

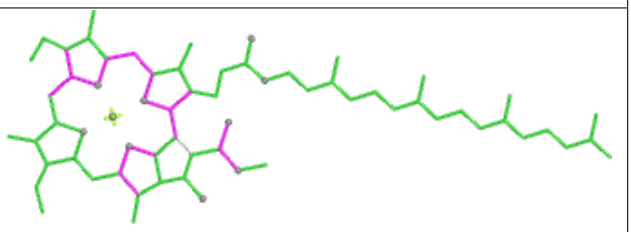


Rings

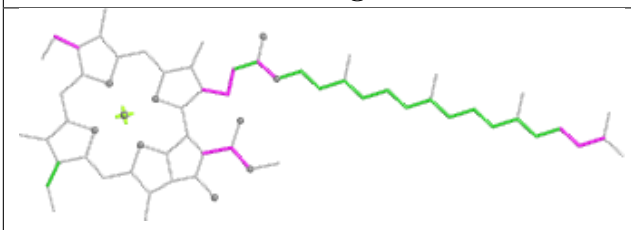
Ligand CLA A 816



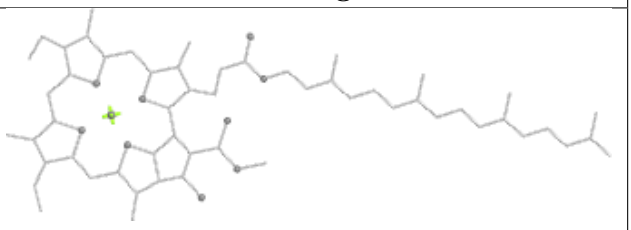
Bond lengths



Bond angles

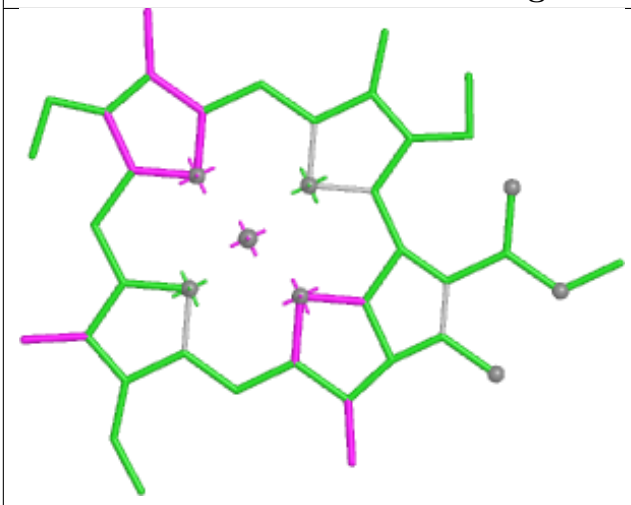


Torsions

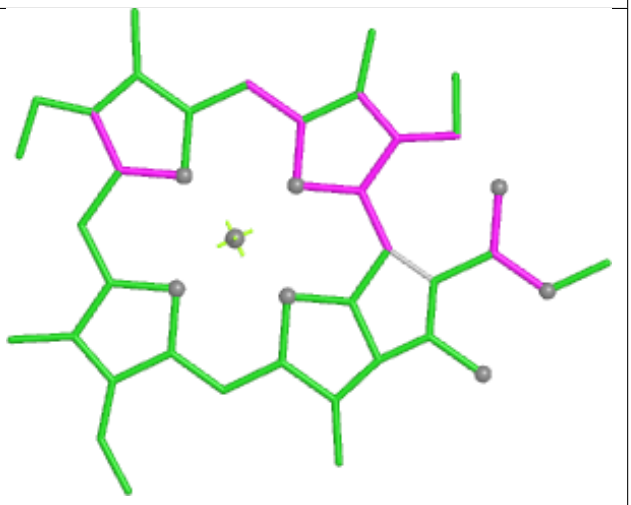


Rings

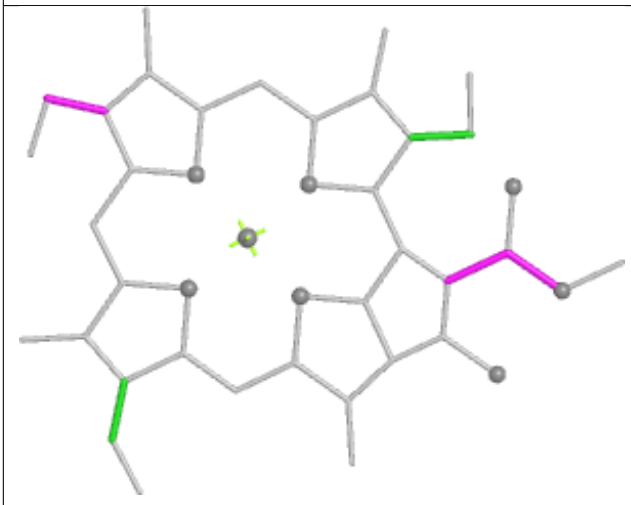
Ligand CLA J 103



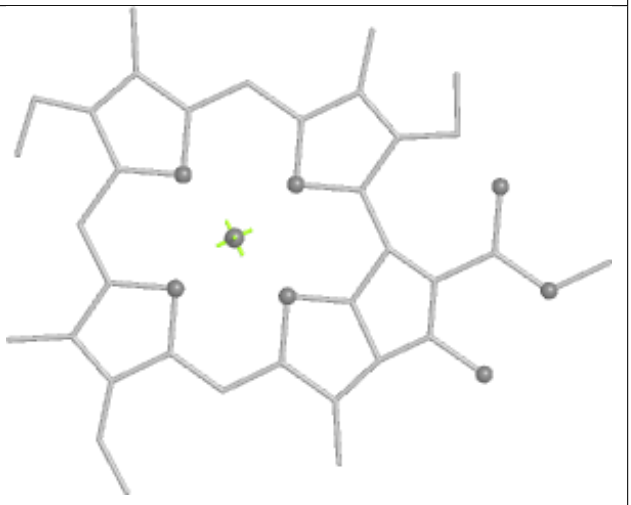
Bond lengths



Bond angles

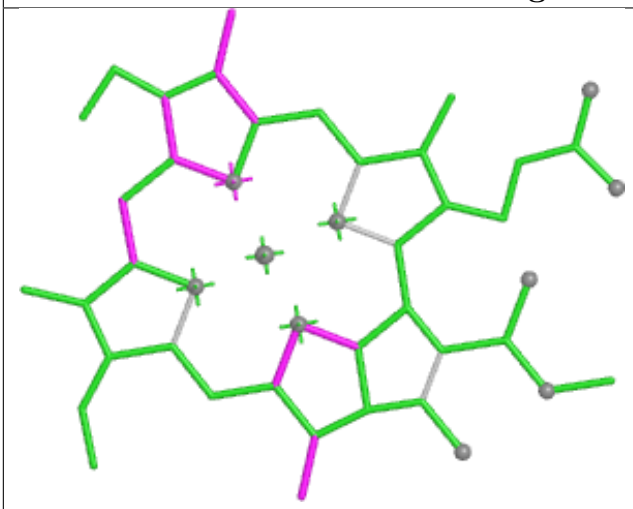


Torsions

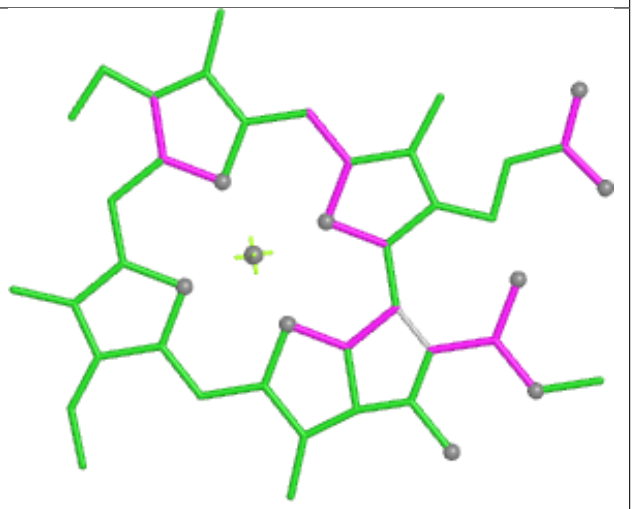


Rings

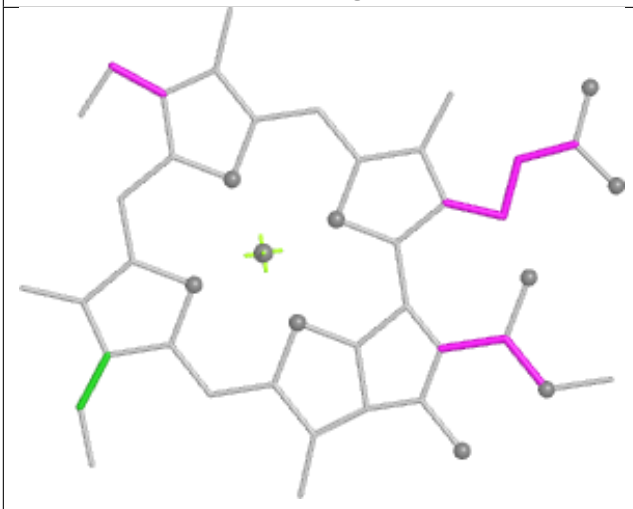
Ligand CLA 4 611



Bond lengths



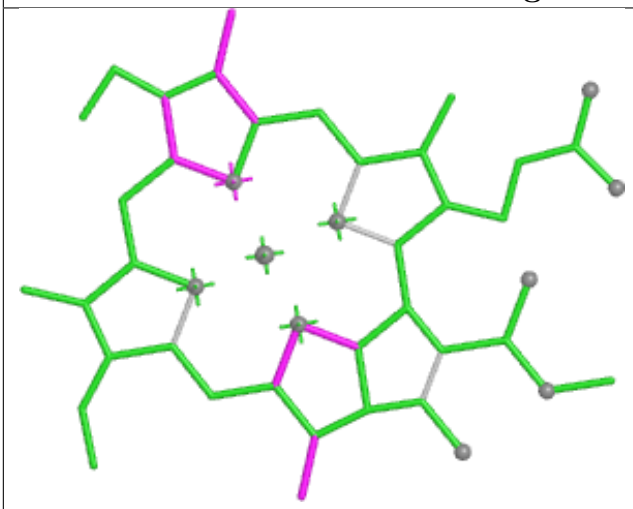
Bond angles



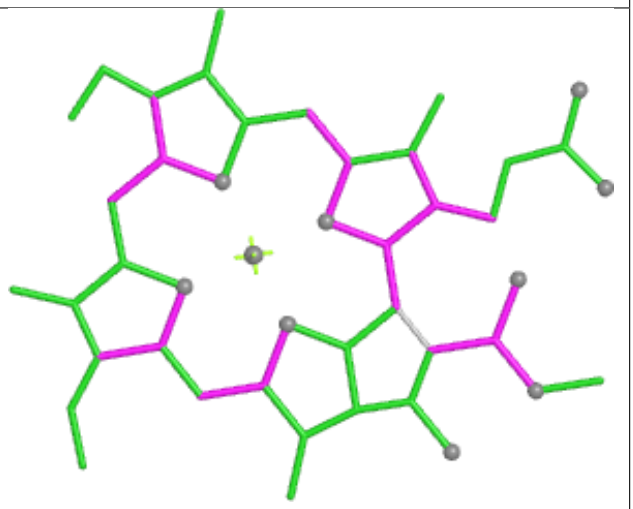
Torsions

Rings

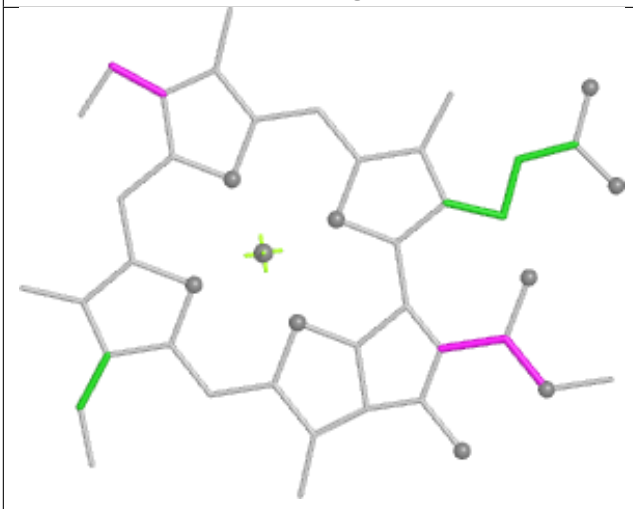
Ligand CLA A 814



Bond lengths



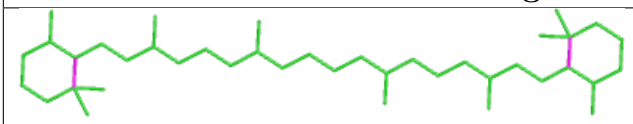
Bond angles



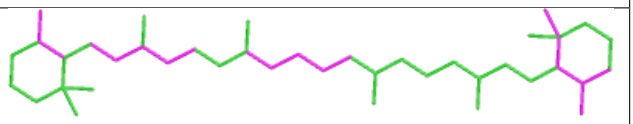
Torsions

Rings

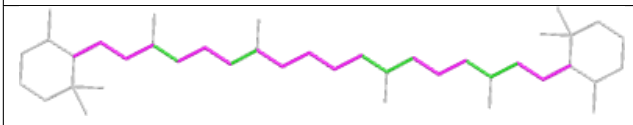
Ligand BCR B 845



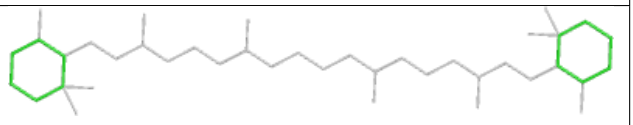
Bond lengths



Bond angles

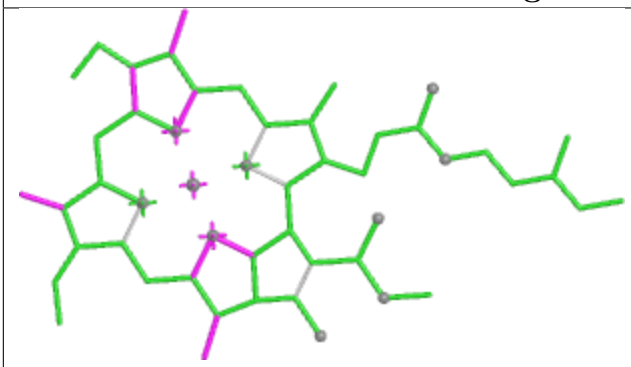


Torsions

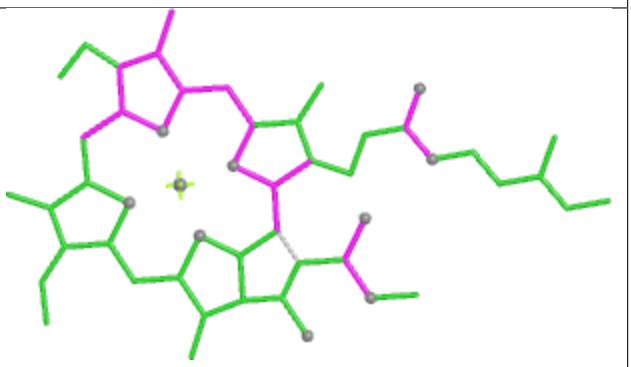


Rings

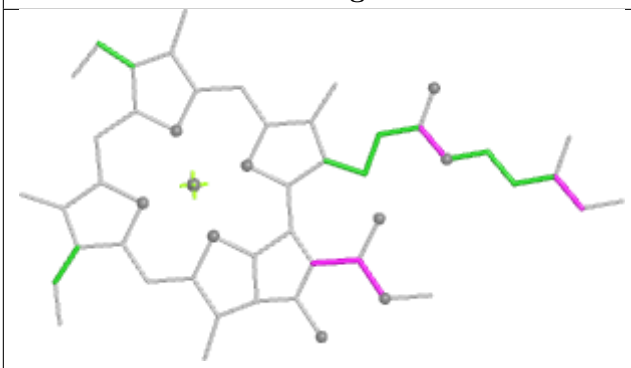
Ligand CLA A 835



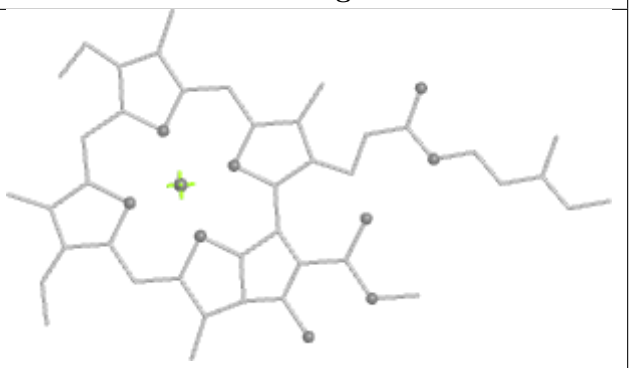
Bond lengths



Bond angles

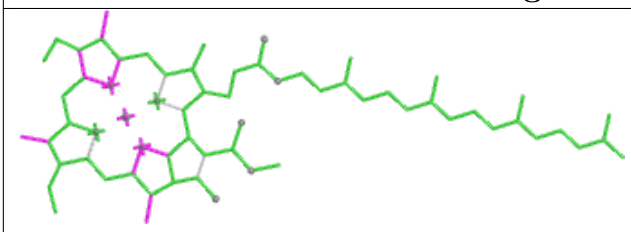


Torsions

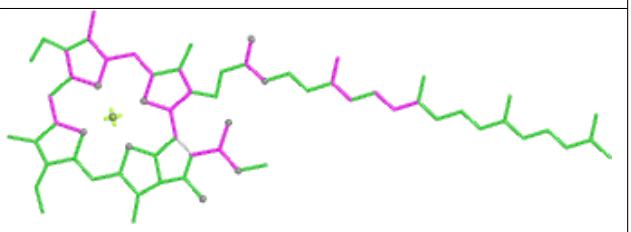


Rings

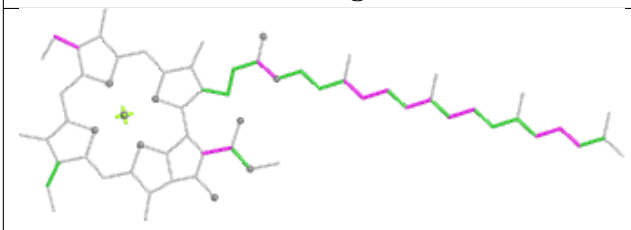
Ligand CLA A 836



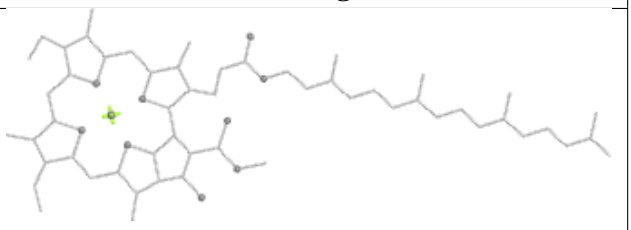
Bond lengths



Bond angles

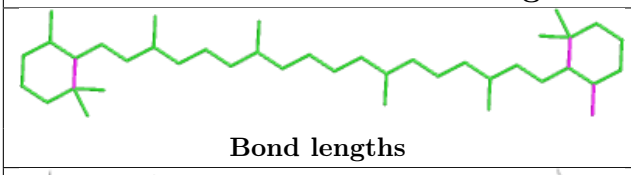


Torsions

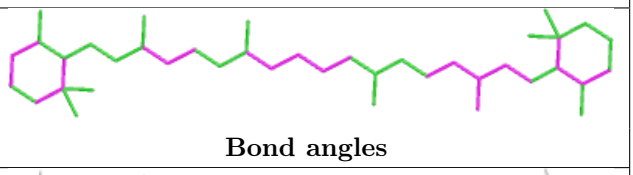


Rings

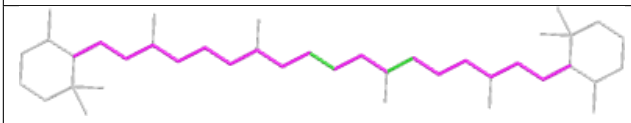
Ligand BCR B 849



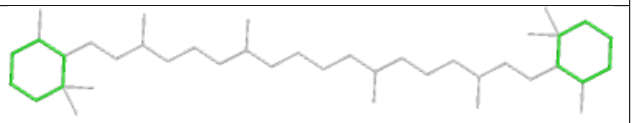
Bond lengths



Bond angles

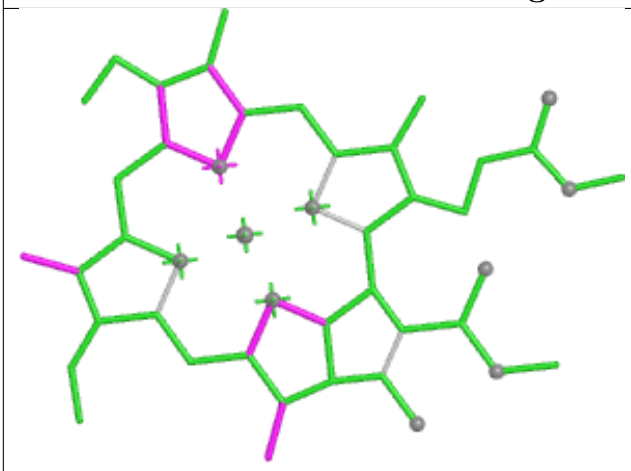


Torsions

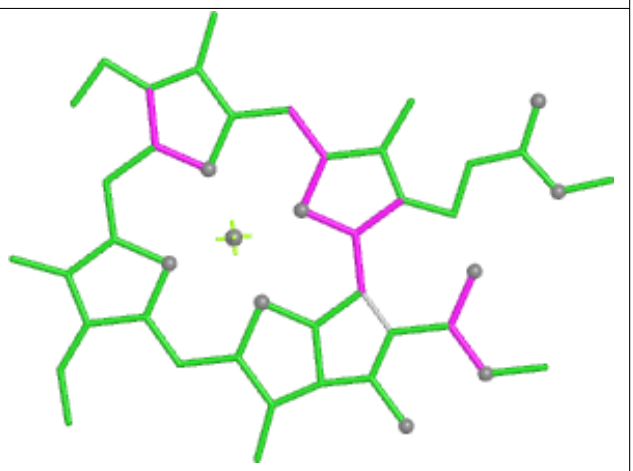


Rings

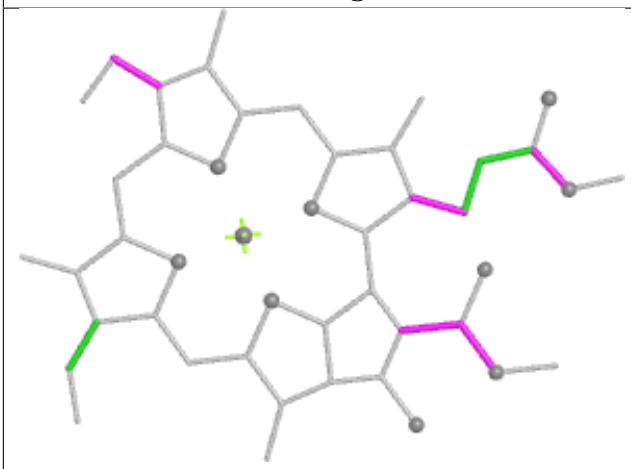
Ligand CLA 3 212



Bond lengths



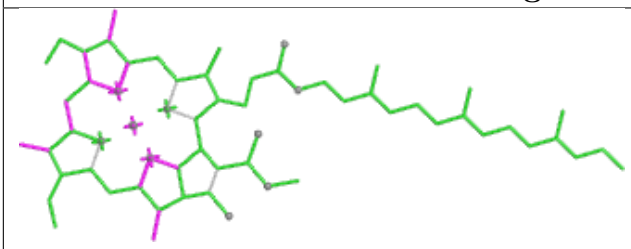
Bond angles



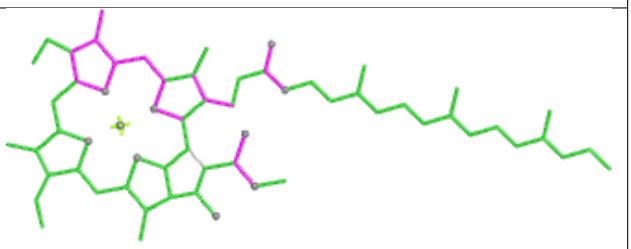
Torsions

Rings

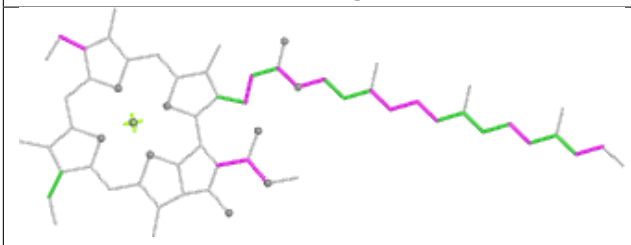
Ligand CLA A 815



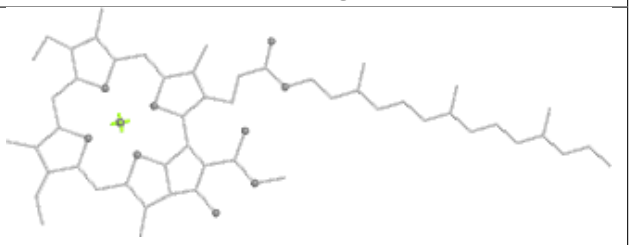
Bond lengths



Bond angles

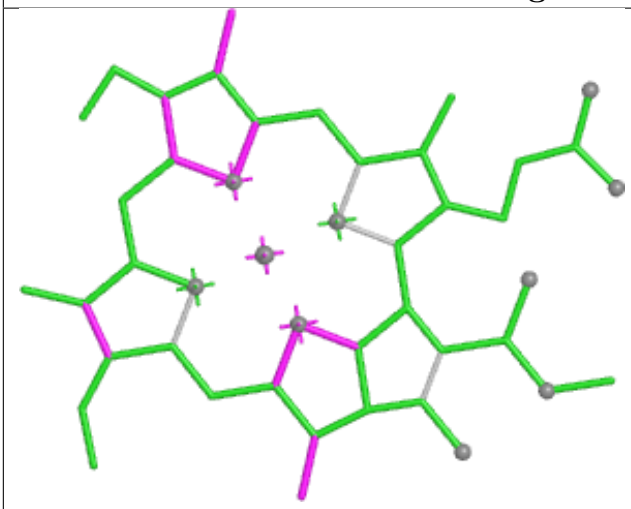


Torsions

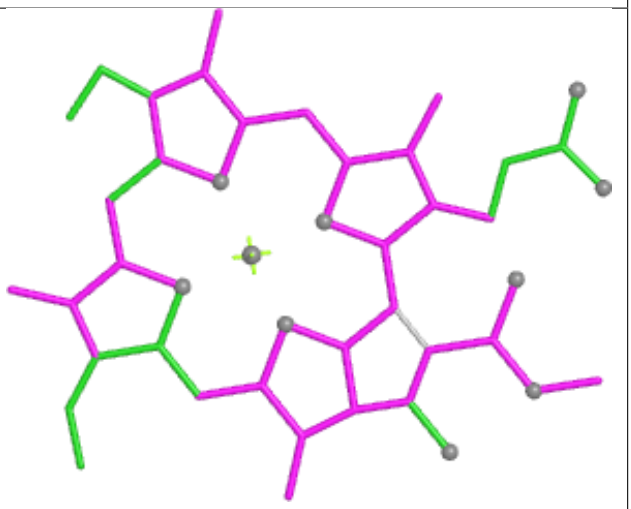


Rings

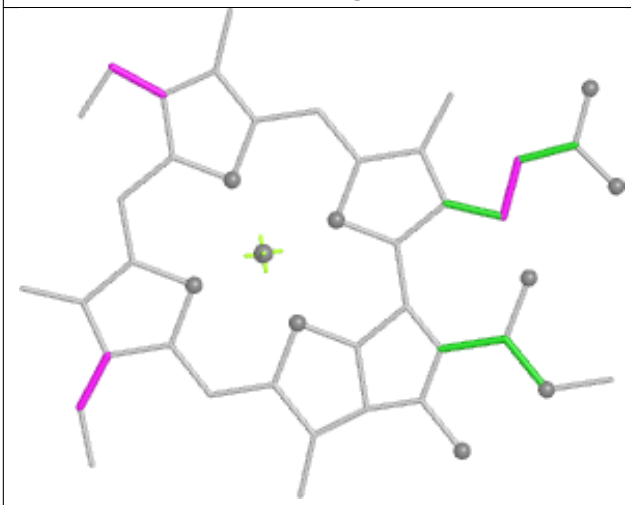
Ligand CLA 5 606



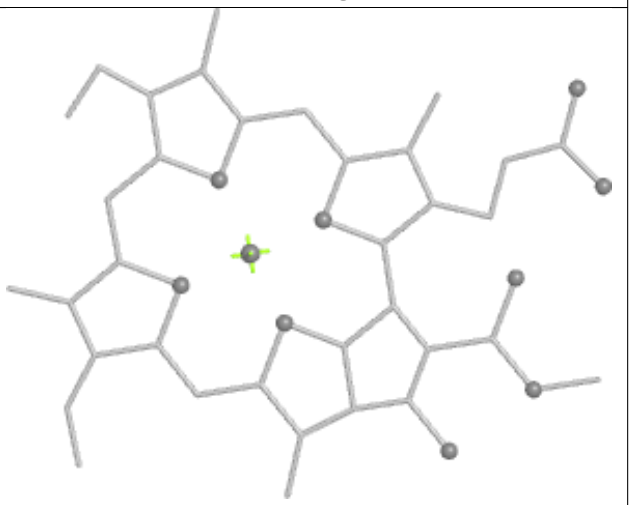
Bond lengths



Bond angles

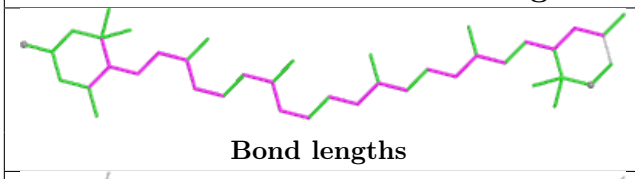


Torsions

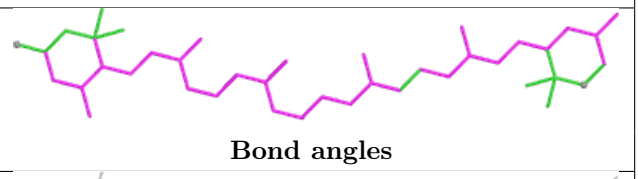


Rings

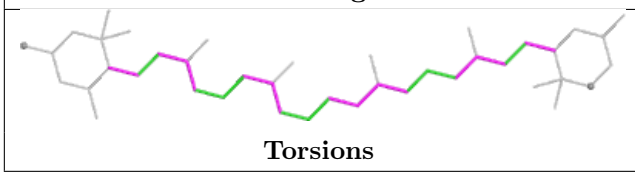
Ligand ZEX 3 214



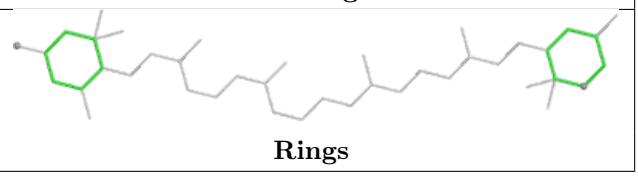
Bond lengths



Bond angles

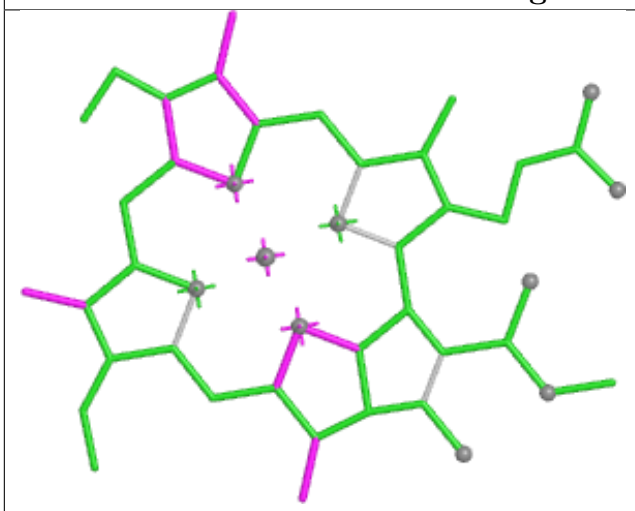


Torsions

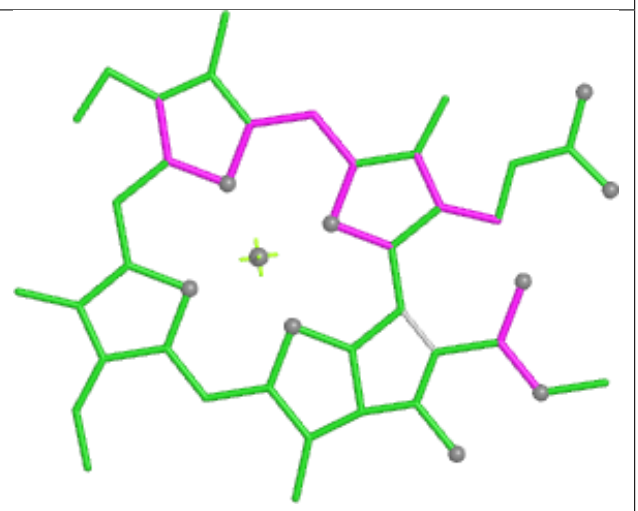


Rings

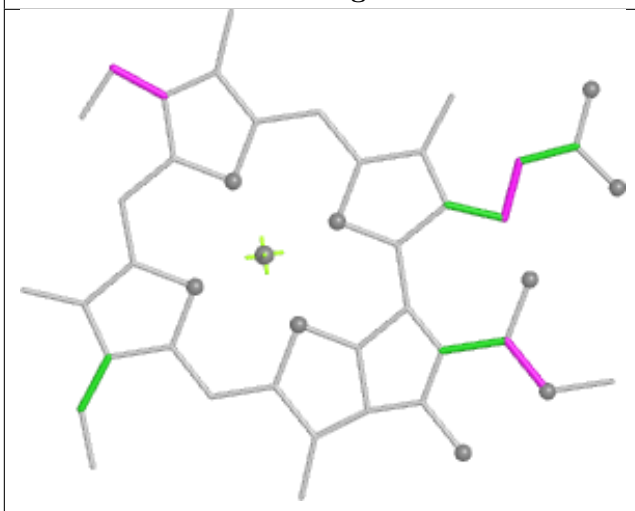
Ligand CLA 2 612



Bond lengths



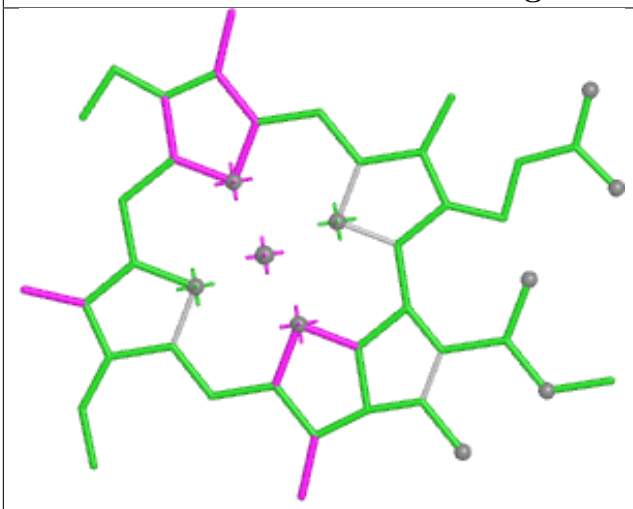
Bond angles



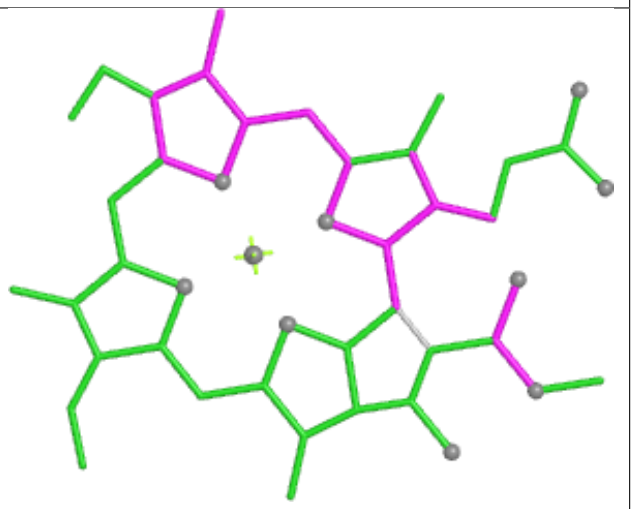
Torsions

Rings

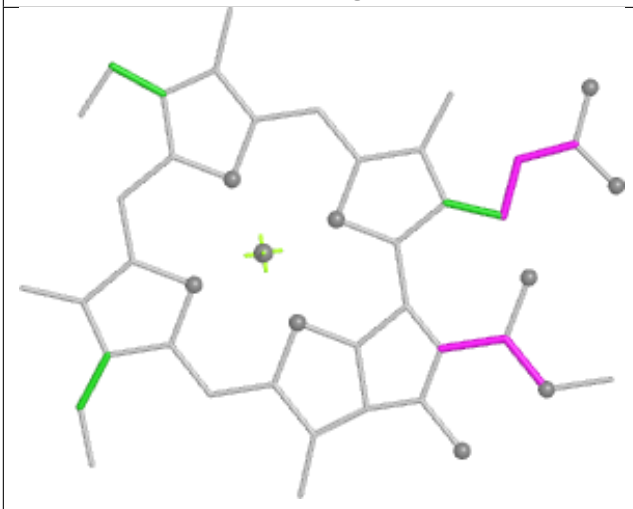
Ligand CLA B 807



Bond lengths



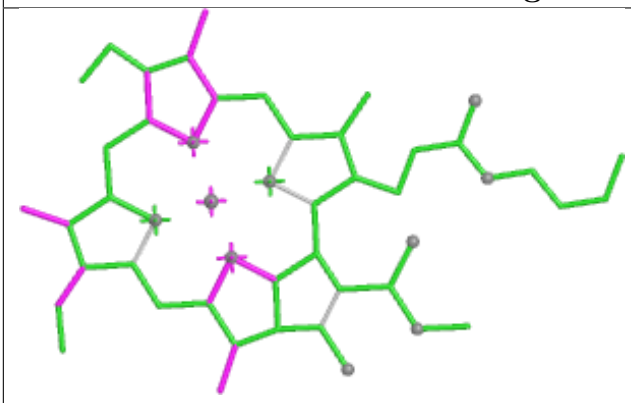
Bond angles



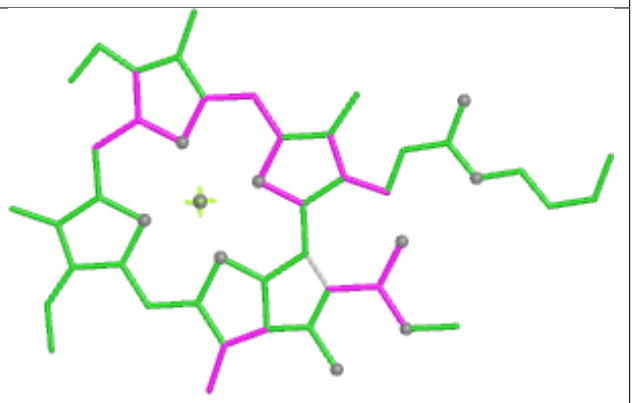
Torsions

Rings

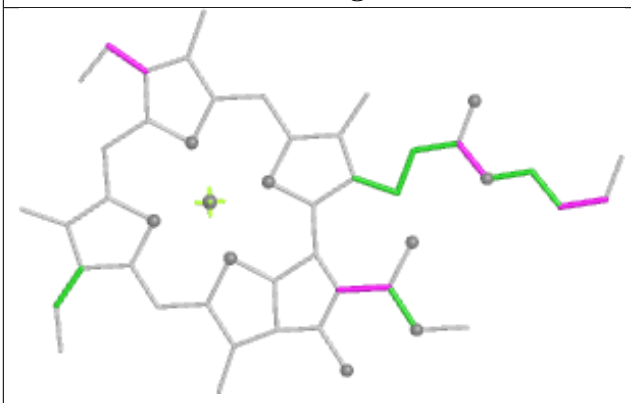
Ligand CLA A 820



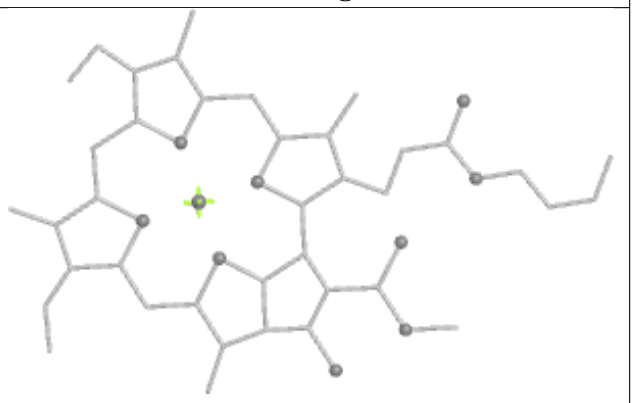
Bond lengths



Bond angles

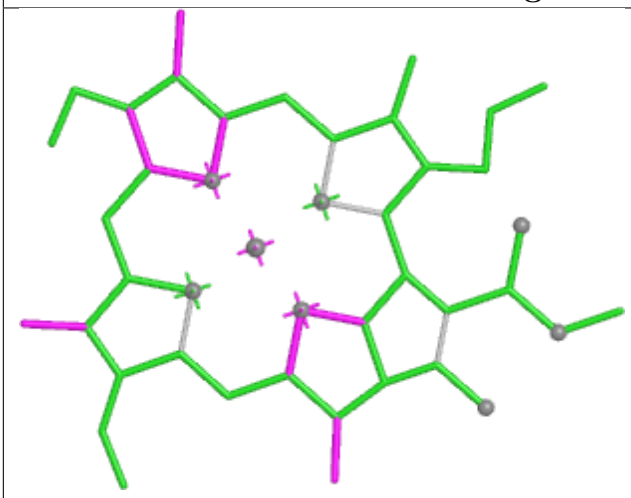


Torsions



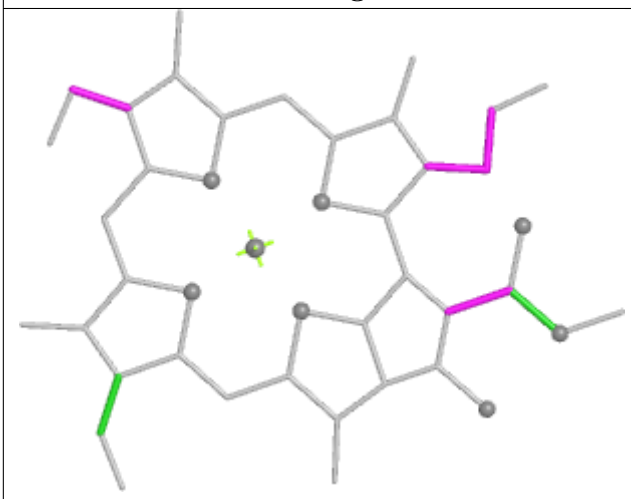
Rings

Ligand CLA B 834

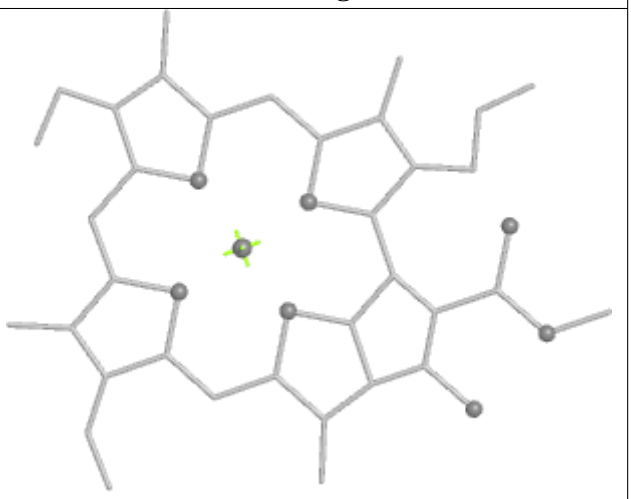


Bond lengths

Bond angles

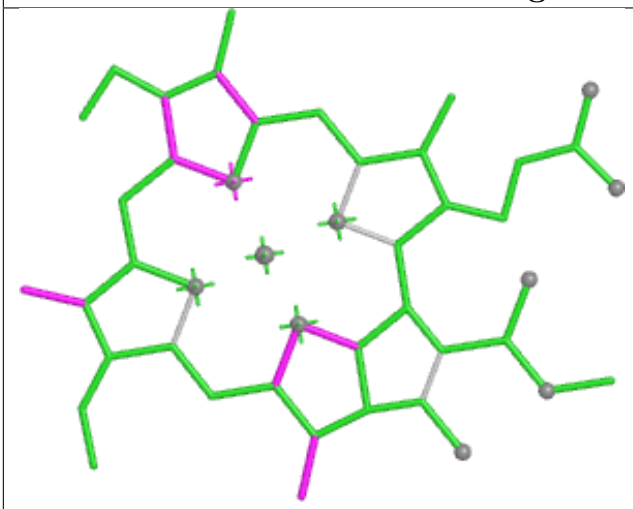


Torsions

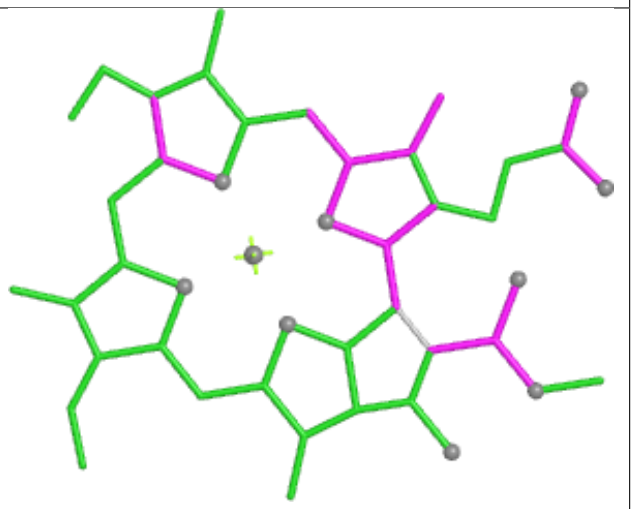


Rings

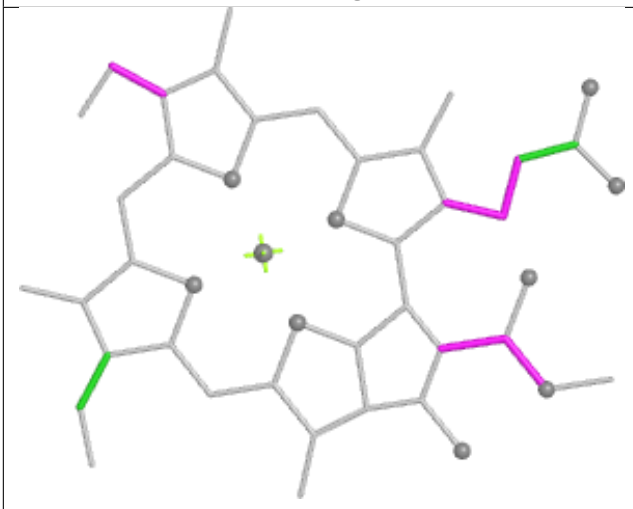
Ligand CLA 4 607



Bond lengths



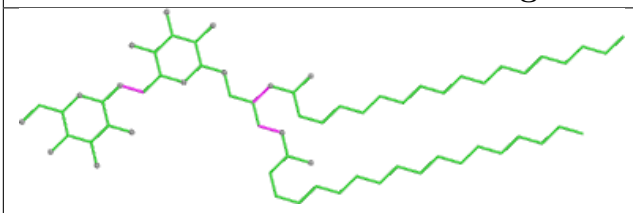
Bond angles



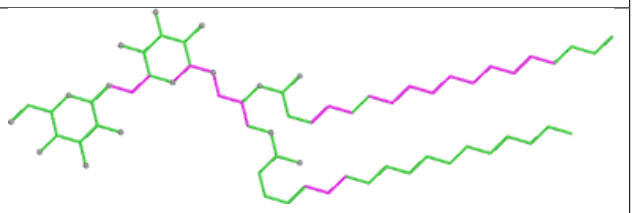
Torsions

Rings

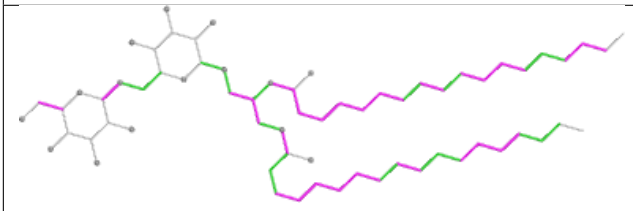
Ligand DGD B 851



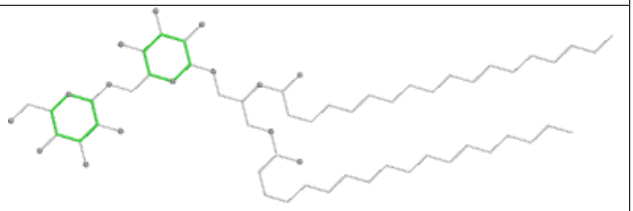
Bond lengths



Bond angles

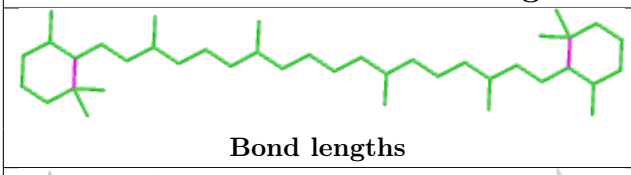


Torsions

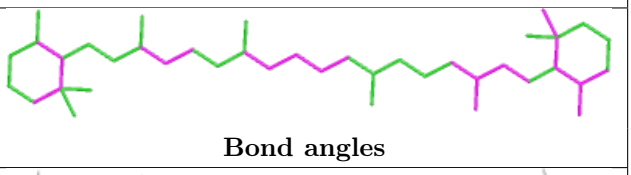


Rings

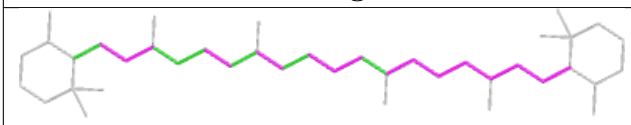
Ligand BCR A 844



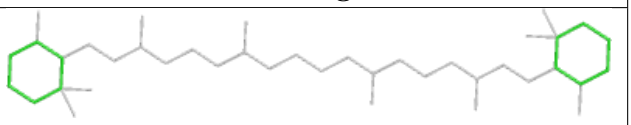
Bond lengths



Bond angles

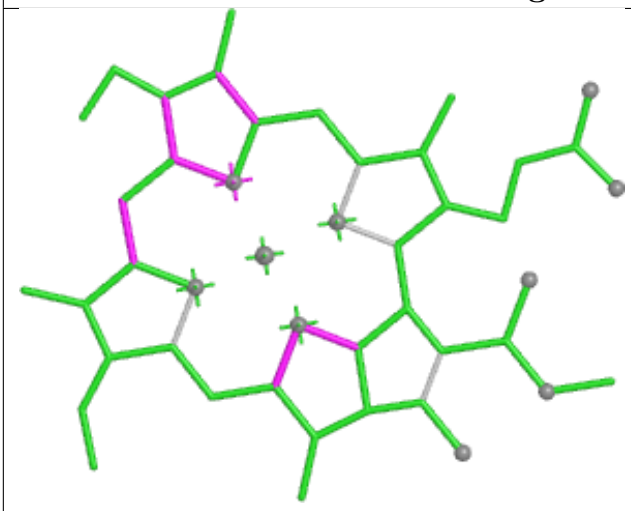


Torsions

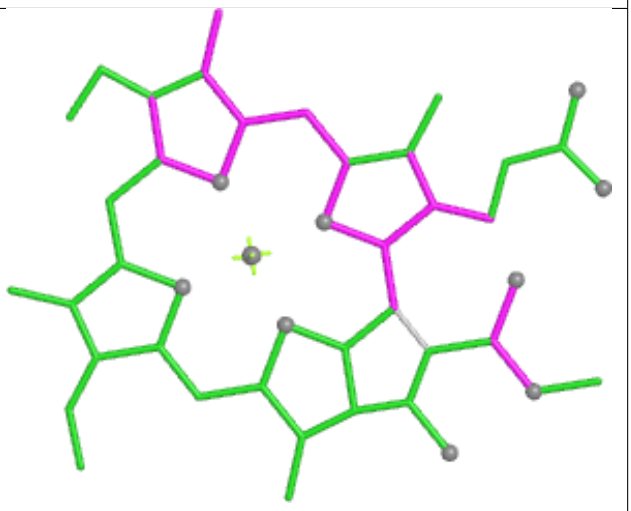


Rings

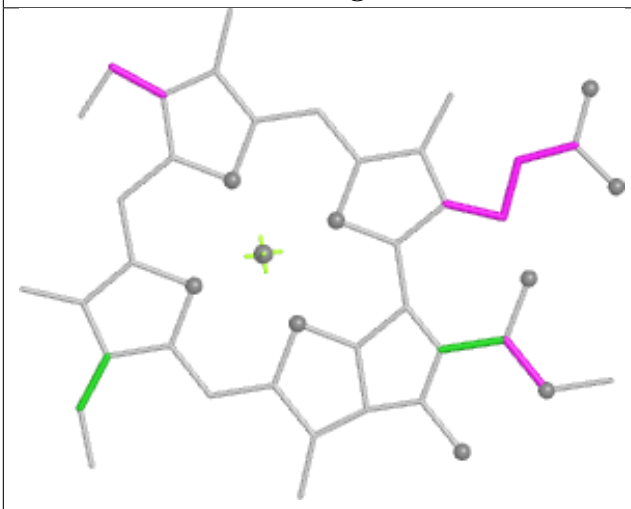
Ligand CLA 5 601



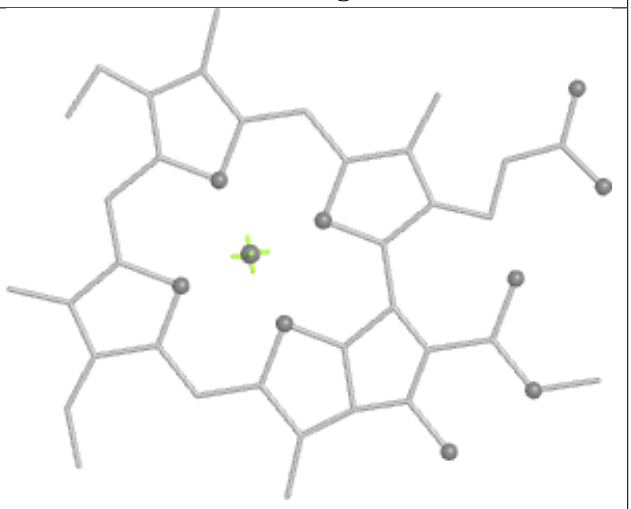
Bond lengths



Bond angles

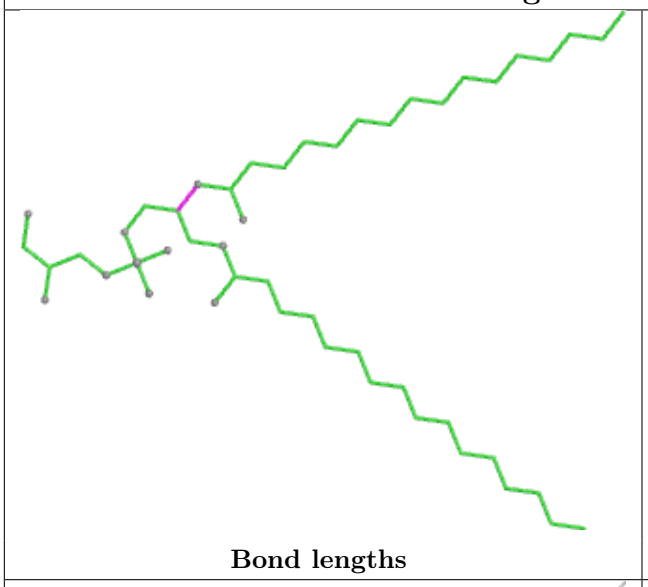


Torsions

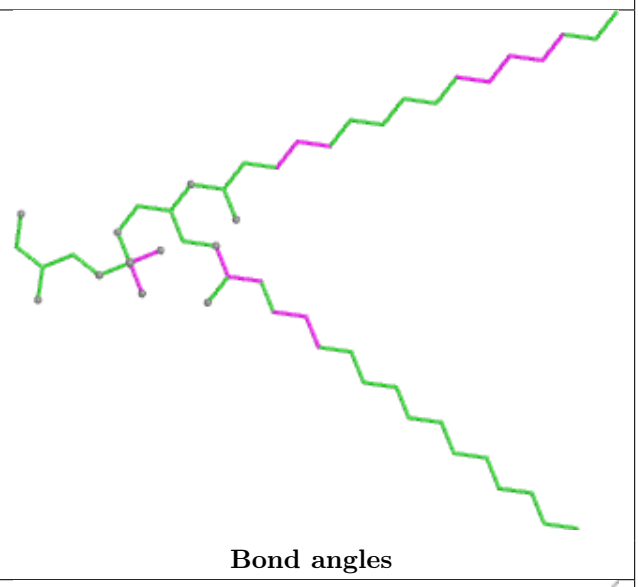


Rings

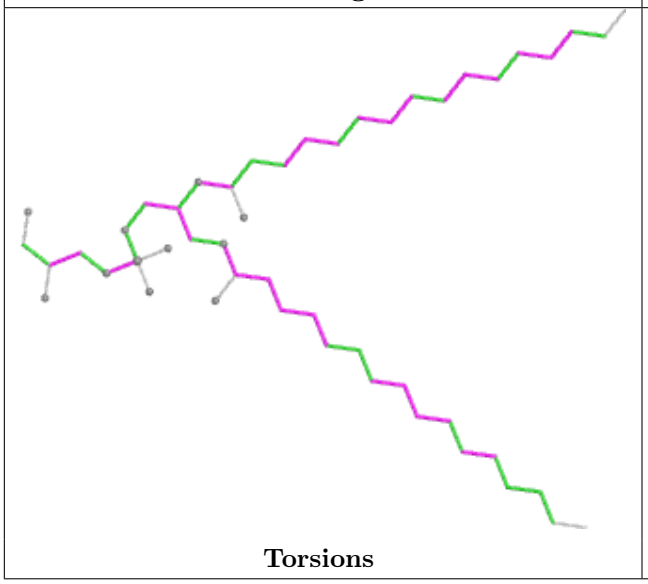
Ligand LHG A 841



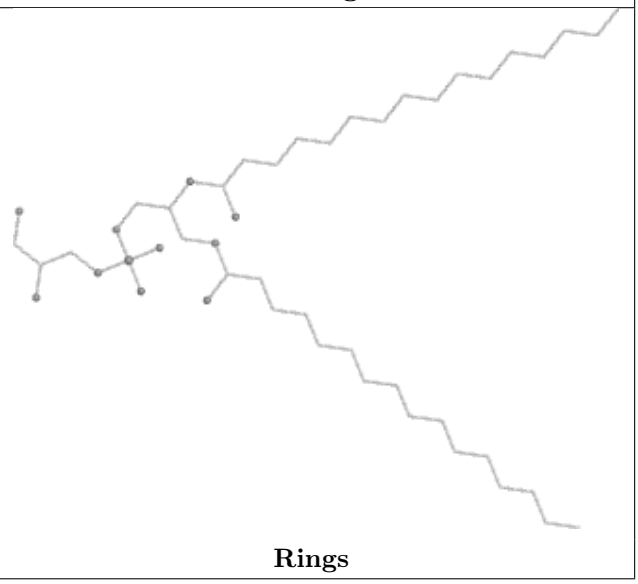
Bond lengths



Bond angles

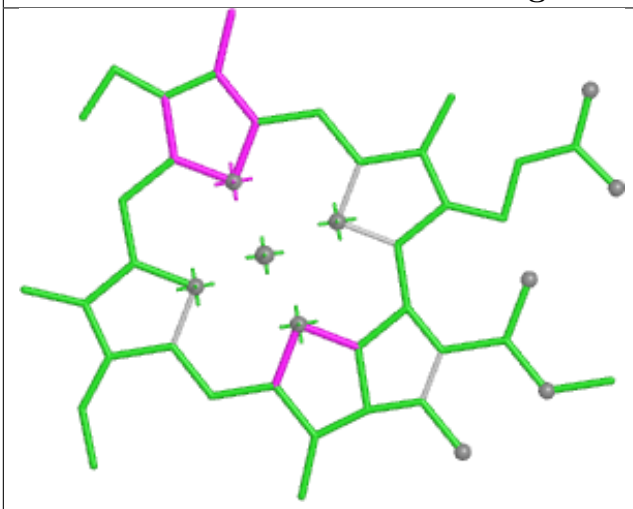


Torsions

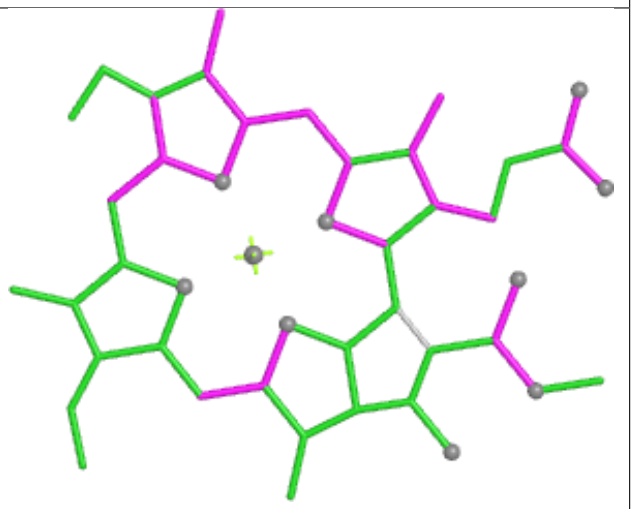


Rings

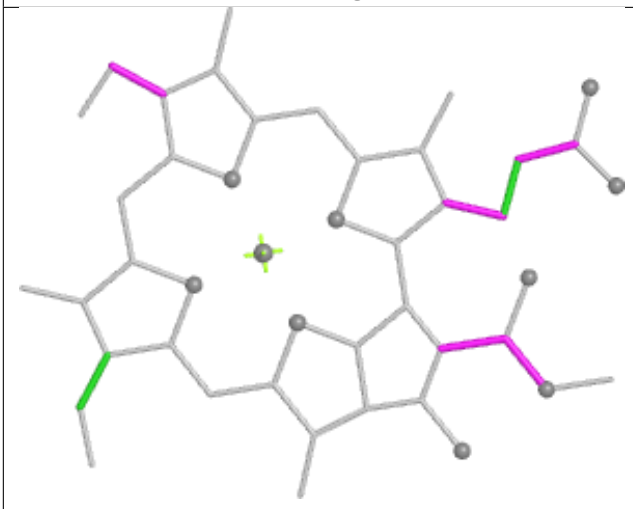
Ligand CLA 5 602



Bond lengths



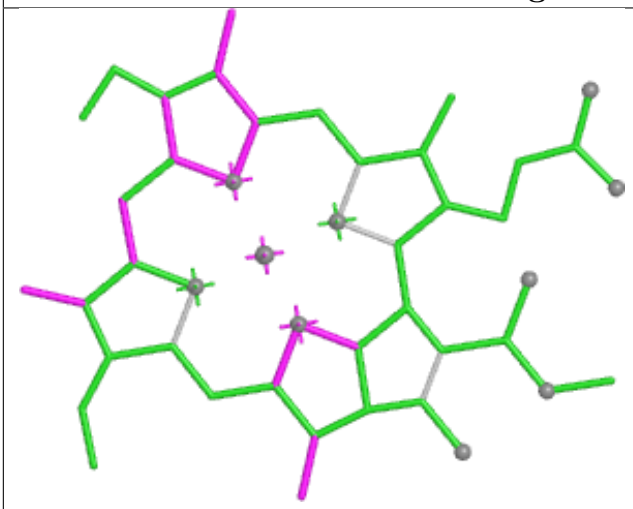
Bond angles



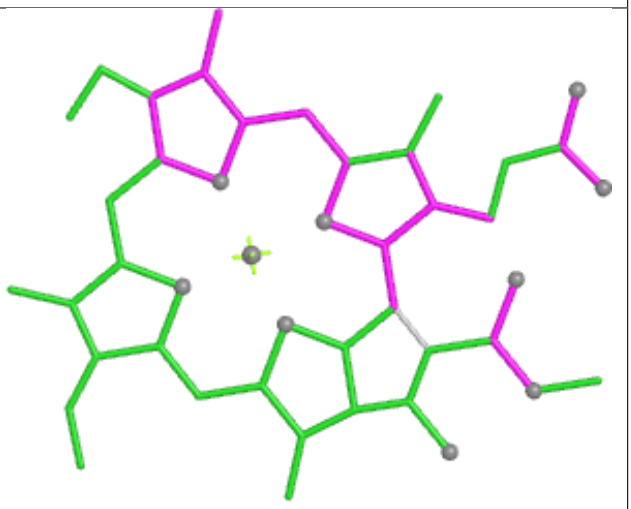
Torsions

Rings

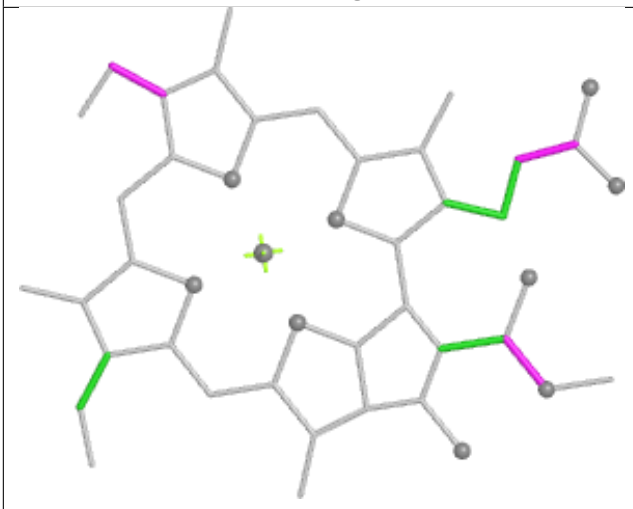
Ligand CLA 1 610



Bond lengths



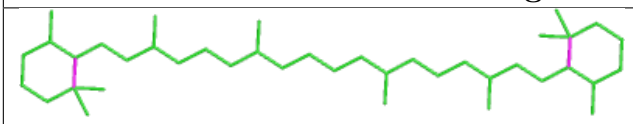
Bond angles



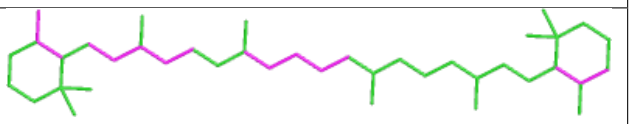
Torsions

Rings

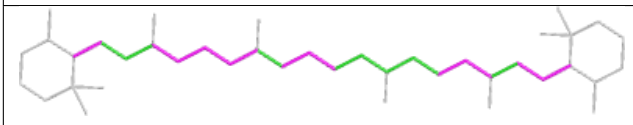
Ligand BCR L 206



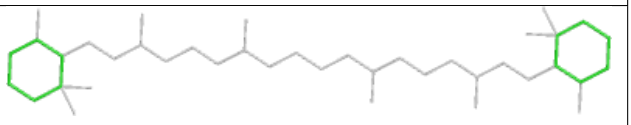
Bond lengths



Bond angles

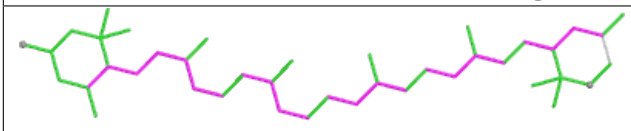


Torsions

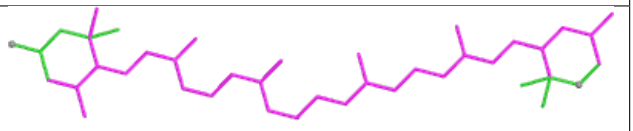


Rings

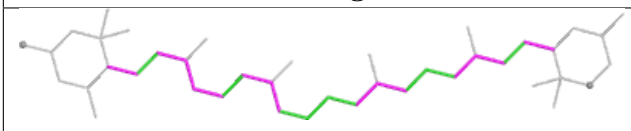
Ligand ZEX 1 613



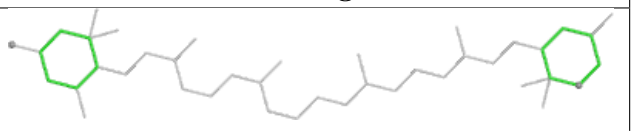
Bond lengths



Bond angles

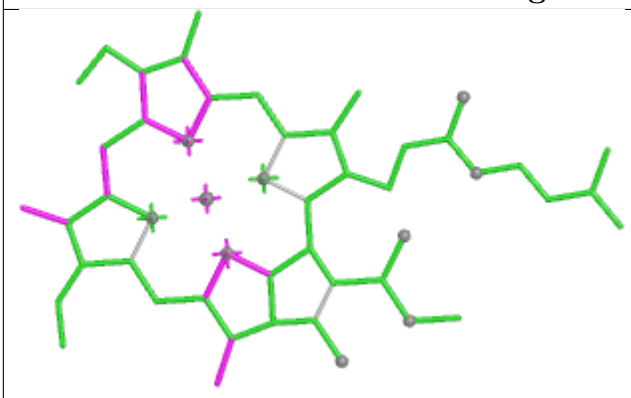


Torsions

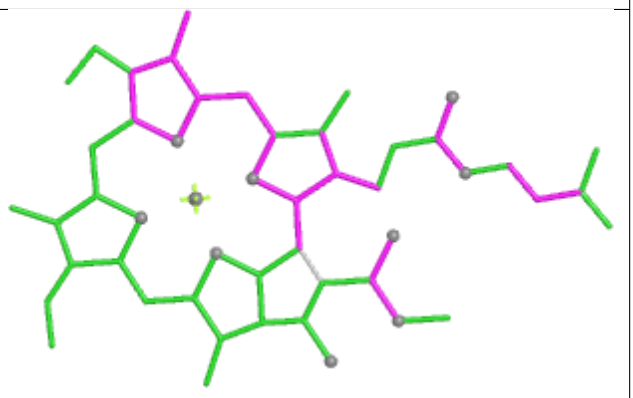


Rings

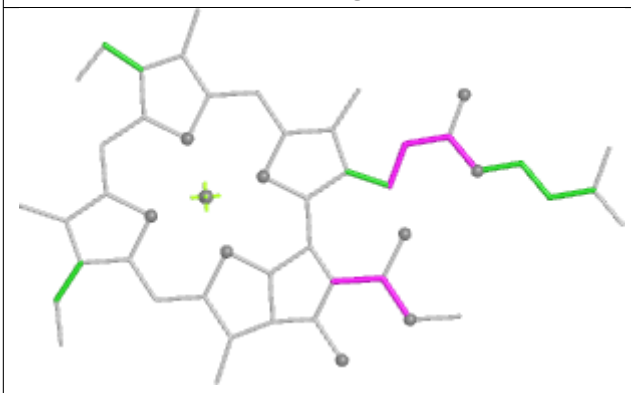
Ligand CLA 2 608



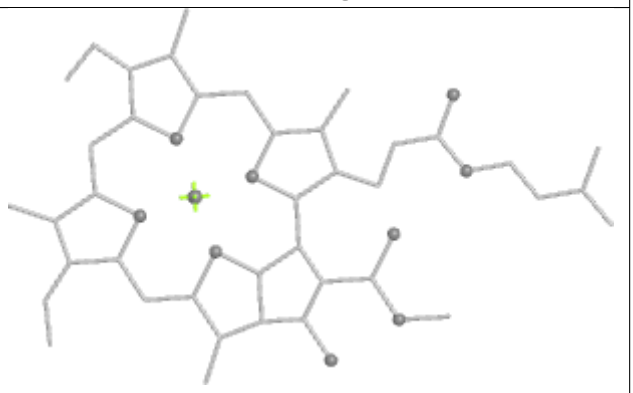
Bond lengths



Bond angles

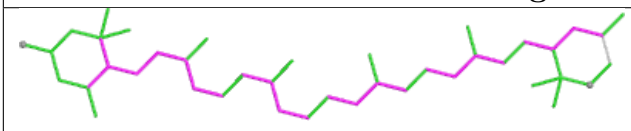


Torsions

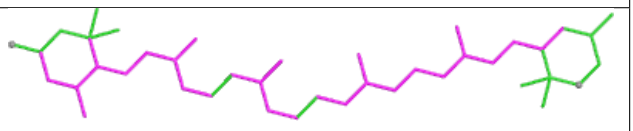


Rings

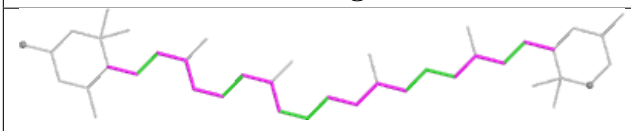
Ligand ZEX 4 615



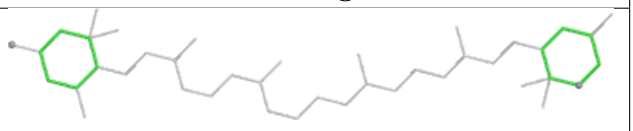
Bond lengths



Bond angles

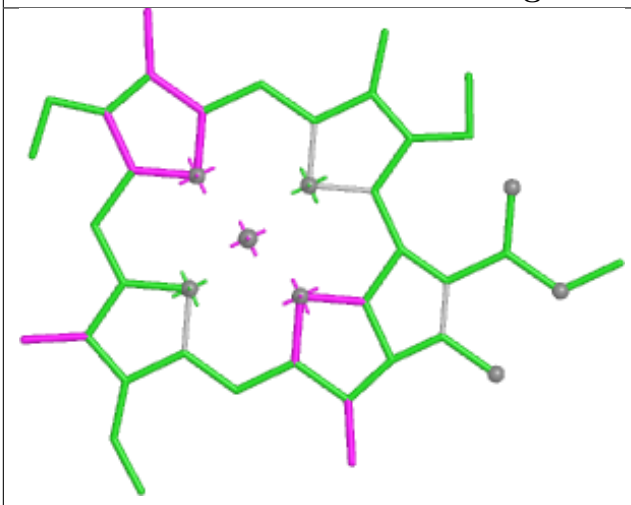


Torsions

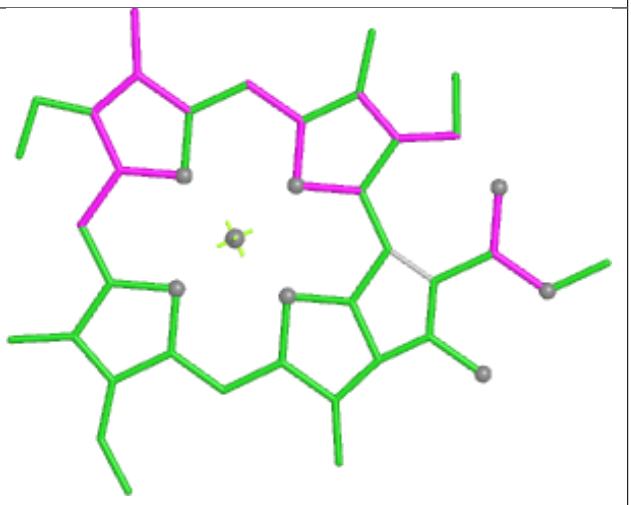


Rings

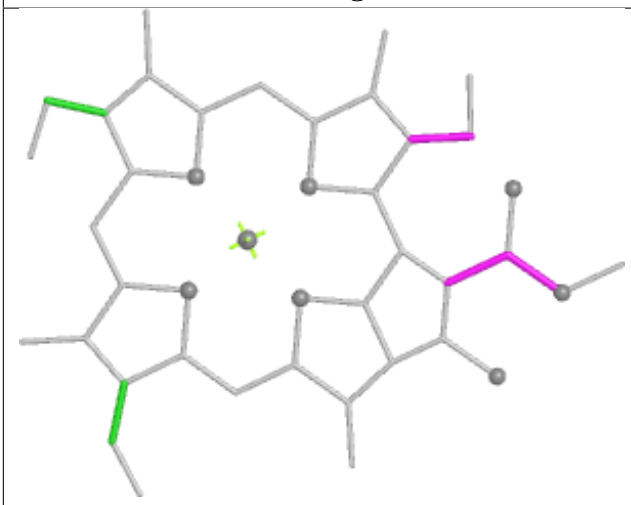
Ligand CLA A 813



Bond lengths



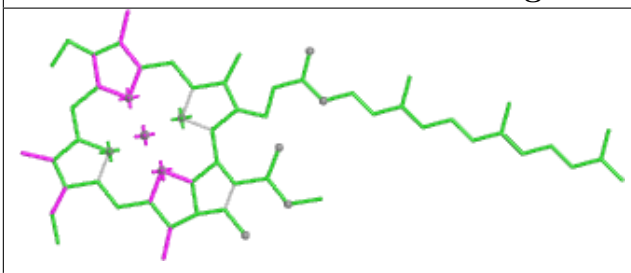
Bond angles



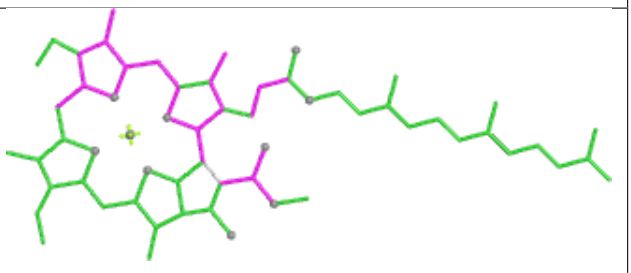
Torsions

Rings

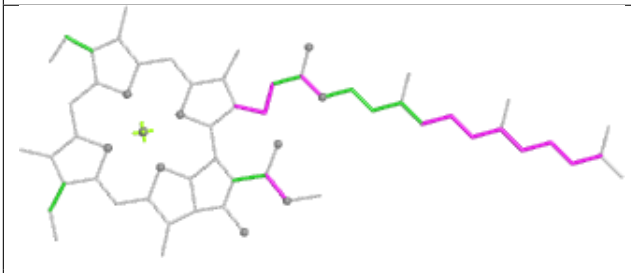
Ligand CLA B 821



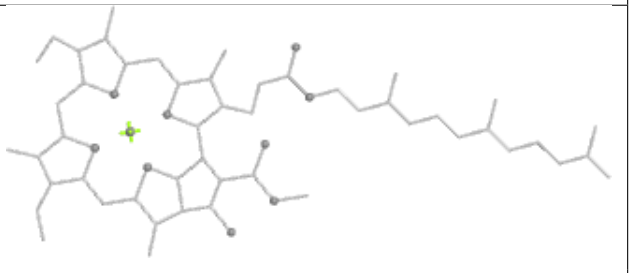
Bond lengths



Bond angles

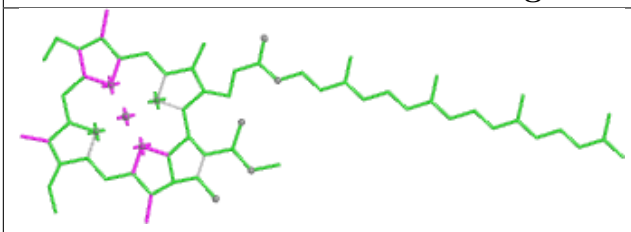


Torsions

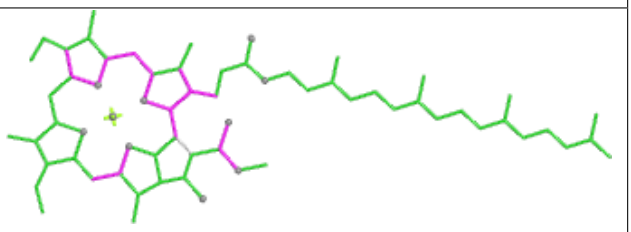


Rings

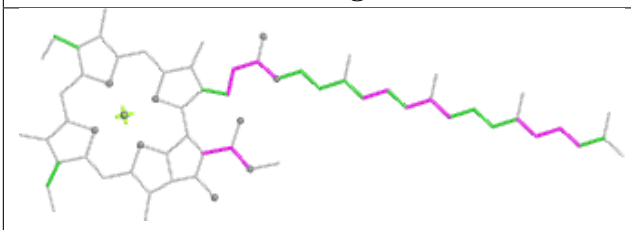
Ligand CLA B 835



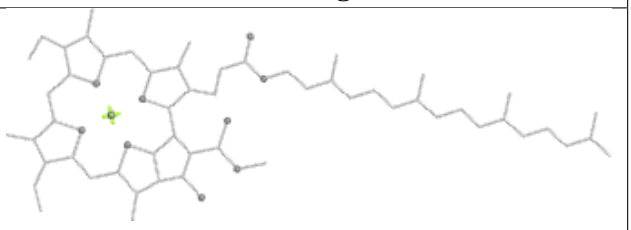
Bond lengths



Bond angles

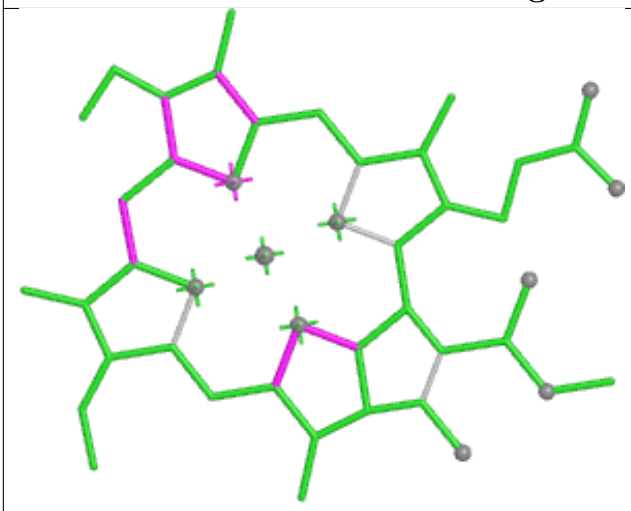


Torsions

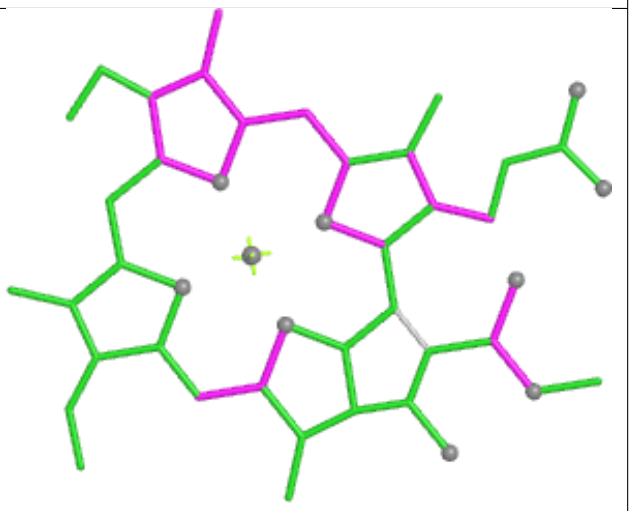


Rings

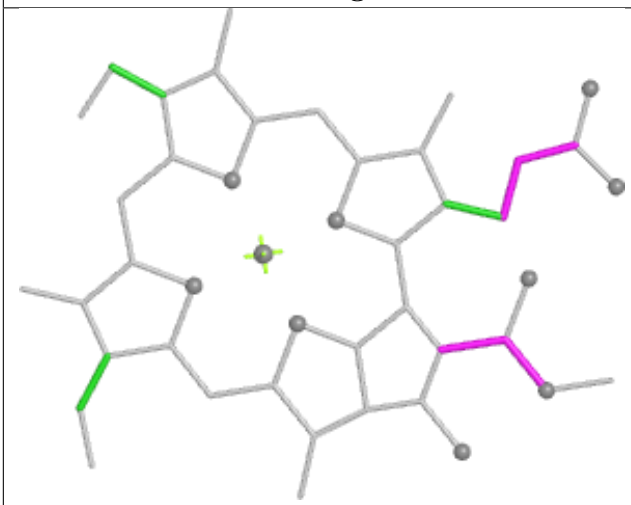
Ligand CLA 5 611



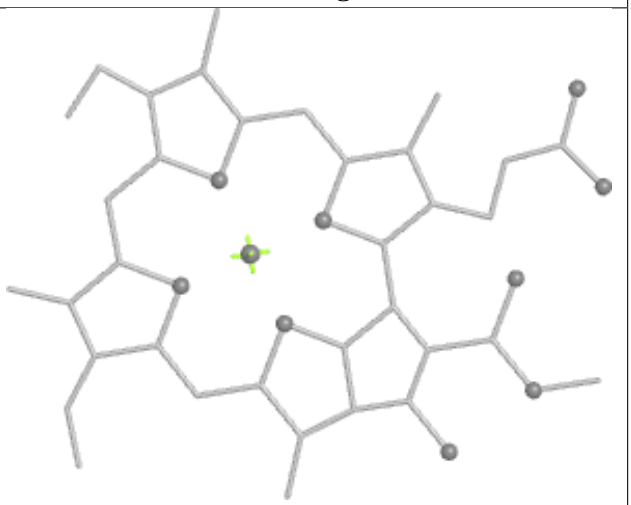
Bond lengths



Bond angles

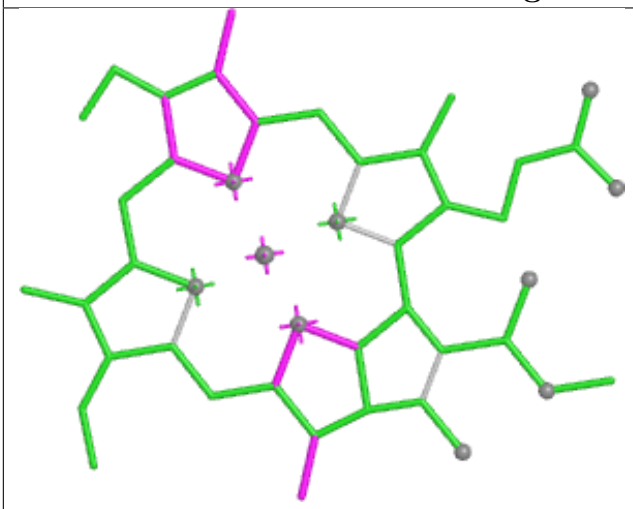


Torsions

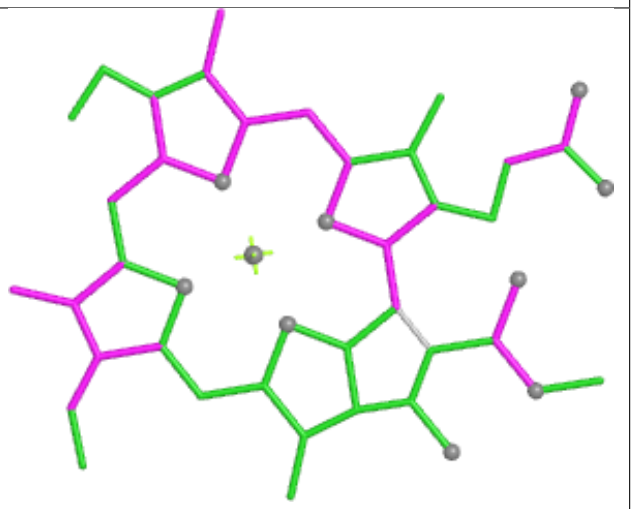


Rings

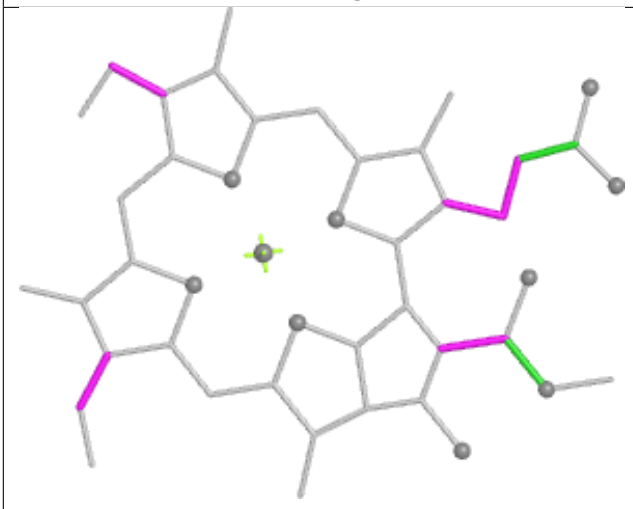
Ligand CLA A 818



Bond lengths



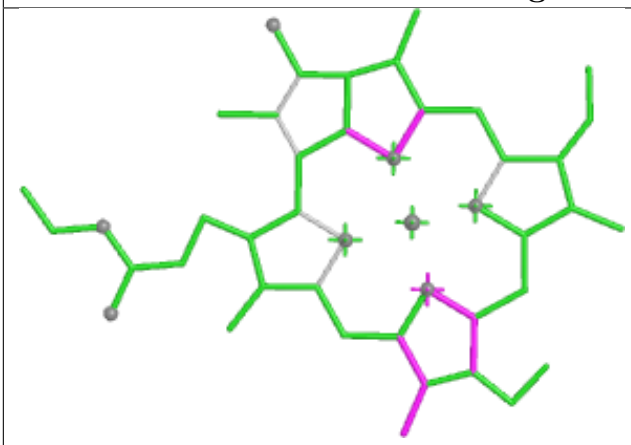
Bond angles



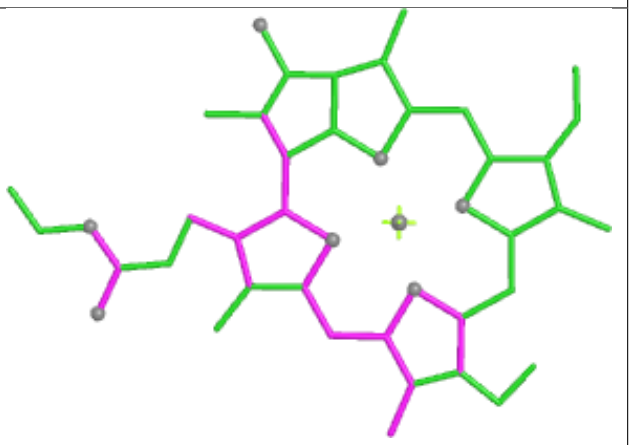
Torsions

Rings

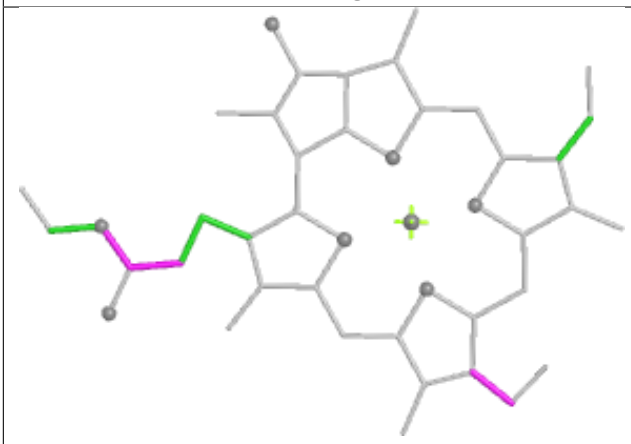
Ligand CLA 5 613



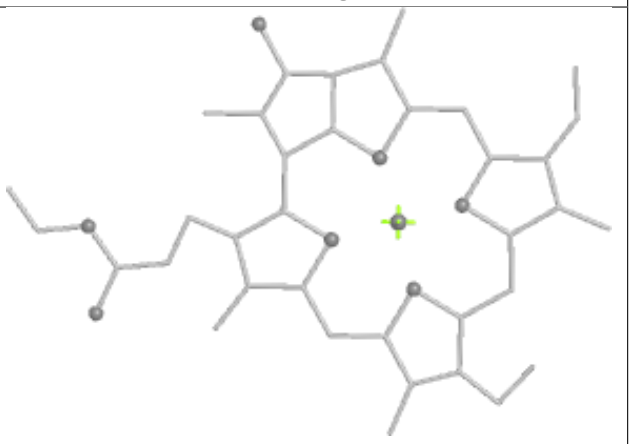
Bond lengths



Bond angles

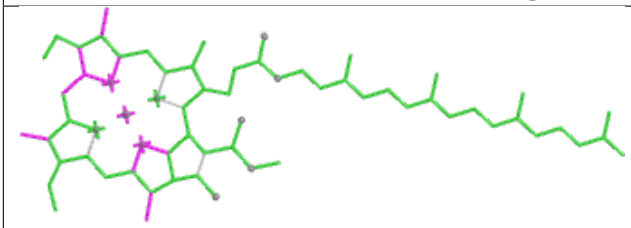


Torsions

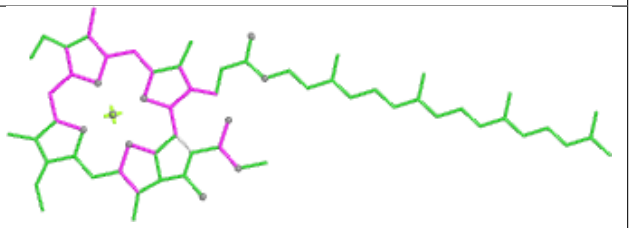


Rings

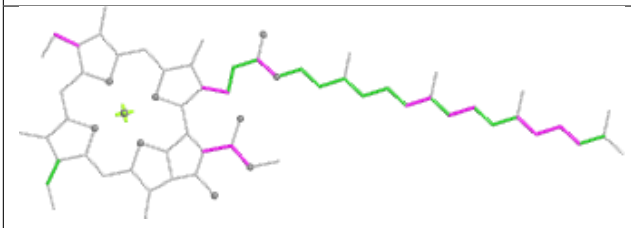
Ligand CLA A 817



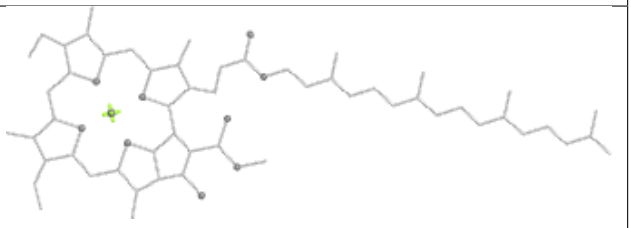
Bond lengths



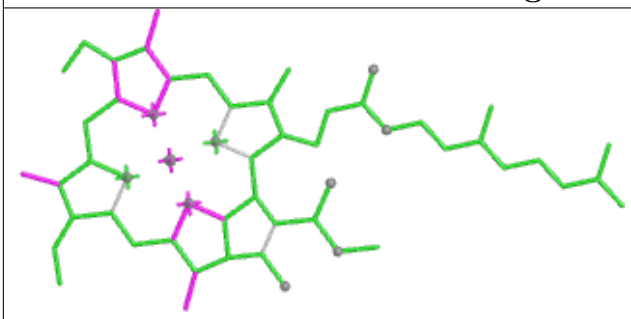
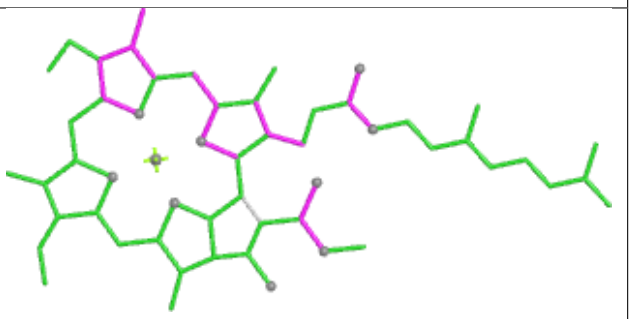
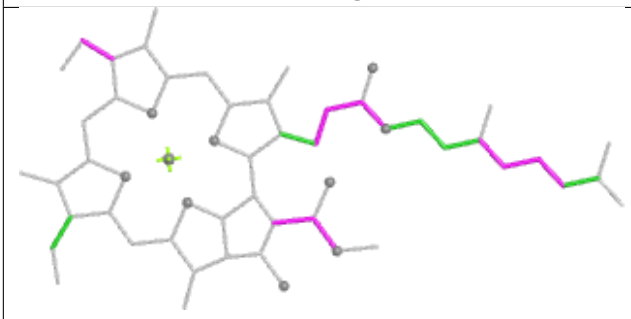
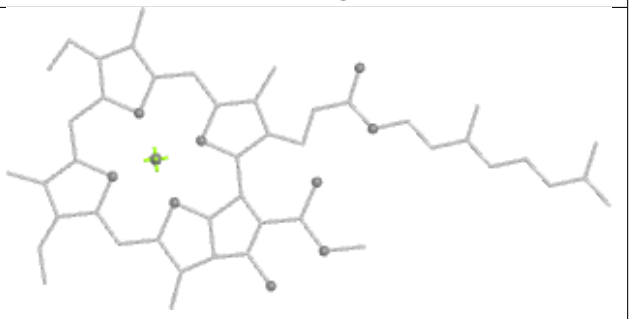
Bond angles

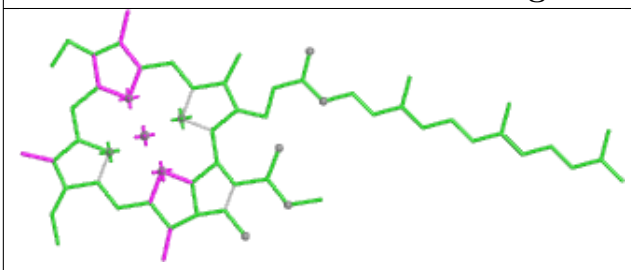
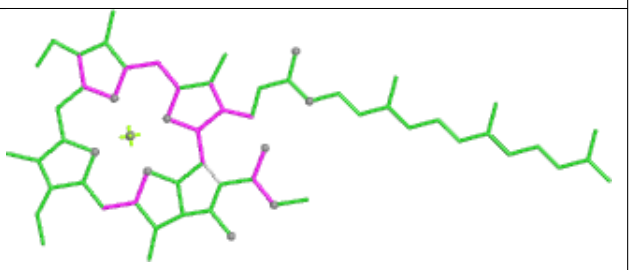
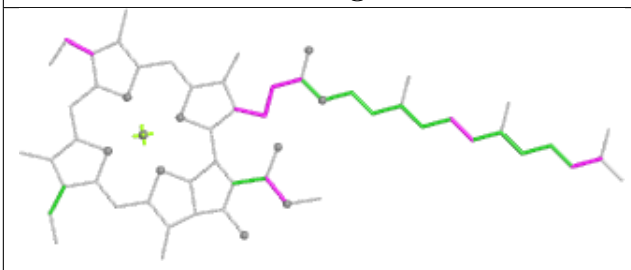
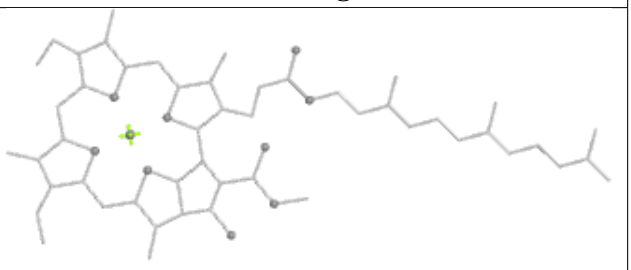


Torsions

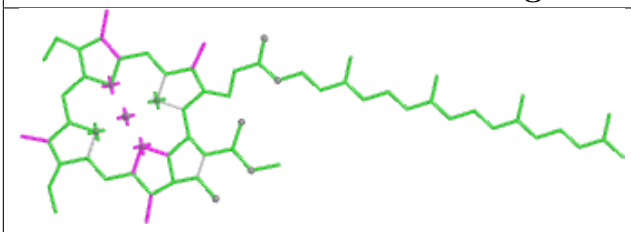


Rings

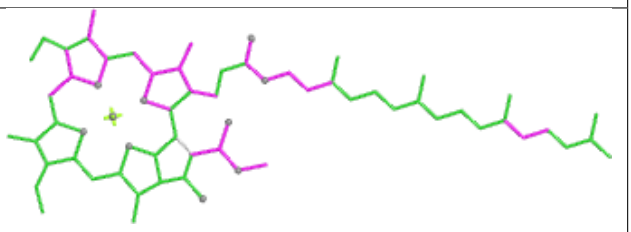
Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

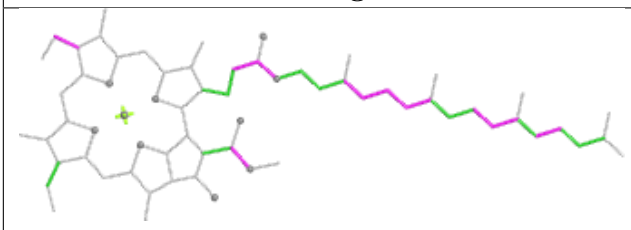
Ligand CLA B 806



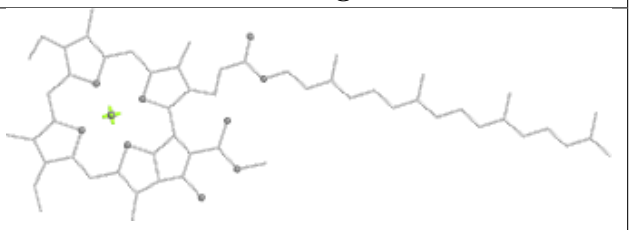
Bond lengths



Bond angles

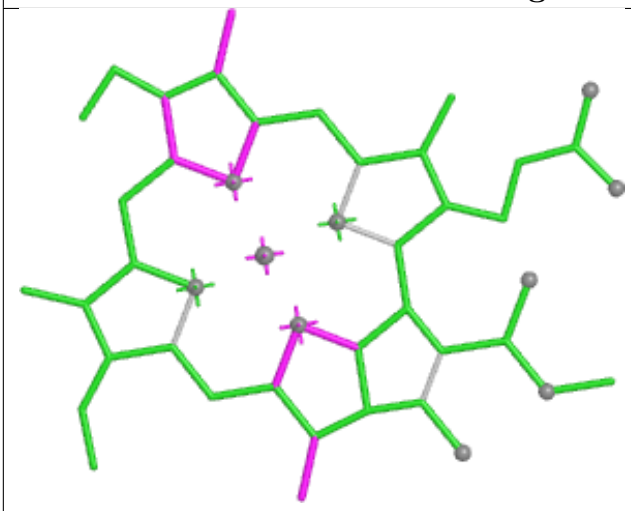


Torsions

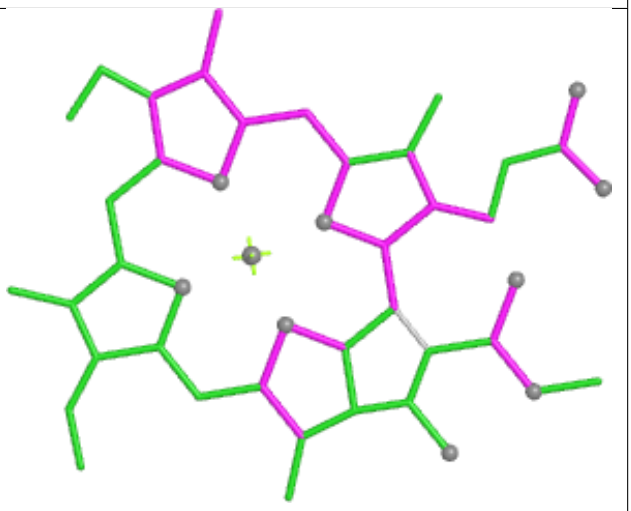


Rings

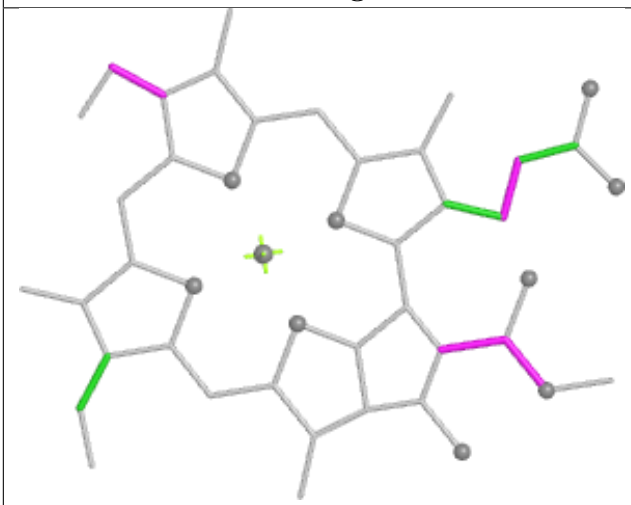
Ligand CLA 3 206



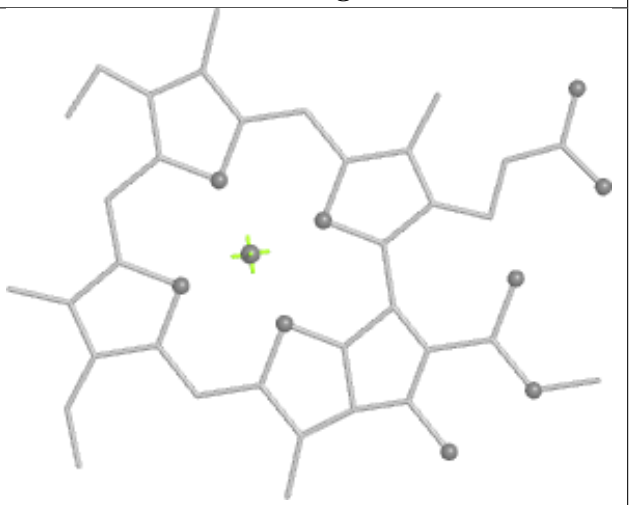
Bond lengths



Bond angles

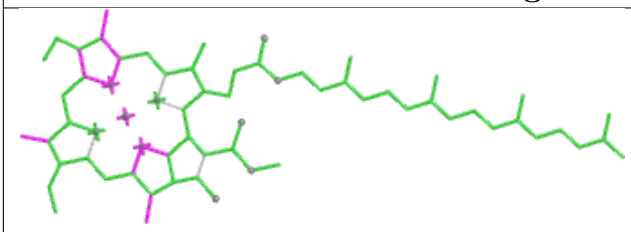


Torsions

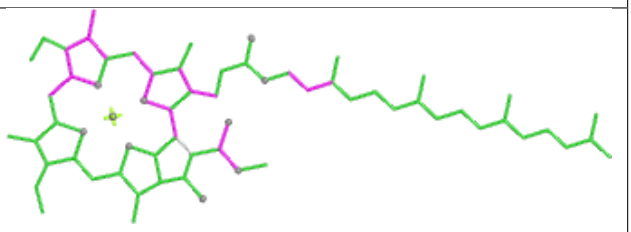


Rings

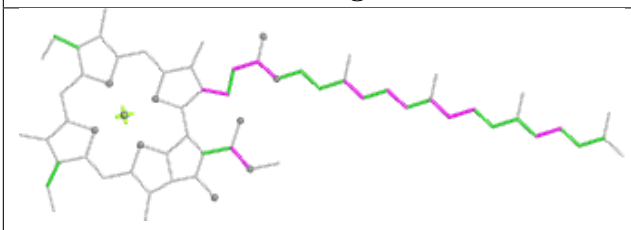
Ligand CLA A 804



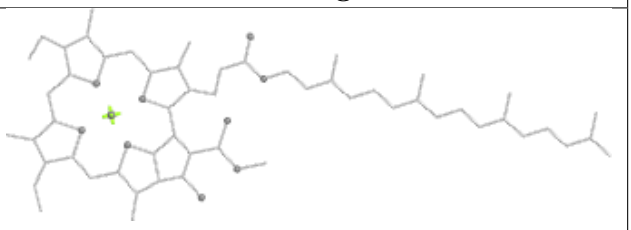
Bond lengths



Bond angles

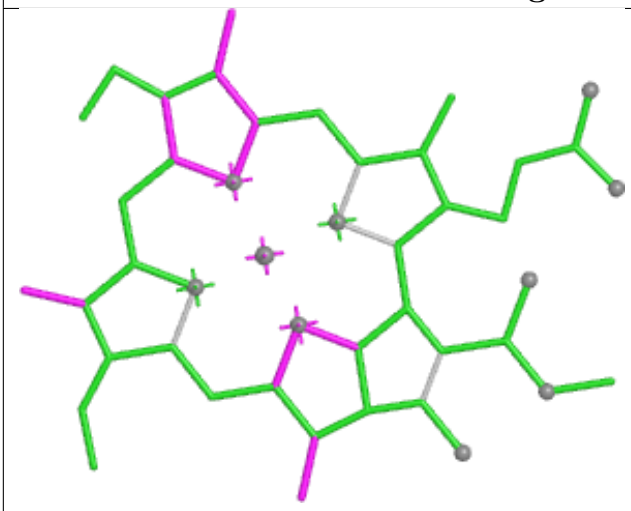


Torsions

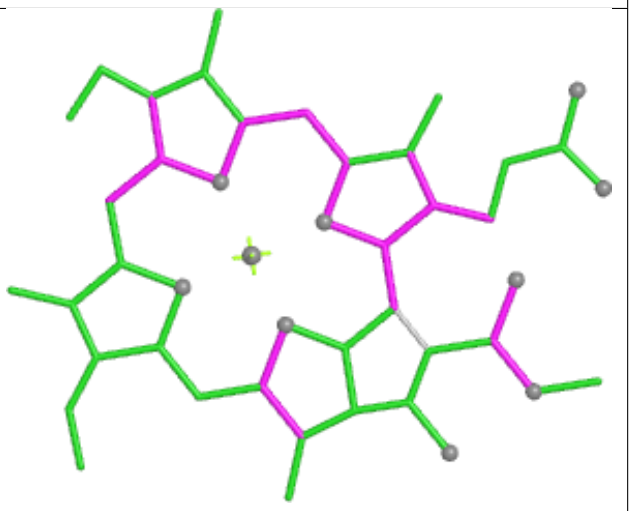


Rings

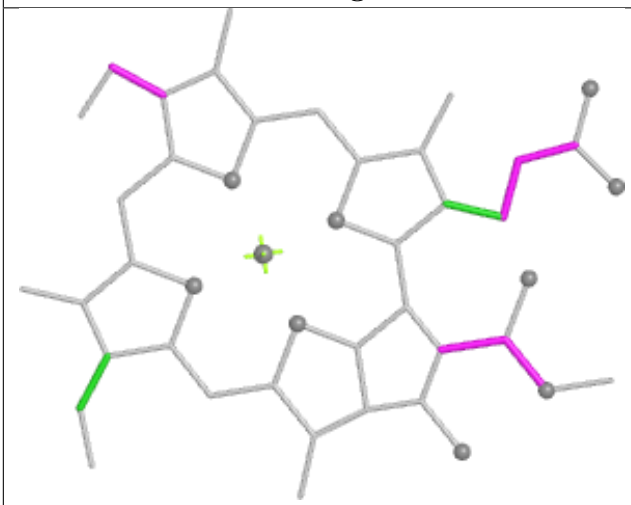
Ligand CLA 1 606



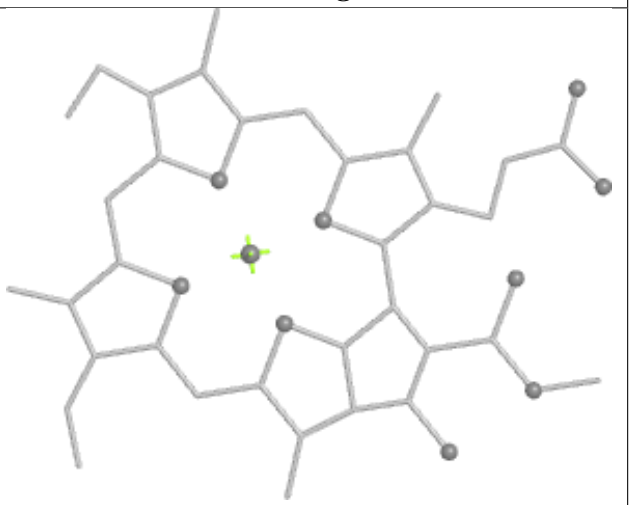
Bond lengths



Bond angles

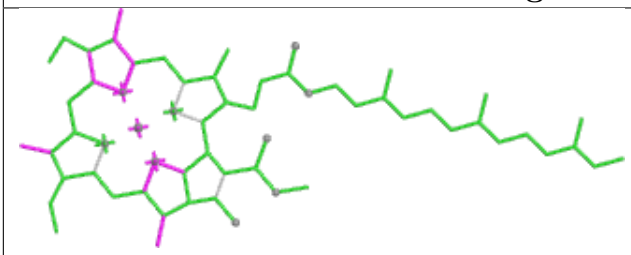


Torsions

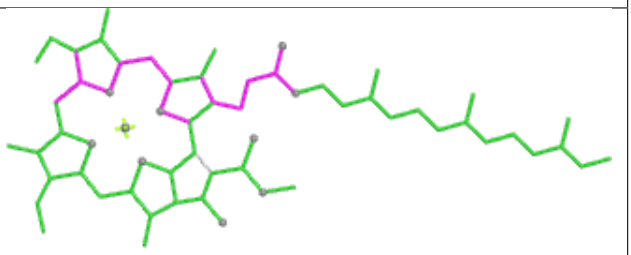


Rings

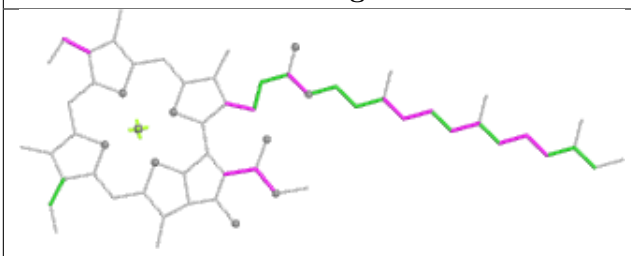
Ligand CLA F 301



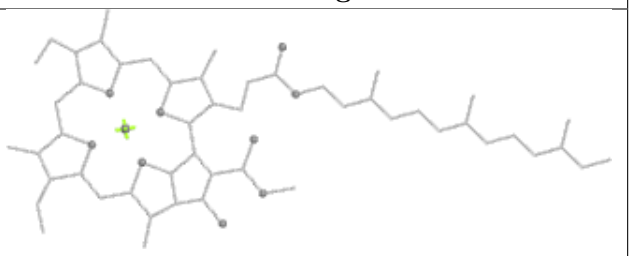
Bond lengths



Bond angles

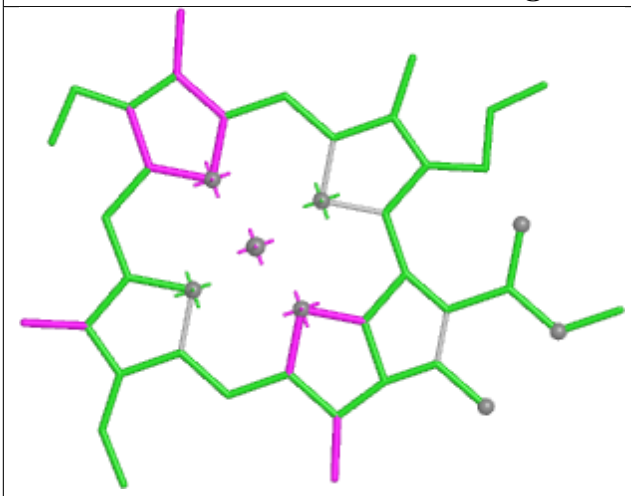


Torsions

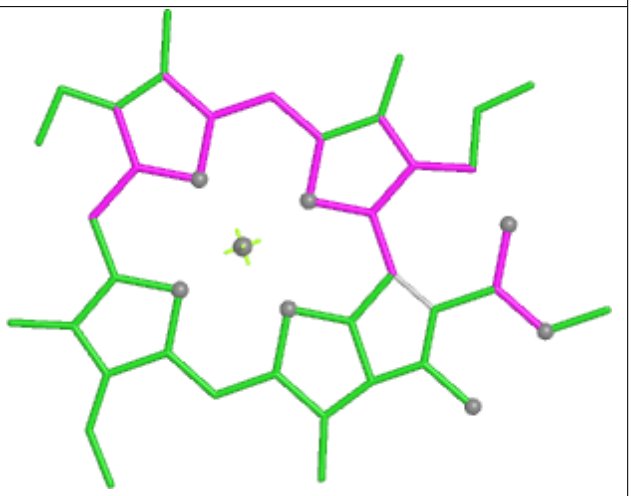


Rings

Ligand CLA B 825

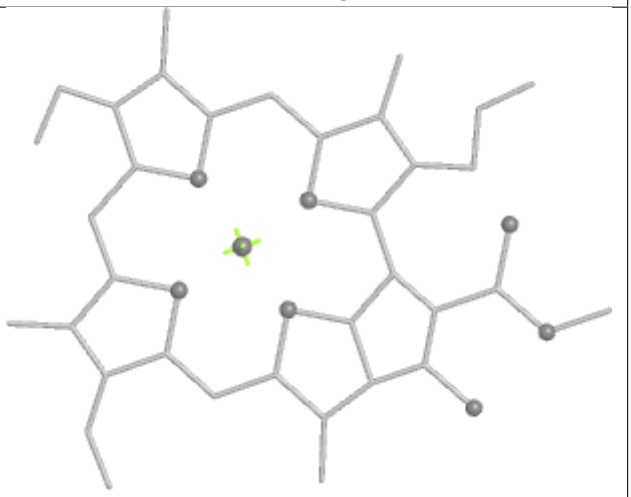


Bond lengths



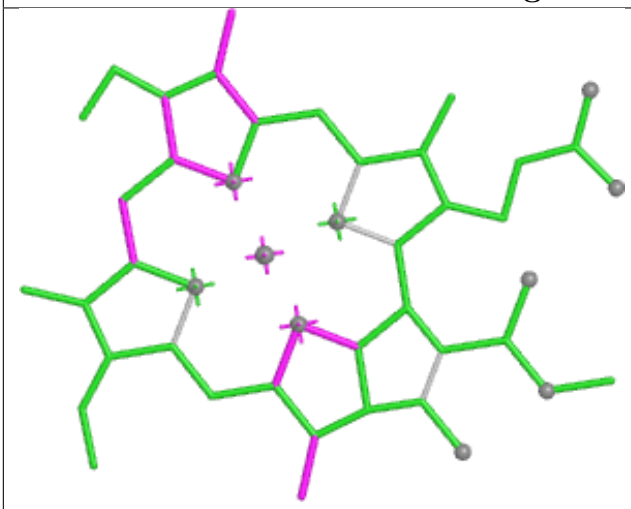
Bond angles

Torsions

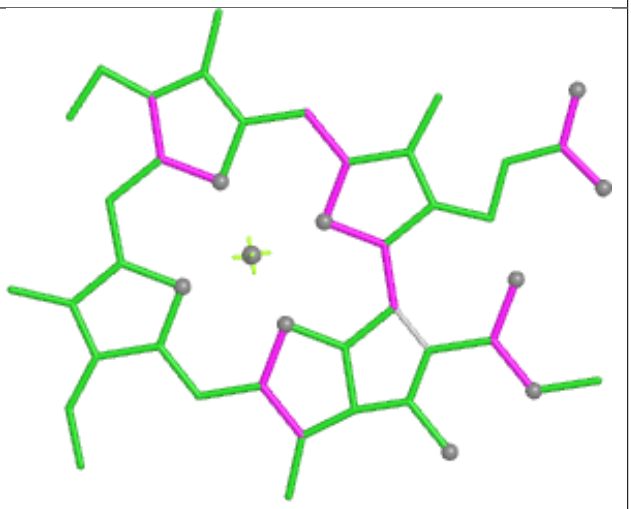


Rings

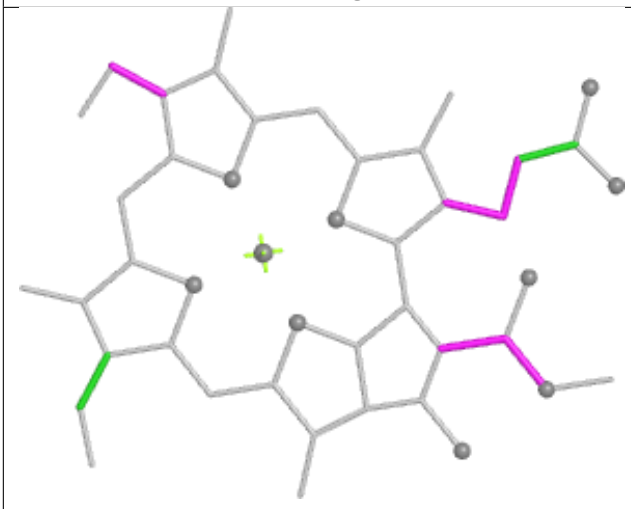
Ligand CLA O 205



Bond lengths



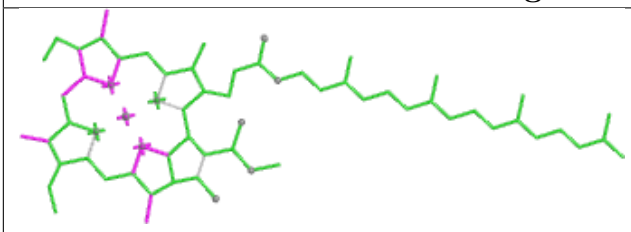
Bond angles



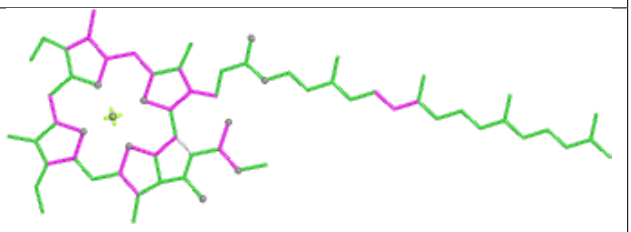
Torsions

Rings

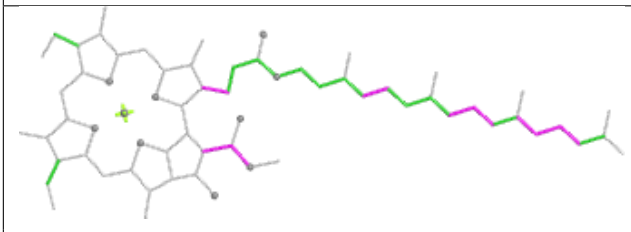
Ligand CLA B 832



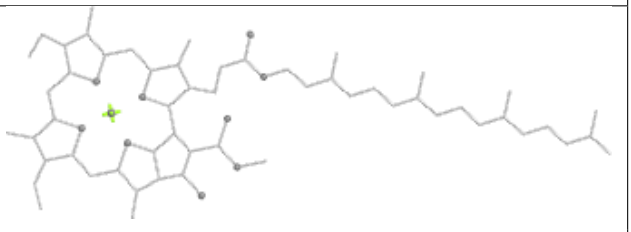
Bond lengths



Bond angles

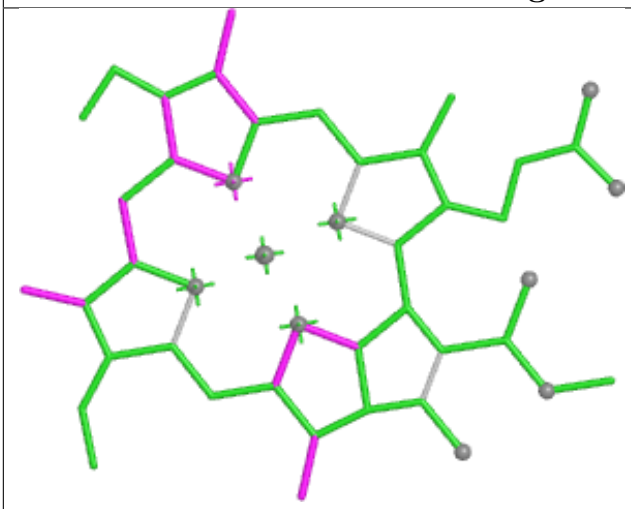


Torsions

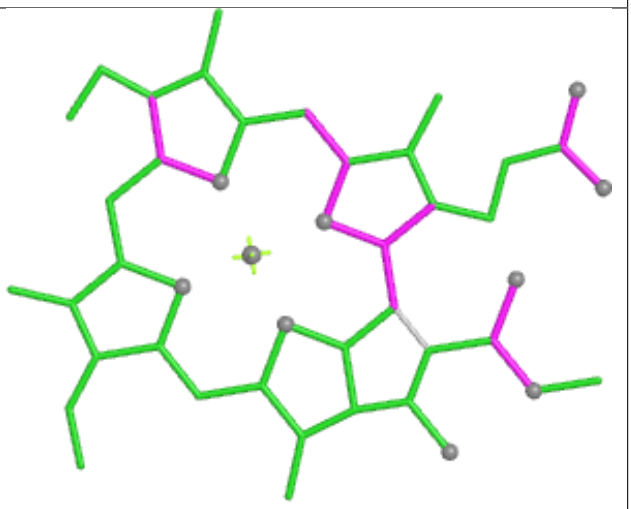


Rings

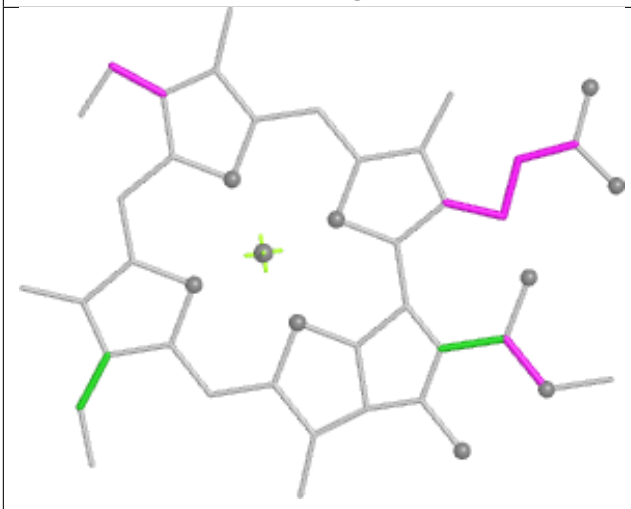
Ligand CLA 4 604



Bond lengths



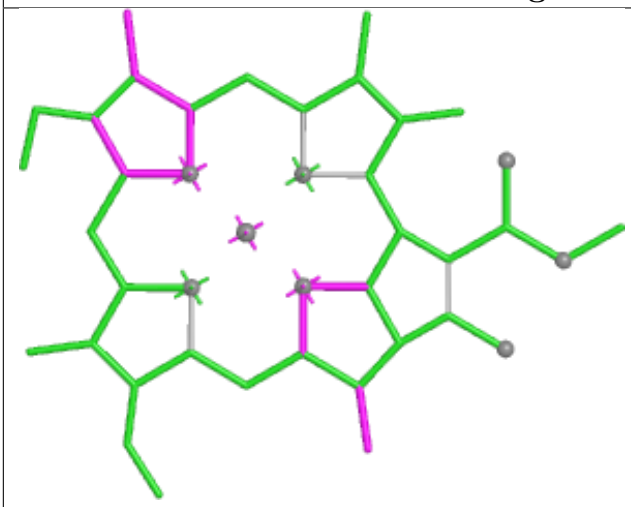
Bond angles



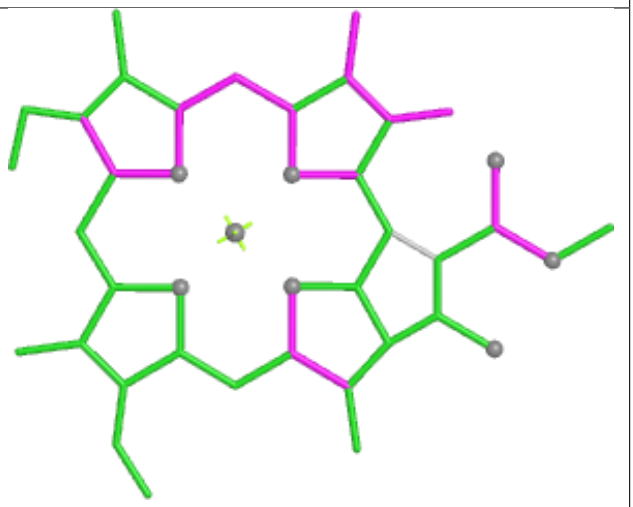
Torsions

Rings

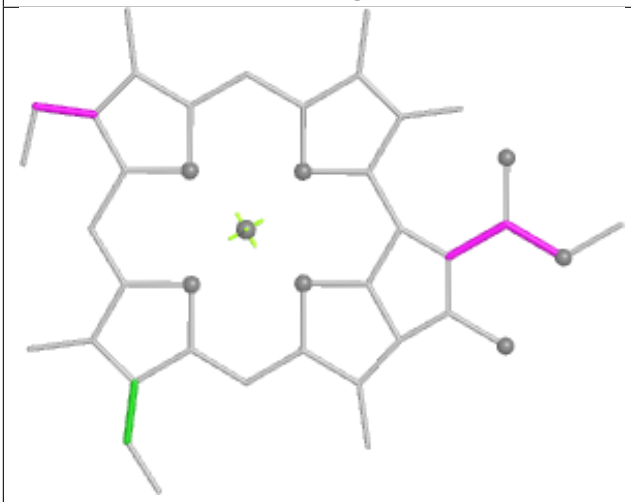
Ligand CLA 2 609



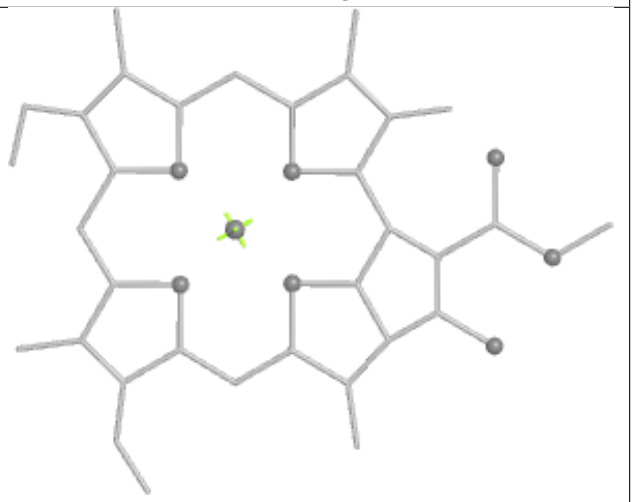
Bond lengths



Bond angles

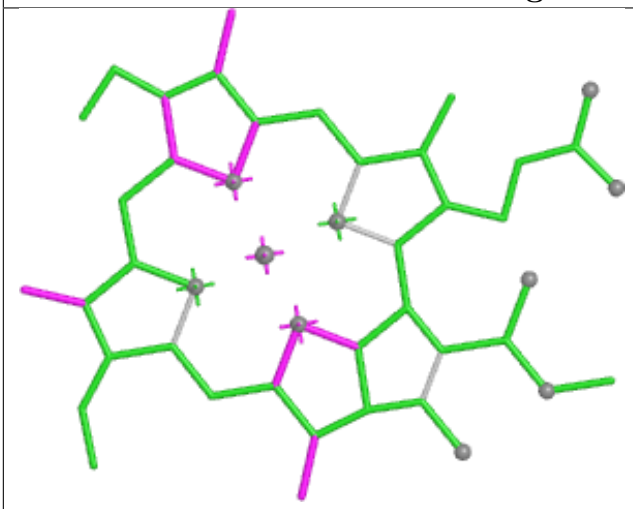


Torsions

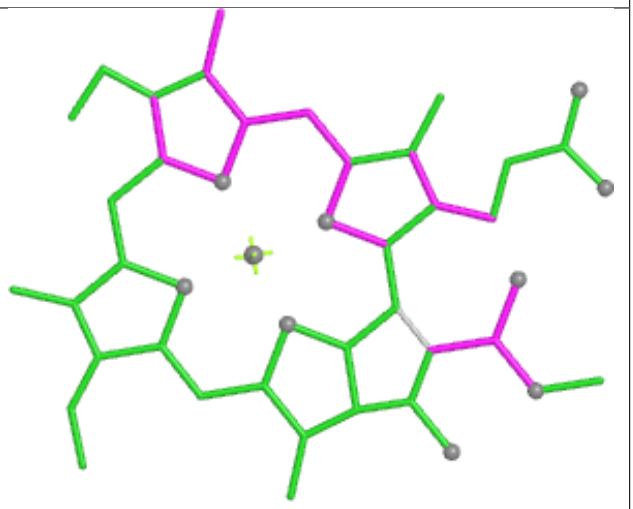


Rings

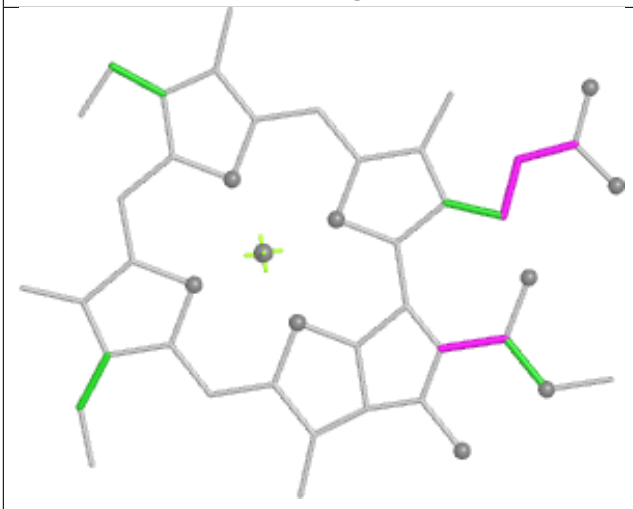
Ligand CLA F 302



Bond lengths



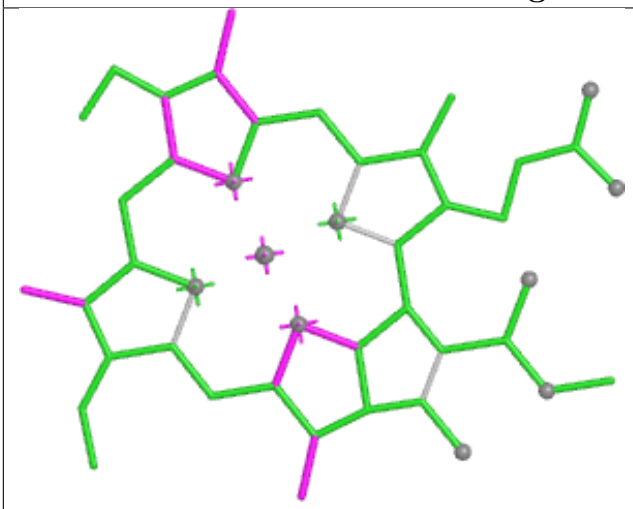
Bond angles



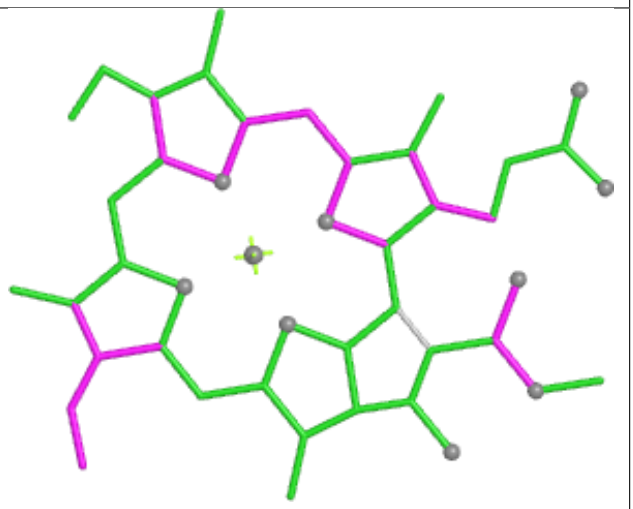
Torsions

Rings

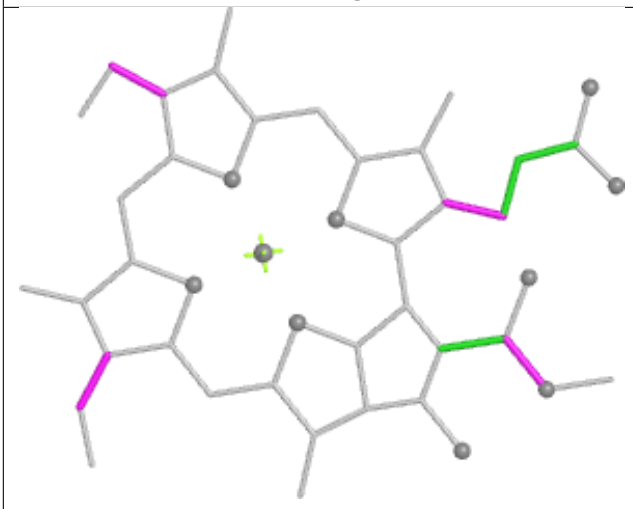
Ligand CLA 2 611



Bond lengths



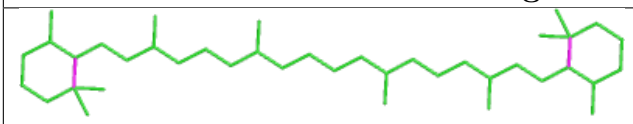
Bond angles



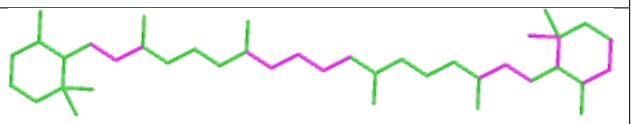
Torsions

Rings

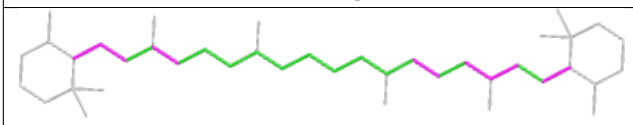
Ligand BCR B 846



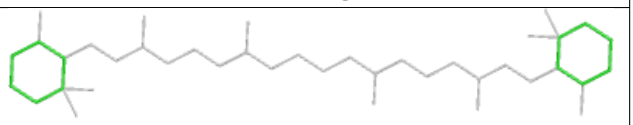
Bond lengths



Bond angles

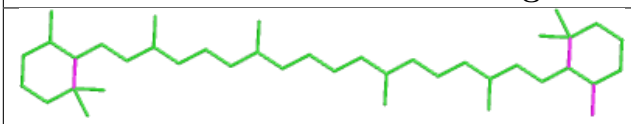


Torsions

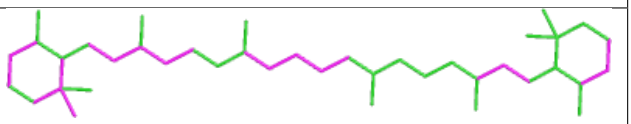


Rings

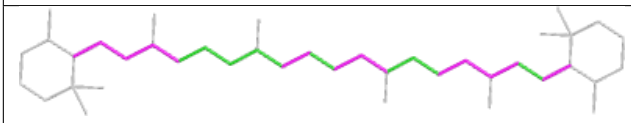
Ligand BCR B 850



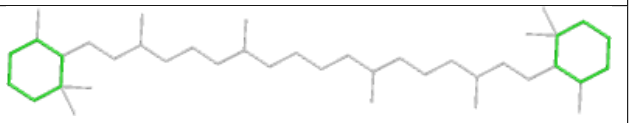
Bond lengths



Bond angles



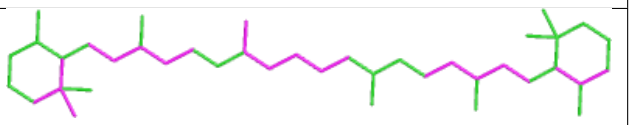
Torsions



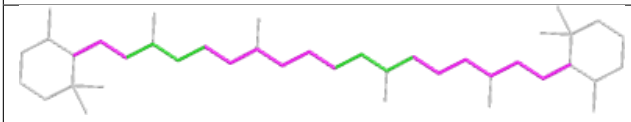
Rings

Ligand BCR F 304

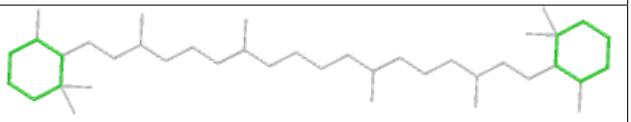
Bond lengths



Bond angles

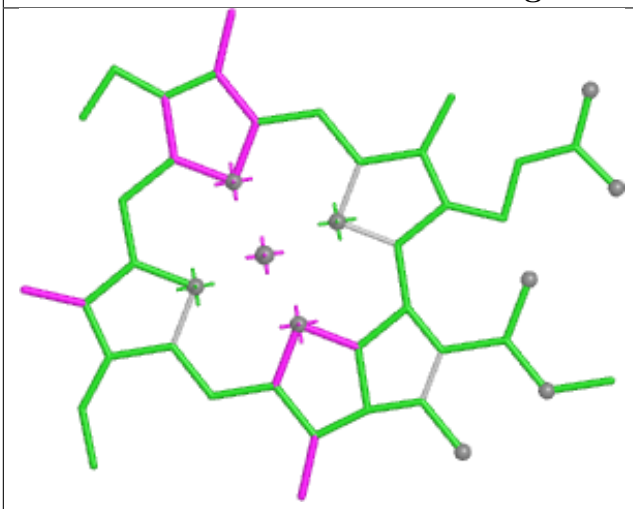


Torsions

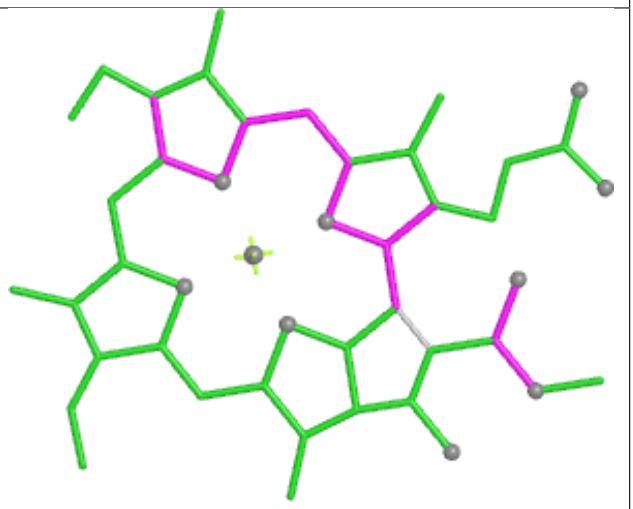


Rings

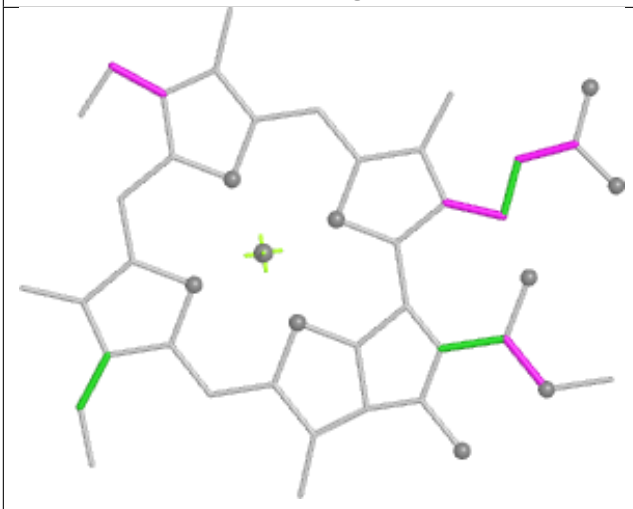
Ligand CLA B 837



Bond lengths



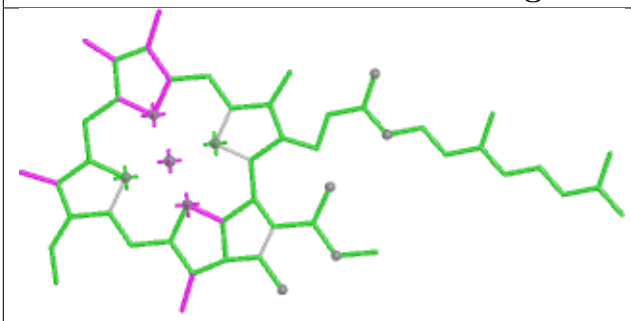
Bond angles



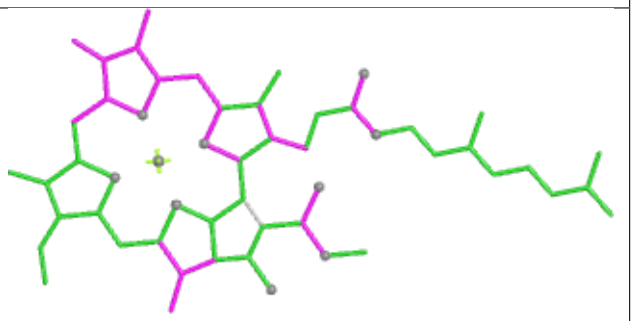
Torsions

Rings

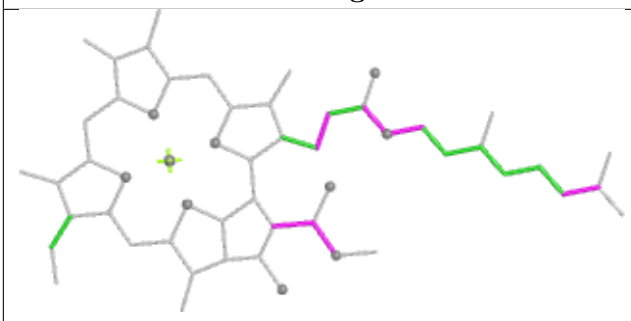
Ligand CLA B 814



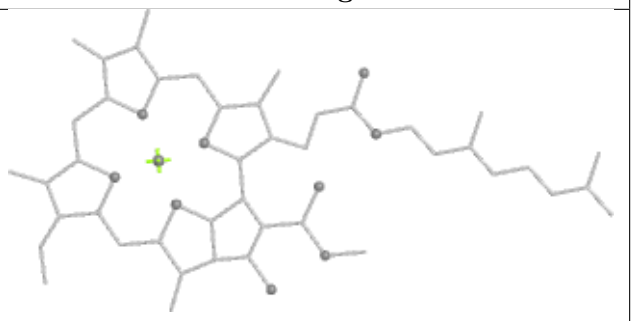
Bond lengths



Bond angles

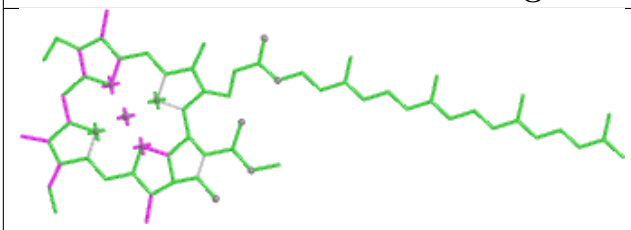


Torsions

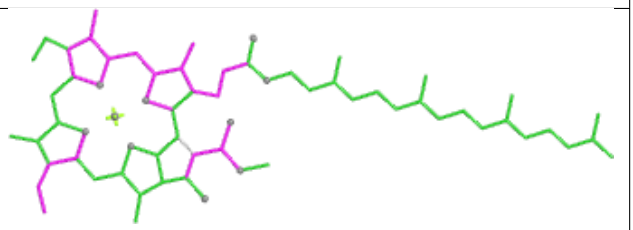


Rings

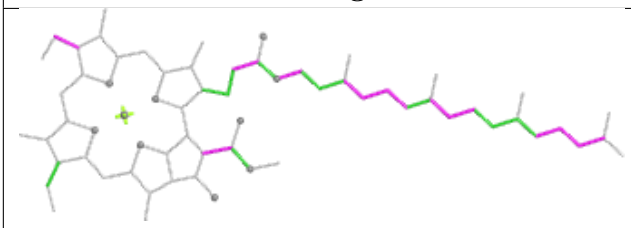
Ligand CLA B 801



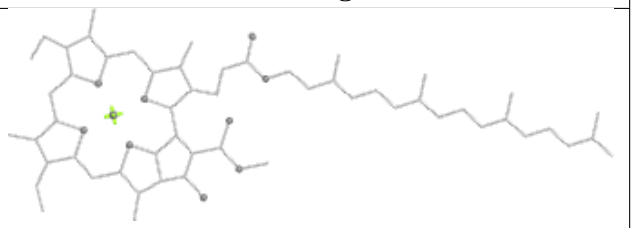
Bond lengths



Bond angles

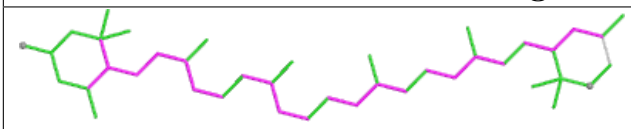


Torsions

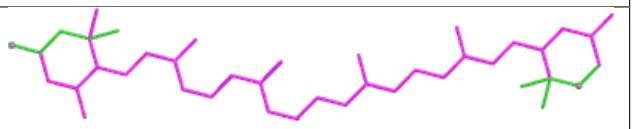


Rings

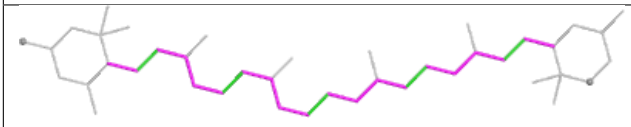
Ligand ZEX 1 615



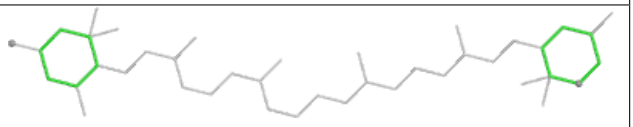
Bond lengths



Bond angles

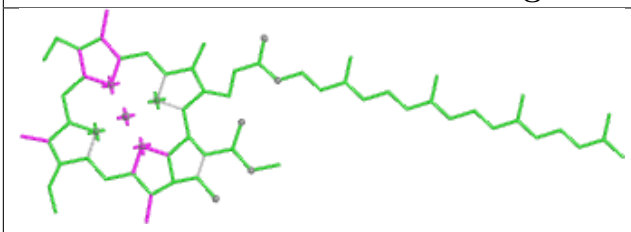


Torsions

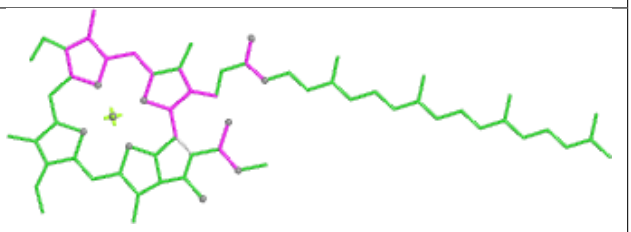


Rings

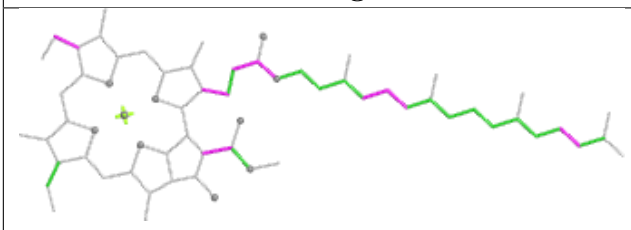
Ligand CLA A 825



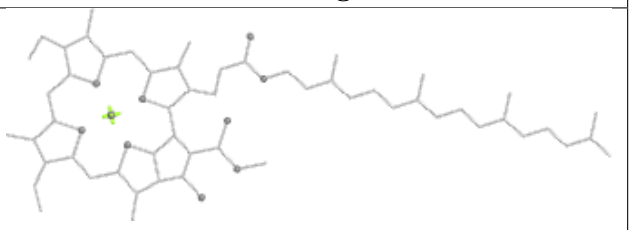
Bond lengths



Bond angles

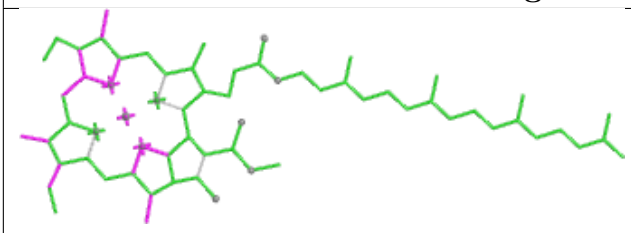


Torsions

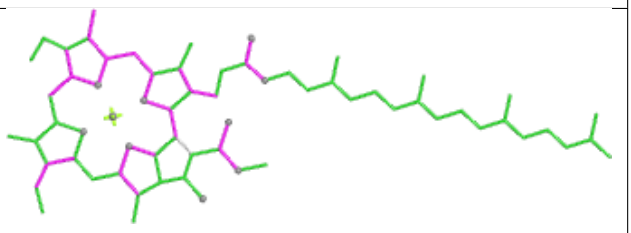


Rings

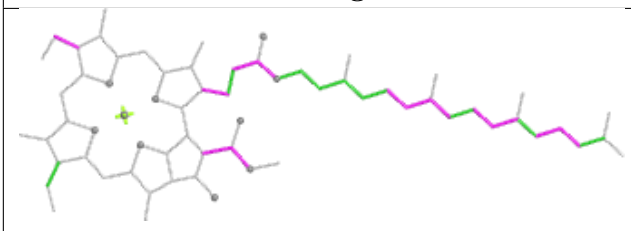
Ligand CLA B 812



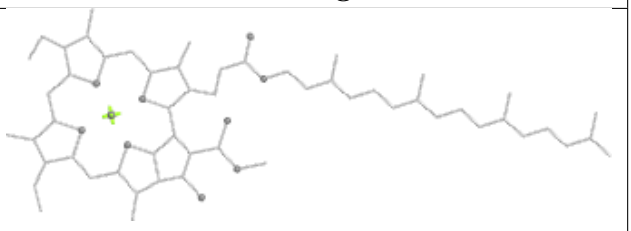
Bond lengths



Bond angles

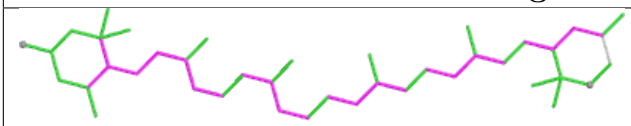


Torsions

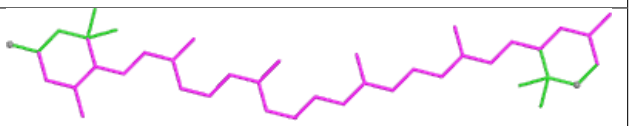


Rings

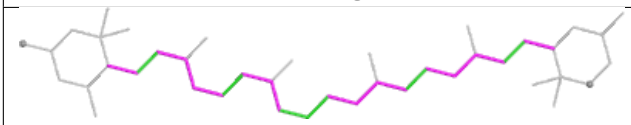
Ligand ZEX 1 616



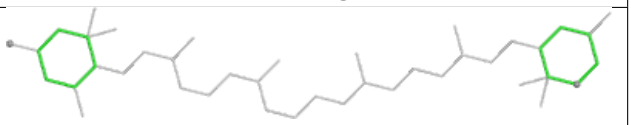
Bond lengths



Bond angles

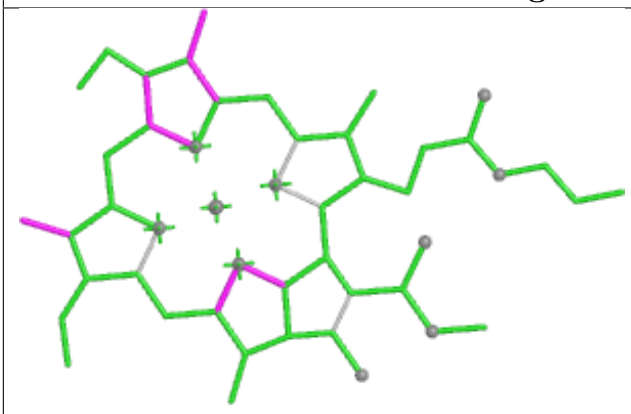


Torsions

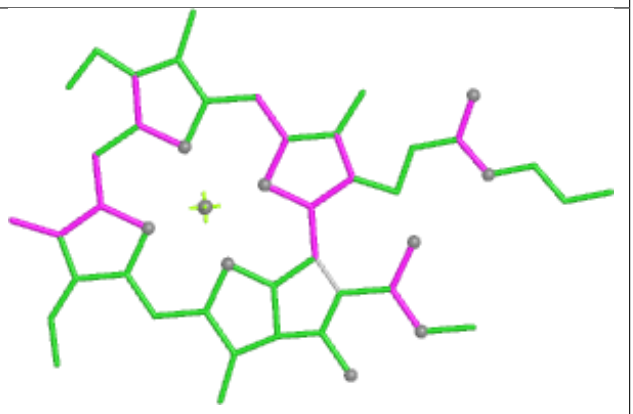


Rings

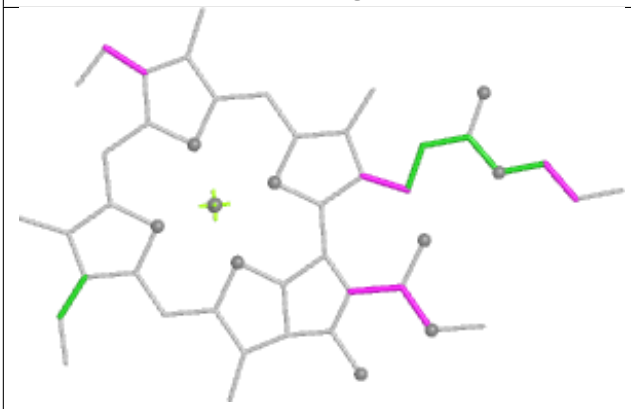
Ligand CLA 4 601



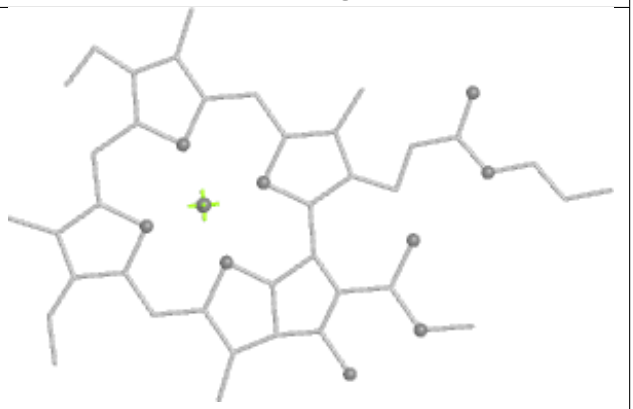
Bond lengths



Bond angles

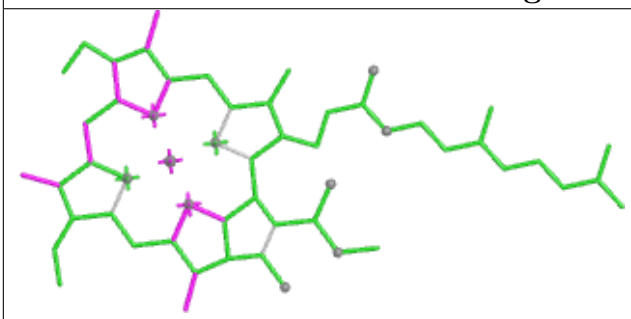


Torsions

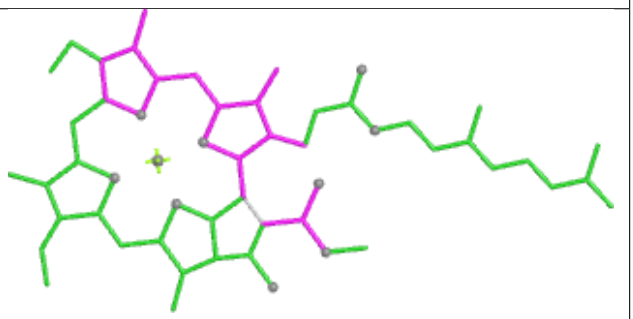


Rings

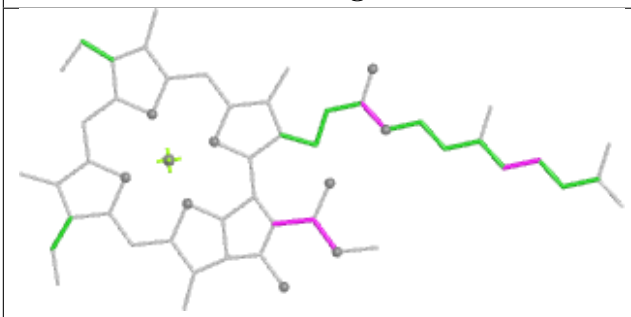
Ligand CLA A 802



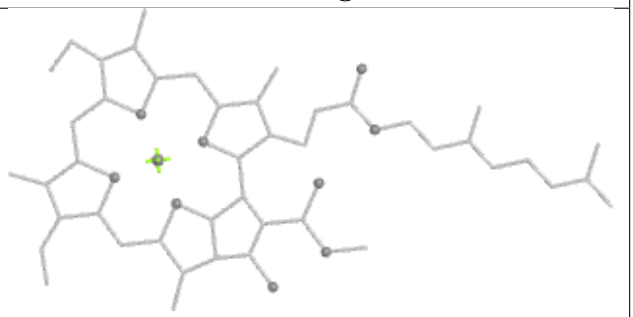
Bond lengths



Bond angles

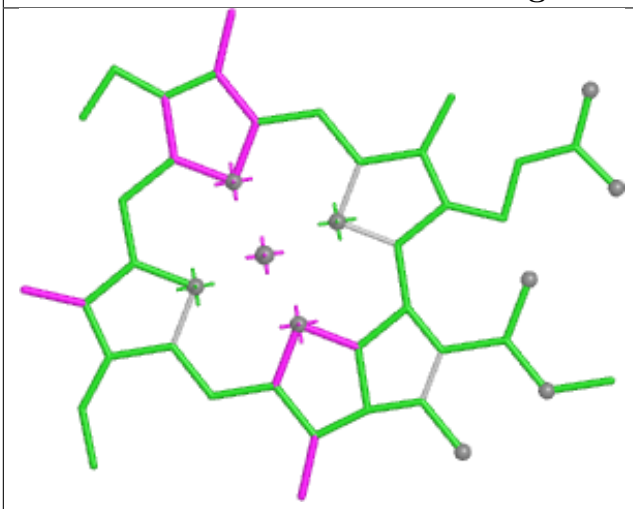


Torsions

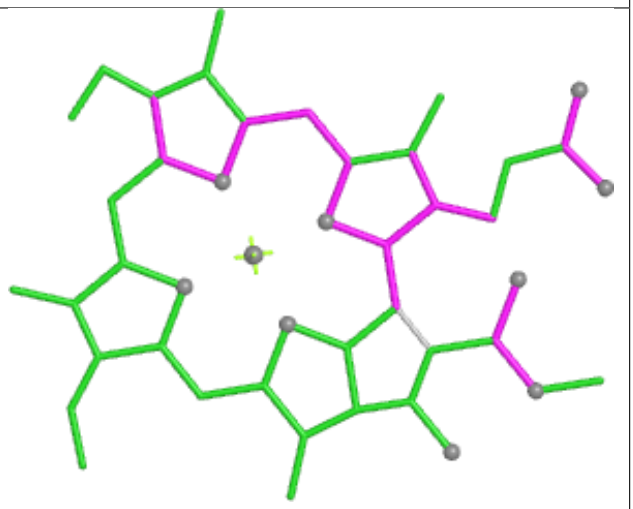


Rings

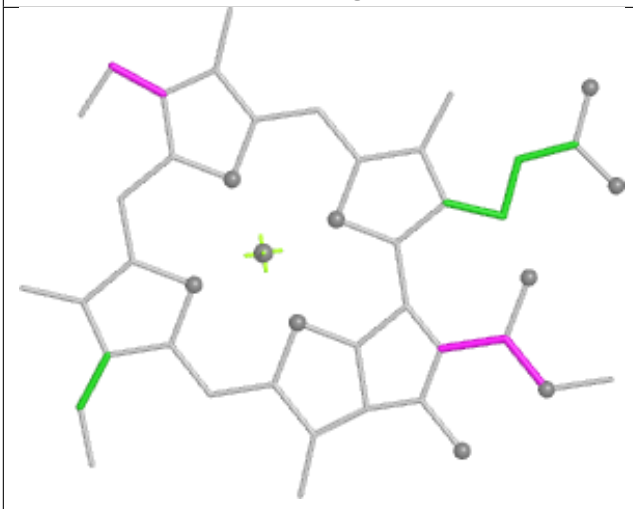
Ligand CLA 2 607



Bond lengths



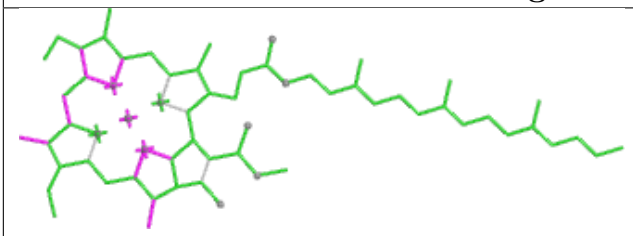
Bond angles



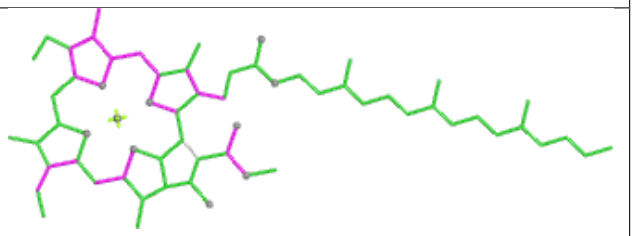
Torsions

Rings

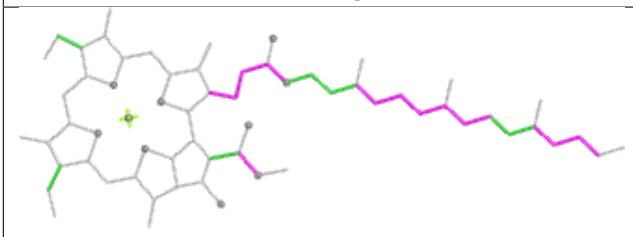
Ligand CLA 3 203



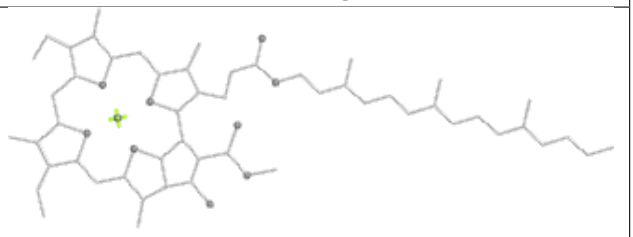
Bond lengths



Bond angles

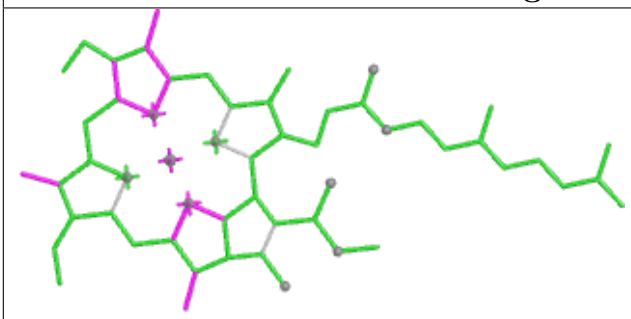


Torsions

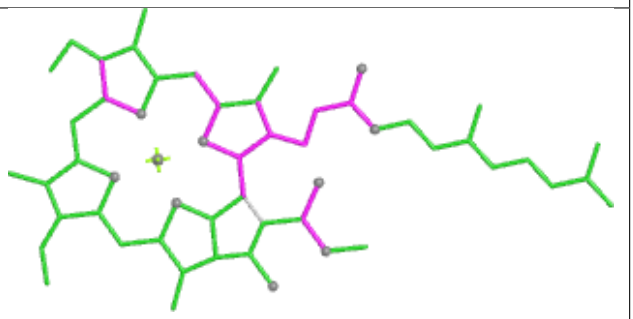


Rings

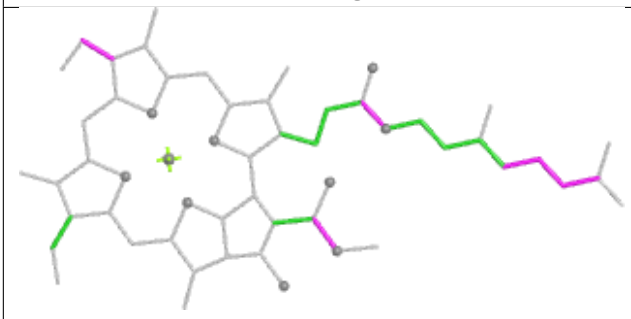
Ligand CLA A 808



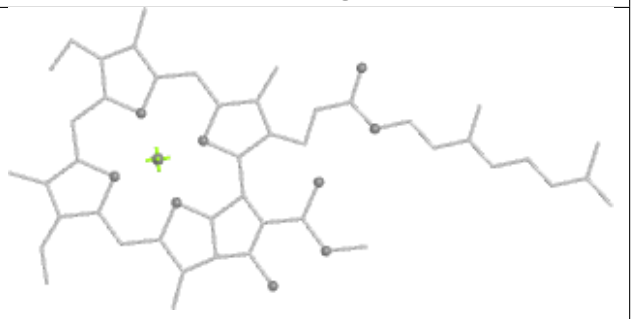
Bond lengths



Bond angles

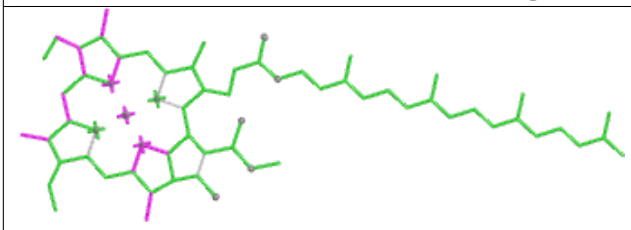


Torsions

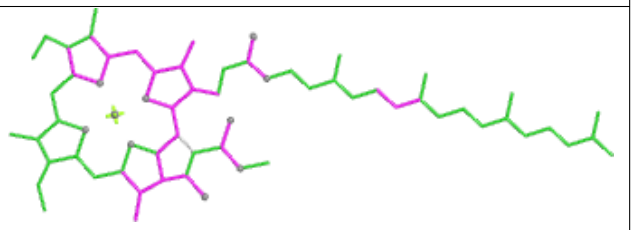


Rings

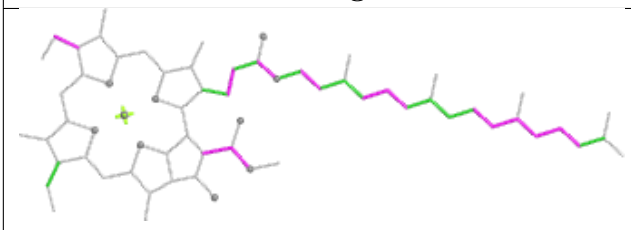
Ligand CLA B 804



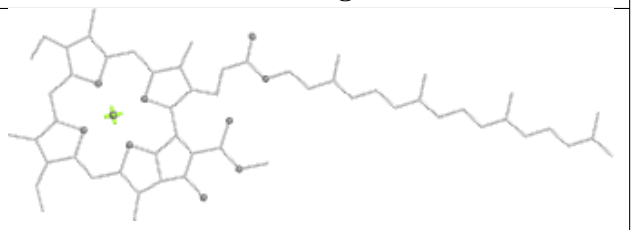
Bond lengths



Bond angles

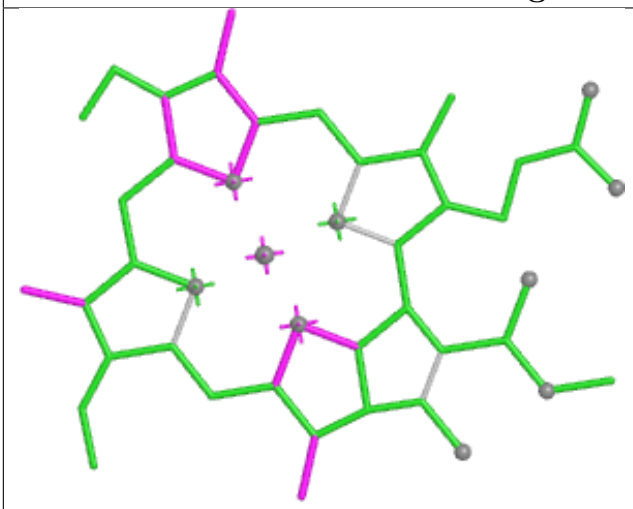


Torsions

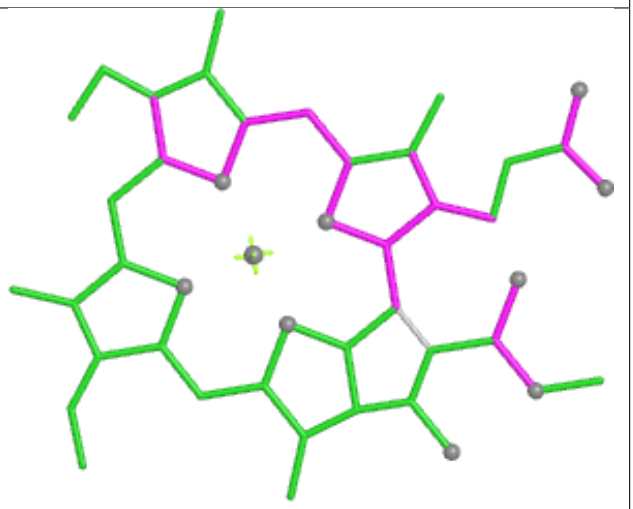


Rings

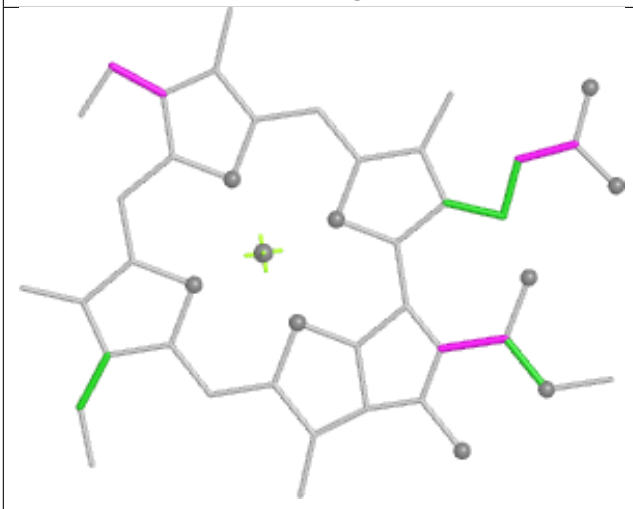
Ligand CLA 3 204



Bond lengths



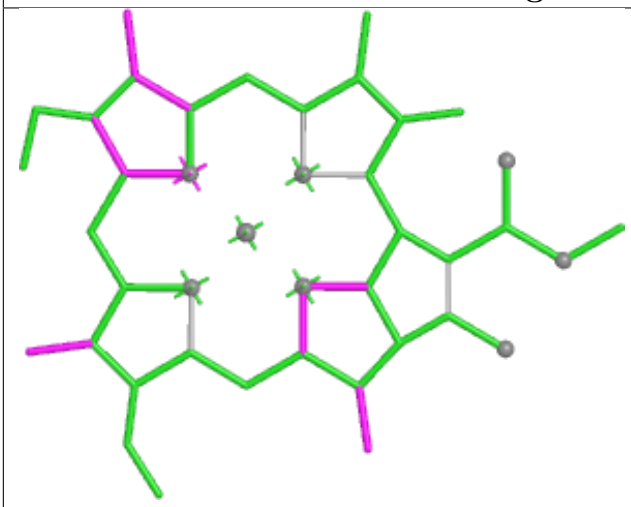
Bond angles



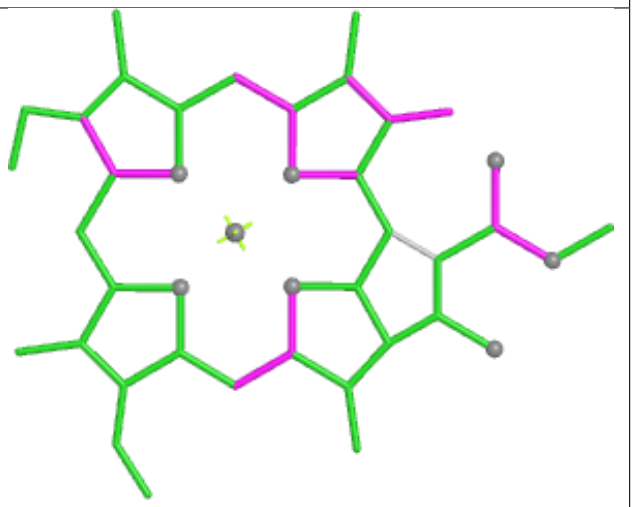
Torsions

Rings

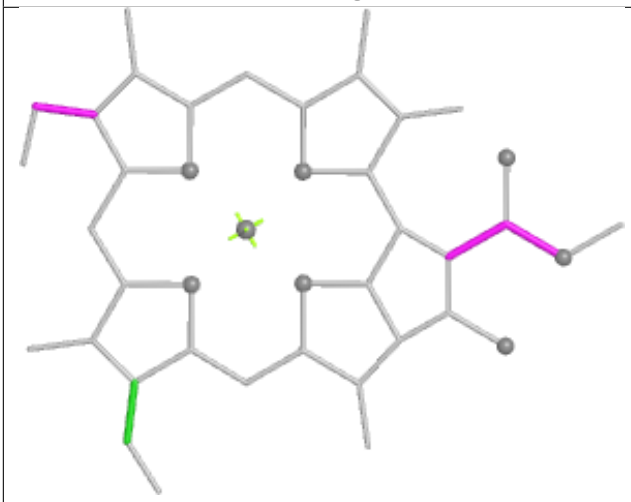
Ligand CLA F 303



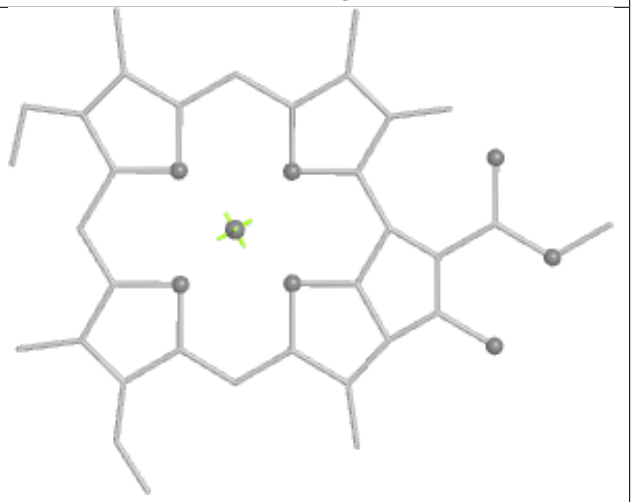
Bond lengths



Bond angles

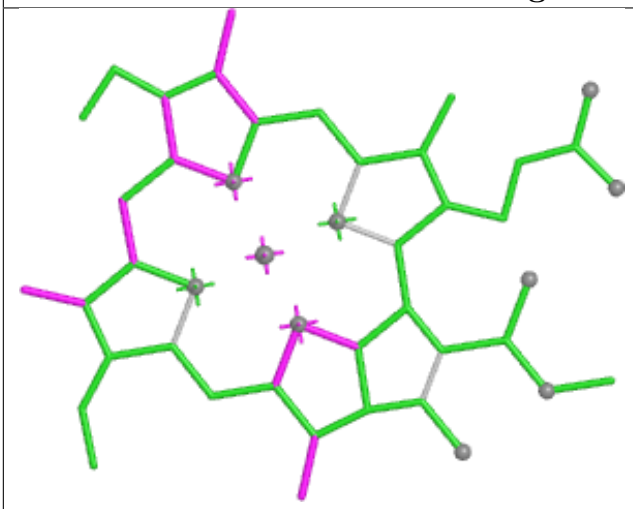


Torsions

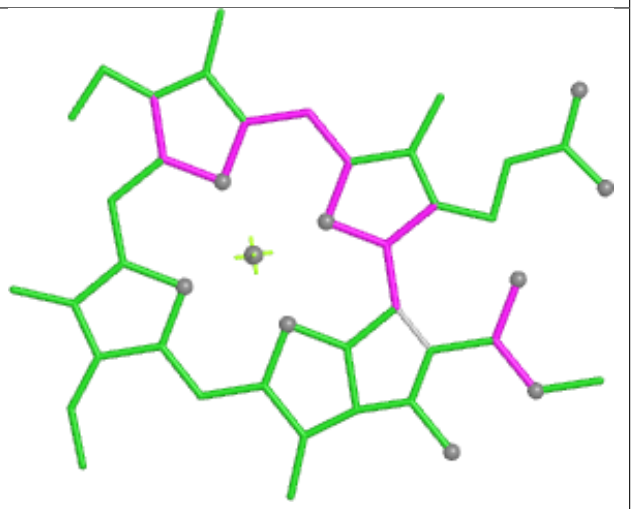


Rings

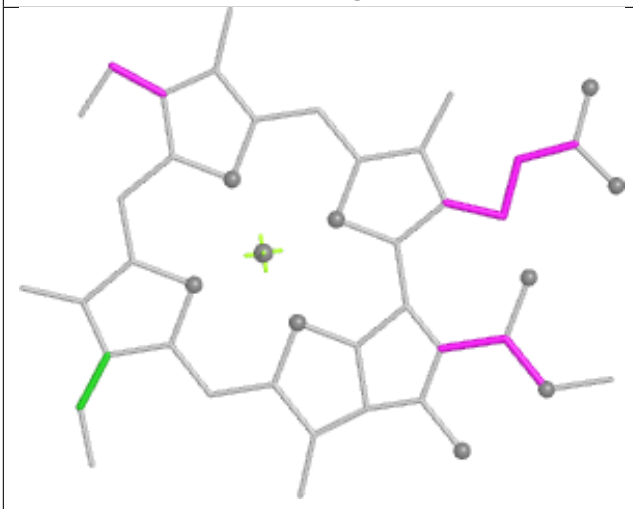
Ligand CLA 3 208



Bond lengths



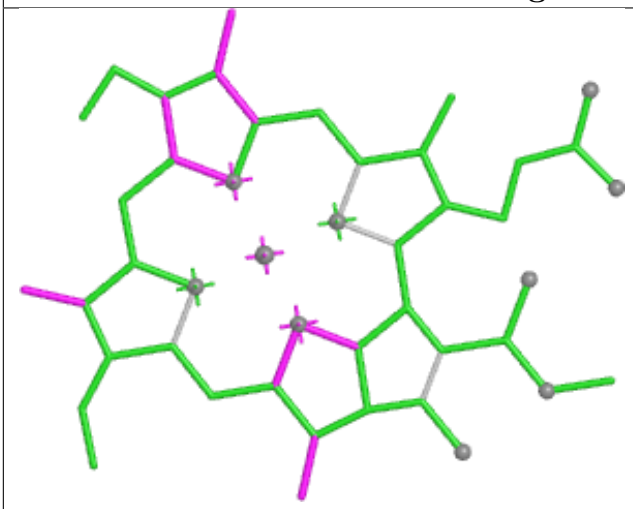
Bond angles



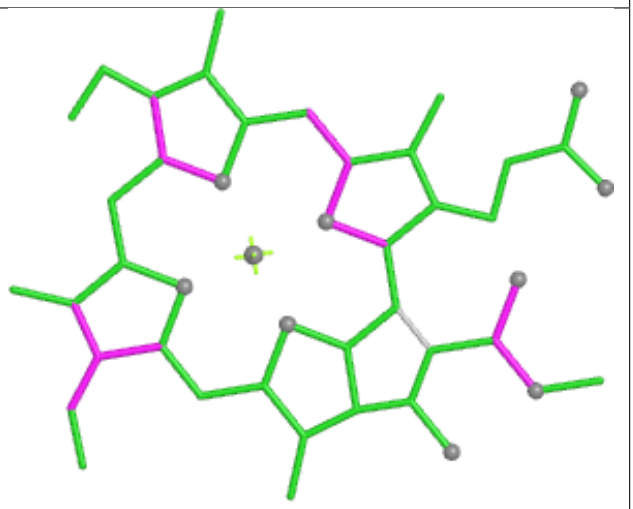
Torsions

Rings

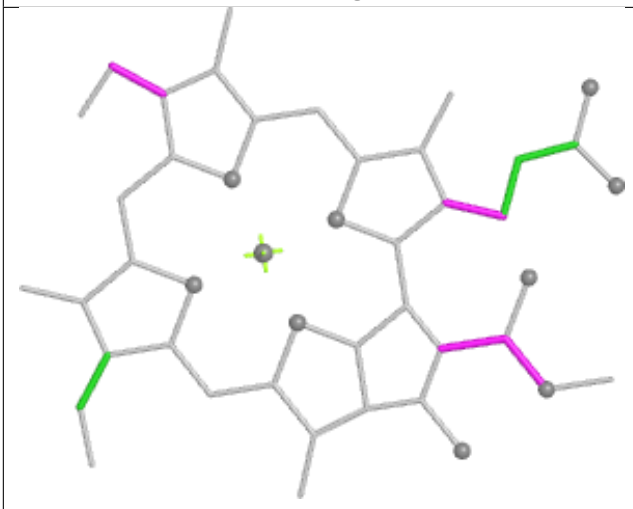
Ligand CLA 4 606



Bond lengths



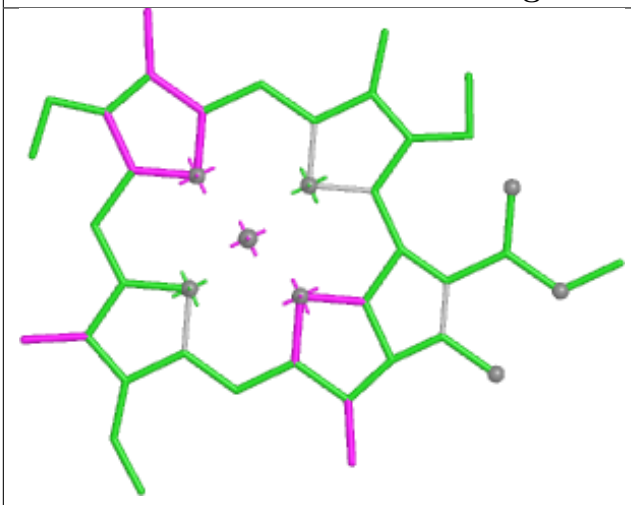
Bond angles



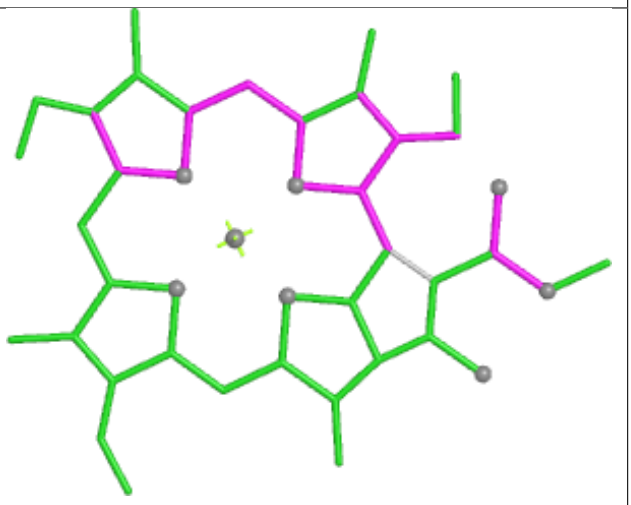
Torsions

Rings

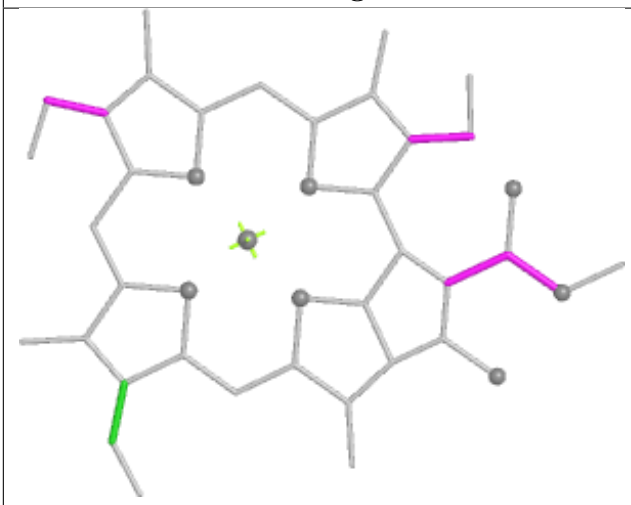
Ligand CLA K 103



Bond lengths



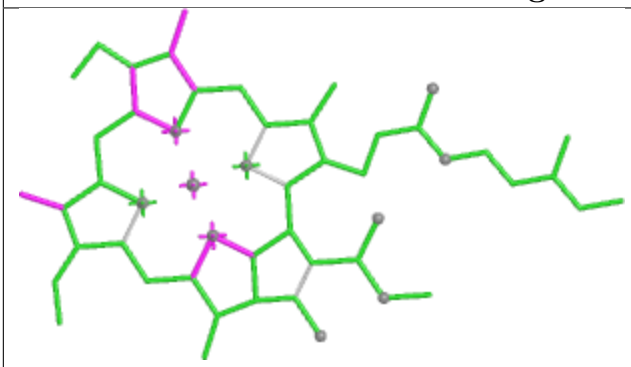
Bond angles



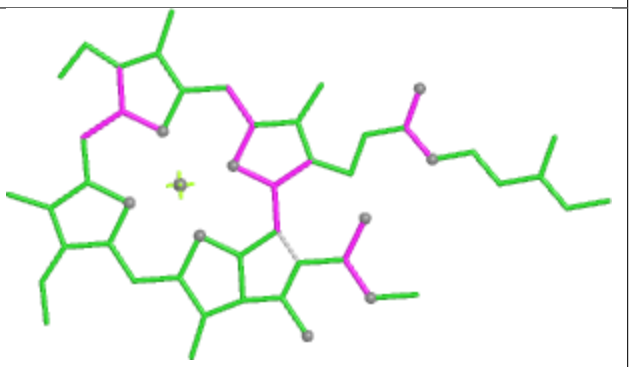
Torsions

Rings

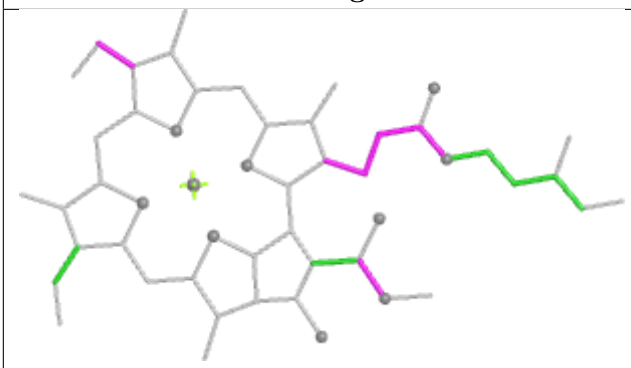
Ligand CLA 3 213



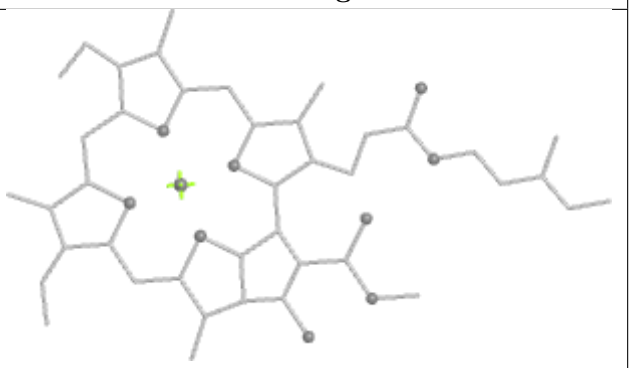
Bond lengths



Bond angles

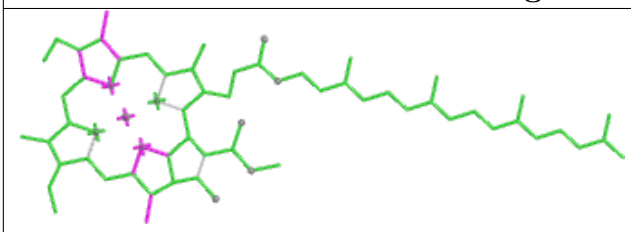


Torsions

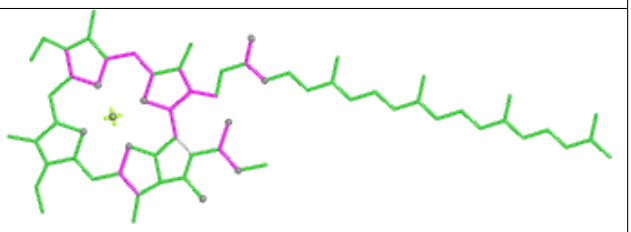


Rings

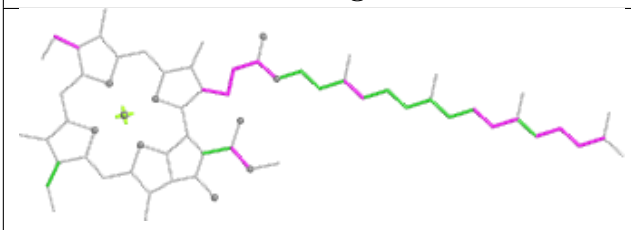
Ligand CLA B 843



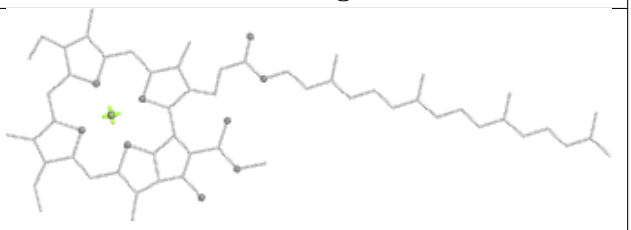
Bond lengths



Bond angles

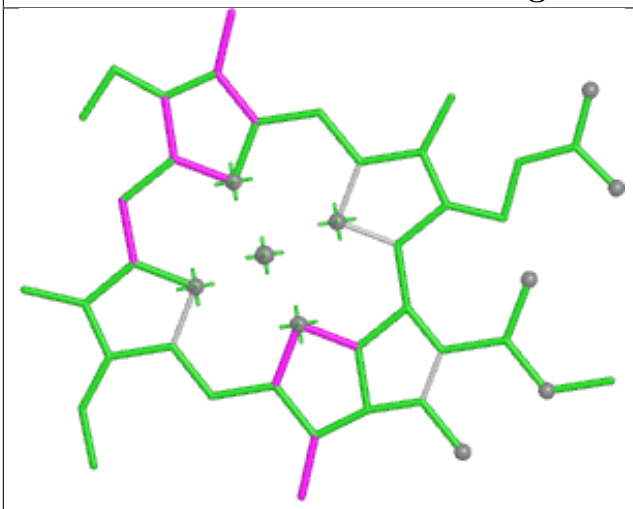


Torsions

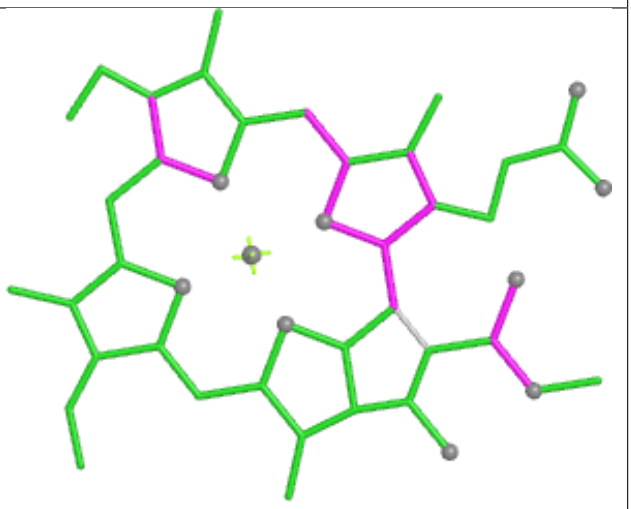


Rings

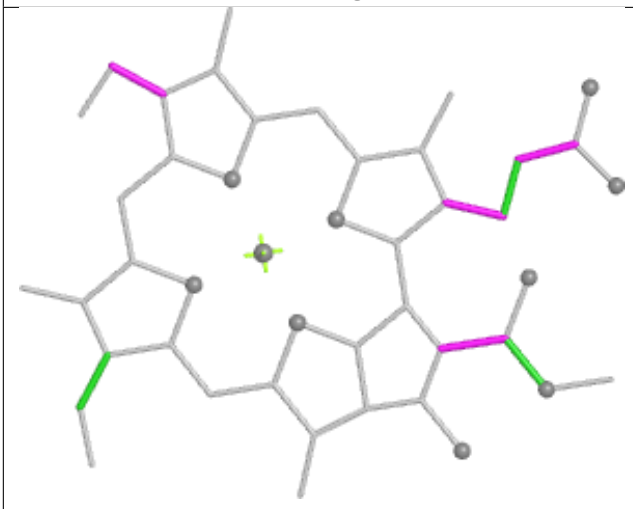
Ligand CLA 4 610



Bond lengths



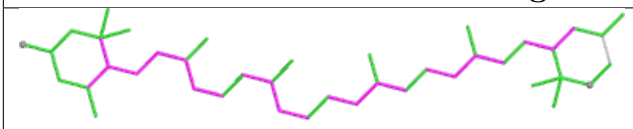
Bond angles



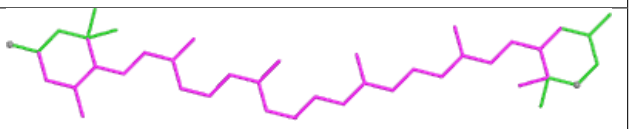
Torsions

Rings

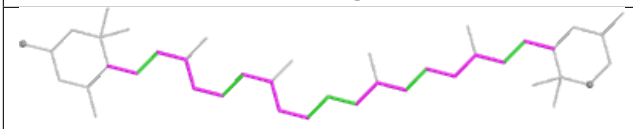
Ligand ZEX 2 615



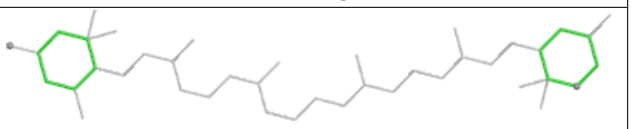
Bond lengths



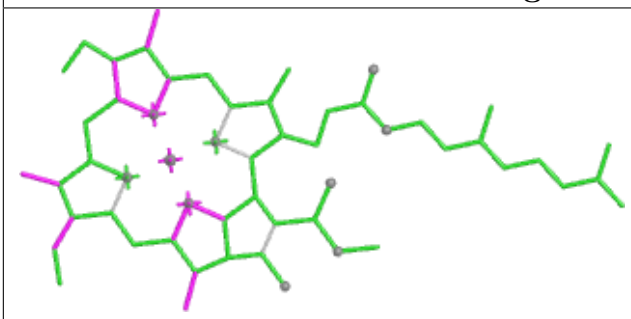
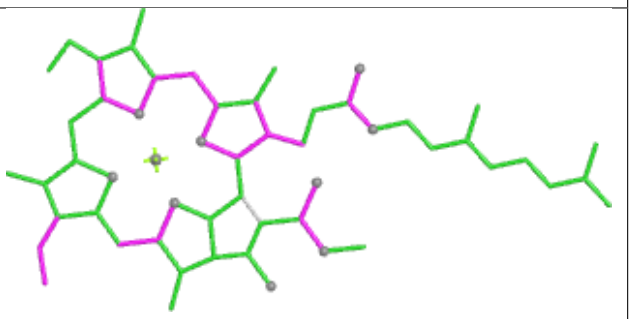
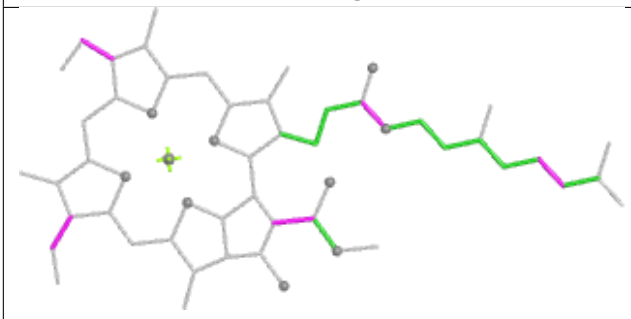
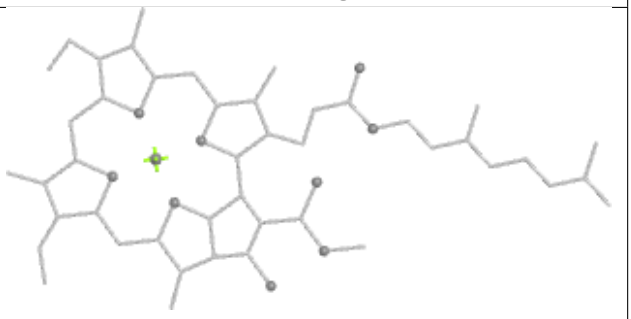
Bond angles



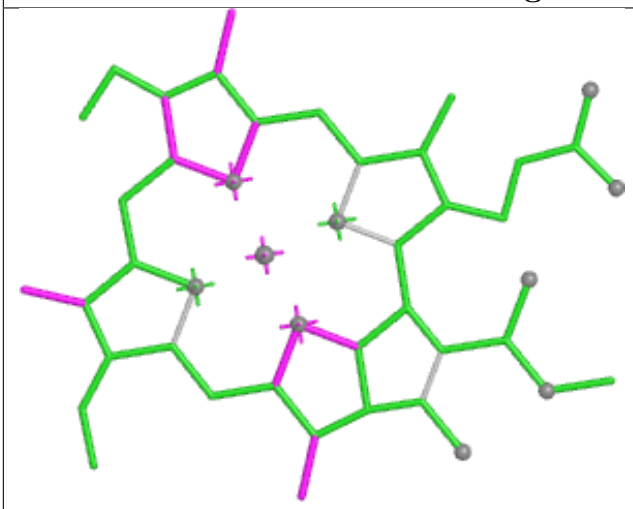
Torsions



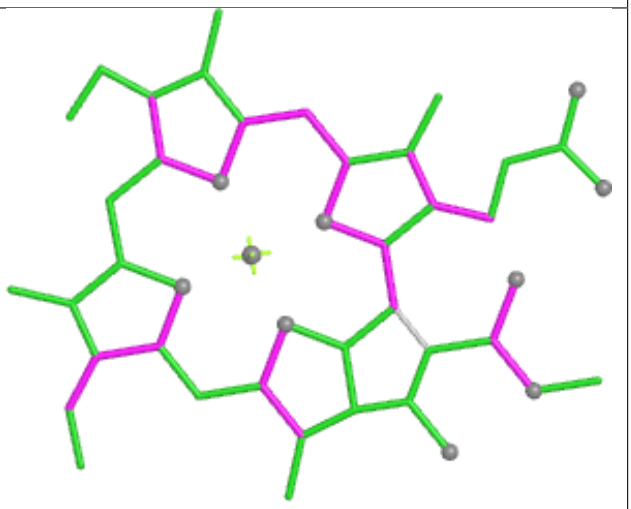
Rings

Ligand CLA A 824	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

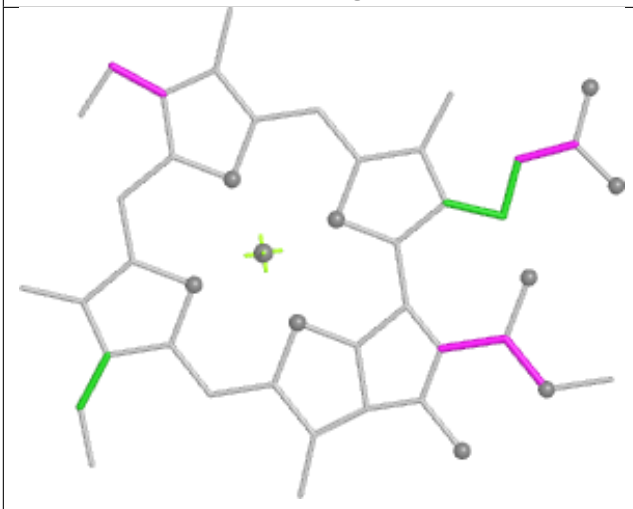
Ligand CLA B 833



Bond lengths



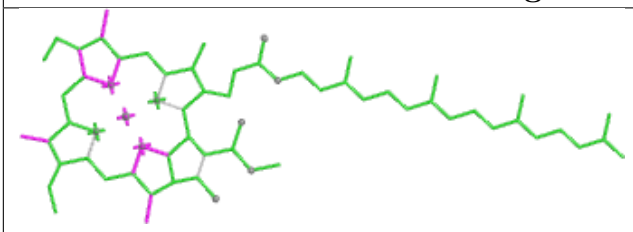
Bond angles



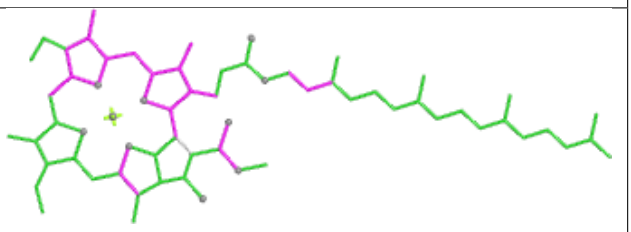
Torsions

Rings

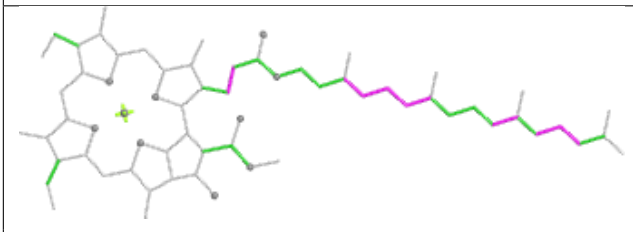
Ligand CLA B 827



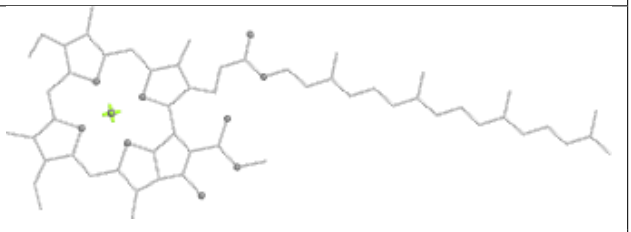
Bond lengths



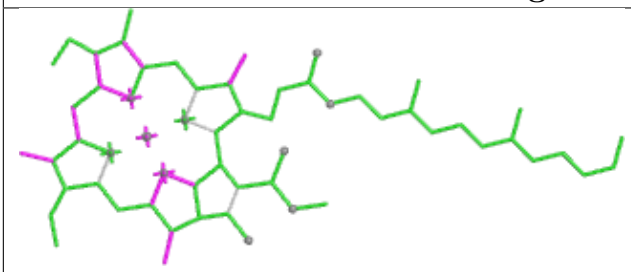
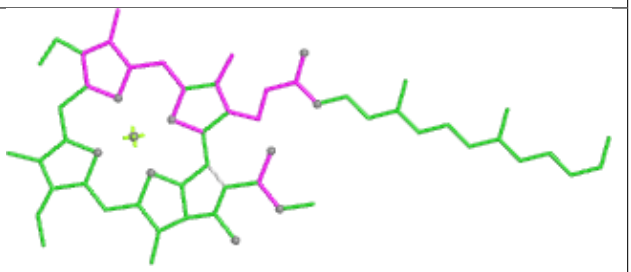
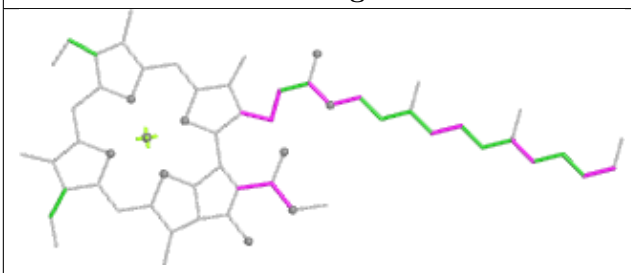
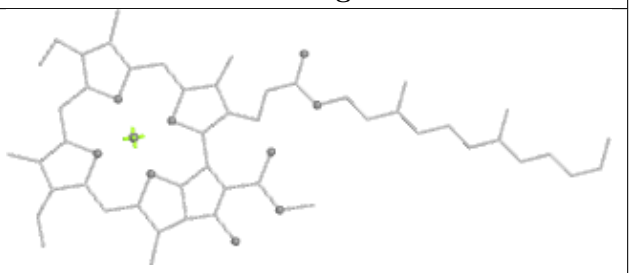
Bond angles

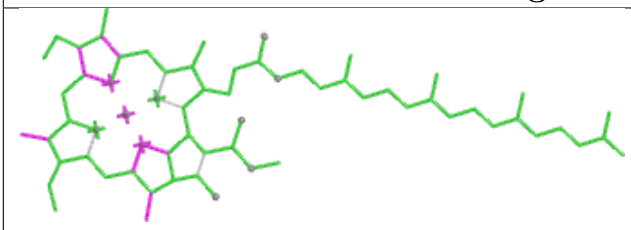
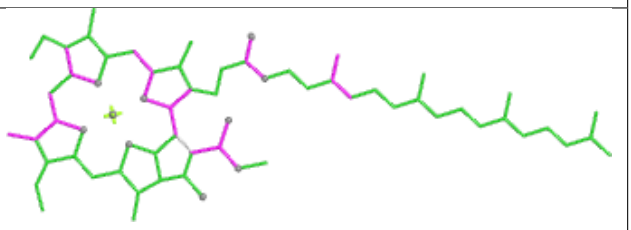
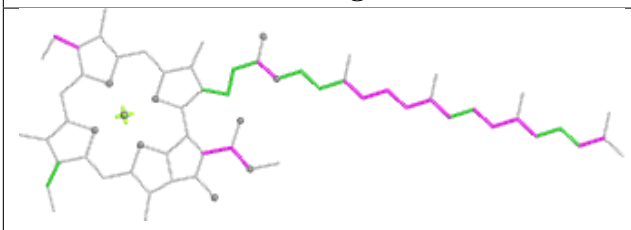
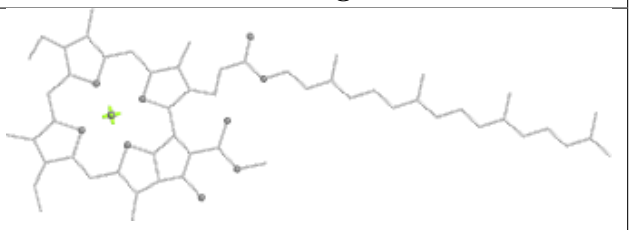


Torsions

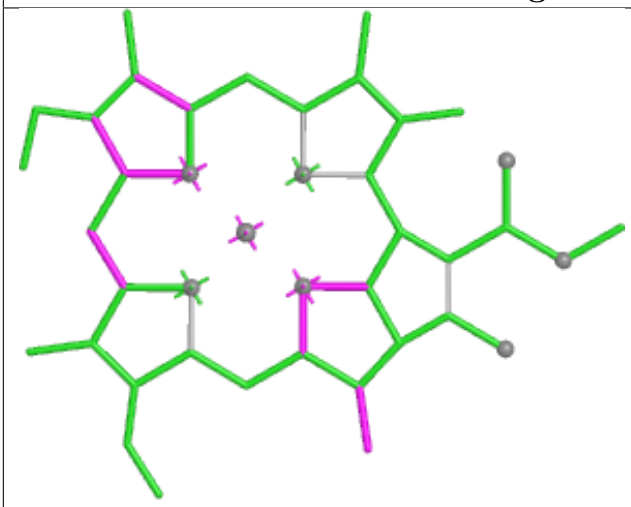


Rings

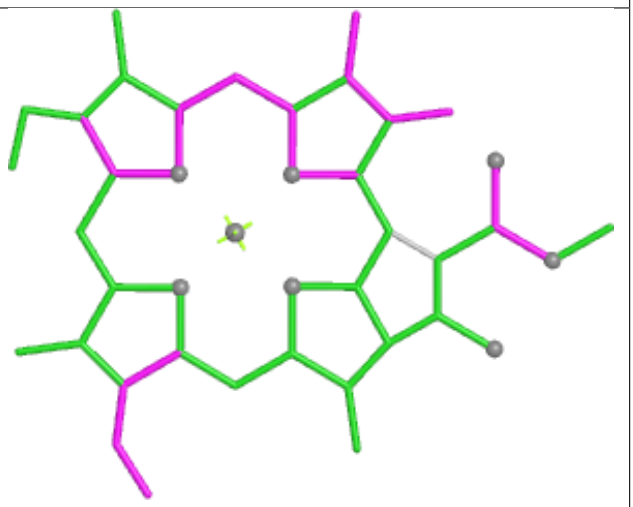
Ligand CLA 4 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

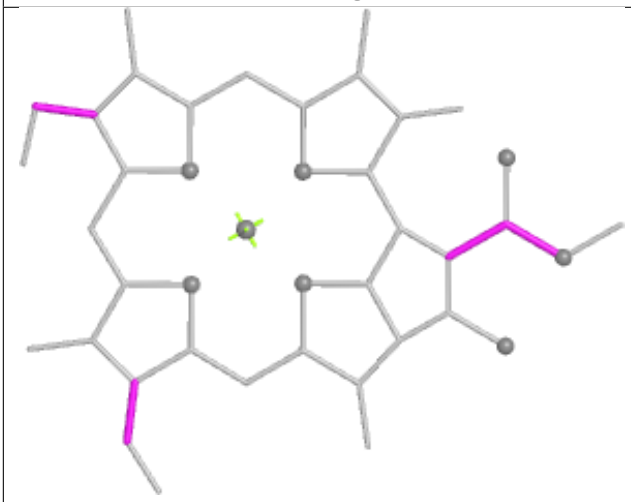
Ligand CLA 3 210



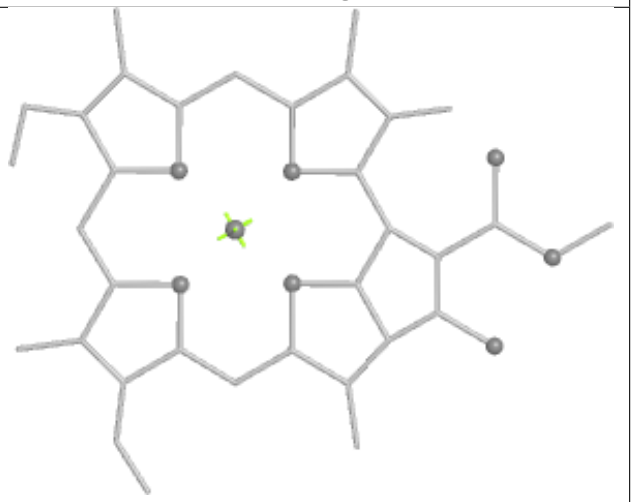
Bond lengths



Bond angles

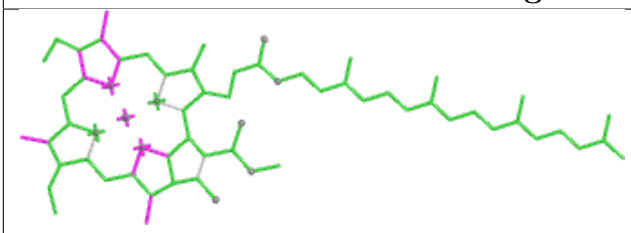


Torsions

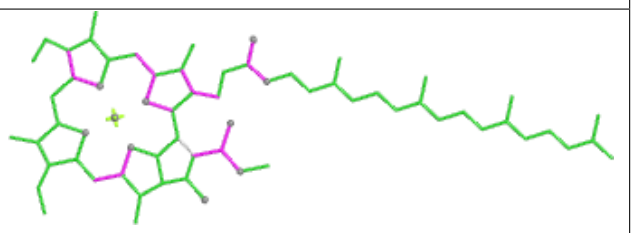


Rings

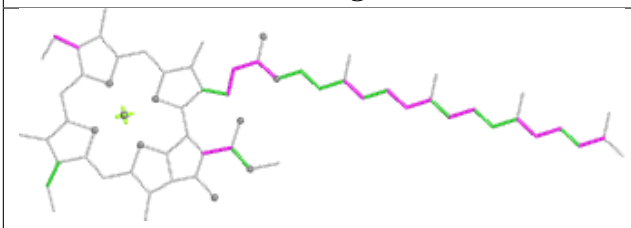
Ligand CLA B 810



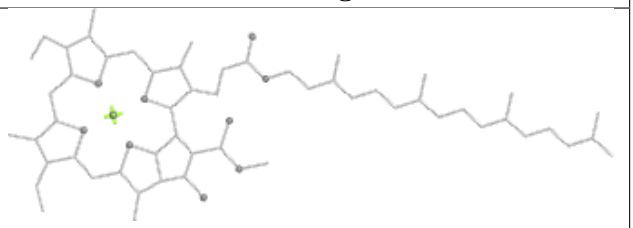
Bond lengths



Bond angles

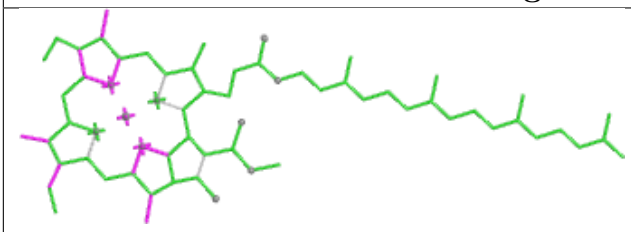


Torsions

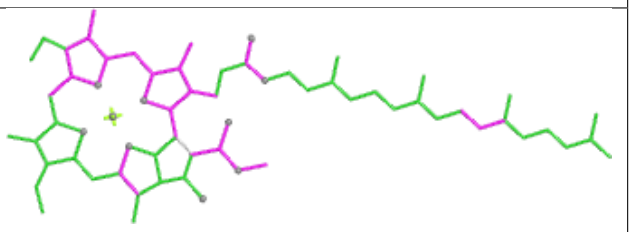


Rings

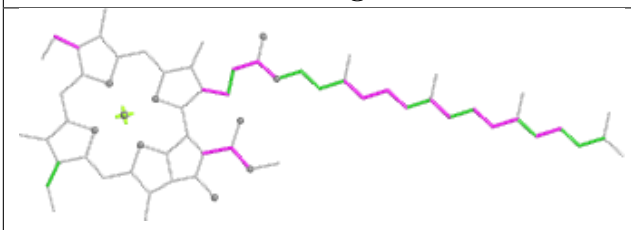
Ligand CLA A 807



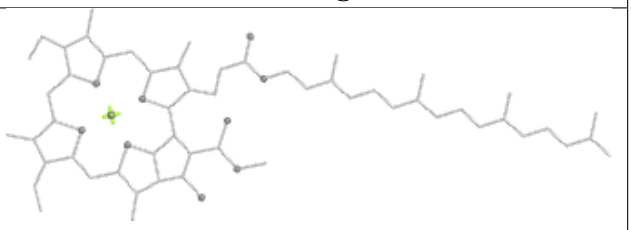
Bond lengths



Bond angles

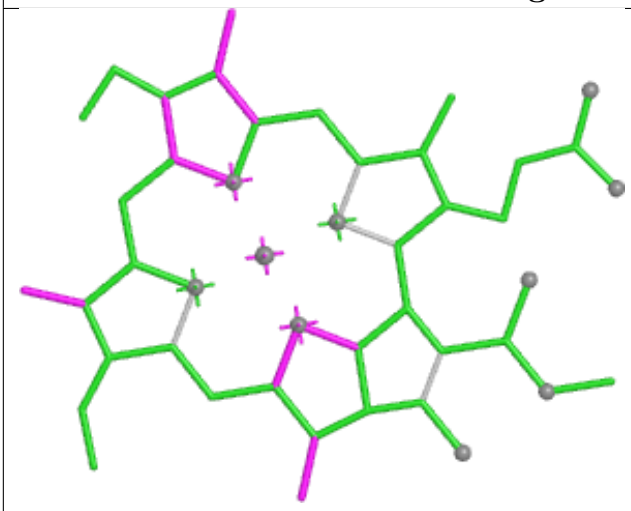


Torsions

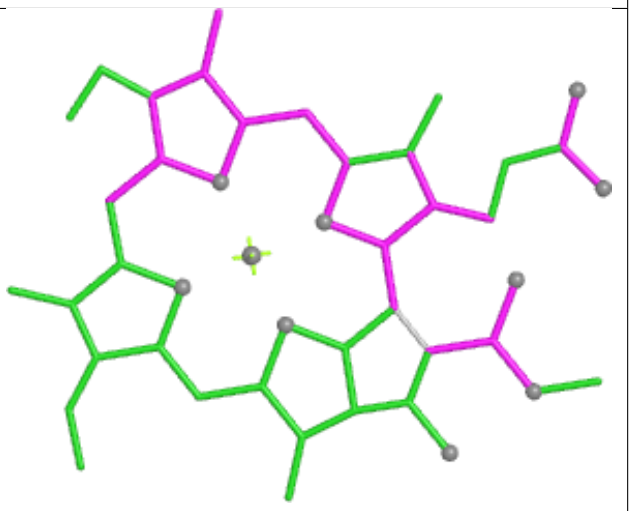


Rings

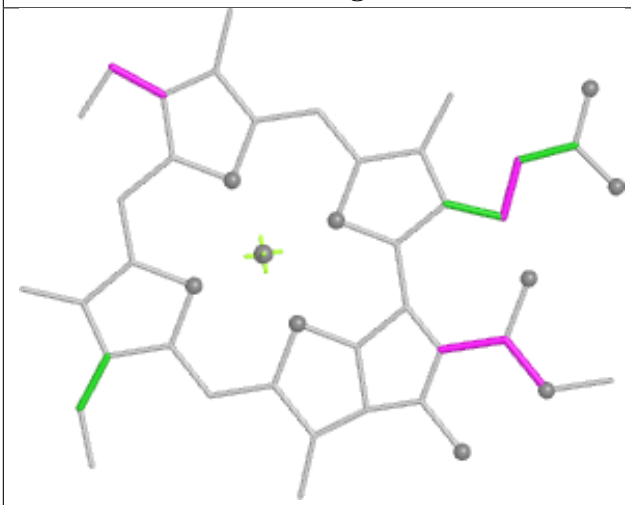
Ligand CLA 5 608



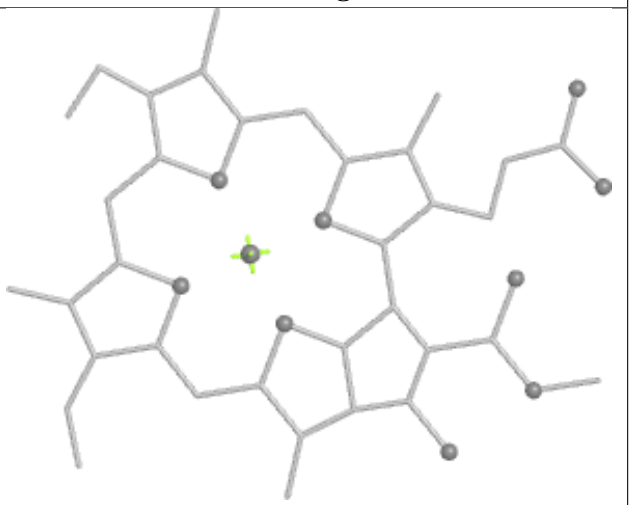
Bond lengths



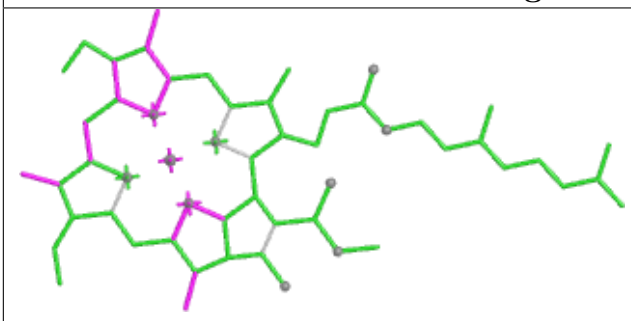
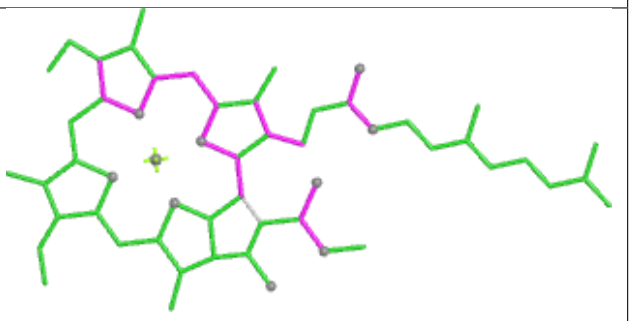
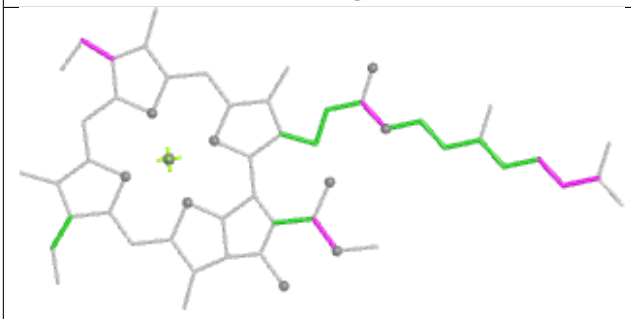
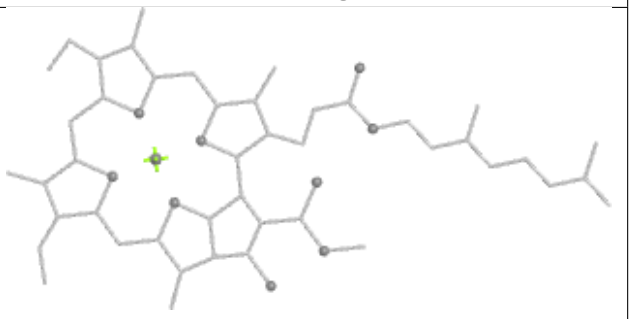
Bond angles

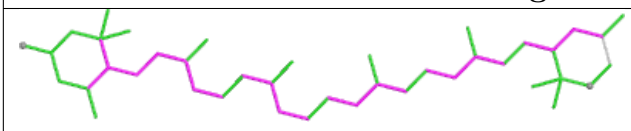
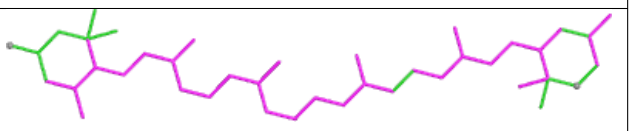
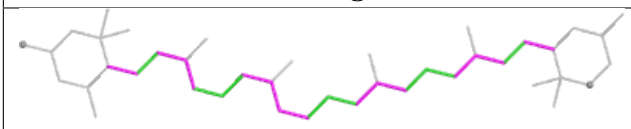
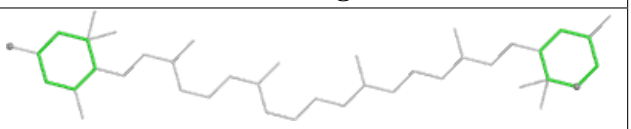


Torsions

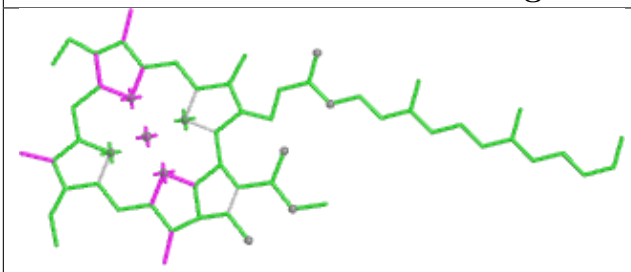


Rings

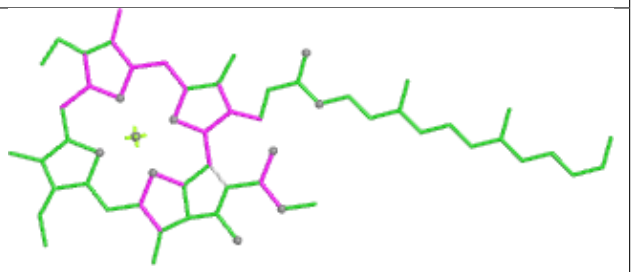
Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZEX 4 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

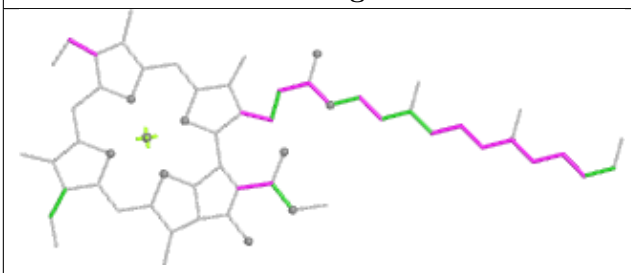
Ligand CLA B 820



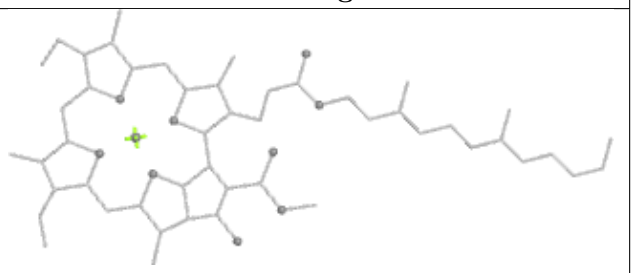
Bond lengths



Bond angles

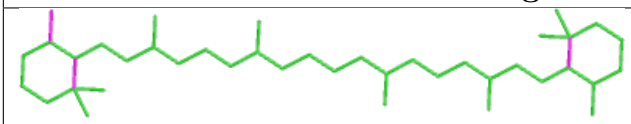


Torsions

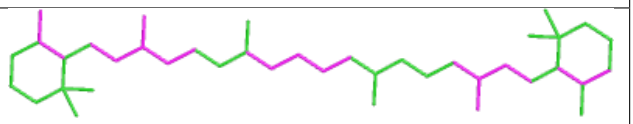


Rings

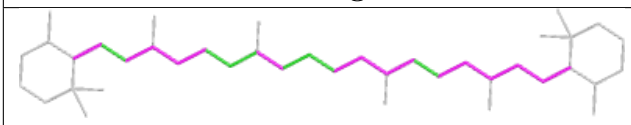
Ligand BCR A 845



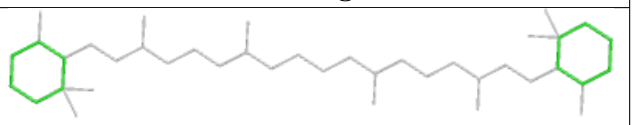
Bond lengths



Bond angles

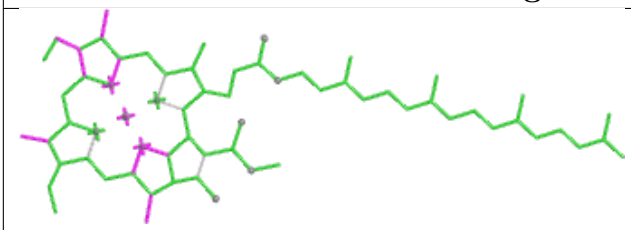


Torsions

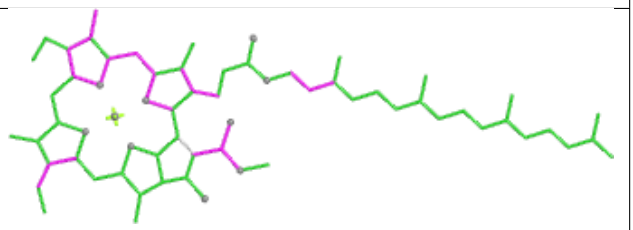


Rings

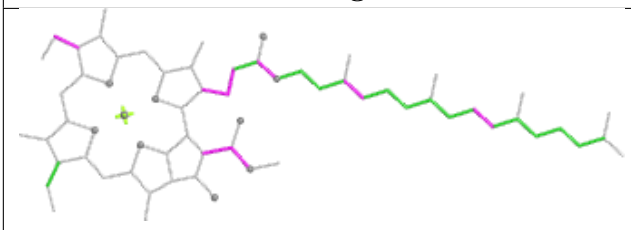
Ligand CLA A 826



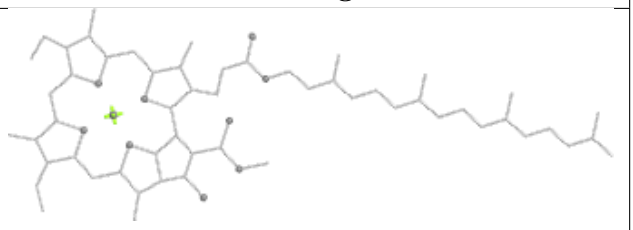
Bond lengths



Bond angles

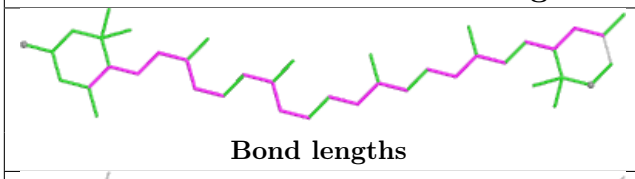


Torsions

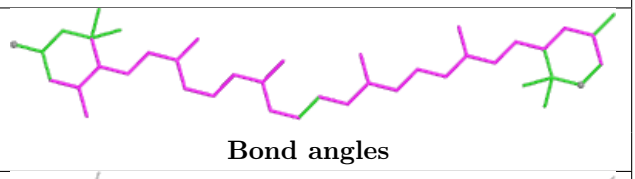


Rings

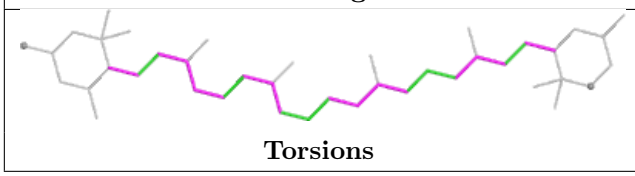
Ligand ZEX 1 617



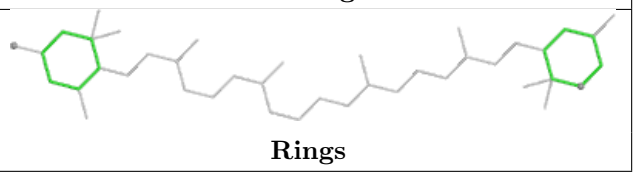
Bond lengths



Bond angles

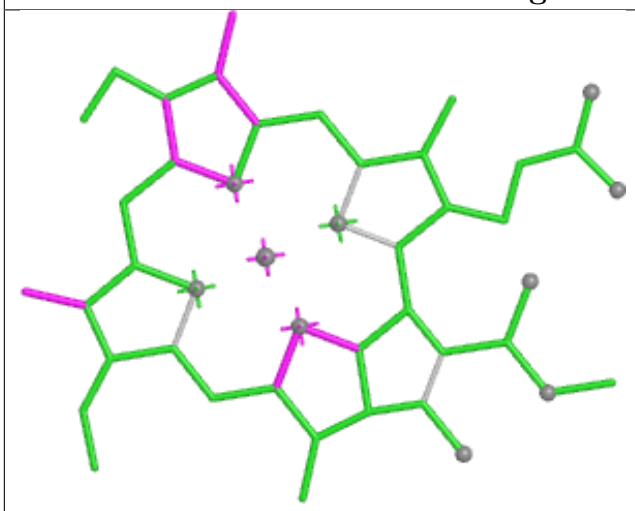


Torsions

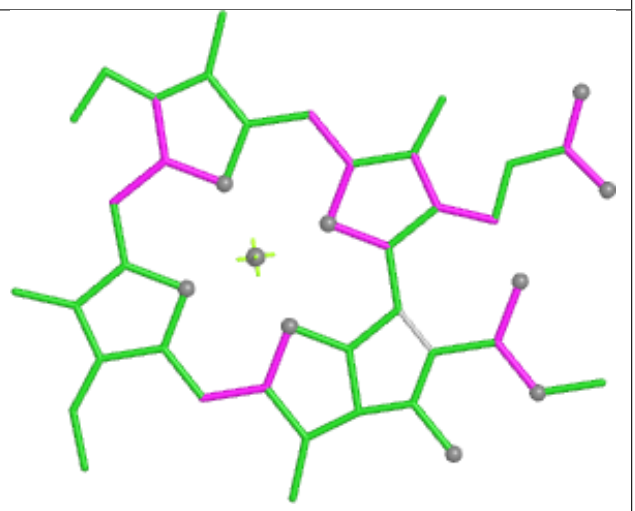


Rings

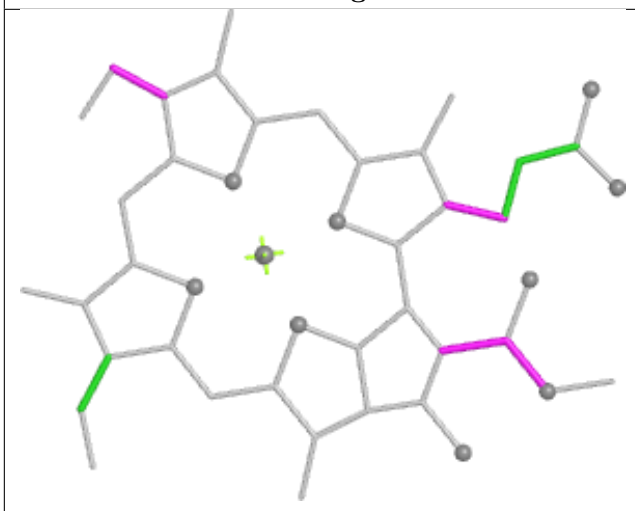
Ligand CLA 2 613



Bond lengths



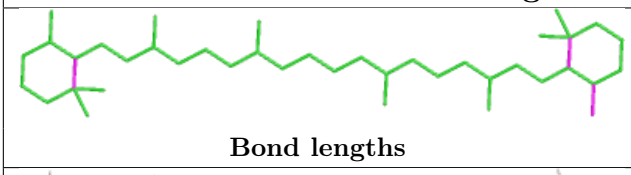
Bond angles



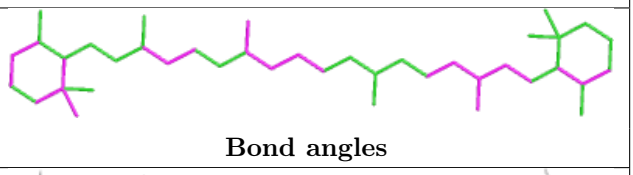
Torsions

Rings

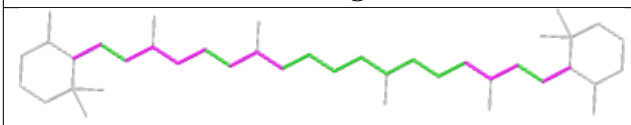
Ligand BCR B 805



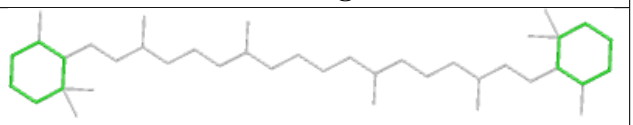
Bond lengths



Bond angles

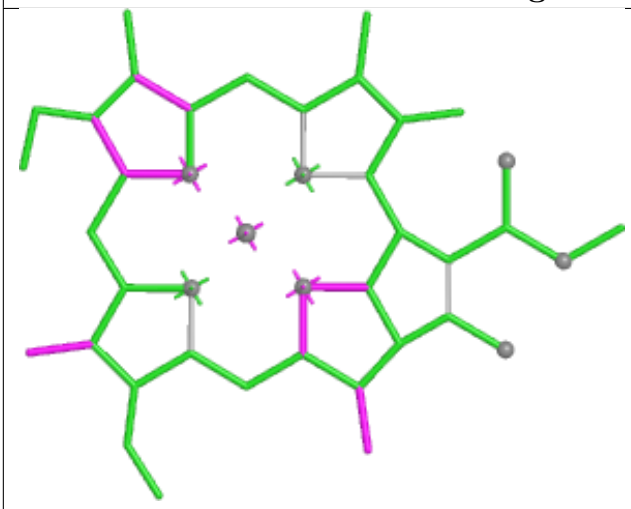


Torsions

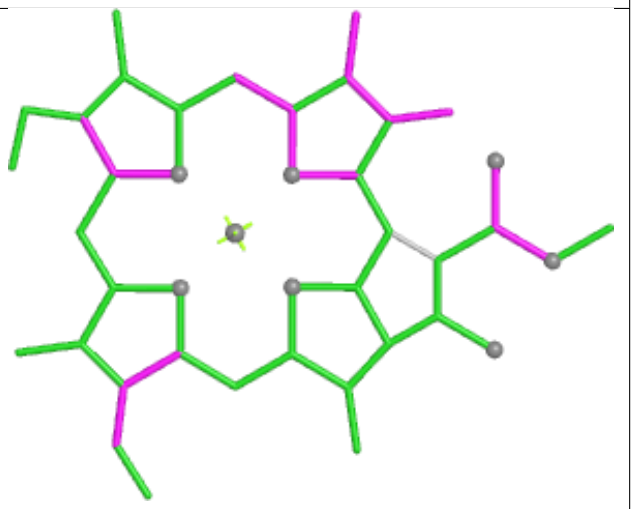


Rings

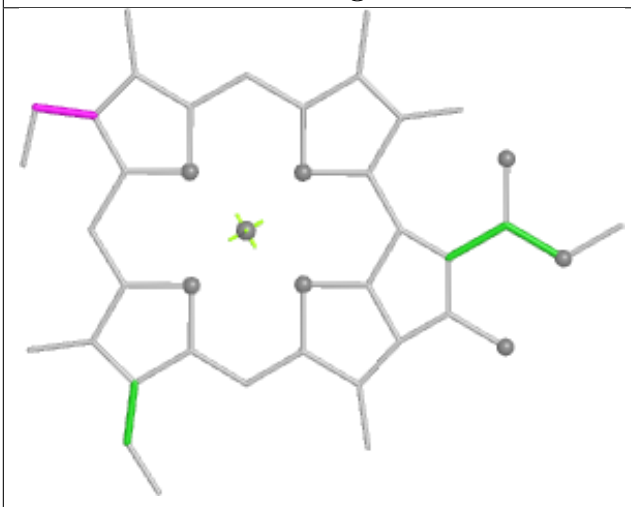
Ligand CLA 1 609



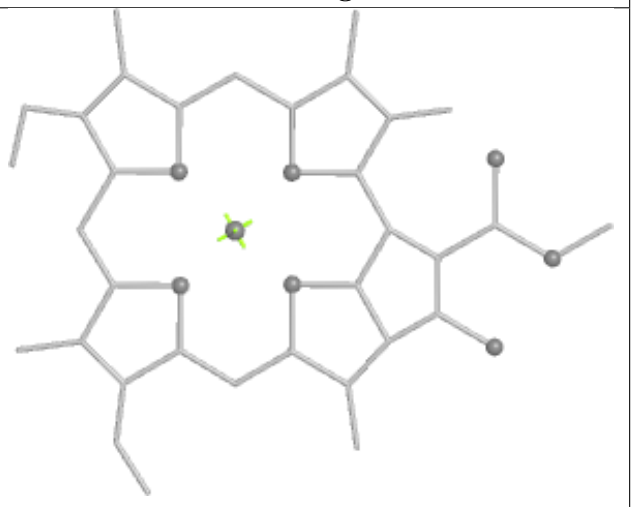
Bond lengths



Bond angles

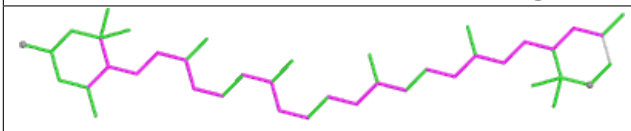


Torsions

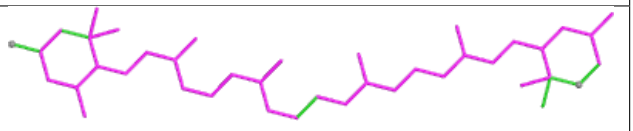


Rings

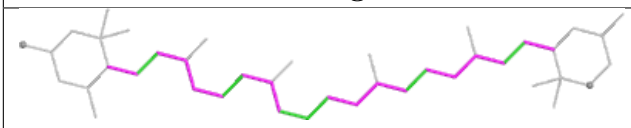
Ligand ZEX 3 218



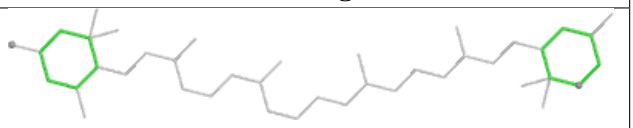
Bond lengths



Bond angles

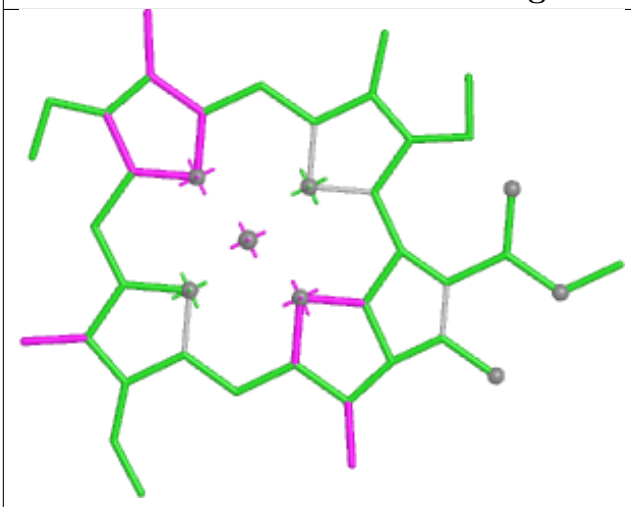


Torsions

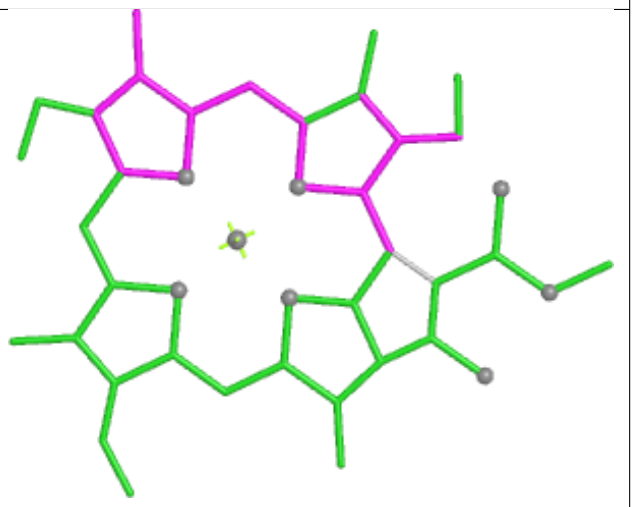


Rings

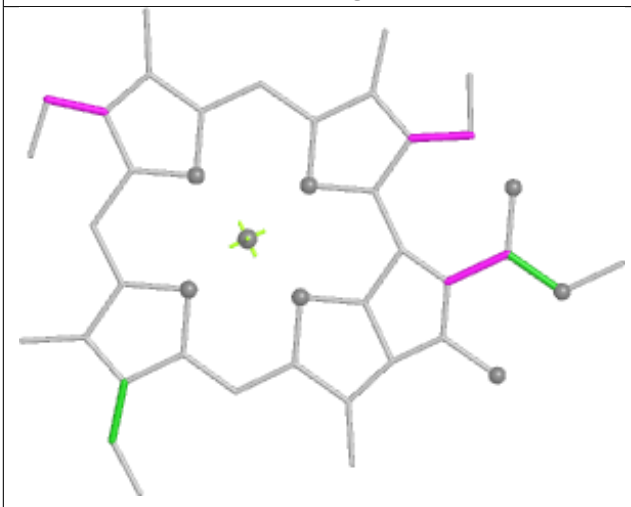
Ligand CLA 2 604



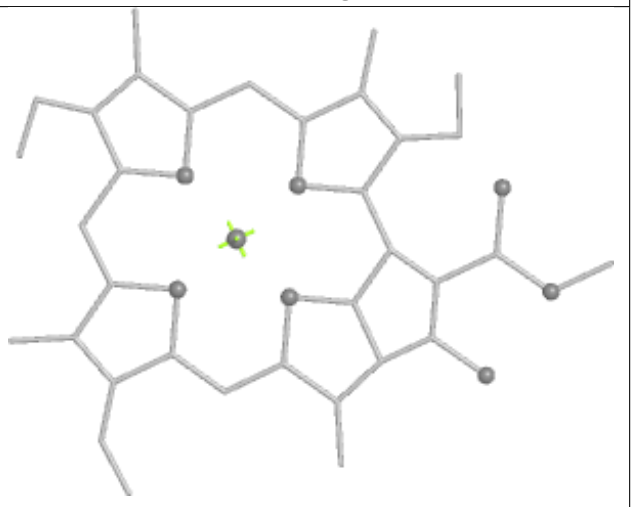
Bond lengths



Bond angles

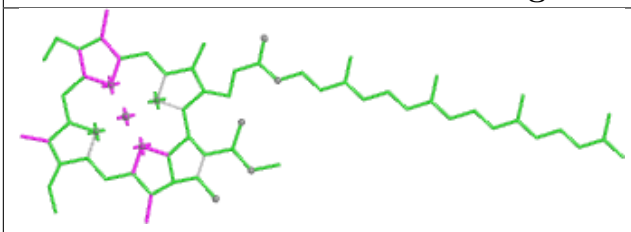


Torsions

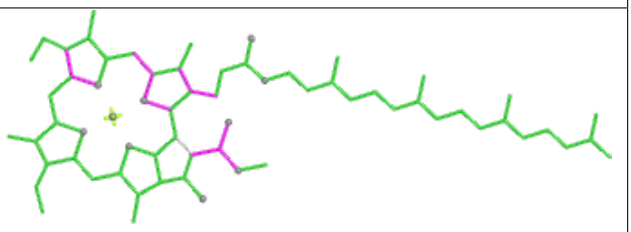


Rings

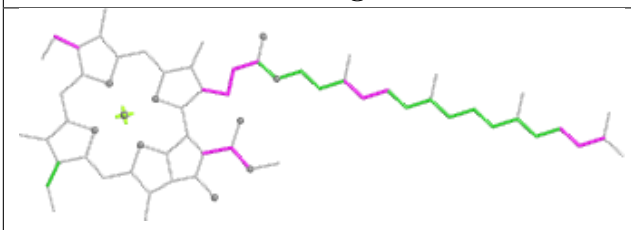
Ligand CLA 2 602



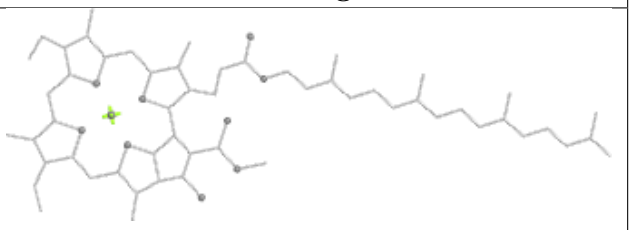
Bond lengths



Bond angles

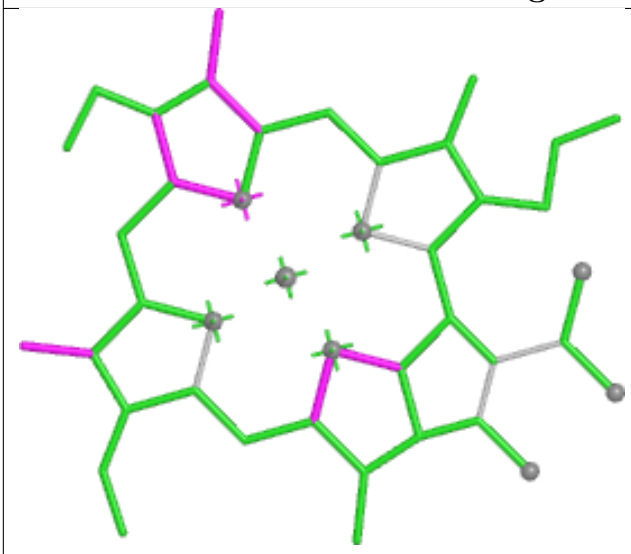


Torsions



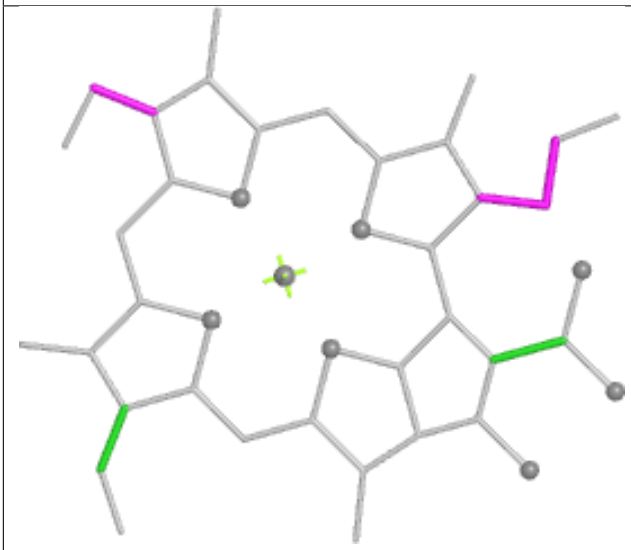
Rings

Ligand CLA 1 605



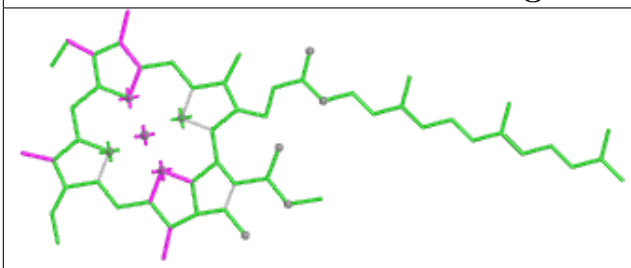
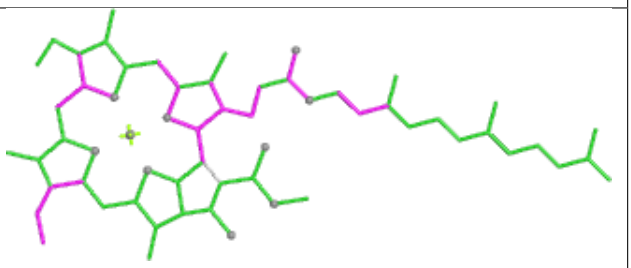
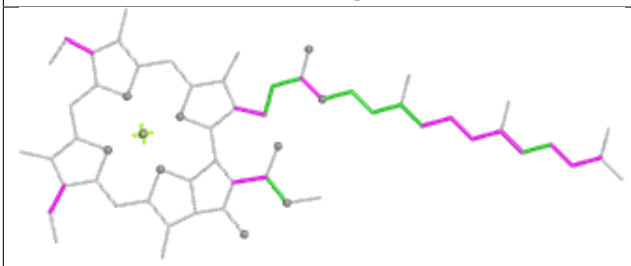
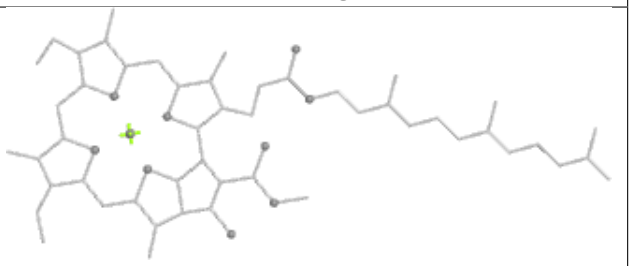
Bond lengths

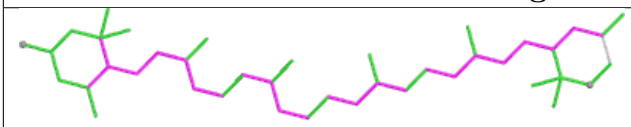
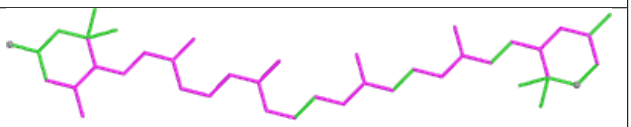
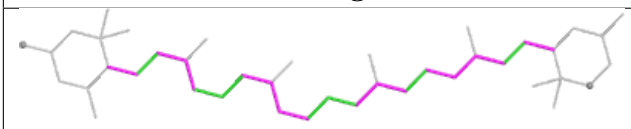
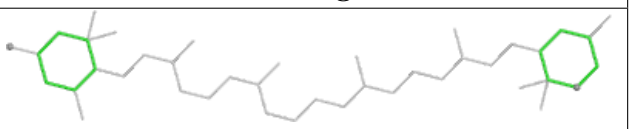
Bond angles



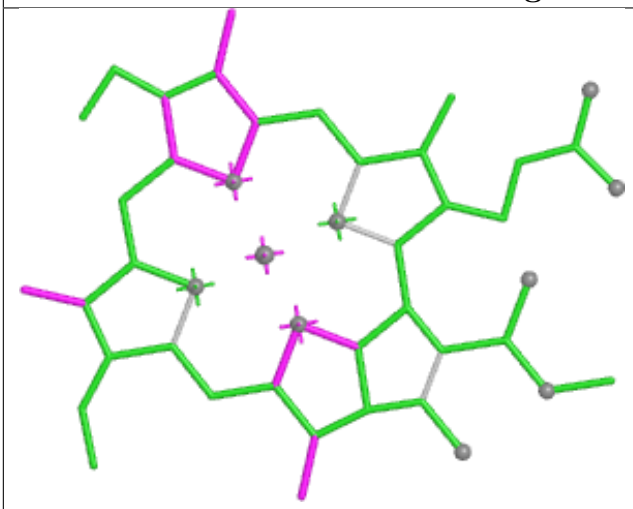
Torsions

Rings

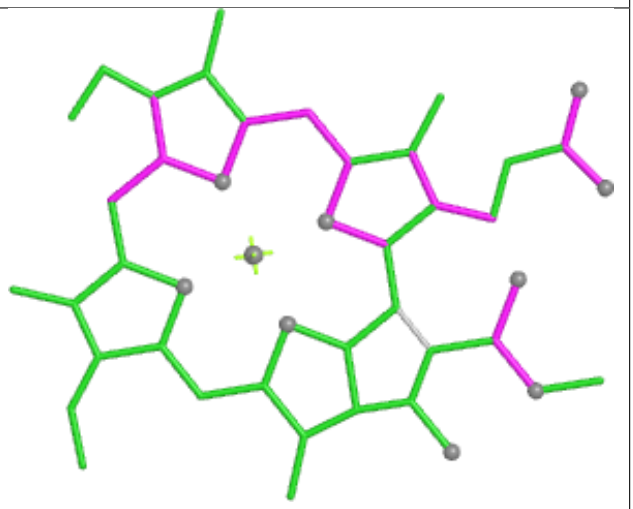
Ligand CLA B 838	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand ZEX 3 217	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

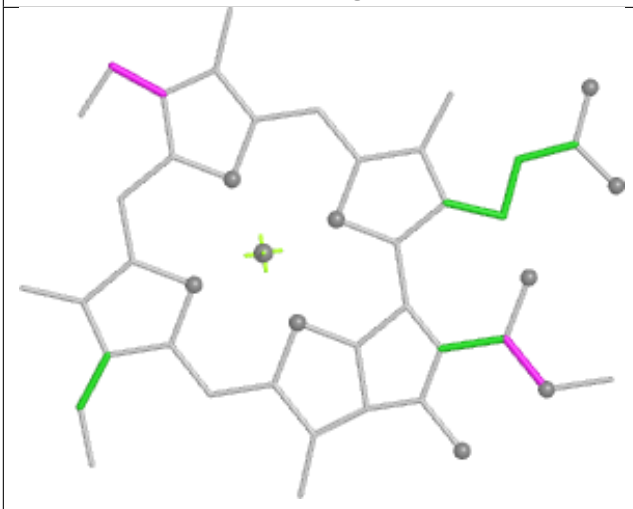
Ligand CLA B 823



Bond lengths



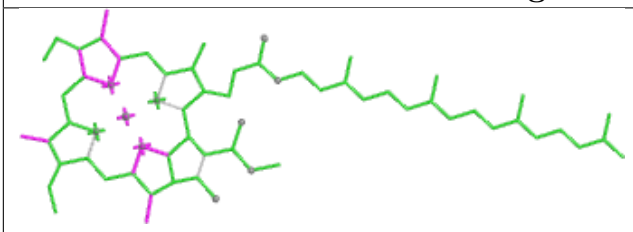
Bond angles



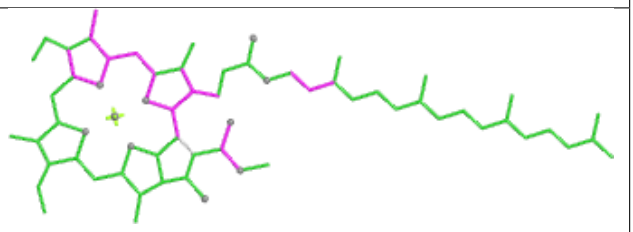
Torsions

Rings

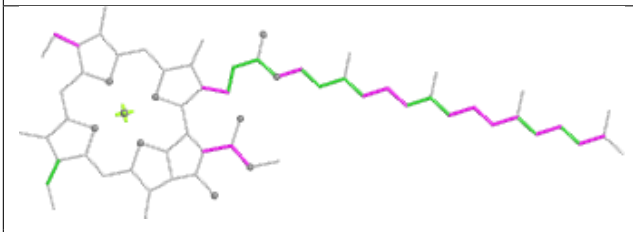
Ligand CLA J 101



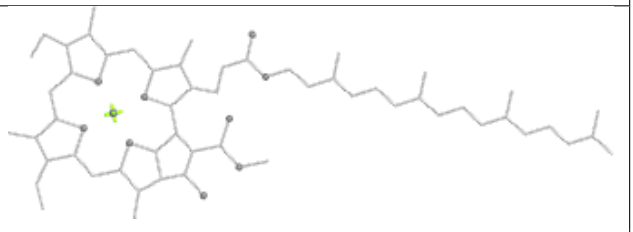
Bond lengths



Bond angles

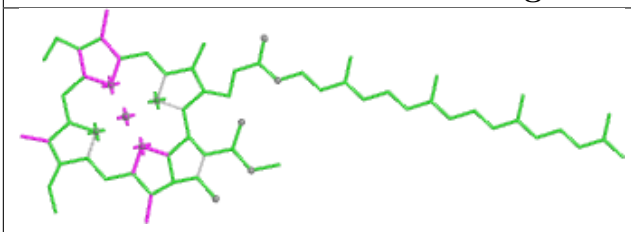


Torsions

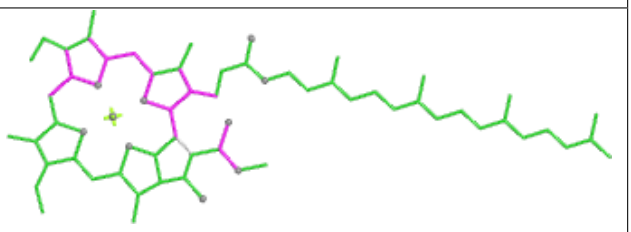


Rings

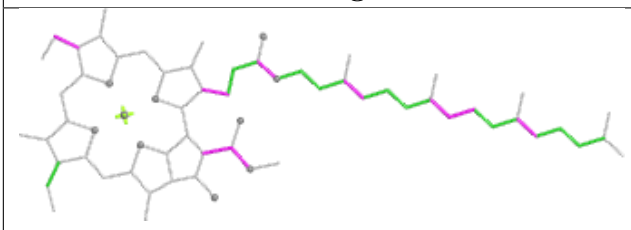
Ligand CLA B 842



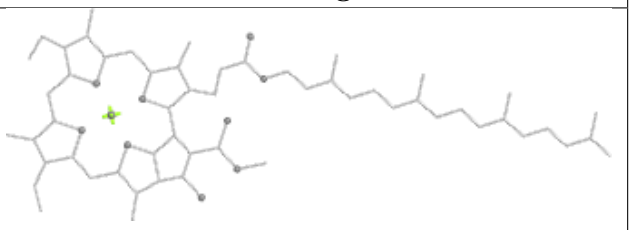
Bond lengths



Bond angles

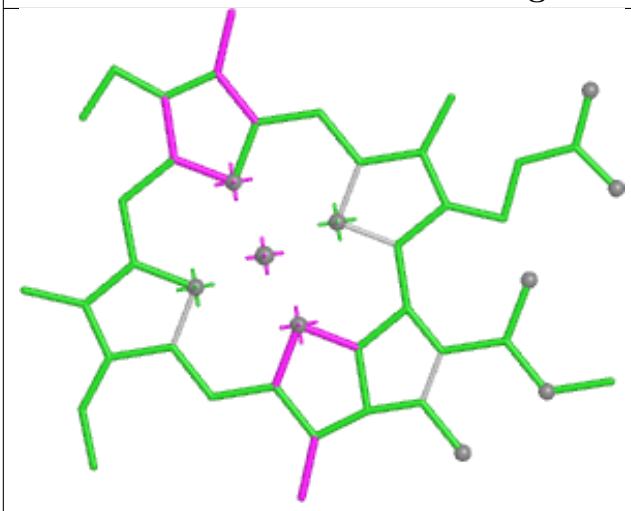


Torsions

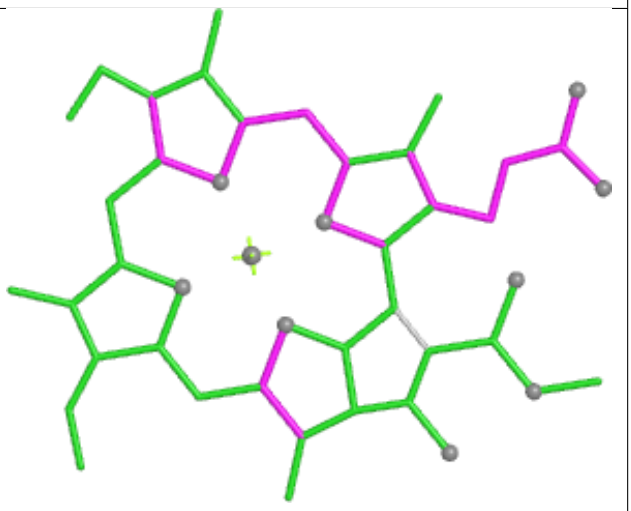


Rings

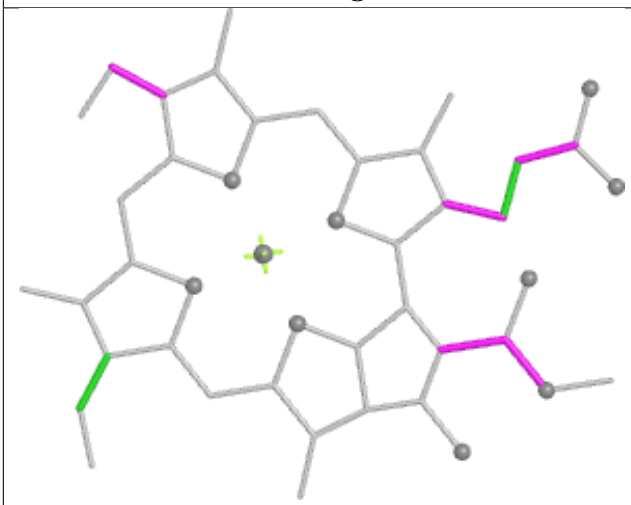
Ligand CLA 1 607



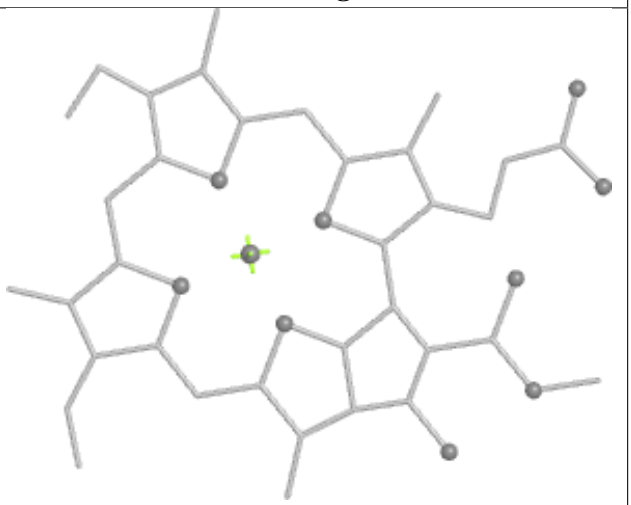
Bond lengths



Bond angles

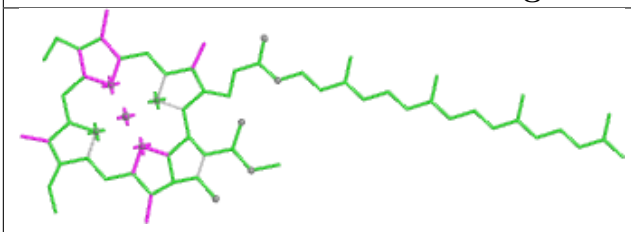


Torsions

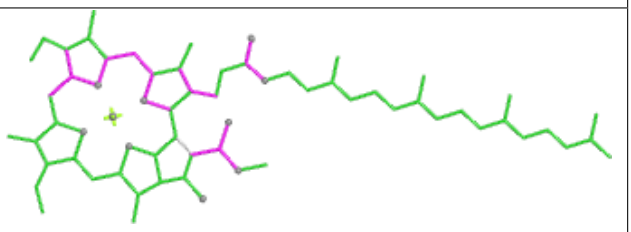


Rings

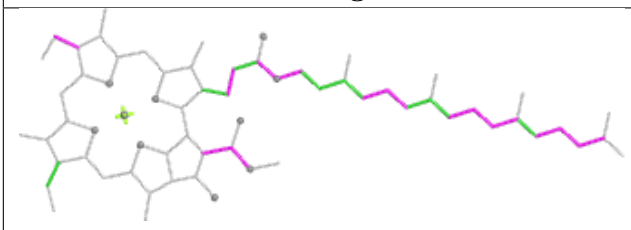
Ligand CLA A 839



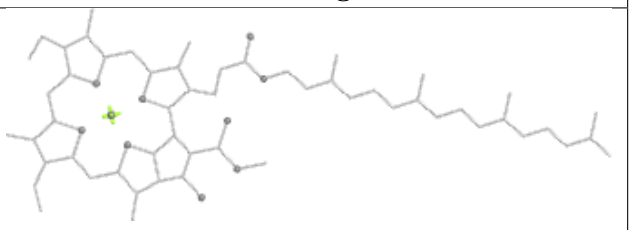
Bond lengths



Bond angles

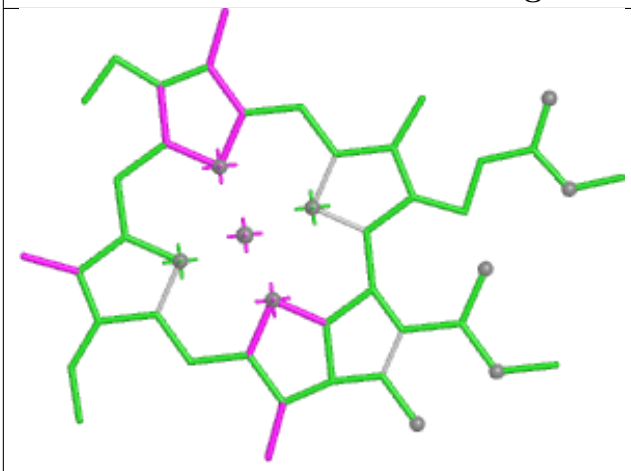


Torsions

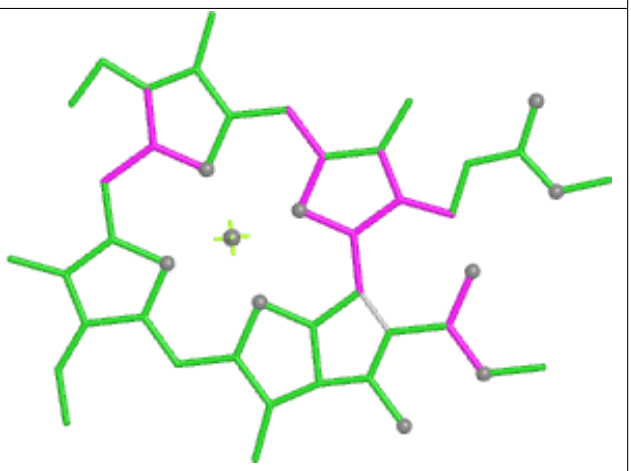


Rings

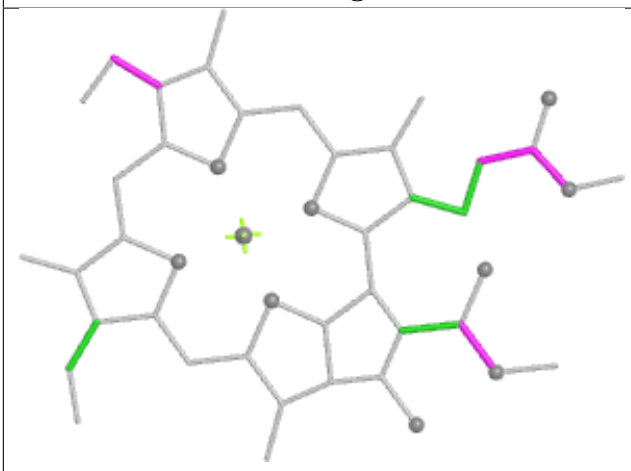
Ligand CLA B 824



Bond lengths



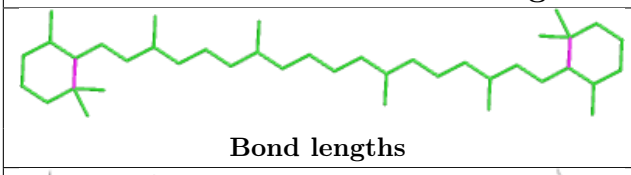
Bond angles



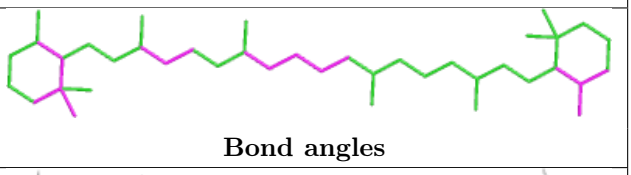
Torsions

Rings

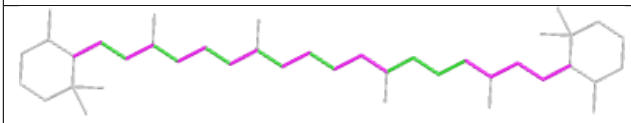
Ligand BCR I 101



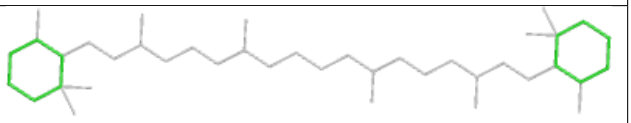
Bond lengths



Bond angles



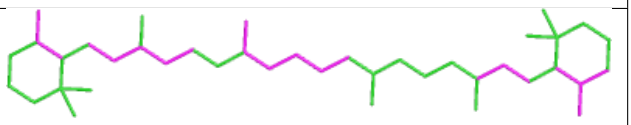
Torsions



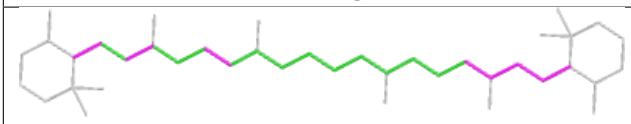
Rings

Ligand BCR K 101

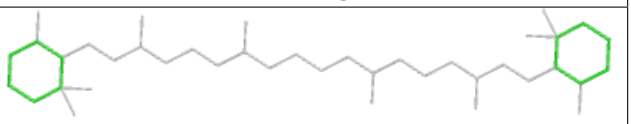
Bond lengths



Bond angles

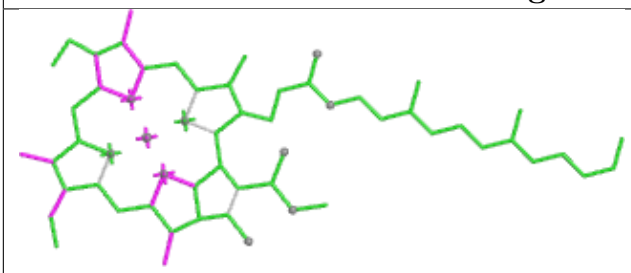


Torsions

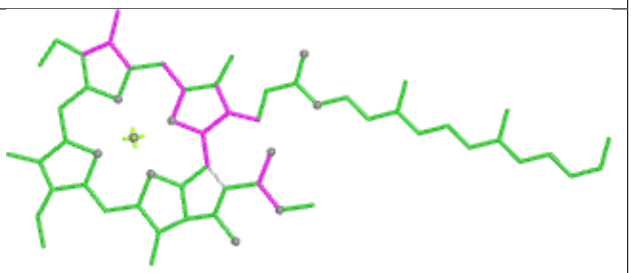


Rings

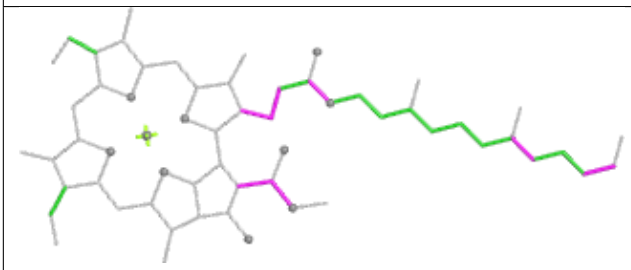
Ligand CLA 1 602



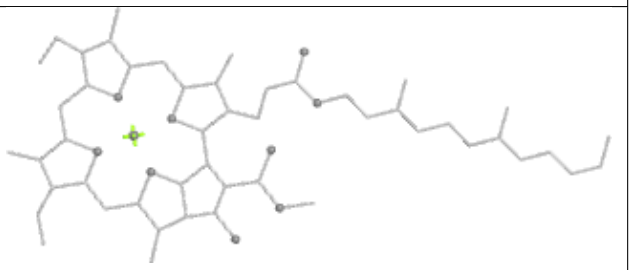
Bond lengths



Bond angles

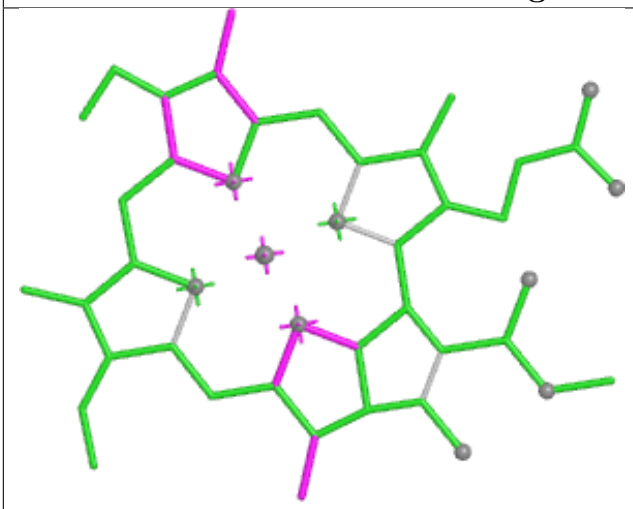


Torsions

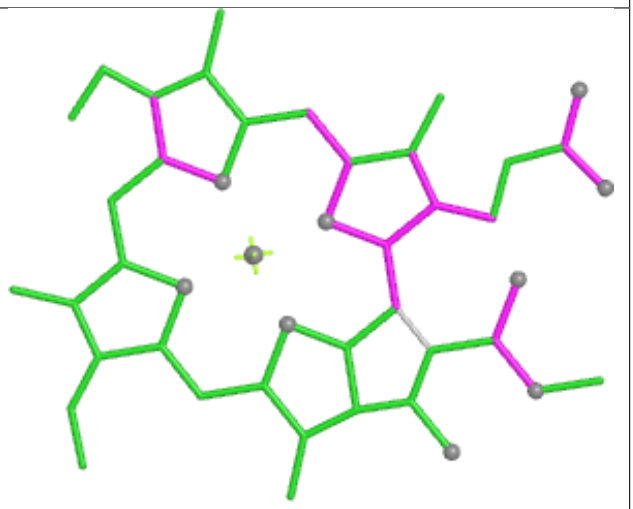


Rings

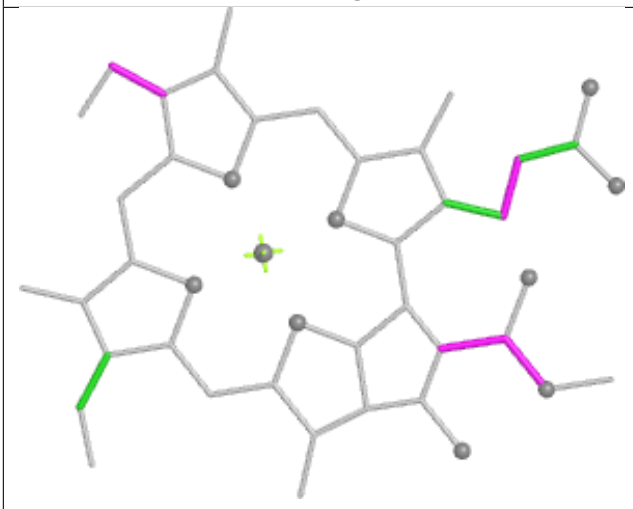
Ligand CLA 3 202



Bond lengths



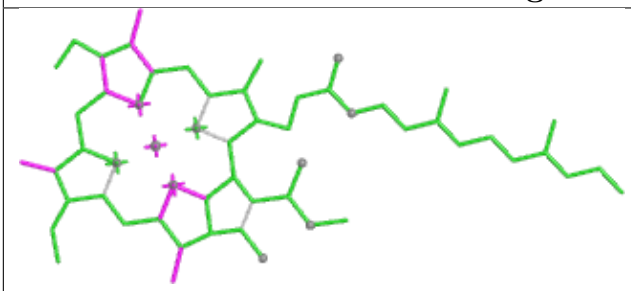
Bond angles



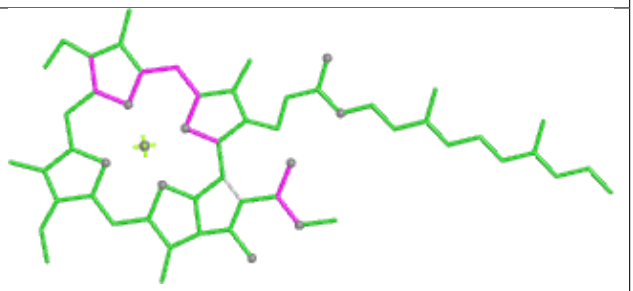
Torsions

Rings

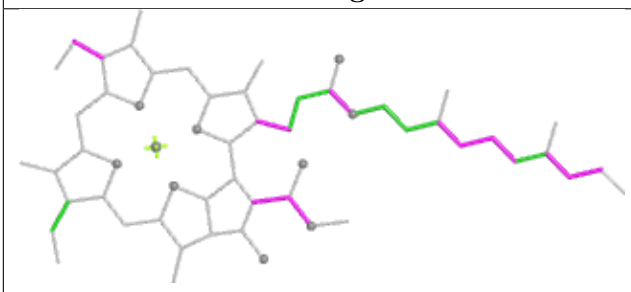
Ligand CLA L 202



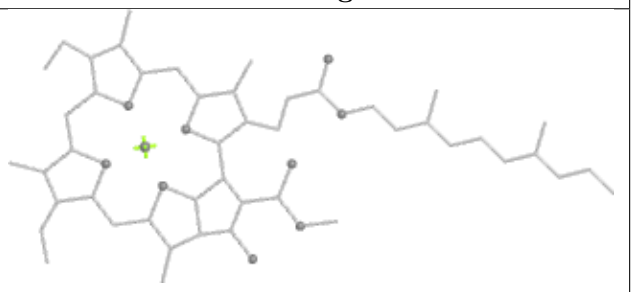
Bond lengths



Bond angles

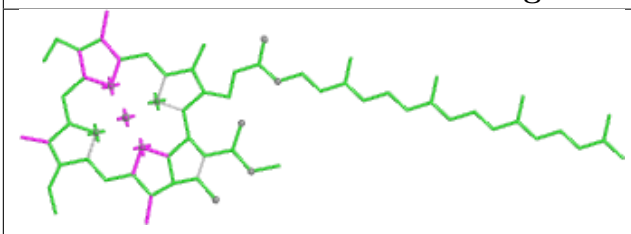


Torsions

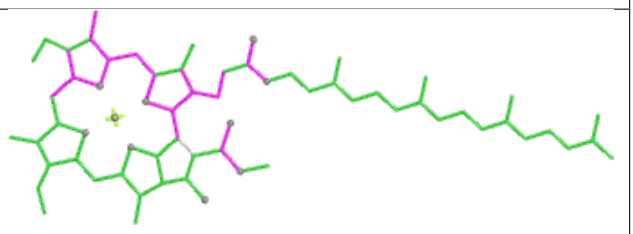


Rings

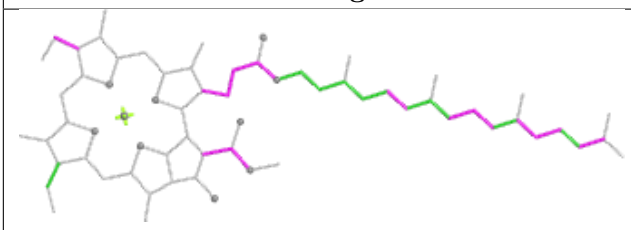
Ligand CLA A 831



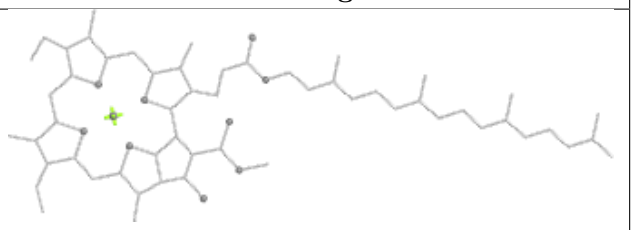
Bond lengths



Bond angles

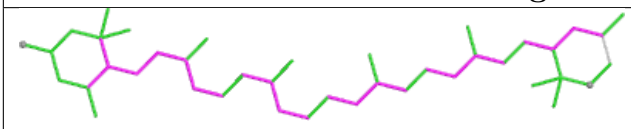


Torsions

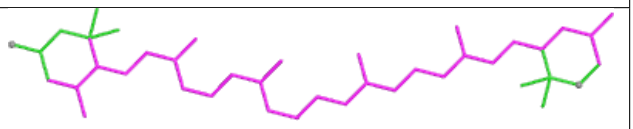


Rings

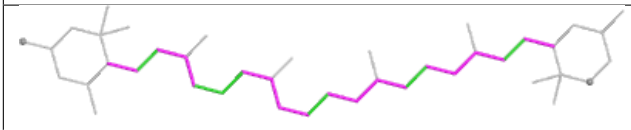
Ligand ZEX 1 614



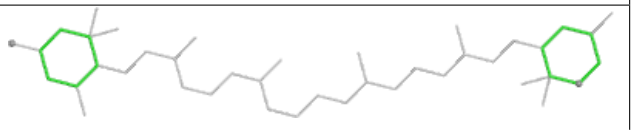
Bond lengths



Bond angles

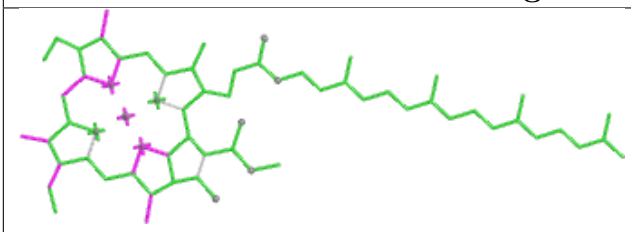


Torsions

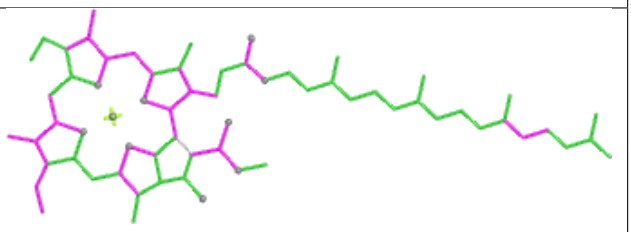


Rings

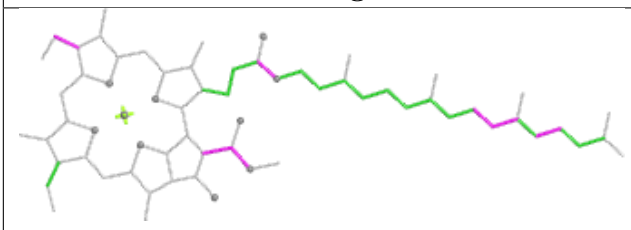
Ligand CLA A 828



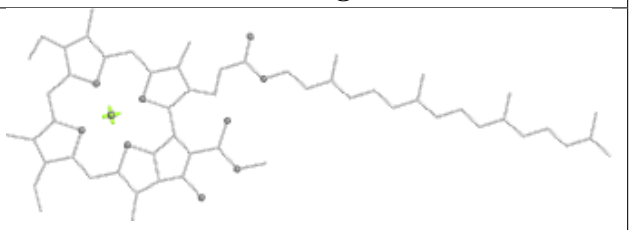
Bond lengths



Bond angles

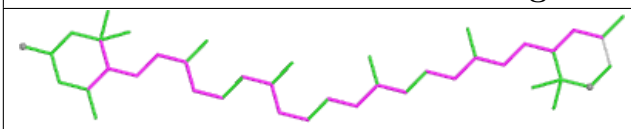


Torsions

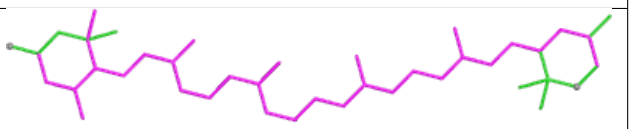


Rings

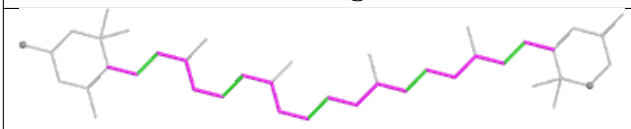
Ligand ZEX 5 615



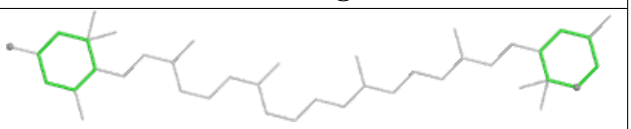
Bond lengths



Bond angles

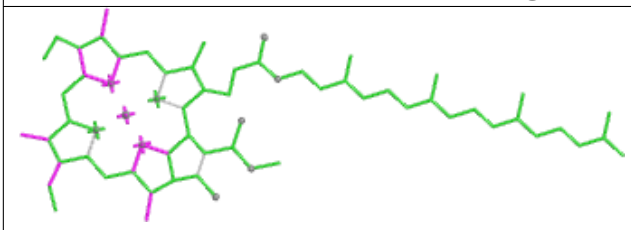


Torsions

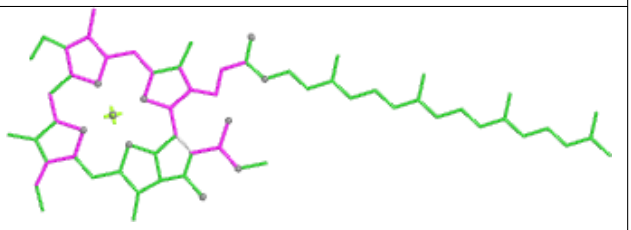


Rings

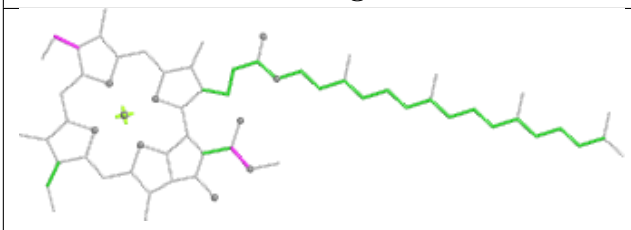
Ligand CLA A 803



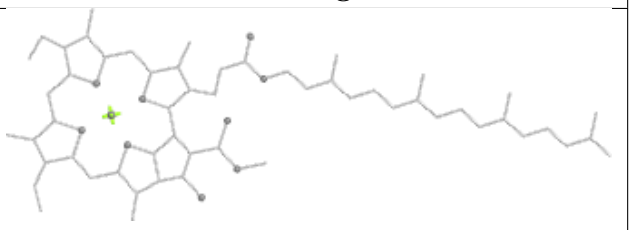
Bond lengths



Bond angles

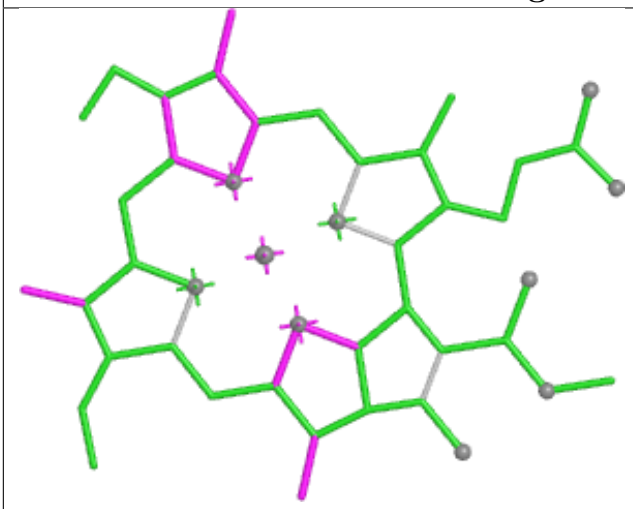


Torsions

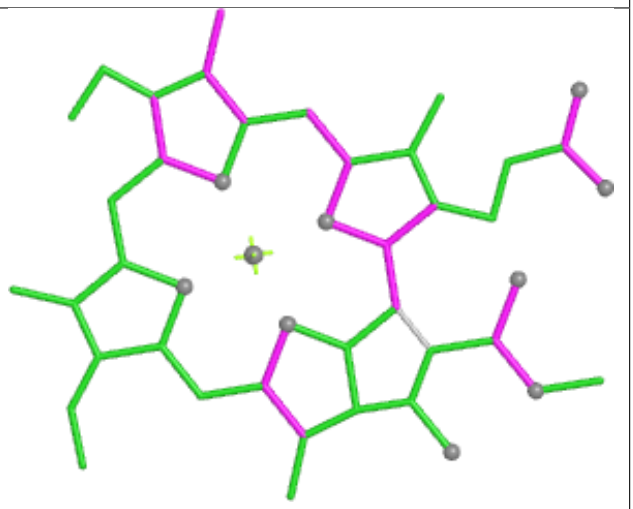


Rings

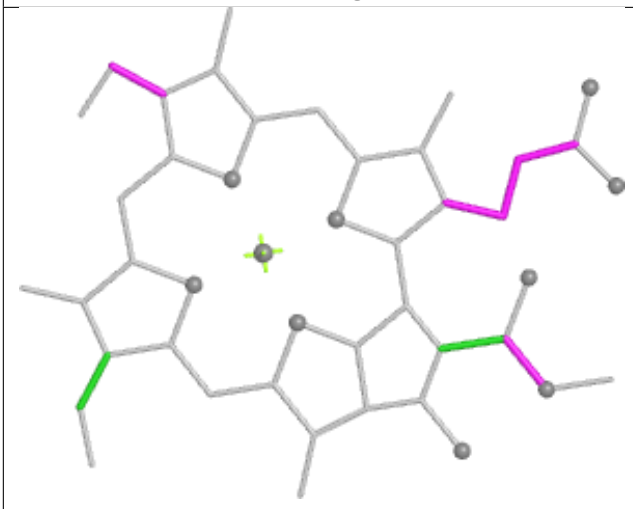
Ligand CLA 1 612



Bond lengths



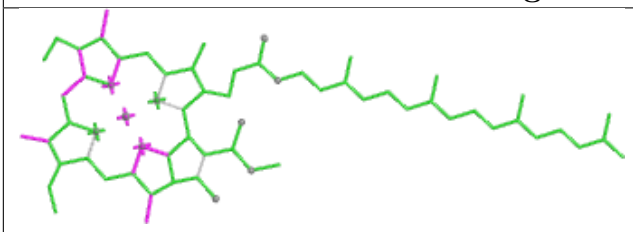
Bond angles



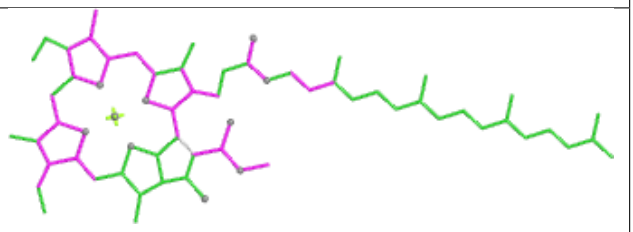
Torsions

Rings

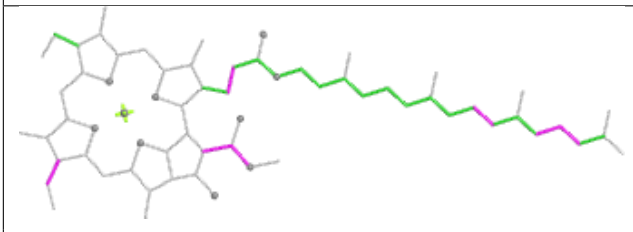
Ligand CLA A 848



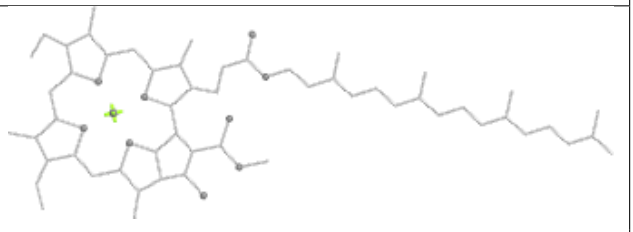
Bond lengths



Bond angles

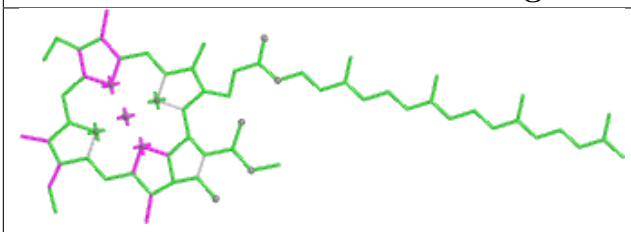


Torsions

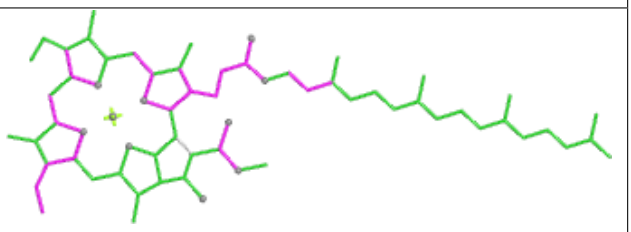


Rings

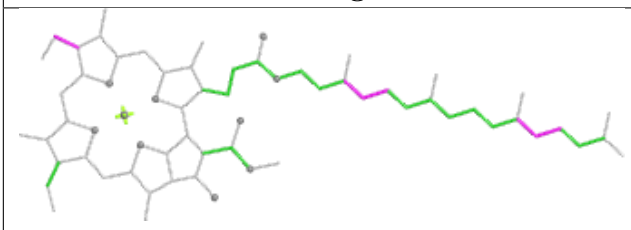
Ligand CLA B 811



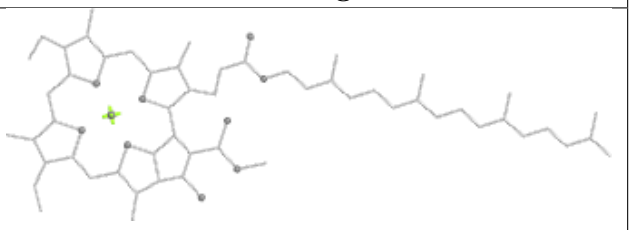
Bond lengths



Bond angles

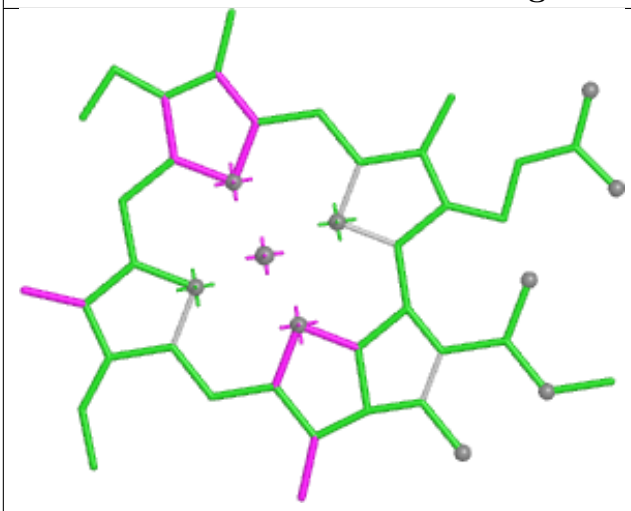


Torsions

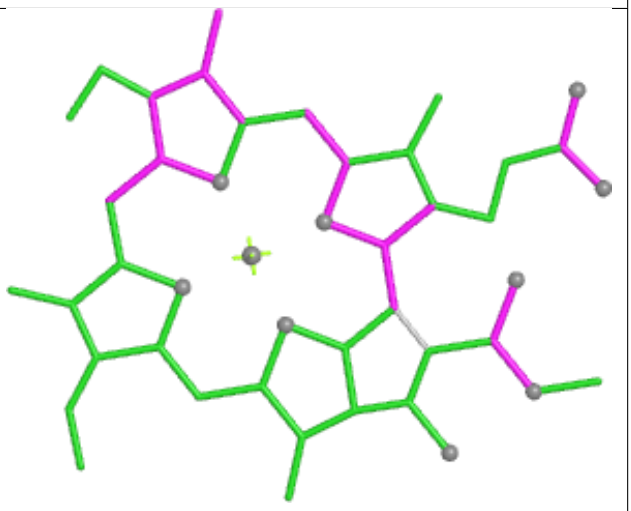


Rings

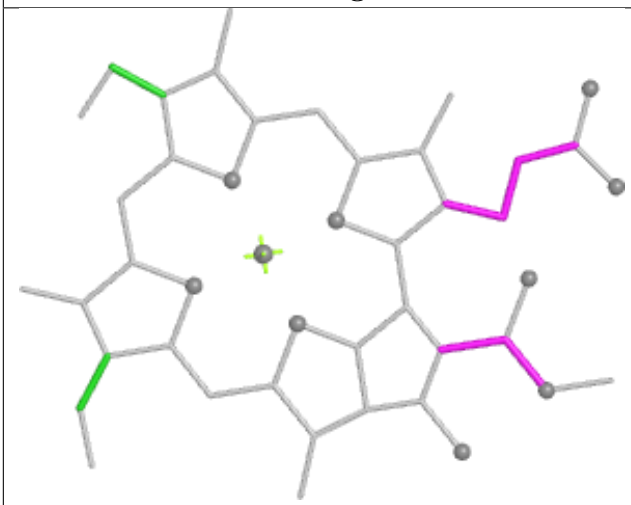
Ligand CLA 4 603



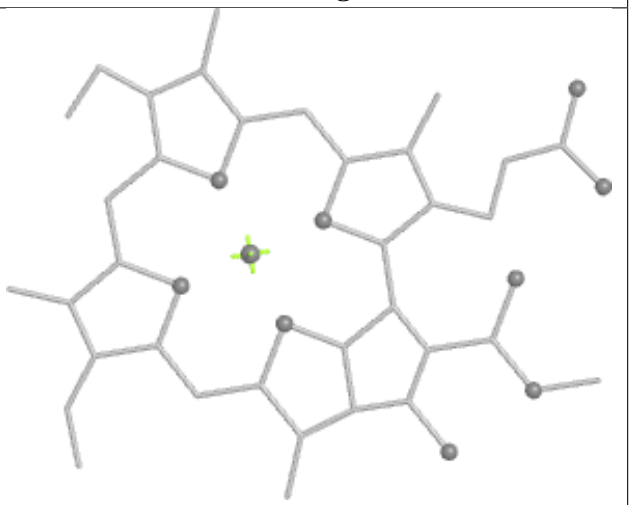
Bond lengths



Bond angles

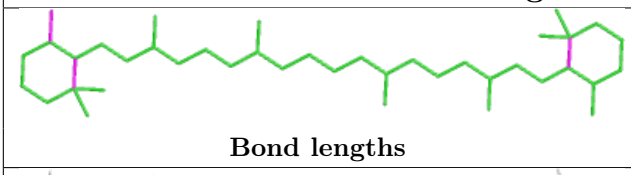


Torsions

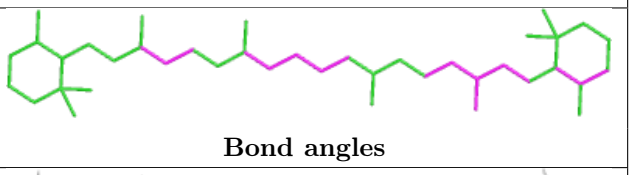


Rings

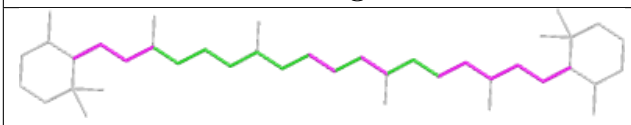
Ligand BCR J 105



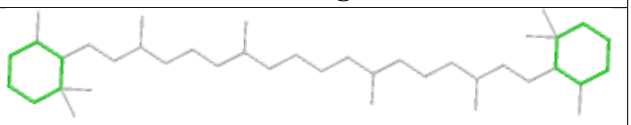
Bond lengths



Bond angles

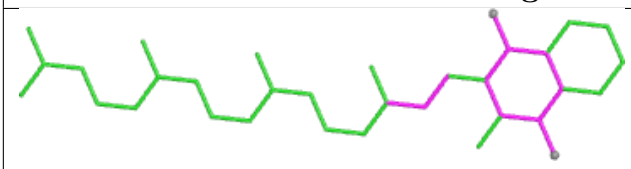


Torsions

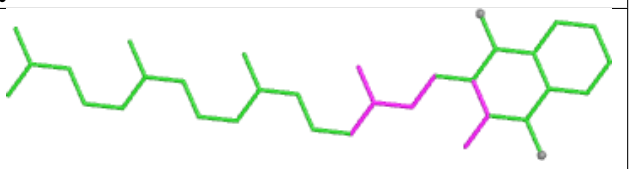


Rings

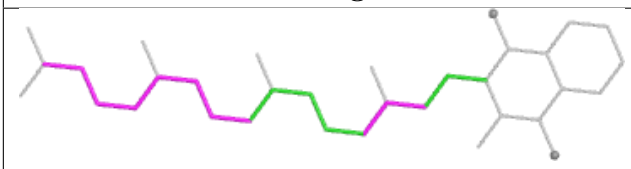
Ligand PQN A 840



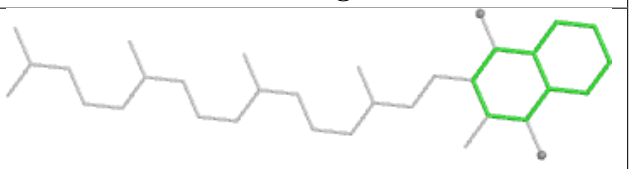
Bond lengths



Bond angles

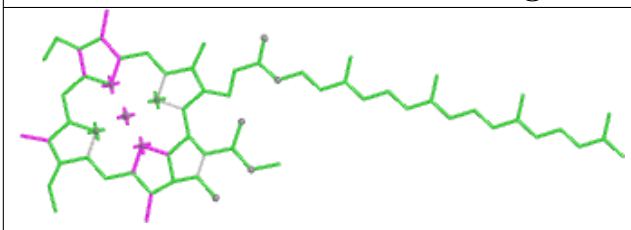


Torsions

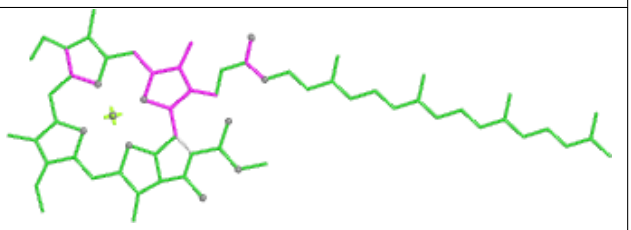


Rings

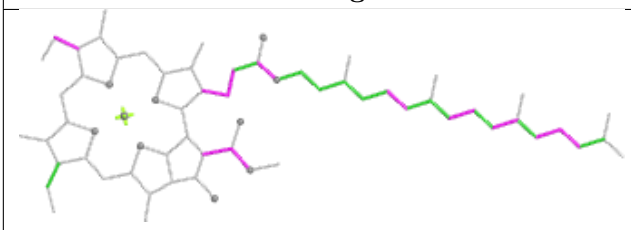
Ligand CLA A 811



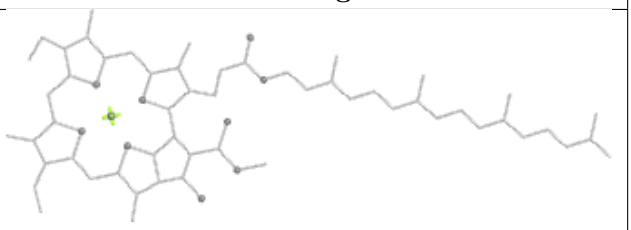
Bond lengths



Bond angles

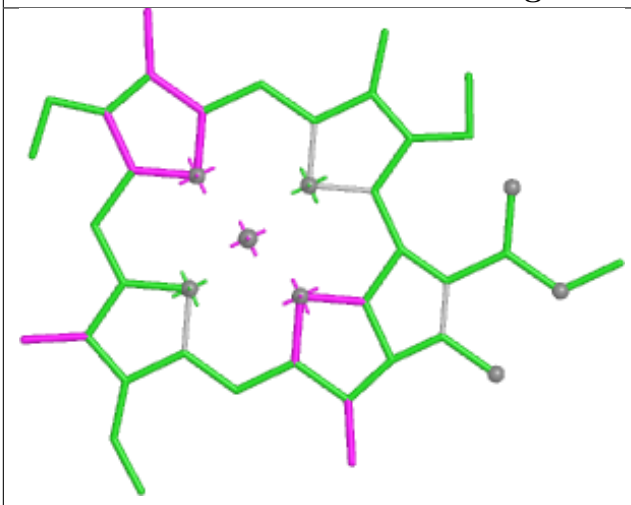


Torsions

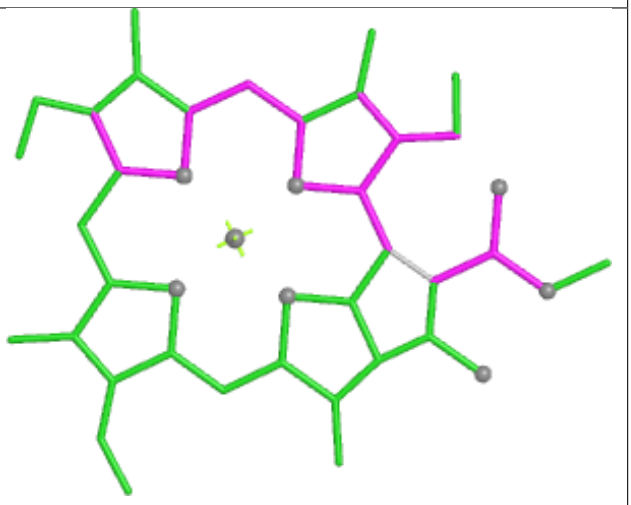


Rings

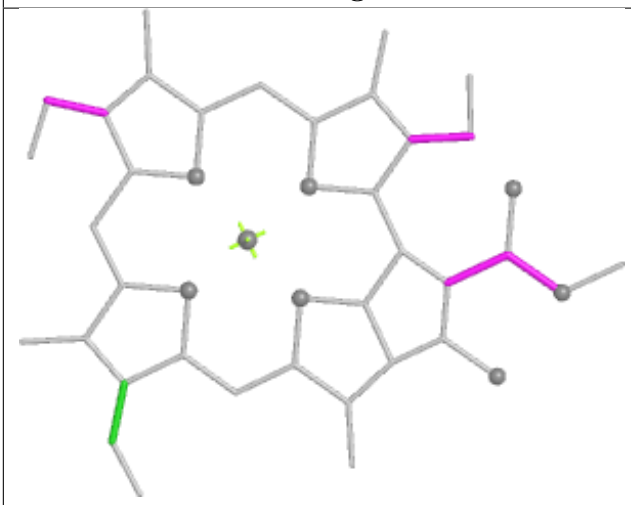
Ligand CLA B 818



Bond lengths



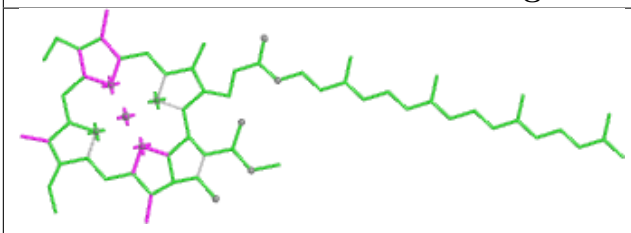
Bond angles



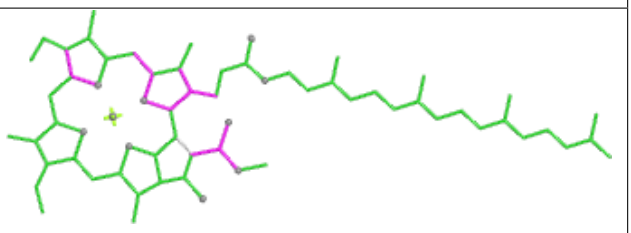
Torsions

Rings

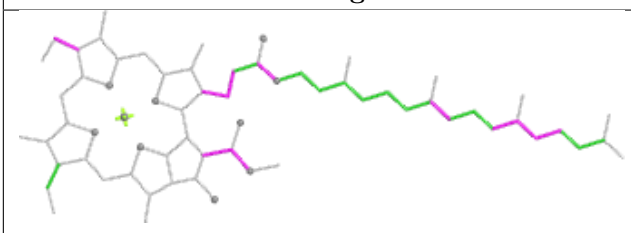
Ligand CLA A 806



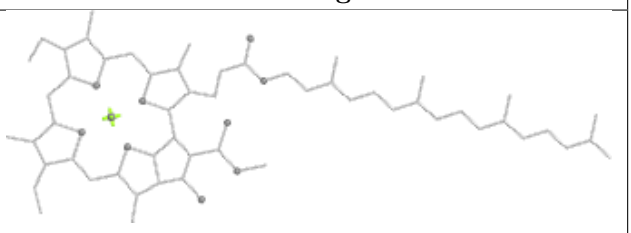
Bond lengths



Bond angles

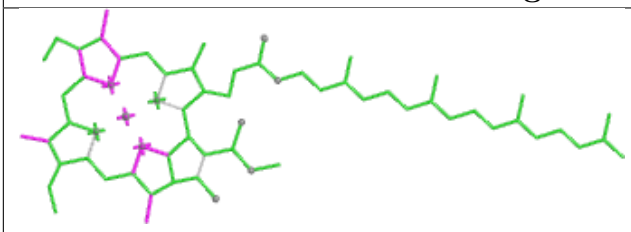


Torsions

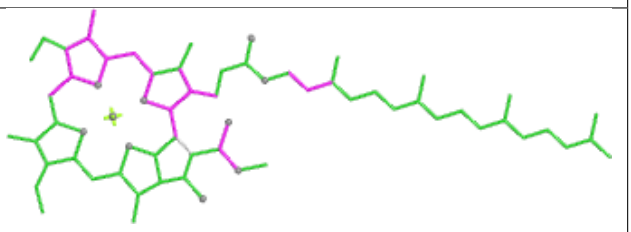


Rings

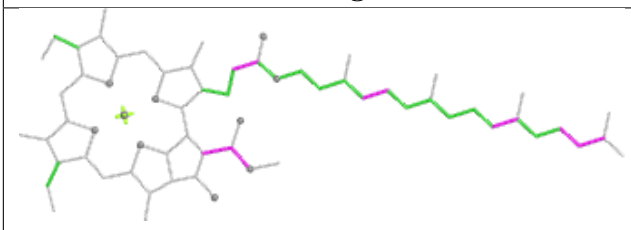
Ligand CLA A 837



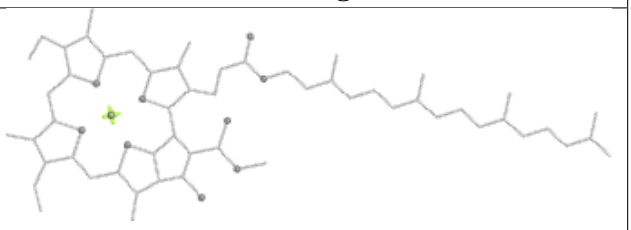
Bond lengths



Bond angles

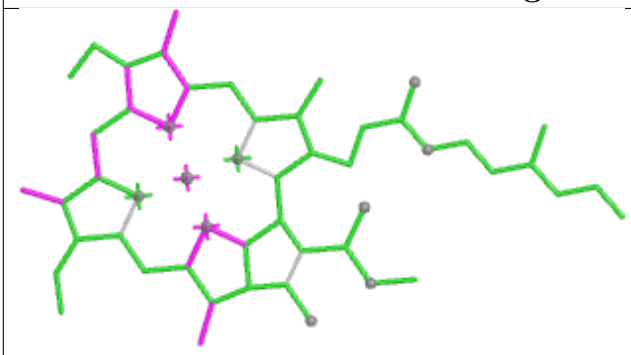


Torsions

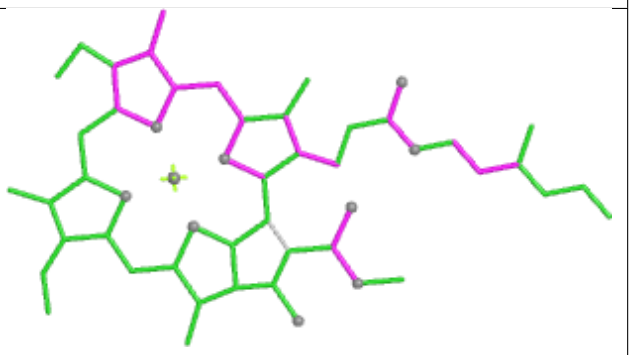


Rings

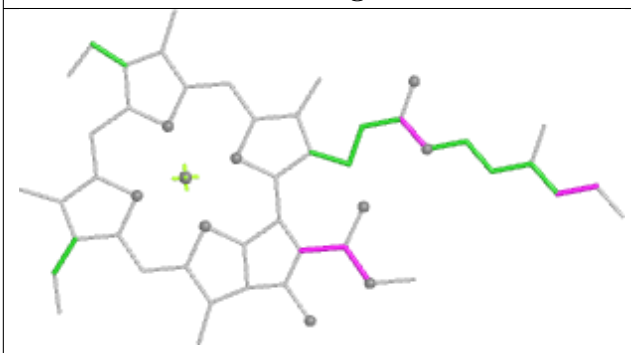
Ligand CLA O 201



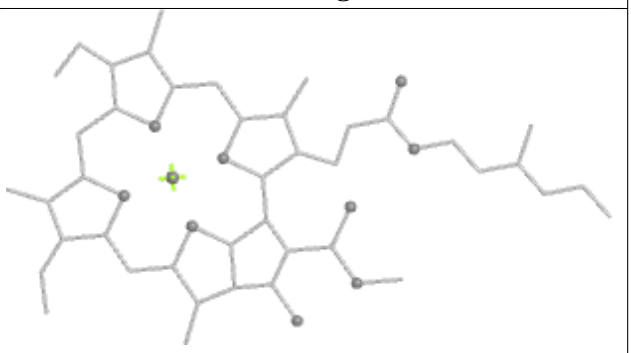
Bond lengths



Bond angles

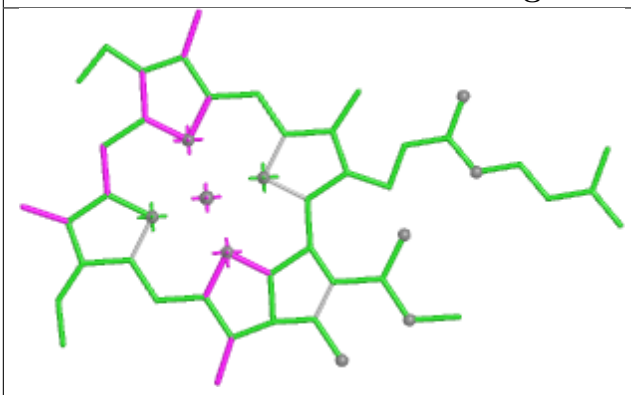


Torsions

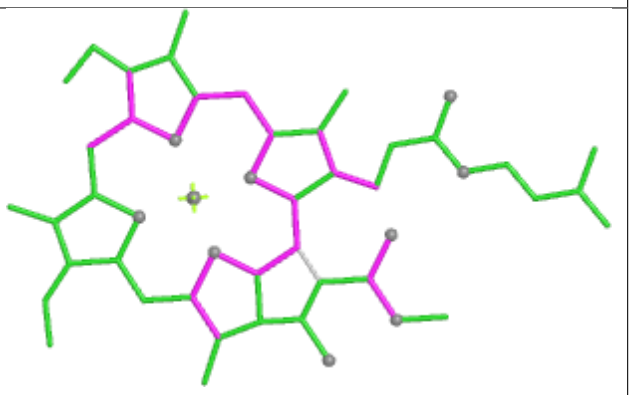


Rings

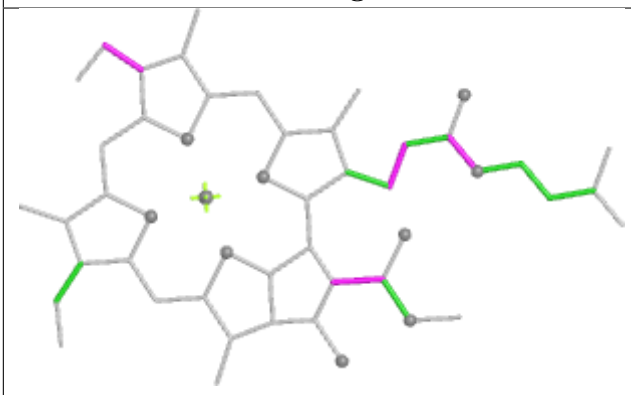
Ligand CLA A 829



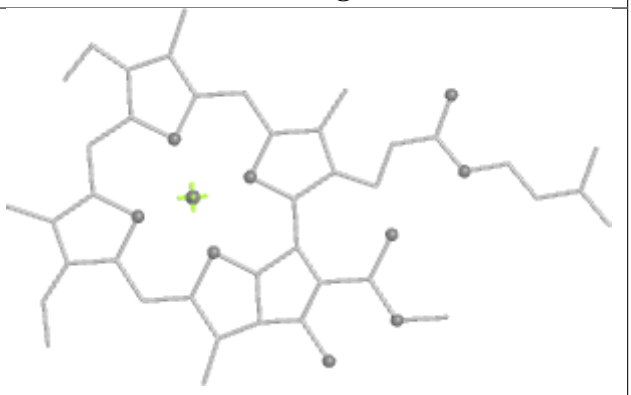
Bond lengths



Bond angles

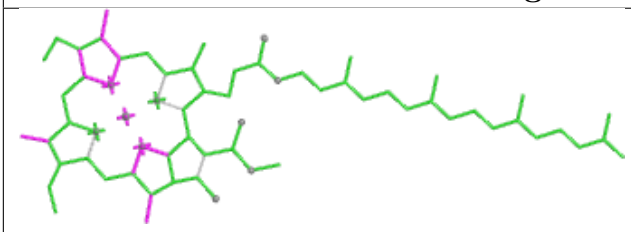


Torsions

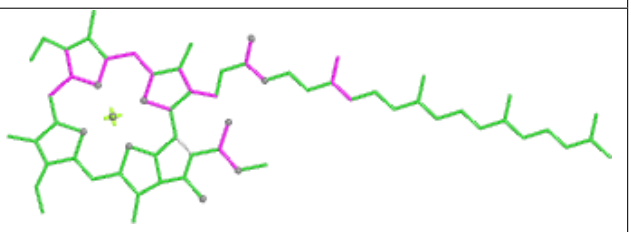


Rings

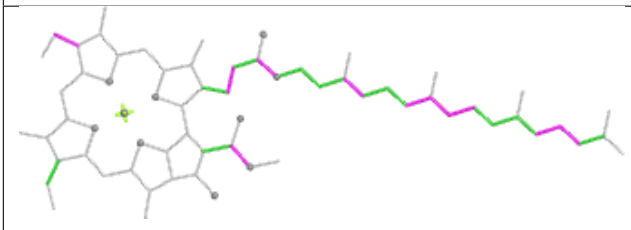
Ligand CLA B 841



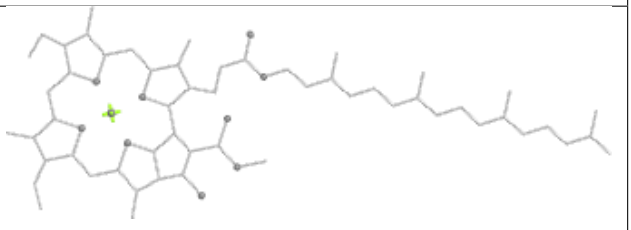
Bond lengths



Bond angles

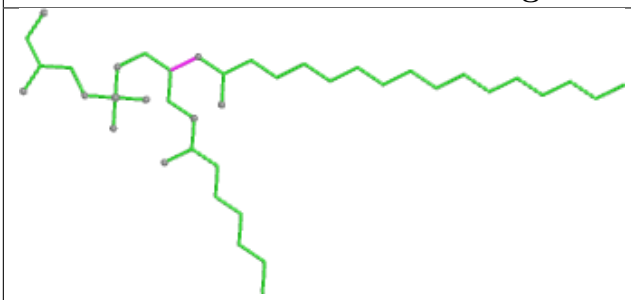


Torsions

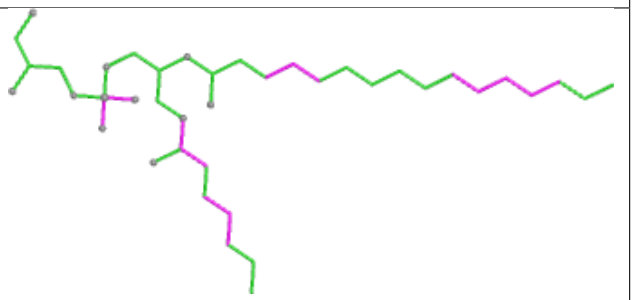


Rings

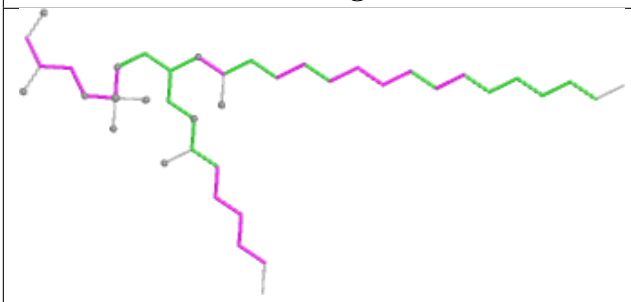
Ligand LHG A 842



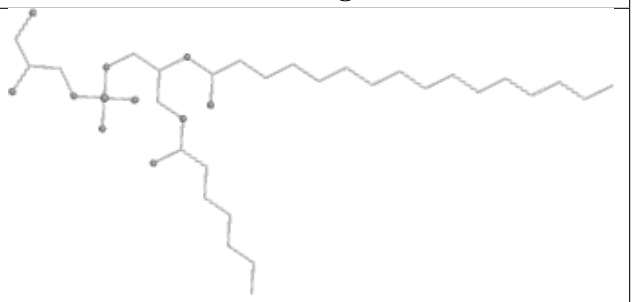
Bond lengths



Bond angles

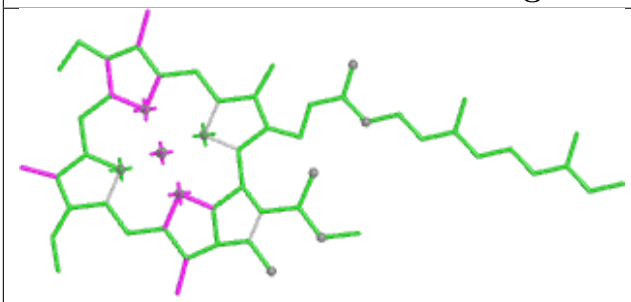


Torsions

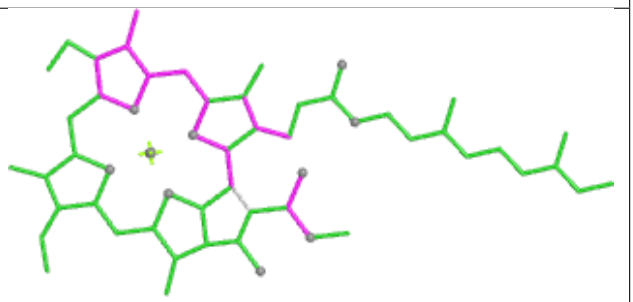


Rings

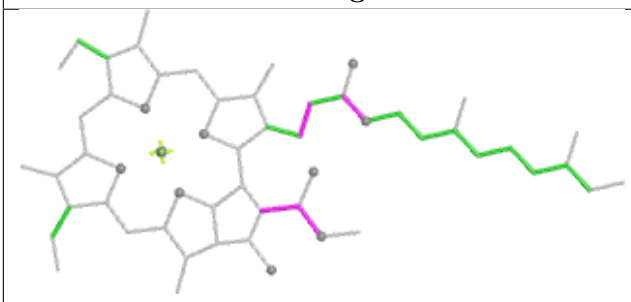
Ligand CLA A 830



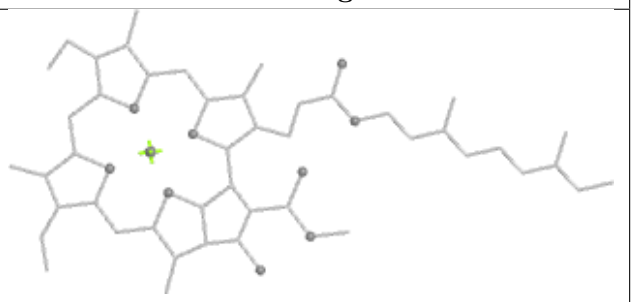
Bond lengths



Bond angles

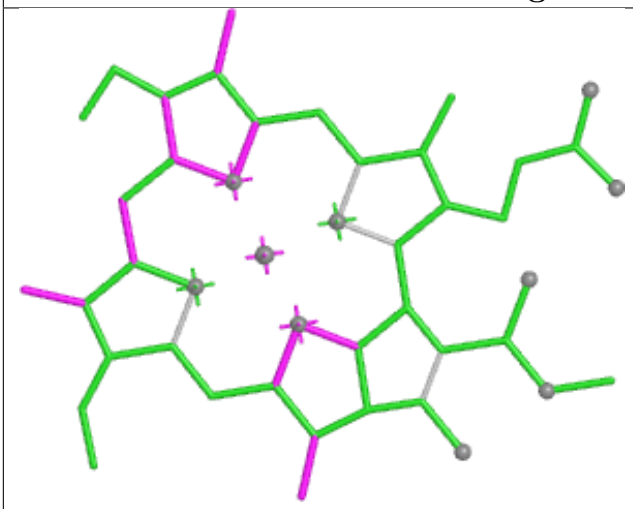


Torsions

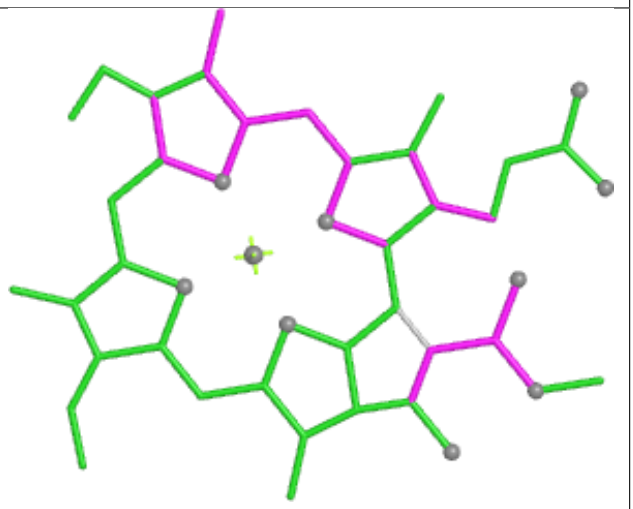


Rings

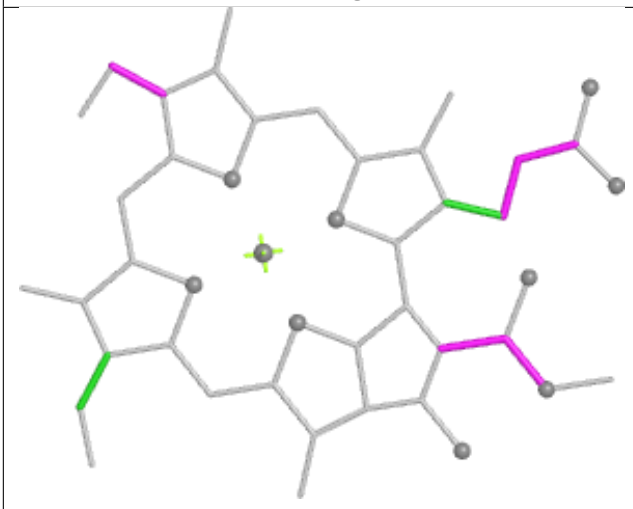
Ligand CLA 3 205



Bond lengths



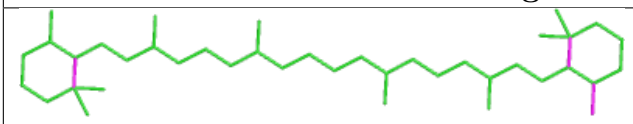
Bond angles



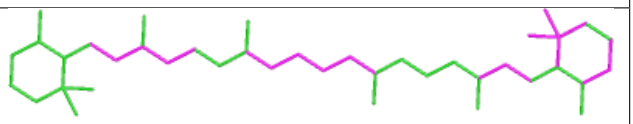
Torsions

Rings

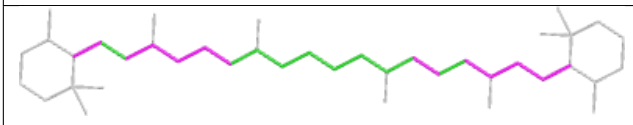
Ligand BCR O 202



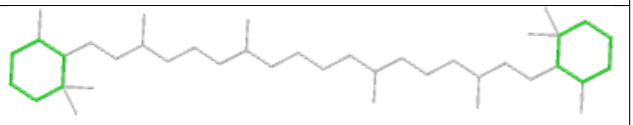
Bond lengths



Bond angles

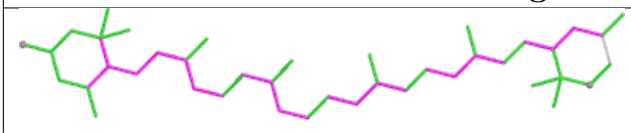


Torsions

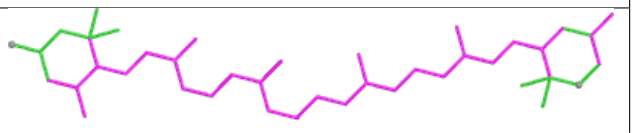


Rings

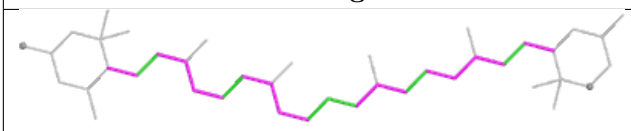
Ligand ZEX 4 612



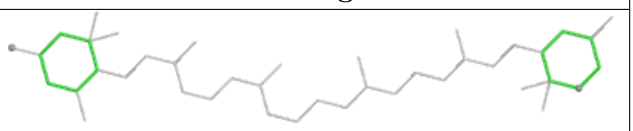
Bond lengths



Bond angles

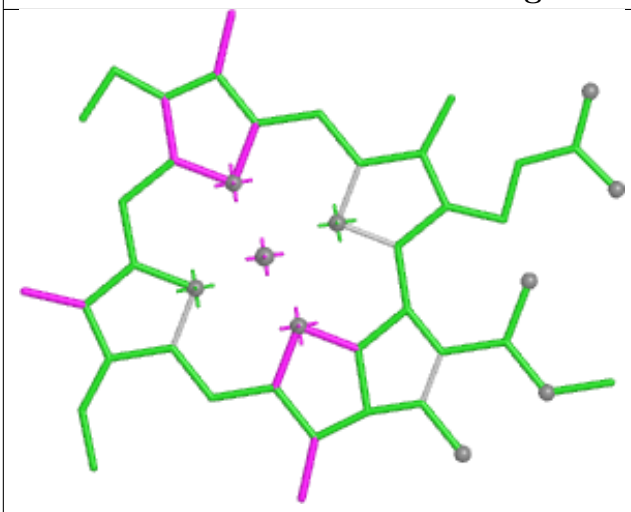


Torsions

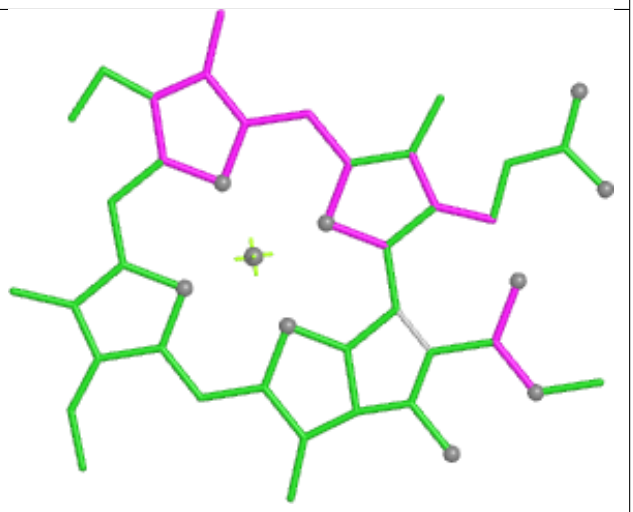


Rings

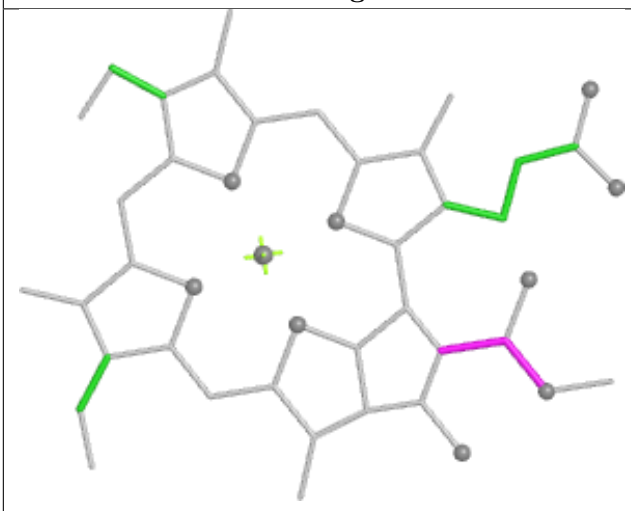
Ligand CLA B 817



Bond lengths



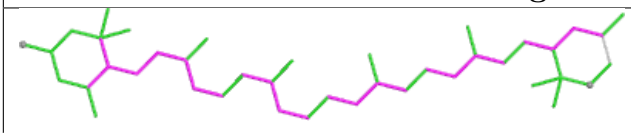
Bond angles



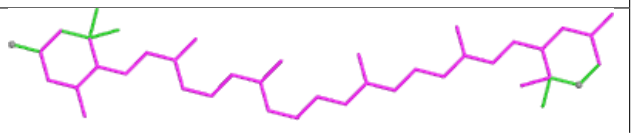
Torsions

Rings

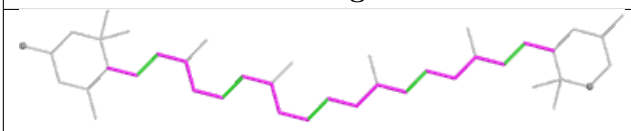
Ligand ZEX 2 614



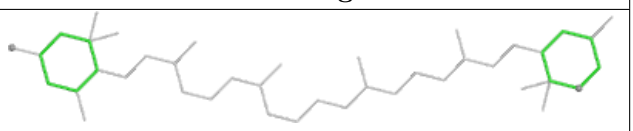
Bond lengths



Bond angles

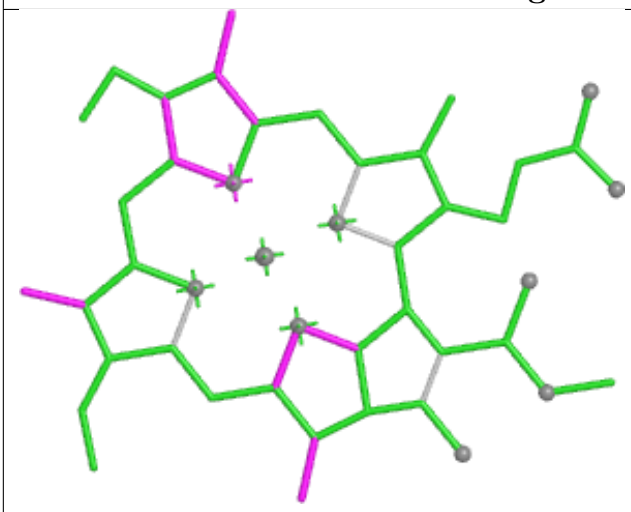


Torsions

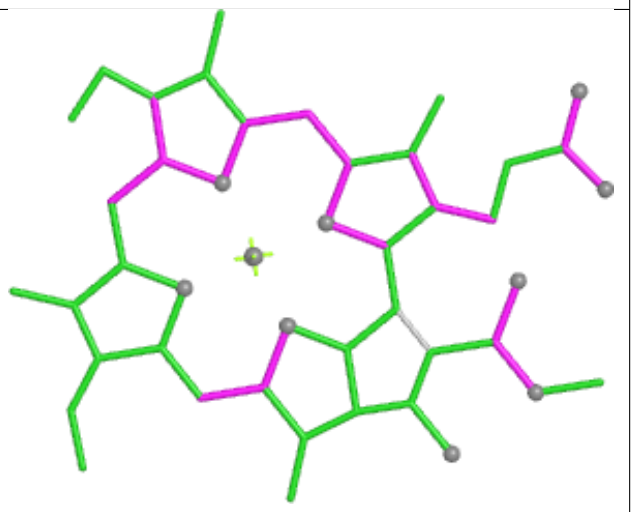


Rings

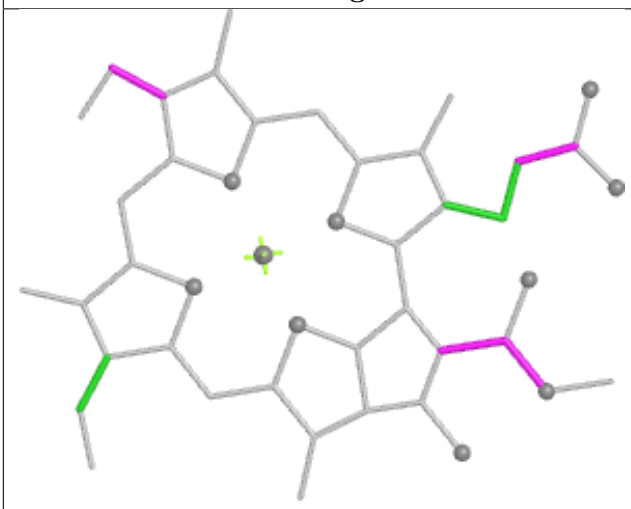
Ligand CLA 3 207



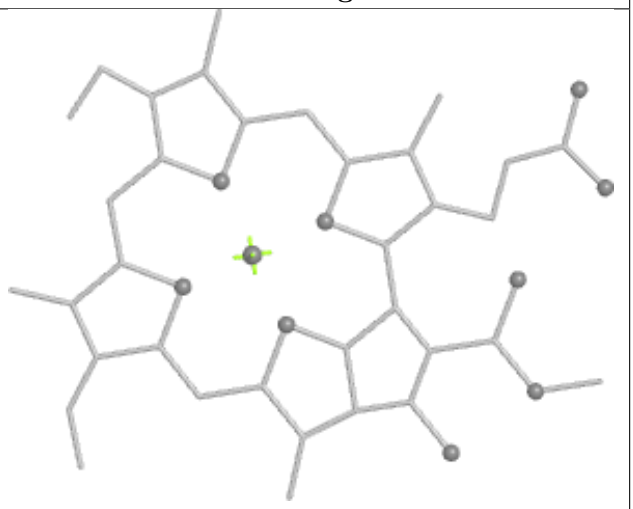
Bond lengths



Bond angles

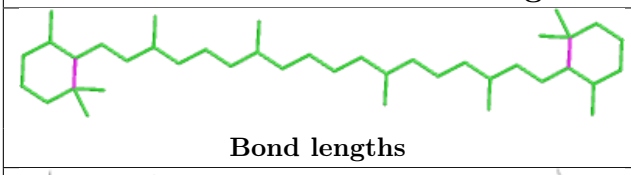


Torsions

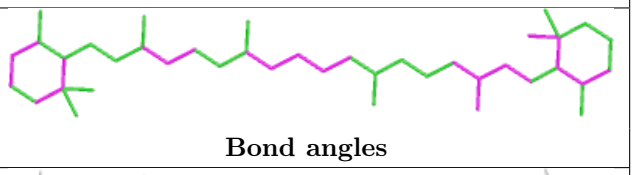


Rings

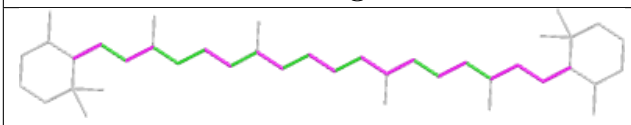
Ligand BCR L 205



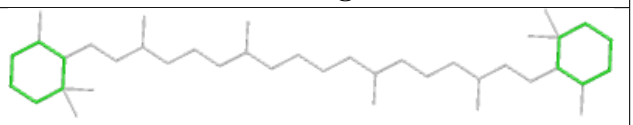
Bond lengths



Bond angles

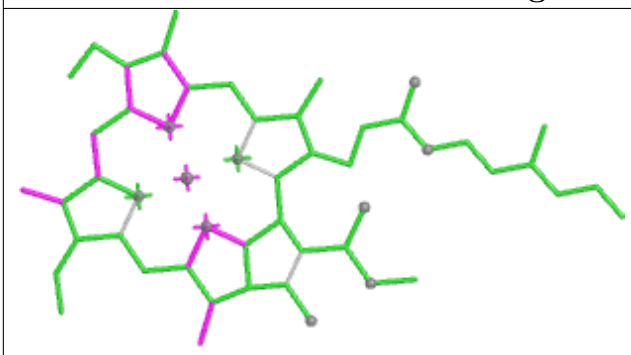


Torsions

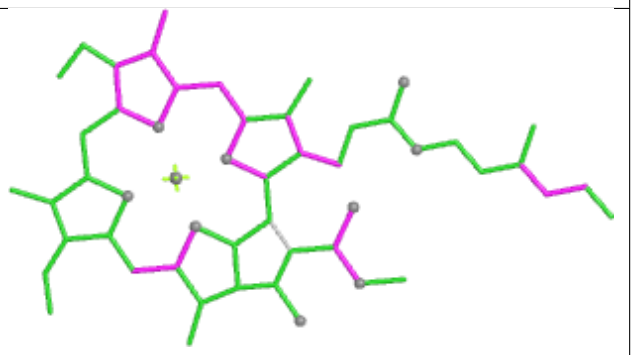


Rings

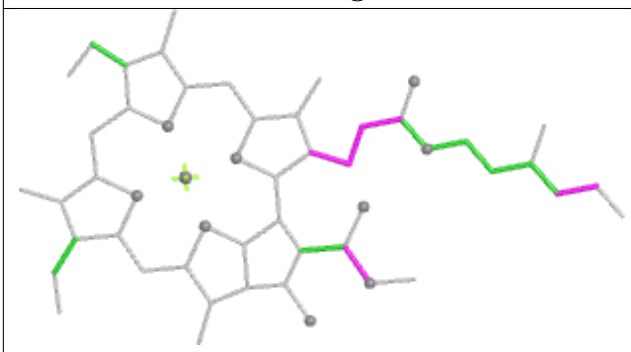
Ligand CLA 3 209



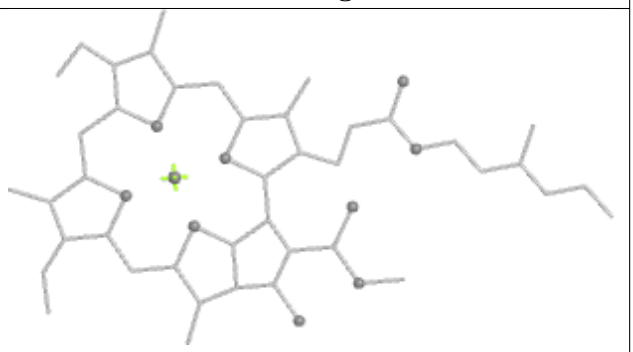
Bond lengths



Bond angles

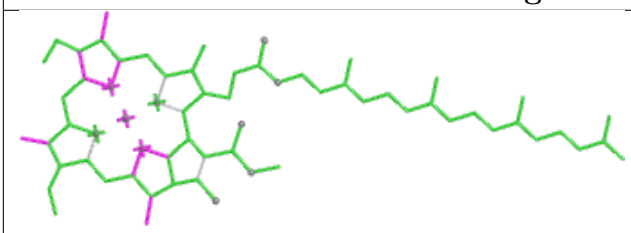


Torsions

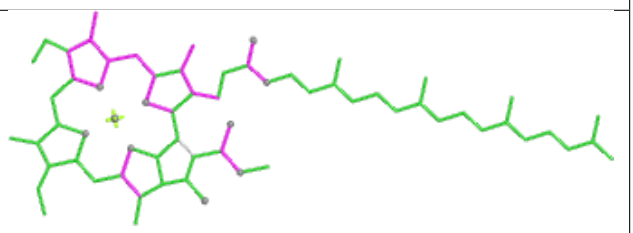


Rings

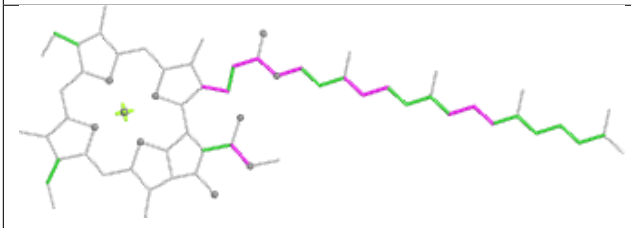
Ligand CLA B 831



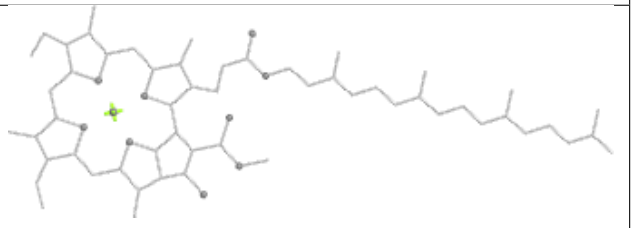
Bond lengths



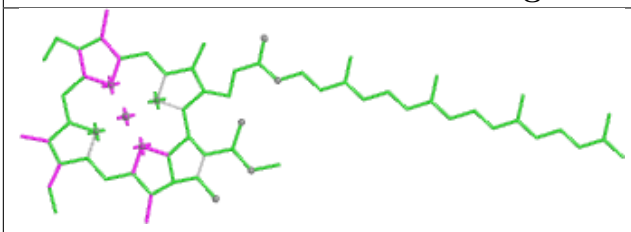
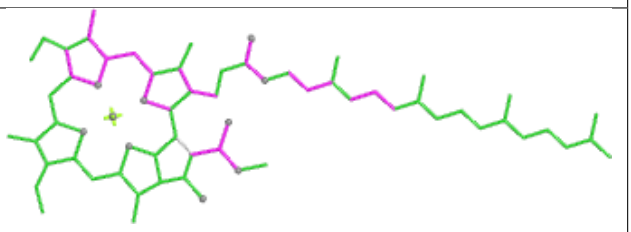
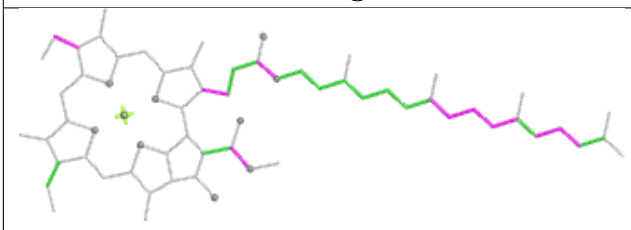
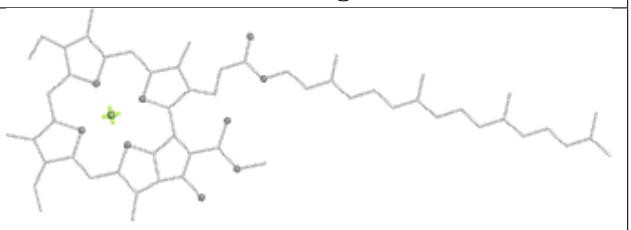
Bond angles



Torsions



Rings

Ligand CLA A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

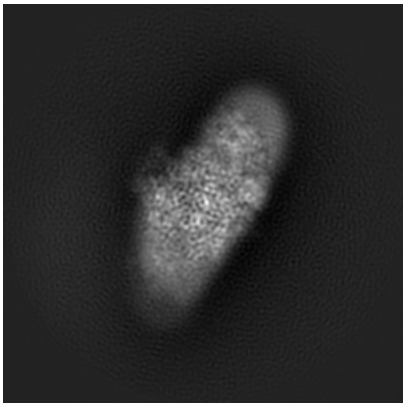
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6929. These allow visual inspection of the internal detail of the map and identification of artifacts.

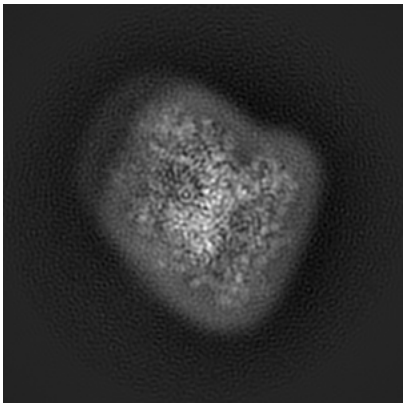
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

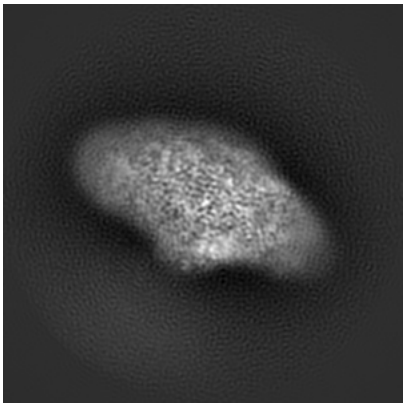
6.1.1 Primary map



X



Y

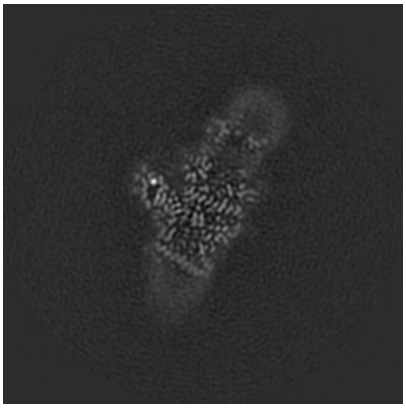


Z

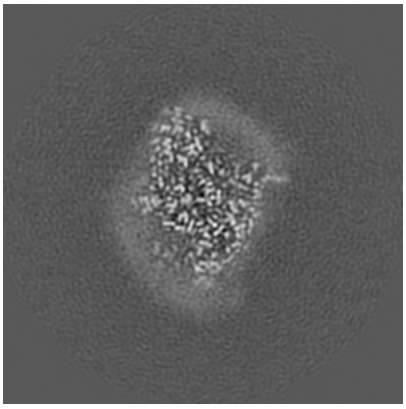
The images above show the map projected in three orthogonal directions.

6.2 Central slices

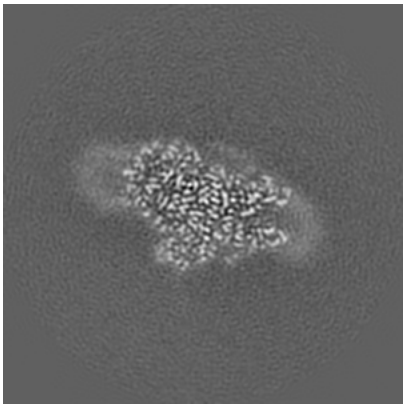
6.2.1 Primary map



X Index: 140



Y Index: 140

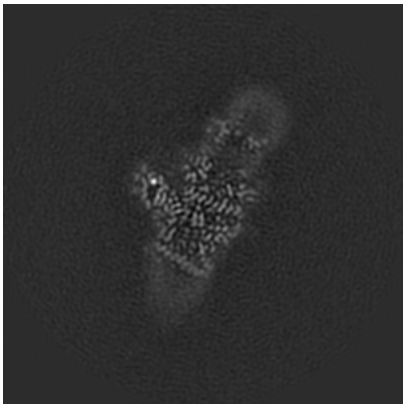


Z Index: 140

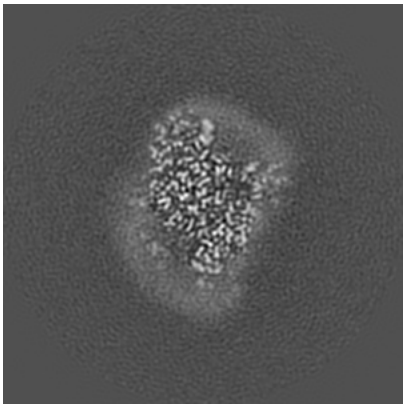
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

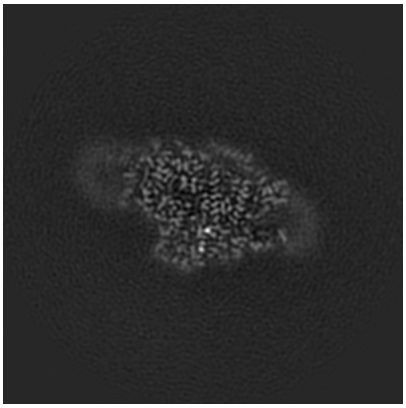
6.3.1 Primary map



X Index: 140



Y Index: 142

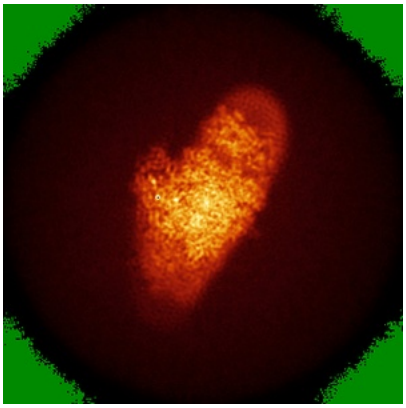


Z Index: 143

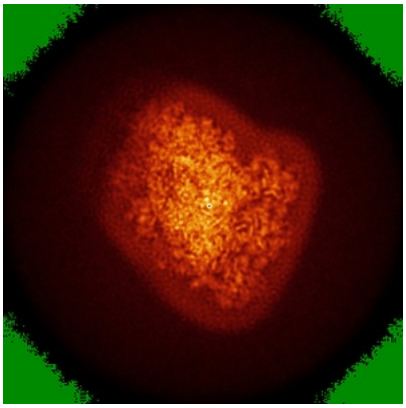
The images above show the largest variance slices of the map in three orthogonal directions.

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

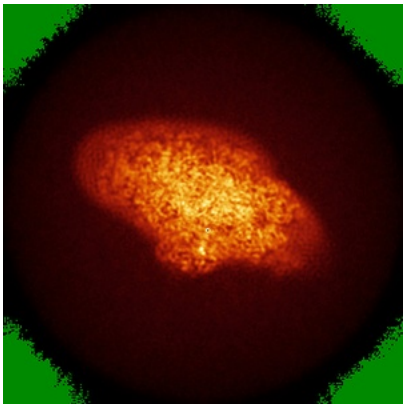
6.4.1 Primary map



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 0.0562. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

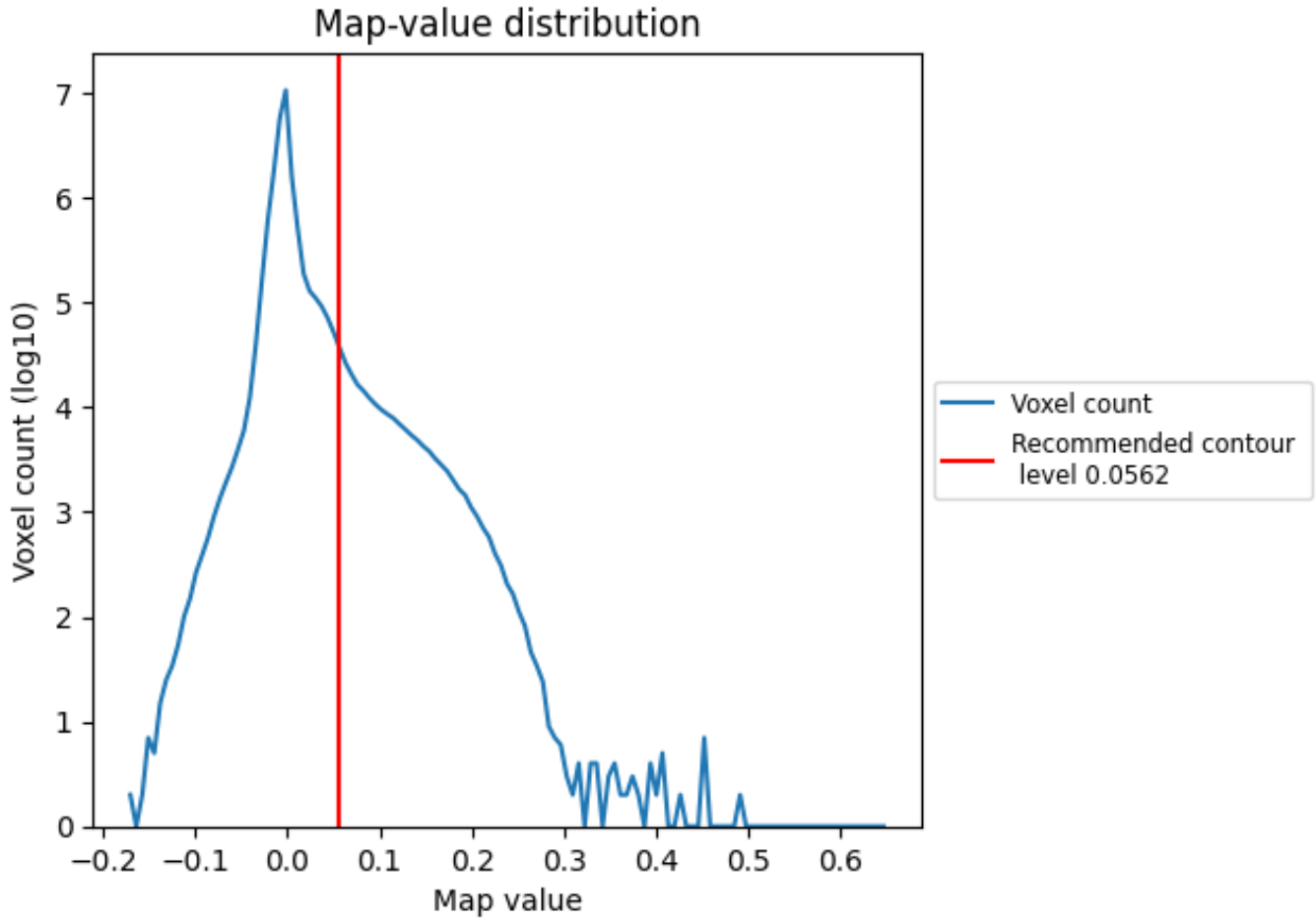
6.6 Mask visualisation (i)

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

7 Map analysis

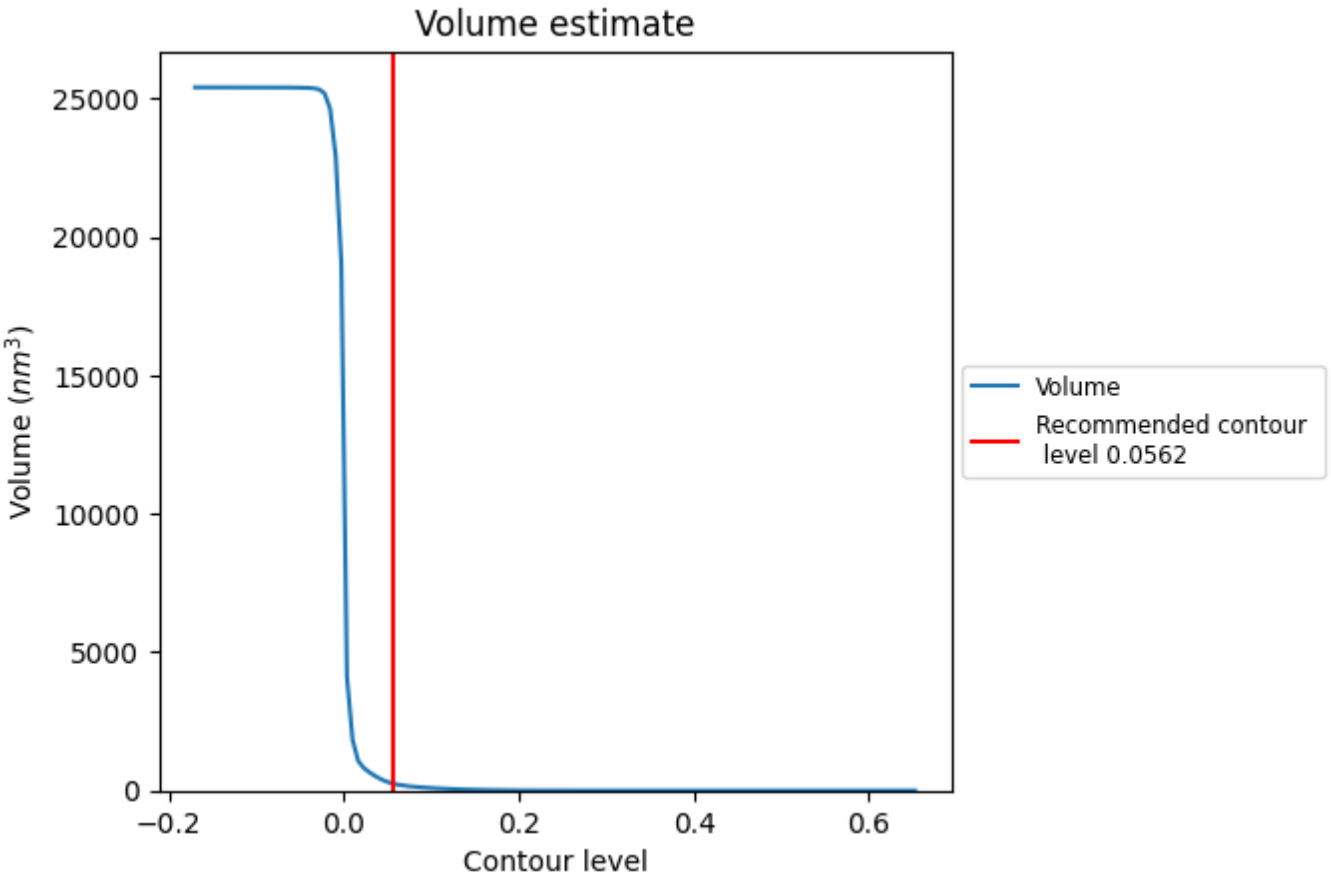
This section contains the results of statistical analysis of the map.

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.

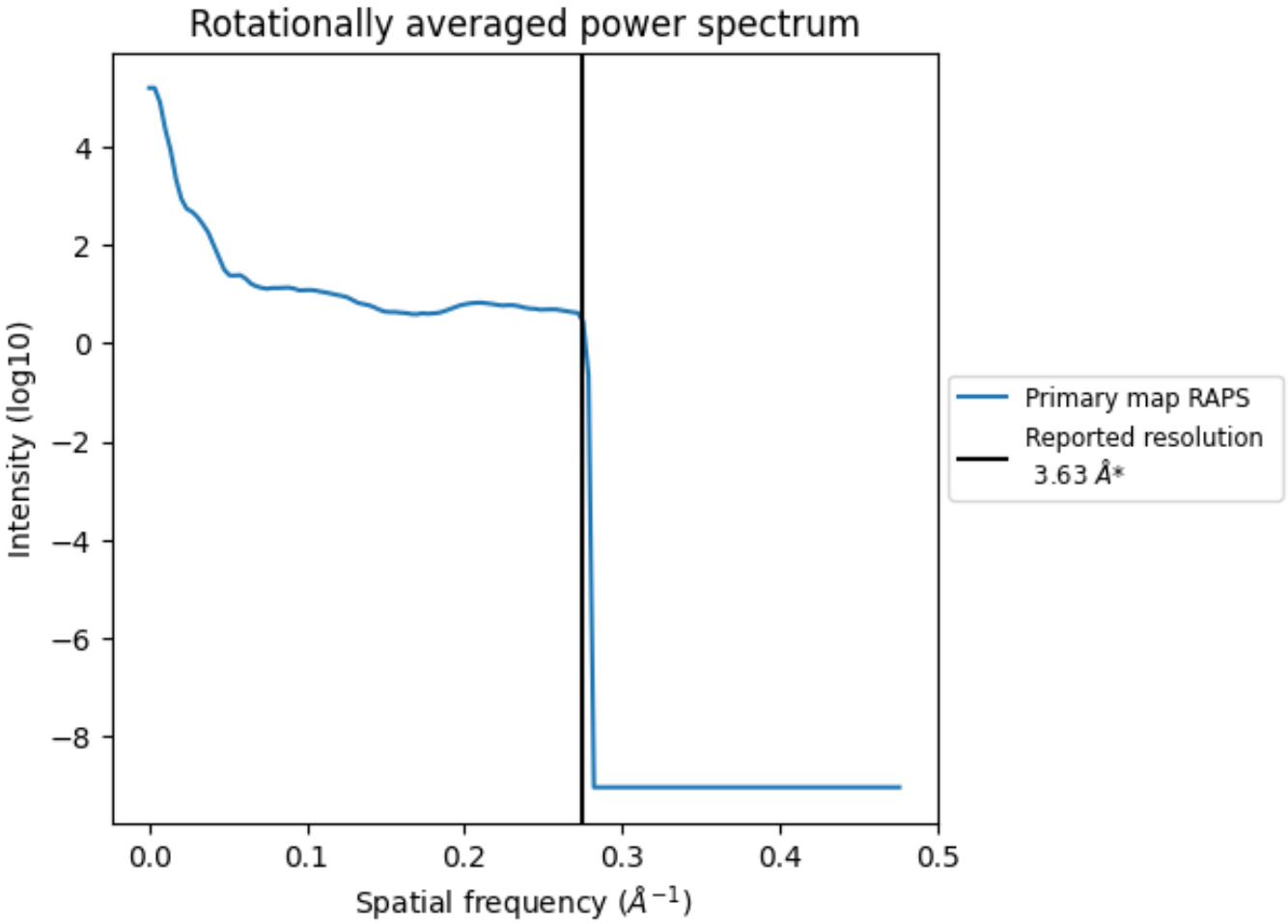
7.2 Volume estimate (i)



The volume at the recommended contour level is 253 nm^3; this corresponds to an approximate mass of 228 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 0.275 Å^{-1}

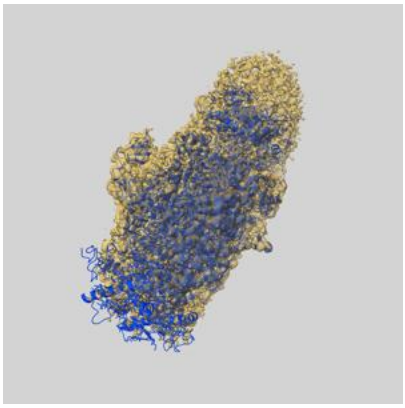
8 Fourier-Shell correlation

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

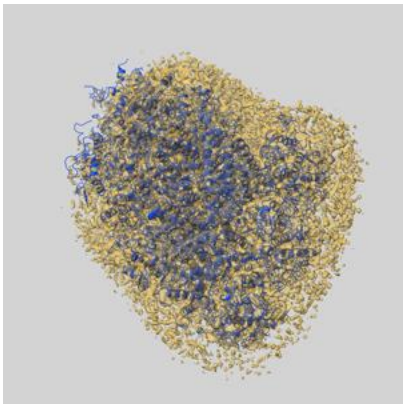
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6929 and PDB model 5ZGB. Per-residue inclusion information can be found in section 3 on page 23.

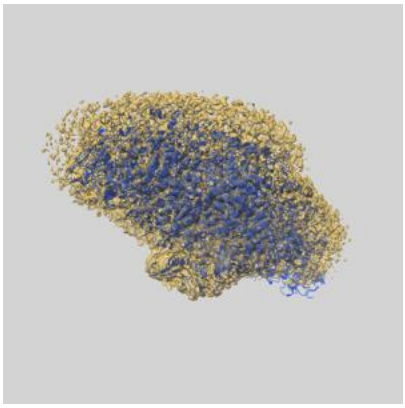
9.1 Map-model overlay



X



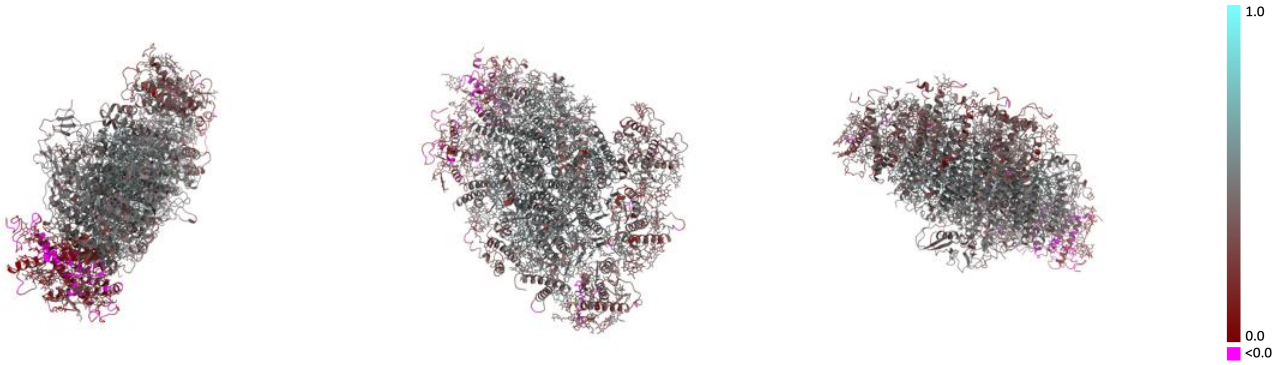
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0562 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

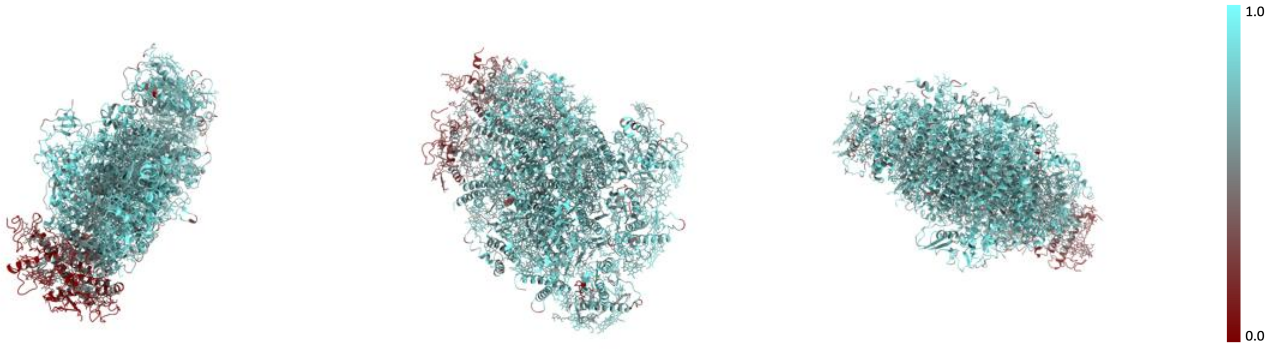
9.2 Q-score mapped to coordinate model



X Y Z

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

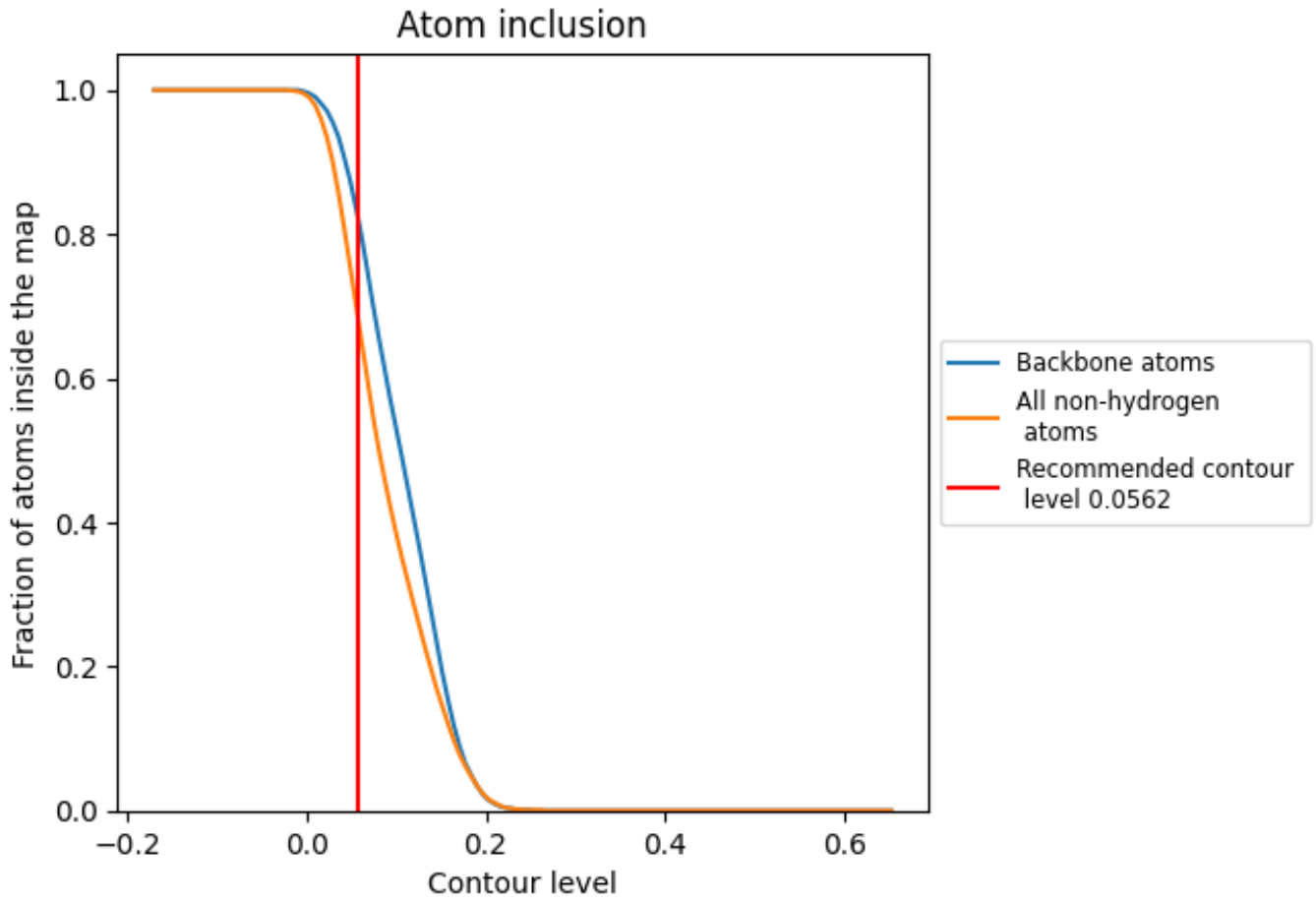
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0562).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.0562) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.3990
1	0.7130	0.3420
2	0.7000	0.3450
3	0.6950	0.3520
4	0.2510	0.1760
5	0.2330	0.0920
A	0.7890	0.4840
B	0.7740	0.4690
C	0.8660	0.4550
D	0.7660	0.4340
E	0.7590	0.4220
F	0.7560	0.4220
I	0.6880	0.4310
J	0.7200	0.4820
K	0.6950	0.3850
L	0.7080	0.4100
M	0.6450	0.3860
O	0.6730	0.3670