wwPDB EM Validation Summary Report (i)

Sep 14, 2026 – 01:11 PM JST

PDB ID	:	7F9O / pdb_00007f9o
EMDB ID	:	EMD-31498
Title	:	PSI-NDH supercomplex of Barley
Authors	:	Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on	:	2021-07-04
Resolution	:	4.50 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:

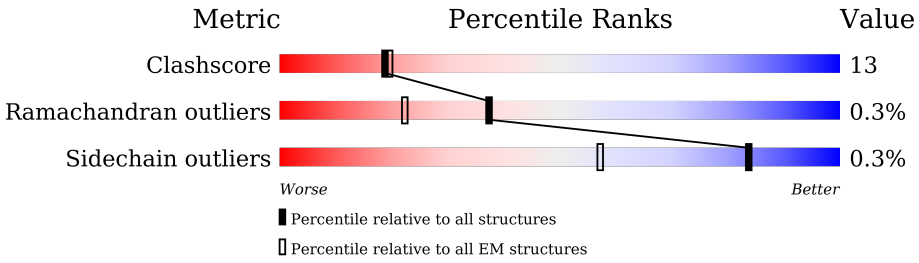
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

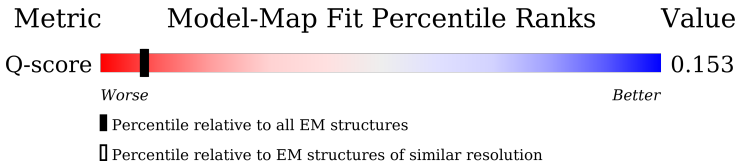
1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	750	78% 21%
1	e	750	19% 72% 27%
2	B	734	84% 16%
2	f	734	12% 72% 28%

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Mol	Chain	Length	Quality of chain
3	C	81	72% 28%
3	g	81	12% 62% 38%
4	D	205	50% 19% 31%
4	h	205	44% 47% 22% 31%
5	E	147	38% 8% 54%
5	i	147	26% 35% 12% 54%
6	F	235	49% 18% 33%
6	j	235	9% 42% 25% 33%
7	H	143	9% 36% 6% 57%
7	k	143	26% 34% 9% 57%
8	I	36	64% 19% 17%
8	l	36	14% 67% 17% 17%
9	J	42	5% 67% 33%
9	m	42	21% 67% 29% 5%
10	K	131	22% 47% 18% 36%
10	n	131	46% 46% 18% 36%
11	L	209	16% 54% 15% 30%
11	o	209	40% 54% 16% 30%
12	1	247	53% 25% 23%
12	p	247	19% 48% 30% 22%
13	2	255	56% 23% 20%
14	3	269	9% 61% 21% 17%
14	q	269	12% 54% 28% 17%
15	5	257	52% 28% 20%
16	G	346	11% 67% 33%

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Mol	Chain	Length	Quality of chain
17	M	483	76% 23%
18	N	117	11% 79% 20%
19	O	499	74% 26%
20	P	100	78% 22%
21	Q	777	65% 21% 14%
22	R	176	80% 20%
23	S	383	63% 60% 40%
24	T	165	52% 76% 23%
25	U	159	58% 64% 36%
26	V	245	27% 51% 28% 21%
27	W	192	22% 17% 18% 64%
28	X	213	28% 37% 15% 47%
29	Y	233	22% 40% 20% 39%
30	Z	61	93% 7%
31	a	154	68% 29%
32	b	216	51% 9% 40%
33	c	227	45% 14% 41%
34	4	130	77% 23%
35	d	243	56% 14% 29%
36	6	469	49% 23% 27%
37	7	361	55% 33% 12%
38	8	119	75% 23%
39	9	83	71% 28%
40	0	155	85% 12%
41	r	197	7% 69% 31%

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Mol	Chain	Length	Quality of chain
42	s	211	

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
44	CLA	2	507	X	-	-	-
51	LUT	p	502	X	-	-	-

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 106329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5813	3812	983	1000	18		
1	e	742	Total	C	N	O	S	0	0
			5798	3797	987	996	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5851	3835	995	1007	14		
2	f	733	Total	C	N	O	S	0	0
			5840	3832	991	1003	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			610	376	105	117	12		
3	g	81	Total	C	N	O	S	0	0
			613	377	105	119	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1113	716	193	201	3		
4	h	142	Total	C	N	O	S	0	0
			1111	714	195	199	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			538	341	98	99		
5	i	68	Total	C	N	O	0	0
			539	341	99	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1204	774	208	219	3		
6	j	158	Total	C	N	O	S	0	0
			1188	768	203	216	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			454	303	76	75		
7	k	61	Total	C	N	O	0	0
			447	298	73	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	30	Total	C	N	O		0	0
			232	161	35	36			
8	l	30	Total	C	N	O	S	0	0
			235	163	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			333	228	51	53	1		
9	m	42	Total	C	N	O	S	0	0
			332	225	51	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			565	359	94	108	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	n	84	Total	C	N	O	S	0	0
			576	361	101	110	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	146	Total	C	N	O	S	0	0
			1088	716	174	197	1		
11	o	146	Total	C	N	O		0	0
			1089	720	174	195			

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	191	Total	C	N	O	S	0	0
			1422	921	239	258	4		
12	p	193	Total	C	N	O	S	0	0
			1484	965	248	269	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	73	PHE	UNK	conflict	UNP A0A287WC32
1	74	GLU	UNK	conflict	UNP A0A287WC32
1	75	ARG	UNK	conflict	UNP A0A287WC32
p	73	PHE	UNK	conflict	UNP A0A287WC32
p	74	GLU	UNK	conflict	UNP A0A287WC32
p	75	ARG	UNK	conflict	UNP A0A287WC32

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2	203	Total	C	N	O	S	0	0
			1554	1012	257	282	3		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	222	Total	C	N	O	S	0	0
			1631	1064	271	293	3		
14	q	222	Total	C	N	O	S	0	0
			1672	1097	272	298	5		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	205	Total	C	N	O	S	0	0
			1486	962	247	270	7		

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	346	Total	C	N	O	S	0	0
			2602	1741	390	463	8		

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	478	Total	C	N	O	S	0	0
			3646	2400	557	665	24		

- Molecule 18 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	116	Total	C	N	O	S	0	0
			841	575	124	140	2		

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	499	Total	C	N	O	S	0	0
			3874	2614	598	639	23		

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	100	Total	C	N	O	S	0	0
			750	486	127	135	2		

- Molecule 21 is a protein called NADH-plastoquinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	671	Total	C	N	O	S	0	0
			5041	3367	784	870	20		

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	176	Total	C	N	O	S	0	0
			1260	841	194	220	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	383	Total	C	N	O	S	0	0
			2991	1944	493	543	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	165	Total	C	N	O	S	0	0
			1229	772	214	231	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	159	Total	C	N	O	S	0	0
			1258	808	213	233	4		

- Molecule 26 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	194	Total	C	N	O	S	0	0
			1473	931	250	282	10		

- Molecule 27 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	69	Total	C	N	O	S	0	0
			572	399	89	81	3		

- Molecule 28 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	112	Total	C	N	O	S	0	0
			876	558	150	162	6		

- Molecule 29 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	142	Total	C	N	O	S	0	0
			1135	741	197	195	2		

- Molecule 30 is a protein called Unidentified stromal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	61	Total	C	N	O	0	0
			305	183	61	61		

- Molecule 31 is a protein called Photosynthetic NDH subunit of subcomplex L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	a	150	Total	C	N	O	0	0
			1185	752	206	227		

- Molecule 32 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	129	Total	C	N	O	S	0	0
			915	580	156	175	4		

- Molecule 33 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	134	Total	C	N	O	S	0	0
			989	634	164	187	4		

- Molecule 34 is a protein called Photosynthetic NDH subunit of subcomplex L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4	130	Total	C	N	O	S	0	0
			878	553	153	163	9		

- Molecule 35 is a protein called Photosynthetic NDH subunit of subcomplex L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	172	Total	C	N	O	S	0	0
			1289	812	229	241	7		

- Molecule 36 is a protein called Photosynthetic NDH subunit of subcomplex B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6	343	Total	C	N	O	S	0	0
			2541	1617	435	474	15		

- Molecule 37 is a protein called Photosynthetic NDH subunit of subcomplex B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7	317	Total	C	N	O	S	0	0
			2302	1436	408	448	10		

- Molecule 38 is a protein called Photosynthetic NDH subunit of subcomplex B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	119	Total	C	N	O	S	0	0
			828	523	151	147	7		

- Molecule 39 is a protein called Photosynthetic NDH subunit of subcomplex B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	9	82	Total	C	N	O	S	0	0
			617	395	101	118	3		

- Molecule 40 is a protein called Photosynthetic NDH subunit of subcomplex B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	0	149	Total	C	N	O	S	0	0
			1089	704	175	204	6		

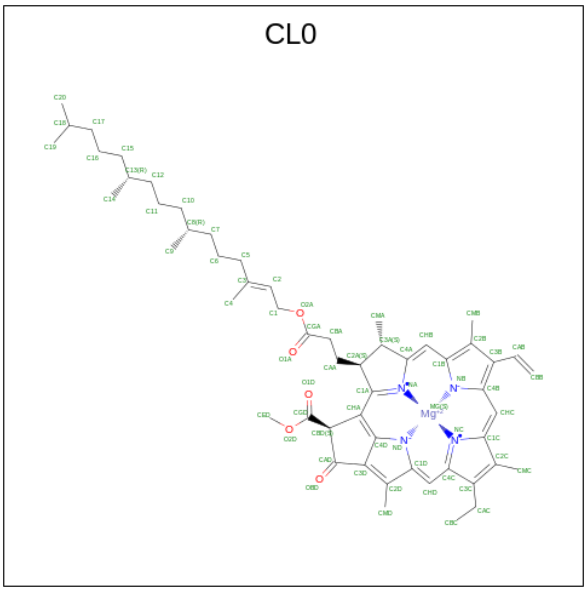
- Molecule 41 is a protein called Chlorophyll a-b binding protein Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	197	Total	C	N	O	S	0	0
			1529	991	253	282	3		

- Molecule 42 is a protein called Chlorophyll a-b binding protein, chloroplastic.

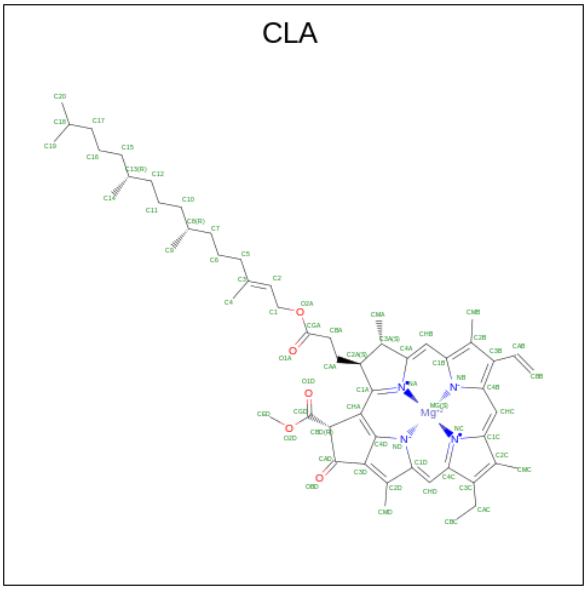
Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	211	Total	C	N	O	S	0	0
			1591	1035	266	283	7		

- Molecule 43 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
43	A	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
43	e	1	Total	C	Mg	N	O	0
			61	52	1	4	4	

- Molecule 44 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			45	37	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
44	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
44	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	K	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
44	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
44	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	2	1	Total	C	Mg	N	O	0
			49	41	1	4	3	
44	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
44	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
44	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	e	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
44	e	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
44	f	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
44	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			58	49	1	4	4	
44	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
44	j	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	m	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	n	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
44	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	n	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	o	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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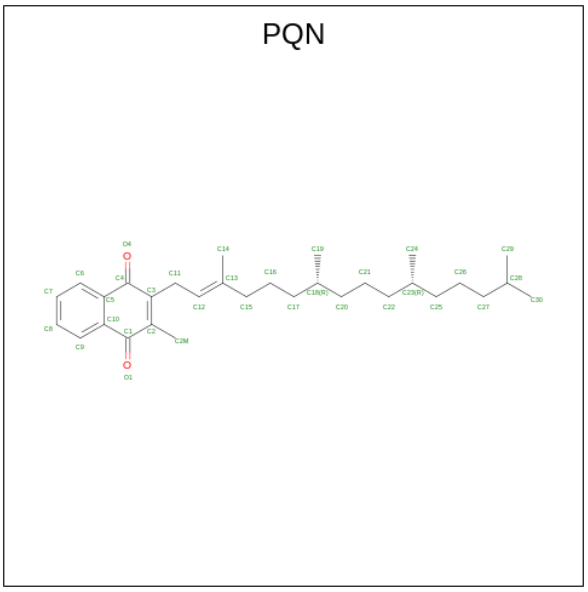
Mol	Chain	Residues	Atoms					AltConf
44	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	p	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			39	31	1	4	3	

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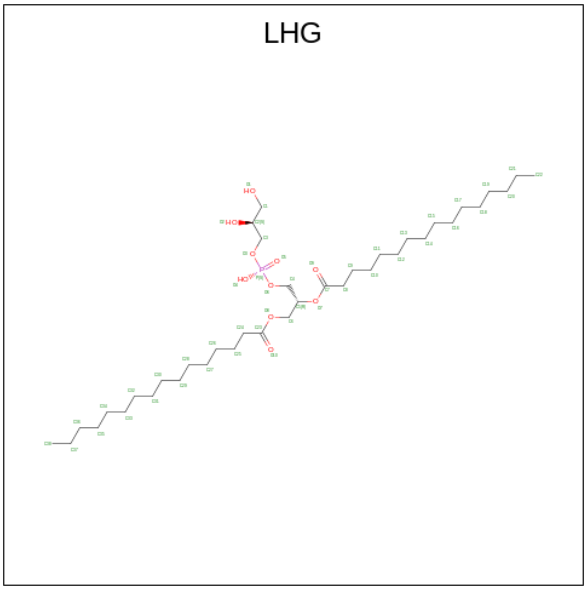
Mol	Chain	Residues	Atoms					AltConf
44	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	s	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

- Molecule 45 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



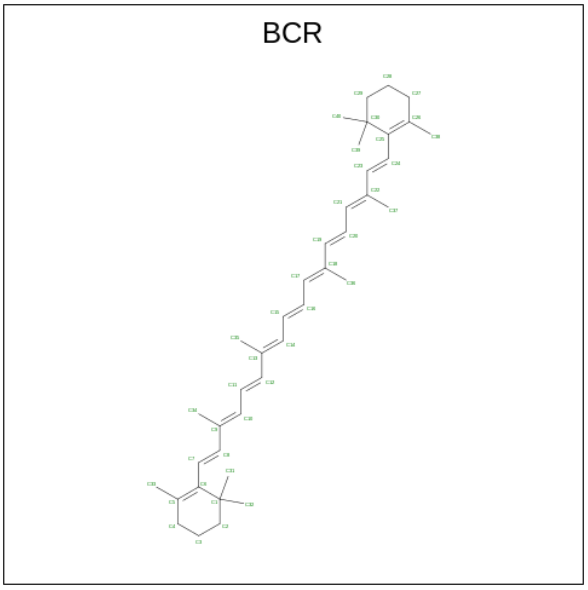
Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total C O 33 31 2	0
45	B	1	Total C O 30 28 2	0
45	e	1	Total C O 14 12 2	0
45	f	1	Total C O 16 14 2	0

- Molecule 46 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
46	A	1	Total	C	O	P	0
			49	38	10	1	
46	A	1	Total	C	O	P	0
			30	19	10	1	
46	B	1	Total	C	O	P	0
			38	27	10	1	
46	1	1	Total	C	O	P	0
			49	38	10	1	
46	2	1	Total	C	O	P	0
			35	24	10	1	
46	O	1	Total	C	O	P	0
			24	15	8	1	
46	e	1	Total	C	O	P	0
			40	29	10	1	
46	e	1	Total	C	O	P	0
			25	15	9	1	
46	f	1	Total	C	O	P	0
			38	27	10	1	
46	p	1	Total	C	O	P	0
			49	38	10	1	
46	s	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 47 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
47	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
47	A	1	Total C 40 40	0
47	A	1	Total C 40 40	0
47	A	1	Total C 40 40	0
47	A	1	Total C 39 39	0
47	A	1	Total C 40 40	0
47	A	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	F	1	Total C 40 40	0
47	F	1	Total C 40 40	0
47	I	1	Total C 40 40	0
47	J	1	Total C 40 40	0
47	K	1	Total C 40 40	0
47	L	1	Total C 40 40	0
47	L	1	Total C 40 40	0
47	1	1	Total C 19 19	0

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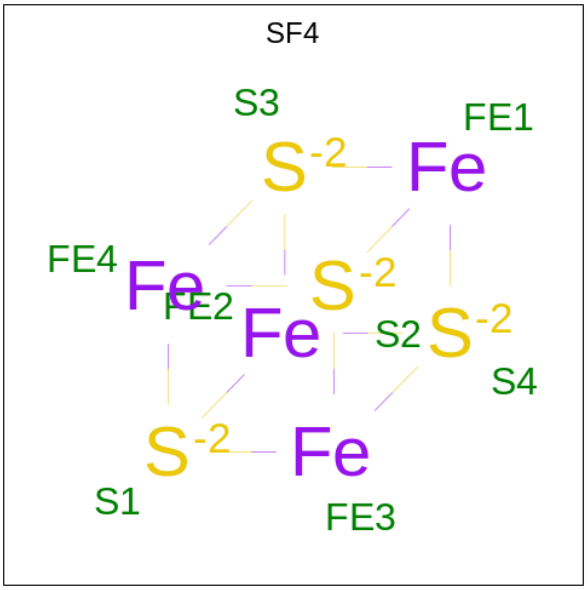
Mol	Chain	Residues	Atoms	AltConf
47	2	1	Total C 40 40	0
47	3	1	Total C 40 40	0
47	5	1	Total C 40 40	0
47	Q	1	Total C 39 39	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 39 39	0
47	j	1	Total C 40 40	0
47	j	1	Total C 40 40	0
47	l	1	Total C 40 40	0
47	l	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
47	m	1	Total C 40 40	0
47	n	1	Total C 40 40	0
47	o	1	Total C 40 40	0
47	o	1	Total C 40 40	0
47	p	1	Total C 11 11	0
47	q	1	Total C 40 40	0
47	r	1	Total C 40 40	0
47	s	1	Total C 40 40	0

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



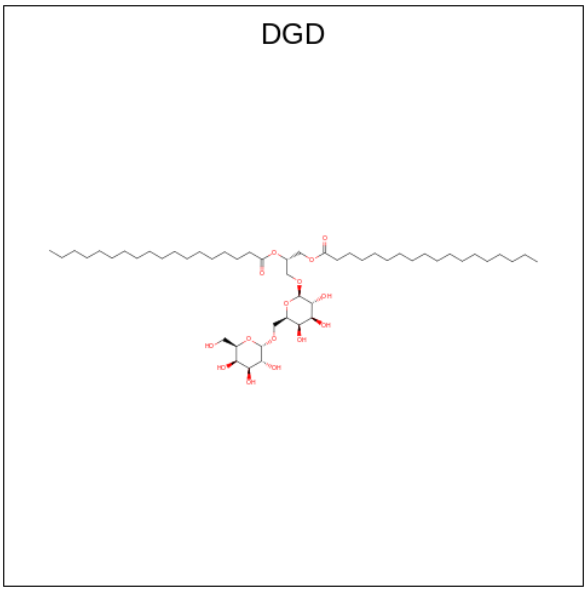
Mol	Chain	Residues	Atoms	AltConf
48	A	1	Total Fe S 8 4 4	0
48	C	1	Total Fe S 8 4 4	0
48	C	1	Total Fe S 8 4 4	0

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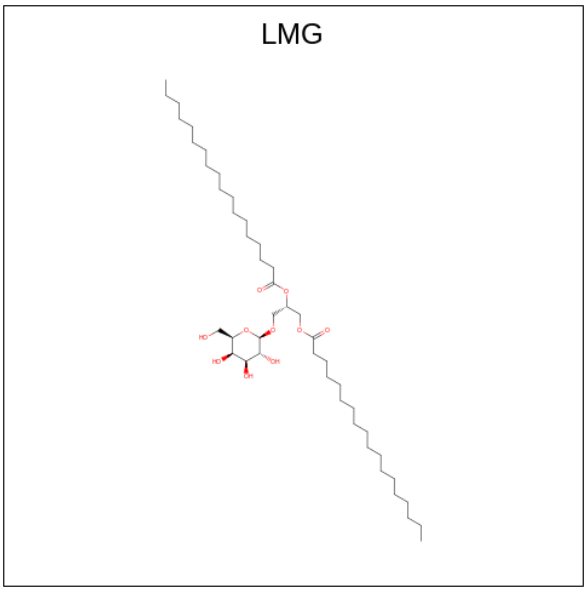
Mol	Chain	Residues	Atoms	AltConf
48	8	1	Total Fe S 8 4 4	0
48	f	1	Total Fe S 8 4 4	0
48	g	1	Total Fe S 8 4 4	0
48	g	1	Total Fe S 8 4 4	0

- Molecule 49 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



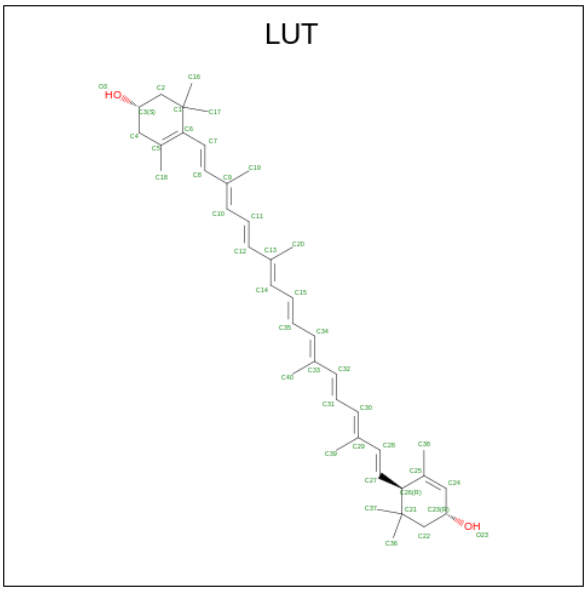
Mol	Chain	Residues	Atoms	AltConf
49	B	1	Total C O 59 44 15	0
49	J	1	Total C O 66 51 15	0
49	f	1	Total C O 52 37 15	0
49	m	1	Total C O 66 51 15	0

- Molecule 50 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



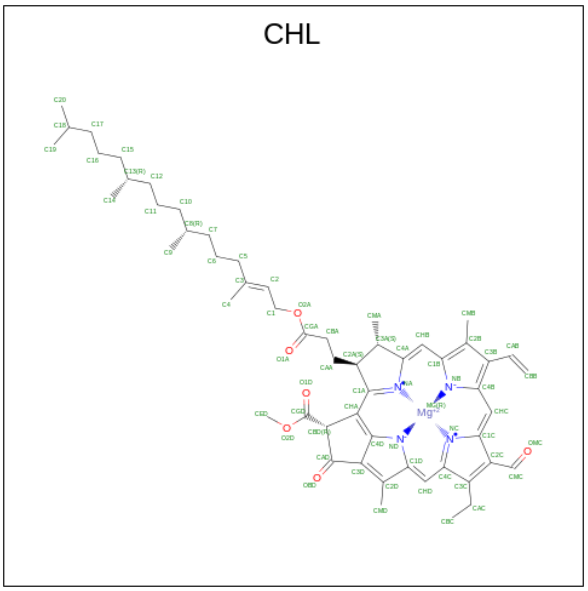
Mol	Chain	Residues	Atoms	AltConf
50	F	1	Total C O 30 20 10	0
50	F	1	Total C O 45 35 10	0
50	2	1	Total C O 16 9 7	0
50	2	1	Total C O 36 26 10	0
50	5	1	Total C O 32 22 10	0
50	m	1	Total C O 30 20 10	0
50	r	1	Total C O 18 10 8	0

- Molecule 51 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
51	1	1	Total C O 42 40 2	0
51	1	1	Total C O 42 40 2	0
51	2	1	Total C O 42 40 2	0
51	3	1	Total C O 42 40 2	0
51	3	1	Total C O 42 40 2	0
51	5	1	Total C O 42 40 2	0
51	p	1	Total C O 42 40 2	0
51	p	1	Total C O 42 40 2	0
51	q	1	Total C O 42 40 2	0
51	q	1	Total C O 42 40 2	0
51	r	1	Total C O 42 40 2	0
51	s	1	Total C O 42 40 2	0

- Molecule 52 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



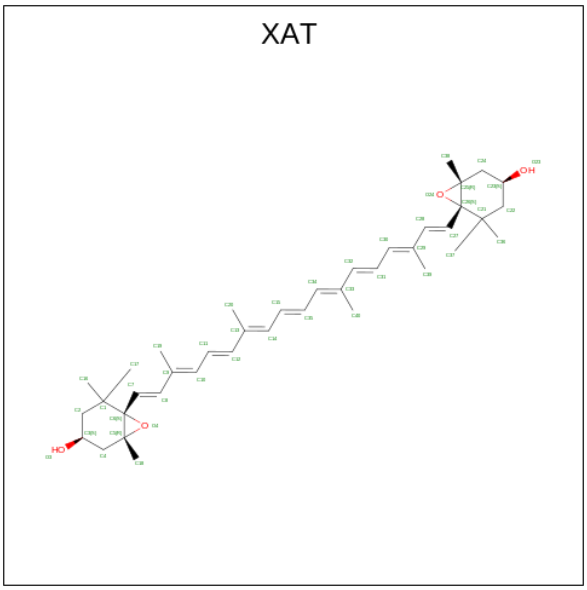
Mol	Chain	Residues	Atoms					AltConf
52	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
52	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
52	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
52	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
52	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
52	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
52	5	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
52	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
52	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
52	r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	r	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
52	r	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	s	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
52	s	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
52	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 53 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



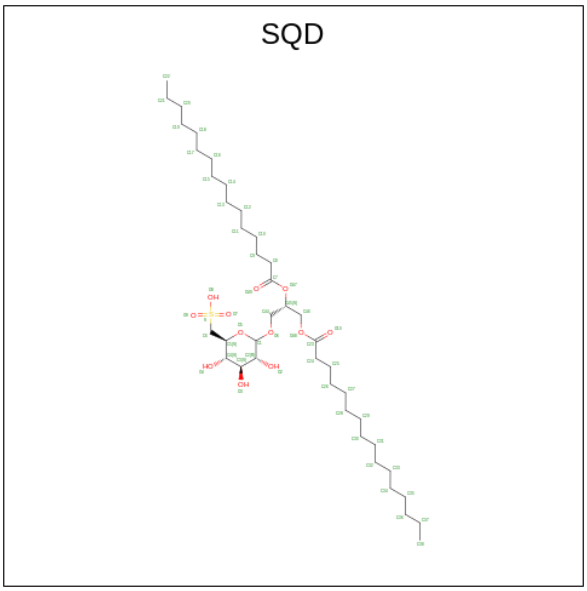
Mol	Chain	Residues	Atoms			AltConf
53	2	1	Total	C	O	0
			44	40	4	
53	5	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
53	r	1	Total 44	C 40	O 4	0
53	s	1	Total 44	C 40	O 4	0

- Molecule 54 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

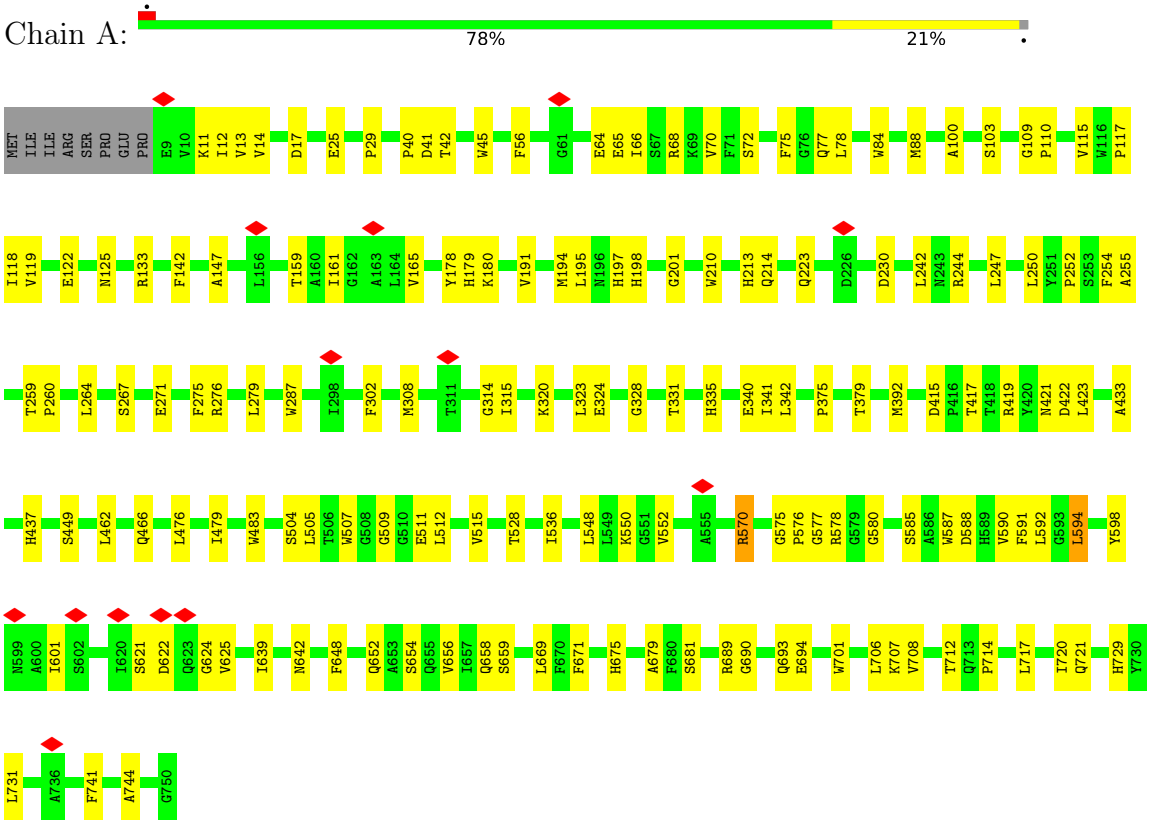


Mol	Chain	Residues	Atoms				AltConf
54	Q	1	Total 54	C 41	O 12	S 1	0
54	Q	1	Total 46	C 33	O 12	S 1	0

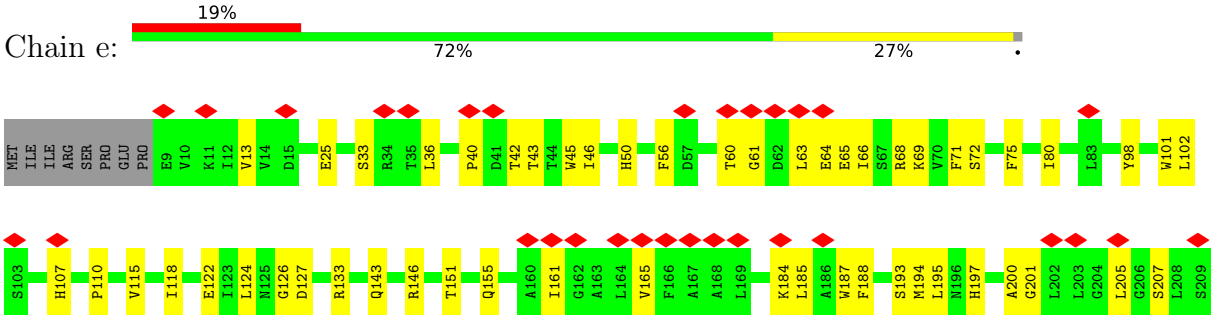
3 Residue-property plots (i)

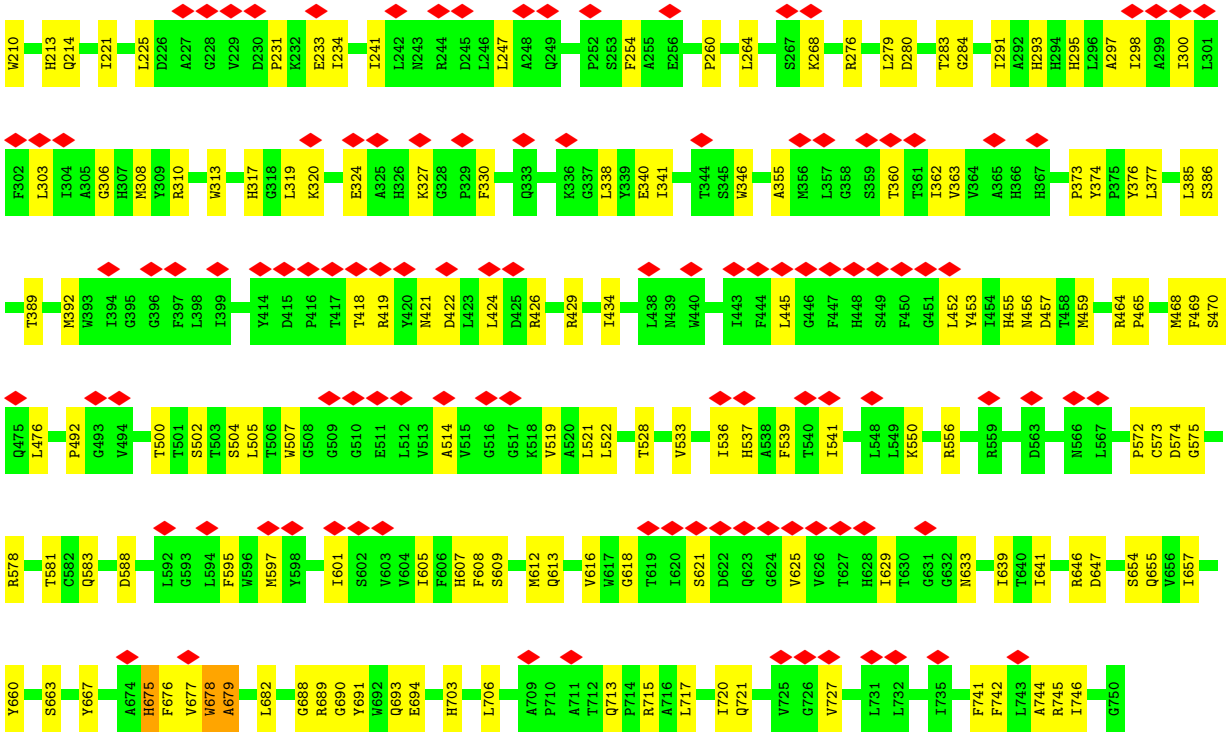
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

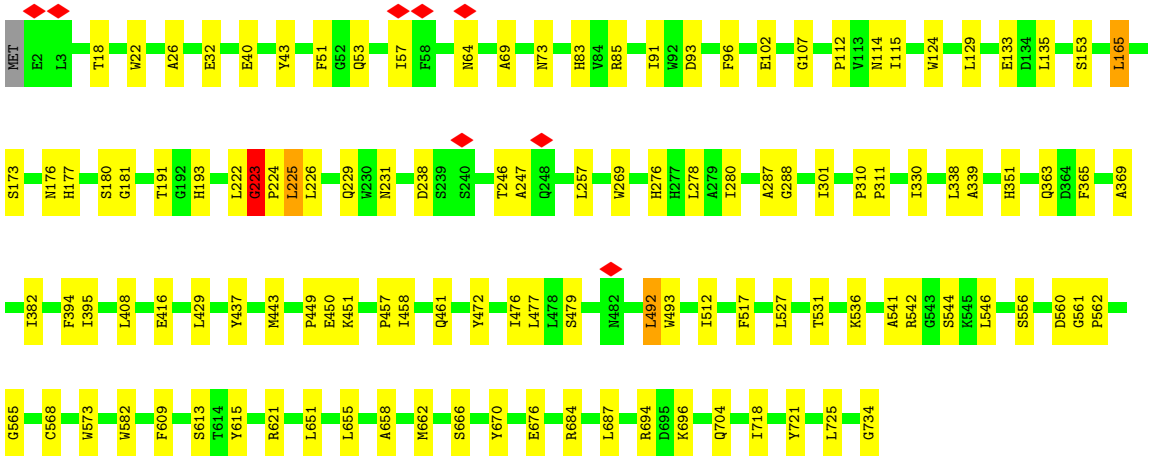




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

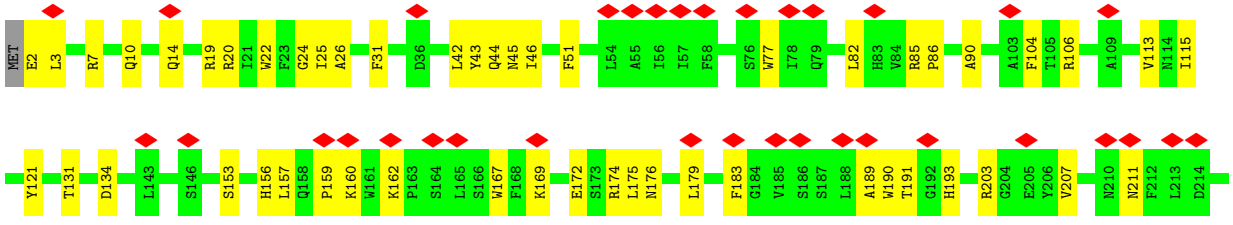


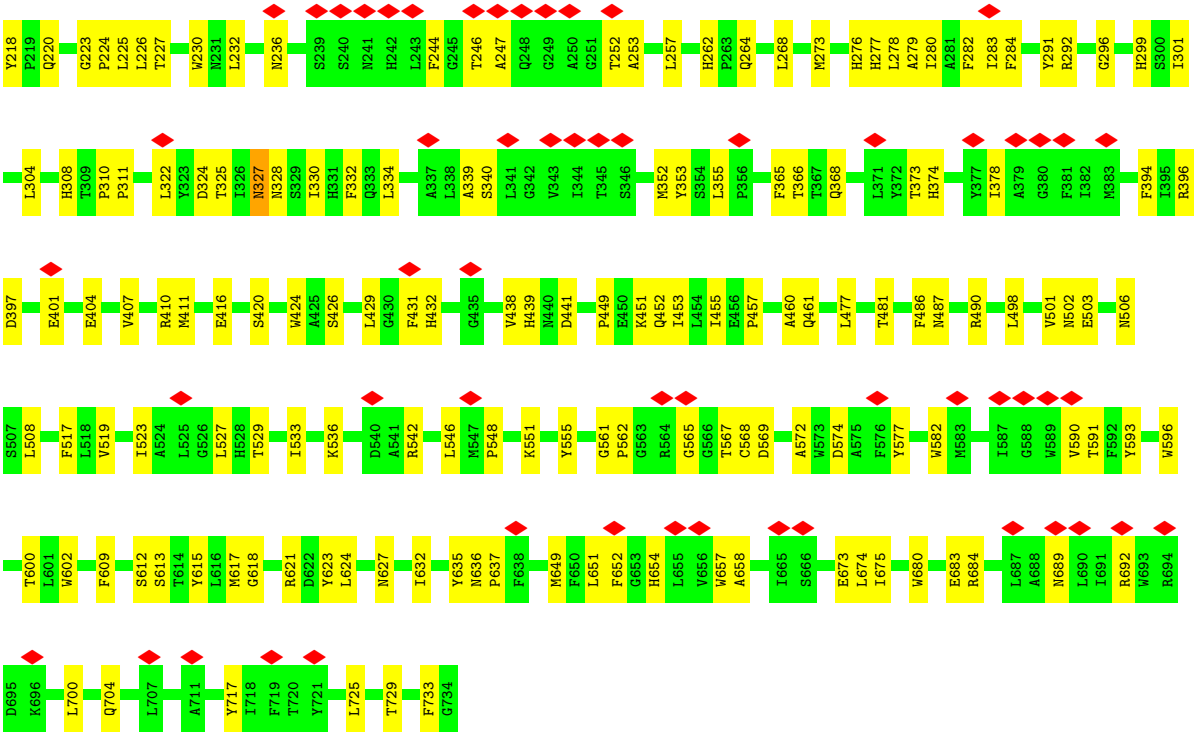


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f:



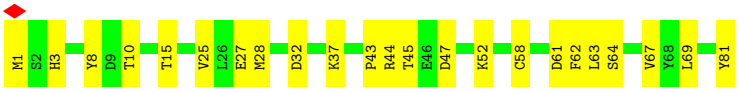




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

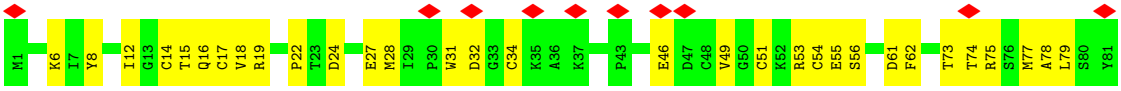




• Molecule 3: Photosystem I iron-sulfur center

Chain g:



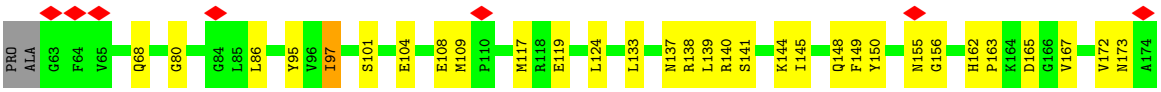


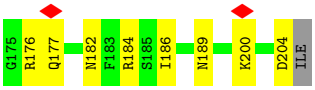
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



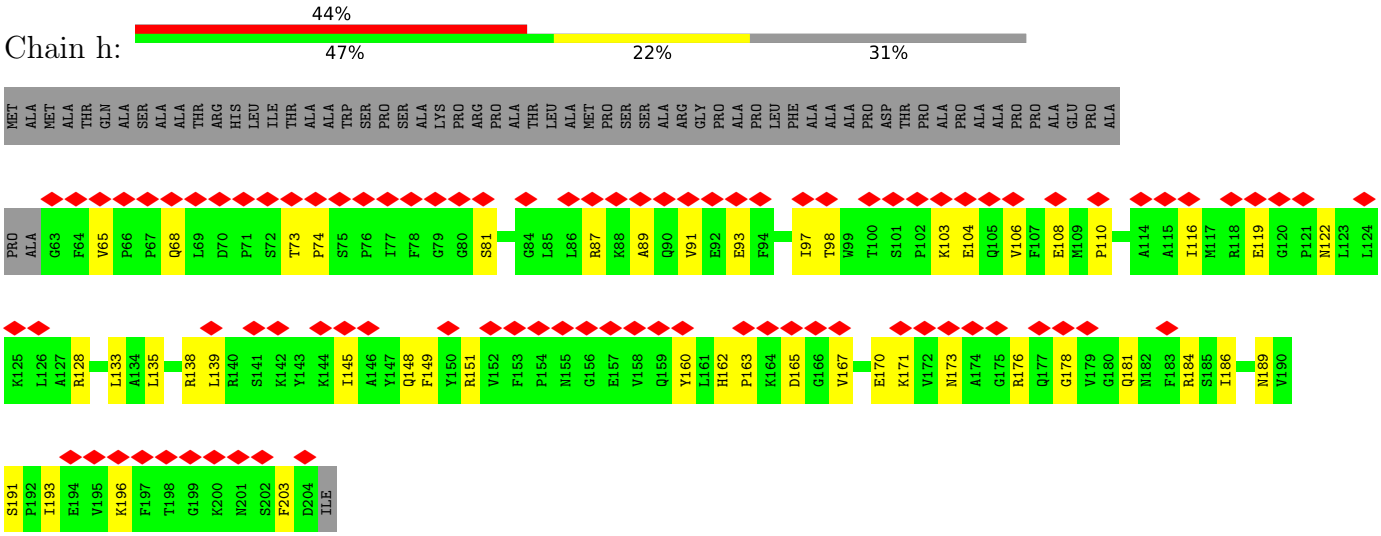






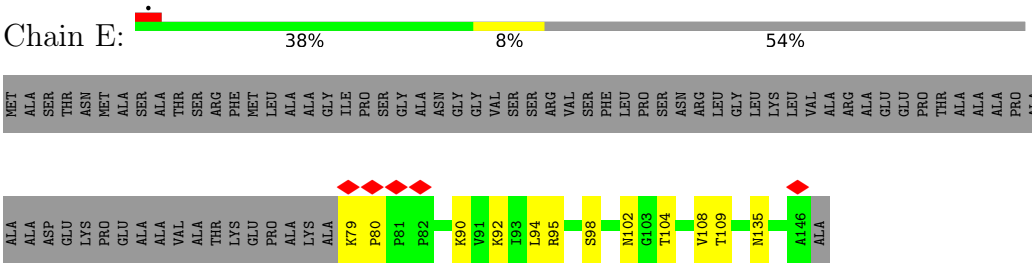
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain h:



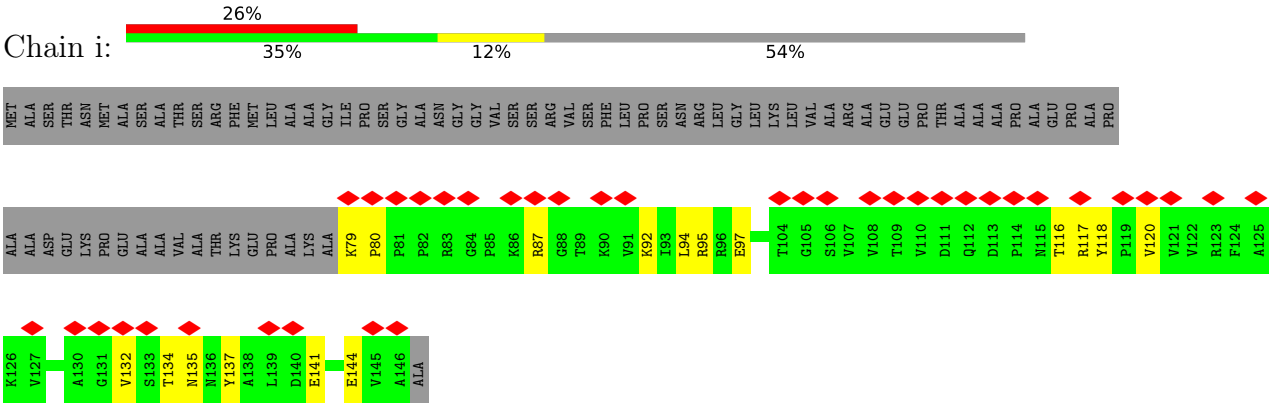
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



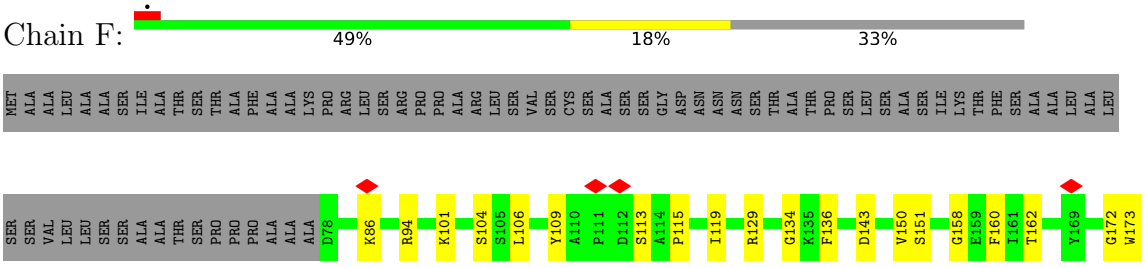
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain i:



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

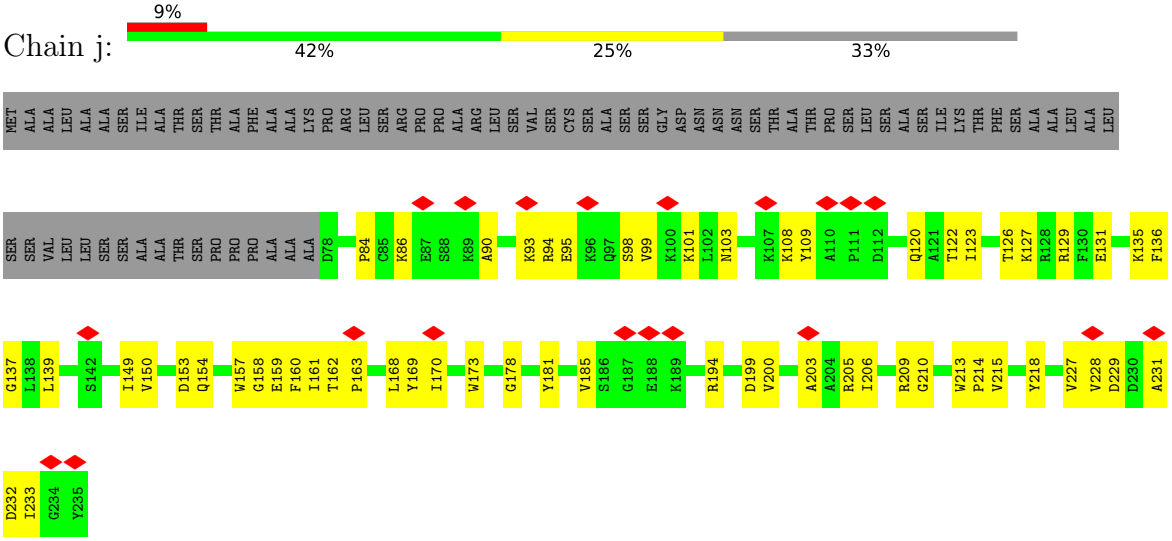
Chain F:





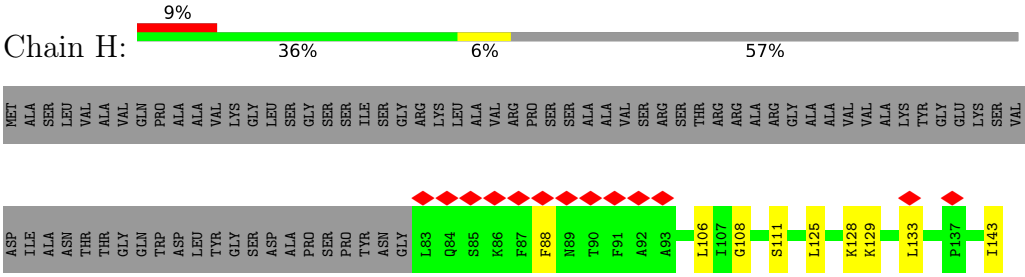
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain j:



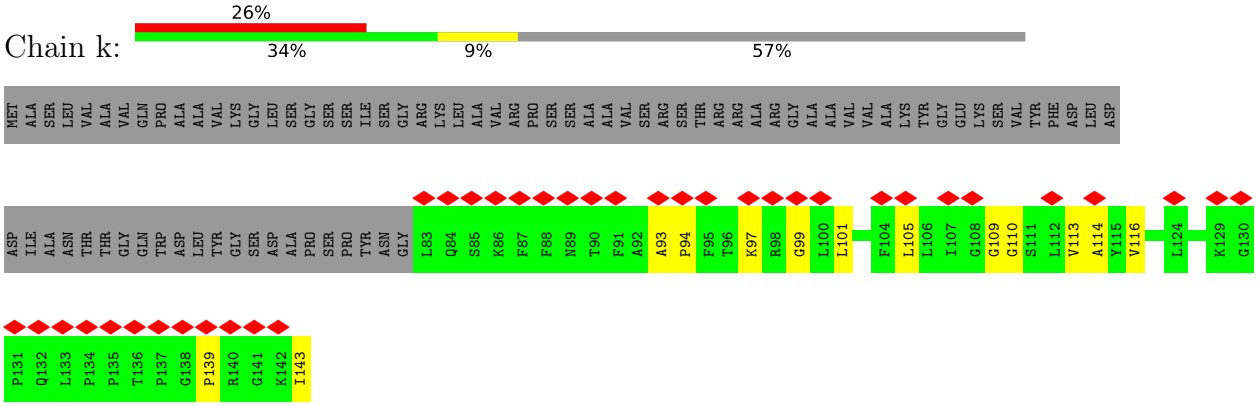
• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic

Chain H:



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

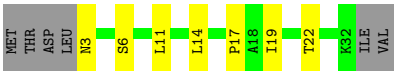
Chain k:



• Molecule 8: Photosystem I reaction center subunit VIII

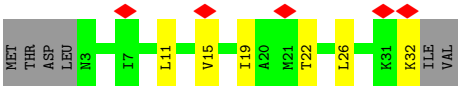
Chain I:





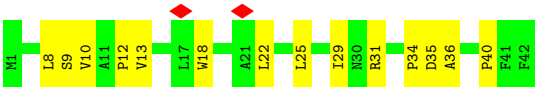
• Molecule 8: Photosystem I reaction center subunit VIII





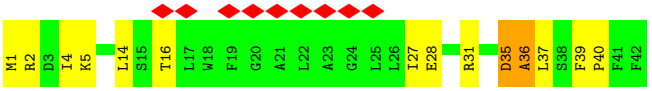
• Molecule 9: Photosystem I reaction center subunit IX





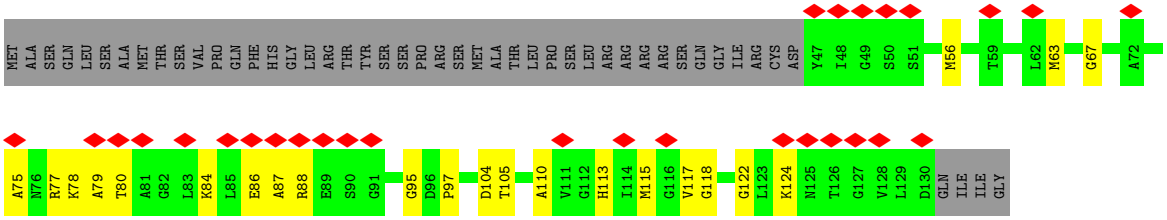
• Molecule 9: Photosystem I reaction center subunit IX





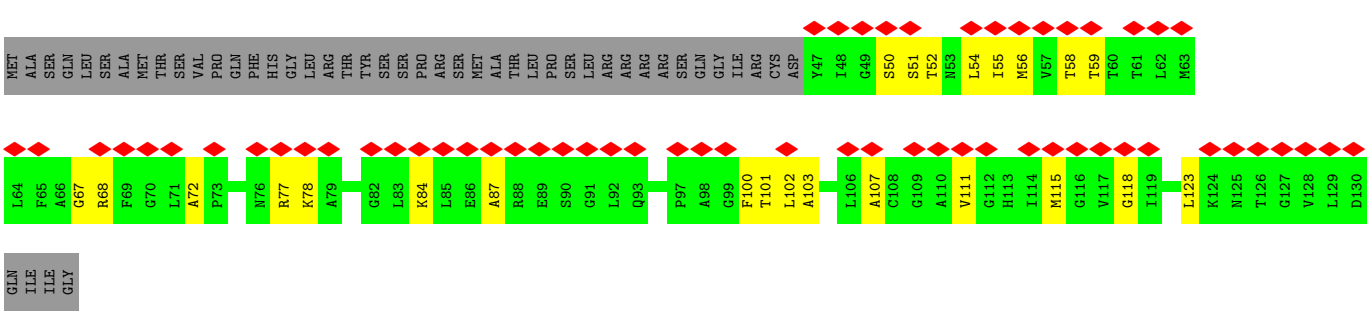
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic





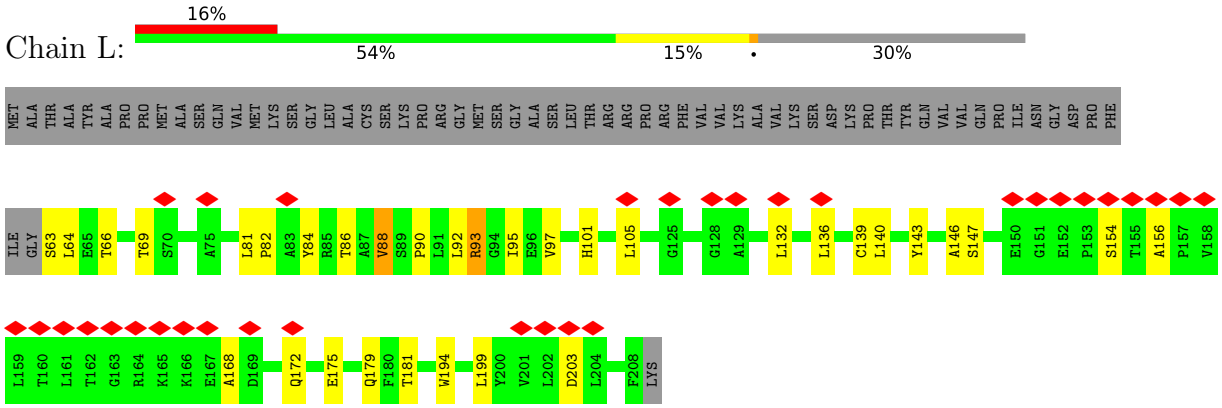
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic





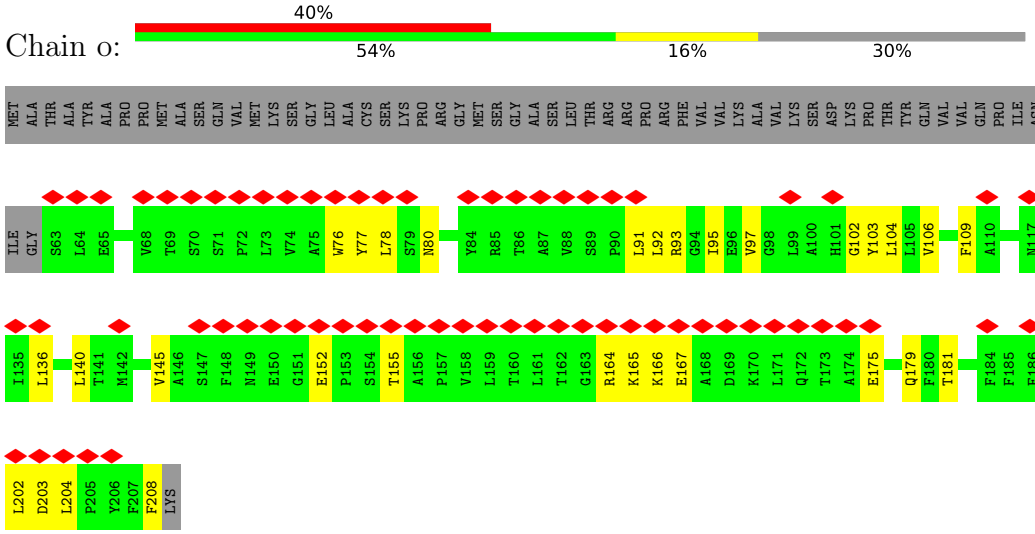
• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

Chain L:



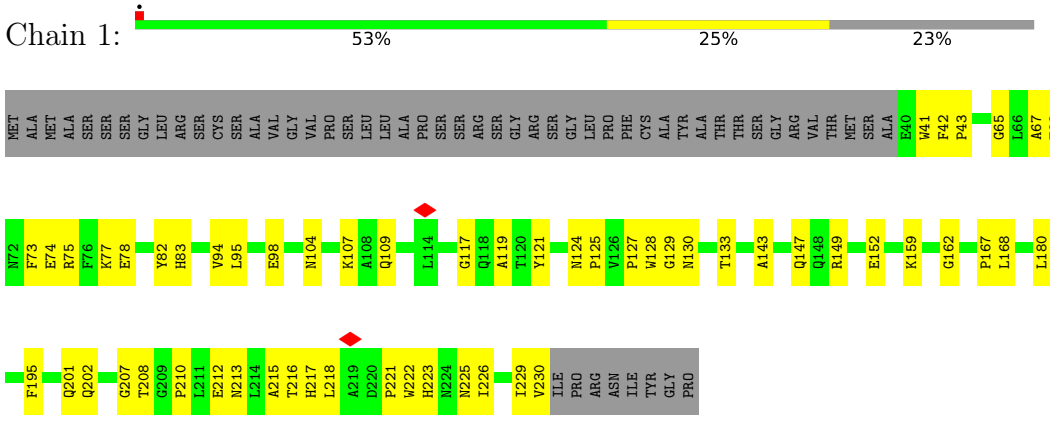
• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

Chain o:



• Molecule 12: Chlorophyll a-b binding protein Lhca1

Chain 1:



• Molecule 12: Chlorophyll a-b binding protein Lhca1

Chain p:

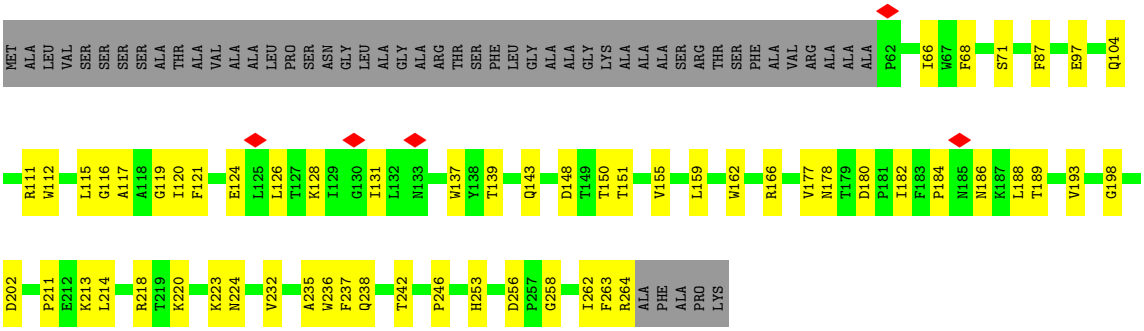




• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

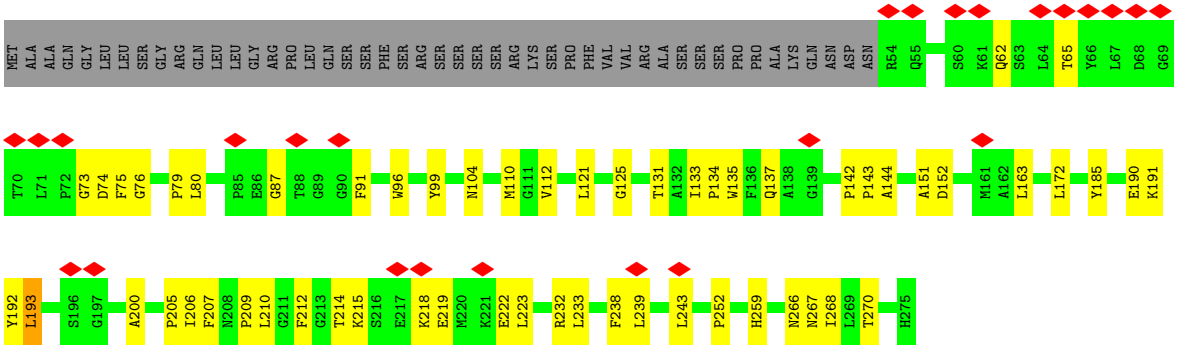




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

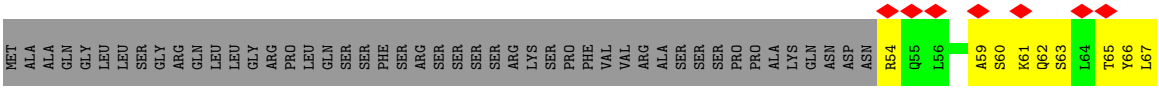


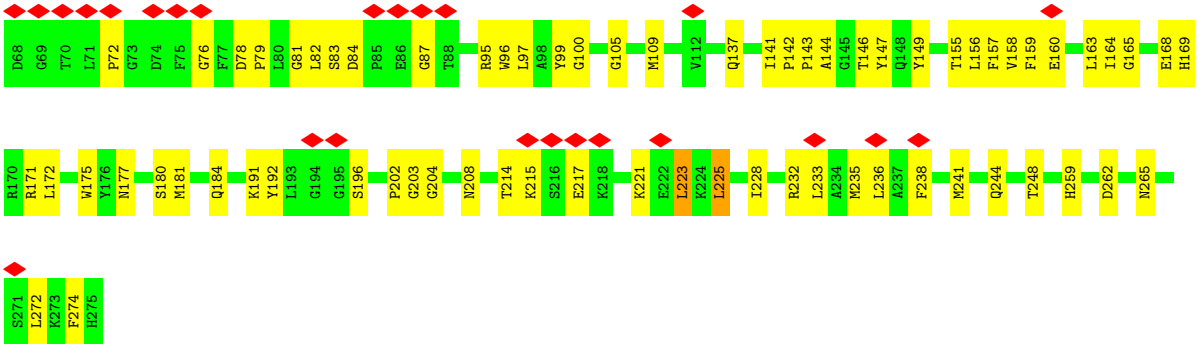


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain q:



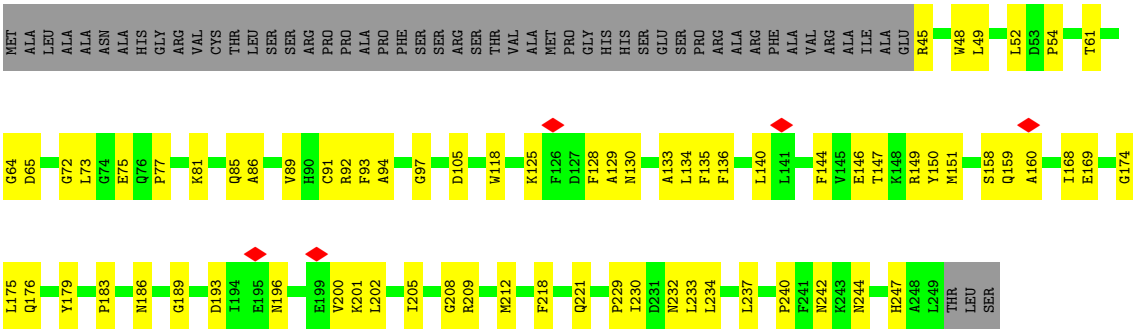




• Molecule 15: Chlorophyll a-b binding protein Lhca5

Chain 5:

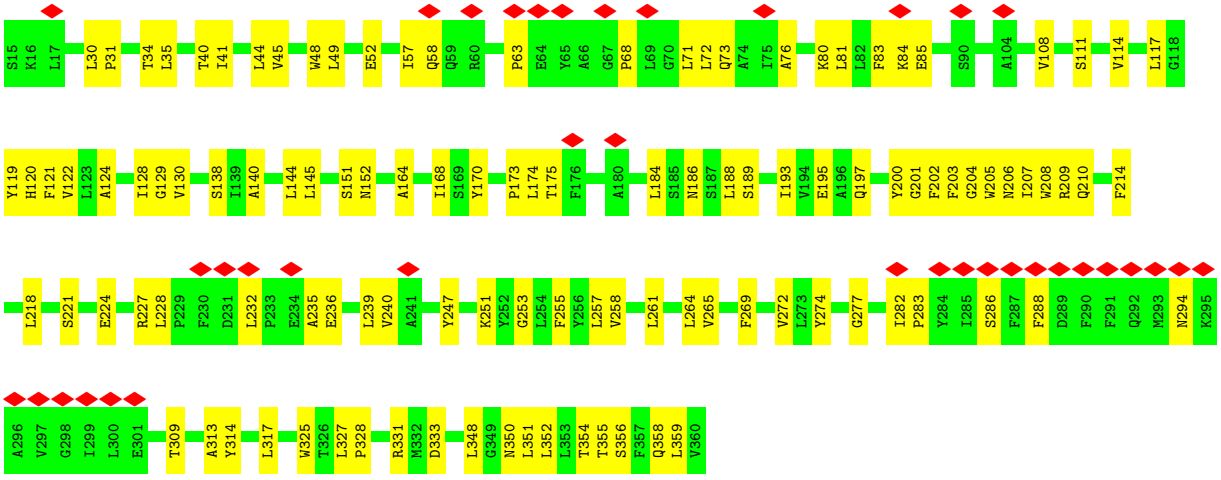




• Molecule 16: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

Chain G:

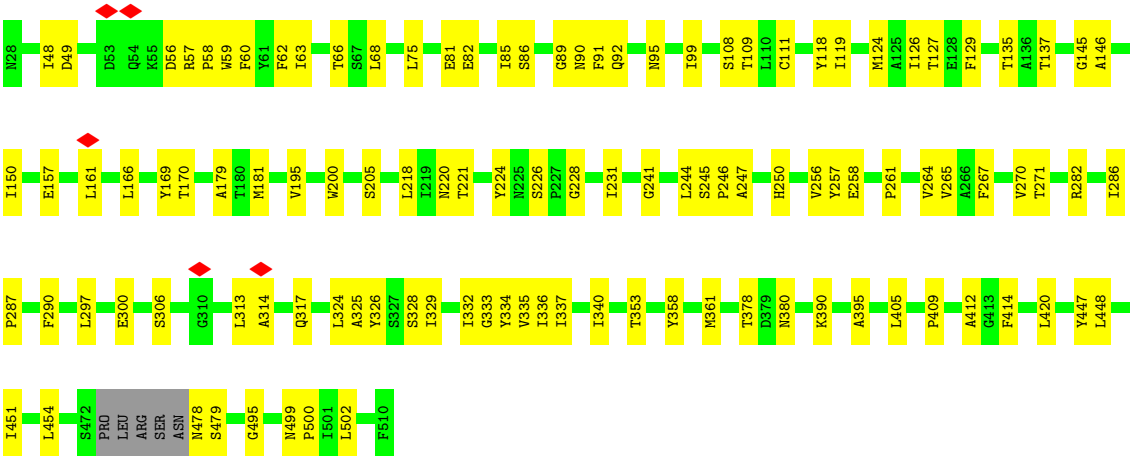




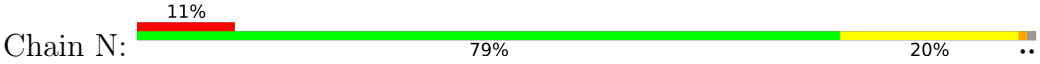
• Molecule 17: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

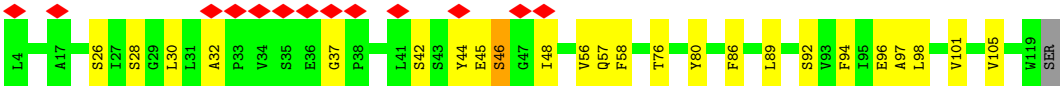
Chain M:





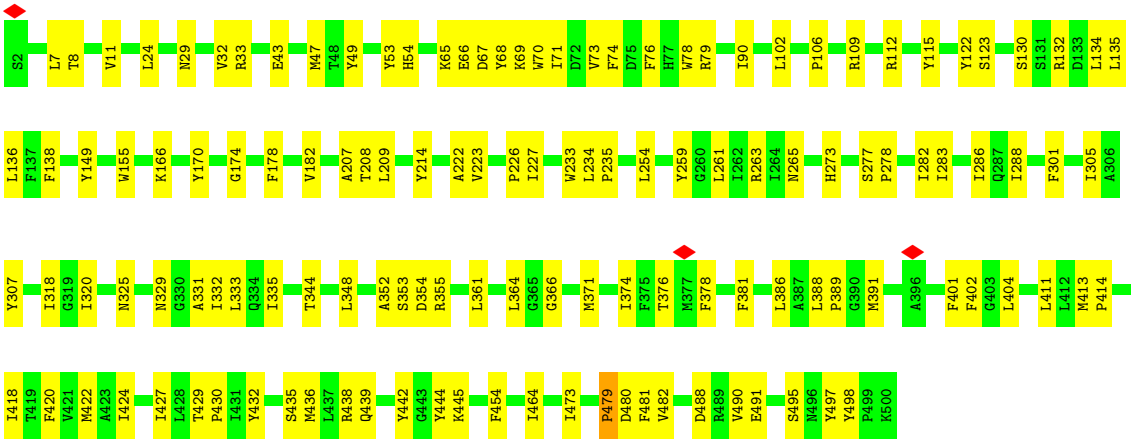
• Molecule 18: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



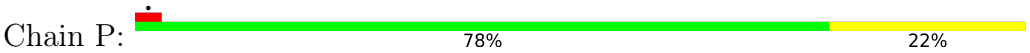


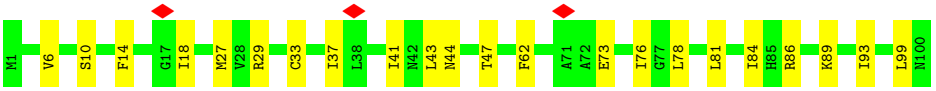
• Molecule 19: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic





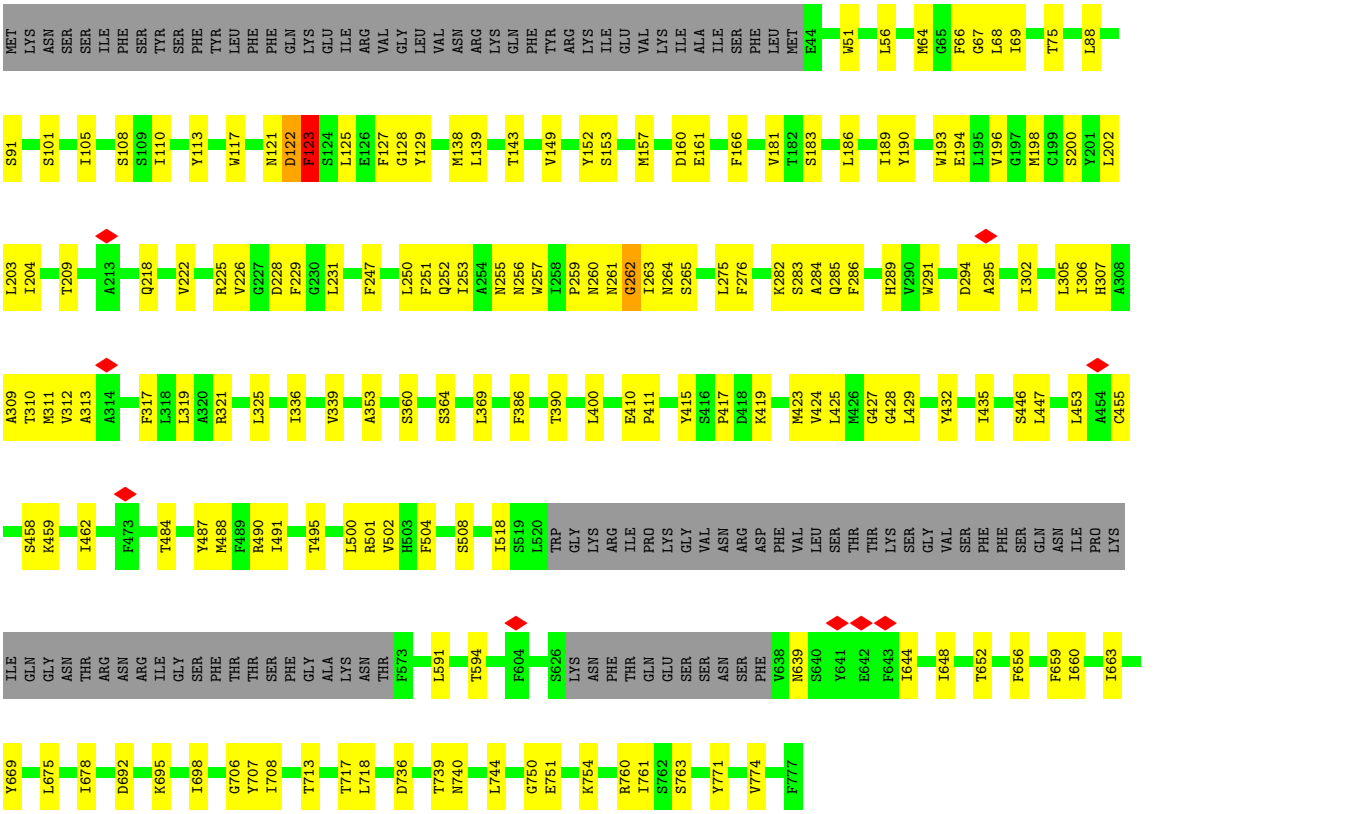
• Molecule 20: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic





• Molecule 21: NADH-plastoquinone oxidoreductase subunit 5

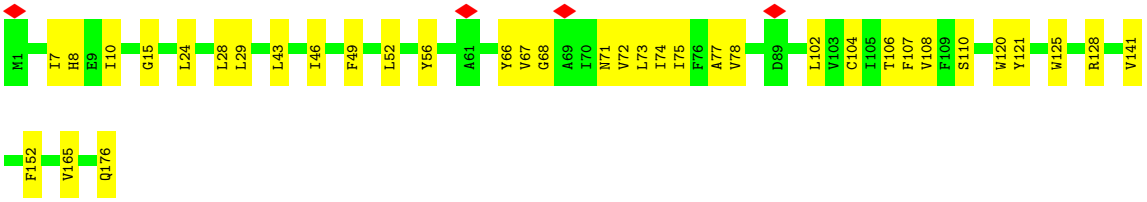




• Molecule 22: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

Chain R:

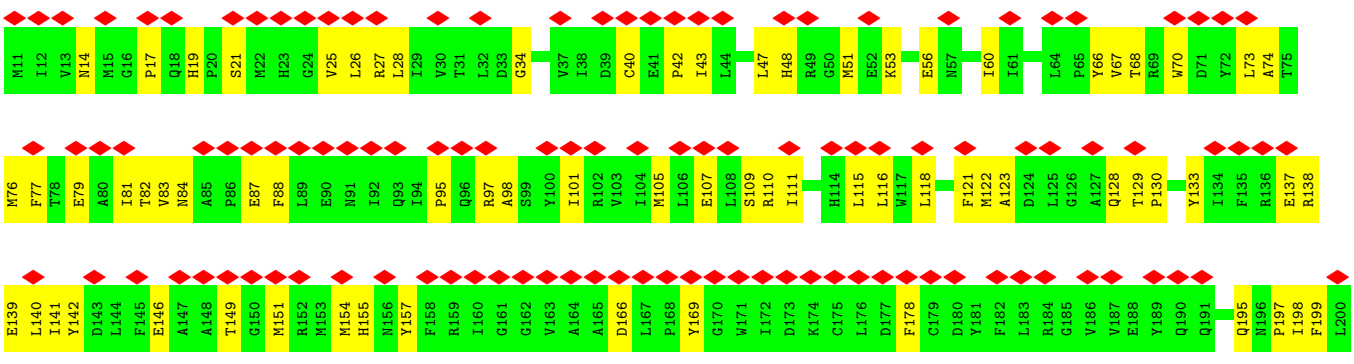


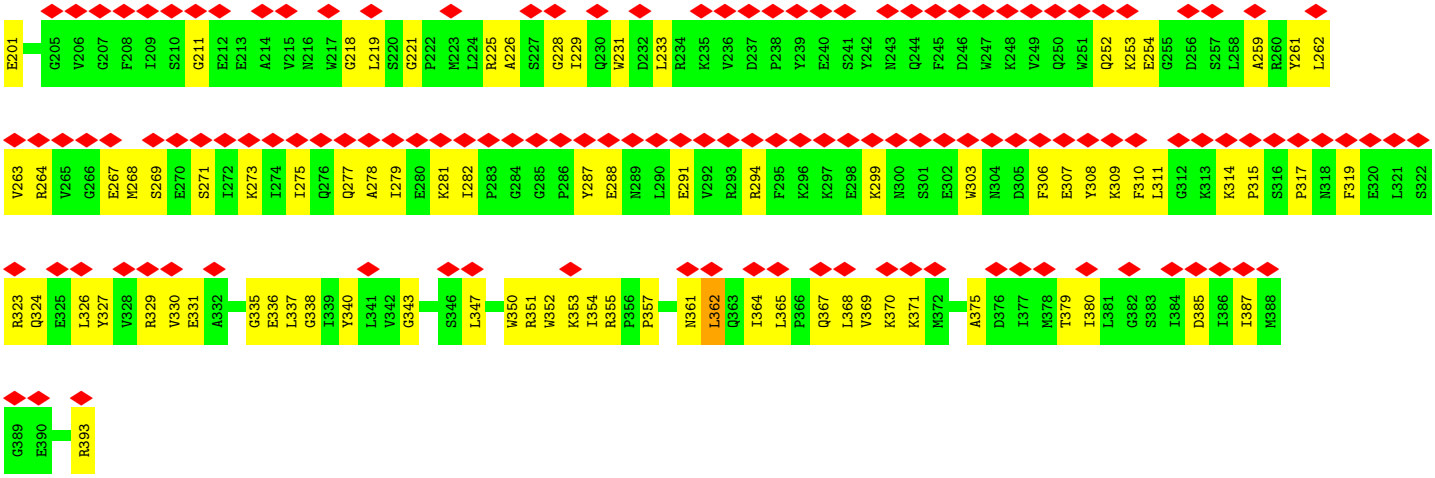


• Molecule 23: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

Chain S:

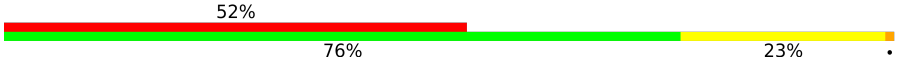


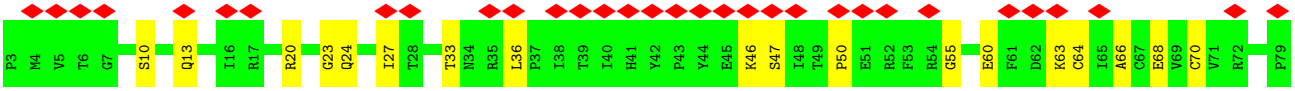




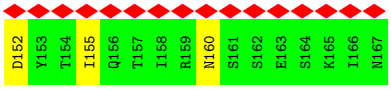
• Molecule 24: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

Chain T:





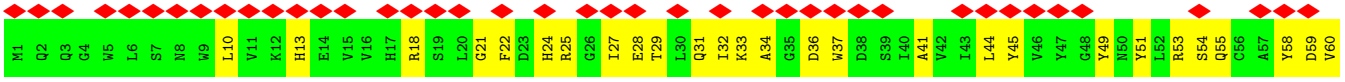


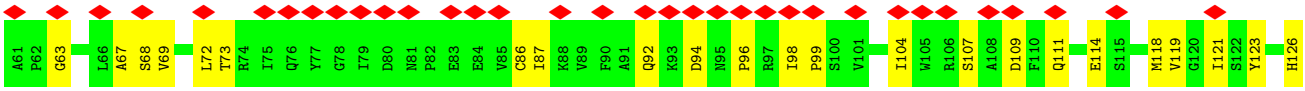


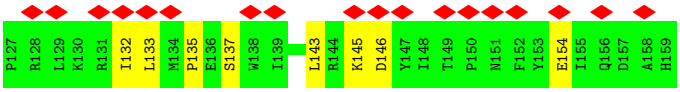
• Molecule 25: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic

Chain U:





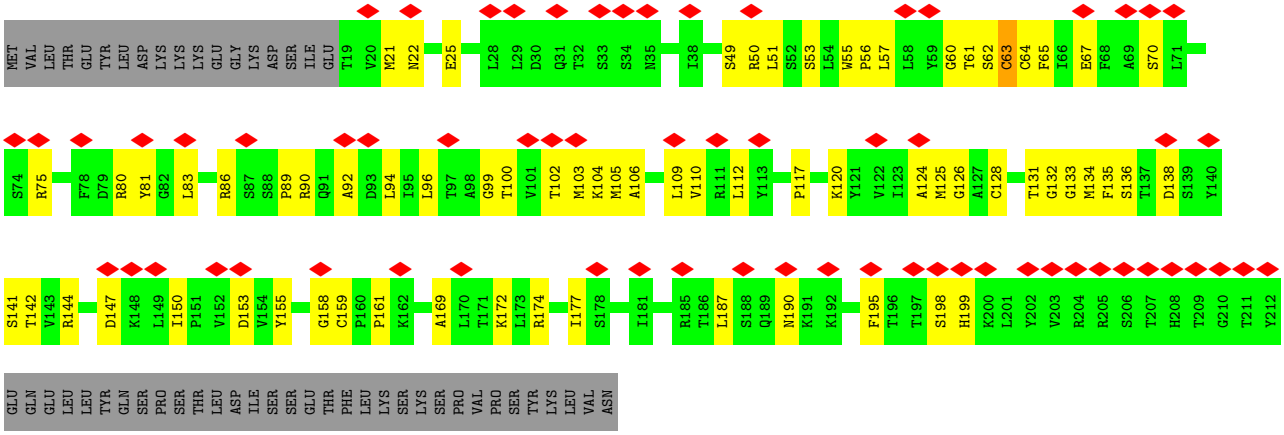




• Molecule 26: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic

Chain V:

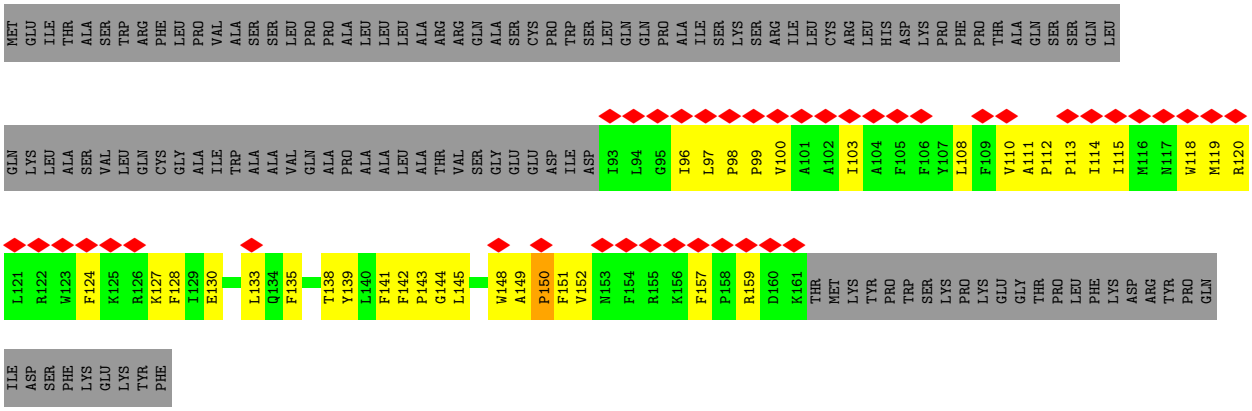




• Molecule 27: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic

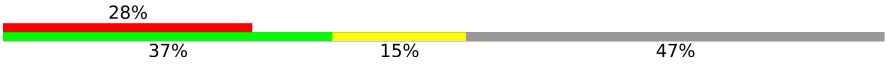
Chain W:

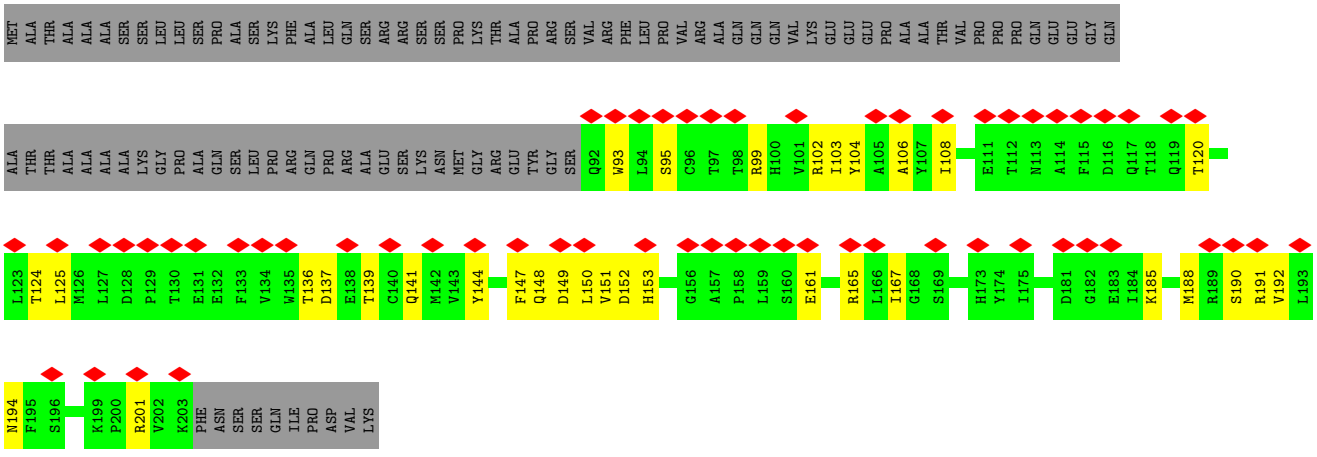




• Molecule 28: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic

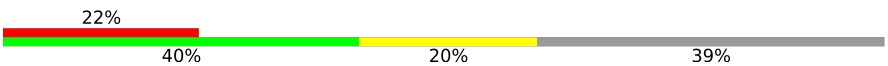
Chain X:

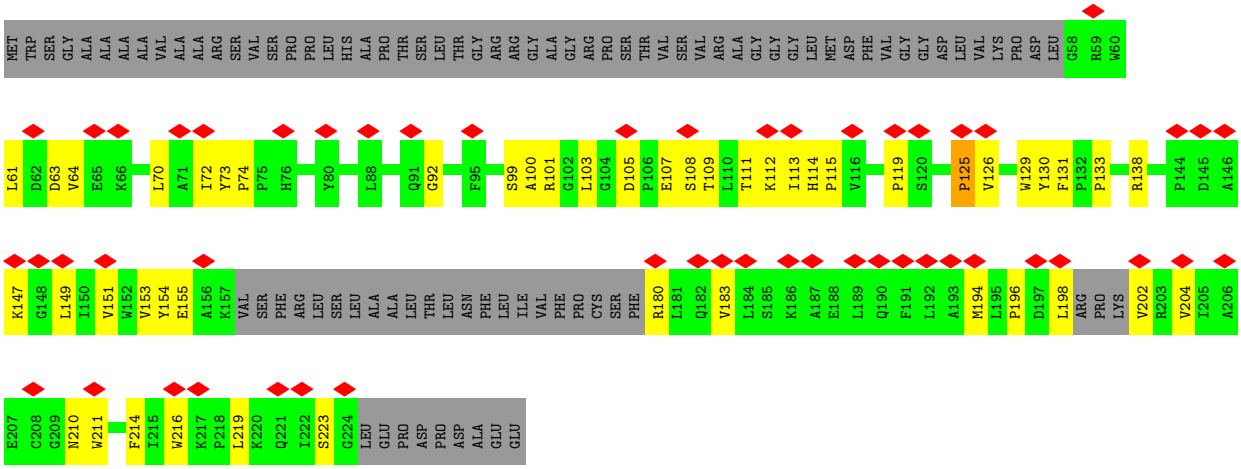




• Molecule 29: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic

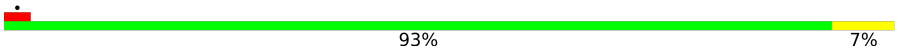
Chain Y:

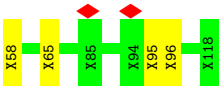




• Molecule 30: Unidentified stromal protein

Chain Z:

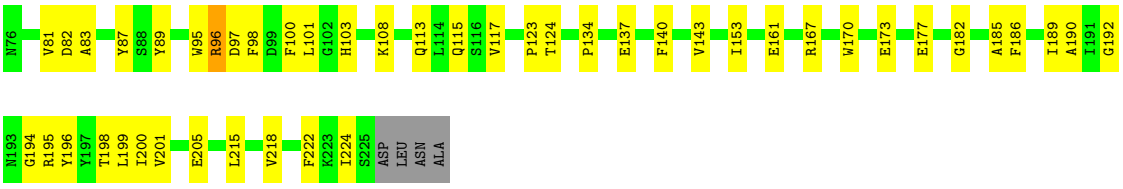




• Molecule 31: Photosynthetic NDH subunit of subcomplex L1

Chain a:

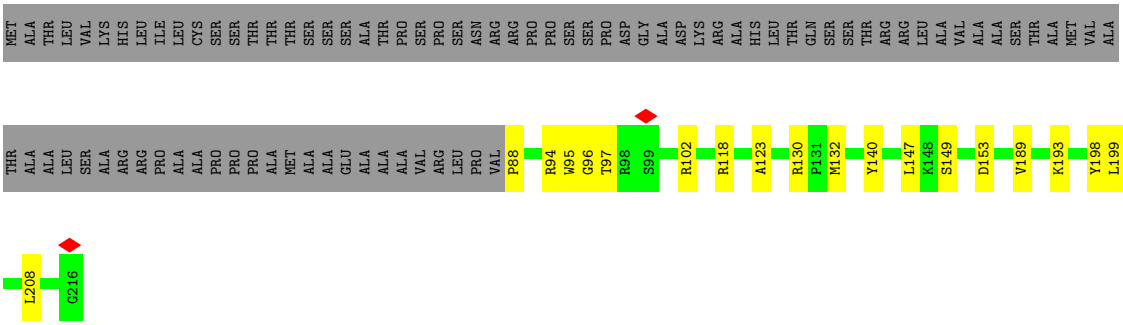




• Molecule 32: Photosynthetic NDH subunit of subcomplex L2

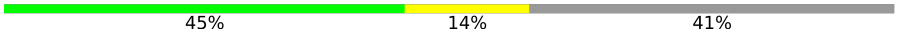
Chain b:

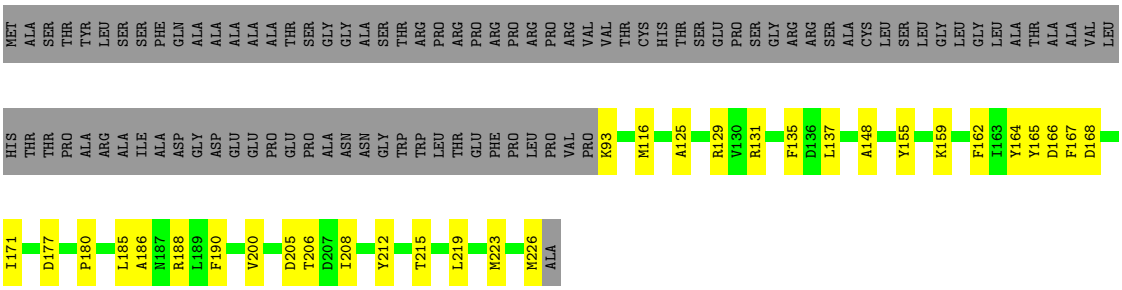




• Molecule 33: Photosynthetic NDH subunit of subcomplex L2

Chain c:





• Molecule 34: Photosynthetic NDH subunit of subcomplex L4

Chain 4:

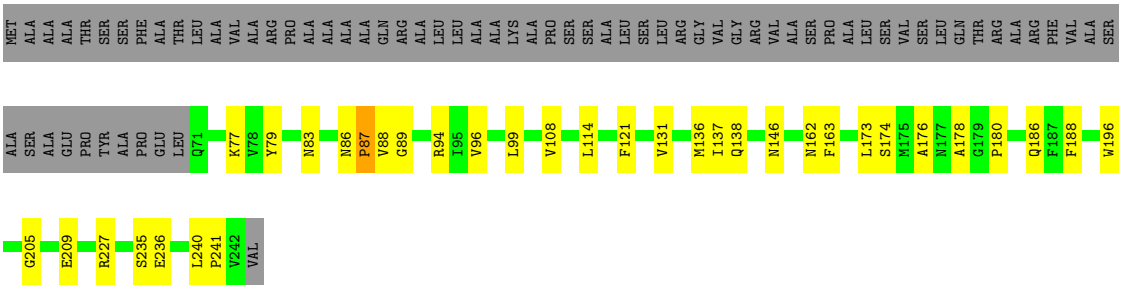




• Molecule 35: Photosynthetic NDH subunit of subcomplex L5

Chain d:

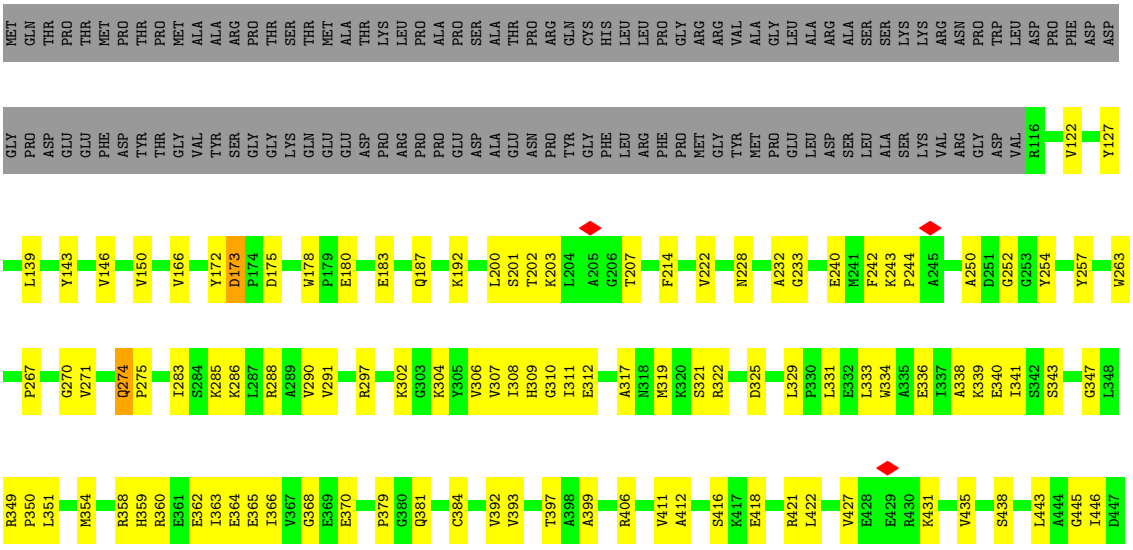




• Molecule 36: Photosynthetic NDH subunit of subcomplex B1

Chain 6:



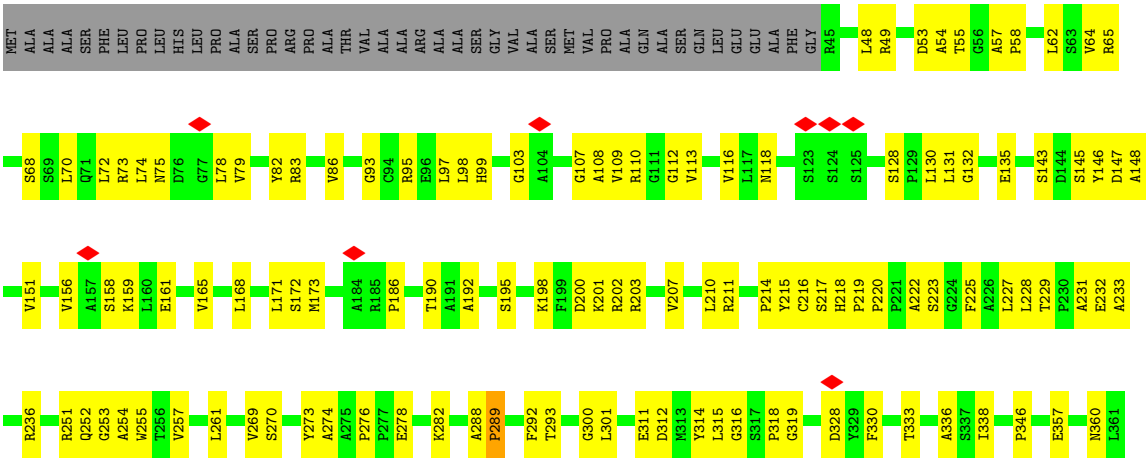




• Molecule 37: Photosynthetic NDH subunit of subcomplex B2

Chain 7:

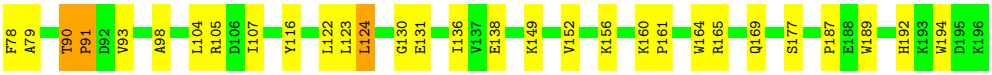




• Molecule 38: Photosynthetic NDH subunit of subcomplex B3

Chain 8:





• Molecule 39: Photosynthetic NDH subunit of subcomplex B4

Chain 9:





• Molecule 40: Photosynthetic NDH subunit of subcomplex B5

Chain 0:

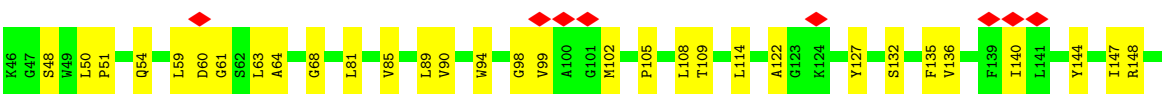


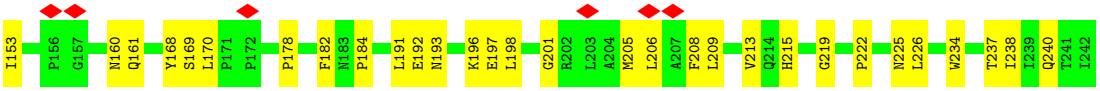


• Molecule 41: Chlorophyll a-b binding protein Lhca4

Chain r:

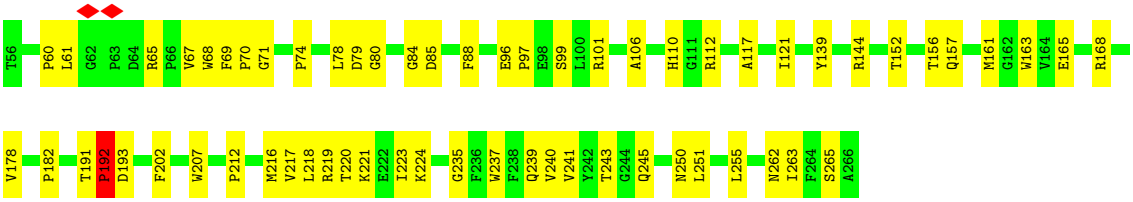






• Molecule 42: Chlorophyll a-b binding protein, chloroplastic





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	32.847	Depositor
Minimum map value	-13.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, SQD, LHG, LUT, PQN, CLA, CHL, CL0, DGD, SF4, XAT, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.64	0/6010	0.42	0/8202
1	e	0.26	4/5993 (0.1%)	0.39	2/8178 (0.0%)
2	B	0.66	0/6060	0.45	3/8276 (0.0%)
2	f	0.31	5/6052 (0.1%)	0.37	1/8267 (0.0%)
3	C	0.65	0/621	0.49	0/840
3	g	0.20	0/624	0.40	0/844
4	D	0.53	0/1142	0.52	0/1542
4	h	0.15	0/1140	0.43	0/1540
5	E	0.52	0/551	0.44	0/751
5	i	0.17	0/552	0.40	0/751
6	F	0.46	0/1230	0.41	0/1665
6	j	0.15	0/1214	0.40	0/1643
7	H	0.34	0/467	0.38	0/631
7	k	0.13	0/460	0.38	0/623
8	I	0.53	0/238	0.41	0/324
8	l	0.21	0/241	0.40	0/327
9	J	0.58	0/343	0.59	2/467 (0.4%)
9	m	0.13	0/342	0.41	0/465
10	K	0.38	0/571	0.43	0/775
10	n	0.16	0/581	0.46	0/786
11	L	0.51	0/1120	0.42	0/1534
11	o	0.15	0/1121	0.34	0/1537
12	1	0.28	0/1467	0.37	0/2008
12	p	0.20	0/1535	0.45	0/2097
13	2	0.36	0/1608	0.39	0/2204
14	3	0.34	0/1684	0.43	0/2298
14	q	0.29	1/1727 (0.1%)	0.52	1/2353 (0.0%)
15	5	0.40	0/1527	0.49	1/2085 (0.0%)
16	G	0.13	0/2664	0.38	0/3637
17	M	0.15	0/3730	0.39	0/5082
18	N	0.29	0/865	0.48	1/1188 (0.1%)
19	O	0.37	6/3987 (0.2%)	0.49	4/5427 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	P	0.14	0/759	0.32	0/1028
21	Q	0.19	0/5180	0.45	3/7068 (0.0%)
22	R	0.15	0/1288	0.45	1/1765 (0.1%)
23	S	0.13	0/3070	0.39	0/4173
24	T	0.22	0/1254	0.54	3/1702 (0.2%)
25	U	0.12	0/1297	0.37	0/1771
26	V	0.13	0/1504	0.40	0/2046
27	W	0.18	0/597	0.46	0/816
28	X	0.12	0/896	0.41	0/1218
29	Y	0.12	0/1170	0.37	0/1592
31	a	0.17	0/1213	0.54	0/1651
32	b	0.13	0/935	0.45	1/1276 (0.1%)
33	c	0.14	0/1006	0.36	0/1365
34	4	0.15	0/894	0.49	0/1216
35	d	0.13	0/1314	0.38	0/1771
36	6	0.19	0/2589	0.58	2/3513 (0.1%)
37	7	0.18	0/2347	0.53	0/3184
38	8	0.19	0/844	0.51	0/1145
39	9	0.14	0/636	0.46	0/868
40	0	0.22	0/1122	0.69	0/1536
41	r	0.16	0/1577	0.38	0/2153
42	s	0.18	0/1650	0.48	3/2255 (0.1%)
All	All	0.34	16/90609 (0.0%)	0.44	28/123459 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
9	m	0	1
12	p	0	1
19	O	0	1
21	Q	0	1
24	T	0	1
29	Y	0	1
31	a	0	1
32	b	0	1
35	d	0	1
36	6	0	4
37	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	8	0	2
40	0	0	3
All	All	0	20

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	657	TRP	C-O	-11.08	1.11	1.24
19	O	479	PRO	CA-C	-9.49	1.39	1.52
2	f	657	TRP	CA-C	-9.13	1.41	1.52
19	O	481	PHE	C-O	-7.58	1.14	1.24
1	e	679	ALA	CA-C	-7.51	1.43	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	6	274	GLN	CA-C-N	12.68	135.69	119.84
36	6	274	GLN	C-N-CA	12.68	135.69	119.84
14	q	225	LEU	N-CA-C	-11.77	98.42	111.14
19	O	481	PHE	N-CA-C	-11.69	96.08	113.61
2	B	223	GLY	CA-C-N	8.07	129.93	119.84

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	LEU	Mainchain
19	O	495	SER	Peptide
21	Q	261	ASN	Peptide
24	T	122	THR	Mainchain
29	Y	125	PRO	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	5813	0	5633	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	5798	0	5613	169	0
2	B	5851	0	5605	95	0
2	f	5840	0	5580	175	0
3	C	610	0	597	23	0
3	g	613	0	607	30	0
4	D	1113	0	1113	32	0
4	h	1111	0	1113	40	0
5	E	538	0	537	8	0
5	i	539	0	539	12	0
6	F	1204	0	1202	35	0
6	j	1188	0	1178	42	0
7	H	454	0	487	7	0
7	k	447	0	472	9	0
8	I	232	0	254	5	0
8	l	235	0	261	6	0
9	J	333	0	347	11	0
9	m	332	0	335	16	0
10	K	565	0	557	19	0
10	n	576	0	584	18	0
11	L	1088	0	1079	29	0
11	o	1089	0	1075	29	0
12	1	1422	0	1324	52	0
12	p	1484	0	1410	61	0
13	2	1554	0	1478	59	0
14	3	1631	0	1501	44	0
14	q	1672	0	1575	66	0
15	5	1486	0	1389	62	0
16	G	2602	0	2598	82	0
17	M	3646	0	3652	83	0
18	N	841	0	761	19	0
19	O	3874	0	3923	94	0
20	P	750	0	760	20	0
21	Q	5041	0	4852	132	0
22	R	1260	0	1197	28	0
23	S	2991	0	2849	131	0
24	T	1229	0	1109	27	0
25	U	1258	0	1151	52	0
26	V	1473	0	1441	56	0
27	W	572	0	559	28	0
28	X	876	0	801	29	0
29	Y	1135	0	1107	31	0
30	Z	305	0	69	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	1185	0	1086	30	0
32	b	915	0	764	14	0
33	c	989	0	927	21	0
34	4	878	0	823	20	0
35	d	1289	0	1247	21	0
36	6	2541	0	2461	75	0
37	7	2302	0	2224	91	0
38	8	828	0	742	21	0
39	9	617	0	520	17	0
40	0	1089	0	901	13	0
41	r	1529	0	1448	49	0
42	s	1591	0	1446	55	0
43	A	61	0	62	2	0
43	e	61	0	62	5	0
44	1	485	0	395	30	0
44	2	454	0	383	20	0
44	3	595	0	452	25	0
44	5	468	0	375	17	0
44	A	2024	0	1724	52	0
44	B	2118	0	1848	66	0
44	F	83	0	60	3	0
44	J	42	0	31	2	0
44	K	157	0	107	6	0
44	L	193	0	152	6	0
44	e	2028	0	1626	68	0
44	f	1921	0	1521	67	0
44	j	41	0	29	1	0
44	m	83	0	59	0	0
44	n	162	0	112	3	0
44	o	145	0	118	6	0
44	p	474	0	373	20	0
44	q	543	0	404	20	0
44	r	525	0	424	21	0
44	s	431	0	349	20	0
45	A	33	0	46	2	0
45	B	30	0	37	1	0
45	e	14	0	7	1	0
45	f	16	0	10	6	0
46	1	49	0	74	5	0
46	2	35	0	40	2	0
46	A	79	0	104	7	0
46	B	38	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	O	24	0	19	1	0
46	e	65	0	77	2	0
46	f	38	0	46	1	0
46	p	49	0	74	7	0
46	s	35	0	40	1	0
47	1	19	0	26	3	0
47	2	40	0	56	4	0
47	3	40	0	56	4	0
47	5	40	0	56	5	0
47	A	279	0	389	18	0
47	B	280	0	392	19	0
47	F	80	0	112	4	0
47	I	40	0	56	4	0
47	J	40	0	56	1	0
47	K	40	0	56	2	0
47	L	80	0	112	10	0
47	Q	39	0	53	6	0
47	e	280	0	392	23	0
47	f	239	0	333	14	0
47	j	80	0	112	2	0
47	l	80	0	112	5	0
47	m	40	0	56	3	0
47	n	40	0	56	1	0
47	o	80	0	112	4	0
47	p	11	0	16	1	0
47	q	40	0	56	3	0
47	r	40	0	56	5	0
47	s	40	0	56	4	0
48	8	8	0	0	1	0
48	A	8	0	0	0	0
48	C	16	0	0	1	0
48	f	8	0	0	0	0
48	g	16	0	0	1	0
49	B	59	0	79	4	0
49	J	66	0	96	3	0
49	f	52	0	62	2	0
49	m	66	0	96	2	0
50	2	52	0	55	3	0
50	5	32	0	34	1	0
50	F	75	0	90	3	0
50	m	30	0	30	1	0
50	r	18	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1	84	0	112	11	0
51	2	42	0	56	8	0
51	3	84	0	112	12	0
51	5	42	0	56	8	0
51	p	84	0	111	11	0
51	q	84	0	112	11	0
51	r	42	0	56	10	0
51	s	42	0	56	5	0
52	1	129	0	83	5	0
52	2	174	0	110	13	0
52	3	90	0	60	1	0
52	5	133	0	80	8	0
52	p	137	0	91	7	0
52	q	46	0	31	1	0
52	r	141	0	97	2	0
52	s	183	0	121	7	0
53	2	44	0	56	7	0
53	5	44	0	56	5	0
53	r	44	0	56	4	0
53	s	44	0	56	8	0
54	Q	100	0	137	6	0
All	All	106329	0	101185	2666	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 13.

The worst 5 of 2666 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)
16:G:240:VAL:HG11	18:N:45:GLU:CB	2.03	0.88
2:f:700:LEU:HB2	45:f:844:PQN:H6	1.62	0.81
33:c:148:ALA:HB3	39:9:105:PHE:HB2	1.67	0.76
18:N:48:ILE:CB	23:S:14:ASN:ND2	2.50	0.75
37:7:68:SER:HA	37:7:83:ARG:O	1.87	0.75

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	740/750 (99%)	690 (93%)	50 (7%)	0	100	100
1	e	740/750 (99%)	684 (92%)	56 (8%)	0	100	100
2	B	731/734 (100%)	688 (94%)	42 (6%)	1 (0%)	48	83
2	f	731/734 (100%)	680 (93%)	51 (7%)	0	100	100
3	C	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
3	g	79/81 (98%)	68 (86%)	11 (14%)	0	100	100
4	D	140/205 (68%)	118 (84%)	22 (16%)	0	100	100
4	h	140/205 (68%)	125 (89%)	15 (11%)	0	100	100
5	E	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
5	i	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
6	F	156/235 (66%)	150 (96%)	6 (4%)	0	100	100
6	j	156/235 (66%)	148 (95%)	8 (5%)	0	100	100
7	H	59/143 (41%)	58 (98%)	1 (2%)	0	100	100
7	k	59/143 (41%)	56 (95%)	3 (5%)	0	100	100
8	I	28/36 (78%)	28 (100%)	0	0	100	100
8	l	28/36 (78%)	28 (100%)	0	0	100	100
9	J	40/42 (95%)	37 (92%)	2 (5%)	1 (2%)	4	26
9	m	40/42 (95%)	38 (95%)	1 (2%)	1 (2%)	4	26
10	K	82/131 (63%)	73 (89%)	9 (11%)	0	100	100
10	n	82/131 (63%)	75 (92%)	7 (8%)	0	100	100
11	L	144/209 (69%)	135 (94%)	9 (6%)	0	100	100
11	o	144/209 (69%)	134 (93%)	10 (7%)	0	100	100
12	1	189/247 (76%)	179 (95%)	10 (5%)	0	100	100
12	p	191/247 (77%)	171 (90%)	18 (9%)	2 (1%)	12	47
13	2	201/255 (79%)	185 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	3	220/269 (82%)	195 (89%)	25 (11%)	0	100 100
14	q	220/269 (82%)	193 (88%)	27 (12%)	0	100 100
15	5	203/257 (79%)	173 (85%)	30 (15%)	0	100 100
16	G	344/346 (99%)	303 (88%)	40 (12%)	1 (0%)	36 71
17	M	474/483 (98%)	424 (90%)	50 (10%)	0	100 100
18	N	114/117 (97%)	96 (84%)	17 (15%)	1 (1%)	14 49
19	O	497/499 (100%)	447 (90%)	48 (10%)	2 (0%)	30 67
20	P	98/100 (98%)	93 (95%)	5 (5%)	0	100 100
21	Q	665/777 (86%)	598 (90%)	64 (10%)	3 (0%)	24 63
22	R	174/176 (99%)	148 (85%)	26 (15%)	0	100 100
23	S	381/383 (100%)	339 (89%)	42 (11%)	0	100 100
24	T	163/165 (99%)	123 (76%)	40 (24%)	0	100 100
25	U	157/159 (99%)	141 (90%)	16 (10%)	0	100 100
26	V	192/245 (78%)	174 (91%)	17 (9%)	1 (0%)	24 63
27	W	67/192 (35%)	59 (88%)	7 (10%)	1 (2%)	8 38
28	X	110/213 (52%)	92 (84%)	18 (16%)	0	100 100
29	Y	136/233 (58%)	114 (84%)	20 (15%)	2 (2%)	8 38
31	a	148/154 (96%)	112 (76%)	35 (24%)	1 (1%)	18 55
32	b	127/216 (59%)	106 (84%)	21 (16%)	0	100 100
33	c	132/227 (58%)	116 (88%)	16 (12%)	0	100 100
34	4	128/130 (98%)	102 (80%)	26 (20%)	0	100 100
35	d	170/243 (70%)	156 (92%)	13 (8%)	1 (1%)	21 58
36	6	341/469 (73%)	249 (73%)	90 (26%)	2 (1%)	21 58
37	7	315/361 (87%)	226 (72%)	88 (28%)	1 (0%)	36 71
38	8	117/119 (98%)	79 (68%)	34 (29%)	4 (3%)	3 21
39	9	80/83 (96%)	65 (81%)	14 (18%)	1 (1%)	9 41
40	0	147/155 (95%)	98 (67%)	48 (33%)	1 (1%)	18 55
41	r	195/197 (99%)	183 (94%)	12 (6%)	0	100 100
42	s	209/211 (99%)	190 (91%)	17 (8%)	2 (1%)	12 47
All	All	11435/13623 (84%)	10134 (89%)	1272 (11%)	29 (0%)	37 71

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	G	84	LYS
19	O	480	ASP
36	6	275	PRO
42	s	191	THR
42	s	192	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	592/608 (97%)	585 (99%)	7 (1%)	63 73
1	e	588/608 (97%)	587 (100%)	1 (0%)	87 85
2	B	595/601 (99%)	590 (99%)	5 (1%)	73 77
2	f	589/601 (98%)	588 (100%)	1 (0%)	87 85
3	C	70/71 (99%)	69 (99%)	1 (1%)	59 71
3	g	71/71 (100%)	71 (100%)	0	100 100
4	D	119/160 (74%)	118 (99%)	1 (1%)	73 77
4	h	118/160 (74%)	118 (100%)	0	100 100
5	E	58/112 (52%)	58 (100%)	0	100 100
5	i	58/112 (52%)	58 (100%)	0	100 100
6	F	121/183 (66%)	121 (100%)	0	100 100
6	j	115/183 (63%)	115 (100%)	0	100 100
7	H	48/110 (44%)	48 (100%)	0	100 100
7	k	47/110 (43%)	47 (100%)	0	100 100
8	I	26/33 (79%)	26 (100%)	0	100 100
8	l	27/33 (82%)	27 (100%)	0	100 100
9	J	35/36 (97%)	35 (100%)	0	100 100
9	m	34/36 (94%)	34 (100%)	0	100 100
10	K	52/102 (51%)	51 (98%)	1 (2%)	50 66
10	n	56/102 (55%)	55 (98%)	1 (2%)	51 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	L	112/166 (68%)	110 (98%)	2 (2%)	51 67
11	o	110/166 (66%)	110 (100%)	0	100 100
12	1	134/196 (68%)	134 (100%)	0	100 100
12	p	147/196 (75%)	147 (100%)	0	100 100
13	2	155/194 (80%)	154 (99%)	1 (1%)	78 80
14	3	148/216 (68%)	147 (99%)	1 (1%)	76 79
14	q	159/216 (74%)	158 (99%)	1 (1%)	78 80
15	5	139/202 (69%)	139 (100%)	0	100 100
16	G	270/301 (90%)	270 (100%)	0	100 100
17	M	397/419 (95%)	397 (100%)	0	100 100
18	N	71/100 (71%)	71 (100%)	0	100 100
19	O	399/427 (93%)	399 (100%)	0	100 100
20	P	78/88 (89%)	78 (100%)	0	100 100
21	Q	495/674 (73%)	494 (100%)	1 (0%)	87 85
22	R	119/154 (77%)	119 (100%)	0	100 100
23	S	298/336 (89%)	297 (100%)	1 (0%)	86 84
24	T	123/155 (79%)	123 (100%)	0	100 100
25	U	126/141 (89%)	126 (100%)	0	100 100
26	V	162/226 (72%)	162 (100%)	0	100 100
27	W	55/167 (33%)	55 (100%)	0	100 100
28	X	86/184 (47%)	86 (100%)	0	100 100
29	Y	115/192 (60%)	115 (100%)	0	100 100
31	a	116/132 (88%)	116 (100%)	0	100 100
32	b	74/181 (41%)	74 (100%)	0	100 100
33	c	92/183 (50%)	92 (100%)	0	100 100
34	4	80/102 (78%)	80 (100%)	0	100 100
35	d	135/191 (71%)	135 (100%)	0	100 100
36	6	250/389 (64%)	250 (100%)	0	100 100
37	7	232/279 (83%)	232 (100%)	0	100 100
38	8	69/102 (68%)	69 (100%)	0	100 100
39	9	55/70 (79%)	54 (98%)	1 (2%)	51 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	0	93/137 (68%)	93 (100%)	0	100 100
41	r	156/164 (95%)	156 (100%)	0	100 100
42	s	151/172 (88%)	151 (100%)	0	100 100
All	All	8820/11250 (78%)	8794 (100%)	26 (0%)	84 84

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	104	ASP
13	2	262	ILE
10	n	123	LEU
11	L	93	ARG
14	3	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
38	8	184	GLN
2	f	220	GLN
42	s	250	ASN
40	0	97	HIS
1	e	642	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)

400 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	$\#\|Z\| > 2$
44	CLA	5	316	-	45,49,73	1.47	10 (22%)	54,84,113	1.59	8 (14%)
44	CLA	3	316	-	42,45,73	1.47	8 (19%)	50,78,113	1.61	8 (16%)
44	CLA	m	102	-	46,50,73	1.52	7 (15%)	55,85,113	1.46	5 (9%)
50	LMG	r	318	-	18,18,55	1.60	2 (11%)	22,23,63	1.61	2 (9%)
44	CLA	e	825	-	45,49,73	1.50	8 (17%)	54,84,113	1.51	8 (14%)
44	CLA	e	831	1	60,64,73	1.32	8 (13%)	72,102,113	1.34	7 (9%)
44	CLA	p	513	-	56,60,73	1.41	7 (12%)	67,97,113	1.34	7 (10%)
44	CLA	s	509	-	54,58,73	1.42	7 (12%)	65,95,113	1.40	8 (12%)
52	CHL	s	512	-	51,55,74	2.41	19 (37%)	57,91,114	2.96	22 (38%)
44	CLA	B	820	-	57,61,73	1.40	11 (19%)	68,98,113	1.38	8 (11%)
44	CLA	1	513	-	69,73,73	1.27	10 (14%)	83,113,113	1.29	7 (8%)
44	CLA	f	810	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	6 (7%)
44	CLA	f	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	7 (8%)
44	CLA	e	838	-	56,60,73	1.37	9 (16%)	67,97,113	1.43	8 (11%)
44	CLA	A	815	-	49,53,73	1.51	11 (22%)	59,89,113	1.46	7 (11%)
44	CLA	f	817	-	47,51,73	1.48	9 (19%)	56,86,113	1.44	5 (8%)
51	LUT	r	302	-	42,43,43	0.76	0	51,60,60	1.90	13 (25%)
47	BCR	e	847	-	41,41,41	0.76	0	56,56,56	1.90	17 (30%)
45	PQN	f	844	-	17,17,34	2.13	2 (11%)	21,24,45	1.20	3 (14%)
44	CLA	2	507	13	51,56,73	1.72	12 (23%)	61,91,113	1.70	10 (16%)
44	CLA	B	838	2	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
47	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	2.07	17 (30%)
47	BCR	o	301	-	41,41,41	0.75	1 (2%)	56,56,56	2.04	17 (30%)
44	CLA	B	832	-	47,51,73	1.44	11 (23%)	56,86,113	1.45	4 (7%)
44	CLA	e	833	1	45,49,73	1.50	9 (20%)	54,84,113	1.50	8 (14%)
44	CLA	f	809	2	56,60,73	1.38	9 (16%)	67,97,113	1.36	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	f	832	-	43,48,73	1.54	10 (23%)	52,82,113	1.60	7 (13%)
44	CLA	B	802	-	68,72,73	1.28	11 (16%)	81,111,113	1.34	9 (11%)
44	CLA	B	807	2	69,73,73	1.30	11 (15%)	83,113,113	1.31	5 (6%)
52	CHL	r	316	-	47,51,74	2.27	17 (36%)	52,86,114	3.06	21 (40%)
44	CLA	q	307	14	43,48,73	1.57	7 (16%)	52,82,113	1.53	7 (13%)
47	BCR	1	503	-	19,19,41	0.67	0	26,26,56	2.04	7 (26%)
44	CLA	f	830	2	42,47,73	1.62	11 (26%)	54,81,113	1.66	9 (16%)
48	SF4	A	850	1,2	0,12,12	-	-	-		
44	CLA	f	822	-	45,49,73	1.53	9 (20%)	54,84,113	1.49	6 (11%)
44	CLA	B	842	-	61,65,73	1.34	11 (18%)	73,103,113	1.36	7 (9%)
44	CLA	f	842	-	45,49,73	1.51	10 (22%)	54,84,113	1.55	7 (12%)
44	CLA	f	834	-	47,51,73	1.47	8 (17%)	56,86,113	1.47	6 (10%)
44	CLA	r	311	41	50,54,73	1.46	9 (18%)	60,90,113	1.37	5 (8%)
52	CHL	p	517	-	47,51,74	2.35	18 (38%)	52,86,114	3.07	23 (44%)
44	CLA	e	830	1	54,58,73	1.41	10 (18%)	65,95,113	1.38	6 (9%)
47	BCR	A	853	-	41,41,41	0.97	2 (4%)	56,56,56	2.24	18 (32%)
44	CLA	2	504	13	37,44,73	1.63	10 (27%)	49,76,113	1.70	9 (18%)
49	DGD	B	850	-	60,60,67	0.88	2 (3%)	74,74,81	1.39	11 (14%)
44	CLA	e	835	1	45,50,73	1.53	9 (20%)	56,85,113	1.39	6 (10%)
44	CLA	B	815	-	69,73,73	1.28	12 (17%)	83,113,113	1.35	8 (9%)
44	CLA	A	819	1	43,48,73	1.54	10 (23%)	52,82,113	1.53	6 (11%)
44	CLA	p	508	12	69,73,73	1.25	8 (11%)	83,113,113	1.23	5 (6%)
50	LMG	F	805	-	30,30,55	1.22	2 (6%)	38,38,63	1.21	3 (7%)
51	LUT	1	501	-	42,43,43	0.89	1 (2%)	51,60,60	1.65	11 (21%)
44	CLA	B	801	-	69,73,73	1.29	12 (17%)	83,113,113	1.31	8 (9%)
44	CLA	B	818	2	63,67,73	1.28	10 (15%)	75,105,113	1.48	9 (12%)
44	CLA	B	808	-	56,60,73	1.41	11 (19%)	67,97,113	1.52	9 (13%)
44	CLA	B	811	2	59,63,73	1.39	11 (18%)	71,101,113	1.40	7 (9%)
51	LUT	p	501	-	42,43,43	0.80	0	51,60,60	1.97	13 (25%)
52	CHL	s	513	-	52,56,74	2.29	19 (36%)	58,92,114	2.97	25 (43%)
44	CLA	J	101	9	46,50,73	1.49	9 (19%)	55,85,113	1.53	6 (10%)
44	CLA	q	311	-	52,56,73	1.44	8 (15%)	62,92,113	1.39	5 (8%)
44	CLA	A	804	1,44	56,60,73	1.36	8 (14%)	67,97,113	1.45	5 (7%)
44	CLA	A	812	-	46,50,73	1.51	11 (23%)	55,85,113	1.61	11 (20%)
47	BCR	B	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.98	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	n	202	-	49,53,73	1.49	7 (14%)	59,89,113	1.46	8 (13%)
47	BCR	j	803	-	41,41,41	0.76	0	56,56,56	2.16	18 (32%)
44	CLA	e	815	-	49,53,73	1.49	9 (18%)	59,89,113	1.41	5 (8%)
51	LUT	q	302	-	42,43,43	0.77	0	51,60,60	1.85	16 (31%)
44	CLA	A	820	-	61,65,73	1.34	9 (14%)	73,103,113	1.54	10 (13%)
44	CLA	3	311	-	54,58,73	1.36	8 (14%)	65,95,113	1.59	9 (13%)
44	CLA	A	852	-	61,65,73	1.37	10 (16%)	73,103,113	1.33	7 (9%)
44	CLA	5	306	-	43,48,73	1.50	8 (18%)	51,83,113	1.60	7 (13%)
44	CLA	f	835	2	49,53,73	1.47	9 (18%)	59,89,113	1.48	7 (11%)
44	CLA	B	803	-	69,73,73	1.28	9 (13%)	83,113,113	1.32	8 (9%)
44	CLA	A	818	1	43,48,73	1.50	9 (20%)	52,82,113	1.57	9 (17%)
51	LUT	1	502	-	42,43,43	0.90	2 (4%)	51,60,60	1.68	11 (21%)
44	CLA	A	816	1	63,67,73	1.30	9 (14%)	75,105,113	1.46	9 (12%)
44	CLA	f	807	2	45,49,73	1.51	9 (20%)	54,84,113	1.50	8 (14%)
52	CHL	q	313	-	51,54,74	2.38	18 (35%)	52,89,114	3.12	22 (42%)
44	CLA	q	312	14	64,68,73	1.30	8 (12%)	77,107,113	1.32	7 (9%)
44	CLA	A	808	1	69,73,73	1.25	10 (14%)	83,113,113	1.36	8 (9%)
44	CLA	q	308	-	46,50,73	1.51	8 (17%)	55,85,113	1.49	7 (12%)
47	BCR	A	847	-	41,41,41	0.97	2 (4%)	56,56,56	2.00	20 (35%)
44	CLA	3	313	14	52,56,73	1.43	8 (15%)	62,92,113	1.53	7 (11%)
46	LHG	f	852	44	37,37,48	1.05	2 (5%)	40,43,54	1.16	3 (7%)
52	CHL	r	314	-	55,59,74	2.13	18 (32%)	62,96,114	3.00	23 (37%)
44	CLA	A	826	-	64,68,73	1.31	11 (17%)	77,107,113	1.43	7 (9%)
44	CLA	5	312	15	50,54,73	1.46	10 (20%)	60,90,113	1.37	5 (8%)
44	CLA	1	510	46	50,54,73	1.46	11 (22%)	60,90,113	1.42	6 (10%)
50	LMG	2	518	-	16,16,55	0.47	0	22,22,63	0.99	2 (9%)
44	CLA	B	821	2	54,58,73	1.44	9 (16%)	65,95,113	1.50	6 (9%)
44	CLA	2	514	-	59,63,73	1.33	11 (18%)	71,101,113	1.40	7 (9%)
44	CLA	A	813	-	49,53,73	1.47	9 (18%)	59,89,113	1.49	5 (8%)
46	LHG	A	843	-	48,48,48	0.90	3 (6%)	51,54,54	1.29	5 (9%)
47	BCR	f	845	-	41,41,41	0.75	0	56,56,56	2.15	19 (33%)
44	CLA	f	806	-	45,49,73	1.51	9 (20%)	54,84,113	1.46	5 (9%)
52	CHL	p	512	-	51,55,74	2.40	19 (37%)	57,91,114	2.94	24 (42%)
44	CLA	A	814	1	46,50,73	1.51	11 (23%)	55,85,113	1.60	8 (14%)
44	CLA	A	836	1	59,63,73	1.38	11 (18%)	71,101,113	1.51	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	f	818	-	59,63,73	1.34	9 (15%)	71,101,113	1.34	6 (8%)
44	CLA	r	305	-	54,58,73	1.43	8 (14%)	65,95,113	1.38	7 (10%)
44	CLA	f	815	-	47,51,73	1.49	8 (17%)	56,86,113	1.36	4 (7%)
46	LHG	A	844	44	29,29,48	1.20	3 (10%)	32,35,54	1.19	3 (9%)
44	CLA	e	832	1	47,51,73	1.49	9 (19%)	56,86,113	1.41	6 (10%)
44	CLA	e	841	-	45,49,73	1.52	9 (20%)	54,84,113	1.53	7 (12%)
44	CLA	p	505	-	50,54,73	1.43	9 (18%)	60,90,113	1.28	8 (13%)
44	CLA	B	823	-	46,50,73	1.51	11 (23%)	55,85,113	1.54	6 (10%)
44	CLA	f	823	-	45,49,73	1.52	10 (22%)	54,84,113	1.53	6 (11%)
44	CLA	B	805	2	45,49,73	1.48	10 (22%)	54,84,113	1.58	8 (14%)
54	SQD	Q	802	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	4 (6%)
44	CLA	s	506	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	5 (6%)
44	CLA	B	819	2	45,49,73	1.53	11 (24%)	54,84,113	1.66	10 (18%)
47	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.17	20 (35%)
44	CLA	K	201	-	42,45,73	1.54	10 (23%)	50,78,113	1.56	7 (14%)
44	CLA	A	821	-	46,50,73	1.47	12 (26%)	55,85,113	1.61	7 (12%)
52	CHL	3	315	-	47,51,74	2.18	17 (36%)	52,86,114	3.25	22 (42%)
44	CLA	f	819	2	45,49,73	1.51	9 (20%)	54,84,113	1.49	6 (11%)
44	CLA	1	507	12	60,64,73	1.30	10 (16%)	72,102,113	1.45	9 (12%)
44	CLA	f	804	2	44,50,73	1.81	7 (15%)	47,83,113	2.08	9 (19%)
47	BCR	B	849	-	41,41,41	1.07	2 (4%)	56,56,56	2.01	17 (30%)
44	CLA	A	806	1	69,73,73	1.27	10 (14%)	83,113,113	1.32	7 (8%)
44	CLA	L	304	-	49,53,73	1.44	11 (22%)	59,89,113	1.69	11 (18%)
44	CLA	s	507	-	45,49,73	1.52	9 (20%)	54,84,113	1.49	7 (12%)
46	LHG	O	601	-	23,23,48	1.32	2 (8%)	26,28,54	1.32	3 (11%)
44	CLA	1	509	-	54,58,73	1.40	8 (14%)	65,95,113	1.45	8 (12%)
44	CLA	q	314	-	43,48,73	1.52	9 (20%)	52,82,113	1.61	8 (15%)
44	CLA	f	814	2	47,51,73	1.48	10 (21%)	56,86,113	1.45	4 (7%)
44	CLA	f	827	-	44,48,73	1.53	10 (22%)	52,82,113	1.52	8 (15%)
44	CLA	s	511	42	54,58,73	1.41	8 (14%)	65,95,113	1.39	6 (9%)
47	BCR	B	846	-	41,41,41	1.05	3 (7%)	56,56,56	2.31	18 (32%)
46	LHG	s	516	-	34,34,48	1.08	2 (5%)	37,40,54	1.14	3 (8%)
44	CLA	F	803	-	45,49,73	1.52	11 (24%)	54,84,113	1.51	7 (12%)
44	CLA	B	833	2	69,73,73	1.23	10 (14%)	83,113,113	1.45	10 (12%)
44	CLA	f	840	2	45,49,73	1.50	9 (20%)	54,84,113	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	A	825	-	63,67,73	1.36	10 (15%)	75,105,113	1.36	7 (9%)
44	CLA	f	801	-	68,72,73	1.29	10 (14%)	85,112,113	1.36	7 (8%)
47	BCR	2	503	-	41,41,41	0.89	1 (2%)	56,56,56	3.62	27 (48%)
44	CLA	A	838	1	69,73,73	1.29	11 (15%)	83,113,113	1.34	11 (13%)
44	CLA	B	824	2	49,53,73	1.50	10 (20%)	59,89,113	1.44	5 (8%)
44	CLA	A	830	1	54,58,73	1.40	9 (16%)	65,95,113	1.52	5 (7%)
44	CLA	A	839	1	46,50,73	1.51	10 (21%)	55,85,113	1.60	6 (10%)
44	CLA	B	836	-	46,50,73	1.51	10 (21%)	55,85,113	1.43	6 (10%)
47	BCR	B	845	-	41,41,41	1.04	1 (2%)	56,56,56	2.07	17 (30%)
44	CLA	F	802	-	46,50,73	1.52	10 (21%)	55,85,113	1.53	6 (10%)
46	LHG	2	517	44	34,34,48	1.07	2 (5%)	37,40,54	1.21	4 (10%)
44	CLA	p	510	-	50,54,73	1.46	10 (20%)	60,90,113	1.36	4 (6%)
44	CLA	q	310	-	45,49,73	1.53	8 (17%)	54,84,113	1.47	4 (7%)
47	BCR	f	848	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	16 (28%)
44	CLA	K	203	-	43,48,73	1.49	11 (25%)	52,82,113	1.50	6 (11%)
47	BCR	l	101	-	41,41,41	0.80	1 (2%)	56,56,56	2.29	21 (37%)
46	LHG	B	851	-	37,37,48	1.08	2 (5%)	40,43,54	1.17	4 (10%)
44	CLA	e	802	-	43,48,73	1.53	9 (20%)	52,82,113	1.55	5 (9%)
44	CLA	5	305	-	40,46,73	1.64	11 (27%)	52,79,113	1.76	12 (23%)
44	CLA	2	511	13	43,48,73	1.51	12 (27%)	52,82,113	1.77	10 (19%)
44	CLA	B	810	2	43,48,73	1.50	11 (25%)	52,82,113	1.63	7 (13%)
44	CLA	B	826	-	66,70,73	1.25	9 (13%)	79,109,113	1.40	11 (13%)
48	SF4	C	102	3	0,12,12	-	-	-		
47	BCR	F	804	-	41,41,41	1.03	1 (2%)	56,56,56	1.97	18 (32%)
51	LUT	q	301	-	42,43,43	0.79	0	51,60,60	2.00	11 (21%)
47	BCR	I	101	-	41,41,41	1.22	3 (7%)	56,56,56	2.08	19 (33%)
44	CLA	B	816	-	47,51,73	1.46	8 (17%)	56,86,113	1.52	5 (8%)
51	LUT	3	303	-	42,43,43	0.89	2 (4%)	51,60,60	1.51	10 (19%)
44	CLA	f	813	-	58,62,73	1.42	9 (15%)	73,100,113	1.39	8 (10%)
44	CLA	p	504	-	45,49,73	1.54	10 (22%)	54,84,113	1.60	8 (14%)
44	CLA	e	829	-	62,66,73	1.32	9 (14%)	74,104,113	1.34	6 (8%)
44	CLA	s	505	-	50,54,73	1.46	9 (18%)	60,90,113	1.44	4 (6%)
44	CLA	e	810	1,44	59,63,73	1.36	10 (16%)	71,101,113	1.37	6 (8%)
47	BCR	e	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.19	18 (32%)
47	BCR	e	850	-	41,41,41	0.81	2 (4%)	56,56,56	2.33	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	BCR	n	204	-	41,41,41	0.70	0	56,56,56	2.09	18 (32%)
43	CL0	e	801	1	64,69,73	1.64	10 (15%)	76,107,113	2.13	17 (22%)
44	CLA	3	307	-	43,48,73	1.65	9 (20%)	52,82,113	1.45	5 (9%)
44	CLA	e	823	1	46,50,73	1.55	9 (19%)	58,85,113	1.55	9 (15%)
52	CHL	1	512	-	51,55,74	2.29	19 (37%)	57,91,114	2.98	23 (40%)
47	BCR	A	848	-	41,41,41	1.06	2 (4%)	56,56,56	2.00	12 (21%)
44	CLA	5	307	15	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
44	CLA	B	829	-	43,48,73	1.51	9 (20%)	52,82,113	1.56	7 (13%)
47	BCR	r	301	-	41,41,41	0.72	0	56,56,56	1.85	14 (25%)
43	CL0	A	801	-	64,69,73	1.64	10 (15%)	76,107,113	2.13	17 (22%)
46	LHG	1	516	44	48,48,48	0.91	2 (4%)	51,54,54	1.16	4 (7%)
47	BCR	J	102	-	41,41,41	1.01	2 (4%)	56,56,56	2.18	24 (42%)
44	CLA	A	822	1	45,49,73	1.51	10 (22%)	54,84,113	1.65	9 (16%)
44	CLA	5	309	15	49,53,73	1.50	11 (22%)	59,89,113	1.48	7 (11%)
44	CLA	e	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.32	8 (9%)
44	CLA	K	205	10	41,47,73	1.54	9 (21%)	49,81,113	1.55	6 (12%)
44	CLA	1	504	-	45,49,73	1.54	10 (22%)	54,84,113	1.44	7 (12%)
47	BCR	f	846	-	41,41,41	0.73	0	56,56,56	1.96	14 (25%)
44	CLA	A	833	1	43,48,73	1.50	10 (23%)	52,82,113	1.58	7 (13%)
44	CLA	A	803	1	45,49,73	1.51	11 (24%)	54,84,113	1.65	10 (18%)
47	BCR	e	849	-	41,41,41	0.74	0	56,56,56	2.06	16 (28%)
50	LMG	m	105	-	30,30,55	1.20	2 (6%)	38,38,63	1.22	3 (7%)
44	CLA	B	827	2	45,49,73	1.52	12 (26%)	54,84,113	1.67	11 (20%)
44	CLA	B	837	-	54,58,73	1.42	12 (22%)	65,95,113	1.48	10 (15%)
51	LUT	p	502	-	42,43,43	2.39	1 (2%)	51,60,60	1.81	9 (17%)
50	LMG	F	806	-	45,45,55	0.95	2 (4%)	53,53,63	1.07	4 (7%)
44	CLA	f	812	2	43,48,73	1.55	10 (23%)	52,82,113	1.58	6 (11%)
44	CLA	3	306	-	56,60,73	1.42	8 (14%)	71,97,113	1.64	10 (14%)
47	BCR	s	503	-	41,41,41	0.71	0	56,56,56	3.61	30 (53%)
44	CLA	5	311	-	46,50,73	1.45	9 (19%)	55,85,113	1.59	7 (12%)
47	BCR	o	305	-	41,41,41	0.71	0	56,56,56	2.18	18 (32%)
44	CLA	B	834	2	49,53,73	1.46	8 (16%)	59,89,113	1.56	9 (15%)
46	LHG	p	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	4 (7%)
44	CLA	A	832	1	48,53,73	1.45	8 (16%)	59,88,113	1.62	6 (10%)
44	CLA	2	506	-	69,73,73	1.22	9 (13%)	83,113,113	1.42	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	f	816	-	43,46,73	1.51	9 (20%)	51,79,113	1.45	5 (9%)
52	CHL	1	514	-	44,49,74	2.51	18 (40%)	49,83,114	3.13	21 (42%)
44	CLA	e	820	-	45,49,73	1.50	9 (20%)	54,84,113	1.53	7 (12%)
44	CLA	K	202	-	45,49,73	1.48	9 (20%)	54,84,113	1.54	6 (11%)
47	BCR	l	102	-	41,41,41	0.70	0	56,56,56	2.15	16 (28%)
44	CLA	f	808	-	58,62,73	1.36	8 (13%)	69,99,113	1.36	7 (10%)
44	CLA	A	842	46	54,58,73	1.39	11 (20%)	65,95,113	1.42	7 (10%)
44	CLA	3	310	-	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
44	CLA	n	203	-	45,49,73	1.52	8 (17%)	54,84,113	1.54	6 (11%)
44	CLA	A	811	1	43,48,73	1.52	9 (20%)	52,82,113	1.57	9 (17%)
47	BCR	q	303	-	41,41,41	0.79	1 (2%)	56,56,56	2.00	18 (32%)
44	CLA	e	840	-	45,49,73	1.50	8 (17%)	54,84,113	1.54	5 (9%)
48	SF4	g	101	-	0,12,12	-	-	-		
44	CLA	1	515	-	49,52,73	1.56	11 (22%)	54,87,113	1.47	7 (12%)
44	CLA	2	508	13	51,55,73	1.48	9 (17%)	61,91,113	1.34	5 (8%)
47	BCR	j	801	-	41,41,41	0.74	0	56,56,56	2.22	21 (37%)
47	BCR	f	849	-	41,41,41	0.79	1 (2%)	56,56,56	2.02	16 (28%)
44	CLA	e	803	1,44	56,60,73	1.38	9 (16%)	67,97,113	1.40	7 (10%)
52	CHL	s	517	42	51,55,74	2.25	19 (37%)	57,91,114	3.08	22 (38%)
44	CLA	f	820	2	54,58,73	1.40	10 (18%)	65,95,113	1.45	6 (9%)
44	CLA	r	315	41	45,49,73	1.52	9 (20%)	54,84,113	1.55	9 (16%)
44	CLA	j	802	-	45,49,73	1.51	9 (20%)	54,84,113	1.45	5 (9%)
52	CHL	s	515	-	44,49,74	2.36	17 (38%)	49,83,114	3.23	22 (44%)
53	XAT	5	304	-	39,47,47	1.24	5 (12%)	54,74,74	2.53	18 (33%)
52	CHL	2	513	-	44,48,74	2.48	19 (43%)	44,81,114	3.40	22 (50%)
44	CLA	n	205	-	41,47,73	1.60	9 (21%)	49,81,113	1.46	6 (12%)
44	CLA	B	817	2	53,57,73	1.42	10 (18%)	62,93,113	1.50	7 (11%)
44	CLA	e	811	-	45,49,73	1.50	10 (22%)	54,84,113	1.51	7 (12%)
49	DGD	J	103	-	67,67,67	0.83	2 (2%)	81,81,81	1.11	4 (4%)
44	CLA	e	809	1	54,58,73	1.39	8 (14%)	65,95,113	1.54	7 (10%)
44	CLA	f	838	-	43,48,73	1.53	10 (23%)	52,82,113	1.55	6 (11%)
44	CLA	f	841	-	45,49,73	1.49	10 (22%)	54,84,113	1.53	5 (9%)
45	PQN	A	841	-	34,34,34	1.38	2 (5%)	42,45,45	1.24	4 (9%)
44	CLA	B	839	2	51,55,73	1.42	10 (19%)	61,91,113	1.57	8 (13%)
44	CLA	A	828	1	45,49,73	1.51	10 (22%)	54,84,113	1.53	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	s	508	-	44,48,73	1.53	8 (18%)	53,83,113	1.52	5 (9%)
44	CLA	2	510	46	64,68,73	1.28	10 (15%)	77,107,113	1.39	9 (11%)
44	CLA	q	316	14	50,54,73	1.47	8 (16%)	60,90,113	1.37	6 (10%)
44	CLA	5	308	-	64,68,73	1.34	10 (15%)	77,107,113	1.43	9 (11%)
44	CLA	e	816	-	64,68,73	1.30	9 (14%)	77,107,113	1.32	5 (6%)
44	CLA	s	514	-	43,48,73	1.54	8 (18%)	52,82,113	1.56	6 (11%)
44	CLA	e	818	1	43,47,73	1.71	7 (16%)	51,81,113	2.01	12 (23%)
47	BCR	B	844	-	41,41,41	0.85	1 (2%)	56,56,56	2.59	19 (33%)
44	CLA	q	304	-	42,46,73	1.75	9 (21%)	48,79,113	1.59	9 (18%)
44	CLA	B	809	2	43,48,73	1.52	11 (25%)	52,82,113	1.57	5 (9%)
44	CLA	e	828	-	47,51,73	1.49	10 (21%)	55,85,113	1.48	5 (9%)
44	CLA	A	831	1	67,71,73	1.37	14 (20%)	83,110,113	1.43	10 (12%)
44	CLA	3	318	14	49,53,73	1.48	8 (16%)	62,89,113	1.49	7 (11%)
47	BCR	Q	801	-	40,40,41	0.77	0	54,54,56	2.99	21 (38%)
44	CLA	3	317	-	45,49,73	1.51	11 (24%)	54,84,113	1.59	8 (14%)
44	CLA	f	821	-	59,63,73	1.35	10 (16%)	71,101,113	1.36	7 (9%)
44	CLA	e	808	1	45,49,73	1.52	9 (20%)	54,84,113	1.55	6 (11%)
52	CHL	3	302	13	51,55,74	2.25	20 (39%)	57,91,114	3.07	21 (36%)
44	CLA	3	312	-	45,49,73	1.53	9 (20%)	54,84,113	1.48	7 (12%)
44	CLA	r	309	-	54,58,73	1.39	8 (14%)	65,95,113	1.31	4 (6%)
44	CLA	f	803	-	44,49,73	1.43	9 (20%)	51,83,113	1.39	4 (7%)
44	CLA	A	810	44	58,62,73	1.38	12 (20%)	69,99,113	1.52	7 (10%)
47	BCR	3	305	-	41,41,41	0.90	2 (4%)	56,56,56	1.98	13 (23%)
44	CLA	r	310	-	46,50,73	1.51	8 (17%)	55,85,113	1.46	6 (10%)
44	CLA	e	814	1	46,50,73	1.51	10 (21%)	55,85,113	1.48	5 (9%)
44	CLA	e	827	-	45,49,73	1.49	9 (20%)	54,84,113	1.47	8 (14%)
44	CLA	A	817	1	43,47,73	1.73	14 (32%)	49,81,113	1.66	7 (14%)
44	CLA	B	835	2	64,68,73	1.30	11 (17%)	77,107,113	1.40	9 (11%)
44	CLA	B	812	2	58,62,73	1.44	12 (20%)	73,100,113	1.46	11 (15%)
52	CHL	2	516	13	47,51,74	2.25	17 (36%)	55,86,114	3.36	23 (41%)
44	CLA	1	508	12	43,48,73	1.50	9 (20%)	52,82,113	1.50	8 (15%)
44	CLA	p	515	-	43,48,73	1.58	9 (20%)	52,82,113	1.57	6 (11%)
49	DGD	f	851	-	53,53,67	0.93	2 (3%)	67,67,81	1.06	3 (4%)
44	CLA	A	802	-	62,66,73	1.34	11 (17%)	74,104,113	1.37	6 (8%)
44	CLA	r	317	41	54,58,73	1.41	9 (16%)	65,95,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	e	837	-	59,63,73	1.34	9 (15%)	71,101,113	1.42	10 (14%)
44	CLA	p	509	-	54,58,73	1.55	7 (12%)	65,95,113	1.98	17 (26%)
48	SF4	C	101	3	0,12,12	-	-	-		
47	BCR	m	103	-	41,41,41	0.77	1 (2%)	56,56,56	2.11	17 (30%)
47	BCR	f	847	-	41,41,41	0.74	0	56,56,56	2.24	18 (32%)
44	CLA	B	806	2	41,47,73	1.57	10 (24%)	53,80,113	1.61	11 (20%)
44	CLA	f	829	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	10 (15%)
44	CLA	2	505	-	56,60,73	1.34	11 (19%)	67,97,113	1.47	7 (10%)
49	DGD	m	104	-	67,67,67	0.84	2 (2%)	81,81,81	0.88	3 (3%)
44	CLA	B	822	-	51,55,73	1.44	12 (23%)	61,91,113	1.58	6 (9%)
44	CLA	r	306	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
44	CLA	p	507	12	44,48,73	1.58	10 (22%)	56,83,113	1.62	9 (16%)
44	CLA	q	305	-	56,60,73	1.40	6 (10%)	67,97,113	1.35	7 (10%)
48	SF4	g	102	-	0,12,12	-	-	-		
47	BCR	K	204	-	41,41,41	0.99	2 (4%)	56,56,56	2.02	16 (28%)
52	CHL	r	313	-	51,55,74	2.36	19 (37%)	57,91,114	2.93	23 (40%)
44	CLA	r	312	-	45,49,73	1.52	8 (17%)	54,84,113	1.51	6 (11%)
44	CLA	5	310	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	7 (10%)
44	CLA	r	308	-	45,49,73	1.52	9 (20%)	54,84,113	1.52	5 (9%)
44	CLA	5	313	15	43,48,73	1.50	9 (20%)	52,82,113	1.54	7 (13%)
44	CLA	B	825	-	46,50,73	1.46	11 (23%)	55,85,113	1.49	8 (14%)
44	CLA	f	825	2	46,50,73	1.50	10 (21%)	55,85,113	1.45	5 (9%)
53	XAT	2	502	-	39,47,47	1.13	4 (10%)	54,74,74	2.84	20 (37%)
44	CLA	o	302	-	44,48,73	1.60	8 (18%)	56,83,113	1.65	7 (12%)
51	LUT	s	501	-	42,43,43	0.78	0	51,60,60	1.89	13 (25%)
47	BCR	5	302	-	41,41,41	0.83	0	56,56,56	1.97	13 (23%)
44	CLA	A	805	1	68,72,73	1.32	13 (19%)	81,111,113	1.47	9 (11%)
44	CLA	B	830	2	60,64,73	1.41	12 (20%)	72,102,113	1.36	6 (8%)
44	CLA	p	506	-	59,63,73	1.34	9 (15%)	71,101,113	1.27	7 (9%)
44	CLA	e	852	-	61,65,73	1.32	9 (14%)	73,103,113	1.35	5 (6%)
44	CLA	f	805	-	41,46,73	1.54	9 (21%)	47,79,113	1.65	8 (17%)
44	CLA	A	835	-	55,59,73	1.42	8 (14%)	66,96,113	1.61	7 (10%)
44	CLA	L	302	-	44,48,73	1.49	8 (18%)	52,82,113	1.67	10 (19%)
44	CLA	f	839	2	45,49,73	1.51	8 (17%)	54,84,113	1.56	6 (11%)
50	LMG	5	301	-	32,32,55	1.18	2 (6%)	40,40,63	1.15	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	e	853	1	49,53,73	1.46	9 (18%)	59,89,113	1.49	8 (13%)
44	CLA	A	834	1	45,49,73	1.52	10 (22%)	54,84,113	1.49	6 (11%)
44	CLA	q	309	-	54,58,73	1.40	7 (12%)	65,95,113	1.41	5 (7%)
45	PQN	B	843	-	31,31,34	1.36	2 (6%)	38,41,45	1.49	5 (13%)
44	CLA	B	814	2	45,49,73	1.57	11 (24%)	54,84,113	1.59	9 (16%)
44	CLA	e	819	-	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
44	CLA	A	840	-	45,49,73	1.54	11 (24%)	54,84,113	1.54	6 (11%)
52	CHL	5	314	-	51,55,74	2.20	19 (37%)	57,91,114	3.04	23 (40%)
44	CLA	f	833	2	47,51,73	1.47	9 (19%)	56,86,113	1.40	4 (7%)
44	CLA	e	822	-	45,49,73	1.50	9 (20%)	54,84,113	1.56	5 (9%)
44	CLA	A	807	1	41,47,73	1.50	10 (24%)	48,80,113	1.60	8 (16%)
51	LUT	3	304	-	42,43,43	0.91	2 (4%)	51,60,60	1.56	10 (19%)
52	CHL	p	514	-	51,55,74	2.38	19 (37%)	57,91,114	2.94	23 (40%)
44	CLA	o	303	-	64,68,73	1.29	8 (12%)	77,107,113	1.33	5 (6%)
52	CHL	2	515	-	49,53,74	2.28	20 (40%)	58,89,114	3.12	24 (41%)
44	CLA	f	843	46	41,46,73	1.56	7 (17%)	51,80,113	1.51	6 (11%)
44	CLA	1	505	-	46,50,73	1.52	8 (17%)	55,85,113	1.45	6 (10%)
44	CLA	A	829	1	59,63,73	1.38	10 (16%)	71,101,113	1.48	9 (12%)
44	CLA	e	817	1	43,47,73	1.53	10 (23%)	49,81,113	1.54	7 (14%)
48	SF4	f	802	-	0,12,12	-	-	-		
44	CLA	e	812	-	41,47,73	1.54	9 (21%)	48,80,113	1.55	8 (16%)
44	CLA	q	306	-	45,49,73	1.52	8 (17%)	54,84,113	1.56	6 (11%)
47	BCR	L	306	-	41,41,41	0.85	1 (2%)	56,56,56	1.96	19 (33%)
44	CLA	e	843	-	53,57,73	1.48	8 (15%)	67,94,113	1.47	8 (11%)
44	CLA	e	805	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	4 (6%)
51	LUT	2	501	-	42,43,43	0.94	1 (2%)	51,60,60	1.94	15 (29%)
44	CLA	f	836	-	62,66,73	1.32	8 (12%)	71,103,113	1.32	6 (8%)
53	XAT	s	502	-	39,47,47	0.91	0	54,74,74	2.89	22 (40%)
44	CLA	B	840	-	45,49,73	1.48	10 (22%)	54,84,113	1.65	7 (12%)
44	CLA	e	804	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	5 (6%)
47	BCR	e	854	-	41,41,41	0.70	0	56,56,56	2.26	19 (33%)
47	BCR	e	851	-	41,41,41	0.71	0	56,56,56	2.16	19 (33%)
47	BCR	L	305	-	41,41,41	1.00	1 (2%)	56,56,56	2.16	18 (32%)
44	CLA	A	823	1	58,62,73	1.42	9 (15%)	67,99,113	1.42	10 (14%)
47	BCR	B	847	-	41,41,41	1.03	2 (4%)	56,56,56	2.35	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	SF4	8	201	38	0,12,12	-	-	-		
44	CLA	e	834	1	49,53,73	1.46	10 (20%)	59,89,113	1.46	6 (10%)
44	CLA	B	804	-	69,73,73	1.30	11 (15%)	83,113,113	1.33	4 (4%)
44	CLA	B	831	2	47,51,73	1.51	10 (21%)	56,86,113	1.49	6 (10%)
44	CLA	f	831	2	60,64,73	1.35	9 (15%)	72,102,113	1.38	7 (9%)
44	CLA	m	101	-	45,49,73	1.60	9 (20%)	57,84,113	1.47	6 (10%)
44	CLA	2	509	-	54,58,73	1.39	9 (16%)	65,95,113	1.50	6 (9%)
46	LHG	e	845	-	24,24,48	0.96	1 (4%)	26,29,54	1.26	3 (11%)
44	CLA	r	304	-	42,47,73	1.60	9 (21%)	54,81,113	1.70	10 (18%)
44	CLA	A	809	1	42,47,73	1.54	10 (23%)	46,80,113	1.48	3 (6%)
47	BCR	p	503	-	10,11,41	0.69	0	15,16,56	1.94	4 (26%)
44	CLA	3	309	-	43,48,73	1.69	10 (23%)	55,82,113	1.60	9 (16%)
50	LMG	2	519	-	36,36,55	1.09	2 (5%)	44,44,63	1.37	8 (18%)
47	BCR	A	849	-	40,40,41	1.04	2 (5%)	54,54,56	1.90	15 (27%)
47	BCR	e	848	-	41,41,41	0.80	1 (2%)	56,56,56	2.15	20 (35%)
44	CLA	e	813	1	46,50,73	1.52	9 (19%)	55,85,113	1.43	6 (10%)
46	LHG	e	844	-	39,39,48	1.00	2 (5%)	42,45,54	1.23	4 (9%)
52	CHL	2	512	-	50,54,74	2.22	17 (34%)	59,90,114	3.20	24 (40%)
44	CLA	A	837	1	45,49,73	1.53	11 (24%)	54,84,113	1.68	12 (22%)
44	CLA	e	836	-	55,59,73	1.40	9 (16%)	66,96,113	1.38	6 (9%)
51	LUT	5	303	-	42,43,43	0.95	2 (4%)	51,60,60	1.83	13 (25%)
44	CLA	1	511	-	50,54,73	1.47	10 (20%)	60,90,113	1.49	6 (10%)
44	CLA	f	811	2	55,59,73	1.41	8 (14%)	66,96,113	1.42	8 (12%)
44	CLA	B	841	2	58,62,73	1.38	11 (18%)	69,99,113	1.43	7 (10%)
44	CLA	f	837	-	46,50,73	1.51	9 (19%)	55,85,113	1.45	5 (9%)
44	CLA	B	813	2	47,51,73	1.52	9 (19%)	56,86,113	1.53	7 (12%)
44	CLA	3	301	1	45,49,73	1.49	9 (20%)	54,84,113	1.60	9 (16%)
44	CLA	A	824	-	43,48,73	1.52	8 (18%)	52,82,113	1.50	6 (11%)
44	CLA	3	308	14	59,63,73	1.31	9 (15%)	71,101,113	1.44	7 (9%)
44	CLA	f	824	-	46,50,73	1.50	9 (19%)	55,85,113	1.48	5 (9%)
44	CLA	q	315	-	49,53,73	1.47	9 (18%)	59,89,113	1.44	7 (11%)
53	XAT	r	303	-	39,47,47	0.88	0	54,74,74	2.72	20 (37%)
44	CLA	r	307	-	64,68,73	1.30	8 (12%)	77,107,113	1.35	8 (10%)
44	CLA	p	511	-	41,47,73	1.57	9 (21%)	53,80,113	1.56	8 (15%)
54	SQD	Q	803	-	45,46,54	1.28	4 (8%)	54,57,65	1.15	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	e	807	-	46,50,73	1.50	9 (19%)	55,85,113	1.52	5 (9%)
52	CHL	5	317	-	44,48,74	2.31	17 (38%)	49,82,114	3.28	25 (51%)
44	CLA	e	826	1	68,72,73	1.30	11 (16%)	85,112,113	1.38	8 (9%)
44	CLA	s	510	-	64,68,73	1.30	8 (12%)	77,107,113	1.26	4 (5%)
44	CLA	A	827	1	69,73,73	1.28	11 (15%)	83,113,113	1.37	9 (10%)
47	BCR	B	852	-	41,41,41	1.22	3 (7%)	56,56,56	2.06	18 (32%)
44	CLA	L	301	1	60,64,73	1.38	13 (21%)	72,102,113	1.36	7 (9%)
44	CLA	3	314	14	64,68,73	1.28	9 (14%)	77,107,113	1.40	9 (11%)
52	CHL	1	517	12	44,49,74	2.27	16 (36%)	49,83,114	3.35	23 (46%)
47	BCR	A	845	-	41,41,41	1.17	4 (9%)	56,56,56	2.29	20 (35%)
44	CLA	n	201	-	42,45,73	1.57	10 (23%)	50,78,113	1.48	6 (12%)
52	CHL	5	315	-	50,54,74	2.22	19 (38%)	56,90,114	3.10	24 (42%)
47	BCR	f	850	-	40,40,41	0.76	0	54,54,56	2.08	15 (27%)
44	CLA	e	821	-	46,50,73	1.48	9 (19%)	55,85,113	1.47	7 (12%)
47	BCR	F	801	-	41,41,41	0.99	2 (4%)	56,56,56	2.09	17 (30%)
44	CLA	e	824	-	60,64,73	1.33	10 (16%)	72,102,113	1.33	7 (9%)
45	PQN	e	842	-	15,15,34	1.44	2 (13%)	22,22,45	0.87	2 (9%)
44	CLA	1	506	-	59,63,73	1.35	9 (15%)	71,101,113	1.41	7 (9%)
44	CLA	B	828	-	45,49,73	1.49	12 (26%)	54,84,113	1.61	10 (18%)
44	CLA	f	828	2	45,49,73	1.52	10 (22%)	54,84,113	1.59	5 (9%)
44	CLA	o	304	-	49,53,73	1.48	8 (16%)	59,89,113	1.42	5 (8%)
44	CLA	s	504	-	42,47,73	1.63	7 (16%)	54,81,113	1.70	10 (18%)
44	CLA	e	806	-	45,49,73	1.51	10 (22%)	54,84,113	1.54	8 (14%)
44	CLA	L	303	11	56,60,73	1.37	9 (16%)	67,97,113	1.59	10 (14%)

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
44	CLA	5	316	-	-	2/10/86/115	-
44	CLA	3	316	-	-	0/4/76/115	-
44	CLA	m	102	-	-	6/12/88/115	-
50	LMG	r	318	-	-	11/11/28/70	0/1/1/1
44	CLA	e	825	-	-	0/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	831	1	-	7/29/105/115	-
44	CLA	p	513	-	-	5/24/100/115	-
44	CLA	s	509	-	-	7/21/97/115	-
52	CHL	s	512	-	-	5/19/95/117	-
44	CLA	B	820	-	-	7/25/101/115	-
44	CLA	1	513	-	-	21/39/115/115	-
44	CLA	f	810	-	-	12/39/115/115	-
44	CLA	f	826	-	-	11/39/115/115	-
44	CLA	e	838	-	-	4/24/100/115	-
44	CLA	A	815	-	-	4/15/91/115	-
44	CLA	f	817	-	-	7/13/89/115	-
51	LUT	r	302	-	-	2/29/67/67	0/2/2/2
47	BCR	e	847	-	-	0/29/63/63	0/2/2/2
45	PQN	f	844	-	-	0/3/23/43	0/2/2/2
44	CLA	2	507	13	1/1/11/20	5/16/88/115	-
44	CLA	B	838	2	-	4/39/115/115	-
47	BCR	A	846	-	-	7/29/63/63	0/2/2/2
47	BCR	o	301	-	-	2/29/63/63	0/2/2/2
44	CLA	B	832	-	-	3/13/89/115	-
44	CLA	e	833	1	-	6/10/86/115	-
44	CLA	f	809	2	-	5/24/100/115	-
44	CLA	f	832	-	-	3/10/82/115	-
44	CLA	B	802	-	-	6/37/113/115	-
44	CLA	B	807	2	-	11/39/115/115	-
52	CHL	r	316	-	-	3/14/90/117	-
44	CLA	q	307	14	-	3/10/82/115	-
47	BCR	1	503	-	-	4/11/28/63	0/1/1/2
44	CLA	f	830	2	-	3/8/80/115	-
48	SF4	A	850	1,2	-	-	0/6/5/5
44	CLA	f	822	-	-	2/10/86/115	-
44	CLA	B	842	-	-	15/30/106/115	-
44	CLA	f	842	-	-	2/10/86/115	-
44	CLA	f	834	-	-	3/13/89/115	-
44	CLA	r	311	41	-	6/17/93/115	-
52	CHL	p	517	-	-	5/14/90/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	830	1	-	8/21/97/115	-
47	BCR	A	853	-	-	2/29/63/63	0/2/2/2
44	CLA	2	504	13	-	2/4/73/115	-
49	DGD	B	850	-	-	19/48/88/95	0/2/2/2
44	CLA	e	835	1	-	4/9/85/115	-
44	CLA	B	815	-	-	9/39/115/115	-
44	CLA	A	819	1	-	5/10/82/115	-
44	CLA	p	508	12	-	17/39/115/115	-
50	LMG	F	805	-	-	4/25/45/70	0/1/1/1
51	LUT	1	501	-	-	2/29/67/67	0/2/2/2
44	CLA	B	801	-	-	9/39/115/115	-
44	CLA	B	818	2	-	16/32/108/115	-
44	CLA	B	808	-	-	9/24/100/115	-
44	CLA	B	811	2	-	12/27/103/115	-
51	LUT	p	501	-	-	2/29/67/67	0/2/2/2
52	CHL	s	513	-	-	5/20/96/117	-
44	CLA	J	101	9	-	9/12/88/115	-
44	CLA	q	311	-	-	10/19/95/115	-
44	CLA	A	804	1,44	-	5/24/100/115	-
44	CLA	A	812	-	-	3/12/88/115	-
47	BCR	B	848	-	-	2/29/63/63	0/2/2/2
44	CLA	n	202	-	-	10/15/91/115	-
47	BCR	j	803	-	-	2/29/63/63	0/2/2/2
44	CLA	e	815	-	-	9/15/91/115	-
51	LUT	q	302	-	-	6/29/67/67	0/2/2/2
44	CLA	A	820	-	-	10/30/106/115	-
44	CLA	3	311	-	-	8/21/97/115	-
44	CLA	A	852	-	-	11/30/106/115	-
44	CLA	5	306	-	-	4/8/84/115	-
44	CLA	f	835	2	-	8/15/91/115	-
44	CLA	B	803	-	-	18/39/115/115	-
44	CLA	A	818	1	-	4/10/82/115	-
51	LUT	1	502	-	-	4/29/67/67	0/2/2/2
44	CLA	A	816	1	-	12/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	f	807	2	-	2/10/86/115	-
52	CHL	q	313	-	-	11/19/91/117	-
44	CLA	q	312	14	-	12/33/109/115	-
44	CLA	A	808	1	-	8/39/115/115	-
44	CLA	q	308	-	-	5/12/88/115	-
47	BCR	A	847	-	-	2/29/63/63	0/2/2/2
44	CLA	3	313	14	-	10/19/95/115	-
46	LHG	f	852	44	-	13/42/42/53	-
52	CHL	r	314	-	-	4/23/99/117	-
44	CLA	A	826	-	-	13/33/109/115	-
44	CLA	5	312	15	-	9/17/93/115	-
44	CLA	1	510	46	-	8/17/93/115	-
50	LMG	2	518	-	-	3/7/27/70	0/1/1/1
44	CLA	B	821	2	-	5/21/97/115	-
44	CLA	2	514	-	-	10/27/103/115	-
44	CLA	A	813	-	-	9/15/91/115	-
46	LHG	A	843	-	-	13/53/53/53	-
47	BCR	f	845	-	-	7/29/63/63	0/2/2/2
44	CLA	f	806	-	-	2/10/86/115	-
52	CHL	p	512	-	-	3/19/95/117	-
44	CLA	A	814	1	-	3/12/88/115	-
44	CLA	A	836	1	-	11/27/103/115	-
44	CLA	f	818	-	-	9/27/103/115	-
44	CLA	r	305	-	-	7/21/97/115	-
44	CLA	f	815	-	-	6/13/89/115	-
46	LHG	A	844	44	-	11/34/34/53	-
44	CLA	e	832	1	-	8/13/89/115	-
44	CLA	e	841	-	-	3/10/86/115	-
44	CLA	p	505	-	-	5/17/93/115	-
44	CLA	B	823	-	-	4/12/88/115	-
44	CLA	f	823	-	-	4/10/86/115	-
44	CLA	B	805	2	-	4/10/86/115	-
54	SQD	Q	802	-	-	9/49/69/69	0/1/1/1
44	CLA	s	506	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	B	819	2	-	0/10/86/115	-
47	BCR	A	851	-	-	6/29/63/63	0/2/2/2
44	CLA	K	201	-	-	2/4/76/115	-
44	CLA	A	821	-	-	2/12/88/115	-
52	CHL	3	315	-	-	4/14/90/117	-
44	CLA	f	819	2	-	4/10/86/115	-
44	CLA	1	507	12	-	6/29/105/115	-
44	CLA	f	804	2	-	4/11/84/115	-
47	BCR	B	849	-	-	3/29/63/63	0/2/2/2
44	CLA	A	806	1	-	20/39/115/115	-
44	CLA	L	304	-	-	6/15/91/115	-
44	CLA	s	507	-	-	2/10/86/115	-
46	LHG	O	601	-	-	3/27/27/53	-
44	CLA	1	509	-	-	6/21/97/115	-
44	CLA	q	314	-	-	2/10/82/115	-
44	CLA	f	814	2	-	4/13/89/115	-
44	CLA	f	827	-	-	1/10/82/115	-
44	CLA	s	511	42	-	9/21/97/115	-
47	BCR	B	846	-	-	6/29/63/63	0/2/2/2
46	LHG	s	516	-	-	6/39/39/53	-
44	CLA	F	803	-	-	5/10/86/115	-
44	CLA	B	833	2	-	4/39/115/115	-
44	CLA	f	840	2	-	4/10/86/115	-
44	CLA	A	825	-	-	8/32/108/115	-
44	CLA	f	801	-	-	13/37/113/115	-
47	BCR	2	503	-	-	8/29/63/63	0/2/2/2
44	CLA	A	838	1	-	15/39/115/115	-
44	CLA	B	824	2	-	8/15/91/115	-
44	CLA	A	830	1	-	3/21/97/115	-
44	CLA	A	839	1	-	5/12/88/115	-
44	CLA	B	836	-	-	6/12/88/115	-
47	BCR	B	845	-	-	6/29/63/63	0/2/2/2
44	CLA	F	802	-	-	4/12/88/115	-
46	LHG	2	517	44	-	5/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	p	510	-	-	9/17/93/115	-
44	CLA	q	310	-	-	5/10/86/115	-
47	BCR	f	848	-	-	0/29/63/63	0/2/2/2
44	CLA	K	203	-	-	5/10/82/115	-
47	BCR	l	101	-	-	6/29/63/63	0/2/2/2
46	LHG	B	851	-	-	18/42/42/53	-
44	CLA	e	802	-	-	4/10/82/115	-
44	CLA	5	305	-	-	1/8/80/115	-
44	CLA	2	511	13	-	3/10/82/115	-
44	CLA	B	810	2	-	2/10/82/115	-
44	CLA	B	826	-	-	8/36/112/115	-
48	SF4	C	102	3	-	-	0/6/5/5
47	BCR	F	804	-	-	2/29/63/63	0/2/2/2
51	LUT	q	301	-	-	6/29/67/67	0/2/2/2
47	BCR	I	101	-	-	4/29/63/63	0/2/2/2
44	CLA	B	816	-	-	4/13/89/115	-
51	LUT	3	303	-	-	2/29/67/67	0/2/2/2
44	CLA	f	813	-	-	10/25/101/115	-
44	CLA	p	504	-	-	7/10/86/115	-
44	CLA	e	829	-	-	13/31/107/115	-
44	CLA	s	505	-	-	11/17/93/115	-
44	CLA	e	810	1,44	-	12/27/103/115	-
47	BCR	e	846	-	-	4/29/63/63	0/2/2/2
47	BCR	e	850	-	-	6/29/63/63	0/2/2/2
47	BCR	n	204	-	-	9/29/63/63	0/2/2/2
43	CL0	e	801	1	-	5/33/105/115	-
44	CLA	3	307	-	-	5/10/82/115	-
44	CLA	e	823	1	-	3/11/87/115	-
52	CHL	1	512	-	-	8/19/95/117	-
47	BCR	A	848	-	-	6/29/63/63	0/2/2/2
44	CLA	5	307	15	-	19/39/115/115	-
44	CLA	B	829	-	-	2/10/82/115	-
47	BCR	r	301	-	-	6/29/63/63	0/2/2/2
43	CL0	A	801	-	-	5/33/105/115	-
46	LHG	1	516	44	-	23/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	BCR	J	102	-	-	3/29/63/63	0/2/2/2
44	CLA	A	822	1	-	4/10/86/115	-
44	CLA	5	309	15	-	6/15/91/115	-
44	CLA	e	839	1	-	16/39/115/115	-
44	CLA	K	205	10	-	2/8/80/115	-
44	CLA	1	504	-	-	5/10/86/115	-
47	BCR	f	846	-	-	7/29/63/63	0/2/2/2
44	CLA	A	833	1	-	1/10/82/115	-
44	CLA	A	803	1	-	2/10/86/115	-
47	BCR	e	849	-	-	7/29/63/63	0/2/2/2
50	LMG	m	105	-	-	5/25/45/70	0/1/1/1
44	CLA	B	827	2	-	3/10/86/115	-
44	CLA	B	837	-	-	5/21/97/115	-
51	LUT	p	502	-	1/1/12/27	9/29/67/67	0/2/2/2
50	LMG	F	806	-	-	18/40/60/70	0/1/1/1
44	CLA	f	812	2	-	4/10/82/115	-
44	CLA	3	306	-	-	14/23/99/115	-
47	BCR	s	503	-	-	7/29/63/63	0/2/2/2
44	CLA	5	311	-	-	4/12/88/115	-
47	BCR	o	305	-	-	2/29/63/63	0/2/2/2
44	CLA	B	834	2	-	8/15/91/115	-
46	LHG	p	516	-	-	12/53/53/53	-
44	CLA	A	832	1	-	5/13/89/115	-
44	CLA	2	506	-	-	16/39/115/115	-
44	CLA	f	816	-	-	1/6/78/115	-
52	CHL	1	514	-	-	4/12/84/117	-
44	CLA	e	820	-	-	3/10/86/115	-
44	CLA	K	202	-	-	4/10/86/115	-
47	BCR	l	102	-	-	8/29/63/63	0/2/2/2
44	CLA	f	808	-	-	6/25/101/115	-
44	CLA	A	842	46	-	11/21/97/115	-
44	CLA	3	310	-	-	5/15/91/115	-
44	CLA	n	203	-	-	4/10/86/115	-
44	CLA	A	811	1	-	2/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	BCR	q	303	-	-	7/29/63/63	0/2/2/2
44	CLA	e	840	-	-	1/10/86/115	-
48	SF4	g	101	-	-	-	0/6/5/5
44	CLA	1	515	-	-	6/15/87/115	-
44	CLA	2	508	13	-	4/17/93/115	-
47	BCR	j	801	-	-	2/29/63/63	0/2/2/2
47	BCR	f	849	-	-	0/29/63/63	0/2/2/2
44	CLA	e	803	1,44	-	5/24/100/115	-
52	CHL	s	517	42	-	5/19/95/117	-
44	CLA	f	820	2	-	13/21/97/115	-
44	CLA	r	315	41	-	2/10/86/115	-
44	CLA	j	802	-	-	4/10/86/115	-
52	CHL	s	515	-	-	4/12/84/117	-
53	XAT	5	304	-	-	2/31/93/93	0/4/4/4
52	CHL	2	513	-	-	5/12/80/117	-
44	CLA	n	205	-	-	2/8/80/115	-
44	CLA	B	817	2	-	7/20/96/115	-
44	CLA	e	811	-	-	6/10/86/115	-
49	DGD	J	103	-	-	26/55/95/95	0/2/2/2
44	CLA	e	809	1	-	6/21/97/115	-
44	CLA	f	838	-	-	5/10/82/115	-
44	CLA	f	841	-	-	3/10/86/115	-
45	PQN	A	841	-	-	13/23/43/43	0/2/2/2
44	CLA	B	839	2	-	5/18/94/115	-
44	CLA	A	828	1	-	2/10/86/115	-
44	CLA	s	508	-	-	2/8/84/115	-
44	CLA	2	510	46	-	16/33/109/115	-
44	CLA	q	316	14	-	9/17/93/115	-
44	CLA	5	308	-	-	14/33/109/115	-
44	CLA	e	816	-	-	13/33/109/115	-
44	CLA	s	514	-	-	2/10/82/115	-
44	CLA	e	818	1	-	4/8/80/115	-
47	BCR	B	844	-	-	4/29/63/63	0/2/2/2
44	CLA	q	304	-	-	1/7/84/115	-
44	CLA	B	809	2	-	4/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	828	-	-	5/12/88/115	-
44	CLA	A	831	1	-	17/35/111/115	-
44	CLA	3	318	14	-	6/15/91/115	-
47	BCR	Q	801	-	-	10/27/61/63	0/2/2/2
44	CLA	3	317	-	-	4/10/86/115	-
44	CLA	f	821	-	-	8/27/103/115	-
44	CLA	e	808	1	-	6/10/86/115	-
52	CHL	3	302	13	-	5/19/95/117	-
44	CLA	3	312	-	-	7/10/86/115	-
44	CLA	r	309	-	-	7/21/97/115	-
44	CLA	f	803	-	-	3/12/88/115	-
44	CLA	A	810	44	-	5/26/102/115	-
47	BCR	3	305	-	-	8/29/63/63	0/2/2/2
44	CLA	r	310	-	-	5/12/88/115	-
44	CLA	e	814	1	-	7/12/88/115	-
44	CLA	e	827	-	-	1/10/86/115	-
44	CLA	A	817	1	-	2/4/82/115	-
44	CLA	B	835	2	-	6/33/109/115	-
44	CLA	B	812	2	-	6/25/101/115	-
52	CHL	2	516	13	-	8/13/89/117	-
44	CLA	1	508	12	-	3/10/82/115	-
44	CLA	p	515	-	-	3/10/82/115	-
49	DGD	f	851	-	-	9/41/81/95	0/2/2/2
44	CLA	A	802	-	-	12/31/107/115	-
44	CLA	r	317	41	-	8/21/97/115	-
44	CLA	e	837	-	-	11/27/103/115	-
44	CLA	p	509	-	-	8/21/97/115	-
48	SF4	C	101	3	-	-	0/6/5/5
47	BCR	m	103	-	-	2/29/63/63	0/2/2/2
47	BCR	f	847	-	-	6/29/63/63	0/2/2/2
44	CLA	B	806	2	-	4/10/79/115	-
44	CLA	f	829	-	-	9/21/97/115	-
44	CLA	2	505	-	-	13/24/100/115	-
49	DGD	m	104	-	-	14/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	B	822	-	-	4/18/94/115	-
44	CLA	r	306	-	-	16/39/115/115	-
44	CLA	p	507	12	-	4/8/84/115	-
44	CLA	q	305	-	-	9/24/100/115	-
48	SF4	g	102	-	-	-	0/6/5/5
47	BCR	K	204	-	-	8/29/63/63	0/2/2/2
52	CHL	r	313	-	-	5/19/95/117	-
44	CLA	r	312	-	-	5/10/86/115	-
44	CLA	5	310	-	-	10/21/97/115	-
44	CLA	r	308	-	-	4/10/86/115	-
44	CLA	5	313	15	-	4/10/82/115	-
44	CLA	B	825	-	-	3/12/88/115	-
44	CLA	f	825	2	-	3/12/88/115	-
53	XAT	2	502	-	-	6/31/93/93	0/4/4/4
44	CLA	o	302	-	-	2/8/84/115	-
51	LUT	s	501	-	-	4/29/67/67	0/2/2/2
47	BCR	5	302	-	-	9/29/63/63	0/2/2/2
44	CLA	A	805	1	-	18/38/114/115	-
44	CLA	B	830	2	-	11/29/105/115	-
44	CLA	p	506	-	-	12/27/103/115	-
44	CLA	e	852	-	-	11/30/106/115	-
44	CLA	f	805	-	-	0/4/78/115	-
44	CLA	A	835	-	-	12/23/99/115	-
44	CLA	L	302	-	-	3/10/82/115	-
44	CLA	f	839	2	-	4/10/86/115	-
50	LMG	5	301	-	-	8/27/47/70	0/1/1/1
44	CLA	e	853	1	-	8/15/91/115	-
44	CLA	A	834	1	-	6/10/86/115	-
44	CLA	q	309	-	-	5/21/97/115	-
45	PQN	B	843	-	-	7/20/40/43	0/2/2/2
44	CLA	B	814	2	-	5/10/86/115	-
44	CLA	e	819	-	-	7/15/91/115	-
44	CLA	A	840	-	-	4/10/86/115	-
52	CHL	5	314	-	-	7/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	f	833	2	-	3/13/89/115	-
44	CLA	e	822	-	-	3/10/86/115	-
44	CLA	A	807	1	-	3/7/79/115	-
51	LUT	3	304	-	-	2/29/67/67	0/2/2/2
52	CHL	p	514	-	-	7/19/95/117	-
44	CLA	o	303	-	-	12/33/109/115	-
52	CHL	2	515	-	-	6/15/91/117	-
44	CLA	f	843	46	-	0/4/80/115	-
44	CLA	1	505	-	-	4/12/88/115	-
44	CLA	A	829	1	-	6/27/103/115	-
44	CLA	e	817	1	-	0/4/82/115	-
48	SF4	f	802	-	-	-	0/6/5/5
44	CLA	e	812	-	-	3/7/79/115	-
44	CLA	q	306	-	-	4/10/86/115	-
47	BCR	L	306	-	-	6/29/63/63	0/2/2/2
44	CLA	e	843	-	-	9/19/95/115	-
44	CLA	e	805	-	-	5/17/93/115	-
51	LUT	2	501	-	-	0/29/67/67	0/2/2/2
44	CLA	f	836	-	-	13/31/103/115	-
53	XAT	s	502	-	-	6/31/93/93	0/4/4/4
44	CLA	B	840	-	-	3/10/86/115	-
44	CLA	e	804	-	-	16/39/115/115	-
47	BCR	e	854	-	-	4/29/63/63	0/2/2/2
47	BCR	e	851	-	-	4/29/63/63	0/2/2/2
47	BCR	L	305	-	-	9/29/63/63	0/2/2/2
44	CLA	A	823	1	-	15/27/99/115	-
47	BCR	B	847	-	-	5/29/63/63	0/2/2/2
48	SF4	8	201	38	-	-	0/6/5/5
44	CLA	e	834	1	-	5/15/91/115	-
44	CLA	B	804	-	-	14/39/115/115	-
44	CLA	B	831	2	-	1/13/89/115	-
44	CLA	f	831	2	-	5/29/105/115	-
44	CLA	m	101	-	-	6/10/86/115	-
44	CLA	2	509	-	-	10/21/97/115	-
46	LHG	e	845	-	-	10/28/28/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	r	304	-	-	3/8/80/115	-
44	CLA	A	809	1	-	3/6/84/115	-
47	BCR	p	503	-	-	1/1/19/63	0/1/1/2
44	CLA	3	309	-	-	4/10/86/115	-
50	LMG	2	519	-	-	14/31/51/70	0/1/1/1
47	BCR	A	849	-	-	2/27/61/63	0/2/2/2
47	BCR	e	848	-	-	6/29/63/63	0/2/2/2
44	CLA	e	813	1	-	4/12/88/115	-
46	LHG	e	844	-	-	8/44/44/53	-
52	CHL	2	512	-	-	3/17/93/117	-
44	CLA	A	837	1	-	4/10/86/115	-
44	CLA	e	836	-	-	6/23/99/115	-
51	LUT	5	303	-	-	2/29/67/67	0/2/2/2
44	CLA	1	511	-	-	7/17/93/115	-
44	CLA	f	811	2	-	8/23/99/115	-
44	CLA	B	841	2	-	10/26/102/115	-
44	CLA	f	837	-	-	5/12/88/115	-
44	CLA	B	813	2	-	3/13/89/115	-
44	CLA	3	301	1	-	4/10/86/115	-
44	CLA	A	824	-	-	5/10/82/115	-
44	CLA	3	308	14	-	14/27/103/115	-
44	CLA	f	824	-	-	6/12/88/115	-
44	CLA	q	315	-	-	8/15/91/115	-
53	XAT	r	303	-	-	2/31/93/93	0/4/4/4
44	CLA	r	307	-	-	12/33/109/115	-
44	CLA	p	511	-	-	4/10/79/115	-
54	SQD	Q	803	-	-	9/41/61/69	0/1/1/1
44	CLA	e	807	-	-	4/12/88/115	-
52	CHL	5	317	-	-	4/10/82/117	-
44	CLA	e	826	1	-	18/37/113/115	-
44	CLA	s	510	-	-	11/33/109/115	-
44	CLA	A	827	1	-	17/39/115/115	-
47	BCR	B	852	-	-	6/29/63/63	0/2/2/2
44	CLA	L	301	1	-	5/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	3	314	14	-	15/33/109/115	-
52	CHL	1	517	12	-	5/12/84/117	-
47	BCR	A	845	-	-	6/29/63/63	0/2/2/2
44	CLA	n	201	-	-	2/4/76/115	-
52	CHL	5	315	-	-	4/17/93/117	-
47	BCR	f	850	-	-	2/27/61/63	0/2/2/2
44	CLA	e	821	-	-	5/12/88/115	-
47	BCR	F	801	-	-	6/29/63/63	0/2/2/2
44	CLA	e	824	-	-	9/29/105/115	-
45	PQN	e	842	-	-	-	0/2/2/2
44	CLA	1	506	-	-	9/27/103/115	-
44	CLA	B	828	-	-	3/10/86/115	-
44	CLA	f	828	2	-	6/10/86/115	-
44	CLA	o	304	-	-	6/15/91/115	-
44	CLA	s	504	-	-	3/8/84/115	-
44	CLA	e	806	-	-	1/10/86/115	-
44	CLA	L	303	11	-	12/24/100/115	-

The worst 5 of 3157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	p	502	LUT	C24-C25	14.61	1.51	1.33
43	A	801	CL0	MG-NA	7.46	2.24	2.06
43	e	801	CL0	MG-NA	7.46	2.24	2.06
45	f	844	PQN	C3-C2	7.19	1.48	1.35
45	A	841	PQN	C3-C2	6.73	1.47	1.35

The worst 5 of 3725 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	503	BCR	C40-C30-C25	-12.70	89.71	110.30
47	s	503	BCR	C40-C30-C25	-12.39	90.20	110.30
43	A	801	CL0	C4A-NA-C1A	10.86	111.59	106.71
43	e	801	CL0	C4A-NA-C1A	10.83	111.58	106.71
47	Q	801	BCR	C11-C10-C9	-10.58	112.21	127.31

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
44	2	507	CLA	C8
51	p	502	LUT	C26

5 of 2528 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	801	CL0	C1A-C2A-CAA-CBA
43	A	801	CL0	CHA-CBD-CGD-O2D
43	e	801	CL0	C1A-C2A-CAA-CBA
43	e	801	CL0	CHA-CBD-CGD-O2D
44	A	802	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

318 monomers are involved in 743 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	5	316	CLA	3	0
44	3	316	CLA	2	0
44	e	825	CLA	2	0
44	p	513	CLA	1	0
44	s	509	CLA	2	0
52	s	512	CHL	3	0
44	B	820	CLA	4	0
44	1	513	CLA	6	0
44	f	810	CLA	3	0
44	f	826	CLA	3	0
44	e	838	CLA	6	0
44	A	815	CLA	1	0
51	r	302	LUT	10	0
47	e	847	BCR	2	0
45	f	844	PQN	6	0
44	2	507	CLA	2	0
44	B	838	CLA	5	0
47	A	846	BCR	3	0
47	o	301	BCR	1	0
44	B	832	CLA	1	0
44	e	833	CLA	2	0
44	f	809	CLA	1	0
44	f	832	CLA	2	0
44	B	802	CLA	6	0
44	B	807	CLA	3	0
52	r	316	CHL	1	0
44	q	307	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	1	503	BCR	3	0
44	B	842	CLA	2	0
44	f	842	CLA	1	0
44	f	834	CLA	2	0
52	p	517	CHL	2	0
44	e	830	CLA	2	0
47	A	853	BCR	4	0
44	2	504	CLA	2	0
49	B	850	DGD	4	0
44	B	815	CLA	4	0
50	F	805	LMG	1	0
51	1	501	LUT	4	0
44	B	801	CLA	1	0
44	B	818	CLA	4	0
44	B	808	CLA	2	0
44	B	811	CLA	5	0
51	p	501	LUT	5	0
52	s	513	CHL	2	0
44	J	101	CLA	2	0
44	q	311	CLA	1	0
44	A	804	CLA	1	0
47	B	848	BCR	3	0
44	n	202	CLA	1	0
47	j	803	BCR	1	0
44	e	815	CLA	1	0
51	q	302	LUT	6	0
44	A	820	CLA	4	0
44	3	311	CLA	5	0
44	A	852	CLA	2	0
44	f	835	CLA	4	0
44	B	803	CLA	1	0
51	1	502	LUT	7	0
44	A	816	CLA	2	0
44	f	807	CLA	4	0
52	q	313	CHL	1	0
44	q	312	CLA	2	0
44	A	808	CLA	2	0
47	A	847	BCR	1	0
44	3	313	CLA	4	0
46	f	852	LHG	1	0
44	A	826	CLA	1	0
44	1	510	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	2	518	LMG	1	0
44	B	821	CLA	1	0
44	2	514	CLA	3	0
44	A	813	CLA	2	0
46	A	843	LHG	4	0
47	f	845	BCR	1	0
44	f	806	CLA	1	0
52	p	512	CHL	1	0
44	A	836	CLA	3	0
44	f	818	CLA	4	0
44	r	305	CLA	2	0
44	f	815	CLA	1	0
46	A	844	LHG	3	0
44	p	505	CLA	1	0
44	B	823	CLA	1	0
44	f	823	CLA	1	0
44	B	805	CLA	1	0
54	Q	802	SQD	1	0
44	s	506	CLA	6	0
47	A	851	BCR	4	0
44	K	201	CLA	3	0
44	A	821	CLA	2	0
52	3	315	CHL	1	0
44	f	819	CLA	5	0
44	1	507	CLA	3	0
44	f	804	CLA	7	0
47	B	849	BCR	2	0
44	A	806	CLA	5	0
44	L	304	CLA	2	0
46	O	601	LHG	1	0
44	1	509	CLA	4	0
44	q	314	CLA	5	0
44	f	827	CLA	1	0
44	s	511	CLA	6	0
47	B	846	BCR	1	0
46	s	516	LHG	1	0
44	B	833	CLA	2	0
44	f	840	CLA	3	0
44	A	825	CLA	1	0
44	f	801	CLA	4	0
47	2	503	BCR	4	0
44	A	838	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	B	824	CLA	3	0
47	B	845	BCR	1	0
44	F	802	CLA	3	0
46	2	517	LHG	2	0
44	p	510	CLA	2	0
44	q	310	CLA	1	0
47	f	848	BCR	4	0
47	l	101	BCR	1	0
44	5	305	CLA	2	0
44	B	810	CLA	1	0
44	B	826	CLA	2	0
48	C	102	SF4	1	0
47	F	804	BCR	3	0
51	q	301	LUT	5	0
47	I	101	BCR	4	0
44	B	816	CLA	1	0
51	3	303	LUT	7	0
44	f	813	CLA	2	0
44	p	504	CLA	5	0
44	e	829	CLA	1	0
44	s	505	CLA	1	0
44	e	810	CLA	5	0
47	e	846	BCR	5	0
47	e	850	BCR	2	0
47	n	204	BCR	1	0
43	e	801	CL0	5	0
44	3	307	CLA	1	0
47	A	848	BCR	2	0
44	5	307	CLA	4	0
47	r	301	BCR	5	0
43	A	801	CL0	2	0
46	1	516	LHG	5	0
47	J	102	BCR	1	0
44	5	309	CLA	1	0
44	e	839	CLA	4	0
44	K	205	CLA	1	0
44	1	504	CLA	3	0
44	A	803	CLA	3	0
47	e	849	BCR	4	0
50	m	105	LMG	1	0
44	B	837	CLA	1	0
51	p	502	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	F	806	LMG	2	0
44	3	306	CLA	3	0
47	s	503	BCR	4	0
47	o	305	BCR	3	0
46	p	516	LHG	7	0
44	2	506	CLA	5	0
44	f	816	CLA	2	0
44	K	202	CLA	2	0
47	l	102	BCR	4	0
44	f	808	CLA	3	0
44	n	203	CLA	1	0
47	q	303	BCR	3	0
48	g	101	SF4	1	0
44	1	515	CLA	3	0
44	2	508	CLA	3	0
47	j	801	BCR	1	0
47	f	849	BCR	4	0
44	e	803	CLA	3	0
52	s	517	CHL	1	0
44	f	820	CLA	2	0
44	j	802	CLA	1	0
52	s	515	CHL	1	0
53	5	304	XAT	5	0
52	2	513	CHL	4	0
44	n	205	CLA	1	0
44	B	817	CLA	1	0
44	e	811	CLA	1	0
49	J	103	DGD	3	0
44	e	809	CLA	5	0
44	f	838	CLA	2	0
45	A	841	PQN	2	0
44	A	828	CLA	1	0
44	2	510	CLA	4	0
44	q	316	CLA	1	0
44	5	308	CLA	5	0
44	e	816	CLA	1	0
44	s	514	CLA	2	0
44	e	818	CLA	3	0
47	B	844	BCR	9	0
44	q	304	CLA	3	0
44	e	828	CLA	2	0
44	A	831	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	Q	801	BCR	6	0
44	f	821	CLA	5	0
44	e	808	CLA	1	0
44	r	309	CLA	1	0
44	f	803	CLA	2	0
44	A	810	CLA	2	0
47	3	305	BCR	4	0
44	r	310	CLA	1	0
44	e	814	CLA	1	0
44	e	827	CLA	2	0
44	A	817	CLA	3	0
44	B	835	CLA	1	0
44	B	812	CLA	1	0
52	2	516	CHL	3	0
44	p	515	CLA	3	0
49	f	851	DGD	2	0
44	A	802	CLA	2	0
44	r	317	CLA	1	0
44	e	837	CLA	3	0
44	p	509	CLA	3	0
47	m	103	BCR	3	0
47	f	847	BCR	1	0
44	B	806	CLA	4	0
44	f	829	CLA	1	0
44	2	505	CLA	3	0
49	m	104	DGD	2	0
44	B	822	CLA	3	0
44	r	306	CLA	7	0
44	p	507	CLA	1	0
44	q	305	CLA	1	0
47	K	204	BCR	2	0
52	r	313	CHL	1	0
44	r	312	CLA	2	0
44	5	310	CLA	2	0
44	r	308	CLA	2	0
44	B	825	CLA	2	0
53	2	502	XAT	7	0
44	o	302	CLA	2	0
51	s	501	LUT	5	0
47	5	302	BCR	5	0
44	A	805	CLA	4	0
44	B	830	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	p	506	CLA	5	0
44	e	852	CLA	4	0
44	f	805	CLA	2	0
44	A	835	CLA	2	0
44	L	302	CLA	1	0
44	f	839	CLA	3	0
50	5	301	LMG	1	0
44	e	853	CLA	2	0
45	B	843	PQN	1	0
44	e	819	CLA	1	0
44	A	840	CLA	1	0
52	5	314	CHL	2	0
44	f	833	CLA	1	0
51	3	304	LUT	5	0
52	p	514	CHL	4	0
44	o	303	CLA	1	0
52	2	515	CHL	2	0
44	f	843	CLA	1	0
44	A	829	CLA	1	0
44	e	817	CLA	2	0
44	e	812	CLA	5	0
47	L	306	BCR	2	0
44	e	843	CLA	2	0
44	e	805	CLA	1	0
51	2	501	LUT	8	0
53	s	502	XAT	8	0
44	e	804	CLA	3	0
47	e	854	BCR	4	0
47	e	851	BCR	5	0
47	L	305	BCR	8	0
47	B	847	BCR	2	0
48	8	201	SF4	1	0
44	e	834	CLA	1	0
44	B	804	CLA	4	0
44	B	831	CLA	1	0
44	f	831	CLA	2	0
44	2	509	CLA	1	0
46	e	845	LHG	1	0
44	r	304	CLA	2	0
47	p	503	BCR	1	0
44	3	309	CLA	2	0
50	2	519	LMG	2	0

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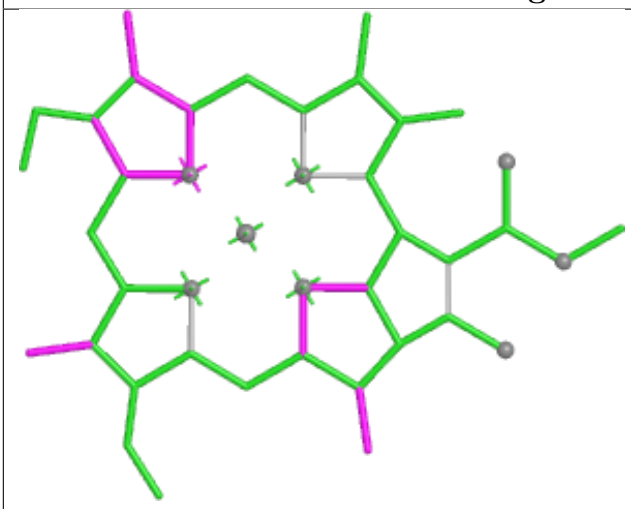
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	A	849	BCR	1	0
47	e	848	BCR	2	0
44	e	813	CLA	2	0
46	e	844	LHG	1	0
52	2	512	CHL	4	0
44	e	836	CLA	2	0
51	5	303	LUT	8	0
44	1	511	CLA	2	0
44	B	841	CLA	1	0
44	B	813	CLA	1	0
44	3	301	CLA	2	0
44	A	824	CLA	1	0
44	3	308	CLA	6	0
44	q	315	CLA	4	0
53	r	303	XAT	4	0
44	r	307	CLA	4	0
54	Q	803	SQD	5	0
44	e	807	CLA	1	0
52	5	317	CHL	3	0
44	e	826	CLA	3	0
44	s	510	CLA	4	0
44	A	827	CLA	4	0
47	B	852	BCR	1	0
44	L	301	CLA	2	0
44	3	314	CLA	2	0
52	1	517	CHL	5	0
47	A	845	BCR	4	0
52	5	315	CHL	4	0
47	f	850	BCR	4	0
44	e	821	CLA	2	0
47	F	801	BCR	1	0
44	e	824	CLA	1	0
45	e	842	PQN	1	0
44	1	506	CLA	8	0
44	B	828	CLA	4	0
44	f	828	CLA	1	0
44	o	304	CLA	3	0
44	s	504	CLA	1	0
44	L	303	CLA	2	0

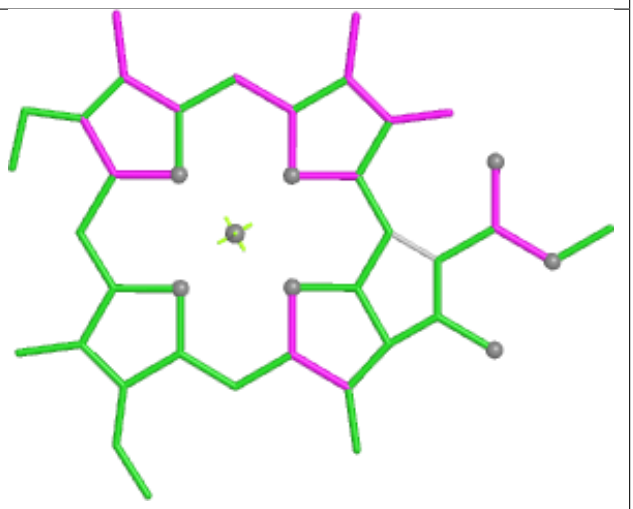
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

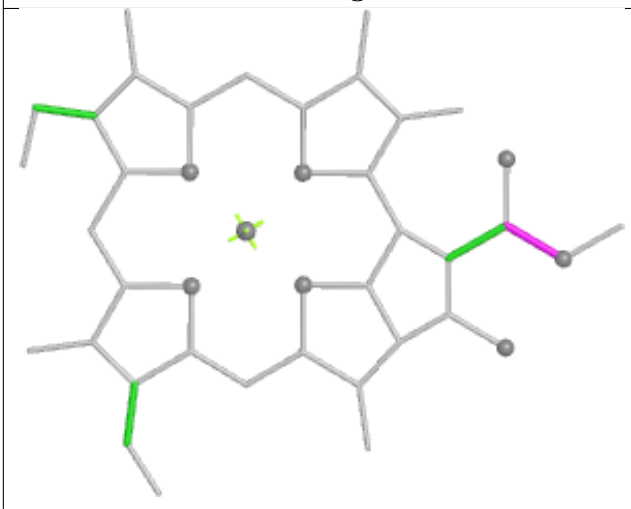
Ligand CLA 5 316



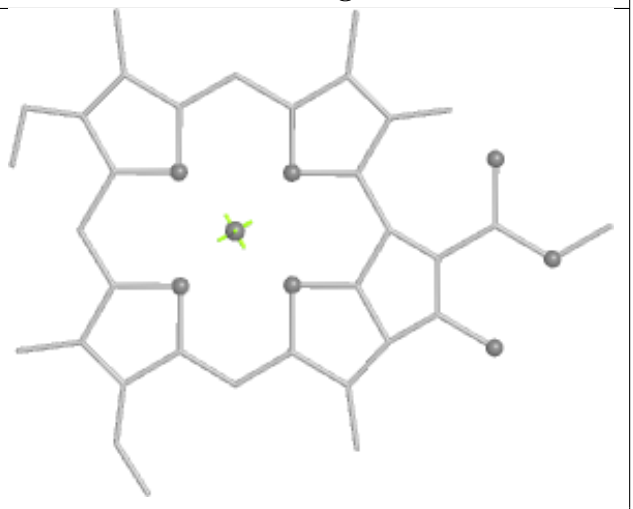
Bond lengths



Bond angles

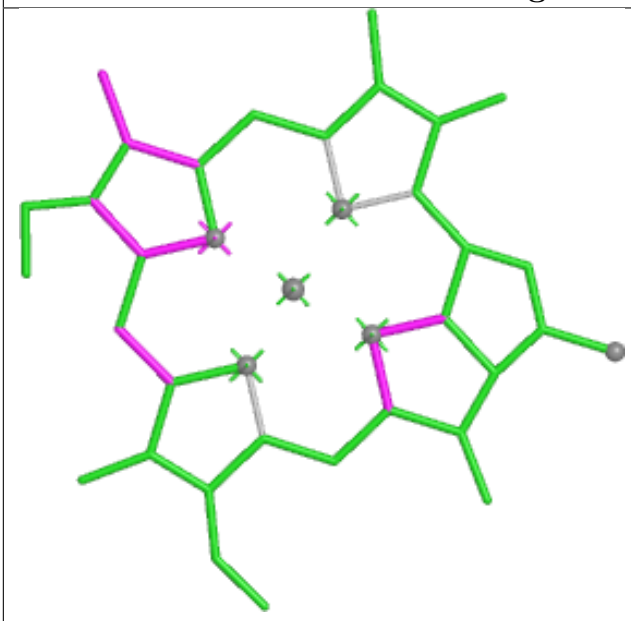


Torsions

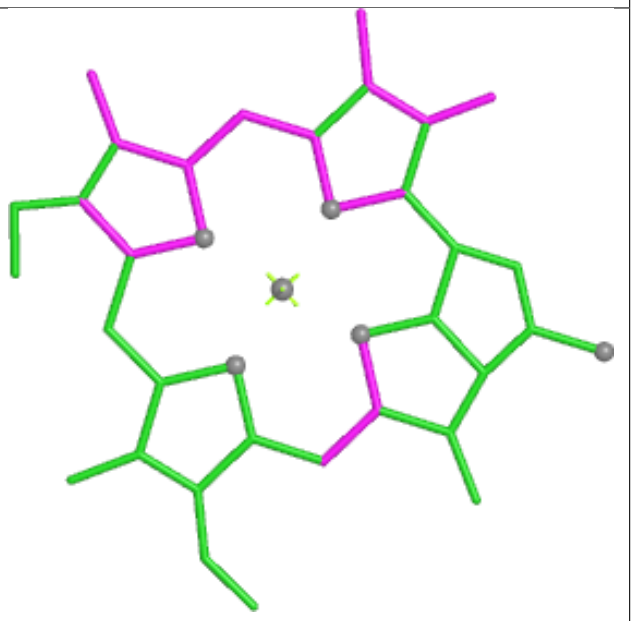


Rings

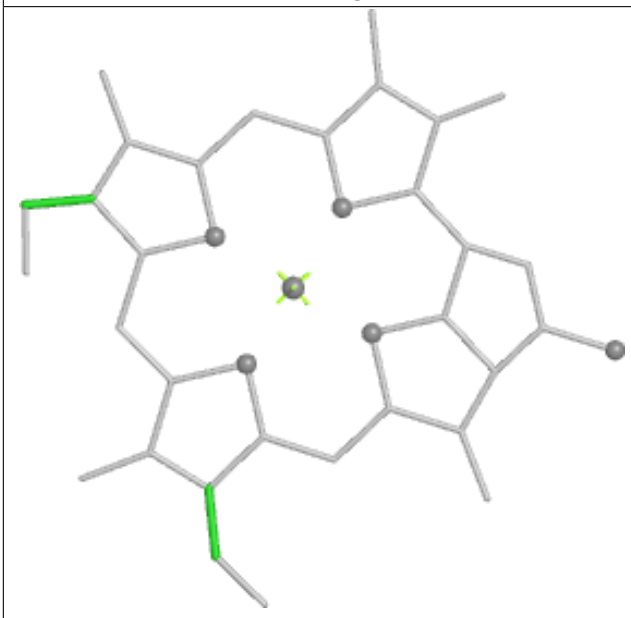
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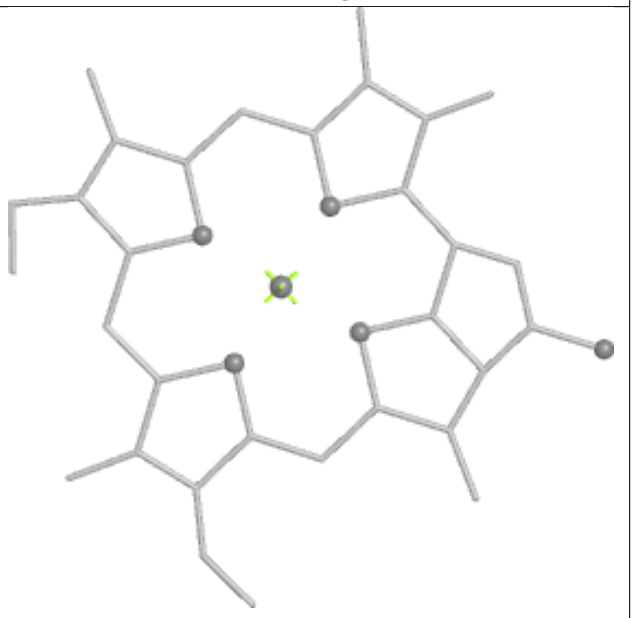
Bond lengths



Bond angles

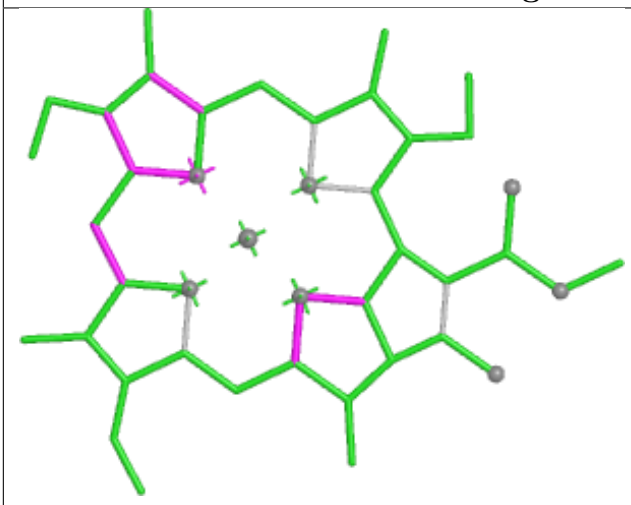


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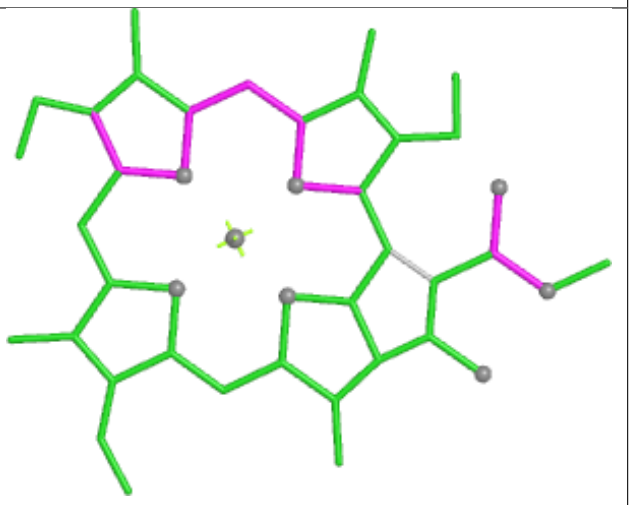


Rings

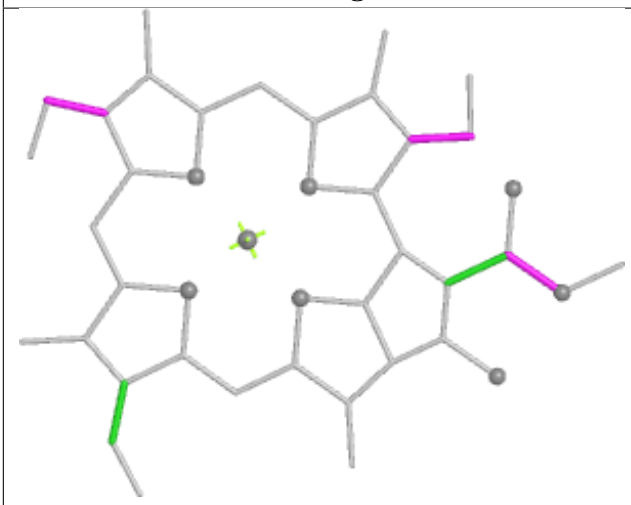
Ligand CLA m 102



Bond lengths



Bond angles

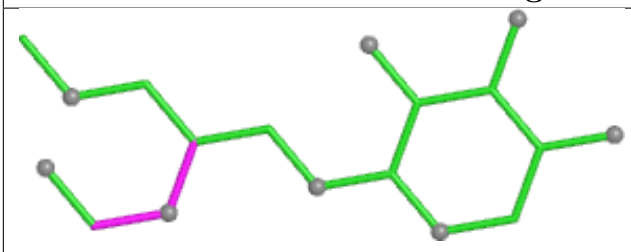


Torsions

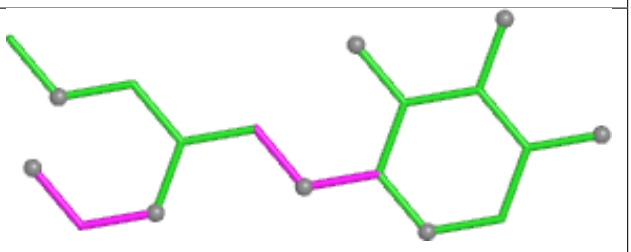


Rings

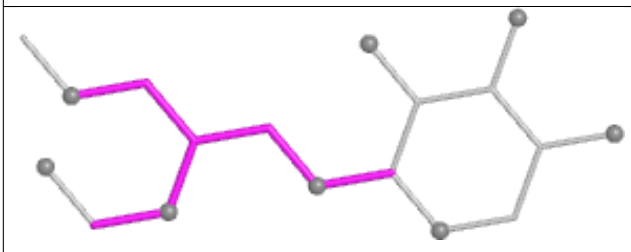
Ligand LMG r 318



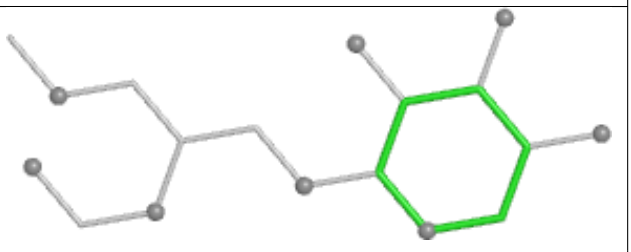
Bond lengths



Bond angles

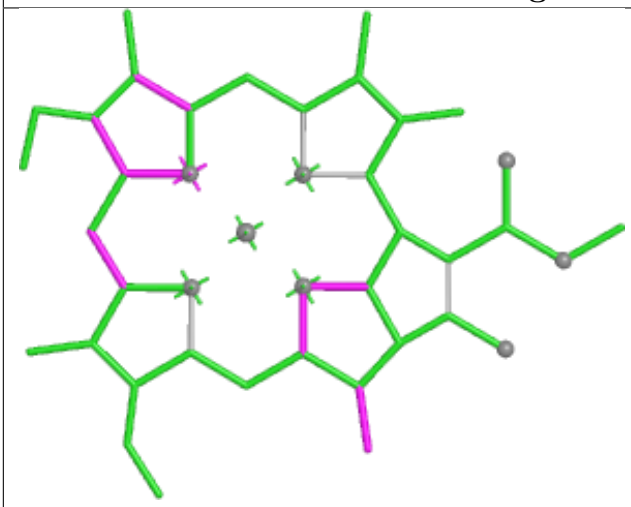


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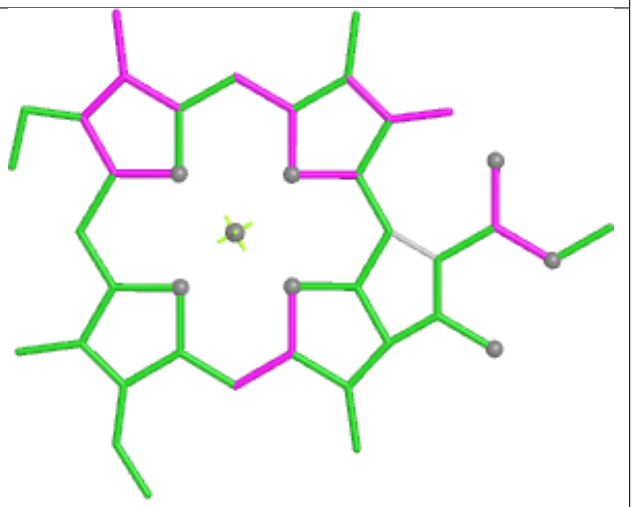


Rings

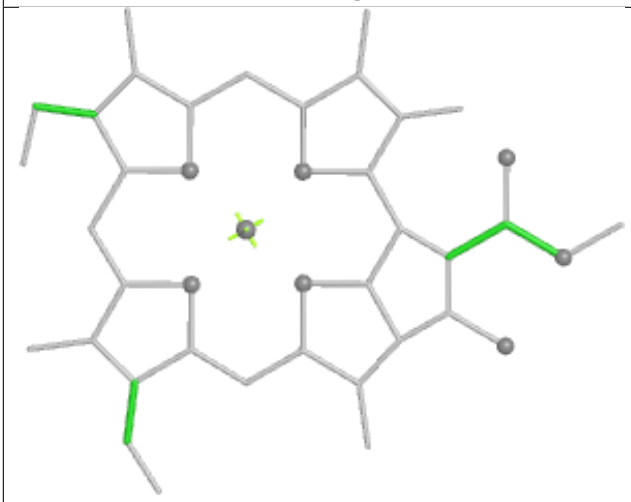
Ligand CLA e 825



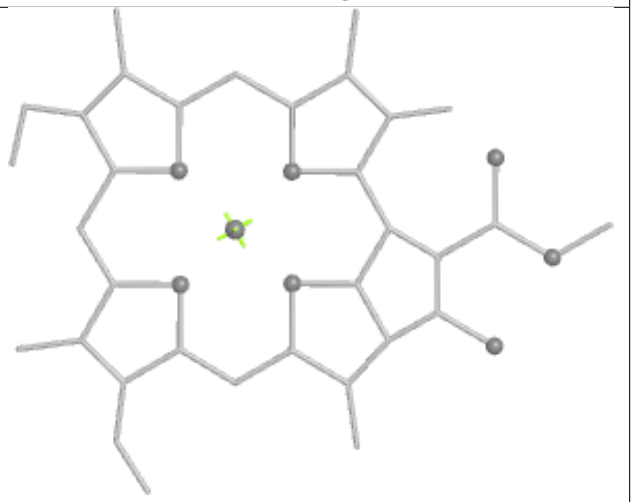
Bond lengths



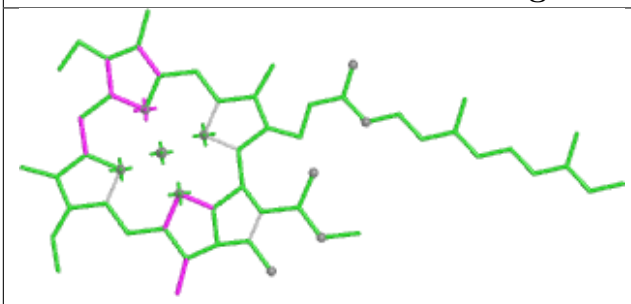
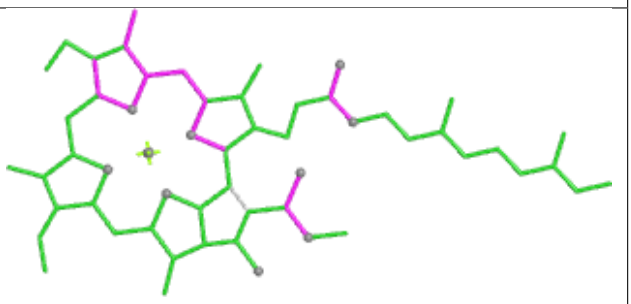
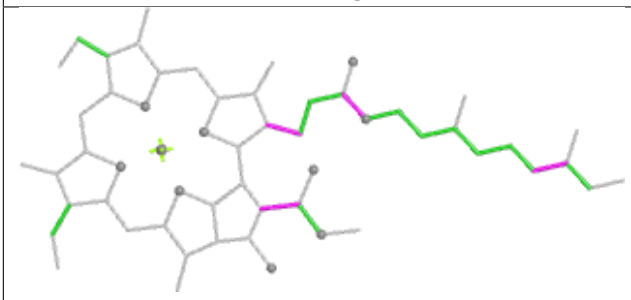
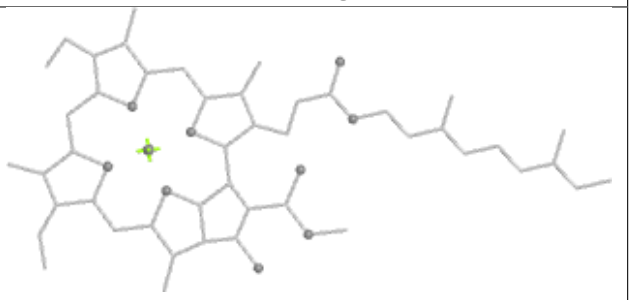
Bond angles

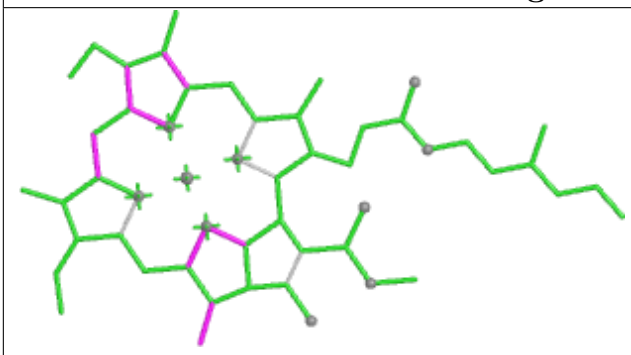
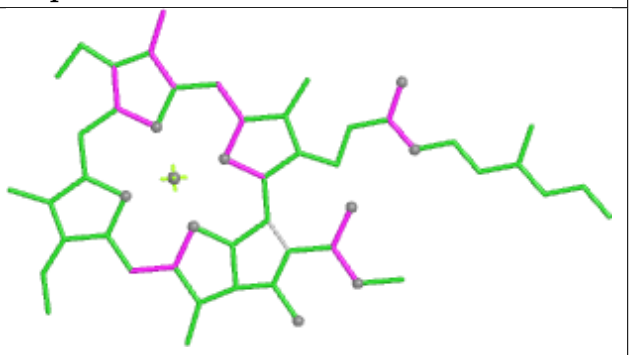
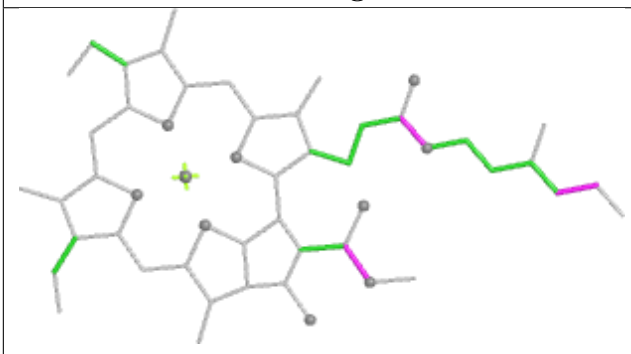
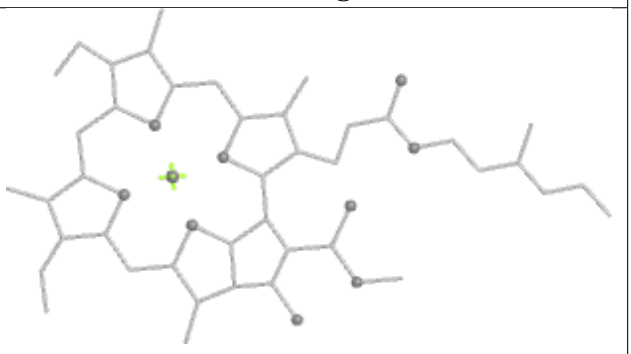


Torsions

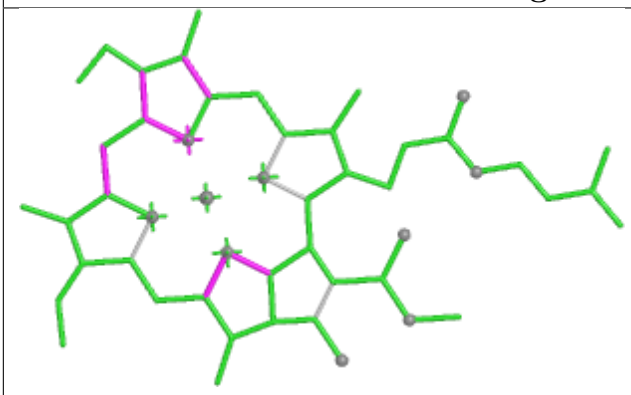


Rings

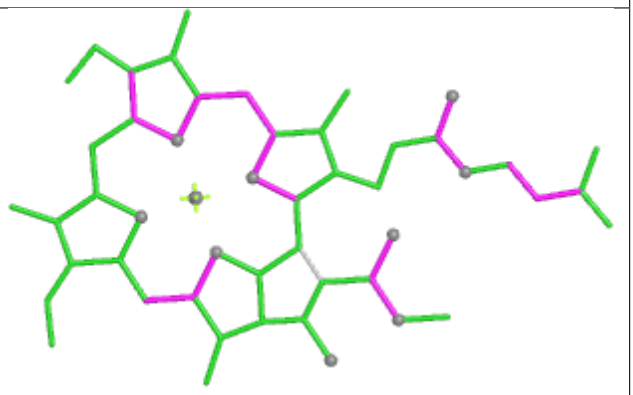
Ligand CLA e 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

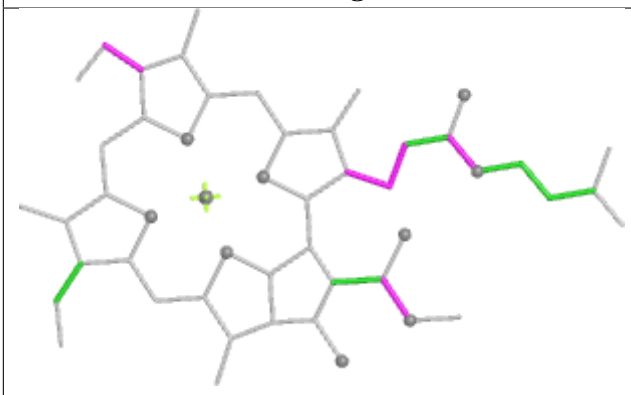
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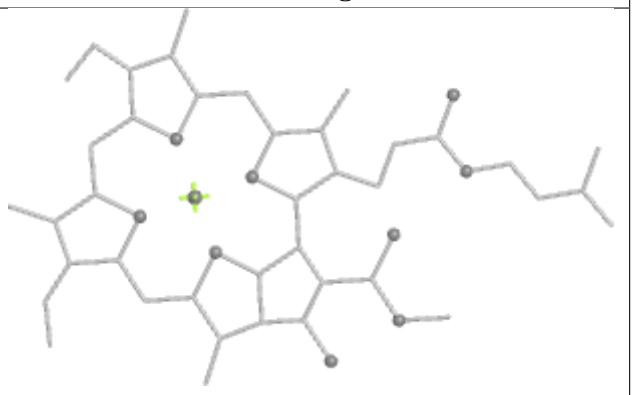
Bond lengths



Bond angles

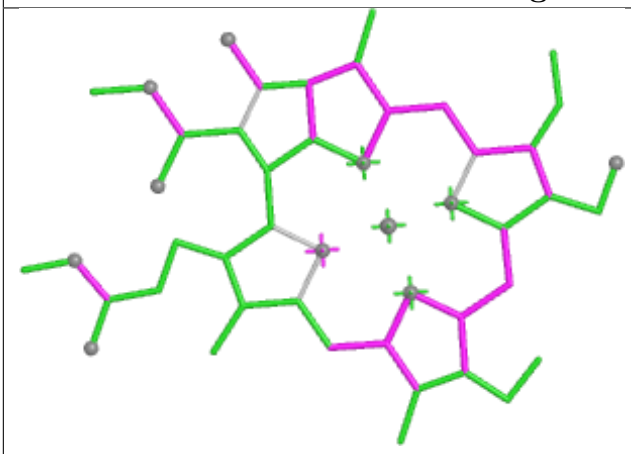


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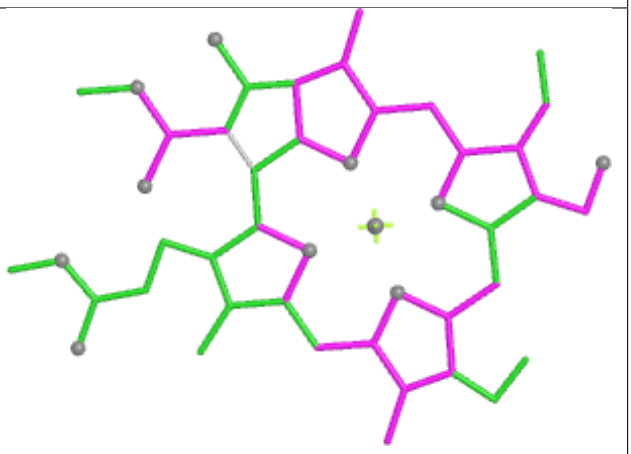


Rings

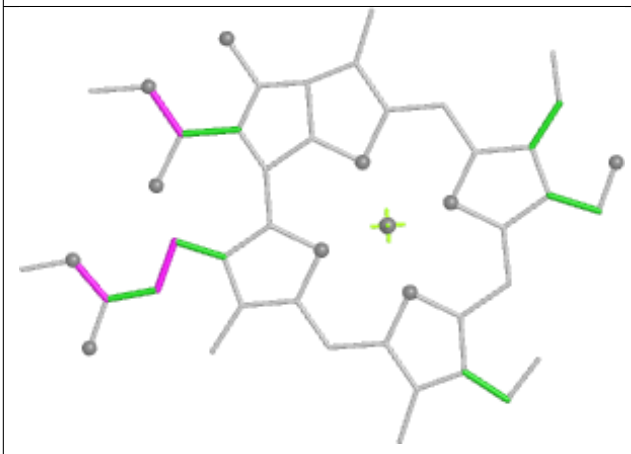
Ligand CHL s 512



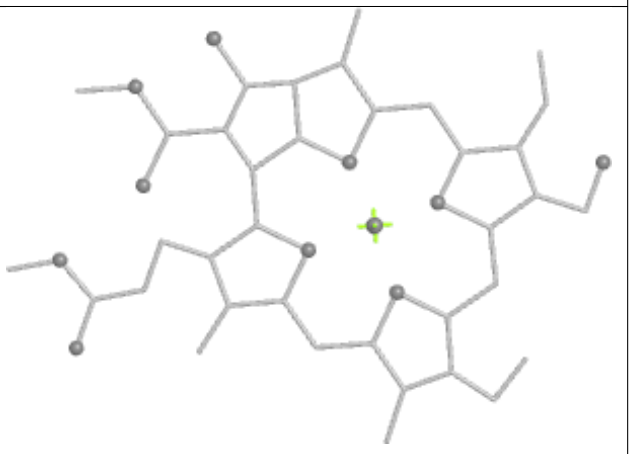
Bond lengths



Bond angles

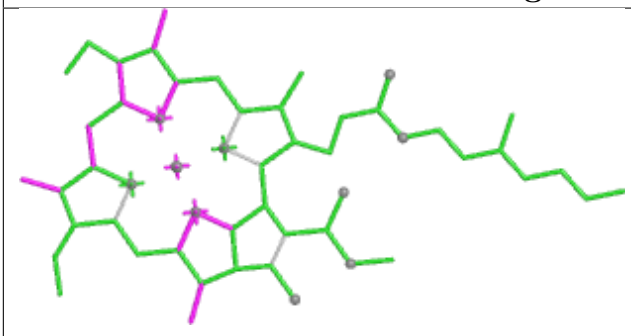


Torsions

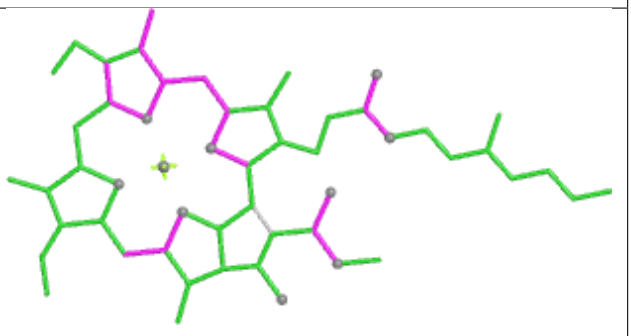


Rings

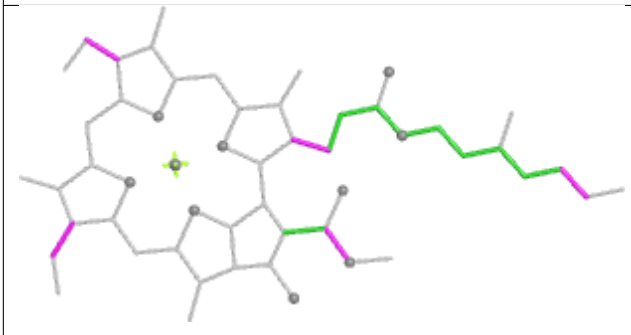
Ligand CLA B 820



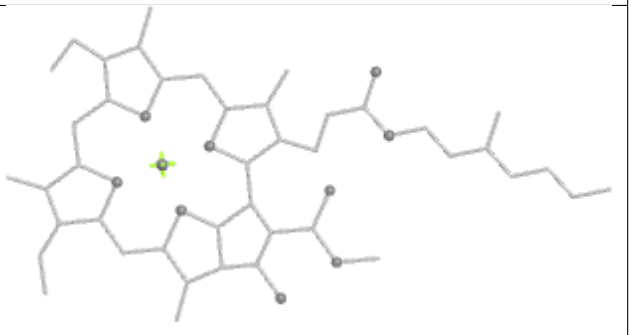
Bond lengths



Bond angles

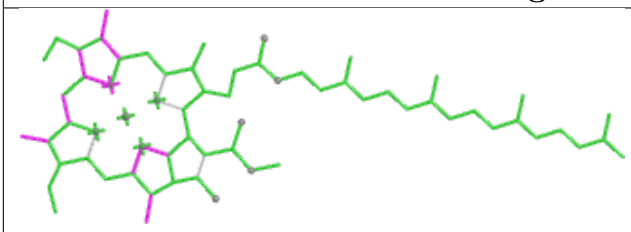


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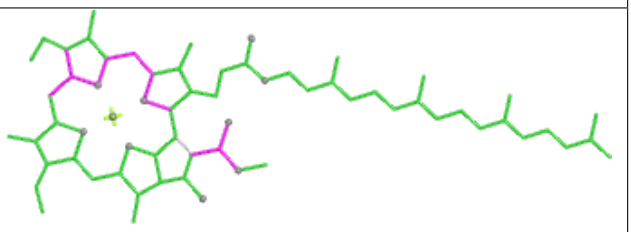


Rings

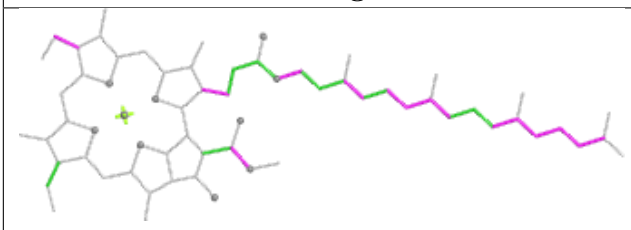
Ligand CLA 1 513



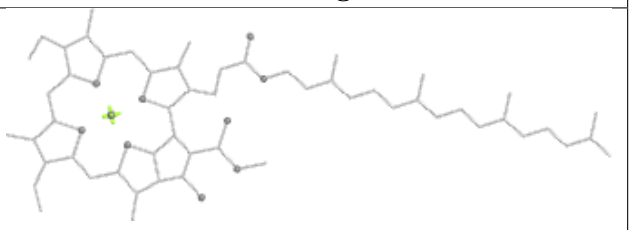
Bond lengths



Bond angles

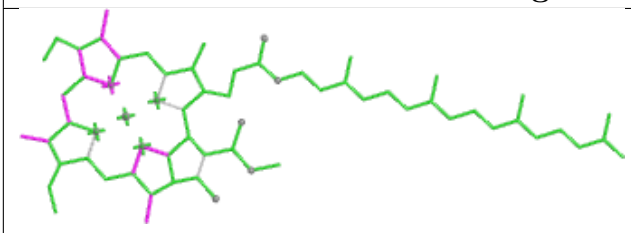


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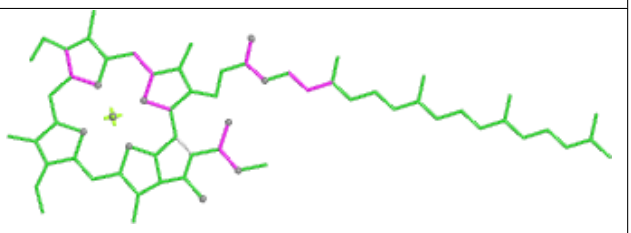


Rings

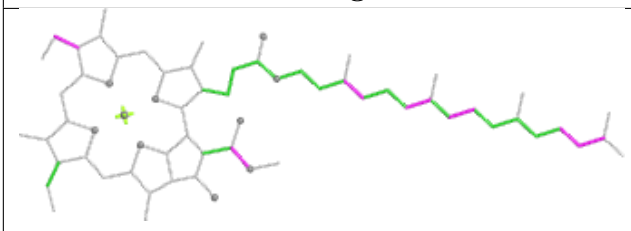
Ligand CLA f 810



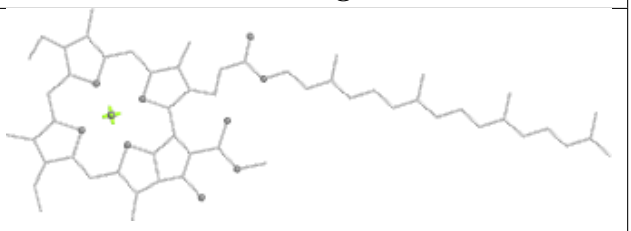
Bond lengths



Bond angles

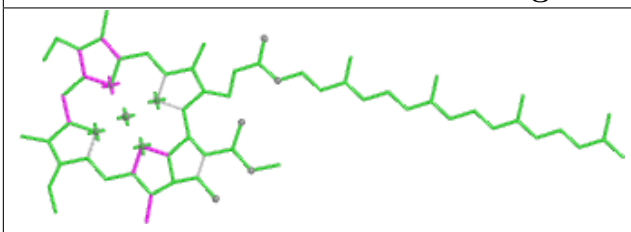


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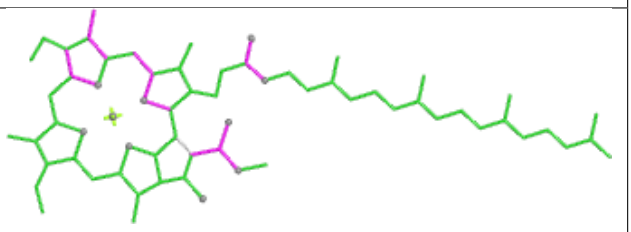


Rings

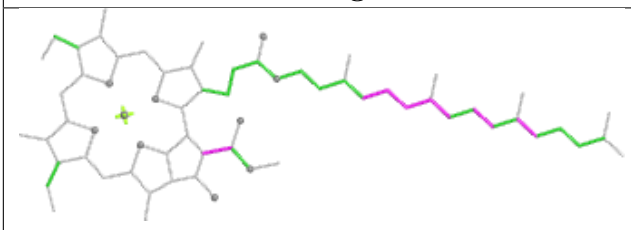
Ligand CLA f 826



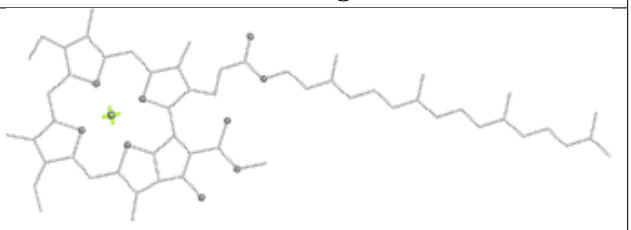
Bond lengths



Bond angles

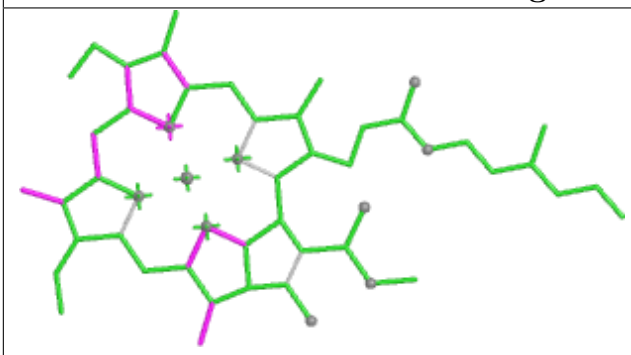


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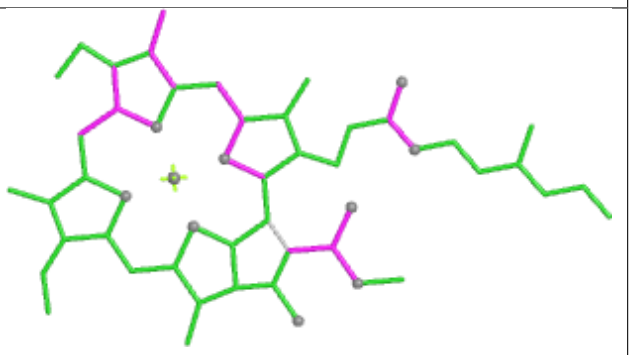


Rings

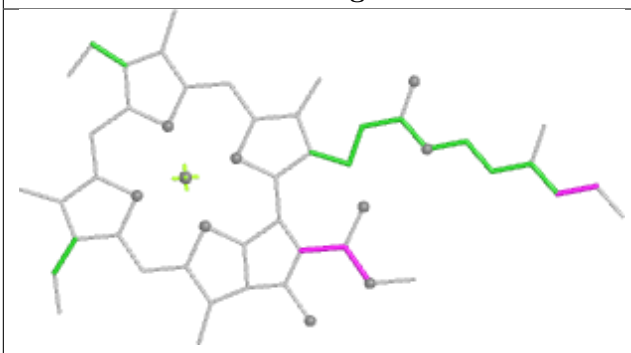
Ligand CLA e 838



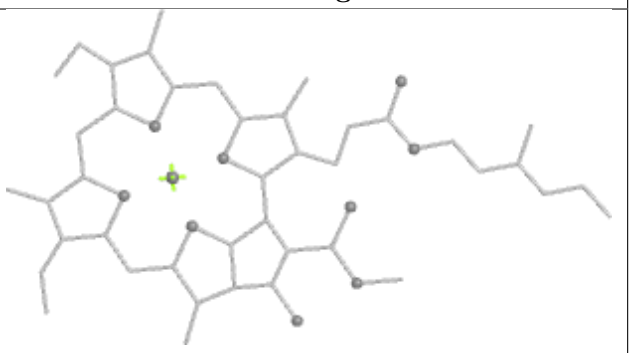
Bond lengths



Bond angles

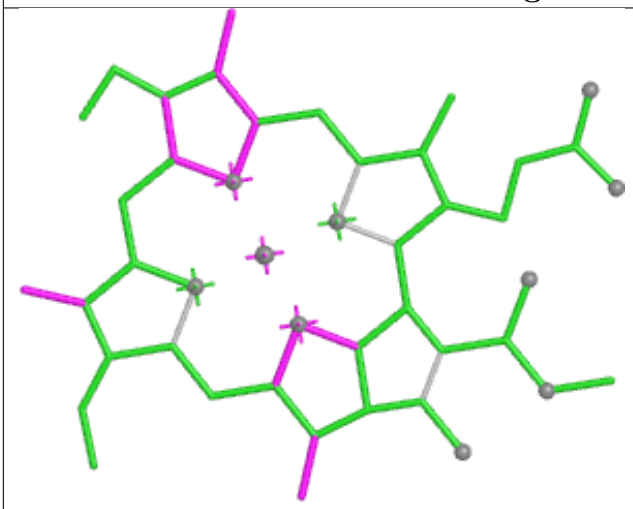


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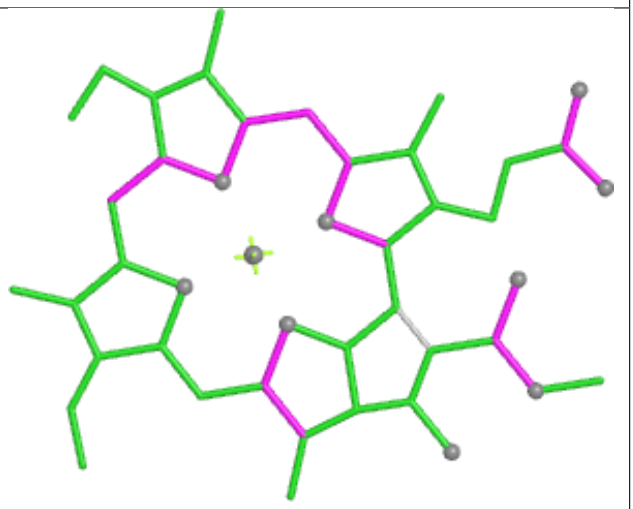


Rings

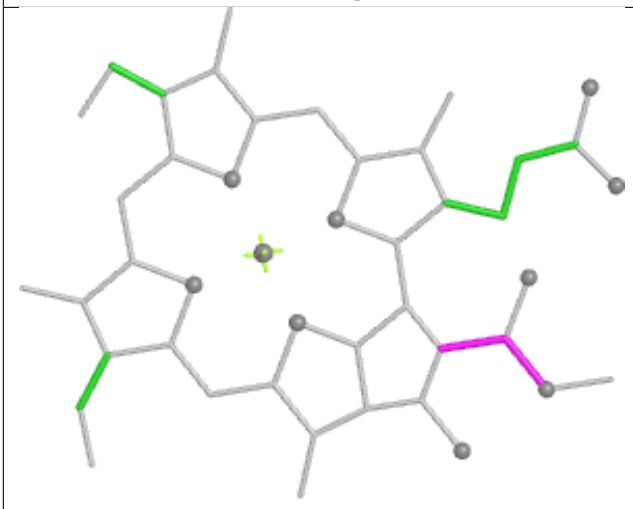
Ligand CLA A 815



Bond lengths



Bond angles

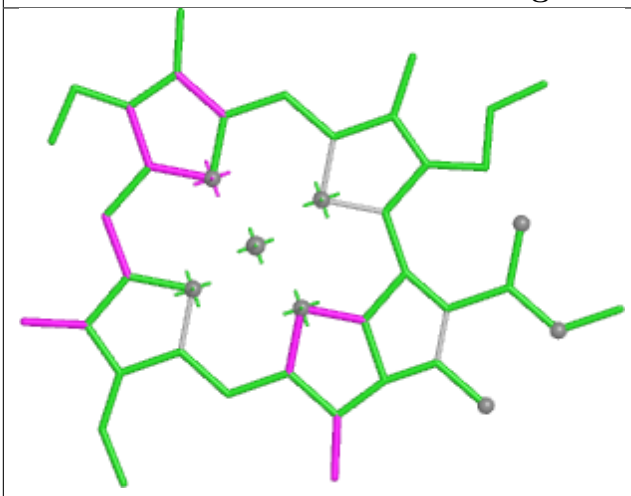


Torsions

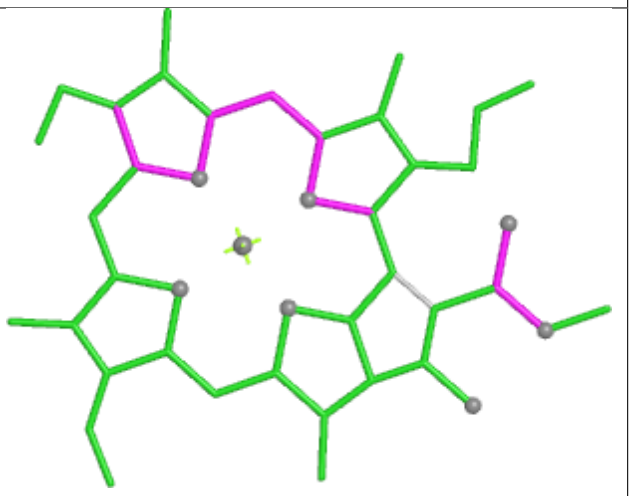


Rings

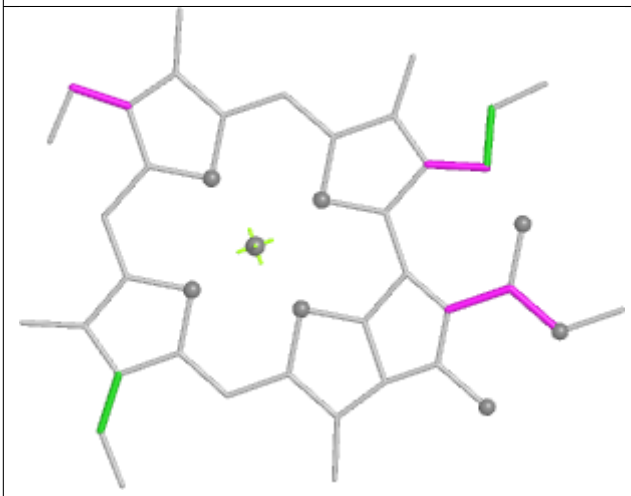
Ligand CLA f 817



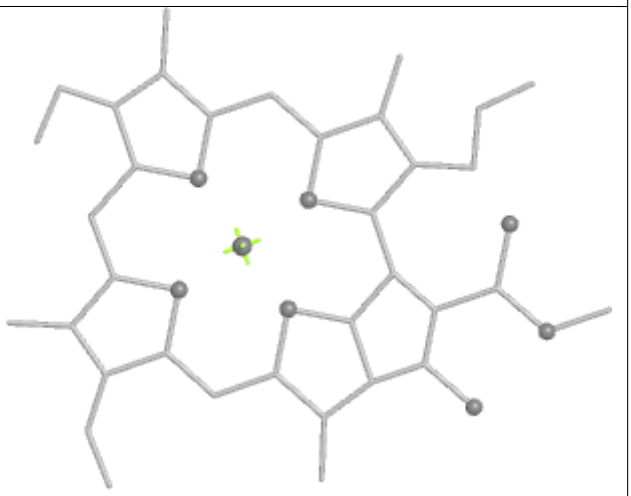
Bond lengths



Bond angles

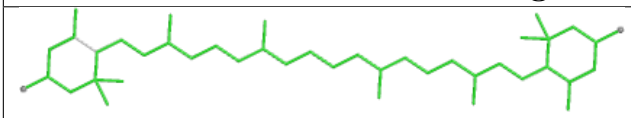


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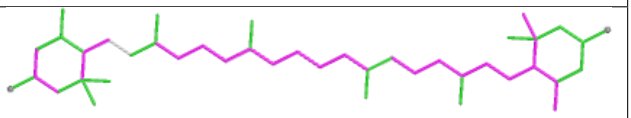


Rings

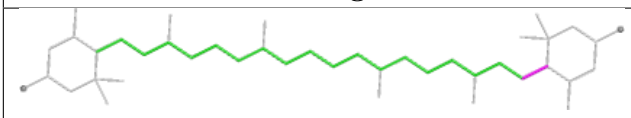
Ligand LUT r 302



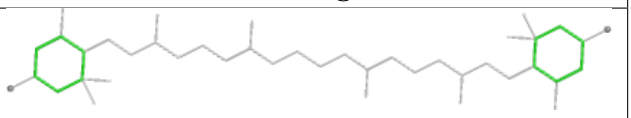
Bond lengths



Bond angles

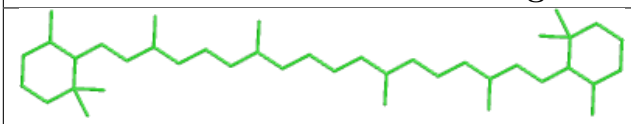


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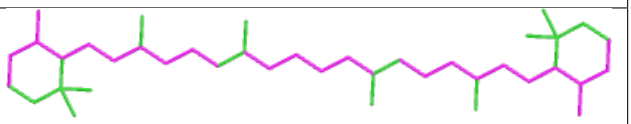


Rings

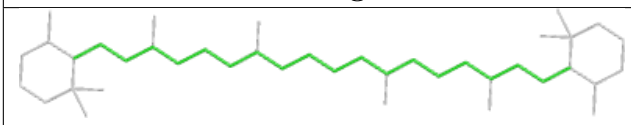
Ligand BCR e 847



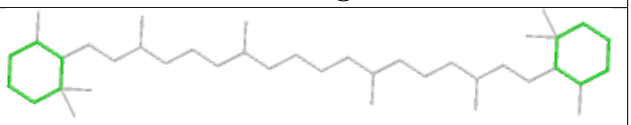
Bond lengths



Bond angles

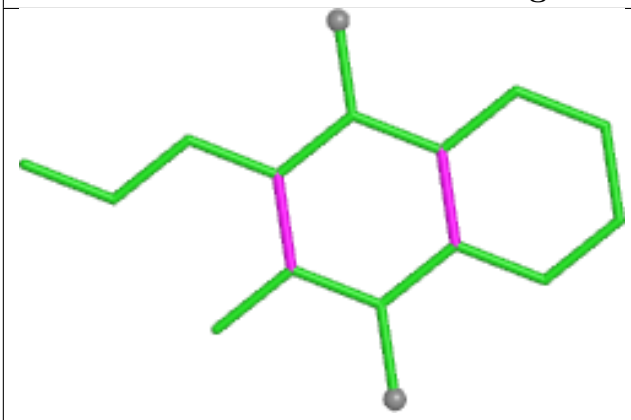


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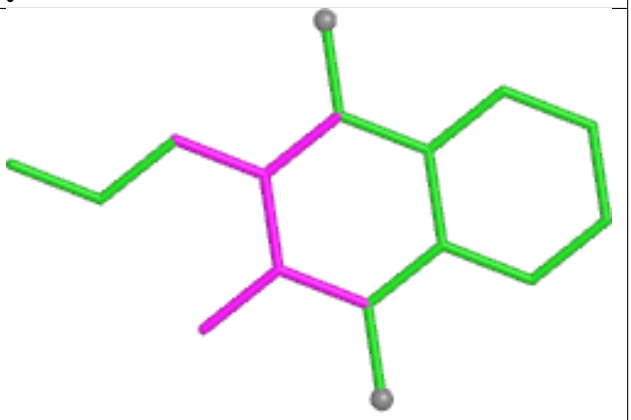


Rings

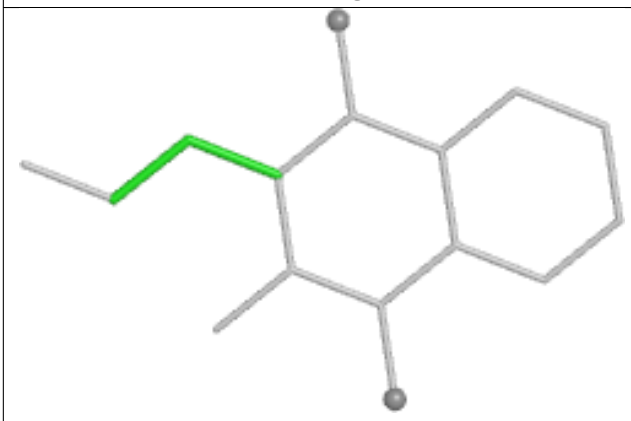
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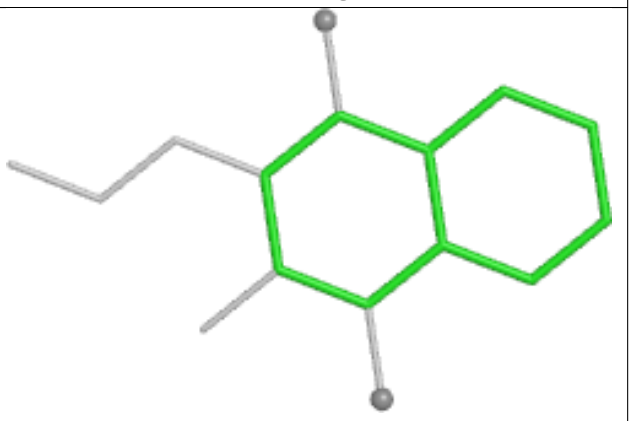
Bond lengths



Bond angles

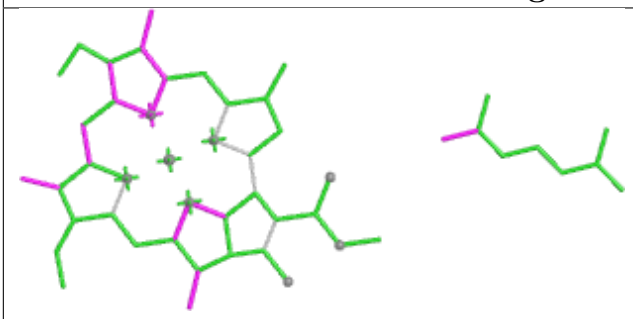


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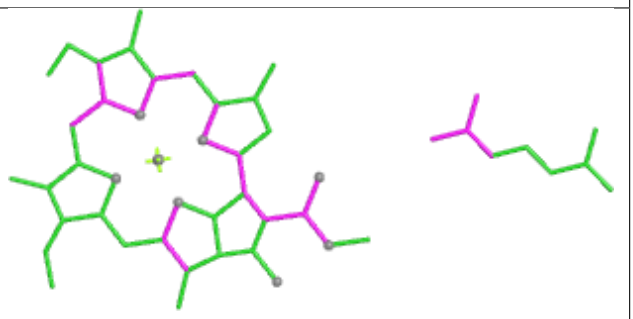


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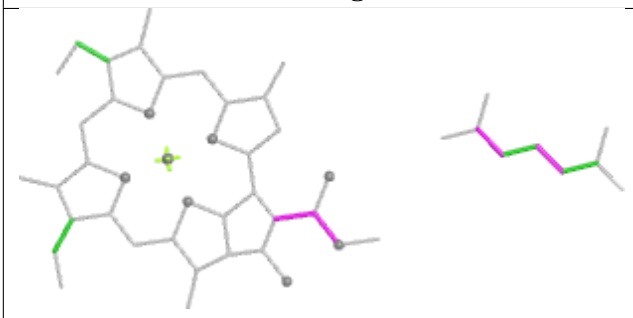
Ligand CLA 2 507



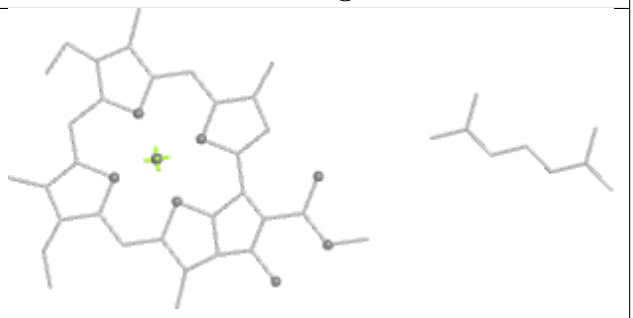
Bond lengths



Bond angles

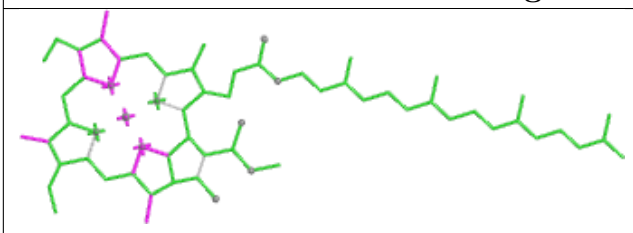


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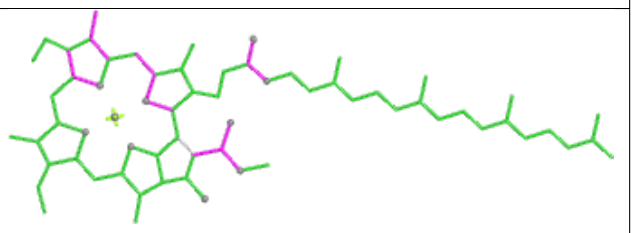


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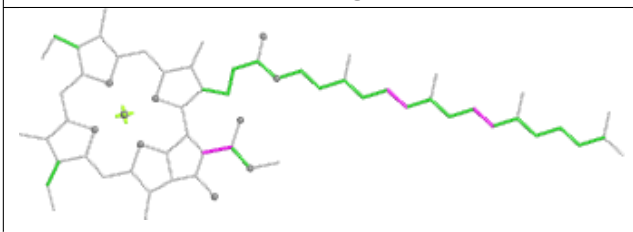
Ligand CLA B 838



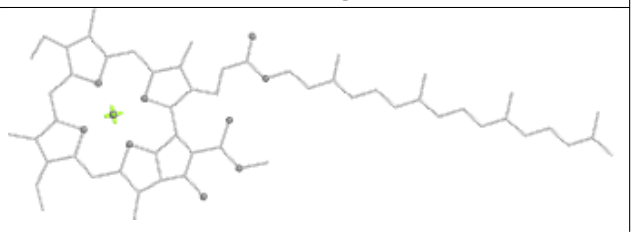
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Bond angles

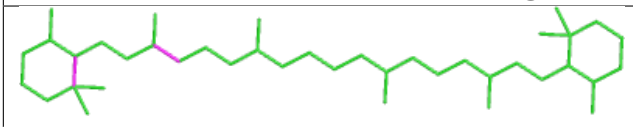


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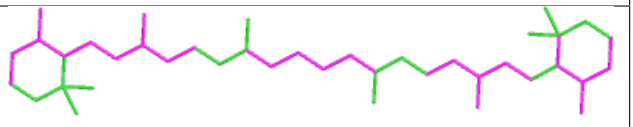


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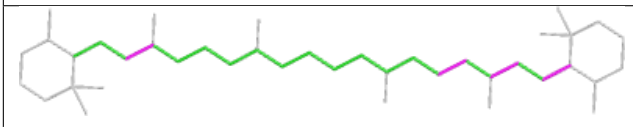
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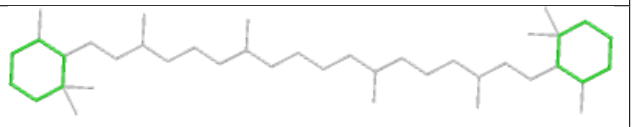
Bond lengths



Bond angles

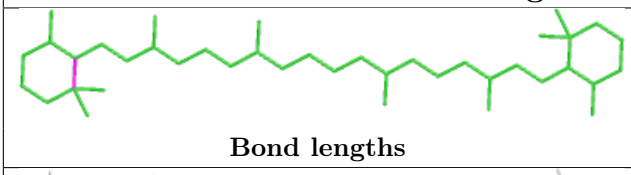


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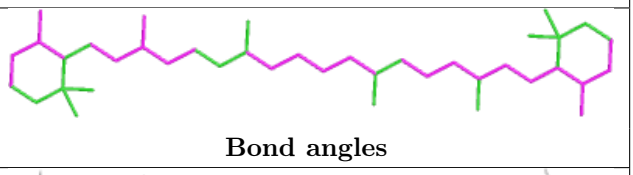


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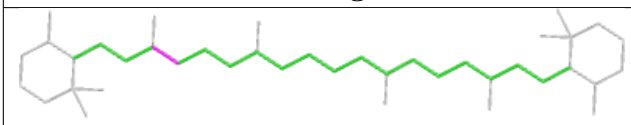
Ligand BCR o 301



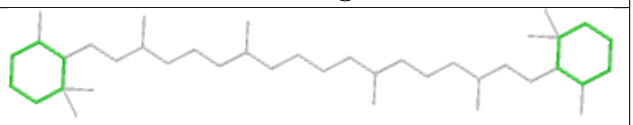
Bond lengths



Bond angles

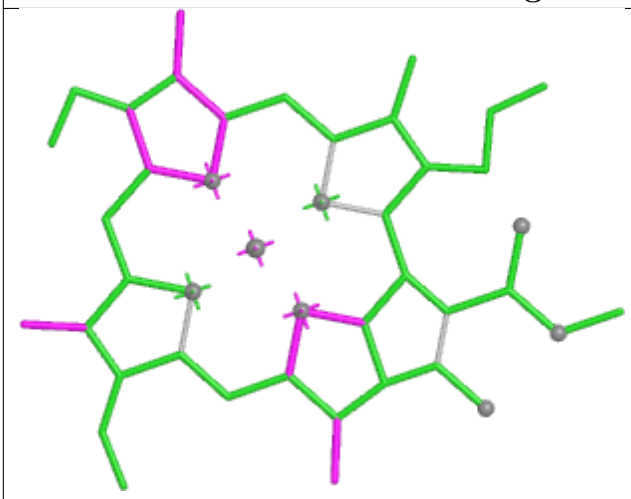


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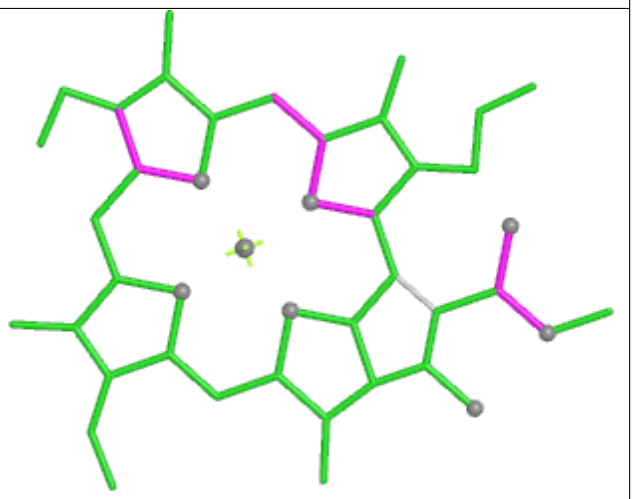


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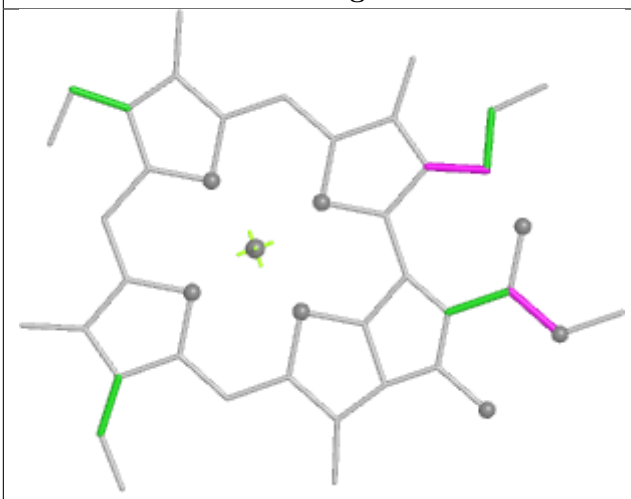
Ligand CLA B 832



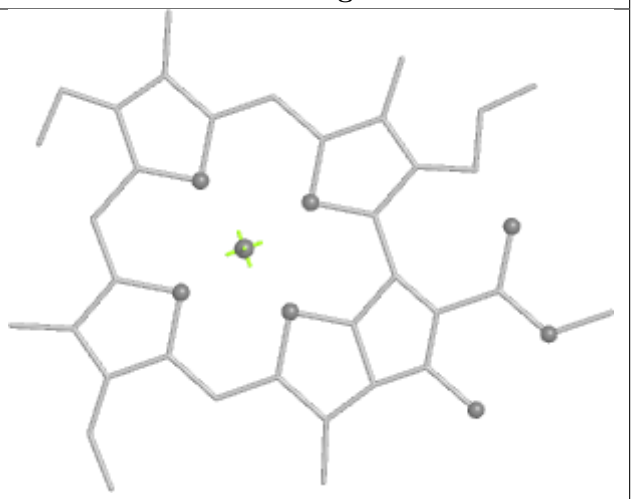
Bond lengths



Bond angles

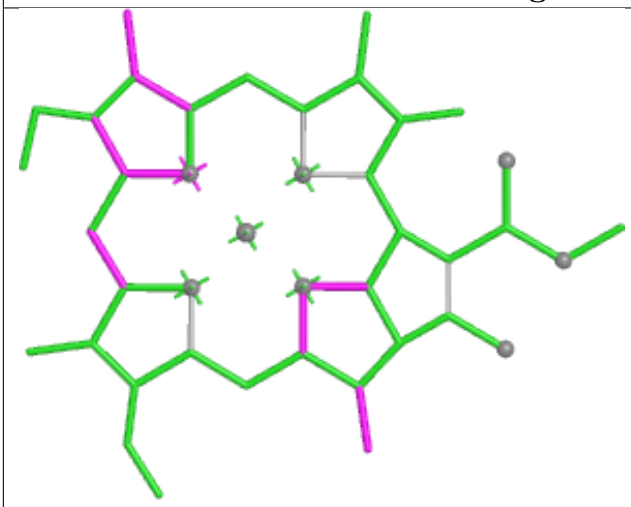


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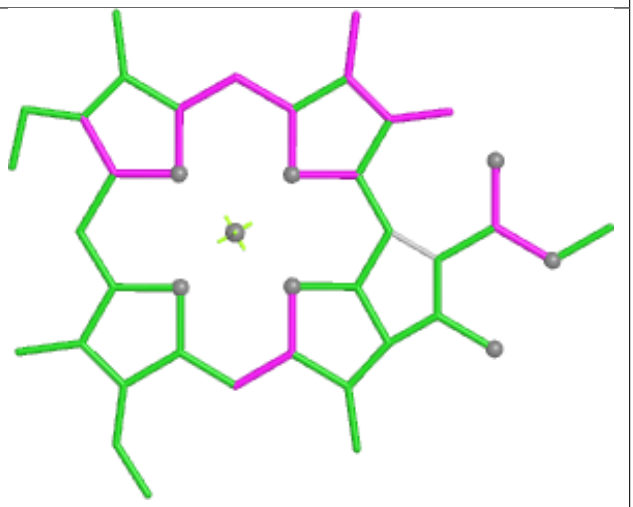


Rings

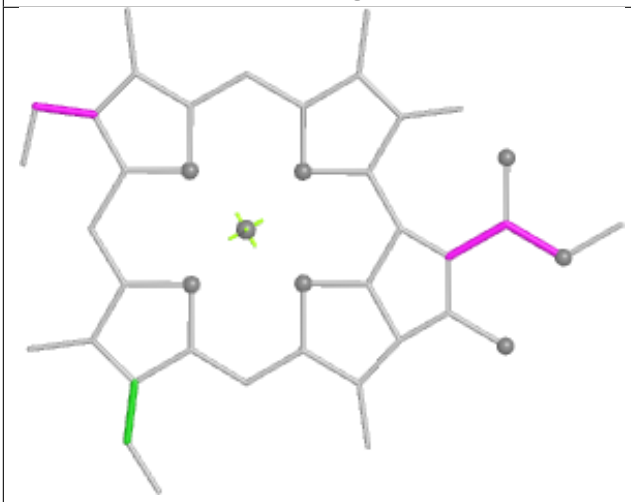
Ligand CLA e 833



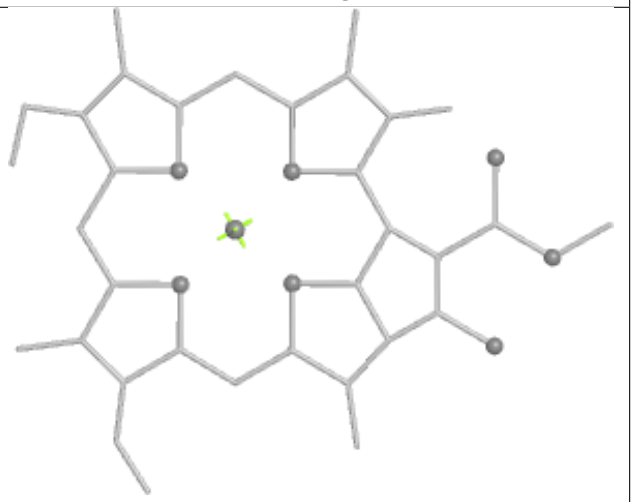
Bond lengths



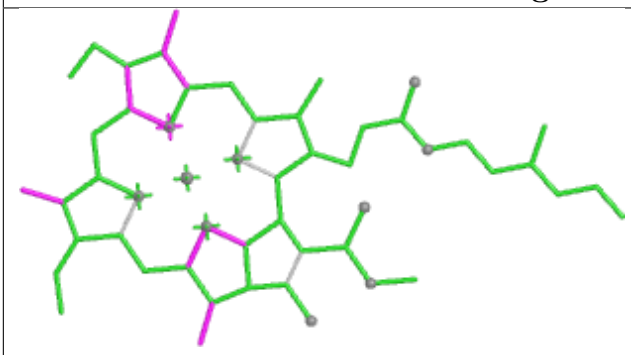
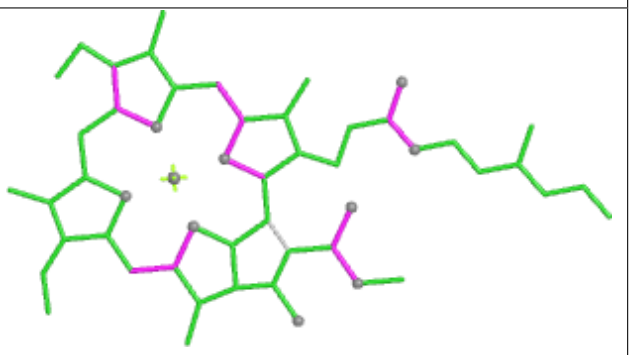
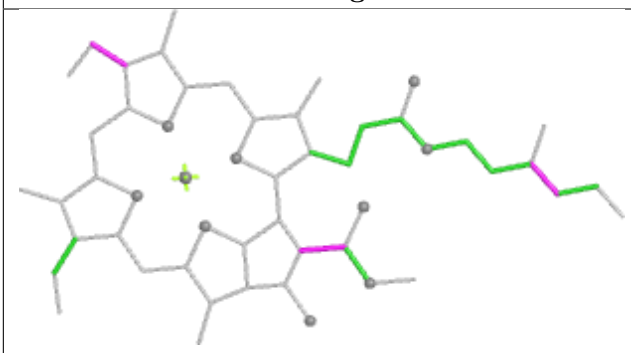
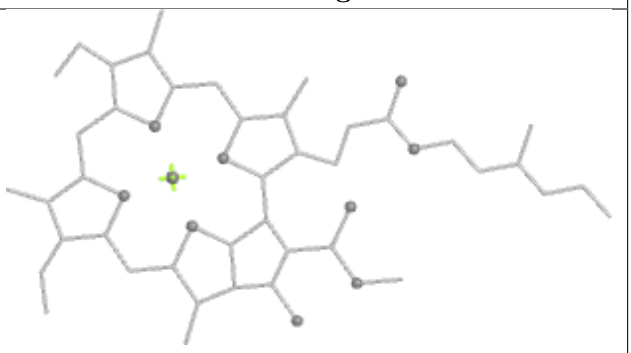
Bond angles



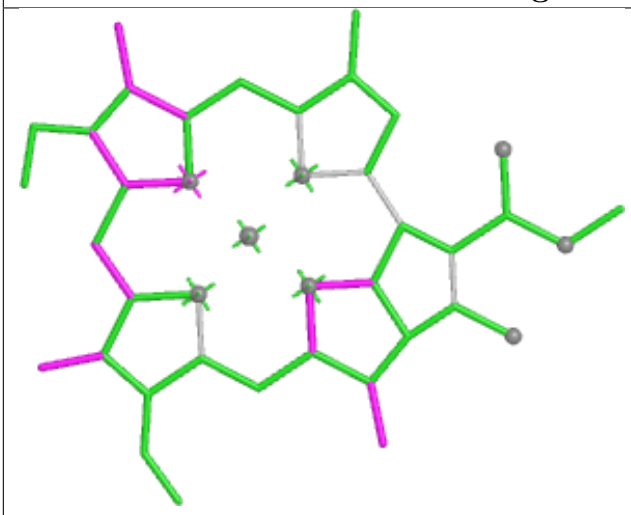
Torsions



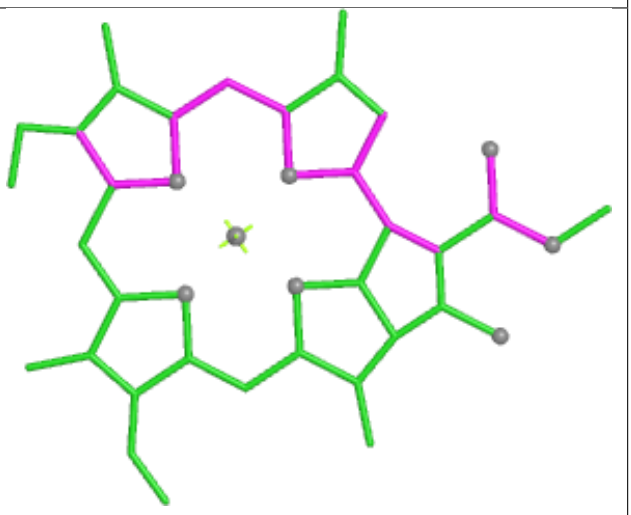
Rings

Ligand CLA f 809	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

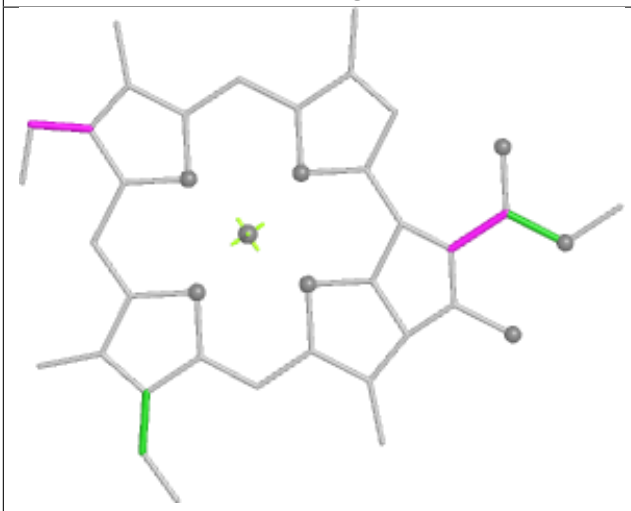
Ligand CLA f 832



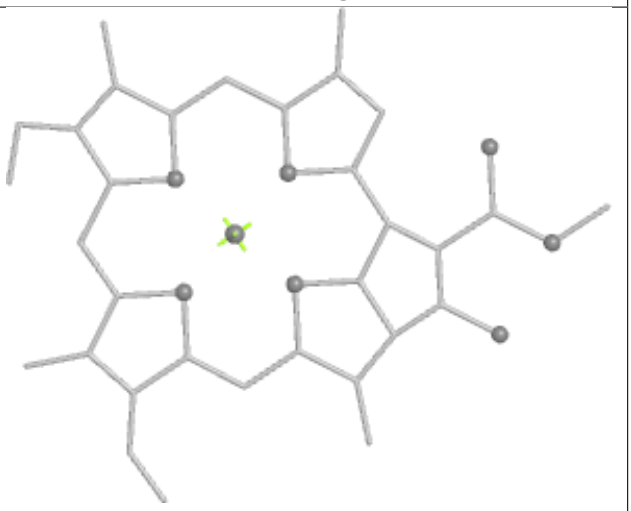
Bond lengths



Bond angles

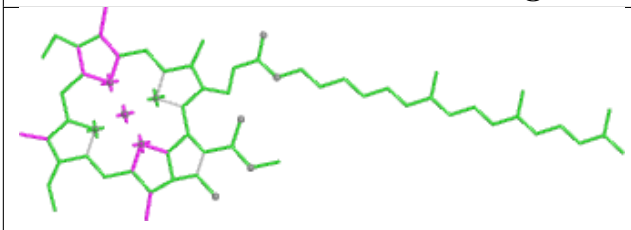


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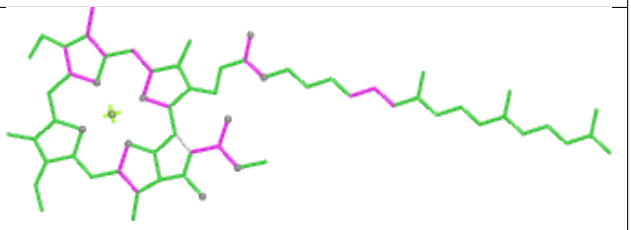


Rings

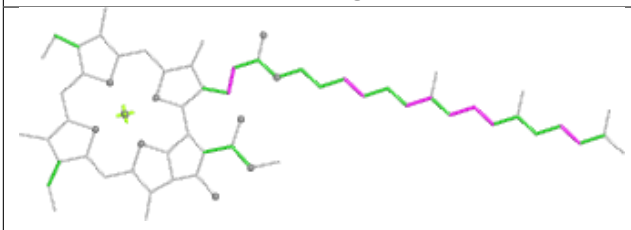
Ligand CLA B 802



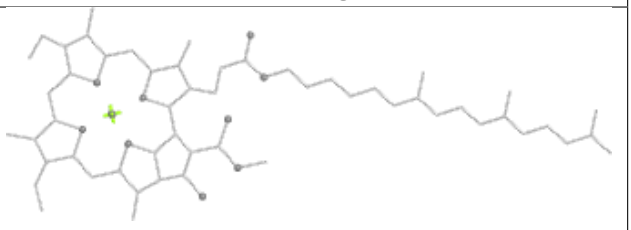
Bond lengths



Bond angles

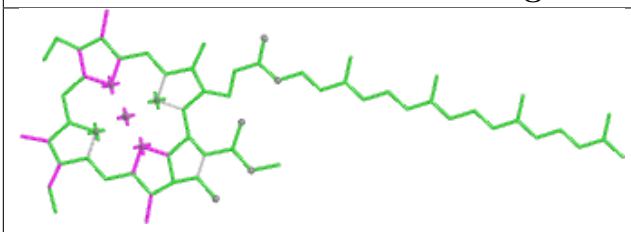


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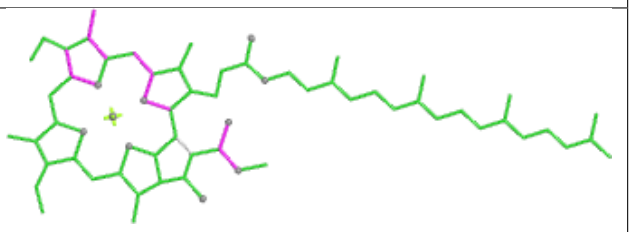


Rings

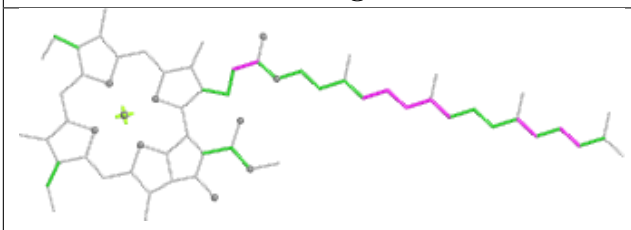
Ligand CLA B 807



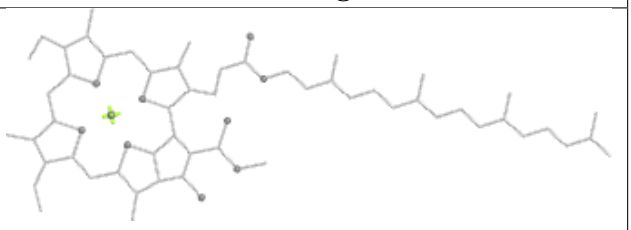
Bond lengths



Bond angles

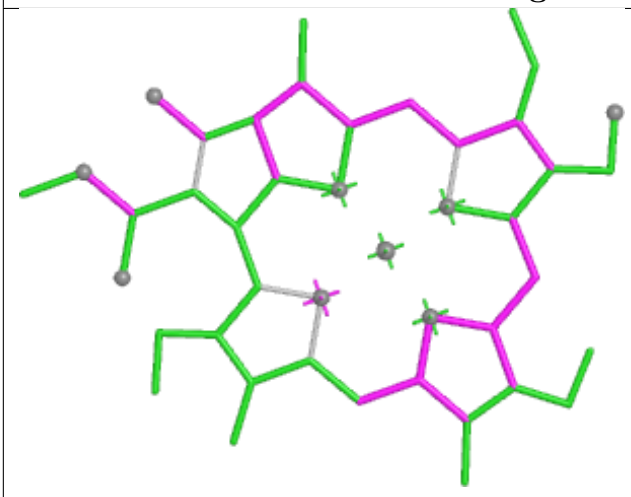


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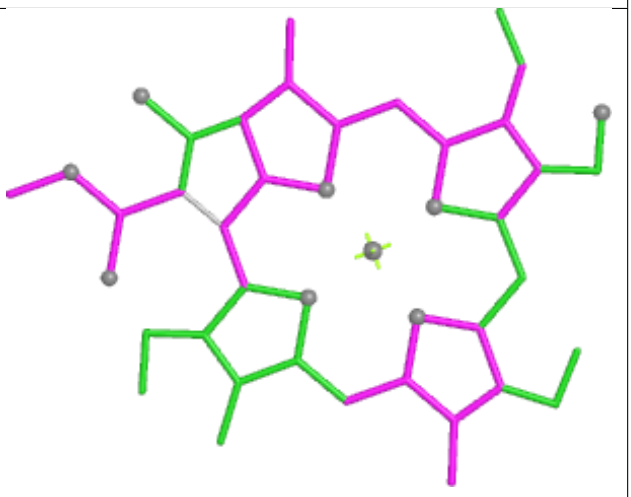


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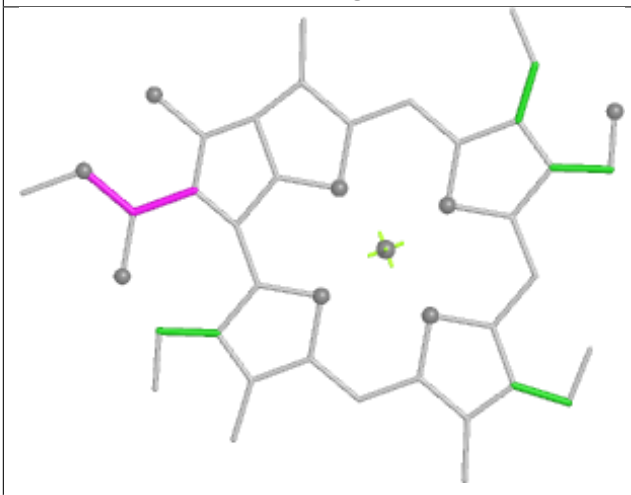
Ligand CHL r 316



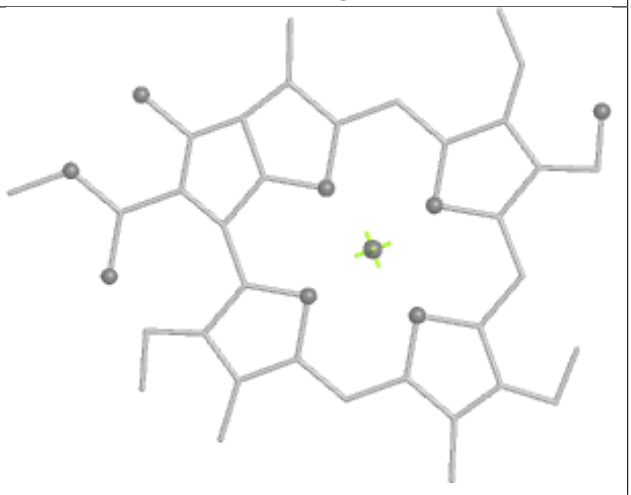
Bond lengths



Bond angles

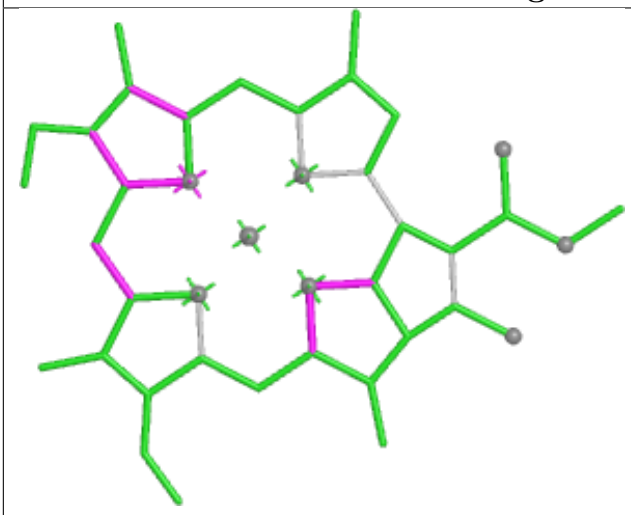


Torsions

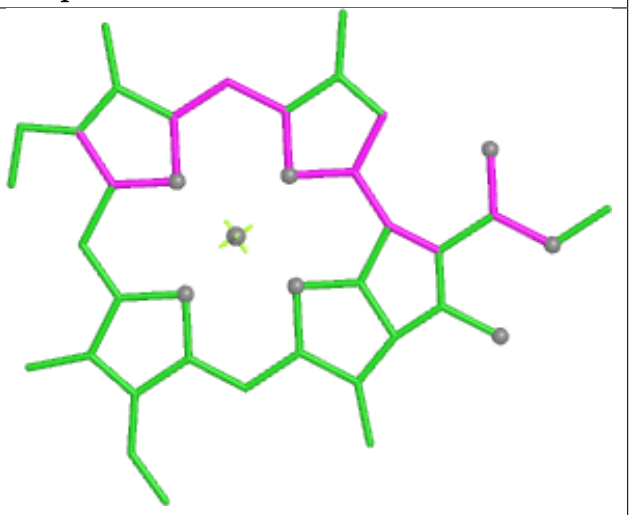


Rings

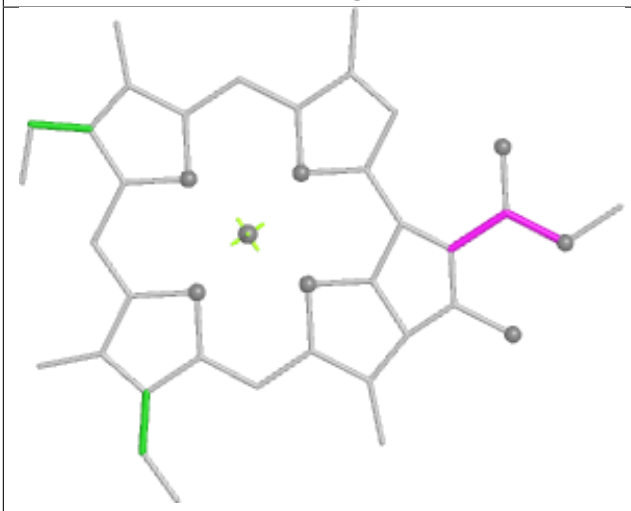
Ligand CLA q 307



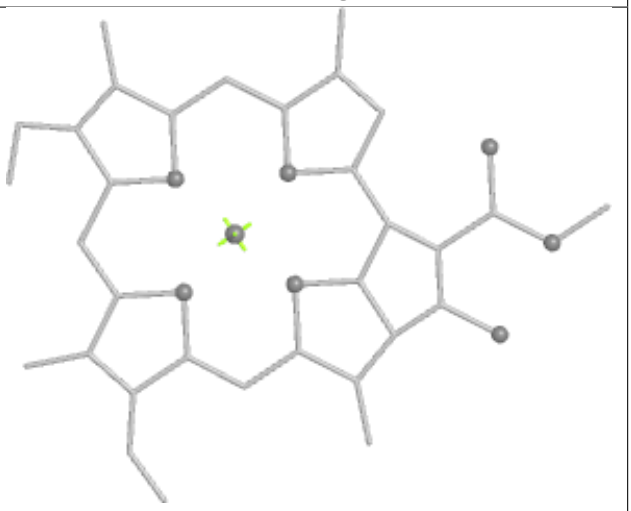
Bond lengths



Bond angles

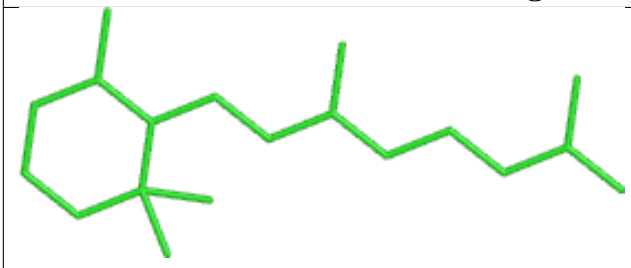


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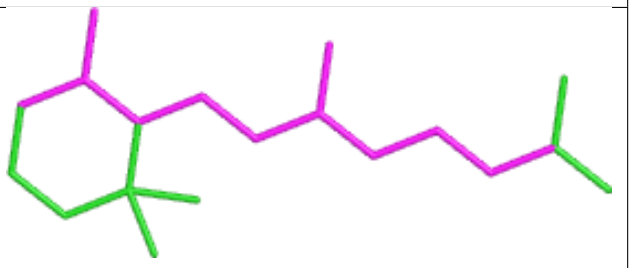


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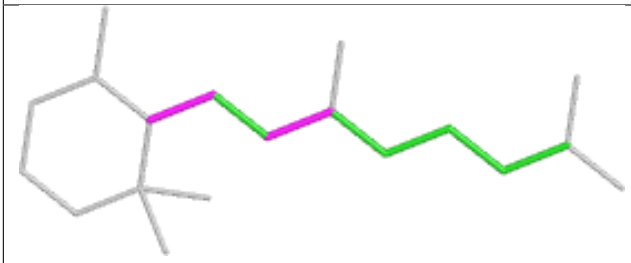
Ligand BCR 1 503



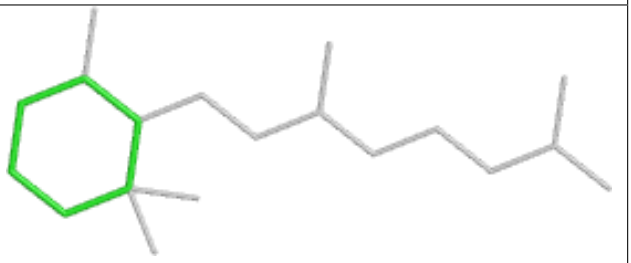
Bond lengths



Bond angles

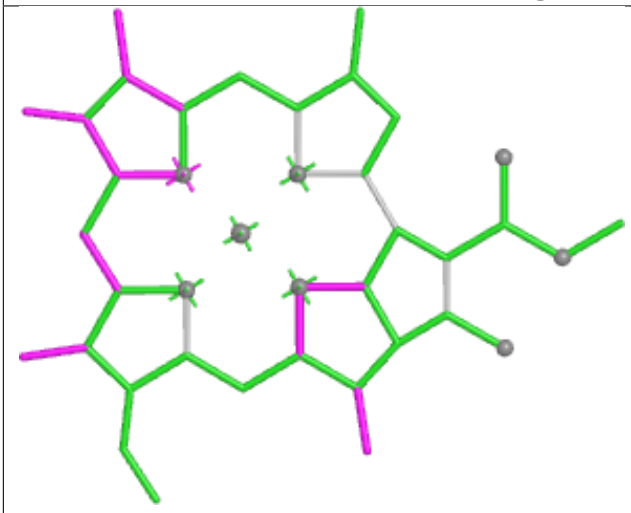


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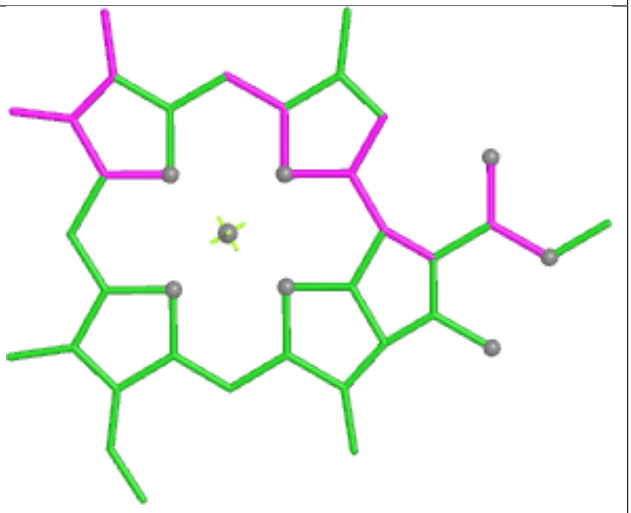


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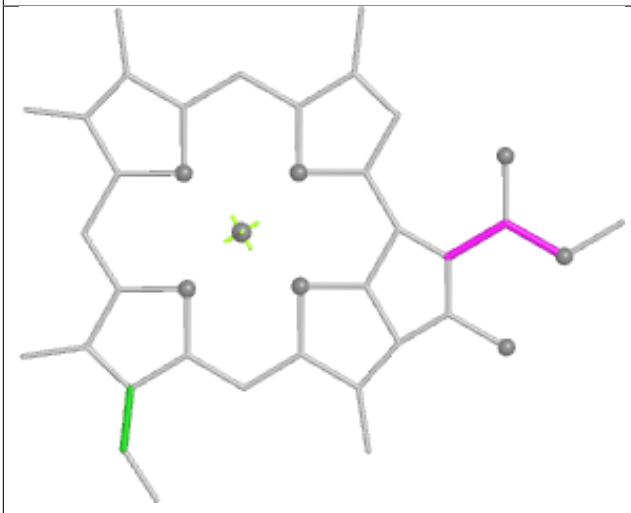
Ligand CLA f 830



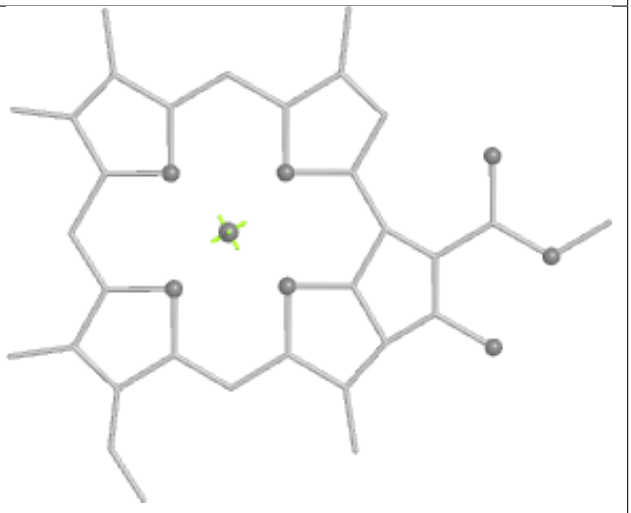
Bond lengths



Bond angles

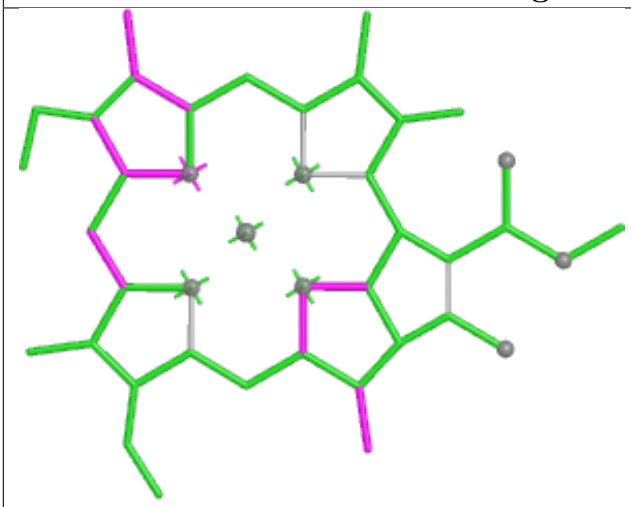


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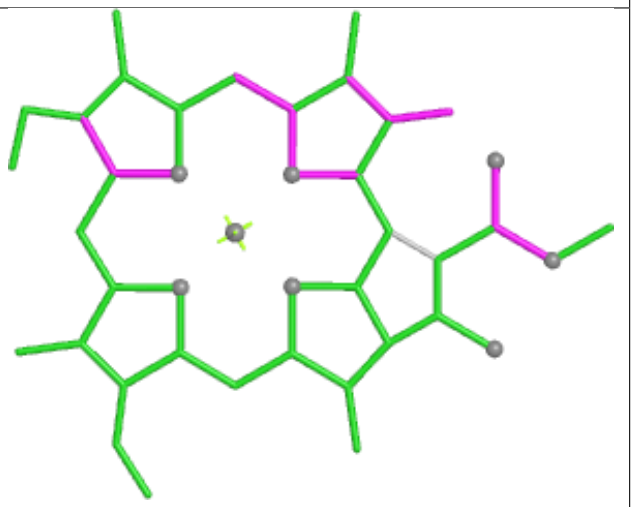


Rings

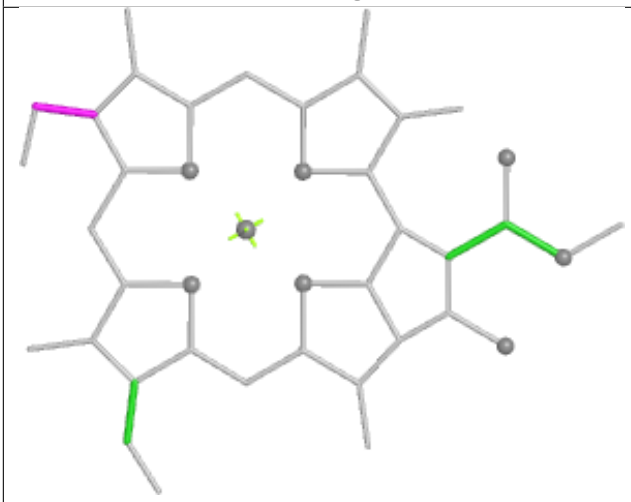
Ligand CLA f 822



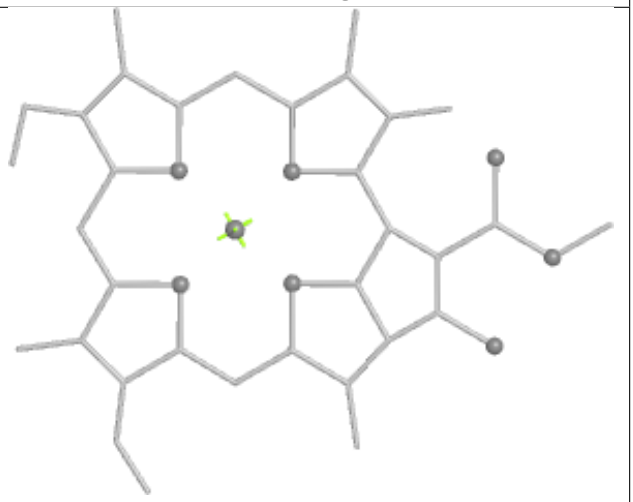
Bond lengths



Bond angles

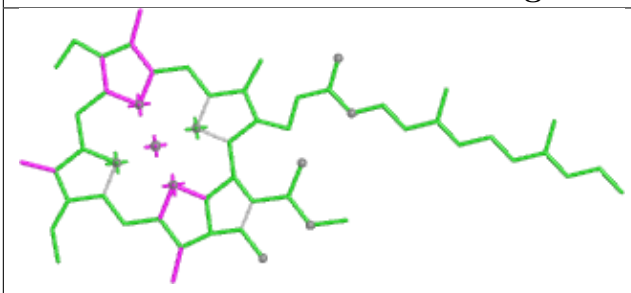


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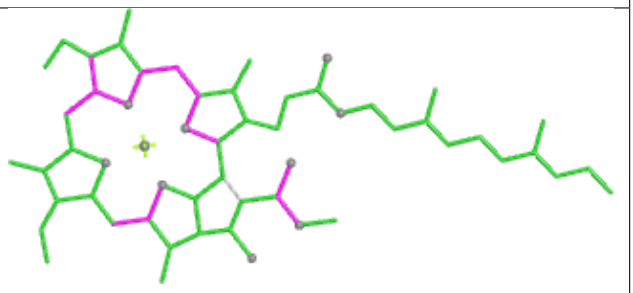


Rings

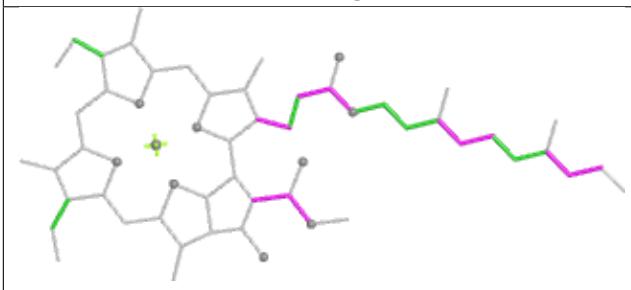
Ligand CLA B 842



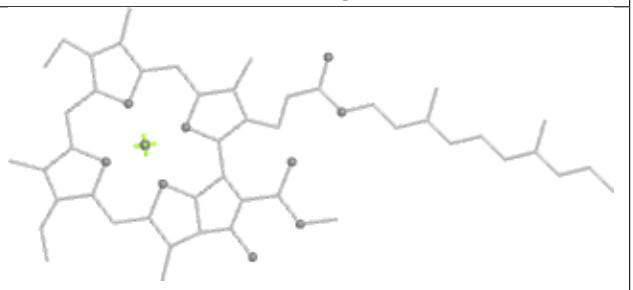
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Bond angles

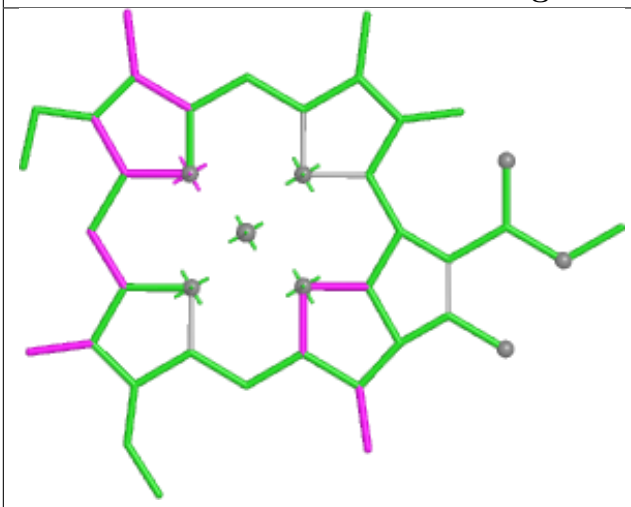


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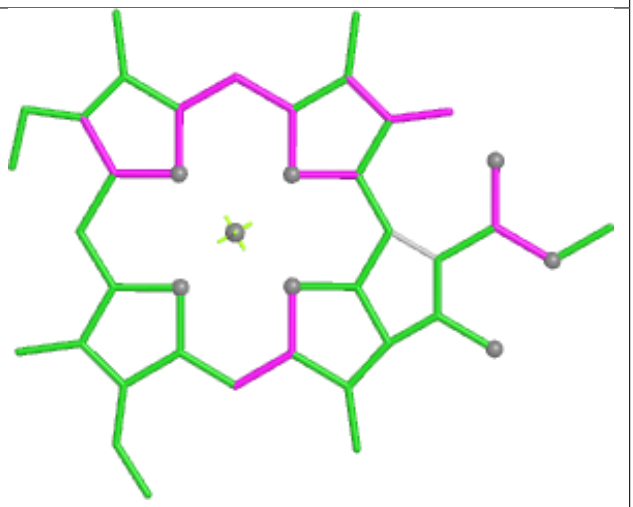


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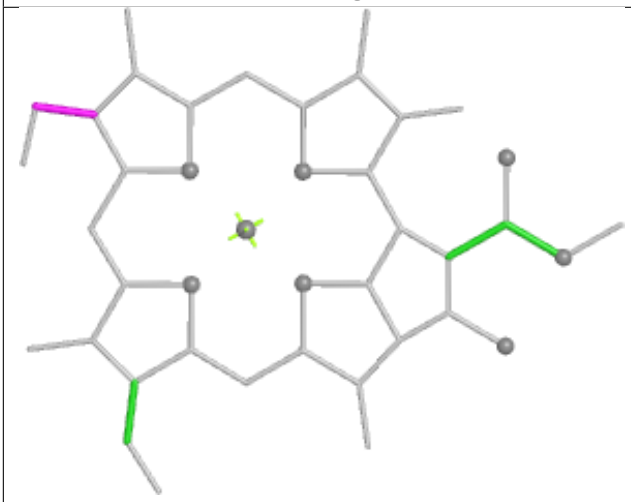
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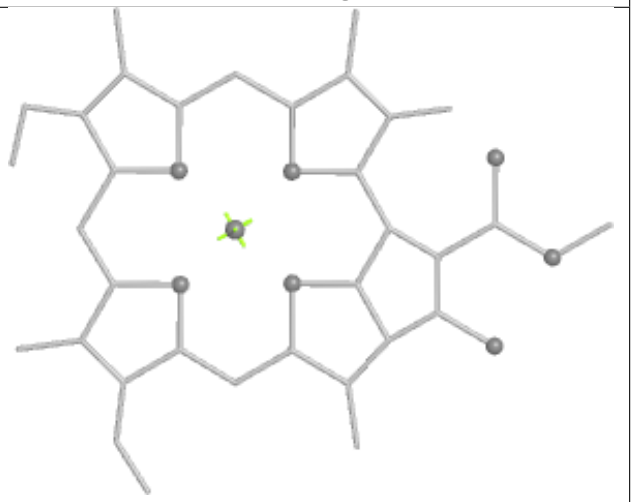
Bond lengths



Bond angles

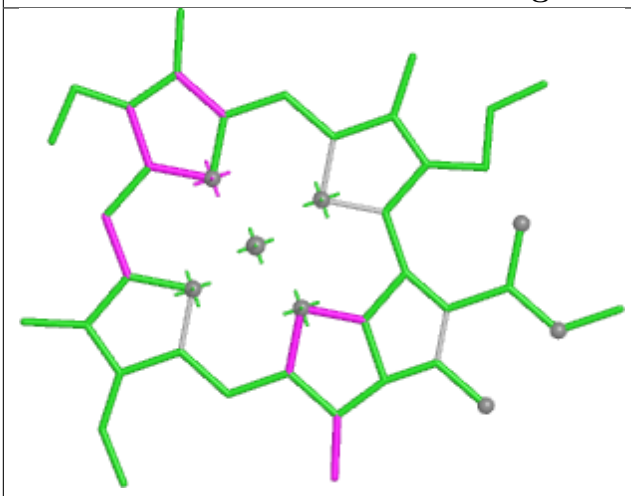


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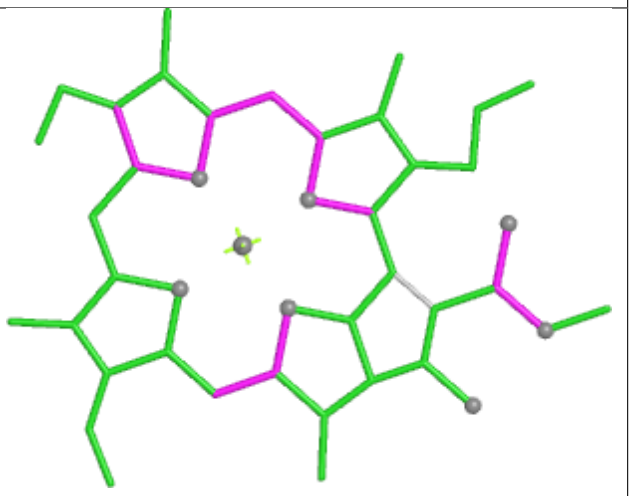


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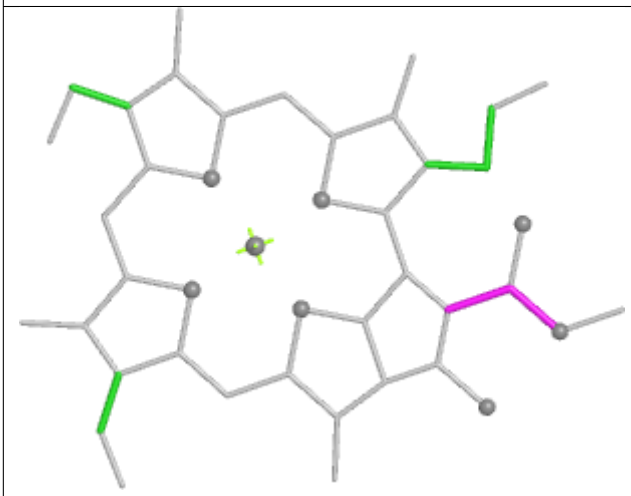
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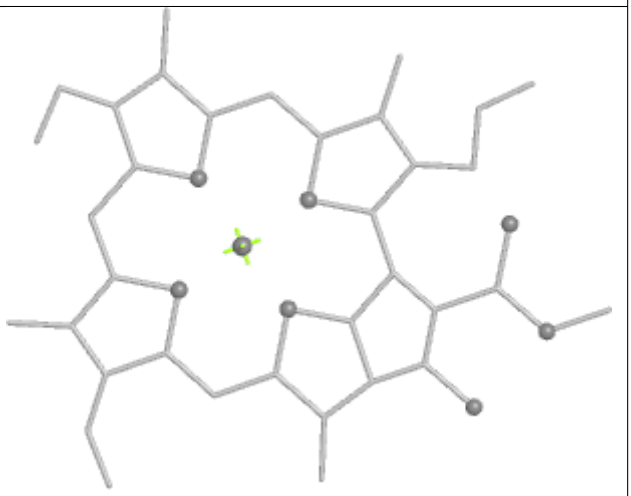
Bond lengths



Bond angles

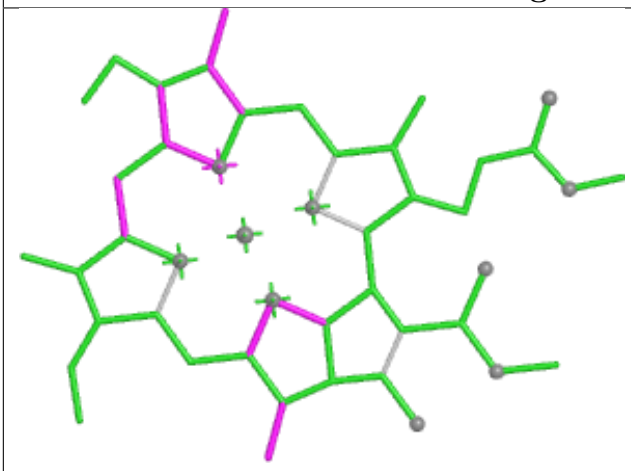


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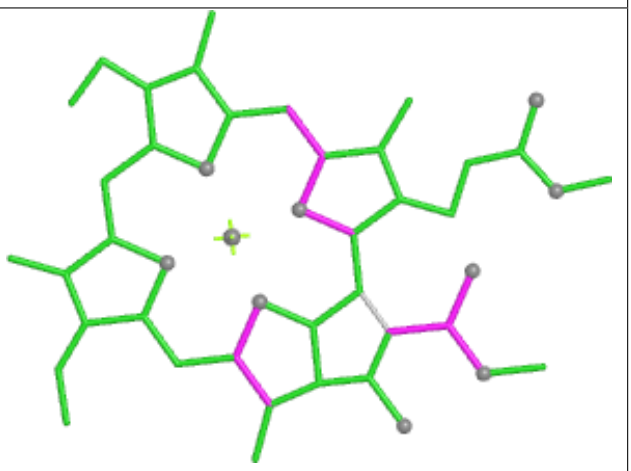


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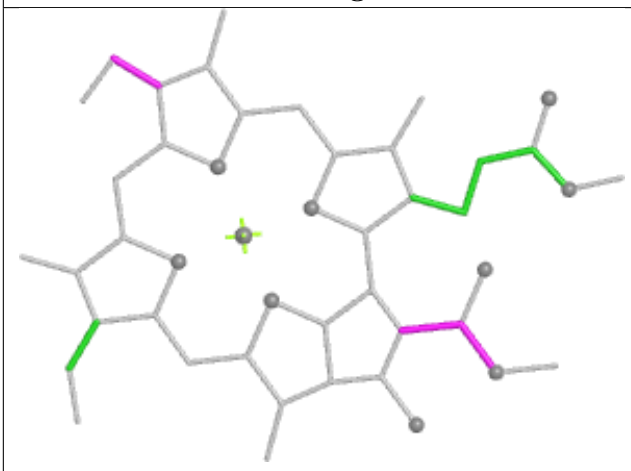
Ligand CLA r 311



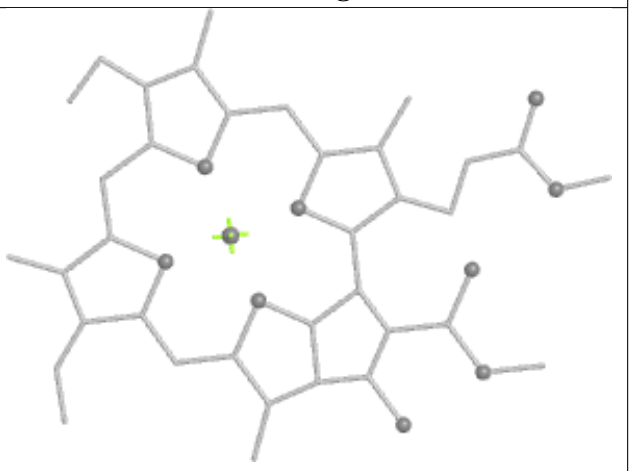
Bond lengths



Bond angles

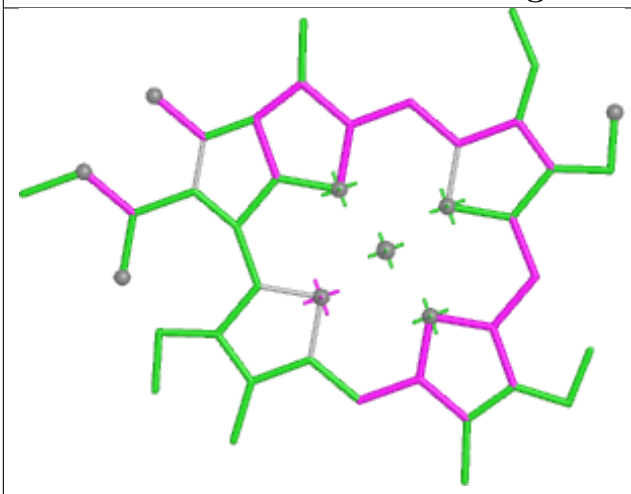


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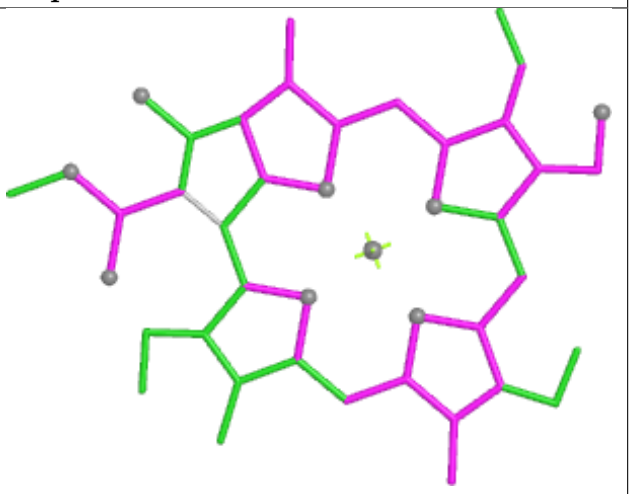


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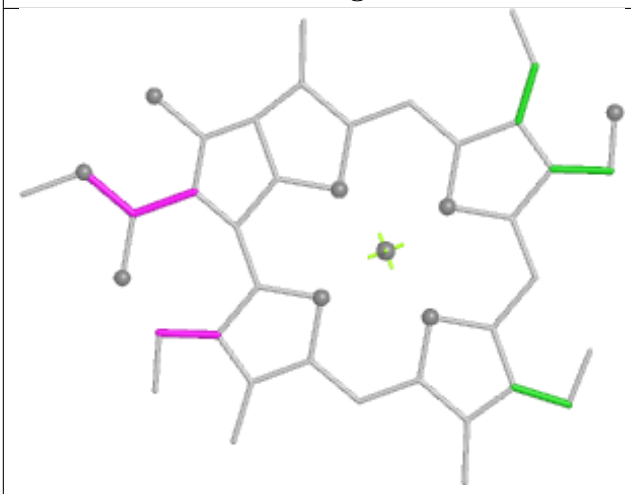
Ligand CHL p 517



Bond lengths



Bond angles

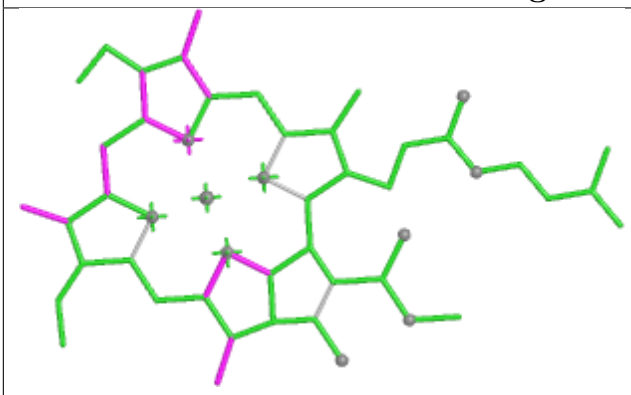


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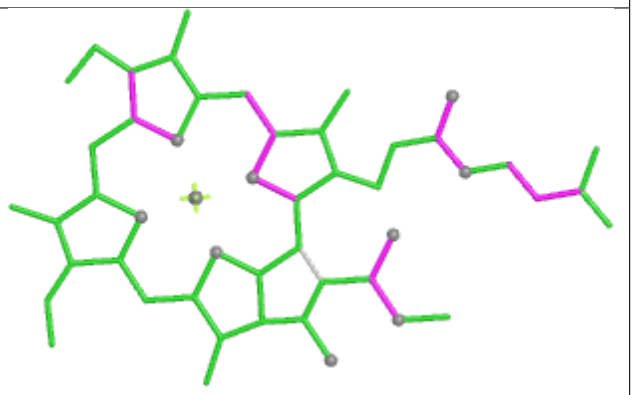


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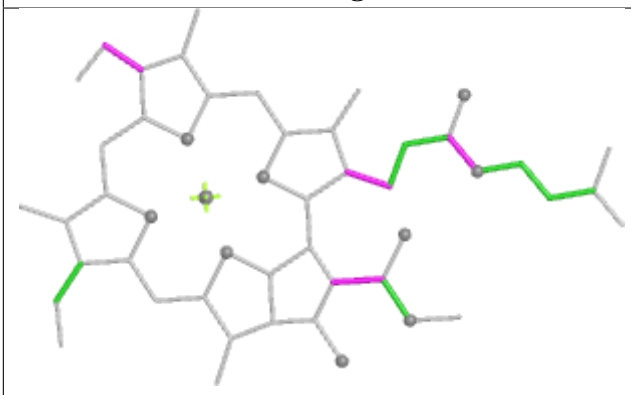
Ligand CLA e 830



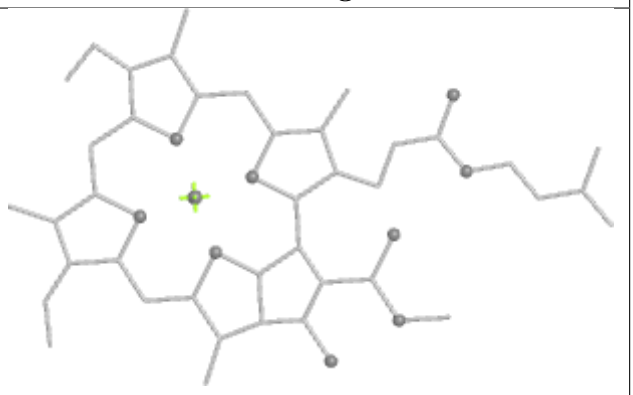
Bond lengths



Bond angles



Torsions

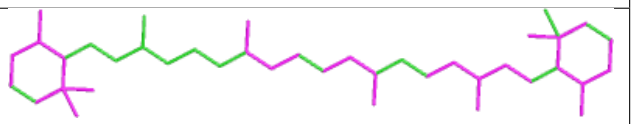


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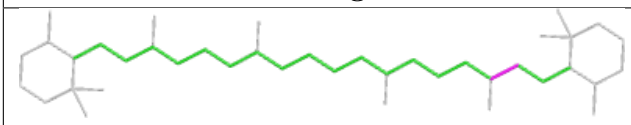
Ligand BCR A 853



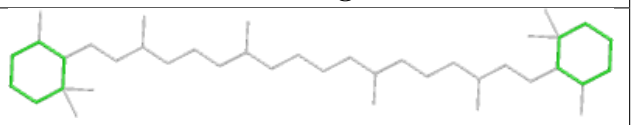
Bond lengths



Bond angles

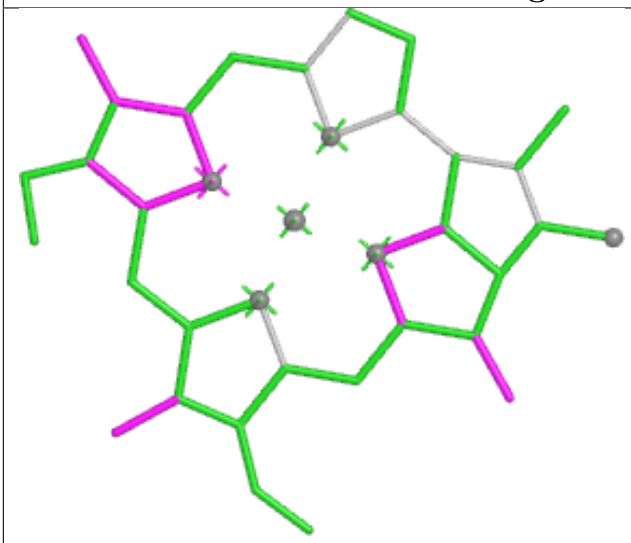


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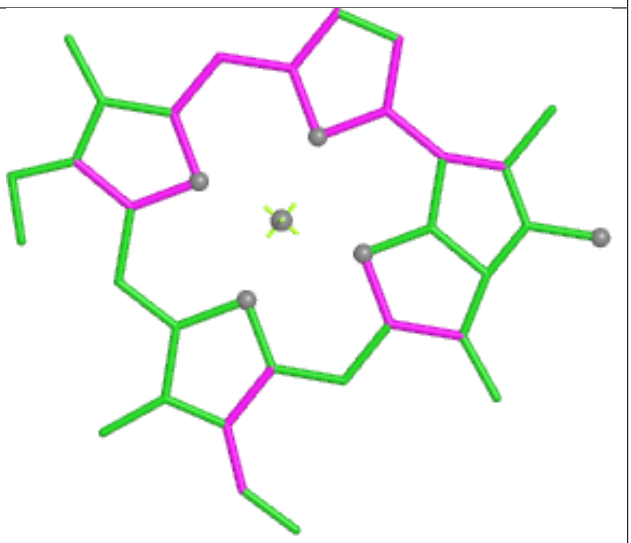


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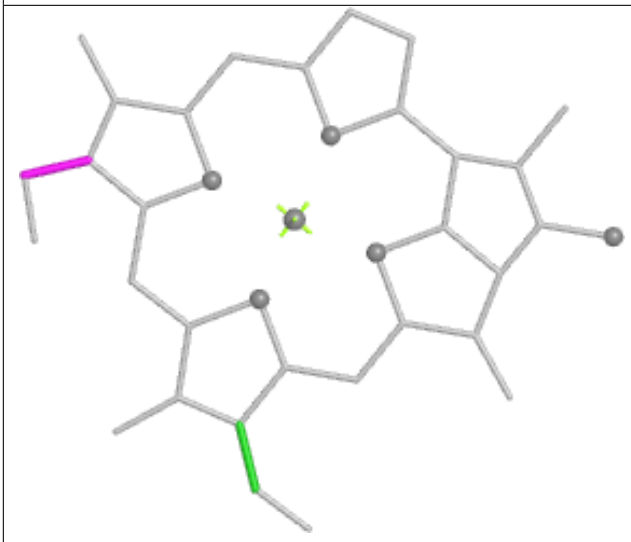
Ligand CLA 2 504



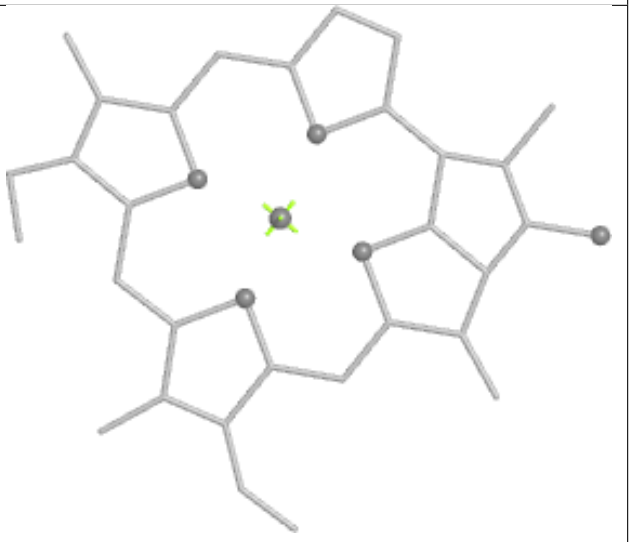
Bond lengths



Bond angles

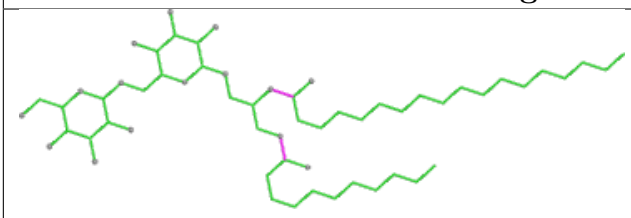


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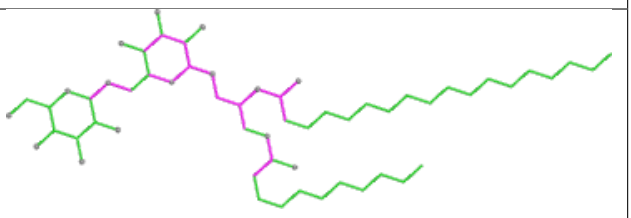


Rings

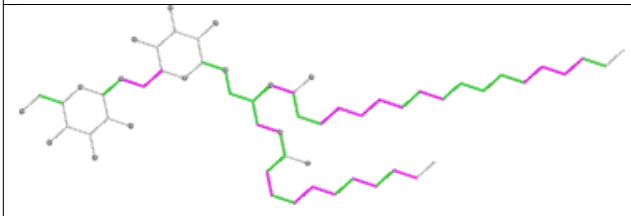
Ligand DGD B 850



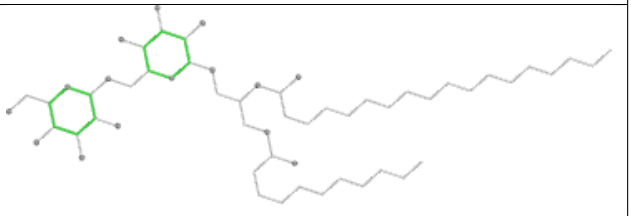
Bond lengths



Bond angles

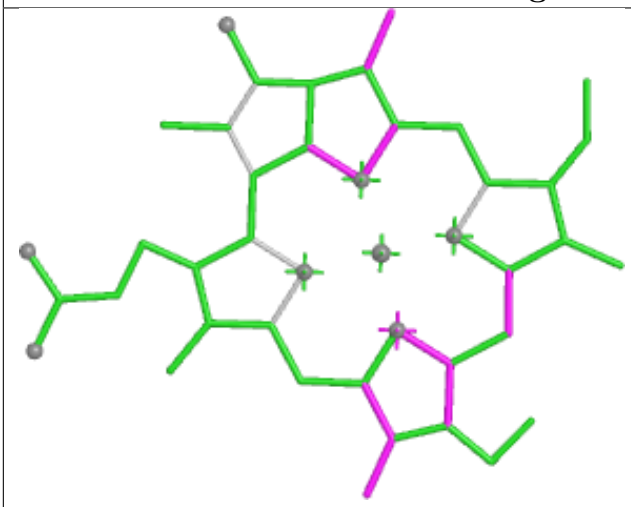


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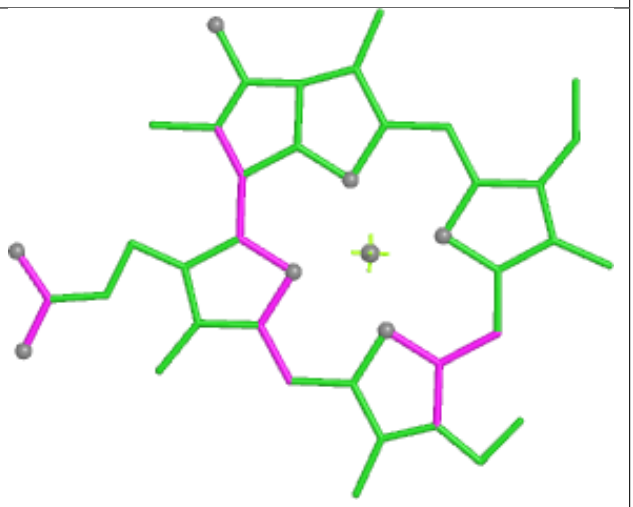


Rings

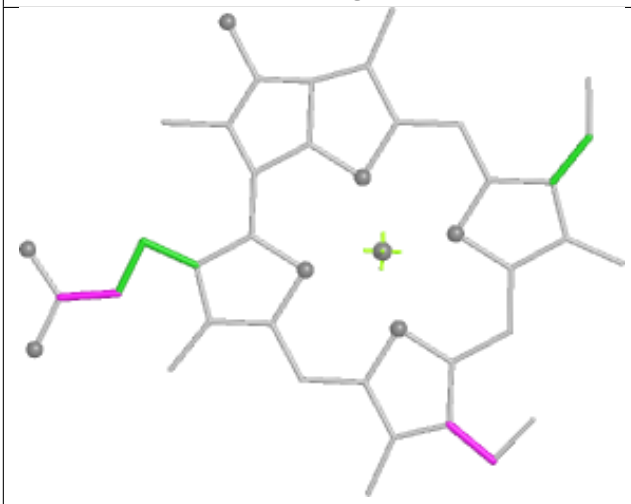
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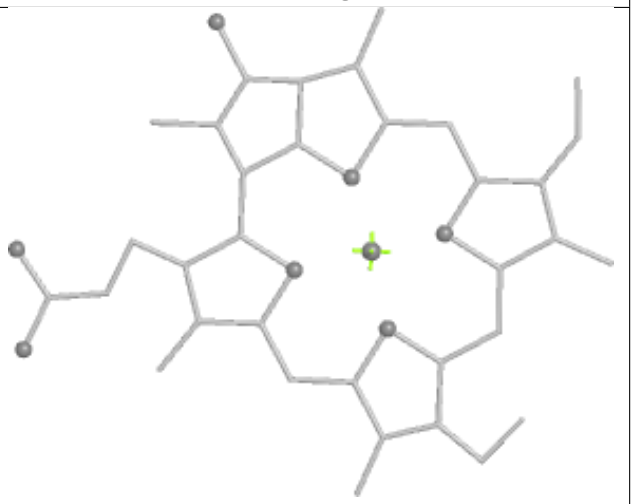
Bond lengths



Bond angles

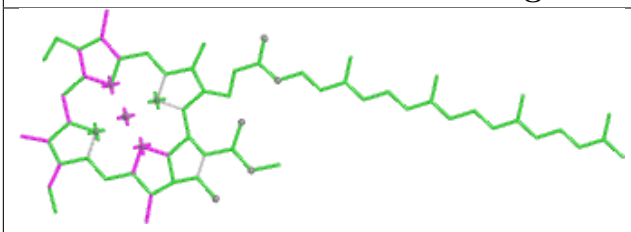


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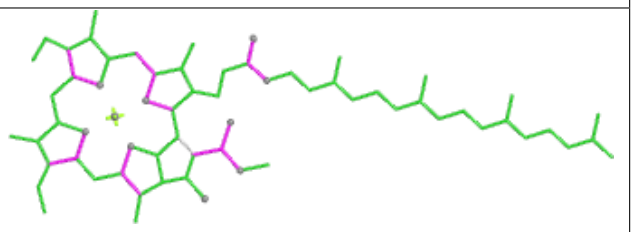


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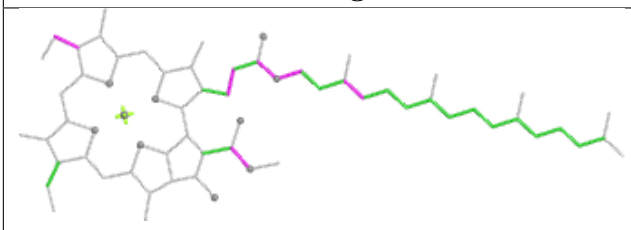
Ligand CLA B 815



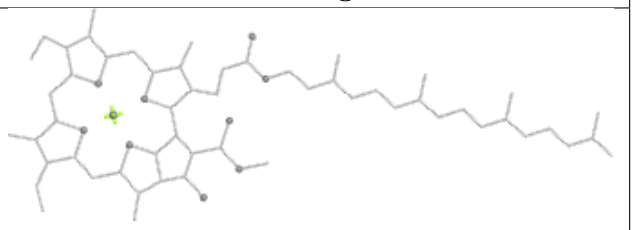
Bond lengths



Bond angles

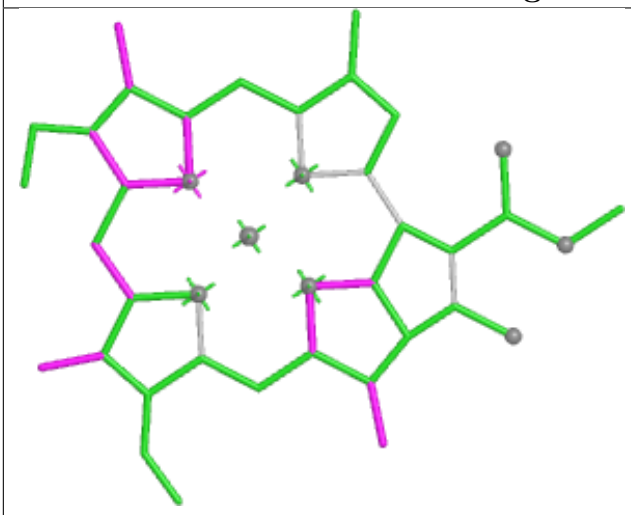


Torsions

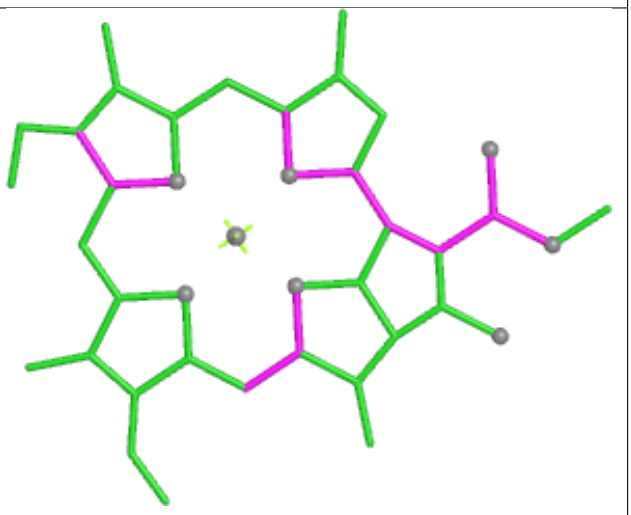


Rings

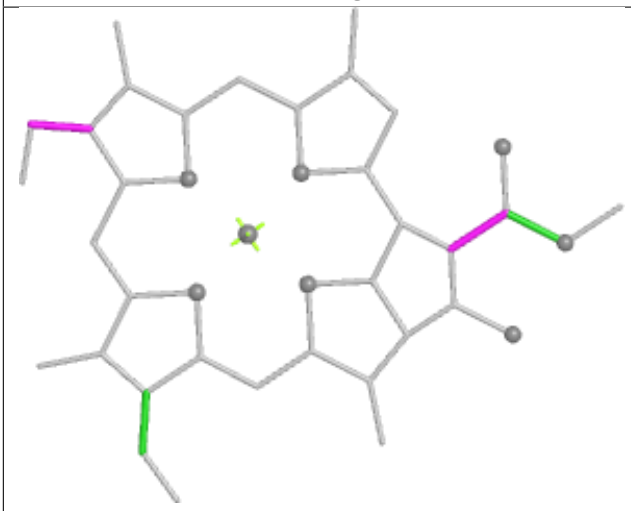
Ligand CLA A 819



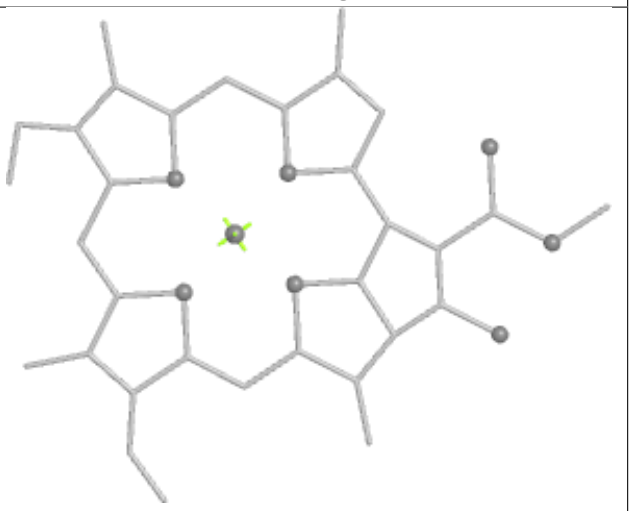
Bond lengths



Bond angles

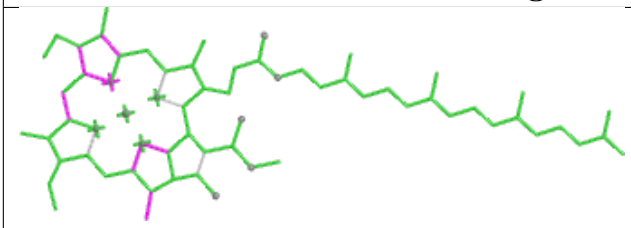


Torsions

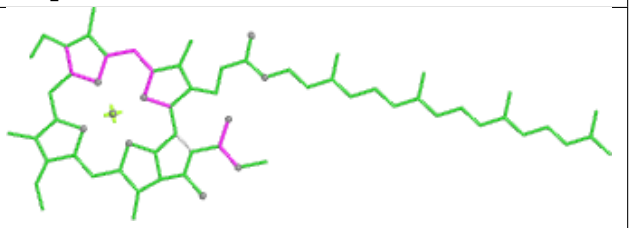


Rings

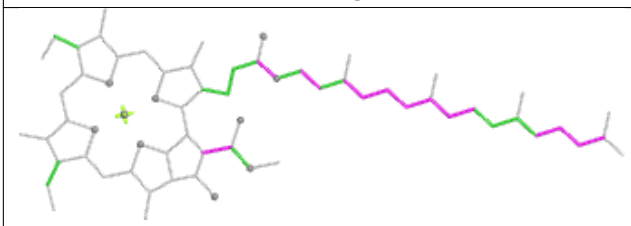
Ligand CLA p 508



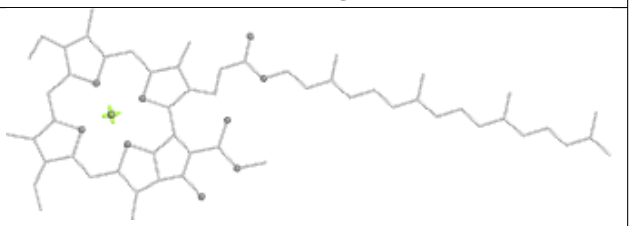
Bond lengths



Bond angles

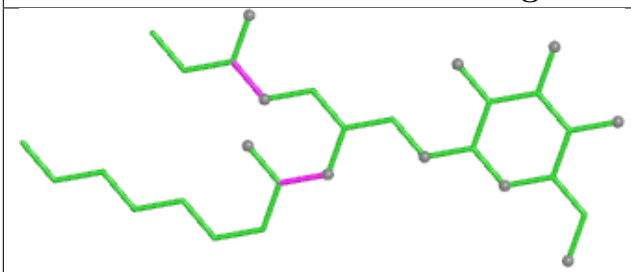


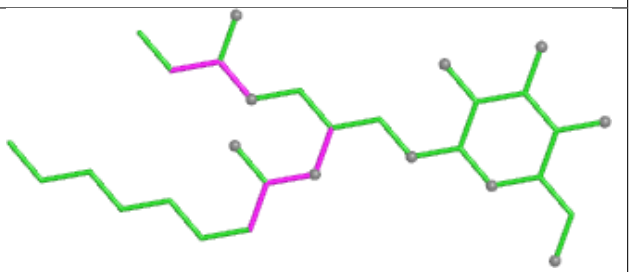
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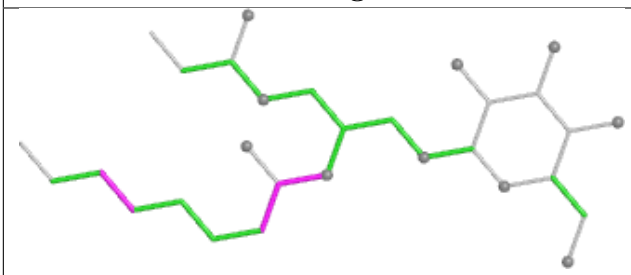


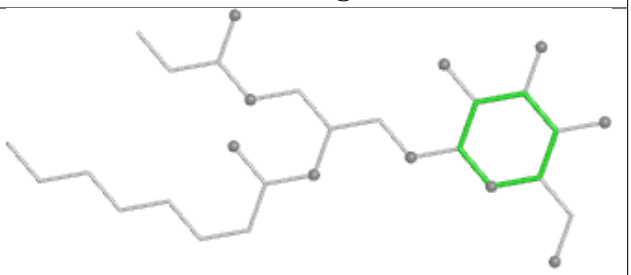
Rings

Ligand LMG F 805


Bond lengths


Bond angles

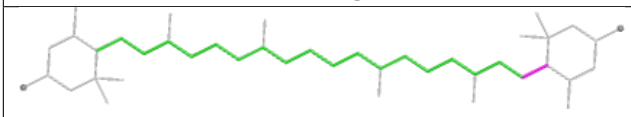

Torsions

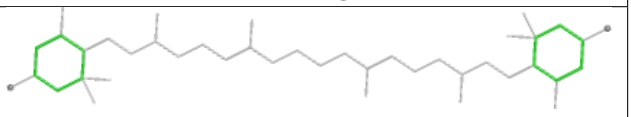

Rings

Ligand LUT 1 501

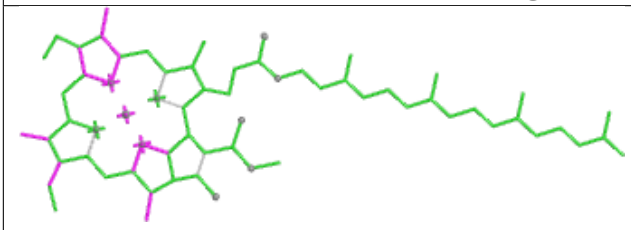

Bond lengths

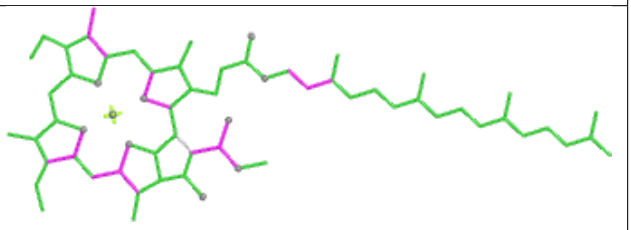

Bond angles

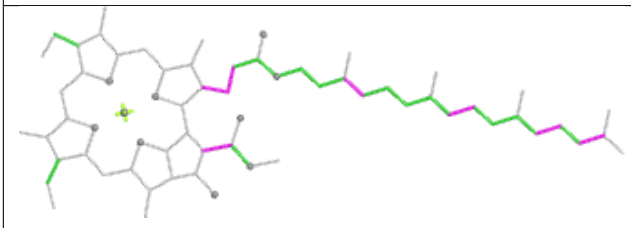

Torsions

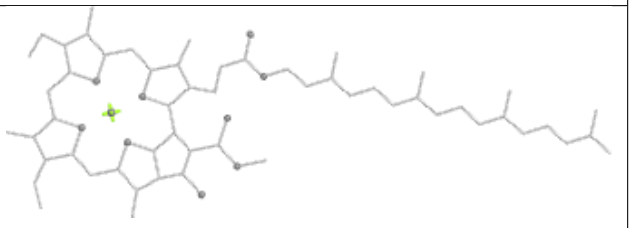

Rings

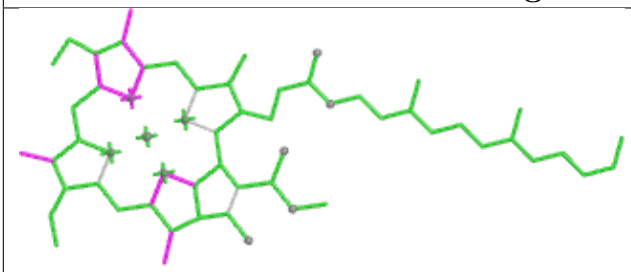
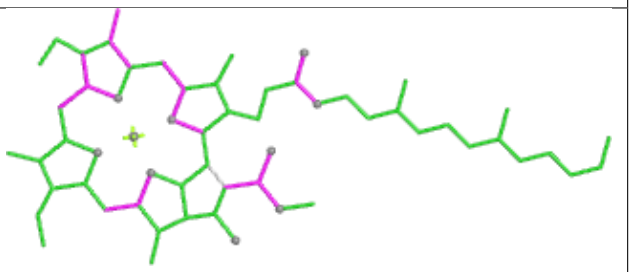
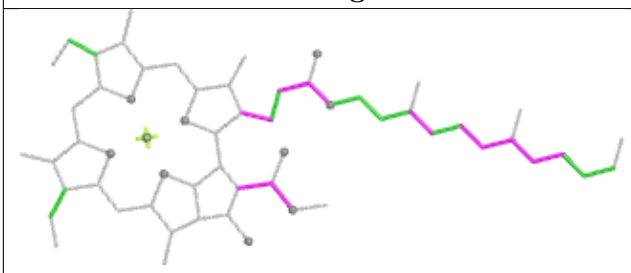
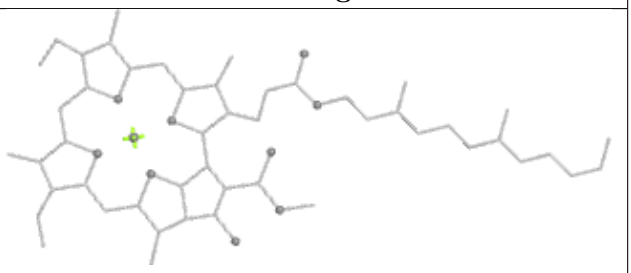
Ligand CLA B 801

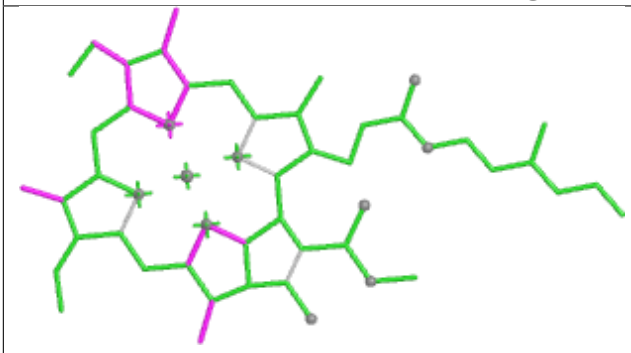
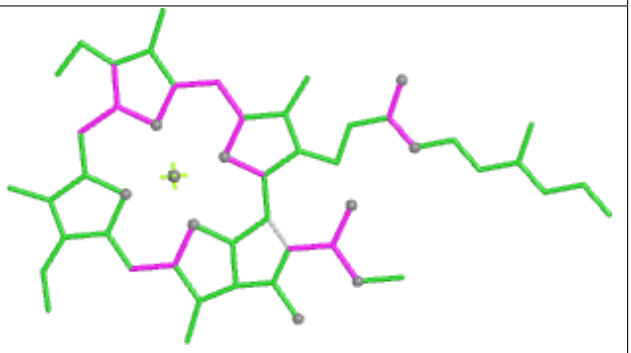
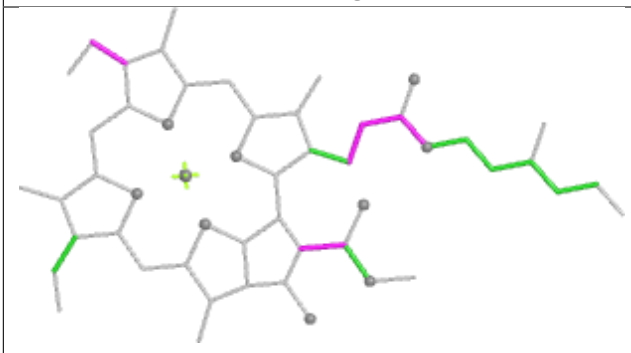
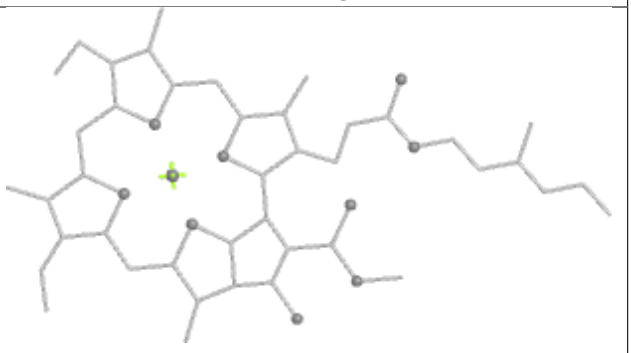

Bond lengths

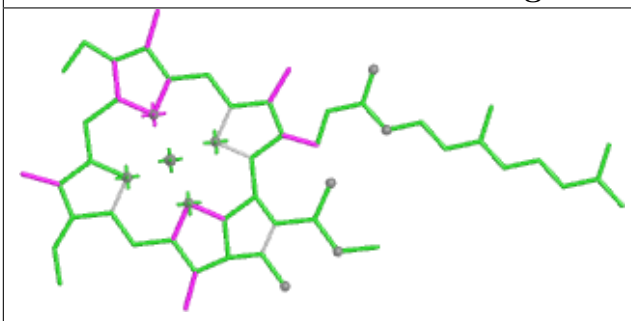
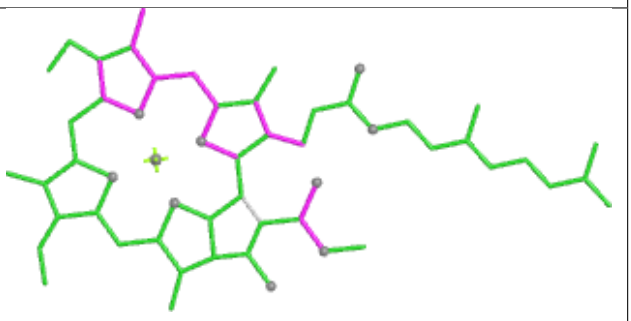
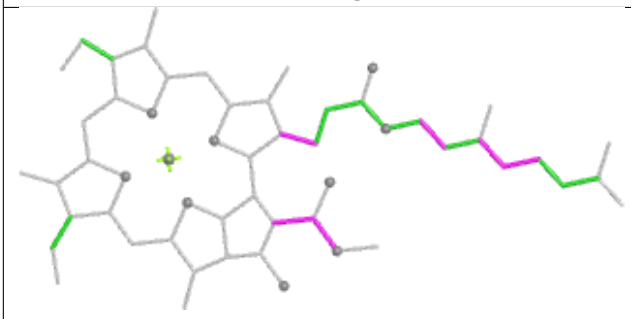
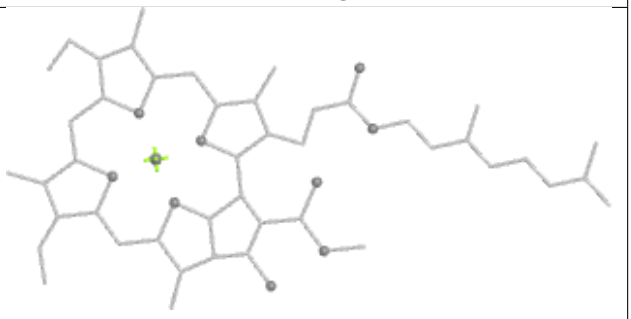

Bond angles

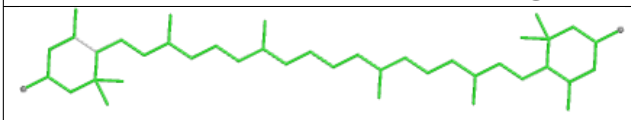
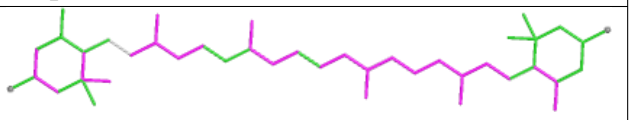
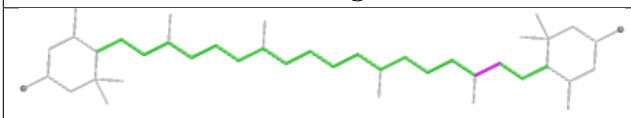
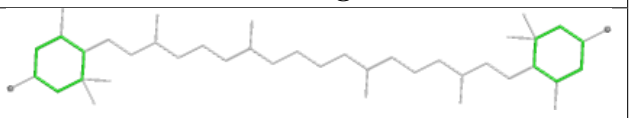

Torsions


Rings

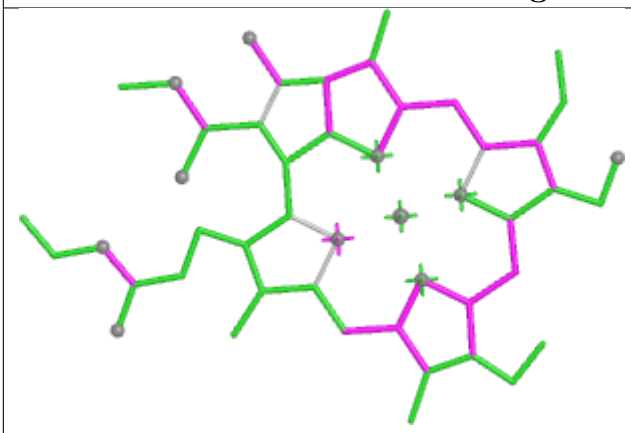
Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

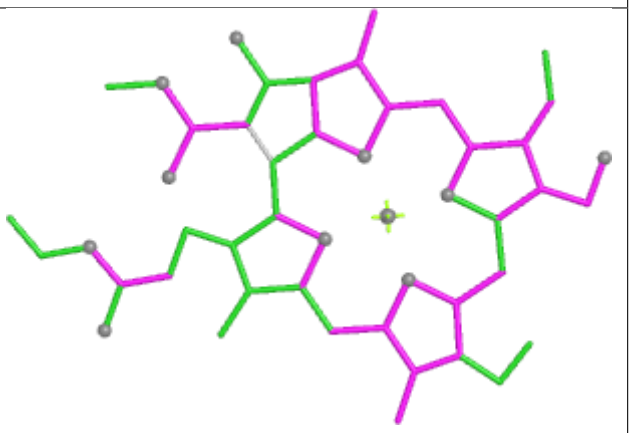
Ligand CLA B 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT p 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

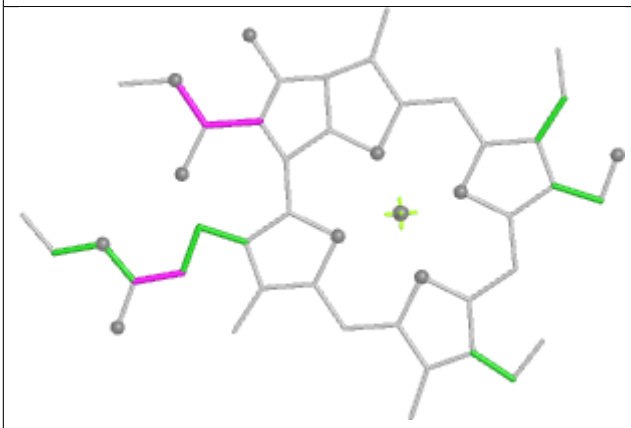
Ligand CHL s 513



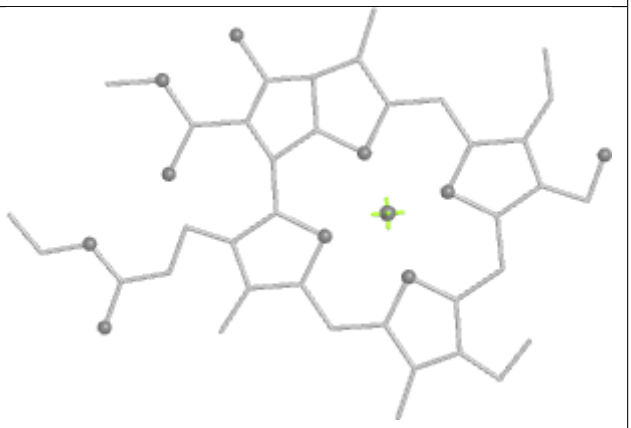
Bond lengths



Bond angles

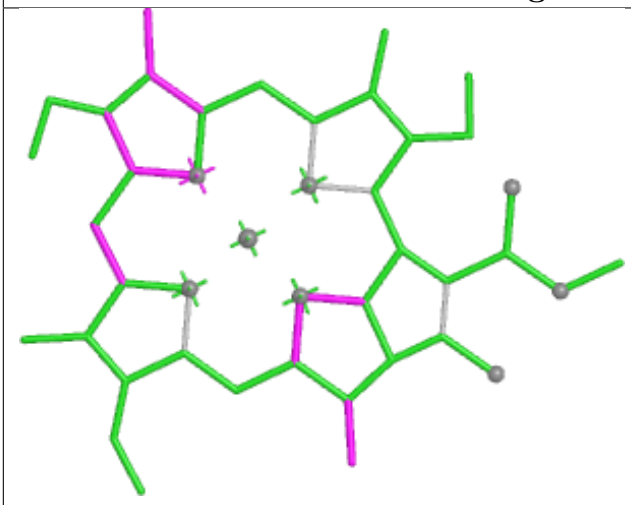


Torsions

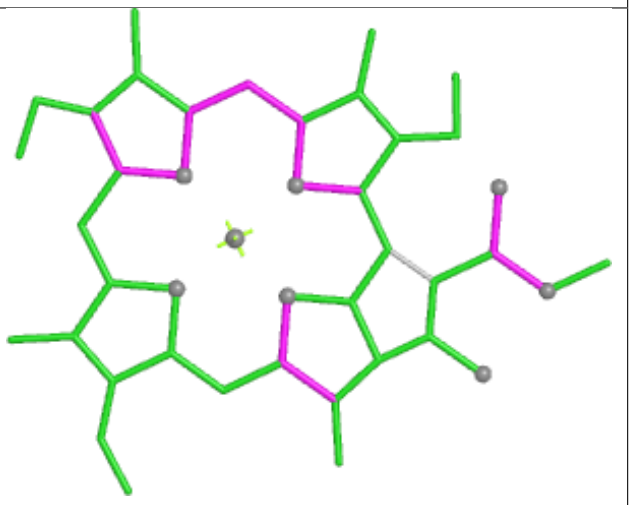


Rings

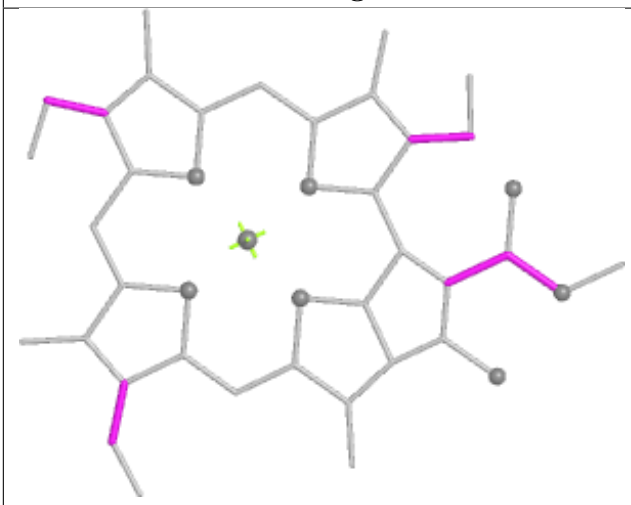
Ligand CLA J 101



Bond lengths



Bond angles

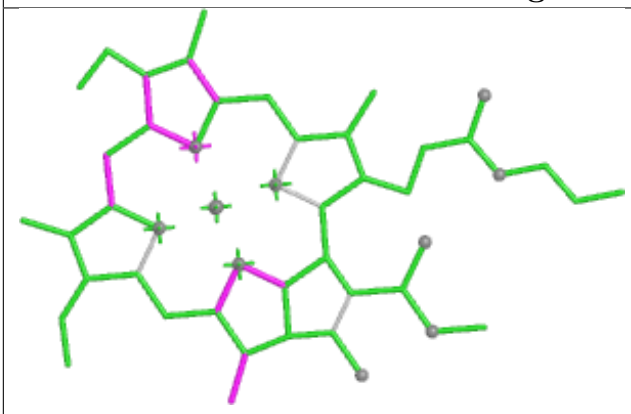


Torsions

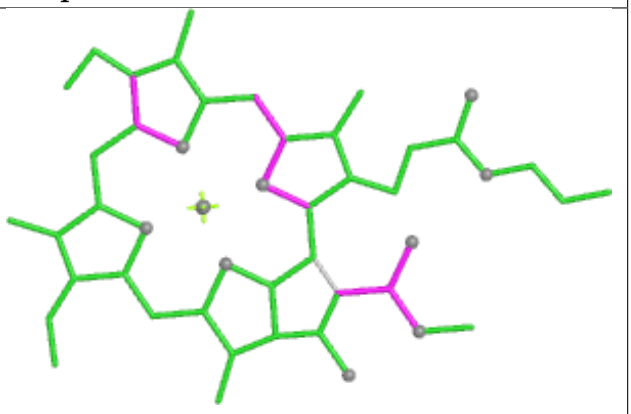


Rings

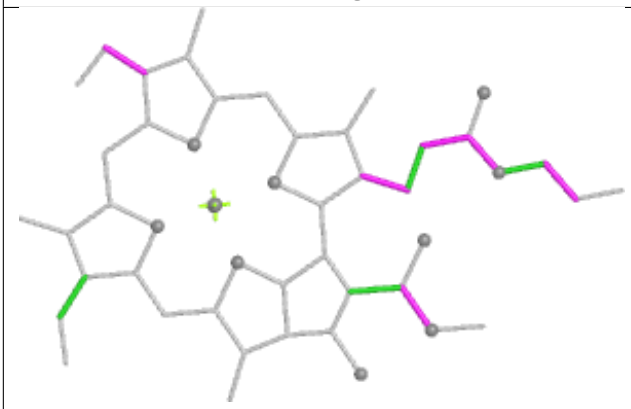
Ligand CLA q 311



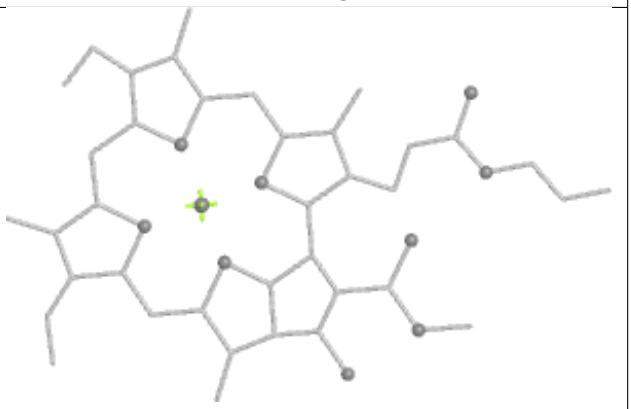
Bond lengths



Bond angles

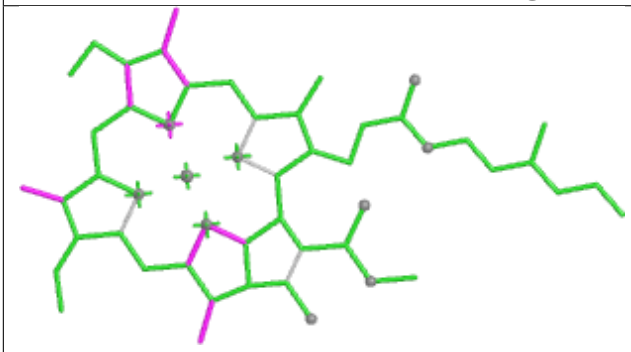


Torsions

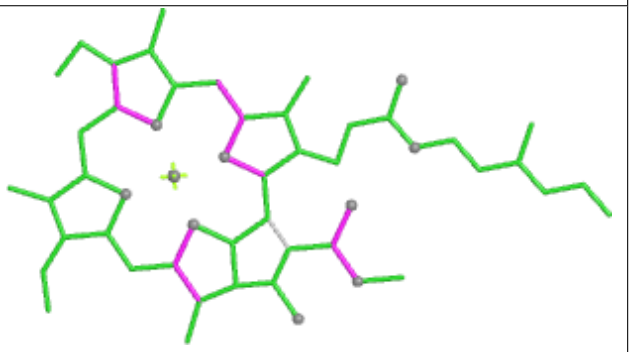


Rings

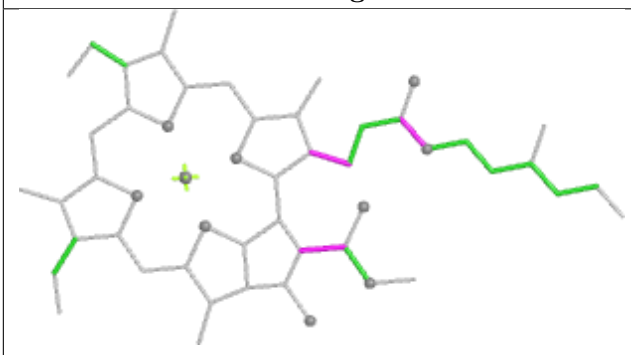
Ligand CLA A 804



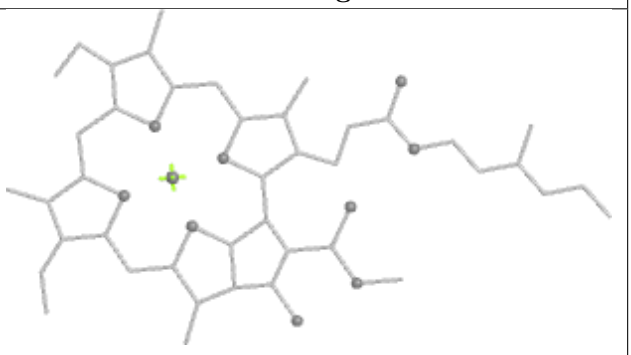
Bond lengths



Bond angles

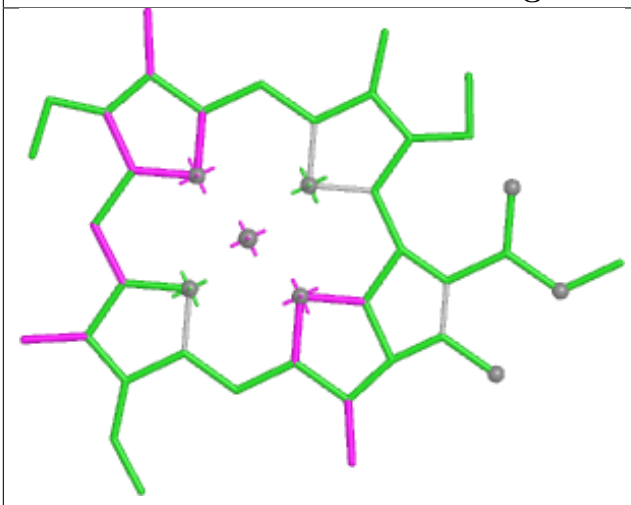


Torsions

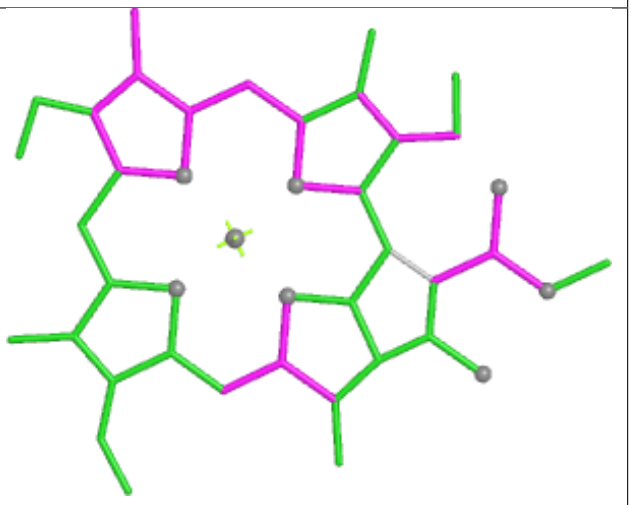


Rings

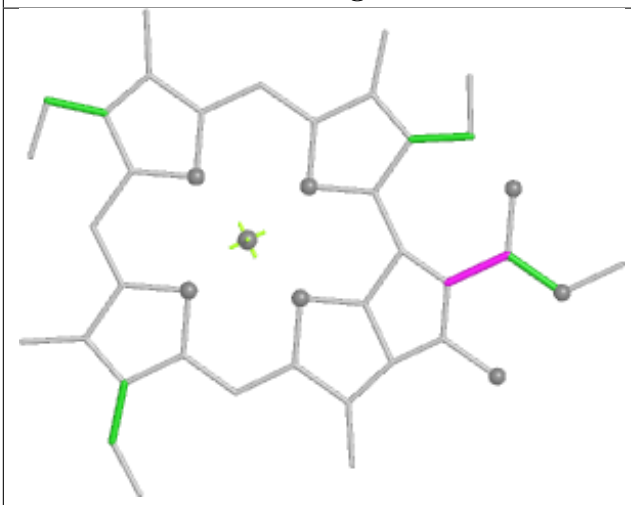
Ligand CLA A 812



Bond lengths



Bond angles



Torsions

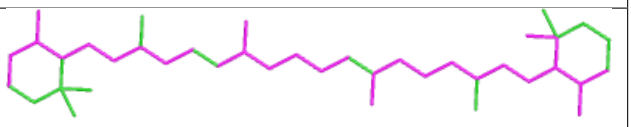


Rings

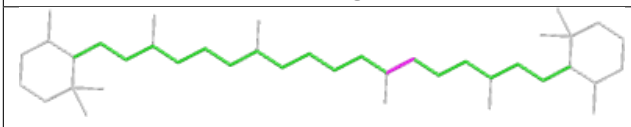
Ligand BCR B 848



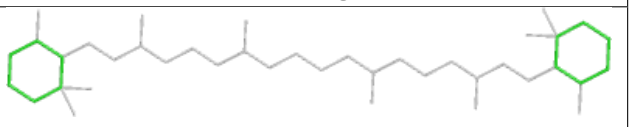
Bond lengths



Bond angles

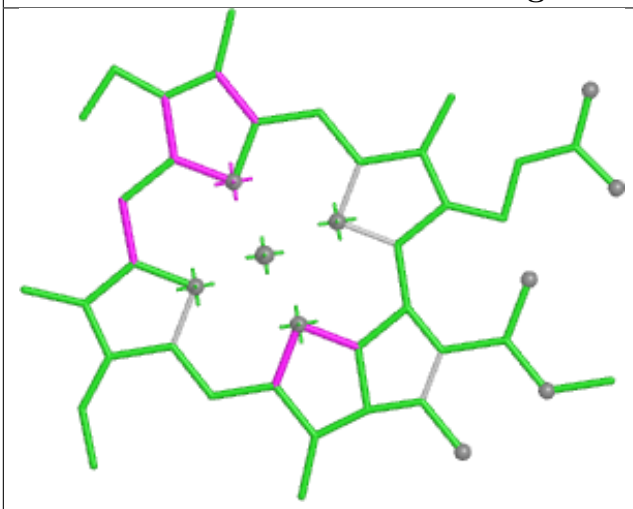


Torsions

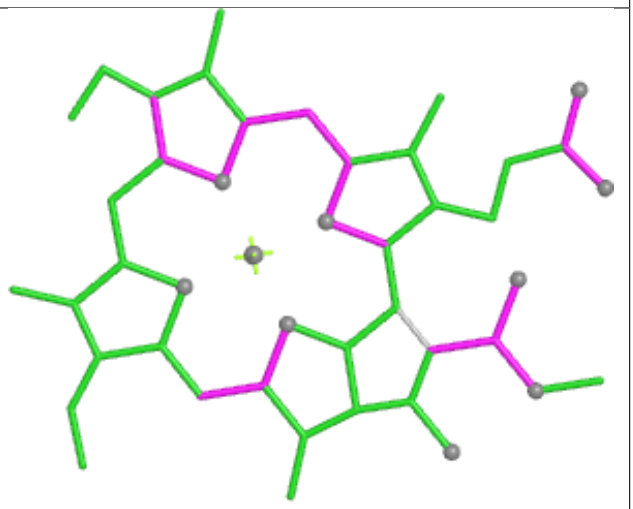


Rings

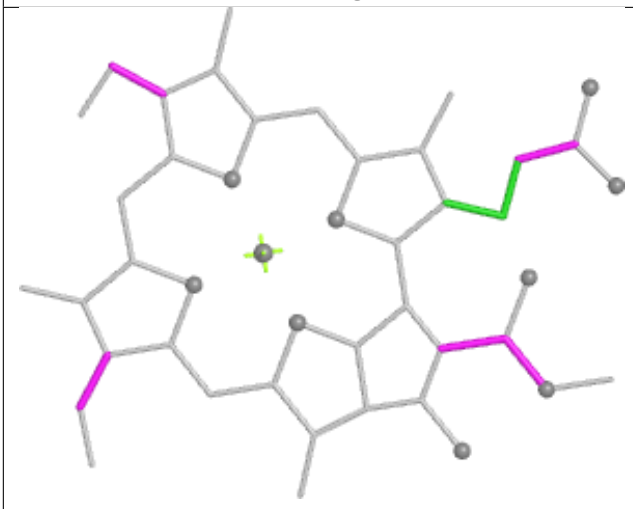
Ligand CLA n 202



Bond lengths



Bond angles

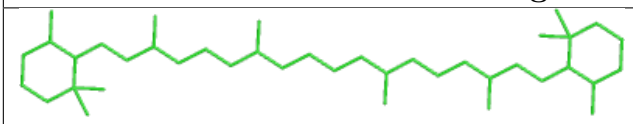


Torsions

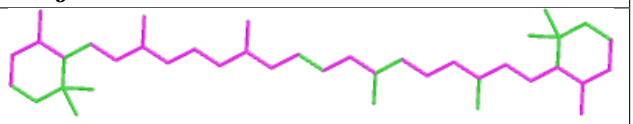


Rings

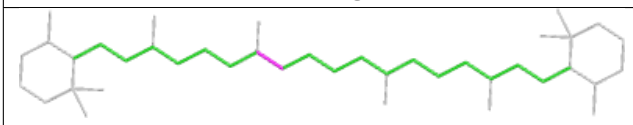
Ligand BCR j 803



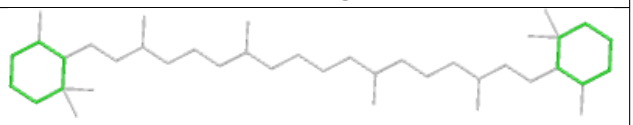
Bond lengths



Bond angles

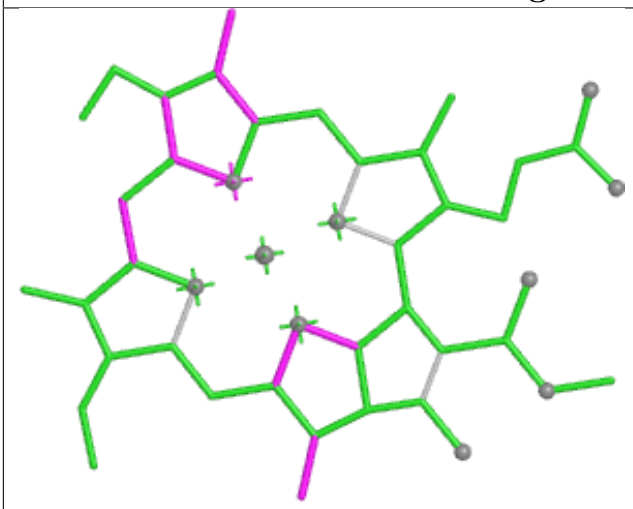


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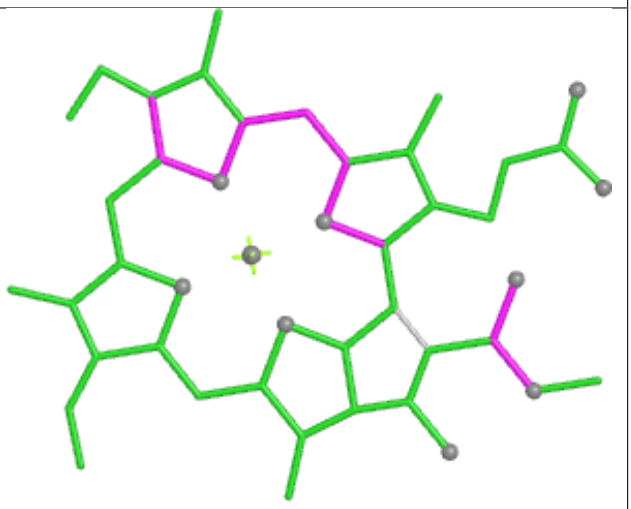


Rings

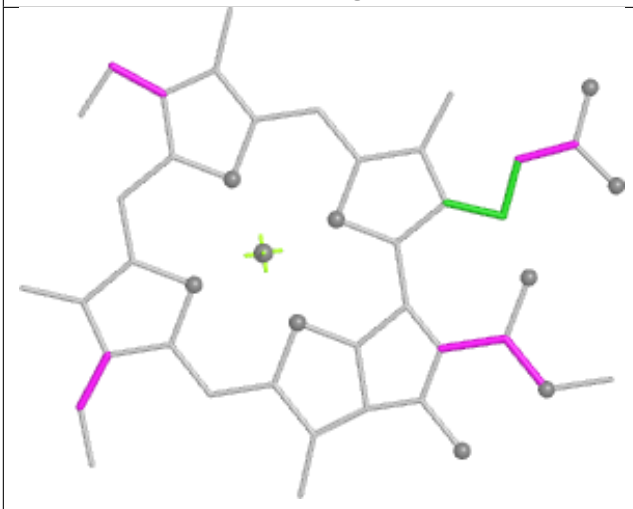
Ligand CLA e 815



Bond lengths



Bond angles

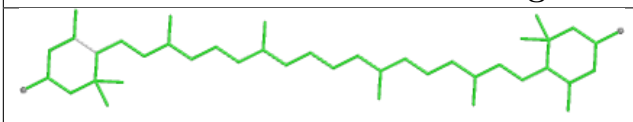


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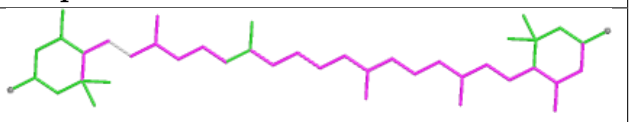


Rings

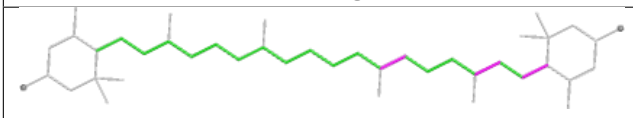
Ligand LUT q 302



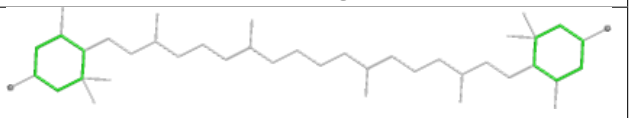
Bond lengths



Bond angles

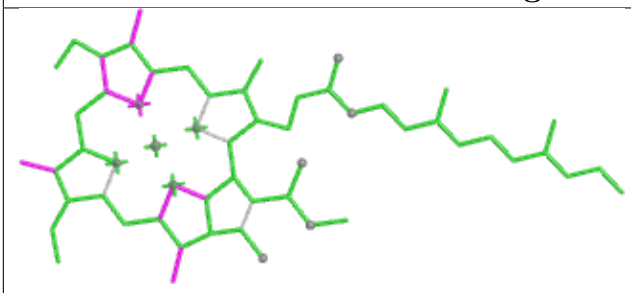


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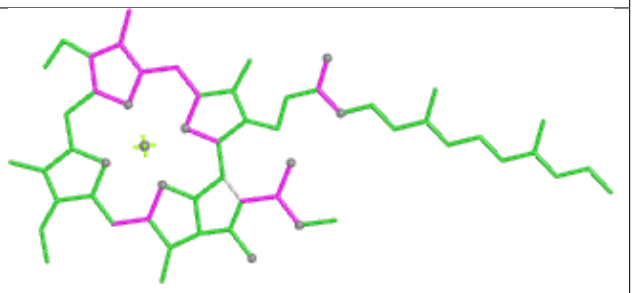


Rings

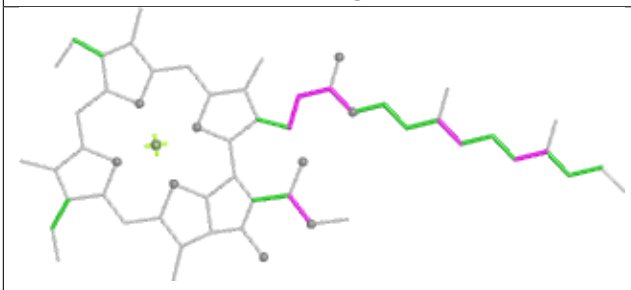
Ligand CLA A 820



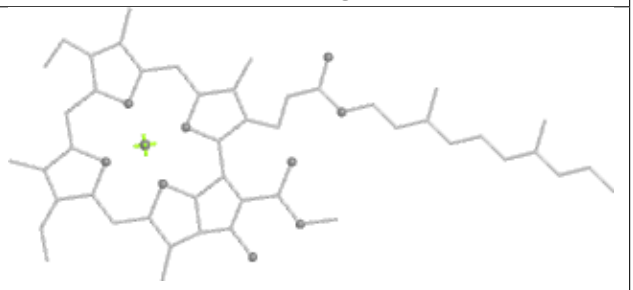
Bond lengths



Bond angles

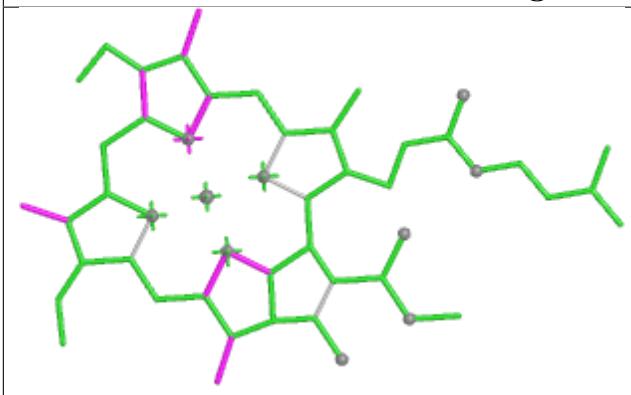


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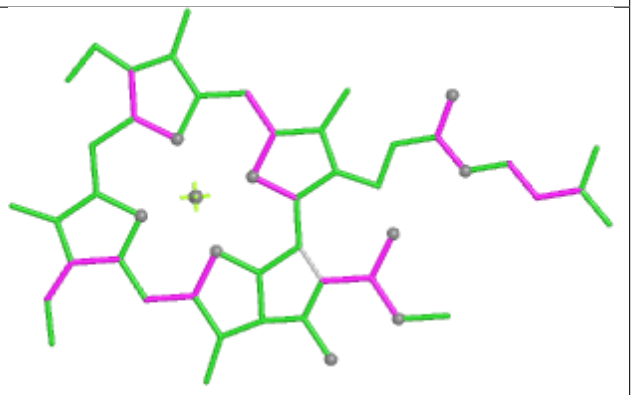


Rings

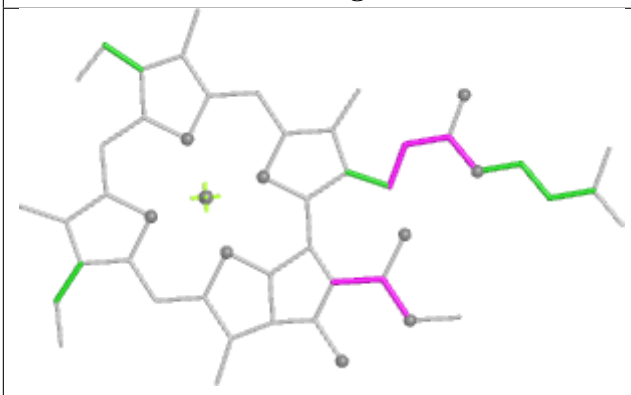
Ligand CLA 3 311



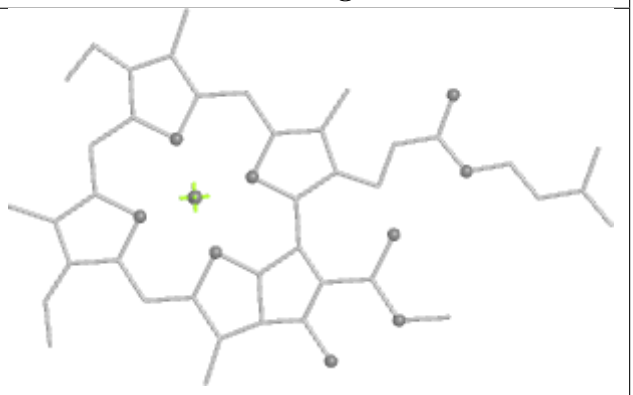
Bond lengths



Bond angles

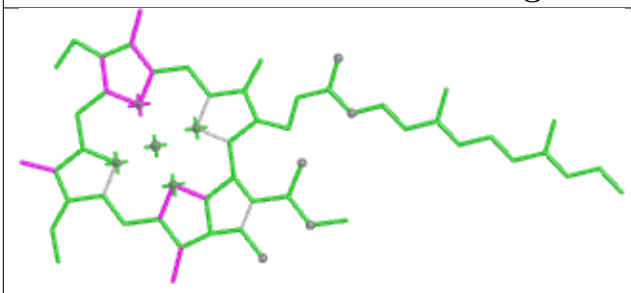


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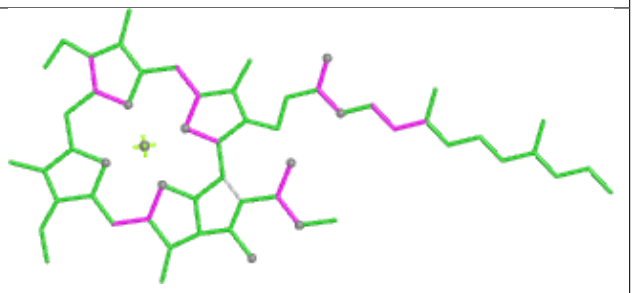


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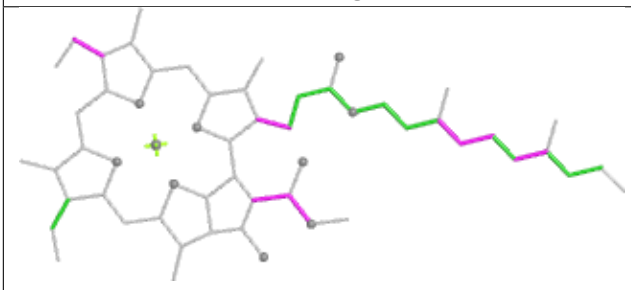
Ligand CLA A 852



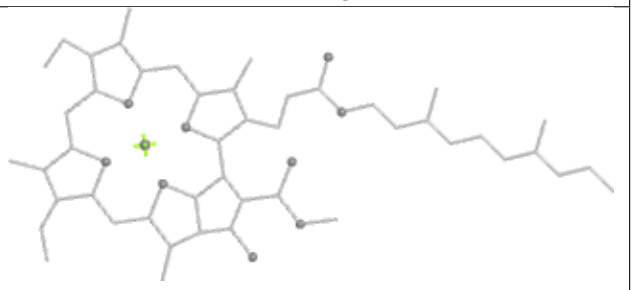
Bond lengths



Bond angles

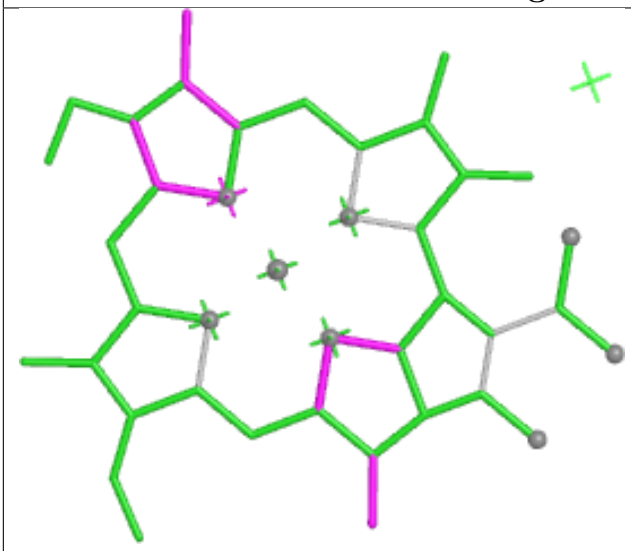


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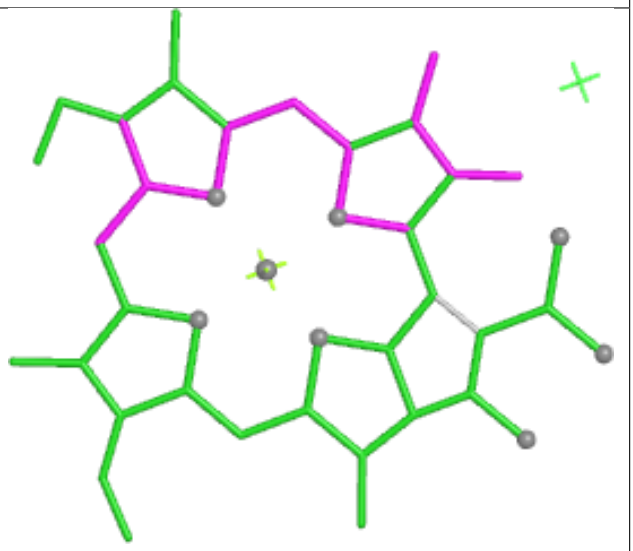


Rings

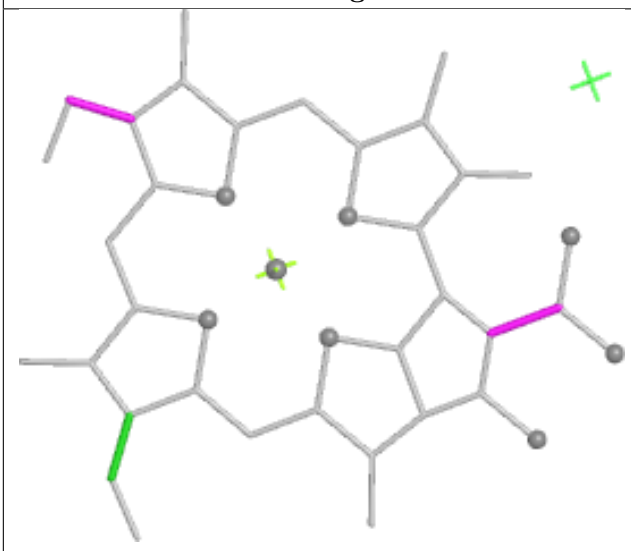
Ligand CLA 5 306



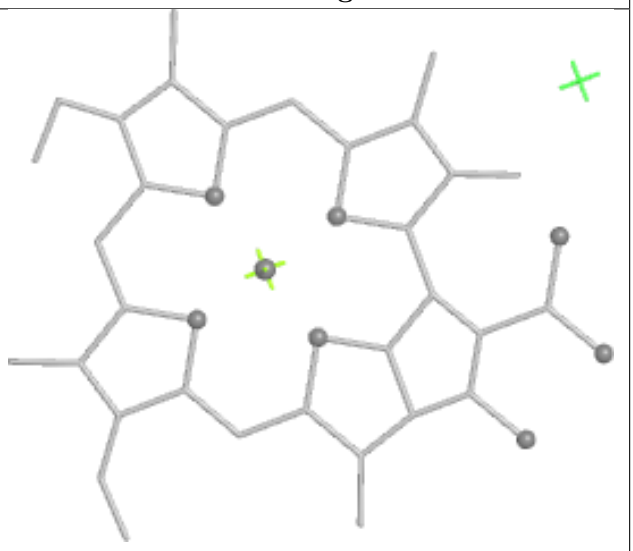
Bond lengths



Bond angles

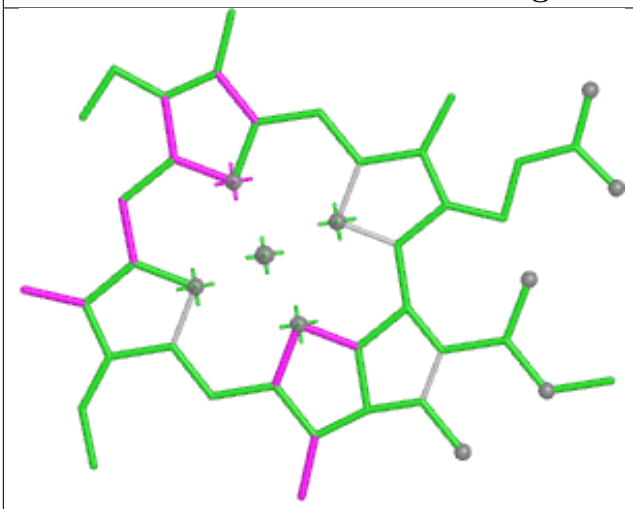


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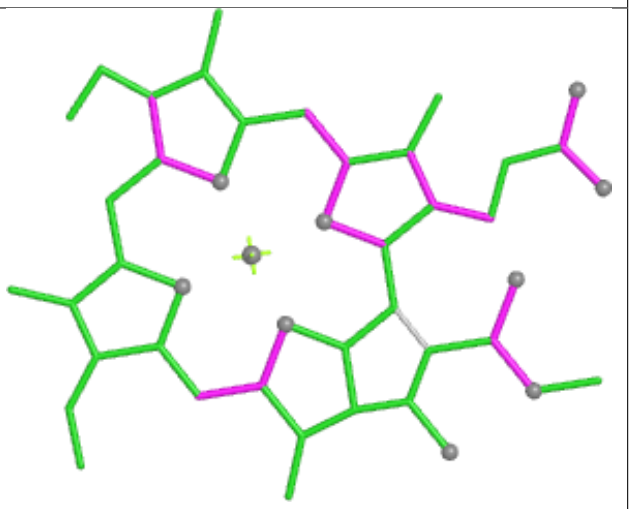


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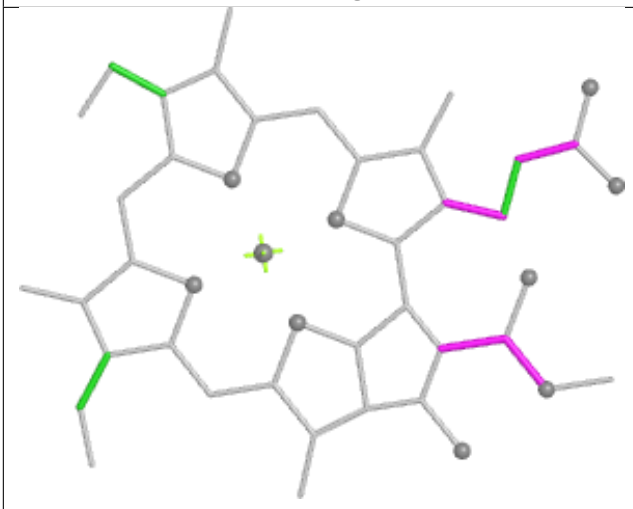
Ligand CLA f 835



Bond lengths



Bond angles

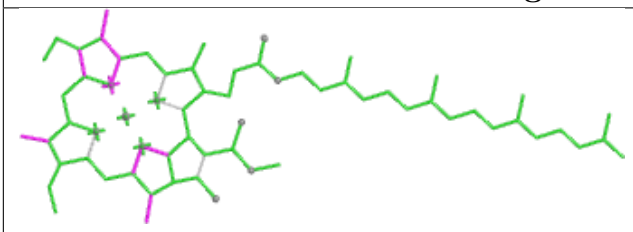


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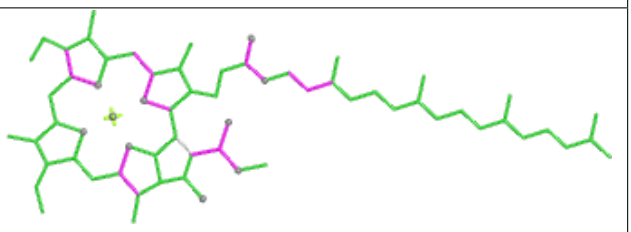


Rings

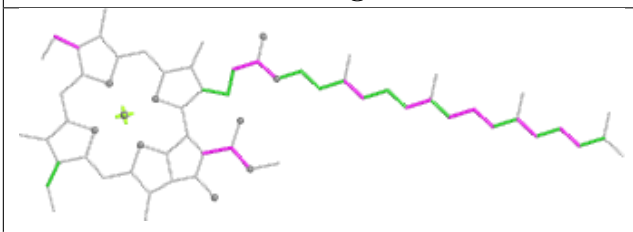
Ligand CLA B 803



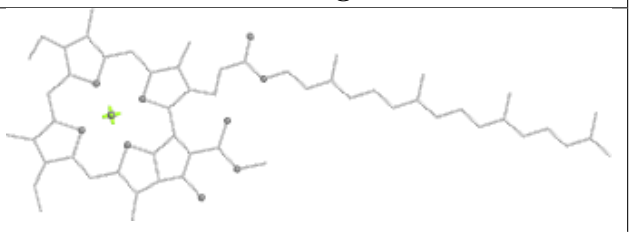
Bond lengths



Bond angles

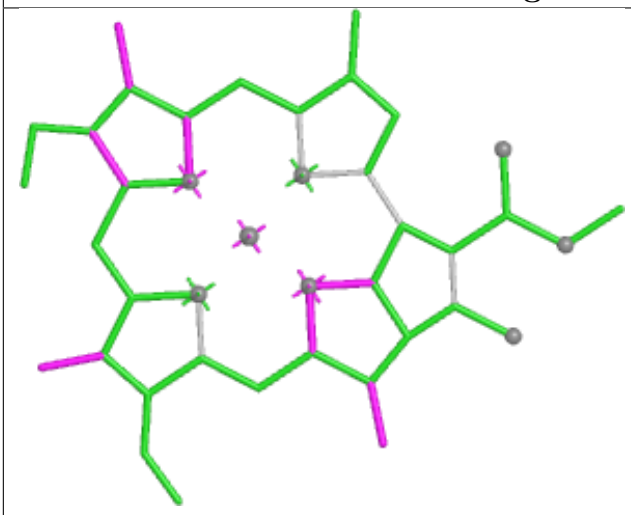


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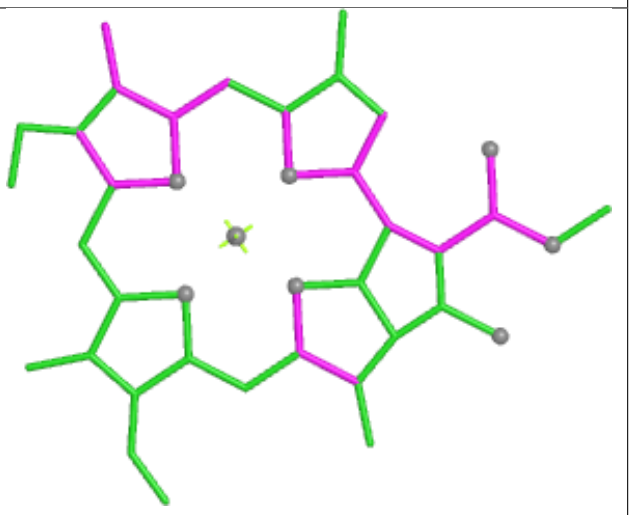


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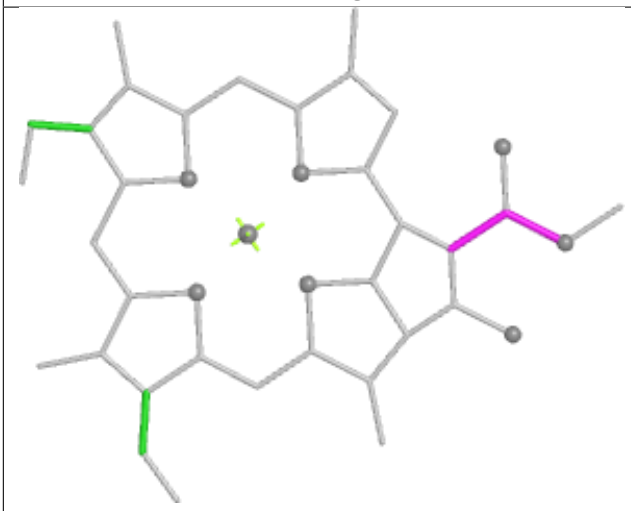
Ligand CLA A 818



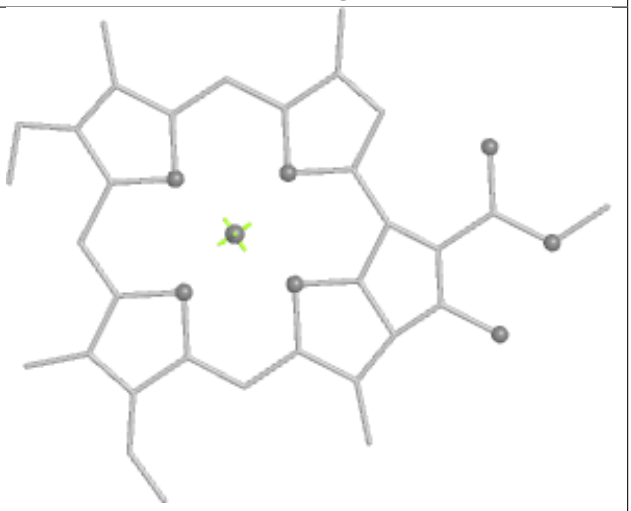
Bond lengths



Bond angles



Torsions

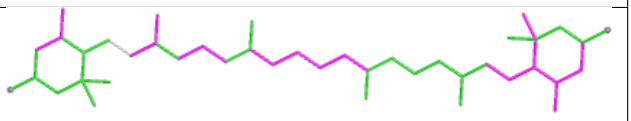


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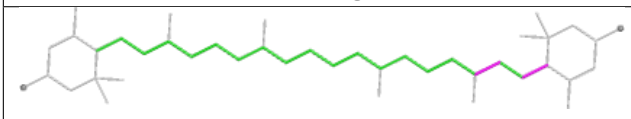
Ligand LUT 1 502



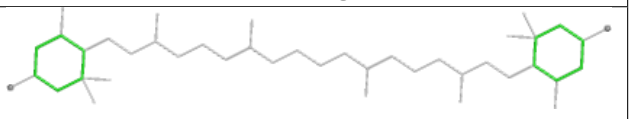
Bond lengths



Bond angles

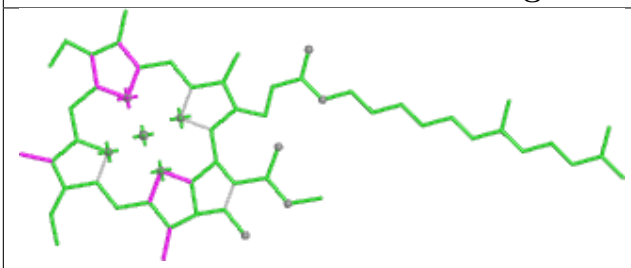


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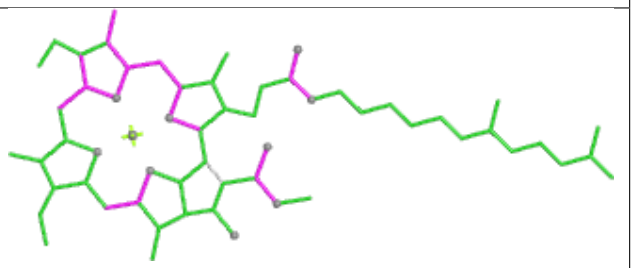


Rings

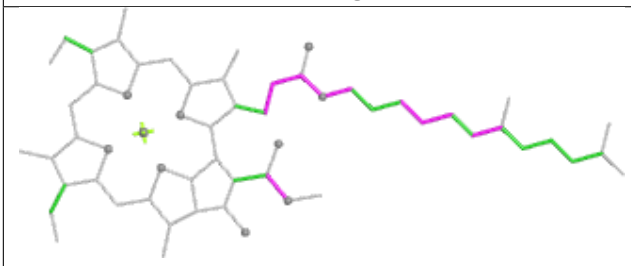
Ligand CLA A 816



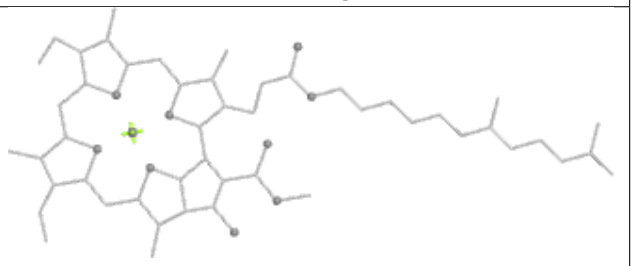
Bond lengths



Bond angles

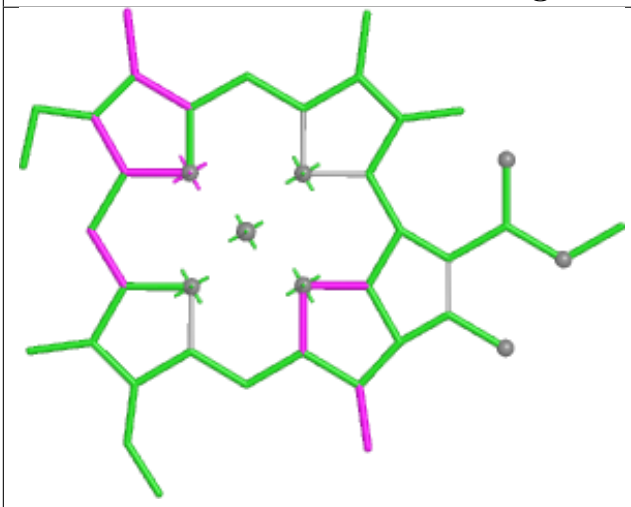


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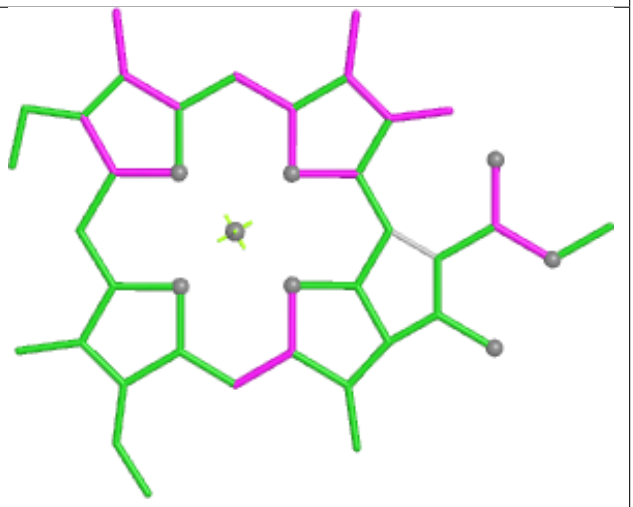


Rings

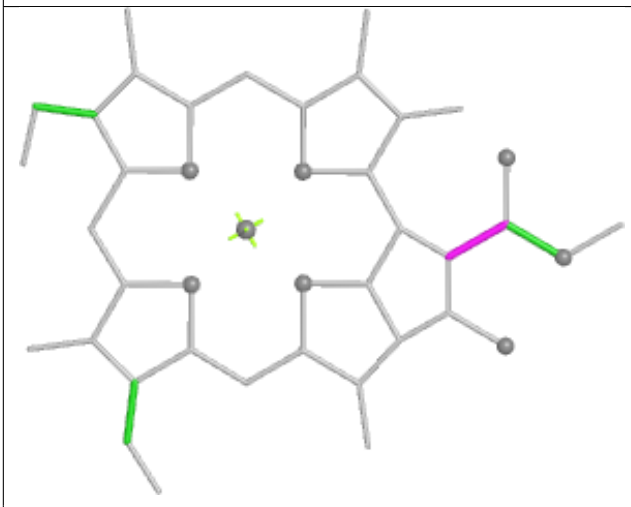
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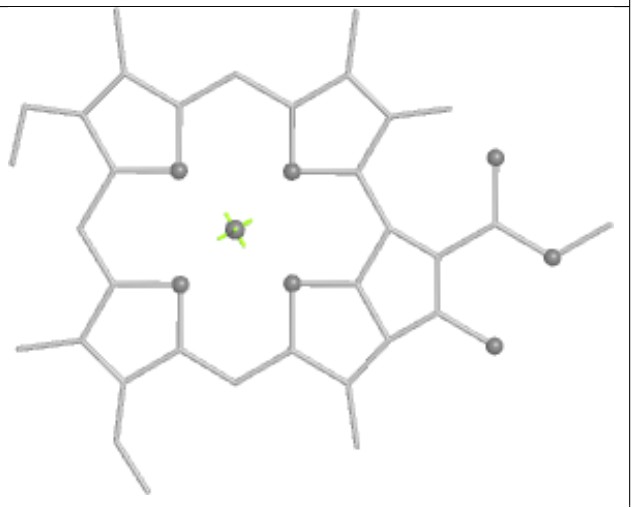
Bond lengths



Bond angles

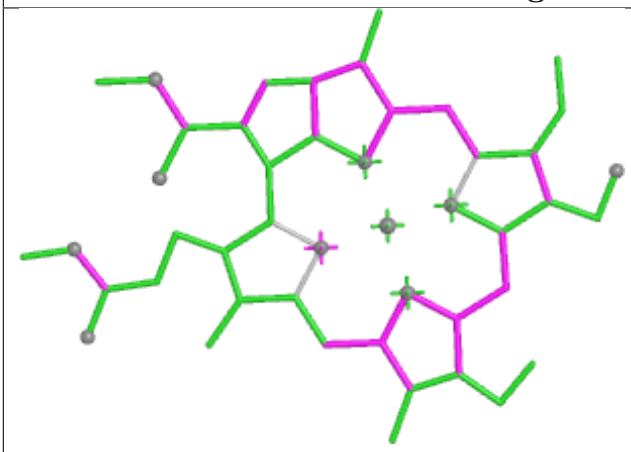


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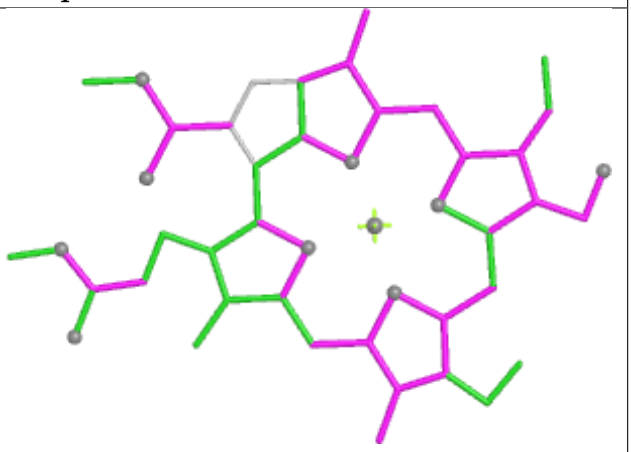


Rings

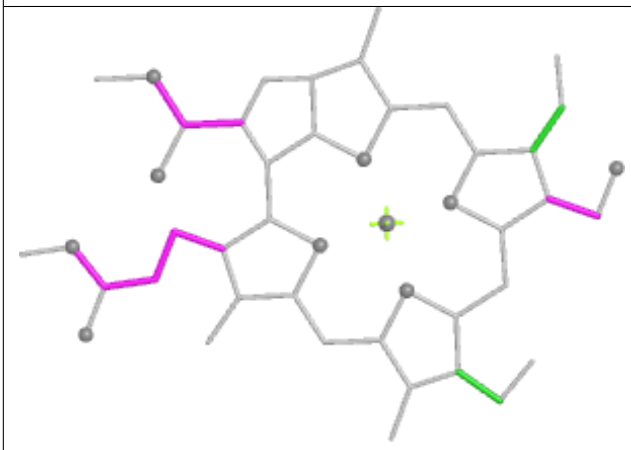
Ligand CHL q 313



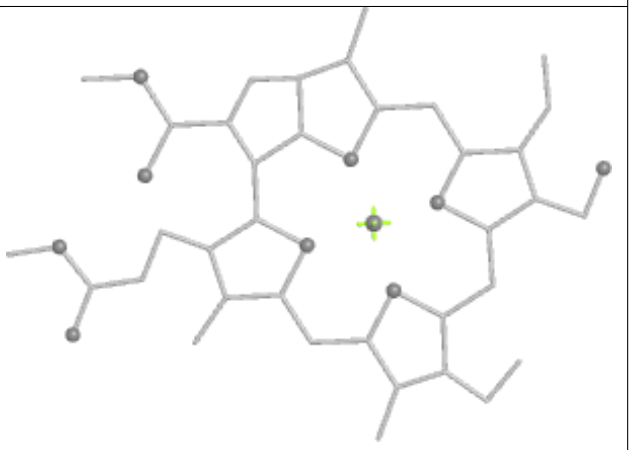
Bond lengths



Bond angles

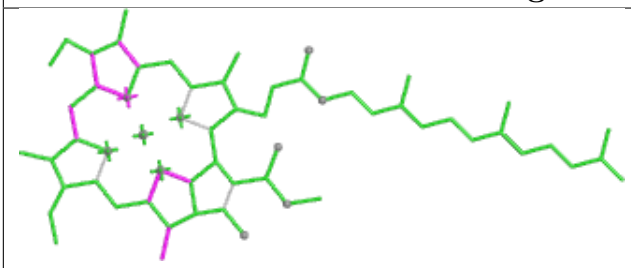


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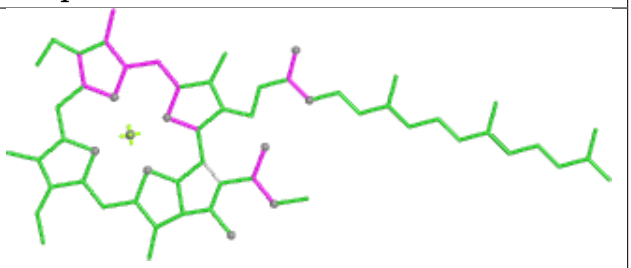


Rings

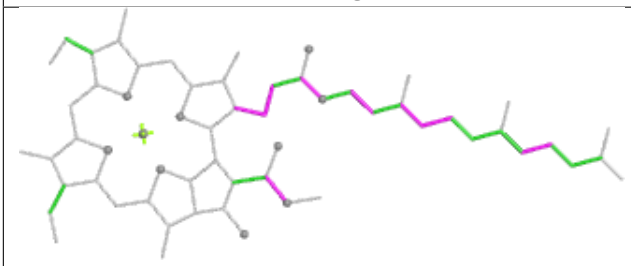
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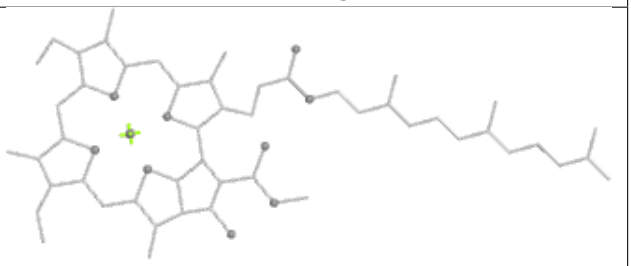
Bond lengths



Bond angles

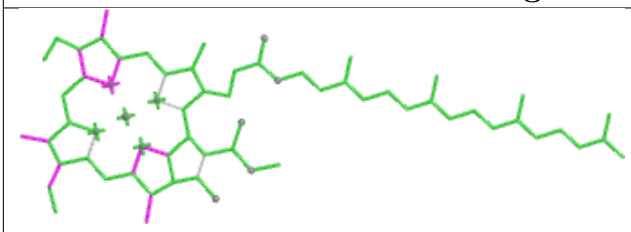


Torsions

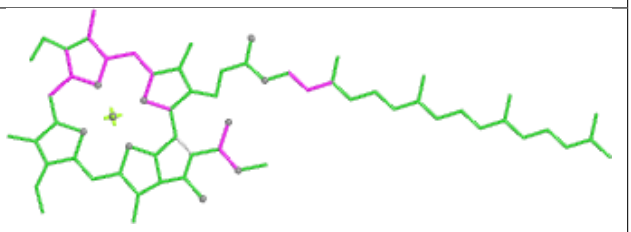


Rings

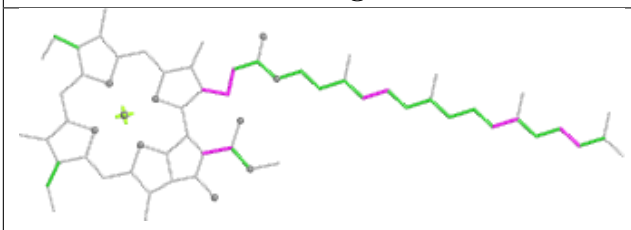
Ligand CLA A 808



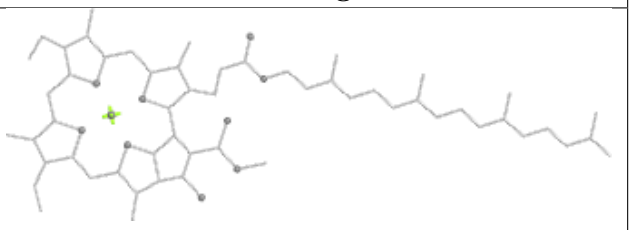
Bond lengths



Bond angles

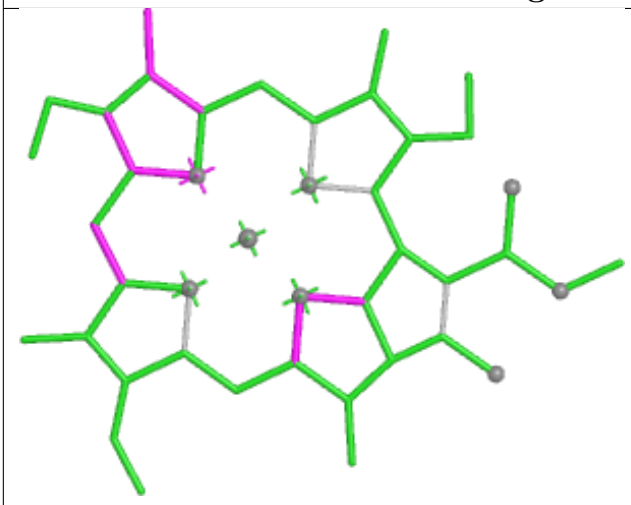


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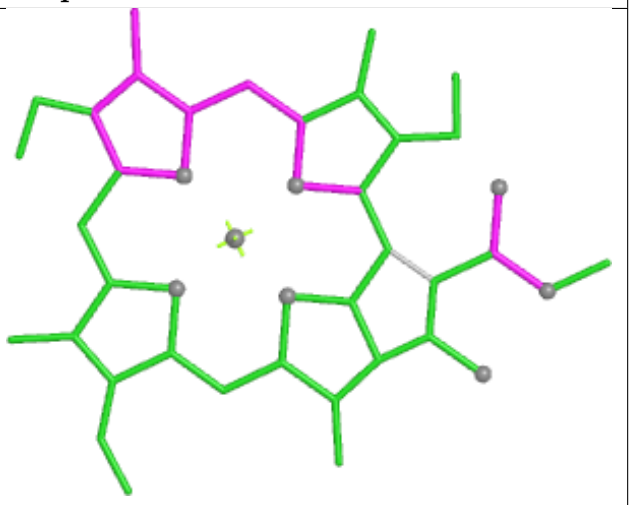


Rings

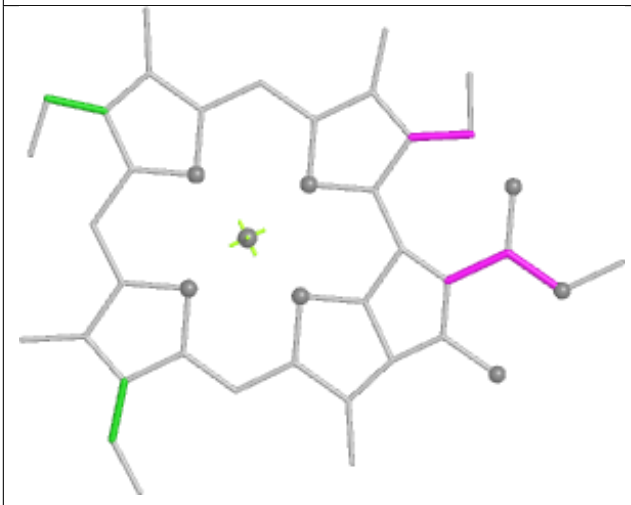
Ligand CLA q 308



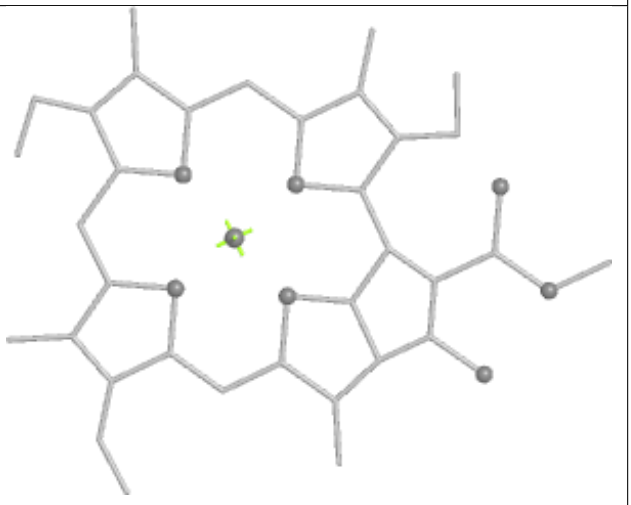
Bond lengths



Bond angles

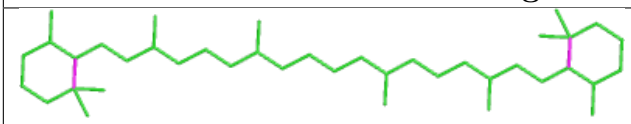


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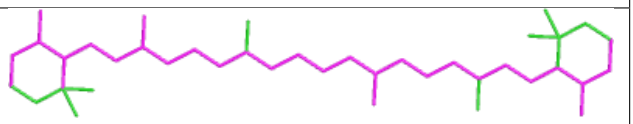


Rings

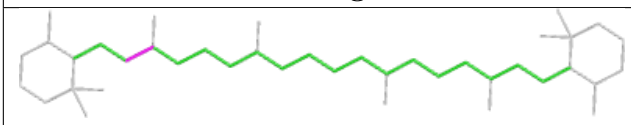
Ligand BCR A 847



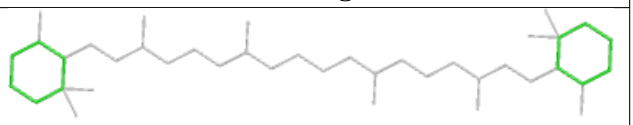
Bond lengths



Bond angles

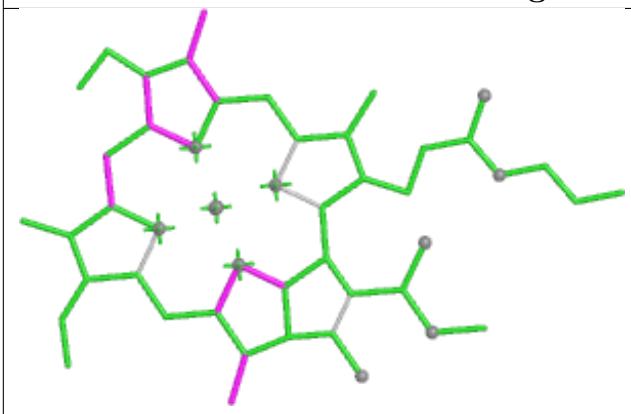


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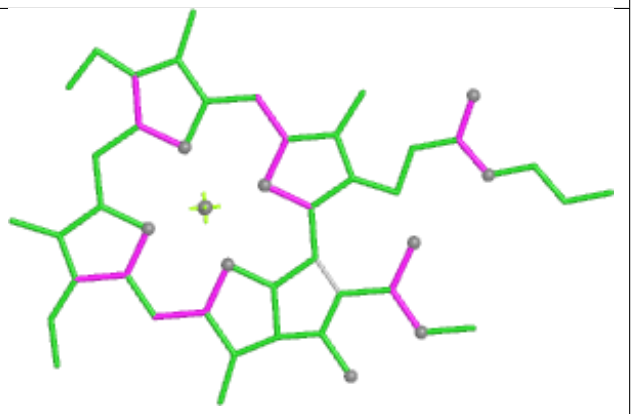


Rings

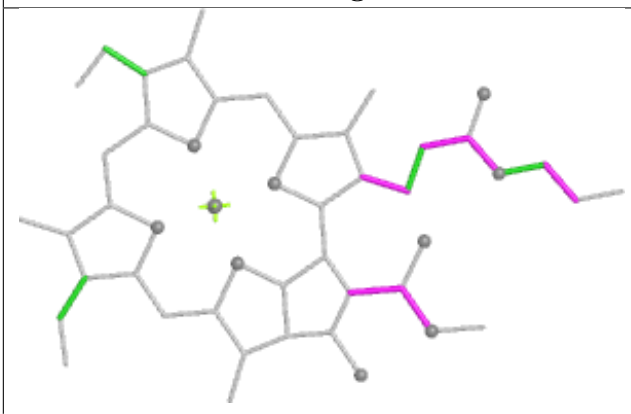
Ligand CLA 3 313



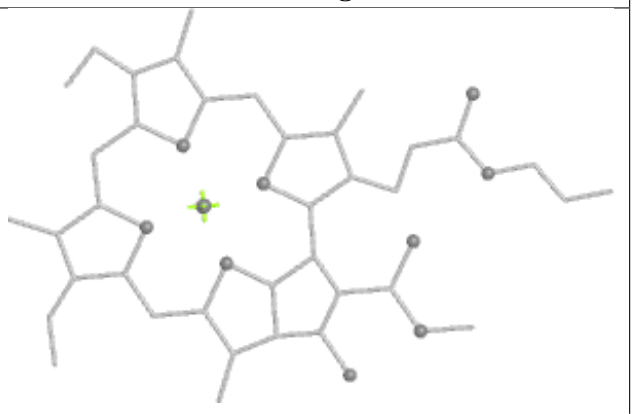
Bond lengths



Bond angles

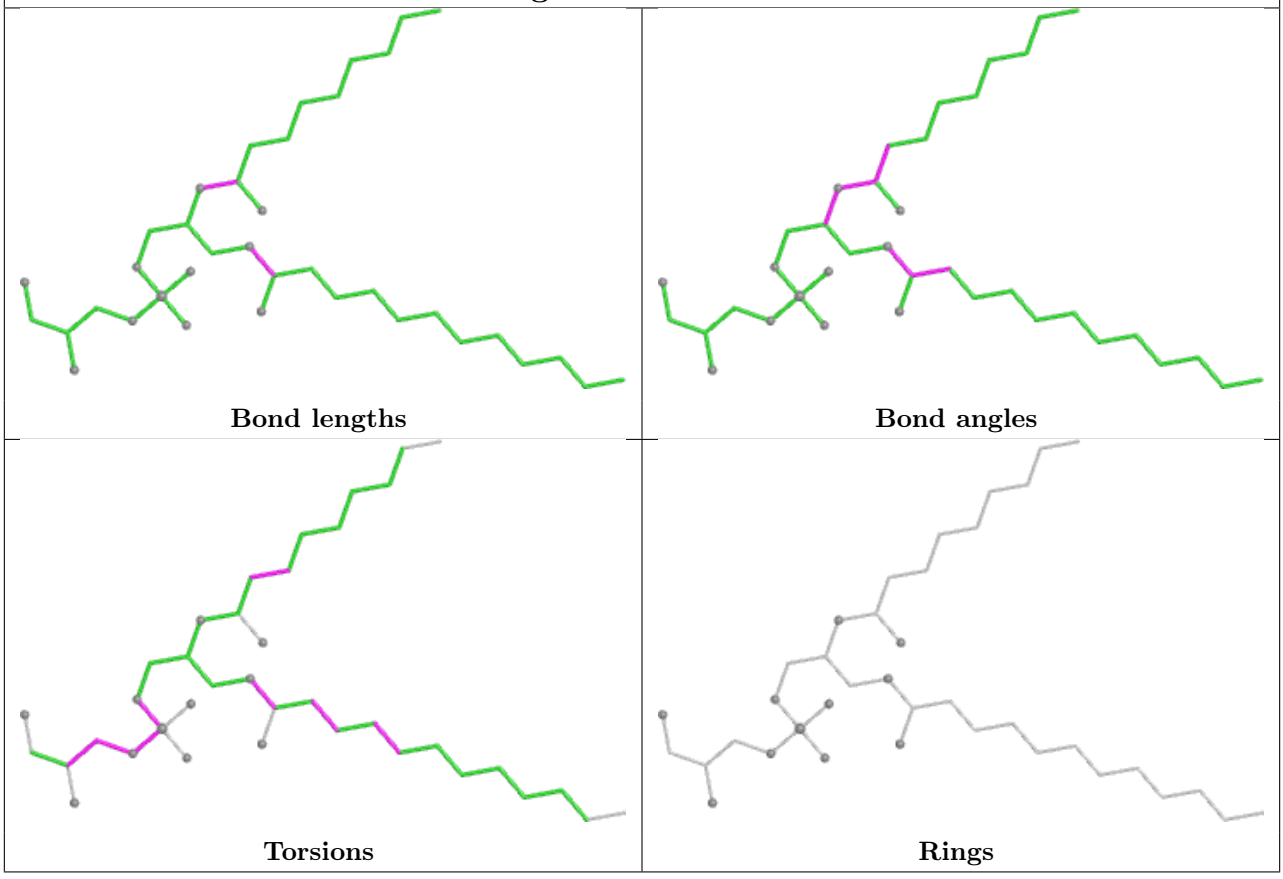


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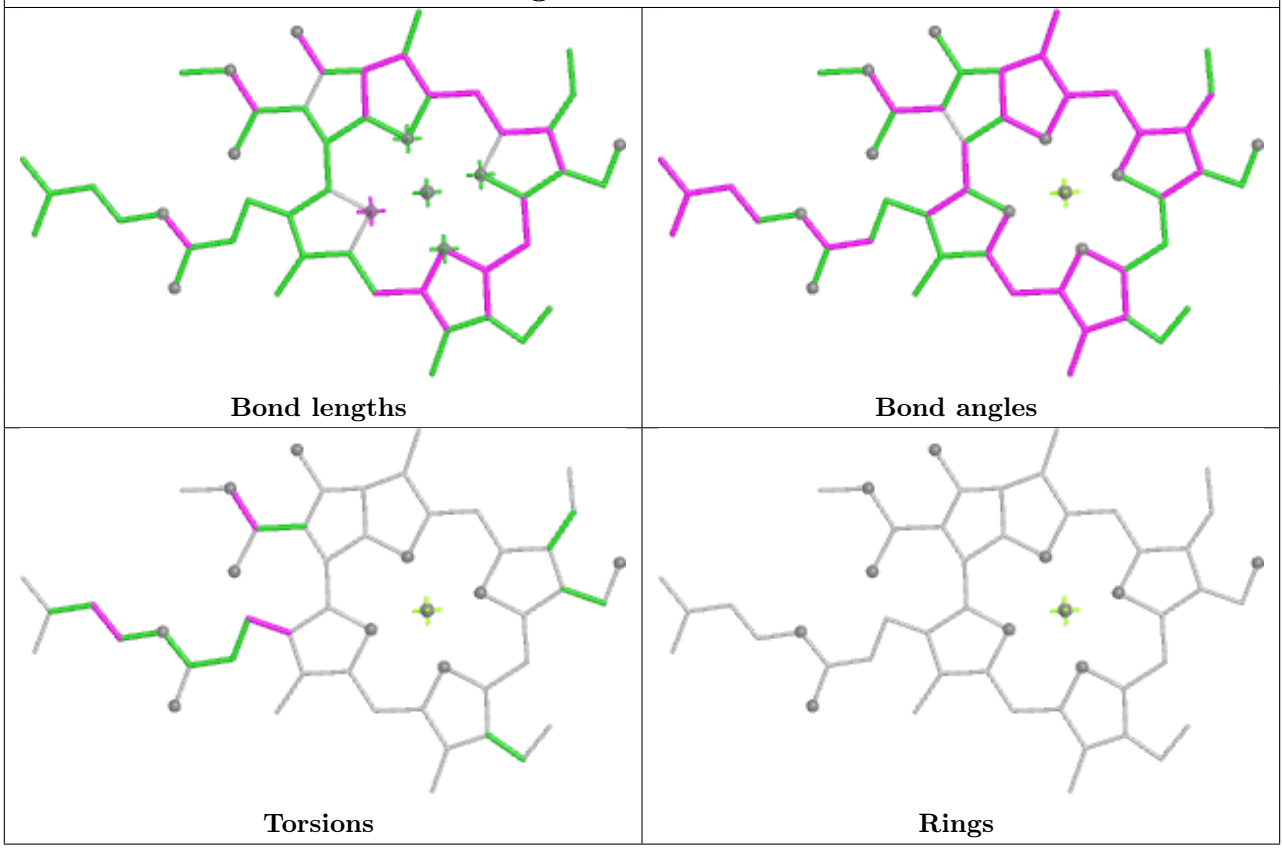


Rings

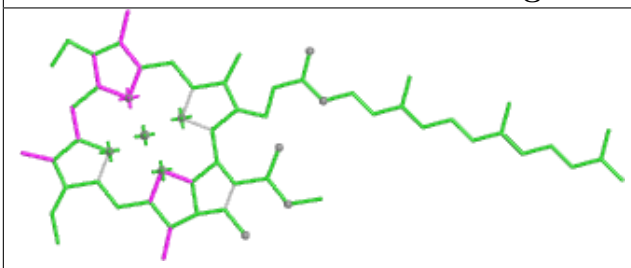
Ligand LHG f 852



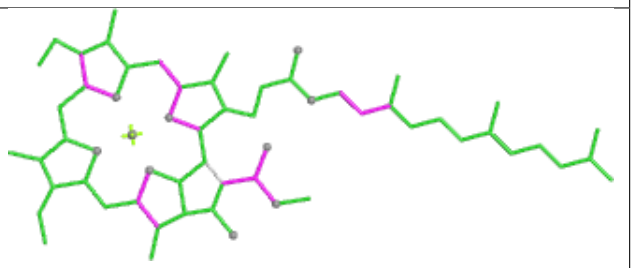
Ligand CHL r 314



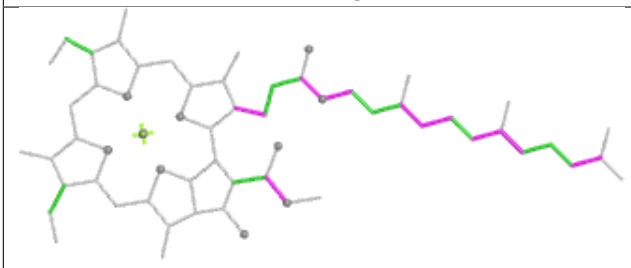
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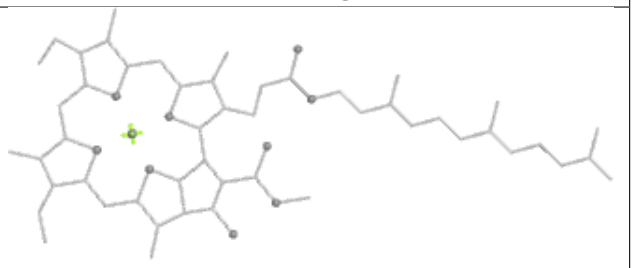
Bond lengths



Bond angles

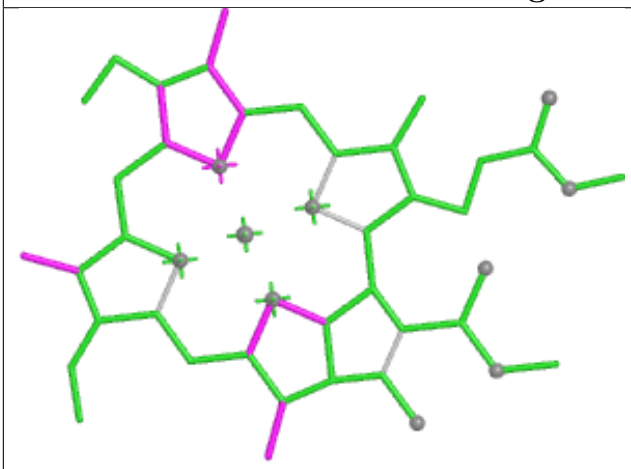


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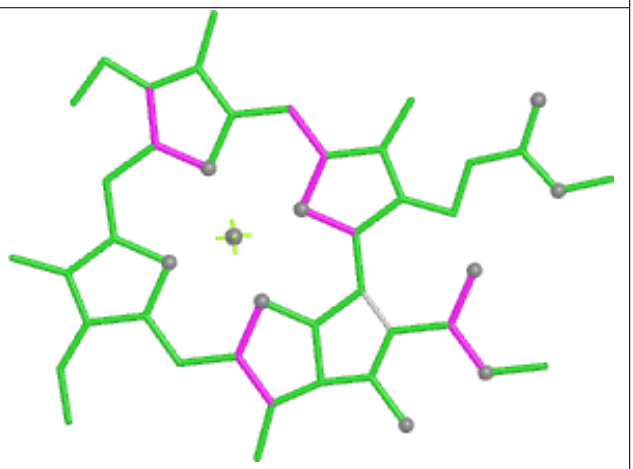


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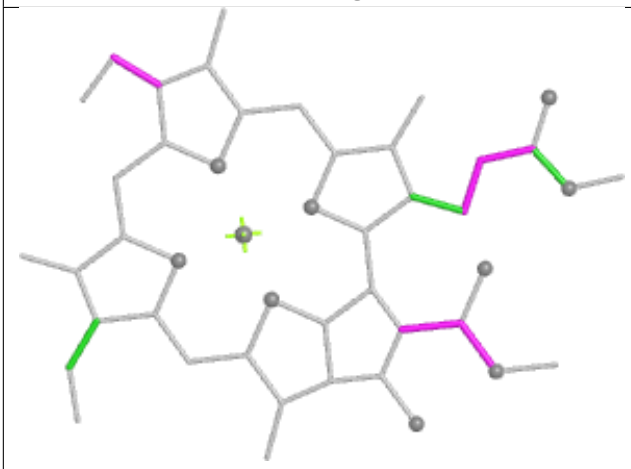
Ligand CLA 5 312



Bond lengths



Bond angles

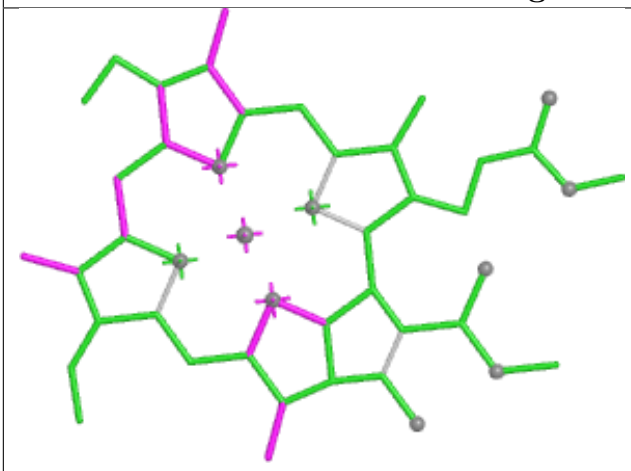


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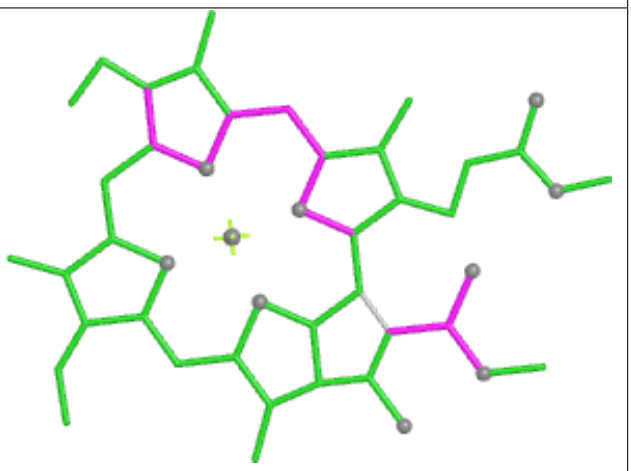


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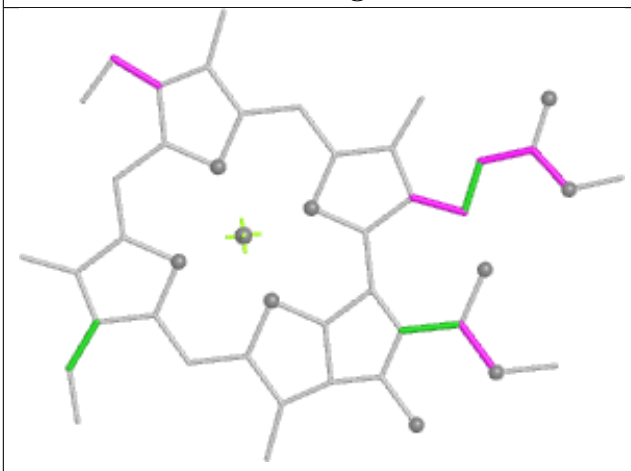
Ligand CLA 1 510



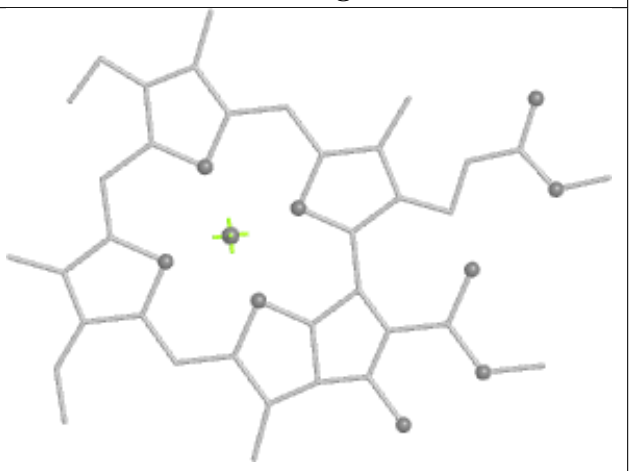
Bond lengths



Bond angles

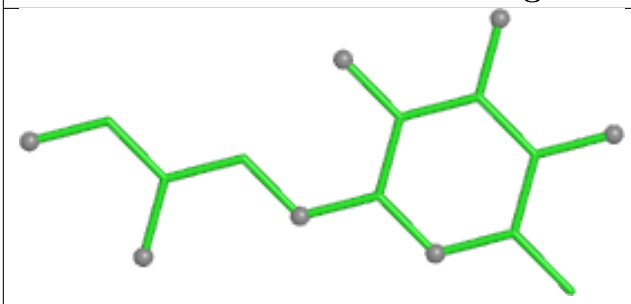


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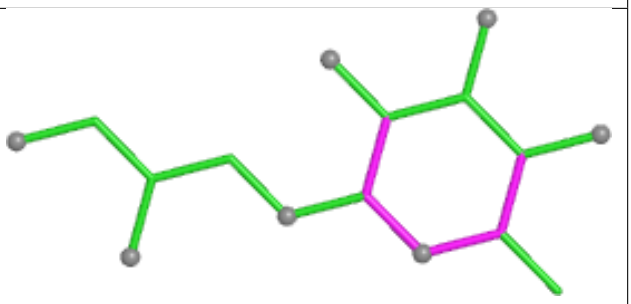


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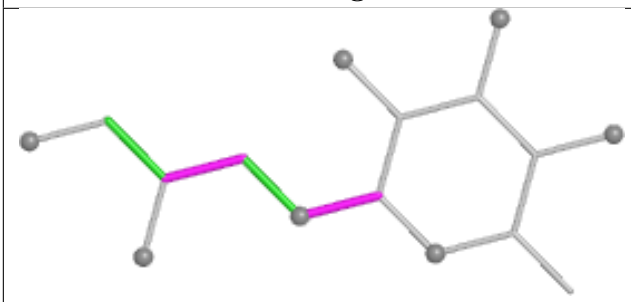
Ligand LMG 2 518



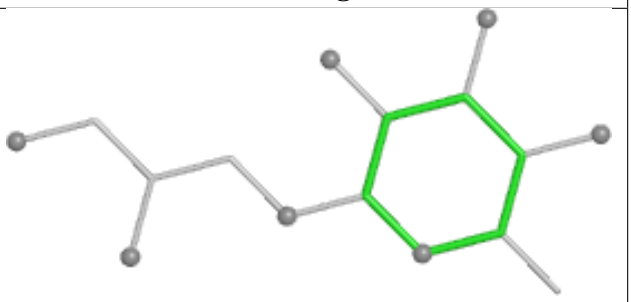
Bond lengths



Bond angles

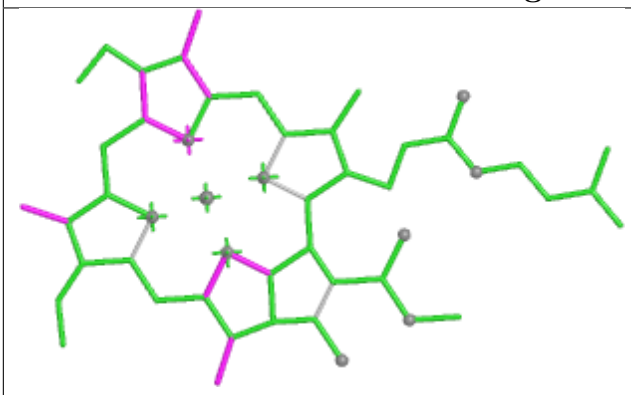


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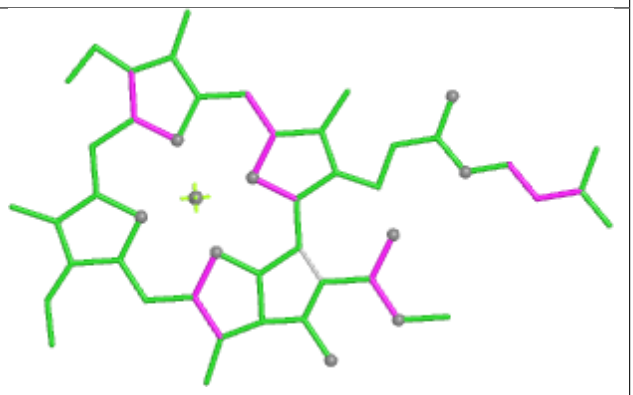


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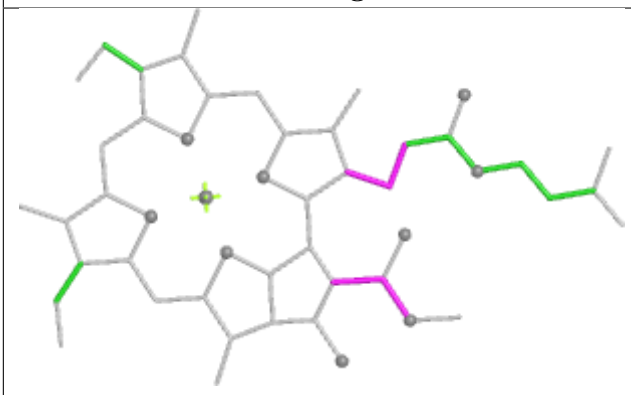
Ligand CLA B 821



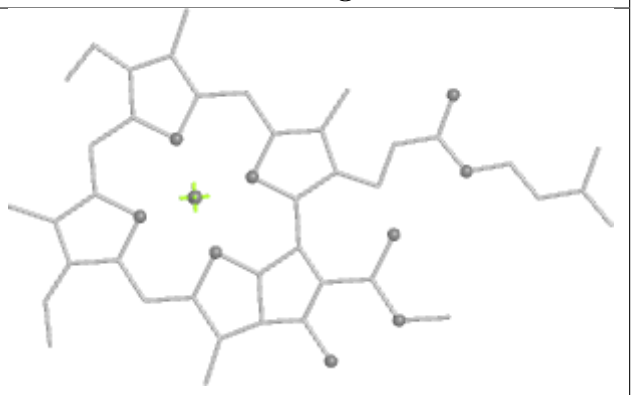
Bond lengths



Bond angles

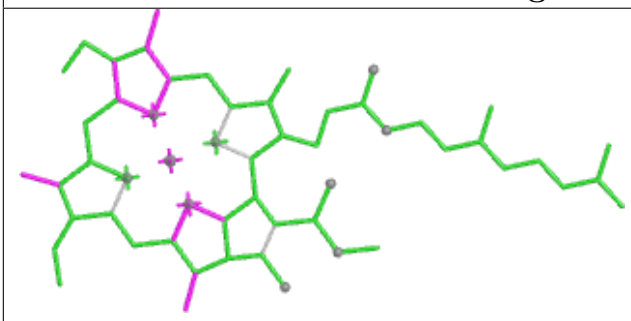


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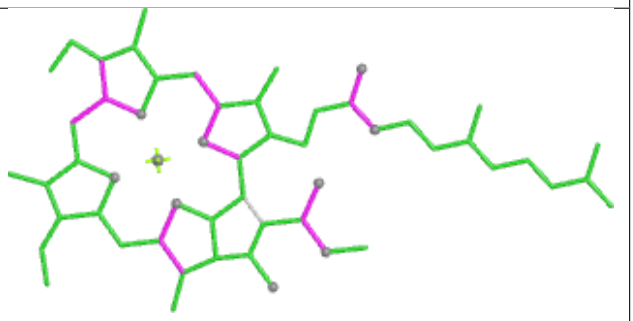


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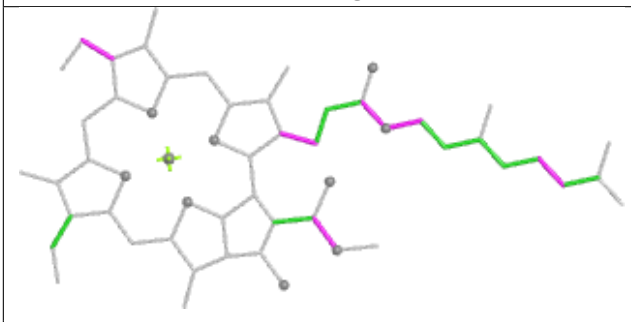
Ligand CLA 2 514



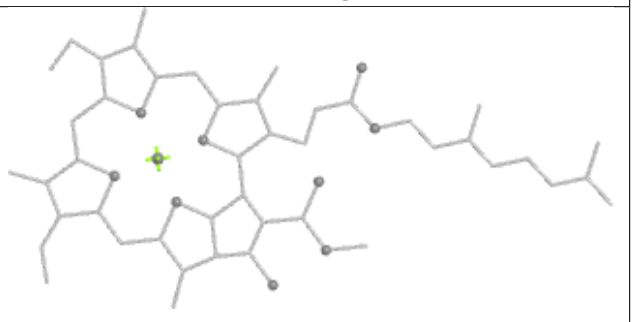
Bond lengths



Bond angles

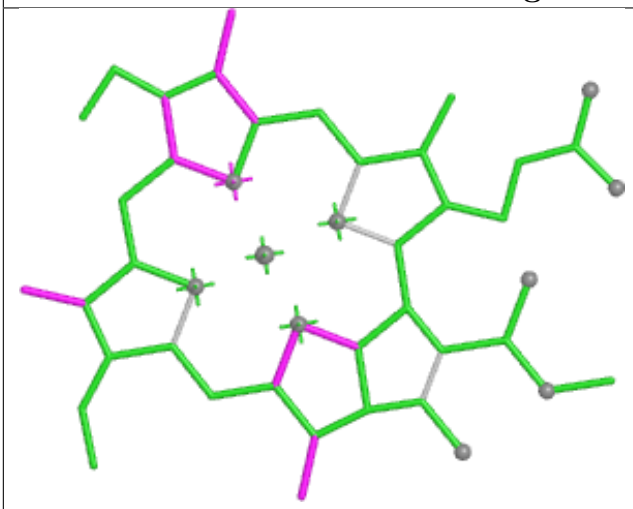


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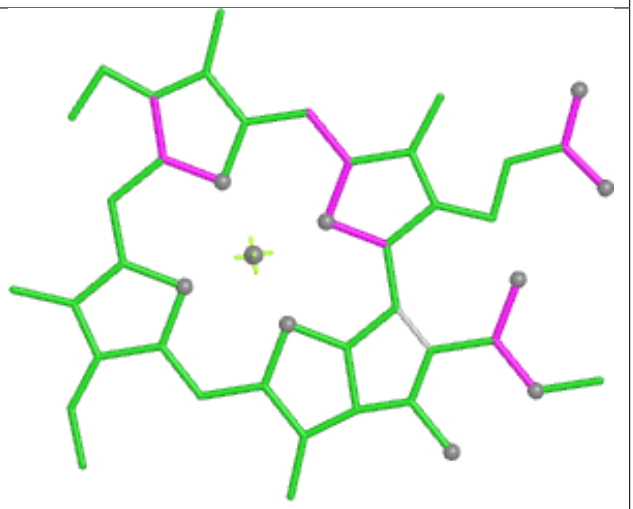


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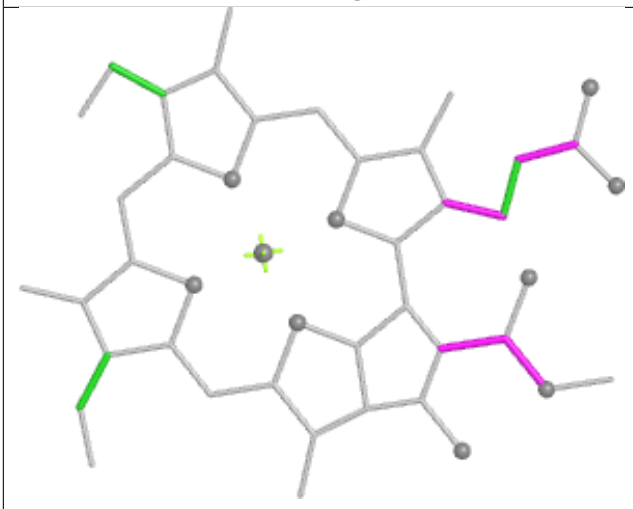
Ligand CLA A 813



Bond lengths



Bond angles

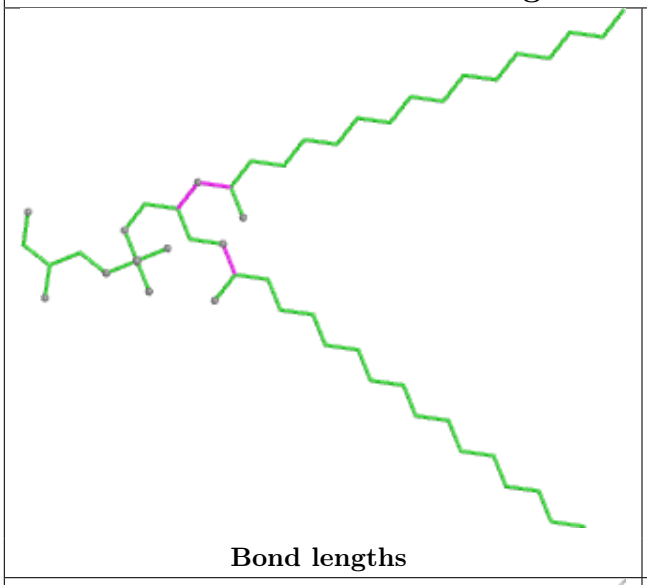


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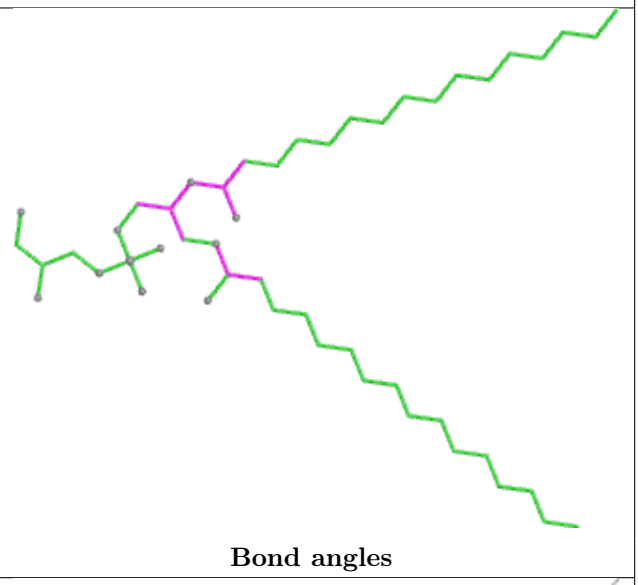


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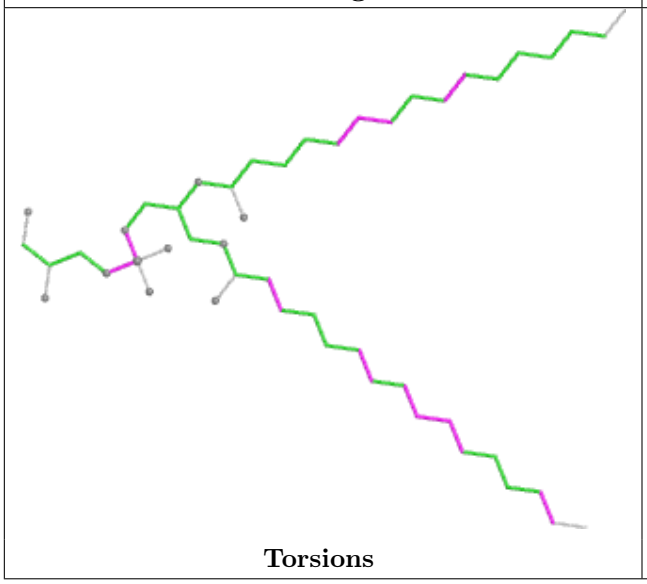
Ligand LHG A 843



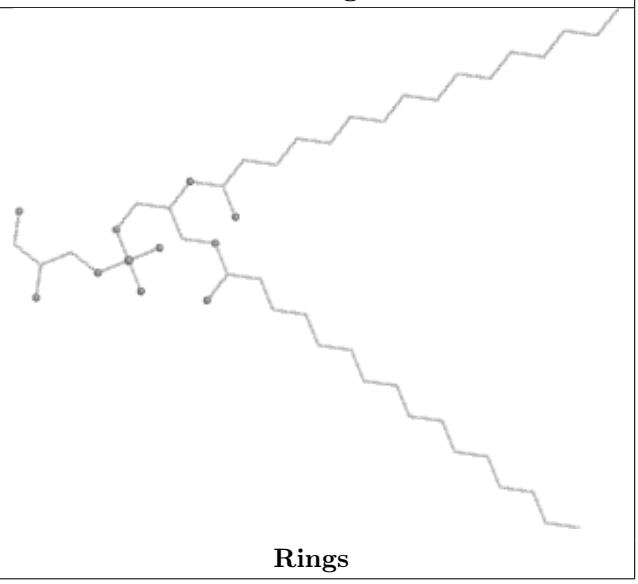
Bond lengths



Bond angles



Torsions



Rings

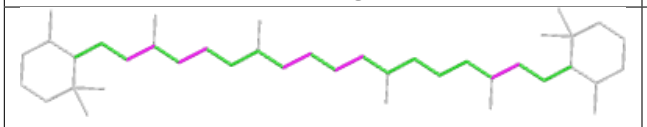
Ligand BCR f 845



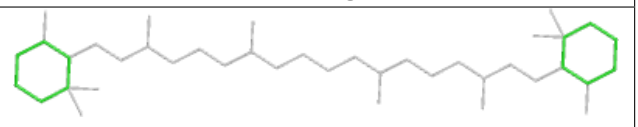
Bond lengths



Bond angles

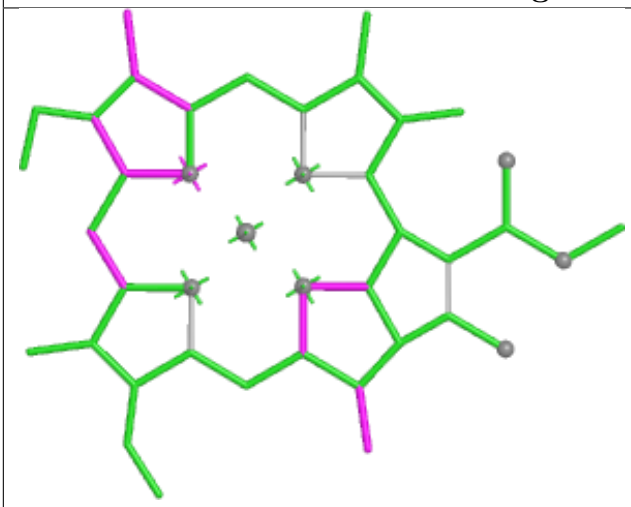


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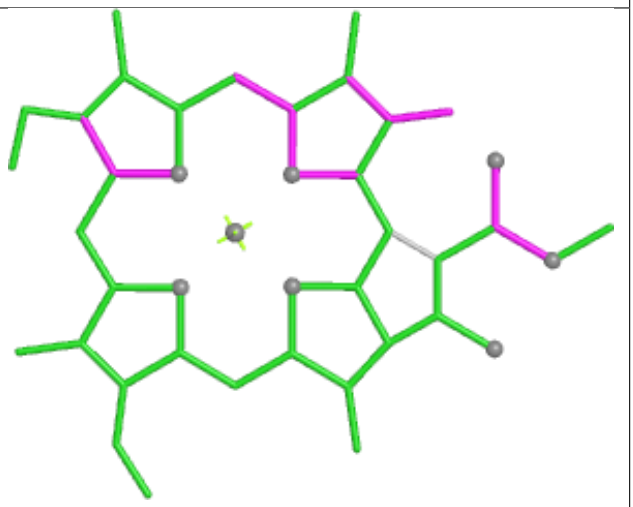


Rings

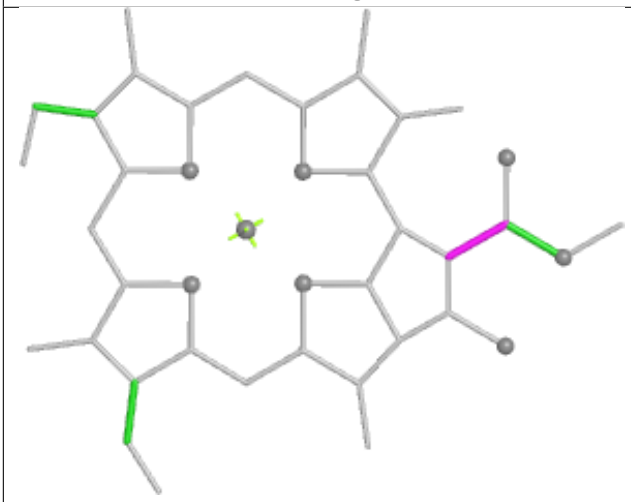
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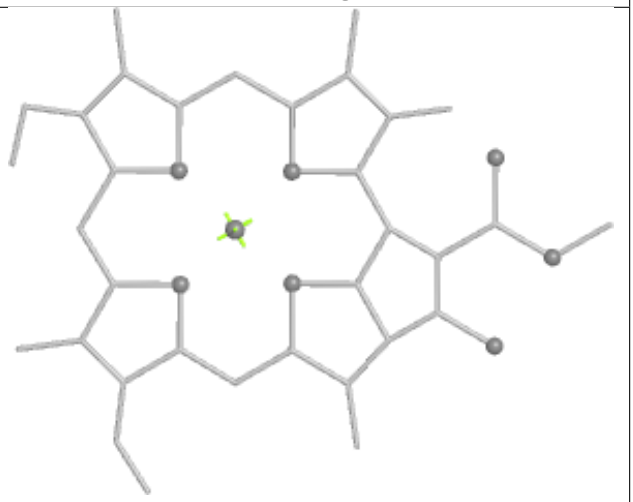
Bond lengths



Bond angles

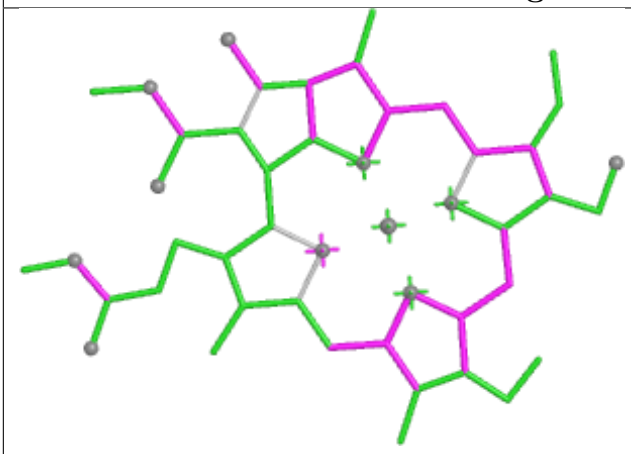


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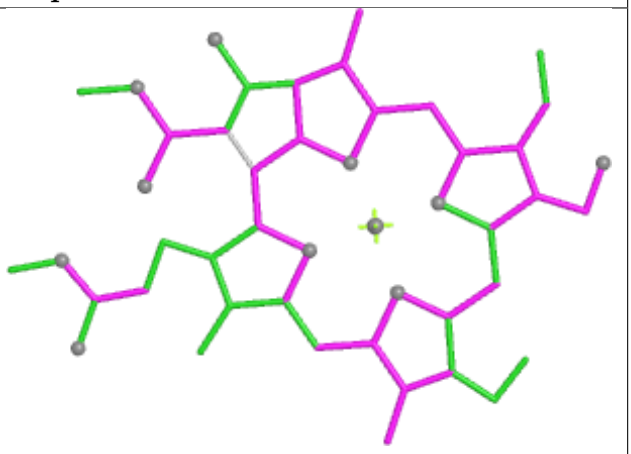


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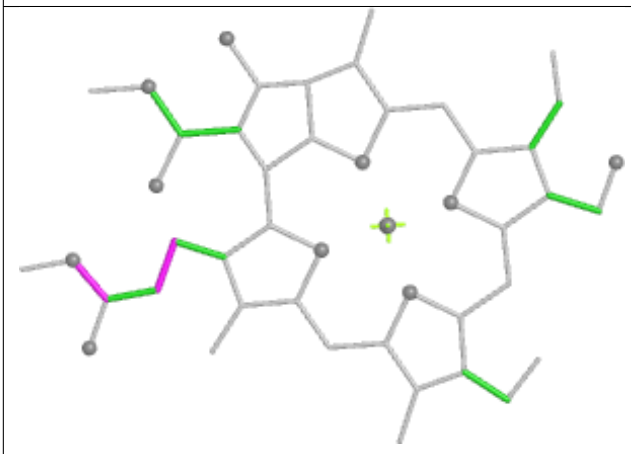
Ligand CHL p 512



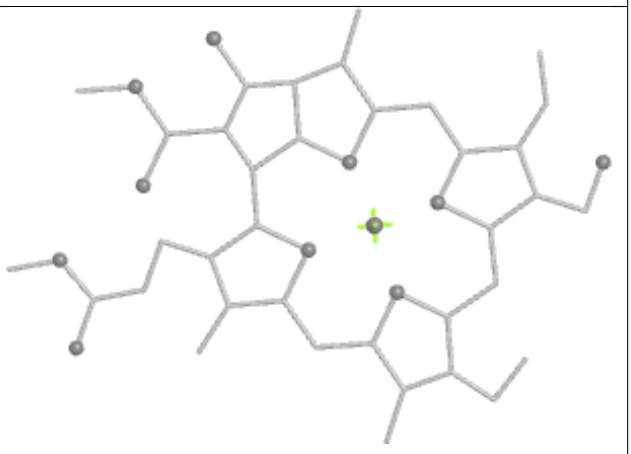
Bond lengths



Bond angles

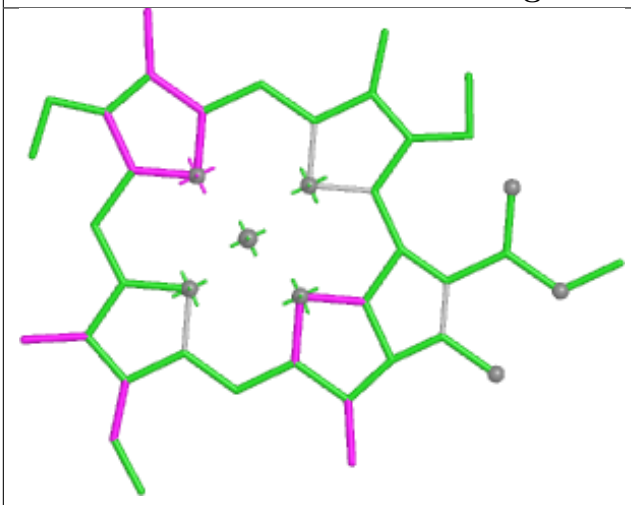


Torsions

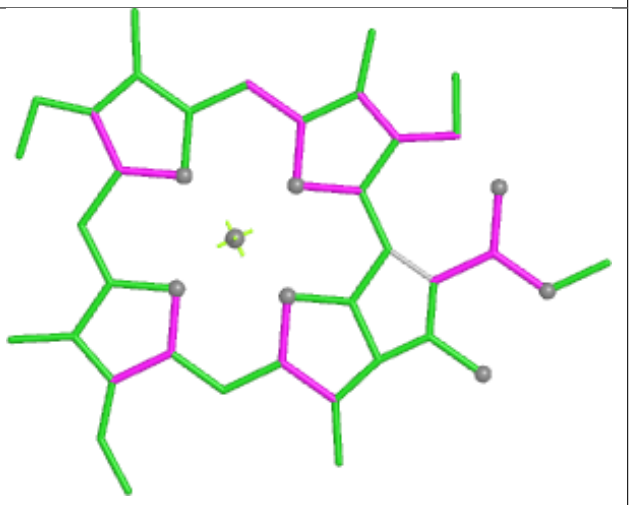


Rings

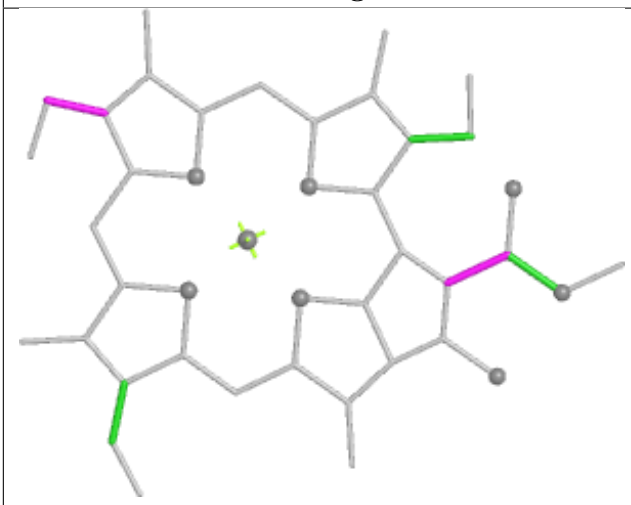
Ligand CLA A 814



Bond lengths



Bond angles

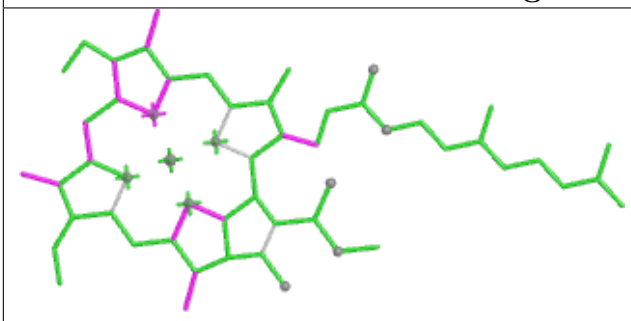


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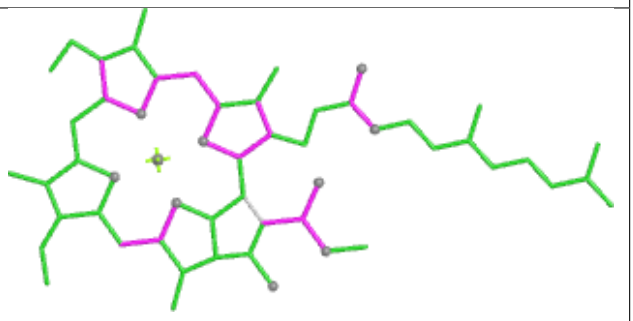


Rings

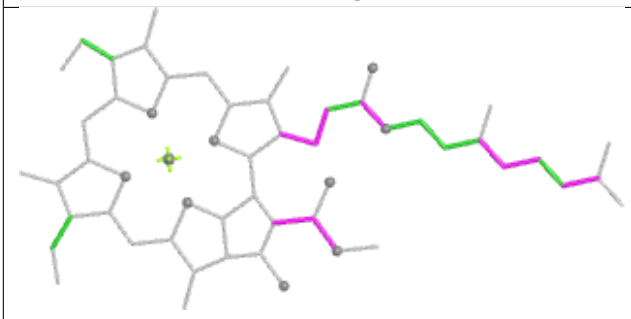
Ligand CLA A 836



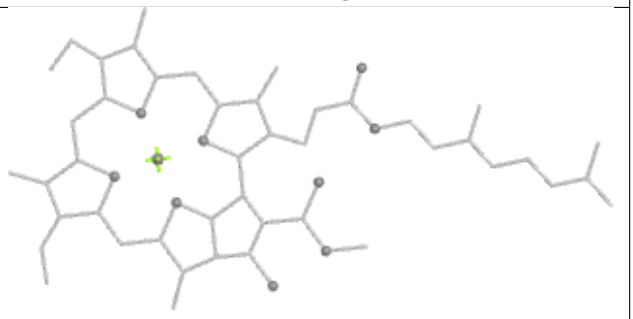
Bond lengths



Bond angles

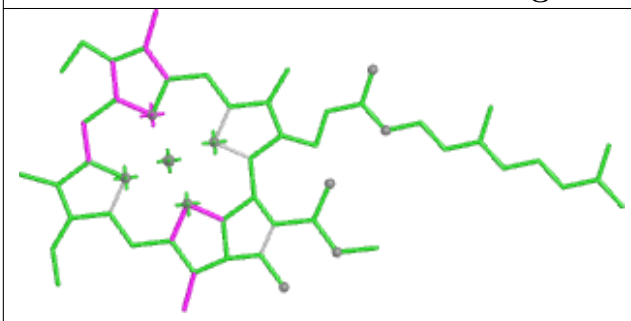


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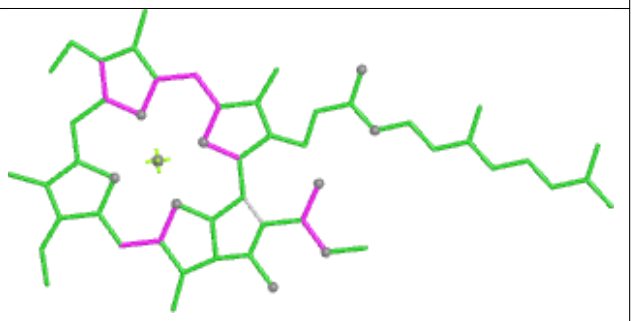


Rings

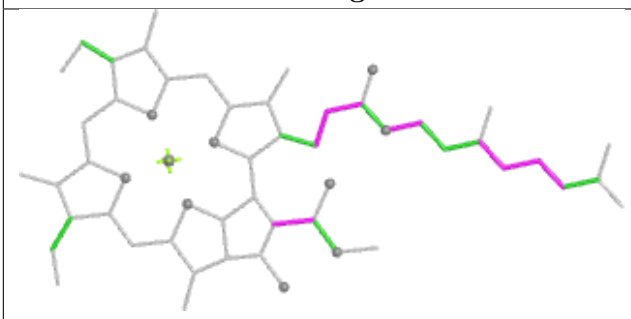
Ligand CLA f 818



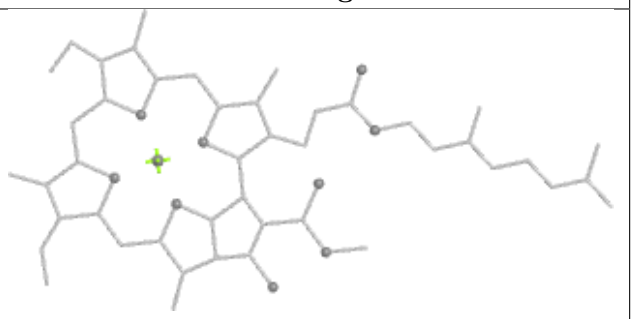
Bond lengths



Bond angles

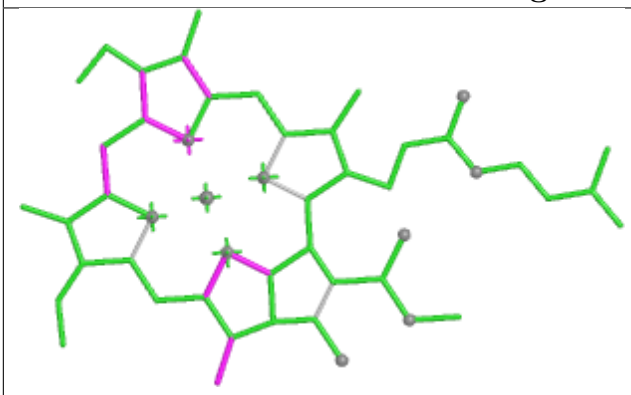


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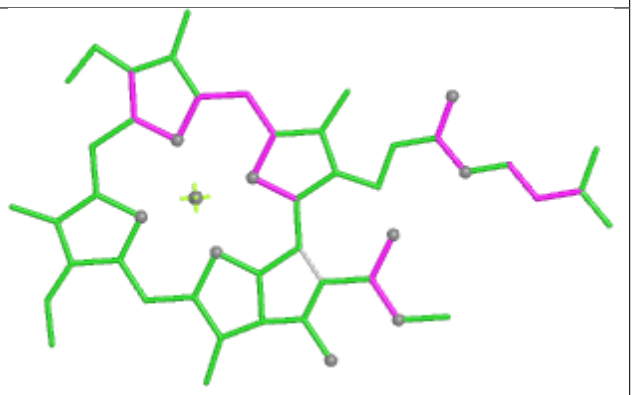


Rings

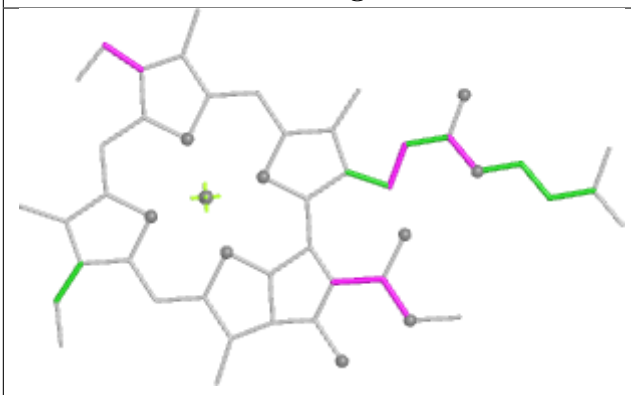
Ligand CLA r 305



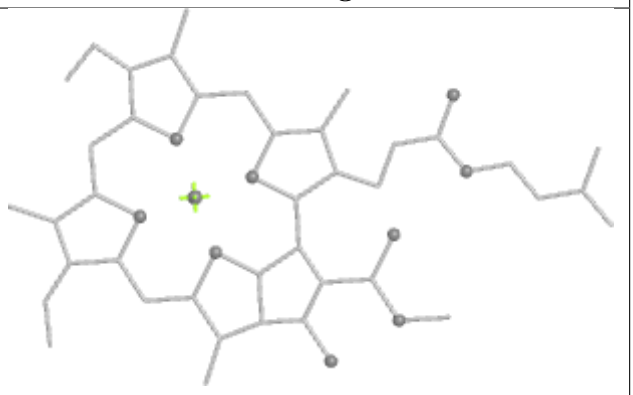
Bond lengths



Bond angles

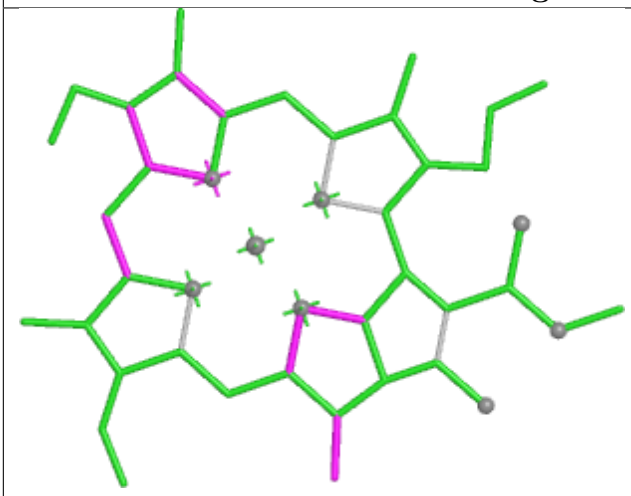


Torsions

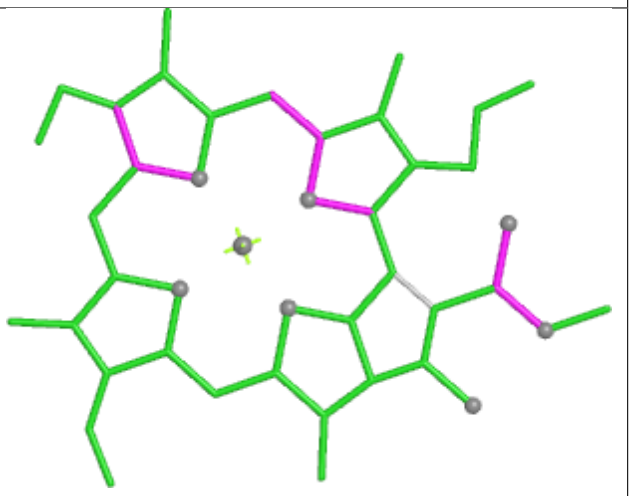


Rings

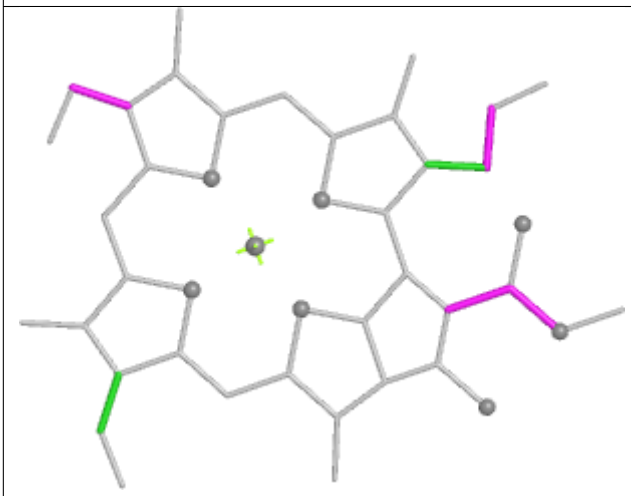
Ligand CLA f 815



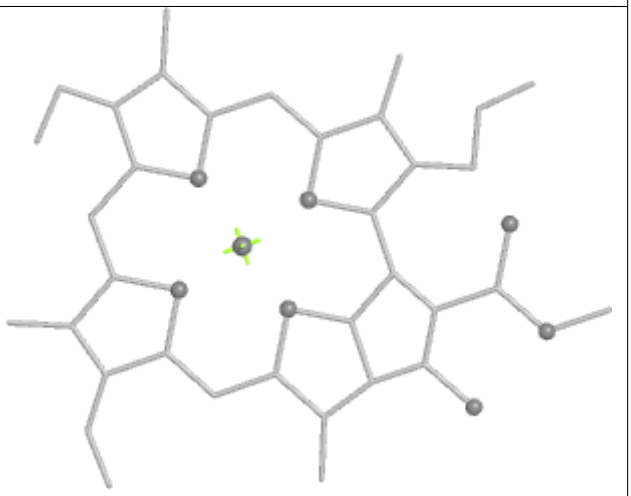
Bond lengths



Bond angles

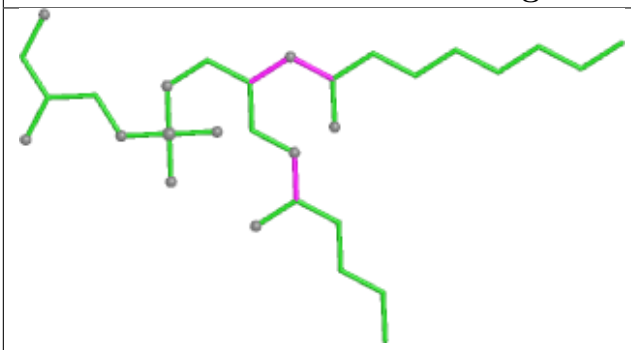


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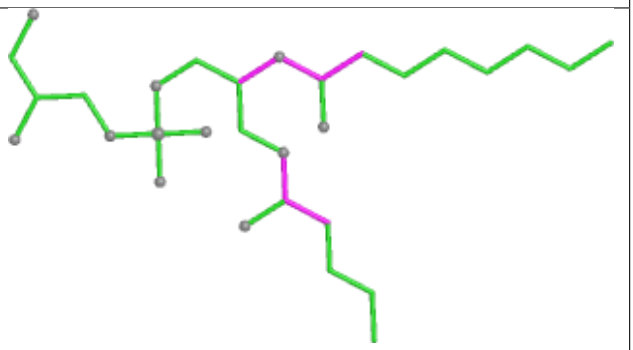


Rings

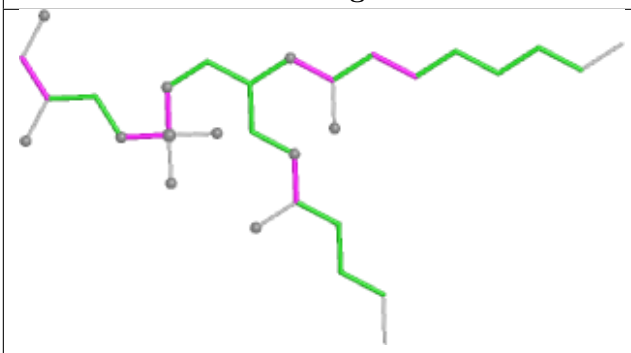
Ligand LHG A 844



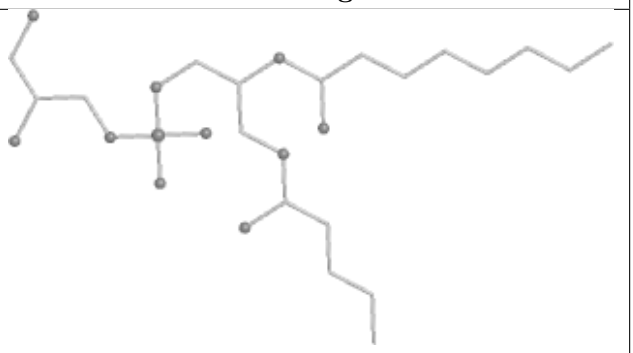
Bond lengths



Bond angles

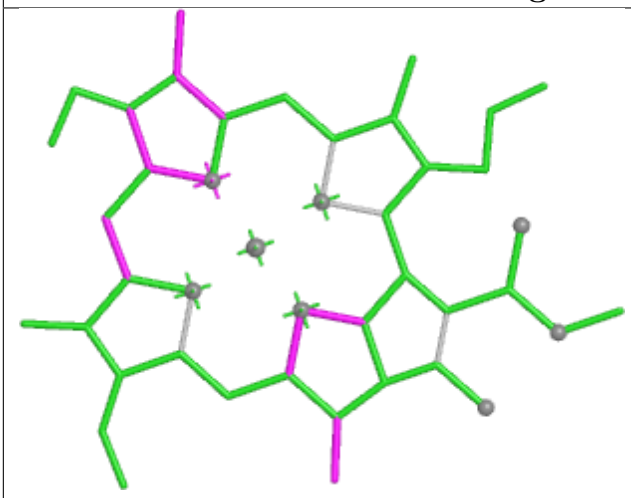


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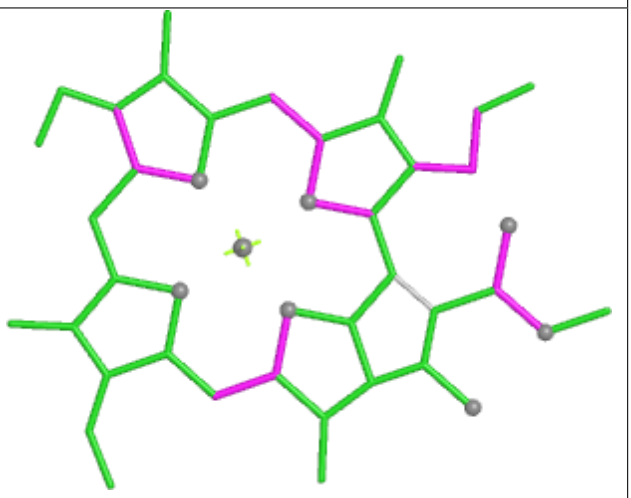


Rings

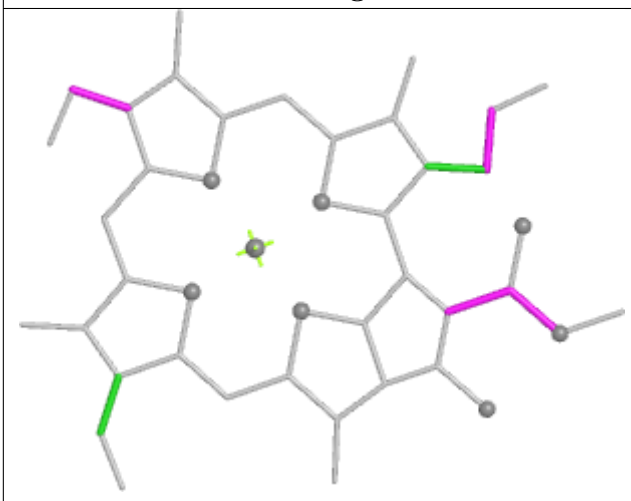
Ligand CLA e 832



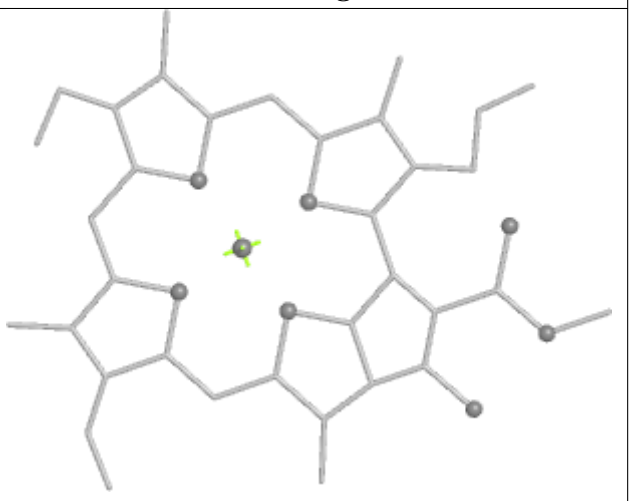
Bond lengths



Bond angles

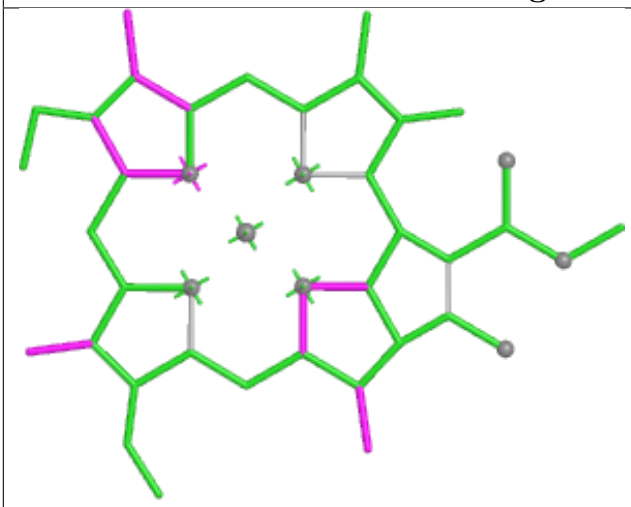


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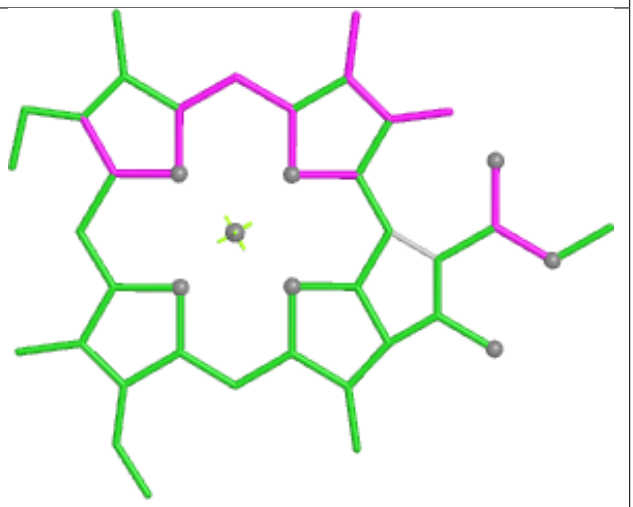


Rings

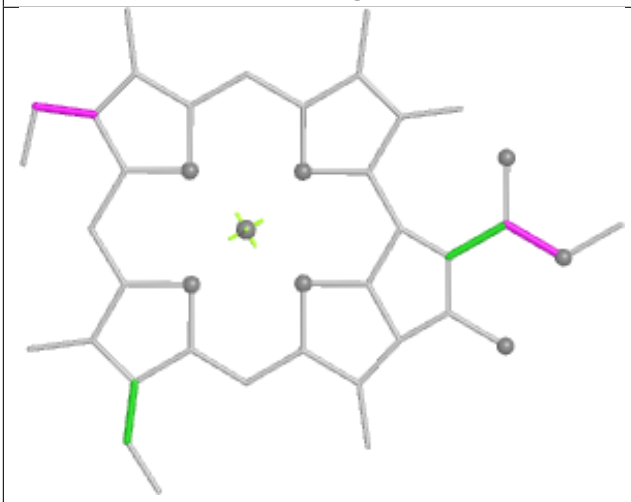
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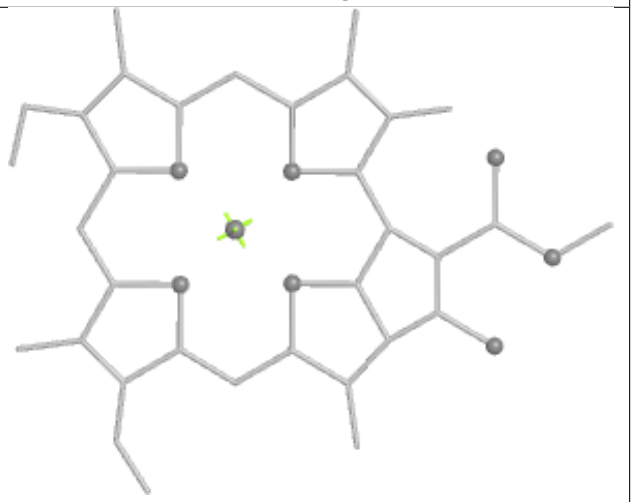
Bond lengths



Bond angles

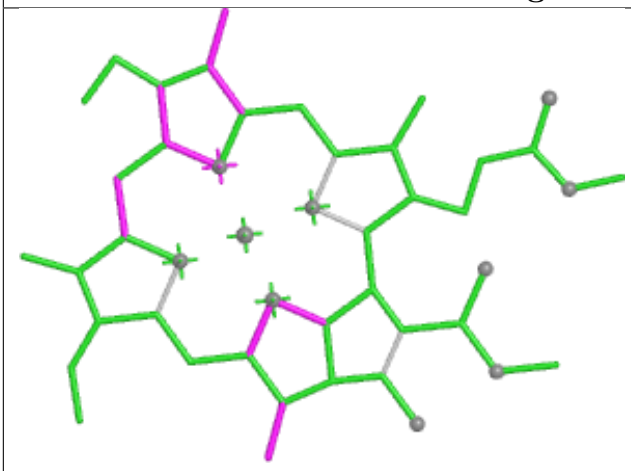


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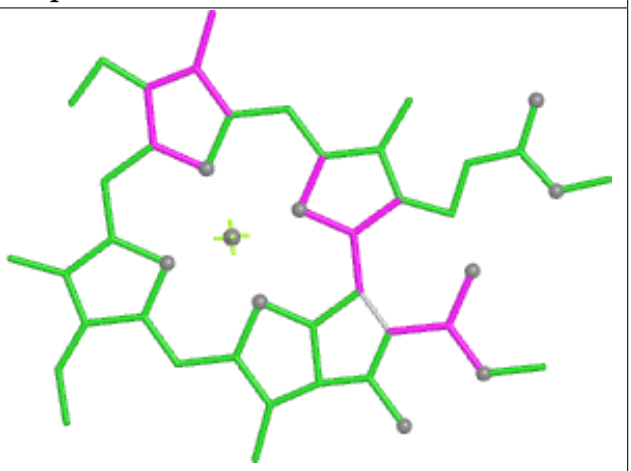


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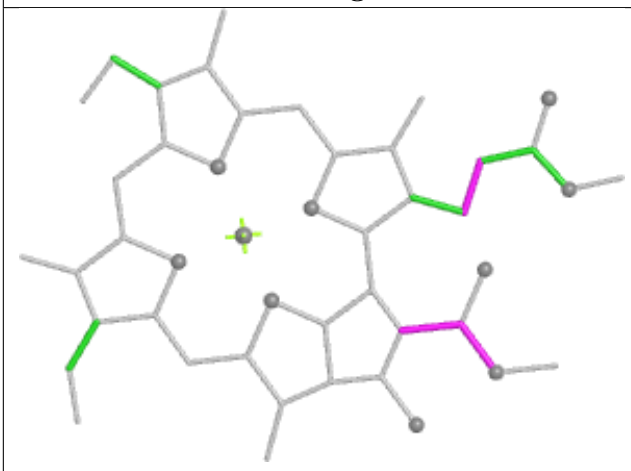
Ligand CLA p 505



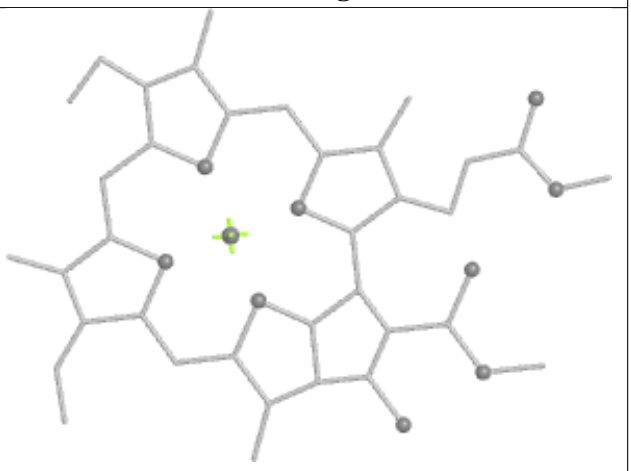
Bond lengths



Bond angles

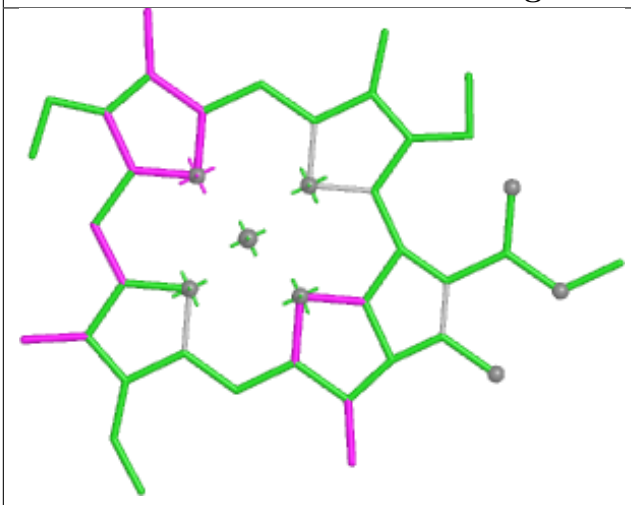


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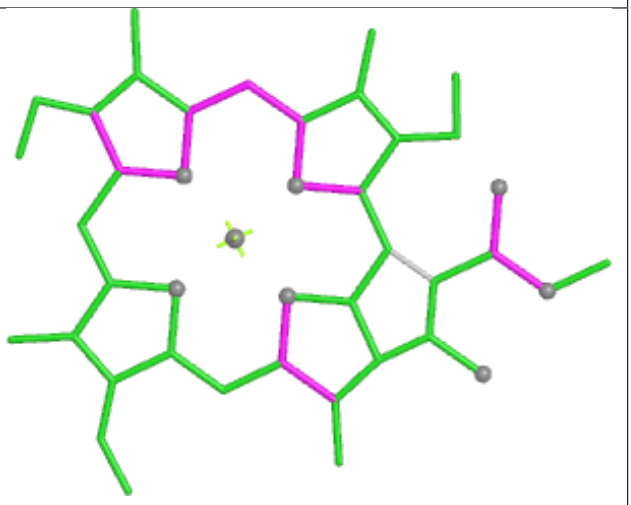


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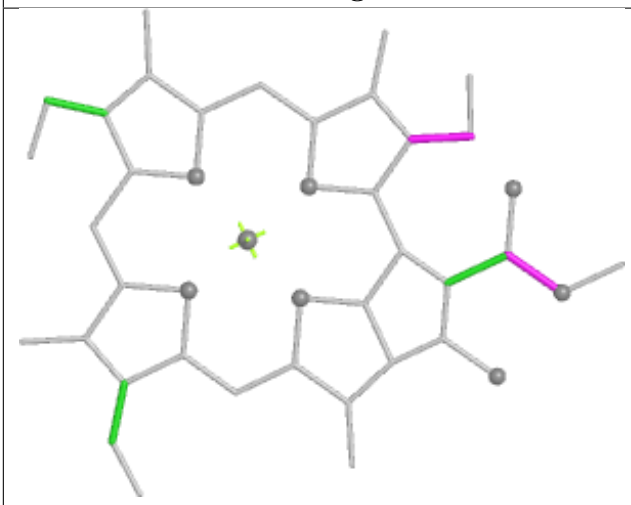
Ligand CLA B 823



Bond lengths



Bond angles

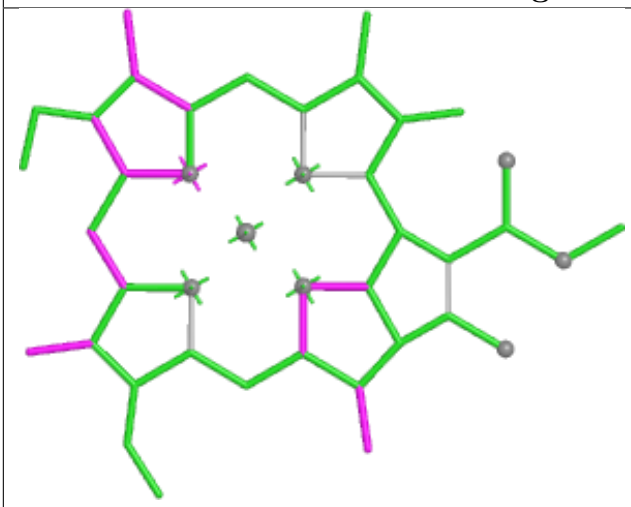


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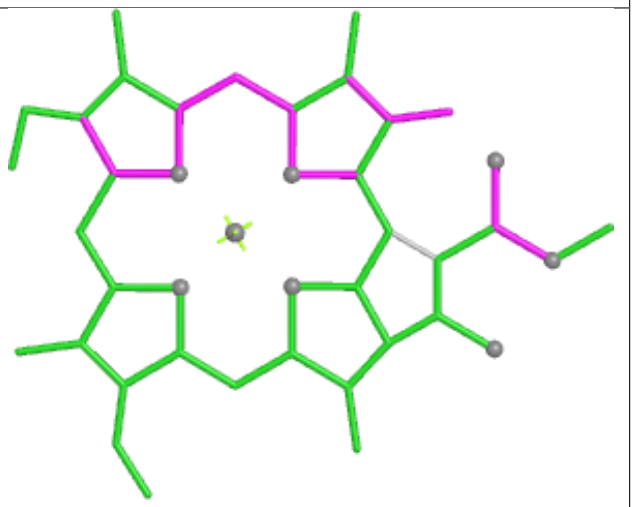


Rings

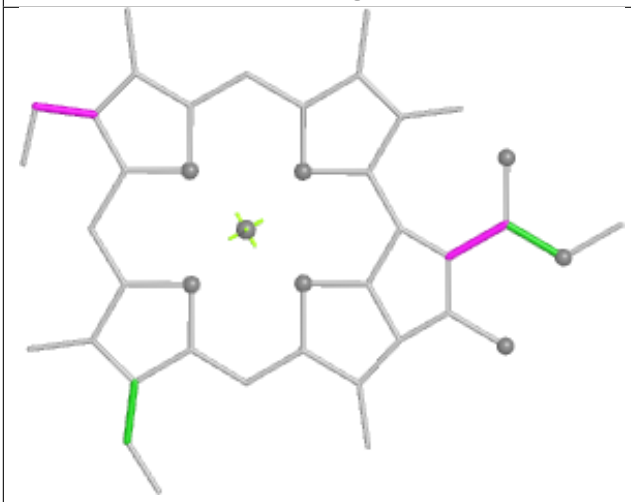
Ligand CLA f 823



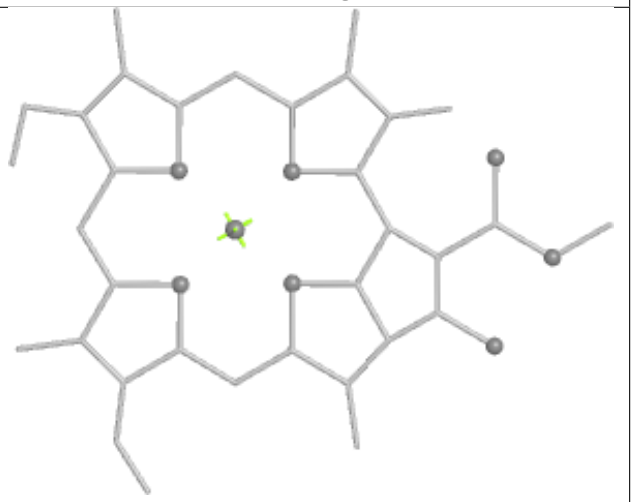
Bond lengths



Bond angles

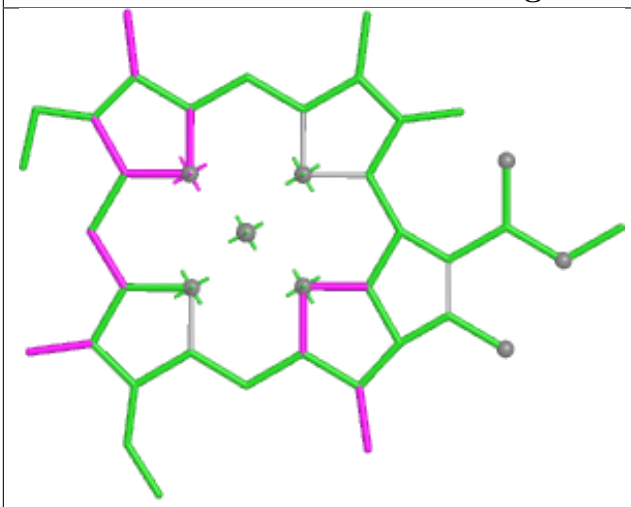


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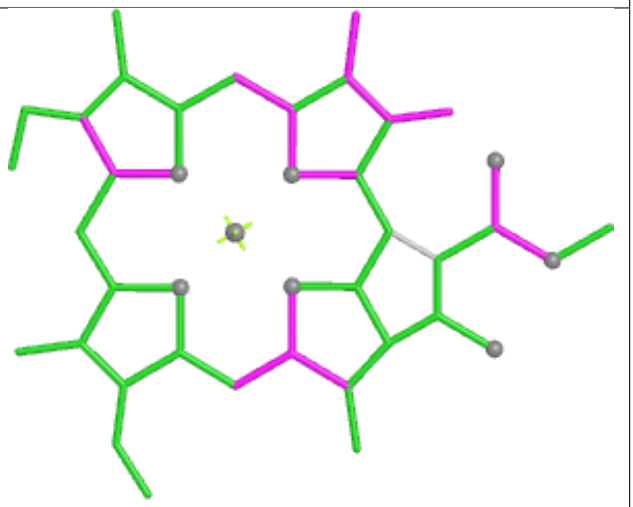


Rings

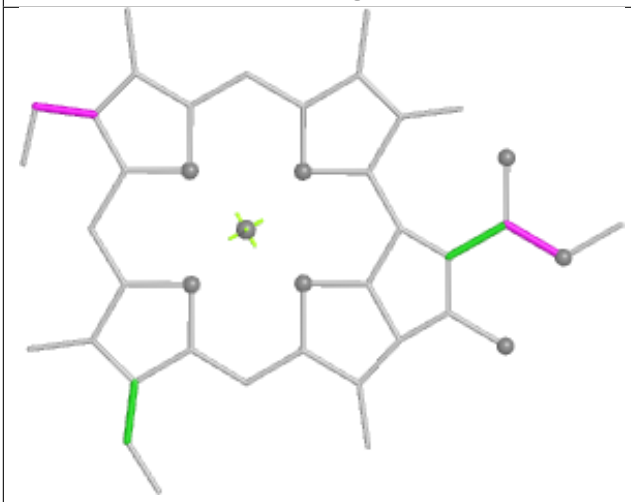
Ligand CLA B 805



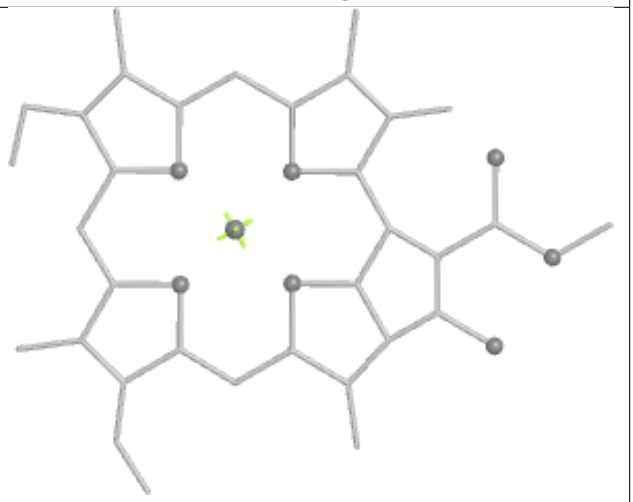
Bond lengths



Bond angles

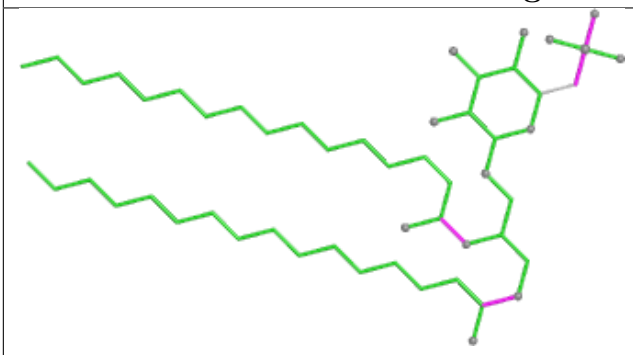


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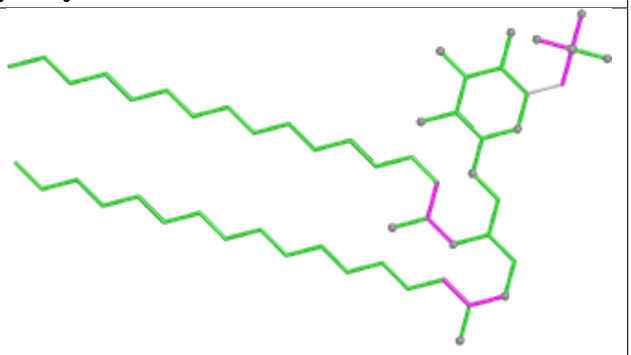


Rings

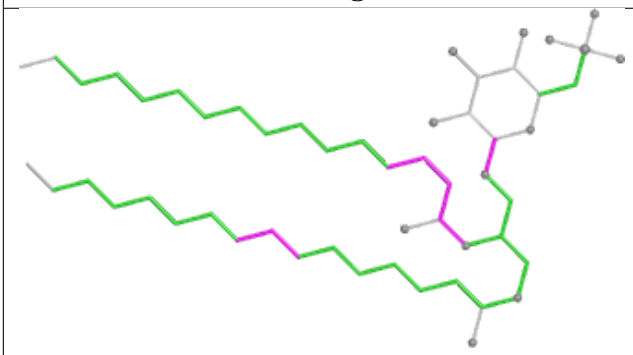
Ligand SQD Q 802



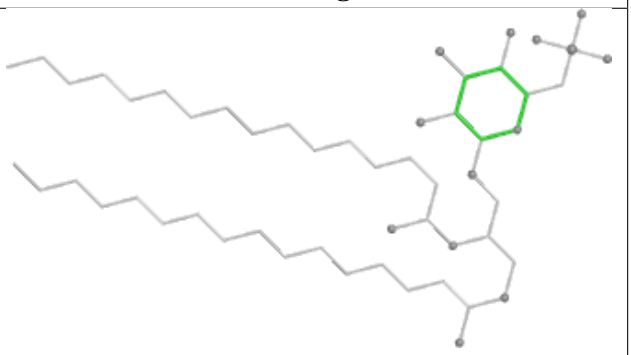
Bond lengths



Bond angles

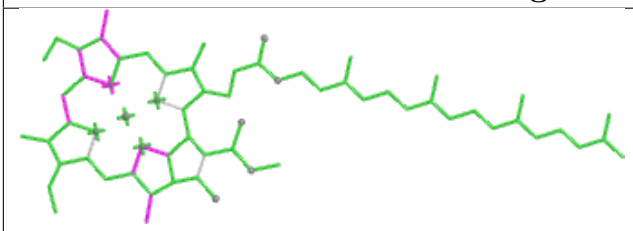


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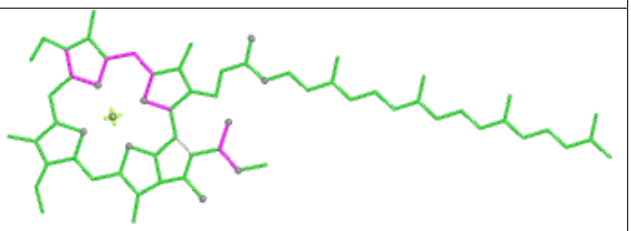


Rings

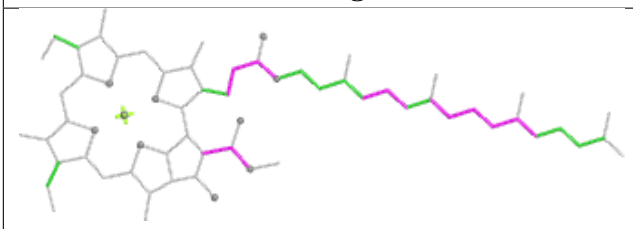
Ligand CLA s 506



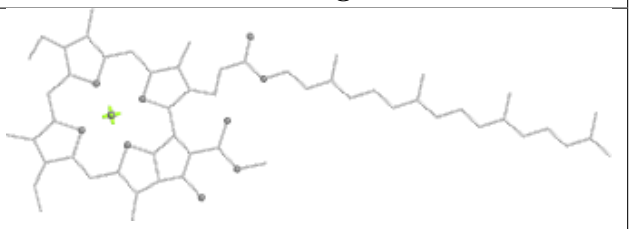
Bond lengths



Bond angles

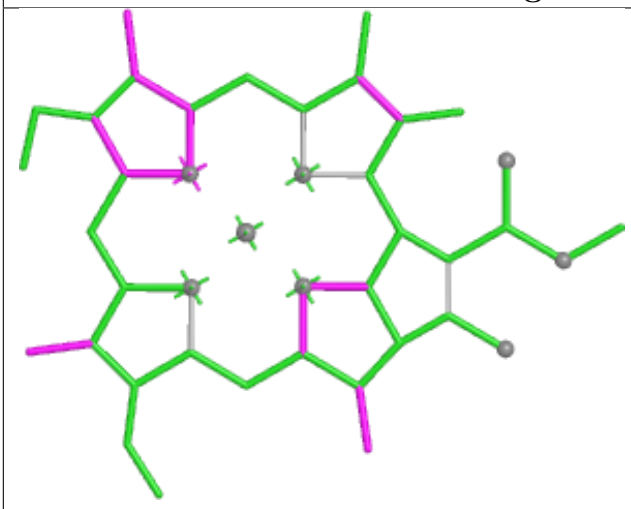


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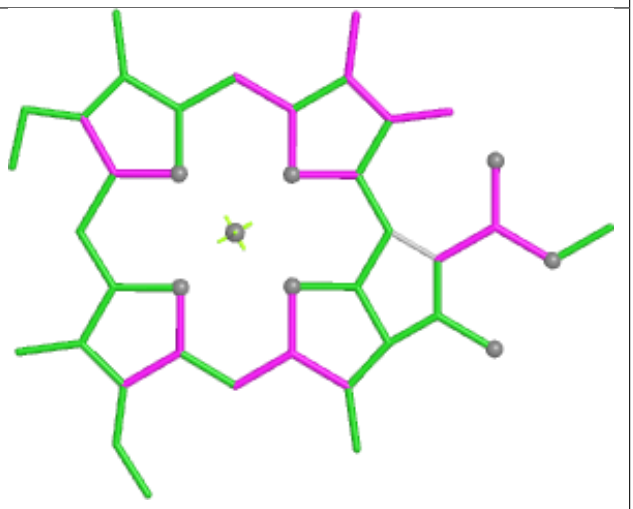


Rings

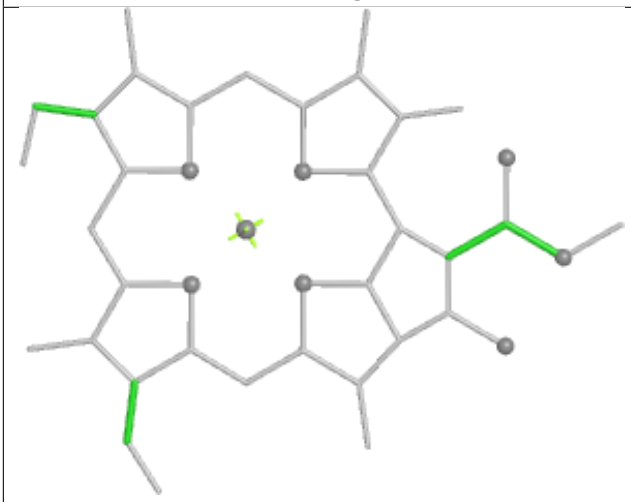
Ligand CLA B 819



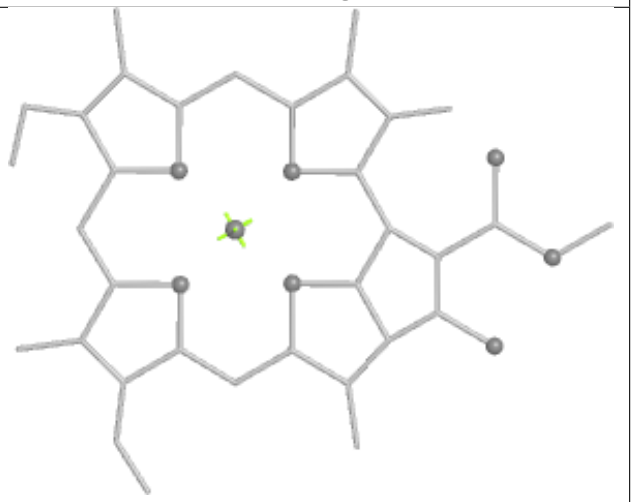
Bond lengths



Bond angles



Torsions

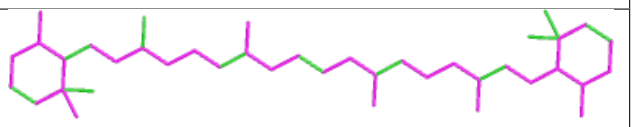


Rings

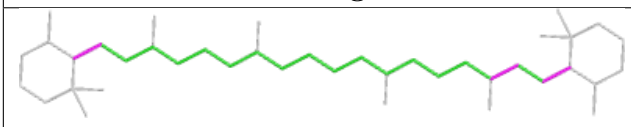
Ligand BCR A 851



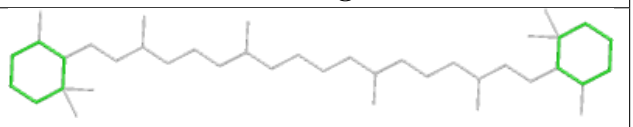
Bond lengths



Bond angles

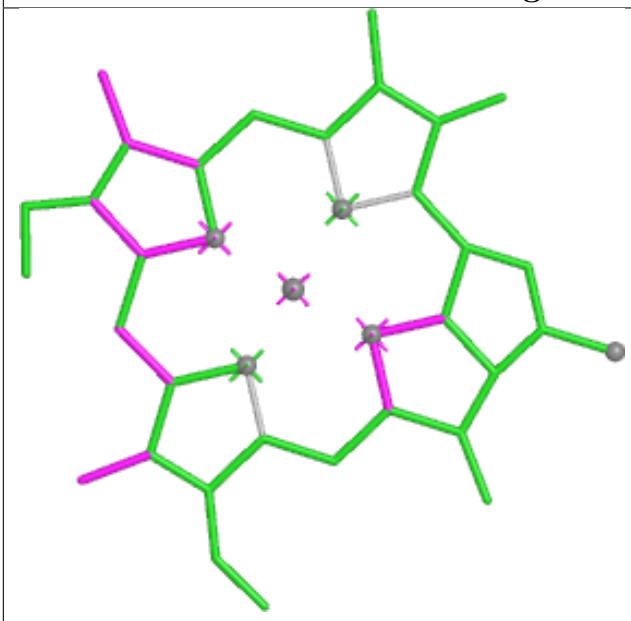


Torsions



Rings

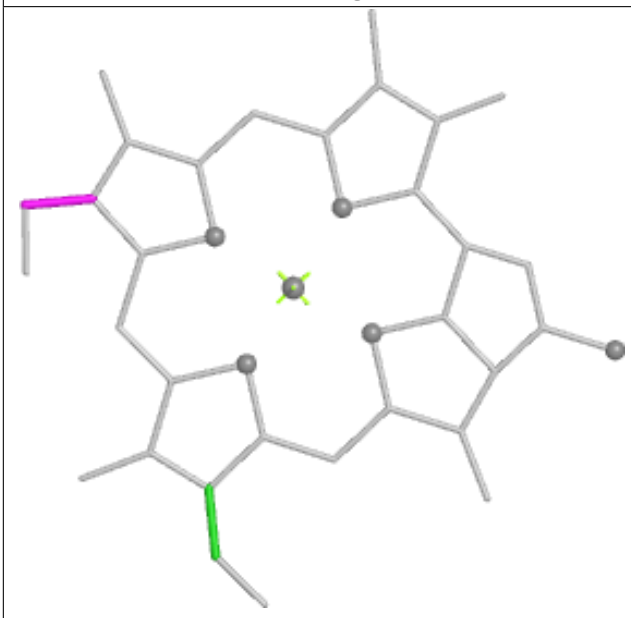
Ligand CLA K 201



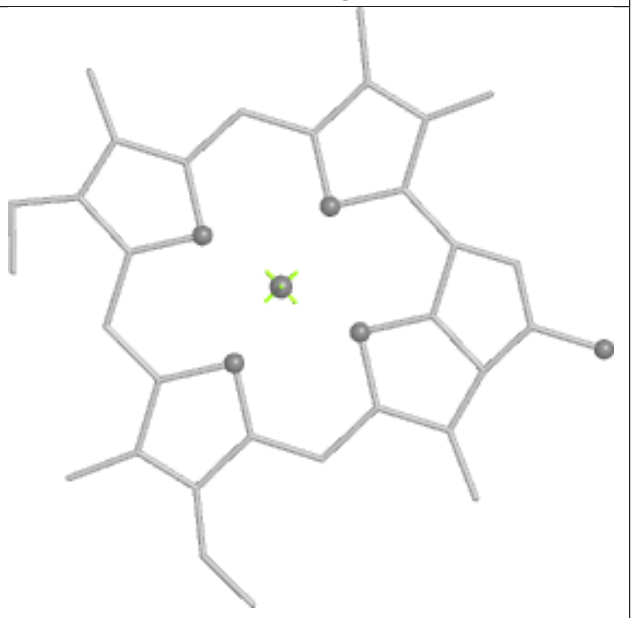
Bond lengths



Bond angles

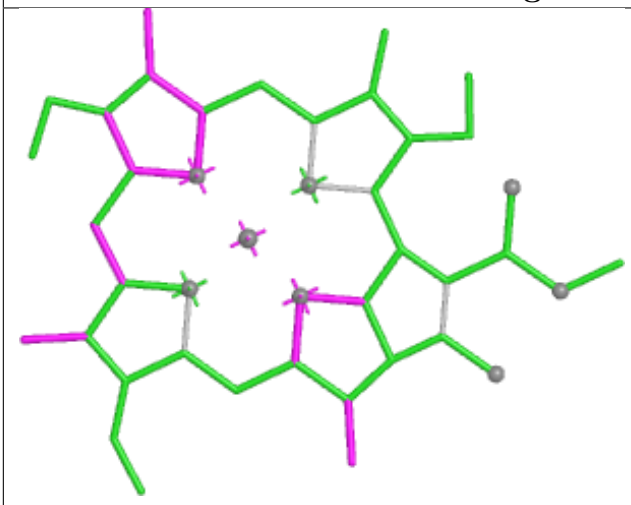


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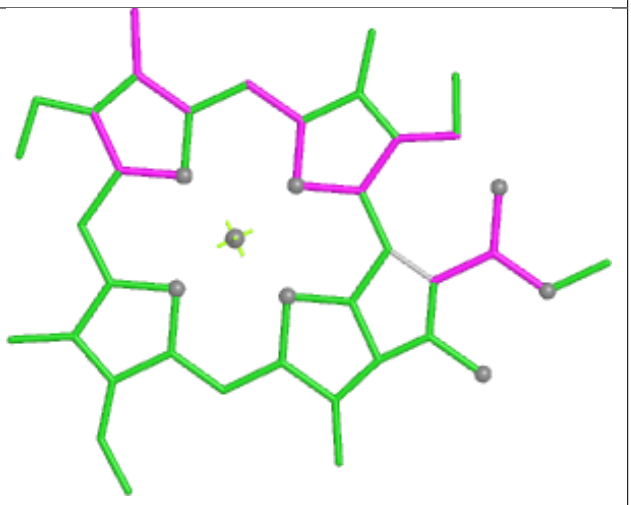


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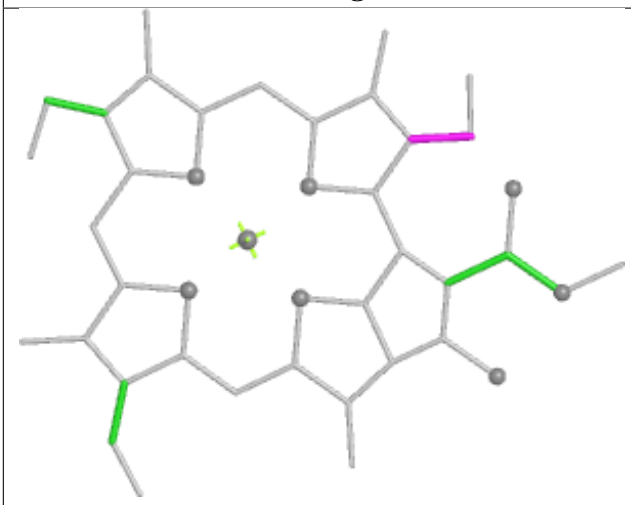
Ligand CLA A 821



Bond lengths



Bond angles

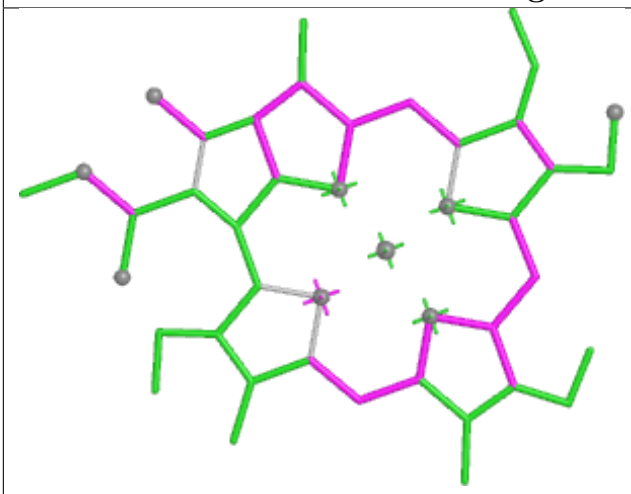


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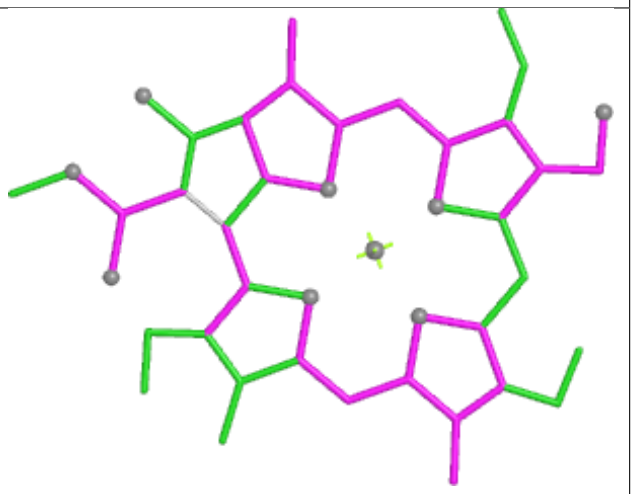


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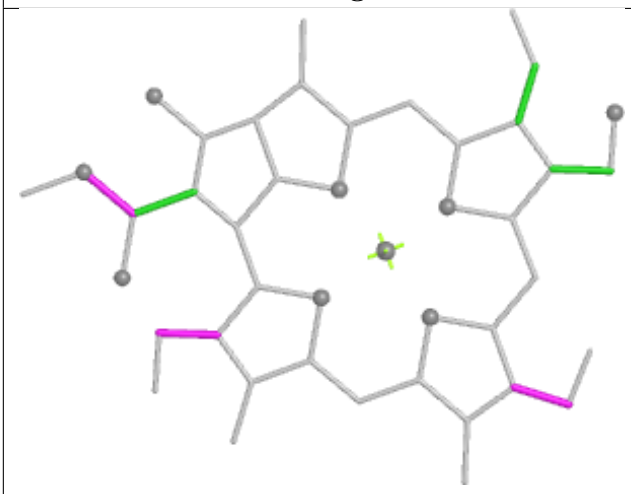
Ligand CHL 3 315



Bond lengths



Bond angles

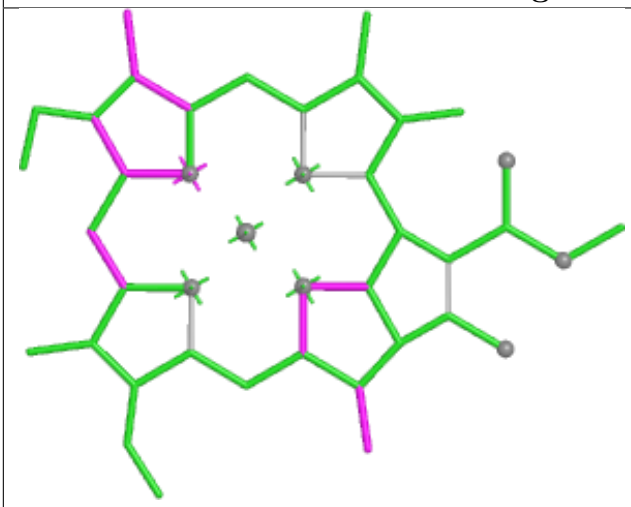


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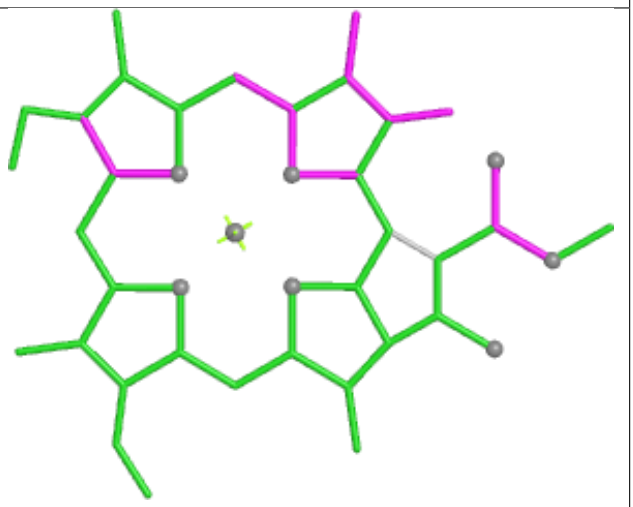


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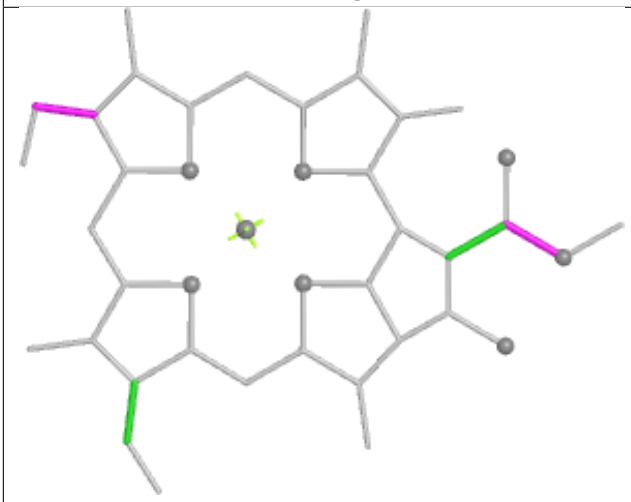
Ligand CLA f 819



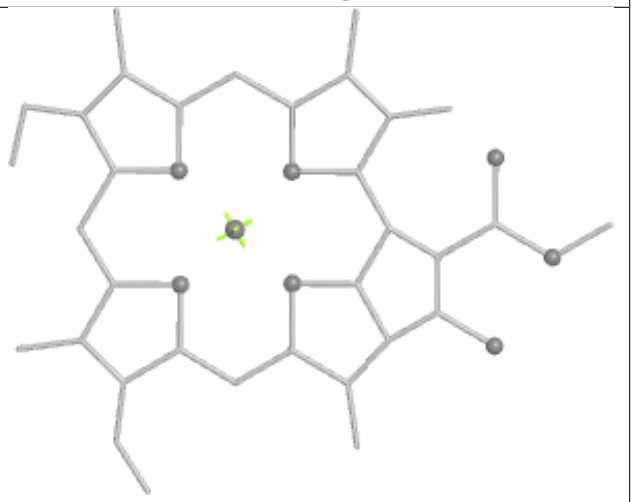
Bond lengths



Bond angles

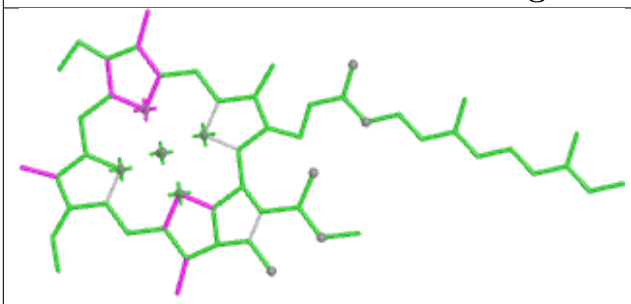


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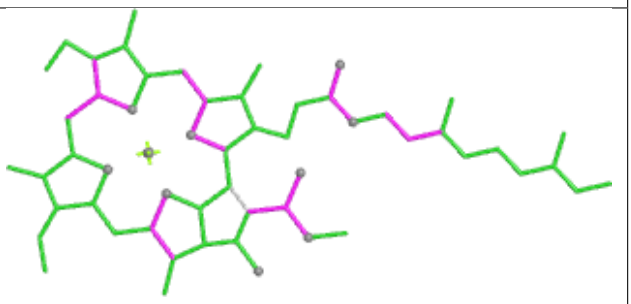


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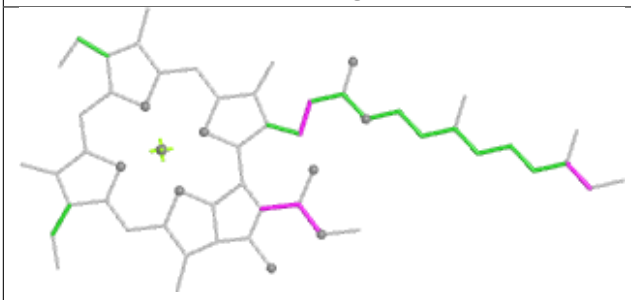
Ligand CLA 1 507



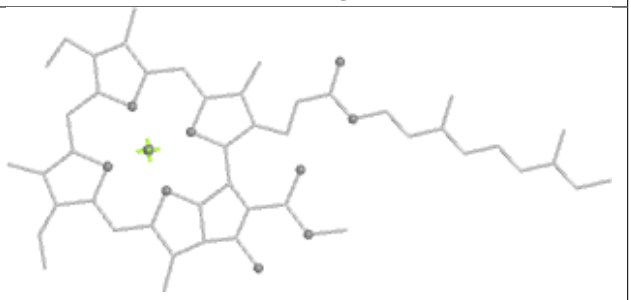
Bond lengths



Bond angles

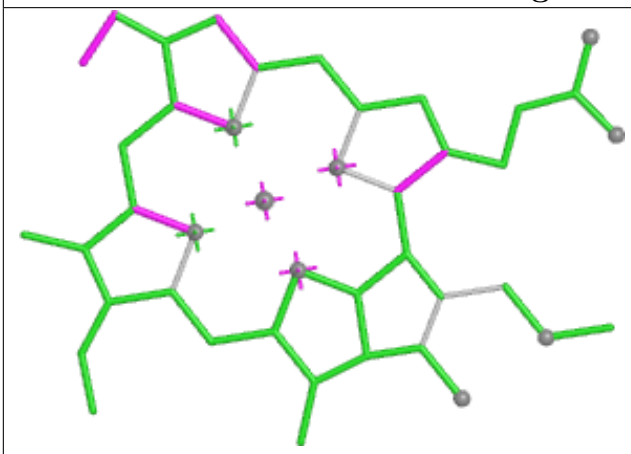


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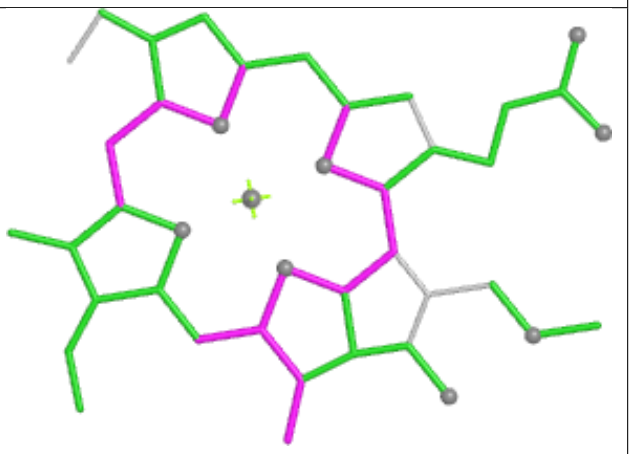


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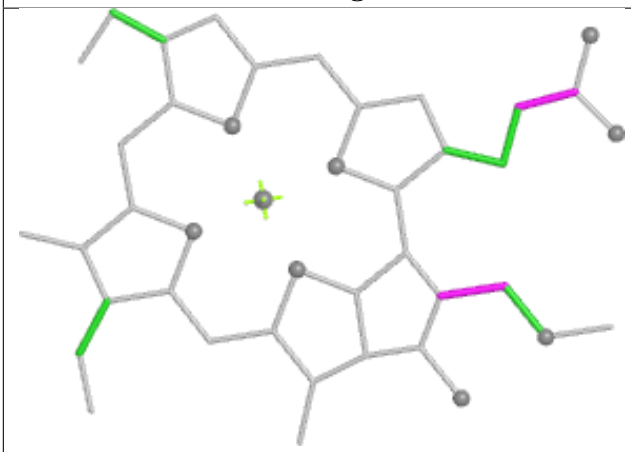
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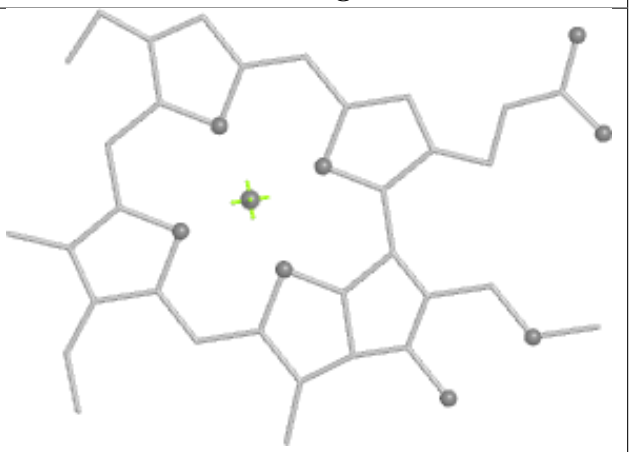
Bond lengths



Bond angles

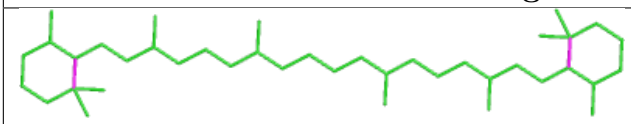


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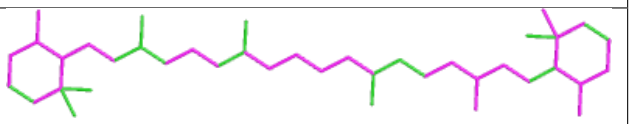


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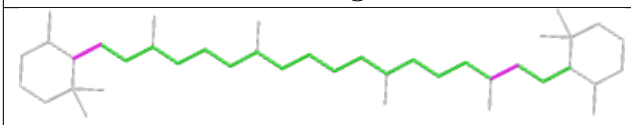
Ligand BCR B 849



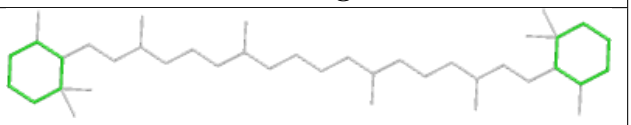
Bond lengths



Bond angles

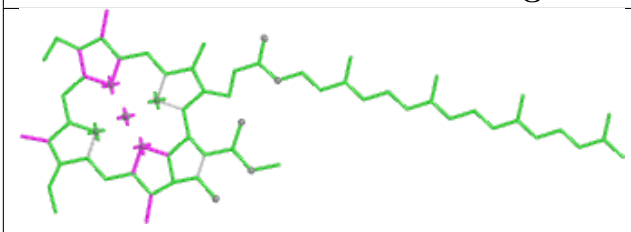


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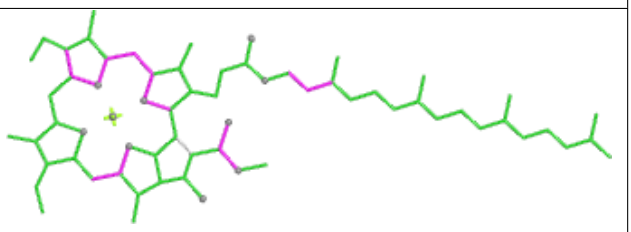


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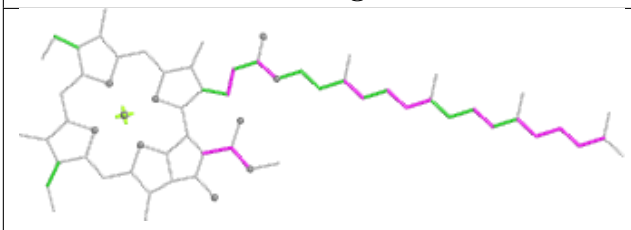
Ligand CLA A 806



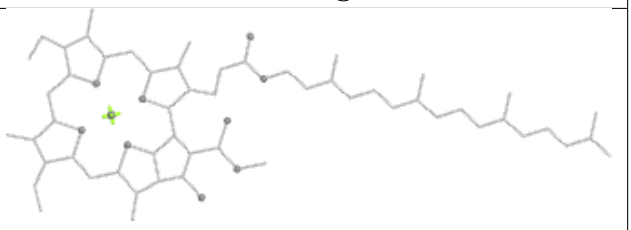
Bond lengths



Bond angles

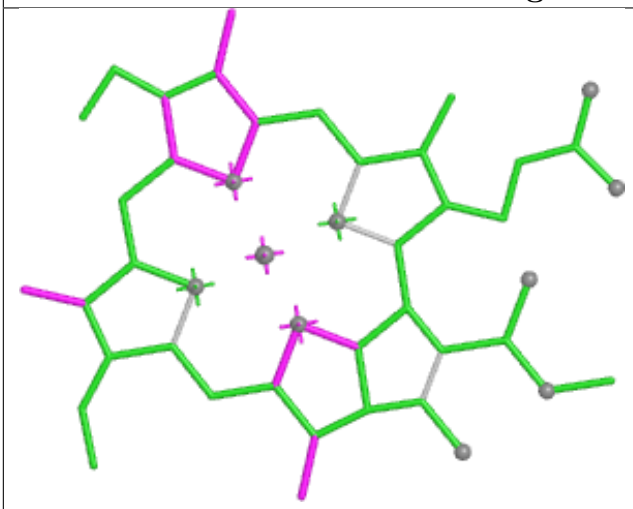


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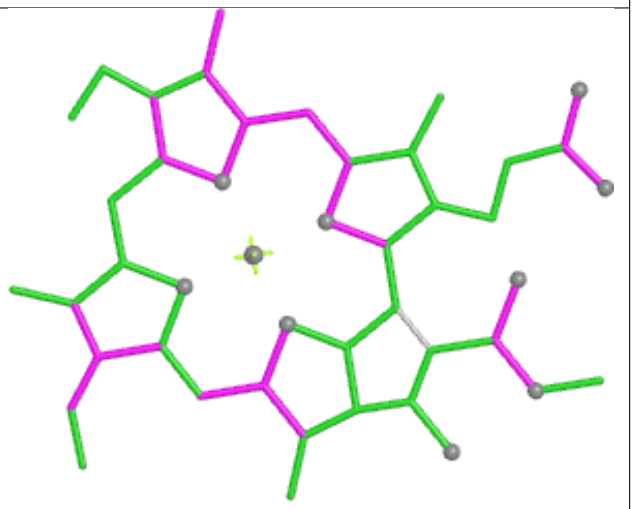


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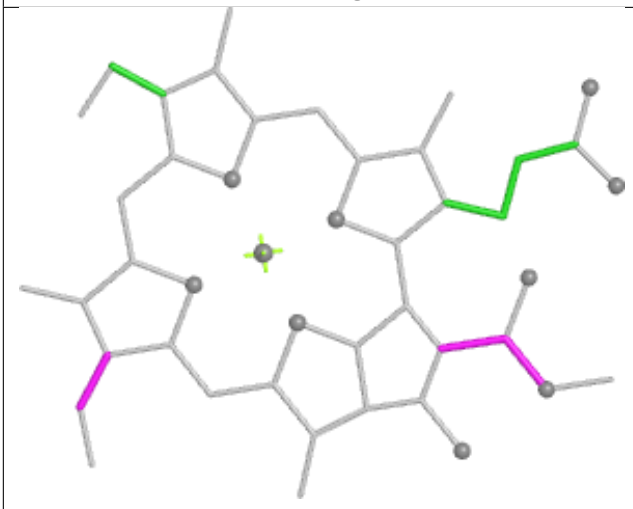
Ligand CLA L 304



Bond lengths



Bond angles

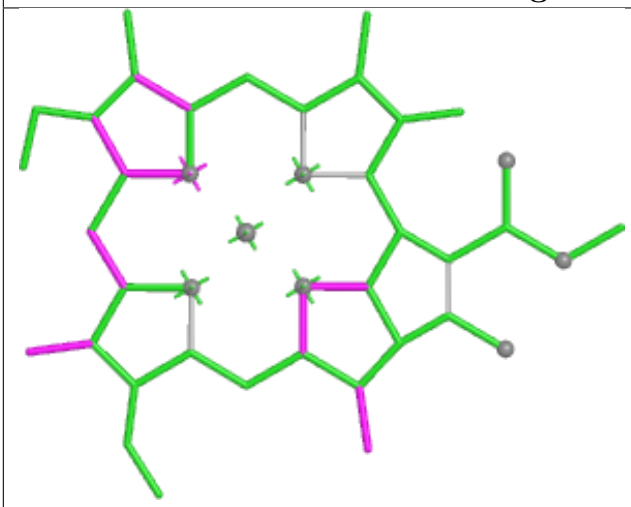


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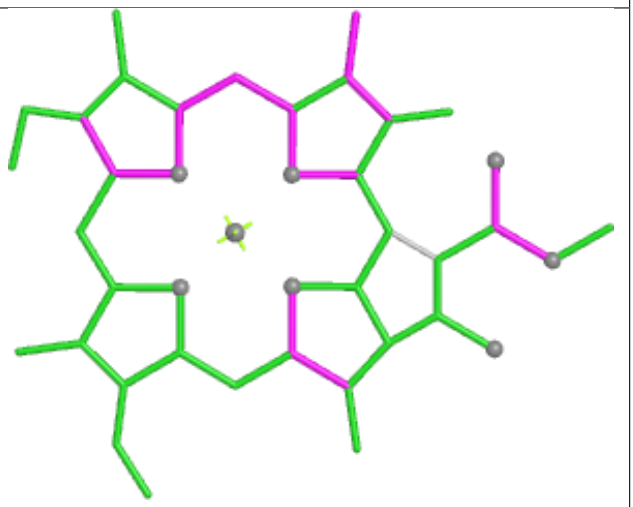


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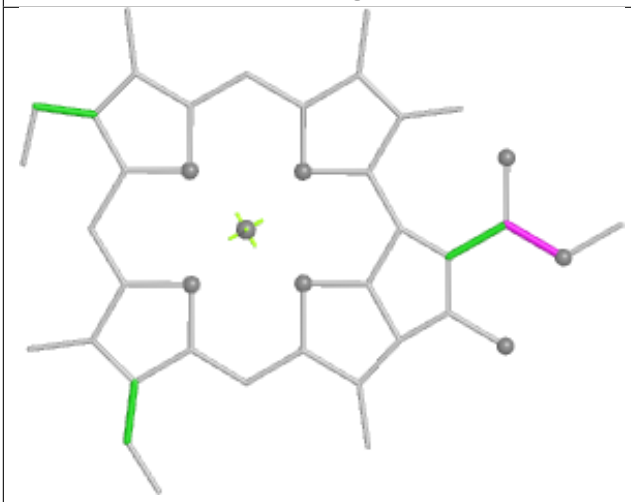
Ligand CLA s 507



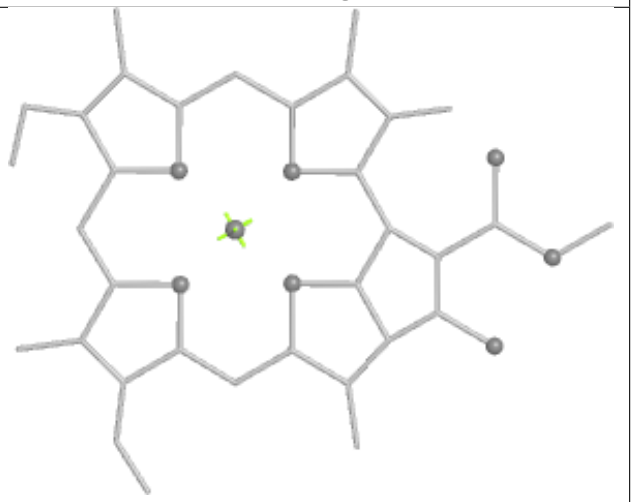
Bond lengths



Bond angles

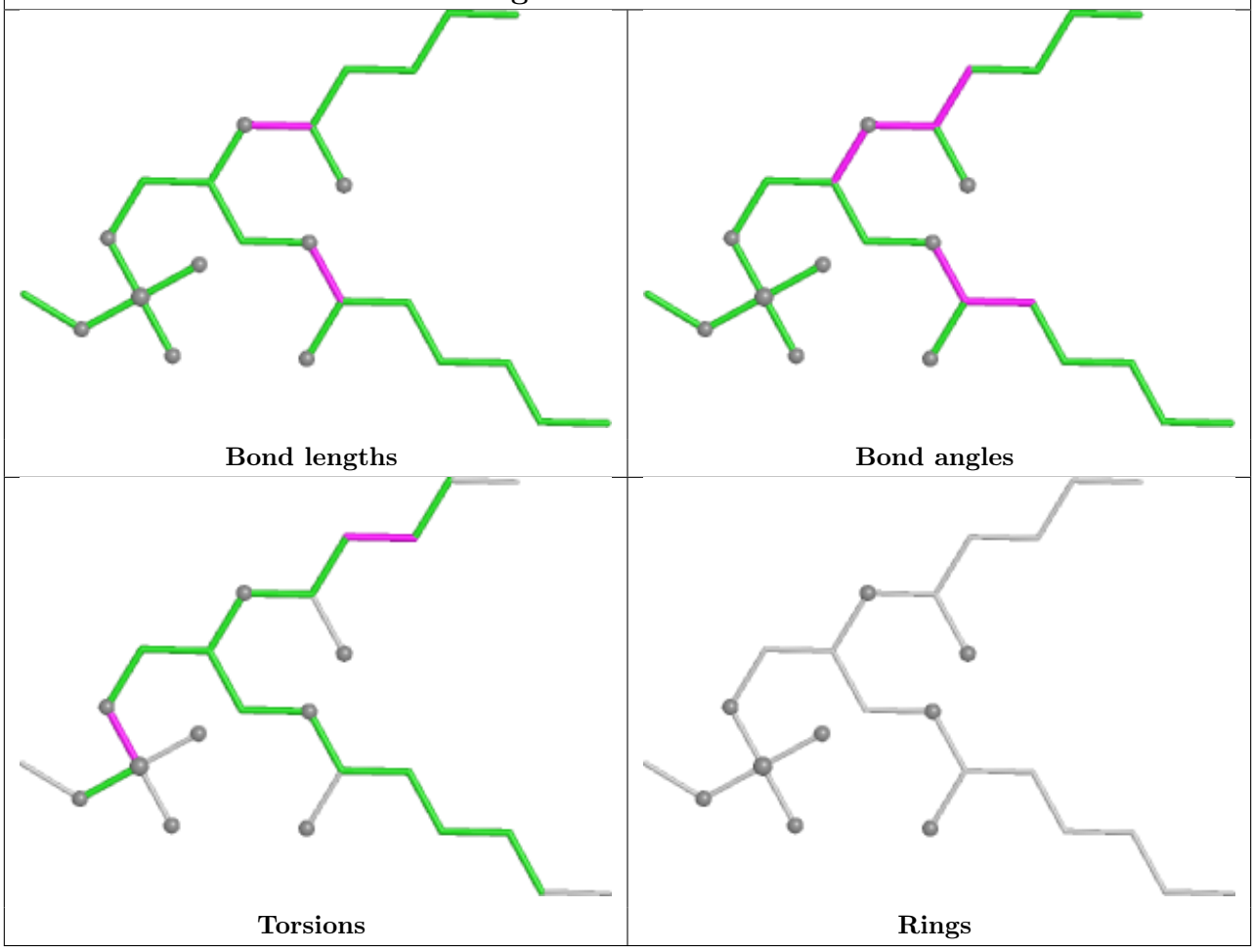


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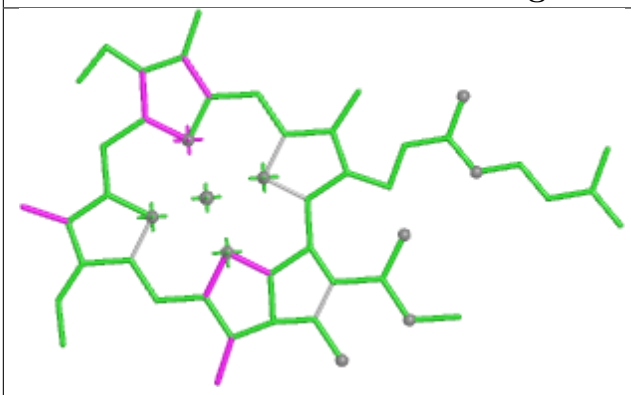


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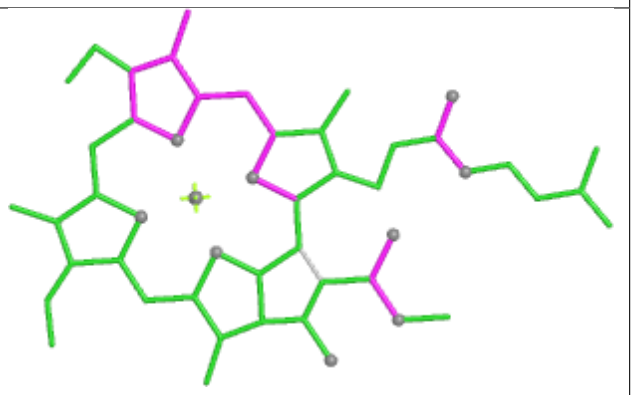
Ligand LHG O 601



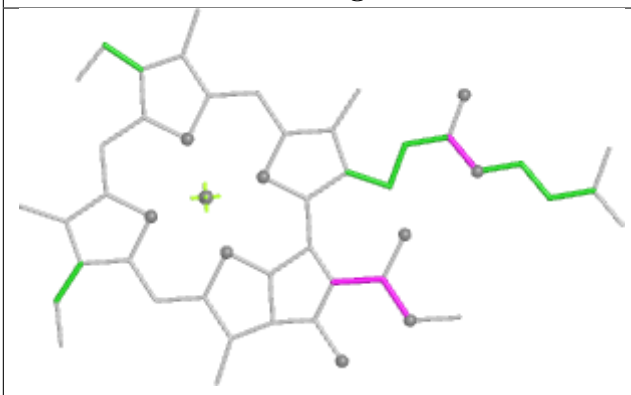
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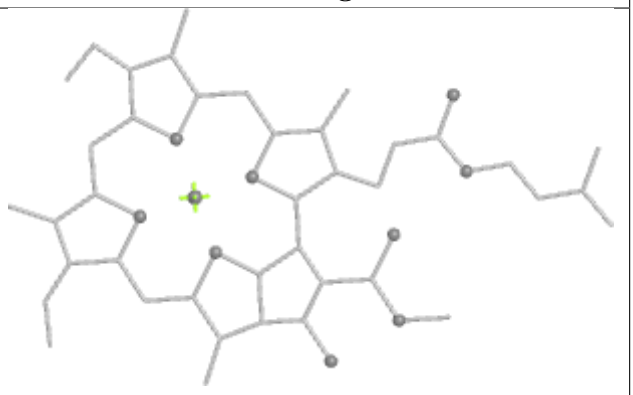
Bond lengths



Bond angles

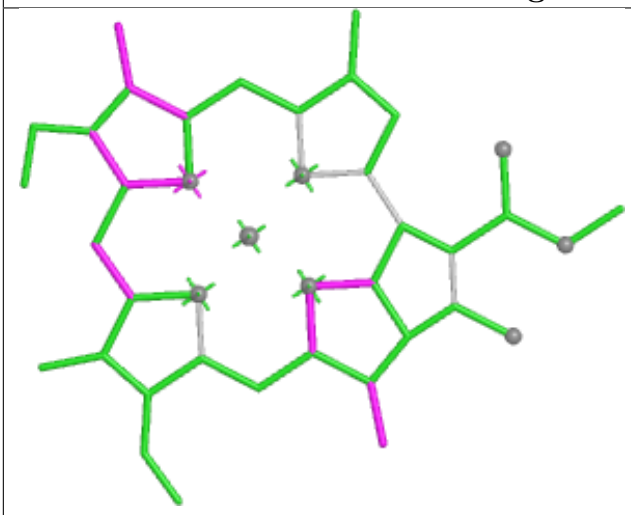


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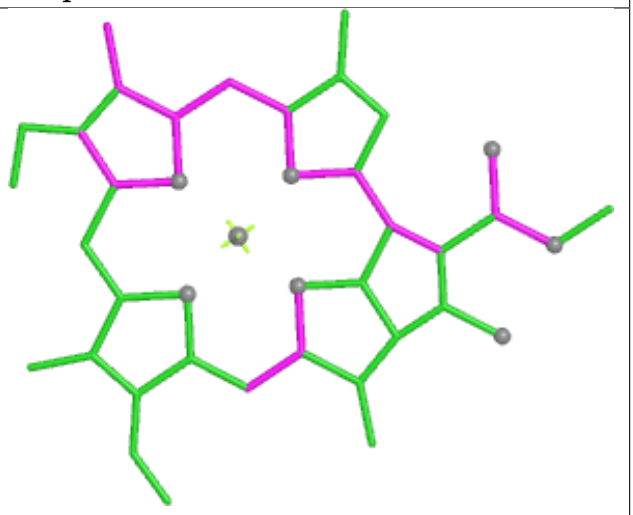


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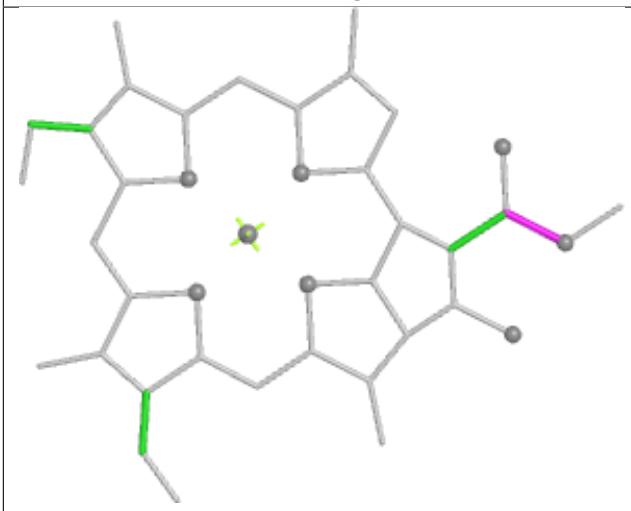
Ligand CLA q 314



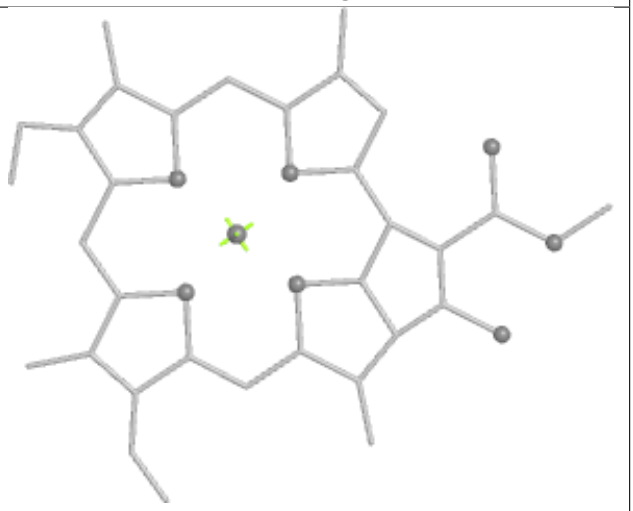
Bond lengths



Bond angles

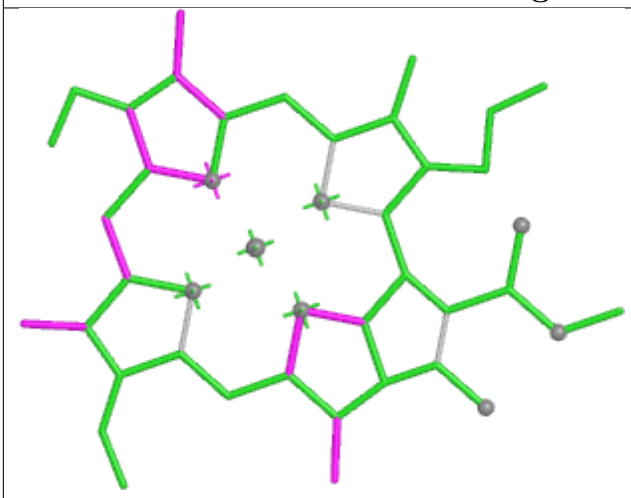


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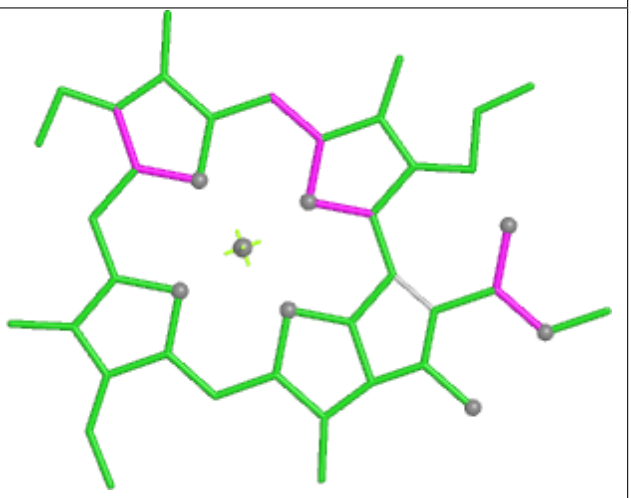


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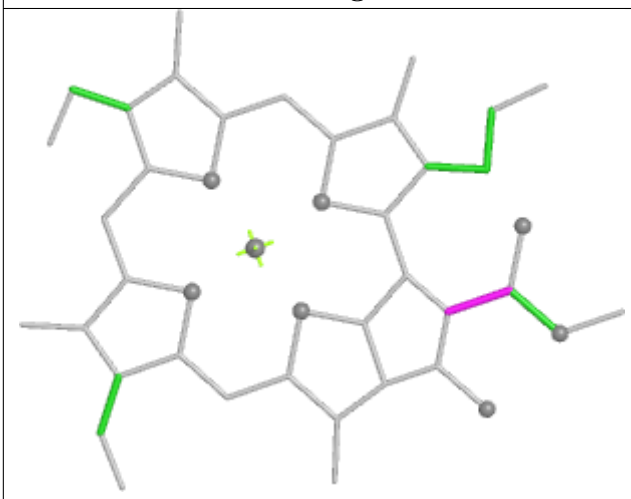
Ligand CLA f 814



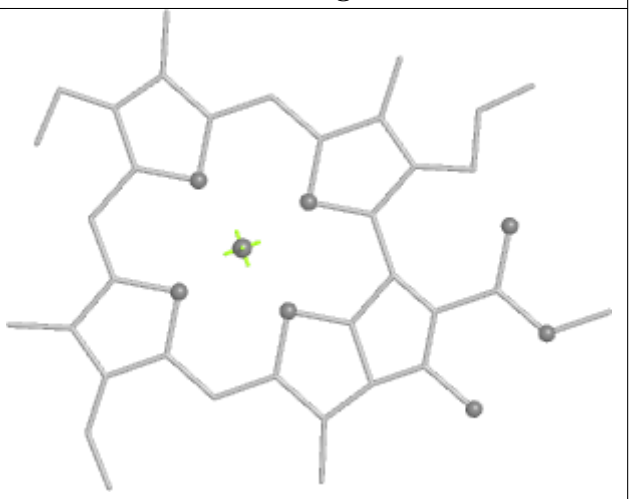
Bond lengths



Bond angles

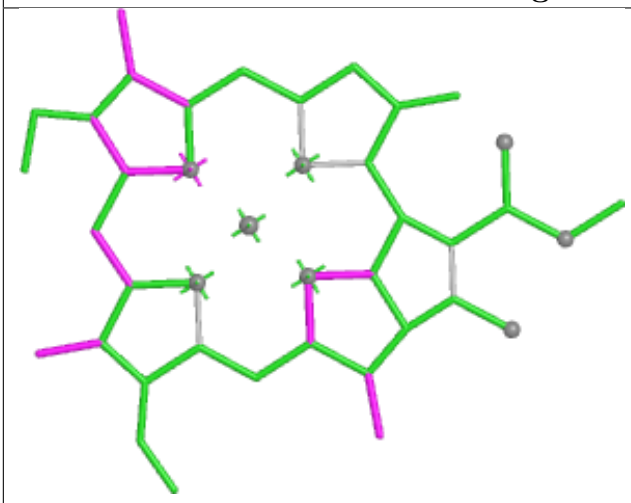


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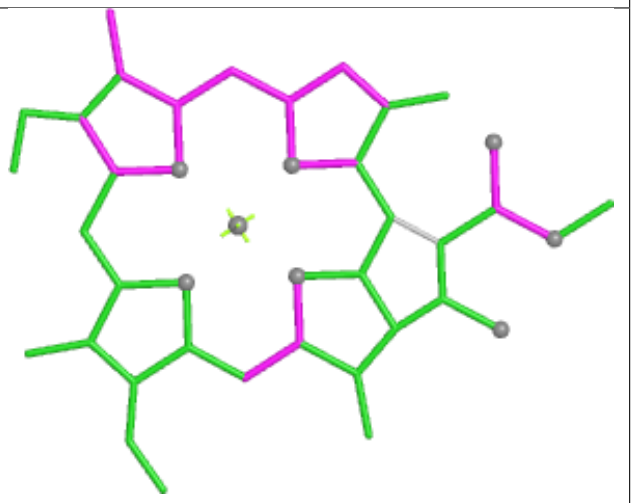


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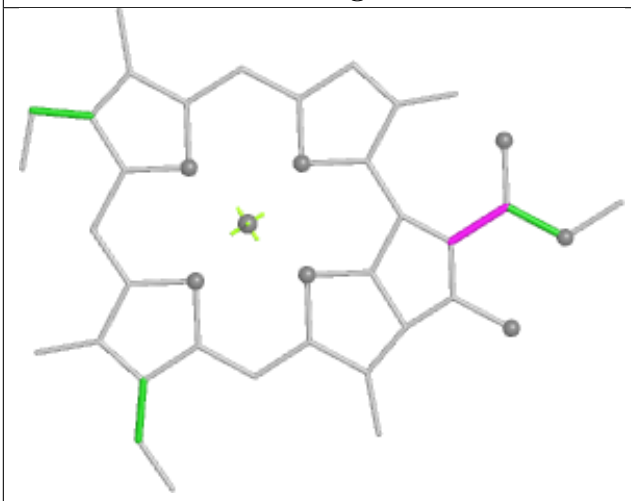
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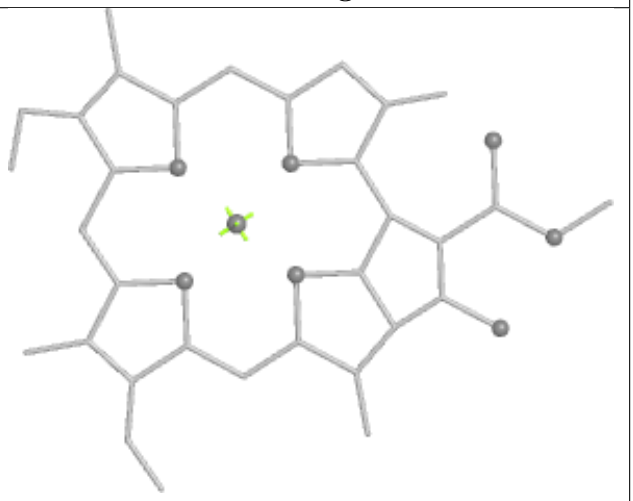
Bond lengths



Bond angles

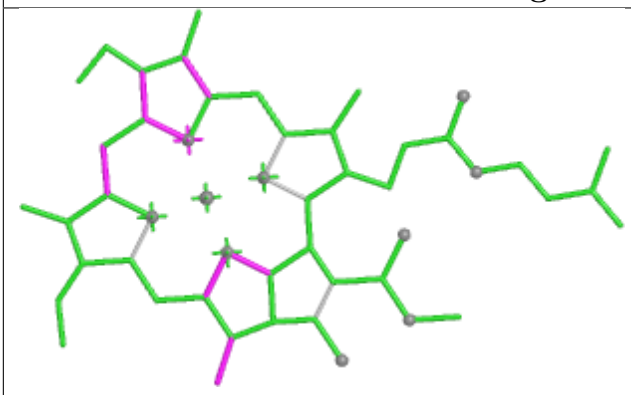


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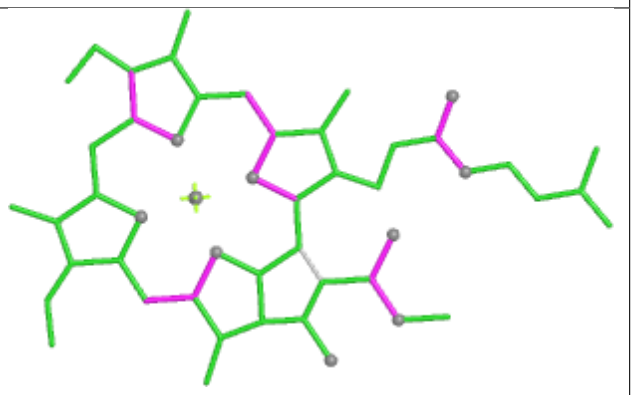


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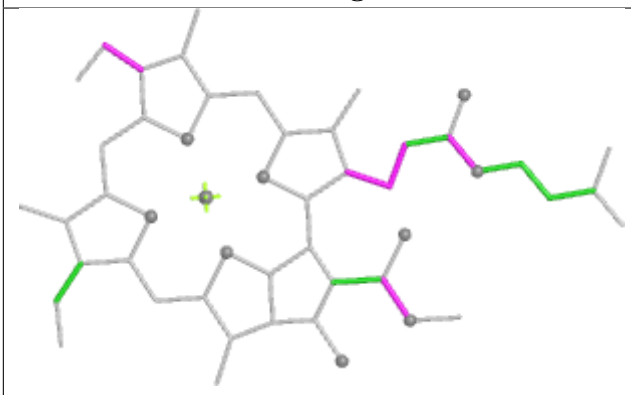
Ligand CLA s 511



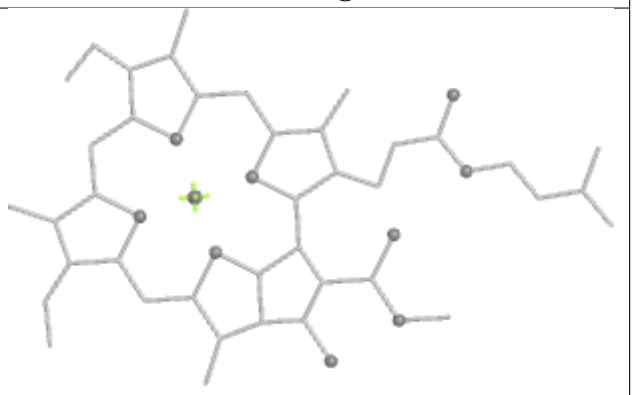
Bond lengths



Bond angles

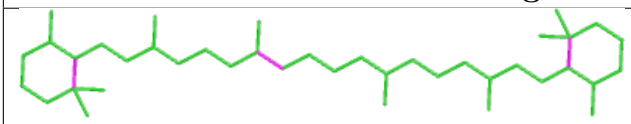


Torsions

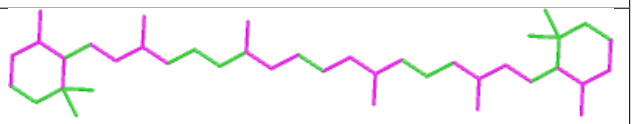


Rings

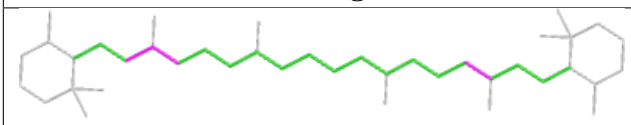
Ligand BCR B 846



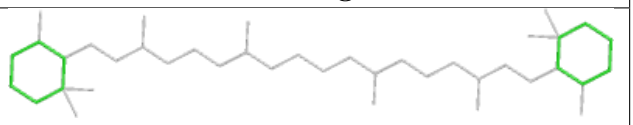
Bond lengths



Bond angles

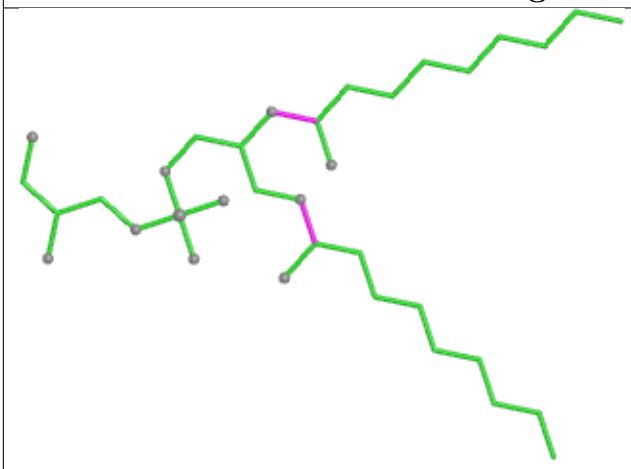


Torsions

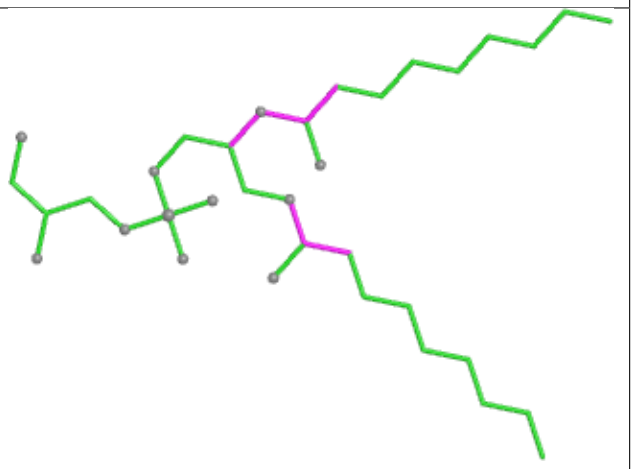


Rings

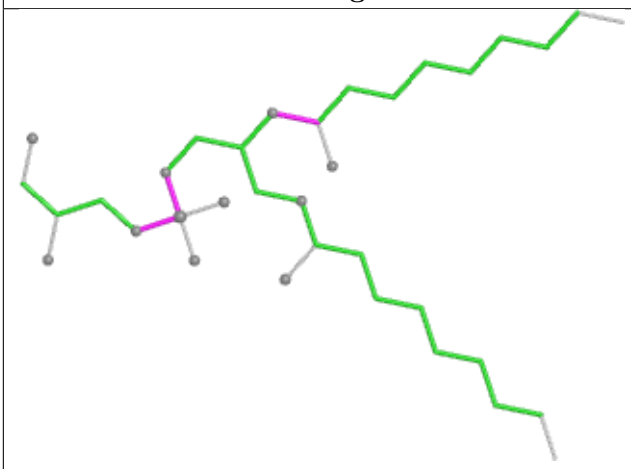
Ligand LHG s 516



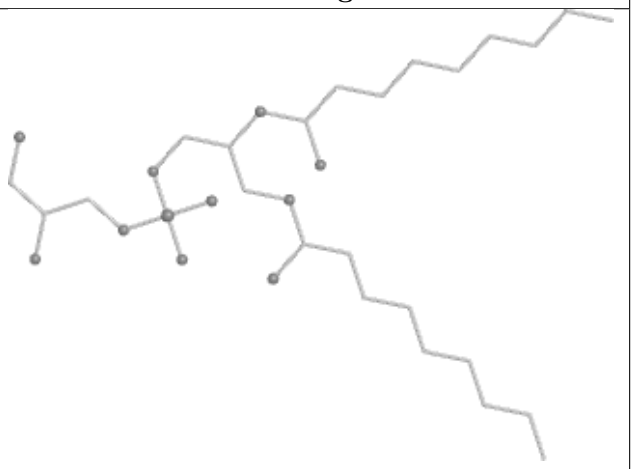
Bond lengths



Bond angles

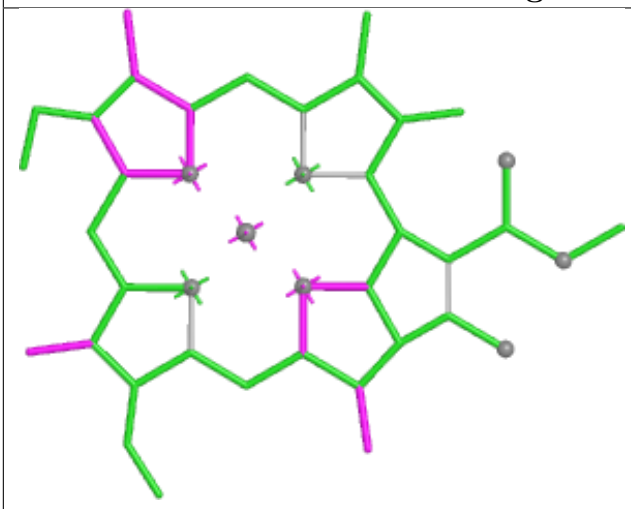


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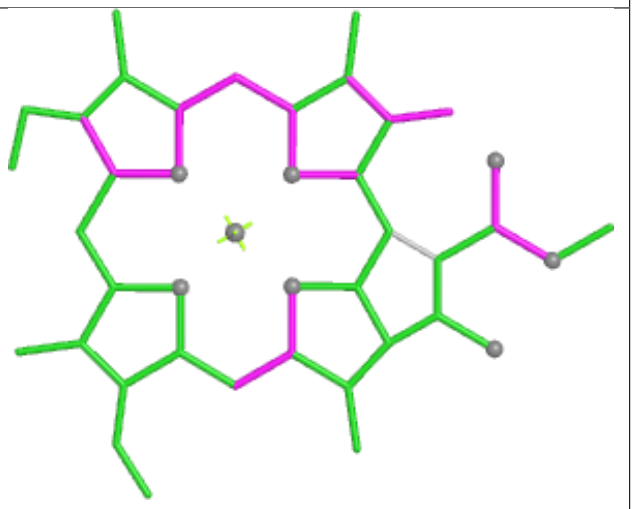


Rings

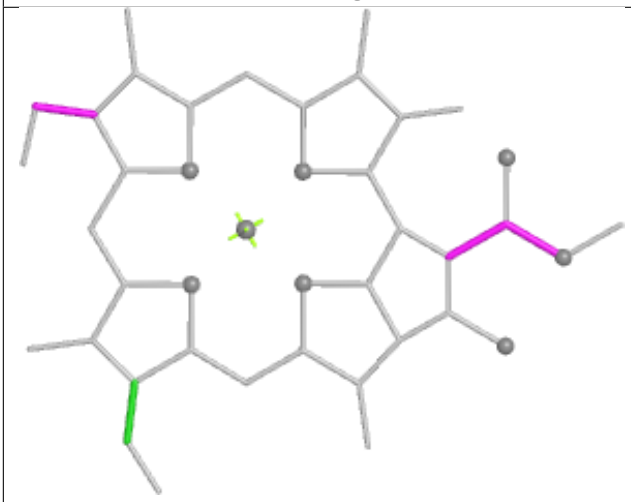
Ligand CLA F 803



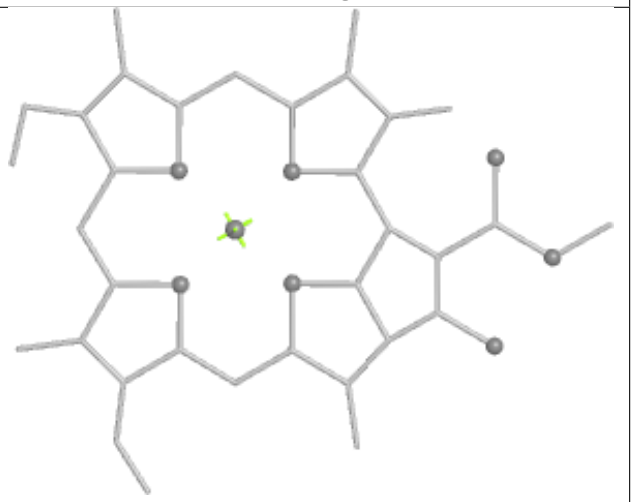
Bond lengths



Bond angles

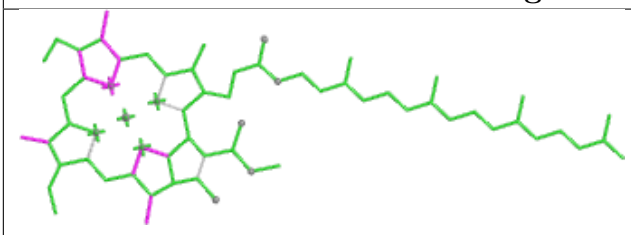


Torsions

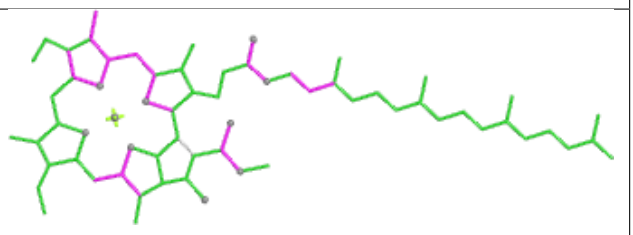


Rings

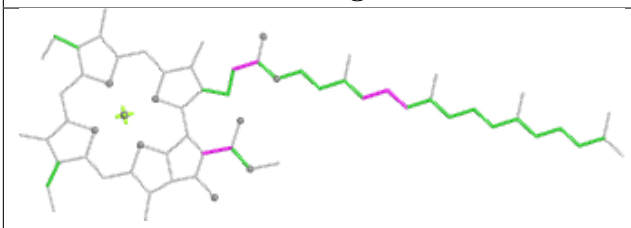
Ligand CLA B 833



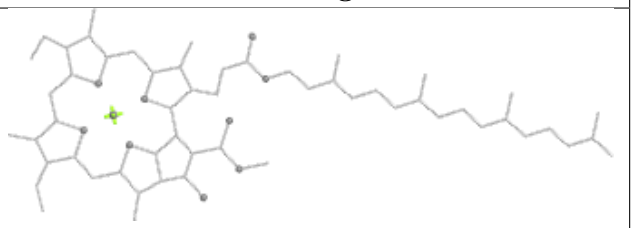
Bond lengths



Bond angles

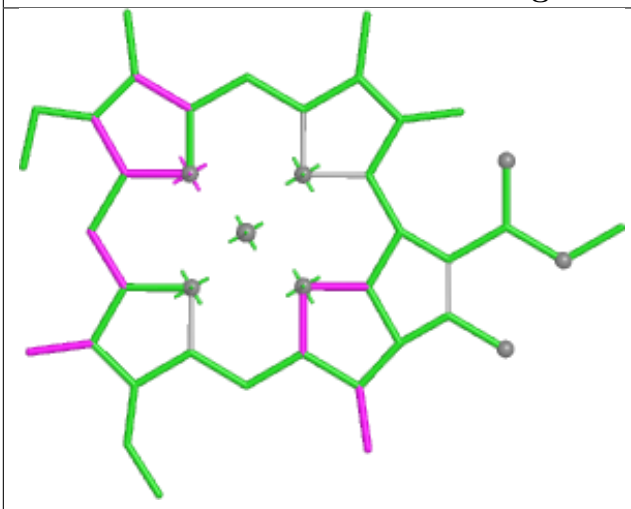


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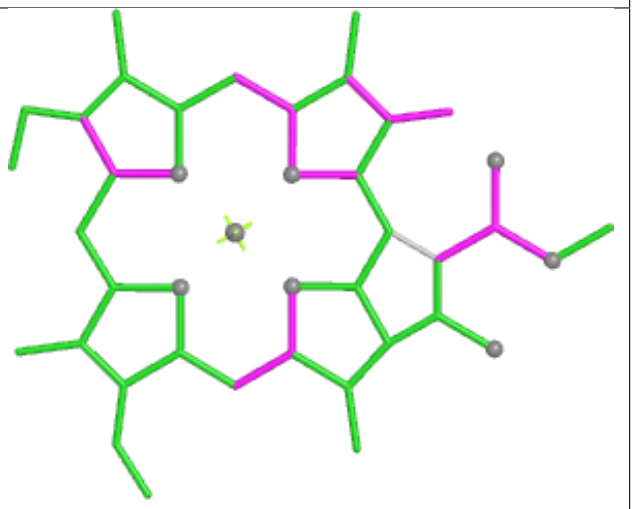


Rings

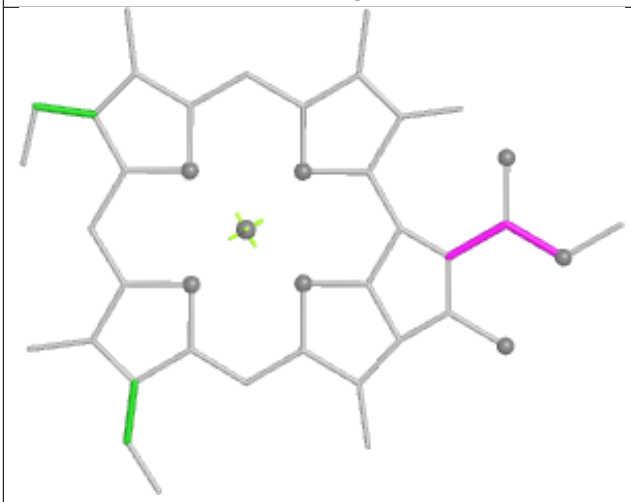
Ligand CLA f 840



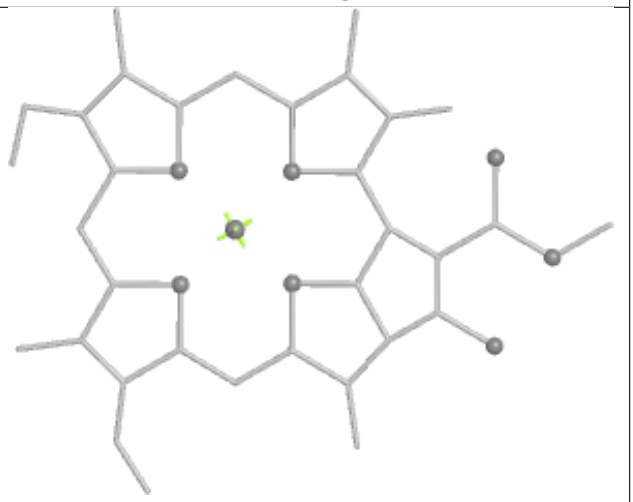
Bond lengths



Bond angles

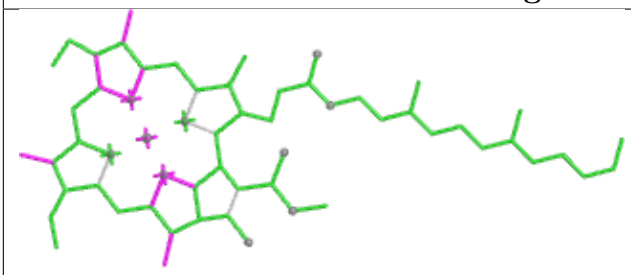


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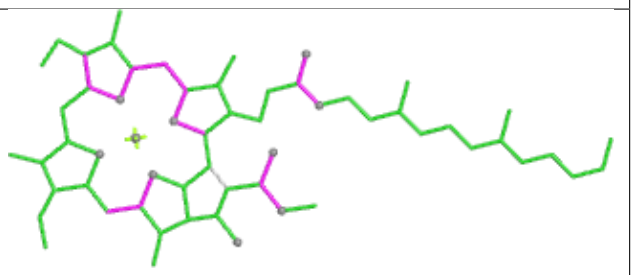


Rings

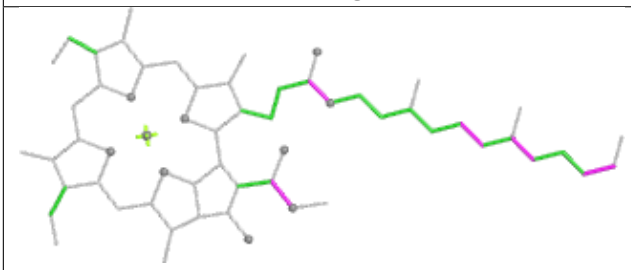
Ligand CLA A 825



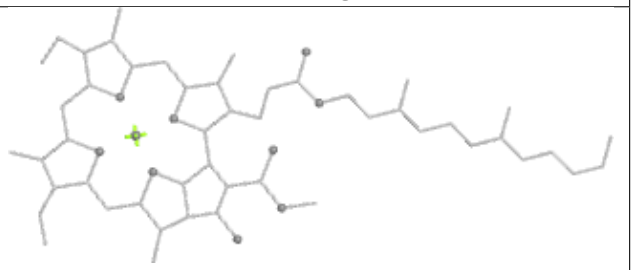
Bond lengths



Bond angles

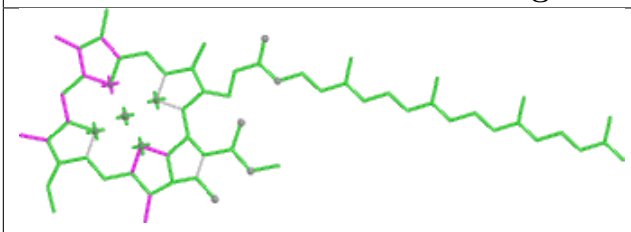


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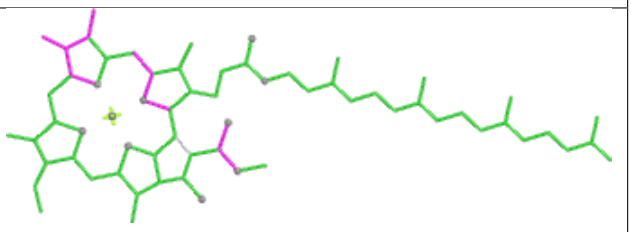


Rings

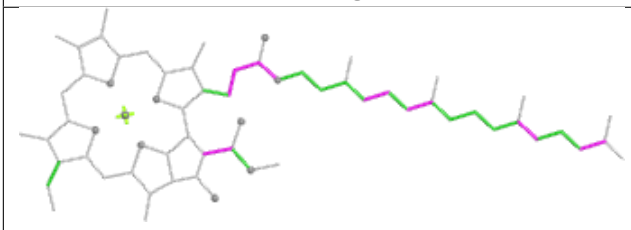
Ligand CLA f 801



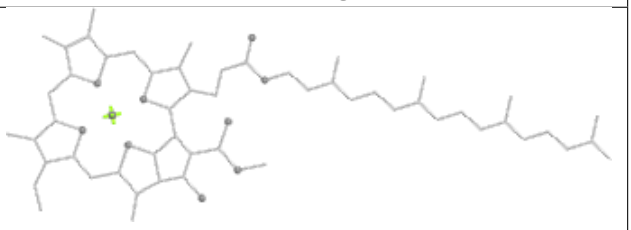
Bond lengths



Bond angles

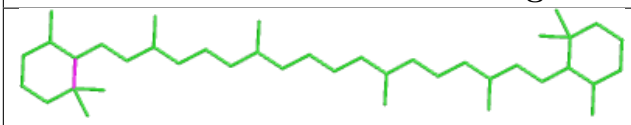


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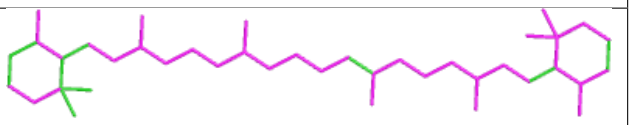


Rings

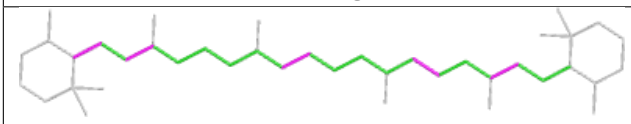
Ligand BCR 2 503



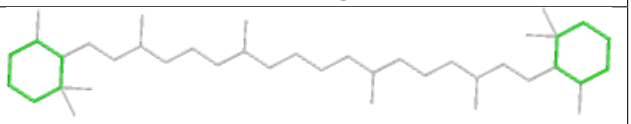
Bond lengths



Bond angles

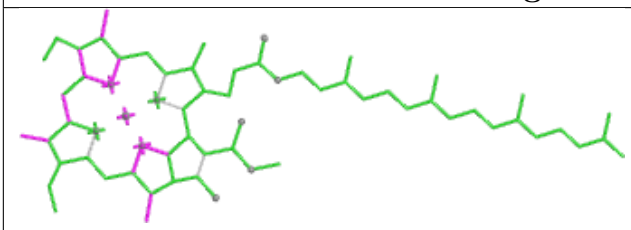


Torsions

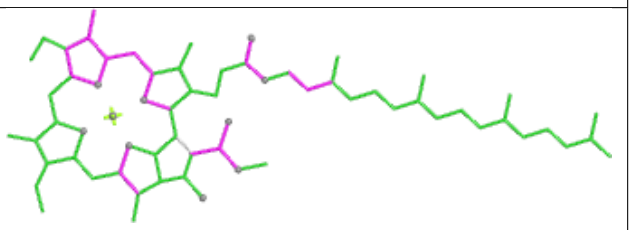


Rings

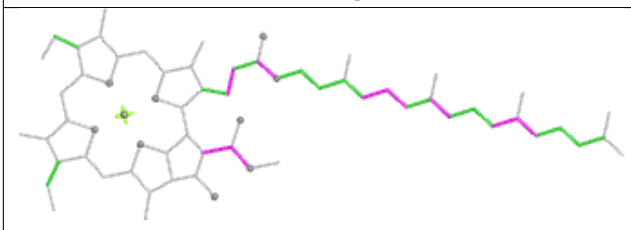
Ligand CLA A 838



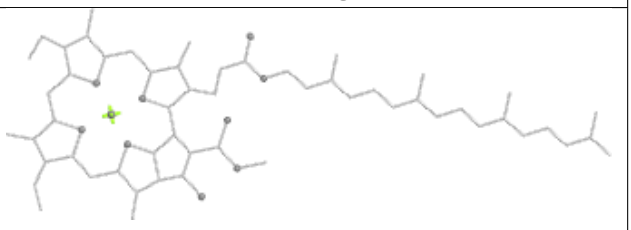
Bond lengths



Bond angles

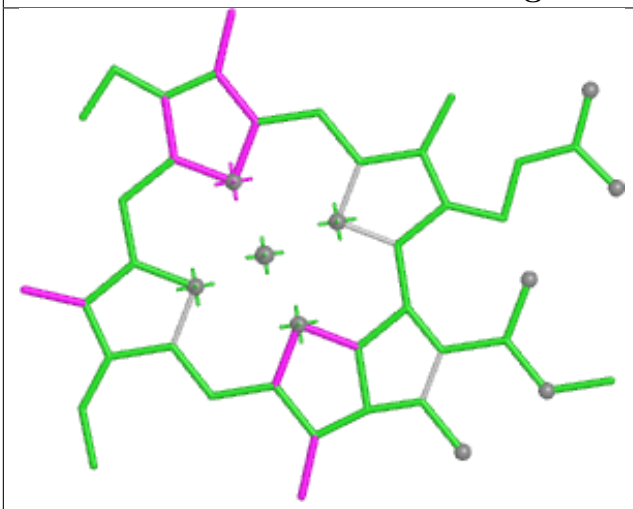


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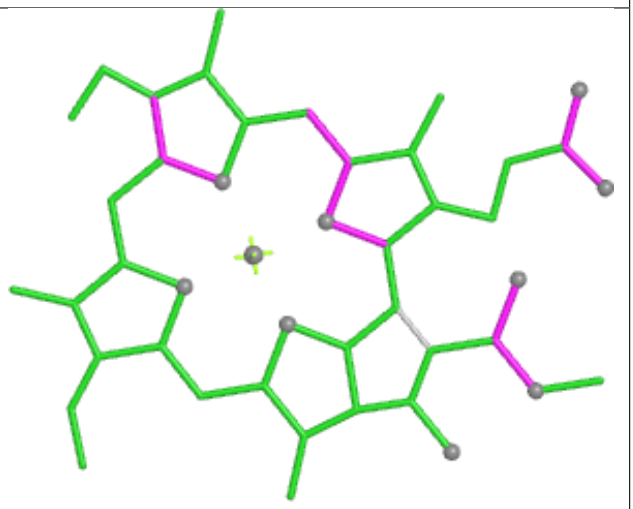


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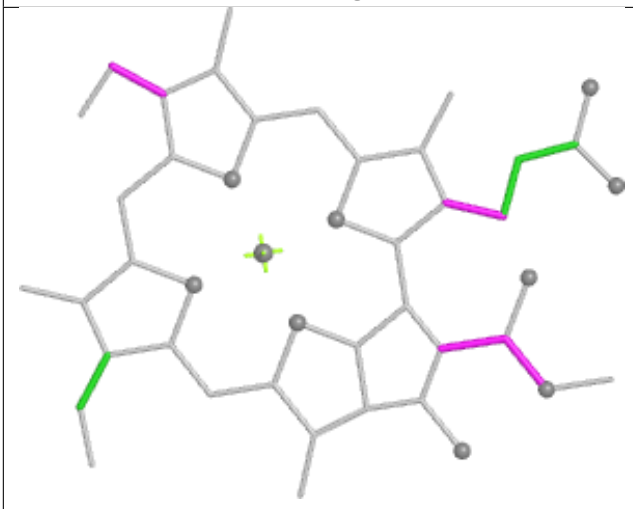
Ligand CLA B 824



Bond lengths



Bond angles

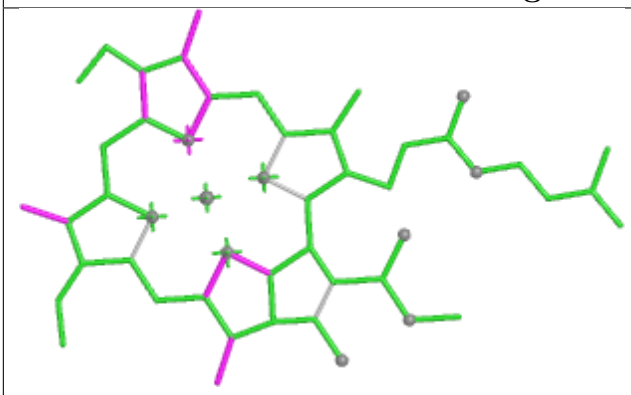


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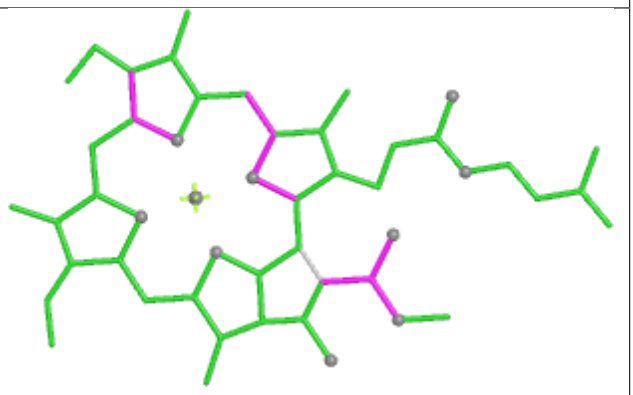


Rings

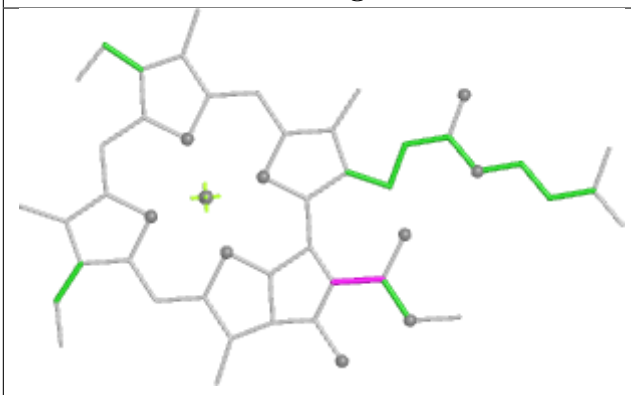
Ligand CLA A 830



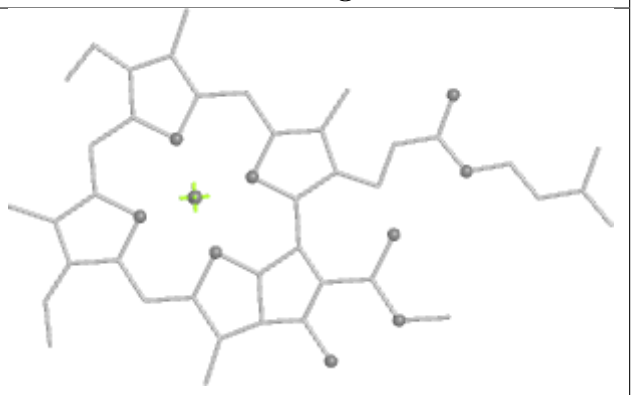
Bond lengths



Bond angles

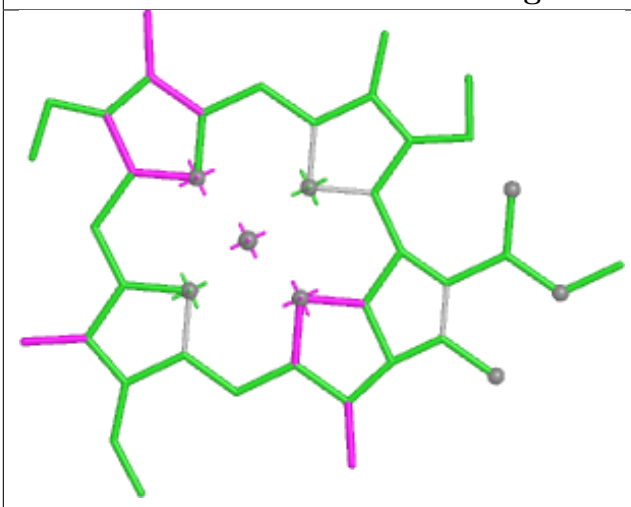


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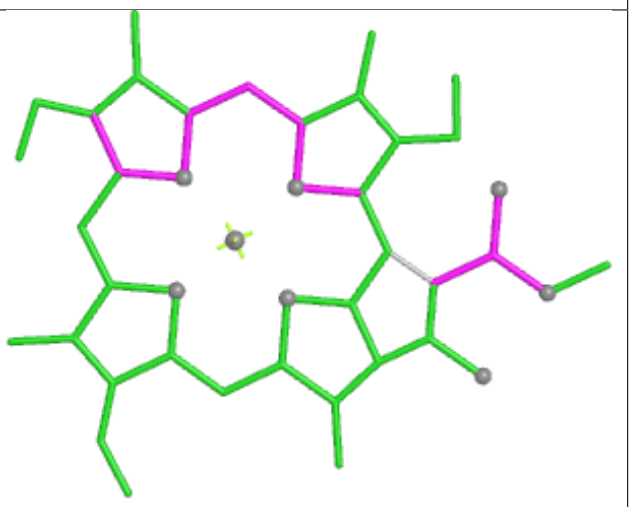


Rings

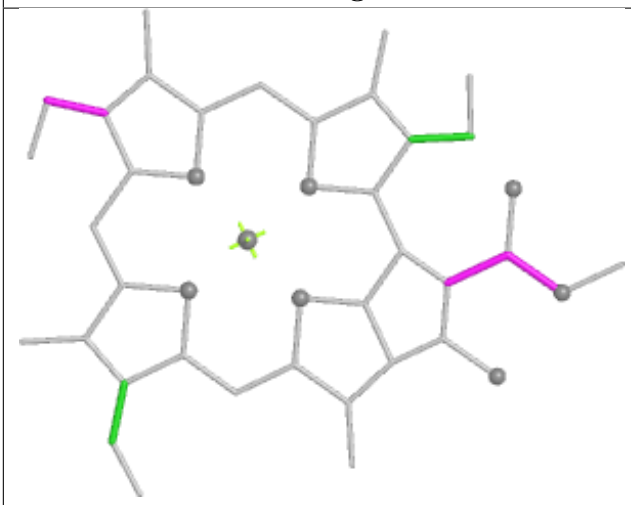
Ligand CLA A 839



Bond lengths



Bond angles

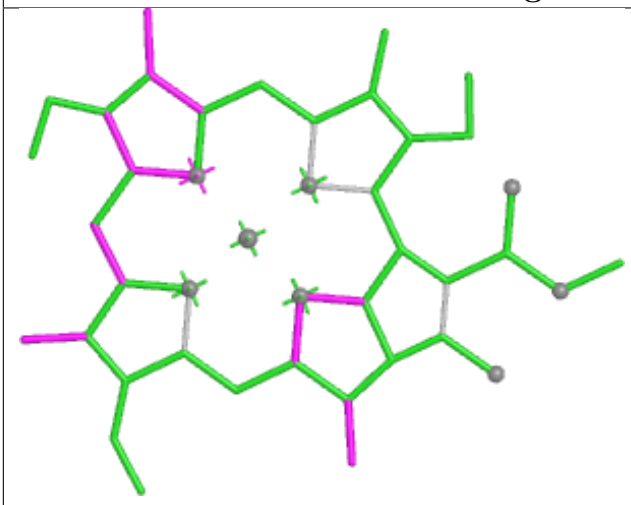


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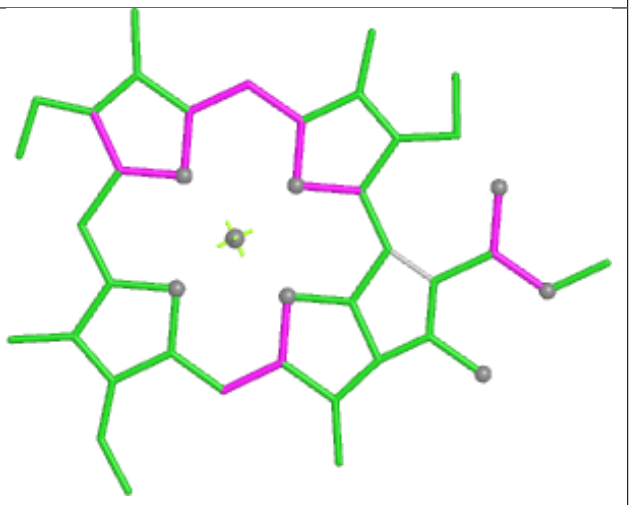


Rings

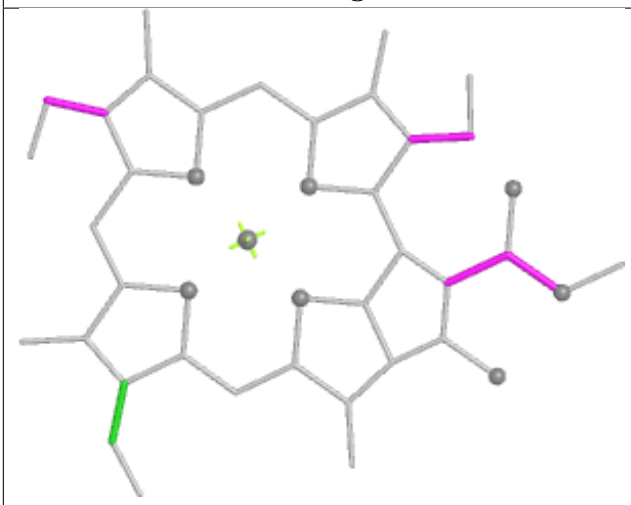
Ligand CLA B 836



Bond lengths



Bond angles



Torsions

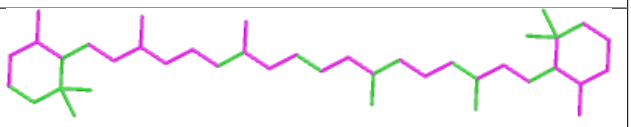


Rings

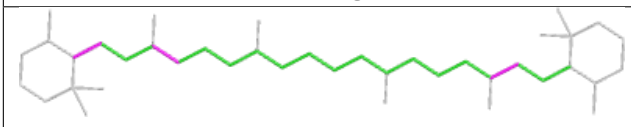
Ligand BCR B 845



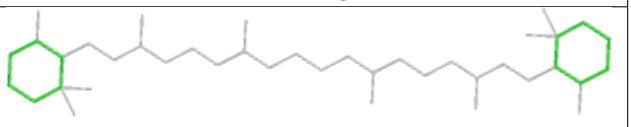
Bond lengths



Bond angles

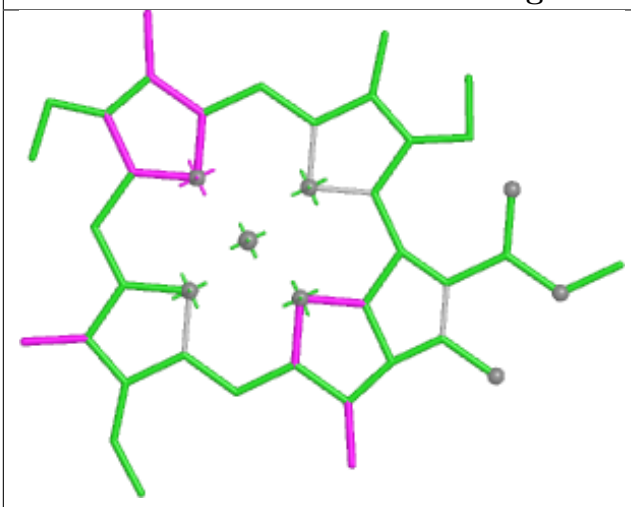


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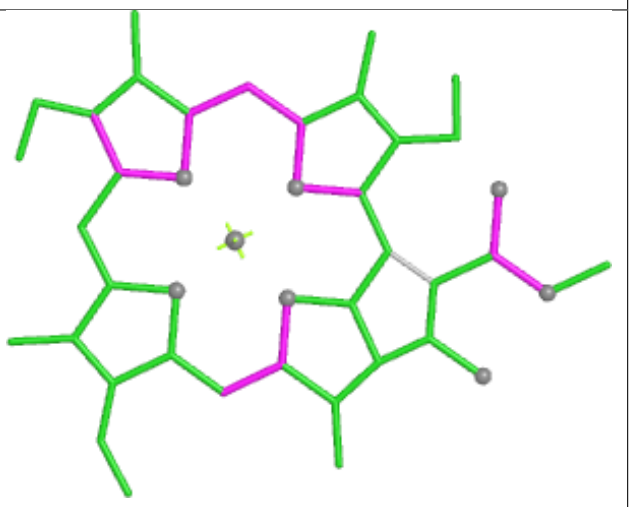


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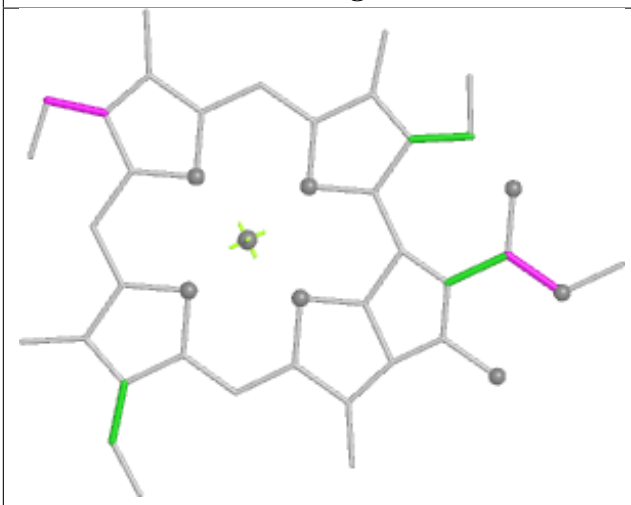
Ligand CLA F 802



Bond lengths



Bond angles

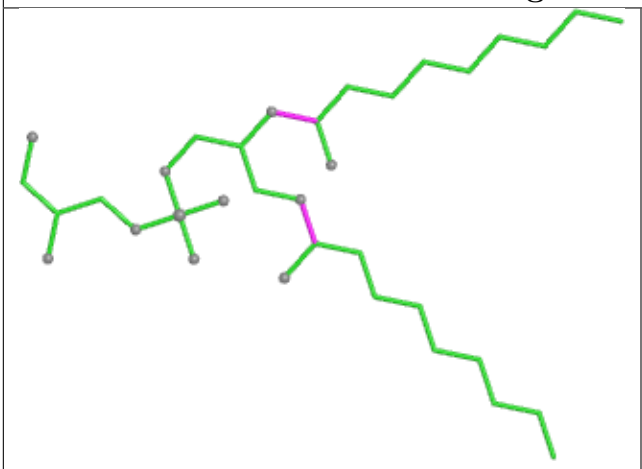


Torsions

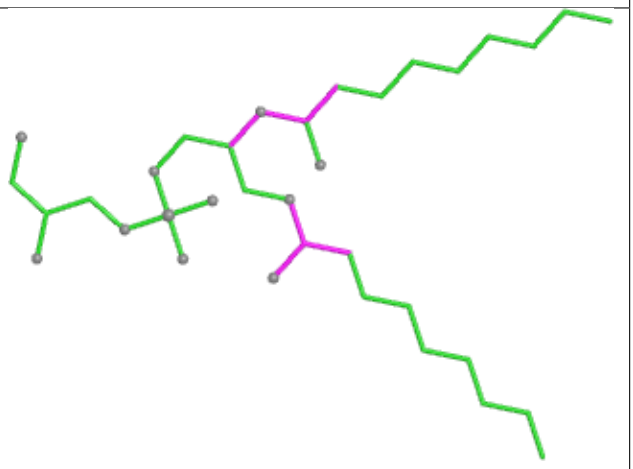


Rings

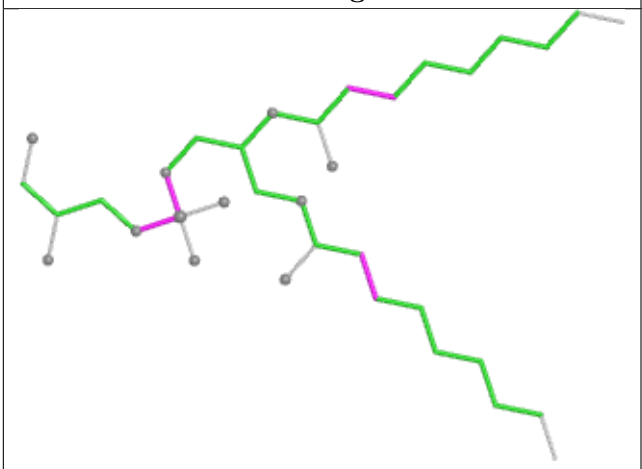
Ligand LHG 2 517



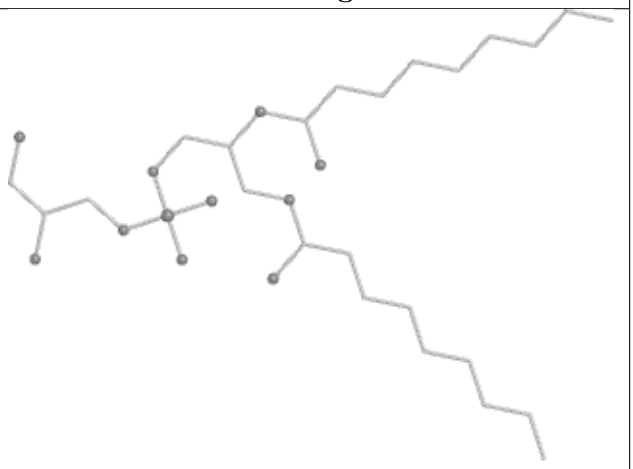
Bond lengths



Bond angles

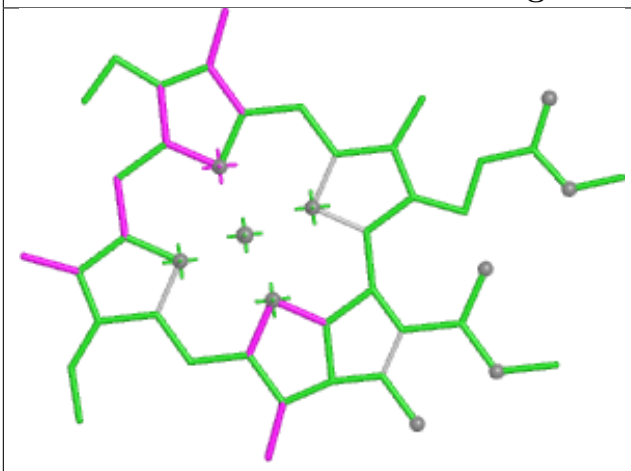


Torsions

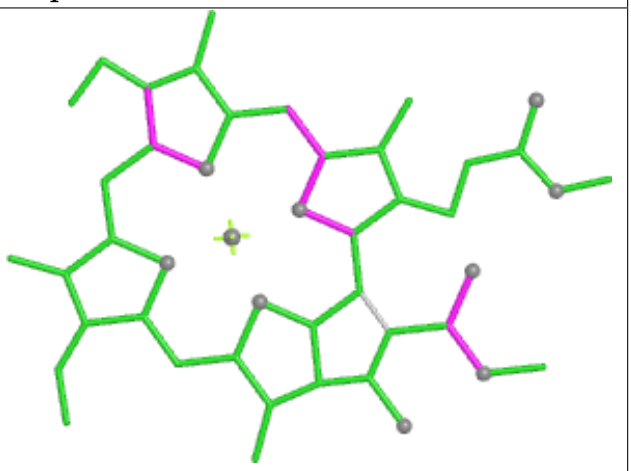


Rings

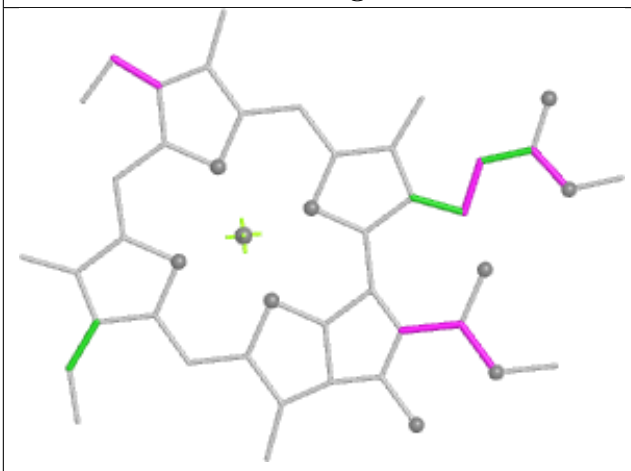
Ligand CLA p 510



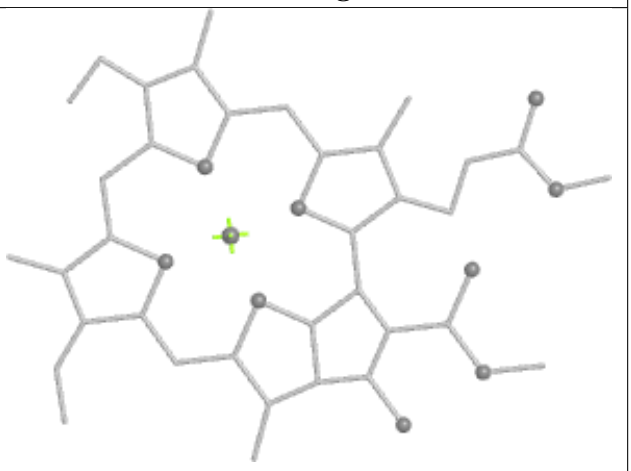
Bond lengths



Bond angles

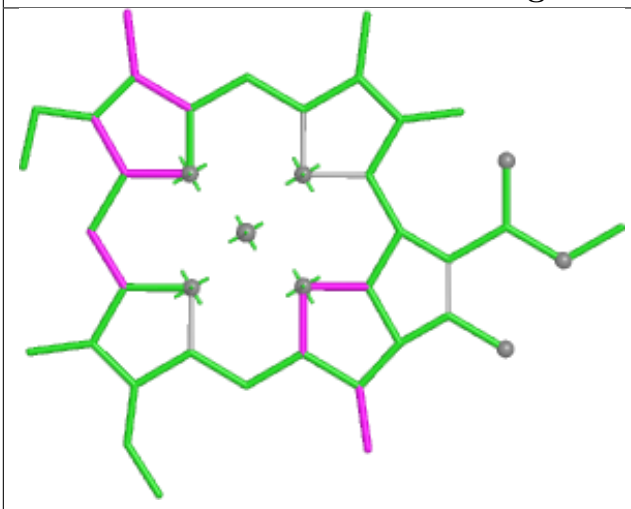


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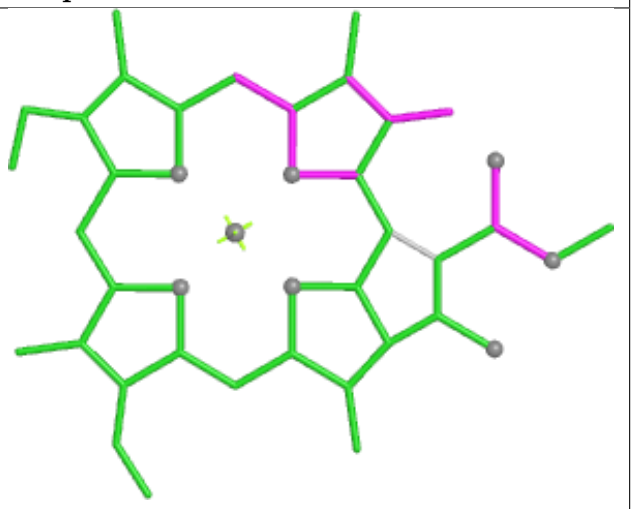


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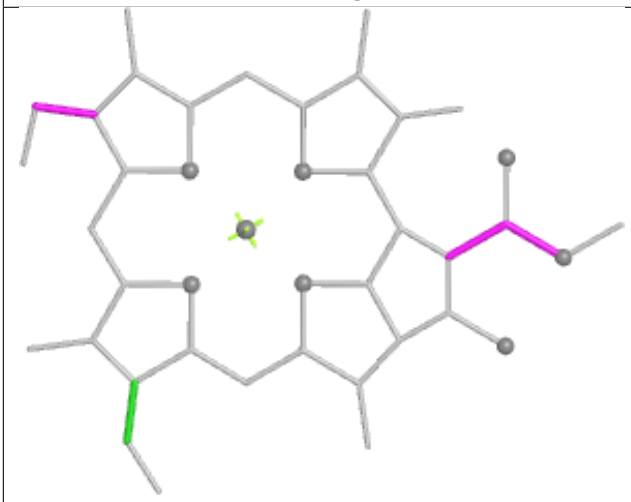
Ligand CLA q 310



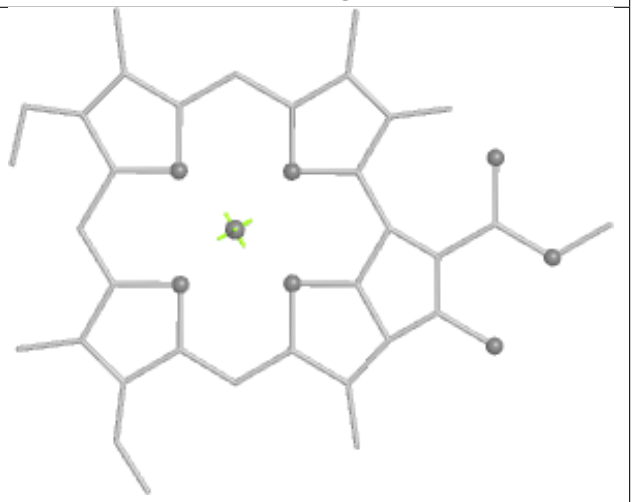
Bond lengths



Bond angles



Torsions

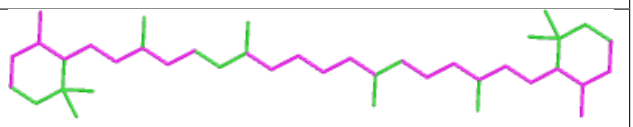


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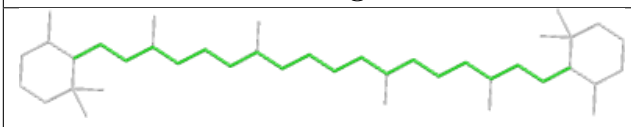
Ligand BCR f 848



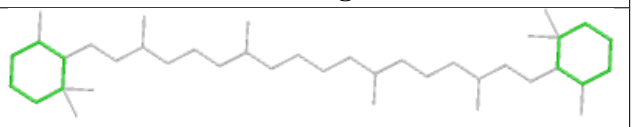
Bond lengths



Bond angles

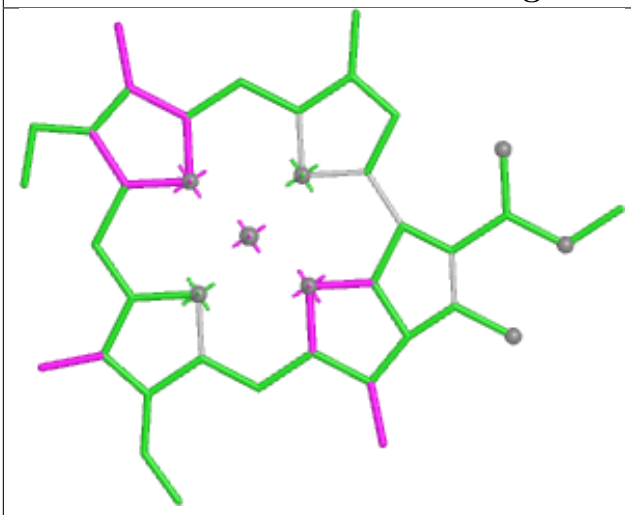


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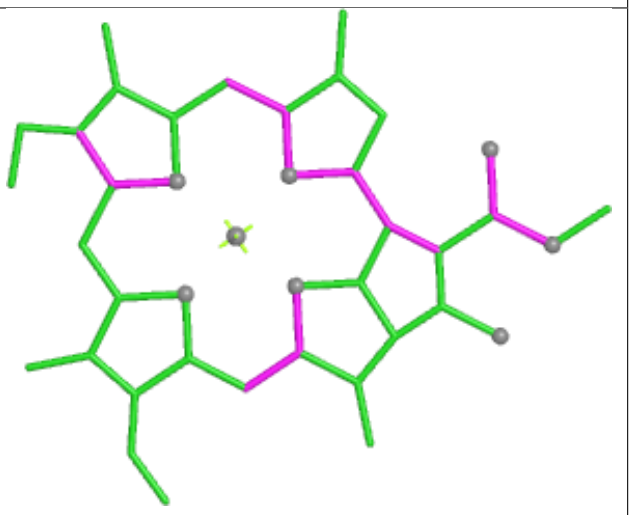


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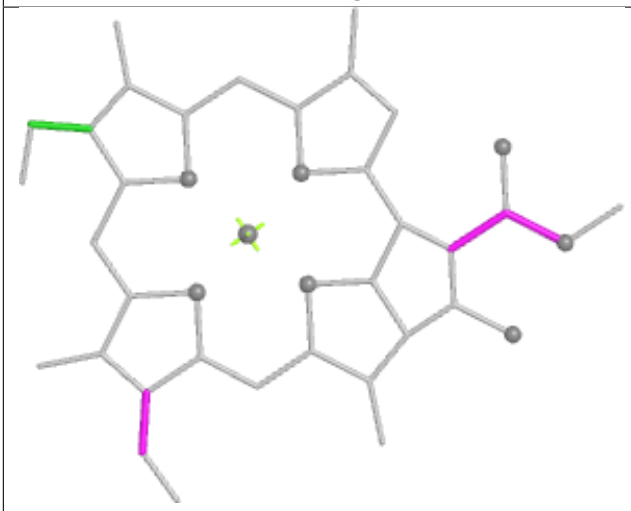
Ligand CLA K 203



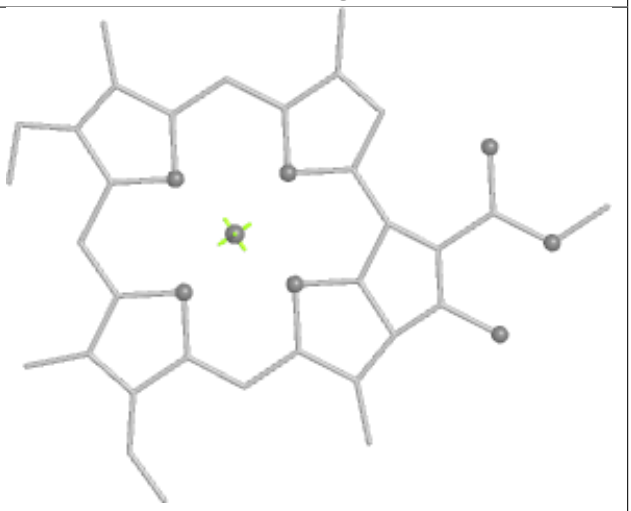
Bond lengths



Bond angles



Torsions



Rings

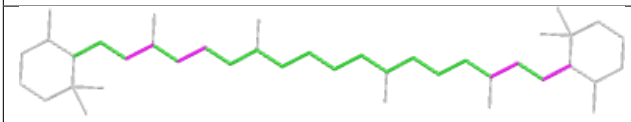
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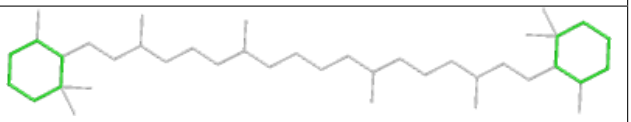
Bond lengths



Bond angles

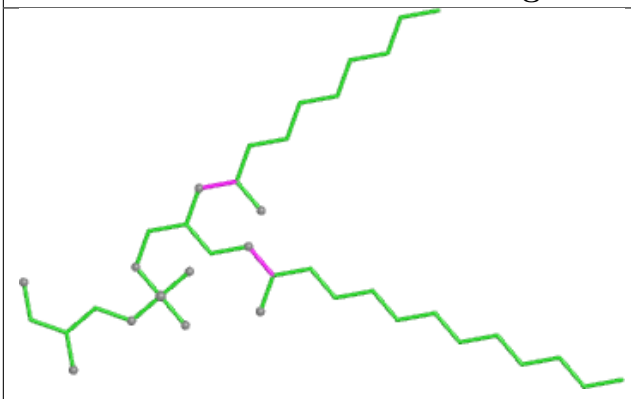


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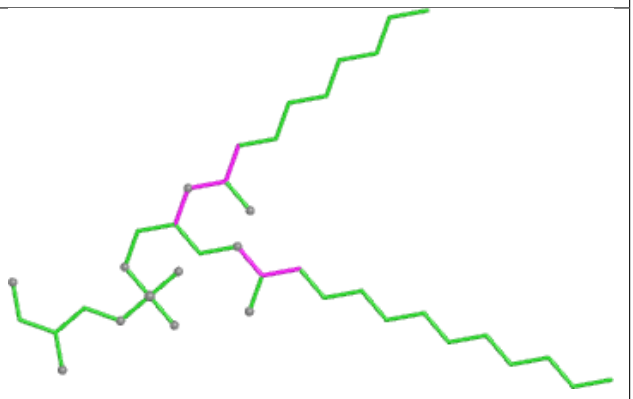


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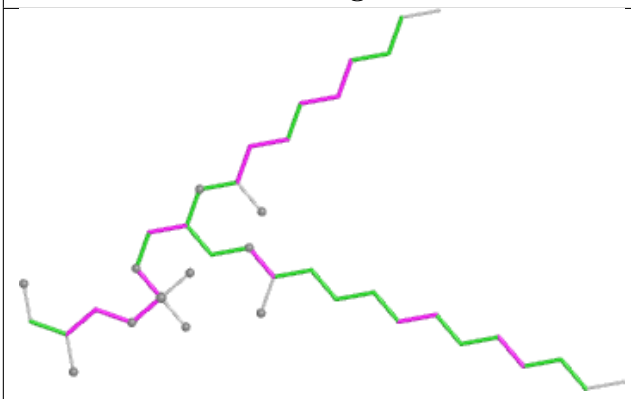
Ligand LHG B 851



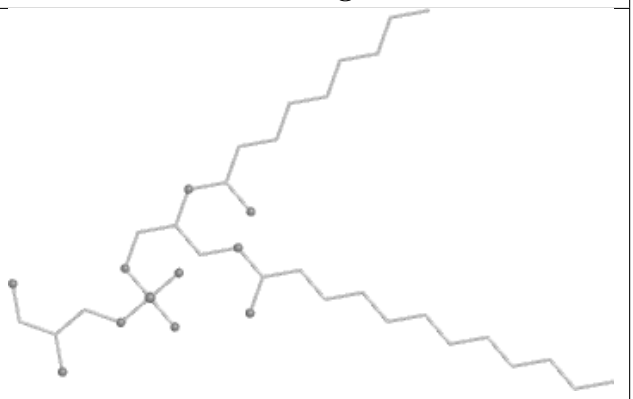
Bond lengths



Bond angles

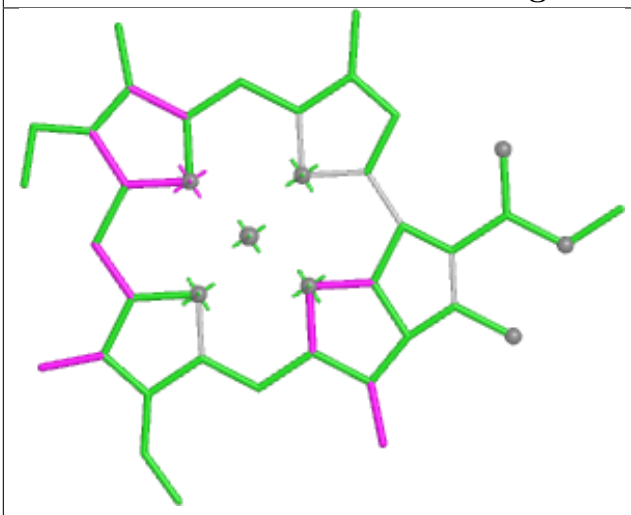


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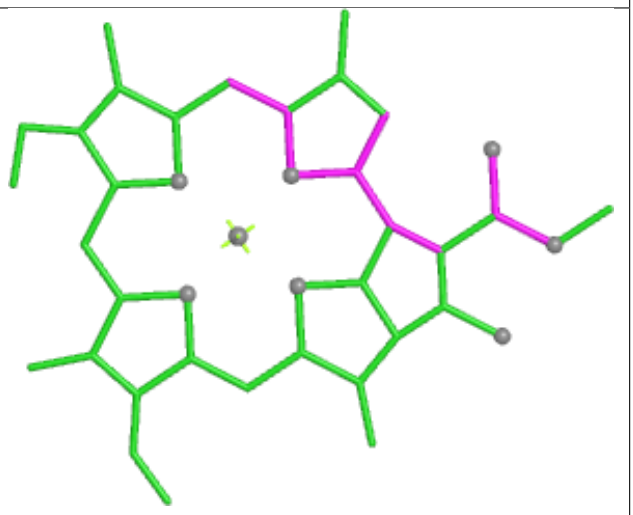


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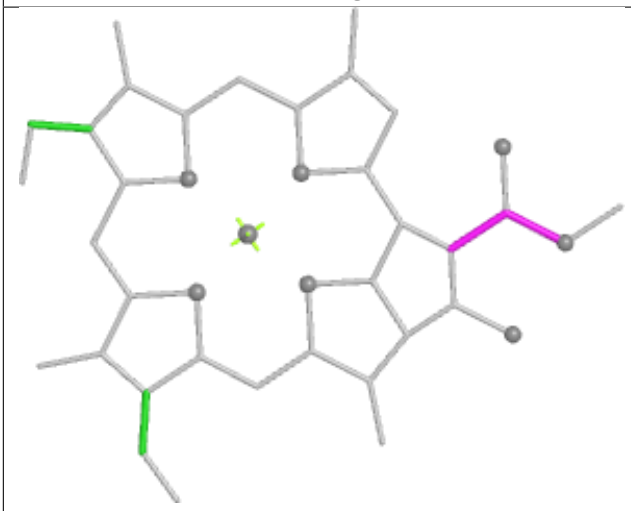
Ligand CLA e 802



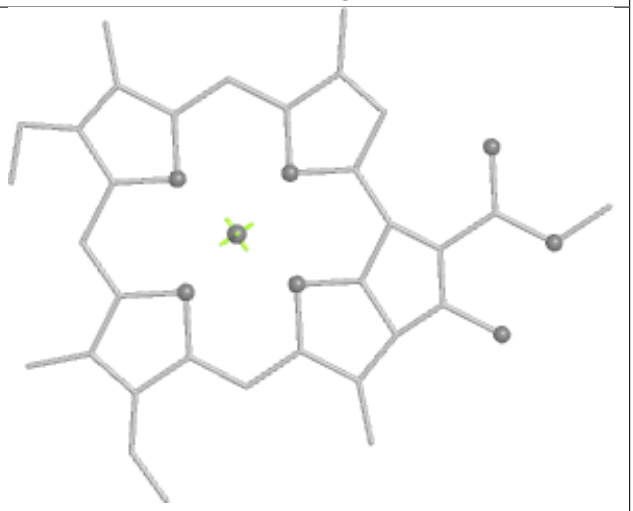
Bond lengths



Bond angles

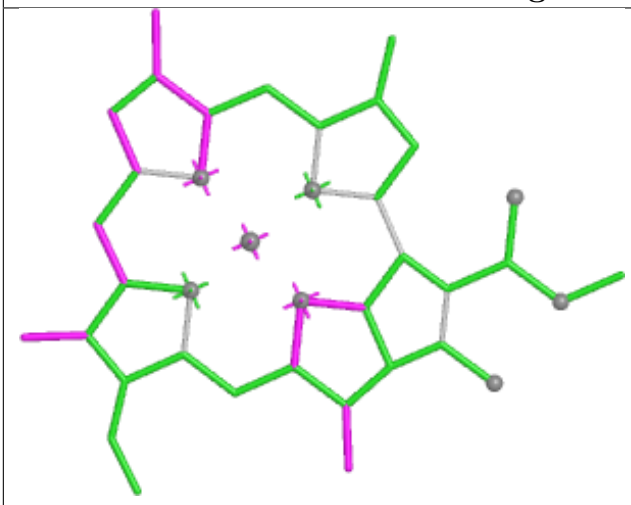


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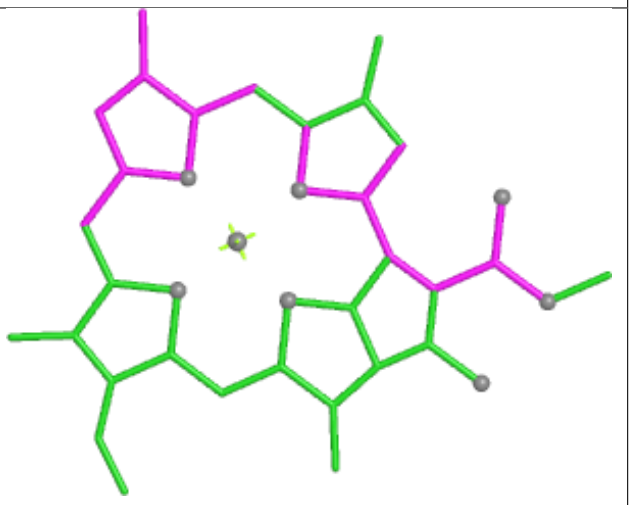


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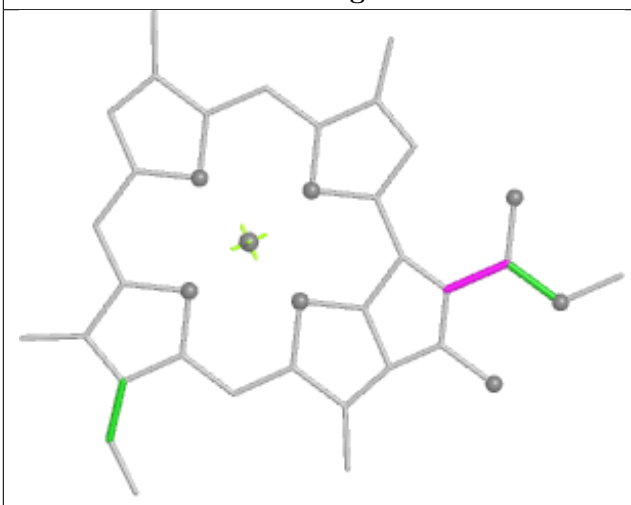
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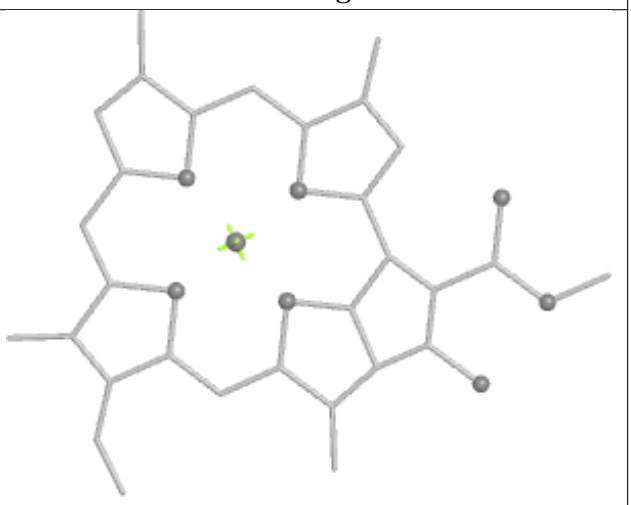
Bond lengths



Bond angles

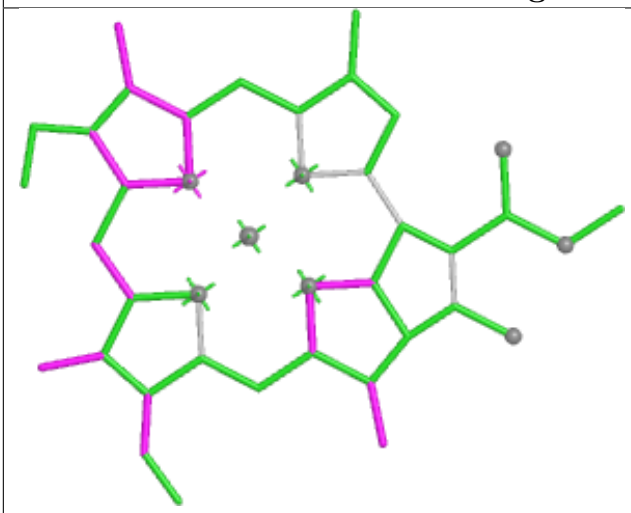


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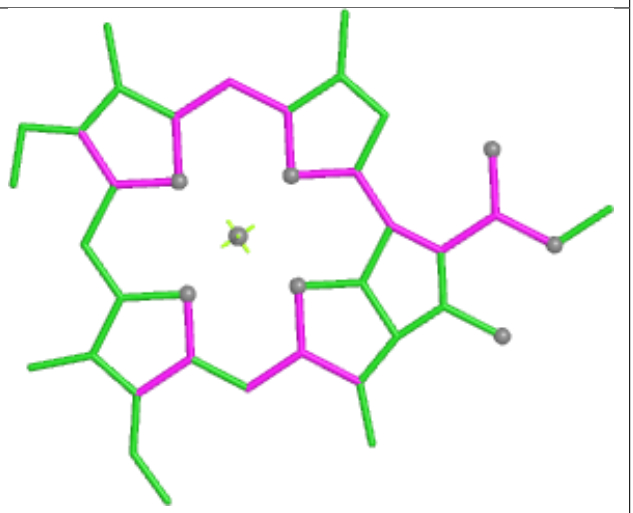


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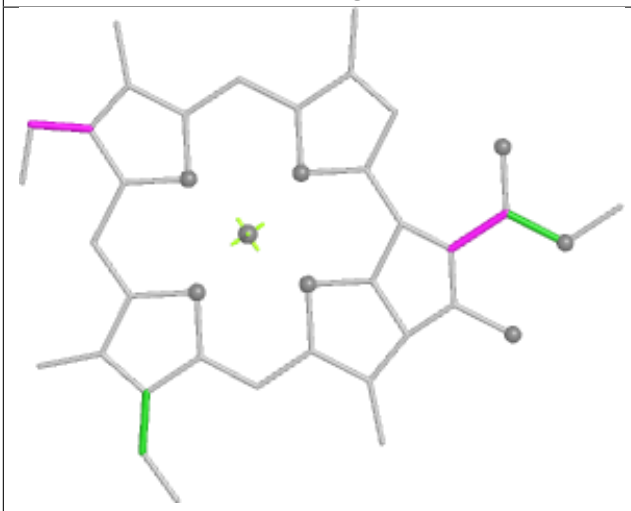
Ligand CLA 2 511



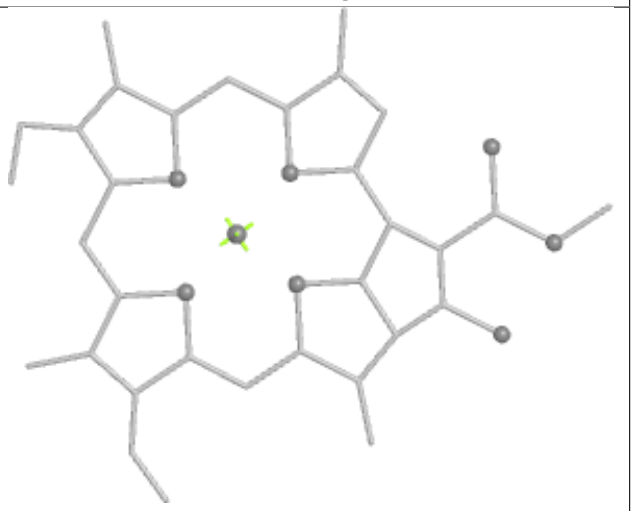
Bond lengths



Bond angles

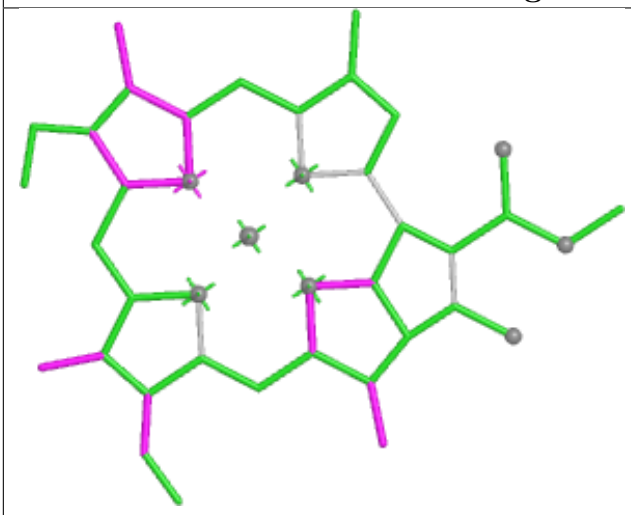


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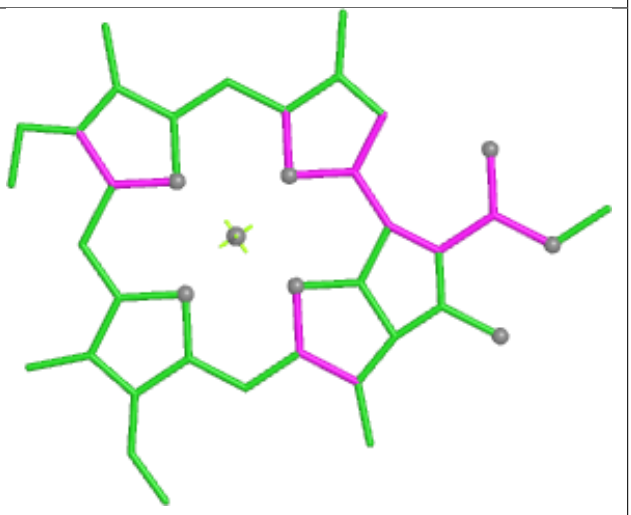


Rings

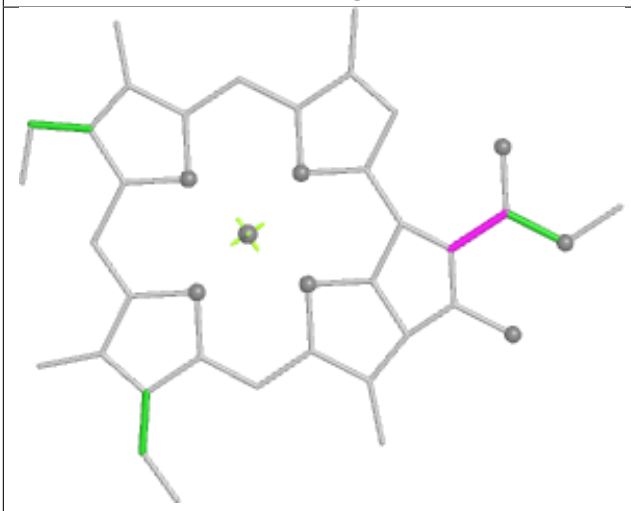
Ligand CLA B 810



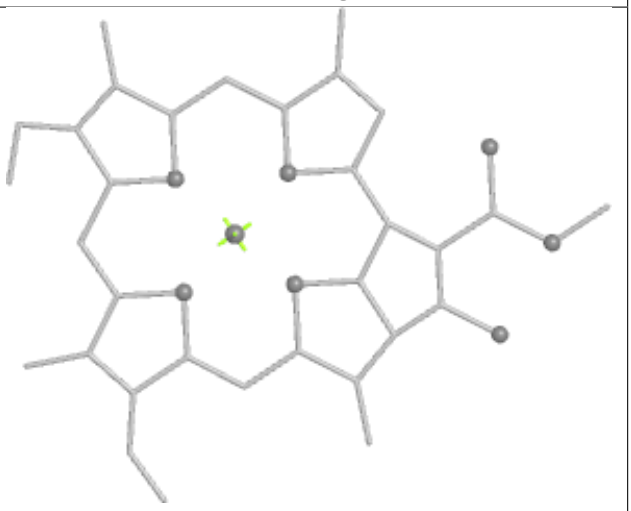
Bond lengths



Bond angles

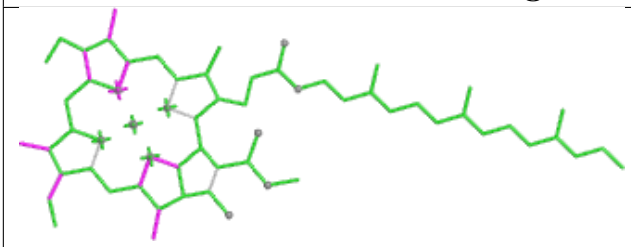


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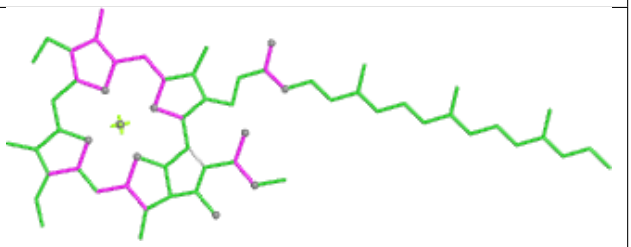


Rings

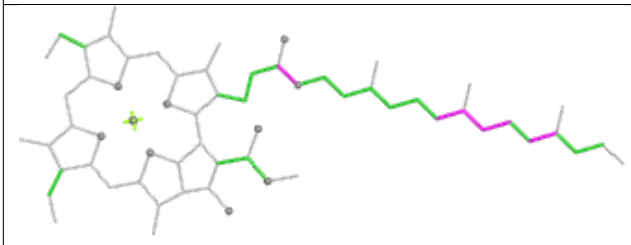
Ligand CLA B 826



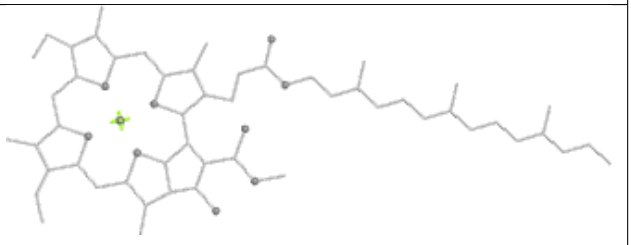
Bond lengths



Bond angles

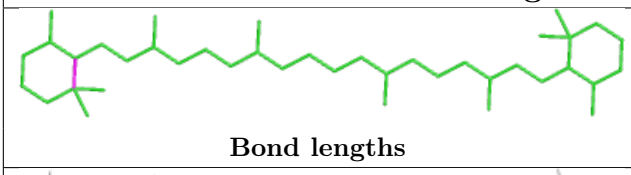


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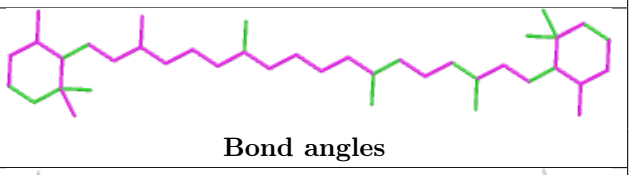


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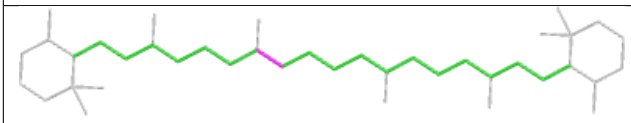
Ligand BCR F 804



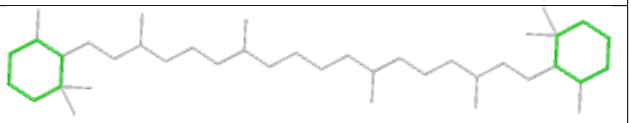
Bond lengths



Bond angles



Torsions

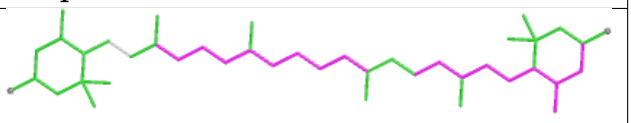


Rings

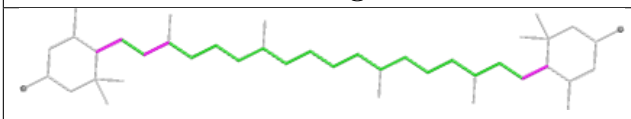
Ligand LUT q 301



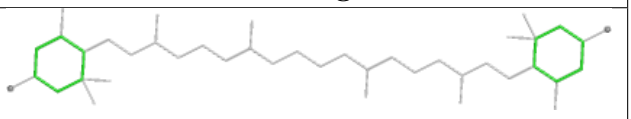
Bond lengths



Bond angles

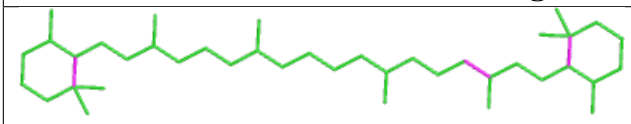


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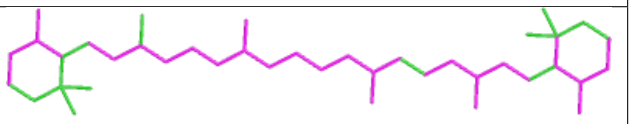


Rings

Ligand BCR I 101



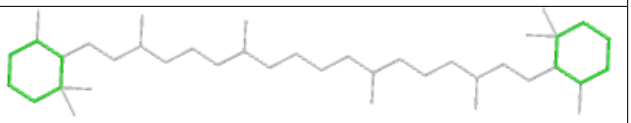
Bond lengths



Bond angles

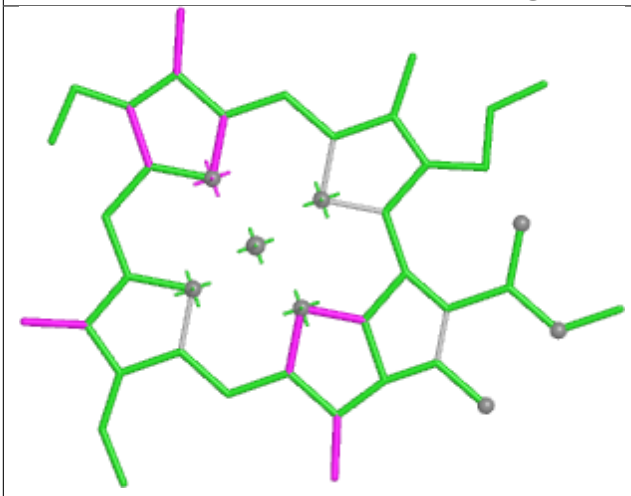


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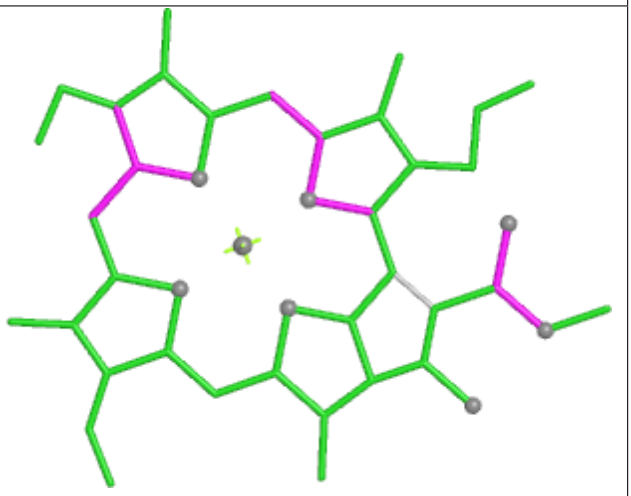


Rings

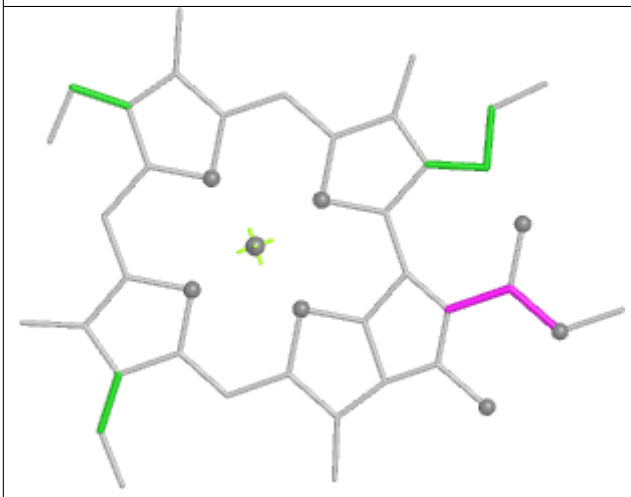
Ligand CLA B 816



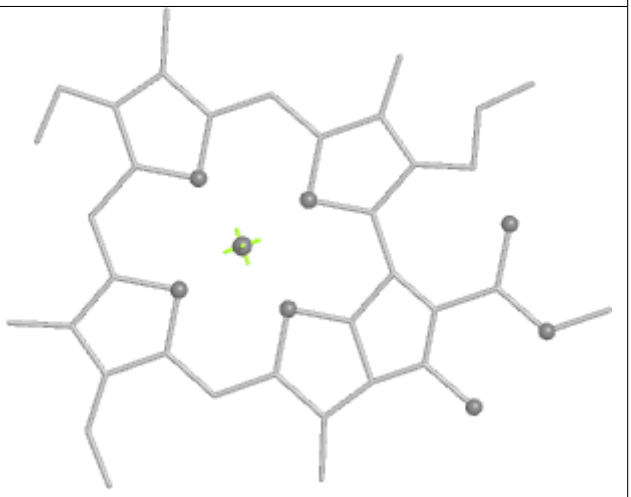
Bond lengths



Bond angles

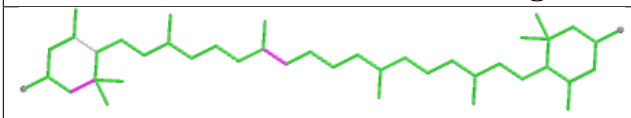


Torsions

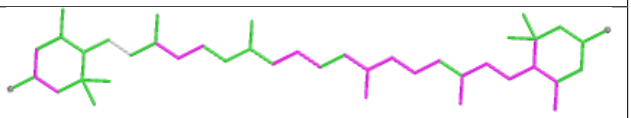


Rings

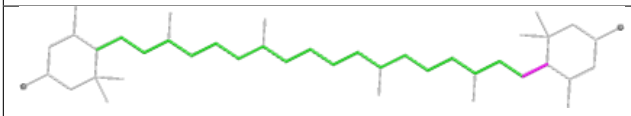
Ligand LUT 3 303



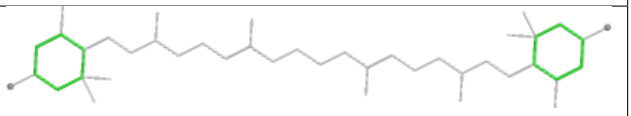
Bond lengths



Bond angles

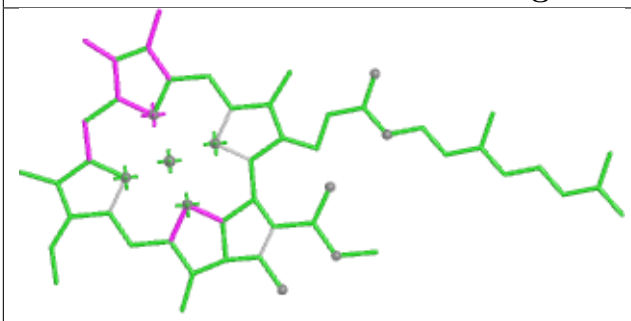


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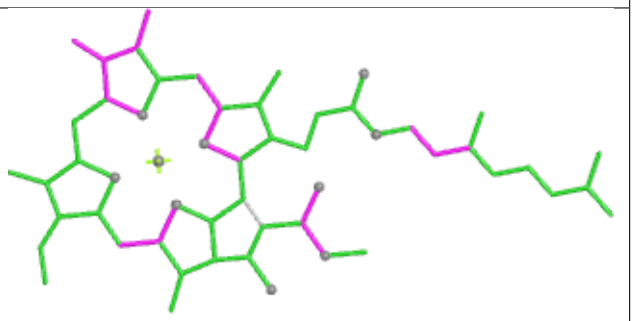


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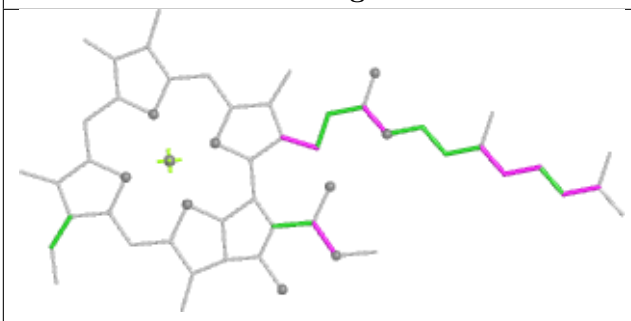
Ligand CLA f 813



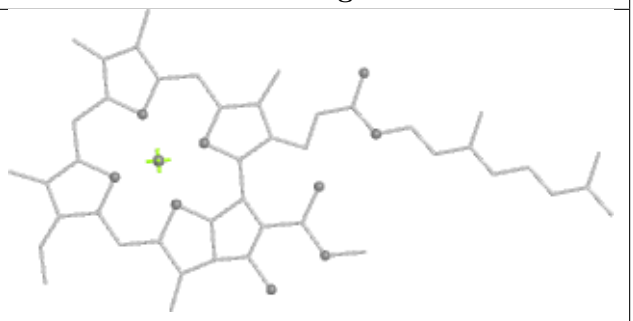
Bond lengths



Bond angles

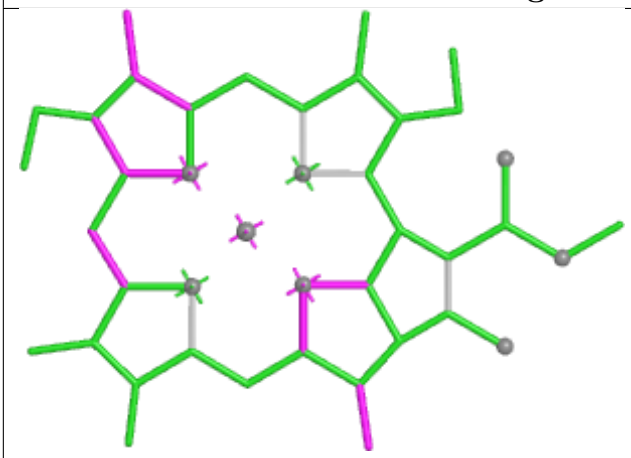


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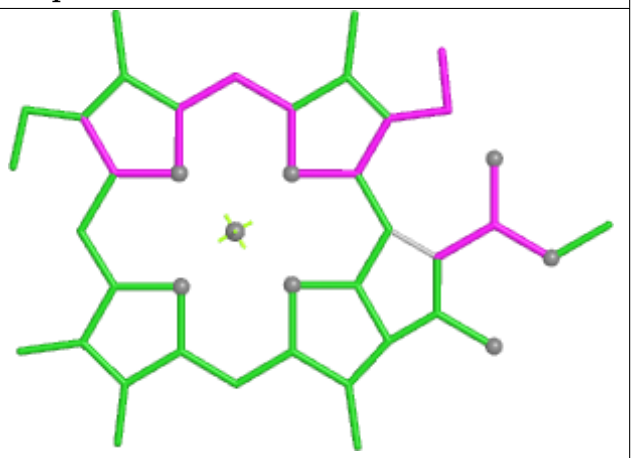


Rings

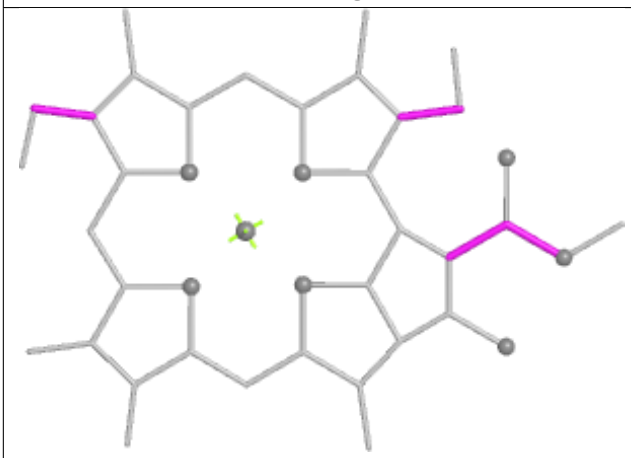
Ligand CLA p 504



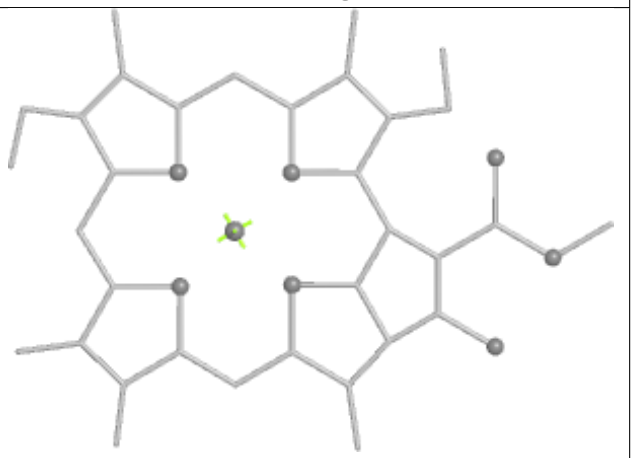
Bond lengths



Bond angles

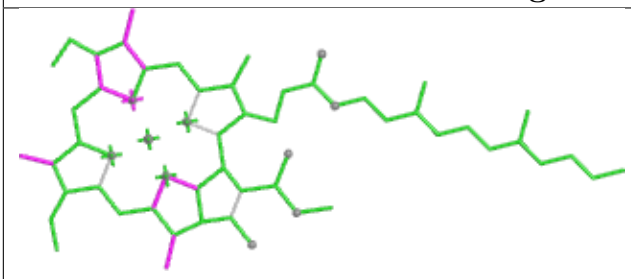


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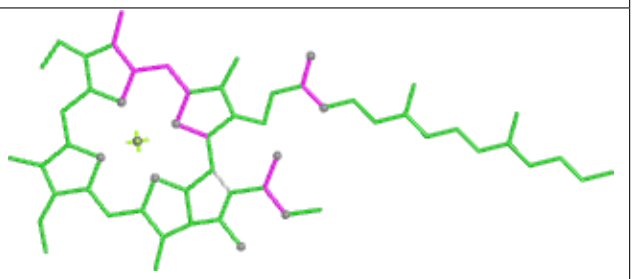


Rings

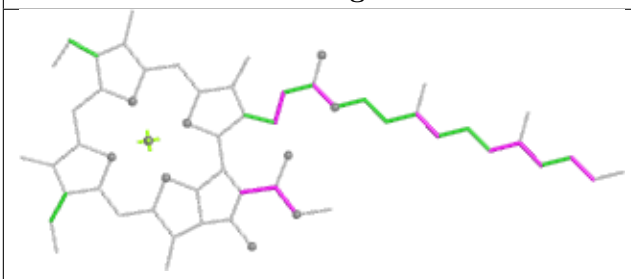
Ligand CLA e 829



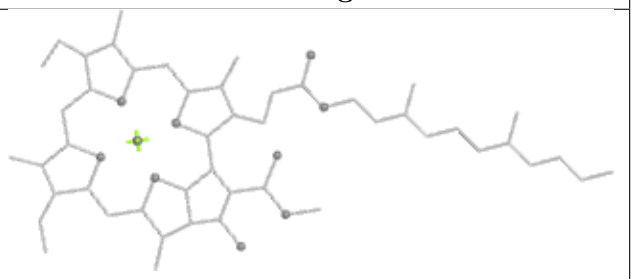
Bond lengths



Bond angles

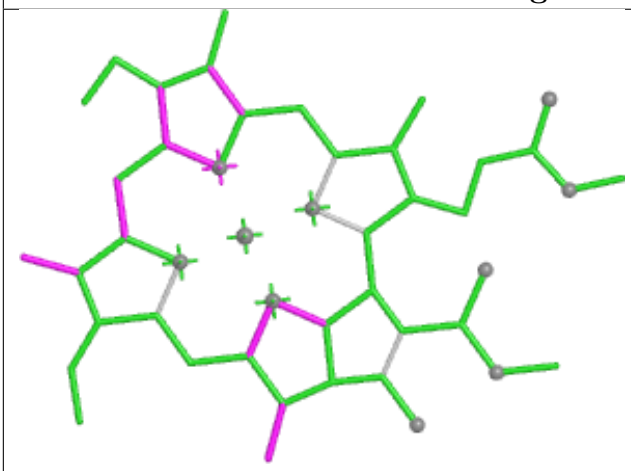


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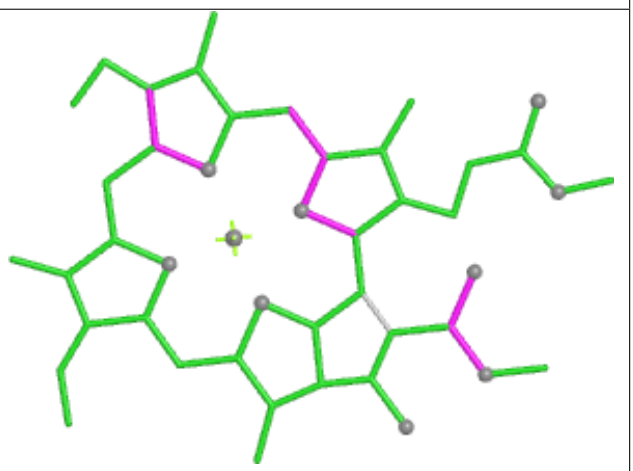


Rings

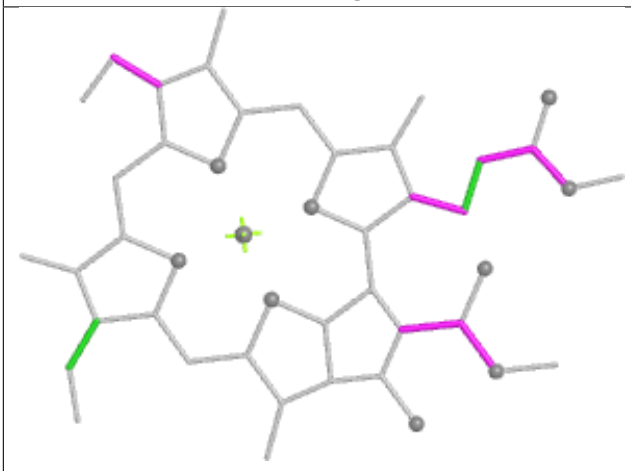
Ligand CLA s 505



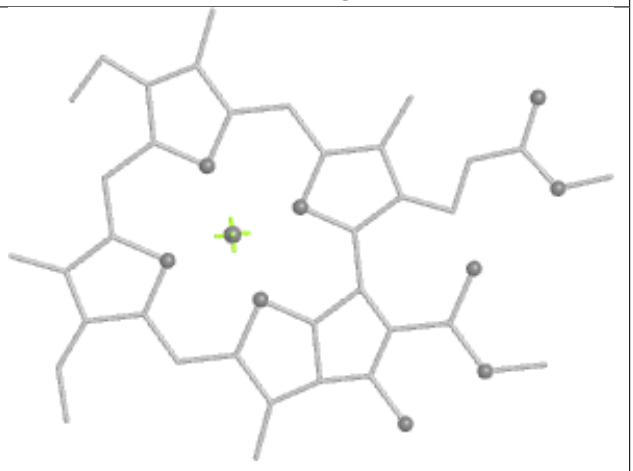
Bond lengths



Bond angles

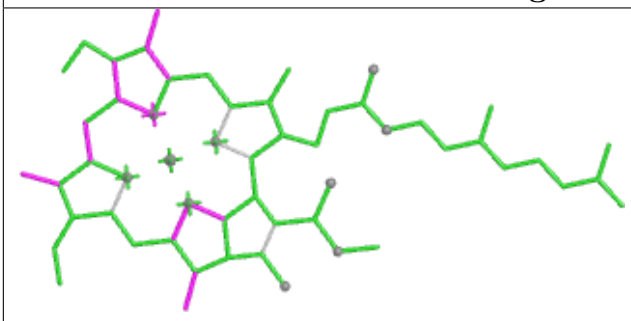


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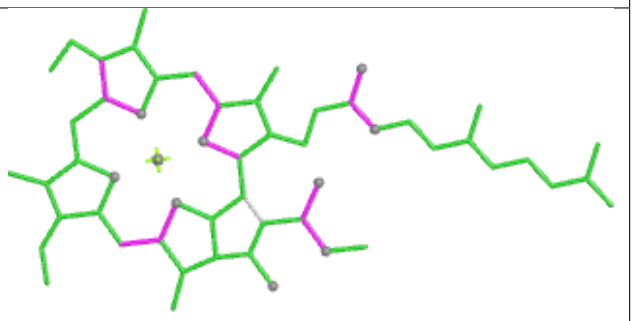


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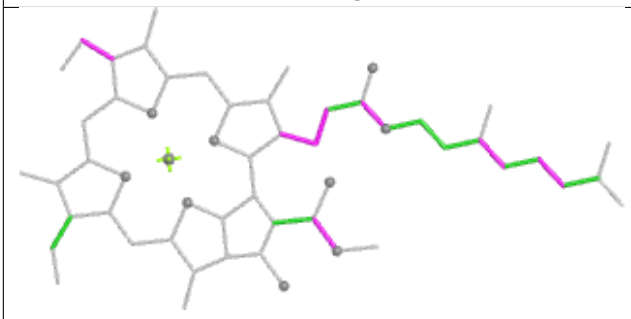
Ligand CLA e 810



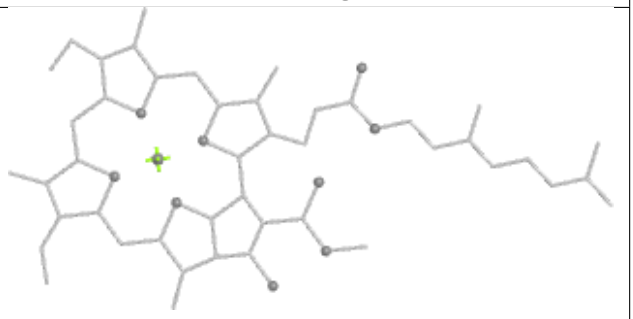
Bond lengths



Bond angles

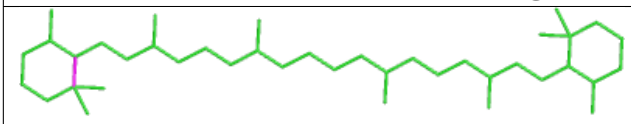


Torsions



Rings

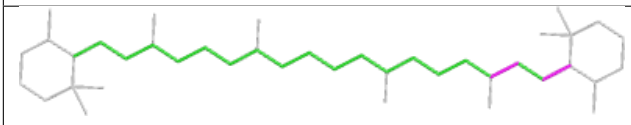
Ligand BCR e 846



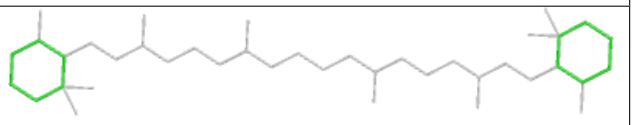
Bond lengths



Bond angles

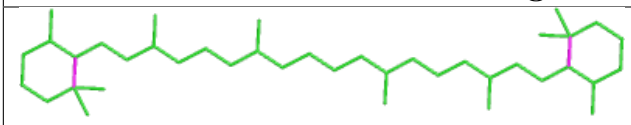


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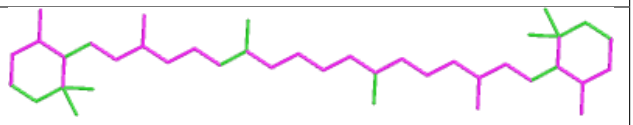


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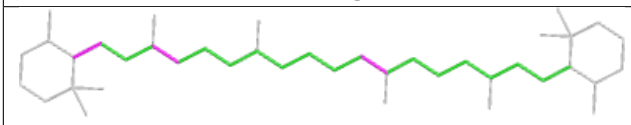
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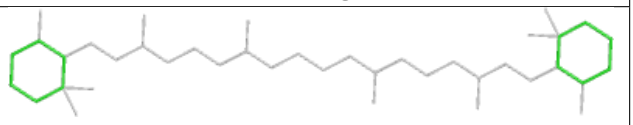
Bond lengths



Bond angles

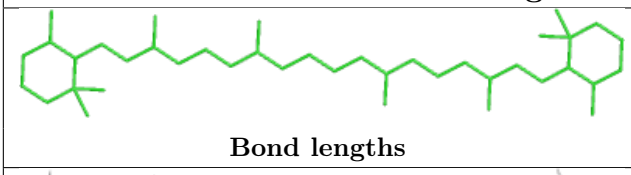


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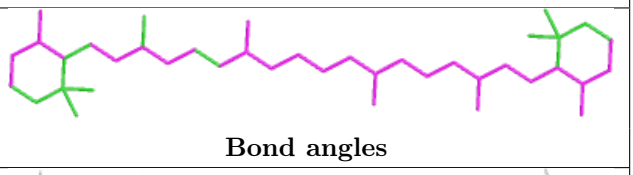


Rings

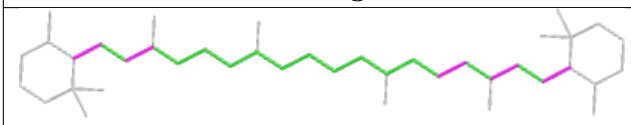
Ligand BCR n 204



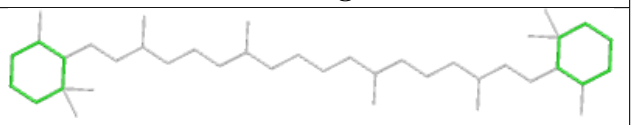
Bond lengths



Bond angles

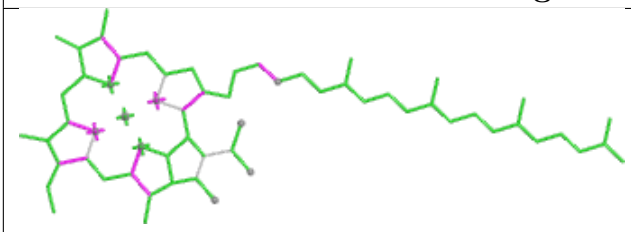


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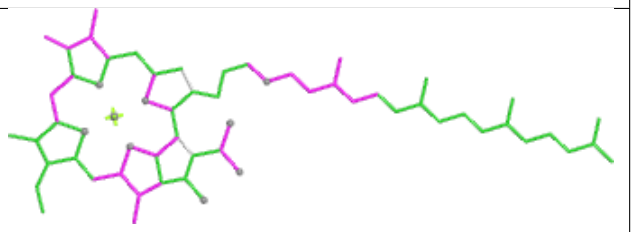


Rings

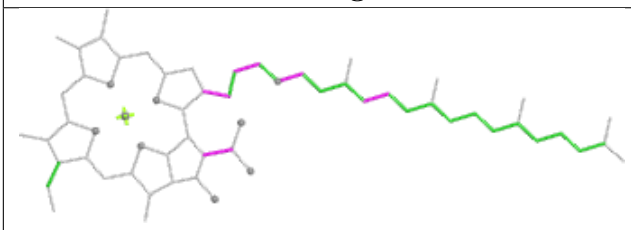
Ligand CL0 e 801



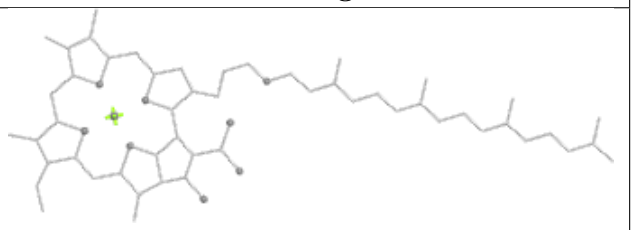
Bond lengths



Bond angles

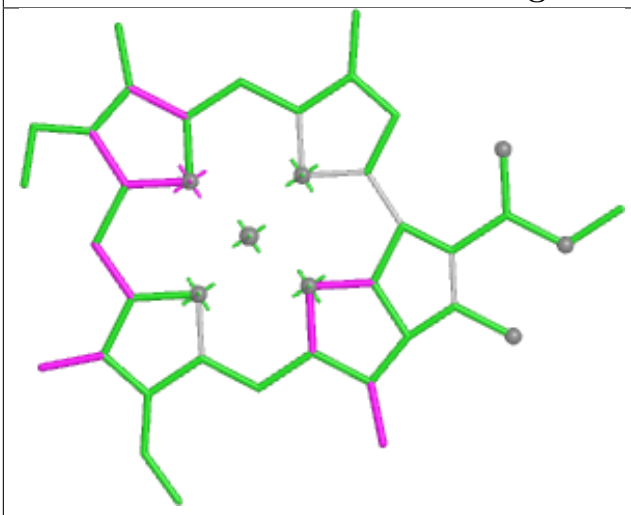


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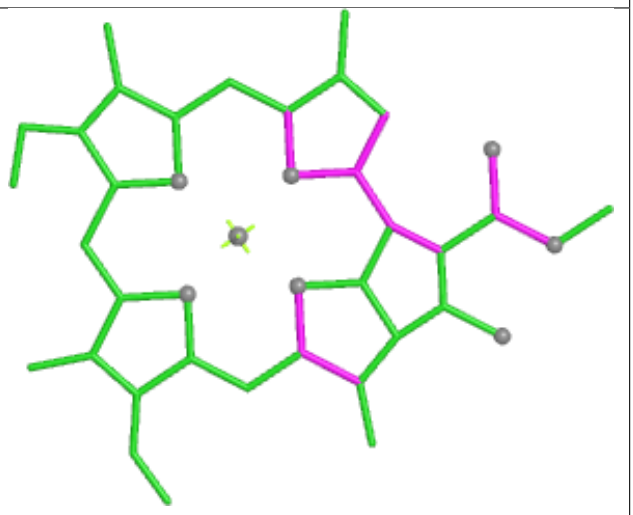


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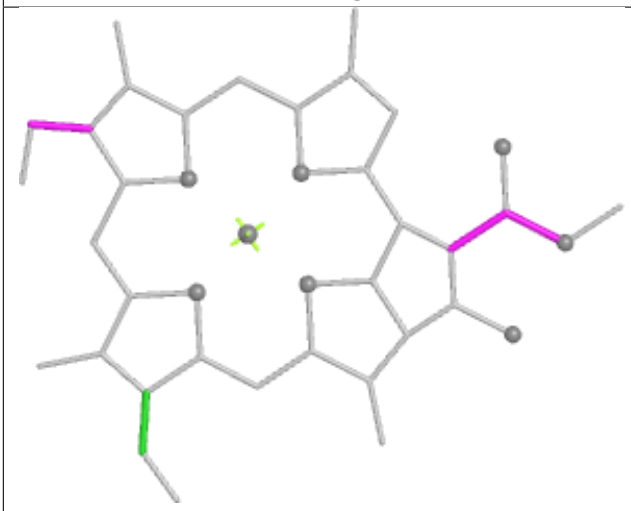
Ligand CLA 3 307



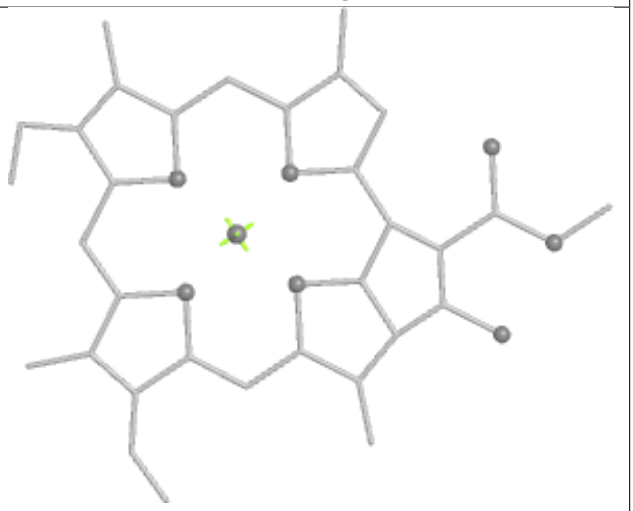
Bond lengths



Bond angles

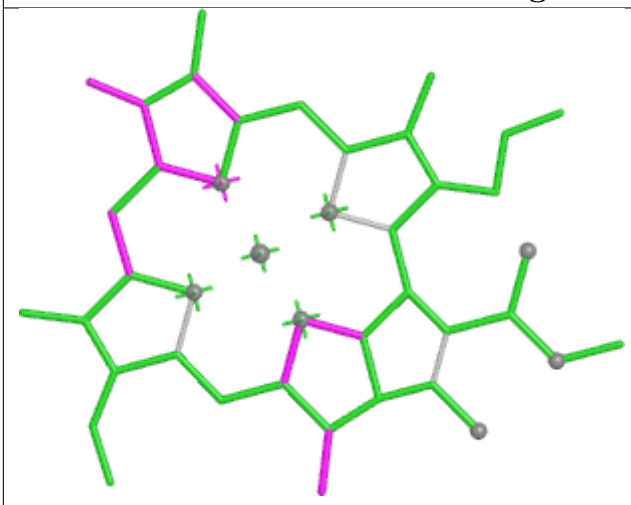


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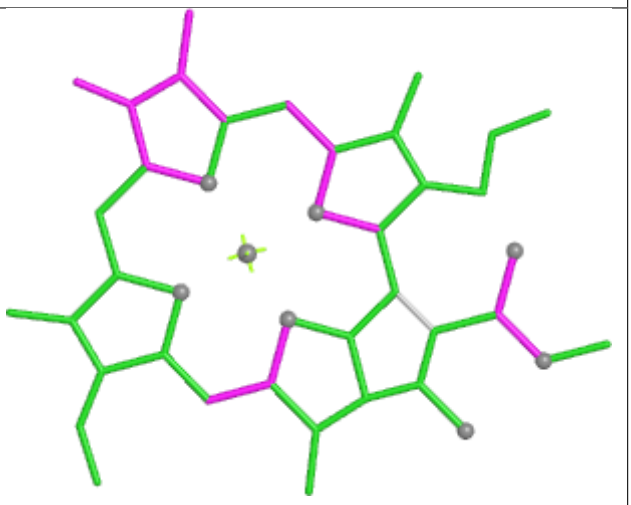


Rings

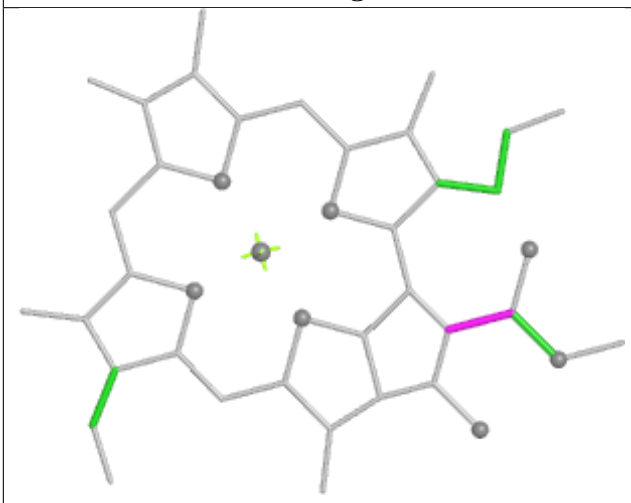
Ligand CLA e 823



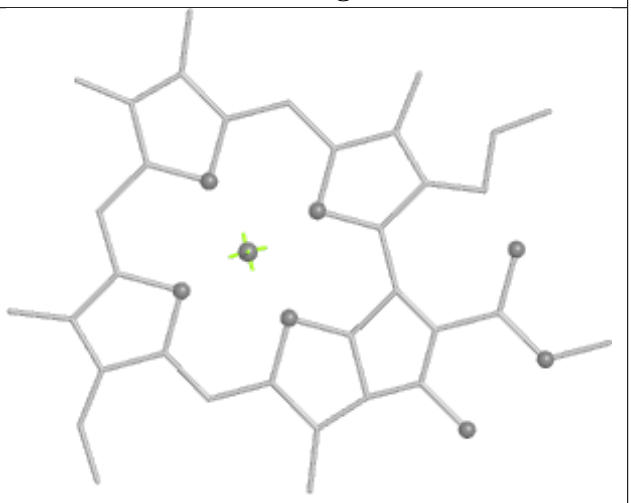
Bond lengths



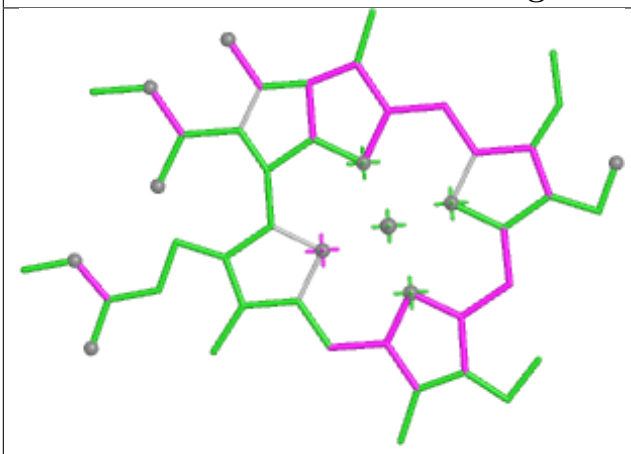
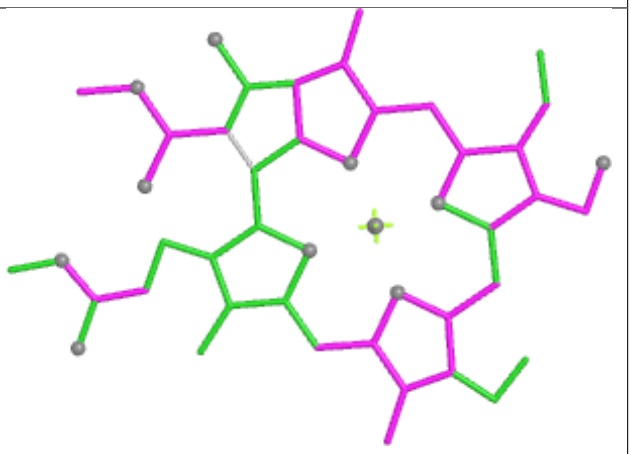
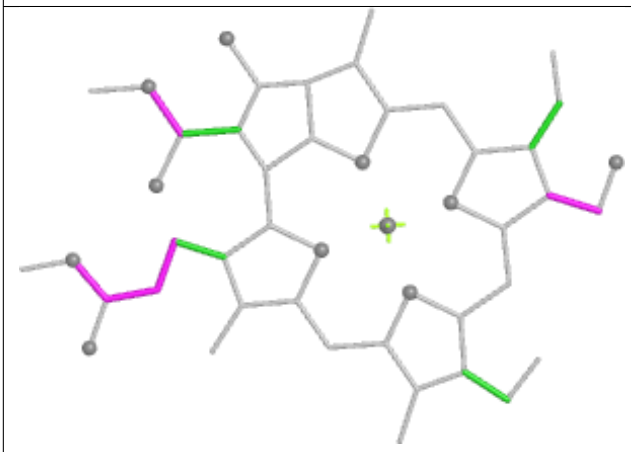
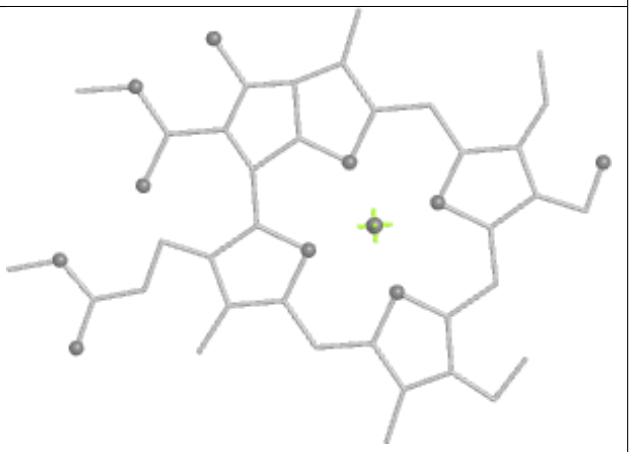
Bond angles

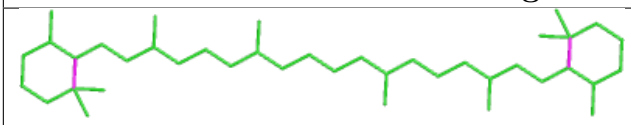
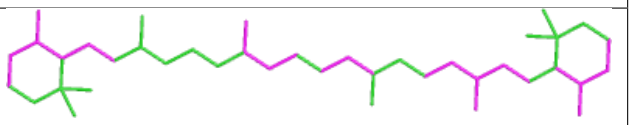
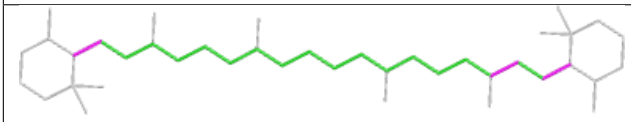
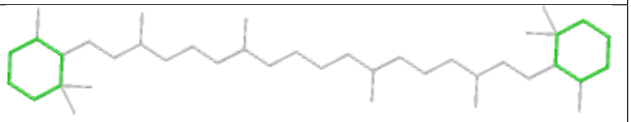


Torsions

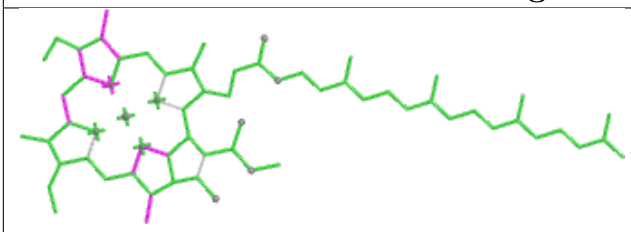


Rings

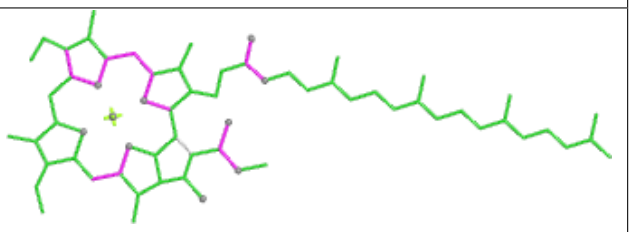
Ligand CHL 1 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

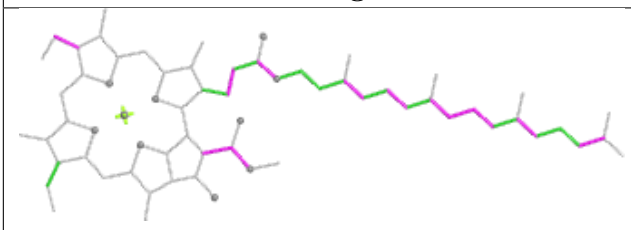
Ligand CLA 5 307



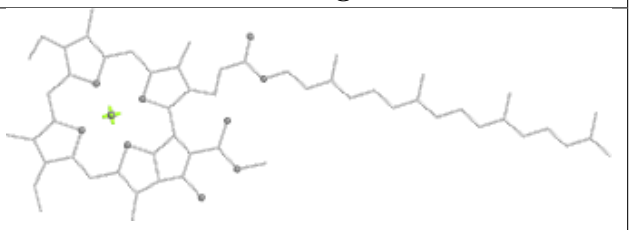
Bond lengths



Bond angles

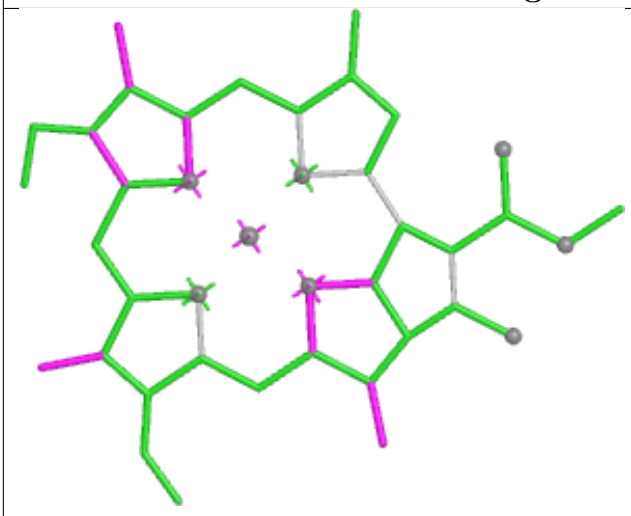


Torsions

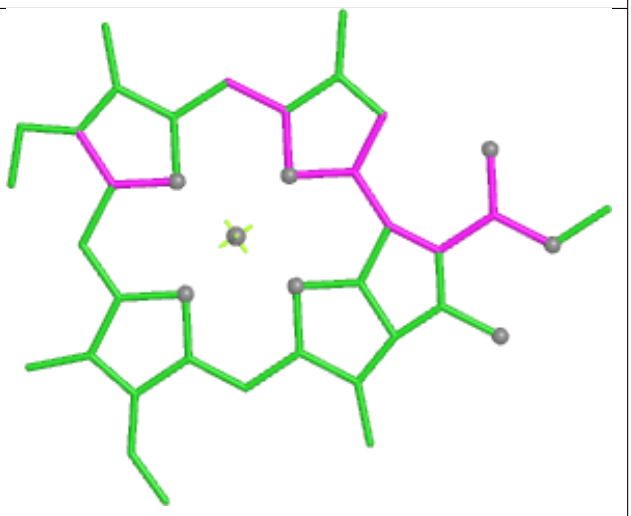


Rings

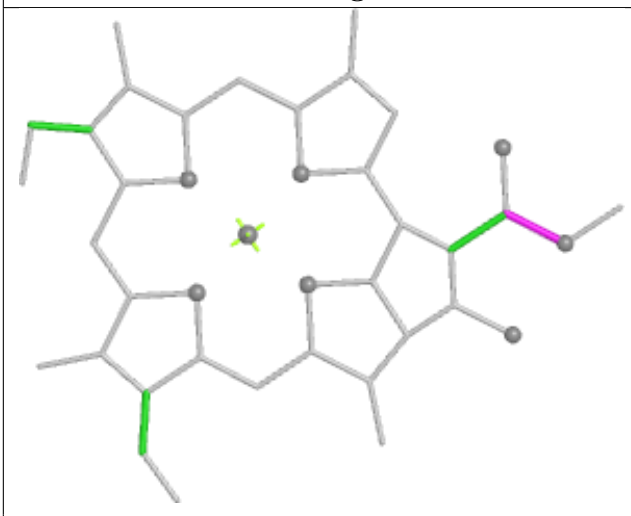
Ligand CLA B 829



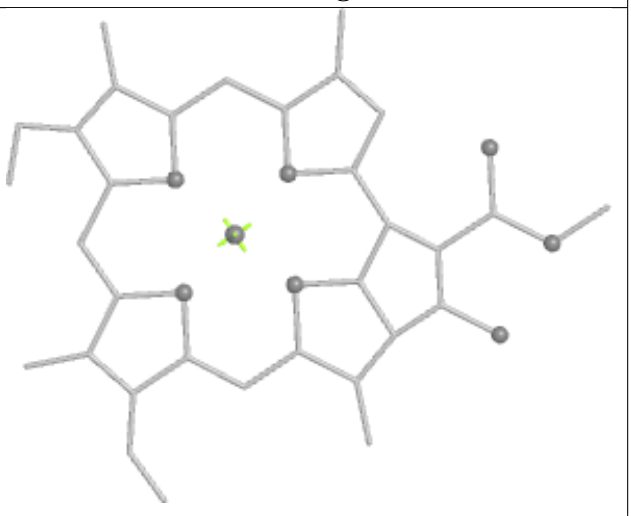
Bond lengths



Bond angles

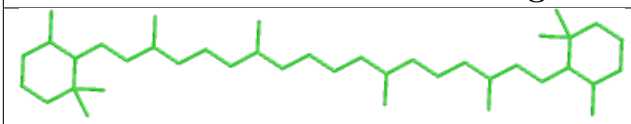


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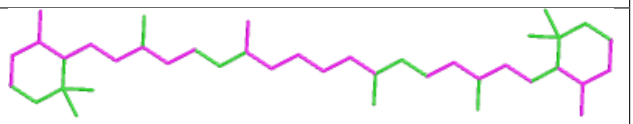


Rings

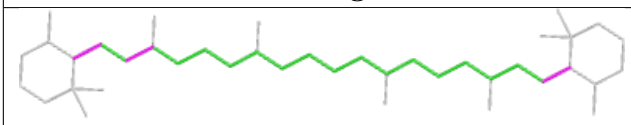
Ligand BCR r 301



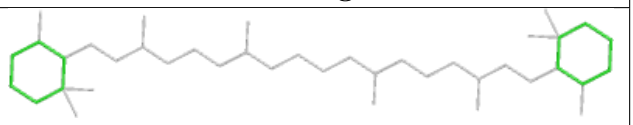
Bond lengths



Bond angles

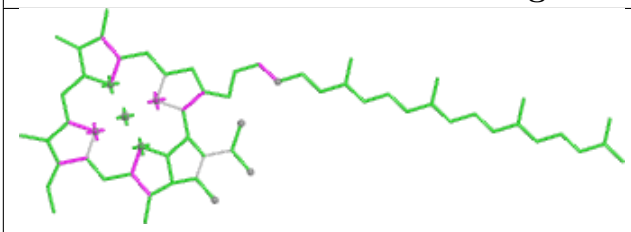


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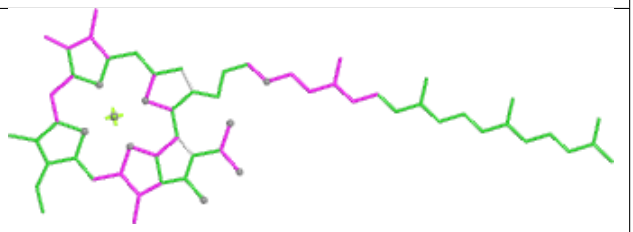


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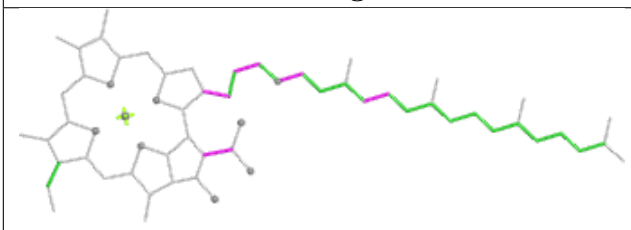
Ligand CL0 A 801



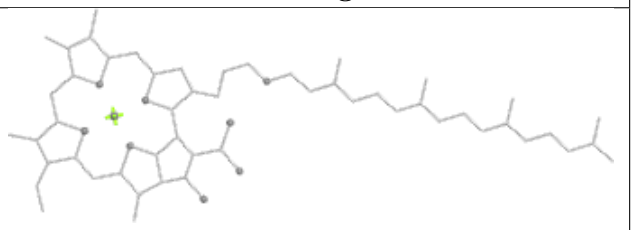
Bond lengths



Bond angles

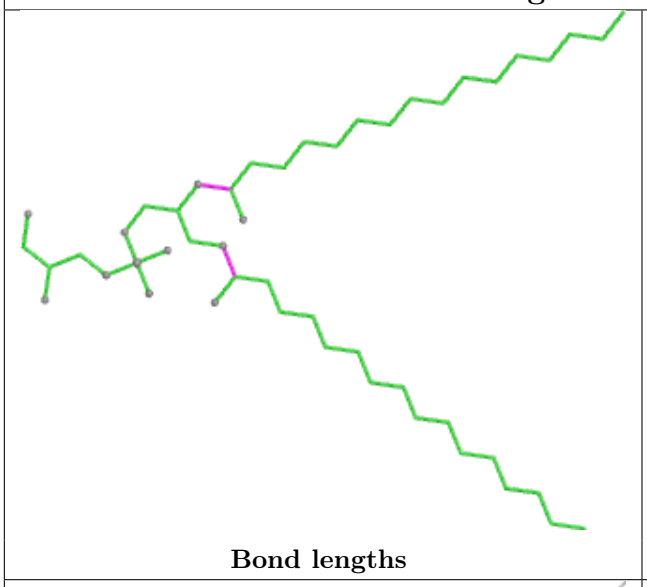


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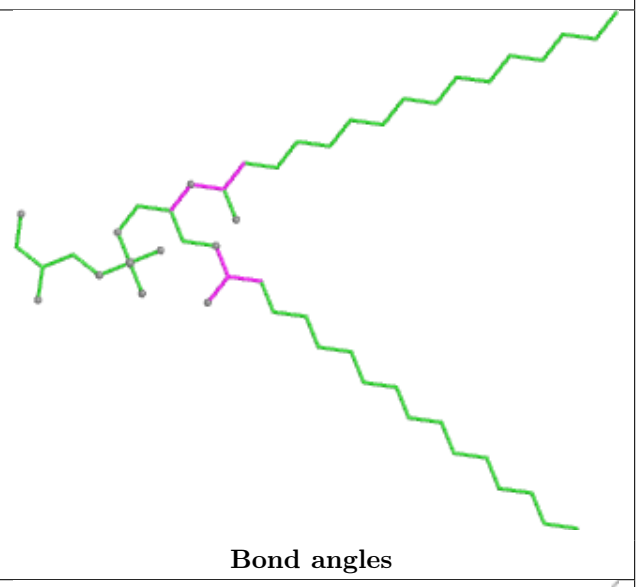


Rings

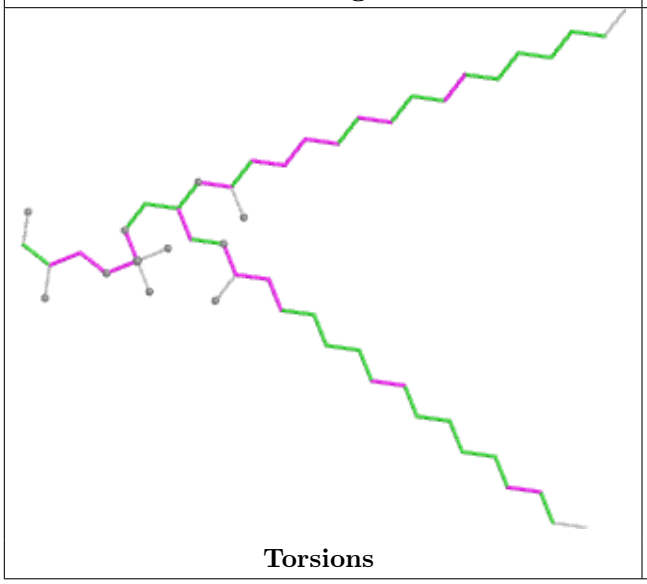
Ligand LHG 1 516



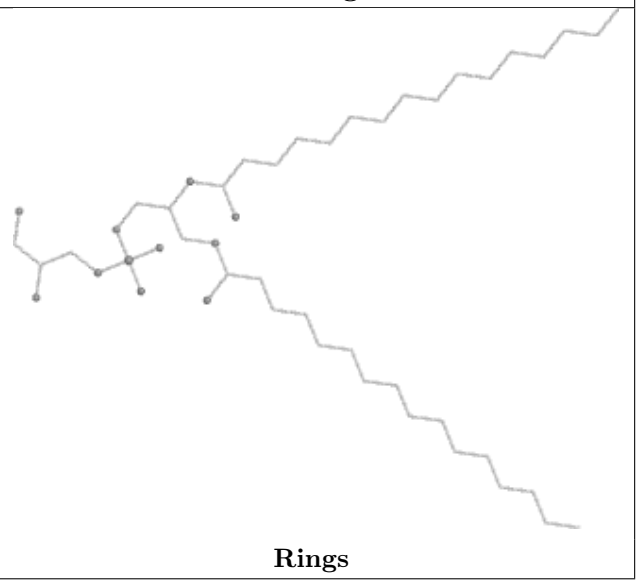
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR J 102



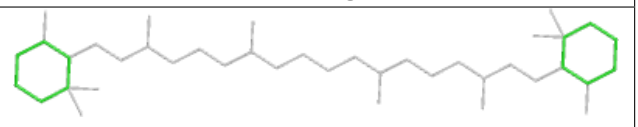
Bond lengths



Bond angles

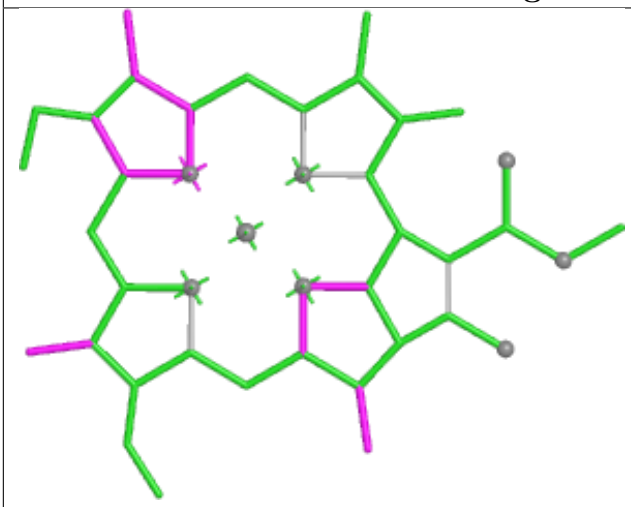


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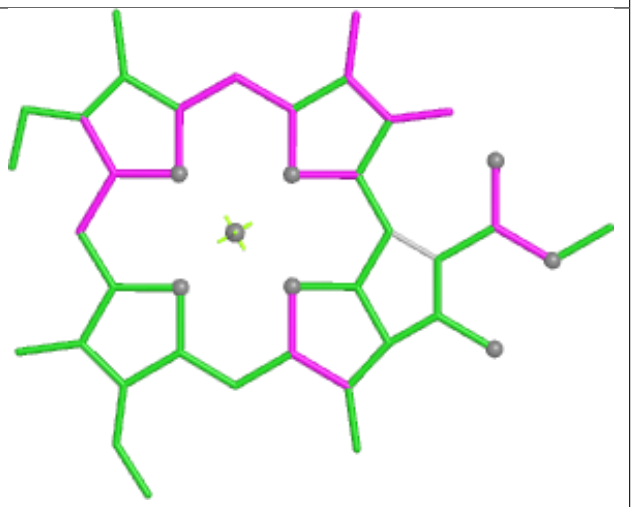


Rings

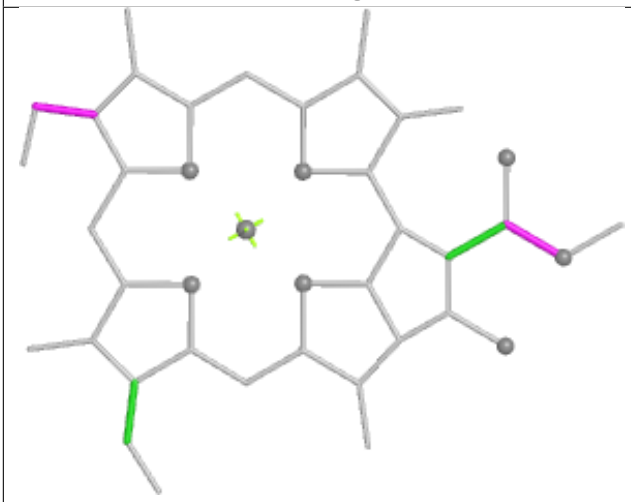
Ligand CLA A 822



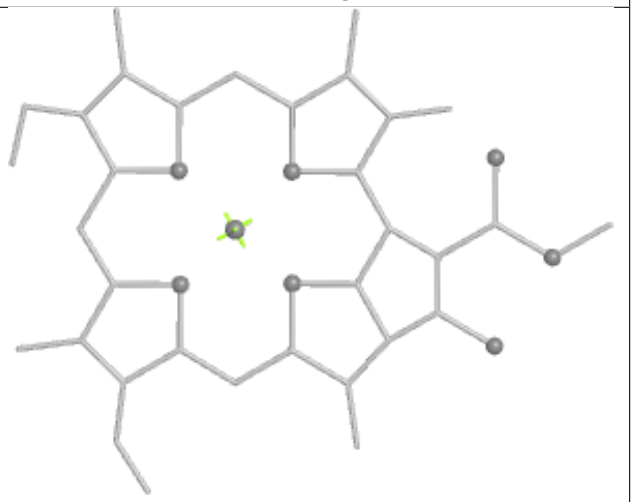
Bond lengths



Bond angles

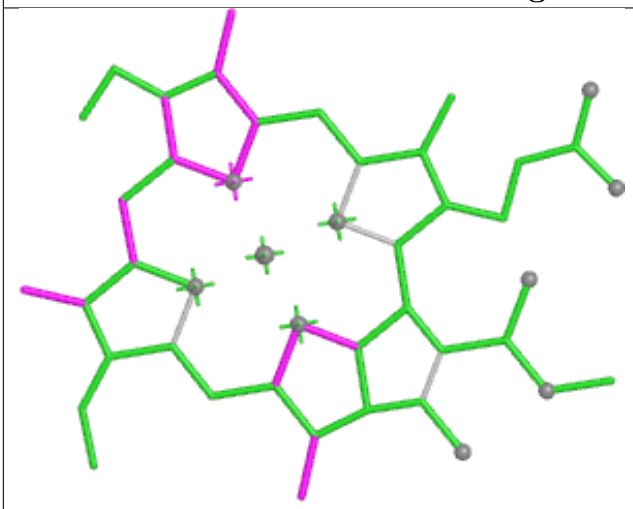


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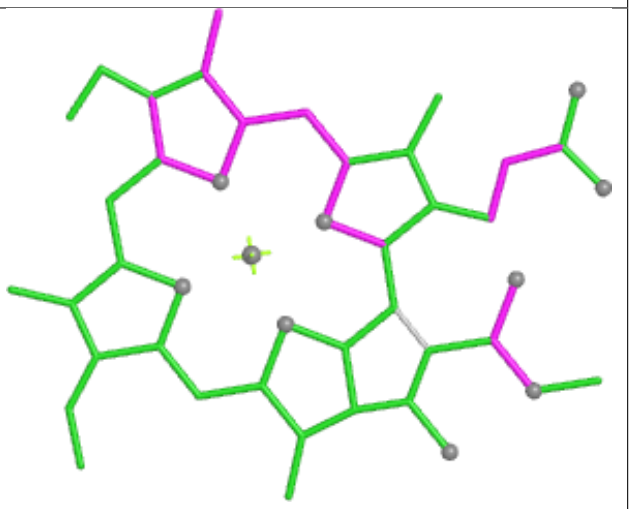


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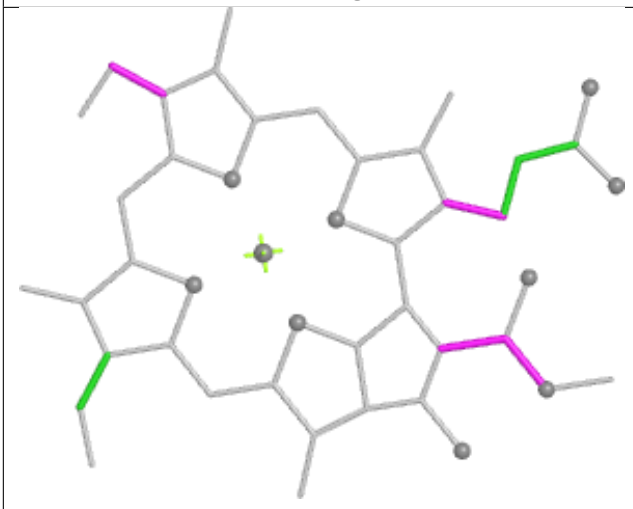
Ligand CLA 5 309



Bond lengths



Bond angles

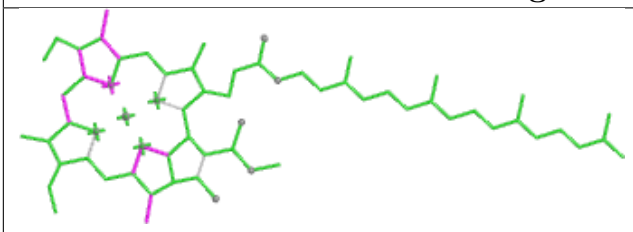


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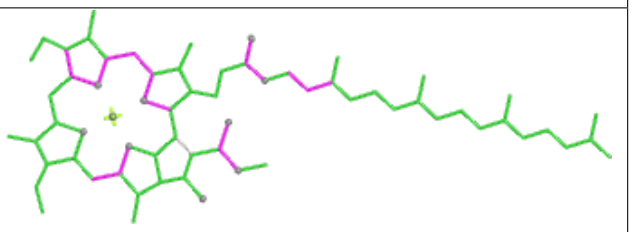


Rings

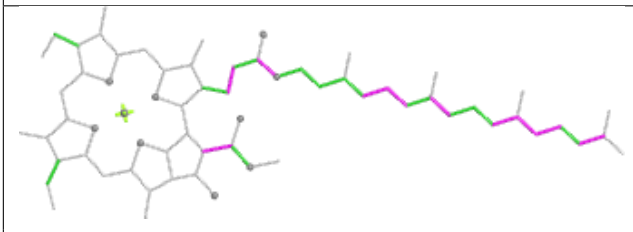
Ligand CLA e 839



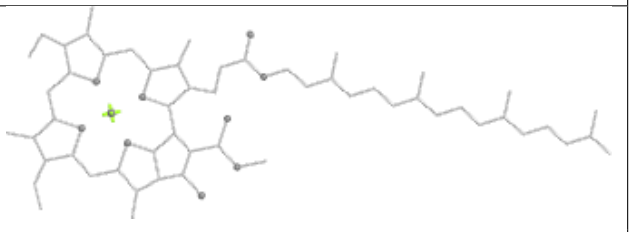
Bond lengths



Bond angles

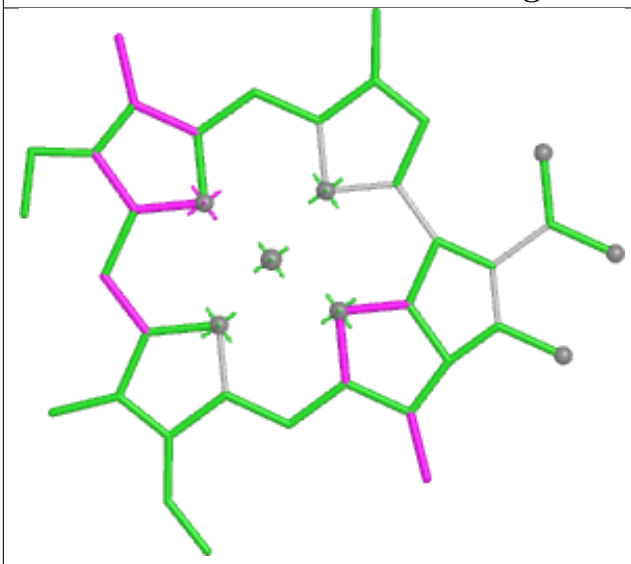


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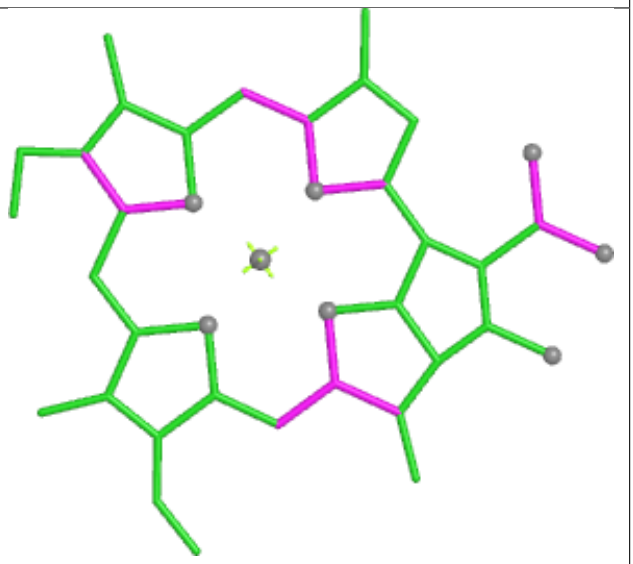


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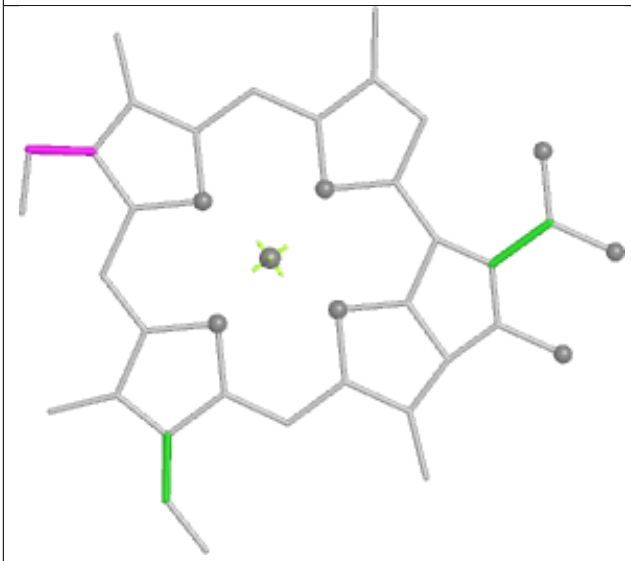
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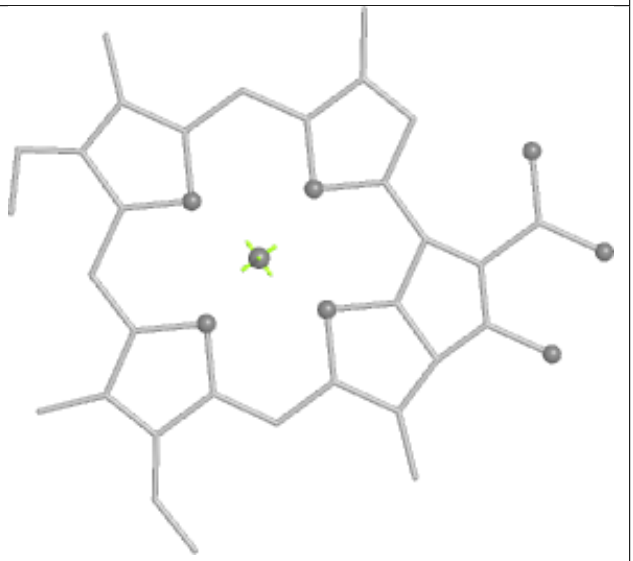
Bond lengths



Bond angles

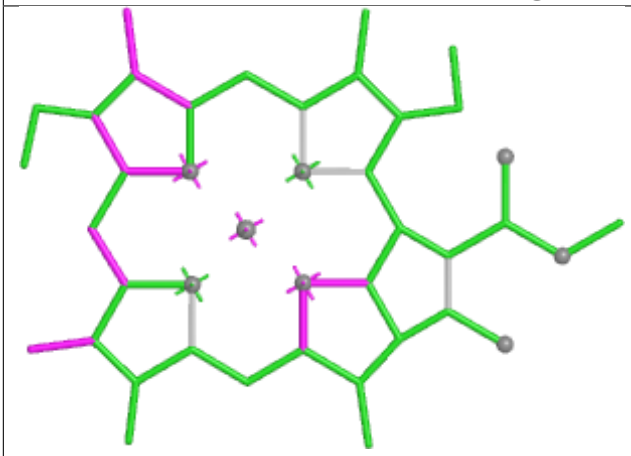


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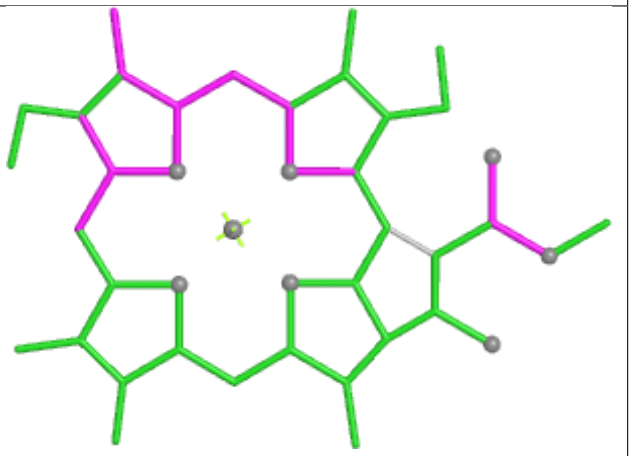


Rings

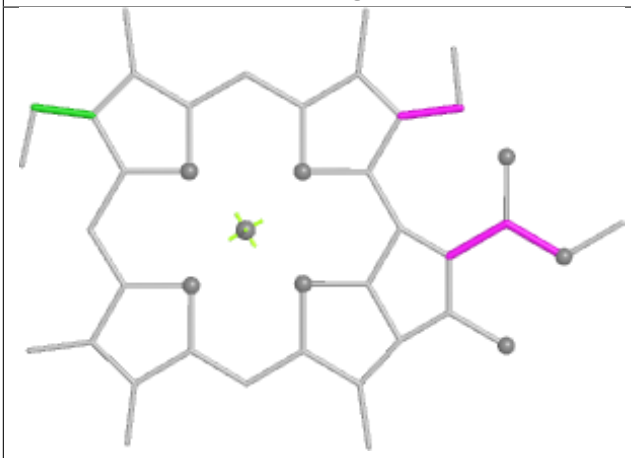
Ligand CLA 1 504



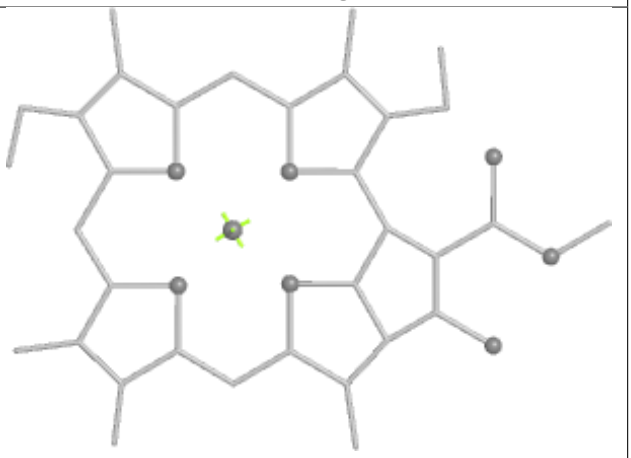
Bond lengths



Bond angles

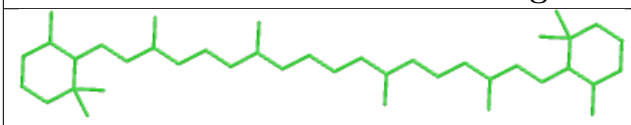


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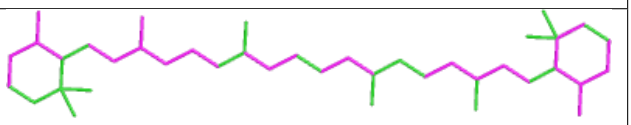


Rings

Ligand BCR f 846



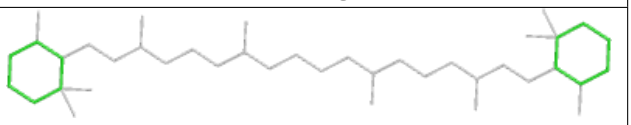
Bond lengths



Bond angles

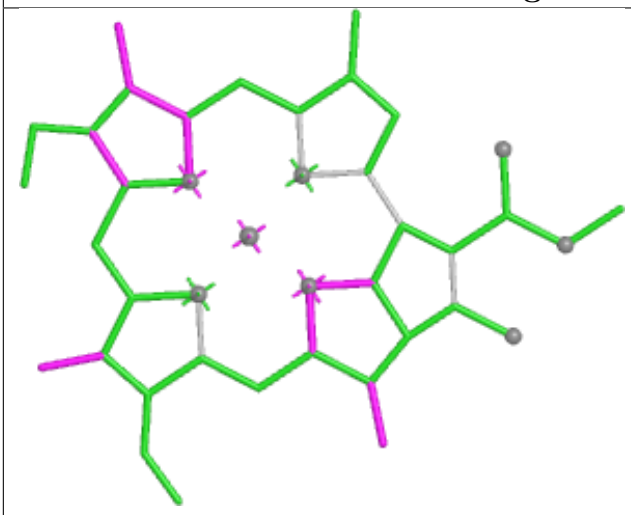


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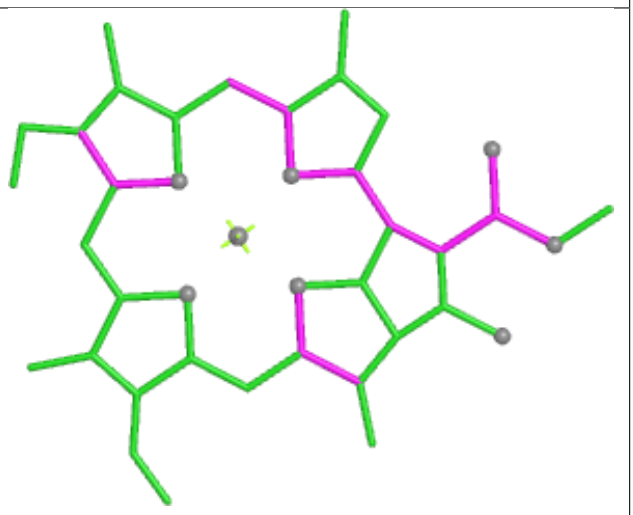


Rings

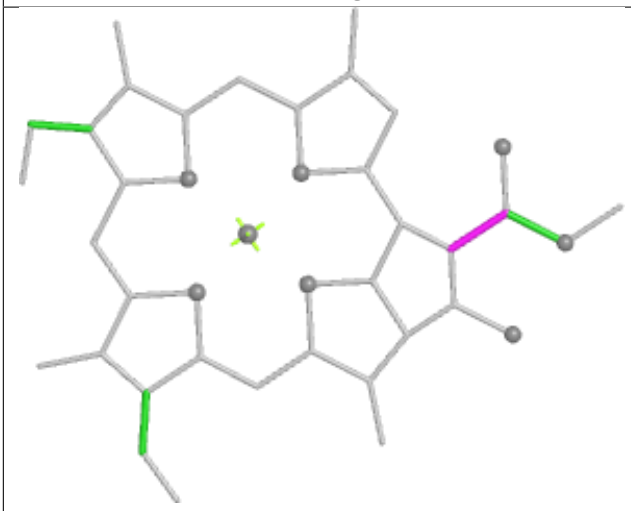
Ligand CLA A 833



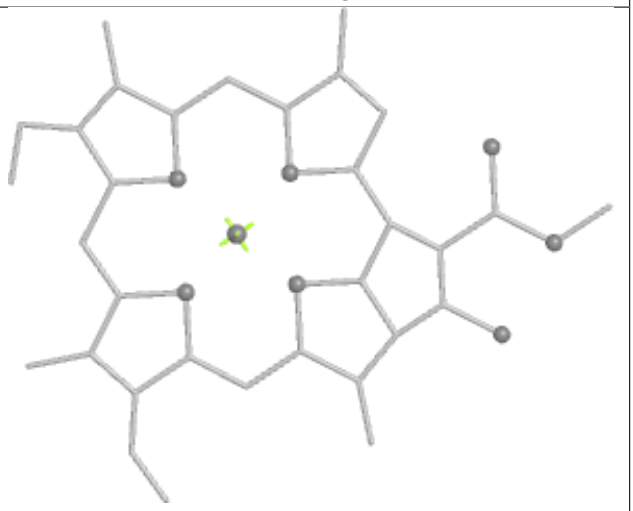
Bond lengths



Bond angles

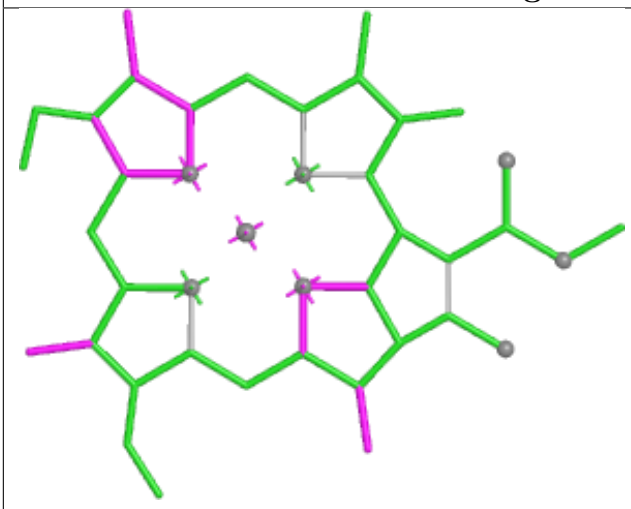


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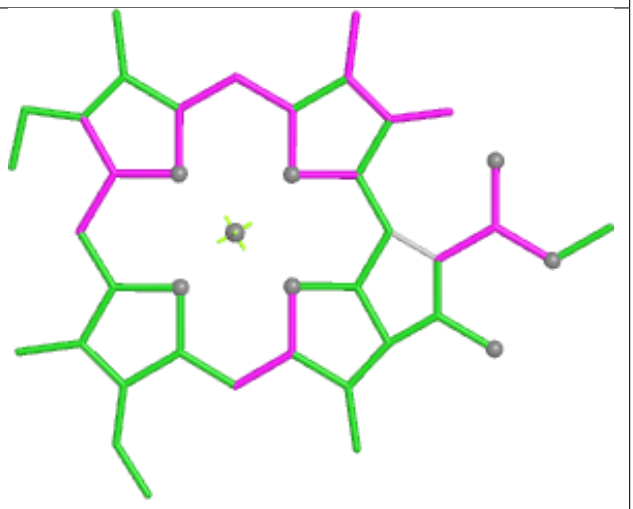


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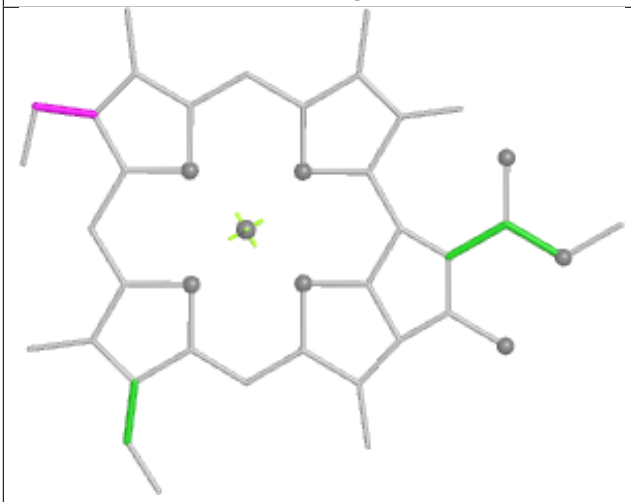
Ligand CLA A 803



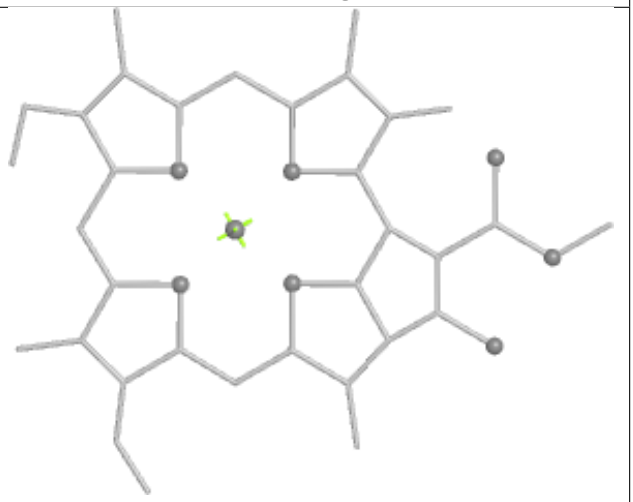
Bond lengths



Bond angles



Torsions

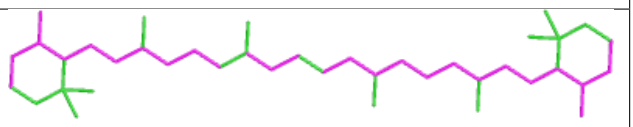


Rings

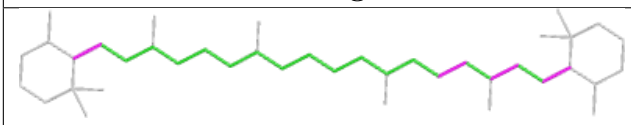
Ligand BCR e 849



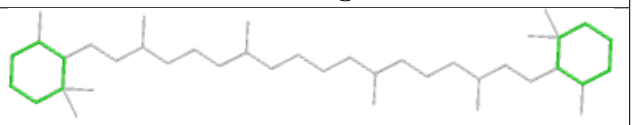
Bond lengths



Bond angles

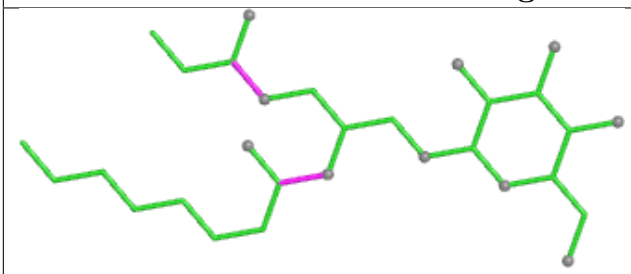


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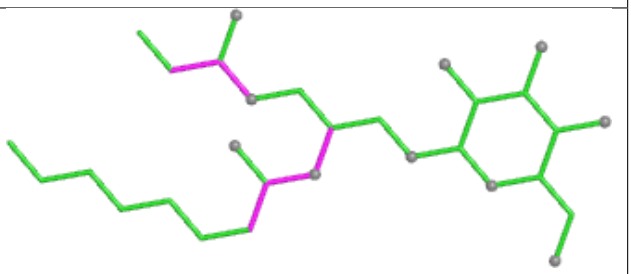


Rings

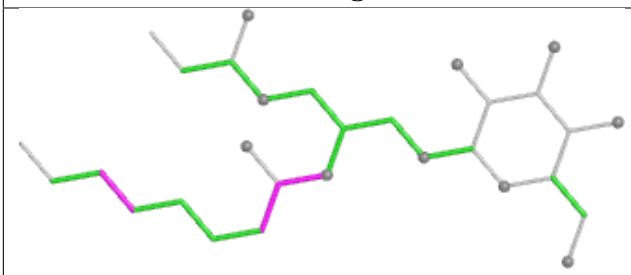
Ligand LMG m 105



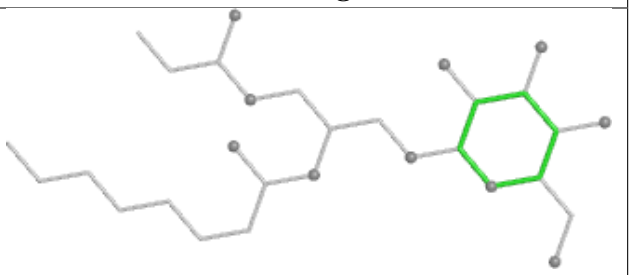
Bond lengths



Bond angles

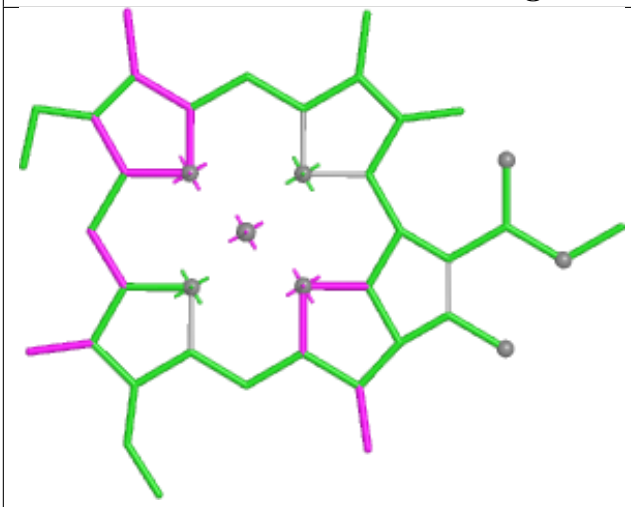


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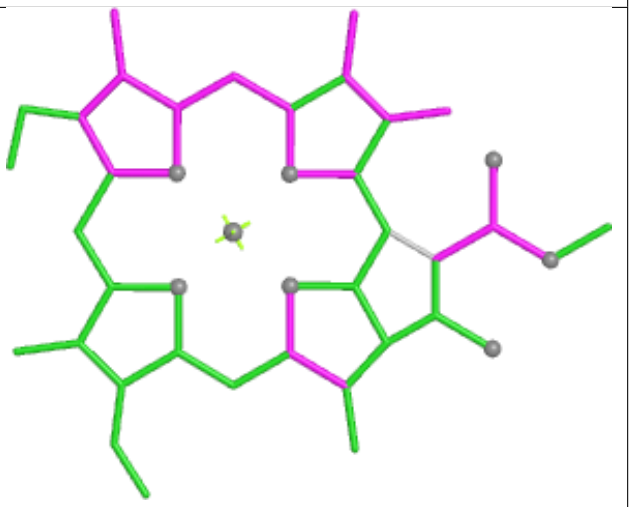


Rings

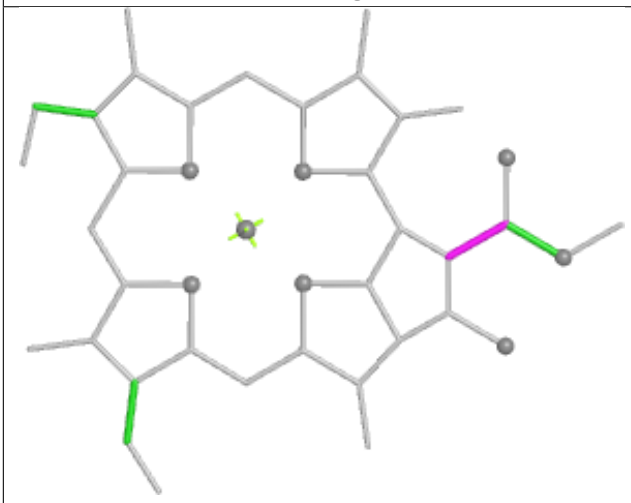
Ligand CLA B 827



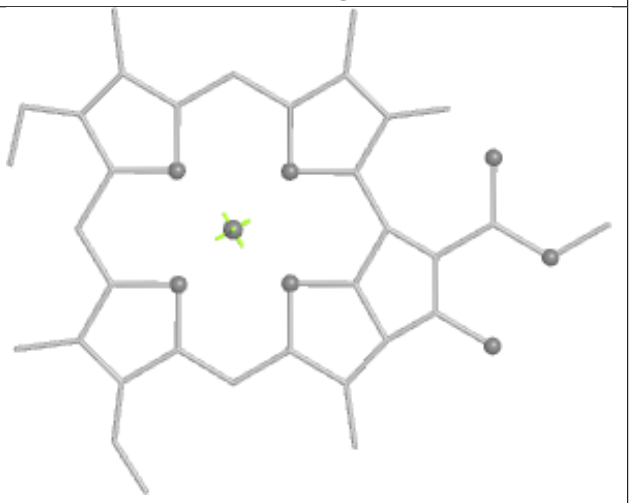
Bond lengths



Bond angles

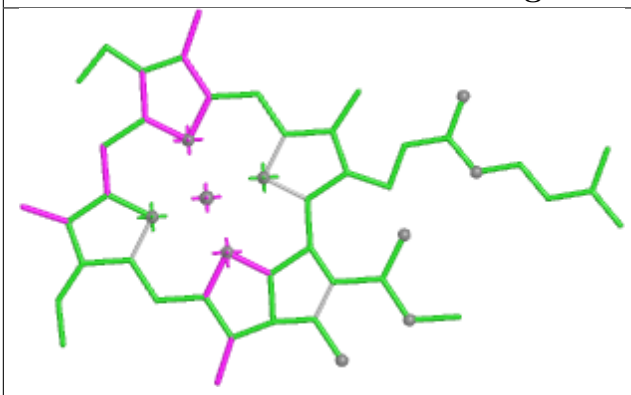


Torsions

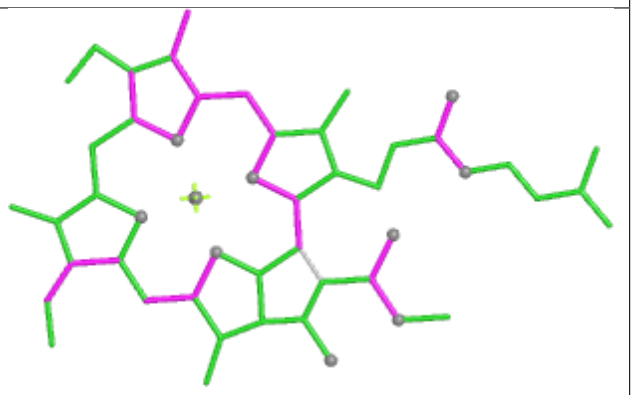


Rings

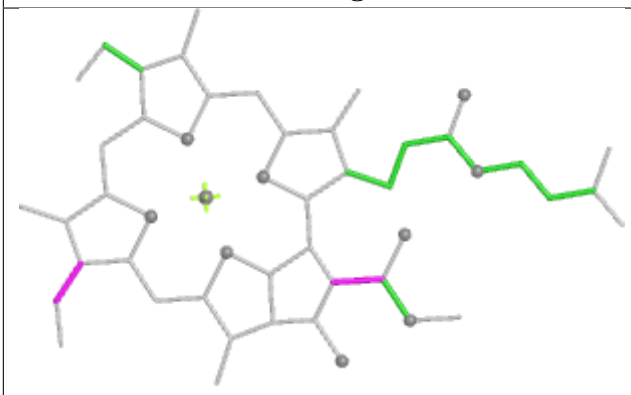
Ligand CLA B 837



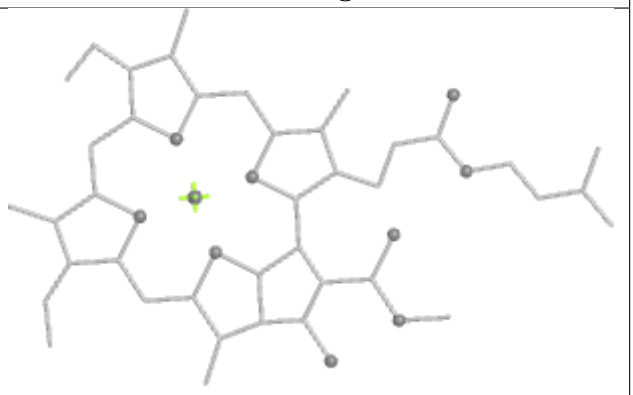
Bond lengths



Bond angles



Torsions

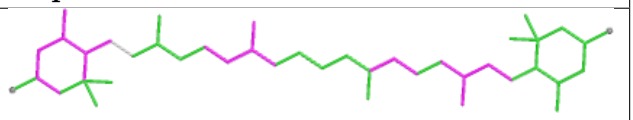


Rings

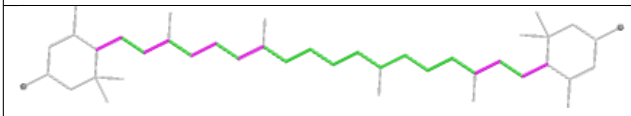
Ligand LUT p 502



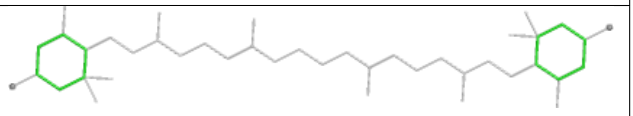
Bond lengths



Bond angles

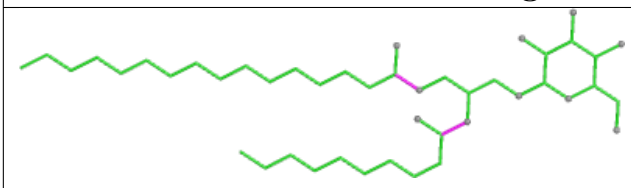


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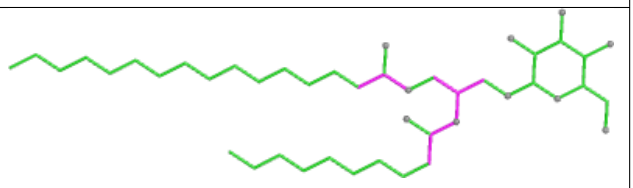


Rings

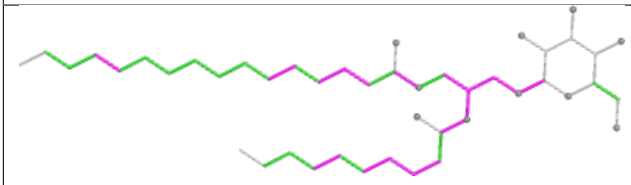
Ligand LMG F 806



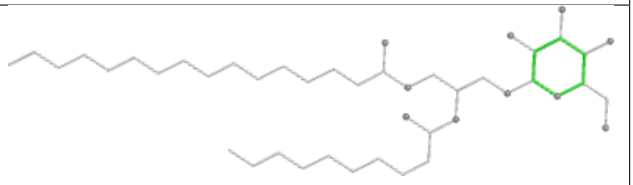
Bond lengths



Bond angles

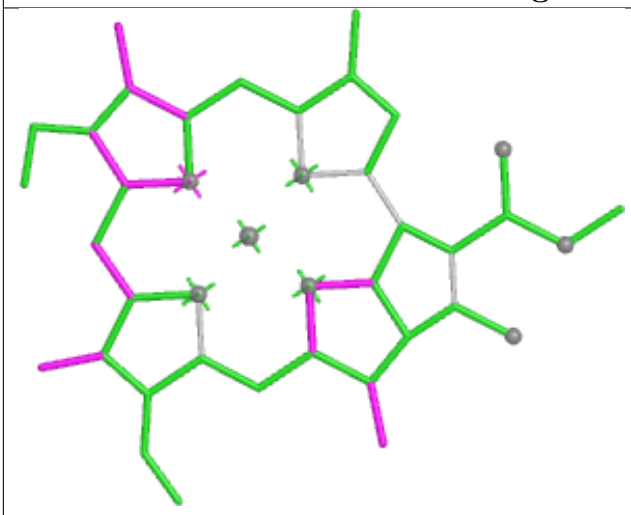


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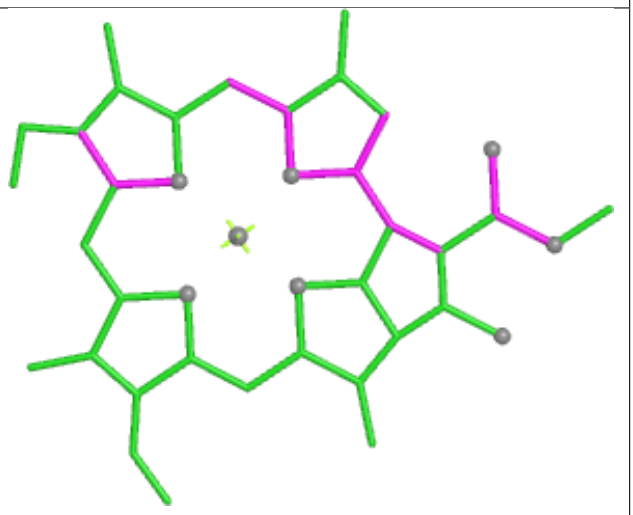


Rings

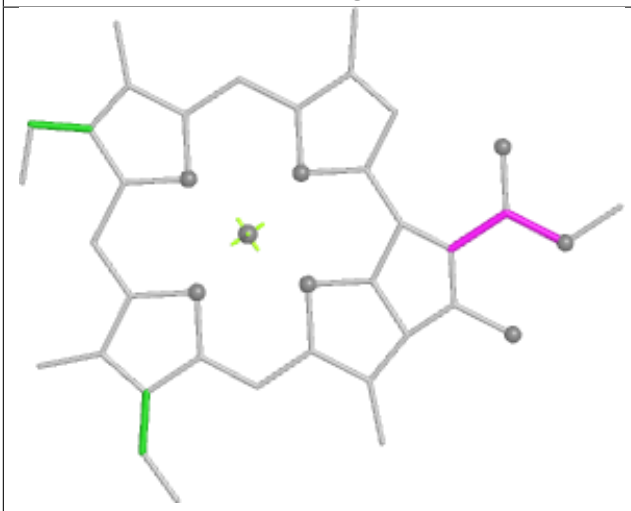
Ligand CLA f 812



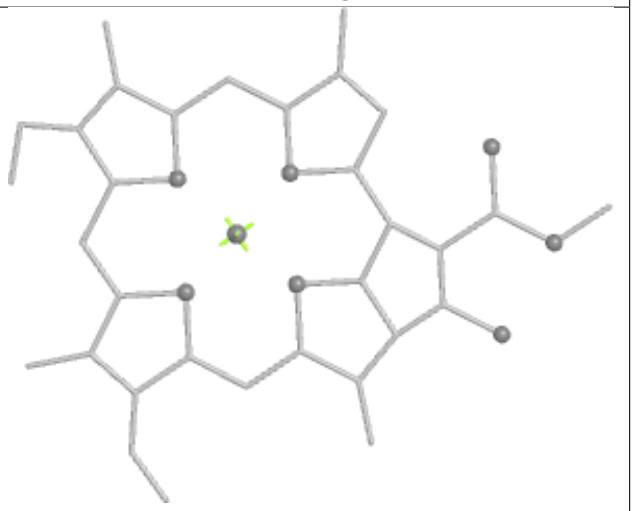
Bond lengths



Bond angles

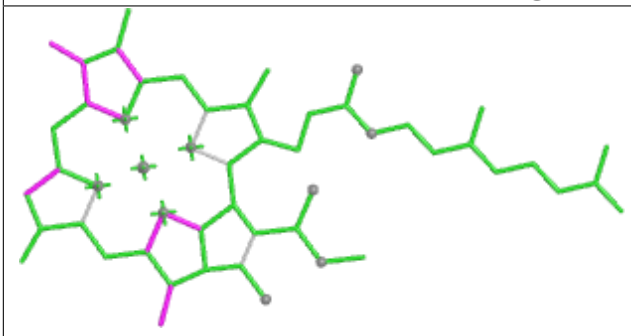


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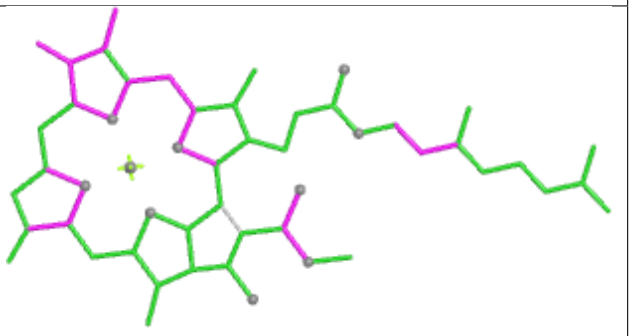


Rings

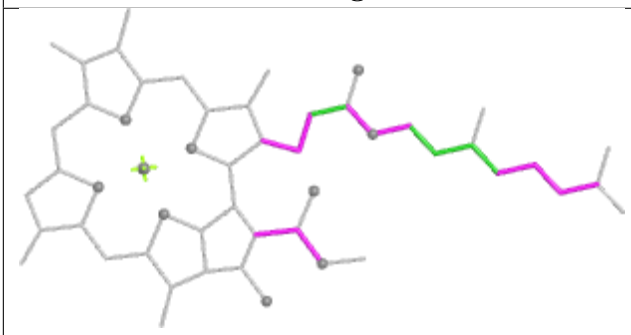
Ligand CLA 3 306



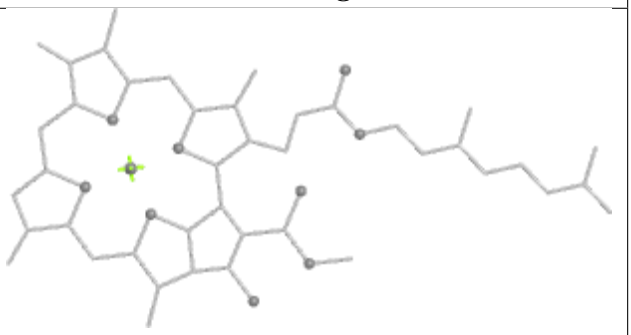
Bond lengths



Bond angles



Torsions

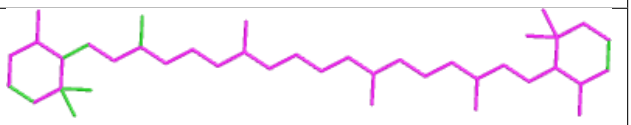


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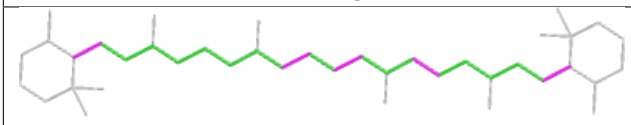
Ligand BCR s 503



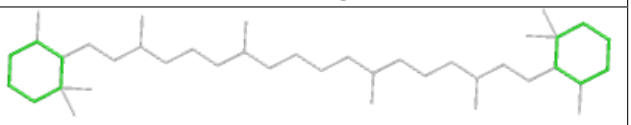
Bond lengths



Bond angles

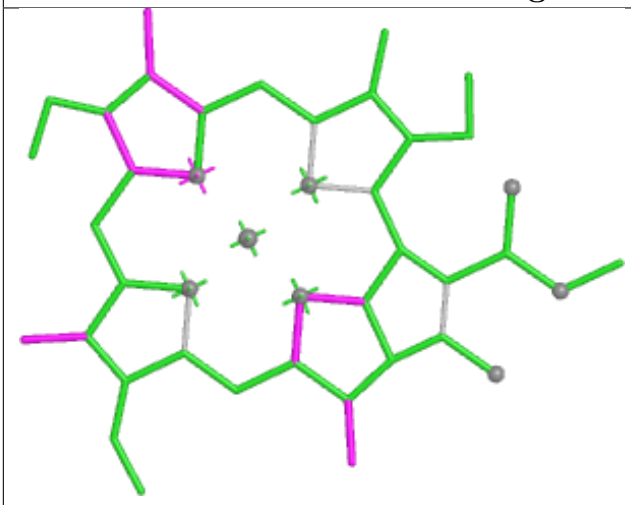


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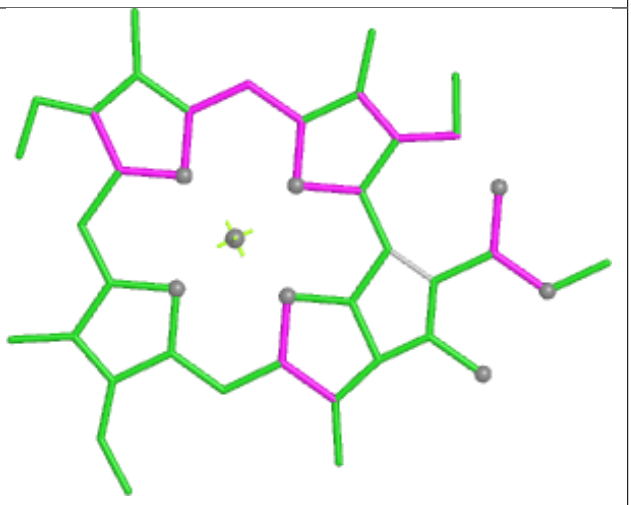


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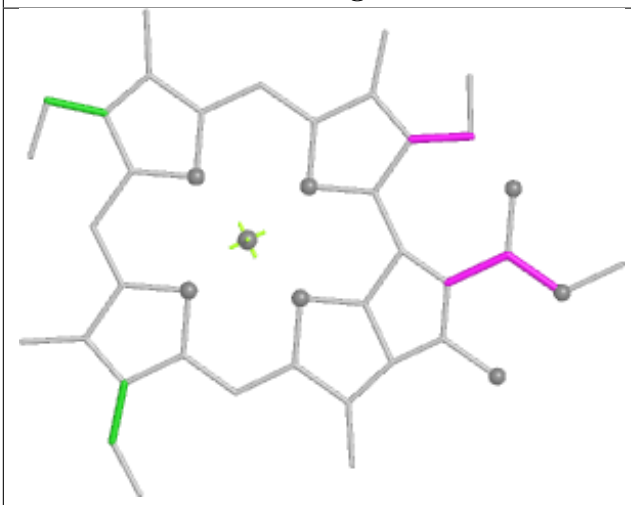
Ligand CLA 5 311



Bond lengths



Bond angles



Torsions

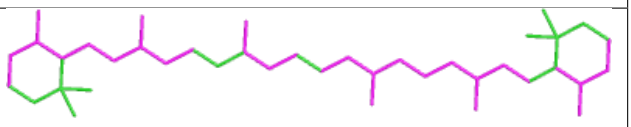


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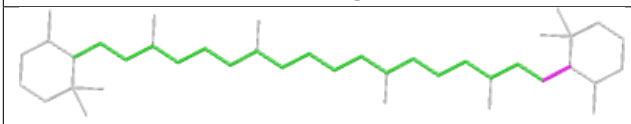
Ligand BCR o 305



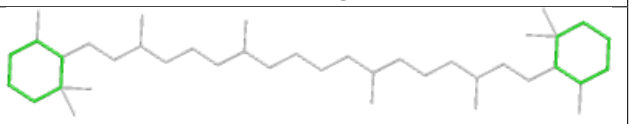
Bond lengths



Bond angles

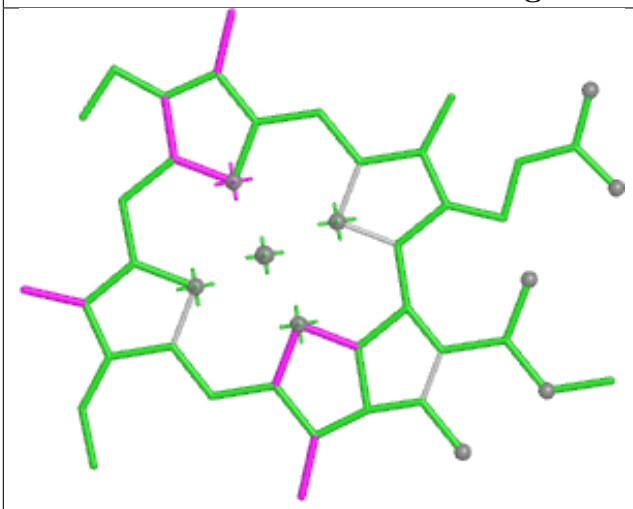


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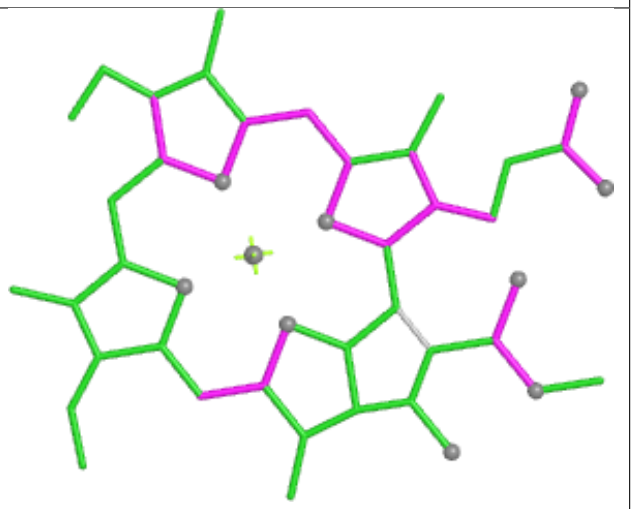


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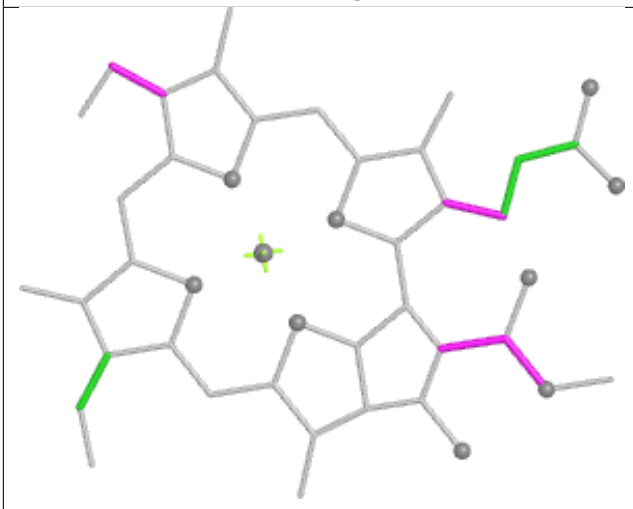
Ligand CLA B 834



Bond lengths



Bond angles

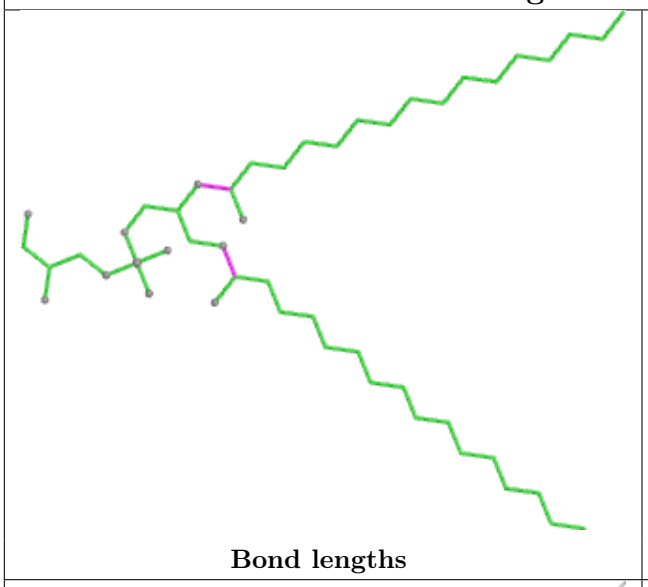


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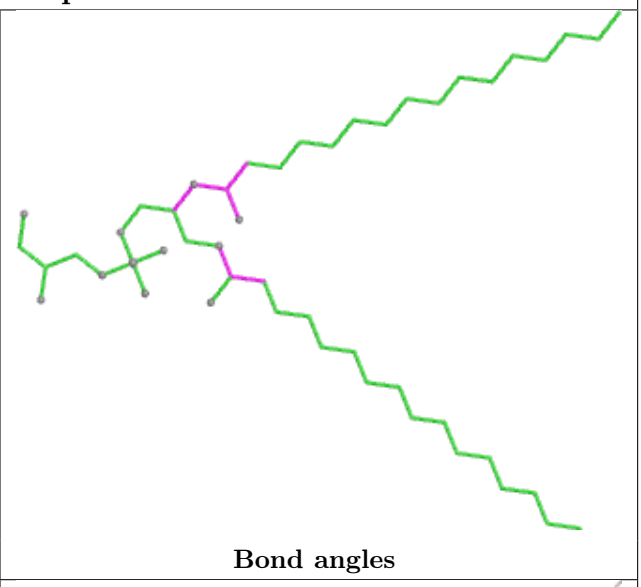


Rings

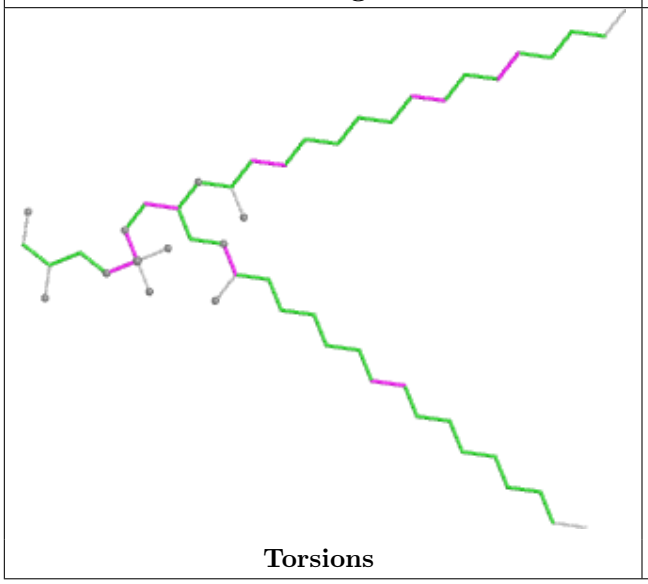
Ligand LHG p 516



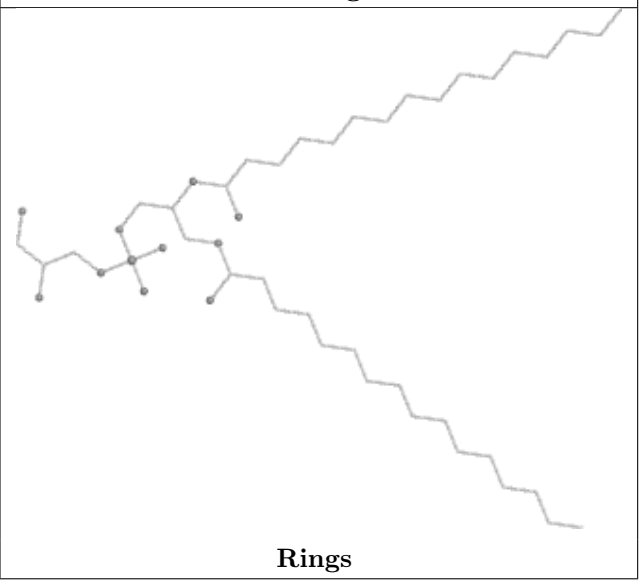
Bond lengths



Bond angles

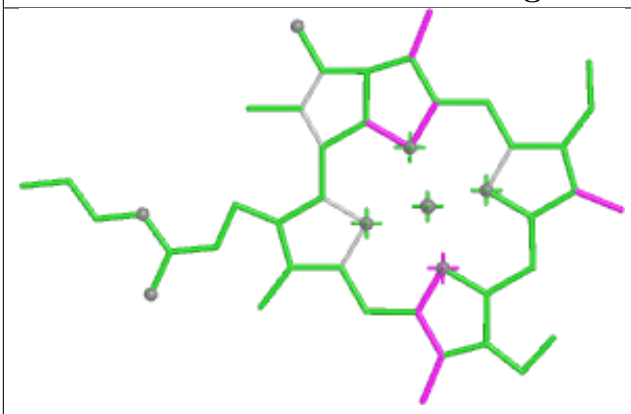


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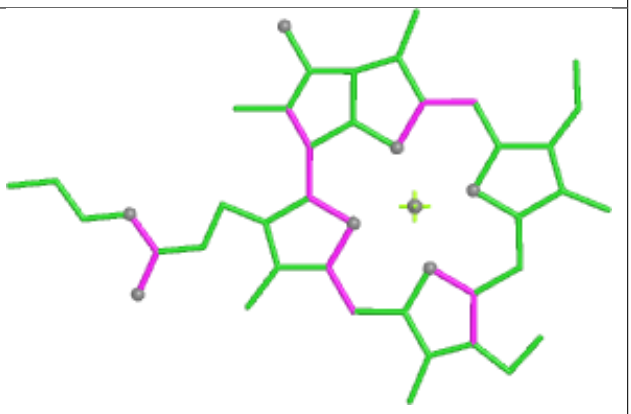


Rings

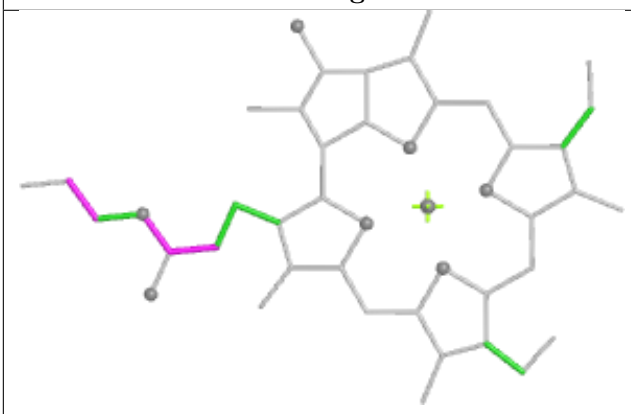
Ligand CLA A 832



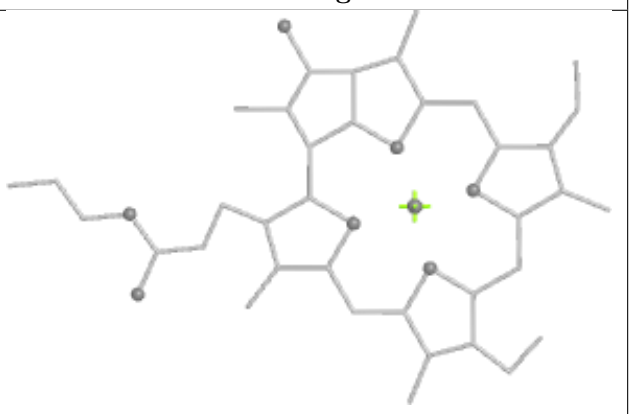
Bond lengths



Bond angles

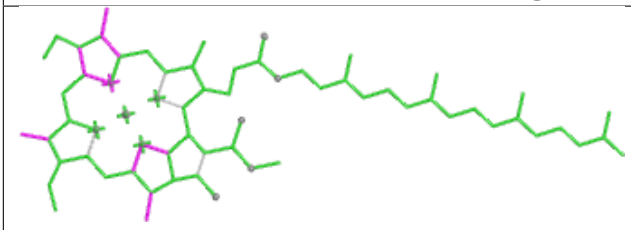


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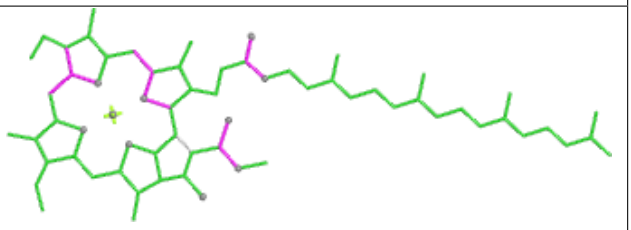


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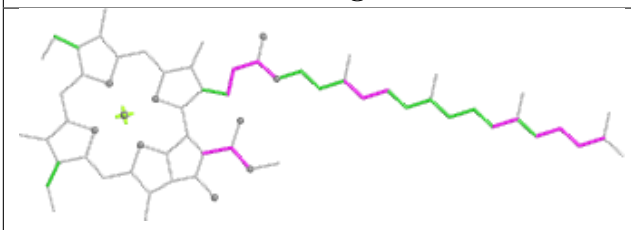
Ligand CLA 2 506



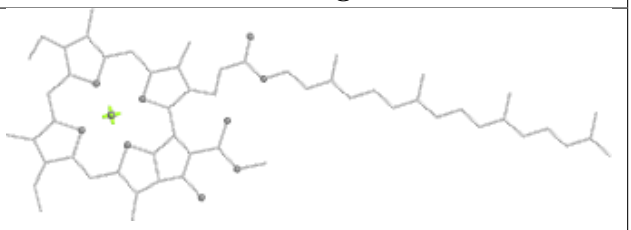
Bond lengths



Bond angles

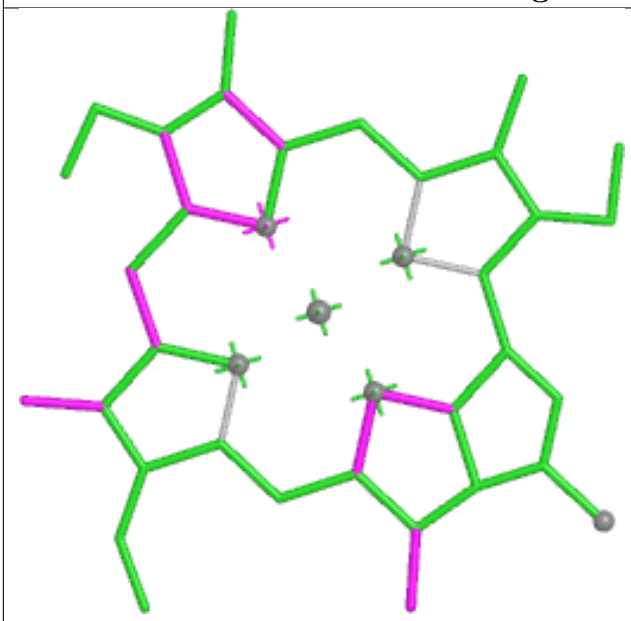


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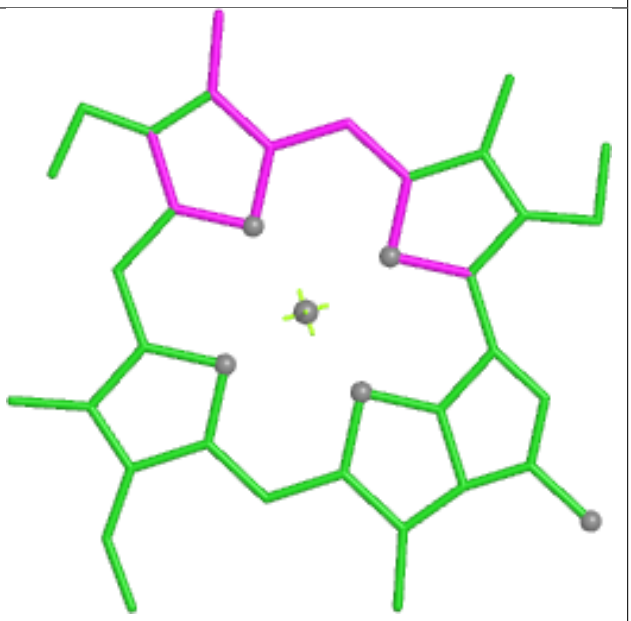


Rings

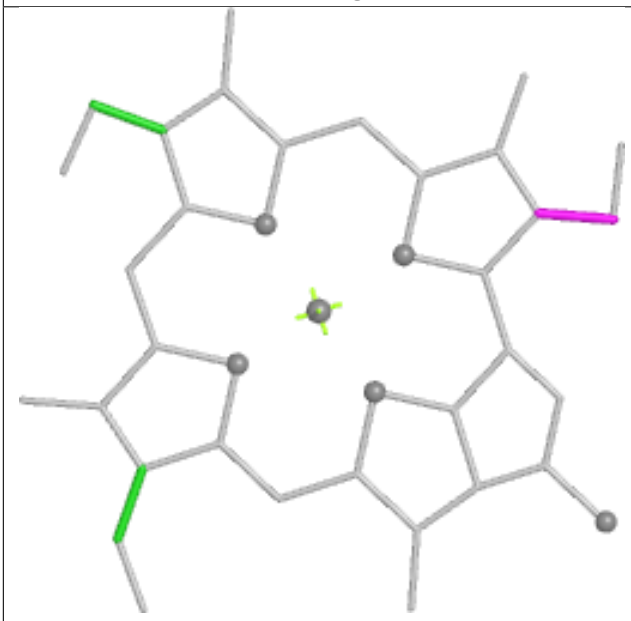
Ligand CLA f 816



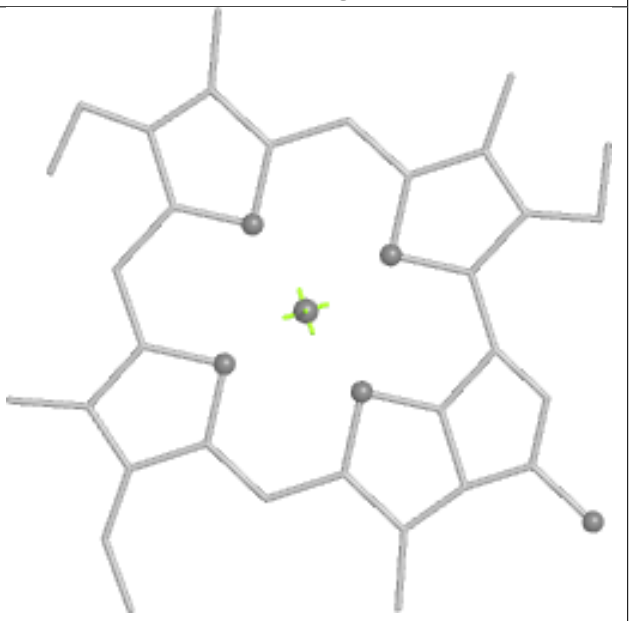
Bond lengths



Bond angles

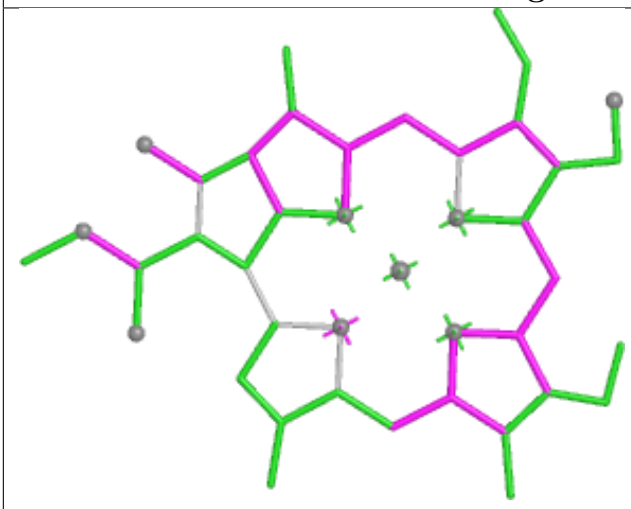


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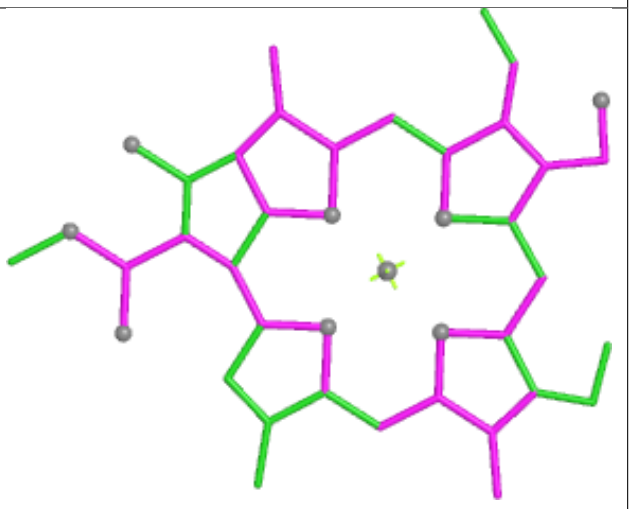


Rings

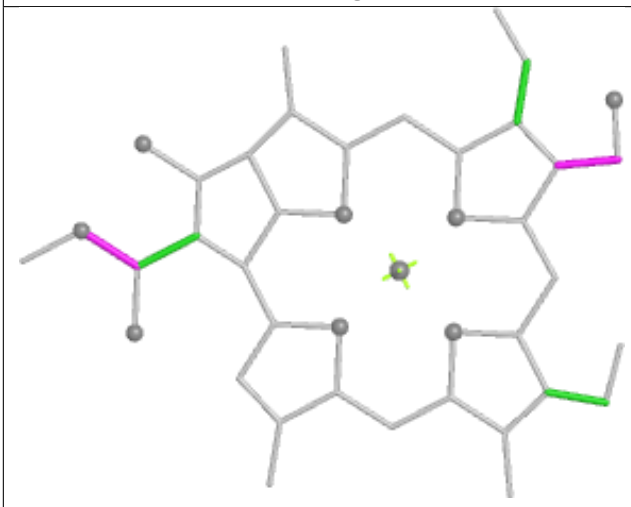
Ligand CHL 1 514



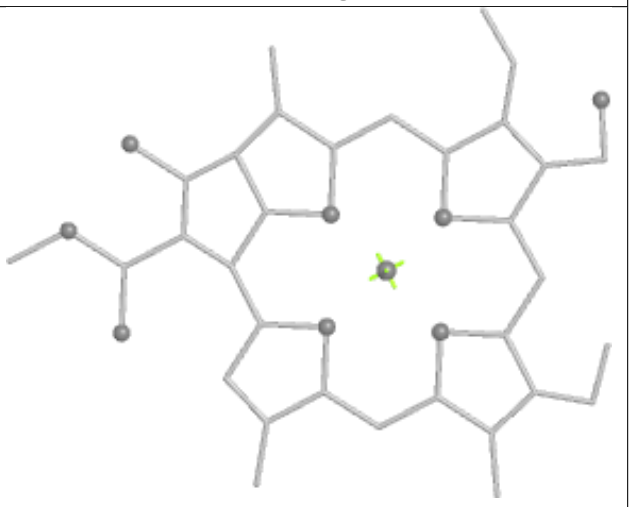
Bond lengths



Bond angles

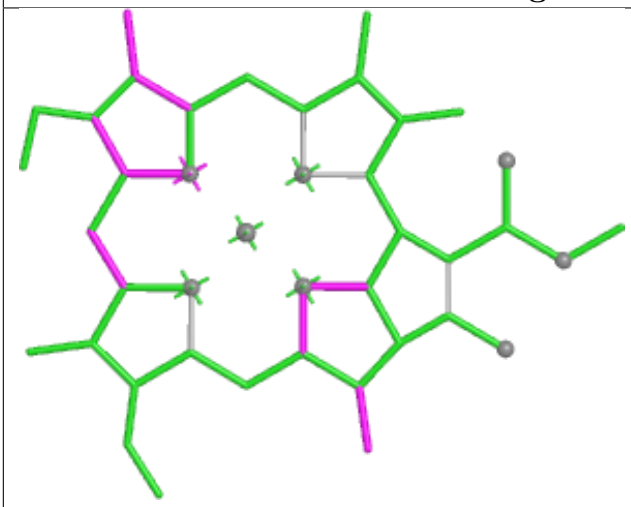


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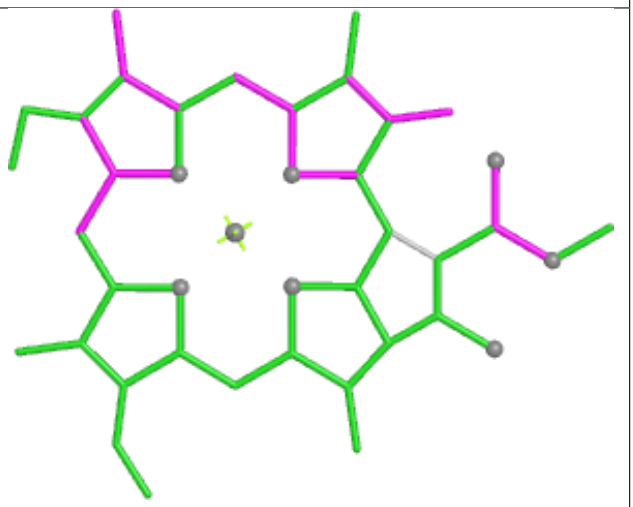


Rings

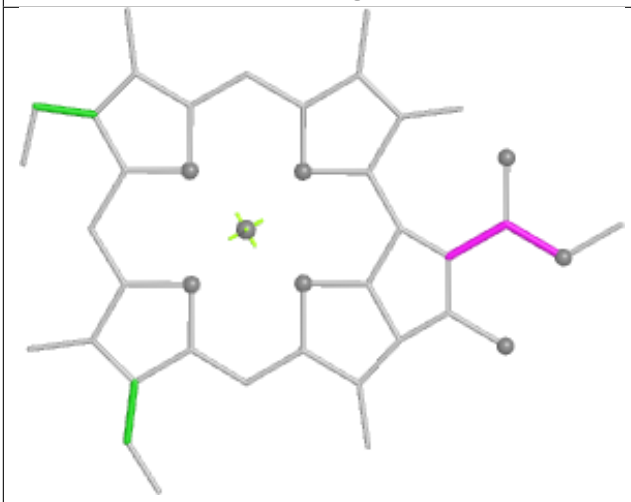
Ligand CLA e 820



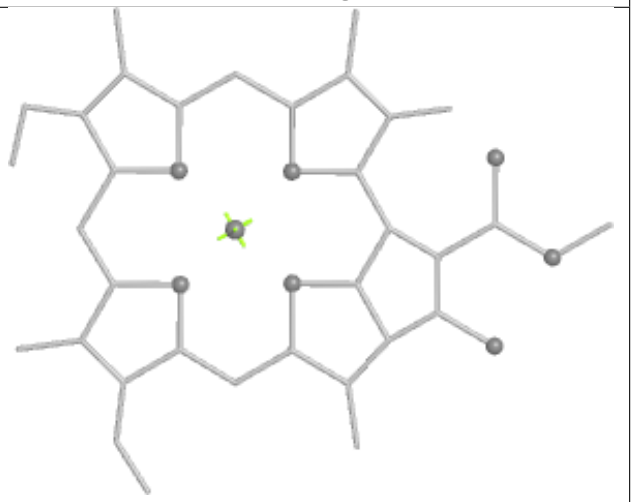
Bond lengths



Bond angles

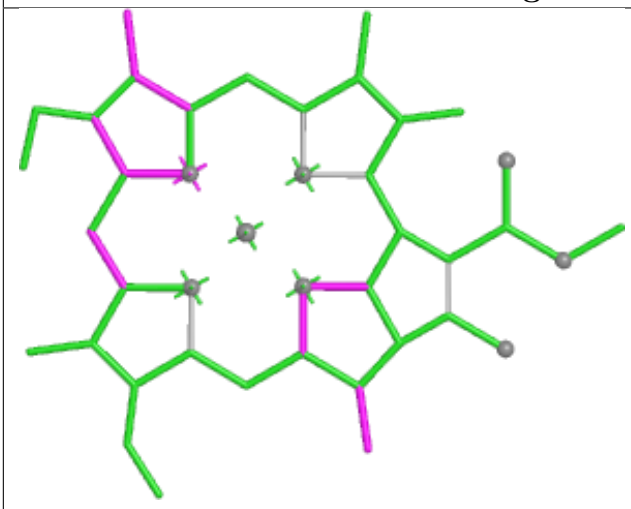


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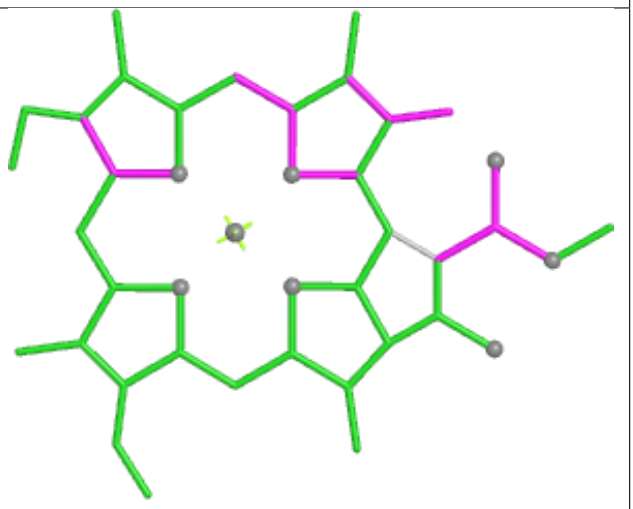


Rings

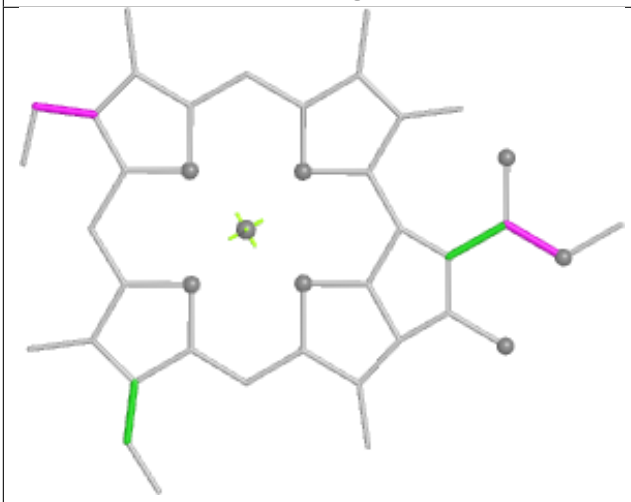
Ligand CLA K 202



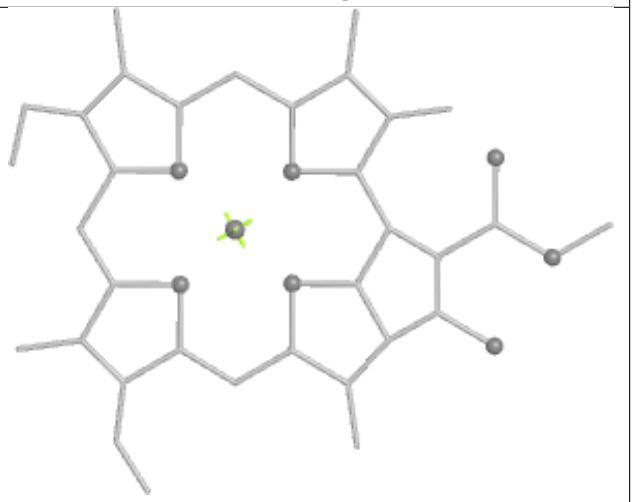
Bond lengths



Bond angles



Torsions

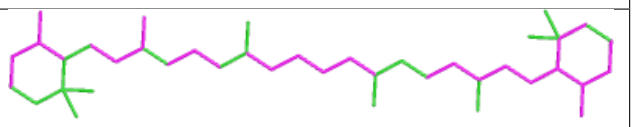


Rings

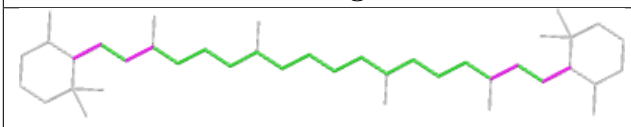
Ligand BCR l 102



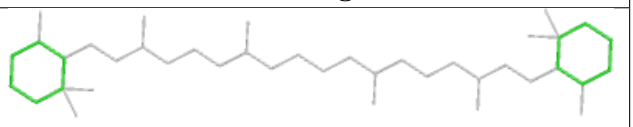
Bond lengths



Bond angles

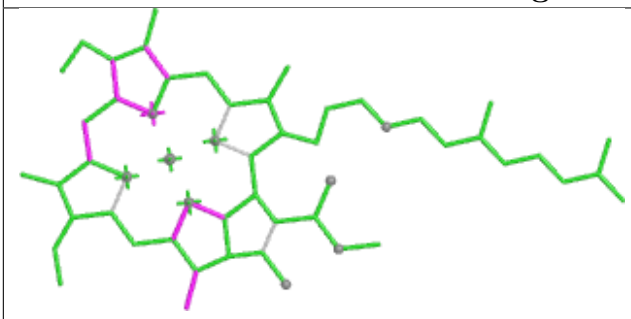


Torsions

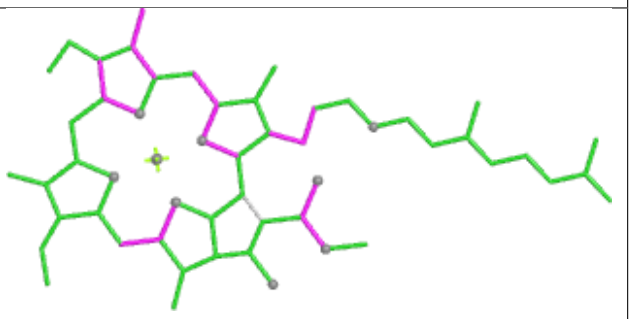


Rings

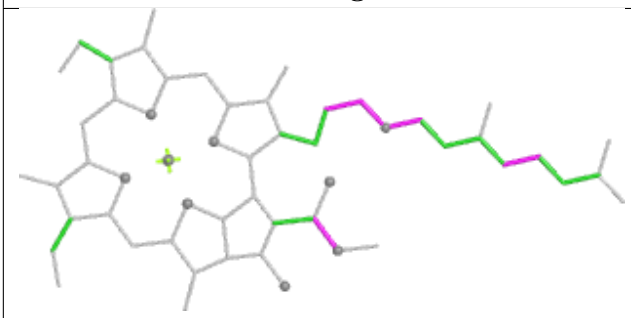
Ligand CLA f 808



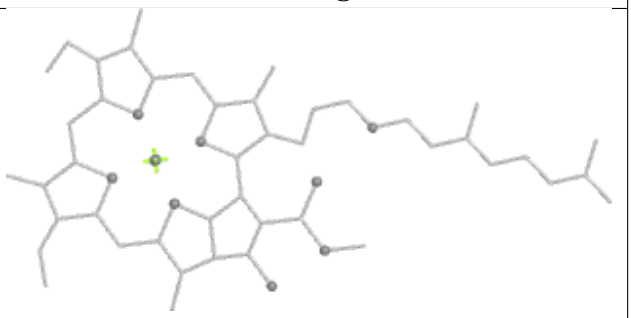
Bond lengths



Bond angles

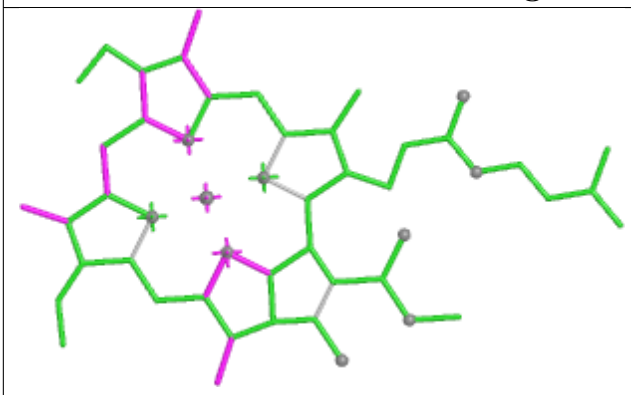


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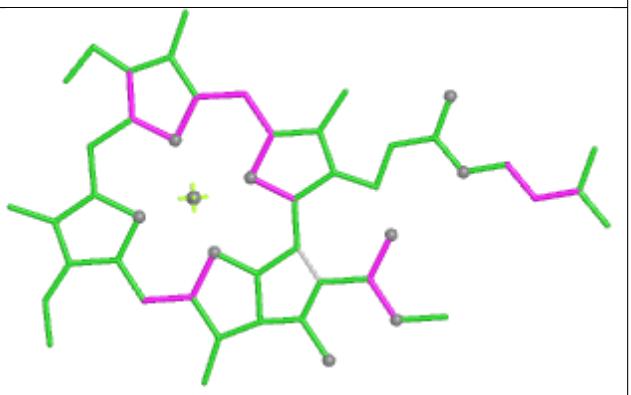


Rings

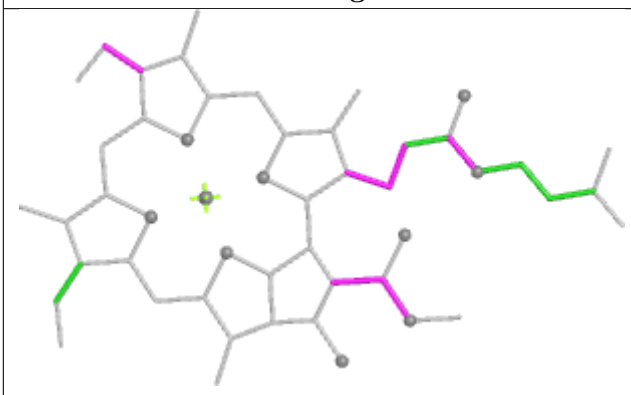
Ligand CLA A 842



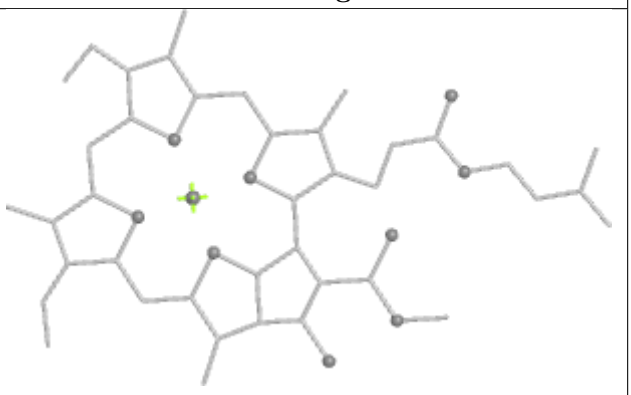
Bond lengths



Bond angles

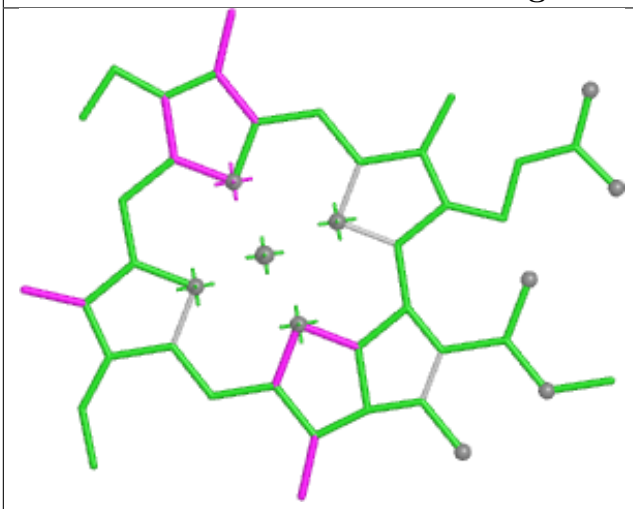


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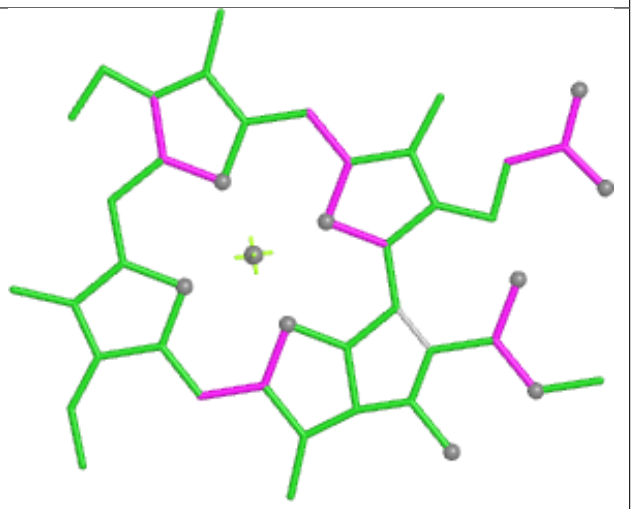


Rings

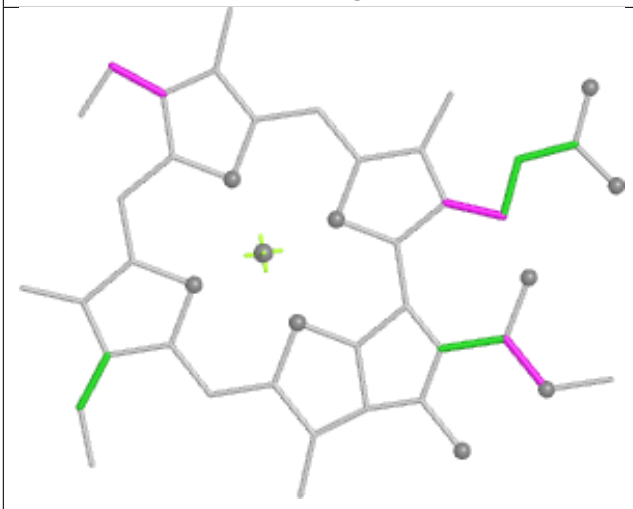
Ligand CLA 3 310



Bond lengths



Bond angles

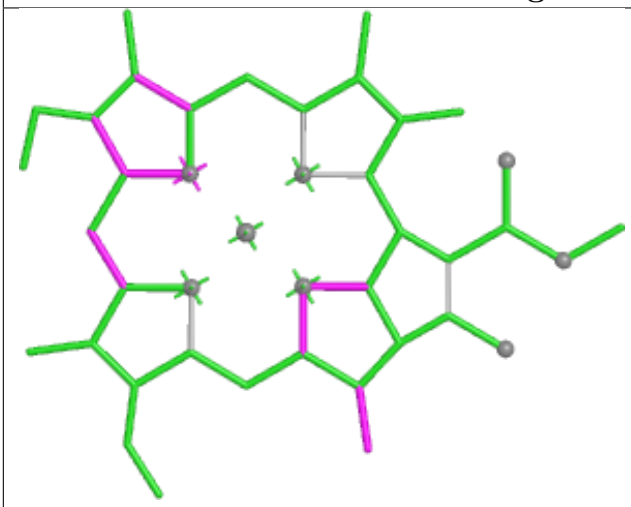


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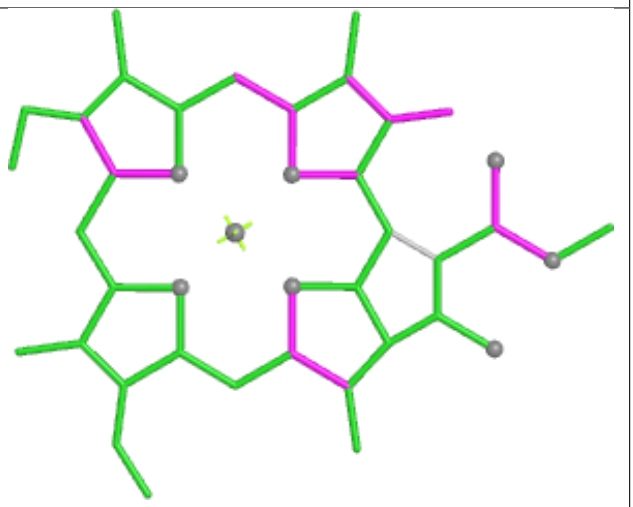


Rings

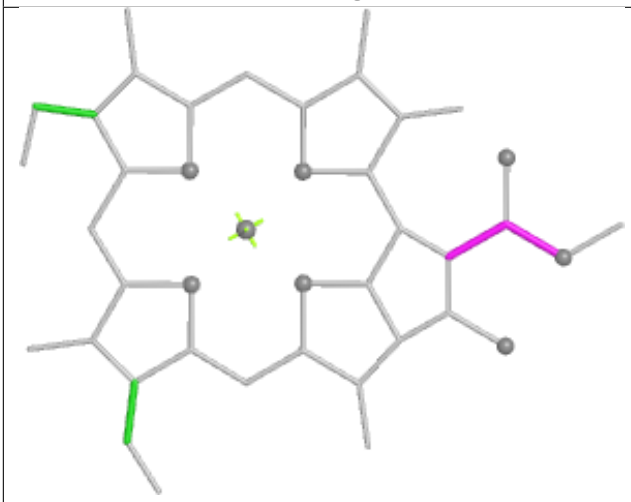
Ligand CLA n 203



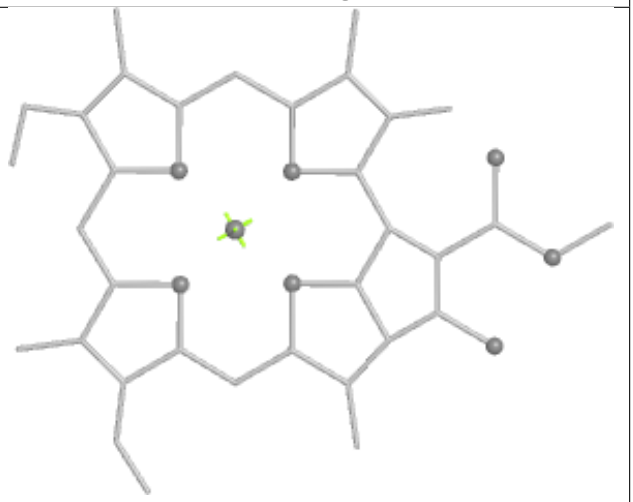
Bond lengths



Bond angles

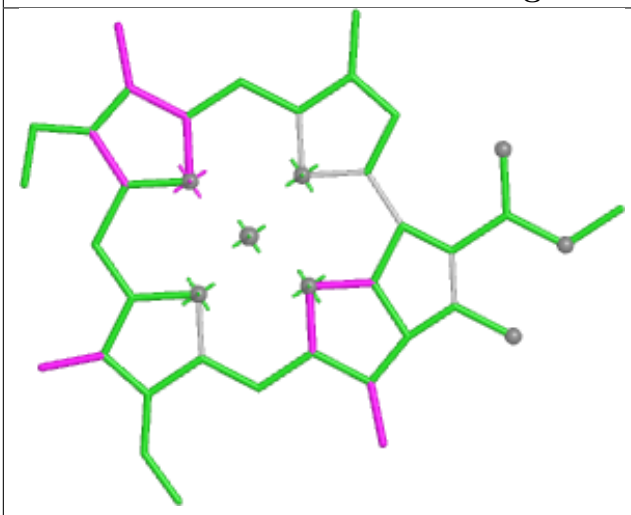


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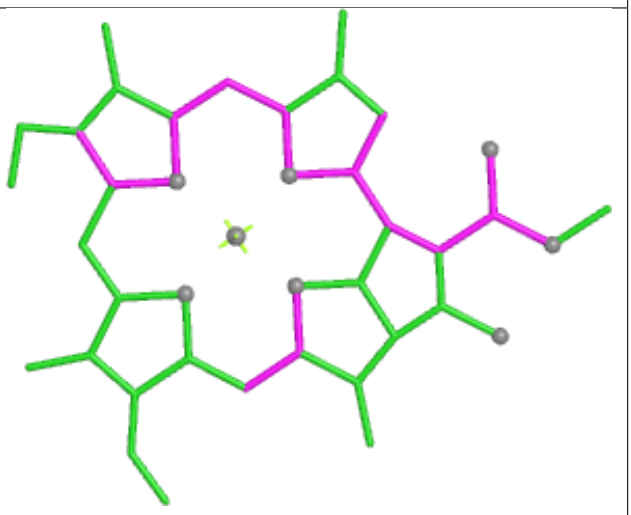


Rings

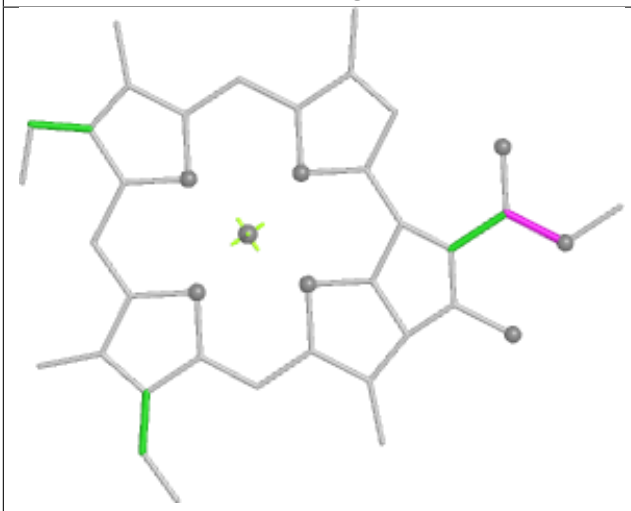
Ligand CLA A 811



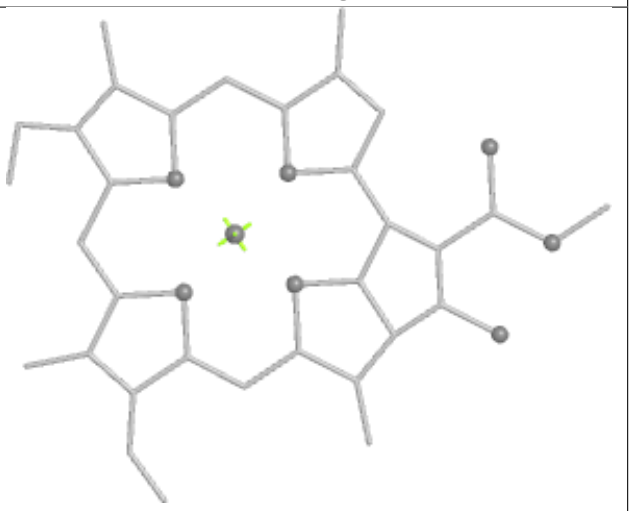
Bond lengths



Bond angles



Torsions



Rings

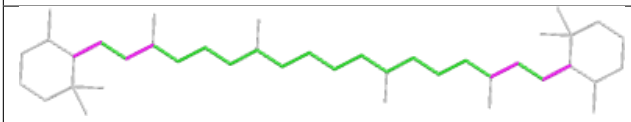
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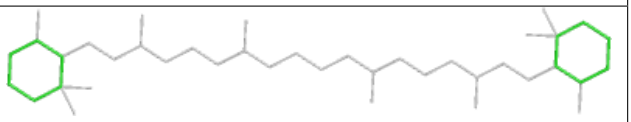
Bond lengths



Bond angles

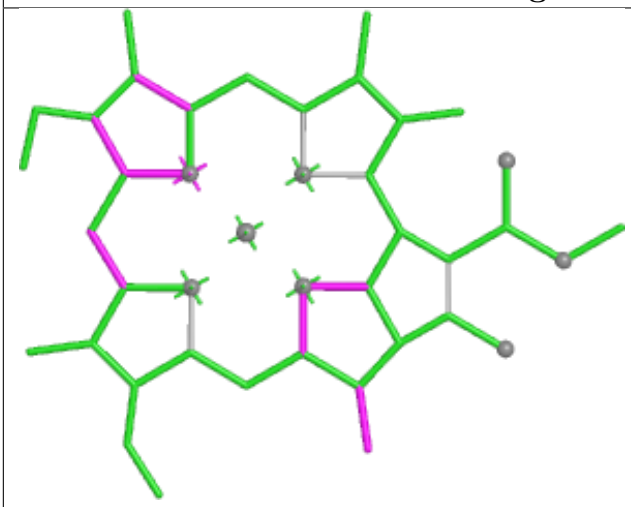


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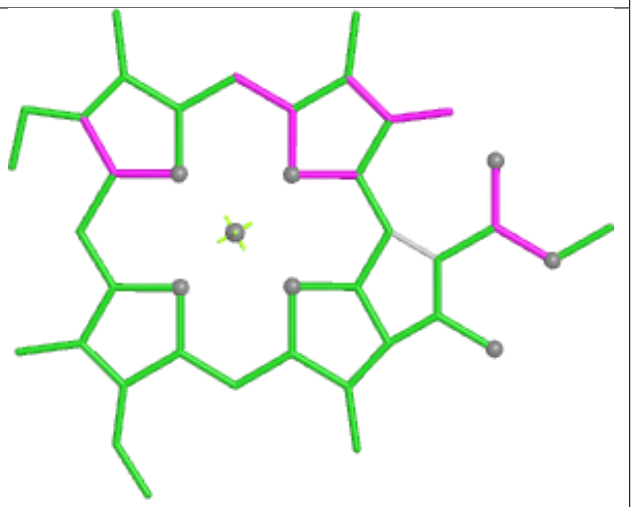


Rings

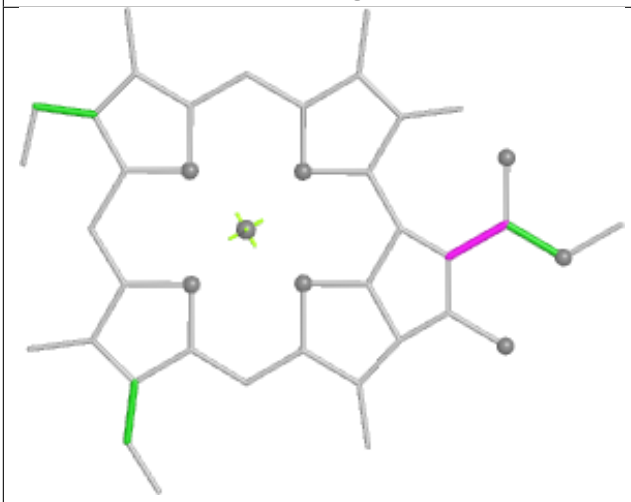
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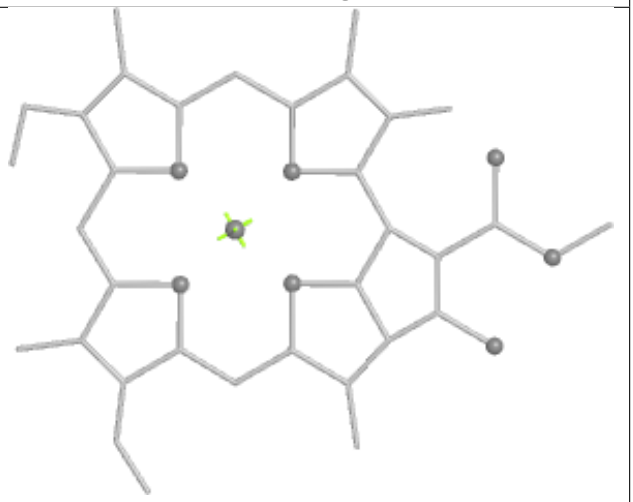
Bond lengths



Bond angles

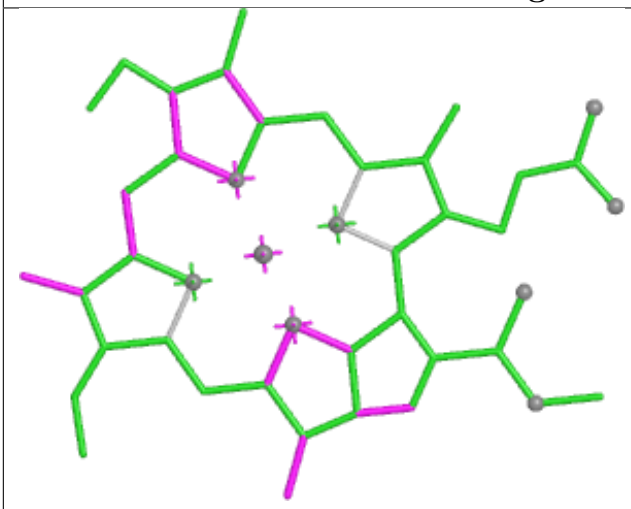


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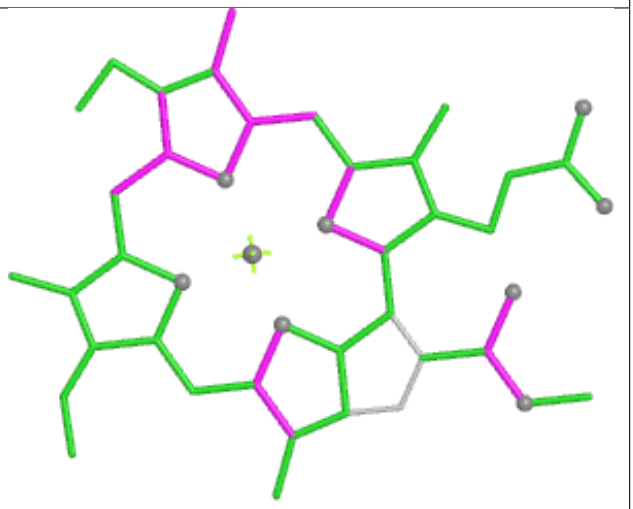


Rings

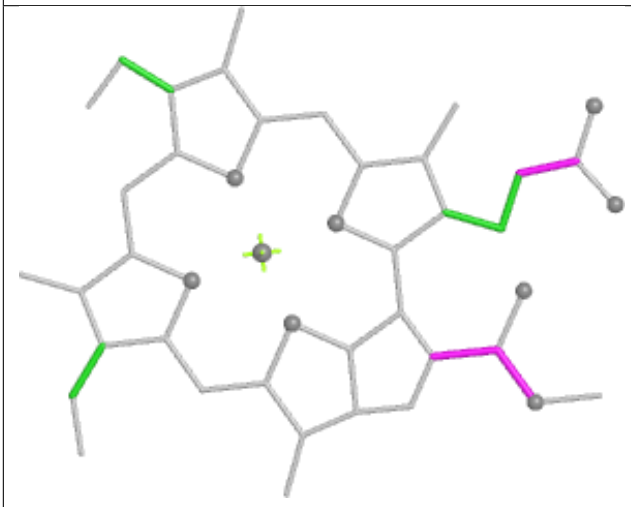
Ligand CLA 1 515



Bond lengths



Bond angles

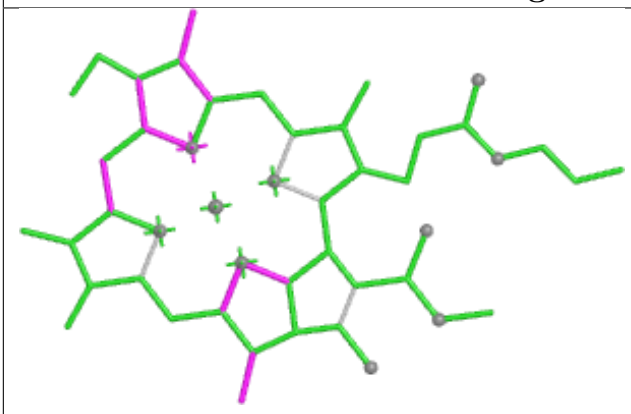


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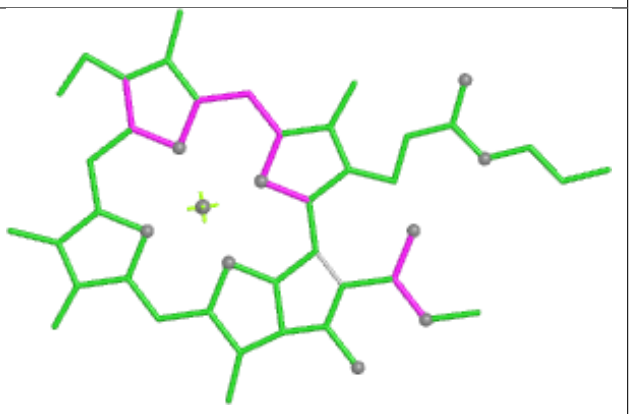


Rings

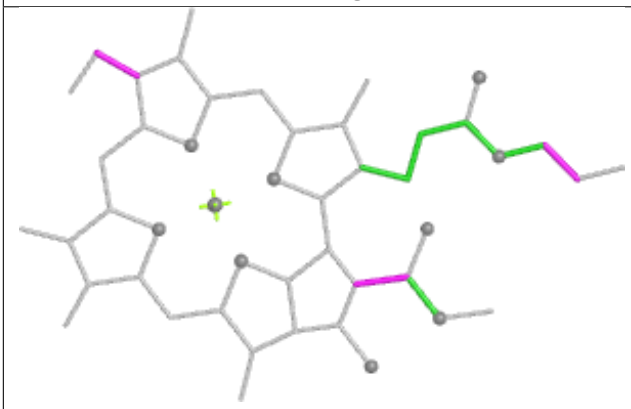
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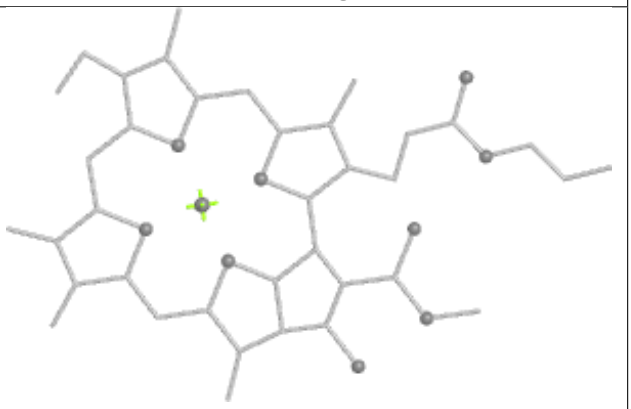
Bond lengths



Bond angles

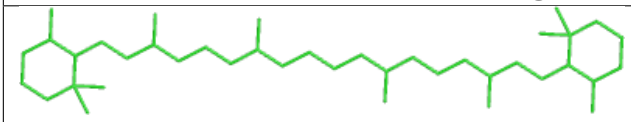


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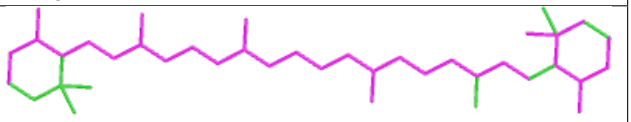


Rings

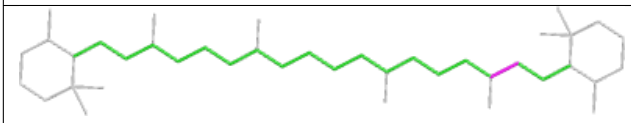
Ligand BCR j 801



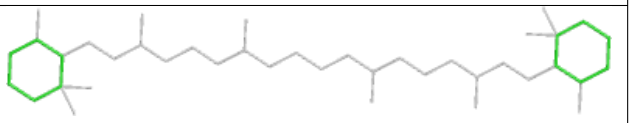
Bond lengths



Bond angles



Torsions



Rings

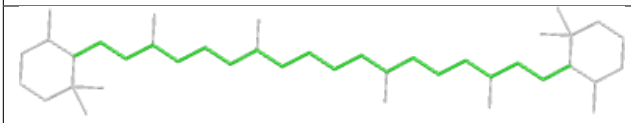
Ligand BCR f 849



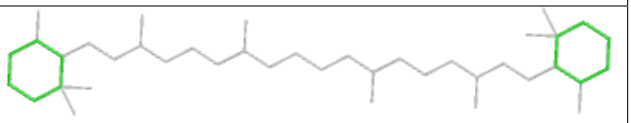
Bond lengths



Bond angles

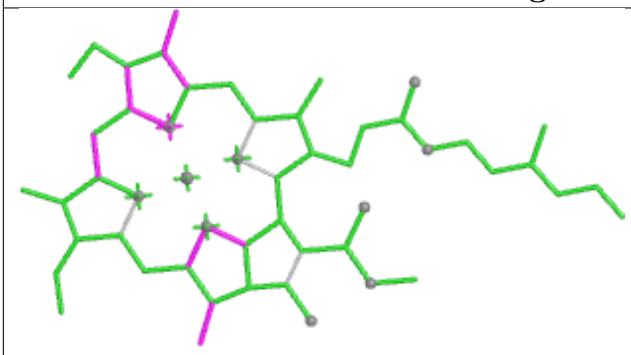


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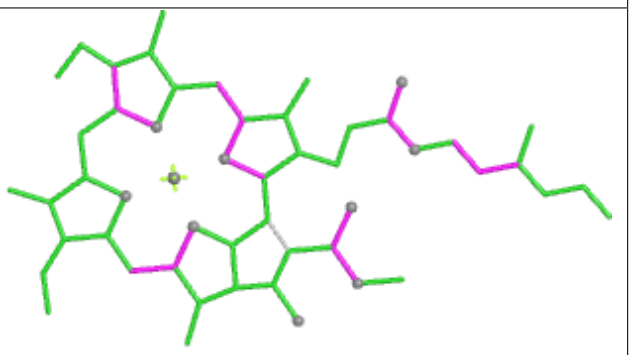


Rings

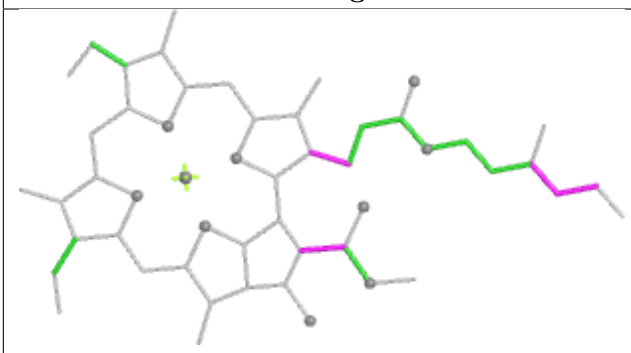
Ligand CLA e 803



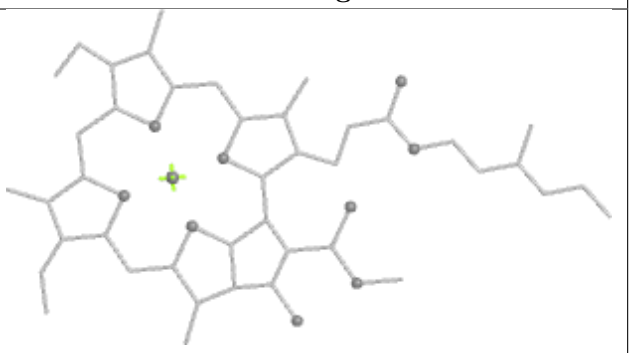
Bond lengths



Bond angles

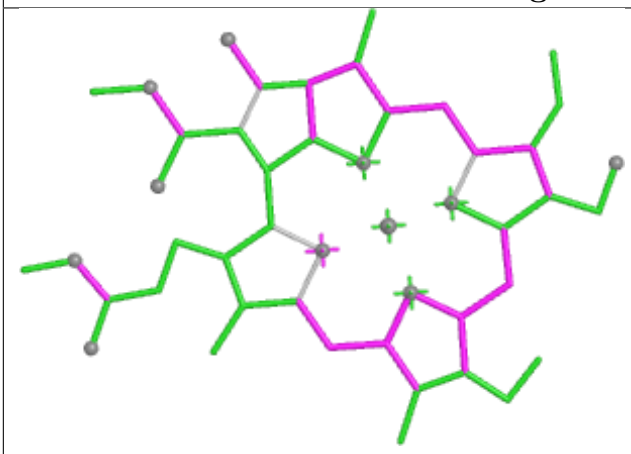


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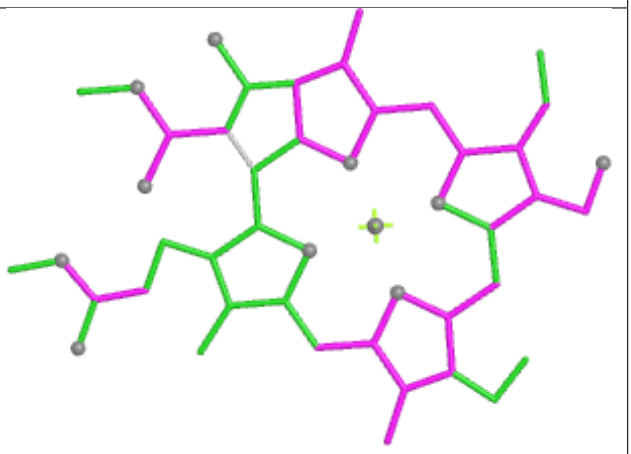


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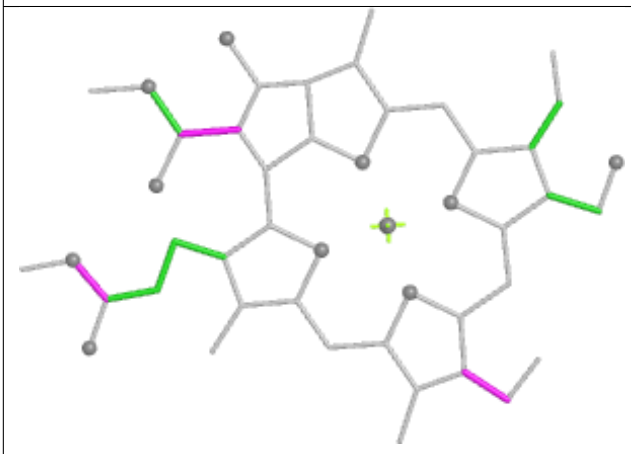
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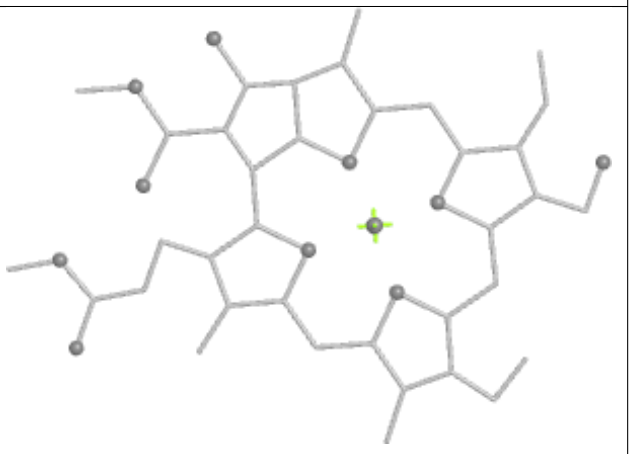
Bond lengths



Bond angles

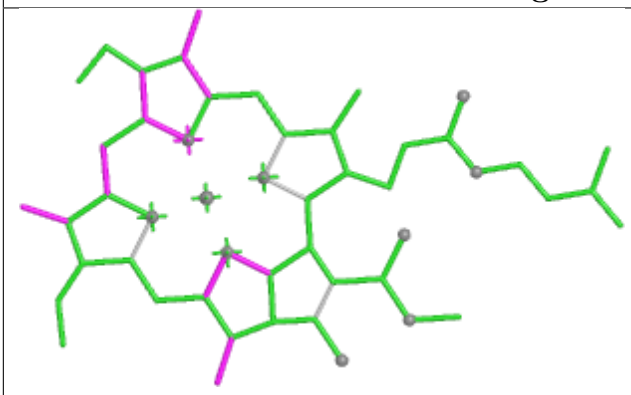


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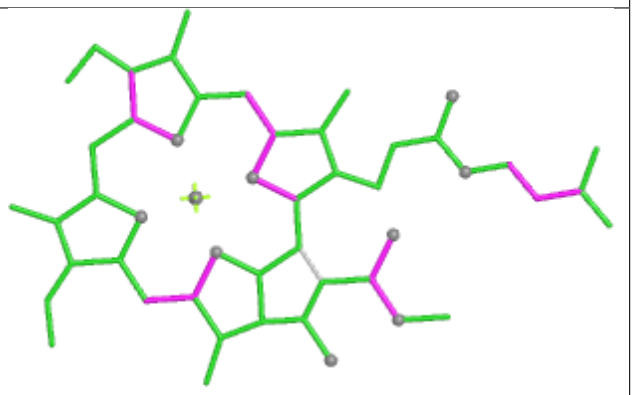


Rings

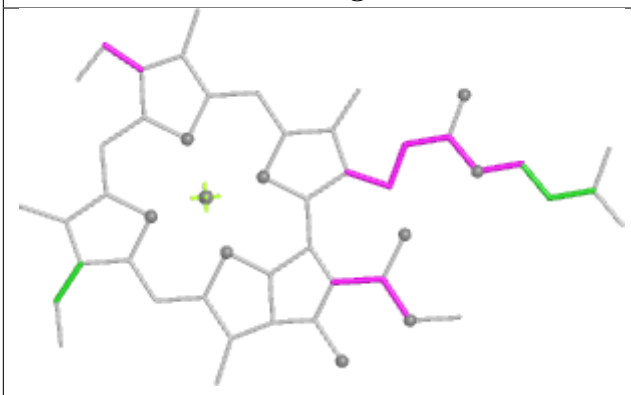
Ligand CLA f 820



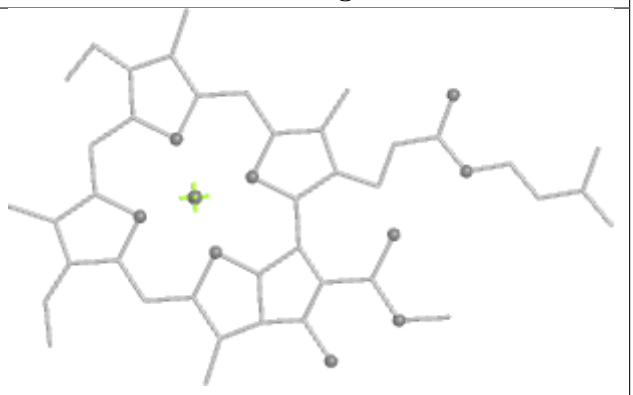
Bond lengths



Bond angles

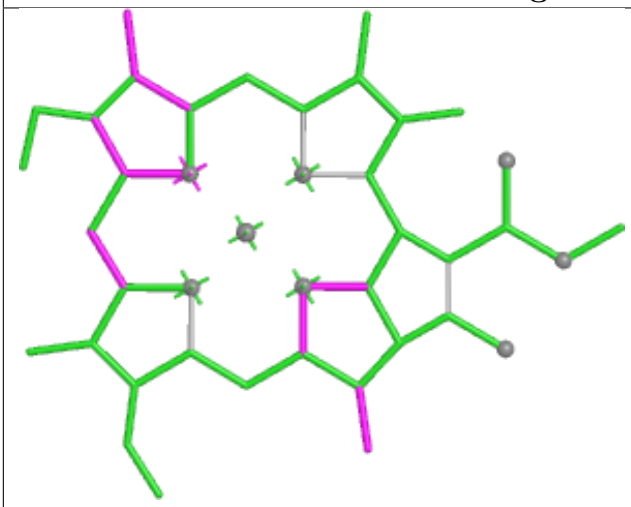


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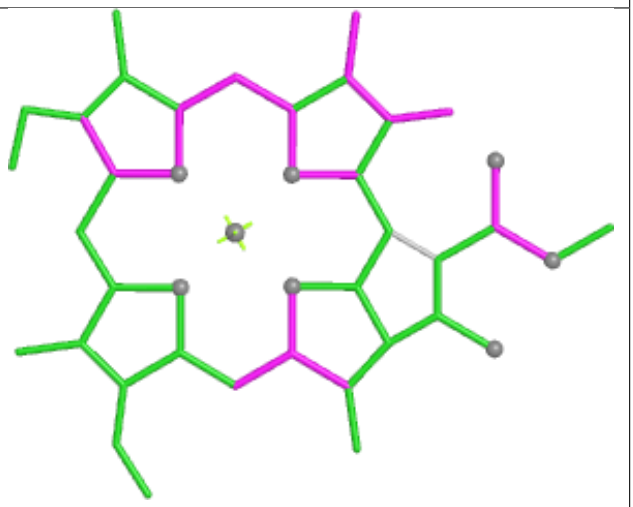


Rings

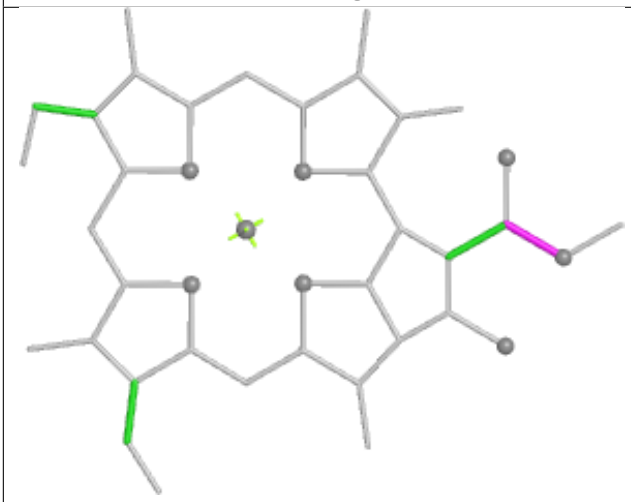
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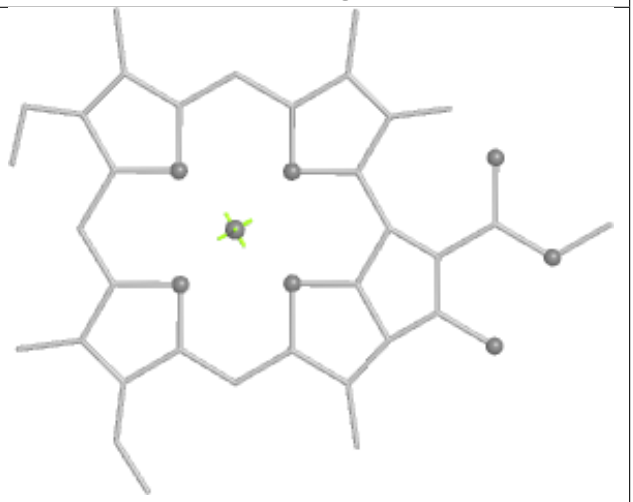
Bond lengths



Bond angles

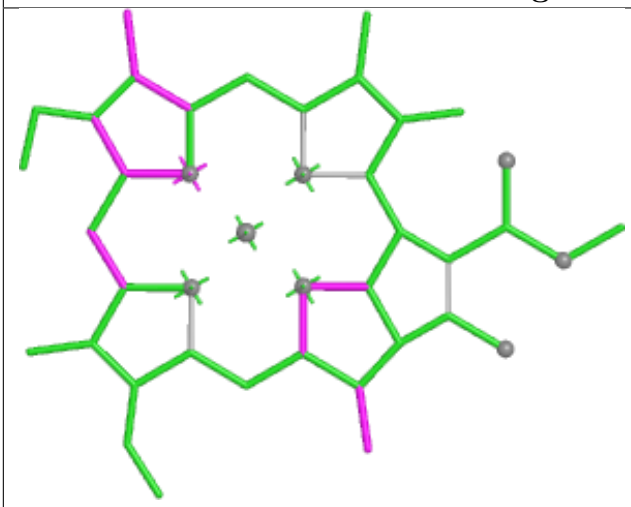


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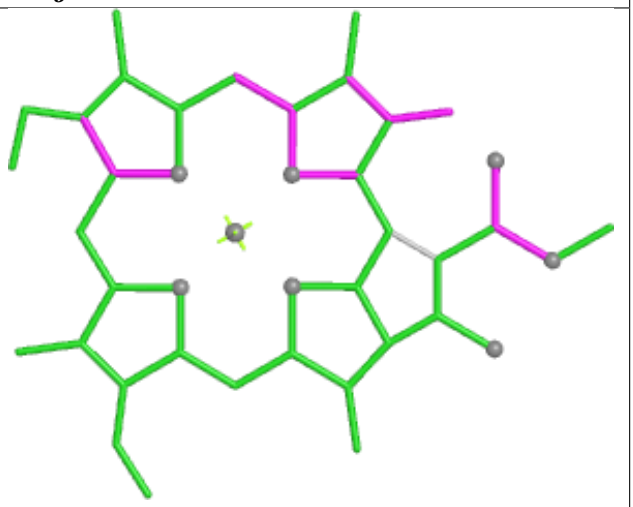


Rings

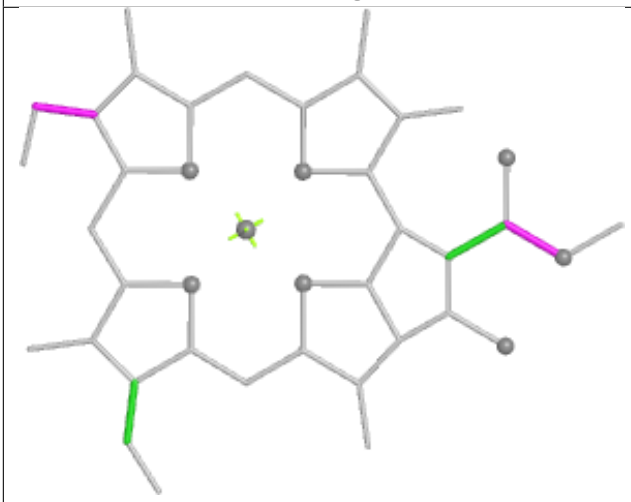
Ligand CLA j 802



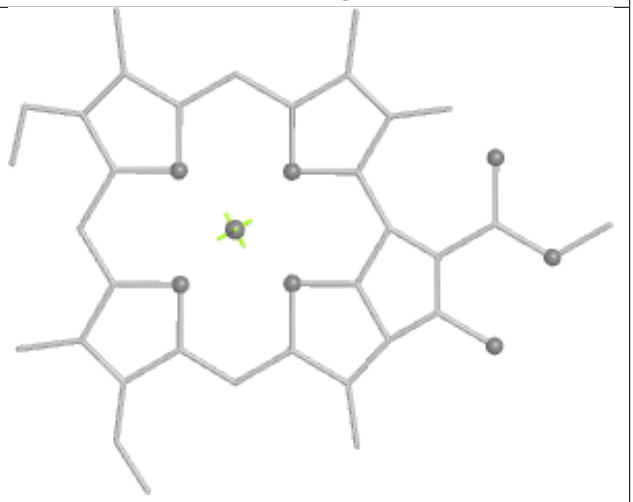
Bond lengths



Bond angles

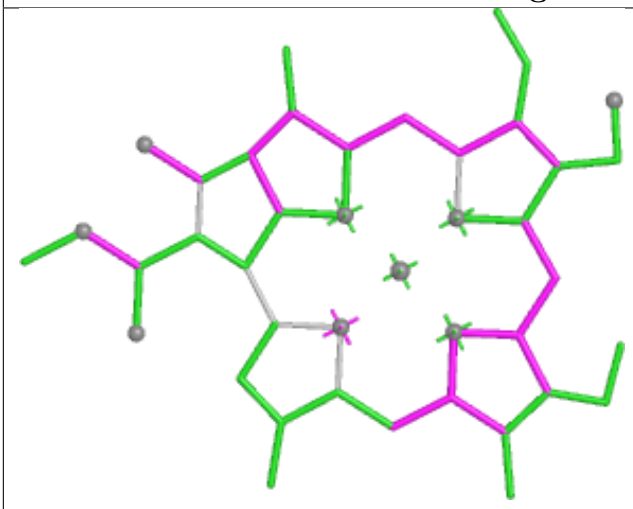


Torsions

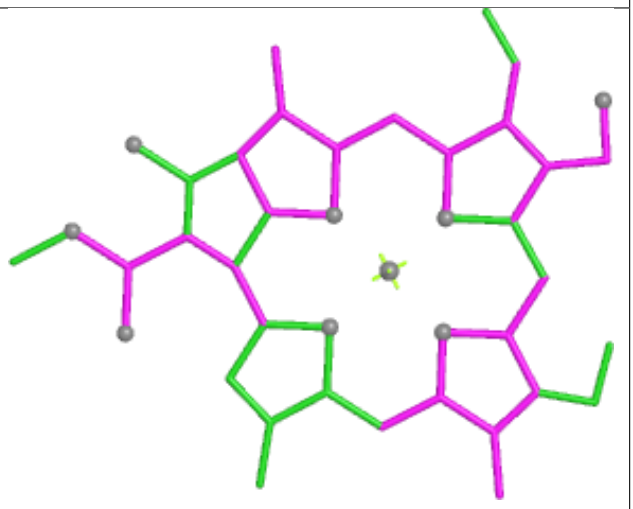


Rings

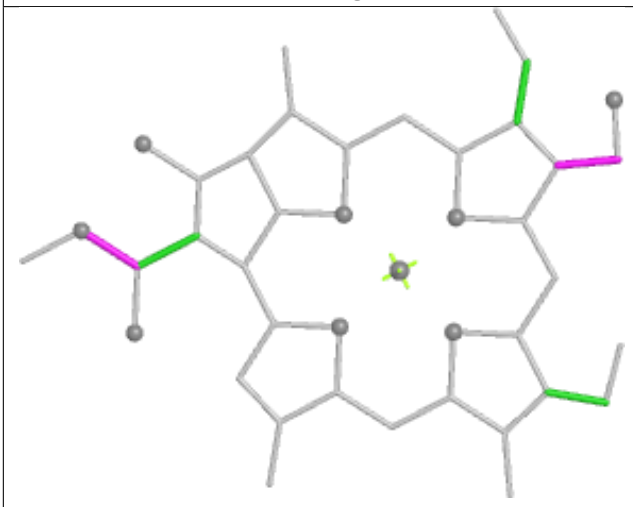
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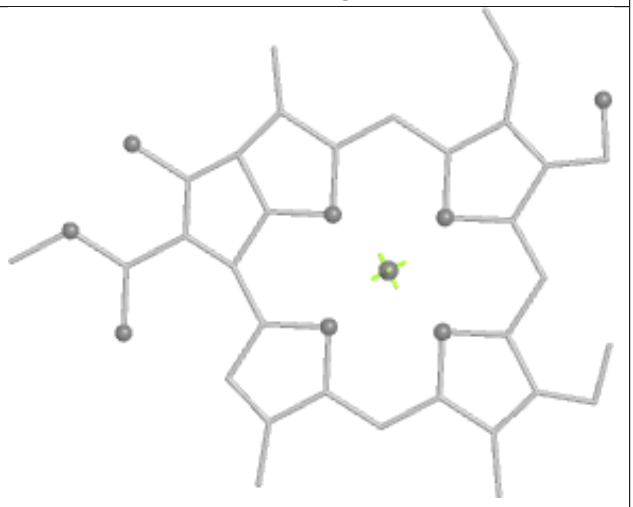
Bond lengths



Bond angles

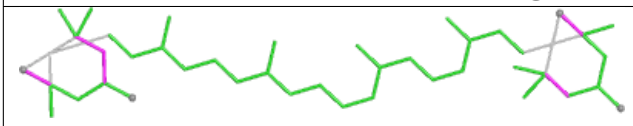


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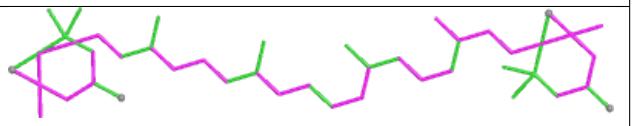


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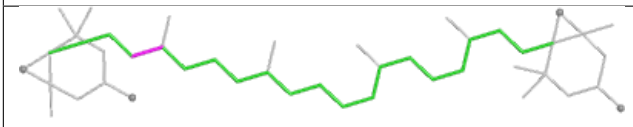
Ligand XAT 5 304



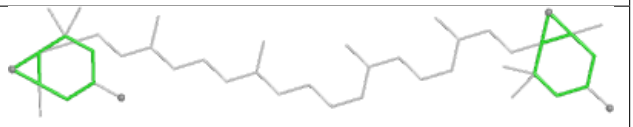
Bond lengths



Bond angles

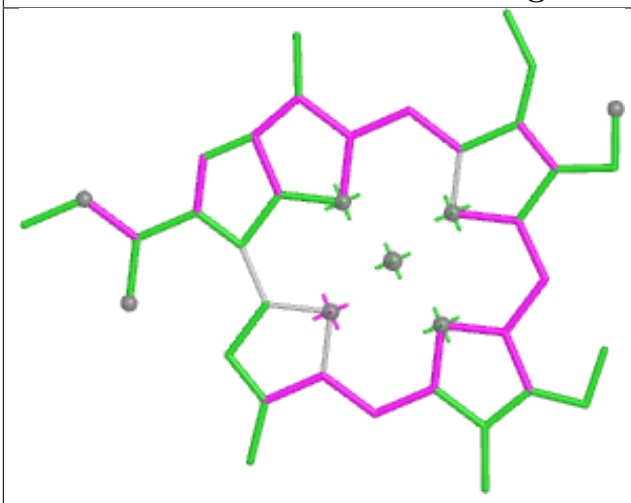


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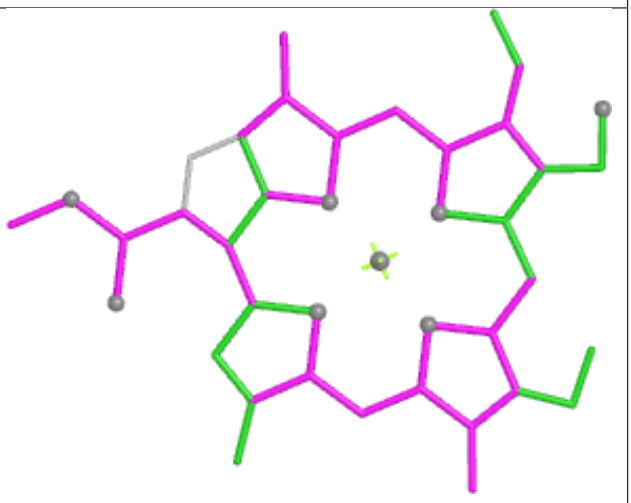


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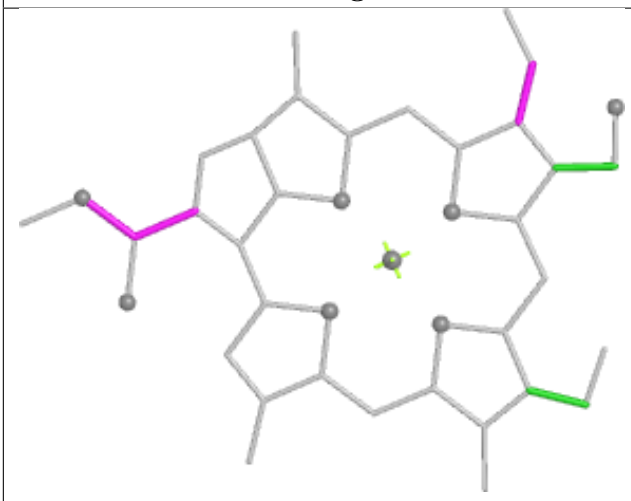
Ligand CHL 2 513



Bond lengths



Bond angles

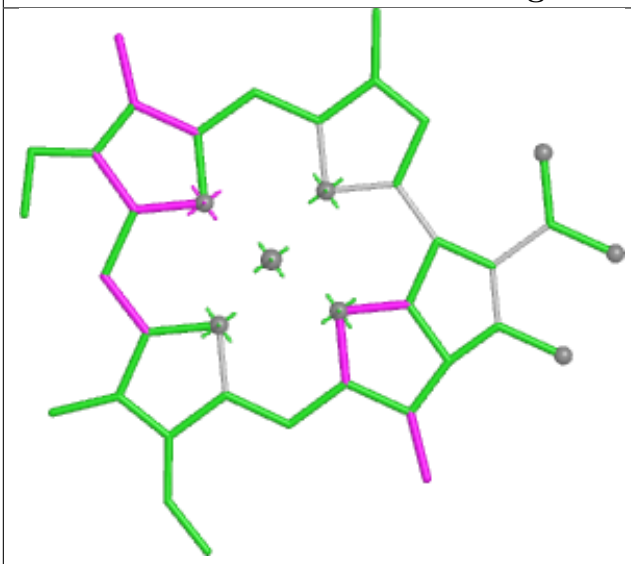


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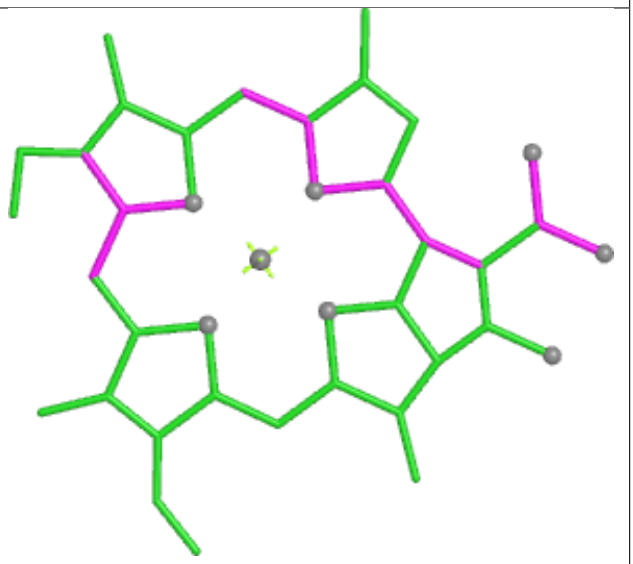


Rings

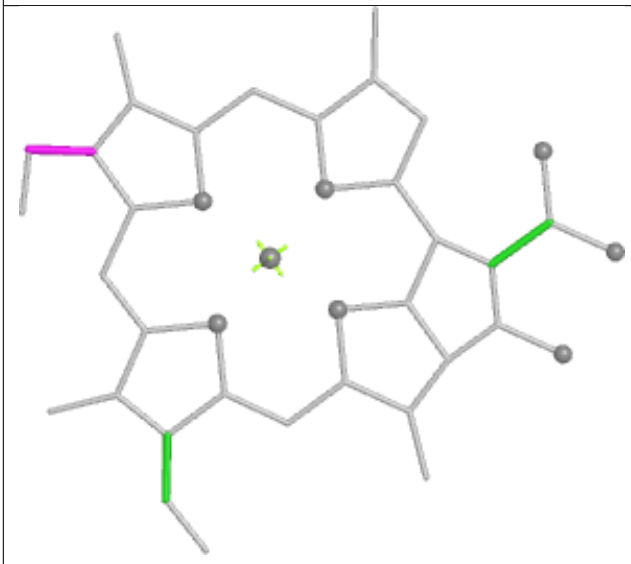
Ligand CLA n 205



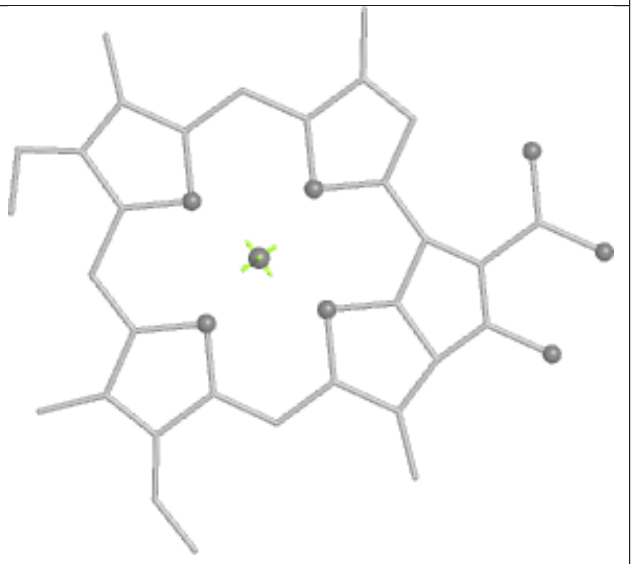
Bond lengths



Bond angles

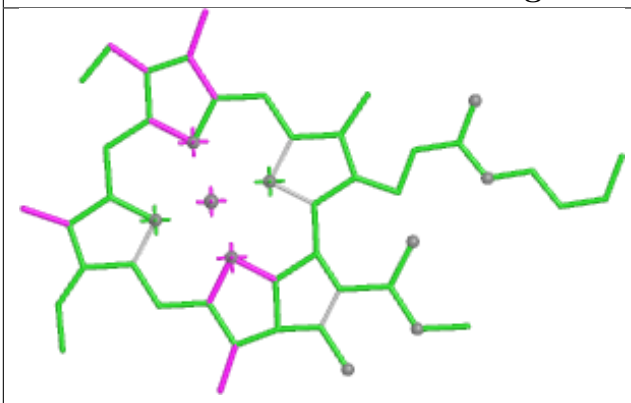


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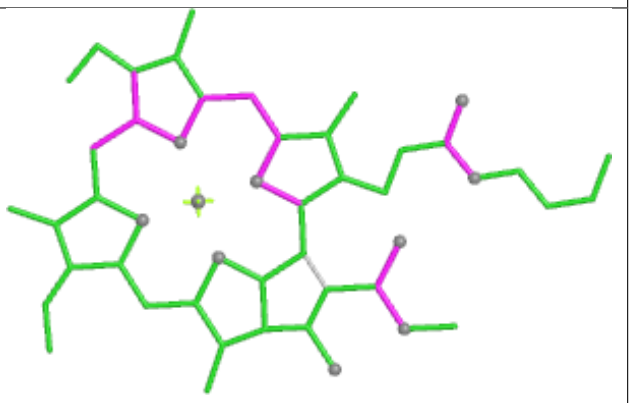


Rings

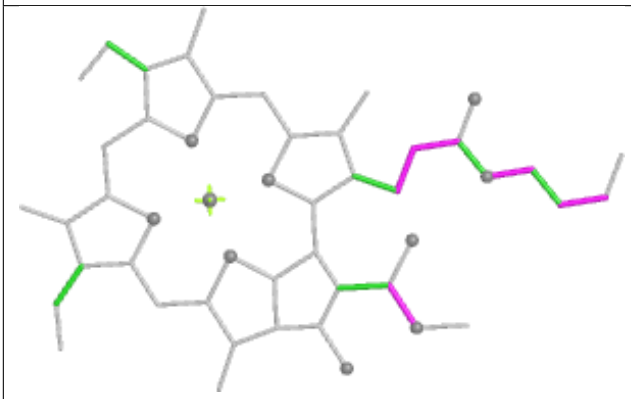
Ligand CLA B 817



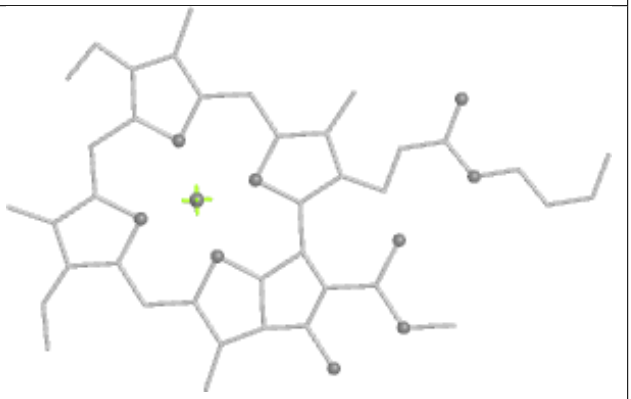
Bond lengths



Bond angles

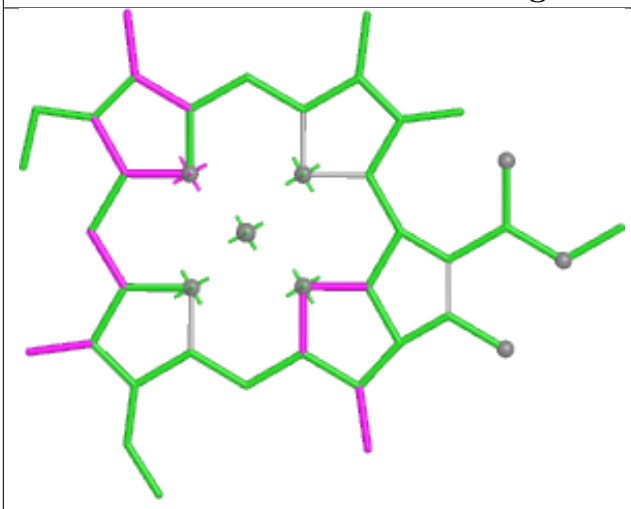


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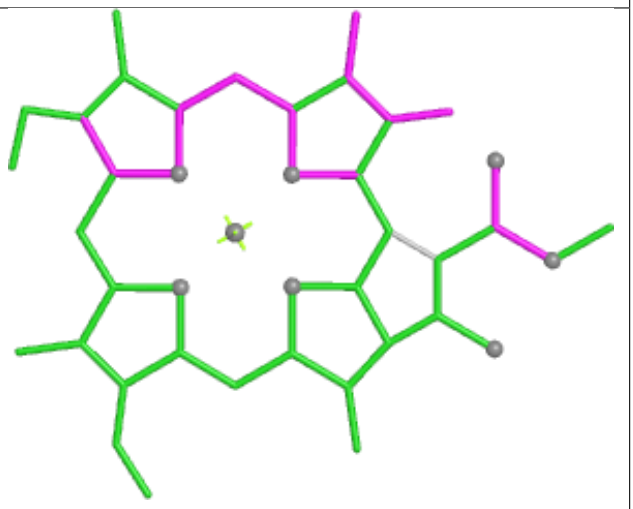


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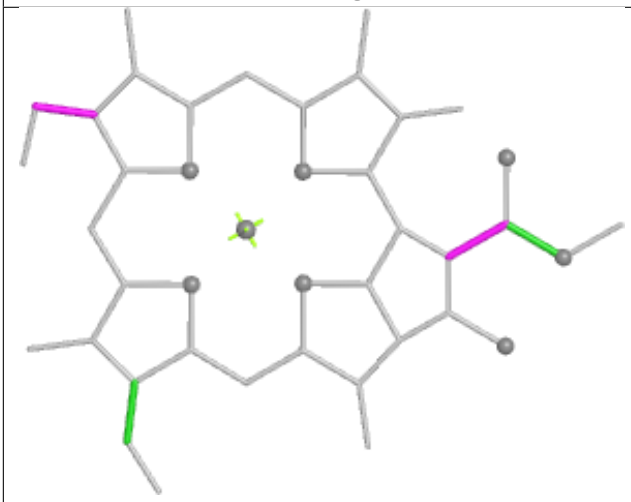
Ligand CLA e 811



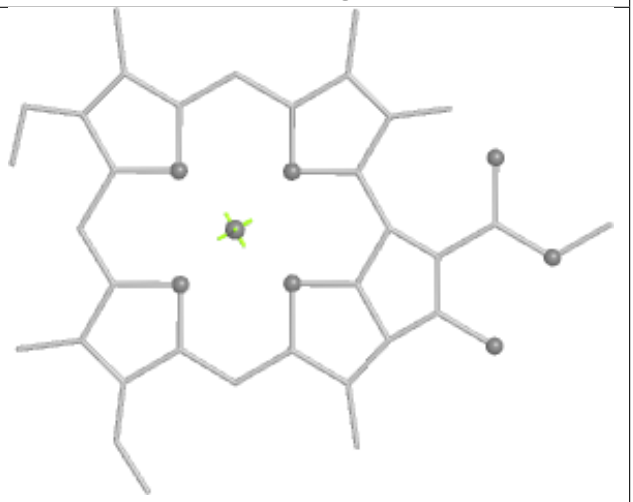
Bond lengths



Bond angles

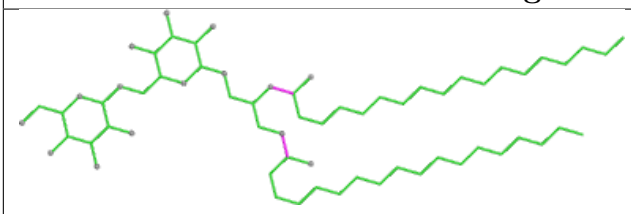


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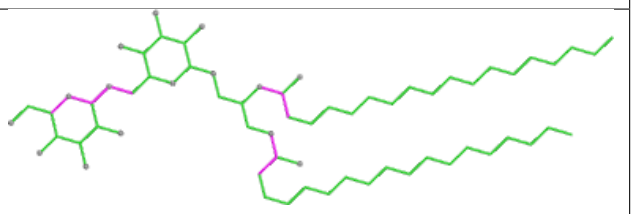


Rings

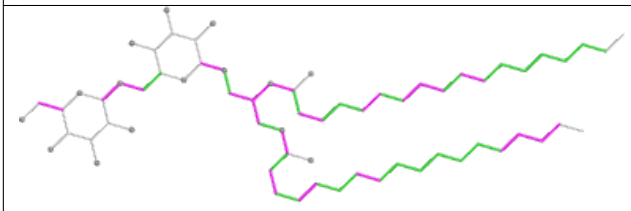
Ligand DGD J 103



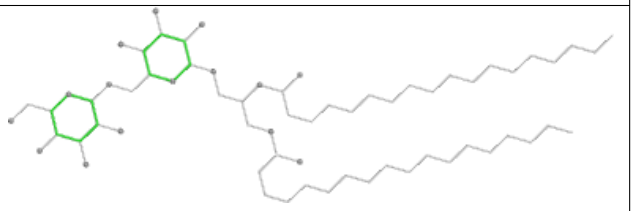
Bond lengths



Bond angles

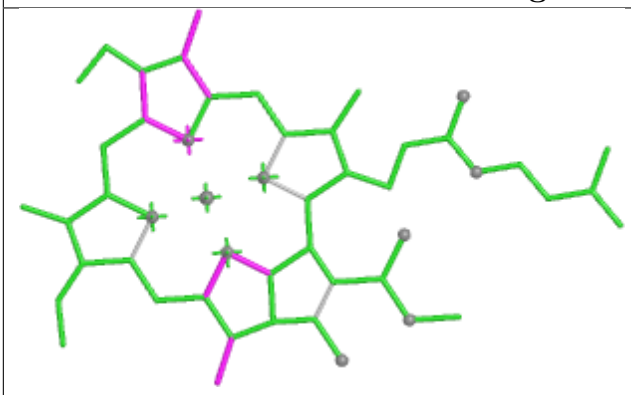


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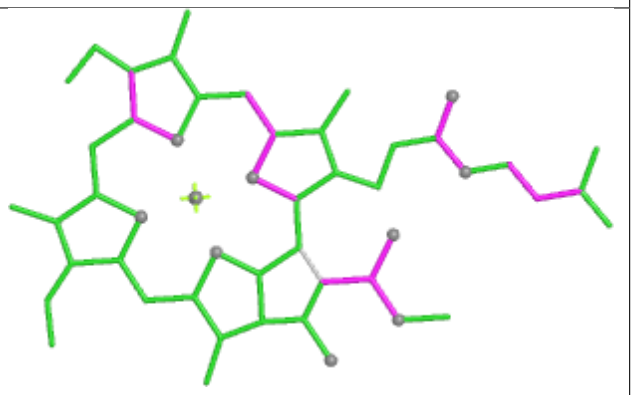


Rings

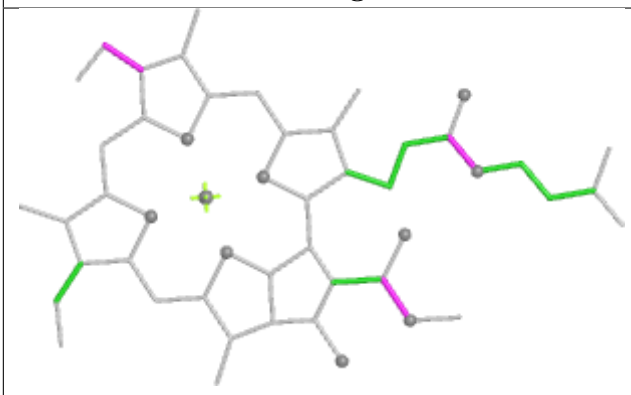
Ligand CLA e 809



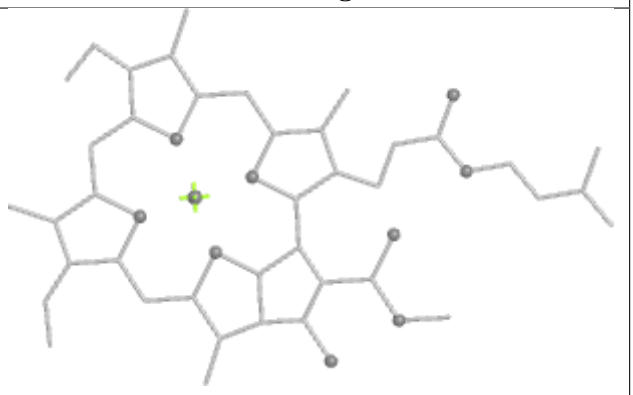
Bond lengths



Bond angles

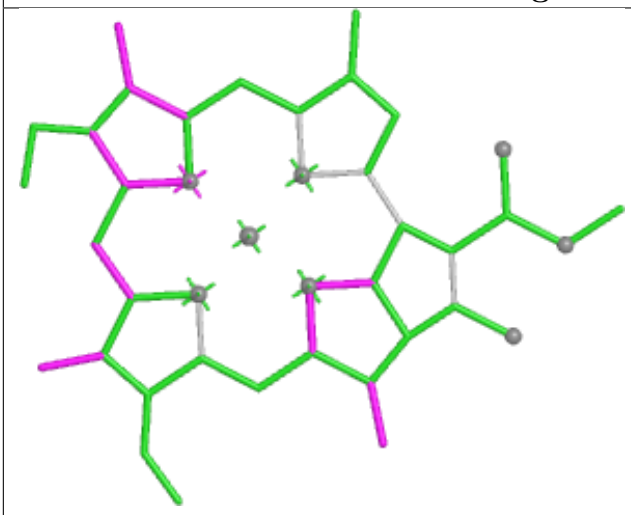


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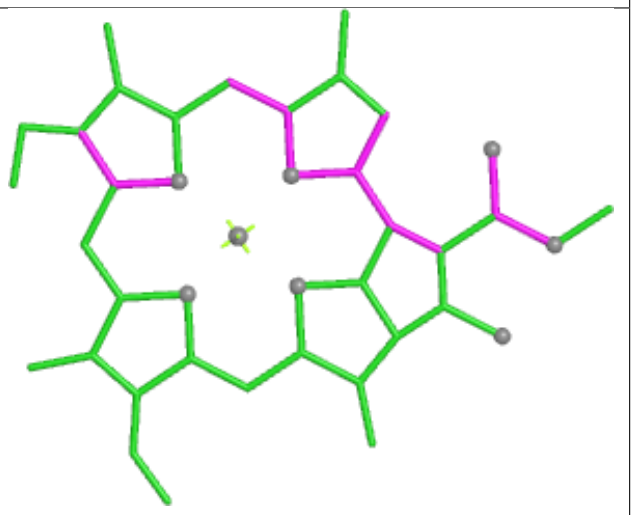


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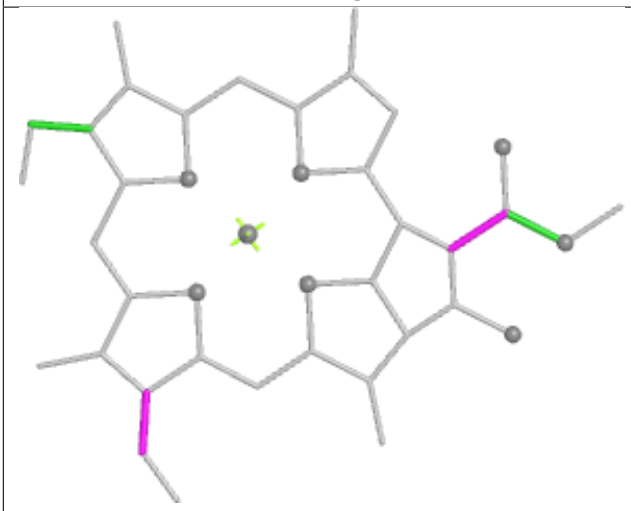
Ligand CLA f 838



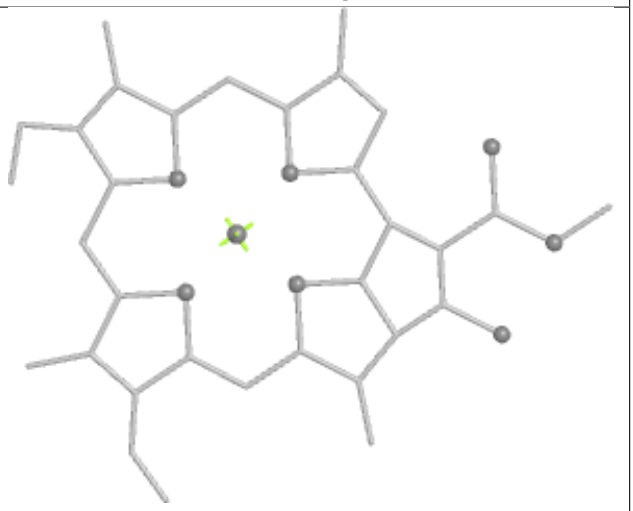
Bond lengths



Bond angles

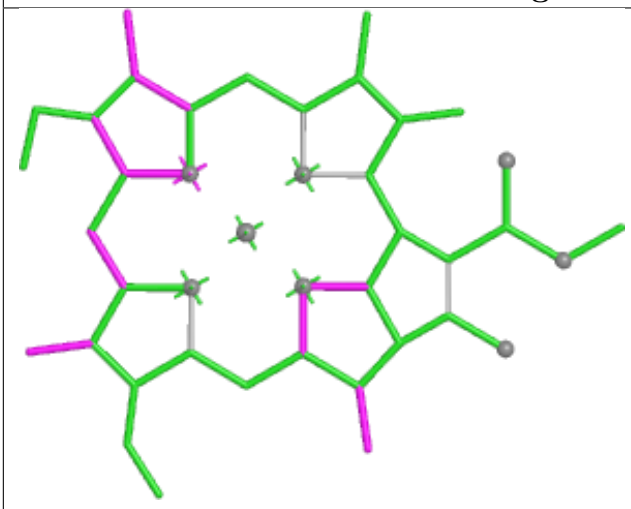


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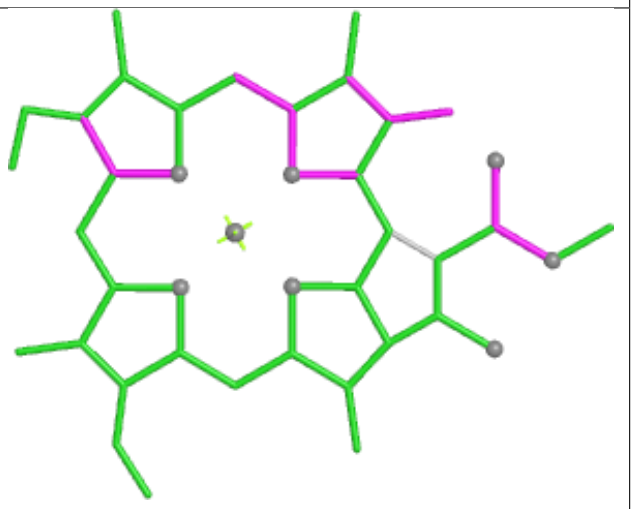


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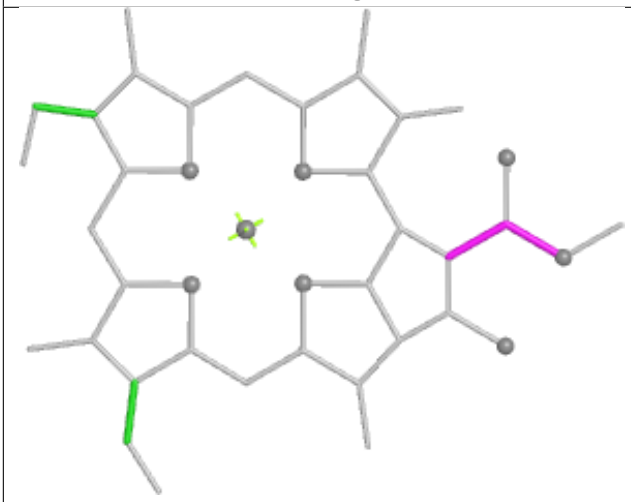
Ligand CLA f 841



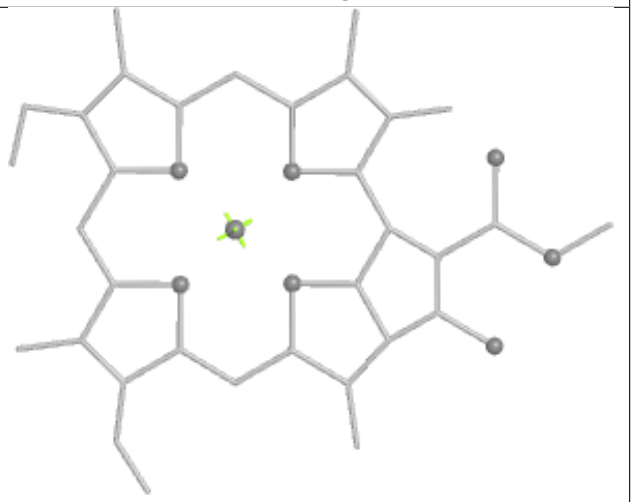
Bond lengths



Bond angles

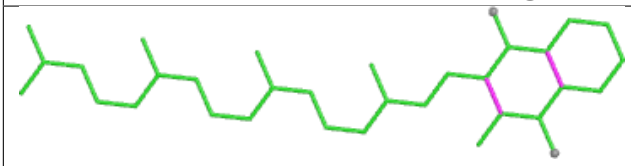


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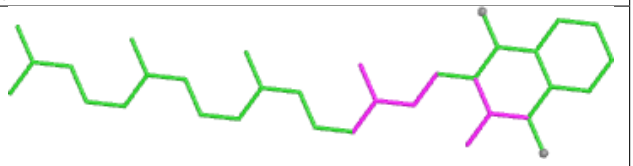


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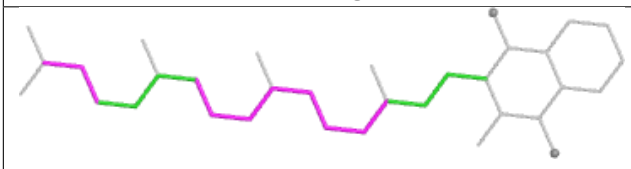
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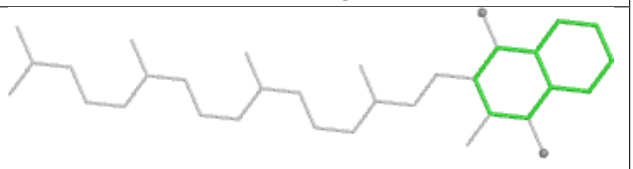
Bond lengths



Bond angles

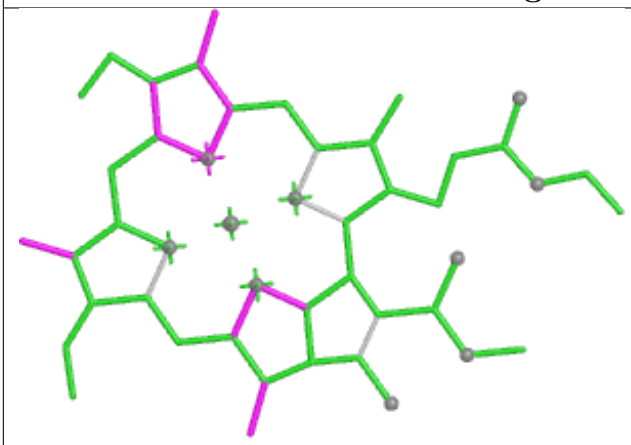


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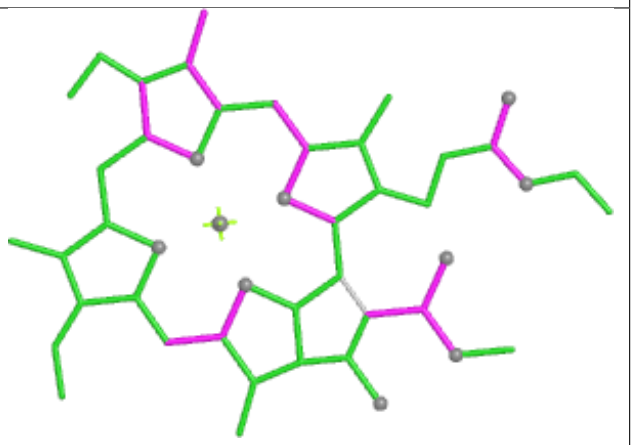


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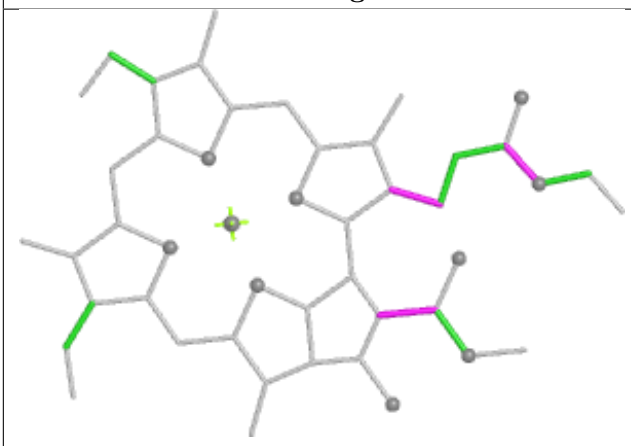
Ligand CLA B 839



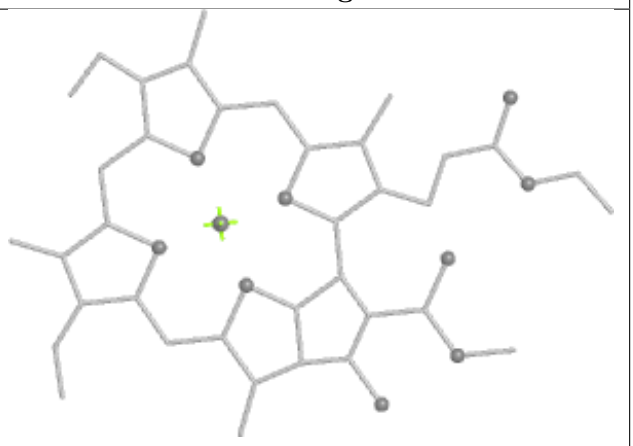
Bond lengths



Bond angles

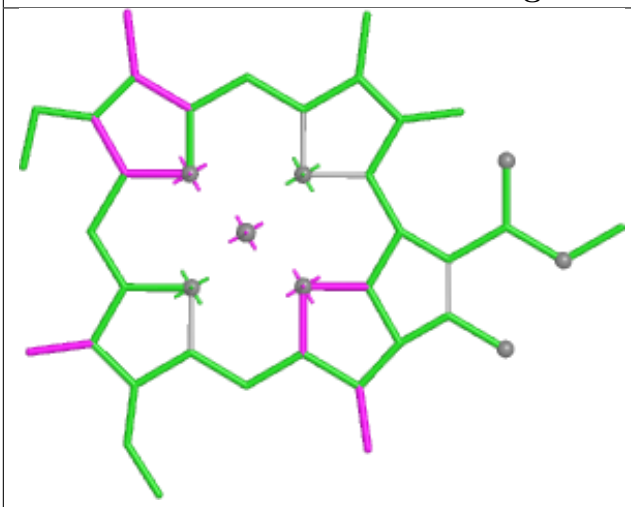


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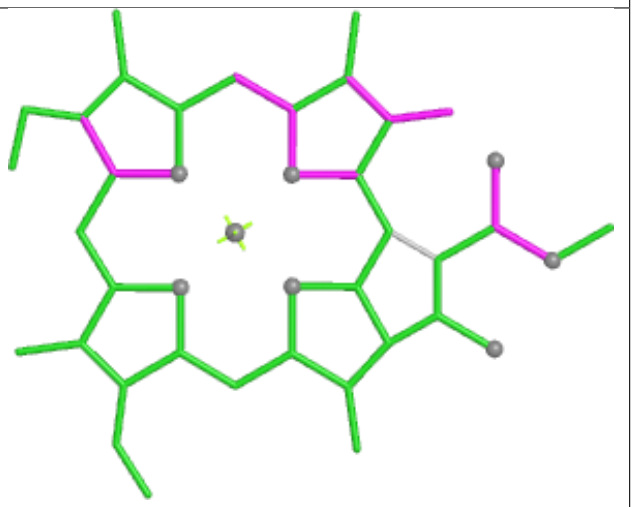


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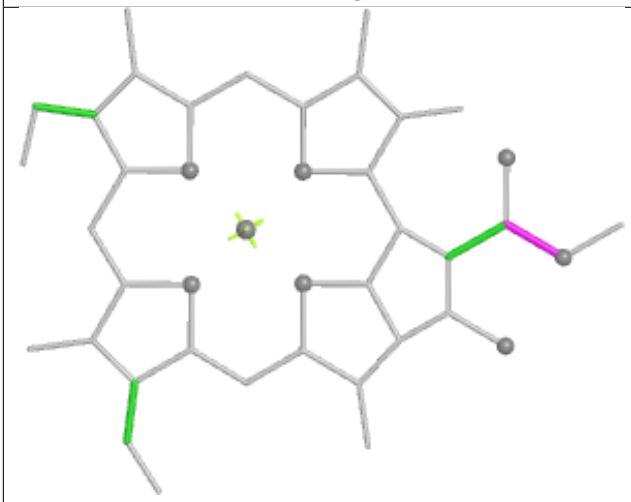
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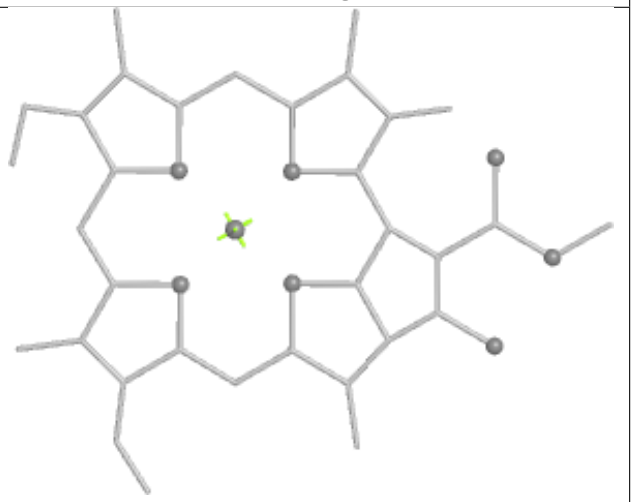
Bond lengths



Bond angles

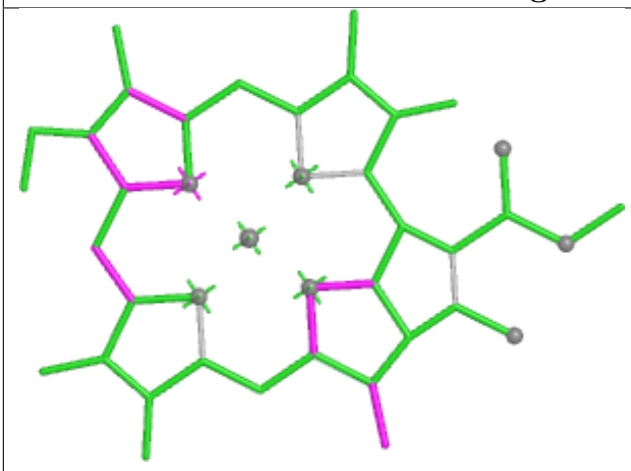


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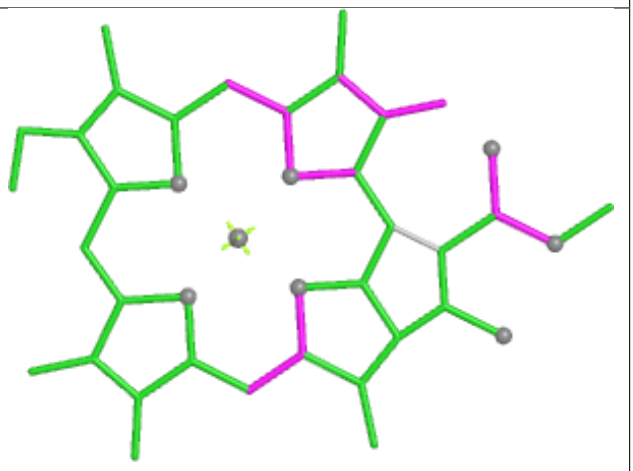


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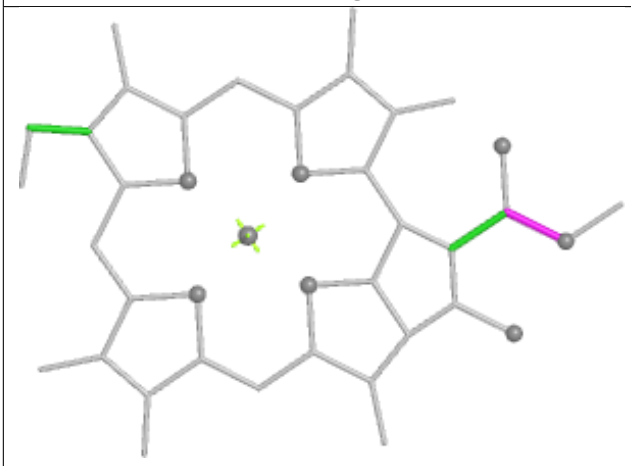
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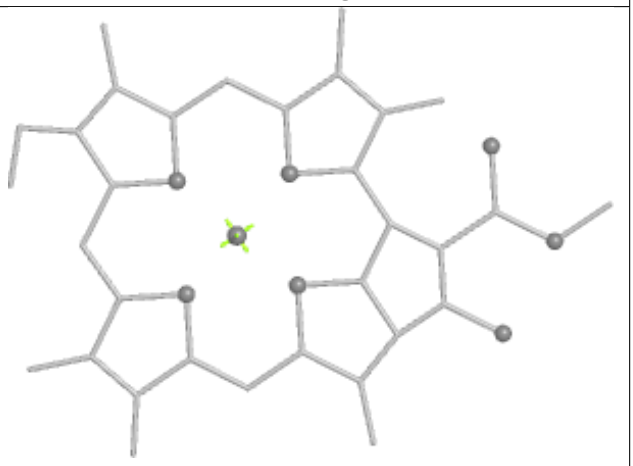
Bond lengths



Bond angles

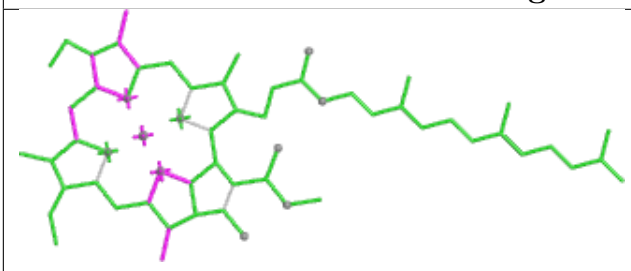


Torsions

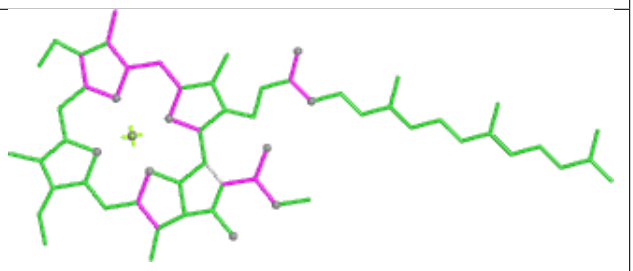


Rings

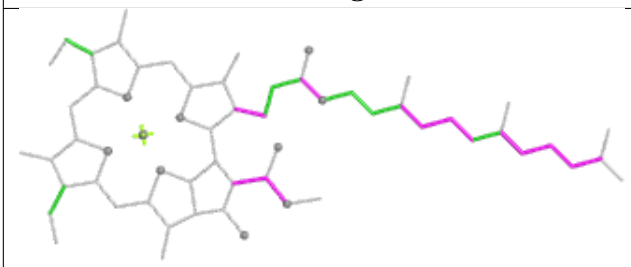
Ligand CLA 2 510



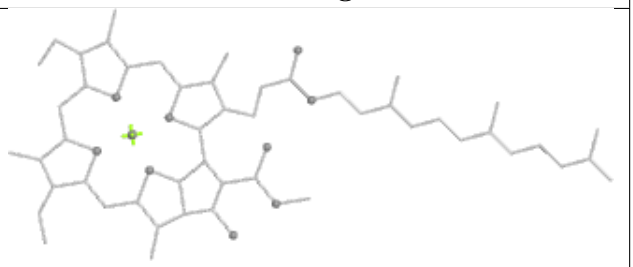
Bond lengths



Bond angles

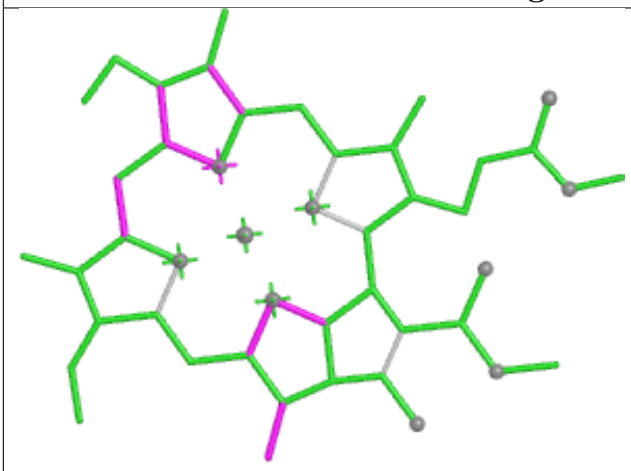


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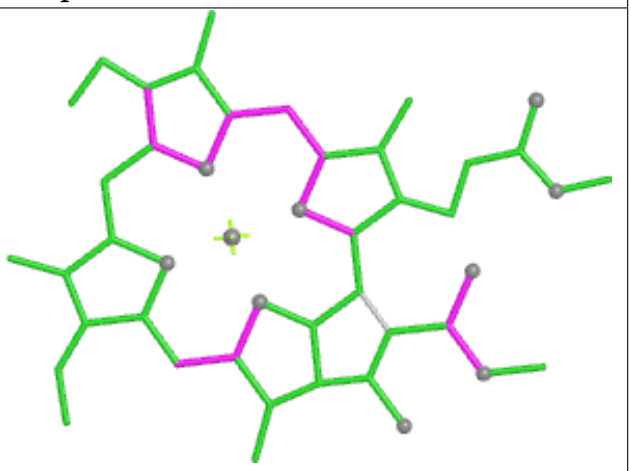


Rings

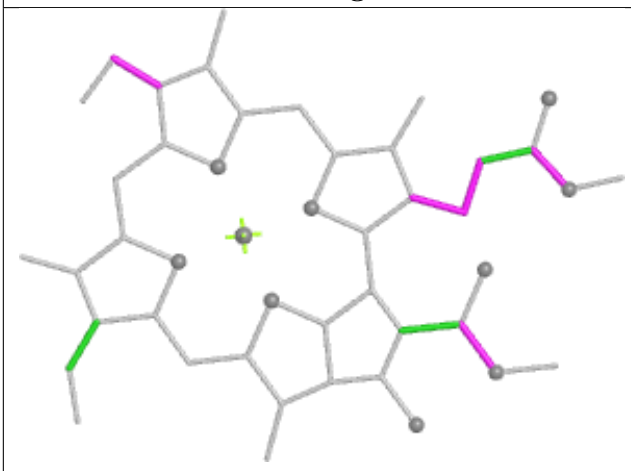
Ligand CLA q 316



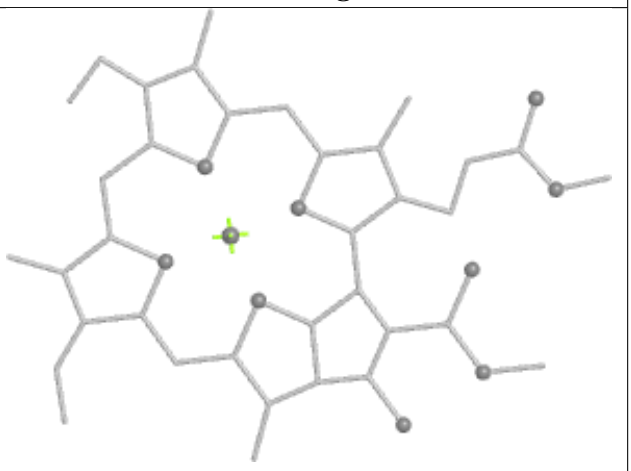
Bond lengths



Bond angles

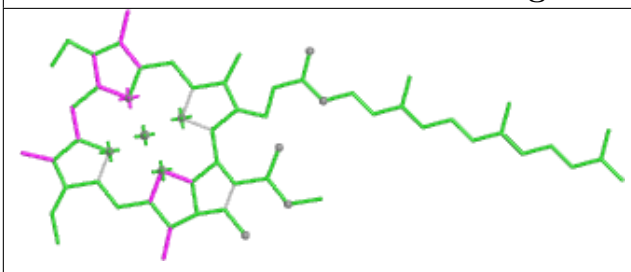


Torsions

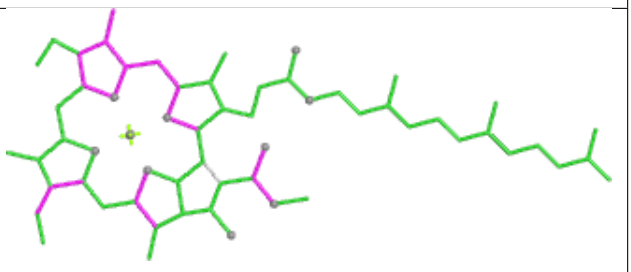


Rings

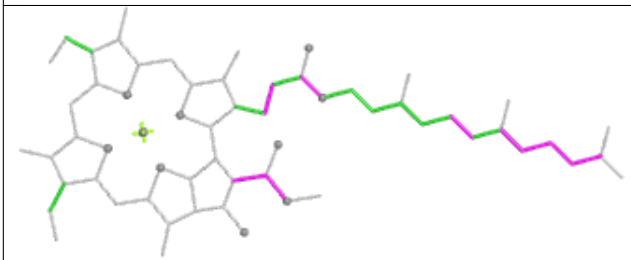
Ligand CLA 5 308



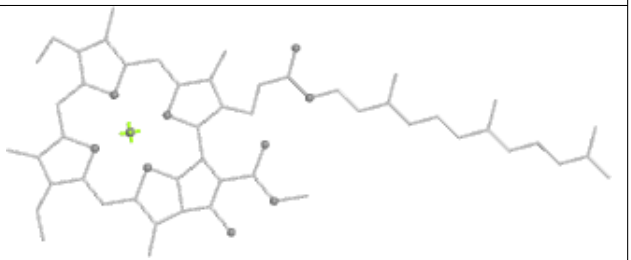
Bond lengths



Bond angles

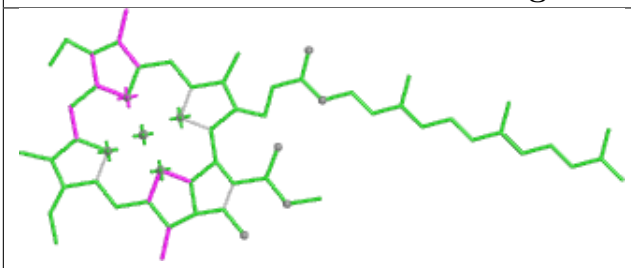


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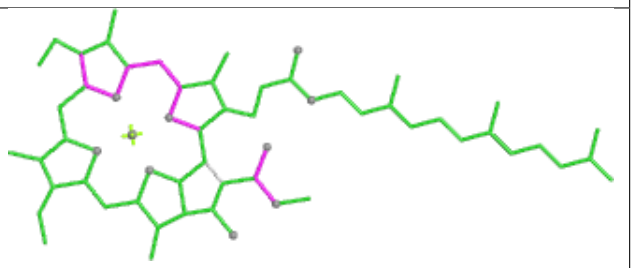


Rings

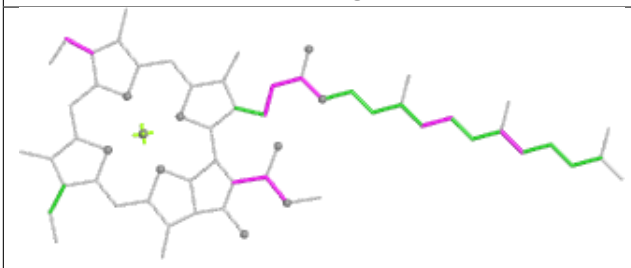
Ligand CLA e 816



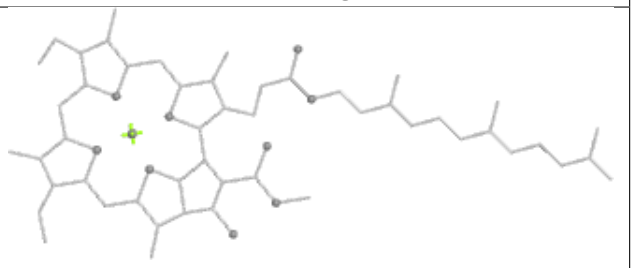
Bond lengths



Bond angles

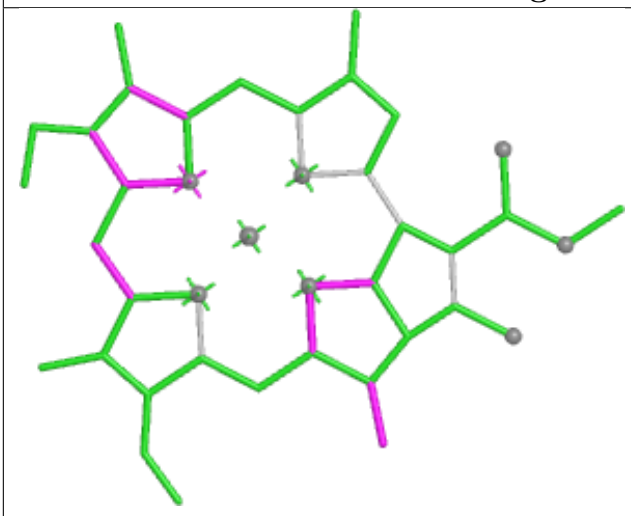


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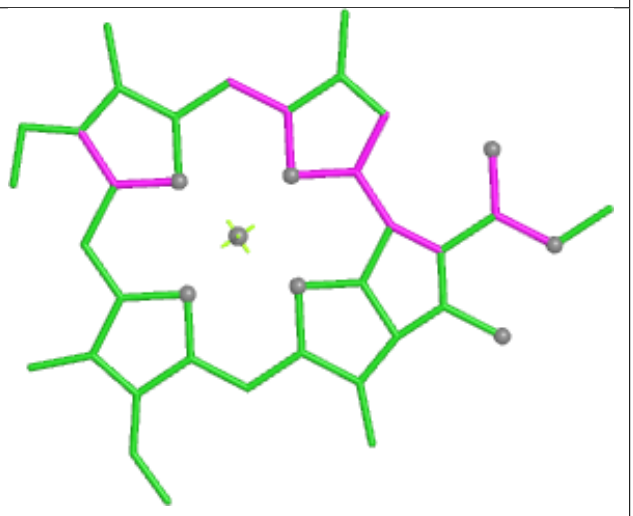


Rings

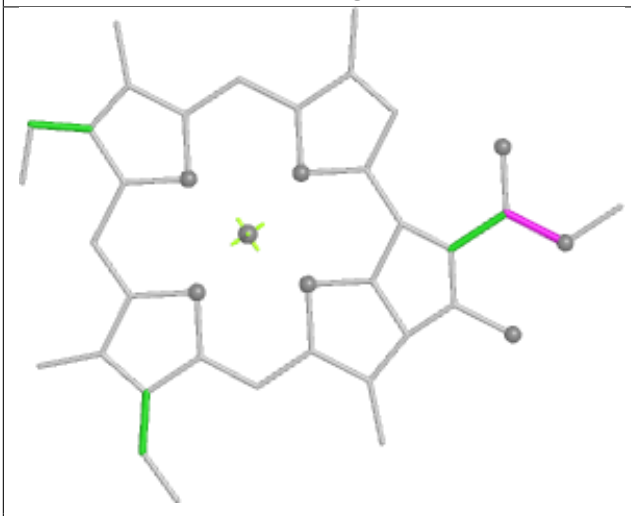
Ligand CLA s 514



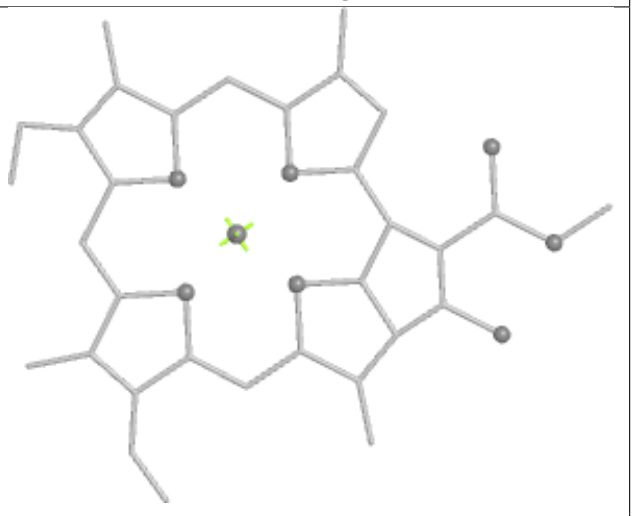
Bond lengths



Bond angles

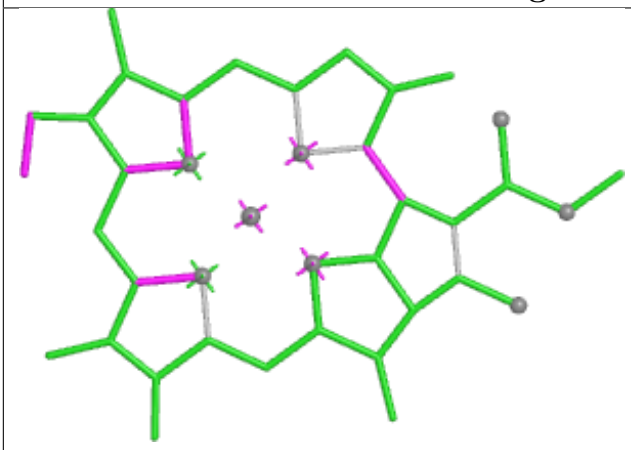


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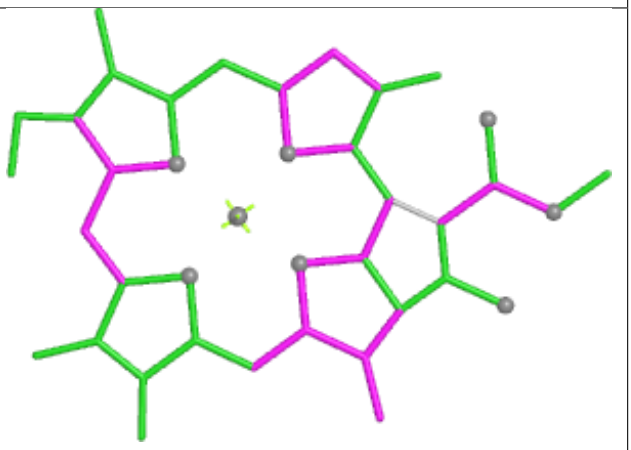


Rings

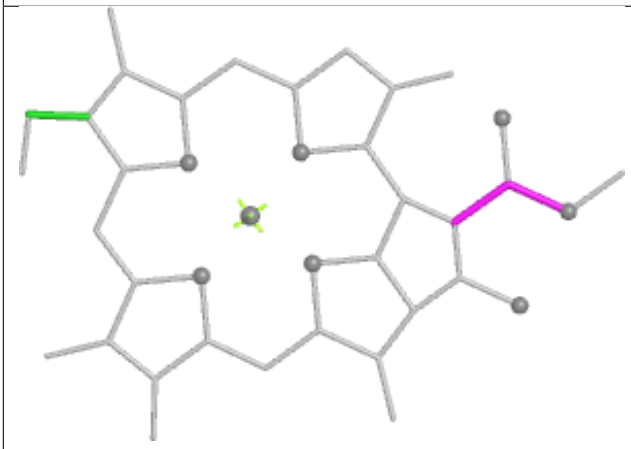
Ligand CLA e 818



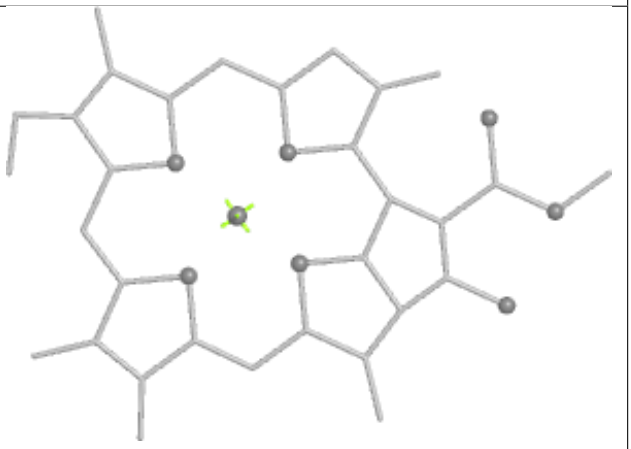
Bond lengths



Bond angles

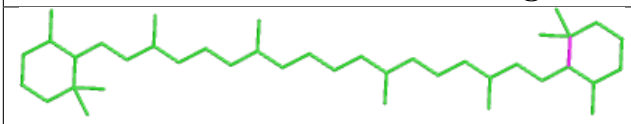


Torsions

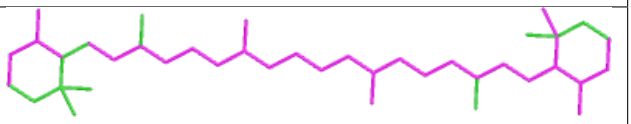


Rings

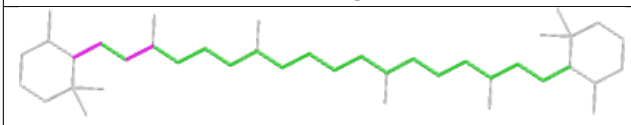
Ligand BCR B 844



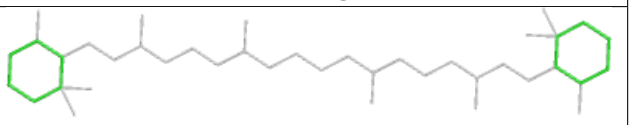
Bond lengths



Bond angles

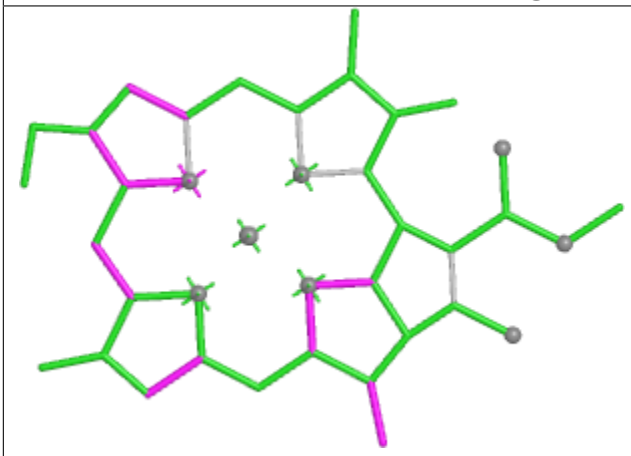


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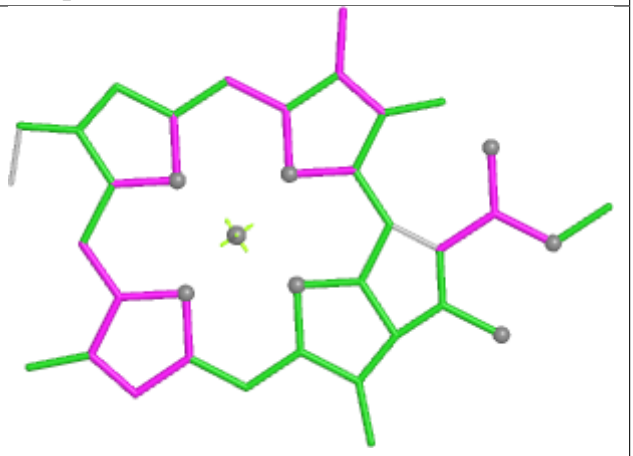


Rings

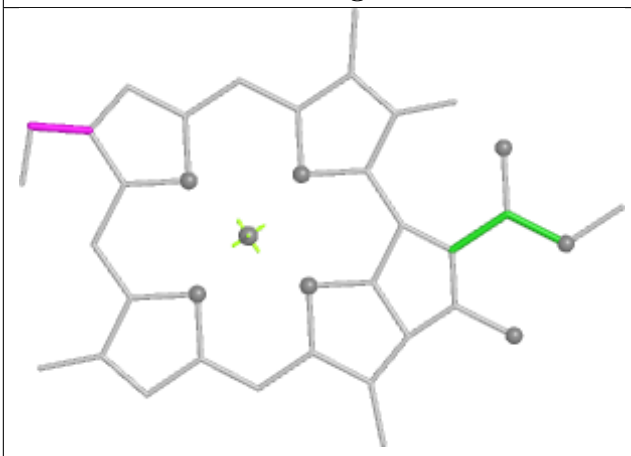
Ligand CLA q 304



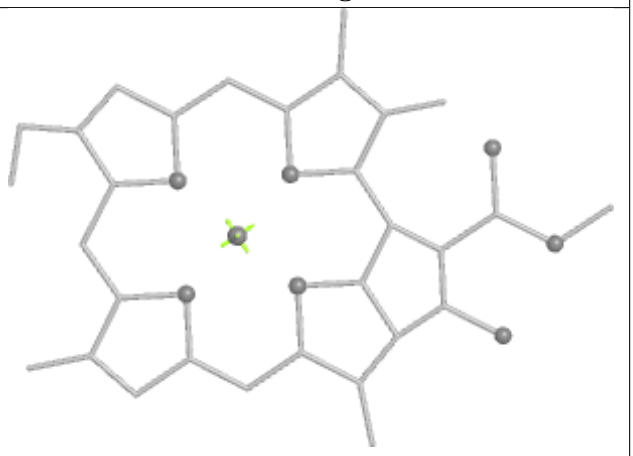
Bond lengths



Bond angles

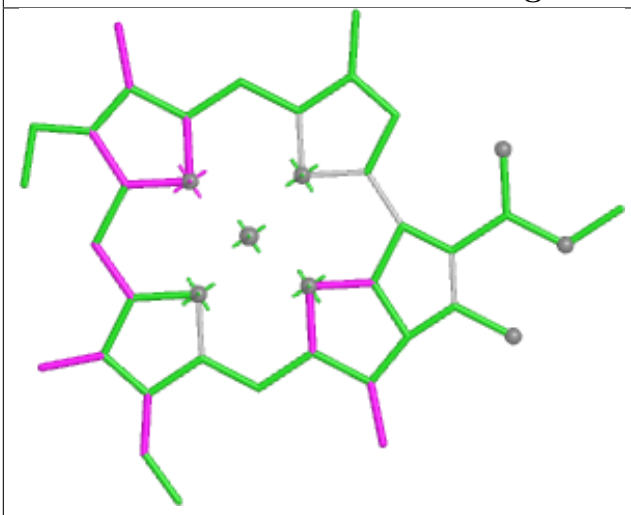


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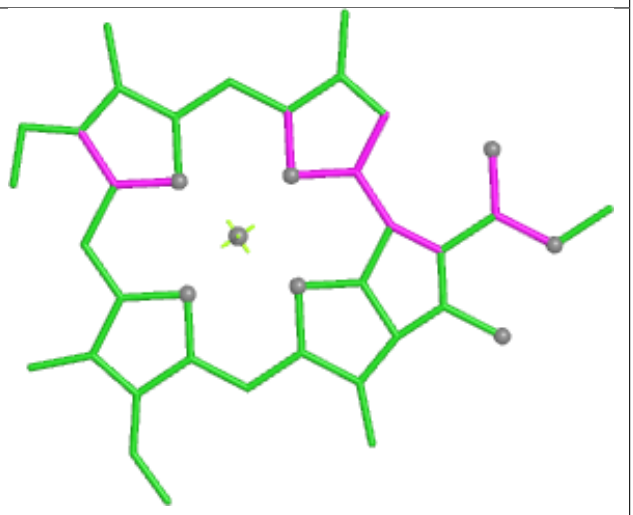


Rings

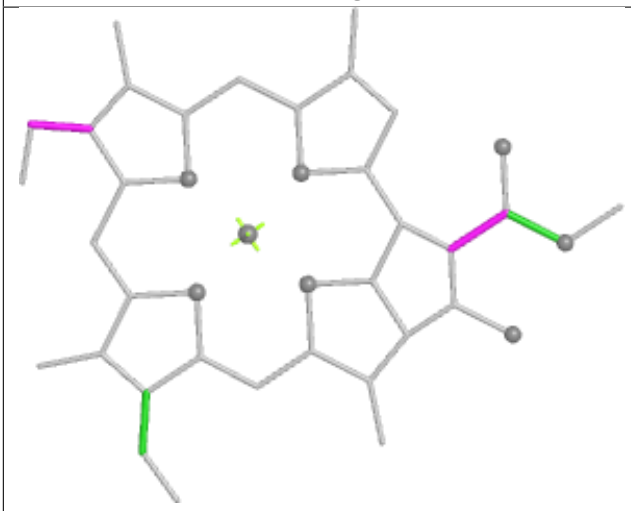
Ligand CLA B 809



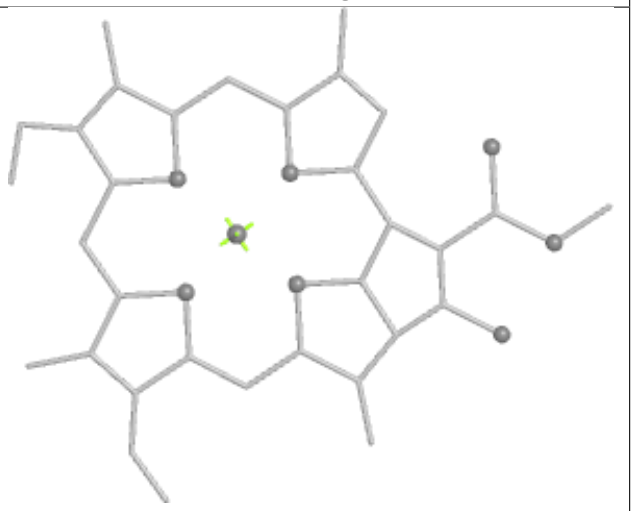
Bond lengths



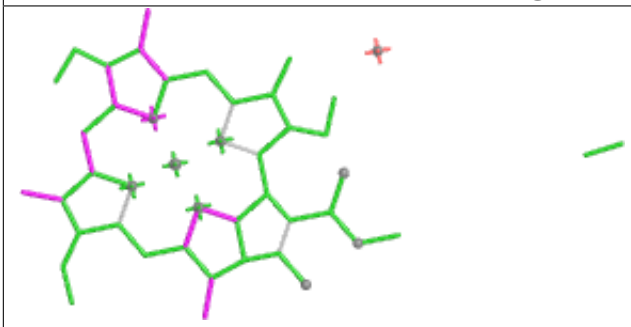
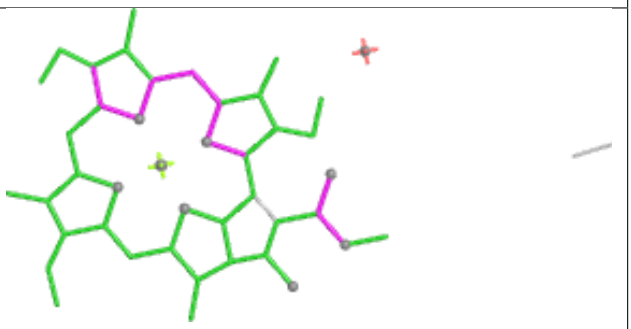
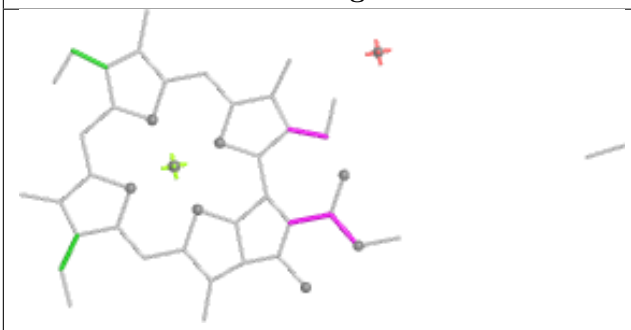
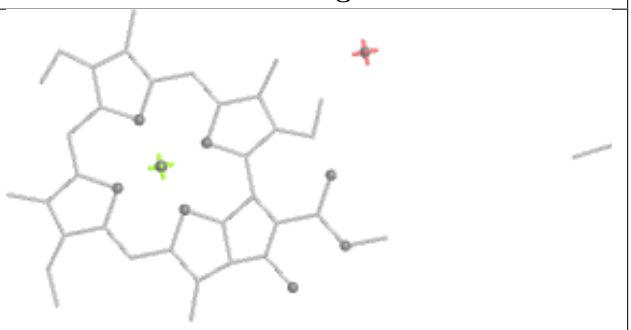
Bond angles

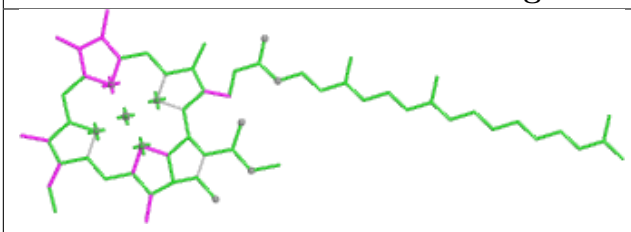
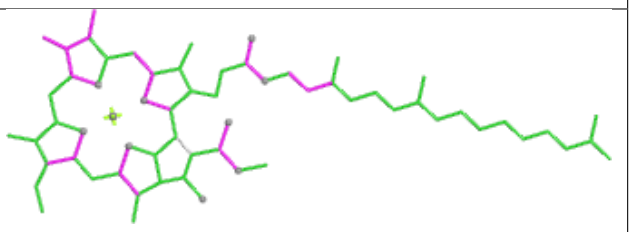
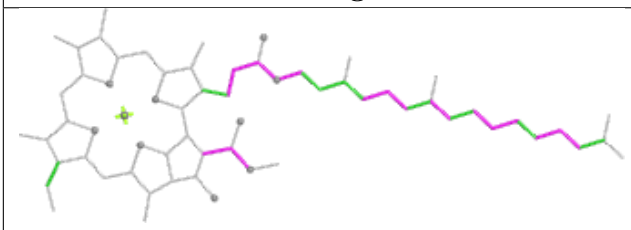
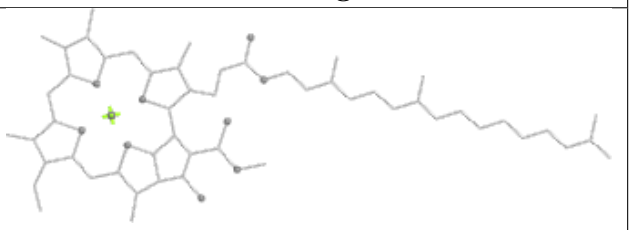


Torsions

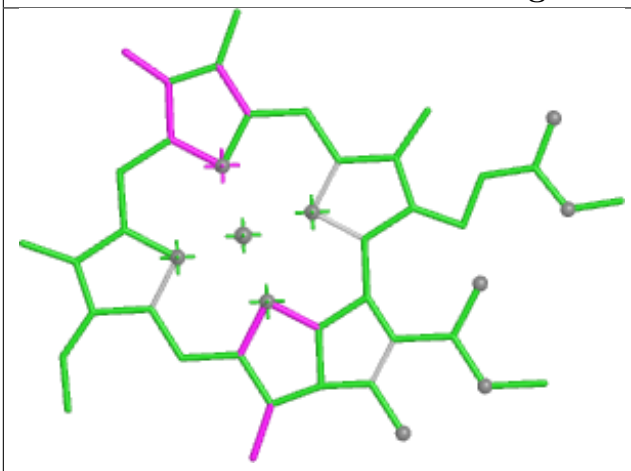


Rings

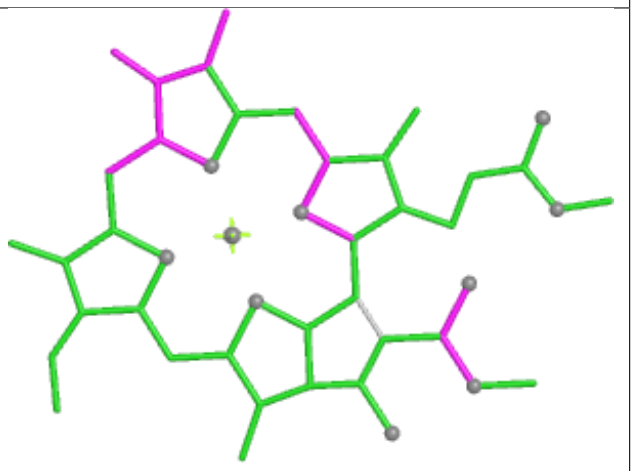
Ligand CLA e 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

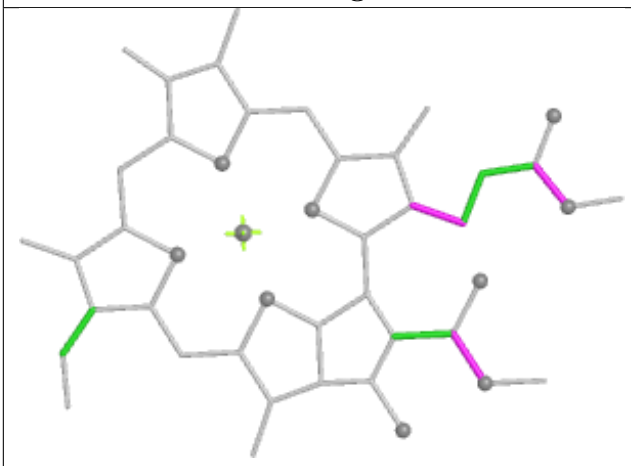
Ligand CLA 3 318



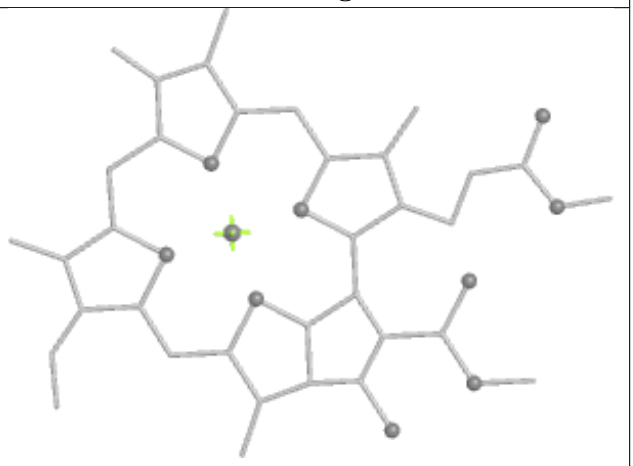
Bond lengths



Bond angles

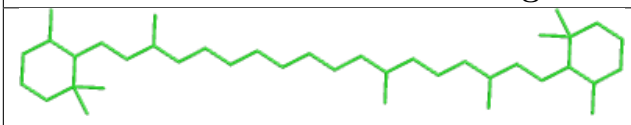


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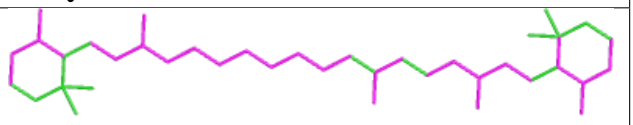


Rings

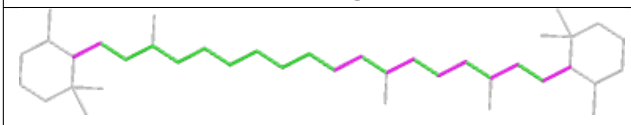
Ligand BCR Q 801



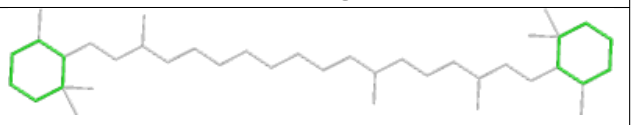
Bond lengths



Bond angles

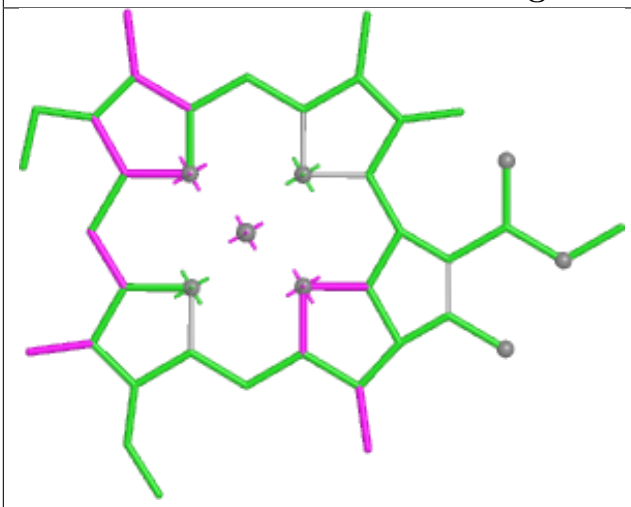


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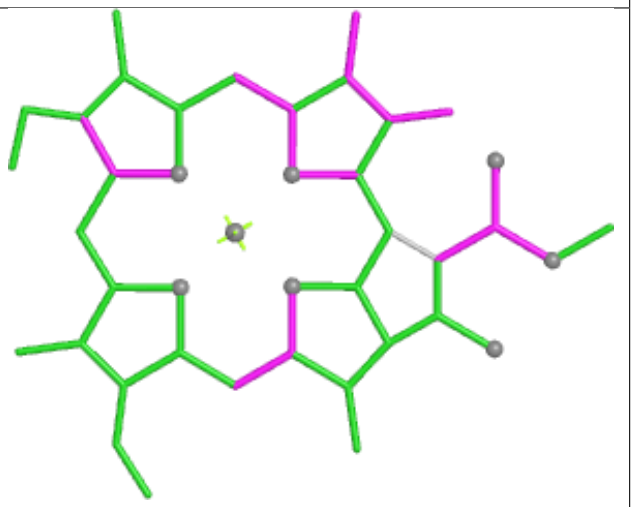


Rings

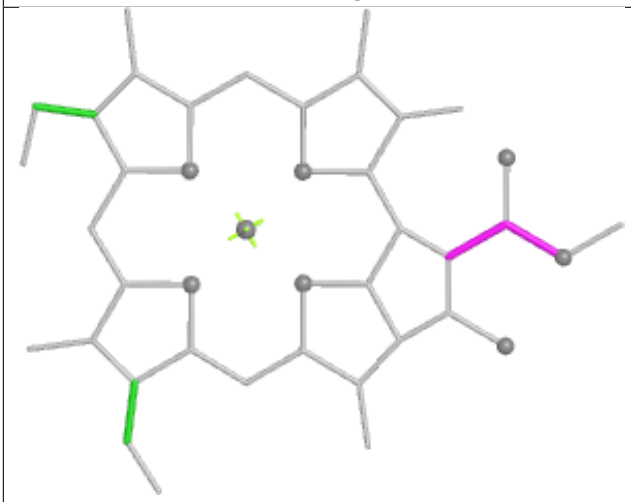
Ligand CLA 3 317



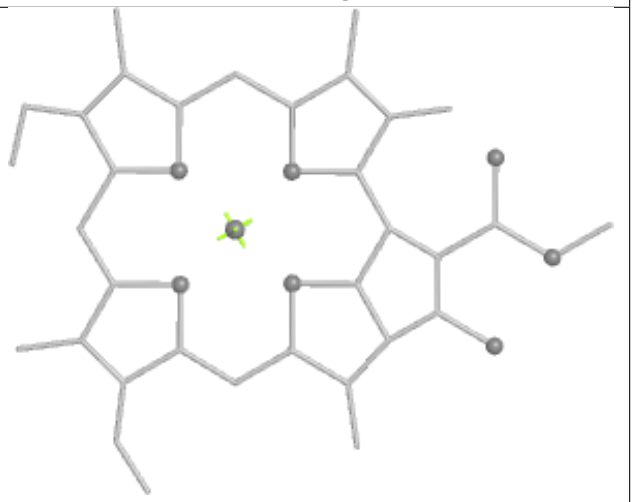
Bond lengths



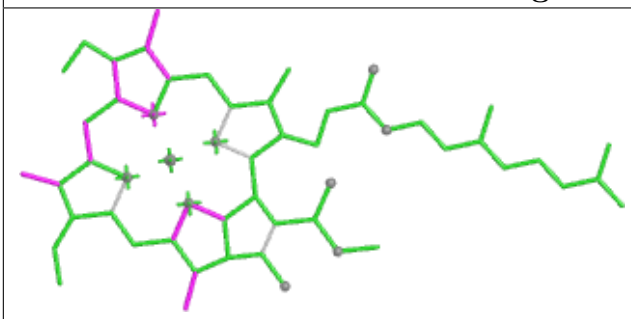
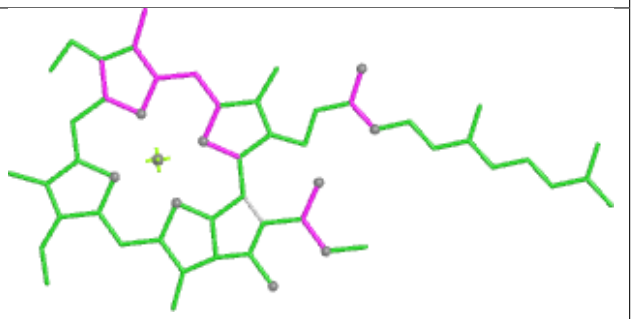
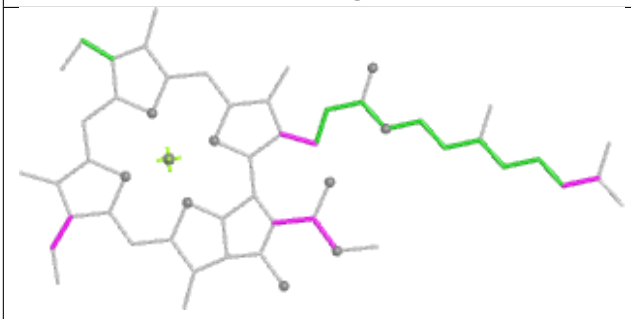
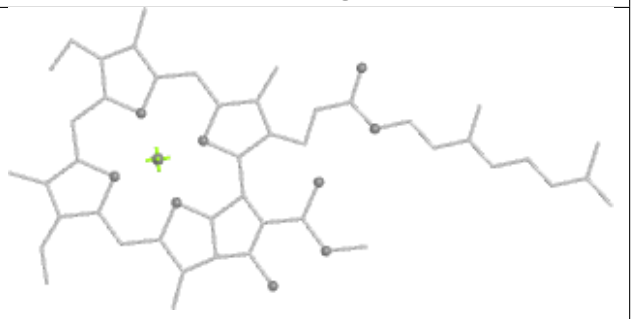
Bond angles



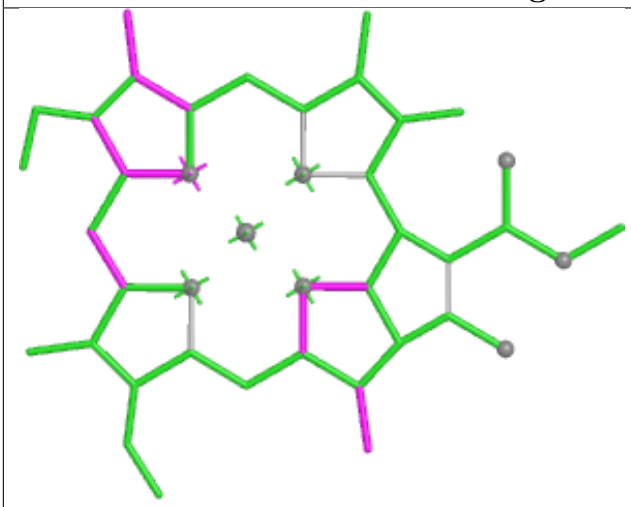
Torsions



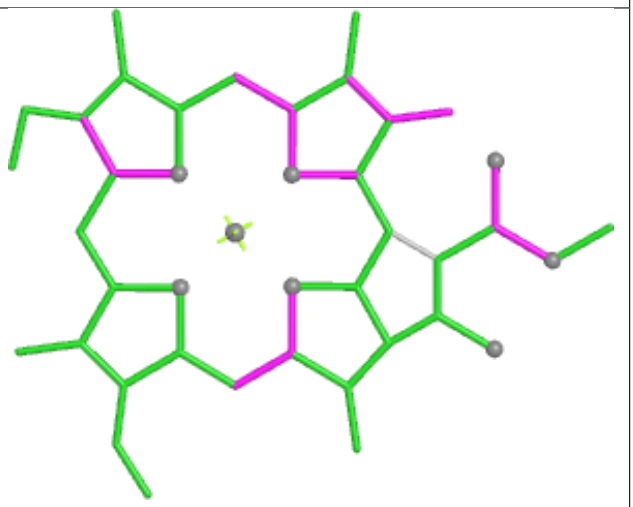
Rings

Ligand CLA f 821	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

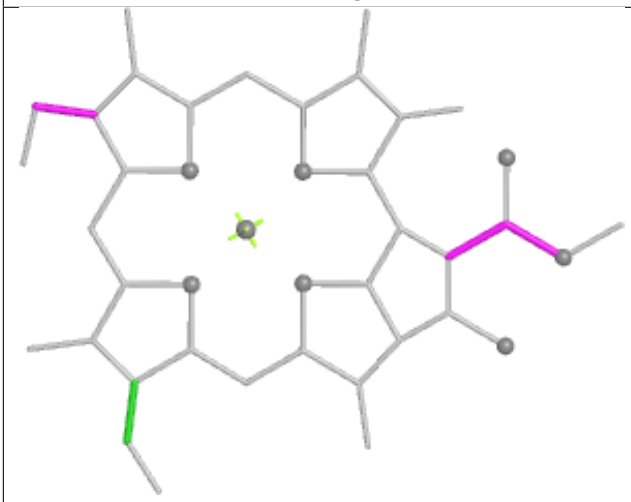
Ligand CLA e 808



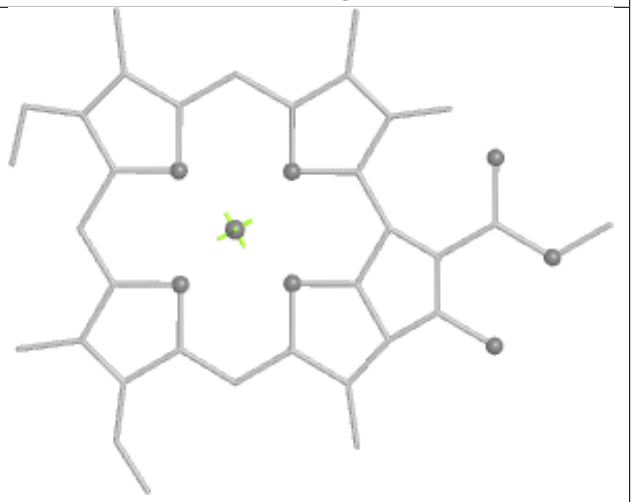
Bond lengths



Bond angles

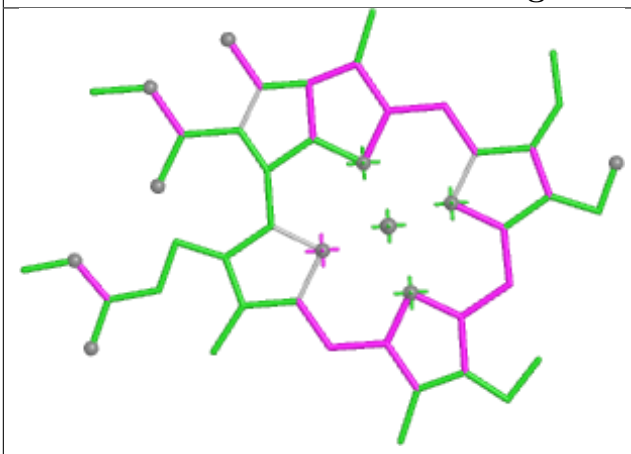


Torsions

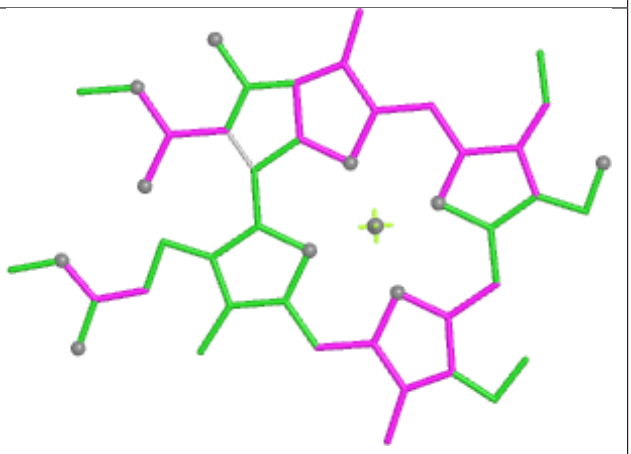


Rings

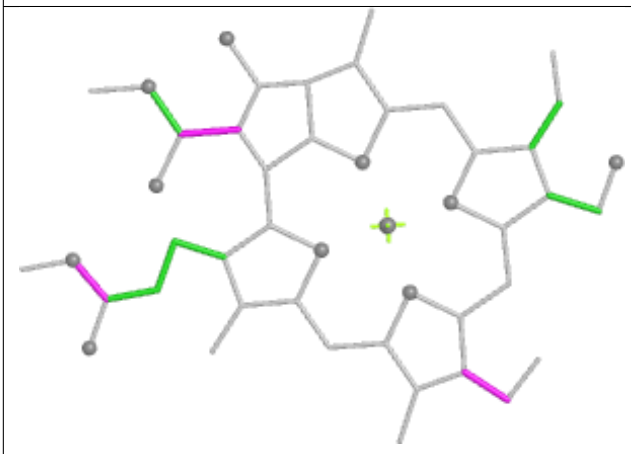
Ligand CHL 3 302



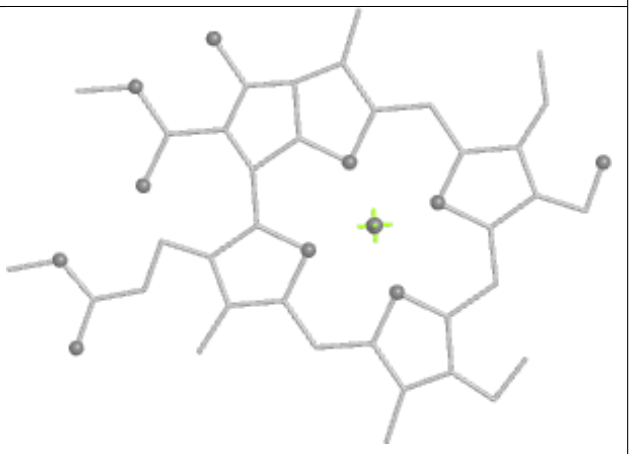
Bond lengths



Bond angles

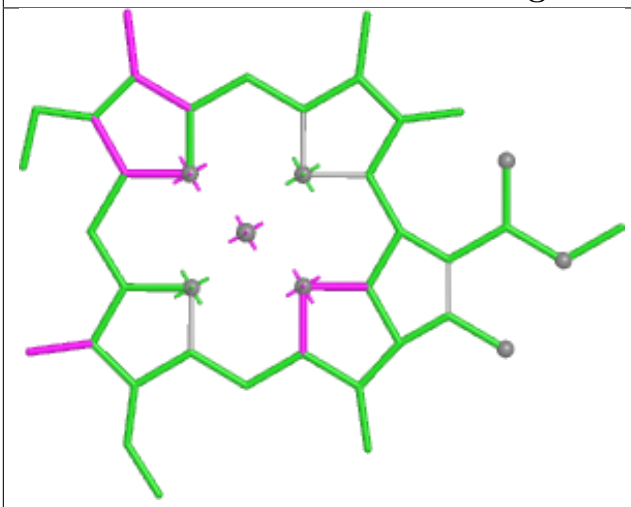


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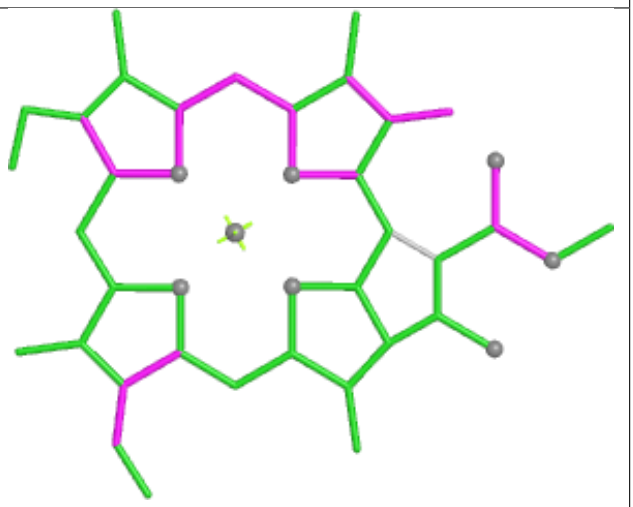


Rings

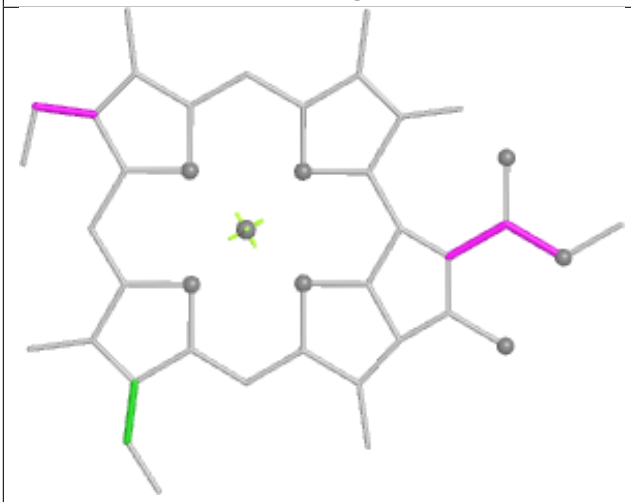
Ligand CLA 3 312



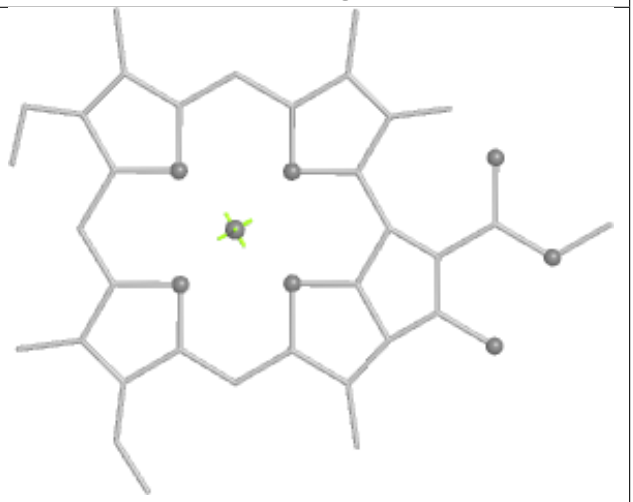
Bond lengths



Bond angles

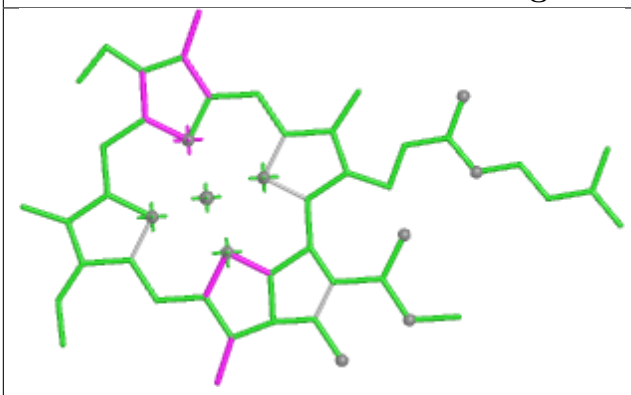


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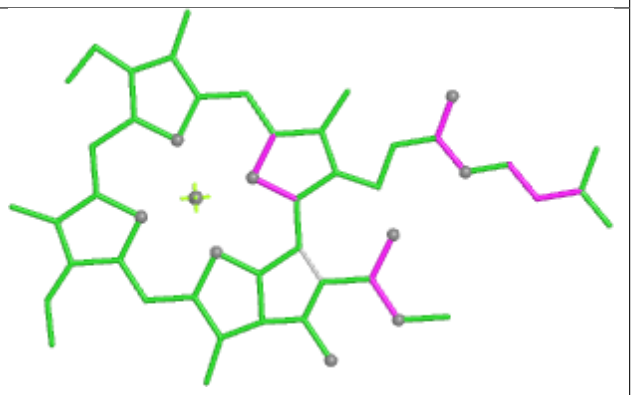


Rings

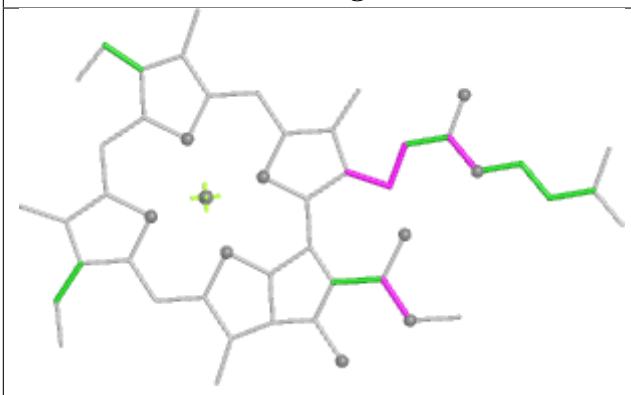
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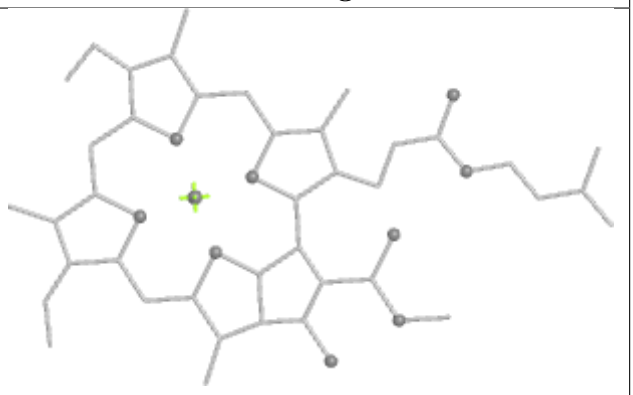
Bond lengths



Bond angles

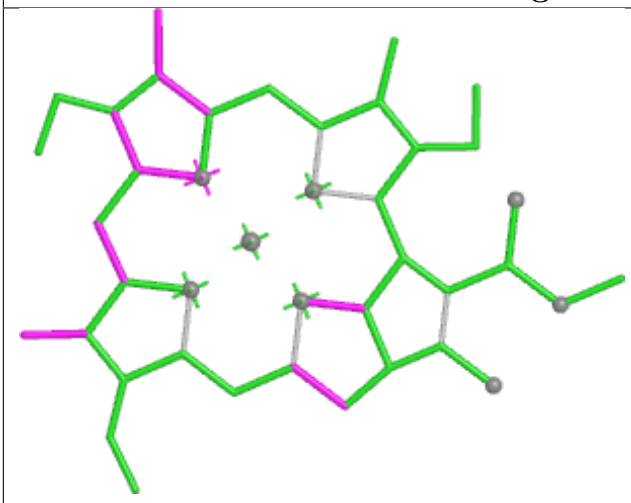


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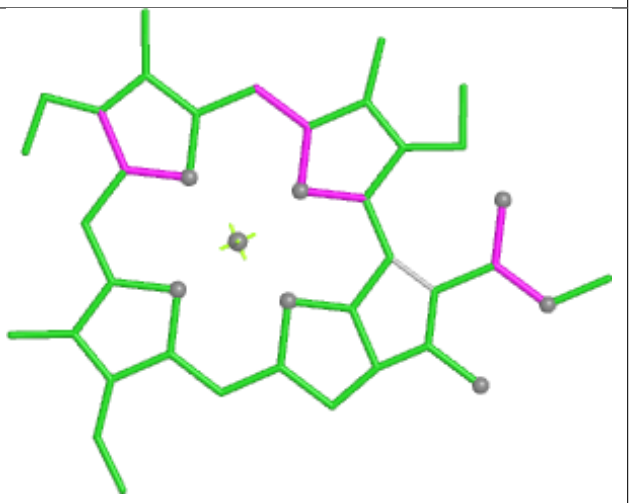


Rings

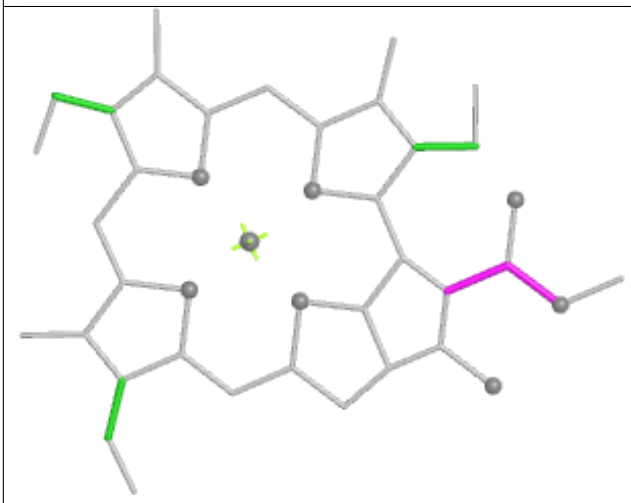
Ligand CLA f 803



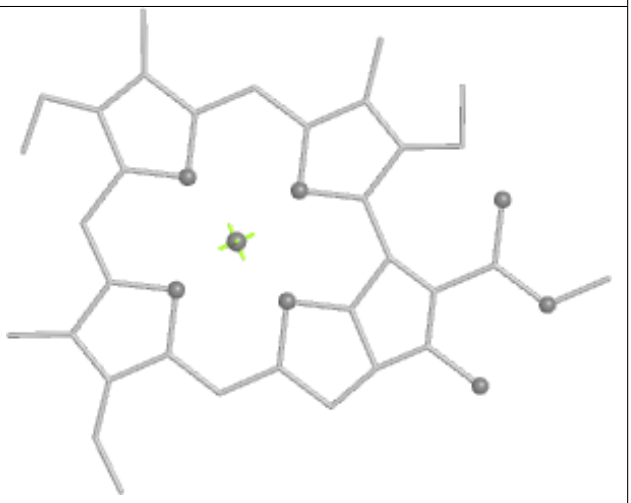
Bond lengths



Bond angles

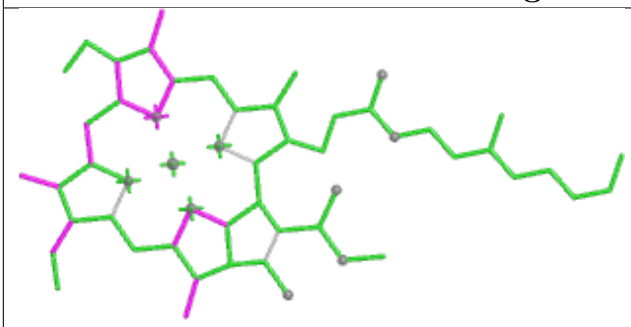


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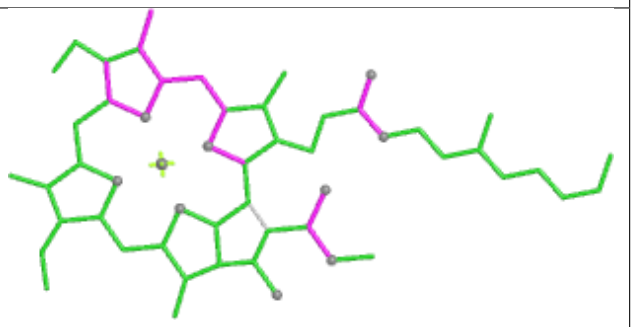


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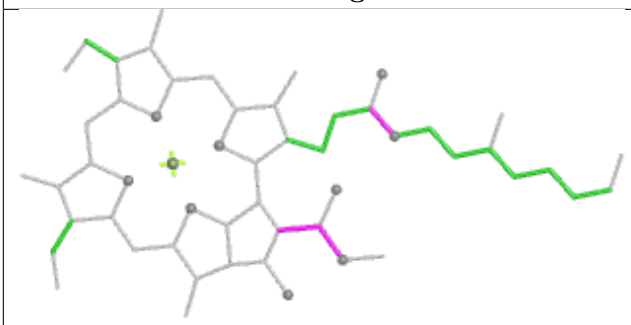
Ligand CLA A 810



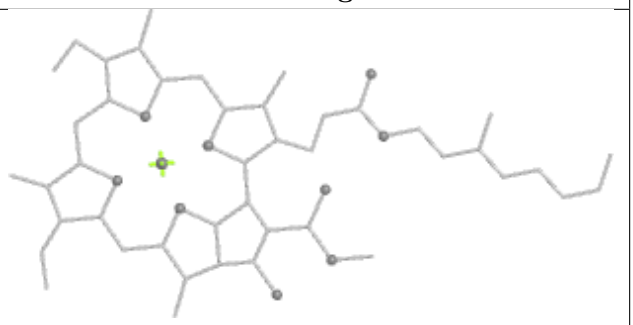
Bond lengths



Bond angles



Torsions

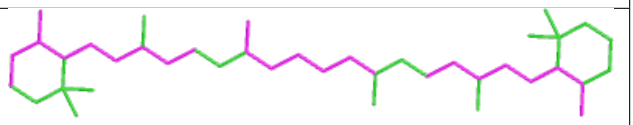


Rings

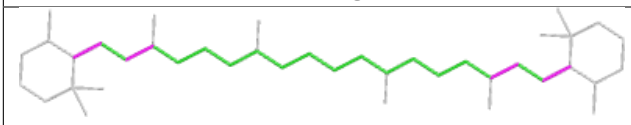
Ligand BCR 3 305



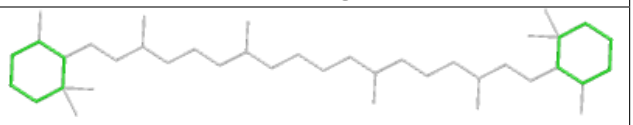
Bond lengths



Bond angles

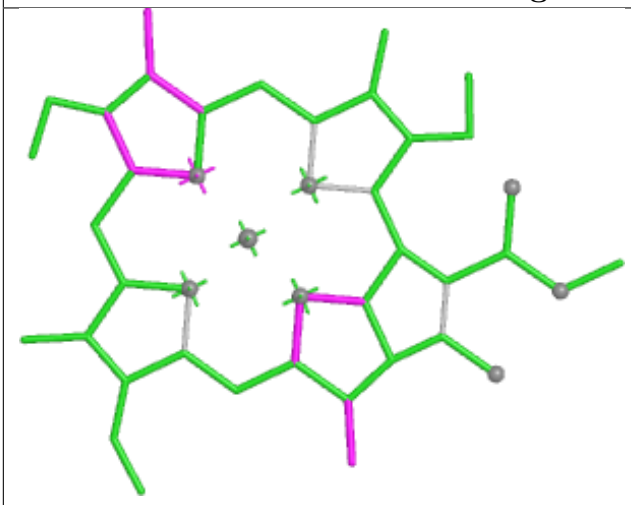


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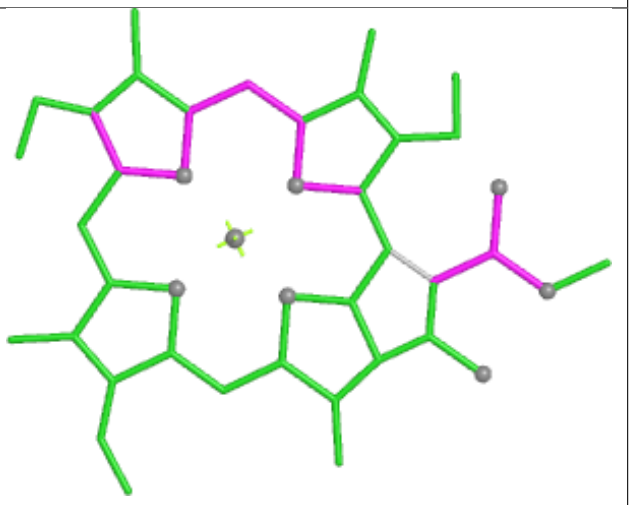


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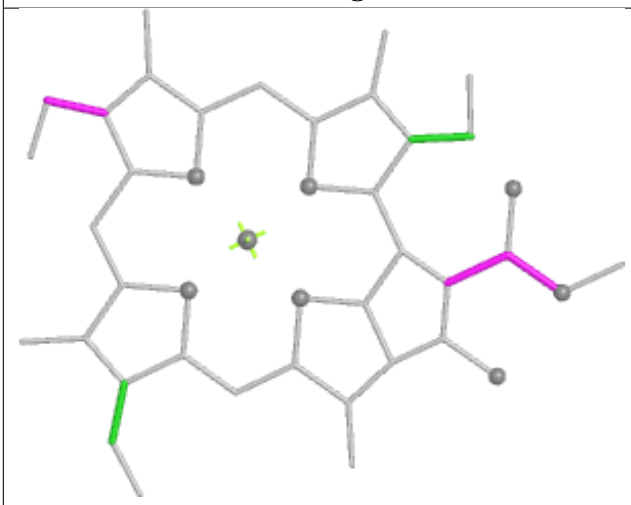
Ligand CLA r 310



Bond lengths



Bond angles

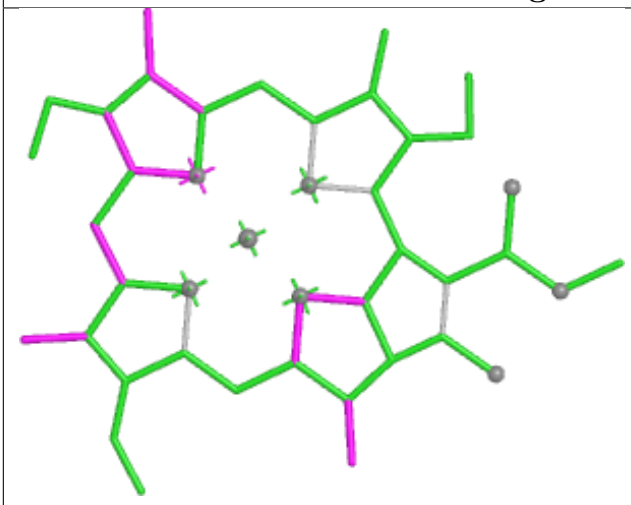


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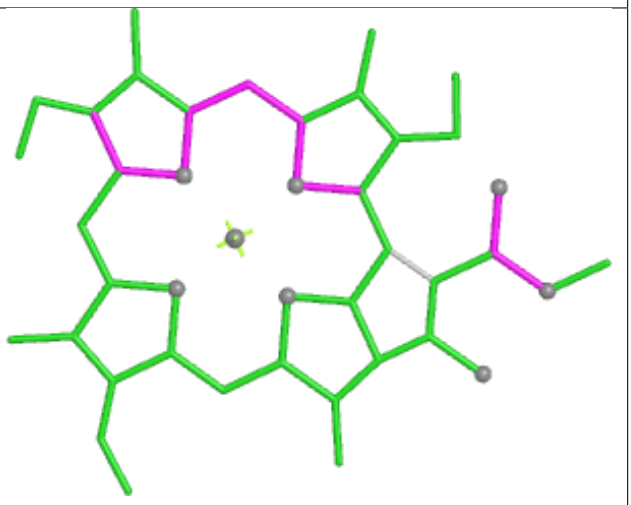


Rings

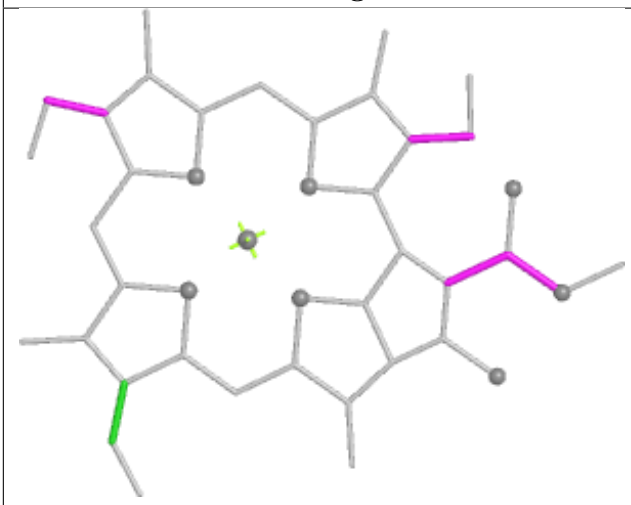
Ligand CLA e 814



Bond lengths



Bond angles

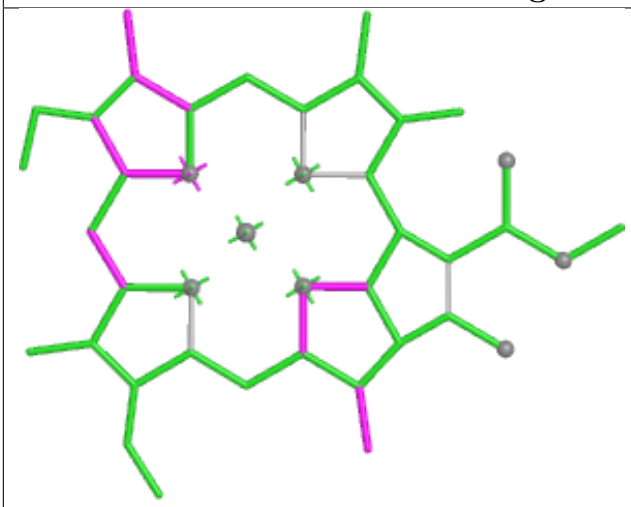


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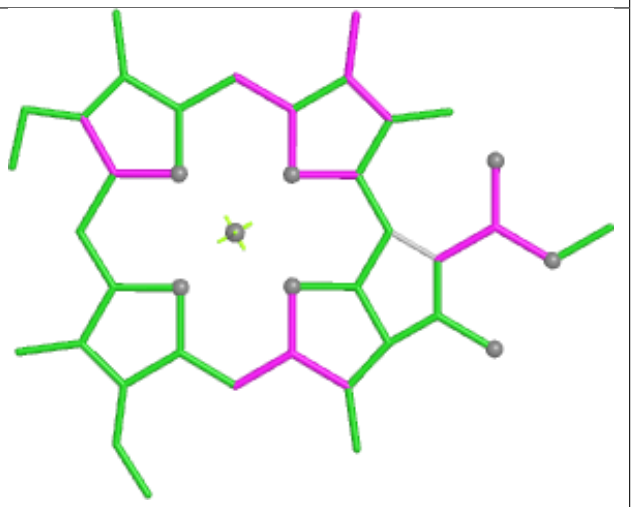


Rings

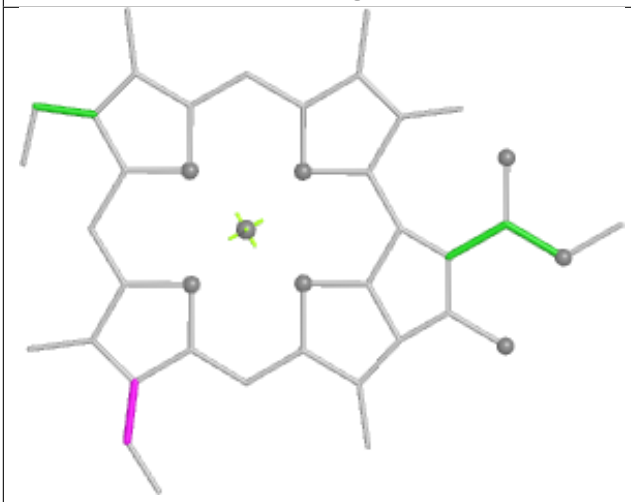
Ligand CLA e 827



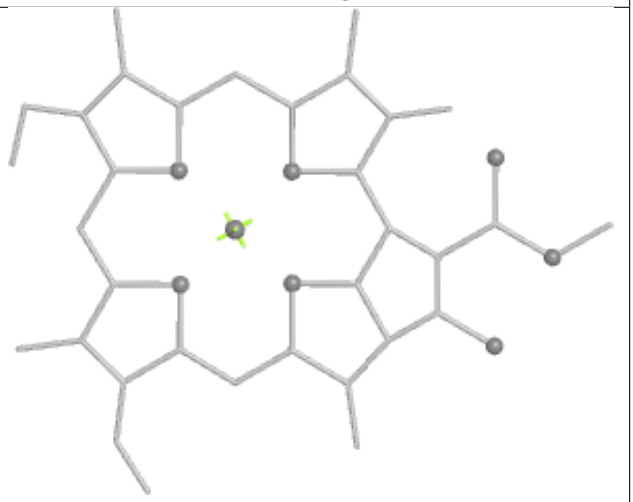
Bond lengths



Bond angles

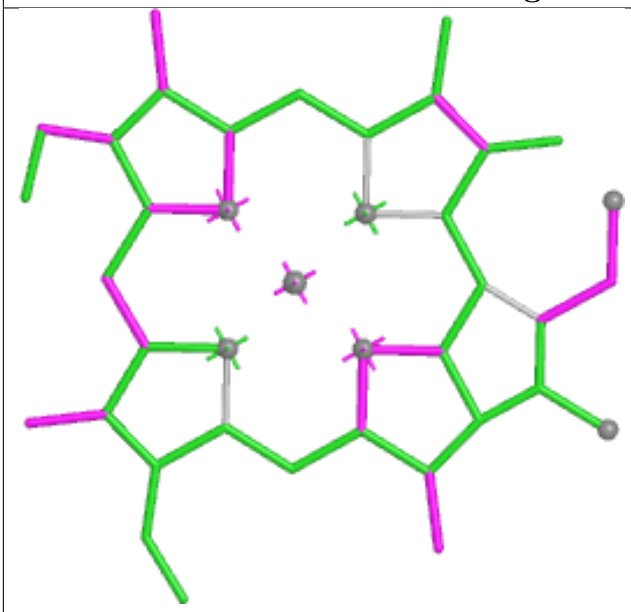


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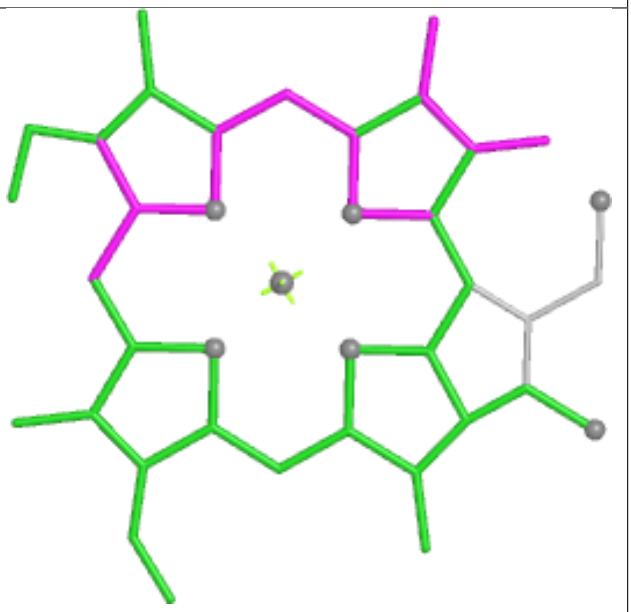


Rings

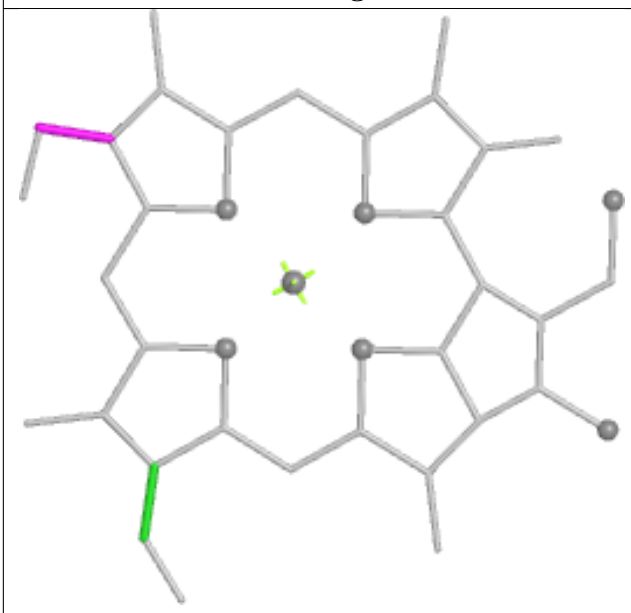
Ligand CLA A 817



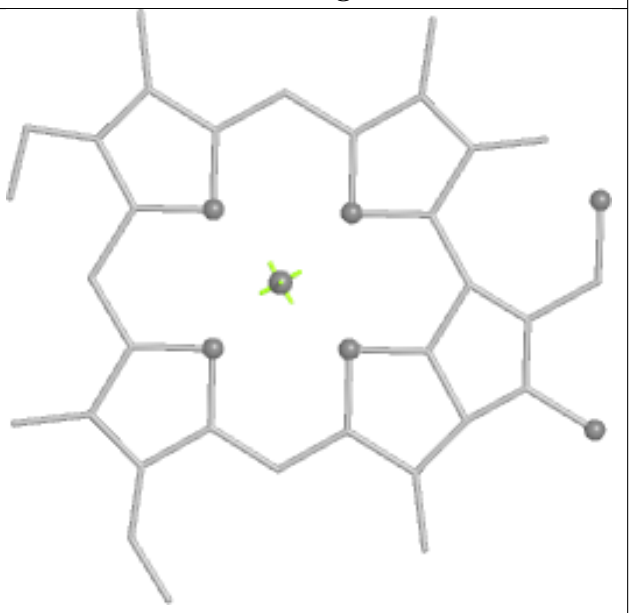
Bond lengths



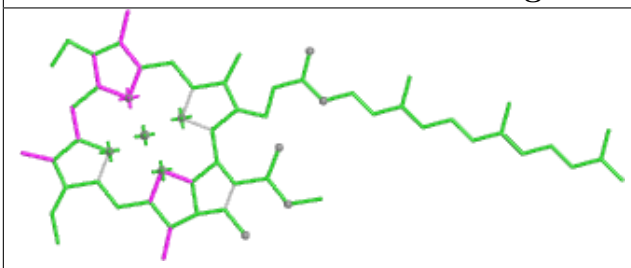
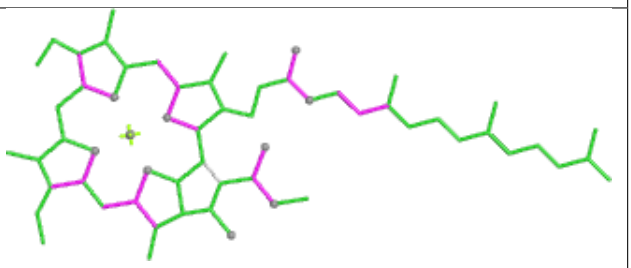
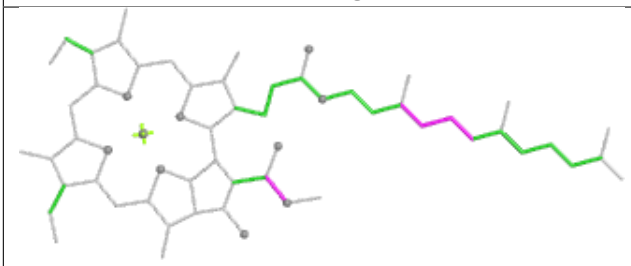
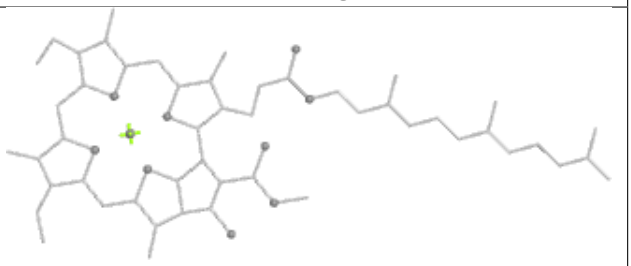
Bond angles

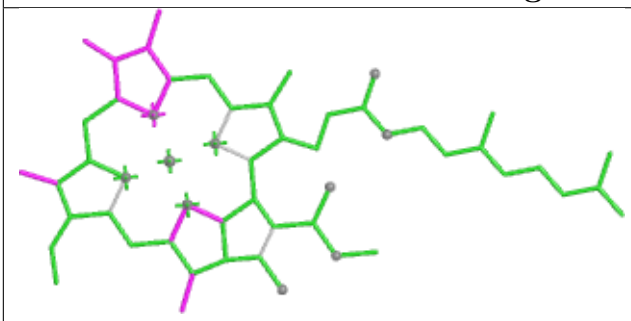
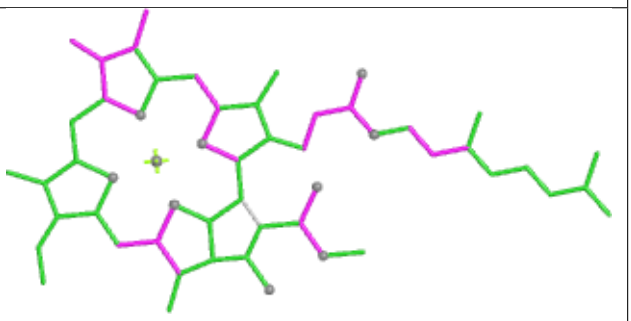
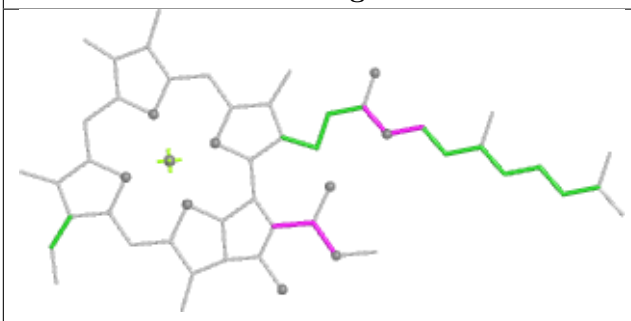
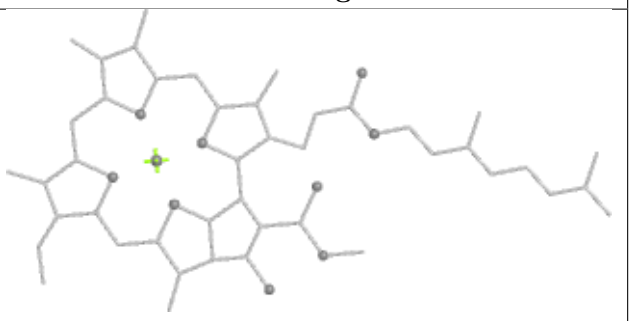


Torsions

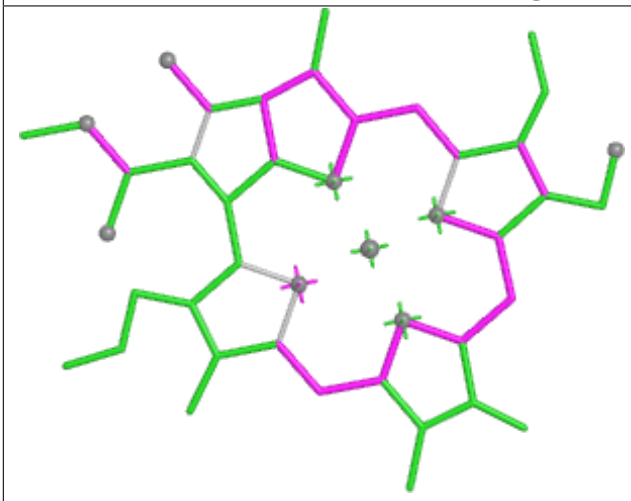


Rings

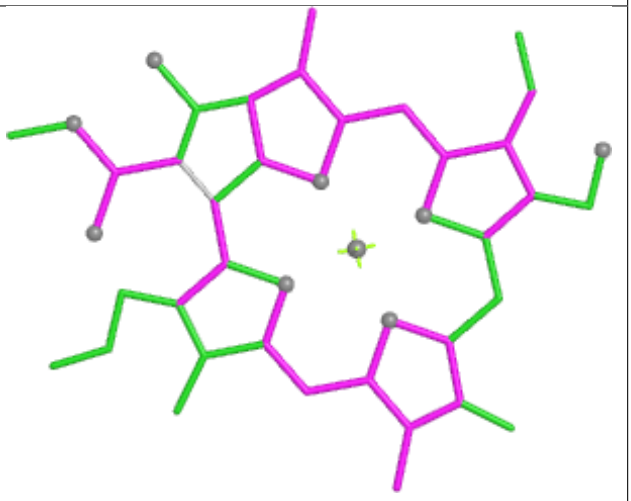
Ligand CLA B 835	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 812	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

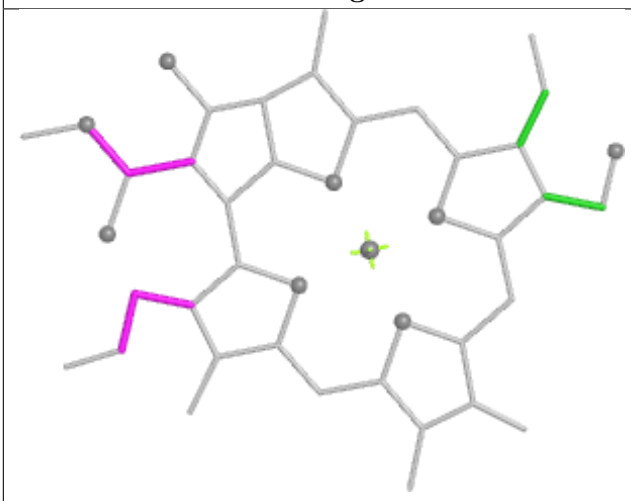
Ligand CHL 2 516



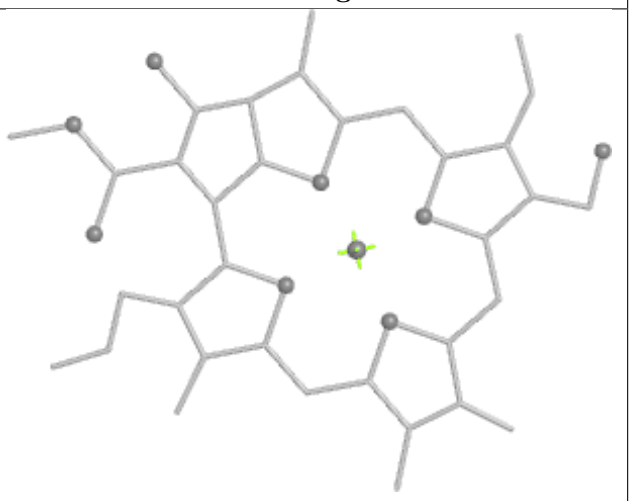
Bond lengths



Bond angles

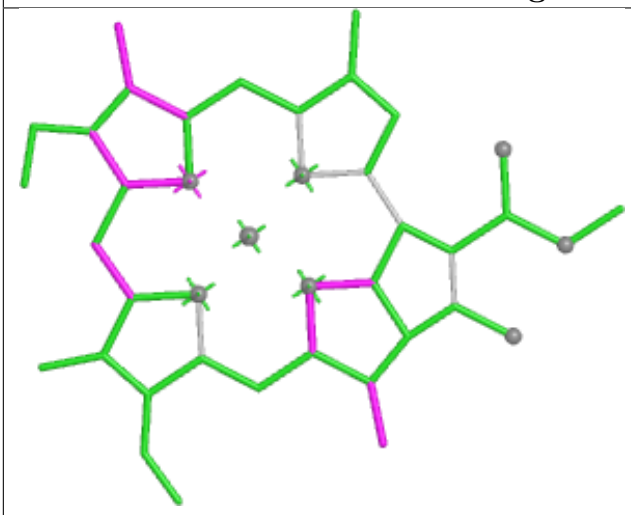


Torsions

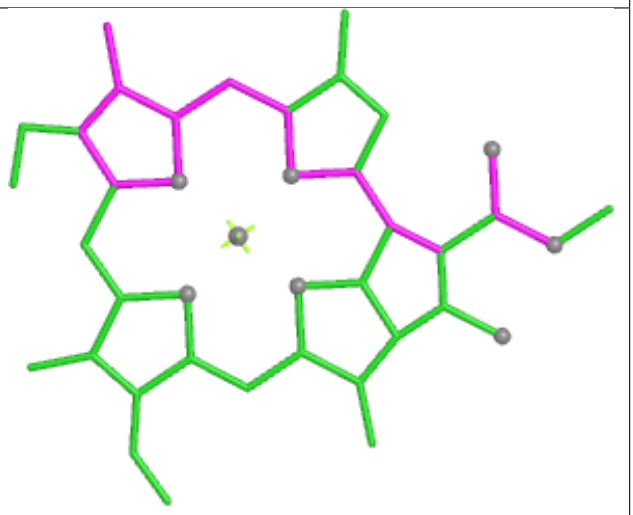


Rings

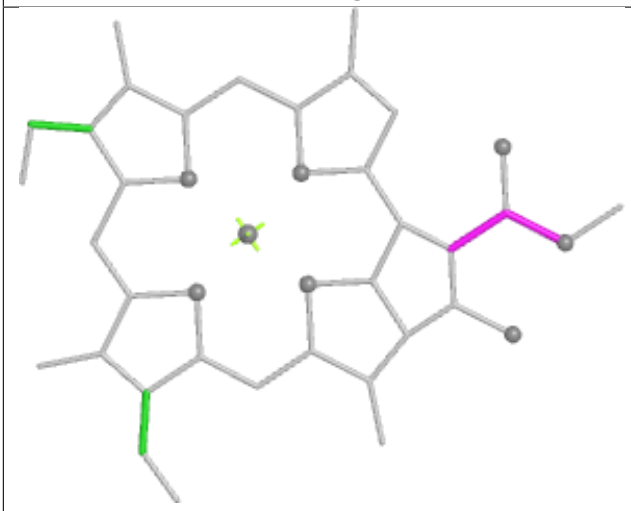
Ligand CLA 1 508



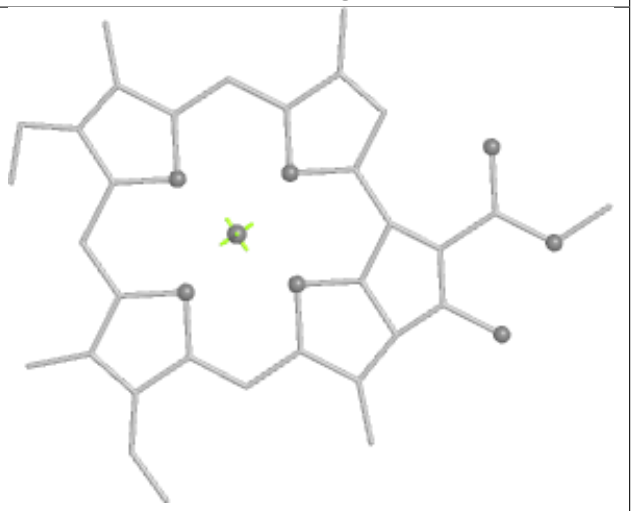
Bond lengths



Bond angles

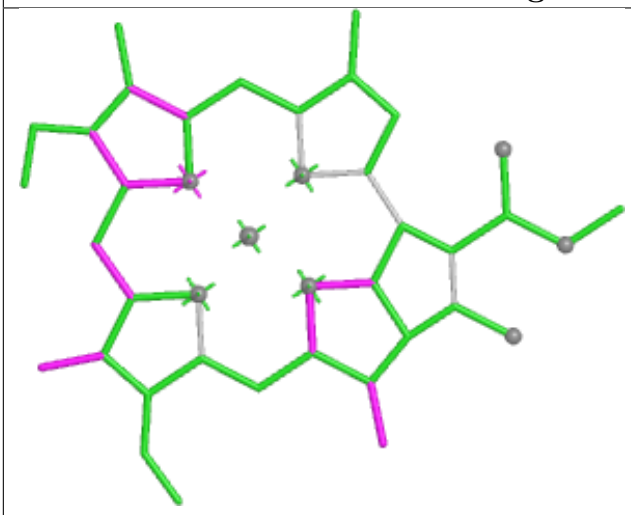


Torsions

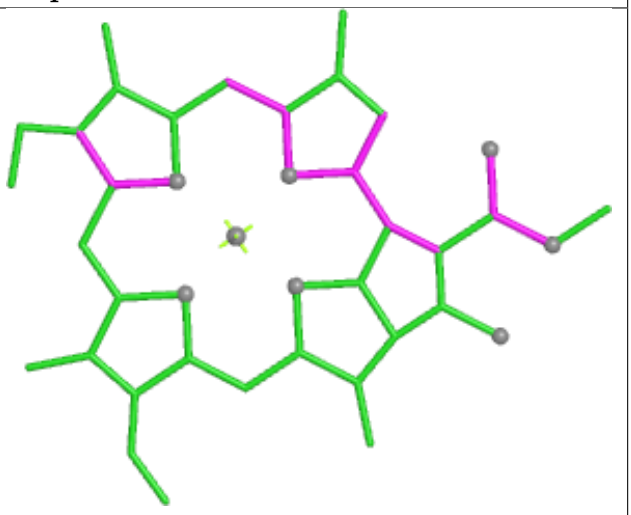


Rings

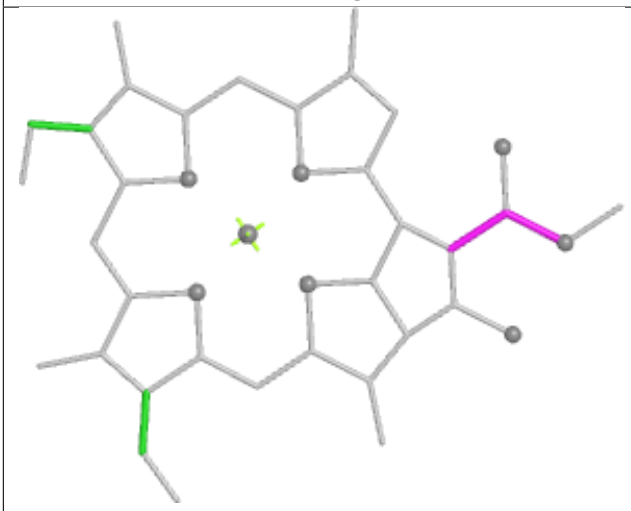
Ligand CLA p 515



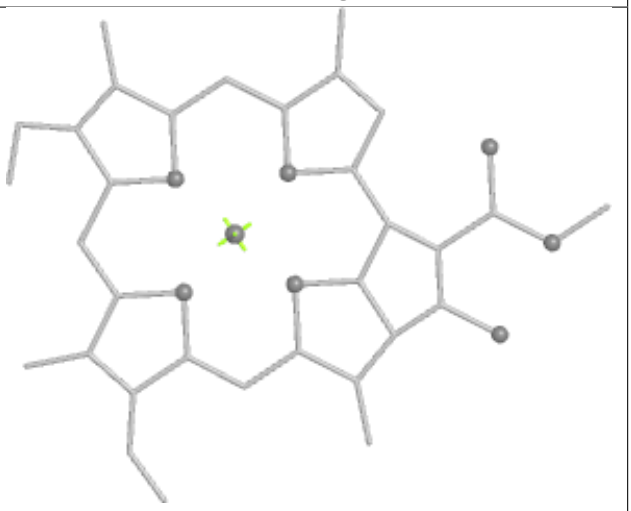
Bond lengths



Bond angles

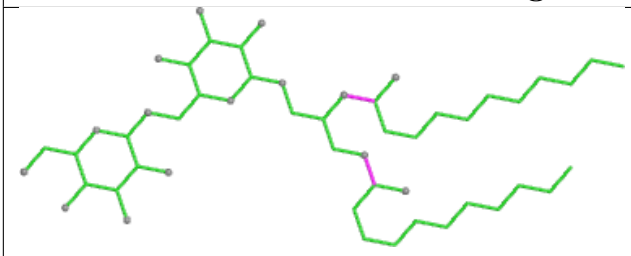


Torsions

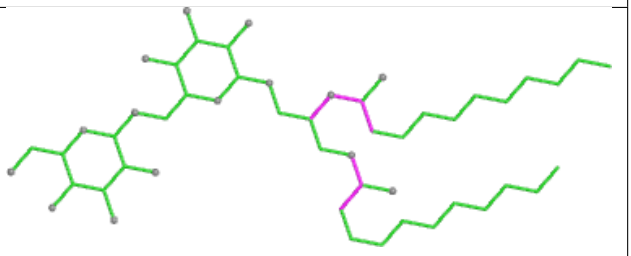


Rings

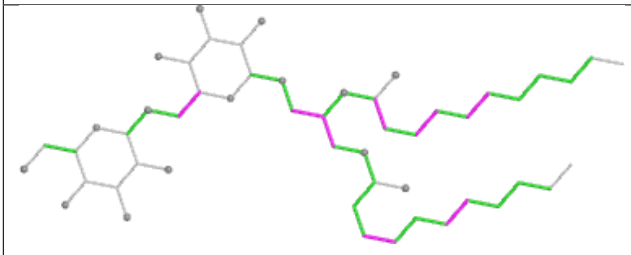
Ligand DGD f 851



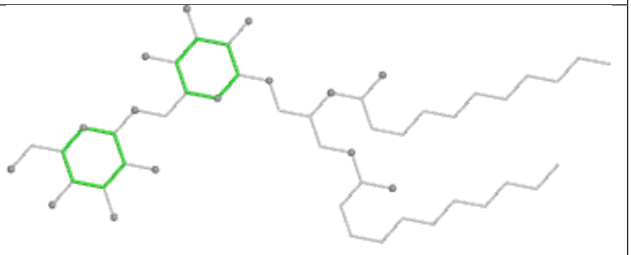
Bond lengths



Bond angles

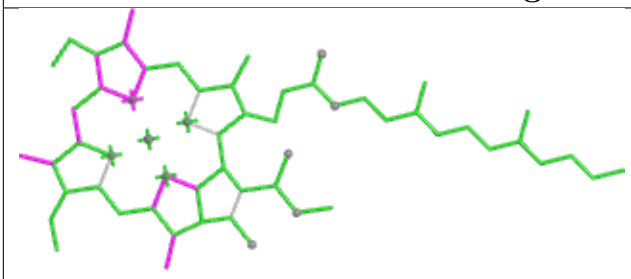


Torsions

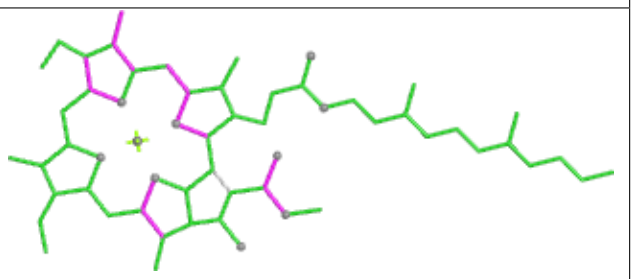


Rings

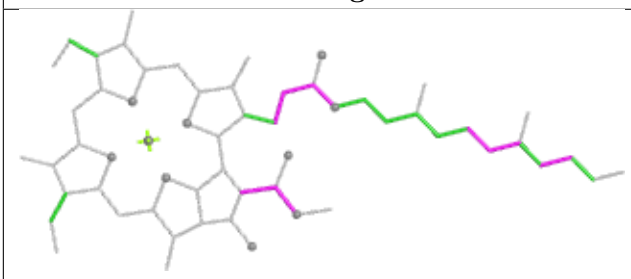
Ligand CLA A 802



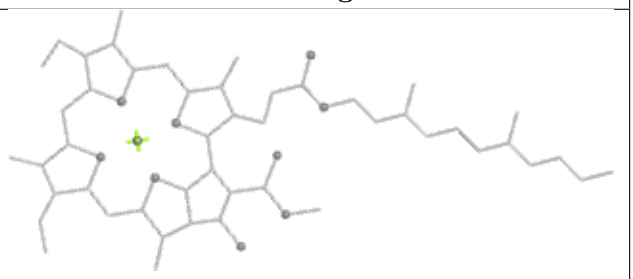
Bond lengths



Bond angles

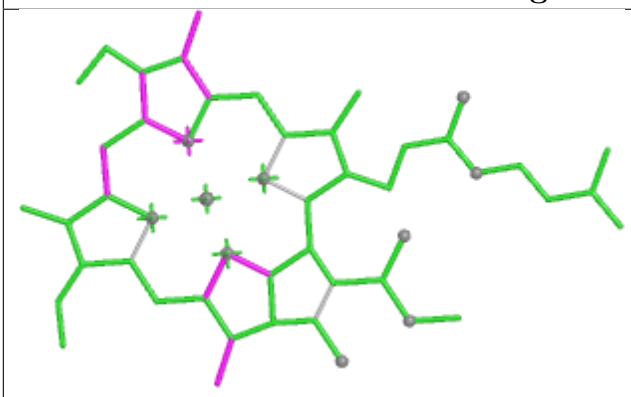


Torsions

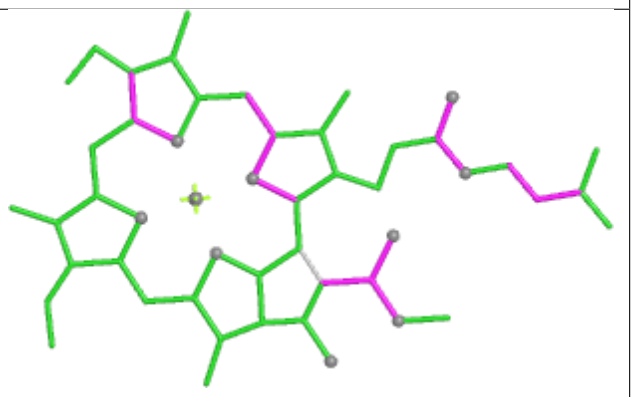


Rings

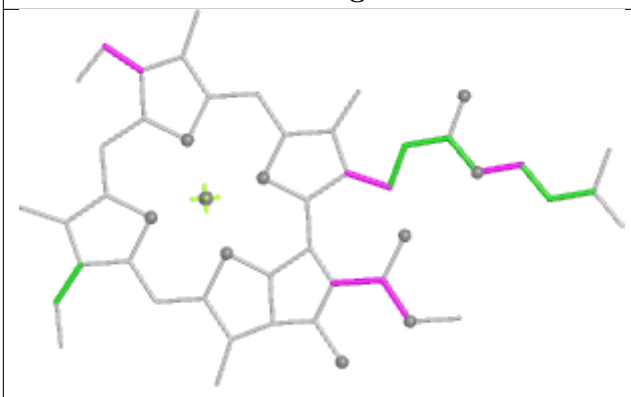
Ligand CLA r 317



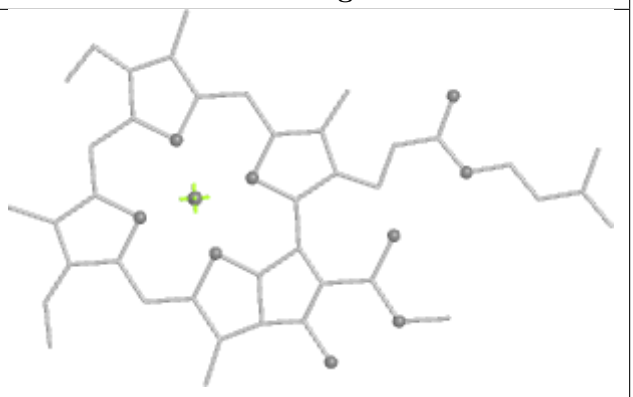
Bond lengths



Bond angles

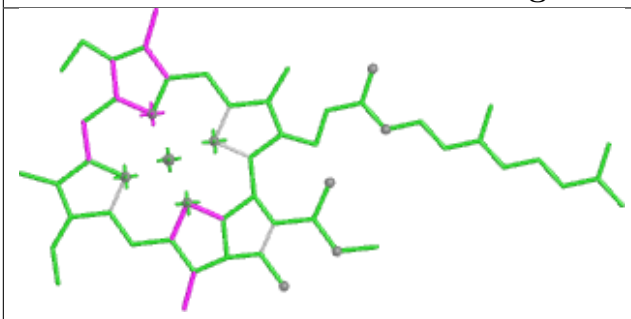


Torsions

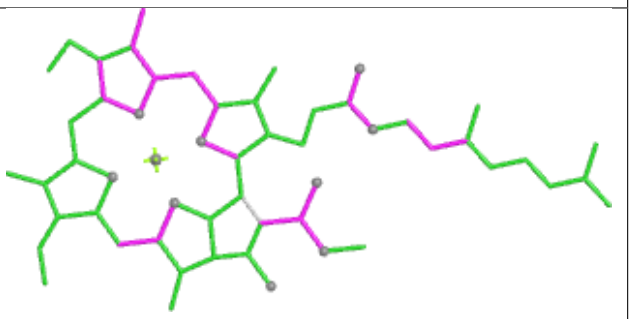


Rings

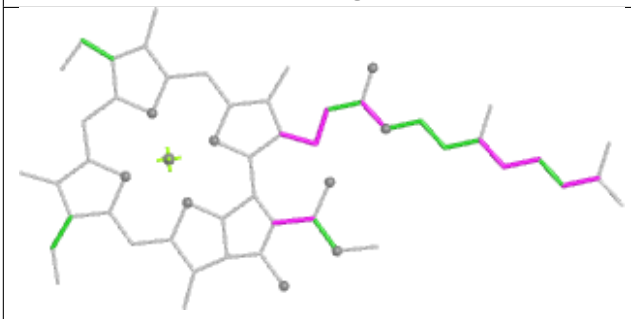
Ligand CLA e 837



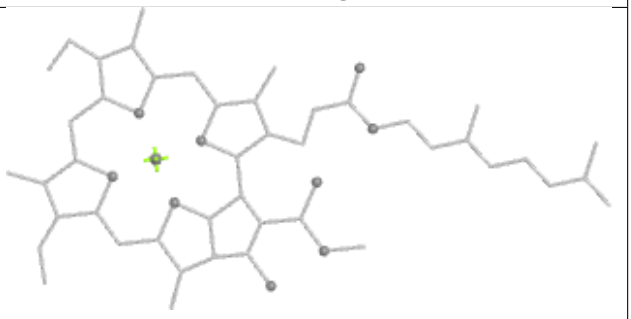
Bond lengths



Bond angles

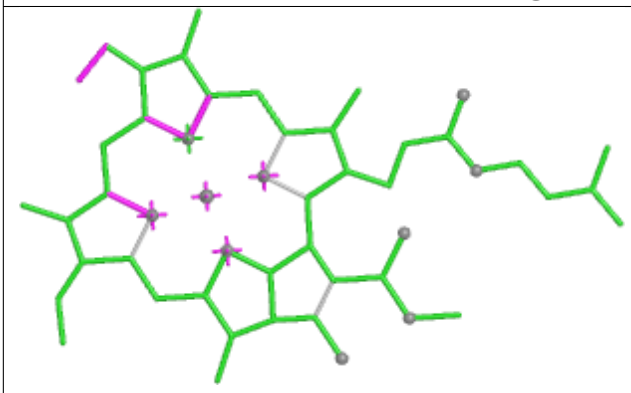


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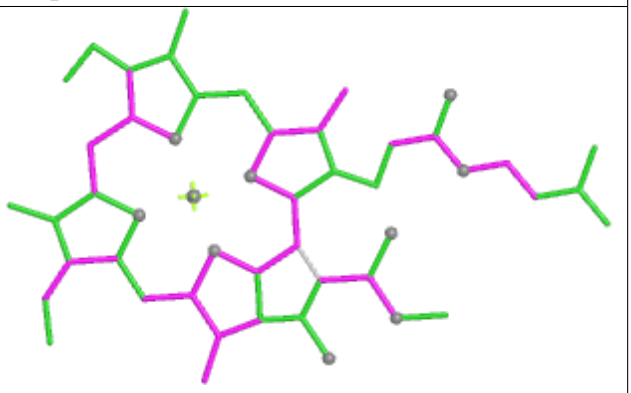


Rings

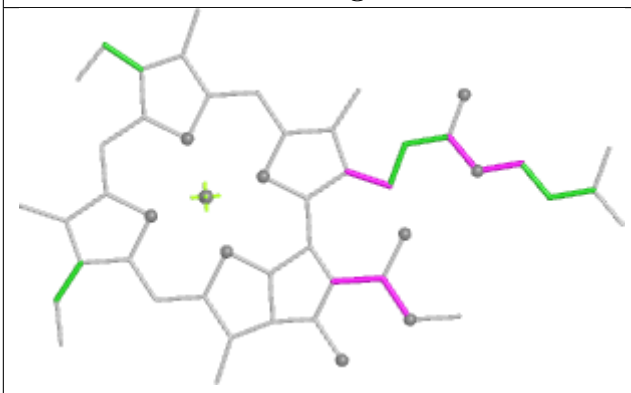
Ligand CLA p 509



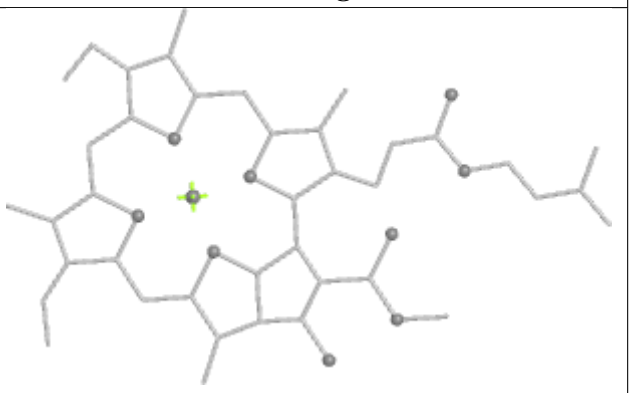
Bond lengths



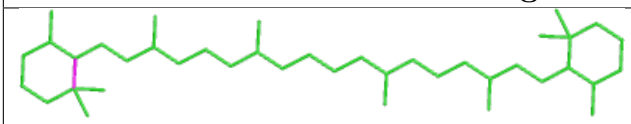
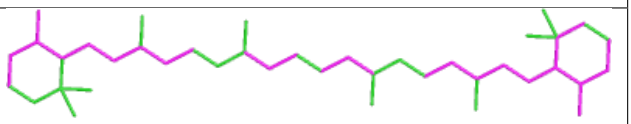
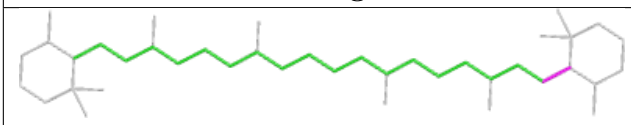
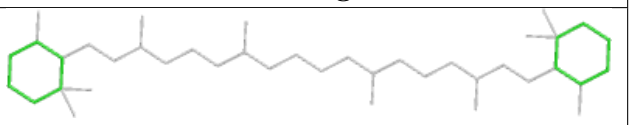
Bond angles

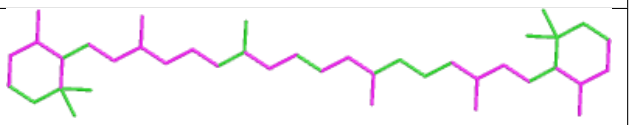
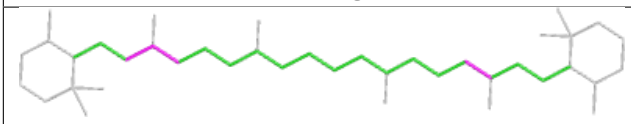
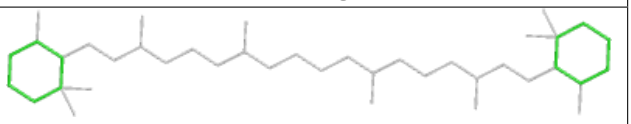


Torsions

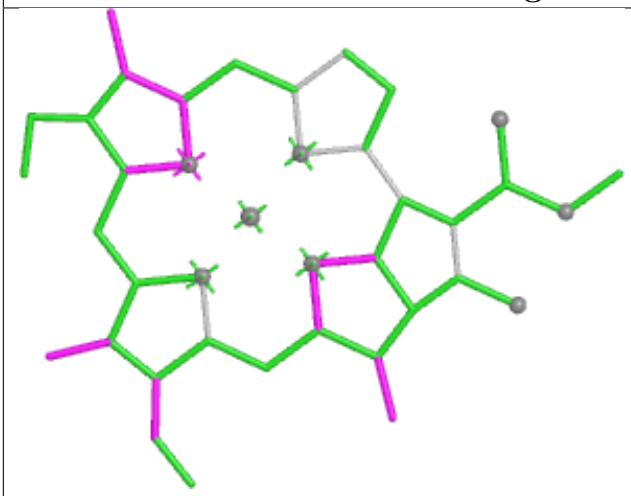


Rings

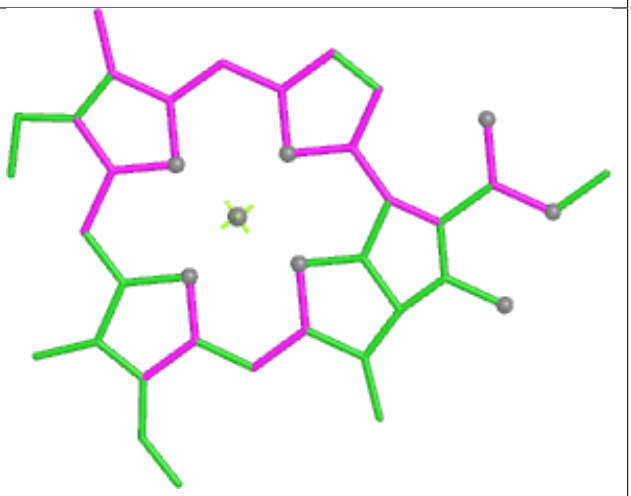
Ligand BCR m 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

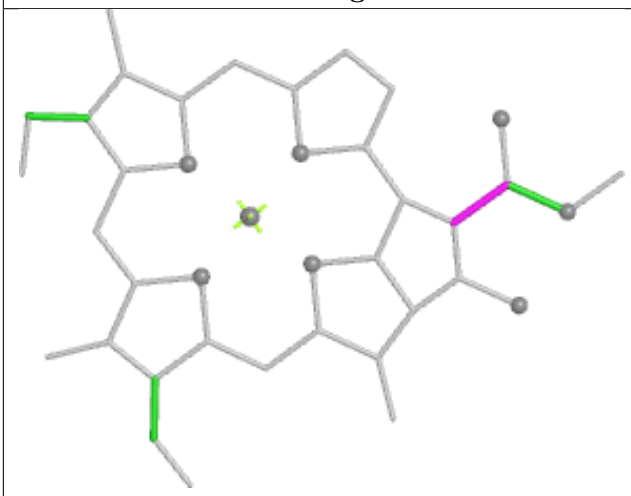
Ligand CLA B 806



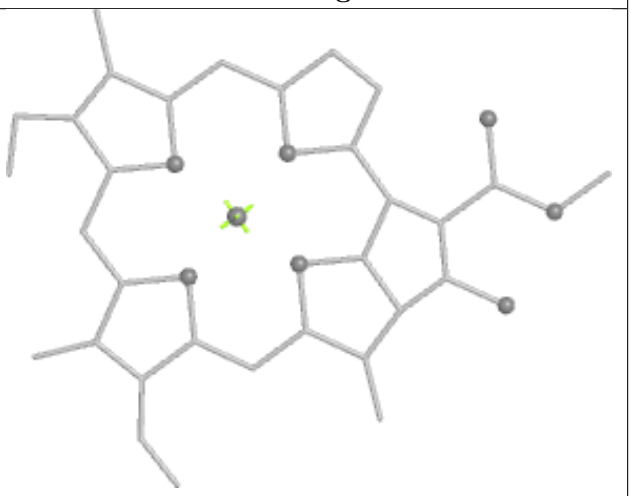
Bond lengths



Bond angles

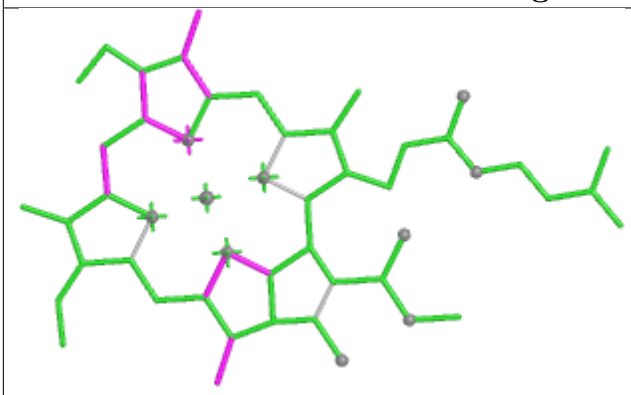


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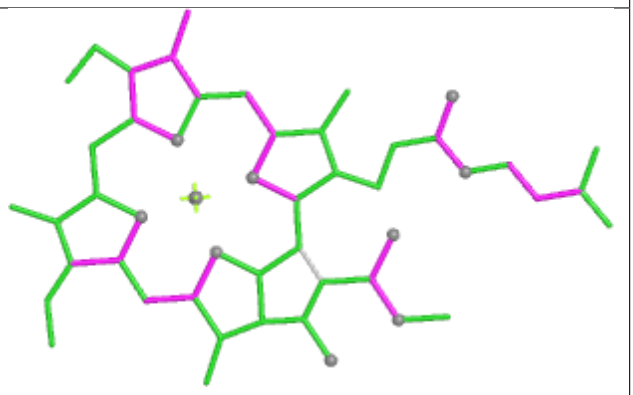


Rings

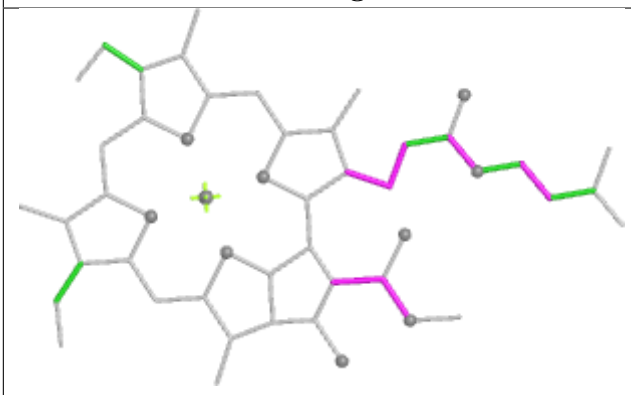
Ligand CLA f 829



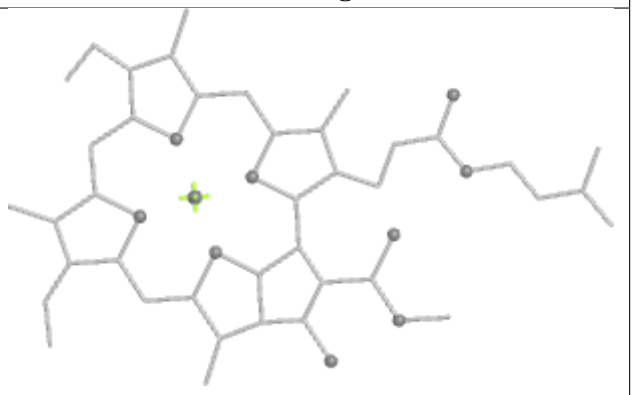
Bond lengths



Bond angles

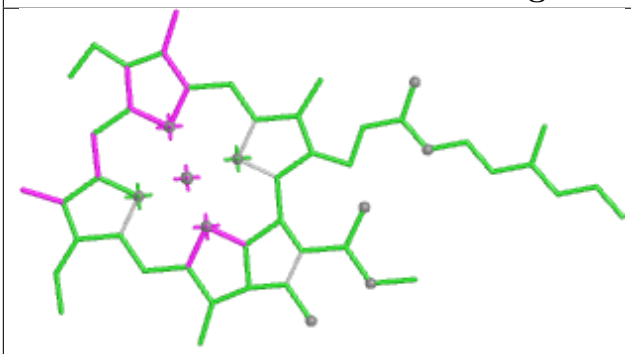


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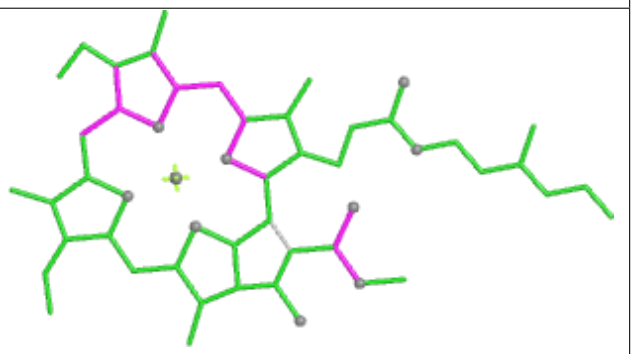


Rings

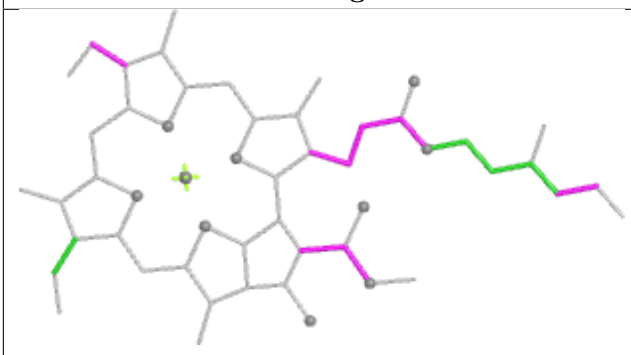
Ligand CLA 2 505



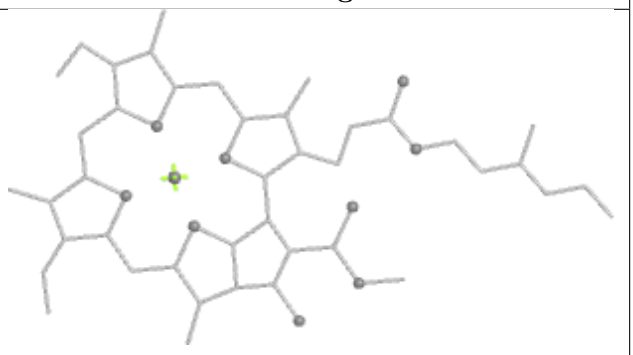
Bond lengths



Bond angles

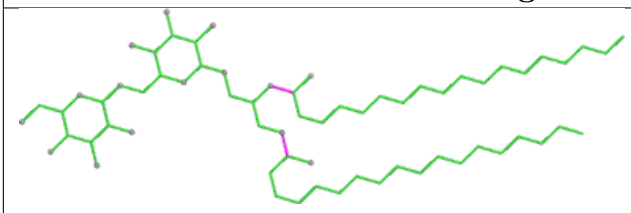


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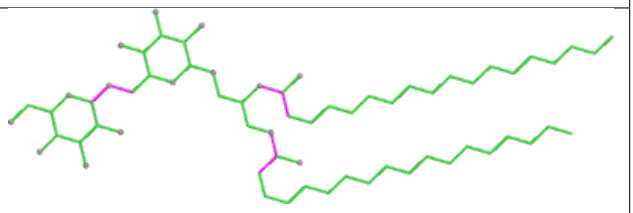


Rings

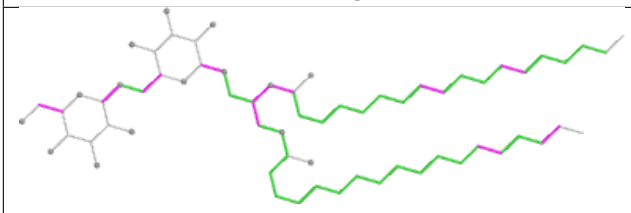
Ligand DGD m 104



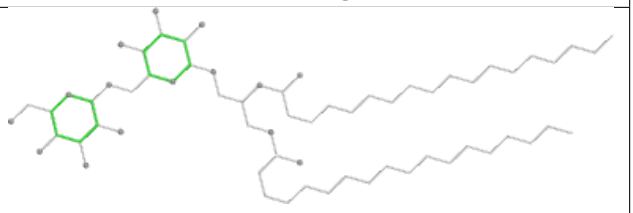
Bond lengths



Bond angles

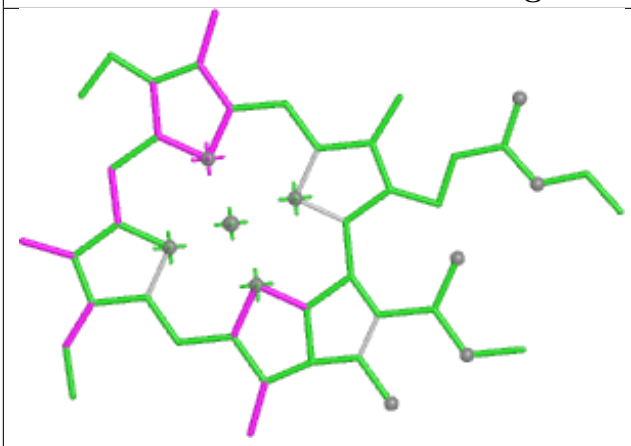


Torsions

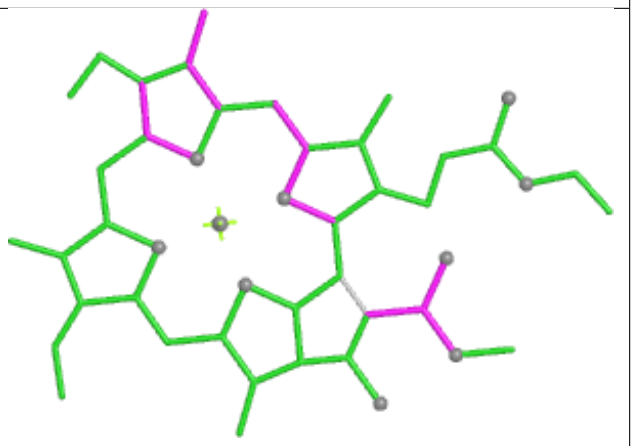


Rings

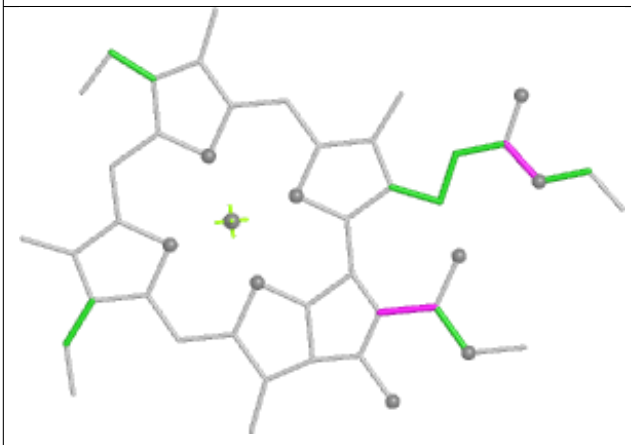
Ligand CLA B 822



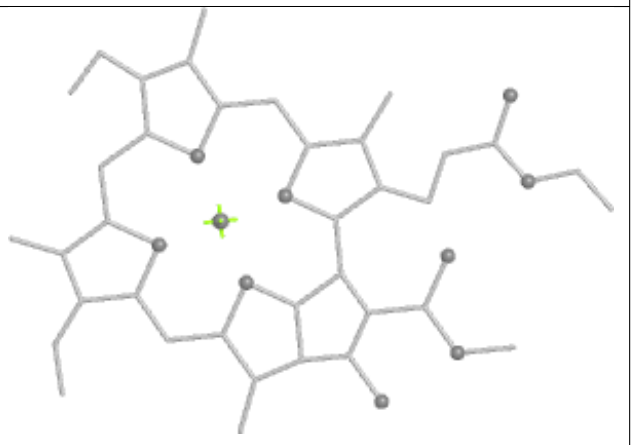
Bond lengths



Bond angles

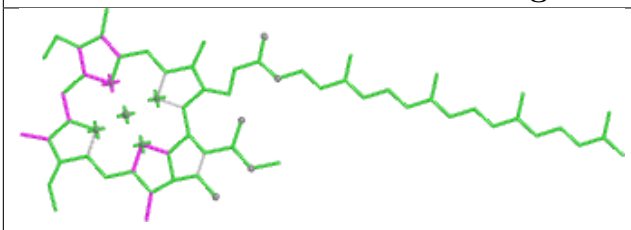


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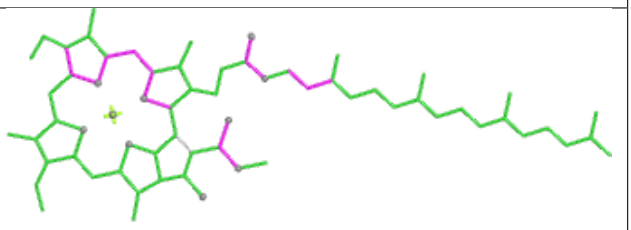


Rings

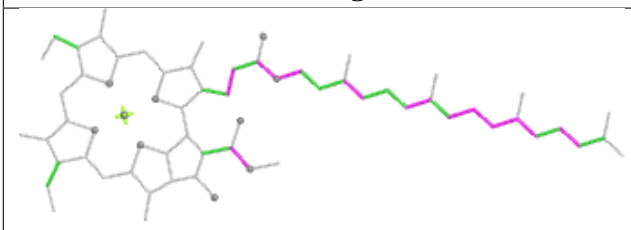
Ligand CLA r 306



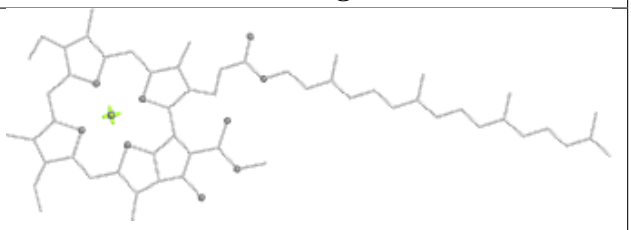
Bond lengths



Bond angles

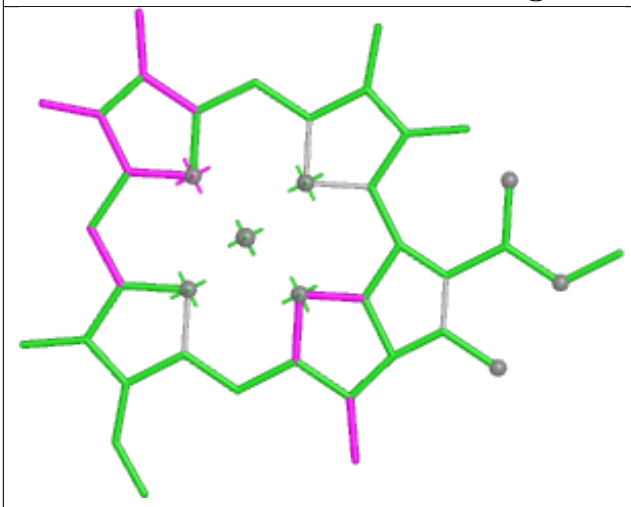


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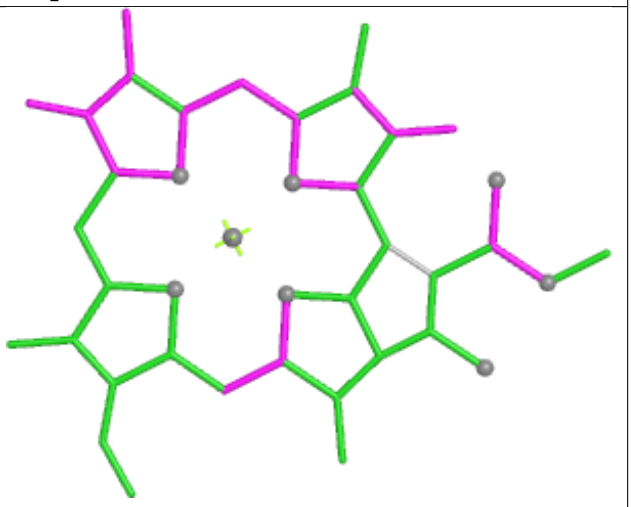


Rings

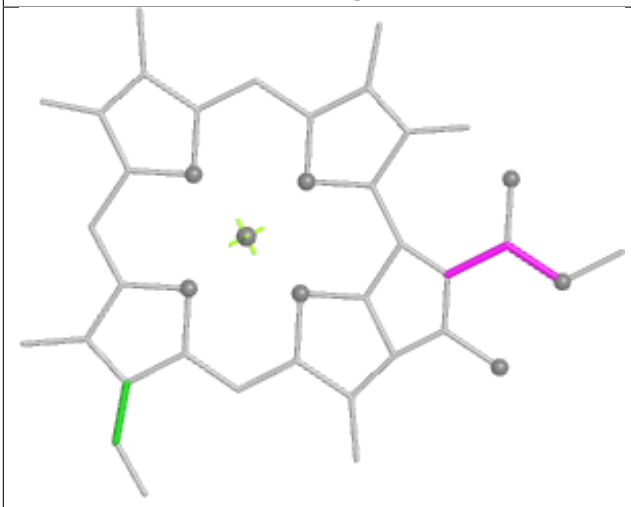
Ligand CLA p 507



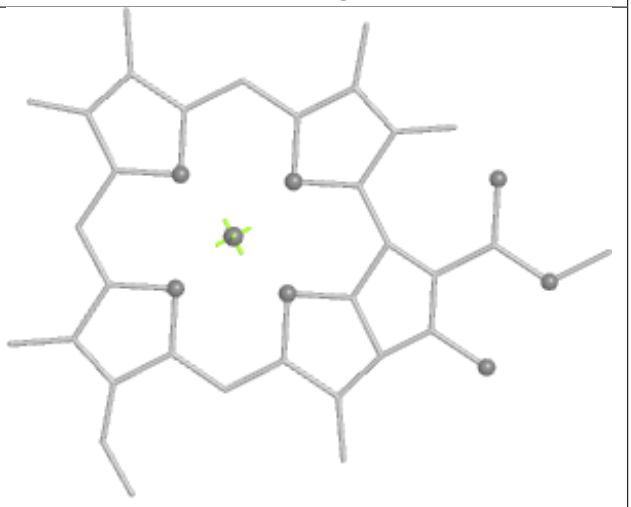
Bond lengths



Bond angles

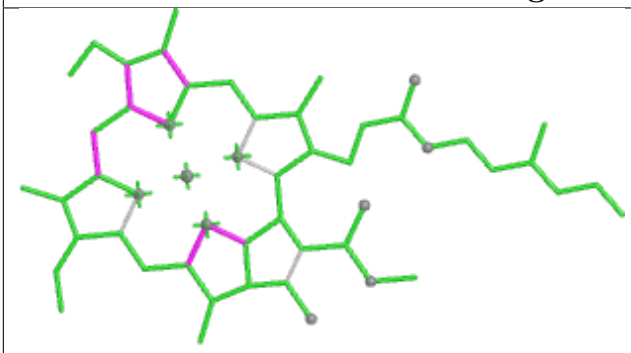


Torsions

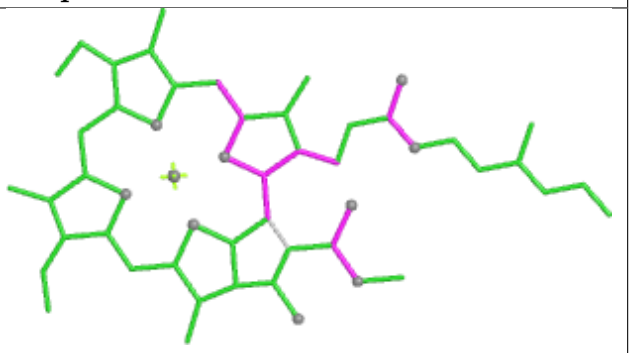


Rings

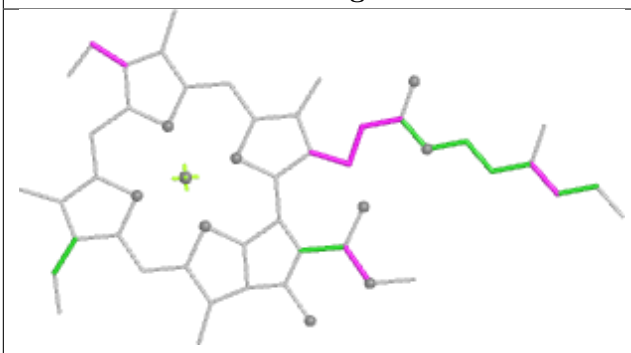
Ligand CLA q 305



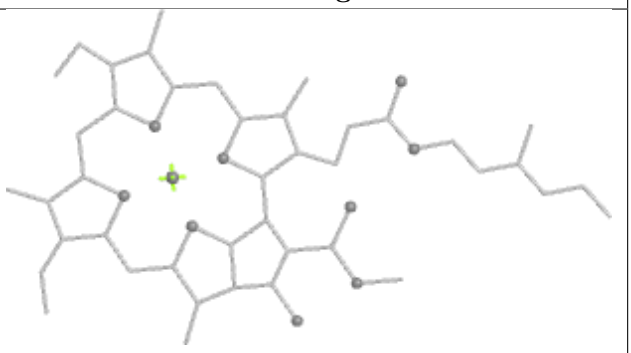
Bond lengths



Bond angles

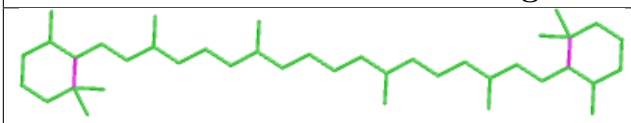


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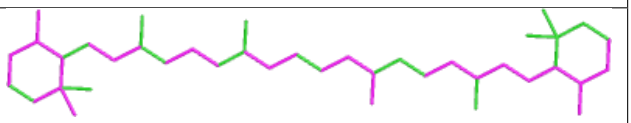


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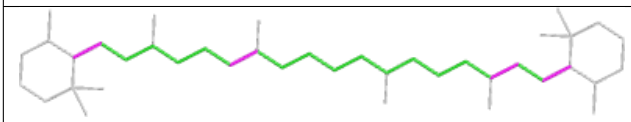
Ligand BCR K 204



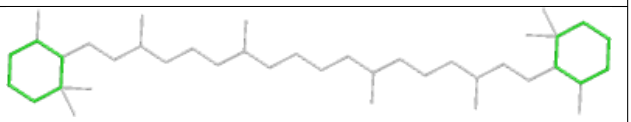
Bond lengths



Bond angles

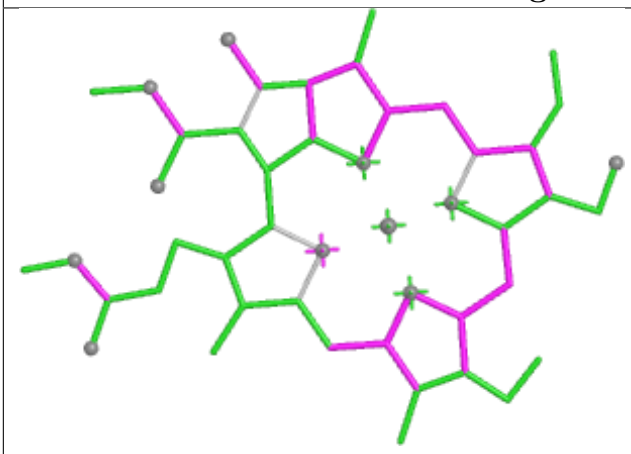


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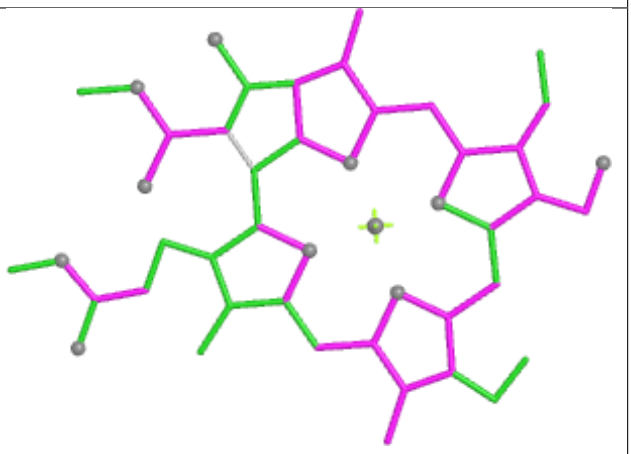


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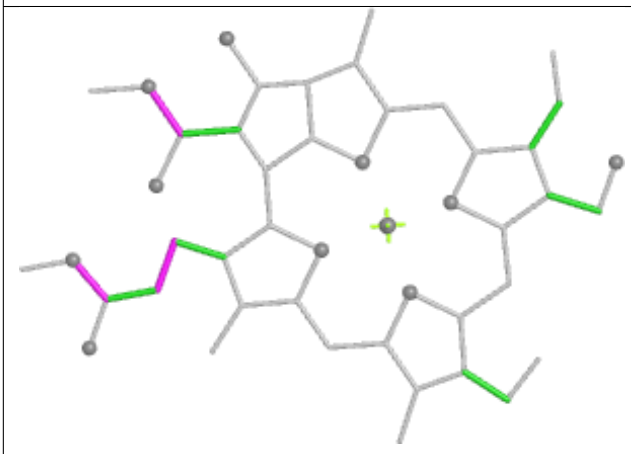
Ligand CHL r 313



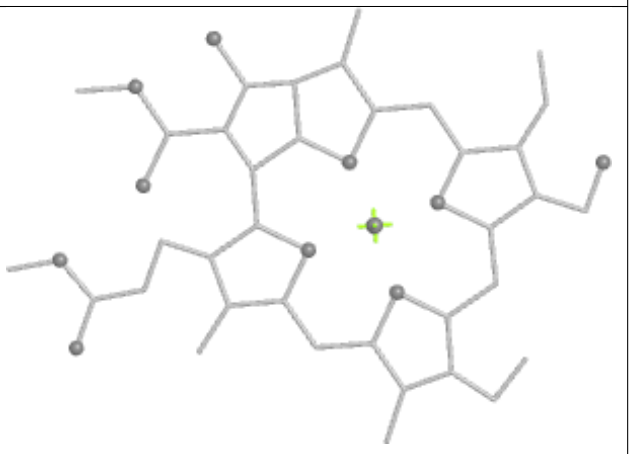
Bond lengths



Bond angles

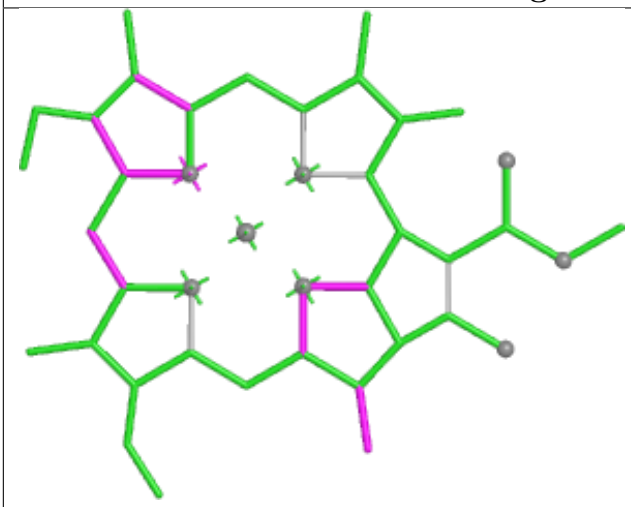


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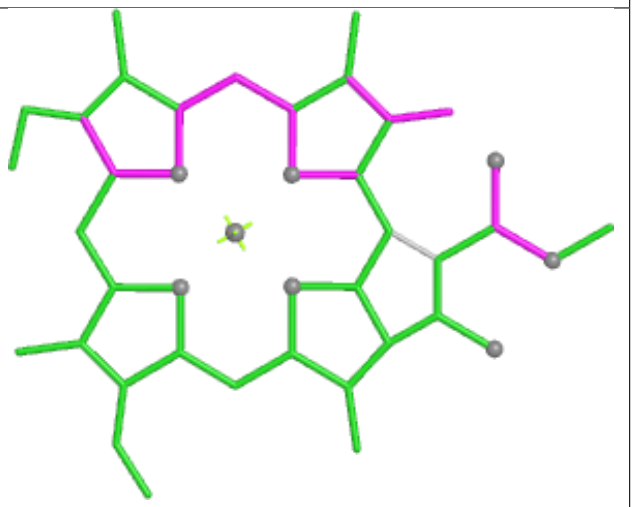


Rings

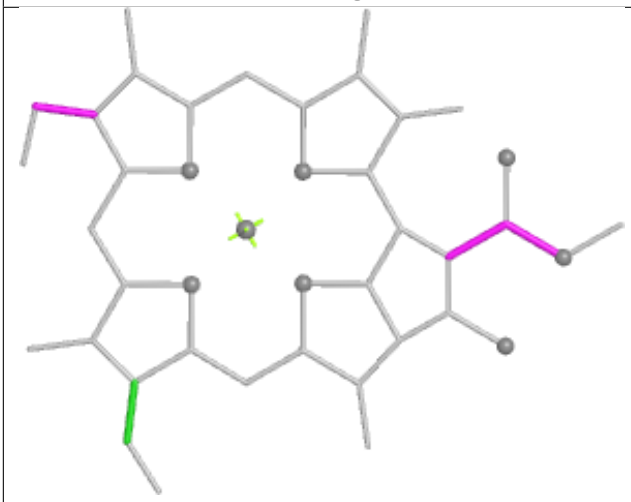
Ligand CLA r 312



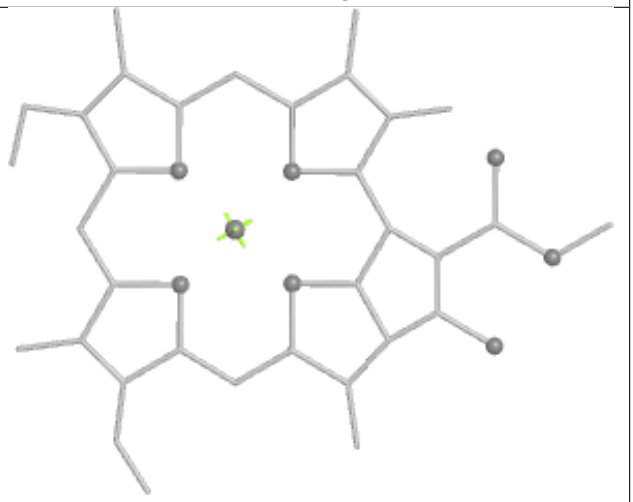
Bond lengths



Bond angles

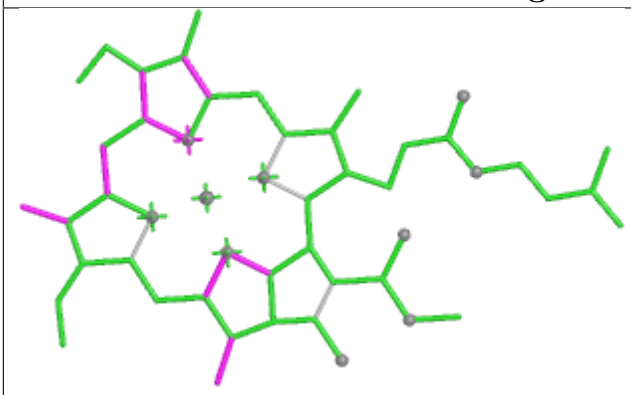


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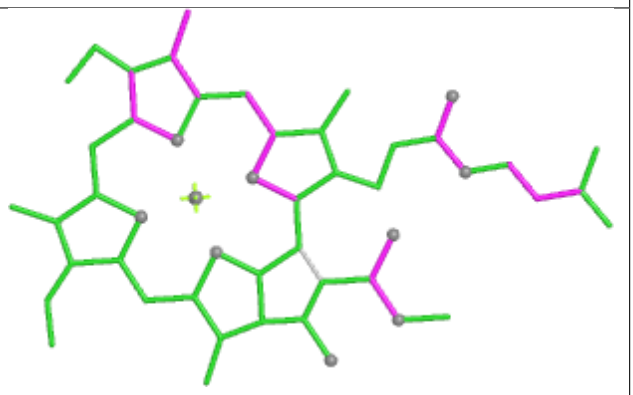


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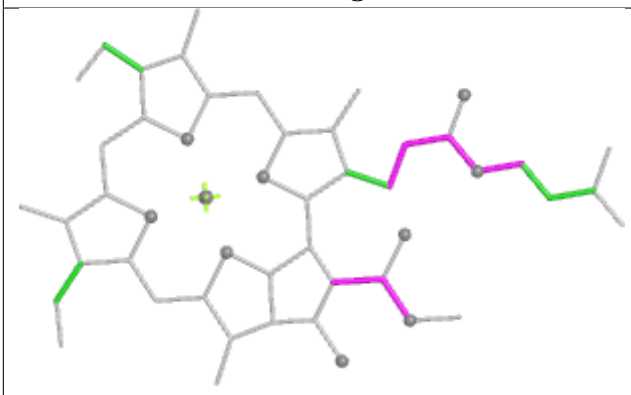
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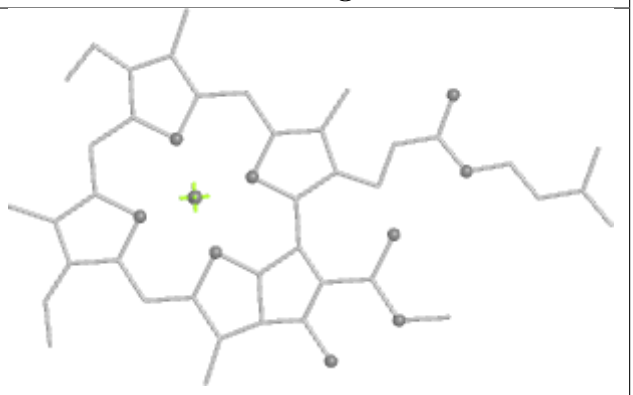
Bond lengths



Bond angles

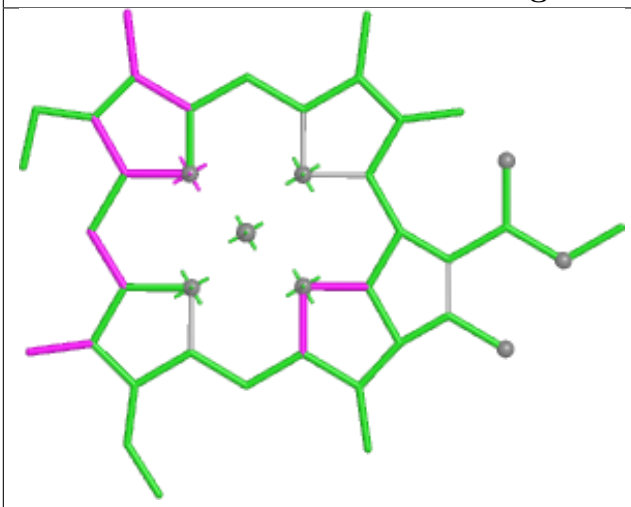


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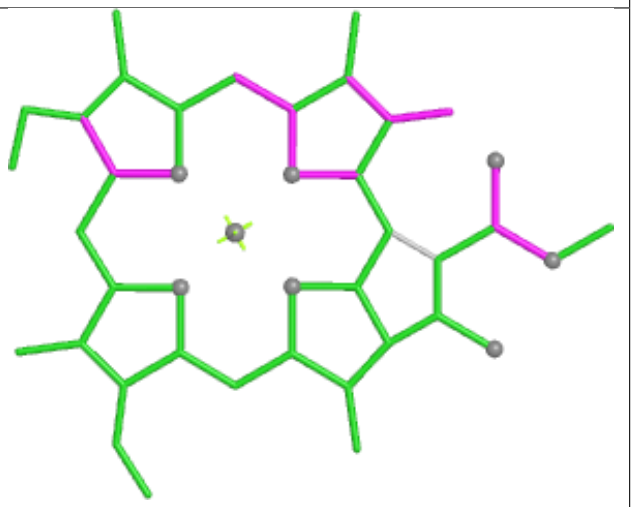


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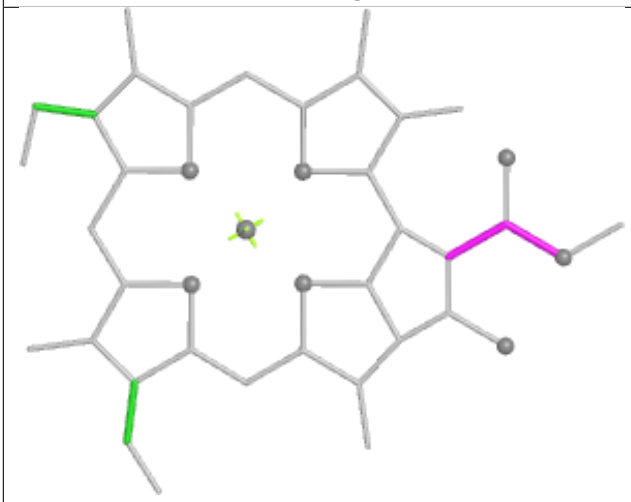
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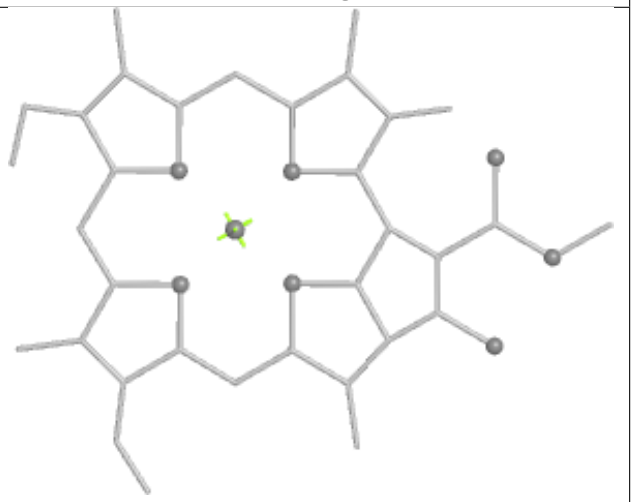
Bond lengths



Bond angles

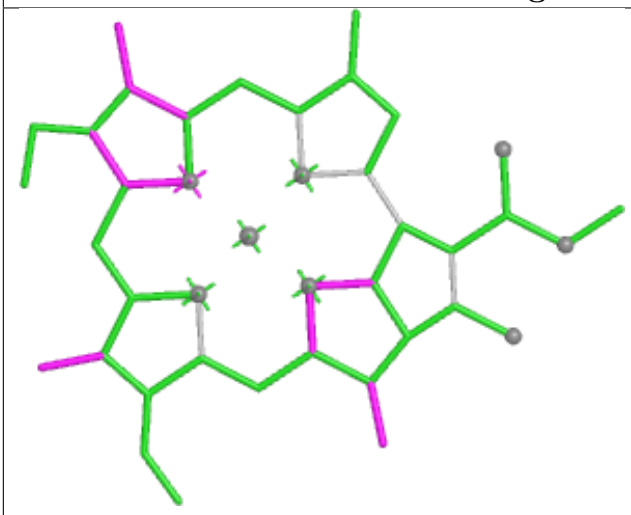


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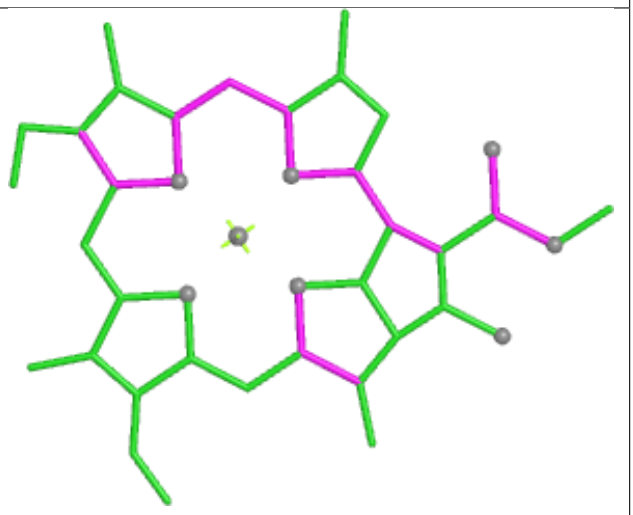


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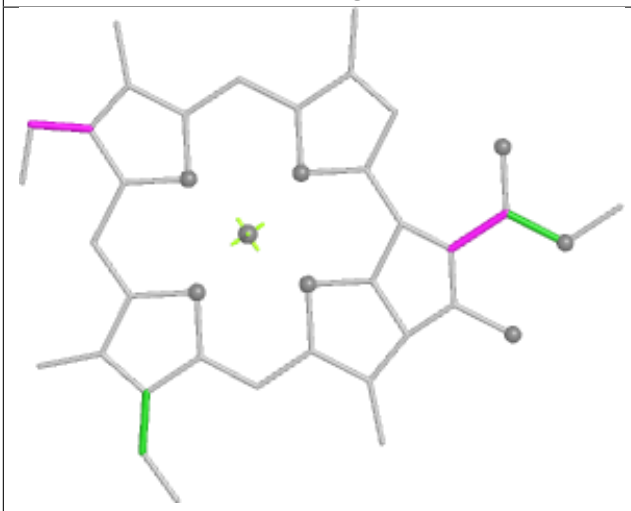
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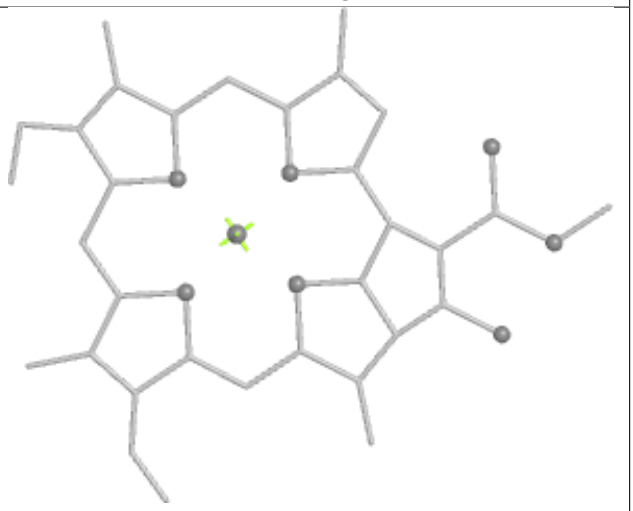
Bond lengths



Bond angles

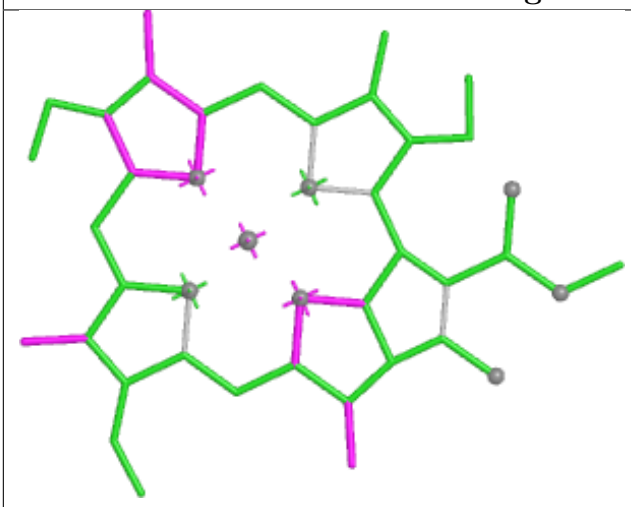


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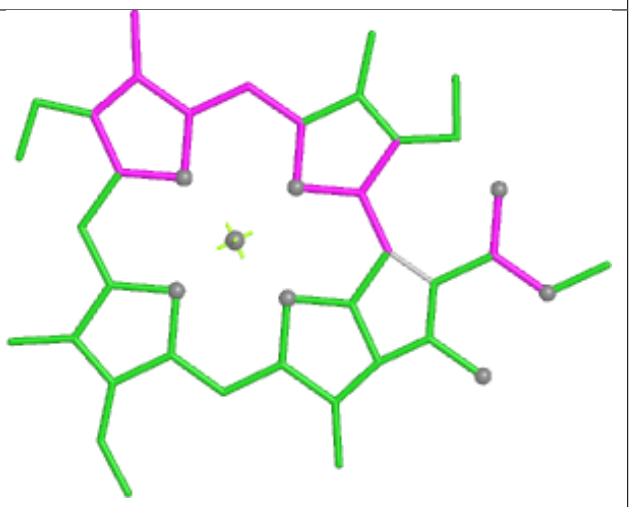


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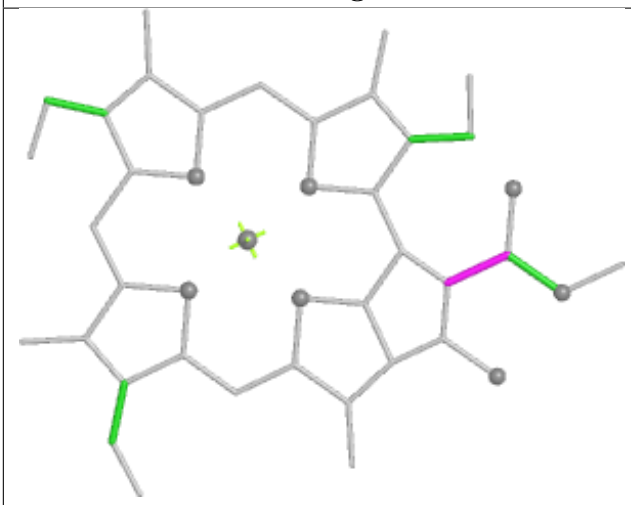
Ligand CLA B 825



Bond lengths



Bond angles

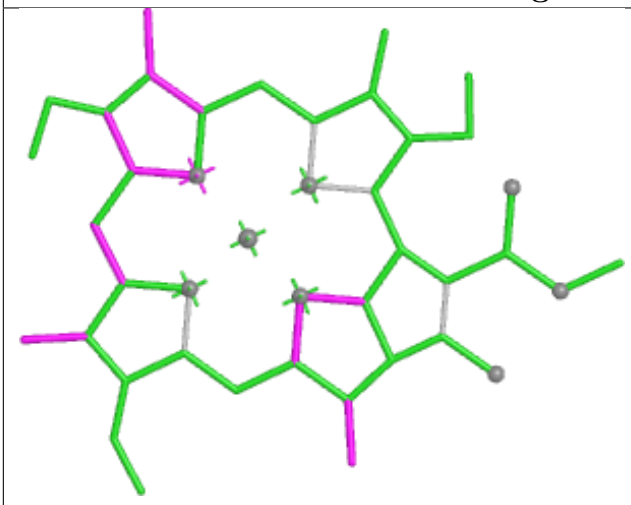


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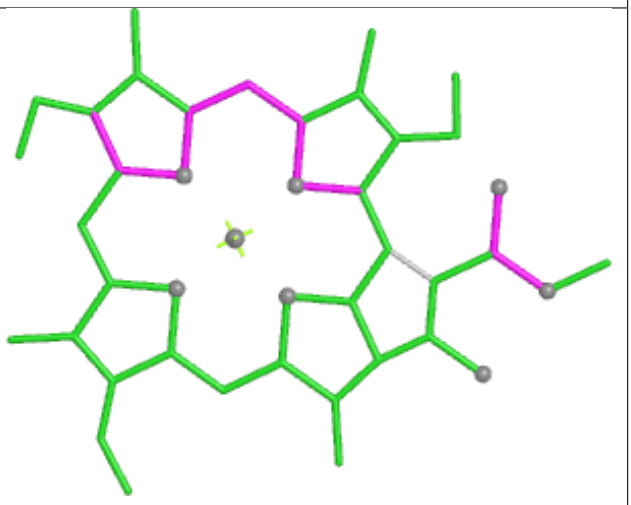


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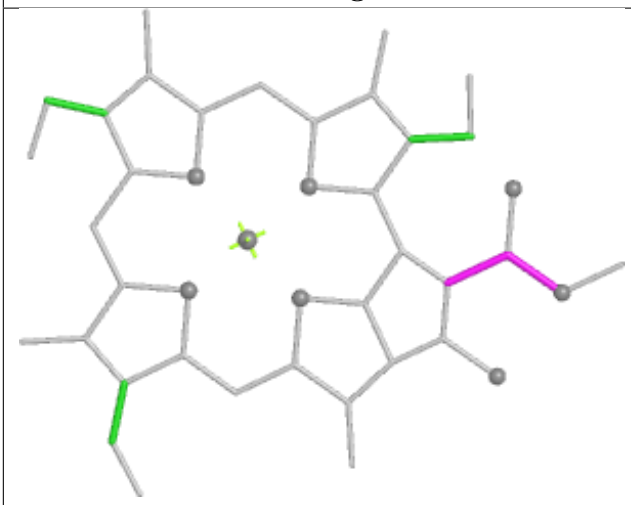
Ligand CLA f 825



Bond lengths



Bond angles

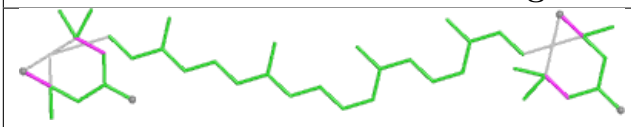


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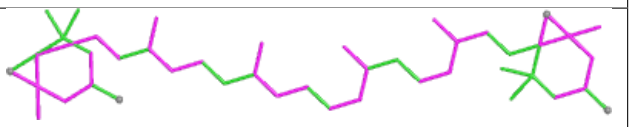


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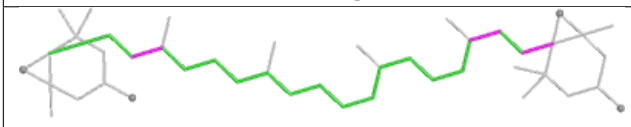
Ligand XAT 2 502



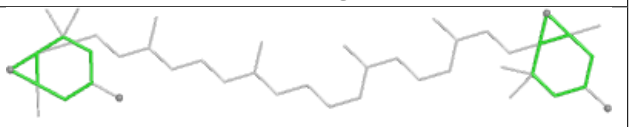
Bond lengths



Bond angles

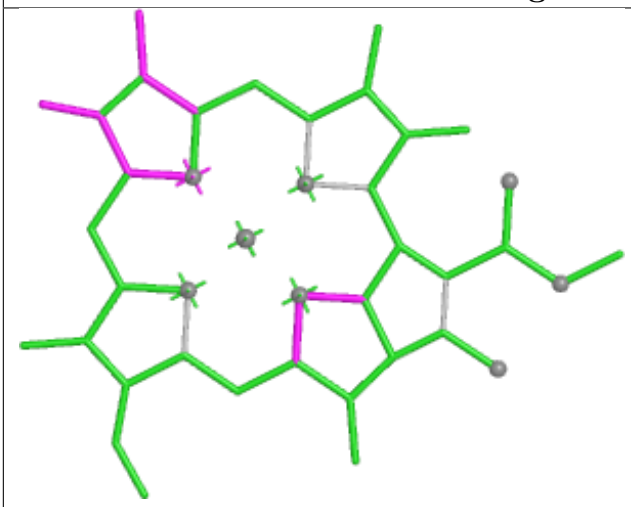


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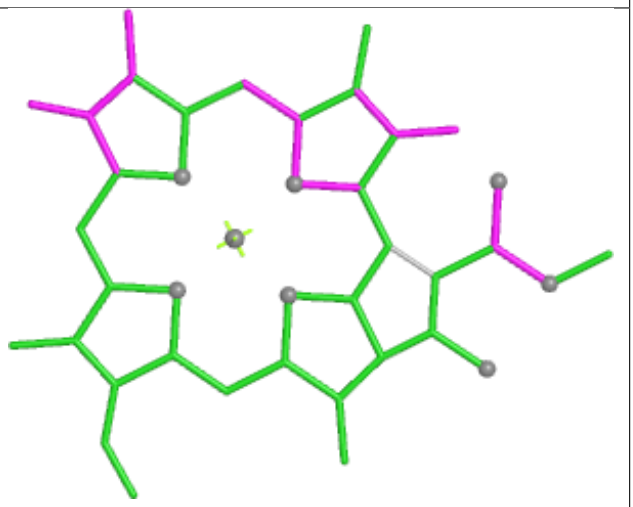


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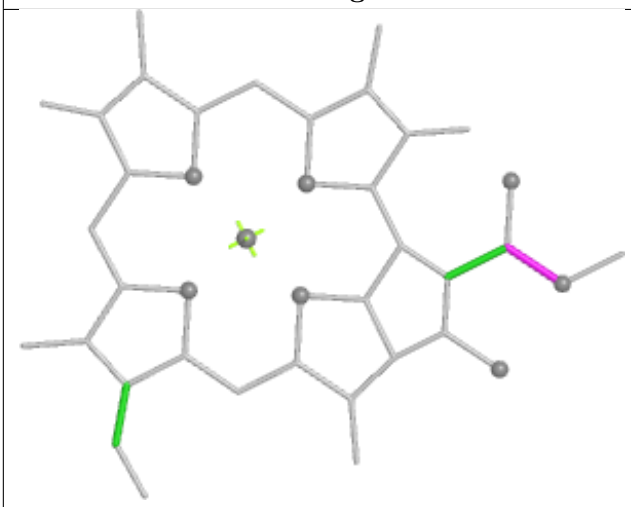
Ligand CLA o 302



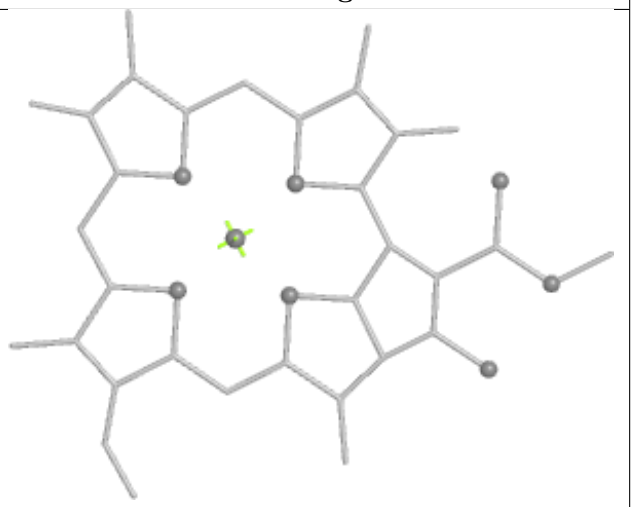
Bond lengths



Bond angles



Torsions

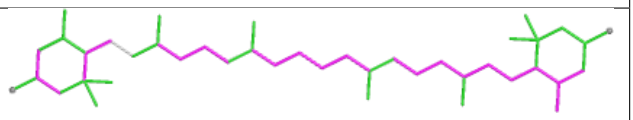


Rings

Ligand LUT s 501



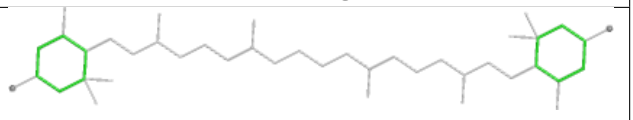
Bond lengths



Bond angles

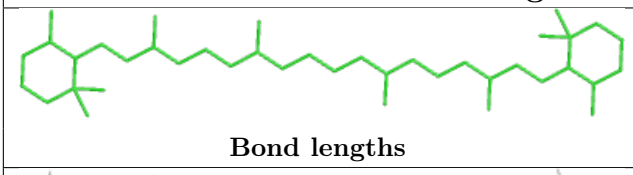


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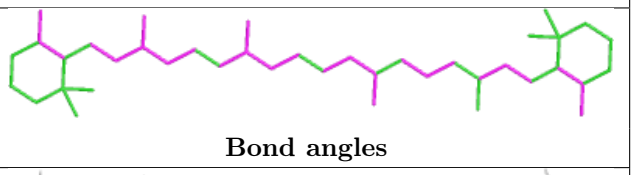


Rings

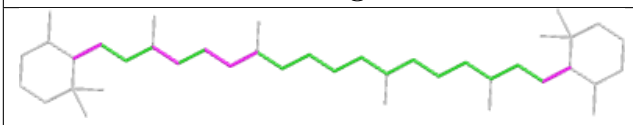
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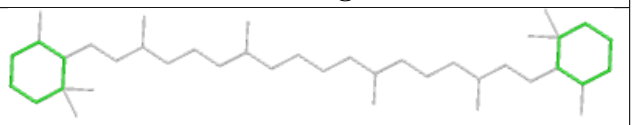
Bond lengths



Bond angles

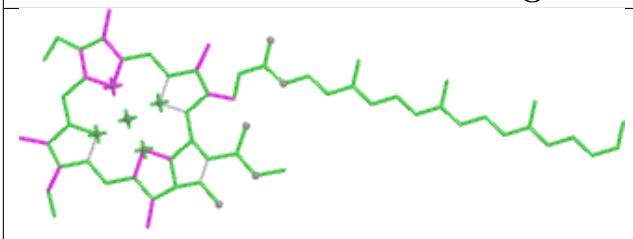


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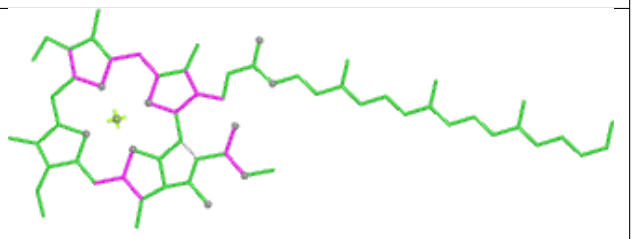


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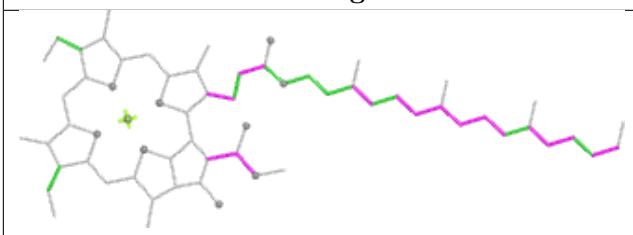
Ligand CLA A 805



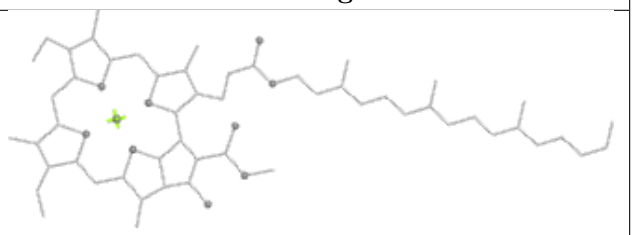
Bond lengths



Bond angles

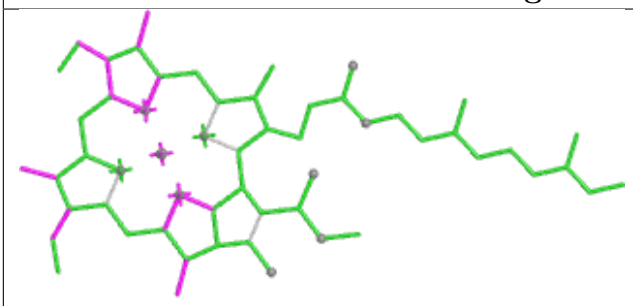


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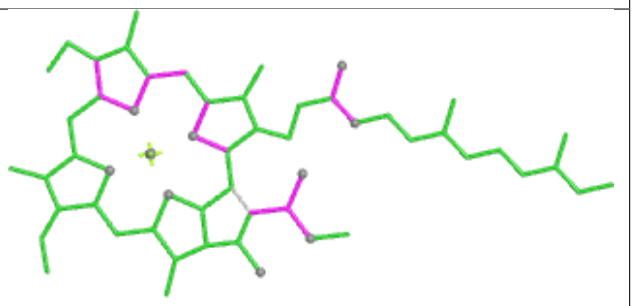


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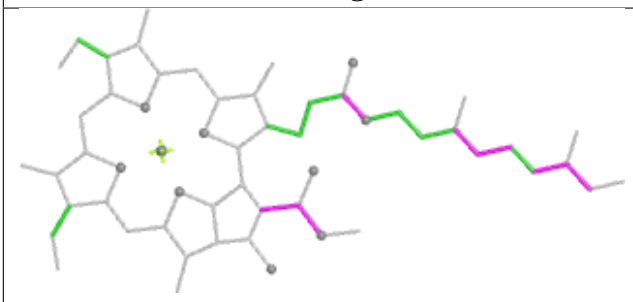
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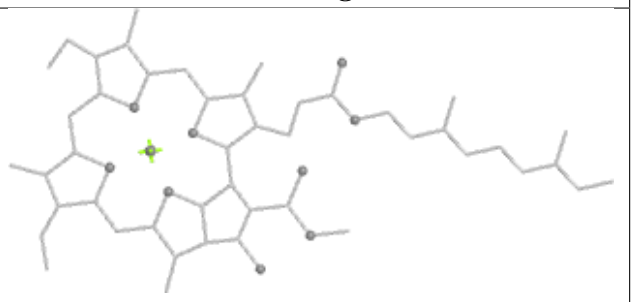
Bond lengths



Bond angles

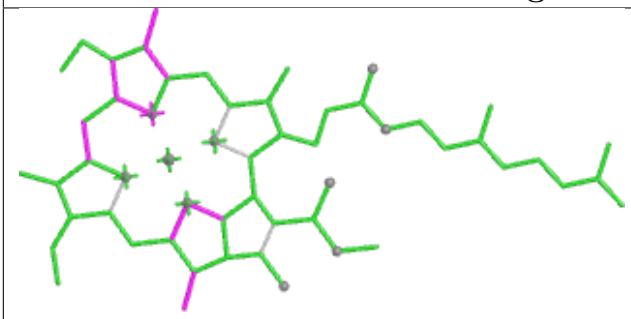


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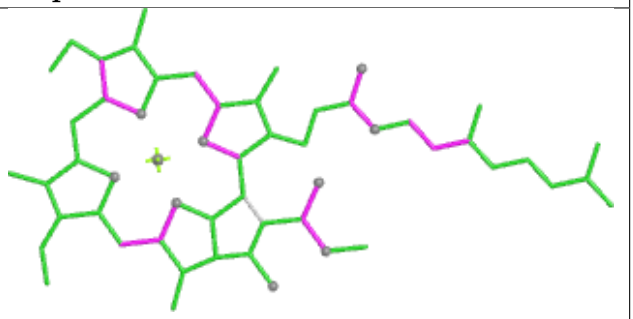


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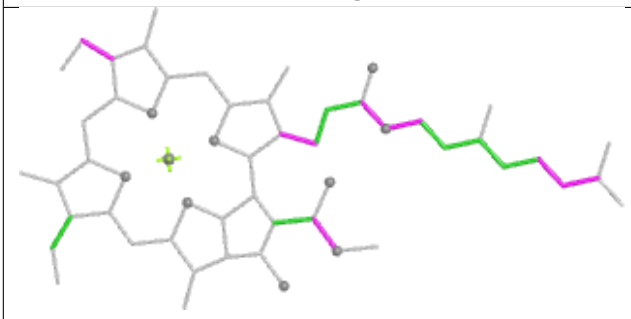
Ligand CLA p 506



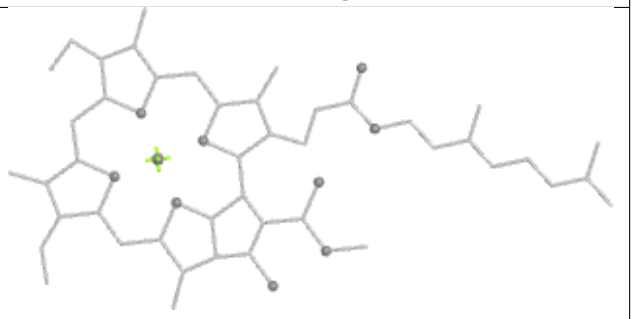
Bond lengths



Bond angles

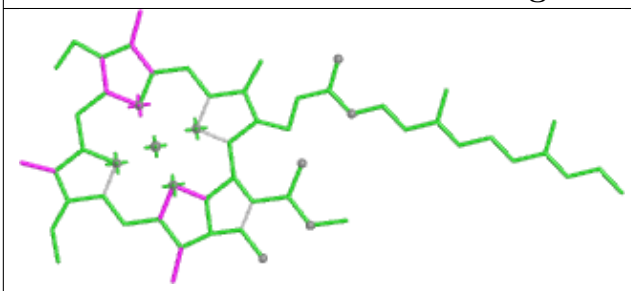


Torsions

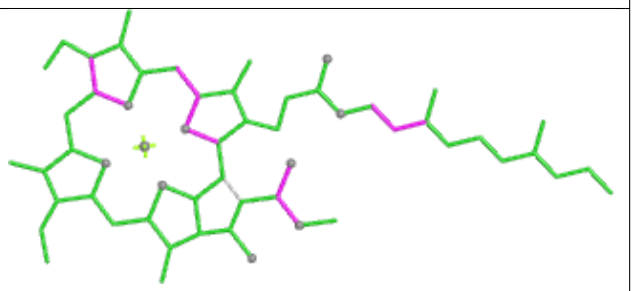


Rings

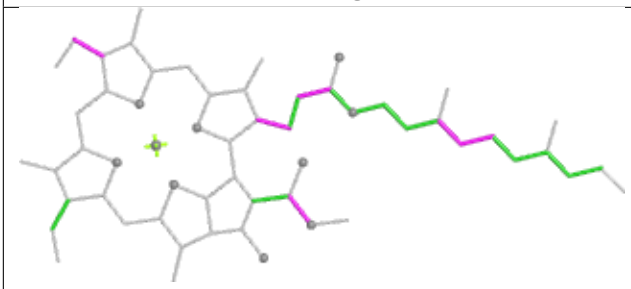
Ligand CLA e 852



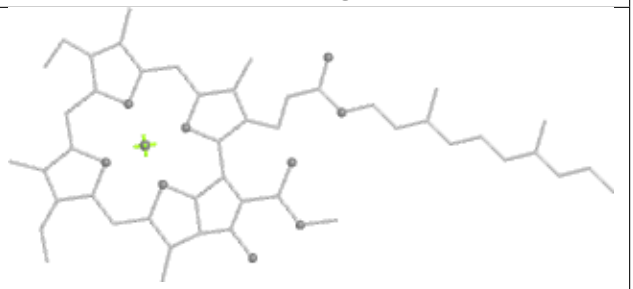
Bond lengths



Bond angles

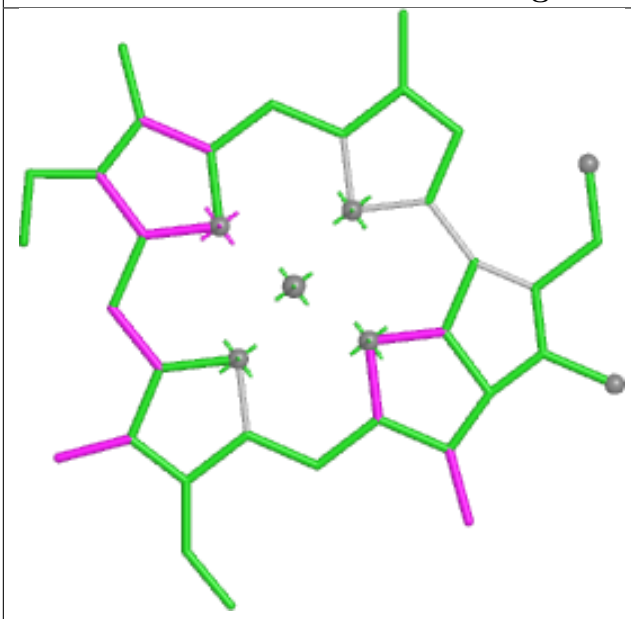


Torsions

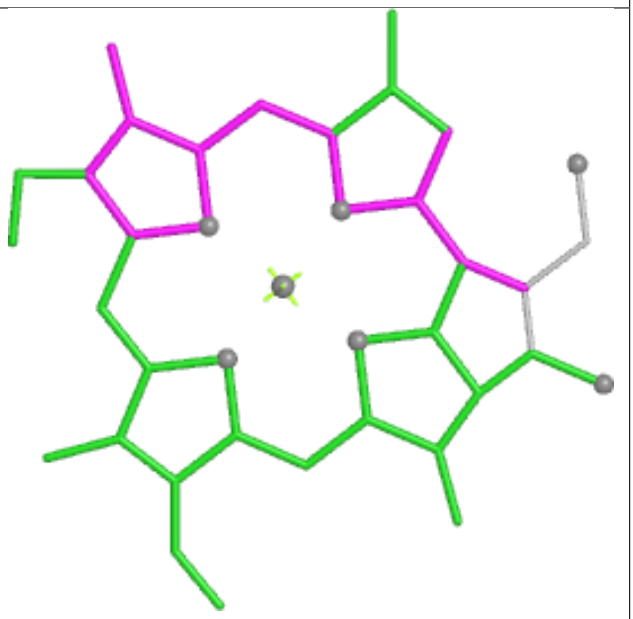


Rings

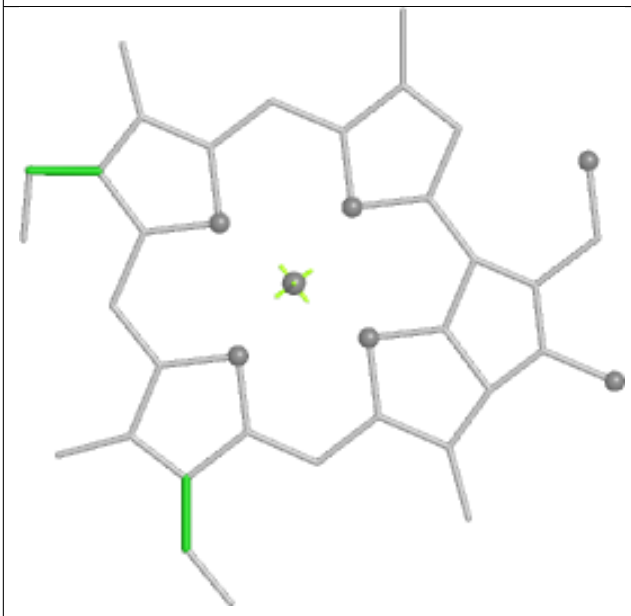
Ligand CLA f 805



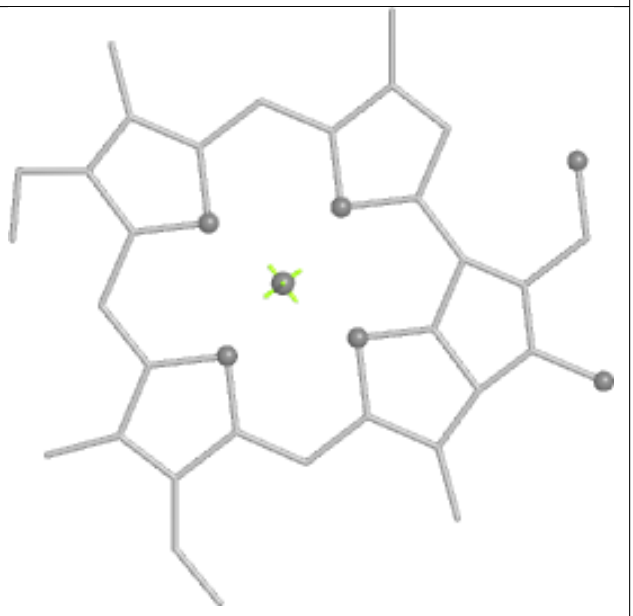
Bond lengths



Bond angles

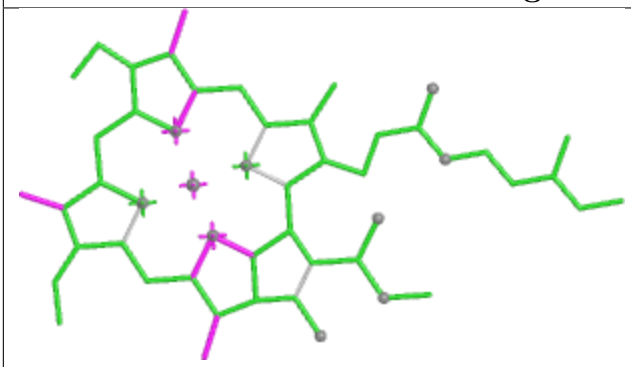


Torsions

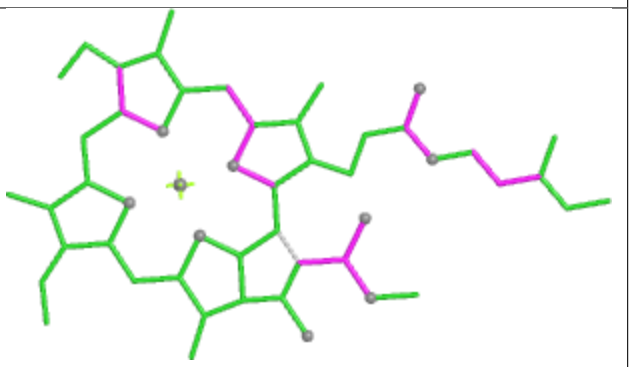


Rings

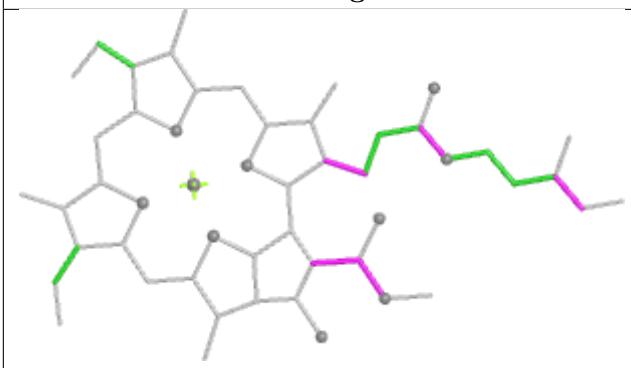
Ligand CLA A 835



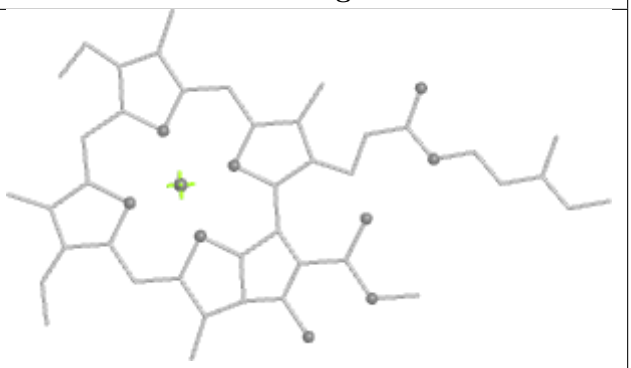
Bond lengths



Bond angles

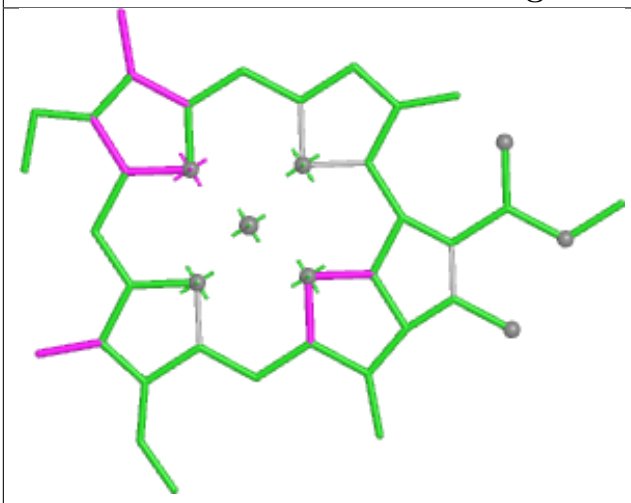


Torsions

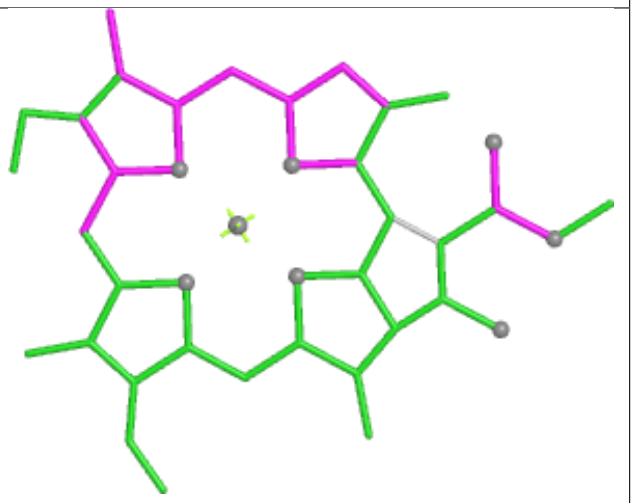


Rings

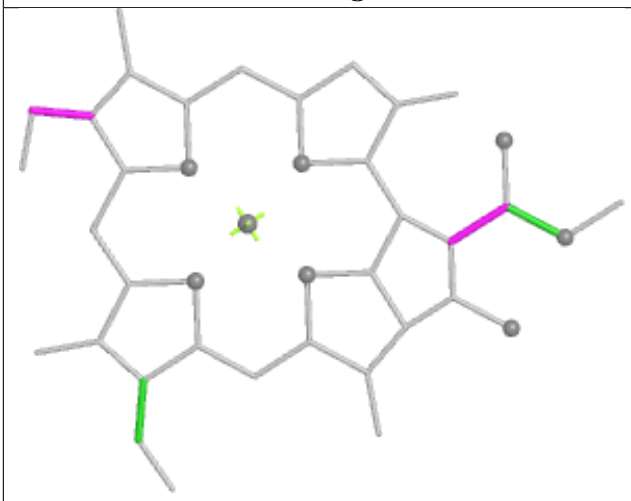
Ligand CLA L 302



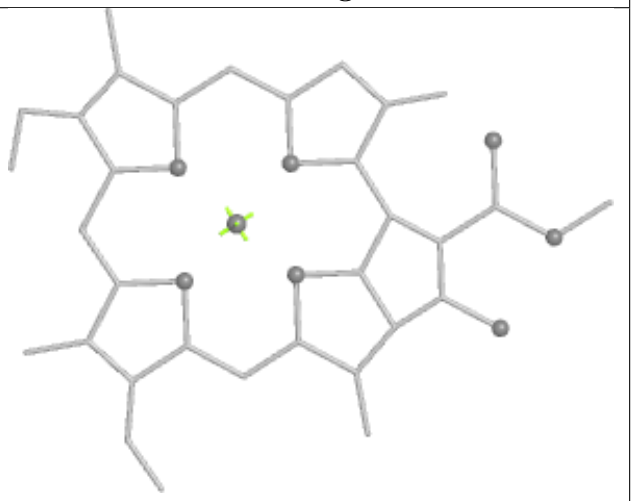
Bond lengths



Bond angles

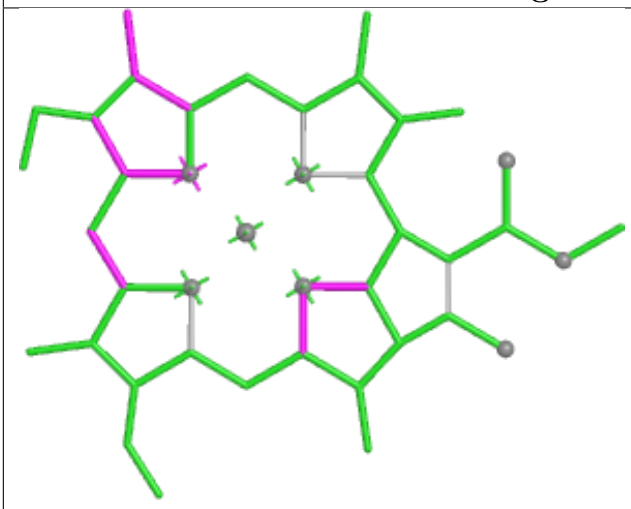


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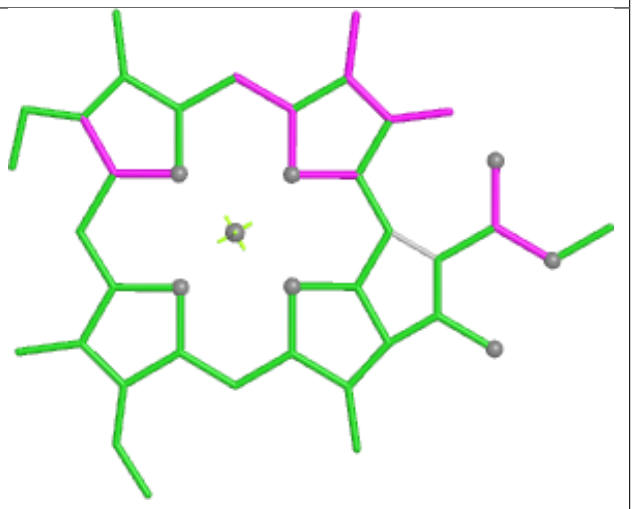


Rings

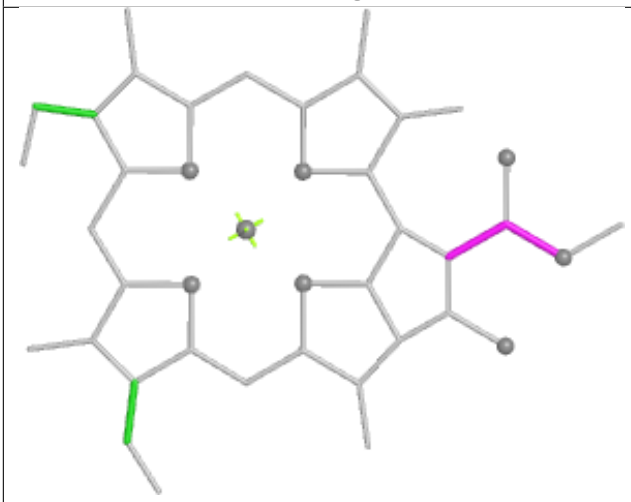
Ligand CLA f 839



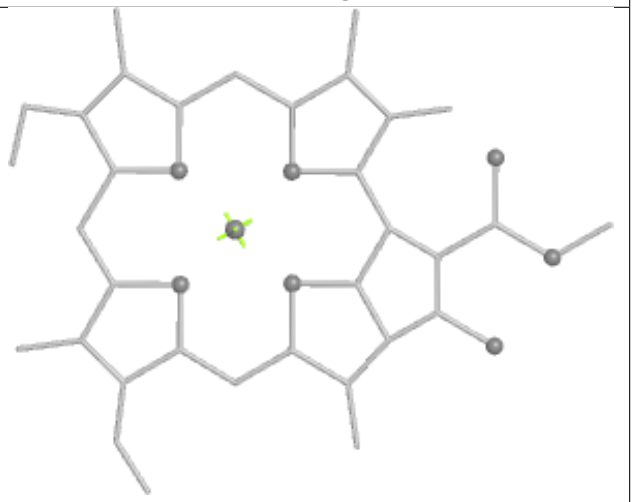
Bond lengths



Bond angles

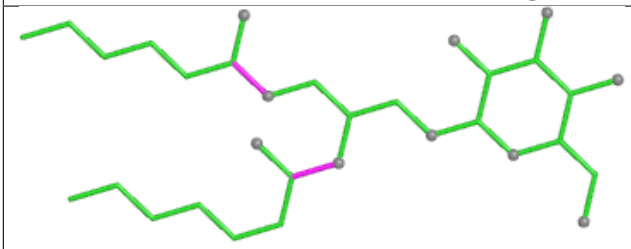


Torsions

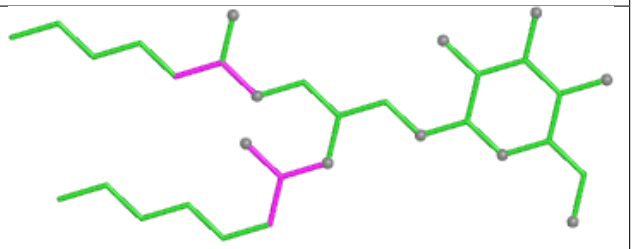


Rings

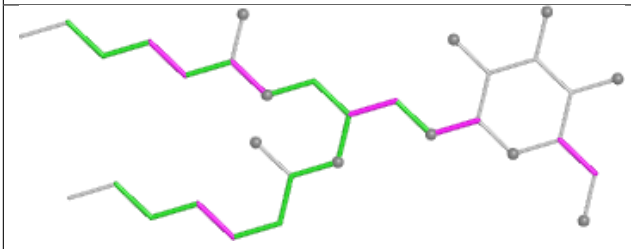
Ligand LMG 5 301



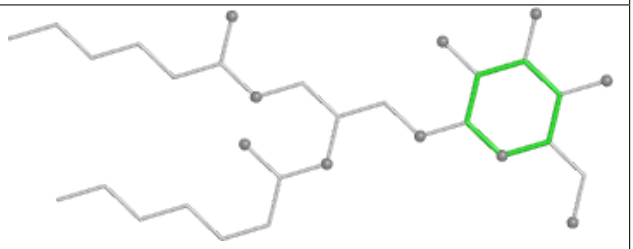
Bond lengths



Bond angles

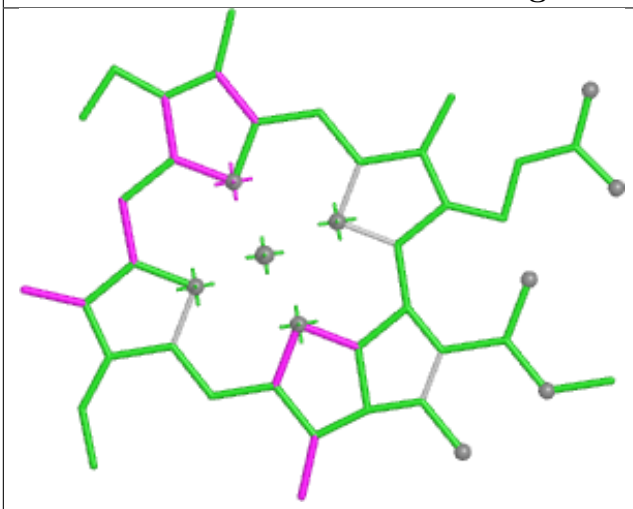


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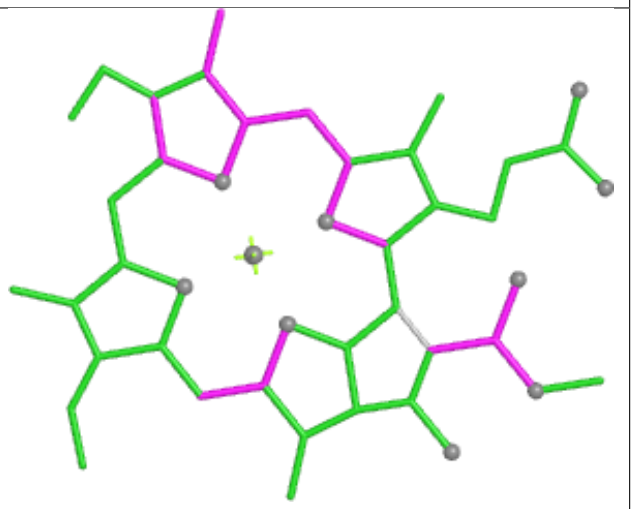


Rings

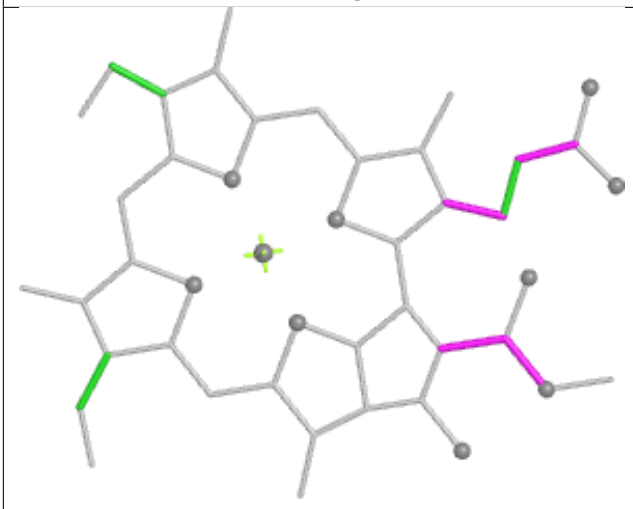
Ligand CLA e 853



Bond lengths



Bond angles

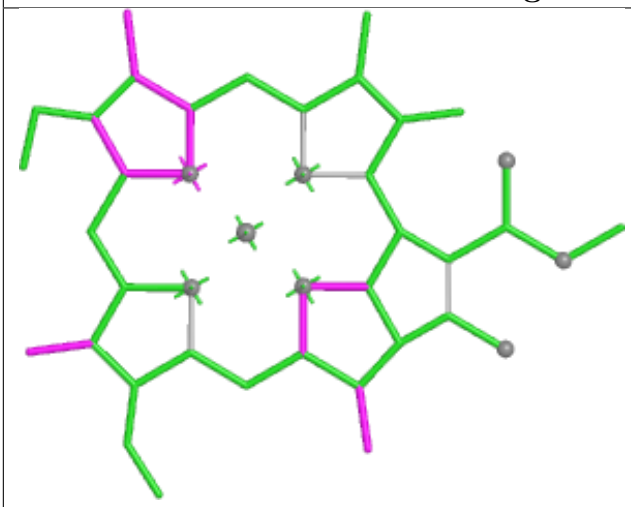


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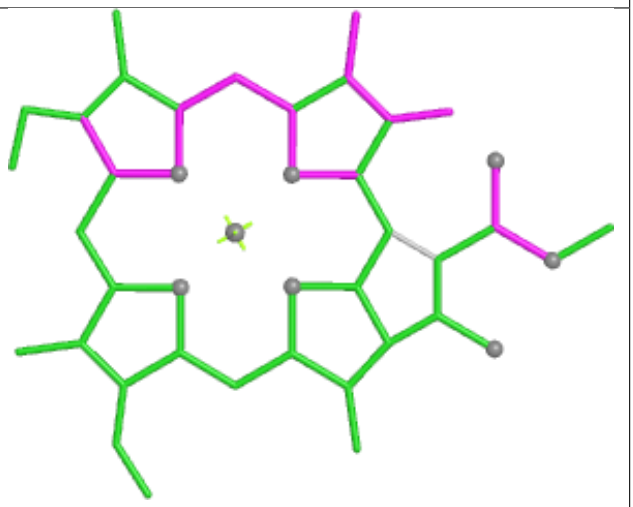


Rings

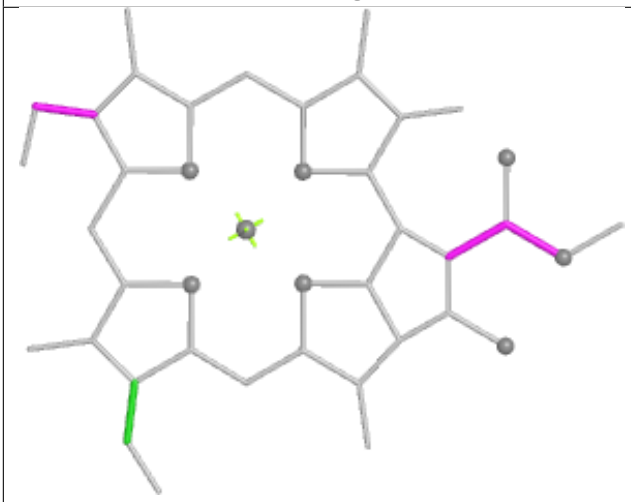
Ligand CLA A 834



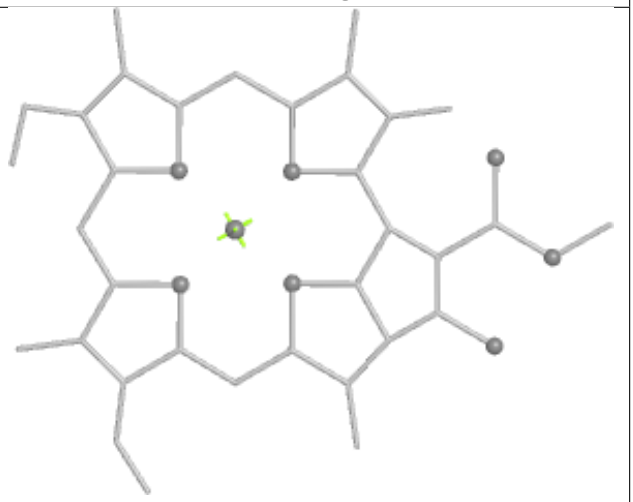
Bond lengths



Bond angles

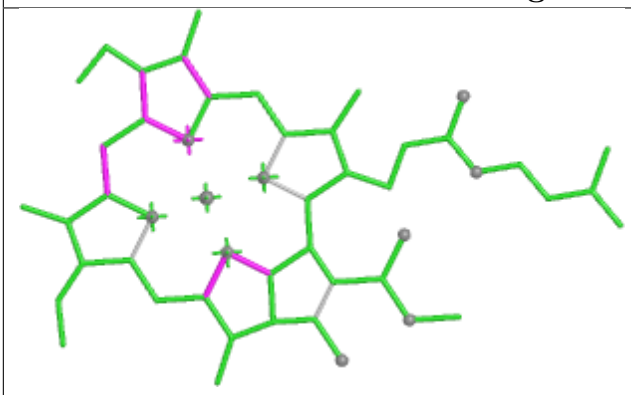


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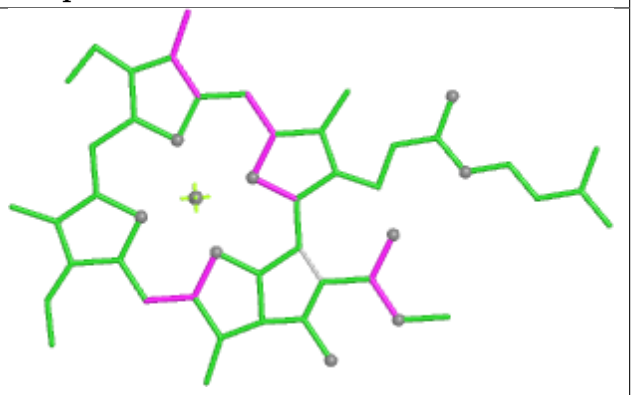


Rings

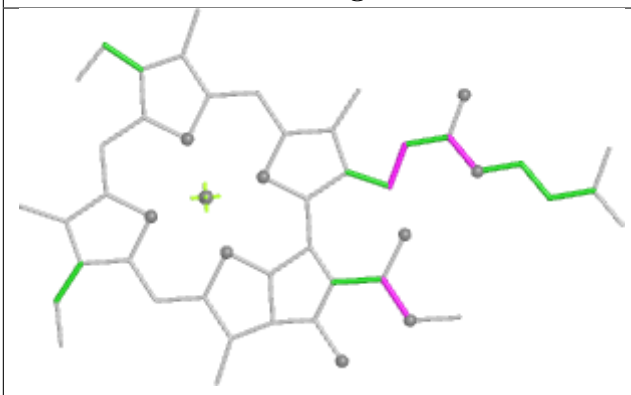
Ligand CLA q 309



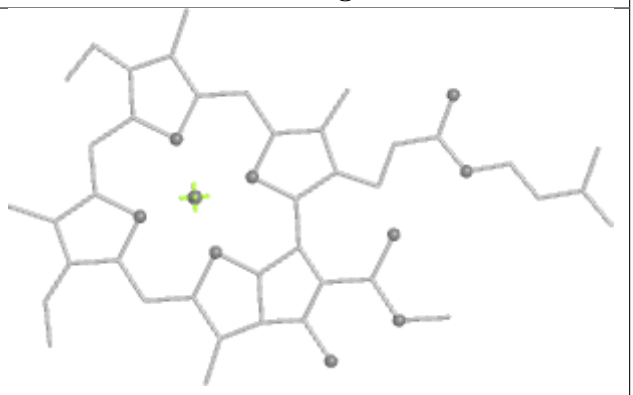
Bond lengths



Bond angles

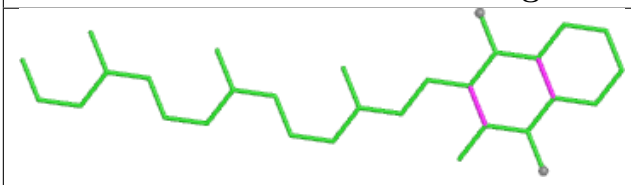


Torsions

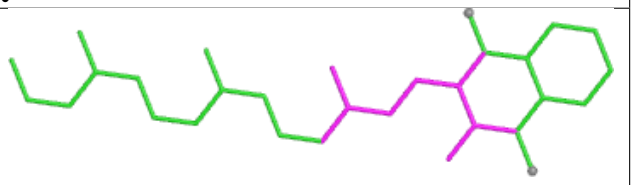


Rings

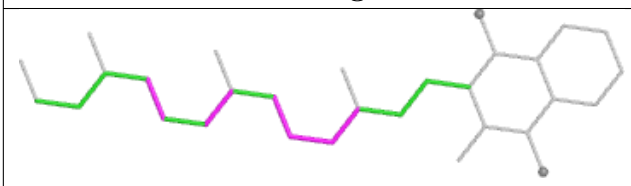
Ligand PQN B 843



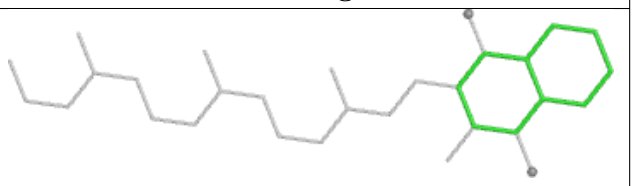
Bond lengths



Bond angles

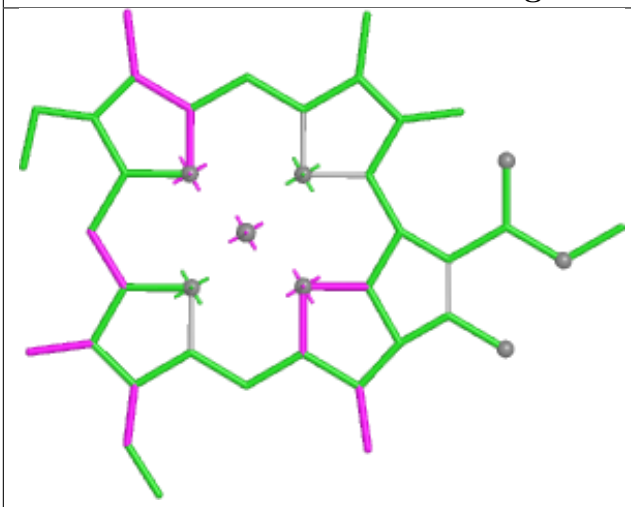


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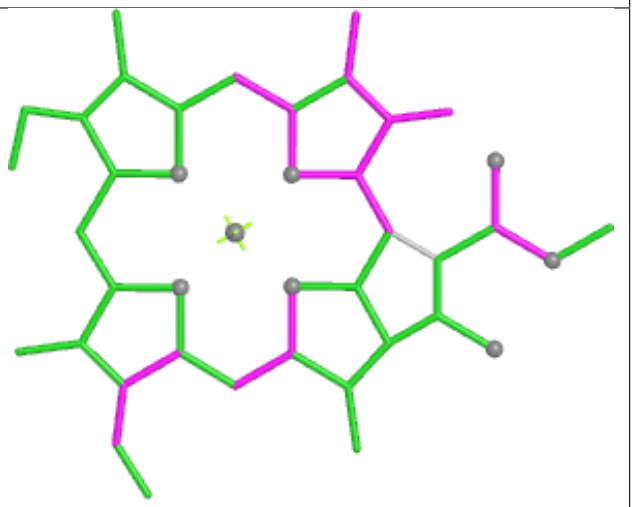


Rings

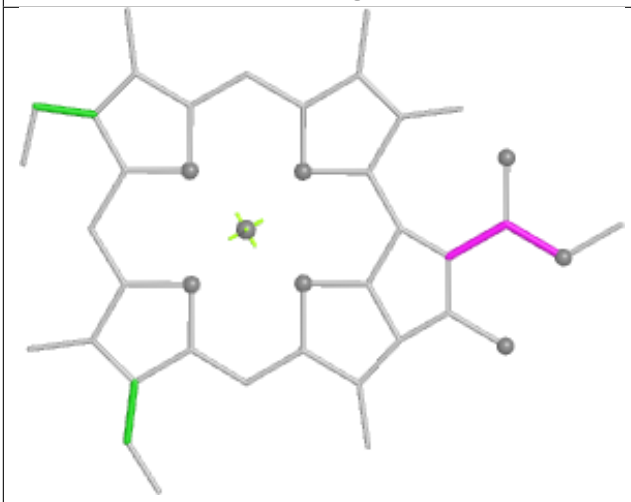
Ligand CLA B 814



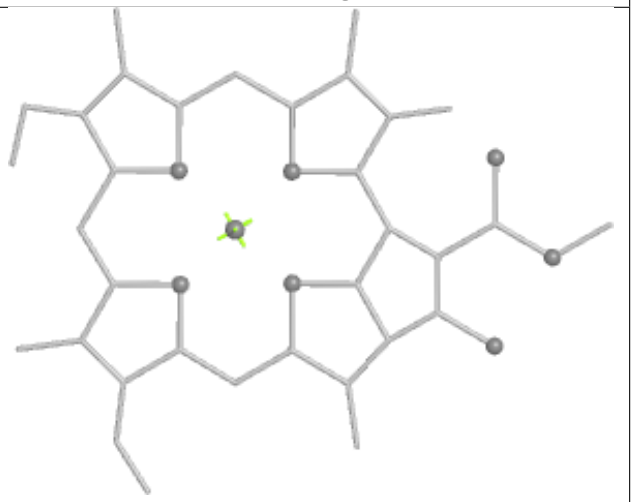
Bond lengths



Bond angles

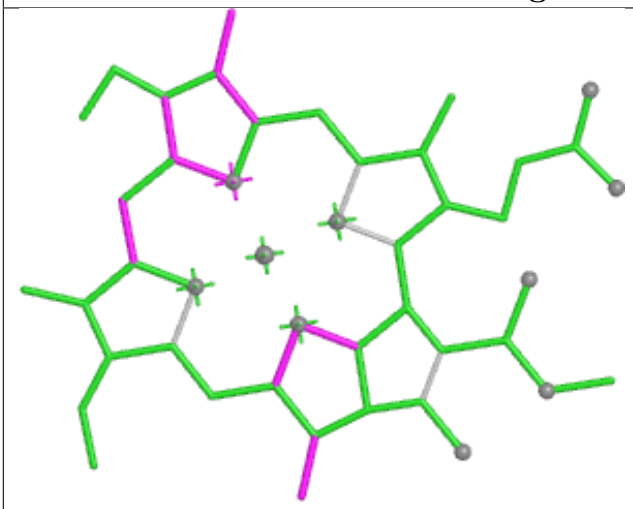


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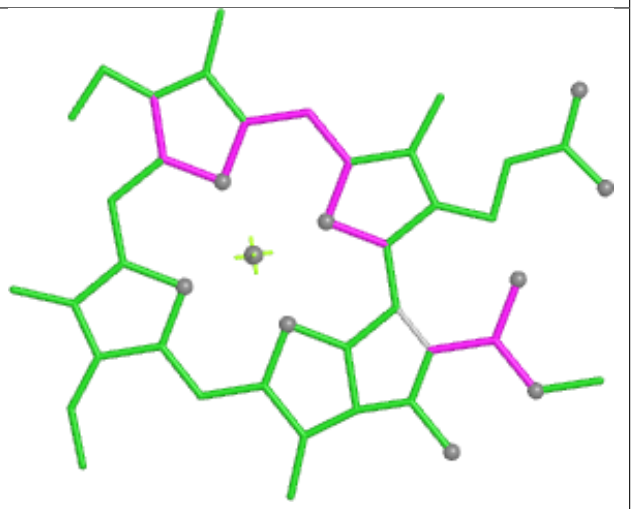


Rings

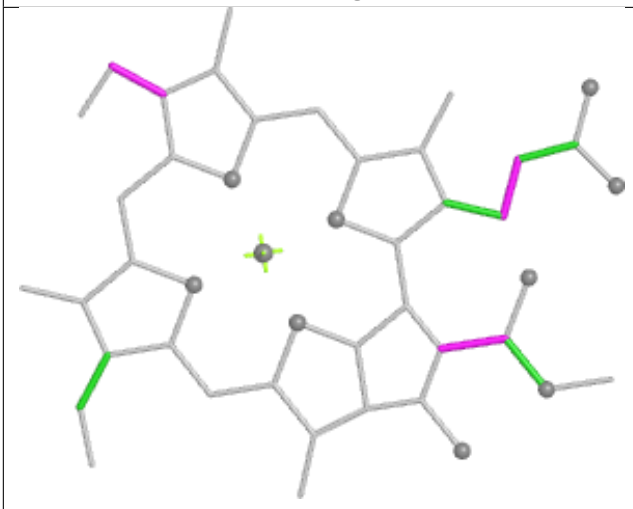
Ligand CLA e 819



Bond lengths



Bond angles

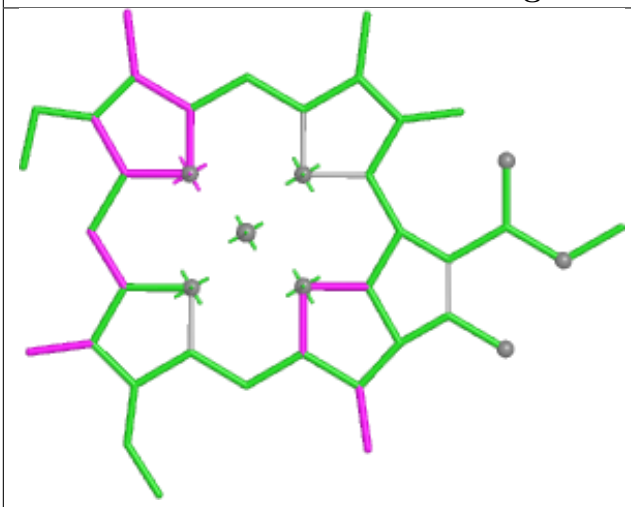


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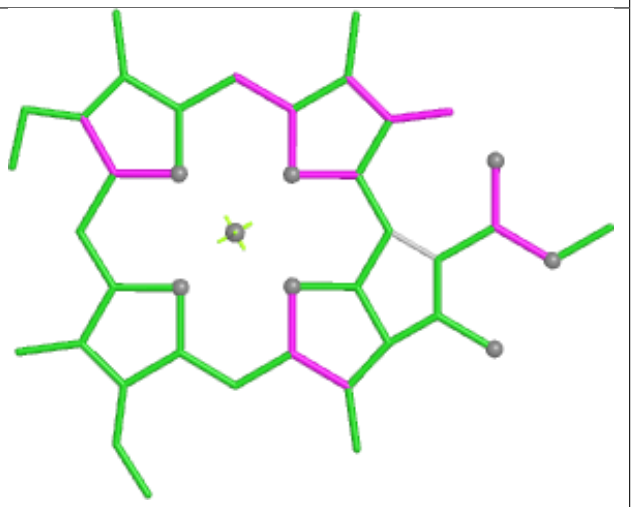


Rings

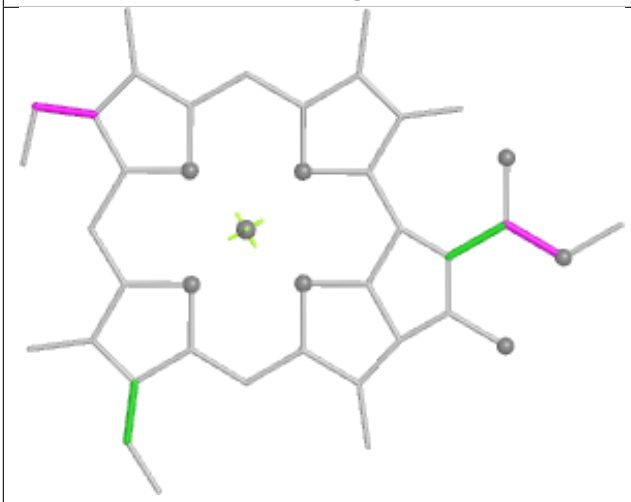
Ligand CLA A 840



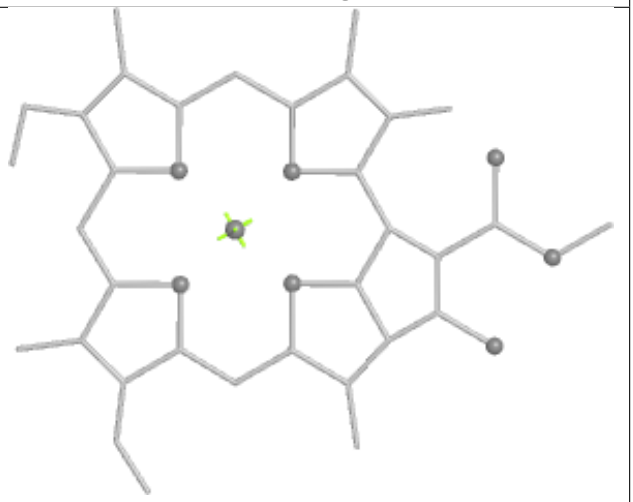
Bond lengths



Bond angles

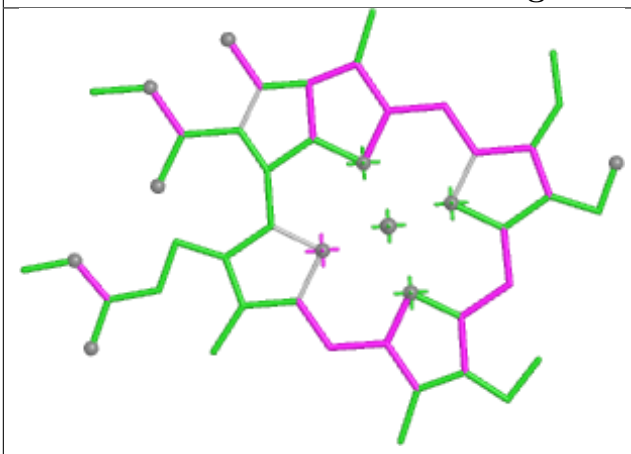


Torsions

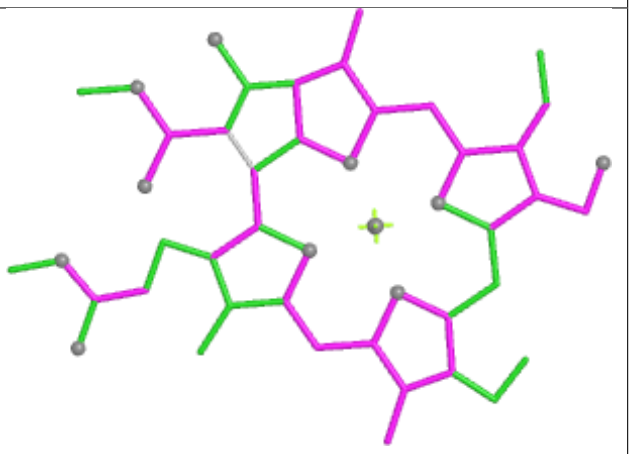


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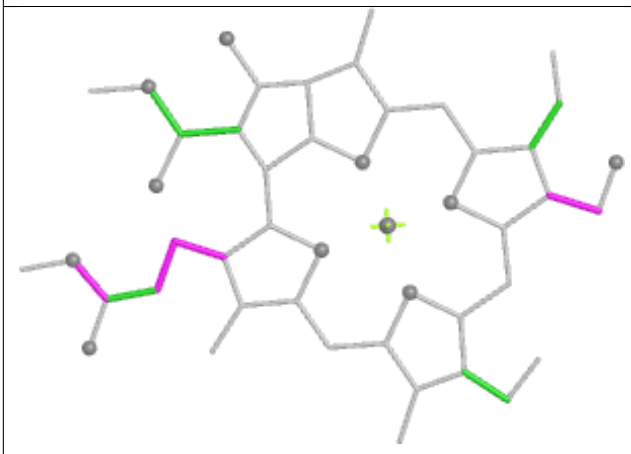
Ligand CHL 5 314



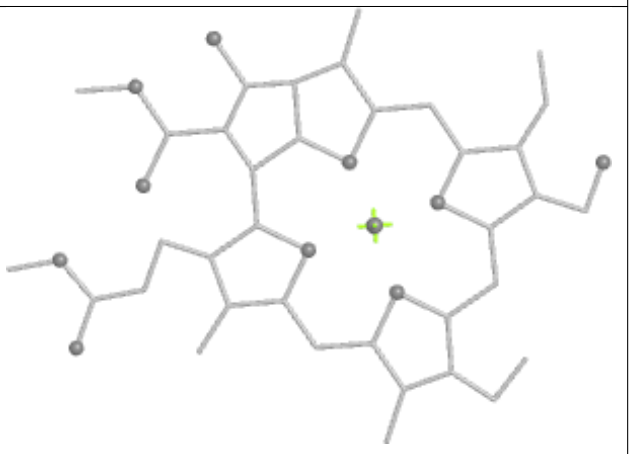
Bond lengths



Bond angles

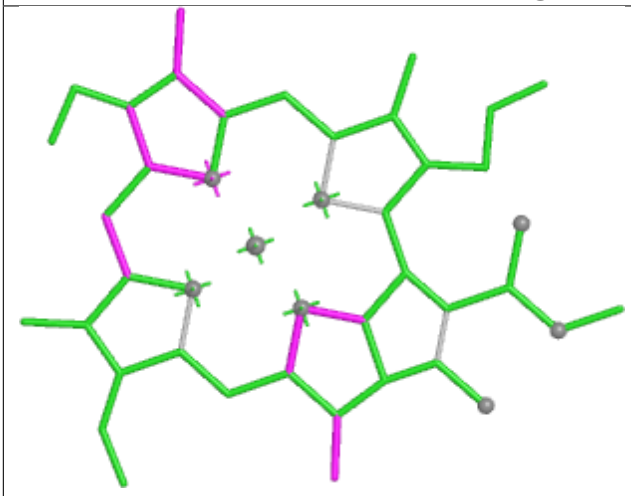


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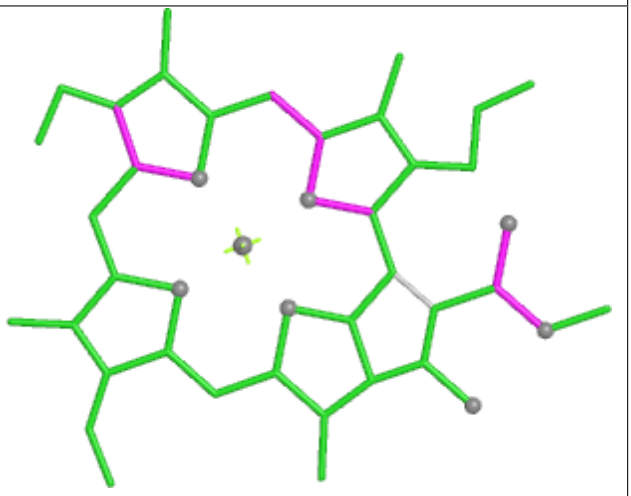


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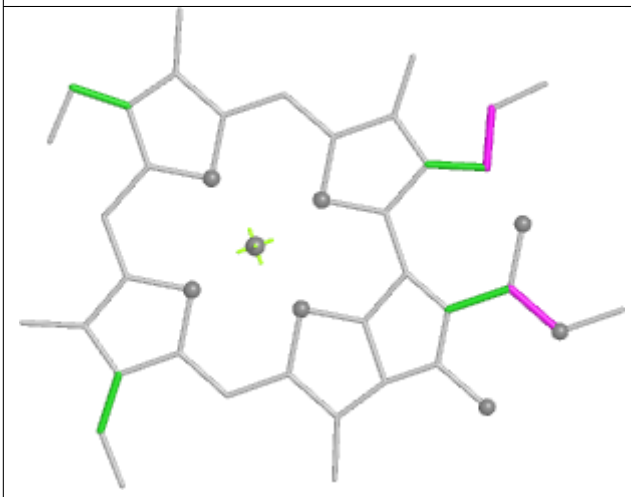
Ligand CLA f 833



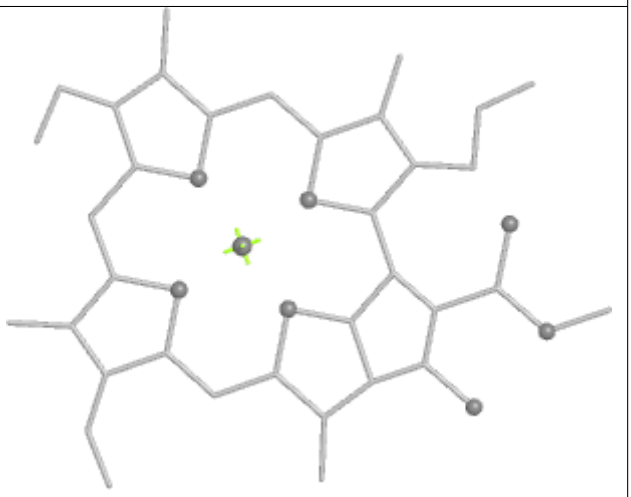
Bond lengths



Bond angles

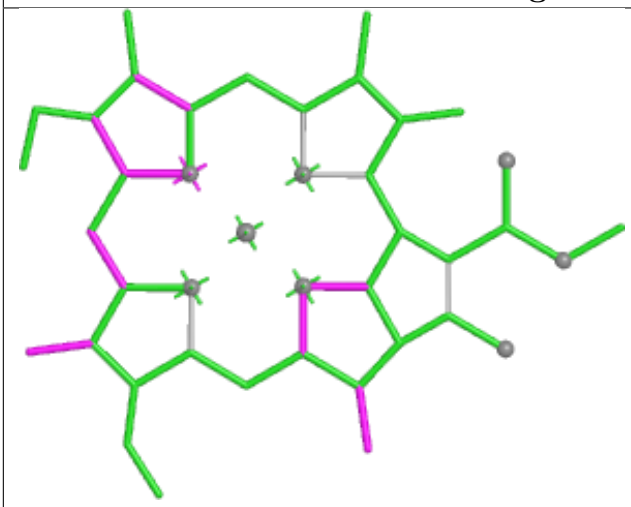


Torsions

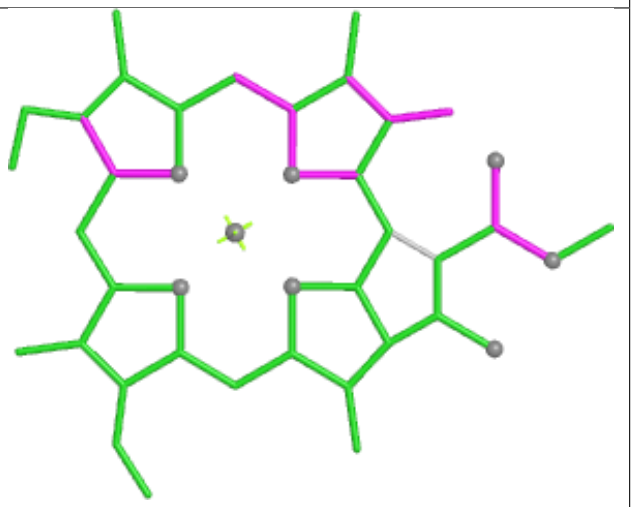


Rings

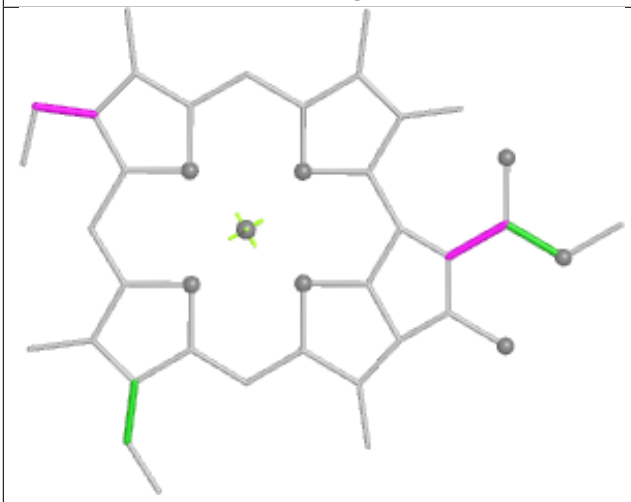
Ligand CLA e 822



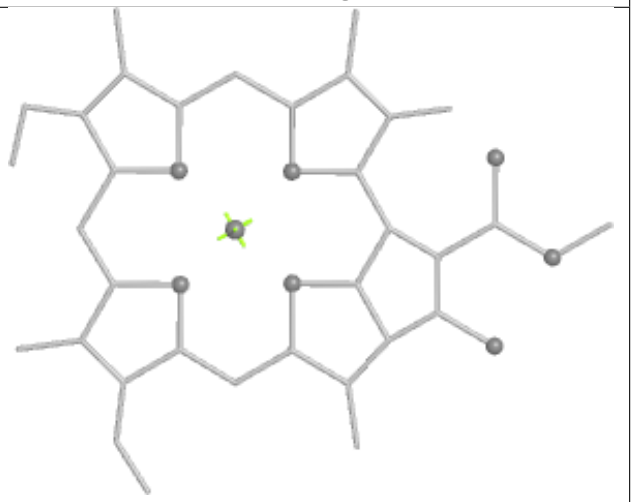
Bond lengths



Bond angles

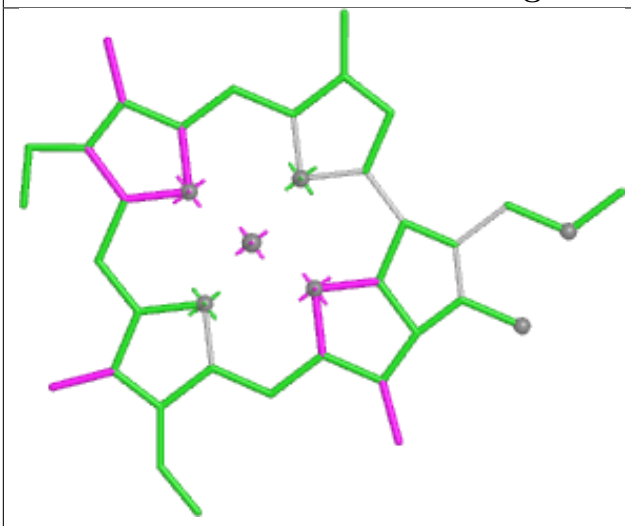


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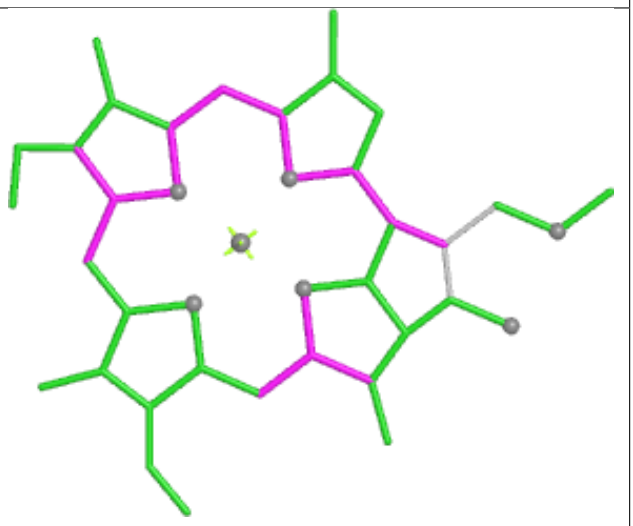


Rings

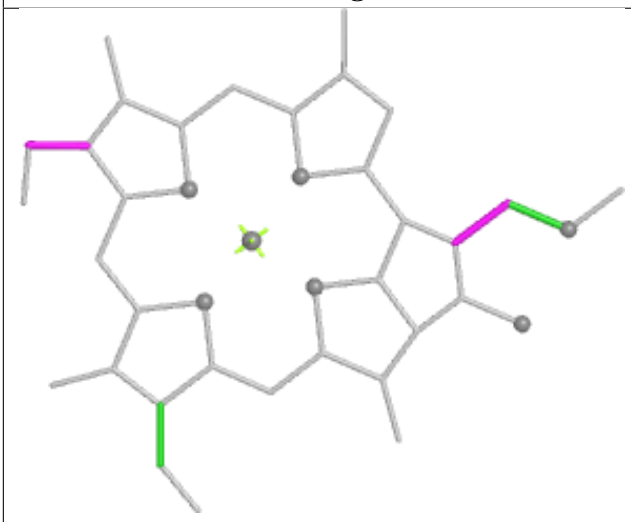
Ligand CLA A 807



Bond lengths



Bond angles

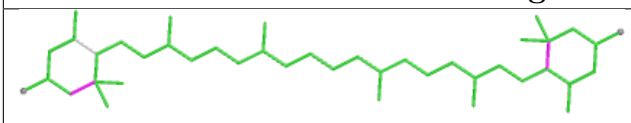


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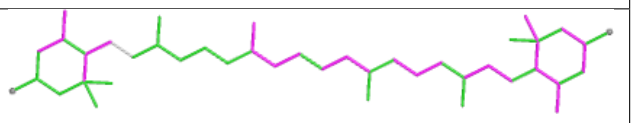


Rings

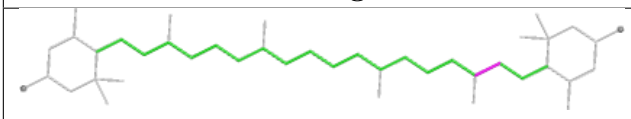
Ligand LUT 3 304



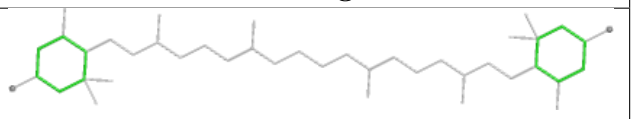
Bond lengths



Bond angles

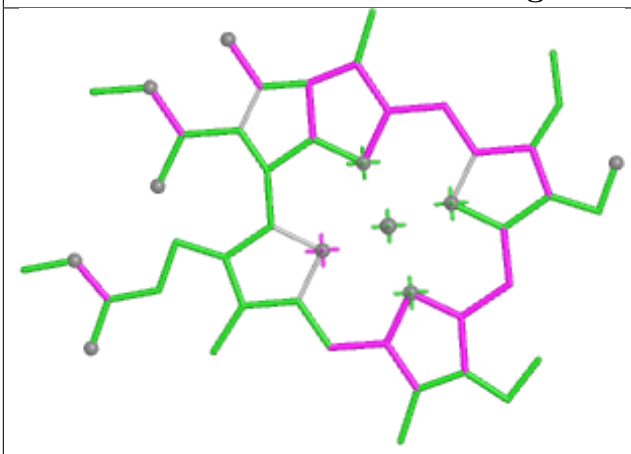


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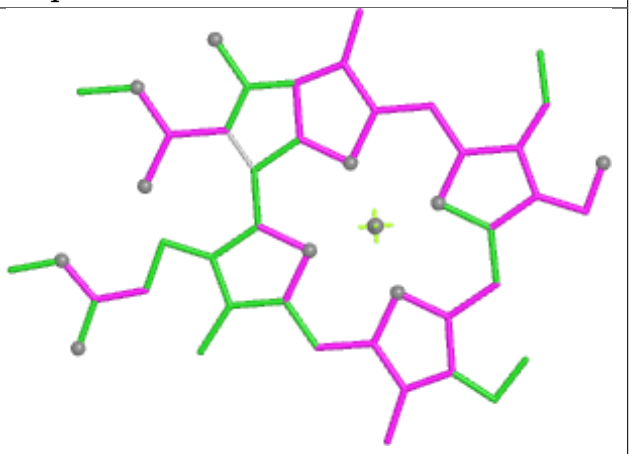


Rings

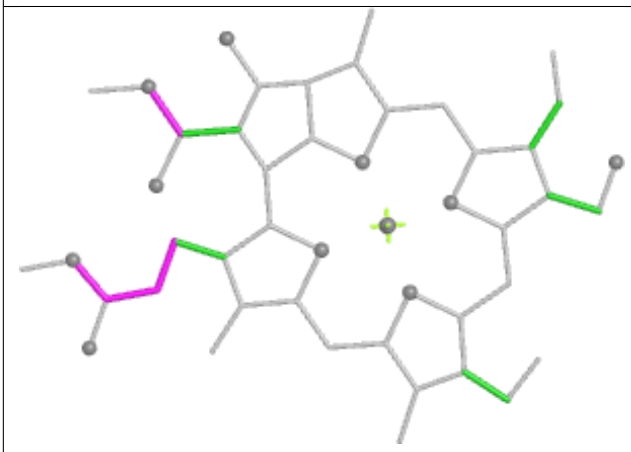
Ligand CHL p 514



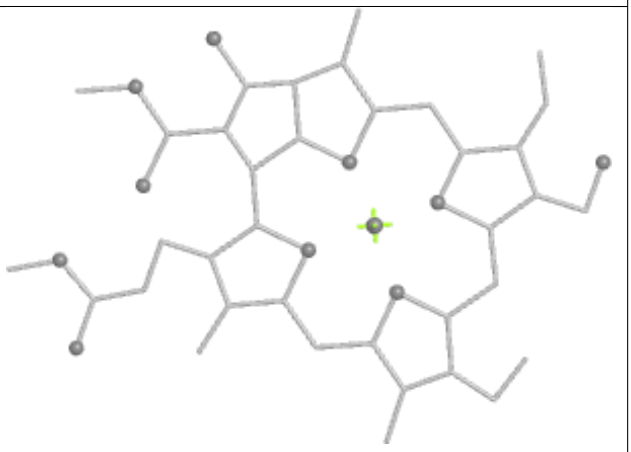
Bond lengths



Bond angles

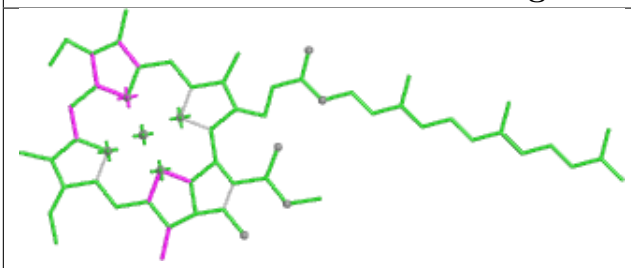


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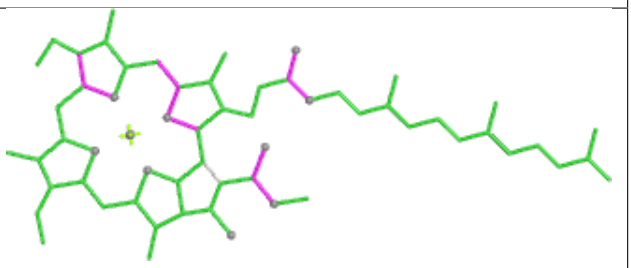


Rings

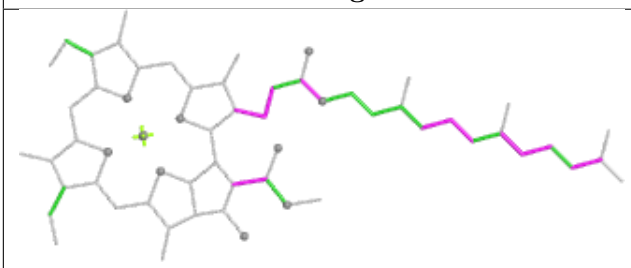
Ligand CLA o 303



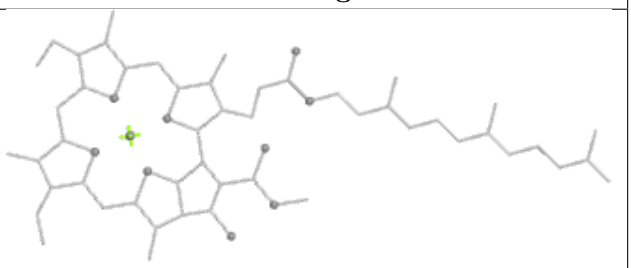
Bond lengths



Bond angles

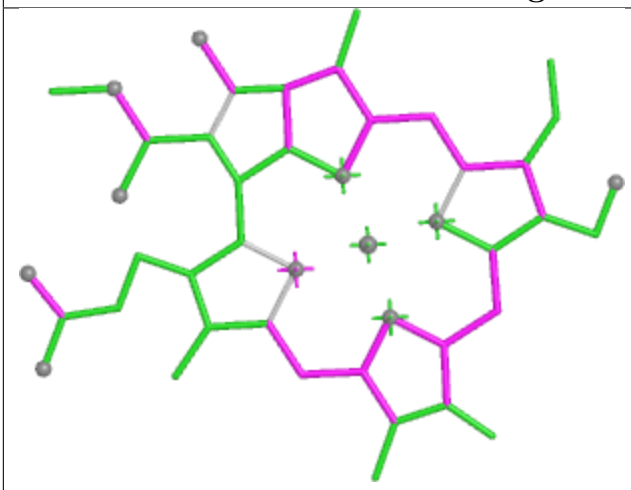


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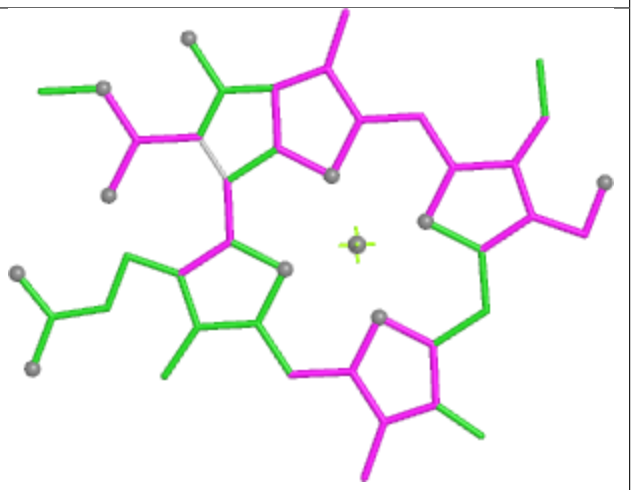


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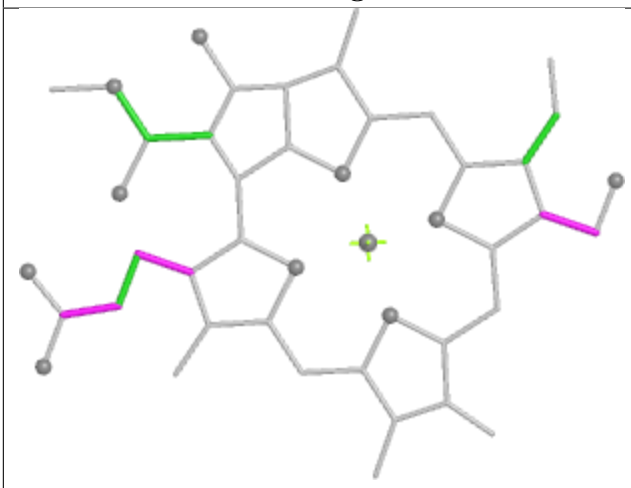
Ligand CHL 2 515



Bond lengths



Bond angles

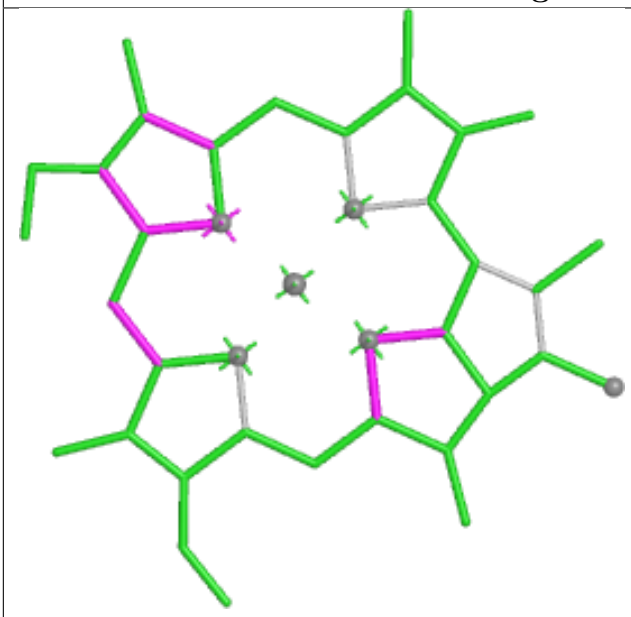


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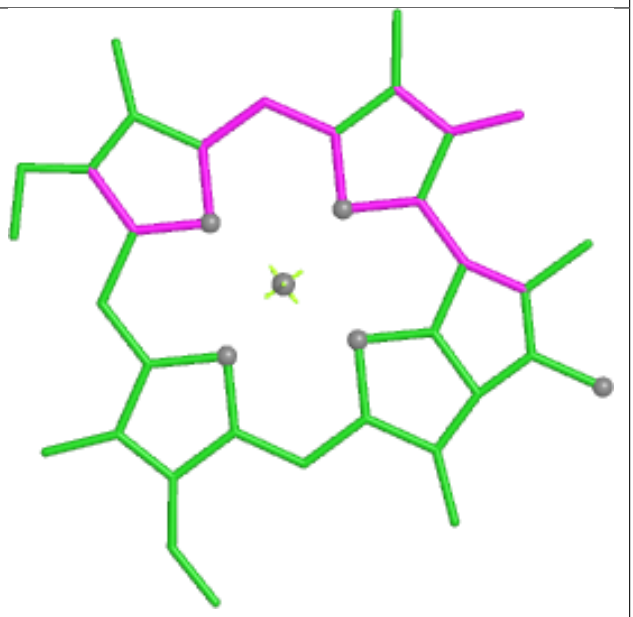


Rings

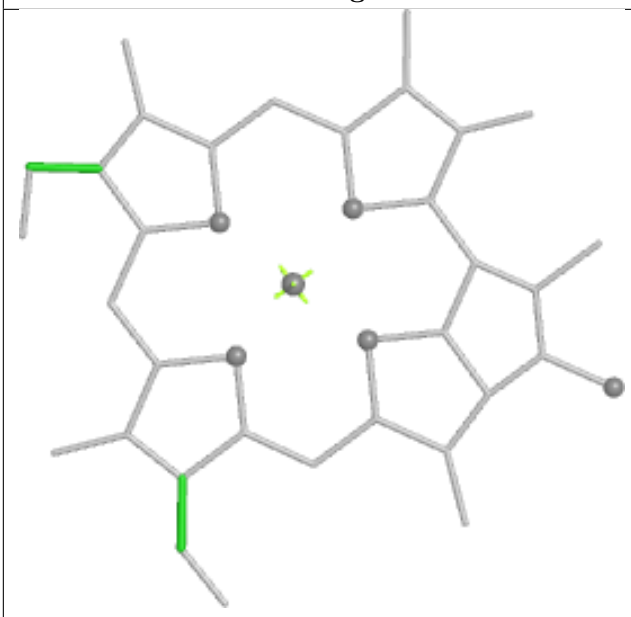
Ligand CLA f 843



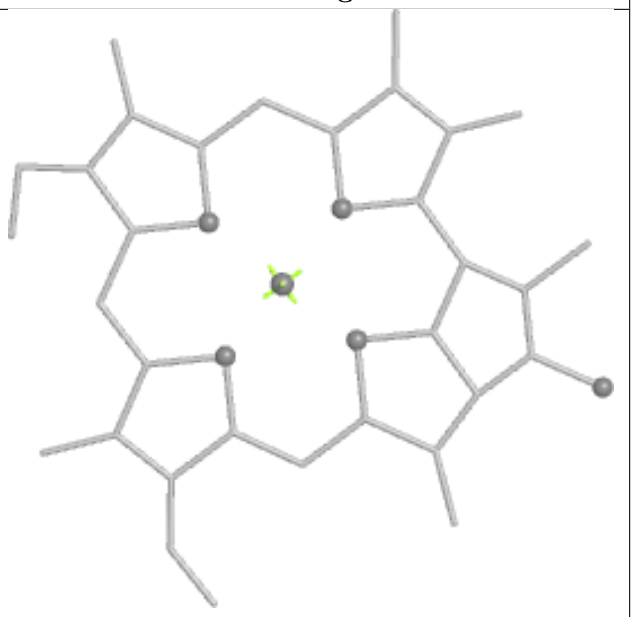
Bond lengths



Bond angles

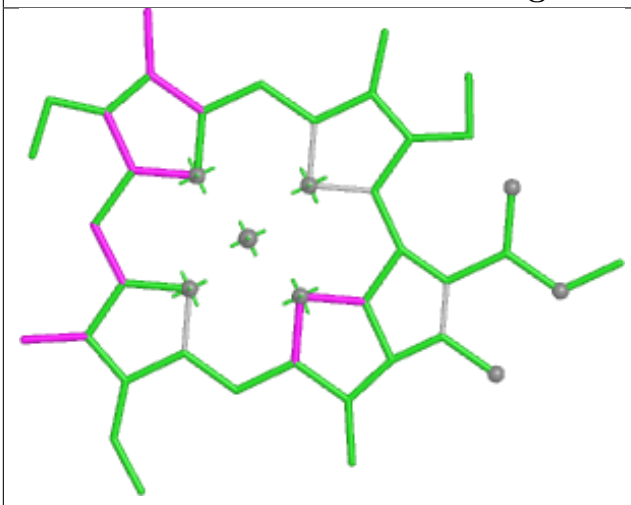


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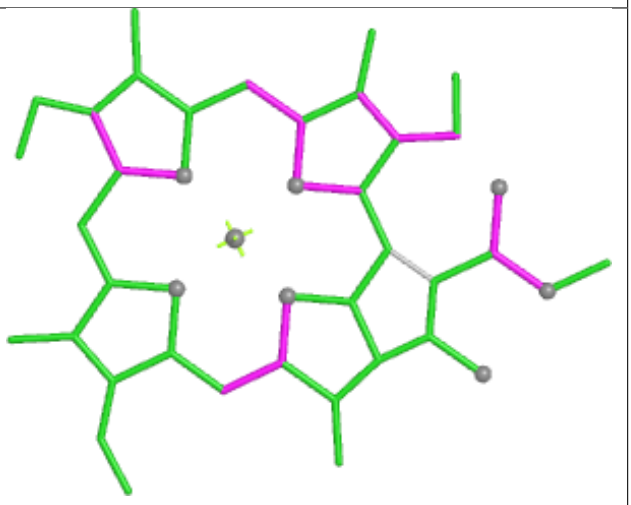


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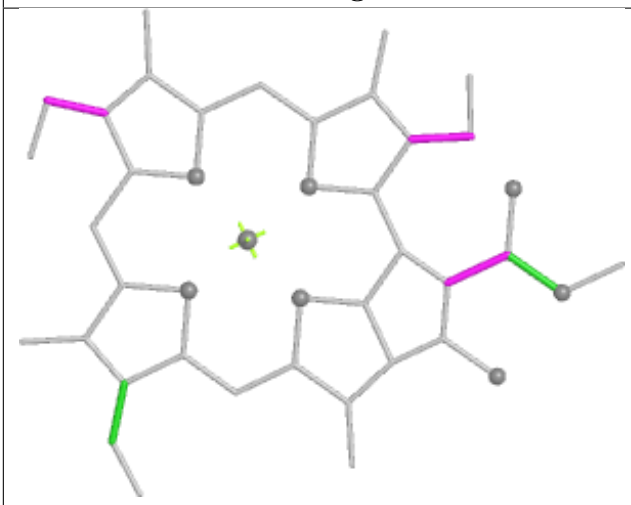
Ligand CLA 1 505



Bond lengths



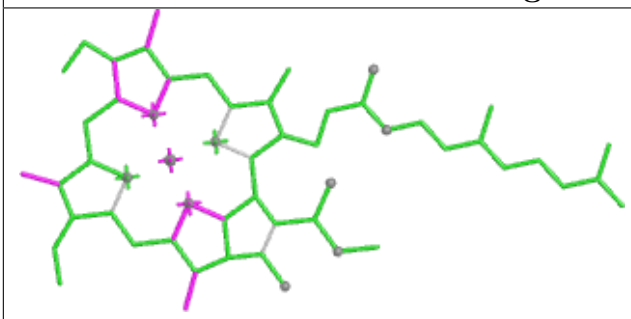
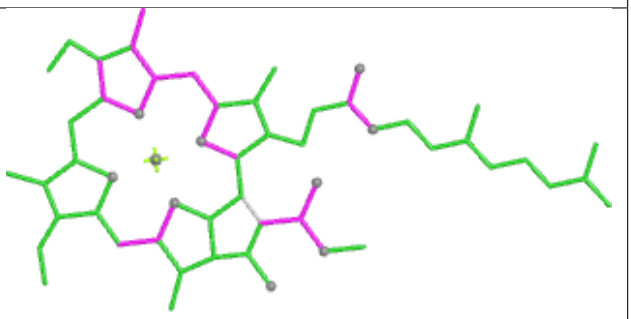
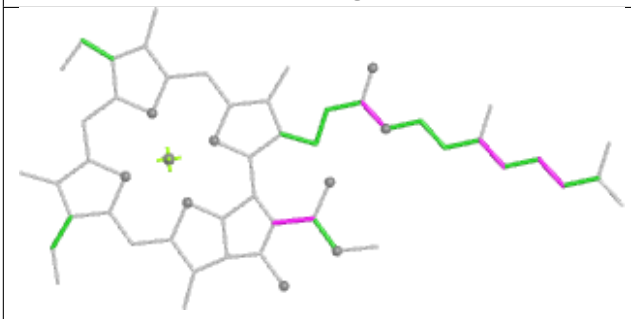
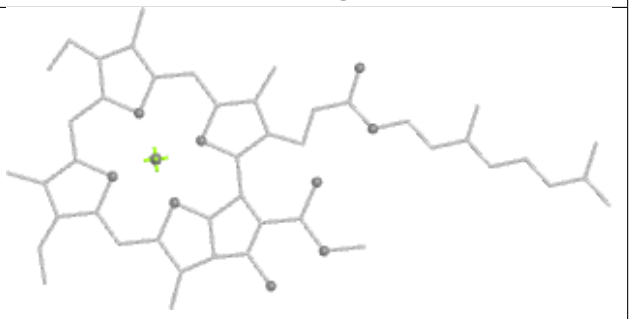
Bond angles



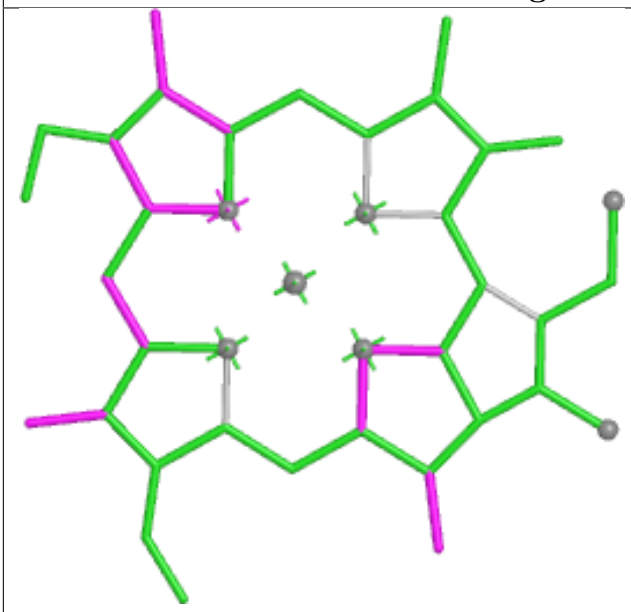
Torsions



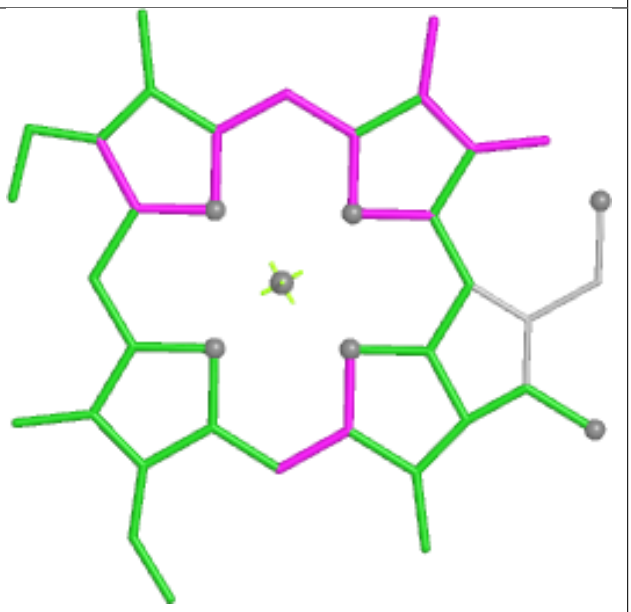
Rings

Ligand CLA A 829	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

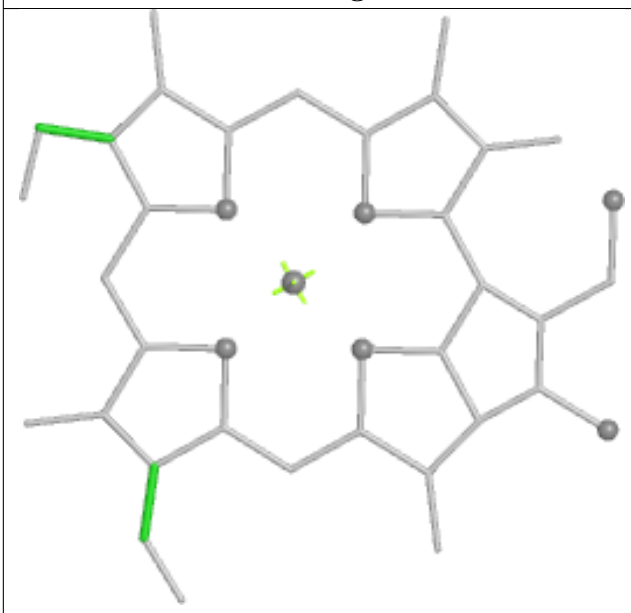
Ligand CLA e 817



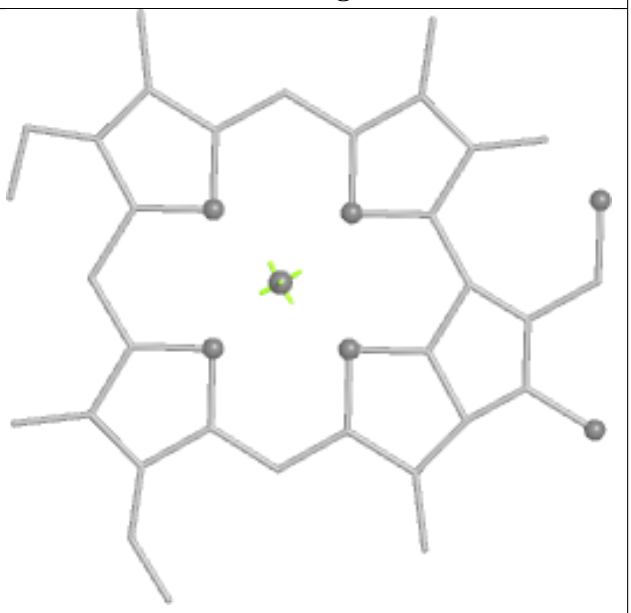
Bond lengths



Bond angles

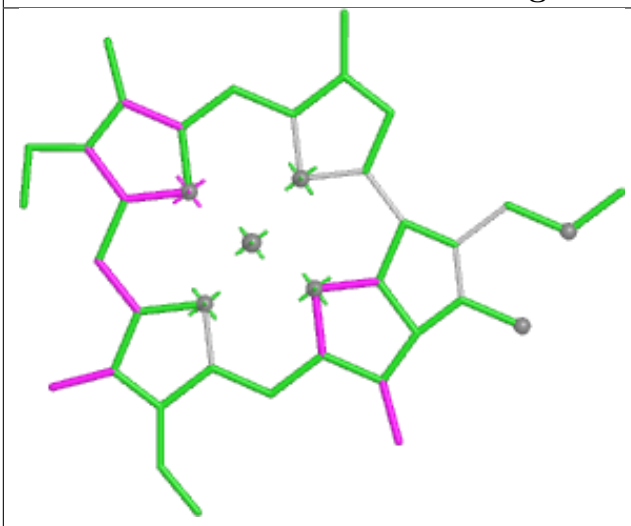


Torsions

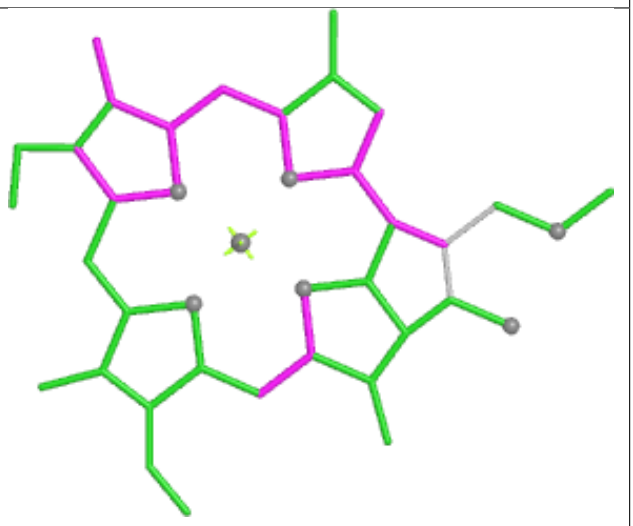


Rings

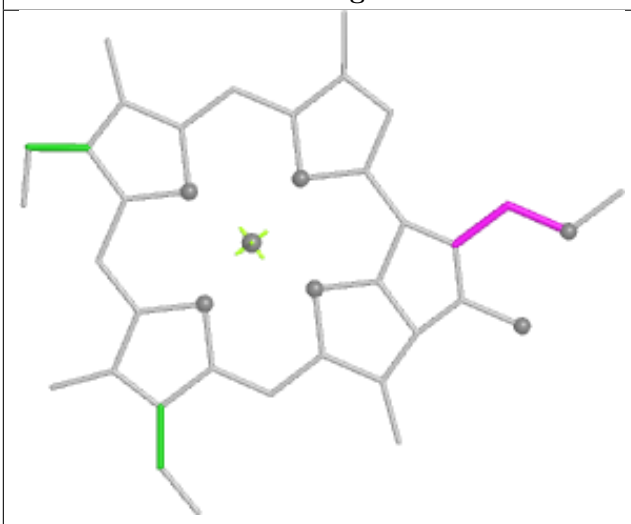
Ligand CLA e 812



Bond lengths



Bond angles

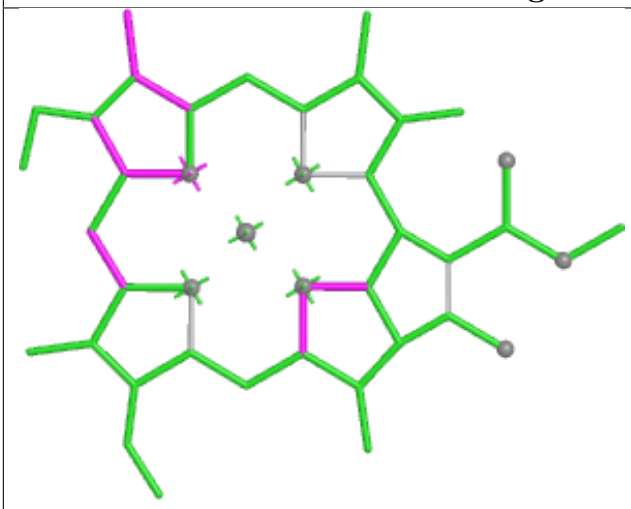


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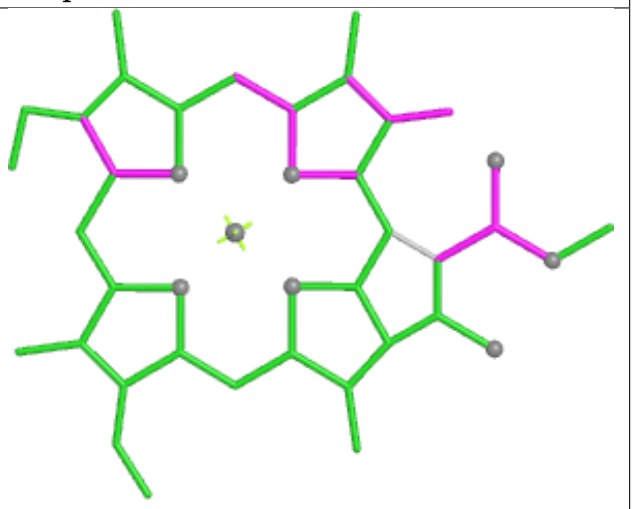


Rings

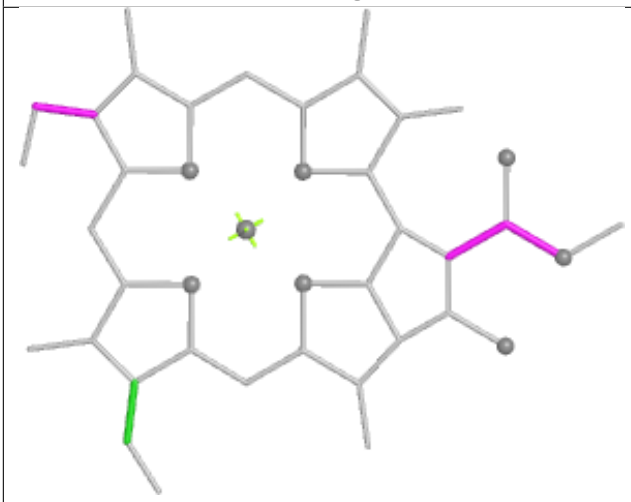
Ligand CLA q 306



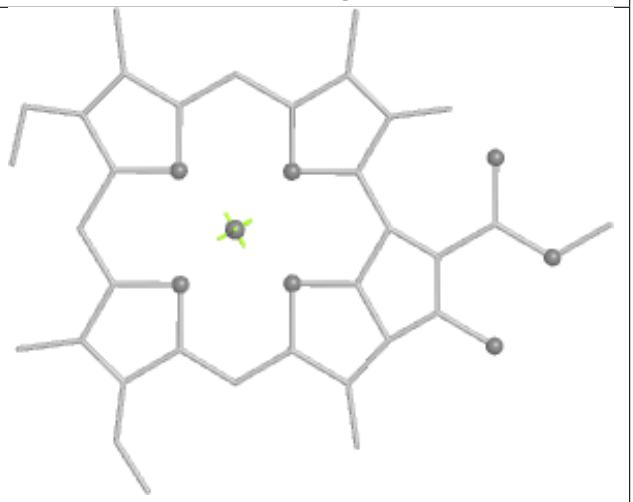
Bond lengths



Bond angles



Torsions

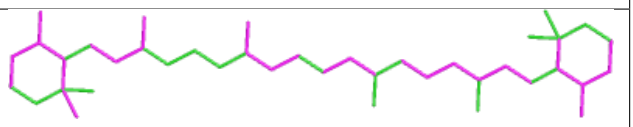


Rings

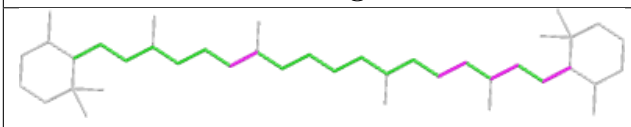
Ligand BCR L 306



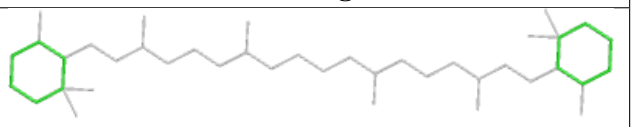
Bond lengths



Bond angles

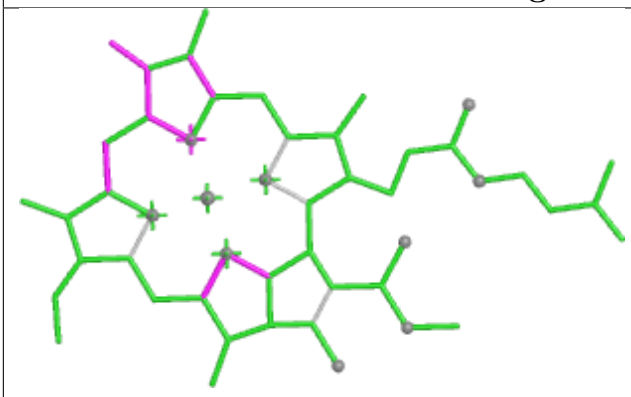


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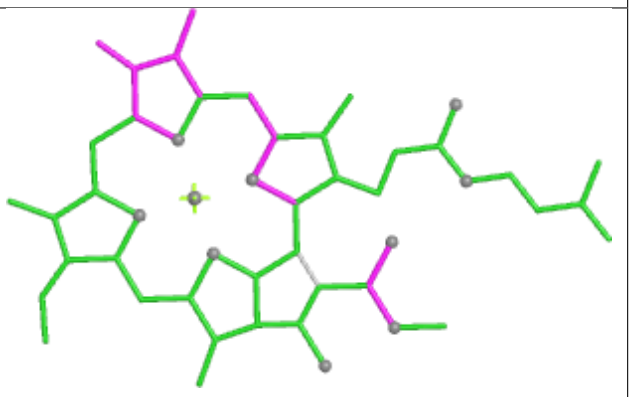


Rings

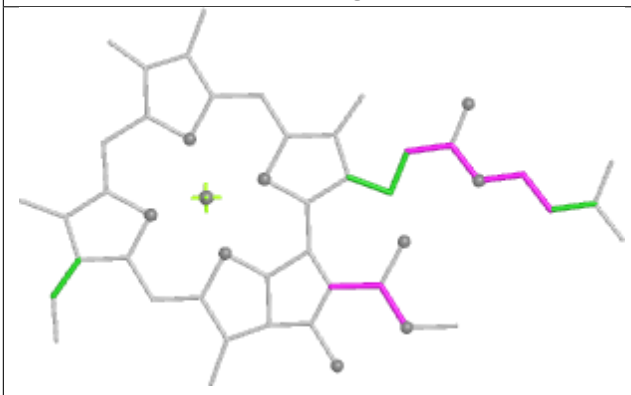
Ligand CLA e 843



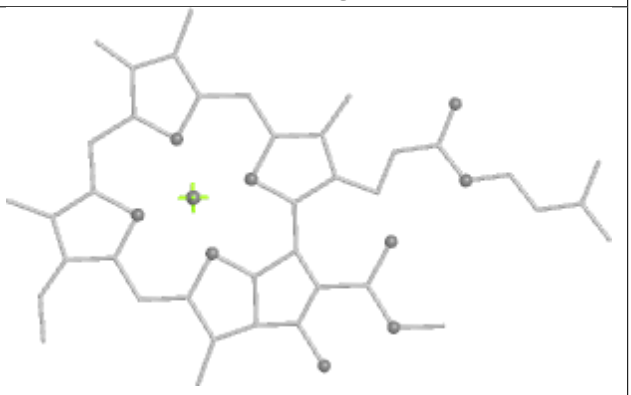
Bond lengths



Bond angles

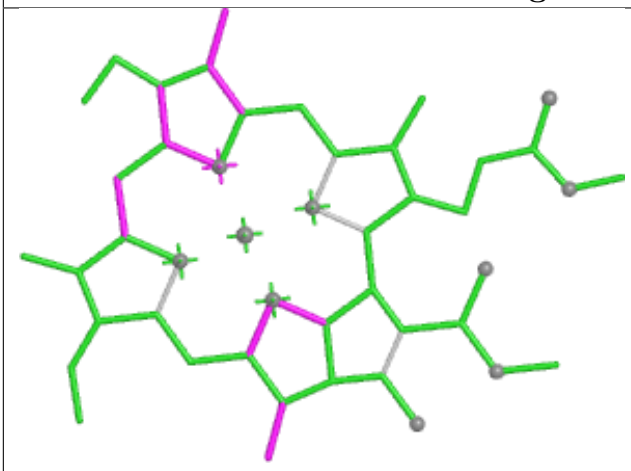


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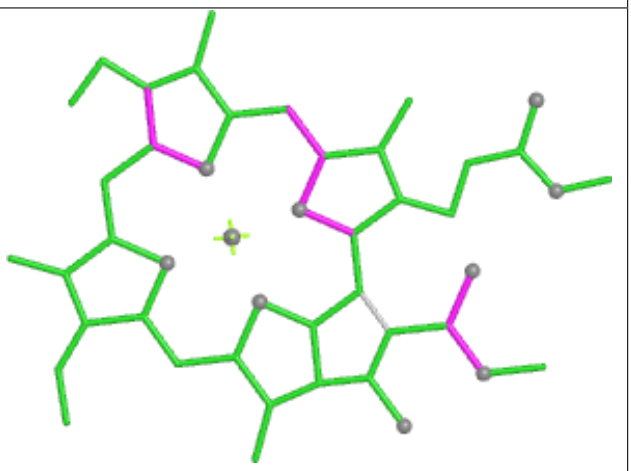


Rings

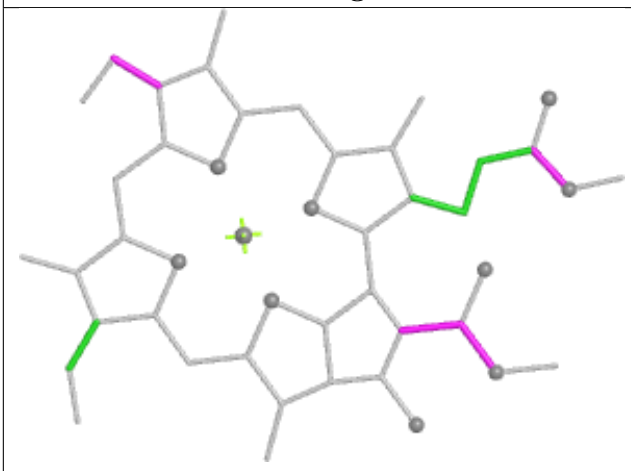
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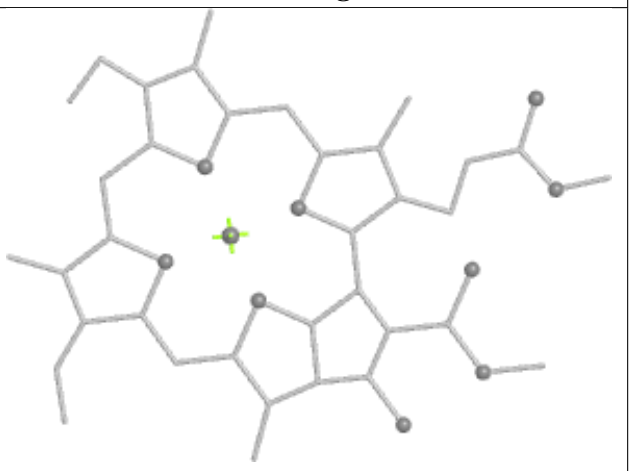
Bond lengths



Bond angles



Torsions

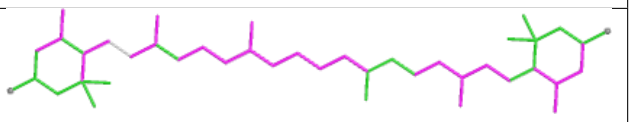


Rings

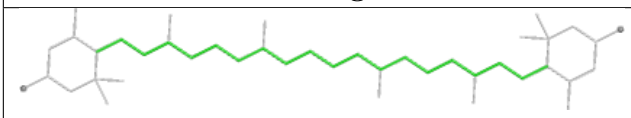
Ligand LUT 2 501



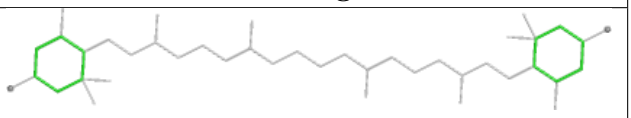
Bond lengths



Bond angles

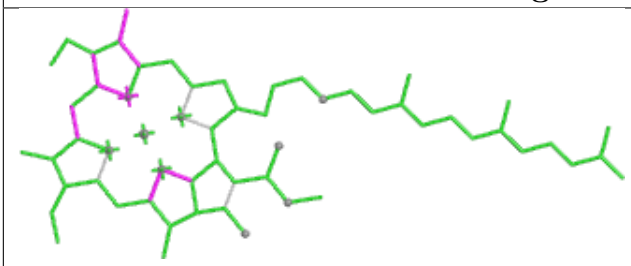


Torsions

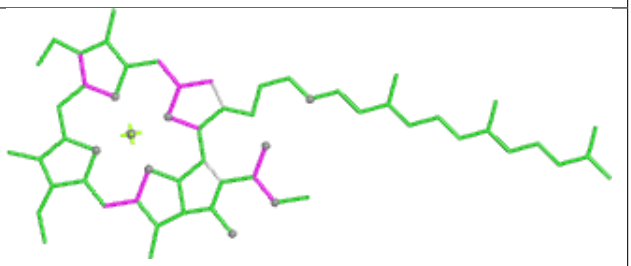


Rings

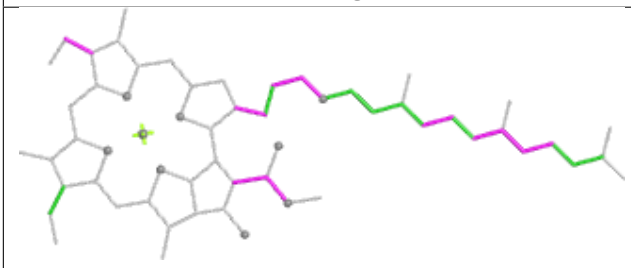
Ligand CLA f 836



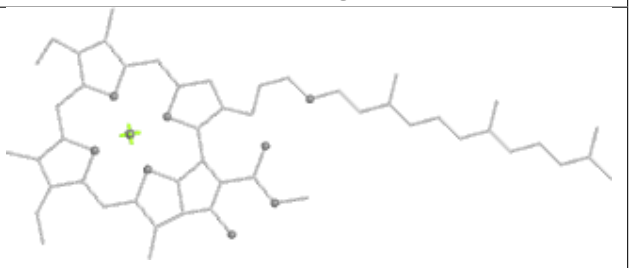
Bond lengths



Bond angles

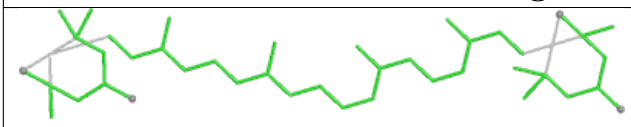


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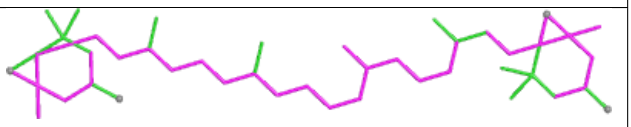


Rings

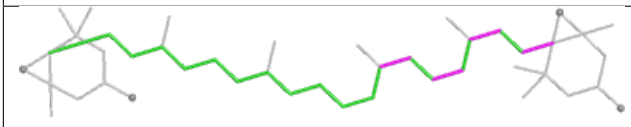
Ligand XAT s 502



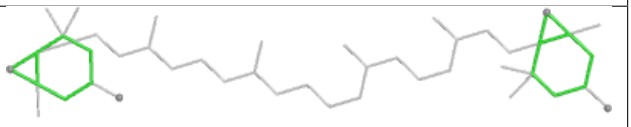
Bond lengths



Bond angles

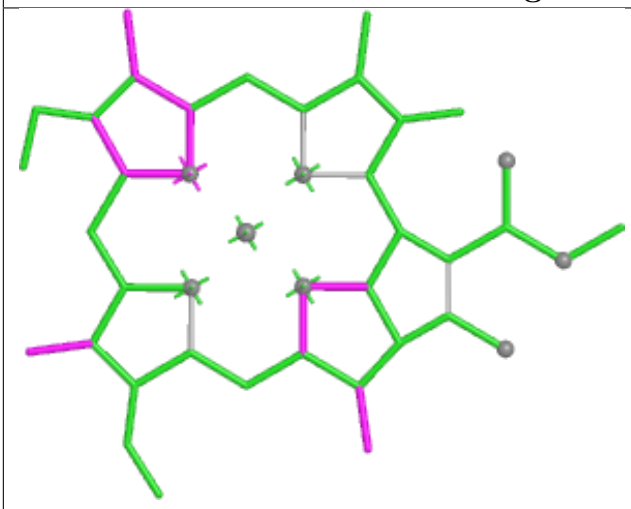


Torsions

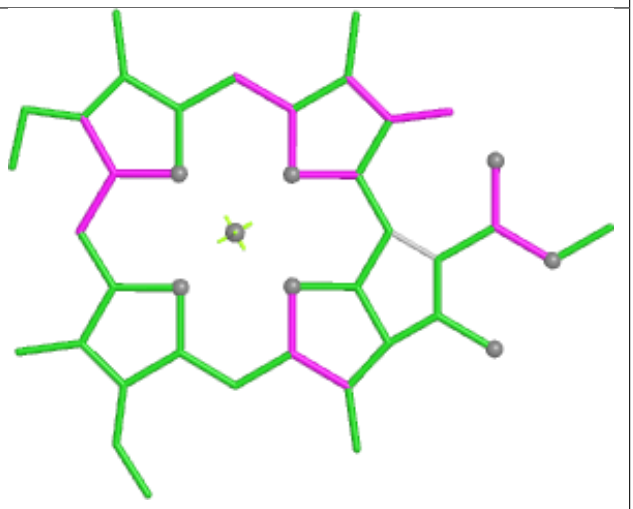


Rings

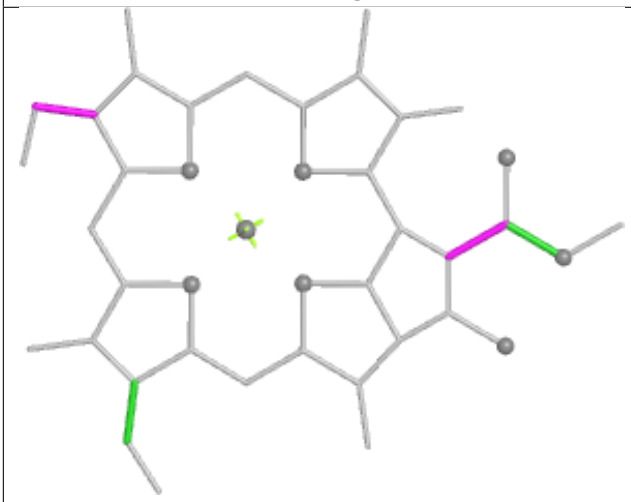
Ligand CLA B 840



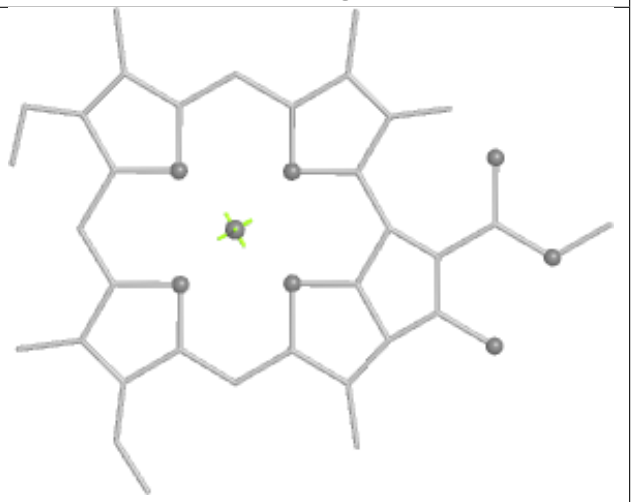
Bond lengths



Bond angles

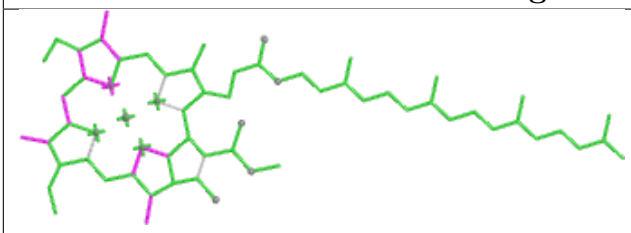


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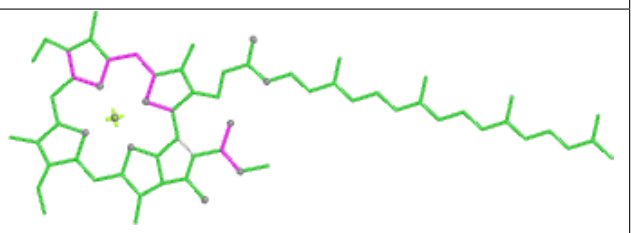


Rings

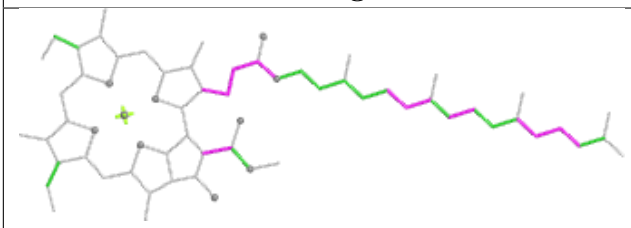
Ligand CLA e 804



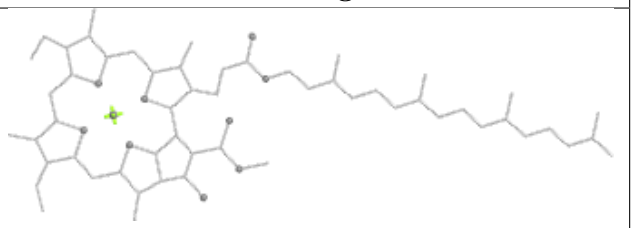
Bond lengths



Bond angles

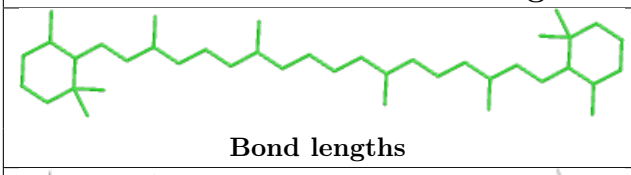


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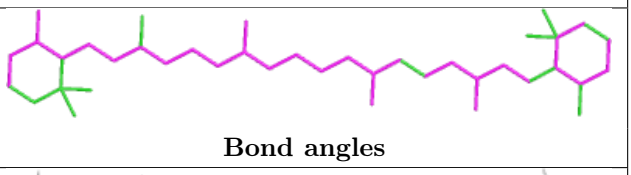


Rings

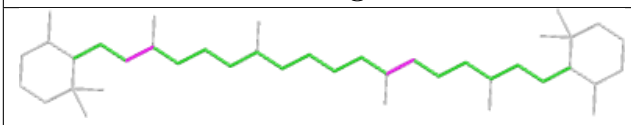
Ligand BCR e 854



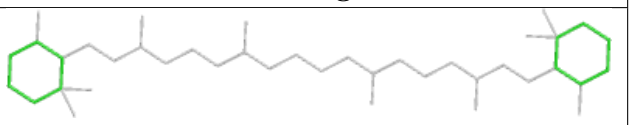
Bond lengths



Bond angles



Torsions

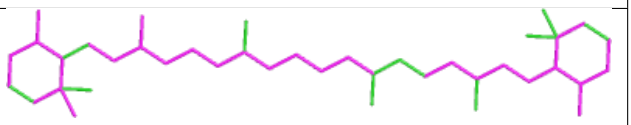


Rings

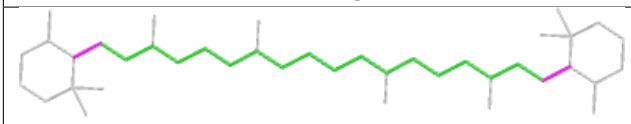
Ligand BCR e 851



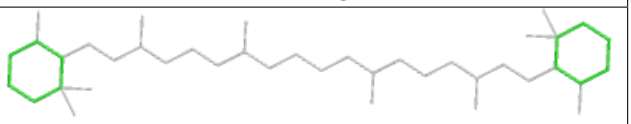
Bond lengths



Bond angles

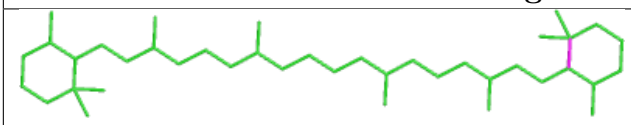


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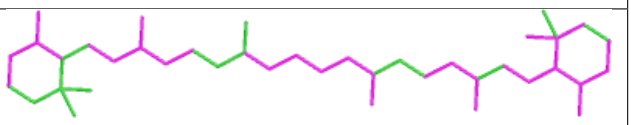


Rings

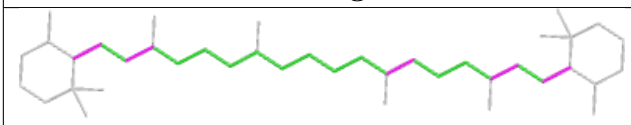
Ligand BCR L 305



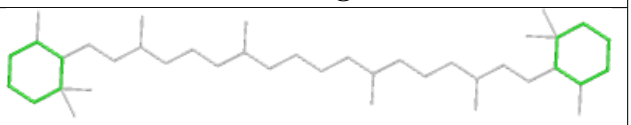
Bond lengths



Bond angles

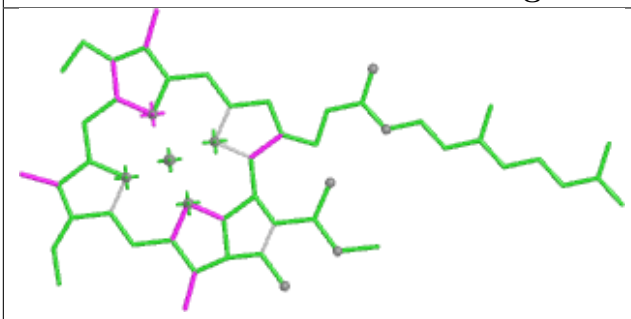


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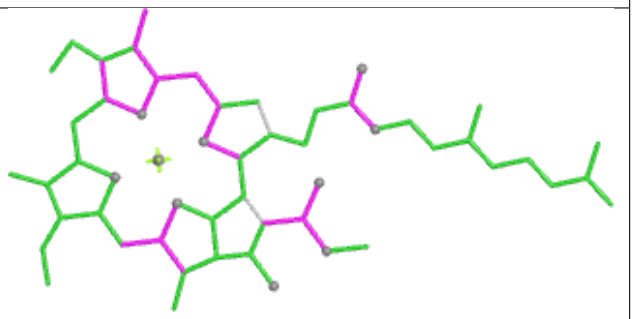


Rings

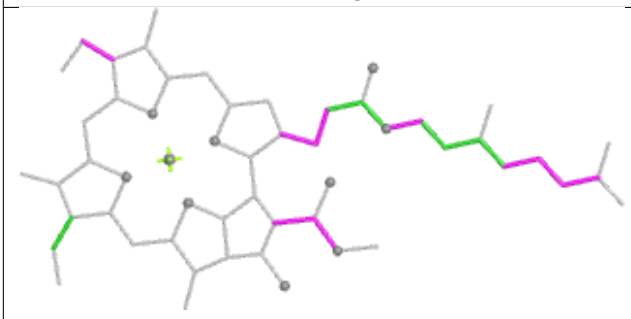
Ligand CLA A 823



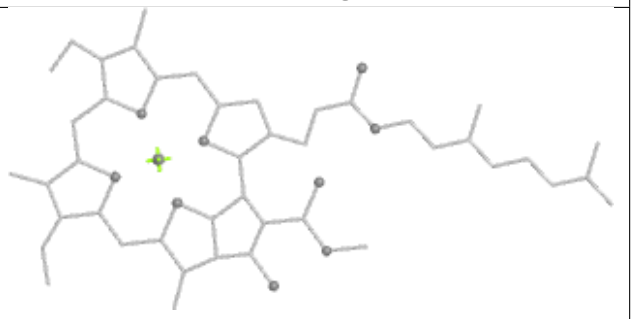
Bond lengths



Bond angles

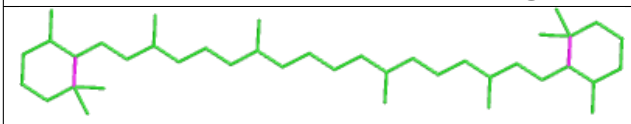


Torsions



Rings

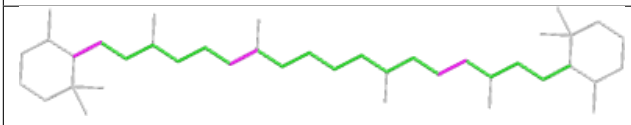
Ligand BCR B 847



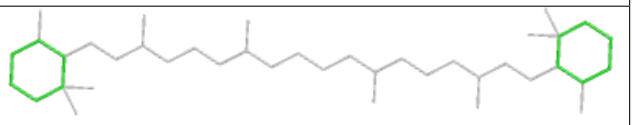
Bond lengths



Bond angles

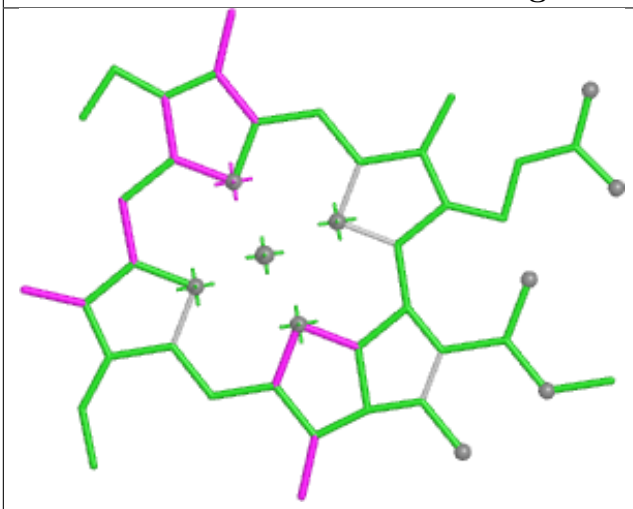


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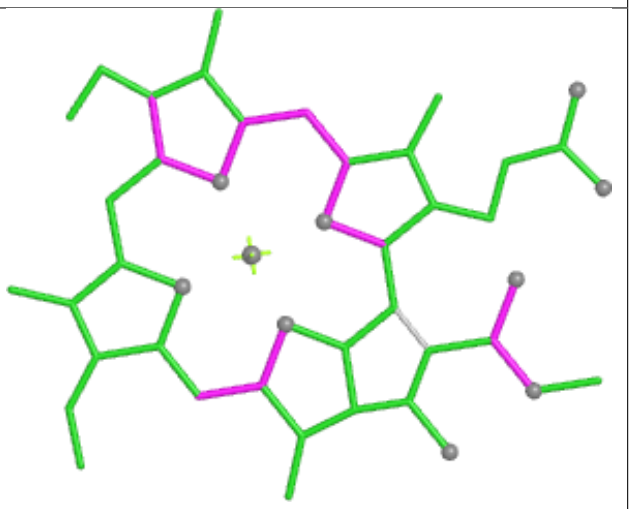


Rings

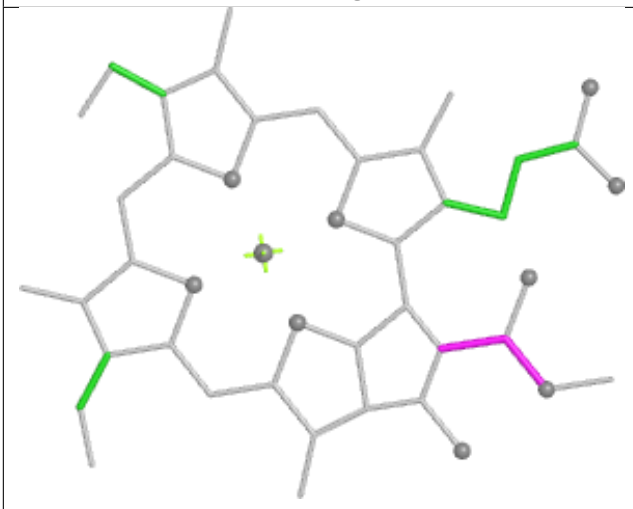
Ligand CLA e 834



Bond lengths



Bond angles

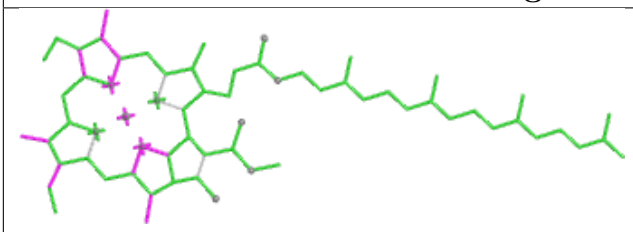


Torsions

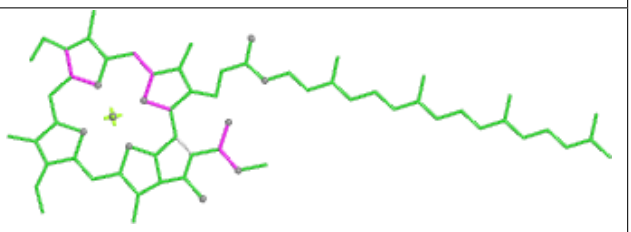


Rings

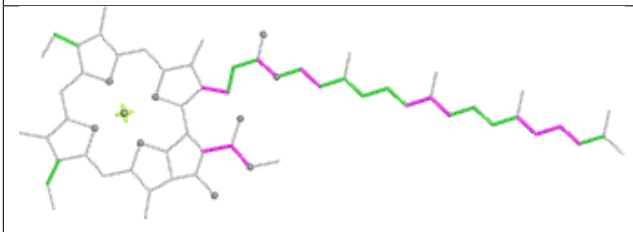
Ligand CLA B 804



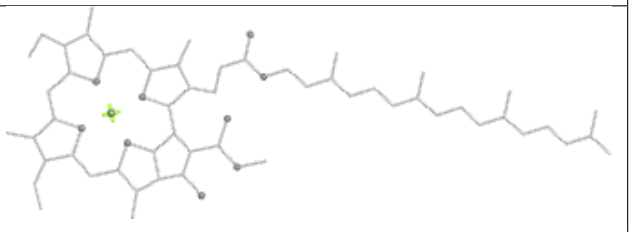
Bond lengths



Bond angles

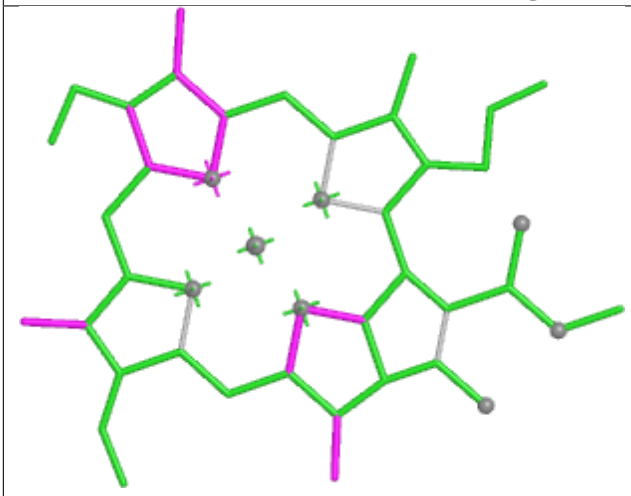


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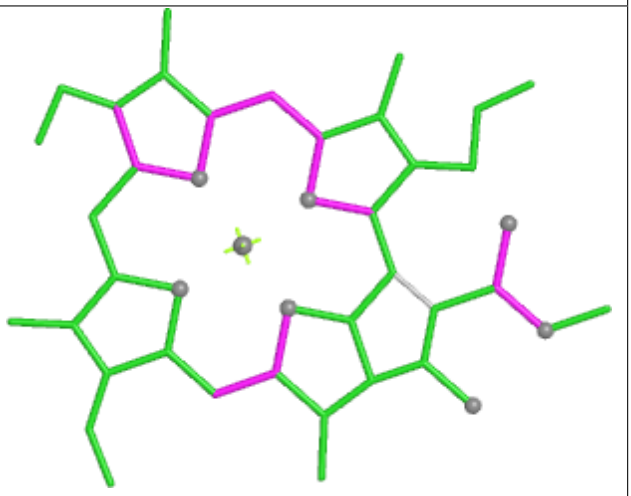


Rings

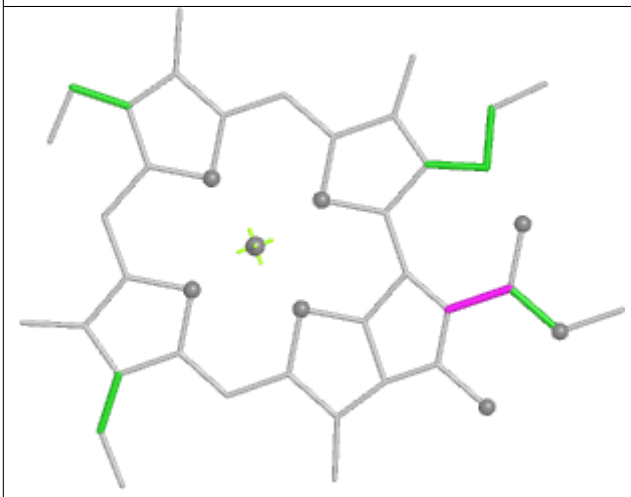
Ligand CLA B 831



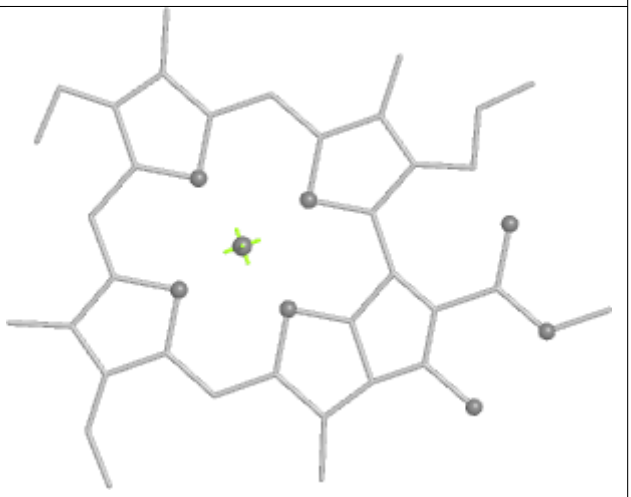
Bond lengths



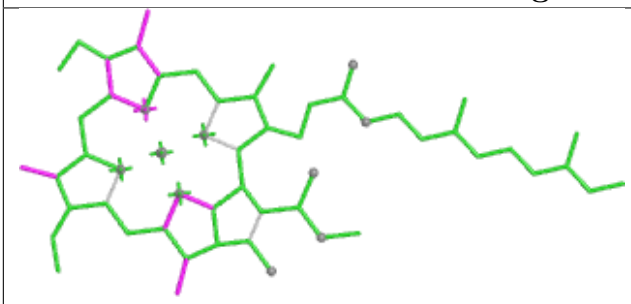
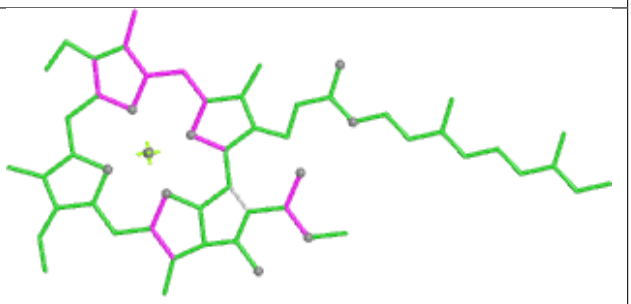
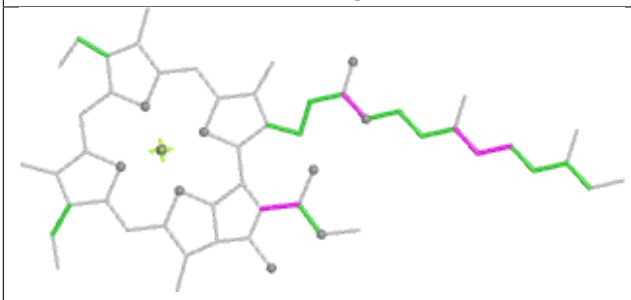
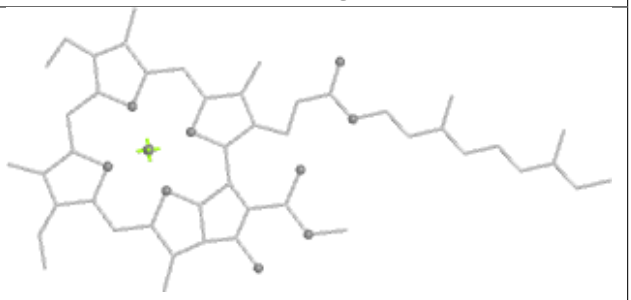
Bond angles



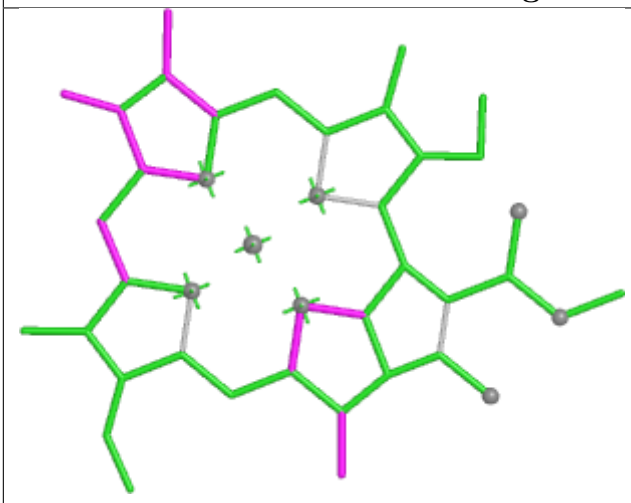
Torsions



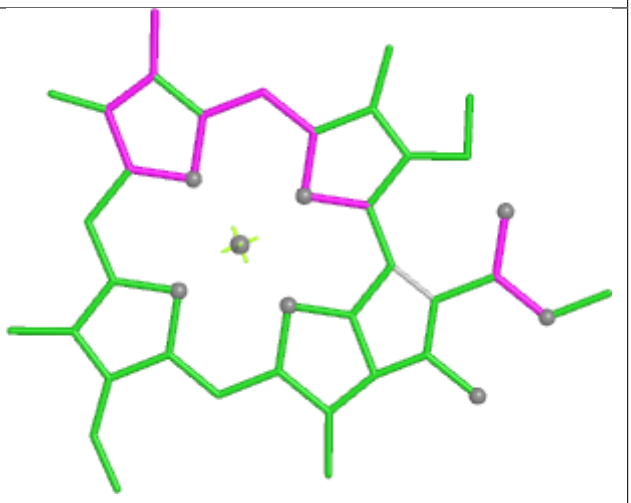
Rings

Ligand CLA f 831	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

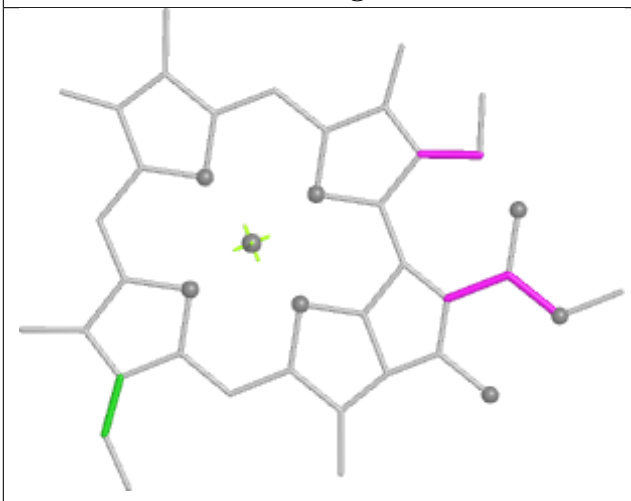
Ligand CLA m 101



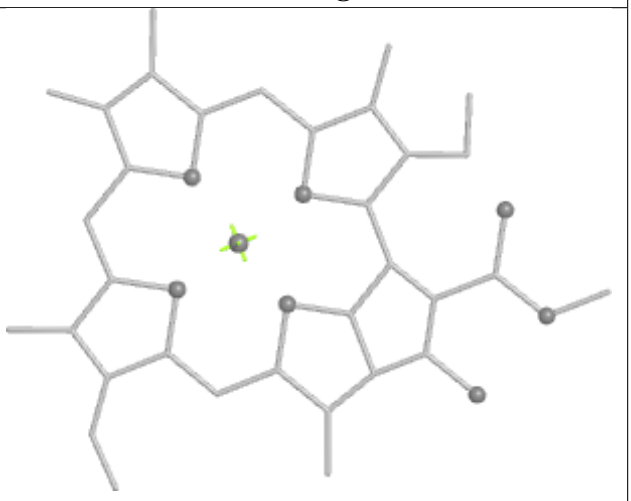
Bond lengths



Bond angles

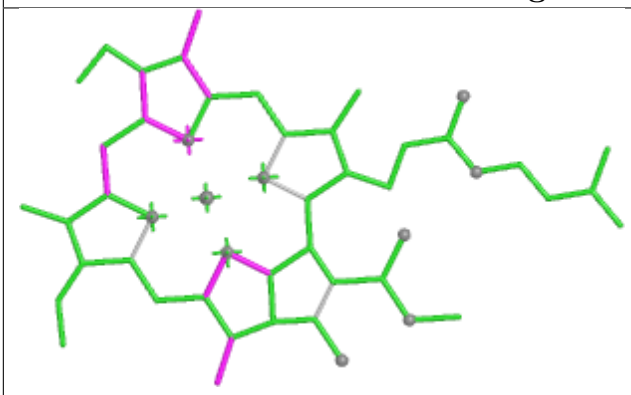


Torsions

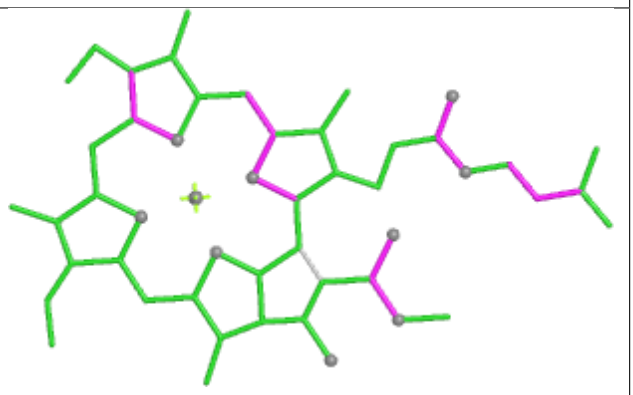


Rings

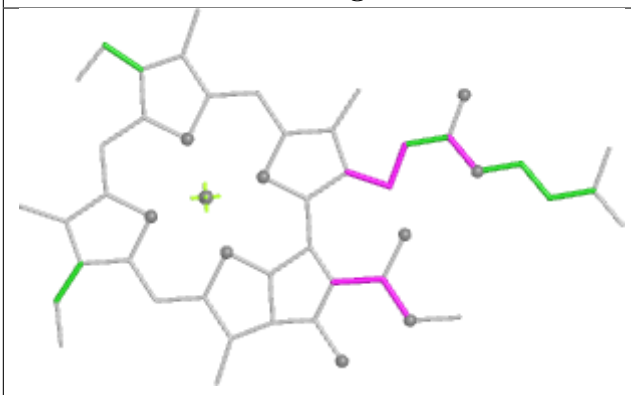
Ligand CLA 2 509



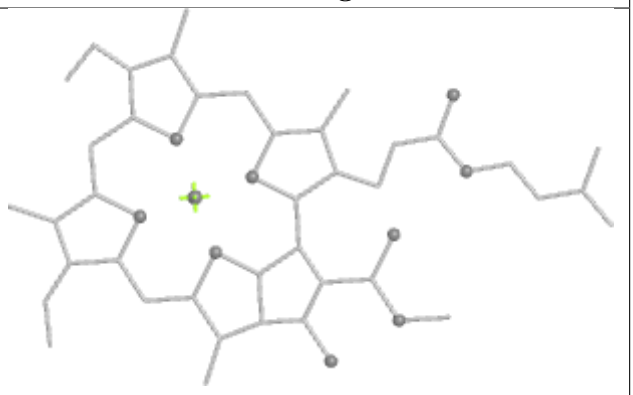
Bond lengths



Bond angles

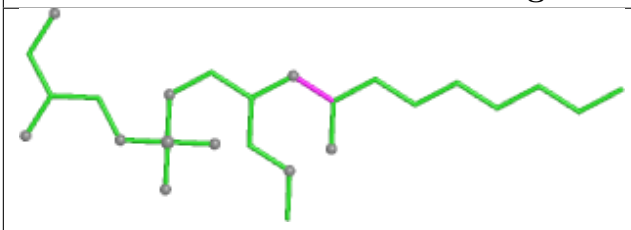


Torsions

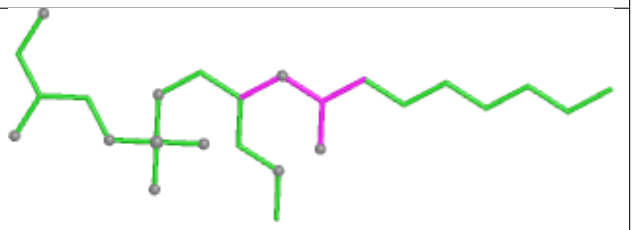


Rings

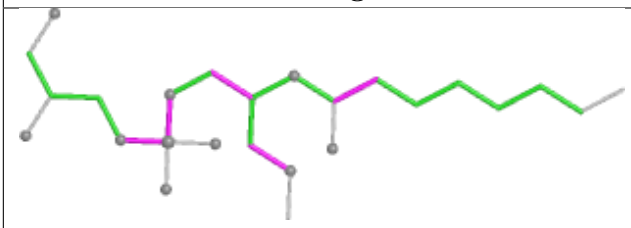
Ligand LHG e 845



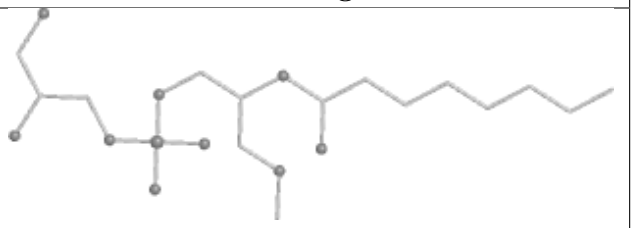
Bond lengths



Bond angles

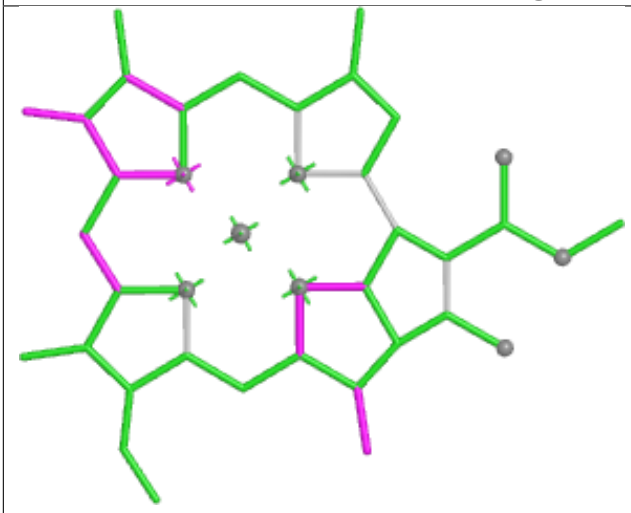


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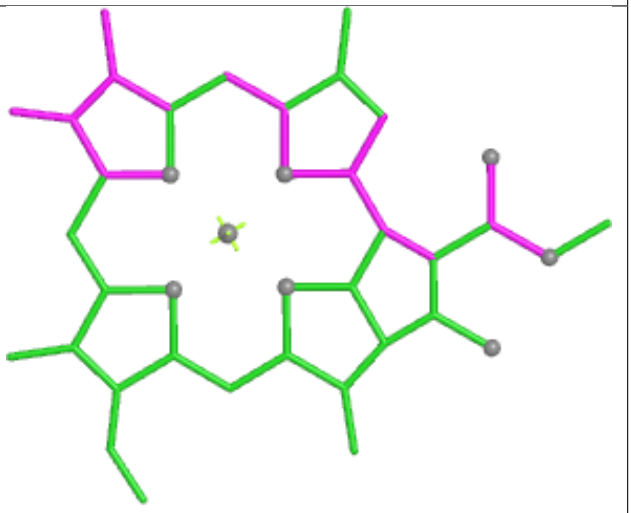


Rings

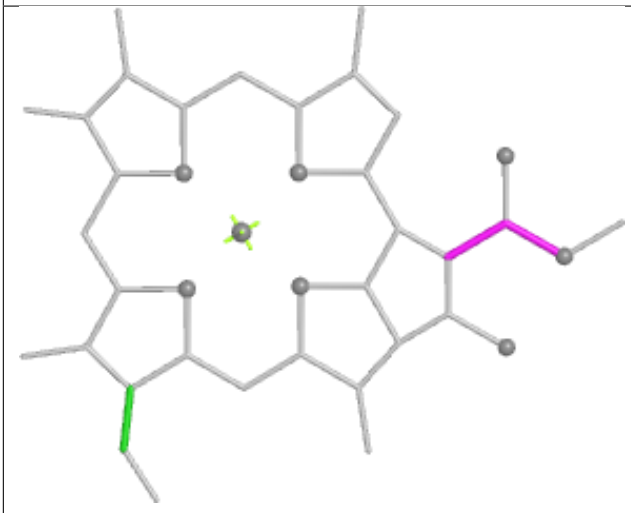
Ligand CLA r 304



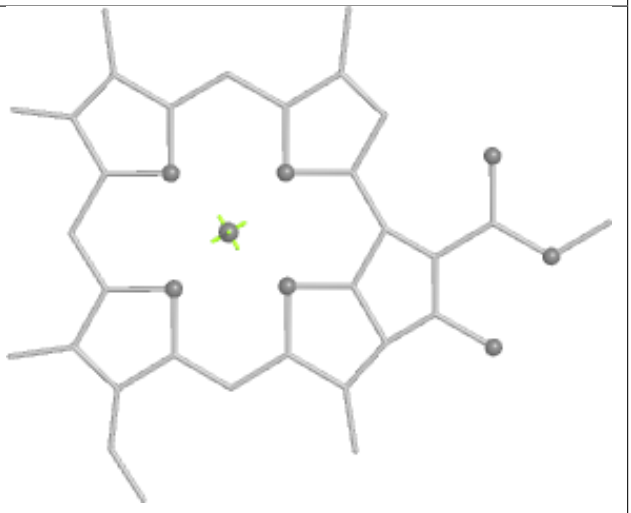
Bond lengths



Bond angles

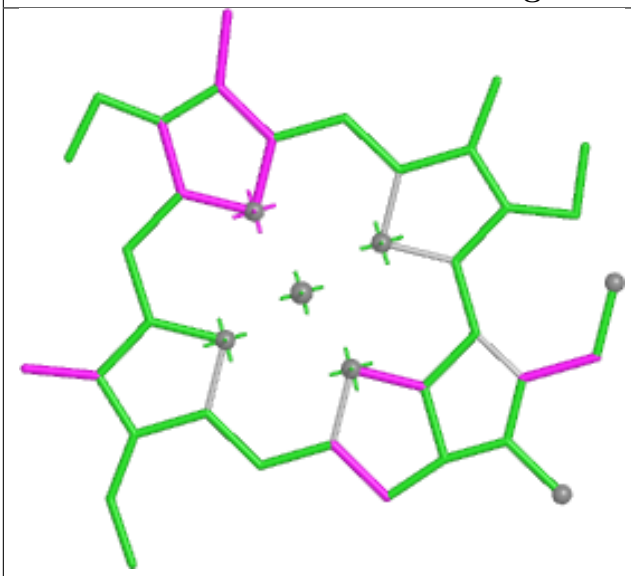


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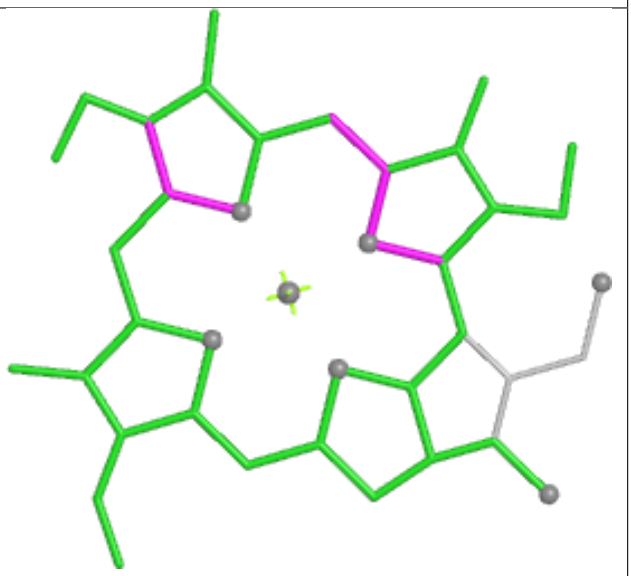


Rings

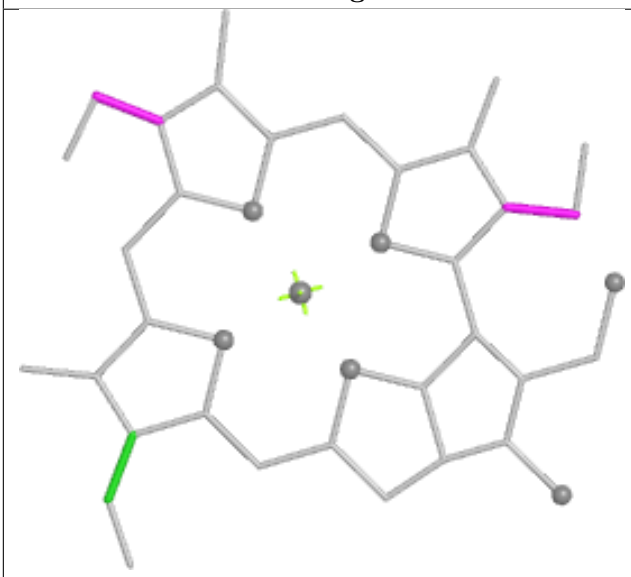
Ligand CLA A 809



Bond lengths



Bond angles

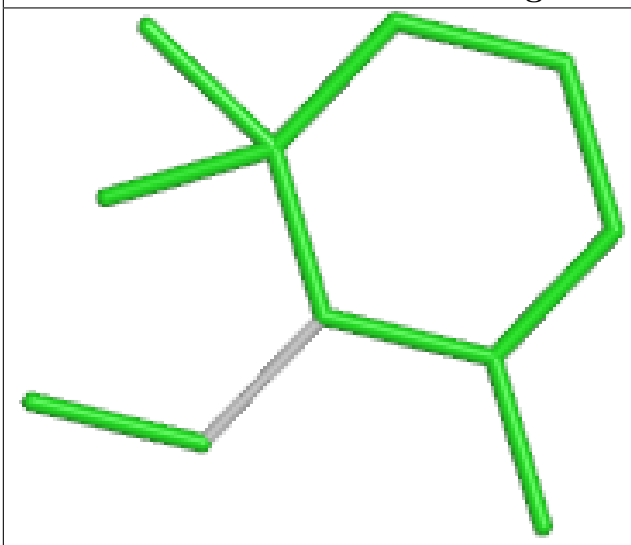


Torsions

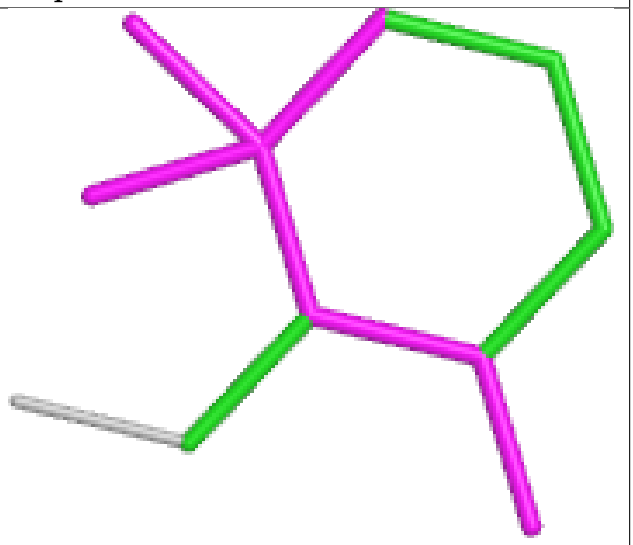


Rings

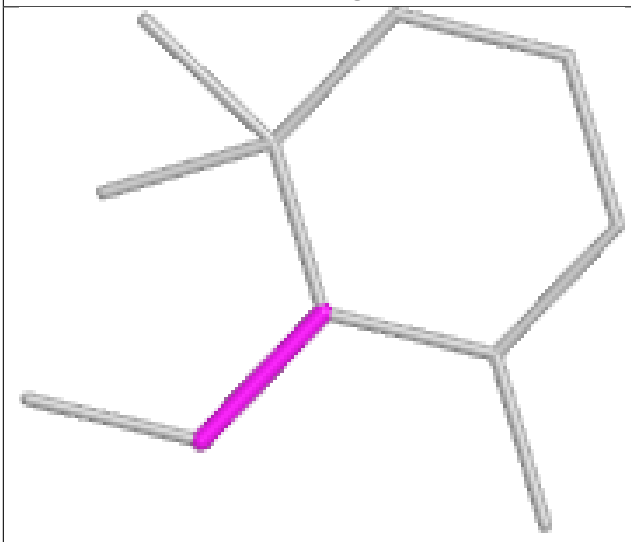
Ligand BCR p 503



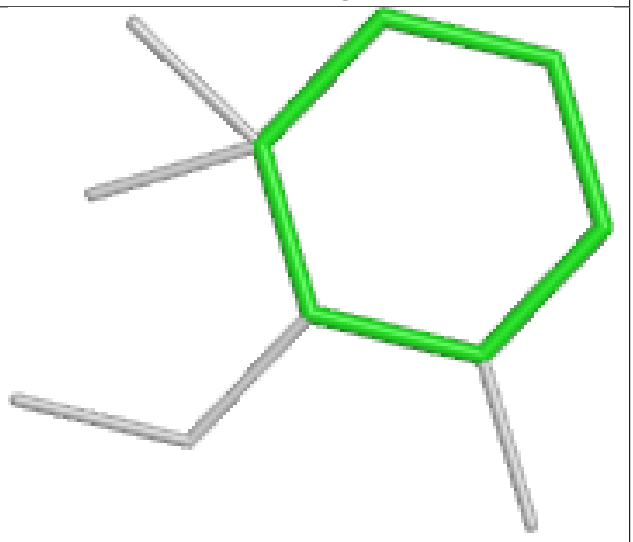
Bond lengths



Bond angles

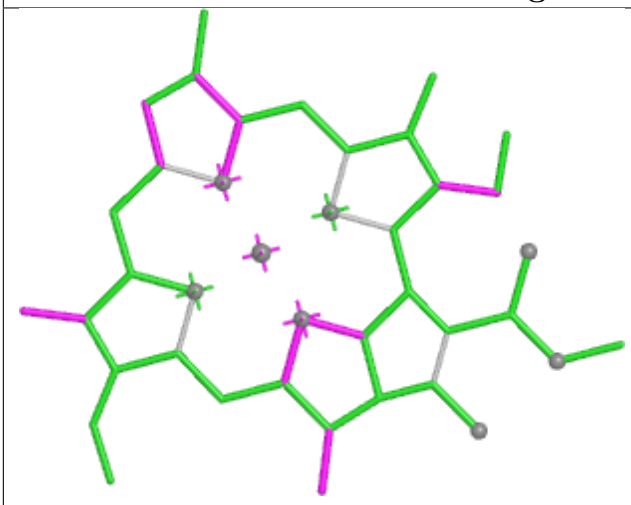


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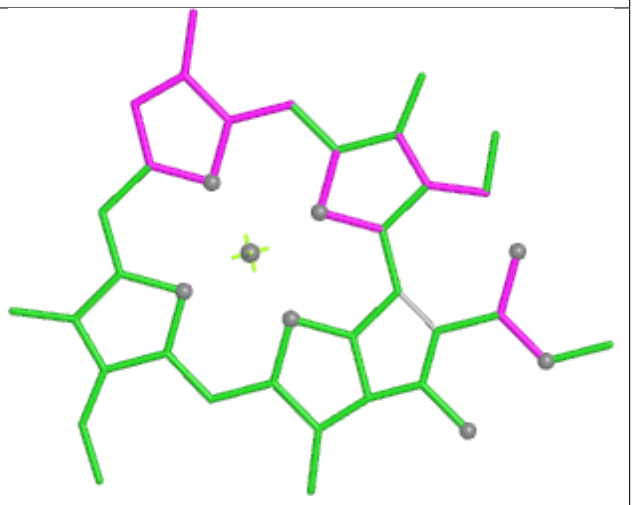


Rings

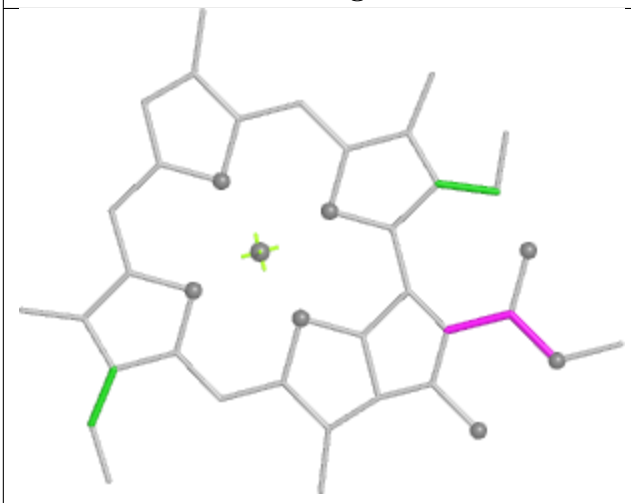
Ligand CLA 3 309



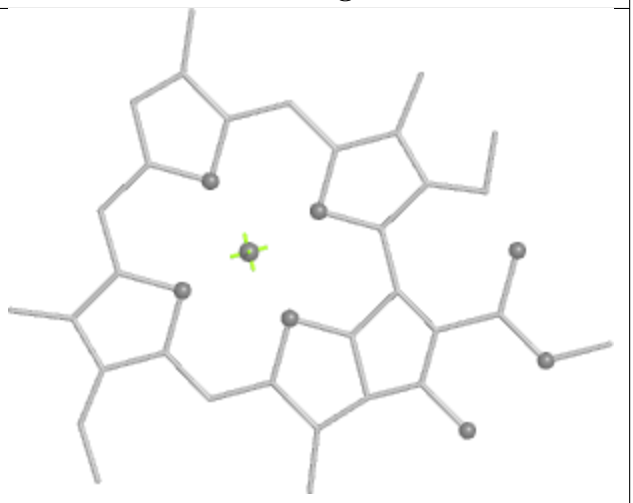
Bond lengths



Bond angles

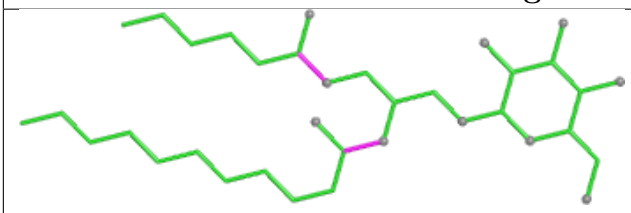


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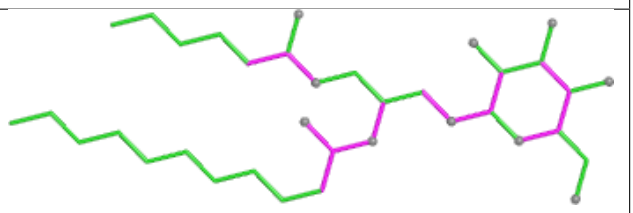


Rings

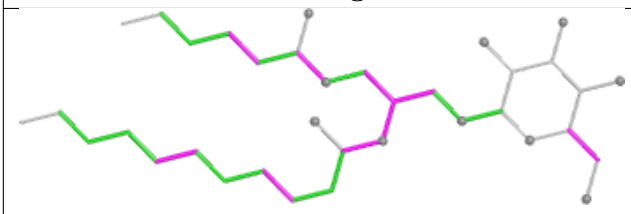
Ligand LMG 2 519



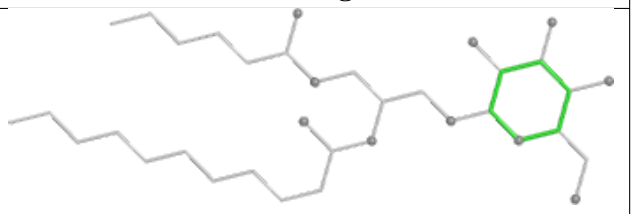
Bond lengths



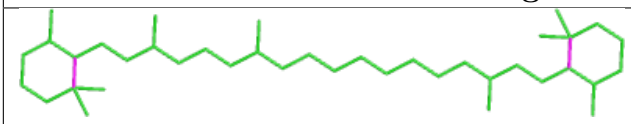
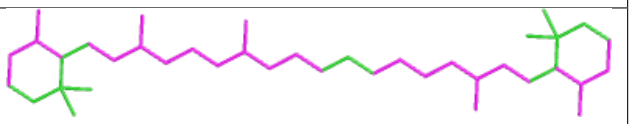
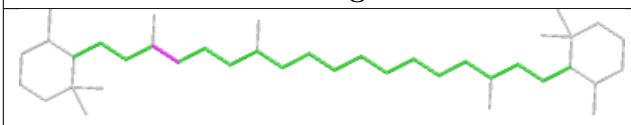
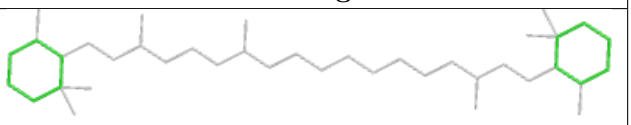
Bond angles

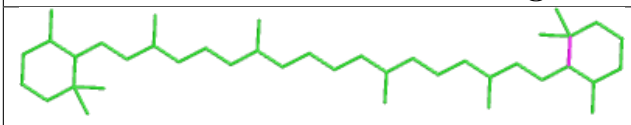
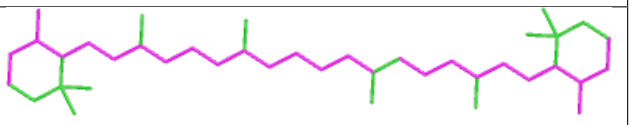
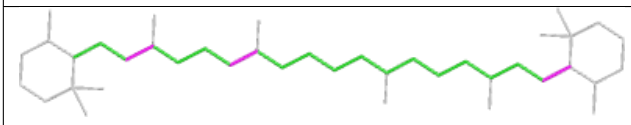
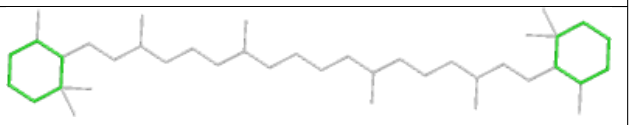


Torsions

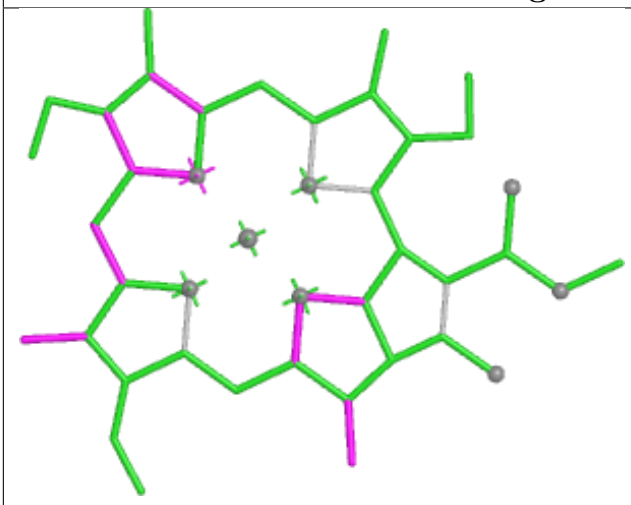


Rings

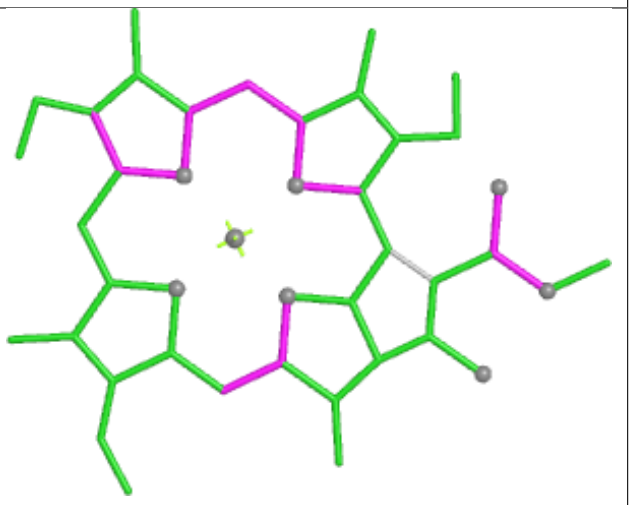
Ligand BCR A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR e 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

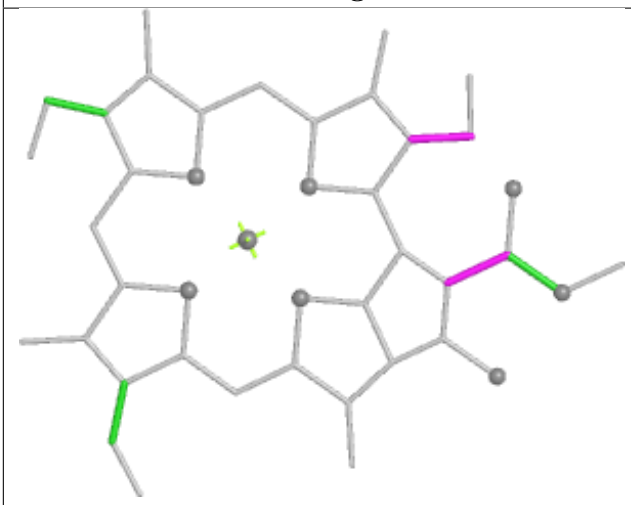
Ligand CLA e 813



Bond lengths



Bond angles

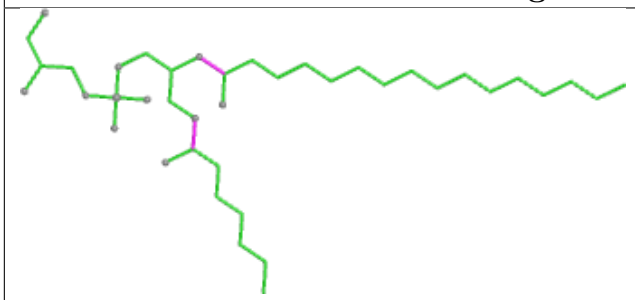


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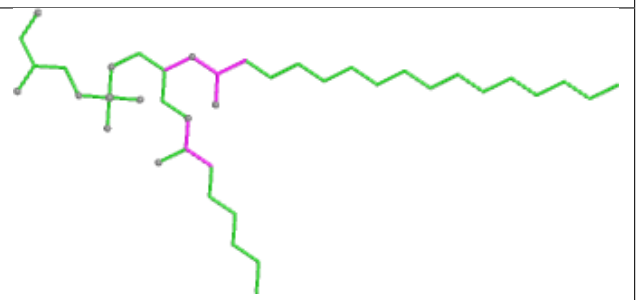


Rings

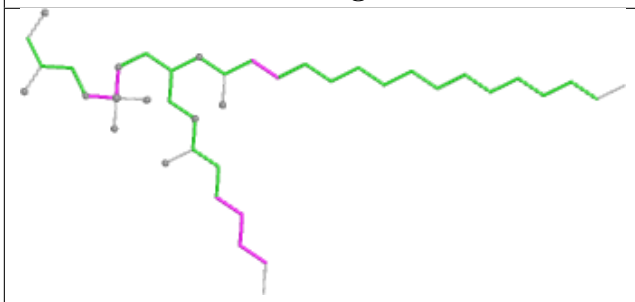
Ligand LHG e 844



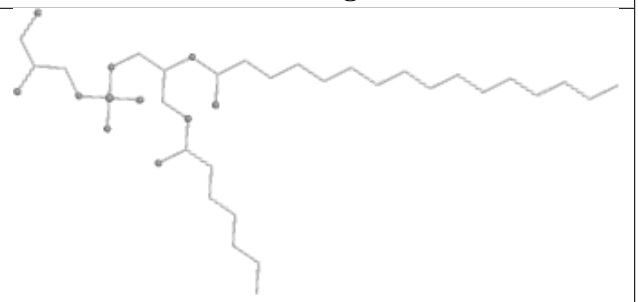
Bond lengths



Bond angles

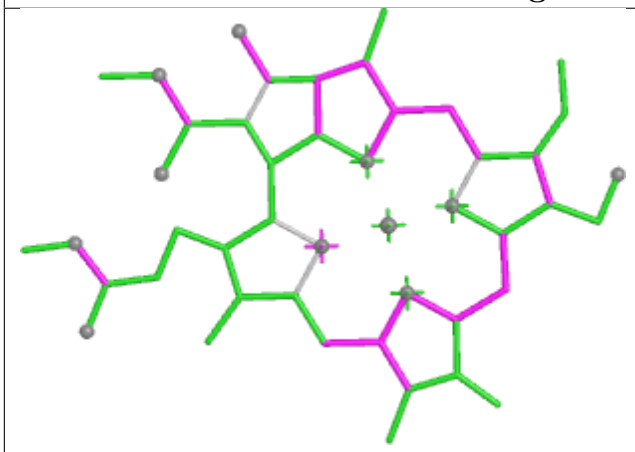


Torsions

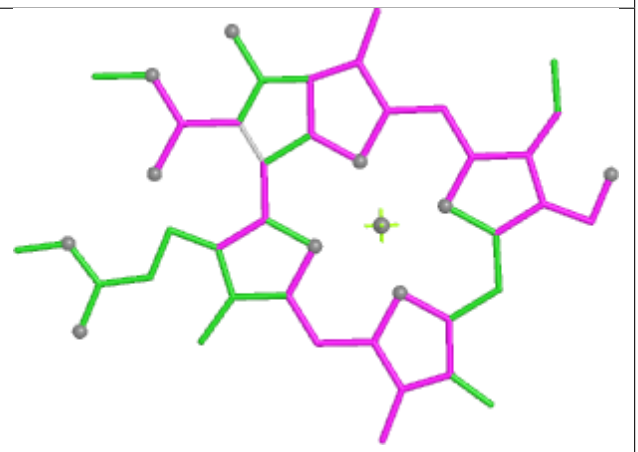


Rings

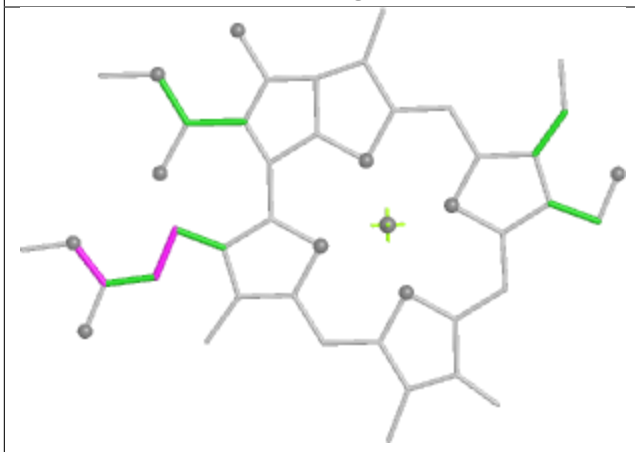
Ligand CHL 2 512



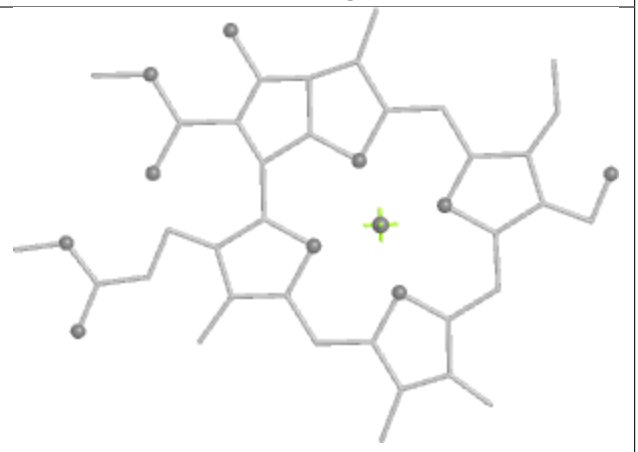
Bond lengths



Bond angles

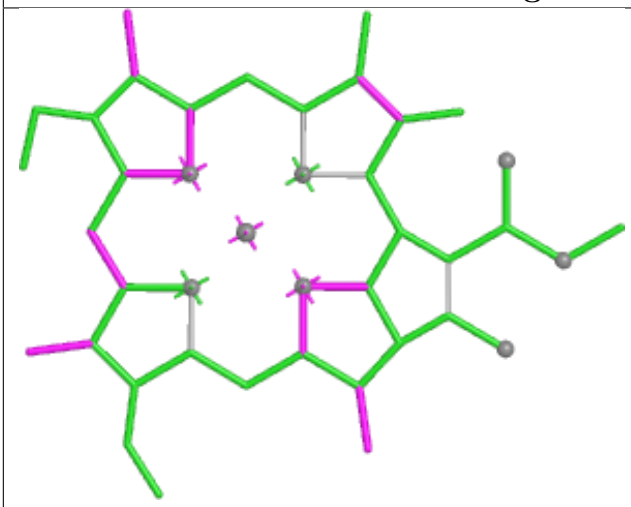


Torsions

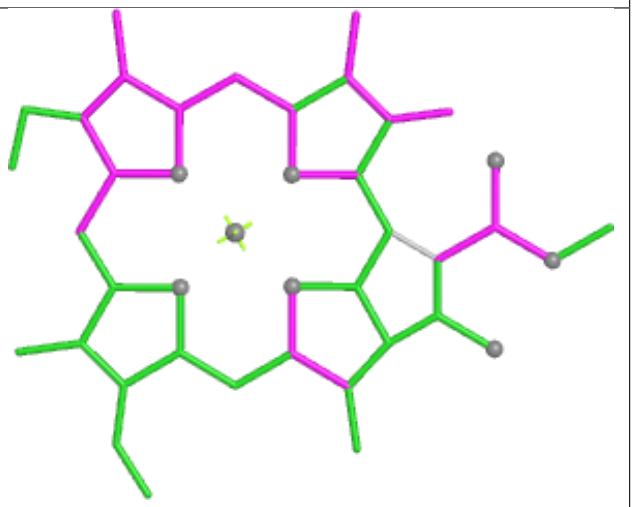


Rings

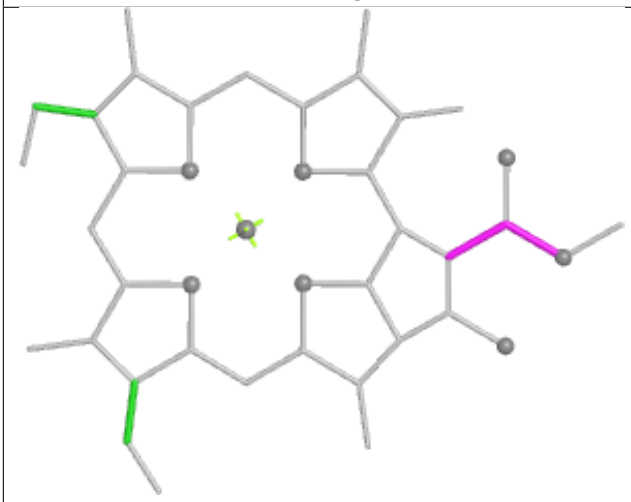
Ligand CLA A 837



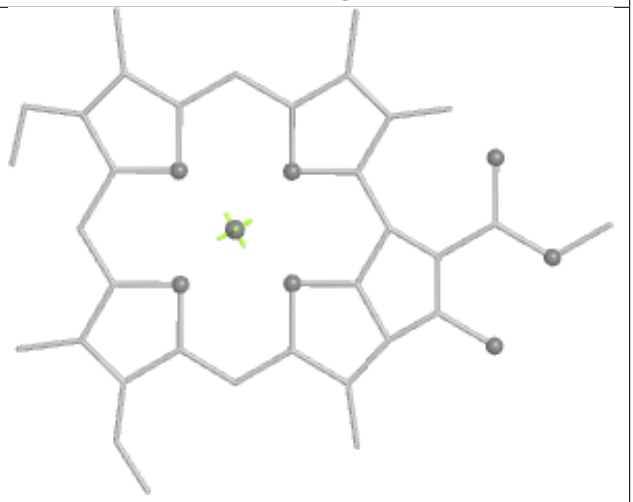
Bond lengths



Bond angles

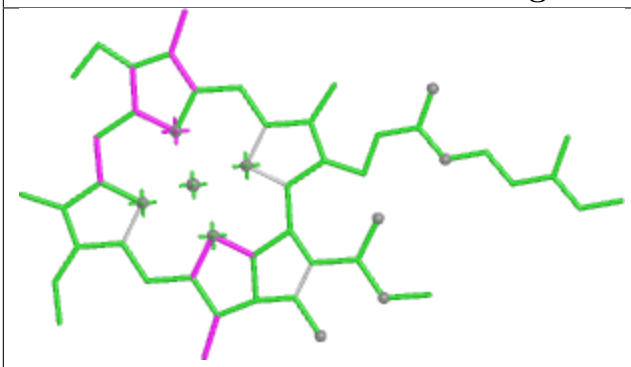


Torsions

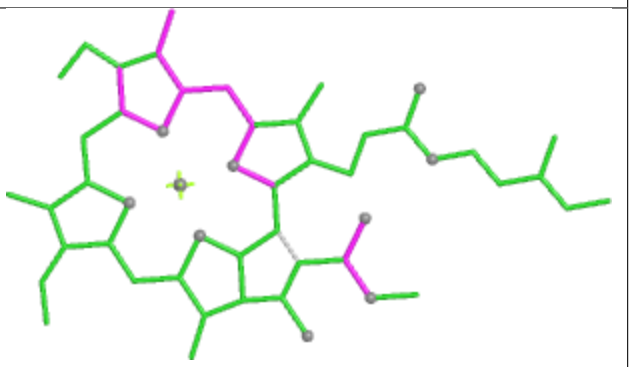


Rings

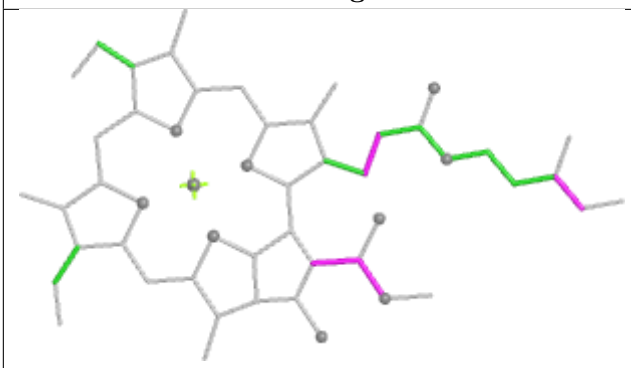
Ligand CLA e 836



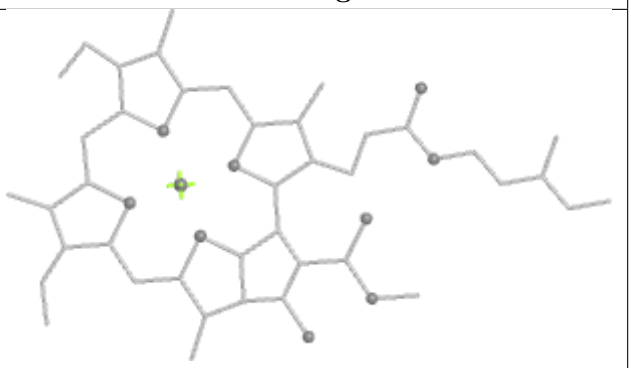
Bond lengths



Bond angles

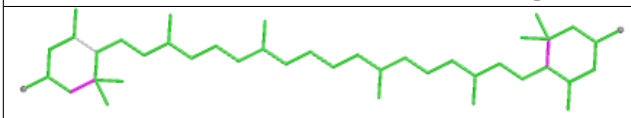


Torsions

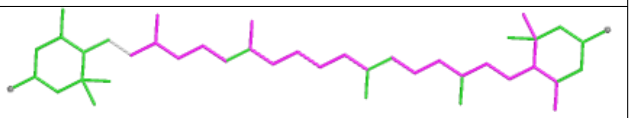


Rings

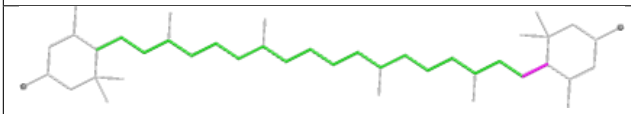
Ligand LUT 5 303



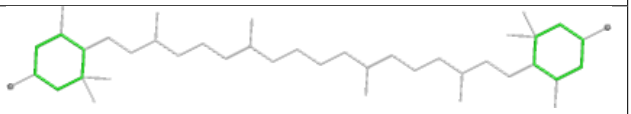
Bond lengths



Bond angles

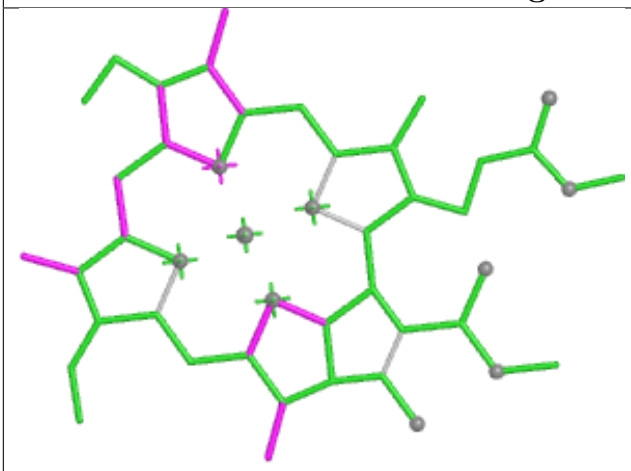


Torsions

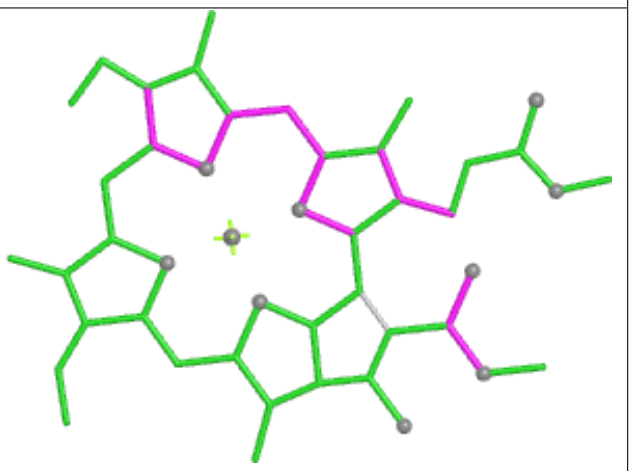


Rings

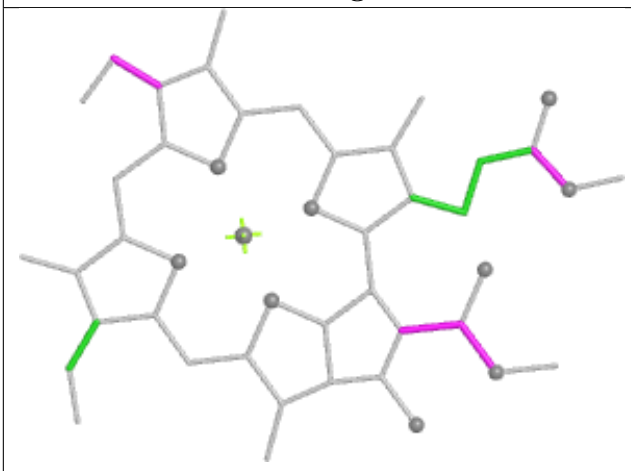
Ligand CLA 1 511



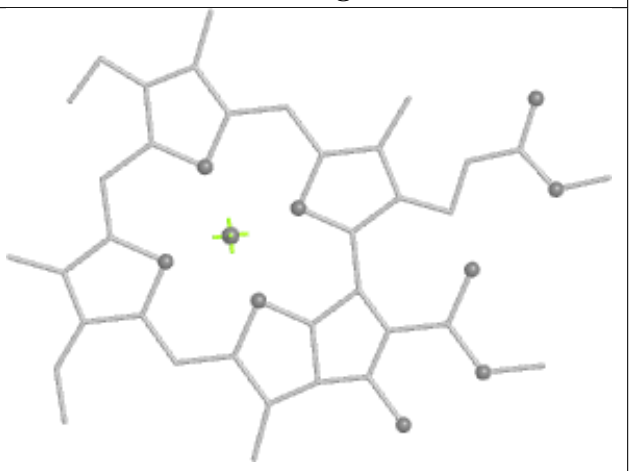
Bond lengths



Bond angles

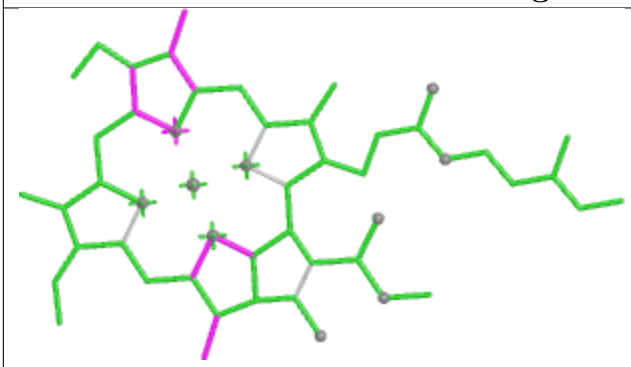


Torsions

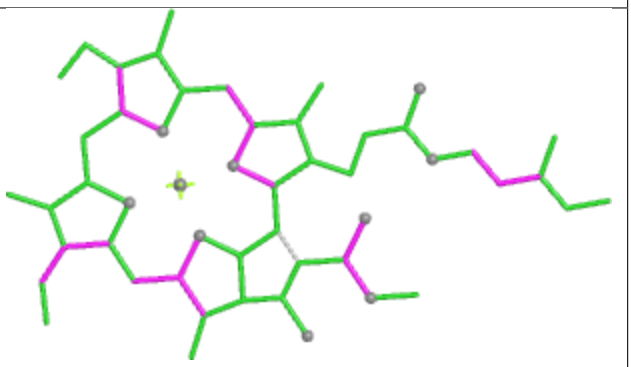


Rings

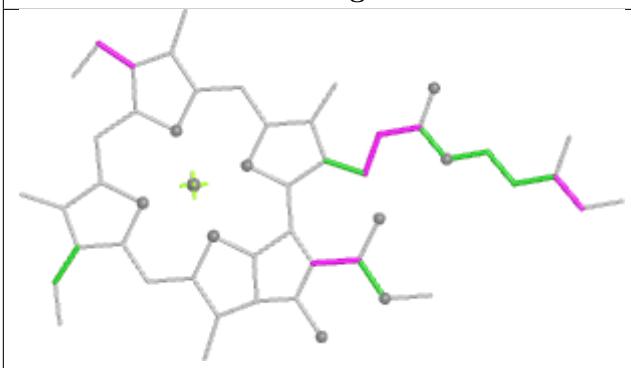
Ligand CLA f 811



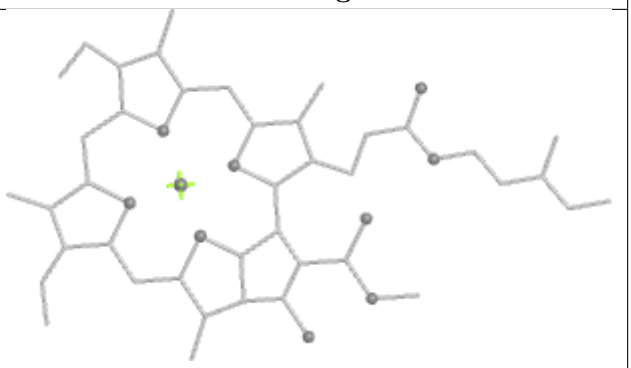
Bond lengths



Bond angles

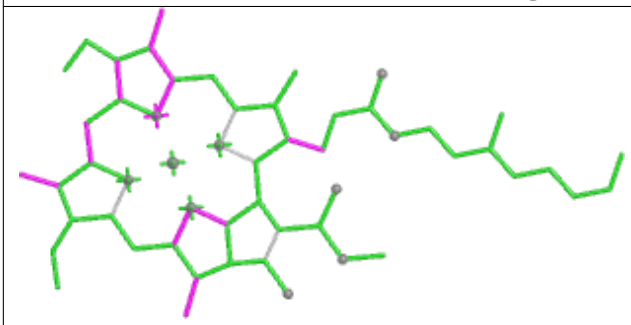


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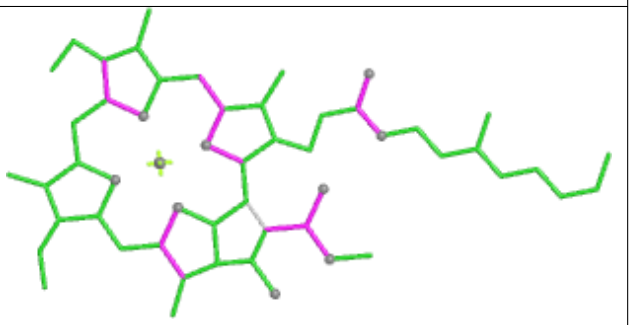


Rings

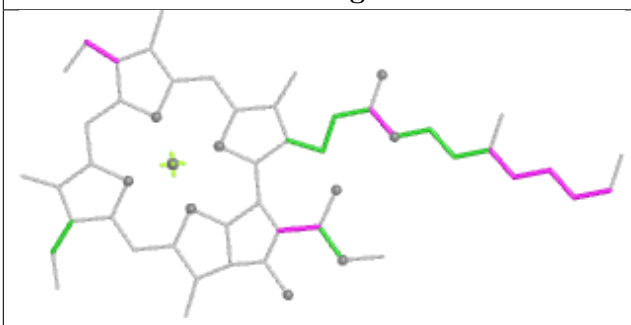
Ligand CLA B 841



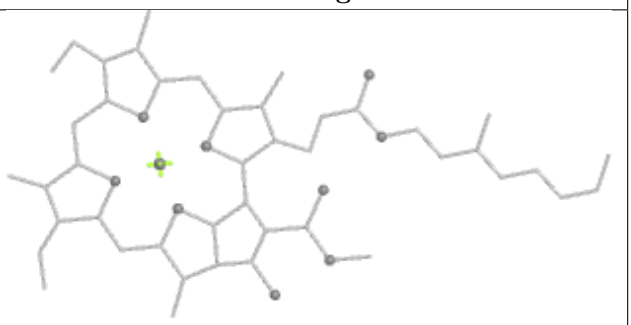
Bond lengths



Bond angles

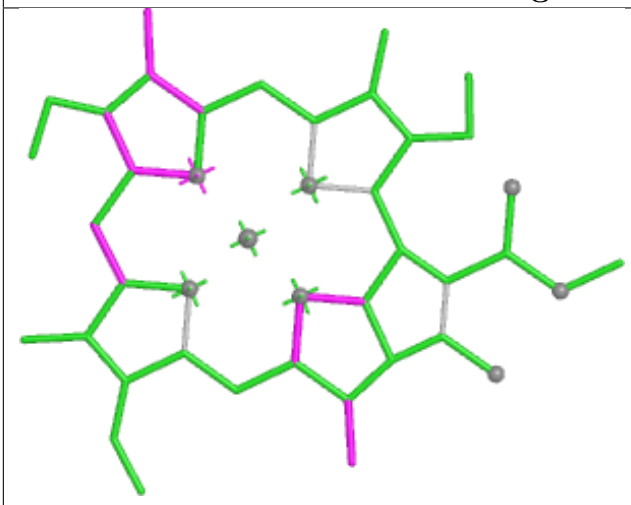


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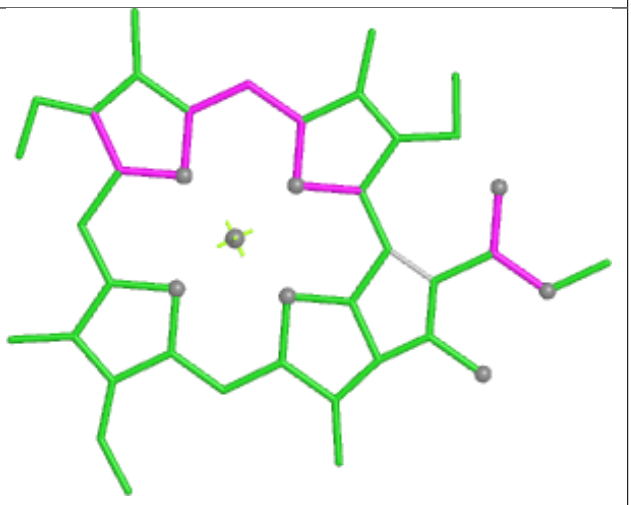


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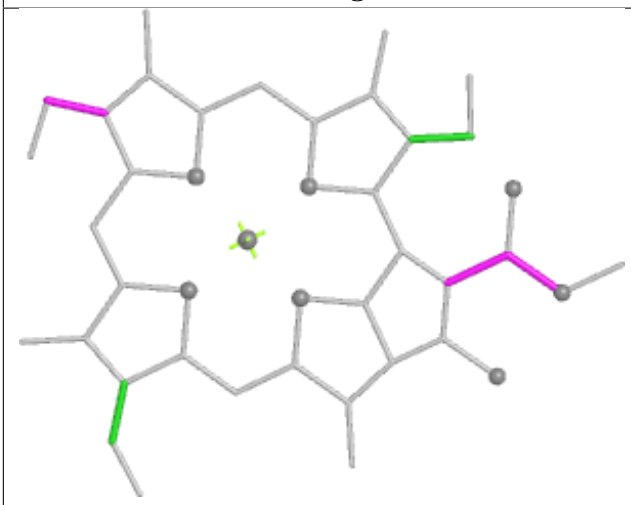
Ligand CLA f 837



Bond lengths



Bond angles

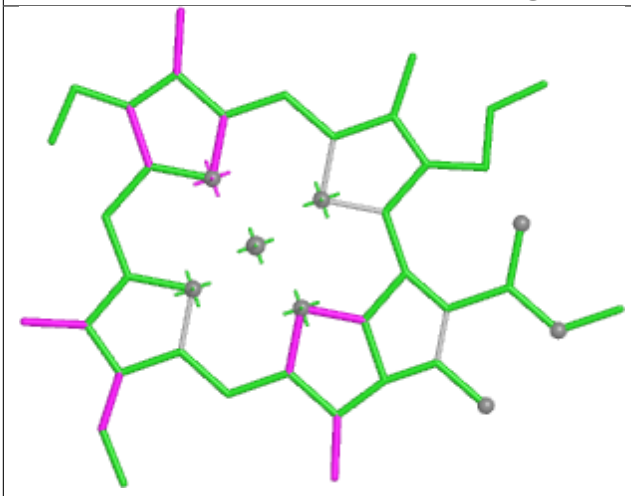


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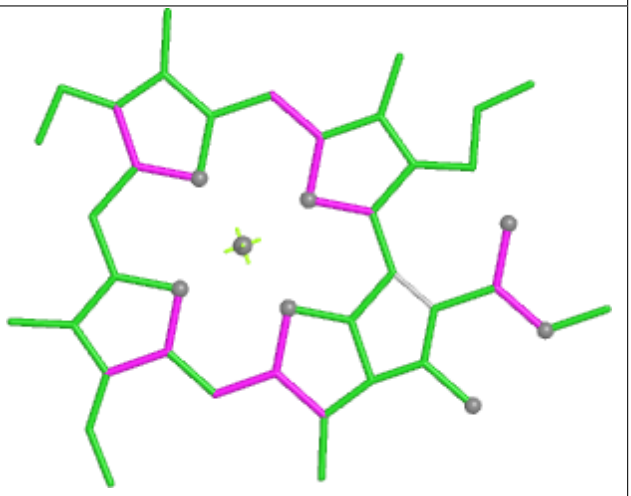


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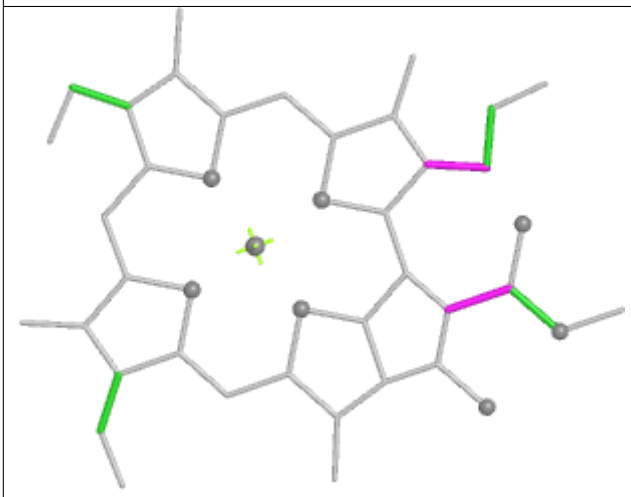
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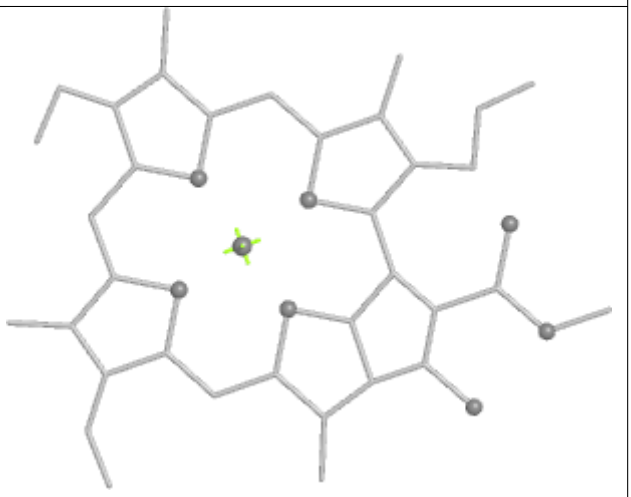
Bond lengths



Bond angles

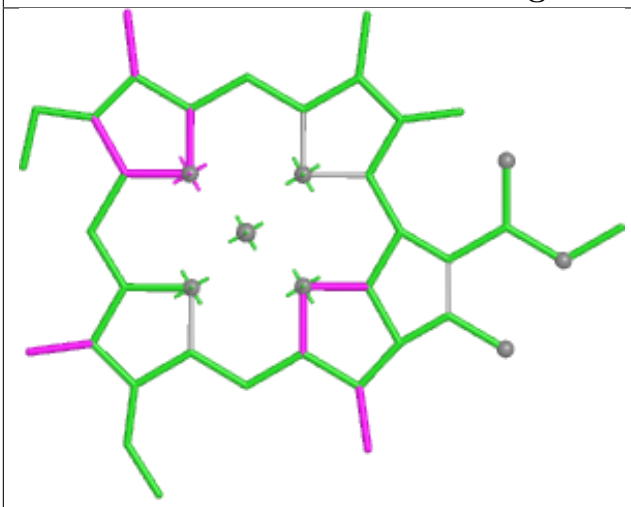


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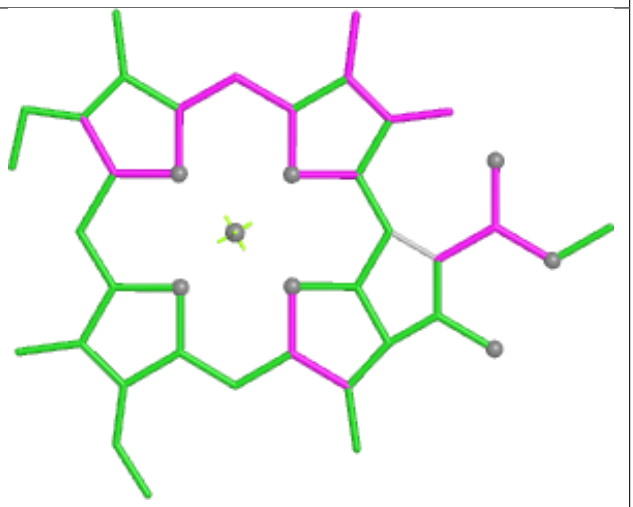


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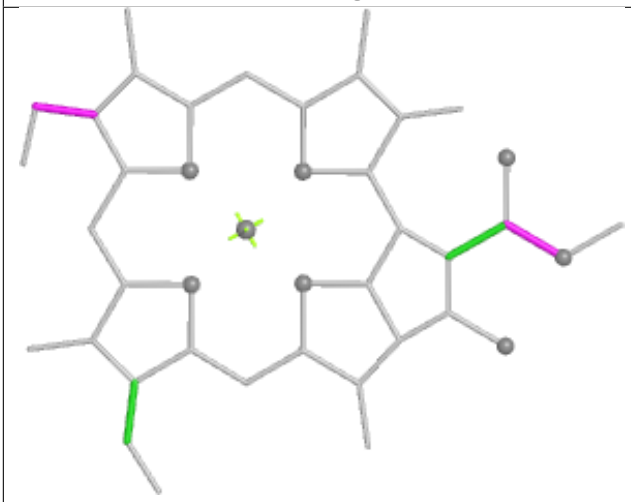
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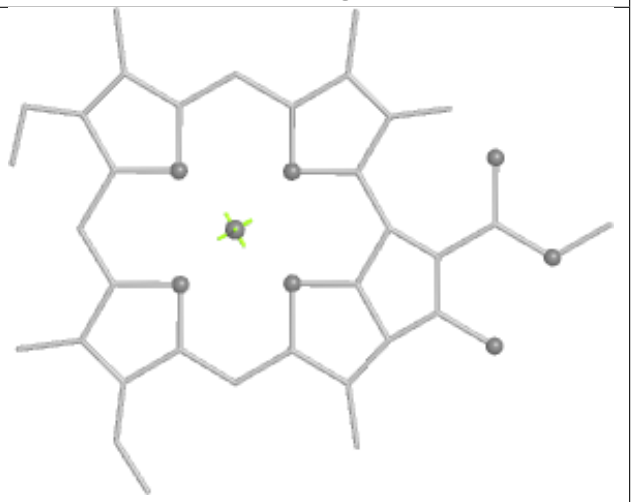
Bond lengths



Bond angles

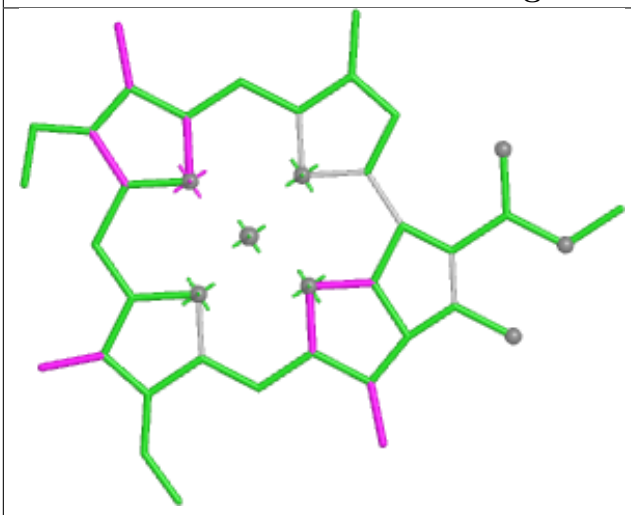


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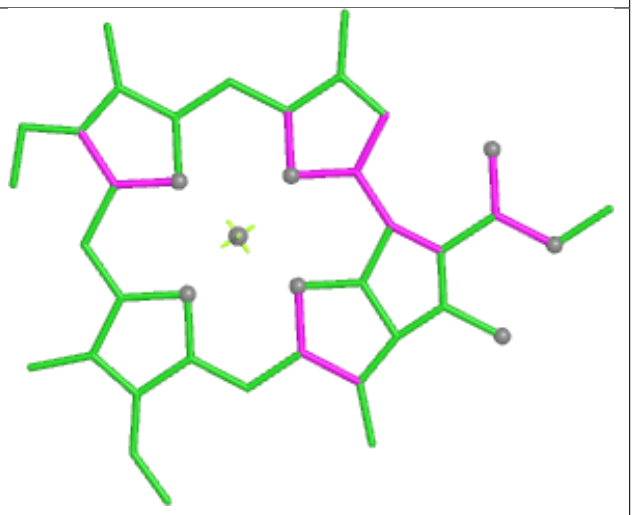


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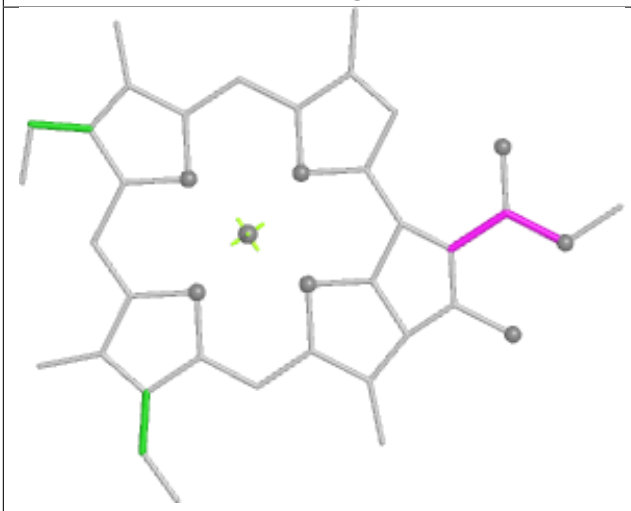
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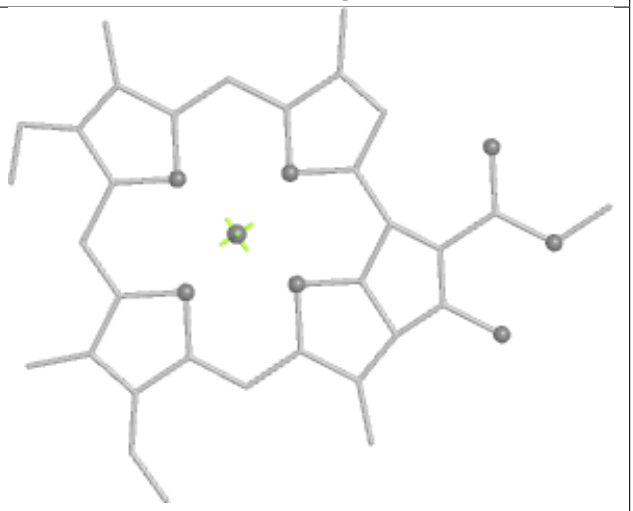
Bond lengths



Bond angles

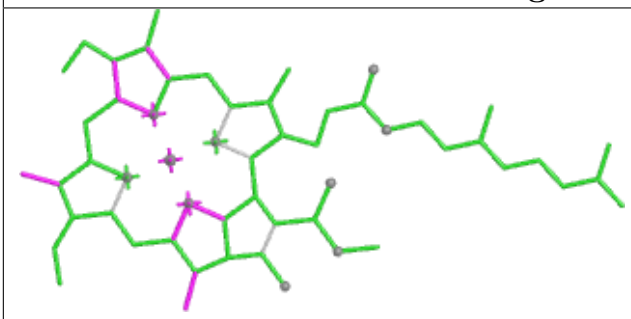


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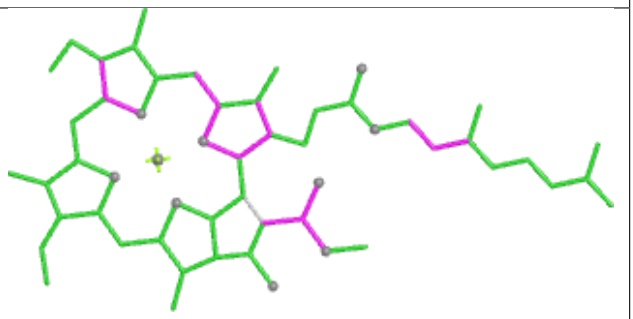


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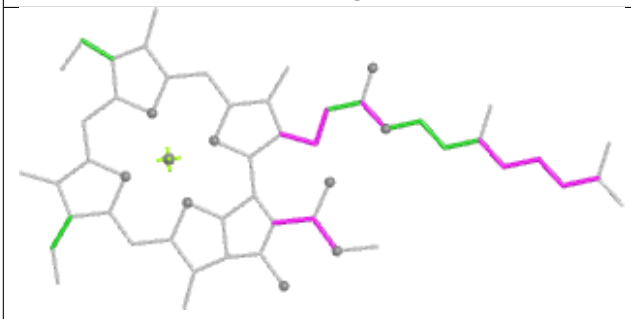
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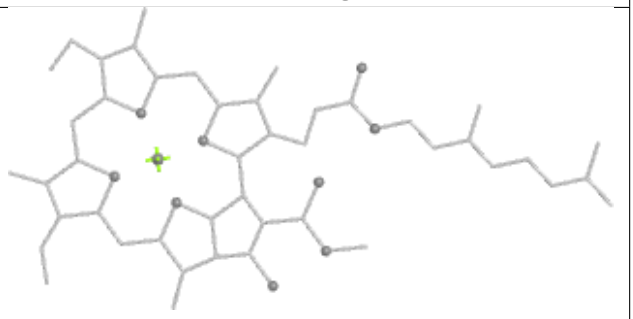
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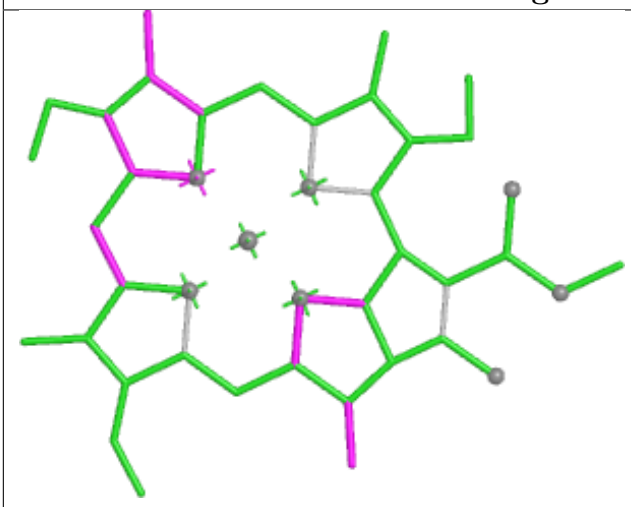


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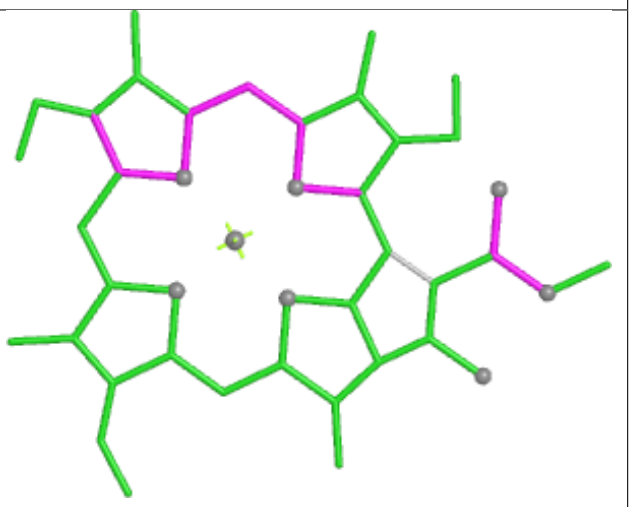


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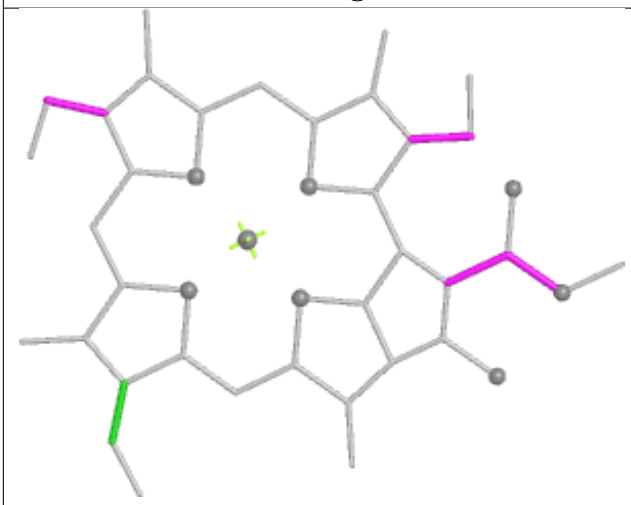
Ligand CLA f 824



Bond lengths



Bond angles

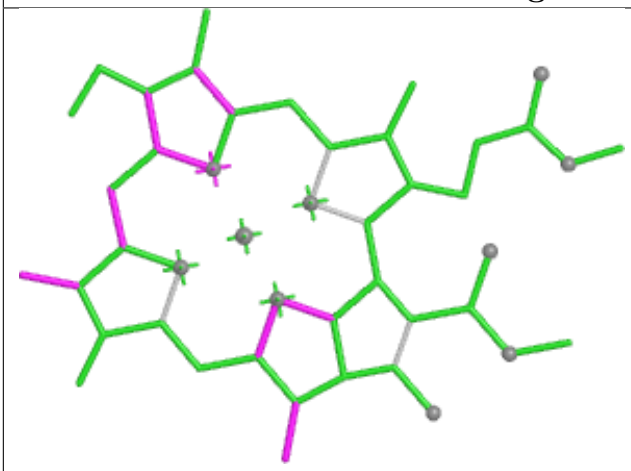


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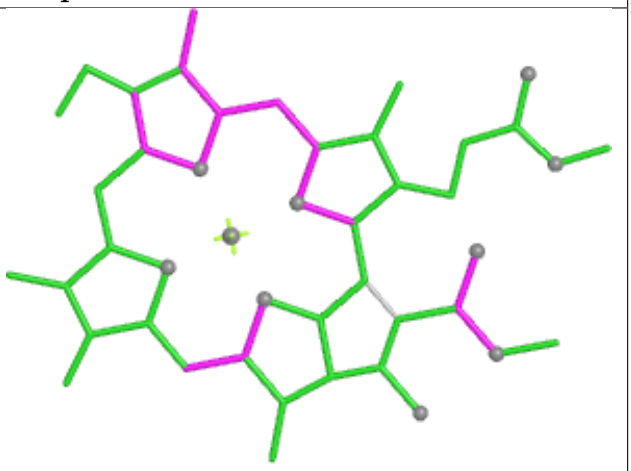


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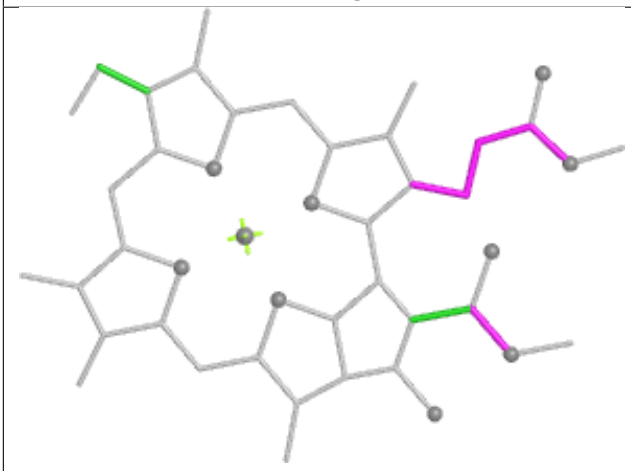
Ligand CLA q 315



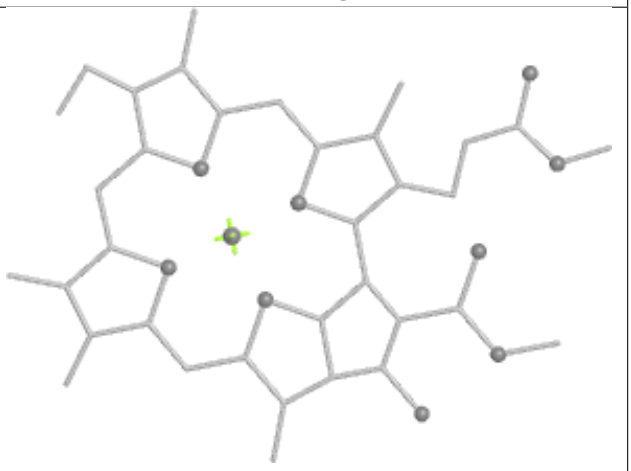
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Bond angles

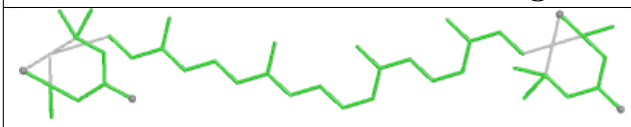


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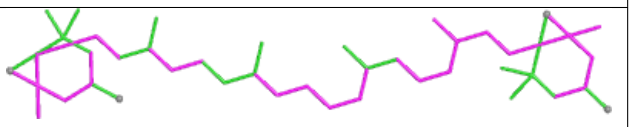


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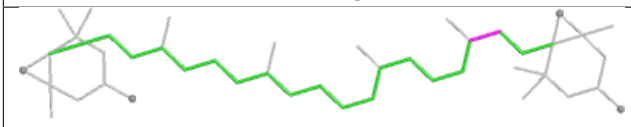
Ligand XAT r 303



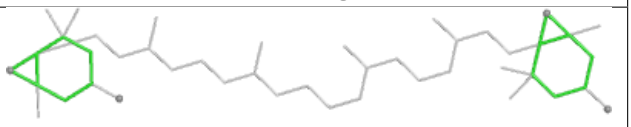
Bond lengths



Bond angles

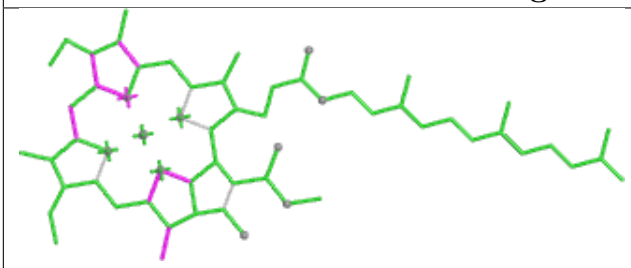


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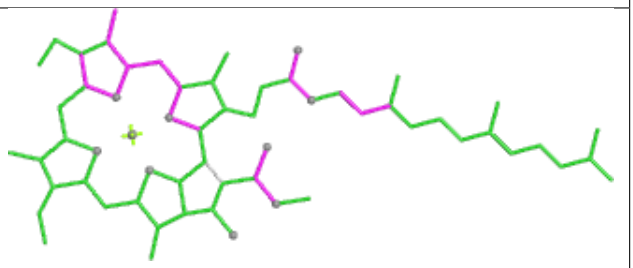


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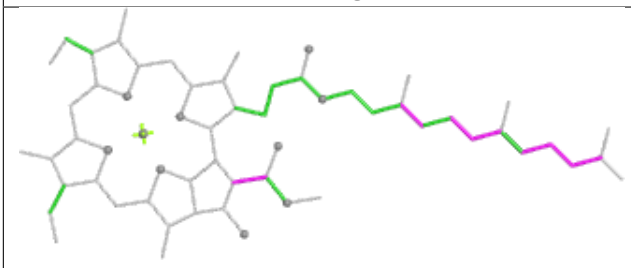
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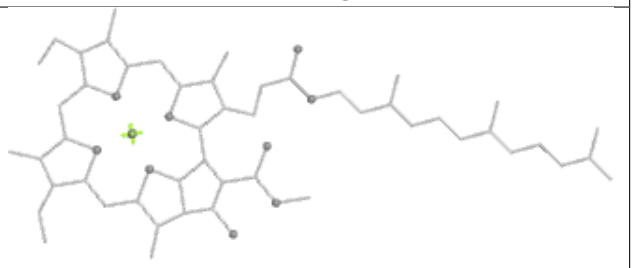
Bond lengths



Bond angles

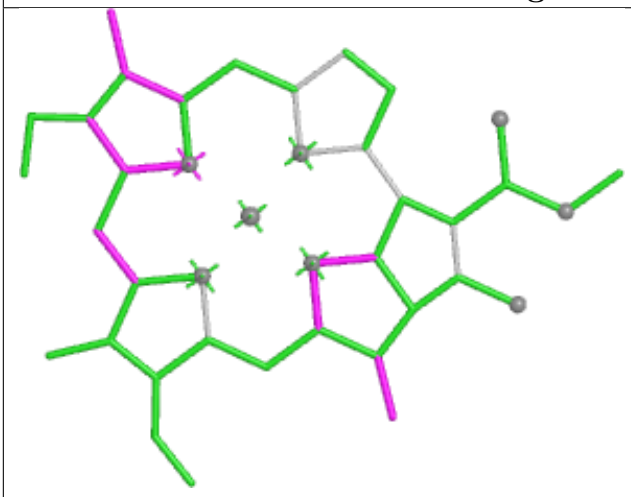


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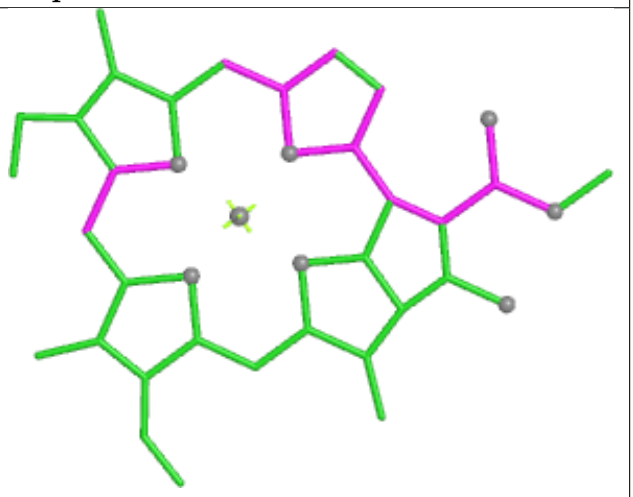


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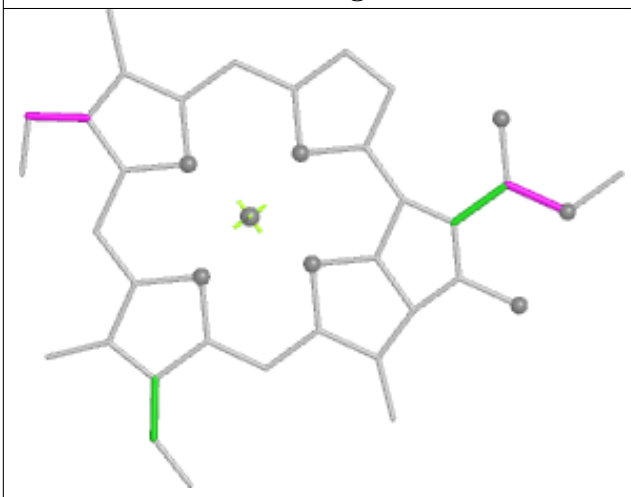
Ligand CLA p 511



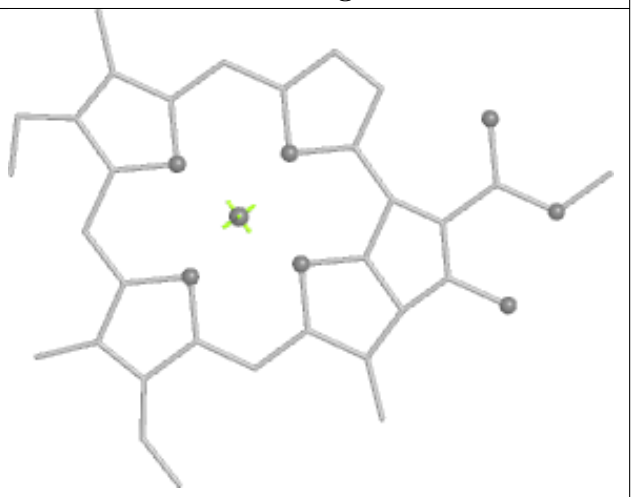
Bond lengths



Bond angles

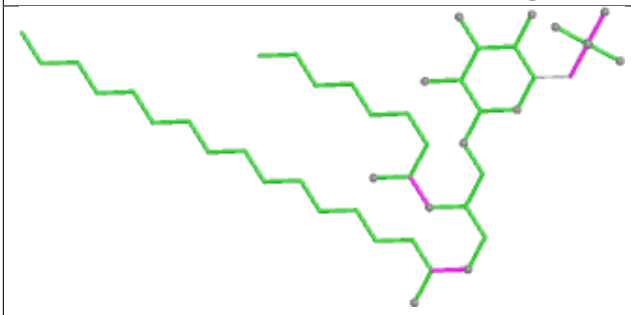


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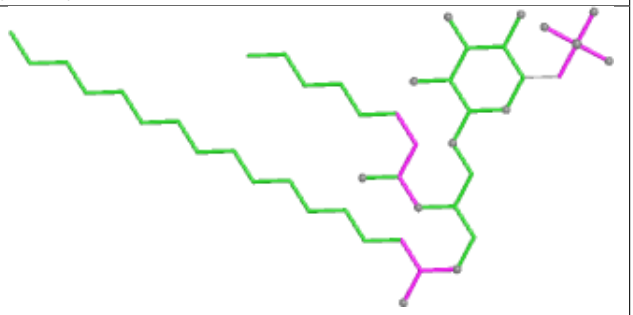


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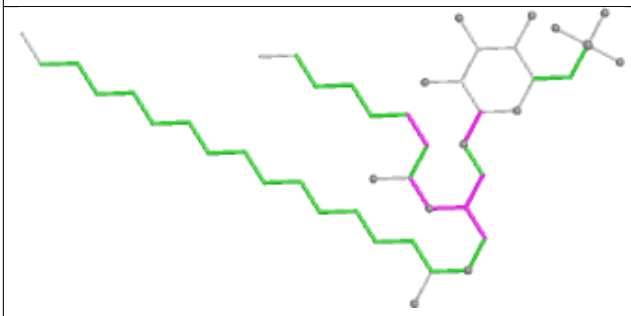
Ligand SQD Q 803



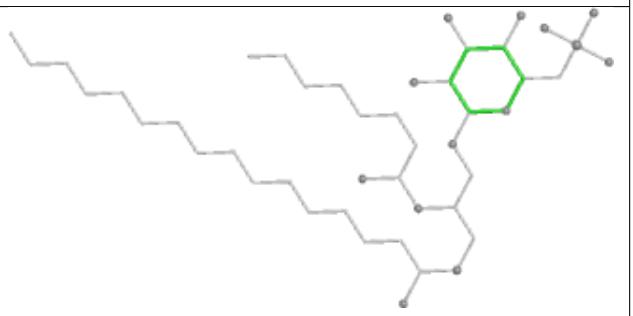
Bond lengths



Bond angles

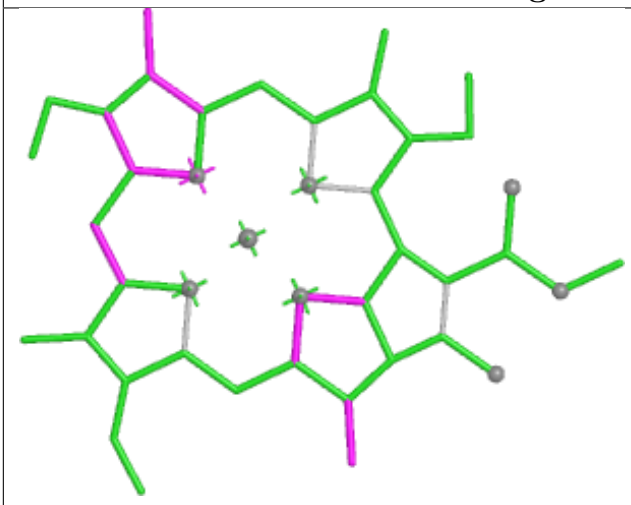


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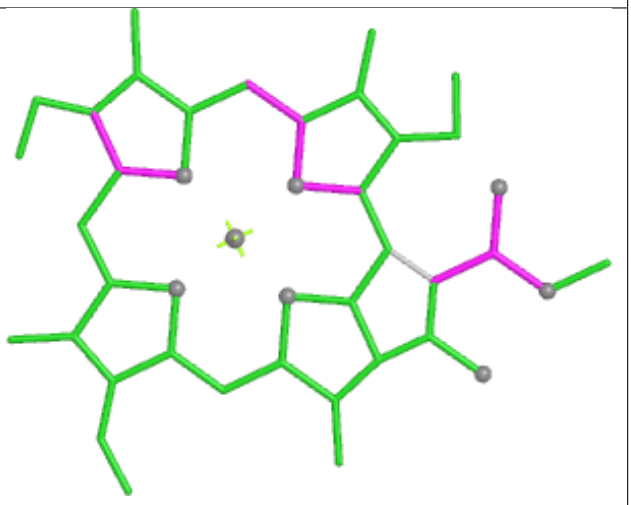


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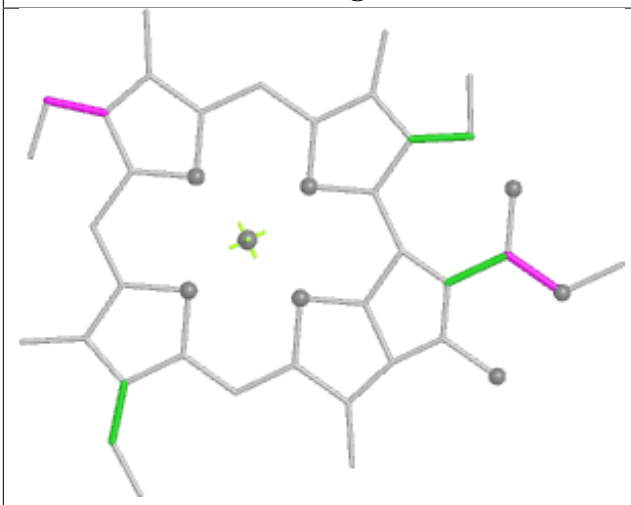
Ligand CLA e 807



Bond lengths



Bond angles

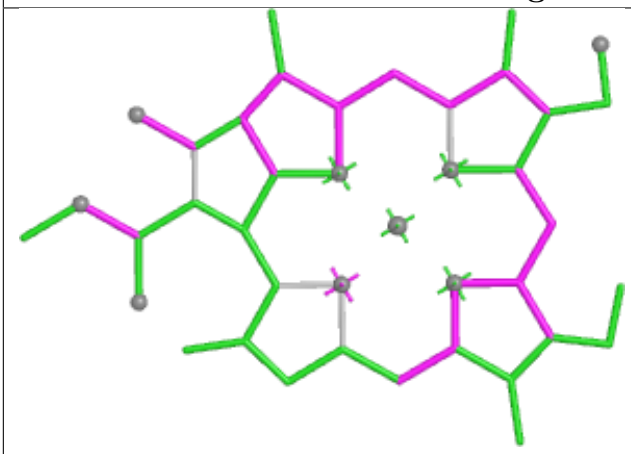


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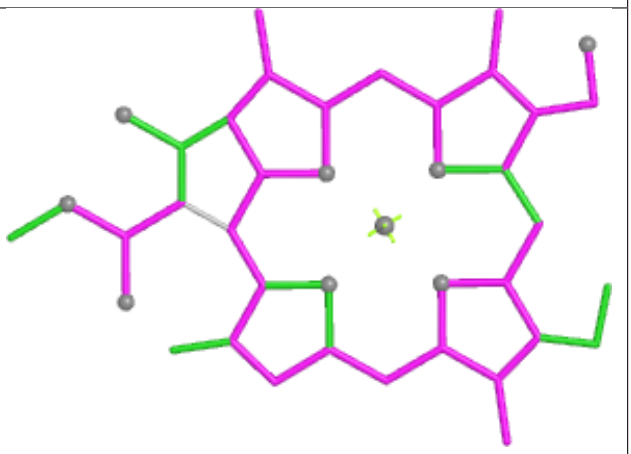


Rings

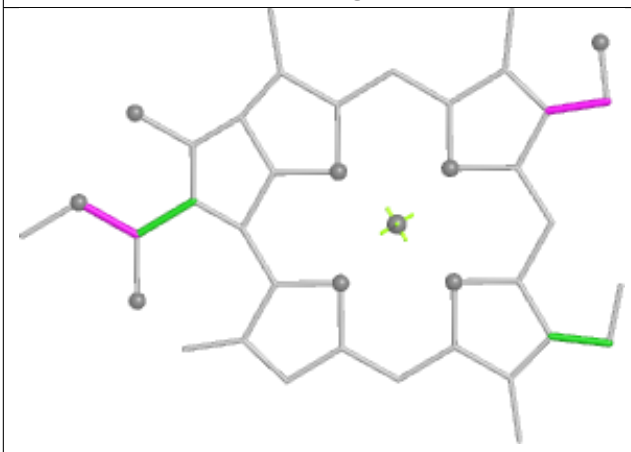
Ligand CHL 5 317



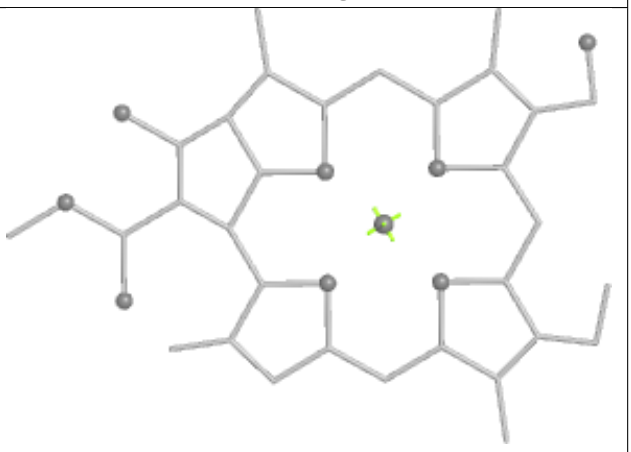
Bond lengths



Bond angles

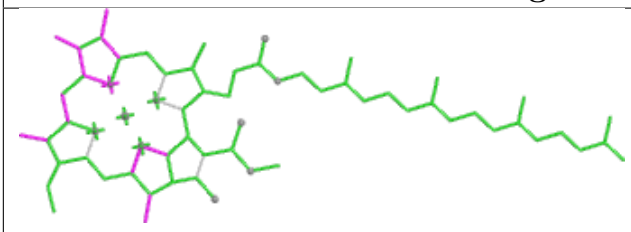


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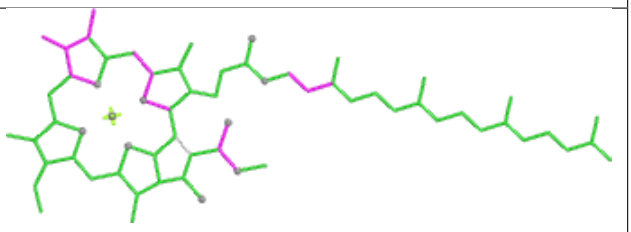


Rings

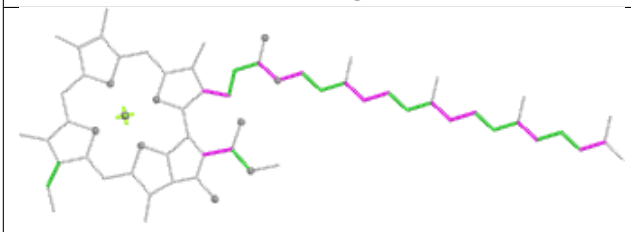
Ligand CLA e 826



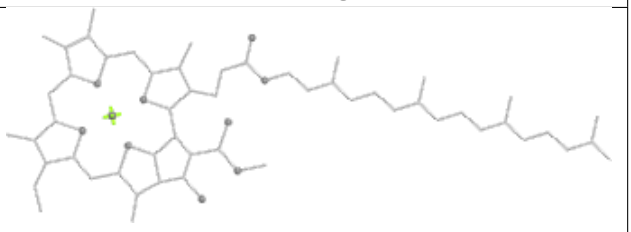
Bond lengths



Bond angles

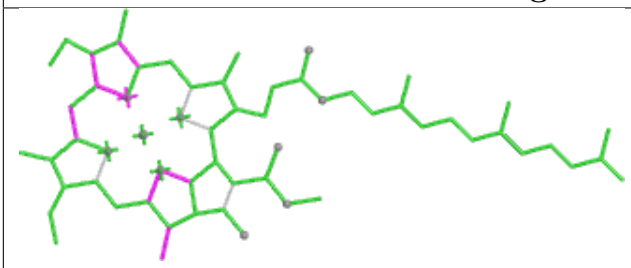


Torsions

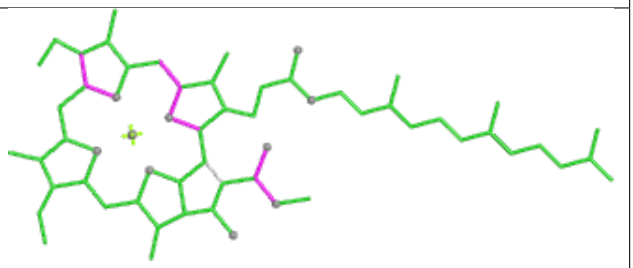


Rings

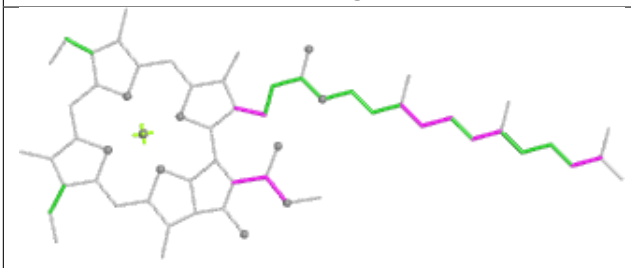
Ligand CLA s 510



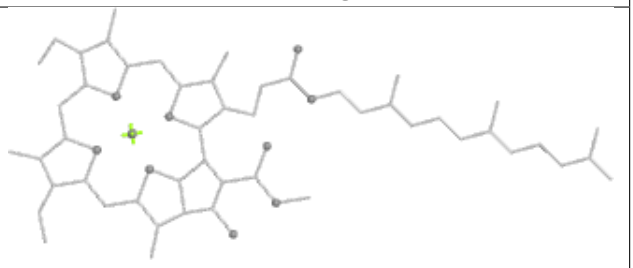
Bond lengths



Bond angles

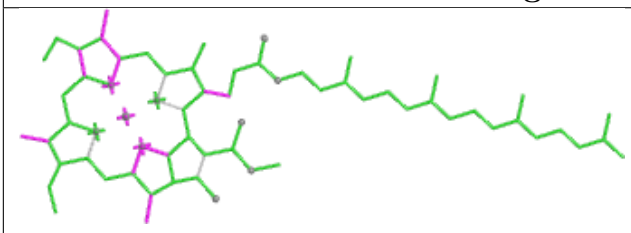


Torsions

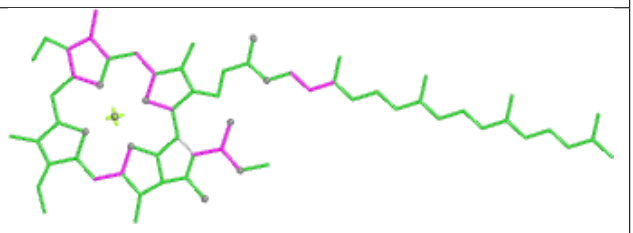


Rings

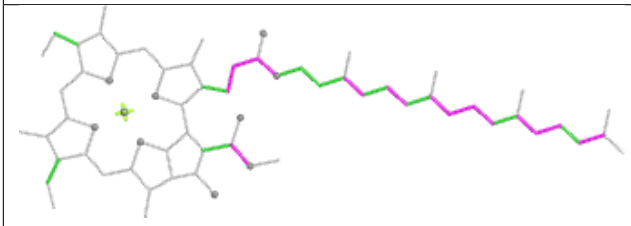
Ligand CLA A 827



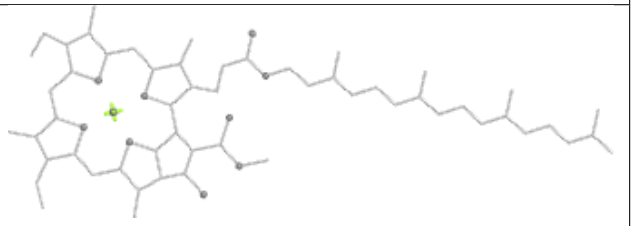
Bond lengths



Bond angles

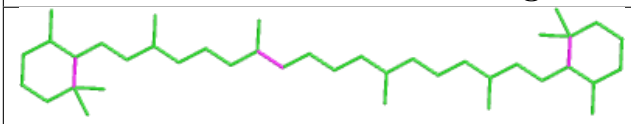


Torsions

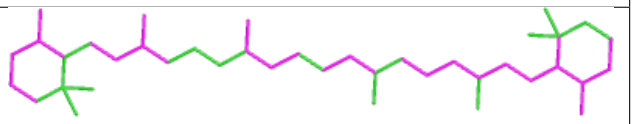


Rings

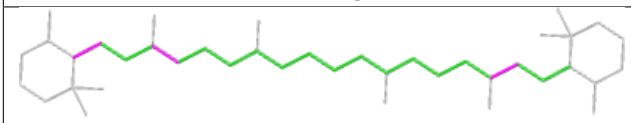
Ligand BCR B 852



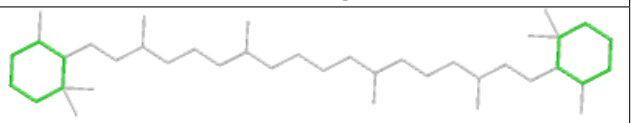
Bond lengths



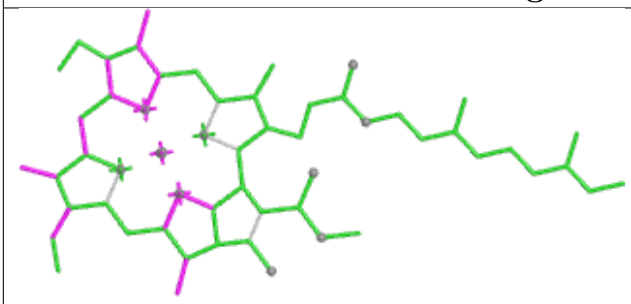
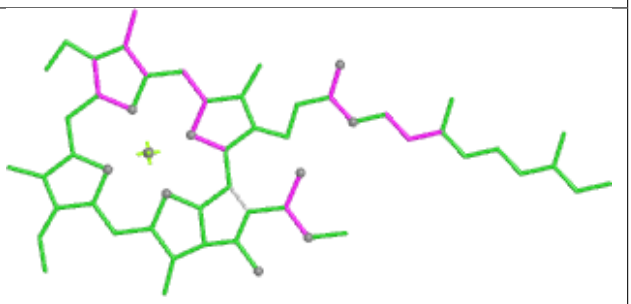
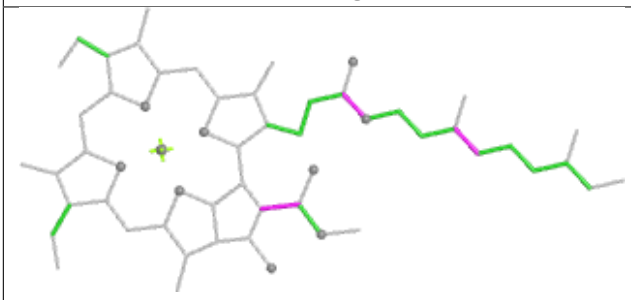
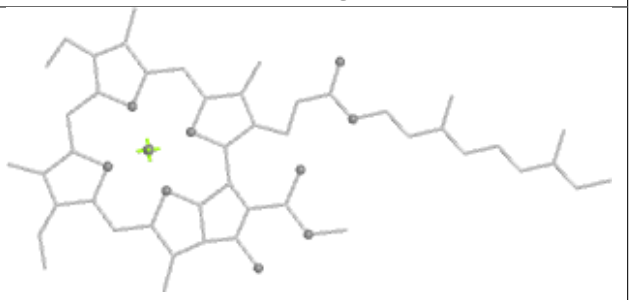
Bond angles

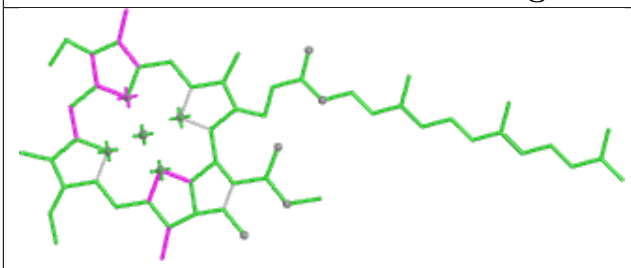
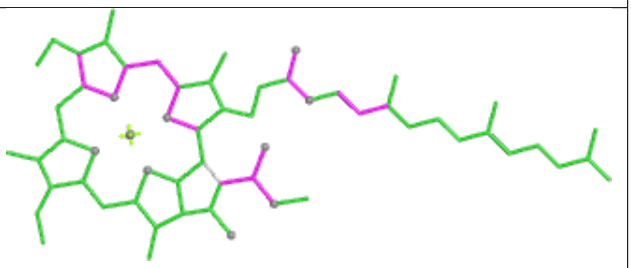
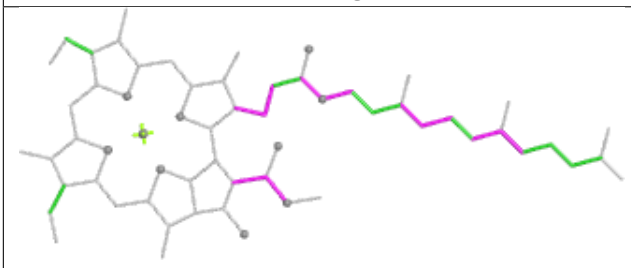
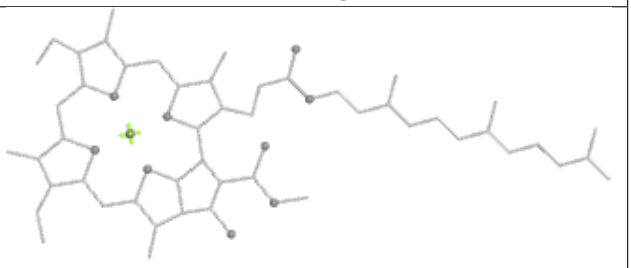


Torsions

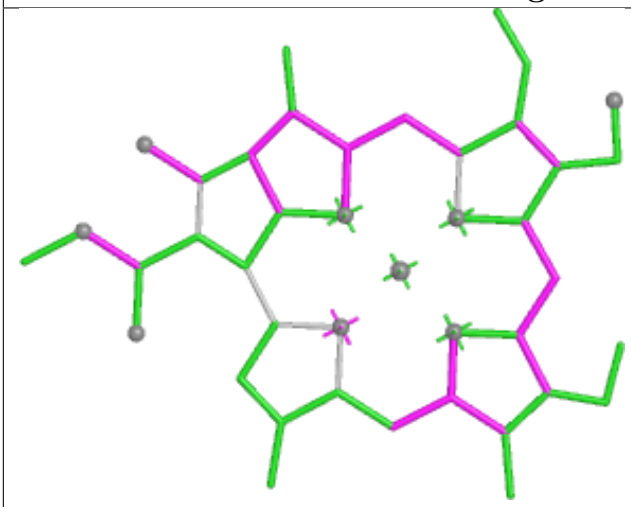


Rings

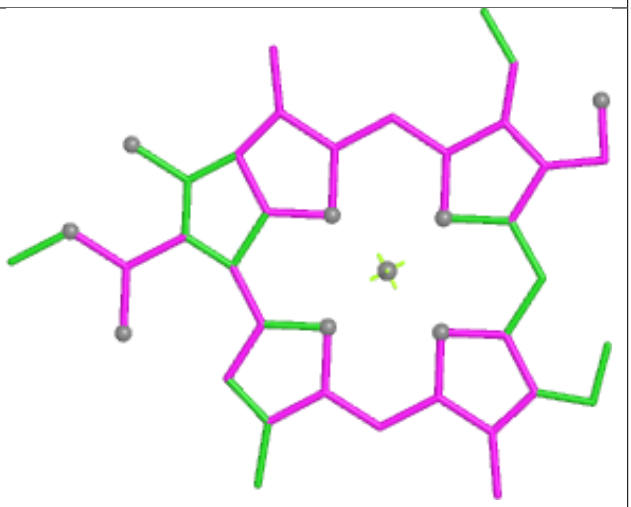
Ligand CLA L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

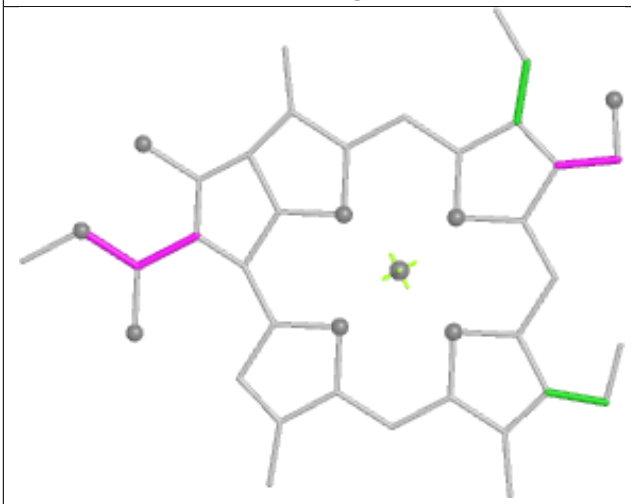
Ligand CHL 1 517



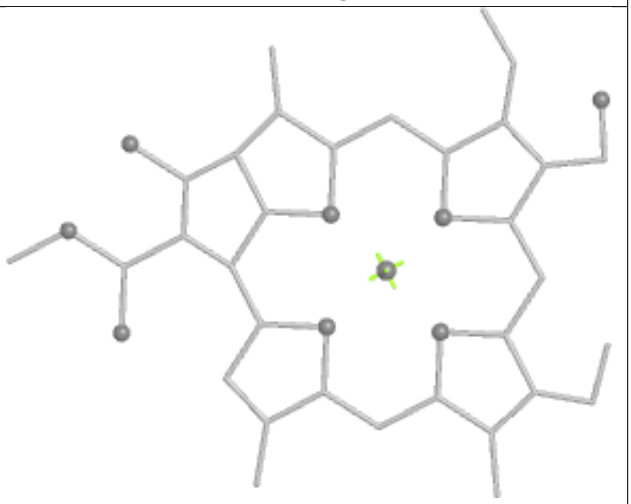
Bond lengths



Bond angles

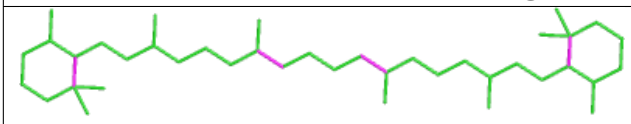


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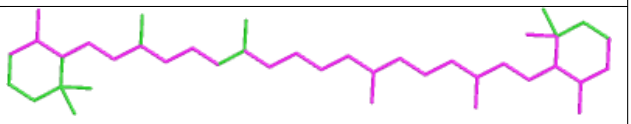


Rings

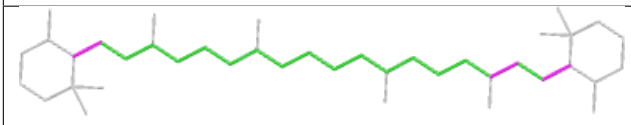
Ligand BCR A 845



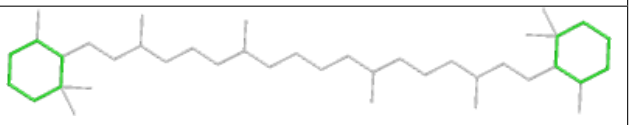
Bond lengths



Bond angles

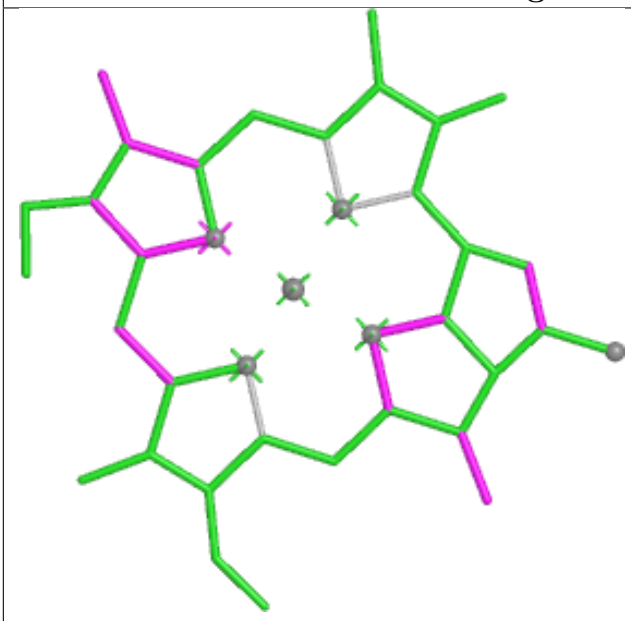


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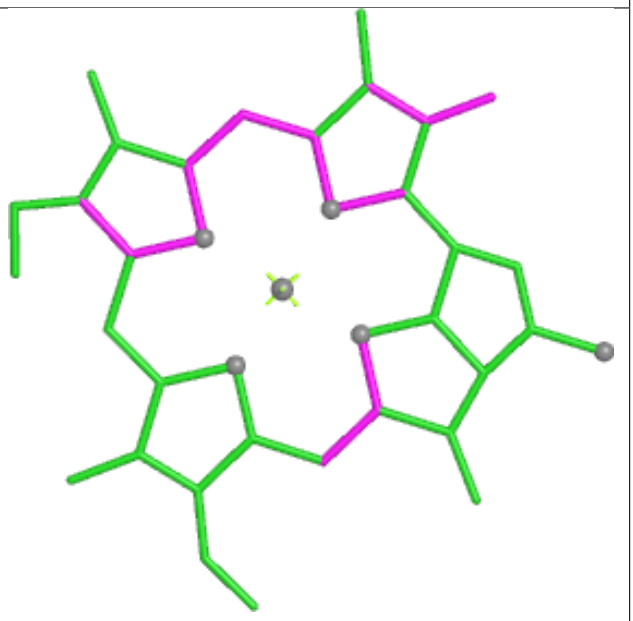


Rings

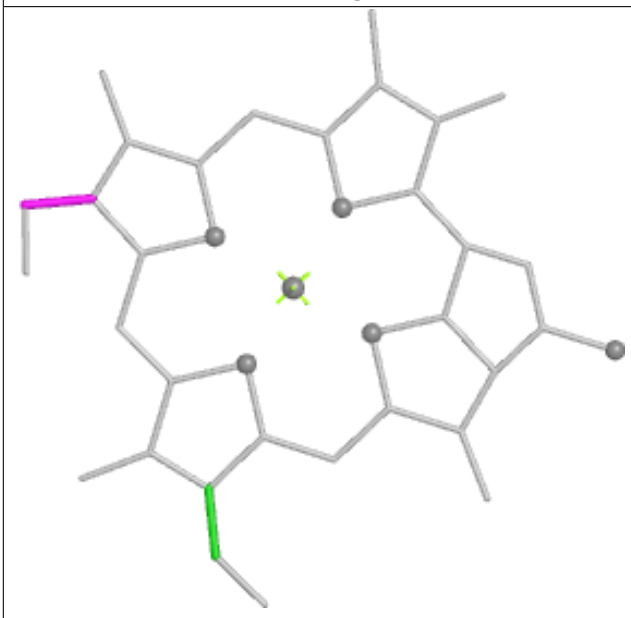
Ligand CLA n 201



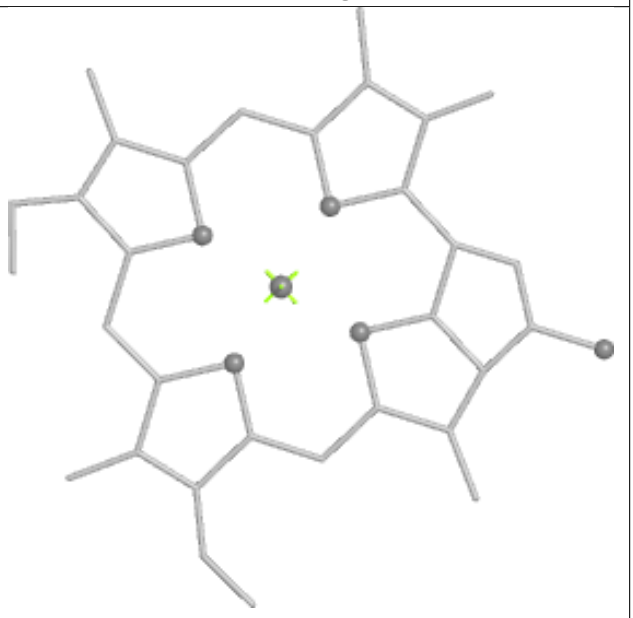
Bond lengths



Bond angles

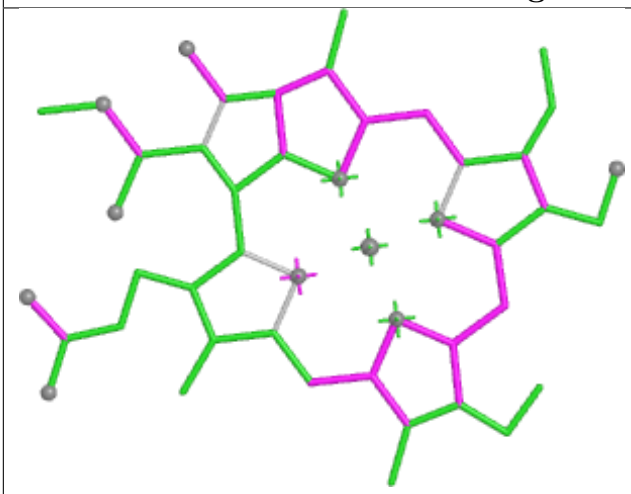


Torsions

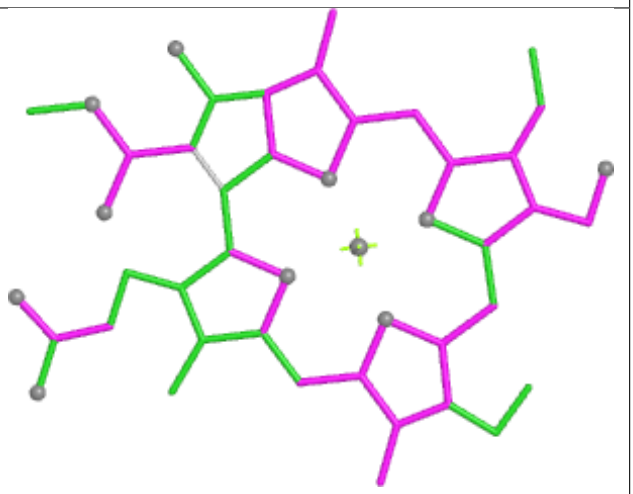


Rings

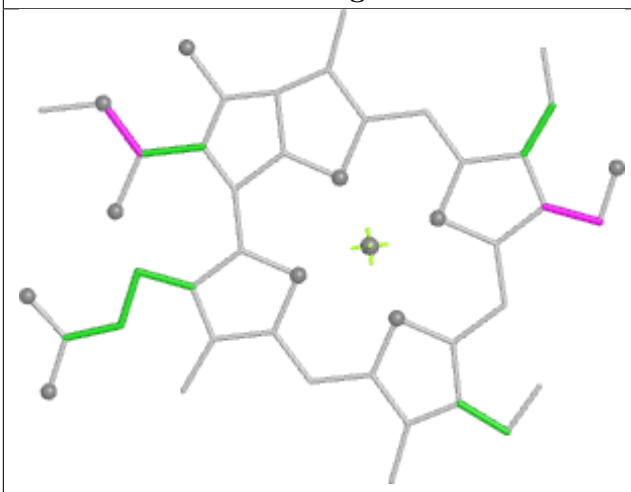
Ligand CHL 5 315



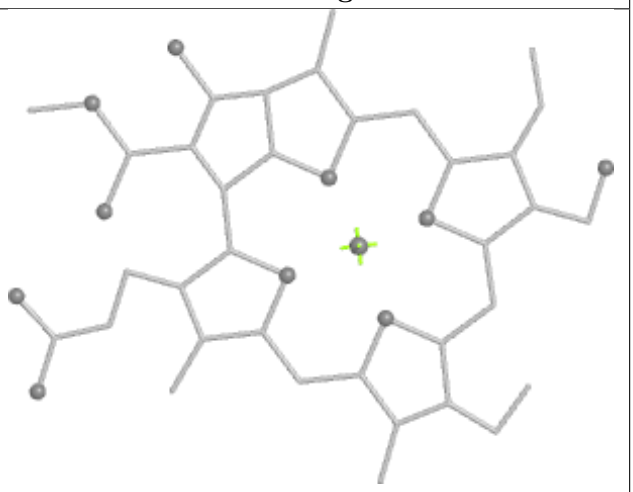
Bond lengths



Bond angles



Torsions



Rings

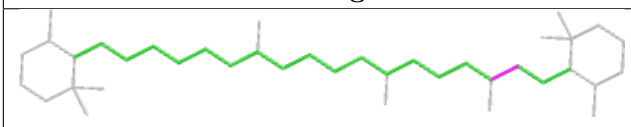
Ligand BCR f 850



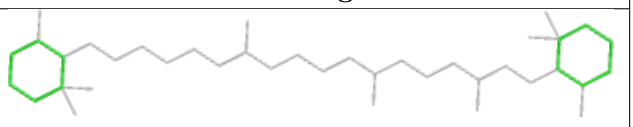
Bond lengths



Bond angles

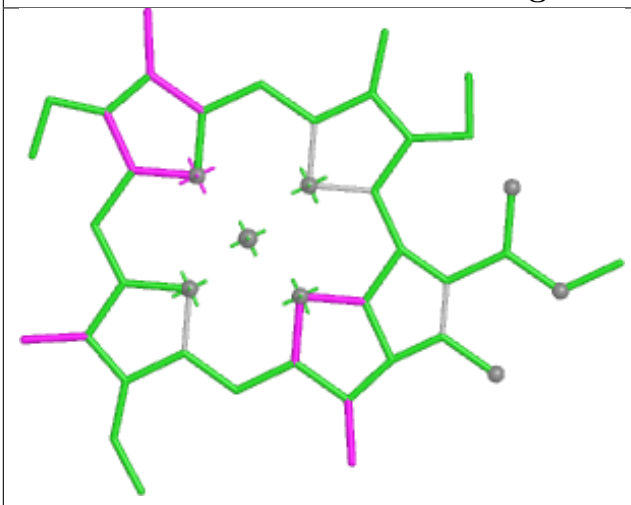


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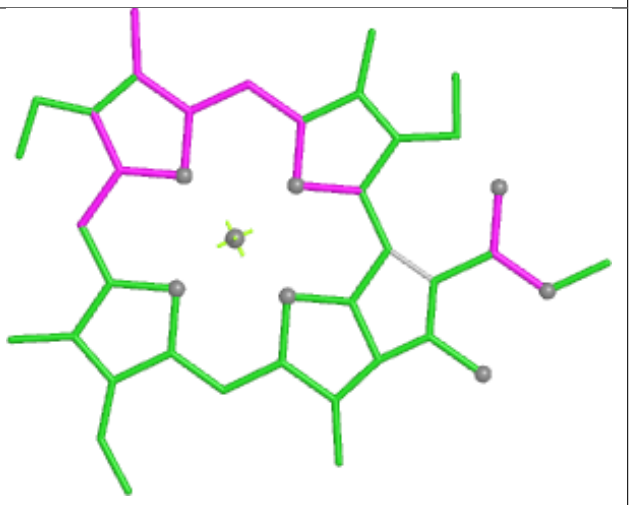


Rings

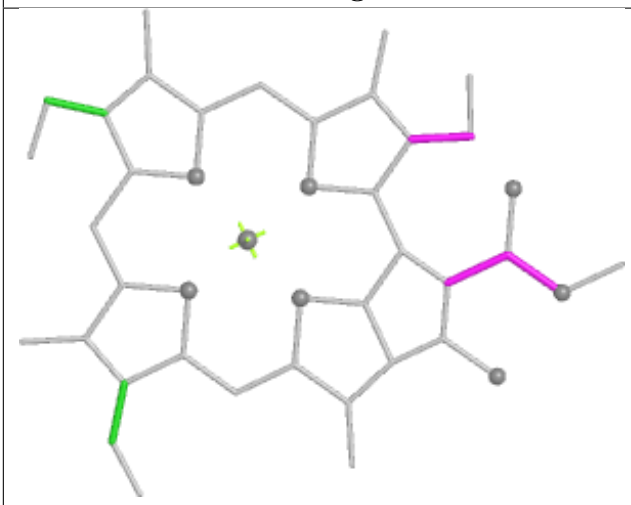
Ligand CLA e 821



Bond lengths



Bond angles



Torsions

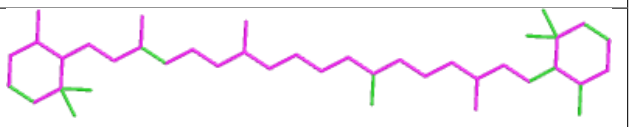


Rings

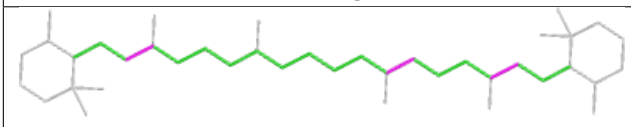
Ligand BCR F 801



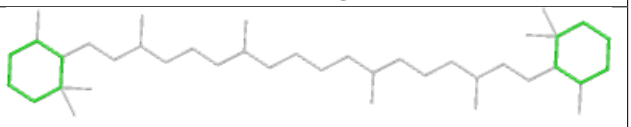
Bond lengths



Bond angles

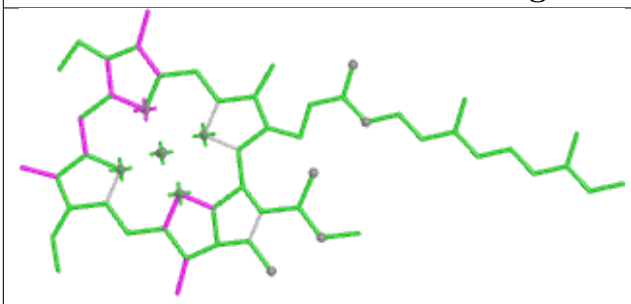


Torsions

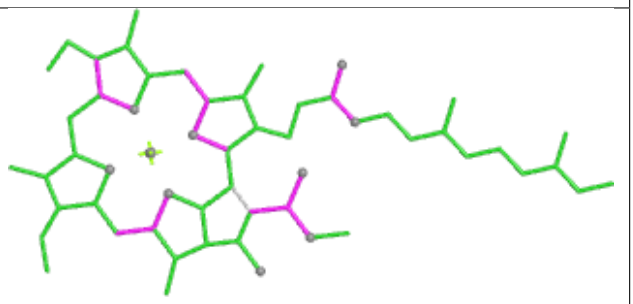


Rings

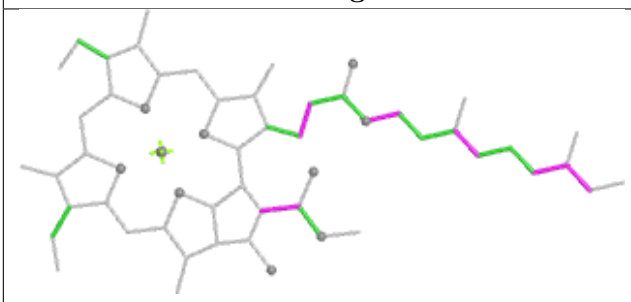
Ligand CLA e 824



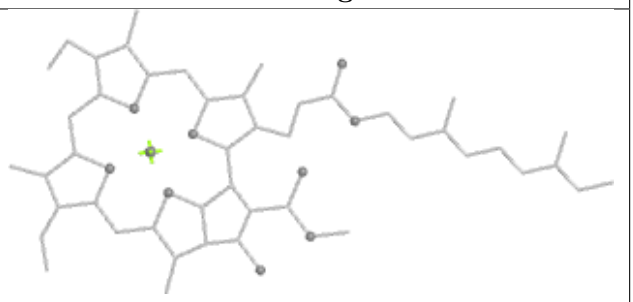
Bond lengths



Bond angles

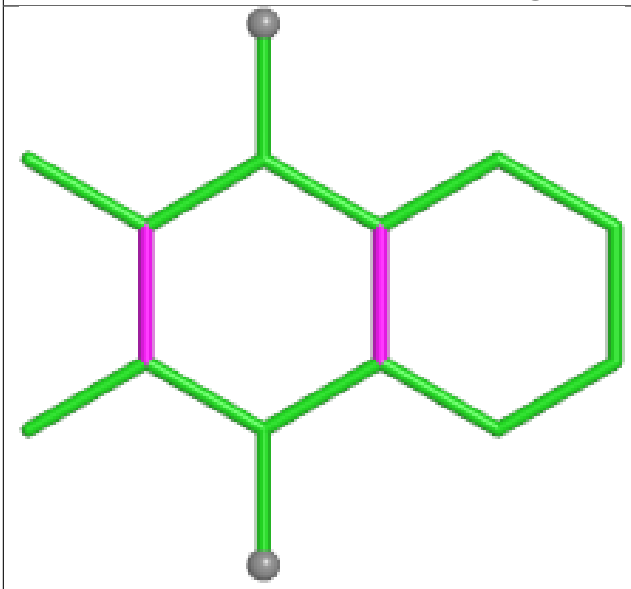


Torsions

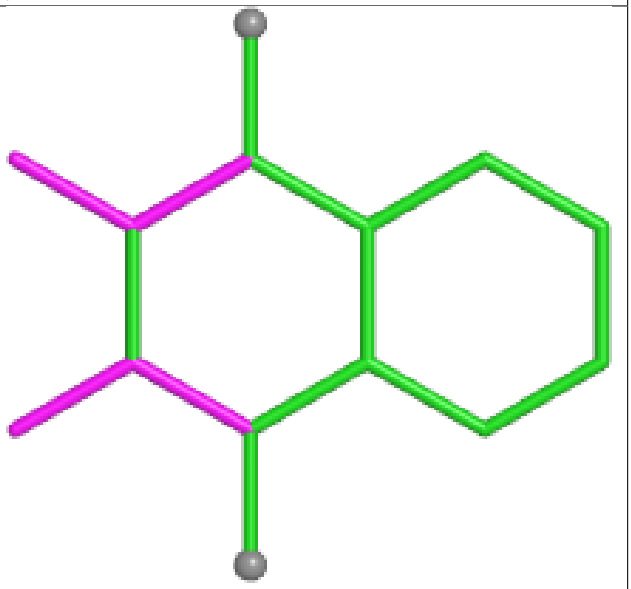


Rings

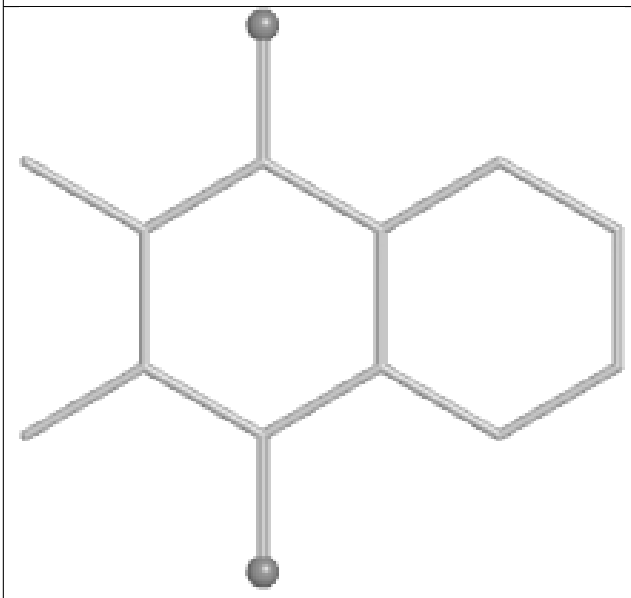
Ligand PQN e 842



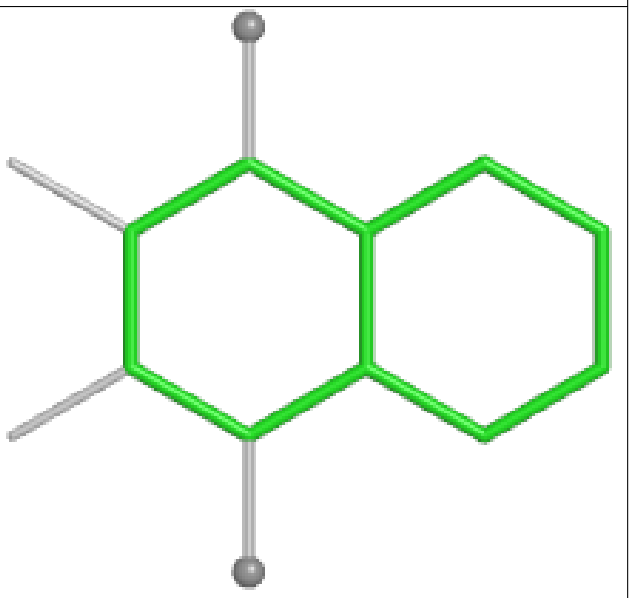
Bond lengths



Bond angles

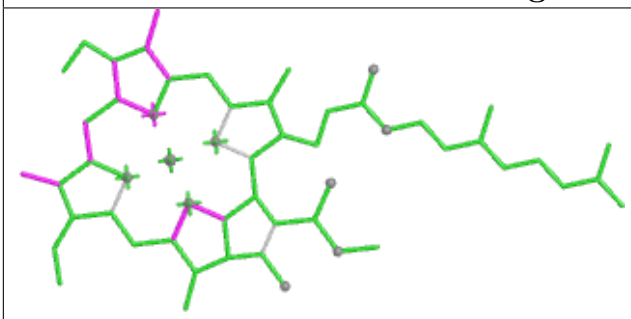


Torsions

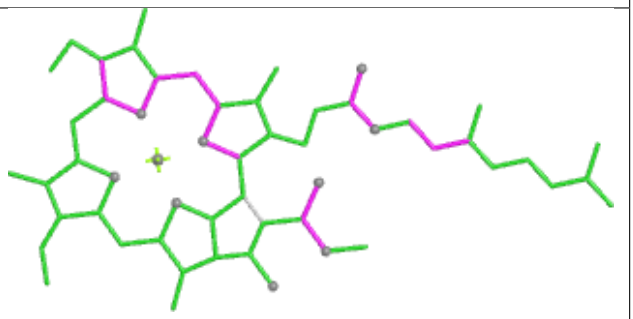


Rings

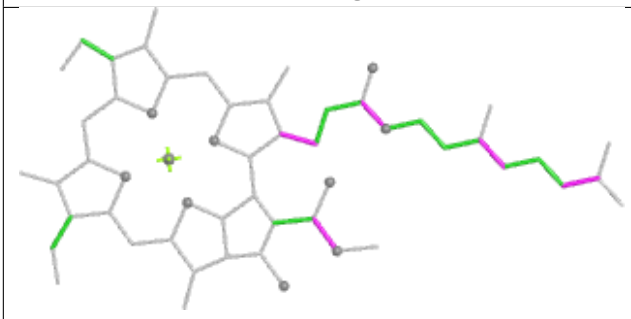
Ligand CLA 1 506



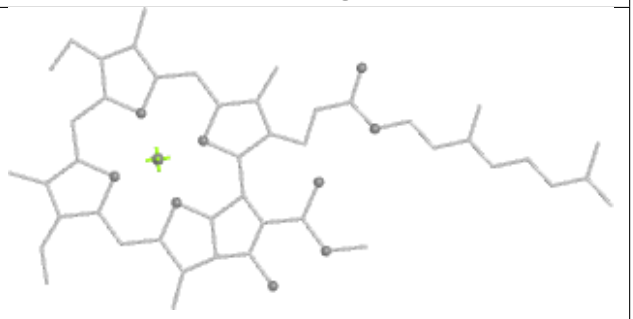
Bond lengths



Bond angles

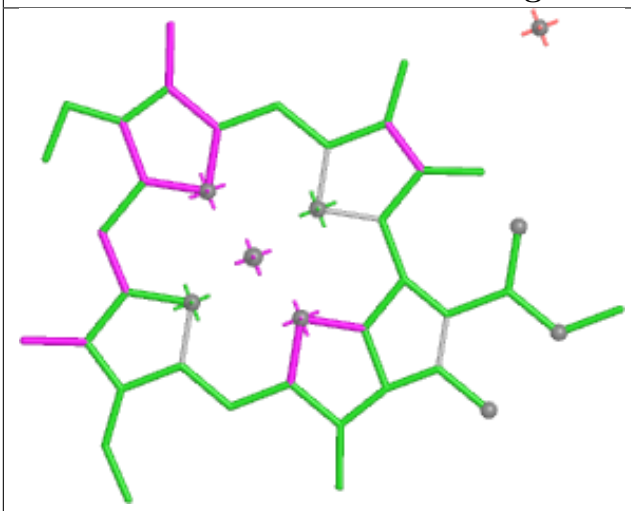


Torsions



Rings

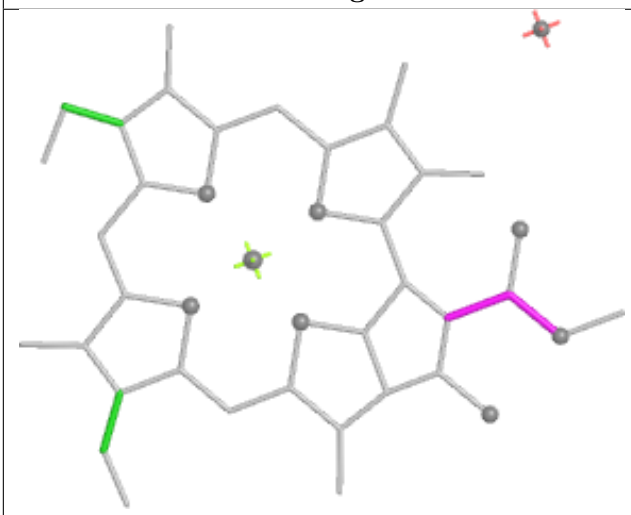
Ligand CLA B 828



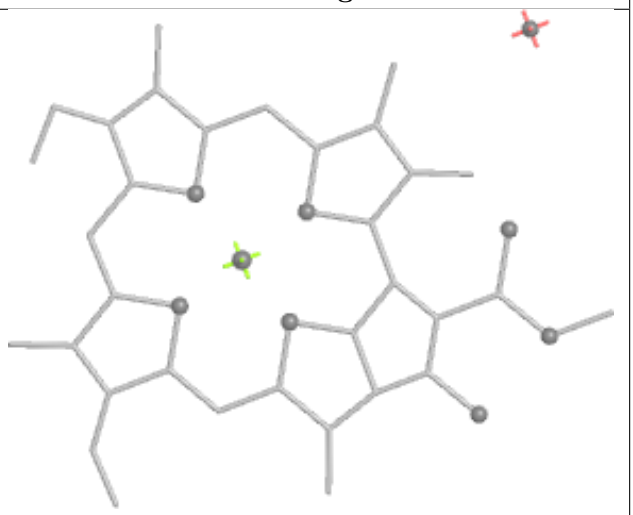
Bond lengths



Bond angles

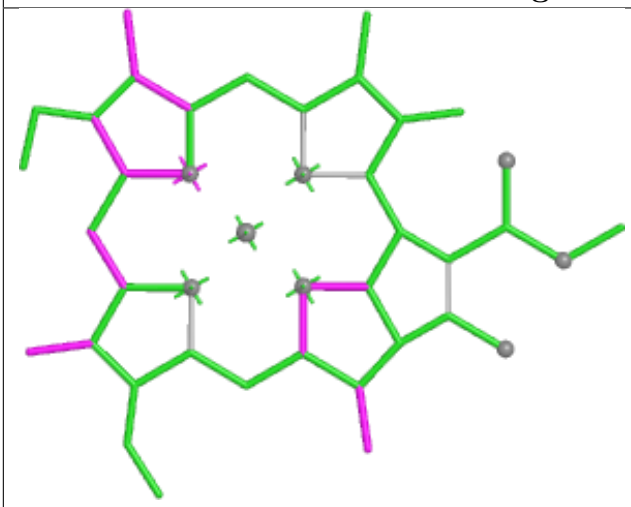


Torsions

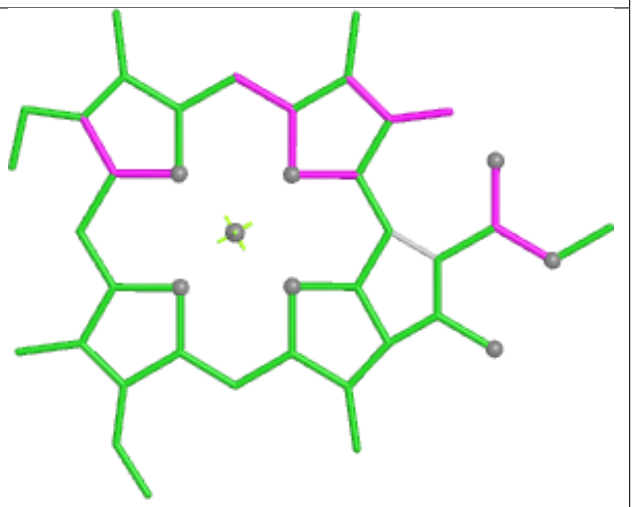


Rings

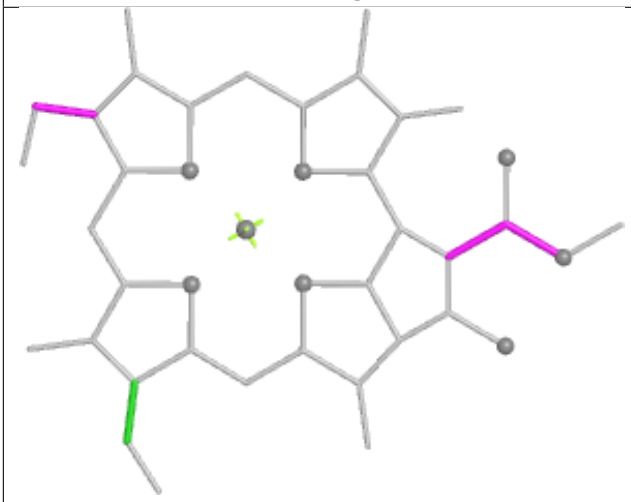
Ligand CLA f 828



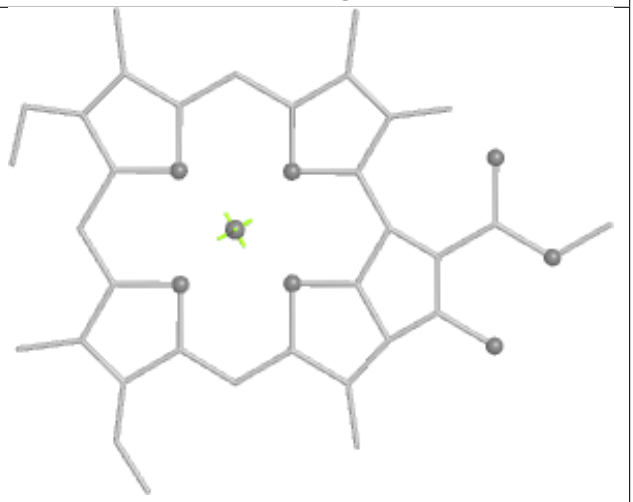
Bond lengths



Bond angles

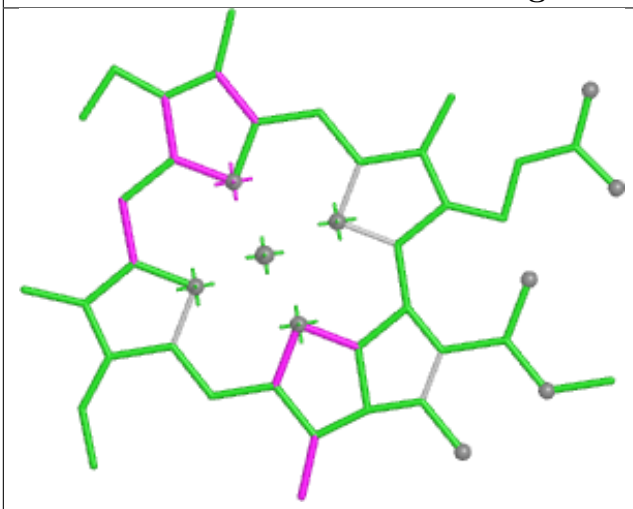


Torsions

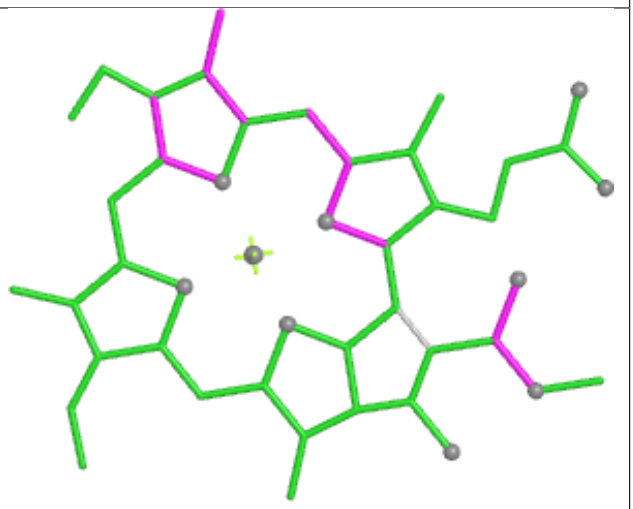


Rings

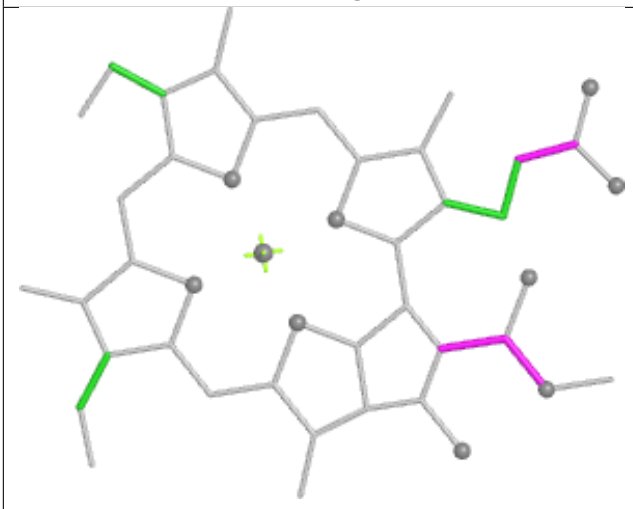
Ligand CLA o 304



Bond lengths



Bond angles

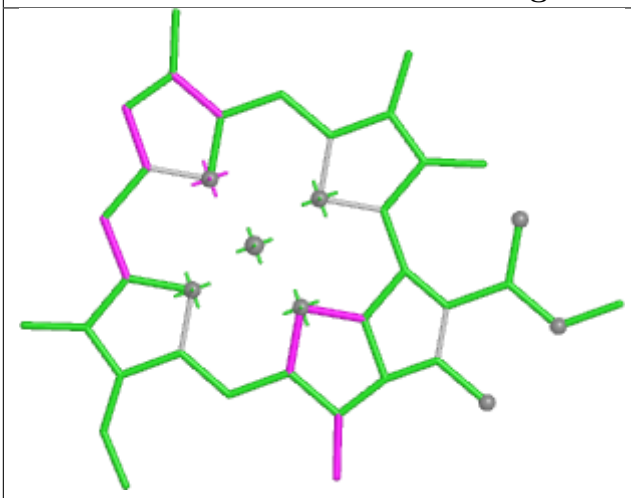


Torsions

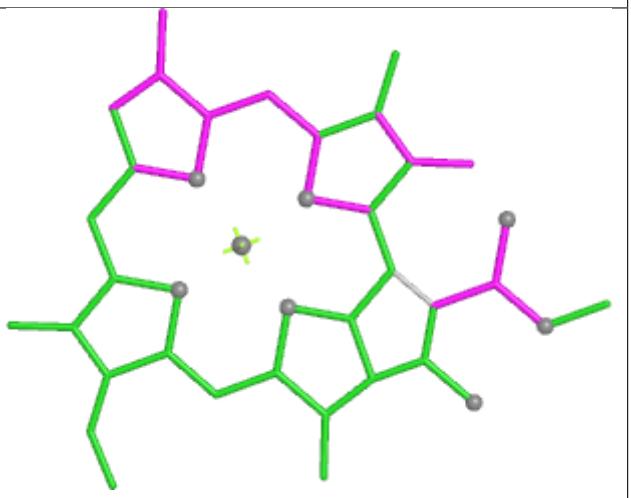


Rings

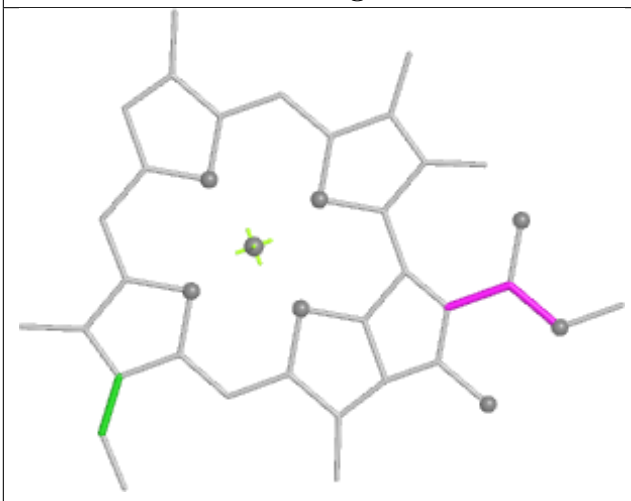
Ligand CLA s 504



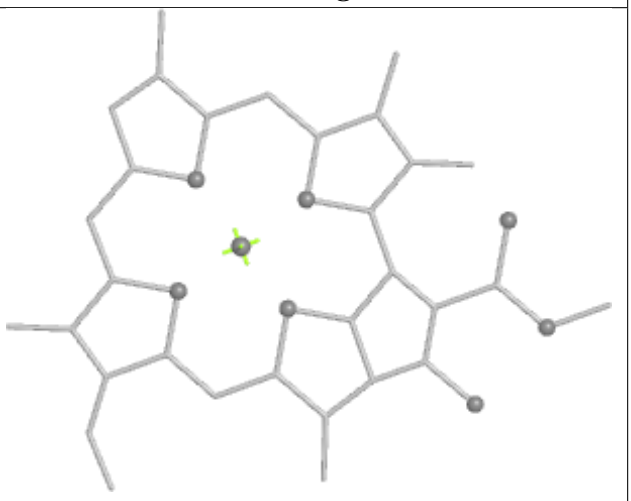
Bond lengths



Bond angles

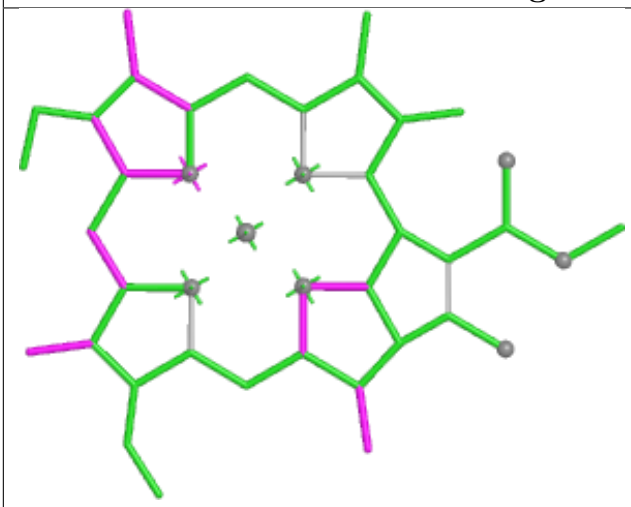


Torsions

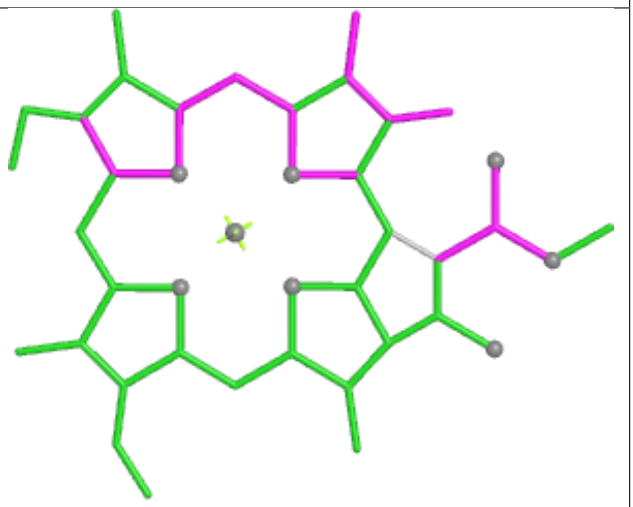


Rings

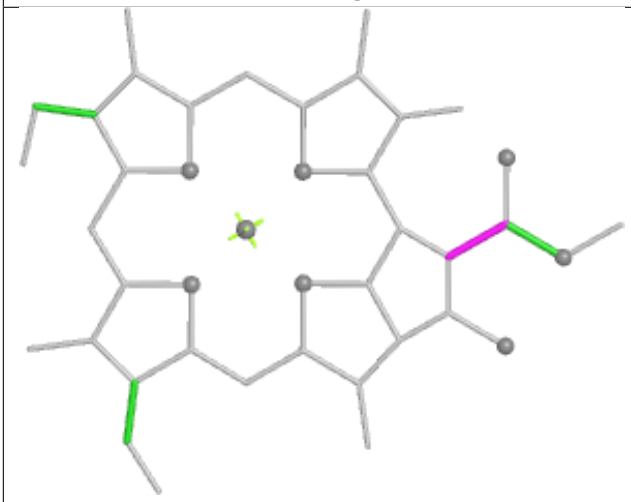
Ligand CLA e 806



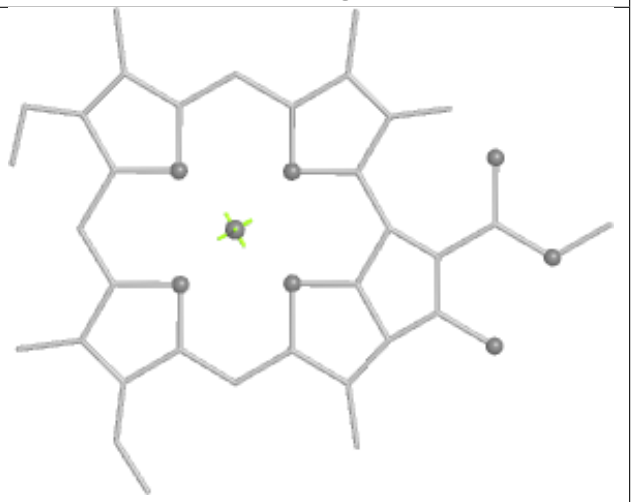
Bond lengths



Bond angles

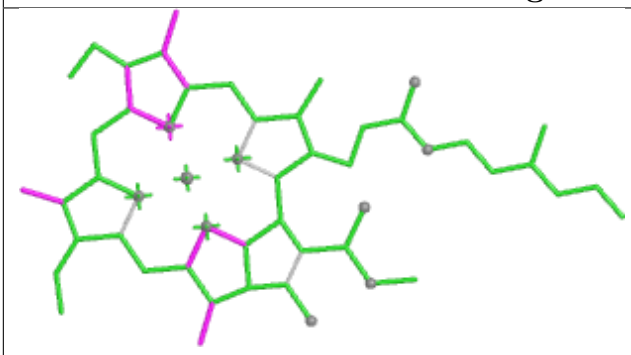


Torsions

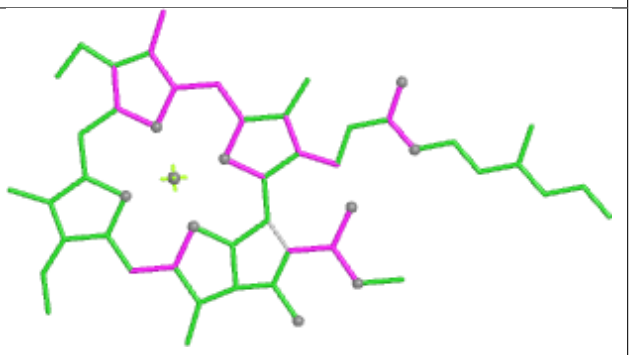


Rings

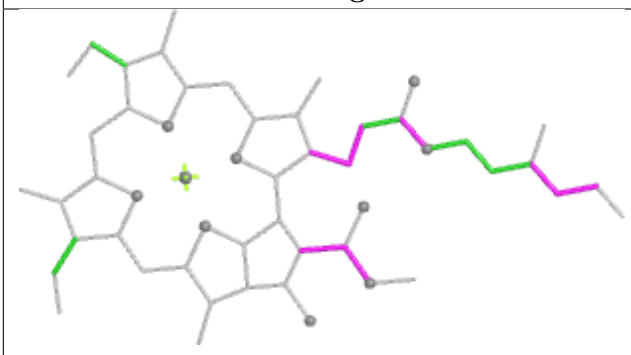
Ligand CLA L 303



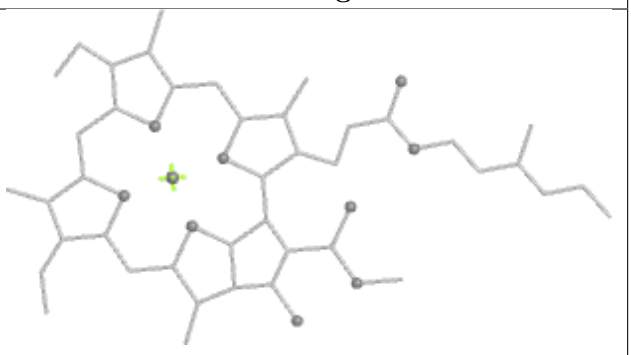
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

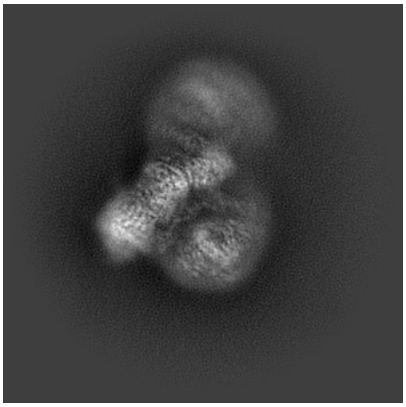
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31498. These allow visual inspection of the internal detail of the map and identification of artifacts.

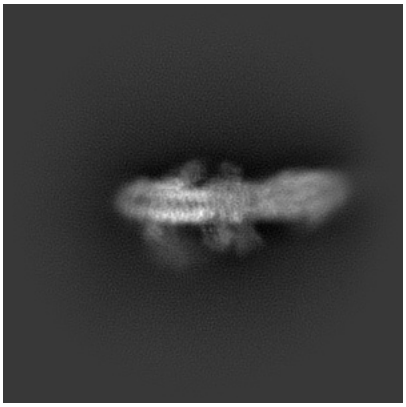
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

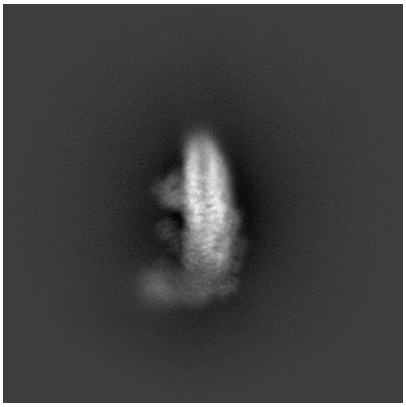
6.1.1 Primary map



X



Y

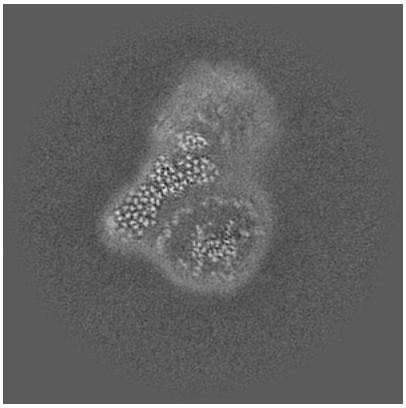


Z

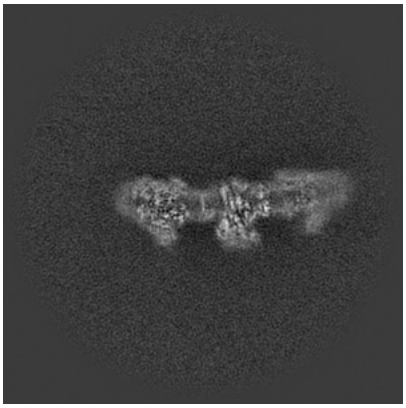
The images above show the map projected in three orthogonal directions.

6.2 Central slices

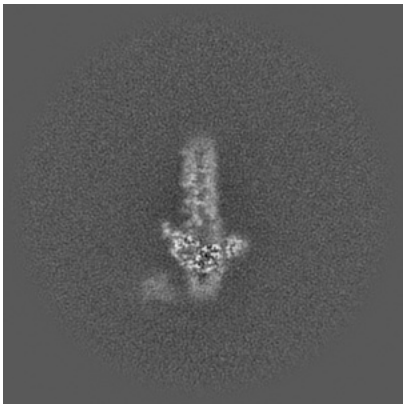
6.2.1 Primary map



X Index: 220



Y Index: 220

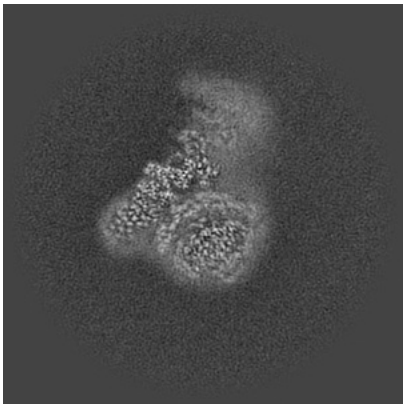


Z Index: 220

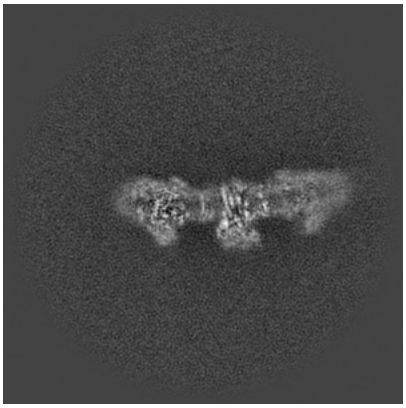
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 209



Y Index: 221

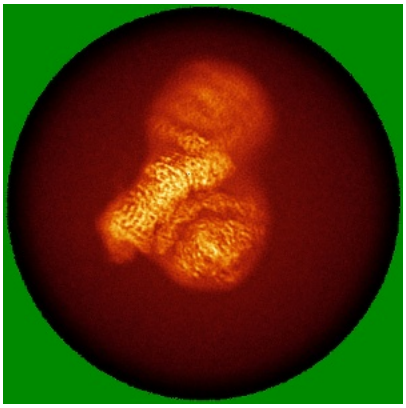


Z Index: 196

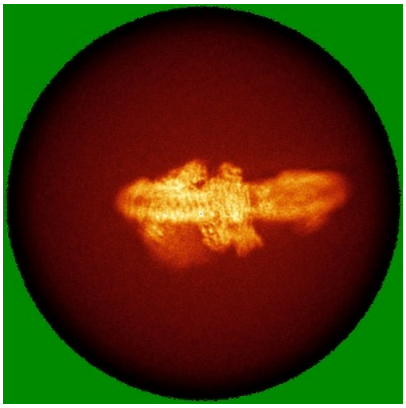
The images above show the largest variance slices of the map in three orthogonal directions.

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

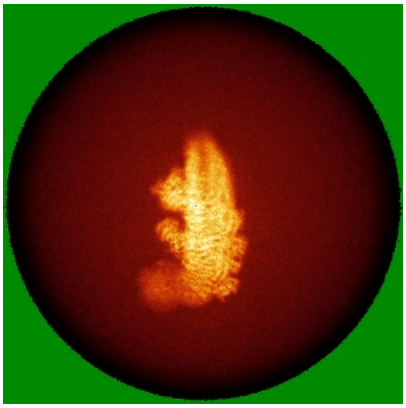
6.4.1 Primary map



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

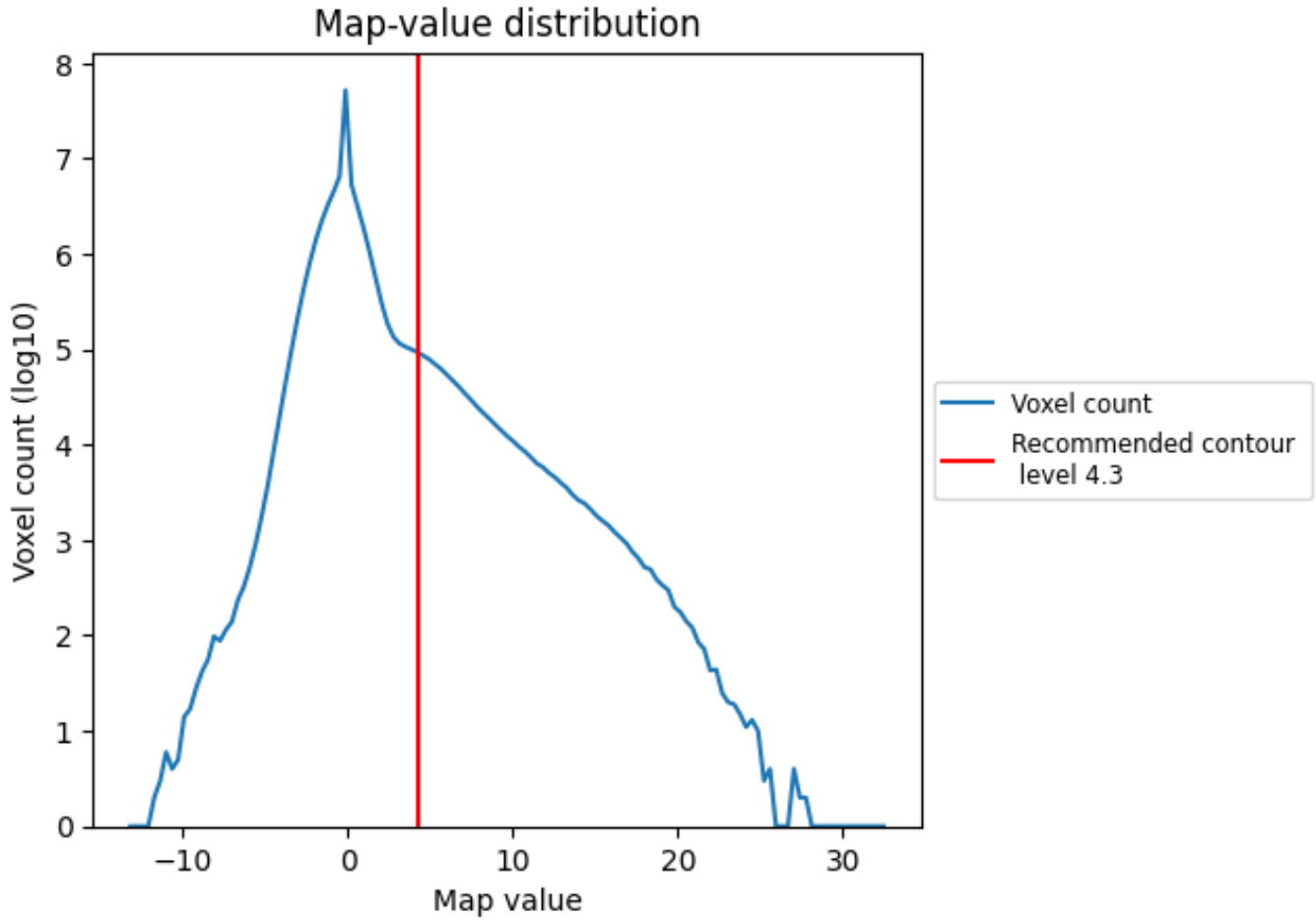
6.6 Mask visualisation (i)

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

7 Map analysis

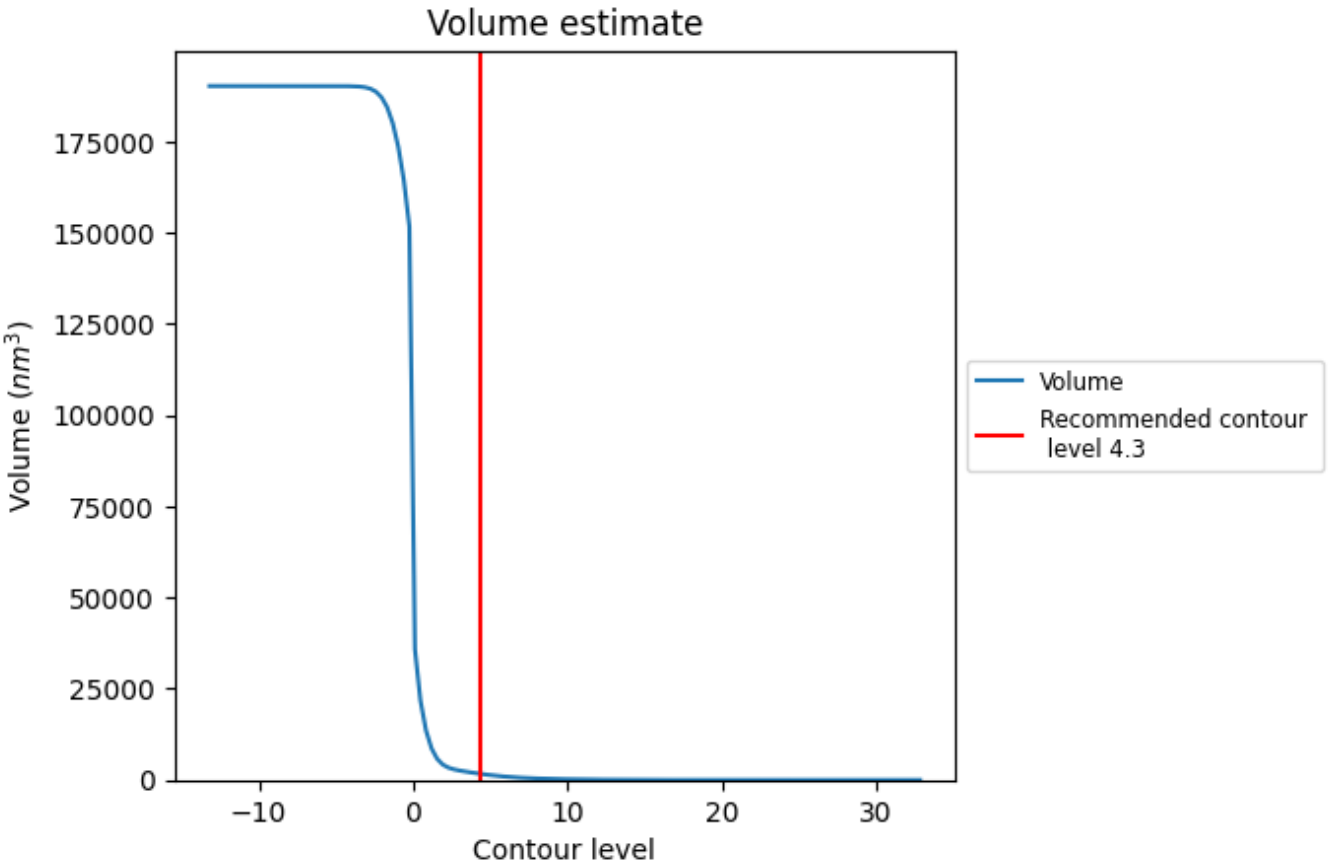
This section contains the results of statistical analysis of the map.

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.

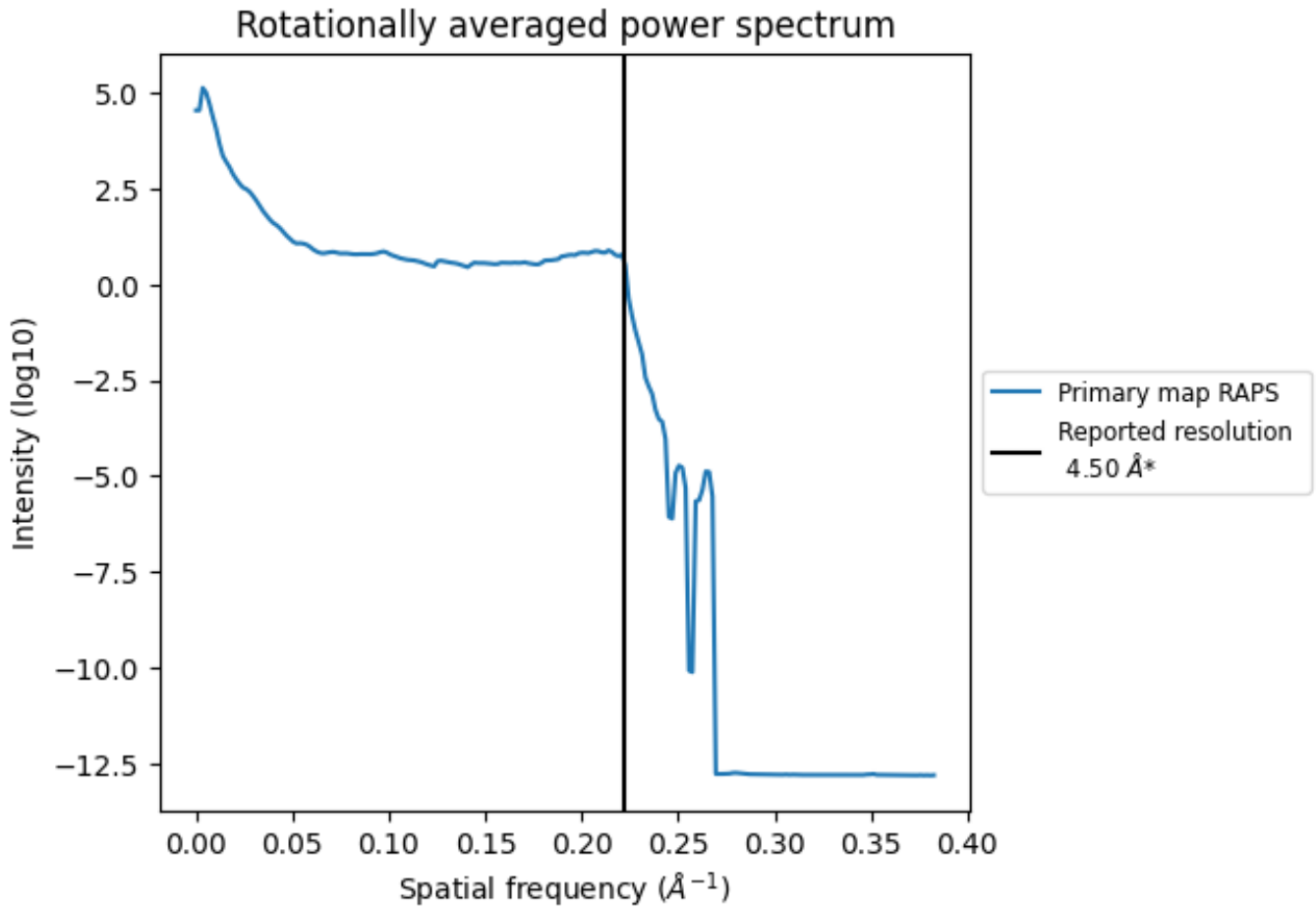
7.2 Volume estimate



The volume at the recommended contour level is 1712 nm^3; this corresponds to an approximate mass of 1547 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 0.222 $Å^{-1}$

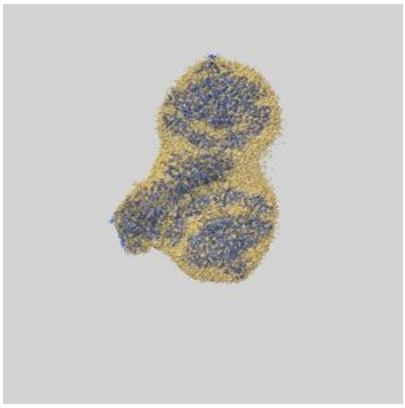
8 Fourier-Shell correlation

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

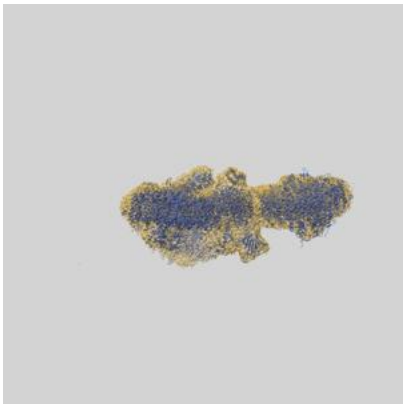
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31498 and PDB model 7F9O. Per-residue inclusion information can be found in section 3 on page 38.

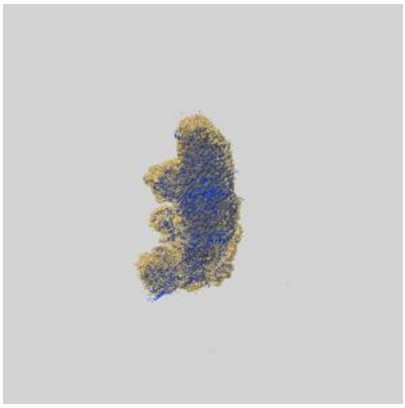
9.1 Map-model overlay



X



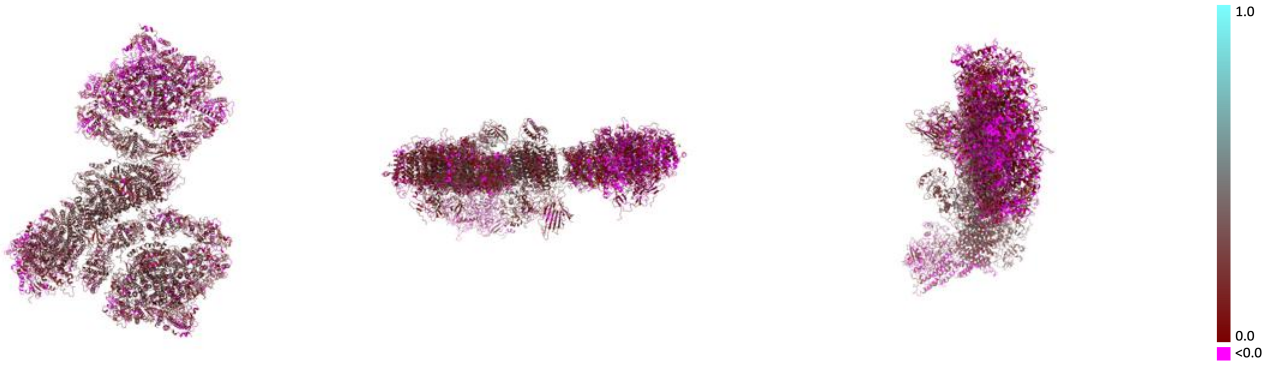
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3 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.

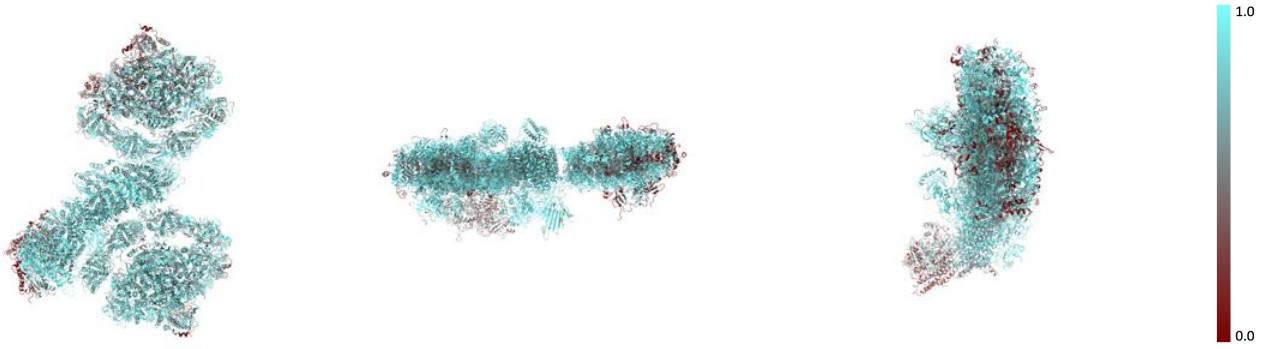
9.2 Q-score mapped to coordinate model



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.

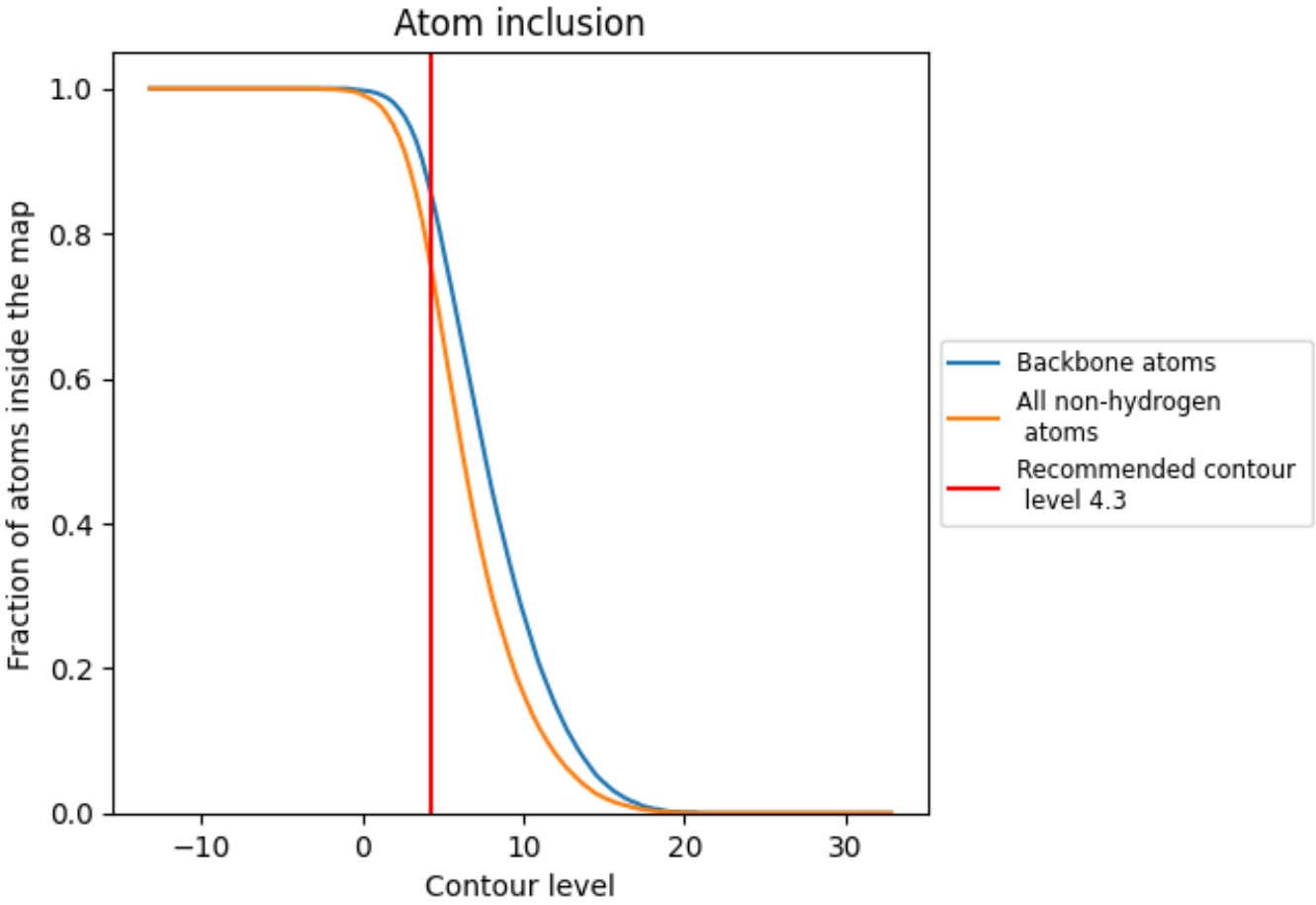
9.3 Atom inclusion mapped to coordinate model



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 (4.3).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 75% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.1530
0	0.9110	0.2790
1	0.8680	0.1670
2	0.8140	0.1560
3	0.7630	0.1310
4	0.9470	0.2970
5	0.8450	0.2040
6	0.9220	0.2590
7	0.9030	0.1660
8	0.9290	0.2190
9	0.9390	0.3030
A	0.7970	0.2100
B	0.8350	0.1920
C	0.9300	0.1900
D	0.8100	0.1390
E	0.8460	0.2510
F	0.7910	0.2080
G	0.7710	0.1410
H	0.6080	0.0710
I	0.7270	0.1620
J	0.7650	0.2130
K	0.5680	0.0740
L	0.6440	0.0840
M	0.8570	0.2760
N	0.8000	0.1930
O	0.8710	0.2910
P	0.8110	0.2610
Q	0.8350	0.2470
R	0.8330	0.2580
S	0.3300	0.0480
T	0.4230	0.0480
U	0.3670	0.0450
V	0.5320	0.0910
W	0.3670	0.0230
X	0.4140	0.0630



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.5340	0.0660
Z	0.9210	0.2760
a	0.9320	0.2200
b	0.9430	0.2340
c	0.9380	0.2400
d	0.9200	0.2580
e	0.6790	0.0550
f	0.7370	0.0470
g	0.7540	0.0570
h	0.3020	0.0450
i	0.3880	0.1030
j	0.7210	0.0960
k	0.2970	0.0220
l	0.5890	0.0150
m	0.6500	0.1240
n	0.2750	0.0030
o	0.3410	0.0070
p	0.6930	0.0230
q	0.7070	0.0930
r	0.7970	0.0940
s	0.8690	0.2290