Full wwPDB EM Validation Report ⓘ

Nov 3, 2026 – 01:19 PM EST

PDB ID	:	9OZ3 / pdb_00009oz3
EMDB ID	:	EMD-71048
Title	:	Structure of a red shifted PSI monomer from 6803
Authors	:	Mazor, Y.; Kahtun, H.; Asido, M.; Gorski, C.; Schlau-Cohen, G.S.
Deposited on	:	2025-06-04
Resolution	:	1.88 Å(reported)

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

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

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

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

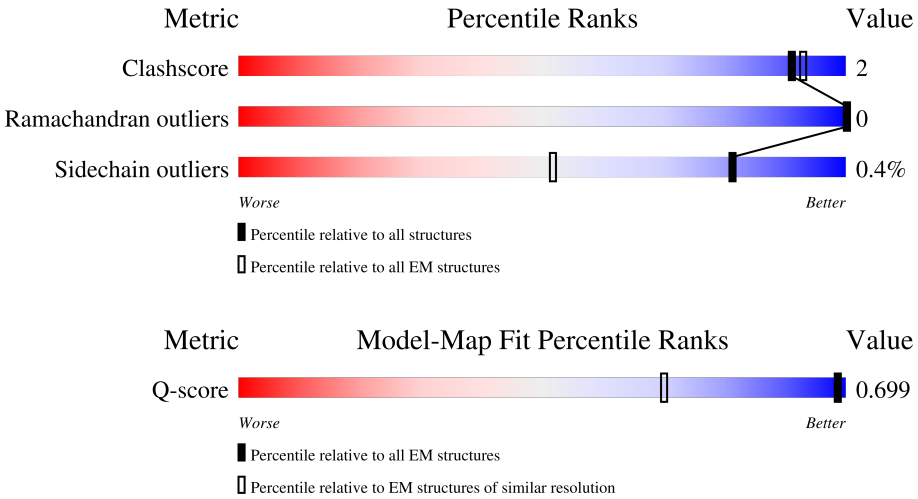
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.88 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	1004 (1.39 - 2.38)

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

Mol	Chain	Length	Quality of chain
1	A	751	97%
1	G	751	97%
1	a	751	96%
2	B	735	97%

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Mol	Chain	Length	Quality of chain
2	H	735	97%
2	b	735	97%
3	C	81	98%
3	N	81	96%
3	c	81	98%
4	D	141	99%
4	P	141	97%
4	d	141	98%
5	E	74	95% 5%
5	O	74	95% 5%
5	e	74	95% 5%
6	F	165	82% 15%
6	Q	165	82% 15%
6	f	165	85% 15%
7	I	40	85% 8% 8%
7	R	40	85% 8% 8%
7	i	40	82% 10% 8%
8	J	40	92% 8%
8	S	40	95%
8	j	40	92% 8%
9	K	86	85% 10%
9	T	86	86% 10%
9	k	86	84% 6% 10%
10	L	157	94%
10	U	157	95%

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Mol	Chain	Length	Quality of chain
10	l	157	96%
11	M	31	100%
11	V	31	100%
11	m	31	100%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 76301 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	741	Total	C	N	O	S	0	0
			5801	3800	987	987	27		
1	G	741	Total	C	N	O	S	0	0
			5801	3800	987	987	27		
1	a	741	Total	C	N	O	S	0	0
			5801	3800	987	987	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5818	3831	974	998	15		
2	H	734	Total	C	N	O	S	0	0
			5818	3831	974	998	15		
2	b	734	Total	C	N	O	S	0	0
			5818	3831	974	998	15		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	95	GLN	HIS	engineered mutation	UNP P29255
B	486	ALA	-	linker	UNP P29255
B	487	TRP	-	linker	UNP P29255
B	488	PRO	-	linker	UNP P29255
B	489	ASN	-	linker	UNP P29255
B	490	TYR	-	linker	UNP P29255
B	491	GLY	-	linker	UNP P29255
B	492	ASN	-	linker	UNP P29255
B	493	VAL	-	linker	UNP P29255
H	95	GLN	HIS	engineered mutation	UNP P29255
H	486	ALA	-	linker	UNP P29255
H	487	TRP	-	linker	UNP P29255
H	488	PRO	-	linker	UNP P29255

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Chain	Residue	Modelled	Actual	Comment	Reference
H	489	ASN	-	linker	UNP P29255
H	490	TYR	-	linker	UNP P29255
H	491	GLY	-	linker	UNP P29255
H	492	ASN	-	linker	UNP P29255
H	493	VAL	-	linker	UNP P29255
b	95	GLN	HIS	engineered mutation	UNP P29255
b	486	ALA	-	linker	UNP P29255
b	487	TRP	-	linker	UNP P29255
b	488	PRO	-	linker	UNP P29255
b	489	ASN	-	linker	UNP P29255
b	490	TYR	-	linker	UNP P29255
b	491	GLY	-	linker	UNP P29255
b	492	ASN	-	linker	UNP P29255
b	493	VAL	-	linker	UNP P29255

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		
4	P	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		
4	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	70	Total	C	N	O	0	0
			547	343	97	107		
5	O	70	Total	C	N	O	0	0
			547	343	97	107		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	70	Total 547	C 343	N 97	O 107	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	40	Total 318	C 215	N 47	O 53	S 3	0	0
8	S	40	Total 318	C 215	N 47	O 53	S 3	0	0
8	j	40	Total 318	C 215	N 47	O 53	S 3	0	0

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

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

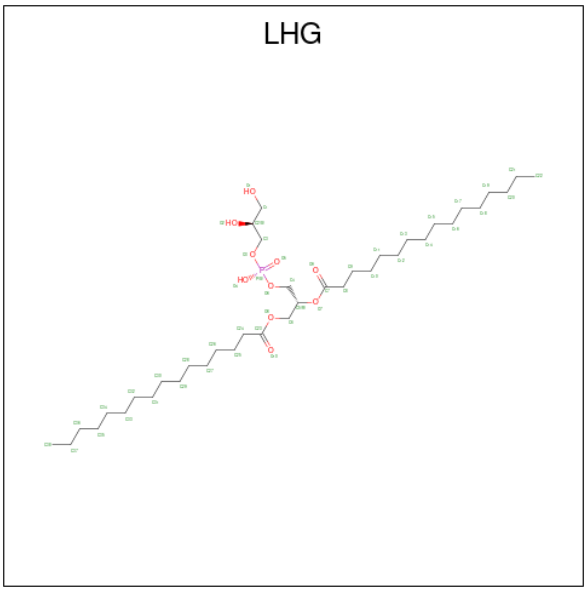
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

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

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

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

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



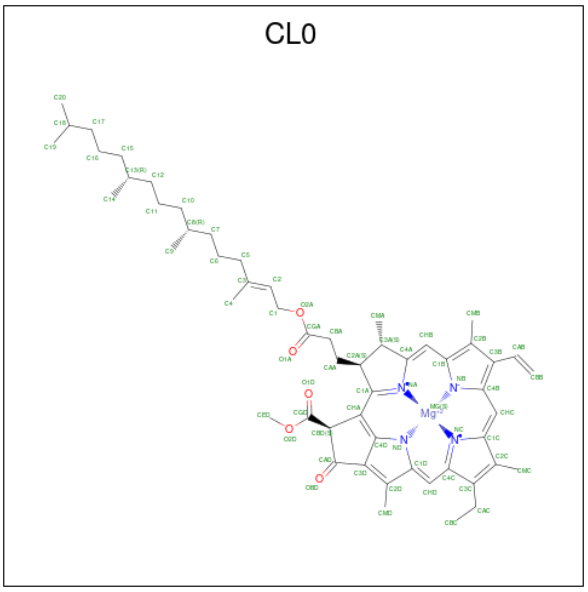
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			48	37	10	1	
12	A	1	Total	C	O	P	0
			49	38	10	1	

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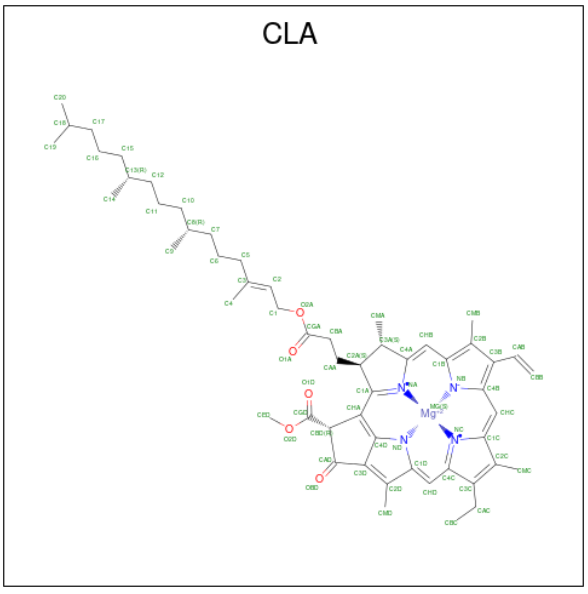
Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	O	P	0
			38	27	10	1	
12	G	1	Total	C	O	P	0
			48	37	10	1	
12	G	1	Total	C	O	P	0
			49	38	10	1	
12	G	1	Total	C	O	P	0
			25	14	10	1	
12	H	1	Total	C	O	P	0
			38	27	10	1	
12	L	1	Total	C	O	P	0
			40	29	10	1	
12	L	1	Total	C	O	P	0
			33	22	10	1	
12	M	1	Total	C	O	P	0
			38	27	10	1	
12	M	1	Total	C	O	P	0
			40	29	10	1	
12	M	1	Total	C	O	P	0
			42	31	10	1	
12	V	1	Total	C	O	P	0
			40	29	10	1	
12	a	1	Total	C	O	P	0
			48	37	10	1	
12	a	1	Total	C	O	P	0
			49	38	10	1	
12	b	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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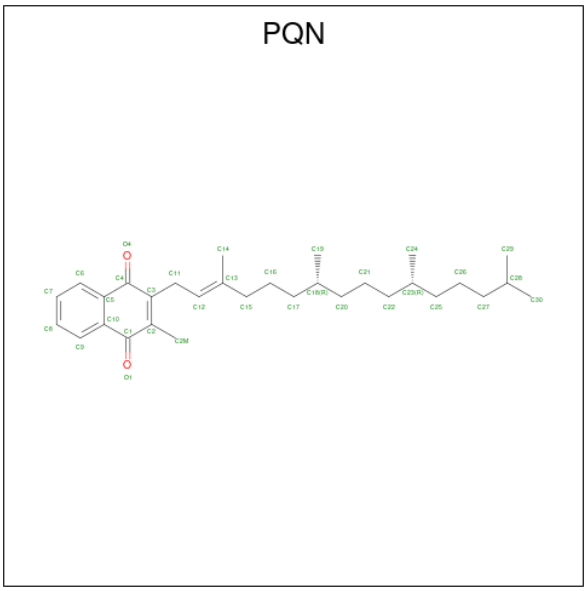
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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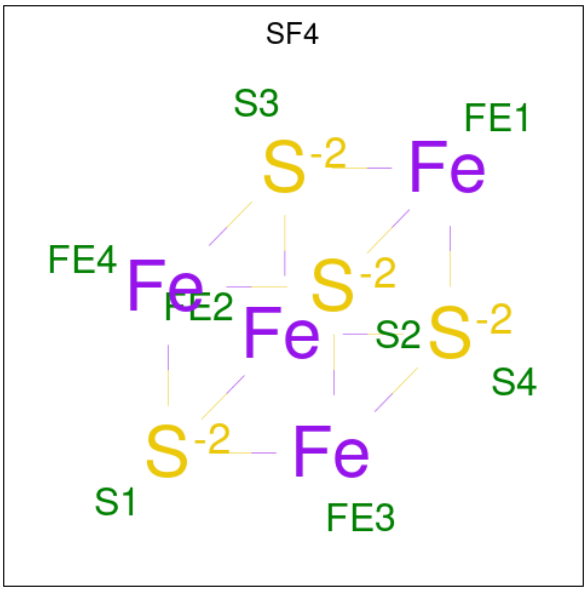
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



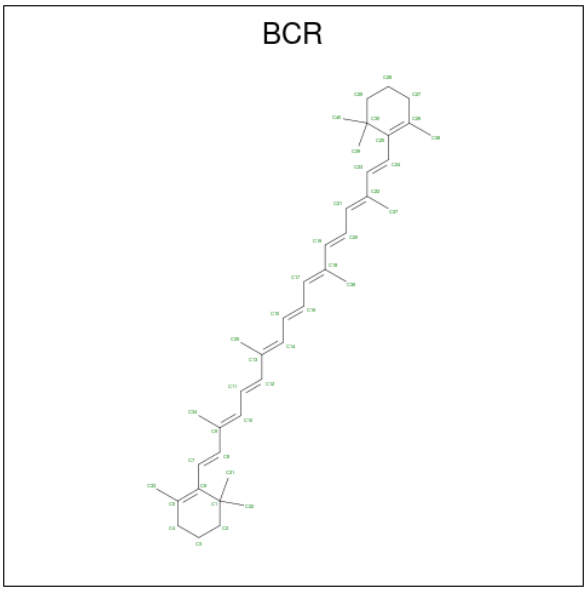
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C O 33 31 2	0
15	B	1	Total C O 33 31 2	0
15	G	1	Total C O 33 31 2	0
15	H	1	Total C O 33 31 2	0
15	a	1	Total C O 33 31 2	0
15	b	1	Total C O 33 31 2	0

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



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

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



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

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

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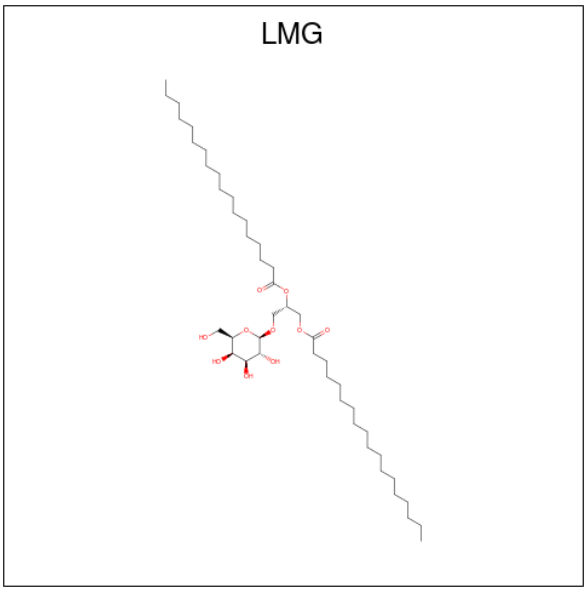
Mol	Chain	Residues	Atoms	AltConf
17	S	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 30 30	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	k	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



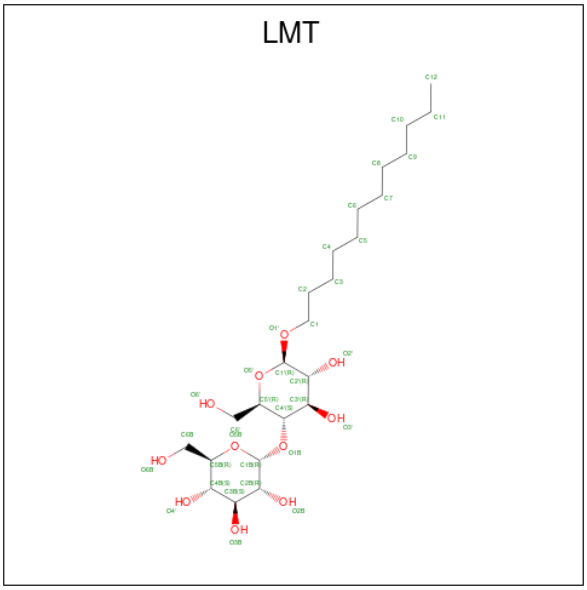
Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O 46 36 10	0
18	A	1	Total C O 42 32 10	0
18	B	1	Total C O 50 40 10	0
18	B	1	Total C O 38 28 10	0
18	B	1	Total C O 49 39 10	0
18	G	1	Total C O 46 36 10	0
18	H	1	Total C O 50 40 10	0
18	H	1	Total C O 36 26 10	0

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Mol	Chain	Residues	Atoms	AltConf
18	K	1	Total C O 35 25 10	0
18	L	1	Total C O 38 28 10	0
18	U	1	Total C O 38 28 10	0
18	a	1	Total C O 46 36 10	0
18	b	1	Total C O 50 40 10	0
18	b	1	Total C O 42 32 10	0
18	l	1	Total C O 38 28 10	0

- Molecule 19 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0

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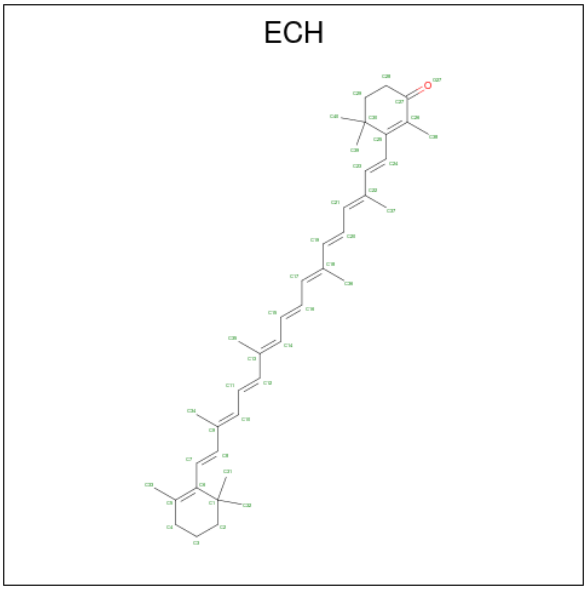
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Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C O 35 24 11	0
19	B	1	Total C O 35 24 11	0
19	G	1	Total C O 35 24 11	0
19	G	1	Total C O 35 24 11	0
19	H	1	Total C O 35 24 11	0
19	H	1	Total C O 35 24 11	0
19	J	1	Total C O 35 24 11	0
19	L	1	Total C O 35 24 11	0
19	Q	1	Total C O 35 24 11	0
19	Q	1	Total C O 35 24 11	0
19	U	1	Total C O 35 24 11	0
19	a	1	Total C O 35 24 11	0
19	a	1	Total C O 35 24 11	0
19	a	1	Total C O 35 24 11	0
19	b	1	Total C O 35 24 11	0
19	b	1	Total C O 35 24 11	0
19	f	1	Total C O 35 24 11	0
19	f	1	Total C O 35 24 11	0
19	l	1	Total C O 35 24 11	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total Ca 1 1	0
20	G	1	Total Ca 1 1	0
20	H	1	Total Ca 1 1	0
20	L	1	Total Ca 1 1	0
20	U	1	Total Ca 1 1	0
20	b	1	Total Ca 1 1	0
20	l	1	Total Ca 1 1	0

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



Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C O 41 40 1	0
21	H	1	Total C O 41 40 1	0
21	I	1	Total C O 41 40 1	0
21	L	1	Total C O 41 40 1	0

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

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	A	105	Total O 105 105	0
22	B	152	Total O 152 152	0
22	C	33	Total O 33 33	0
22	D	24	Total O 24 24	0
22	E	4	Total O 4 4	0
22	F	4	Total O 4 4	0
22	G	104	Total O 104 104	0
22	H	150	Total O 150 150	0
22	I	4	Total O 4 4	0
22	J	2	Total O 2 2	0
22	K	2	Total O 2 2	0
22	L	21	Total O 21 21	0
22	M	3	Total O 3 3	0

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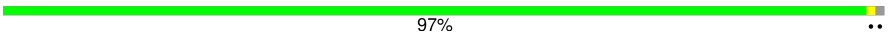
Mol	Chain	Residues	Atoms	AltConf
22	N	30	Total O 30 30	0
22	O	4	Total O 4 4	0
22	P	26	Total O 26 26	0
22	Q	4	Total O 4 4	0
22	R	4	Total O 4 4	0
22	S	3	Total O 3 3	0
22	T	2	Total O 2 2	0
22	U	20	Total O 20 20	0
22	V	3	Total O 3 3	0
22	a	110	Total O 110 110	0
22	b	152	Total O 152 152	0
22	c	29	Total O 29 29	0
22	d	23	Total O 23 23	0
22	e	3	Total O 3 3	0
22	f	4	Total O 4 4	0
22	i	4	Total O 4 4	0
22	j	3	Total O 3 3	0
22	k	2	Total O 2 2	0
22	l	20	Total O 20 20	0
22	m	3	Total O 3 3	0

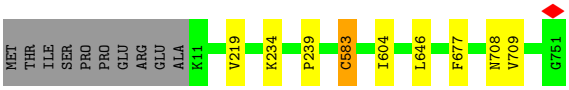
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

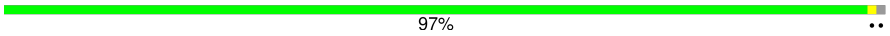
Chain A:





• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

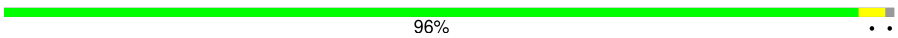
Chain G:





• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

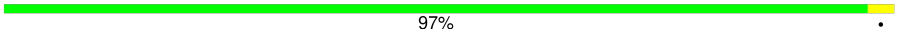
Chain a:

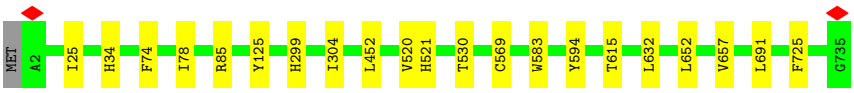




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

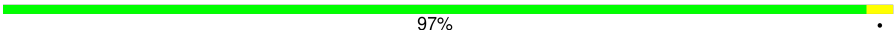
Chain B:

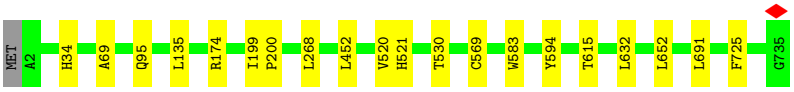




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

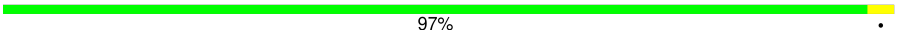
Chain H:

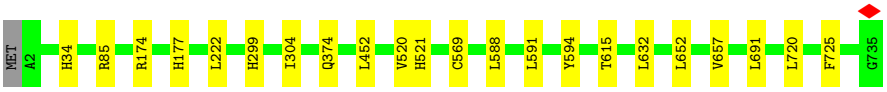




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

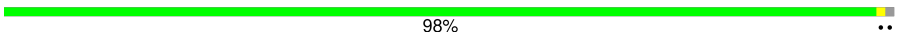
Chain b:

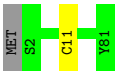




• Molecule 3: Photosystem I iron-sulfur center

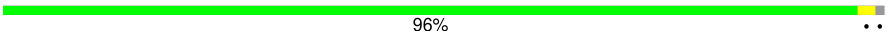
Chain C:

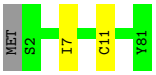




• Molecule 3: Photosystem I iron-sulfur center

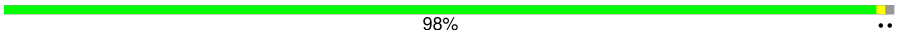
Chain N:





• Molecule 3: Photosystem I iron-sulfur center

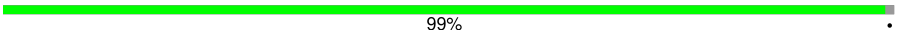
Chain c:





• Molecule 4: Photosystem I reaction center subunit II

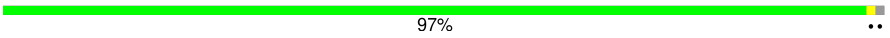
Chain D:

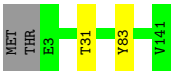




• Molecule 4: Photosystem I reaction center subunit II

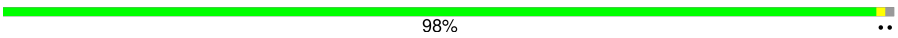
Chain P:

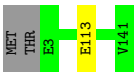




• Molecule 4: Photosystem I reaction center subunit II

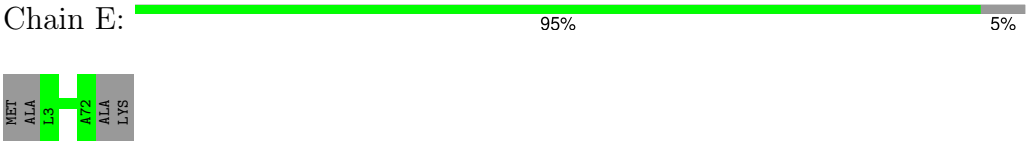
Chain d:





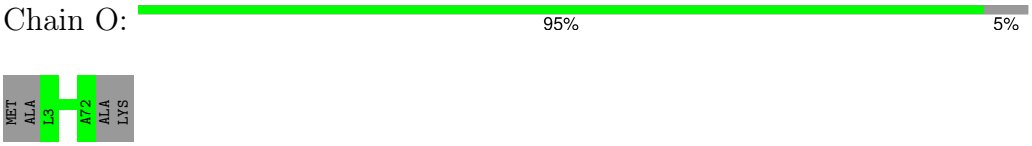
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



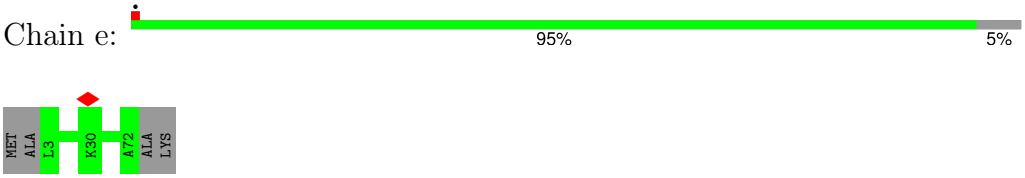
• Molecule 5: Photosystem I reaction center subunit IV

Chain O:



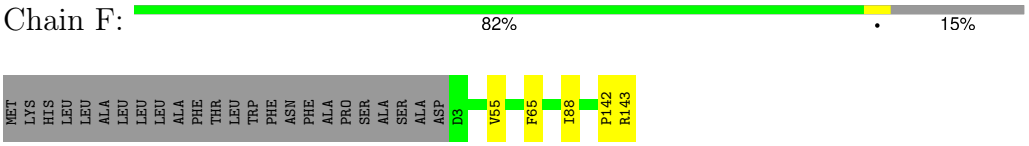
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:



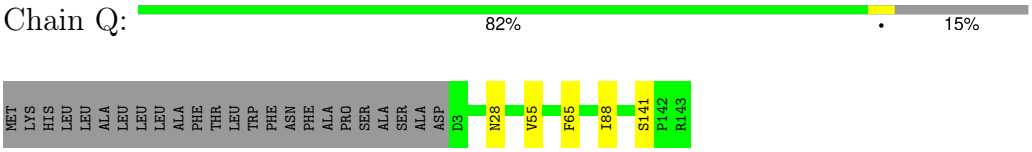
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



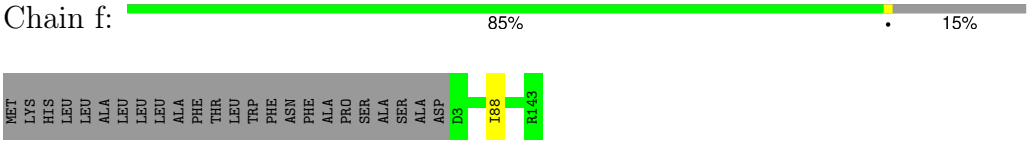
• Molecule 6: Photosystem I reaction center subunit III

Chain Q:



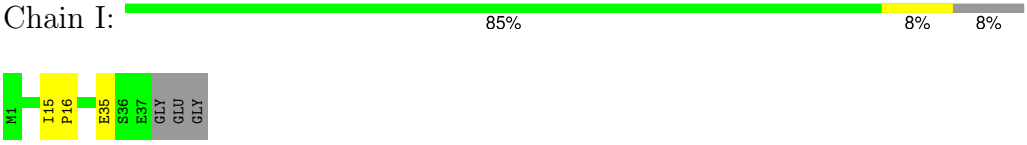
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



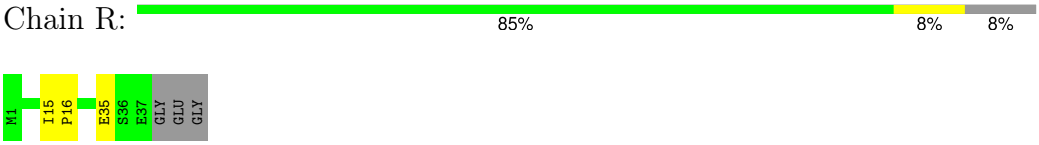
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



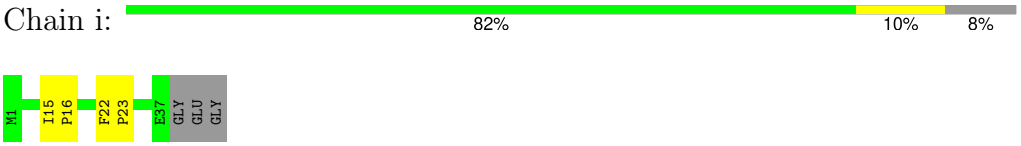
• Molecule 7: Photosystem I reaction center subunit VIII

Chain R:



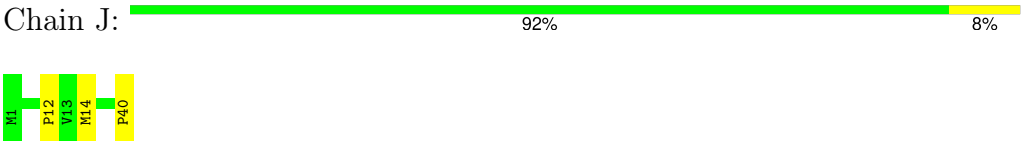
• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:



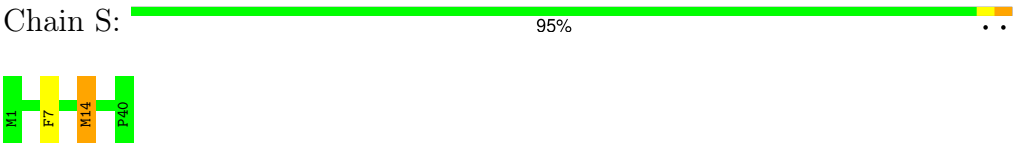
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



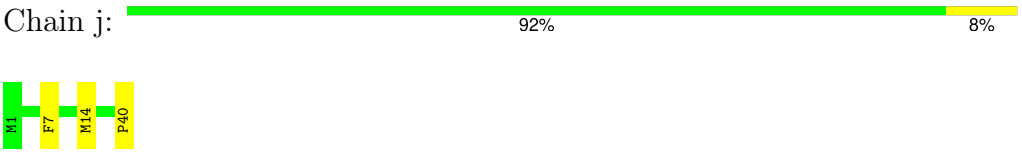
• Molecule 8: Photosystem I reaction center subunit IX

Chain S:



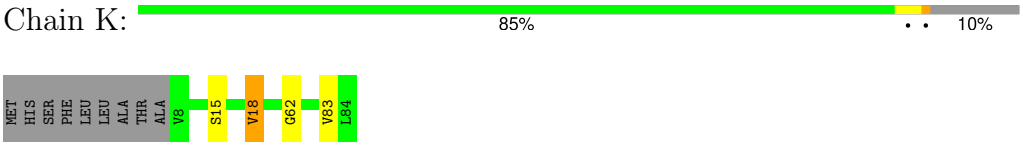
• Molecule 8: Photosystem I reaction center subunit IX

Chain j:



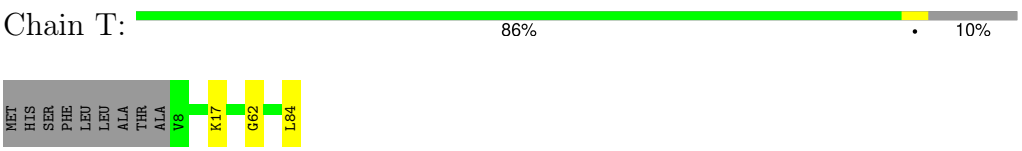
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:



• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain T:



• Molecule 9: Photosystem I reaction center subunit PsaK 1

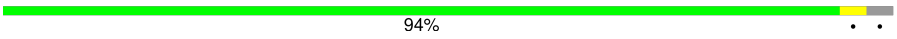
Chain k:

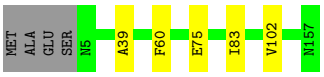




• Molecule 10: Photosystem I reaction center subunit XI

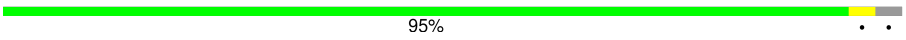
Chain L:

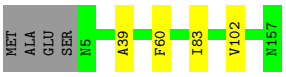




• Molecule 10: Photosystem I reaction center subunit XI

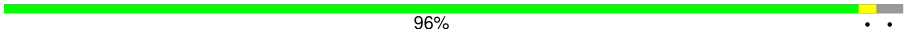
Chain U:

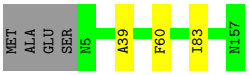




• Molecule 10: Photosystem I reaction center subunit XI

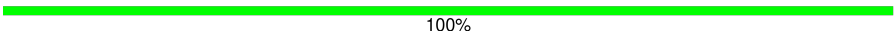
Chain l:





• Molecule 11: Photosystem I reaction center subunit XII

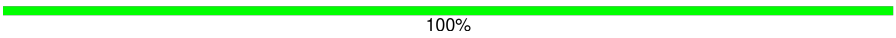
Chain M:



There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem I reaction center subunit XII

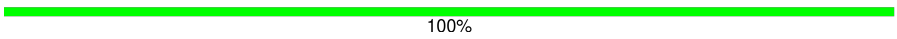
Chain V:



There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem I reaction center subunit XII

Chain m:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	285821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.643	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	321.64, 321.64, 321.64	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.19	0/5999	0.25	0/8176
1	G	0.19	0/5999	0.25	0/8176
1	a	0.19	0/5999	0.25	0/8176
2	B	0.19	0/6032	0.26	0/8250
2	H	0.19	0/6032	0.25	0/8250
2	b	0.20	0/6032	0.26	0/8250
3	C	0.18	0/610	0.30	0/826
3	N	0.19	0/610	0.30	0/826
3	c	0.19	0/610	0.31	0/826
4	D	0.17	0/1111	0.25	0/1497
4	P	0.18	0/1111	0.26	0/1497
4	d	0.17	0/1111	0.25	0/1497
5	E	0.14	0/556	0.22	0/752
5	O	0.15	0/556	0.23	0/752
5	e	0.14	0/556	0.22	0/752
6	F	0.13	0/1130	0.25	0/1535
6	Q	0.15	0/1130	0.26	0/1535
6	f	0.14	0/1130	0.26	0/1535
7	I	0.23	0/304	0.28	0/416
7	R	0.23	0/304	0.30	0/416
7	i	0.24	0/304	0.32	0/416
8	J	0.17	0/327	0.23	0/443
8	S	0.18	0/327	0.23	0/443
8	j	0.17	0/327	0.22	0/443
9	K	0.13	0/549	0.24	0/745
9	T	0.13	0/549	0.32	0/745
9	k	0.13	0/549	0.31	0/745
10	L	0.19	0/1180	0.25	0/1603
10	U	0.19	0/1180	0.26	0/1603
10	l	0.19	0/1180	0.25	0/1603
11	M	0.20	0/241	0.20	0/326
11	V	0.20	0/241	0.18	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	m	0.20	0/241	0.19	0/326
All	All	0.19	0/54117	0.25	0/73707

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5801	0	5664	8	0
1	G	5801	0	5664	11	0
1	a	5801	0	5665	17	0
2	B	5818	0	5589	13	0
2	H	5818	0	5589	12	0
2	b	5818	0	5589	15	0
3	C	600	0	588	0	0
3	N	600	0	587	1	0
3	c	600	0	587	0	0
4	D	1087	0	1082	0	0
4	P	1087	0	1082	1	0
4	d	1087	0	1082	0	0
5	E	547	0	530	0	0
5	O	547	0	530	0	0
5	e	547	0	530	0	0
6	F	1100	0	1096	3	0
6	Q	1100	0	1096	2	0
6	f	1100	0	1096	1	0
7	I	293	0	292	2	0
7	R	293	0	292	2	0
7	i	293	0	292	2	0
8	J	318	0	328	3	0
8	S	318	0	328	2	0
8	j	318	0	328	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	538	0	565	4	0
9	T	538	0	565	2	0
9	k	538	0	565	3	0
10	L	1150	0	1122	5	0
10	U	1150	0	1122	5	0
10	l	1150	0	1122	3	0
11	M	238	0	260	0	0
11	V	238	0	260	0	0
11	m	238	0	260	0	0
12	A	97	0	143	0	0
12	B	38	0	49	0	0
12	G	122	0	163	1	0
12	H	38	0	49	0	0
12	L	73	0	86	0	0
12	M	120	0	153	0	0
12	V	40	0	50	0	0
12	a	97	0	143	0	0
12	b	38	0	49	0	0
13	A	65	0	72	4	0
13	G	65	0	72	6	0
13	a	65	0	72	7	0
14	A	2621	0	2727	19	0
14	B	2530	0	2671	24	0
14	F	156	0	138	3	0
14	G	2639	0	2764	17	0
14	H	2436	0	2540	20	0
14	J	160	0	144	1	0
14	K	155	0	138	0	0
14	L	195	0	216	2	0
14	Q	156	0	138	2	0
14	S	160	0	144	0	0
14	T	155	0	138	1	0
14	U	260	0	288	1	0
14	a	2654	0	2797	18	0
14	b	2576	0	2700	22	0
14	f	156	0	138	1	0
14	j	91	0	66	0	0
14	k	155	0	138	3	0
14	l	195	0	216	1	0
15	A	33	0	46	0	0
15	B	33	0	46	0	0
15	G	33	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	33	0	46	0	0
15	a	33	0	46	0	0
15	b	33	0	46	0	0
16	A	8	0	0	1	0
16	C	16	0	0	0	0
16	G	8	0	0	1	0
16	N	16	0	0	0	0
16	a	8	0	0	0	0
16	c	16	0	0	0	0
17	A	240	0	336	7	0
17	B	230	0	319	6	0
17	F	80	0	112	1	0
17	G	240	0	336	6	0
17	H	230	0	319	3	0
17	I	40	0	56	2	0
17	J	80	0	112	3	0
17	K	40	0	56	0	0
17	L	40	0	56	1	0
17	Q	80	0	112	0	0
17	R	80	0	112	0	0
17	S	80	0	112	0	0
17	T	40	0	56	0	0
17	U	40	0	56	1	0
17	a	240	0	336	6	0
17	b	230	0	319	2	0
17	f	80	0	112	2	0
17	i	40	0	56	1	0
17	j	80	0	112	1	0
17	k	40	0	56	0	0
17	l	80	0	112	4	0
18	A	88	0	116	0	0
18	B	137	0	190	1	0
18	G	46	0	62	0	0
18	H	86	0	115	0	0
18	K	35	0	40	2	0
18	L	38	0	46	0	0
18	U	38	0	46	0	0
18	a	46	0	62	0	0
18	b	92	0	127	1	0
18	l	38	0	46	0	0
19	A	140	0	184	1	0
19	B	70	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	G	70	0	92	0	0
19	H	70	0	92	0	0
19	J	35	0	46	0	0
19	L	35	0	46	0	0
19	Q	70	0	92	0	0
19	U	35	0	46	0	0
19	a	105	0	138	0	0
19	b	70	0	92	0	0
19	f	70	0	92	0	0
19	l	35	0	46	0	0
20	B	1	0	0	0	0
20	G	1	0	0	0	0
20	H	1	0	0	0	0
20	L	1	0	0	0	0
20	U	1	0	0	0	0
20	b	1	0	0	0	0
20	l	1	0	0	0	0
21	B	41	0	54	0	0
21	H	41	0	54	1	0
21	I	41	0	54	0	0
21	L	41	0	54	1	0
21	M	41	0	54	4	0
21	R	41	0	54	0	0
21	V	41	0	54	1	0
21	b	41	0	54	0	0
21	i	41	0	54	0	0
21	m	41	0	54	1	0
22	A	105	0	0	0	0
22	B	152	0	0	0	0
22	C	33	0	0	0	0
22	D	24	0	0	0	0
22	E	4	0	0	0	0
22	F	4	0	0	0	0
22	G	104	0	0	0	0
22	H	150	0	0	0	0
22	I	4	0	0	0	0
22	J	2	0	0	0	0
22	K	2	0	0	0	0
22	L	21	0	0	0	0
22	M	3	0	0	0	0
22	N	30	0	0	0	0
22	O	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	P	26	0	0	0	0
22	Q	4	0	0	0	0
22	R	4	0	0	0	0
22	S	3	0	0	0	0
22	T	2	0	0	0	0
22	U	20	0	0	0	0
22	V	3	0	0	0	0
22	a	110	0	0	0	0
22	b	152	0	0	0	0
22	c	29	0	0	0	0
22	d	23	0	0	0	0
22	e	3	0	0	0	0
22	f	4	0	0	0	0
22	i	4	0	0	0	0
22	j	3	0	0	0	0
22	k	2	0	0	0	0
22	l	20	0	0	0	0
22	m	3	0	0	0	0
All	All	76301	0	76526	248	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 2.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:803:CLA:HMB1	14:A:803:CLA:HBB1	1.71	0.72
9:k:81:MET:HE1	14:k:103:CLA:HMB3	1.70	0.72
14:B:812:CLA:H42	10:L:83:ILE:HG22	1.77	0.67
14:G:829:CLA:HMB1	14:G:829:CLA:HBB1	1.76	0.67
14:a:829:CLA:HBB1	14:a:829:CLA:HMB1	1.77	0.65
14:A:836:CLA:HMB1	17:A:850:BCR:H281	1.79	0.65
1:a:677:PHE:CG	17:a:852:BCR:H363	2.33	0.63
14:G:836:CLA:HMB1	17:G:850:BCR:H281	1.80	0.63
14:B:838:CLA:HMB2	14:B:840:CLA:HED1	1.81	0.62
9:k:46:MET:HE2	9:k:60:VAL:HG21	1.82	0.61
14:B:838:CLA:HBB1	14:B:838:CLA:HMB1	1.82	0.61
8:S:14:MET:HA	8:S:14:MET:HE2	1.83	0.60
2:B:452:LEU:HD22	2:B:615:THR:HG21	1.82	0.60
13:G:801:CL0:H13	14:G:802:CLA:OBD	2.04	0.58
14:A:819:CLA:HBB1	14:A:819:CLA:HMB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:14:MET:HE2	8:j:14:MET:HA	1.86	0.58
17:I:101:BCR:H382	17:I:101:BCR:H23C	1.85	0.57
14:b:813:CLA:H42	10:l:83:ILE:HG22	1.86	0.57
1:A:604:ILE:HD11	13:A:802:CL0:H35	1.87	0.57
14:b:802:CLA:HMB1	14:b:802:CLA:HBB1	1.86	0.57
21:M:103:ECH:H40B	21:M:103:ECH:H23	1.87	0.56
1:A:677:PHE:CG	17:A:851:BCR:H363	2.40	0.56
8:J:14:MET:HA	8:J:14:MET:HE2	1.87	0.56
18:B:803:LMG:C22	14:B:811:CLA:H142	2.35	0.55
2:b:452:LEU:HD22	2:b:615:THR:HG21	1.87	0.55
1:G:604:ILE:HD11	13:G:801:CL0:H35	1.88	0.55
14:G:840:CLA:HBB1	14:G:840:CLA:HMB1	1.88	0.55
9:K:83:VAL:HG22	18:K:105:LMG:C9	2.37	0.54
14:A:813:CLA:HMB1	14:A:813:CLA:HBB1	1.89	0.54
14:a:820:CLA:HMB1	14:a:820:CLA:HBB1	1.90	0.53
13:a:802:CL0:H11	13:a:802:CL0:H15	1.90	0.53
14:G:828:CLA:HMB1	14:G:828:CLA:HBB1	1.90	0.53
14:A:805:CLA:HMB1	14:A:805:CLA:HBB1	1.90	0.53
14:B:814:CLA:HMB1	14:B:814:CLA:HBB1	1.91	0.52
14:H:811:CLA:H42	10:U:83:ILE:HG22	1.91	0.52
14:H:808:CLA:H3A	14:H:809:CLA:HMB3	1.91	0.51
2:B:34:HIS:HE1	14:B:806:CLA:HED1	1.76	0.51
21:m:101:ECH:H40B	21:m:101:ECH:H23	1.91	0.51
14:A:832:CLA:HMB1	14:A:832:CLA:HBB1	1.93	0.51
13:G:801:CL0:H15	13:G:801:CL0:H11	1.93	0.51
14:H:829:CLA:HBB1	14:H:829:CLA:HMB1	1.92	0.51
14:a:807:CLA:HBB1	14:a:807:CLA:HMB1	1.93	0.51
14:A:813:CLA:HMB3	19:A:857:LMT:H123	1.93	0.50
14:L:1501:CLA:HBA2	21:L:1506:ECH:H36B	1.92	0.50
1:a:375:PRO:HB3	14:a:820:CLA:HMA2	1.92	0.50
14:a:833:CLA:HBB1	14:a:833:CLA:HMB1	1.94	0.50
18:b:803:LMG:C22	14:b:812:CLA:H142	2.42	0.50
2:B:25:ILE:HA	14:B:806:CLA:HMD3	1.94	0.50
14:B:840:CLA:HMB1	14:B:840:CLA:HBB1	1.92	0.50
1:a:708:ASN:O	6:f:88:ILE:HD11	2.11	0.50
1:a:604:ILE:HD11	13:a:802:CL0:H35	1.93	0.50
14:G:814:CLA:HBB1	14:G:814:CLA:HMB1	1.93	0.50
14:H:839:CLA:HMB1	14:H:839:CLA:HBB1	1.94	0.50
14:b:822:CLA:HMB2	14:b:827:CLA:HMA3	1.93	0.50
14:H:827:CLA:HBB1	14:H:827:CLA:HMB1	1.92	0.49
1:a:141:SER:HA	14:a:829:CLA:HMA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:828:CLA:HBB1	14:B:828:CLA:HMB1	1.93	0.49
14:G:816:CLA:HBB1	14:G:816:CLA:HMB1	1.94	0.49
14:B:801:CLA:H201	17:J:1104:BCR:H362	1.95	0.49
1:G:646:LEU:HD22	2:H:652:LEU:HD21	1.94	0.49
21:V:102:ECH:H40B	21:V:102:ECH:H23	1.93	0.49
14:H:814:CLA:HBB1	14:H:814:CLA:HMB1	1.93	0.49
2:B:691:LEU:HD11	10:L:39:ALA:HB1	1.94	0.48
14:H:813:CLA:HBB1	14:H:813:CLA:HMB1	1.96	0.48
14:A:815:CLA:HBB1	14:A:815:CLA:HMB1	1.94	0.48
14:b:822:CLA:O2A	14:b:827:CLA:HMB2	2.13	0.48
14:a:816:CLA:HBB1	14:a:816:CLA:HMB1	1.96	0.48
1:A:646:LEU:HD22	2:B:652:LEU:HD21	1.95	0.48
1:a:646:LEU:HD22	2:b:652:LEU:HD21	1.96	0.48
2:b:299:HIS:HB3	2:b:304:ILE:HD11	1.96	0.48
14:G:807:CLA:HBB1	14:G:807:CLA:HMB1	1.96	0.48
2:b:174:ARG:HD2	14:b:827:CLA:OBD	2.14	0.48
14:B:807:CLA:HMB1	14:B:807:CLA:HBB1	1.95	0.48
17:G:858:BCR:H331	17:G:858:BCR:C8	2.44	0.48
13:a:802:CL0:H32	14:a:803:CLA:C1D	2.43	0.48
1:a:370:MET:HE1	14:a:830:CLA:O1D	2.13	0.47
2:H:268:LEU:HD13	14:H:818:CLA:HMA2	1.96	0.47
14:H:818:CLA:HBB1	14:H:818:CLA:HMB1	1.96	0.47
14:a:826:CLA:O1D	14:a:826:CLA:H42	2.13	0.47
14:b:818:CLA:HBB1	14:b:818:CLA:HMB1	1.96	0.47
1:A:708:ASN:O	6:F:88:ILE:HD11	2.14	0.47
14:A:824:CLA:H91	14:A:831:CLA:HBC3	1.97	0.47
2:b:177:HIS:CG	14:b:816:CLA:HMC2	2.50	0.47
2:b:657:VAL:HG22	14:b:843:CLA:HMB3	1.96	0.47
14:A:824:CLA:H91	14:A:831:CLA:CBC	2.45	0.47
2:H:34:HIS:HE1	14:H:805:CLA:HED1	1.80	0.47
13:G:801:CL0:H32	14:G:804:CLA:C1D	2.45	0.47
1:a:709:VAL:O	1:a:709:VAL:HG22	2.15	0.47
13:A:802:CL0:H32	14:A:803:CLA:C1D	2.45	0.46
14:B:841:CLA:H18	17:I:101:BCR:H362	1.97	0.46
14:G:825:CLA:H141	12:G:855:LHG:H152	1.97	0.46
1:A:583:CYS:HB3	16:A:846:SF4:S2	2.55	0.46
2:B:657:VAL:HG22	14:B:842:CLA:HMB3	1.98	0.46
2:H:632:LEU:HD22	2:H:725:PHE:HA	1.96	0.46
2:H:691:LEU:HD11	10:U:39:ALA:HB1	1.97	0.46
14:b:801:CLA:H201	17:j:103:BCR:H362	1.97	0.46
14:b:831:CLA:HMB1	14:b:831:CLA:HBB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:858:BCR:C8	17:a:858:BCR:H331	2.46	0.46
2:b:34:HIS:HE1	14:b:807:CLA:HED1	1.81	0.46
17:A:860:BCR:H372	9:K:62:GLY:HA2	1.98	0.46
7:R:15:ILE:HB	7:R:16:PRO:HD3	1.98	0.46
7:I:35:GLU:HB3	10:L:102:VAL:HG13	1.97	0.46
14:B:817:CLA:HBB1	14:B:817:CLA:HMB1	1.98	0.46
6:F:55:VAL:HG12	6:F:65:PHE:HB2	1.96	0.46
10:L:39:ALA:HB2	14:L:1502:CLA:HMD1	1.96	0.46
14:G:812:CLA:H42	8:S:7:PHE:CE1	2.51	0.46
6:Q:55:VAL:HG12	6:Q:65:PHE:HB2	1.98	0.46
14:b:801:CLA:HMB1	14:b:801:CLA:HBB1	1.98	0.46
14:A:806:CLA:HBB1	14:A:806:CLA:HMB1	1.98	0.45
17:B:856:BCR:H382	8:J:40:PRO:HG2	1.98	0.45
2:H:530:THR:HG21	2:H:583:TRP:CE2	2.51	0.45
14:J:1101:CLA:HBB1	14:J:1101:CLA:HMB1	1.99	0.45
2:b:632:LEU:HD22	2:b:725:PHE:HA	1.98	0.45
7:i:15:ILE:HB	7:i:16:PRO:HD3	1.98	0.45
10:l:60:PHE:CD1	10:l:60:PHE:C	2.94	0.45
17:A:851:BCR:H381	14:F:201:CLA:HMA1	1.98	0.45
2:H:452:LEU:HD22	2:H:615:THR:HG21	1.97	0.45
1:a:677:PHE:CD2	17:a:852:BCR:H363	2.51	0.45
14:A:827:CLA:HBB1	14:A:827:CLA:HMB1	1.97	0.45
1:G:207:LEU:HD21	14:G:821:CLA:HMC1	1.97	0.45
10:U:60:PHE:CD1	10:U:60:PHE:C	2.94	0.45
14:H:830:CLA:HMB1	14:H:830:CLA:HBB1	1.98	0.45
14:A:804:CLA:H191	14:A:809:CLA:C6	2.46	0.45
1:a:221:MET:HE1	1:a:274:PHE:HB2	1.98	0.45
14:F:201:CLA:HBB1	14:F:201:CLA:HMB1	1.99	0.45
1:a:319:HIS:HB3	1:a:324:ILE:HD11	1.98	0.45
2:b:520:VAL:HG21	2:b:594:TYR:HB2	1.98	0.45
14:A:823:CLA:HBB1	14:A:823:CLA:HMB1	1.98	0.45
2:B:521:HIS:CG	14:B:839:CLA:HED3	2.52	0.44
14:B:819:CLA:HBB1	14:B:819:CLA:HMB1	1.99	0.44
17:b:856:BCR:H382	8:j:40:PRO:HG2	1.99	0.44
14:H:811:CLA:H43	14:H:811:CLA:HED2	1.99	0.44
14:Q:202:CLA:HBB1	14:Q:202:CLA:HMB1	1.99	0.44
14:F:201:CLA:HMB2	17:F:202:BCR:H10C	2.00	0.44
14:H:813:CLA:H93	17:H:845:BCR:H332	2.00	0.44
2:B:520:VAL:HG21	2:B:594:TYR:HB2	1.99	0.44
1:G:677:PHE:CG	17:G:851:BCR:H363	2.52	0.44
14:G:825:CLA:H91	14:G:832:CLA:HBC1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:39:ALA:HB2	14:U:205:CLA:HMD1	2.00	0.44
13:a:802:CL0:H35	13:a:802:CL0:H41	1.88	0.44
17:a:852:BCR:H403	17:a:852:BCR:H23C	1.99	0.44
2:B:299:HIS:HB3	2:B:304:ILE:HD11	2.00	0.44
17:B:846:BCR:H331	17:B:846:BCR:C8	2.47	0.44
7:R:35:GLU:HB3	10:U:102:VAL:HG13	2.00	0.44
1:a:58:PHE:CD2	14:a:806:CLA:HMC2	2.53	0.44
13:a:802:CL0:H41	13:a:802:CL0:H49	1.74	0.44
17:G:848:BCR:H24C	17:G:848:BCR:H371	1.86	0.44
17:G:851:BCR:H381	14:Q:202:CLA:HMA1	2.00	0.44
14:H:820:CLA:O2A	14:H:825:CLA:HMB2	2.19	0.43
9:k:26:ASN:O	9:k:30:ILE:HD13	2.18	0.43
17:l:5003:BCR:H363	14:l:5004:CLA:HBA2	2.00	0.43
2:B:74:PHE:O	2:B:78:ILE:HG12	2.18	0.43
2:B:78:ILE:HD12	2:B:125:TYR:CD1	2.52	0.43
7:I:15:ILE:HB	7:I:16:PRO:HD3	1.99	0.43
1:a:609:PHE:O	1:a:613:MET:HG2	2.18	0.43
14:a:828:CLA:HBB1	14:a:828:CLA:HMB1	1.99	0.43
14:a:812:CLA:H42	8:j:7:PHE:CE1	2.53	0.43
2:B:530:THR:HG21	2:B:583:TRP:CE2	2.52	0.43
14:B:814:CLA:C9	17:B:846:BCR:H332	2.48	0.43
14:B:830:CLA:HMB1	14:B:830:CLA:HBB1	1.98	0.43
2:b:374:GLN:O	2:b:588:LEU:HD11	2.18	0.43
14:f:204:CLA:HBB1	14:f:204:CLA:HMB1	2.00	0.43
14:B:812:CLA:HED2	14:B:812:CLA:H43	1.99	0.43
14:a:822:CLA:H122	14:a:825:CLA:H93	2.01	0.43
14:A:823:CLA:HMB3	14:A:844:CLA:C2C	2.48	0.43
1:G:445:ILE:HG22	14:G:834:CLA:HED3	2.01	0.43
14:H:807:CLA:H41	14:H:807:CLA:H71	2.00	0.43
17:H:845:BCR:H331	17:H:845:BCR:C8	2.48	0.43
21:M:103:ECH:H24	21:M:103:ECH:H37	1.87	0.43
2:b:691:LEU:HD11	10:l:39:ALA:HB1	2.01	0.43
21:H:846:ECH:H34A	14:k:103:CLA:HMB2	2.00	0.43
9:K:83:VAL:HG22	18:K:105:LMG:HC92	2.00	0.43
14:B:802:CLA:CGA	14:B:802:CLA:H3A	2.50	0.42
1:G:604:ILE:HD12	13:G:801:CL0:H53	1.99	0.42
14:G:803:CLA:CGA	14:G:803:CLA:H3A	2.48	0.42
1:G:221:MET:HE1	1:G:274:PHE:HB2	2.01	0.42
14:H:813:CLA:C9	17:H:845:BCR:H332	2.49	0.42
1:G:583:CYS:HB3	16:G:846:SF4:S4	2.59	0.42
1:G:709:VAL:HG22	1:G:709:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:142:PRO:O	6:F:143:ARG:HB2	2.19	0.42
1:G:141:SER:HA	14:G:829:CLA:HMA2	2.00	0.42
17:G:858:BCR:H372	9:T:62:GLY:HA2	2.01	0.42
2:H:174:ARG:HD2	14:H:825:CLA:OBD	2.19	0.42
14:a:825:CLA:H91	14:a:832:CLA:CBC	2.49	0.42
14:G:805:CLA:H61	14:G:805:CLA:H41	1.91	0.42
14:b:816:CLA:HBB1	14:b:816:CLA:HMB1	2.01	0.42
17:f:206:BCR:H20C	17:f:206:BCR:H361	1.88	0.42
13:G:801:CL0:H49	13:G:801:CL0:H41	1.82	0.42
14:H:816:CLA:HBB1	14:H:816:CLA:HMB1	2.02	0.42
9:T:17:LYS:HG2	9:T:84:LEU:HD11	2.00	0.42
13:A:802:CL0:H35	13:A:802:CL0:H41	1.79	0.42
17:A:850:BCR:C23	17:A:850:BCR:H403	2.50	0.42
10:L:60:PHE:CD1	10:L:60:PHE:C	2.97	0.42
21:M:103:ECH:H20	21:M:103:ECH:H36	1.94	0.42
14:a:825:CLA:H91	14:a:832:CLA:HBC3	2.00	0.42
2:b:521:HIS:CG	14:b:840:CLA:HED3	2.54	0.42
14:a:822:CLA:HMB2	14:a:826:CLA:HMA3	2.02	0.42
14:b:802:CLA:CGA	14:b:802:CLA:H3A	2.49	0.42
2:H:69:ALA:HB2	2:H:135:LEU:HB2	2.01	0.41
17:a:849:BCR:H383	17:a:849:BCR:H23C	2.02	0.41
17:i:101:BCR:H392	17:i:101:BCR:H24C	1.87	0.41
14:B:820:CLA:O1A	14:B:830:CLA:HMD1	2.20	0.41
8:J:12:PRO:HB2	17:J:1105:BCR:H381	2.02	0.41
17:U:203:BCR:H20C	17:U:203:BCR:H361	1.89	0.41
17:A:851:BCR:C23	17:A:851:BCR:H403	2.50	0.41
2:B:632:LEU:HD22	2:B:725:PHE:HA	2.01	0.41
17:B:850:BCR:H24C	17:B:850:BCR:H371	1.89	0.41
14:H:826:CLA:H43	14:H:831:CLA:H203	2.02	0.41
17:l:5003:BCR:H24C	17:l:5003:BCR:H371	1.88	0.41
2:H:199:ILE:HB	2:H:200:PRO:HD3	2.03	0.41
1:A:604:ILE:CD1	13:A:802:CL0:H35	2.50	0.41
17:a:852:BCR:H403	17:a:852:BCR:C23	2.51	0.41
17:l:5003:BCR:C8	17:l:5003:BCR:H321	2.50	0.41
14:T:102:CLA:HMC1	14:T:102:CLA:HBC2	2.02	0.41
17:f:206:BCR:H24C	17:f:206:BCR:H371	1.94	0.41
2:b:720:LEU:HD23	14:b:830:CLA:H41	2.03	0.41
14:B:823:CLA:C17	14:B:823:CLA:H141	2.51	0.41
3:N:7:ILE:N	3:N:7:ILE:HD12	2.36	0.41
4:P:31:THR:O	4:P:83:TYR:HA	2.20	0.41
1:a:90:MET:N	1:a:90:MET:HE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:840:CLA:HHC	14:a:840:CLA:CBB	2.51	0.41
2:b:222:LEU:HD11	14:b:818:CLA:O1A	2.20	0.41
14:b:802:CLA:HMB1	14:b:802:CLA:CBB	2.50	0.41
1:A:709:VAL:O	1:A:709:VAL:HG22	2.21	0.41
14:A:809:CLA:HMB3	17:J:1104:BCR:C8	2.51	0.41
17:A:860:BCR:C8	17:A:860:BCR:H331	2.50	0.41
14:B:814:CLA:H91	17:B:846:BCR:H332	2.03	0.41
14:B:838:CLA:HMB2	14:B:840:CLA:CED	2.50	0.41
1:a:51:LEU:C	1:a:51:LEU:HD23	2.46	0.41
17:l:5007:BCR:H20C	17:l:5007:BCR:H361	1.89	0.41
1:G:708:ASN:O	6:Q:88:ILE:HD11	2.21	0.41
17:L:1504:BCR:C23	17:L:1504:BCR:H403	2.50	0.41
13:a:802:CL0:H7	14:b:805:CLA:HMB3	2.03	0.41
7:i:22:PHE:HB3	7:i:23:PRO:HD3	2.03	0.40
14:k:102:CLA:HMC1	14:k:102:CLA:HBC2	2.02	0.40
14:A:828:CLA:HBB1	14:A:828:CLA:HMB1	2.03	0.40
14:b:820:CLA:HMB1	14:b:820:CLA:HBB1	2.03	0.40
14:A:858:CLA:H121	17:B:850:BCR:H362	2.04	0.40
21:M:103:ECH:H39A	21:M:103:ECH:C23	2.50	0.40
1:a:604:ILE:CD1	13:a:802:CL0:H35	2.50	0.40
2:b:588:LEU:HD13	2:b:591:LEU:HD21	2.03	0.40
14:b:817:CLA:H202	14:b:817:CLA:H161	1.96	0.40
1:a:219:VAL:HG13	1:a:239:PRO:HB3	2.03	0.40
17:b:856:BCR:H24C	17:b:856:BCR:H371	1.93	0.40
1:A:219:VAL:HG13	1:A:239:PRO:HB3	2.04	0.40
2:H:520:VAL:HG21	2:H:594:TYR:HB2	2.02	0.40
2:H:521:HIS:CG	14:H:838:CLA:HED3	2.56	0.40
9:K:15:SER:O	9:K:18:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	718 (97%)	21 (3%)	0	100	100
1	G	739/751 (98%)	724 (98%)	15 (2%)	0	100	100
1	a	739/751 (98%)	723 (98%)	16 (2%)	0	100	100
2	B	732/735 (100%)	721 (98%)	11 (2%)	0	100	100
2	H	732/735 (100%)	719 (98%)	13 (2%)	0	100	100
2	b	732/735 (100%)	721 (98%)	11 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	N	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/141 (97%)	136 (99%)	1 (1%)	0	100	100
4	P	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
4	d	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
5	O	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
5	e	68/74 (92%)	65 (96%)	3 (4%)	0	100	100
6	F	139/165 (84%)	138 (99%)	1 (1%)	0	100	100
6	Q	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	f	139/165 (84%)	137 (99%)	2 (1%)	0	100	100
7	I	35/40 (88%)	35 (100%)	0	0	100	100
7	R	35/40 (88%)	35 (100%)	0	0	100	100
7	i	35/40 (88%)	35 (100%)	0	0	100	100
8	J	38/40 (95%)	38 (100%)	0	0	100	100
8	S	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	K	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
9	T	75/86 (87%)	72 (96%)	3 (4%)	0	100	100
9	k	75/86 (87%)	72 (96%)	3 (4%)	0	100	100
10	L	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	U	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	l	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	6663/6903 (96%)	6542 (98%)	121 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	594/603 (98%)	592 (100%)	2 (0%)	86	82
1	G	594/603 (98%)	593 (100%)	1 (0%)	87	84
1	a	594/603 (98%)	593 (100%)	1 (0%)	87	84
2	B	587/588 (100%)	585 (100%)	2 (0%)	86	82
2	H	587/588 (100%)	585 (100%)	2 (0%)	86	82
2	b	587/588 (100%)	585 (100%)	2 (0%)	86	82
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	46
3	N	68/69 (99%)	67 (98%)	1 (2%)	57	46
3	c	68/69 (99%)	67 (98%)	1 (2%)	57	46
4	D	114/116 (98%)	114 (100%)	0	100	100
4	P	114/116 (98%)	114 (100%)	0	100	100
4	d	114/116 (98%)	113 (99%)	1 (1%)	70	63
5	E	58/60 (97%)	58 (100%)	0	100	100
5	O	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	118/137 (86%)	118 (100%)	0	100	100
6	Q	118/137 (86%)	116 (98%)	2 (2%)	53	40
6	f	118/137 (86%)	118 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	R	31/32 (97%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	i	31/32 (97%)	31 (100%)	0	100 100
8	J	35/35 (100%)	35 (100%)	0	100 100
8	S	35/35 (100%)	34 (97%)	1 (3%)	37 20
8	j	35/35 (100%)	35 (100%)	0	100 100
9	K	55/62 (89%)	54 (98%)	1 (2%)	51 38
9	T	55/62 (89%)	55 (100%)	0	100 100
9	k	55/62 (89%)	55 (100%)	0	100 100
10	L	115/118 (98%)	114 (99%)	1 (1%)	70 63
10	U	115/118 (98%)	115 (100%)	0	100 100
10	l	115/118 (98%)	115 (100%)	0	100 100
11	M	25/25 (100%)	25 (100%)	0	100 100
11	V	25/25 (100%)	25 (100%)	0	100 100
11	m	25/25 (100%)	25 (100%)	0	100 100
All	All	5400/5535 (98%)	5381 (100%)	19 (0%)	81 79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	LYS
1	A	583	CYS
2	B	85	ARG
2	B	569	CYS
3	C	11	CYS
1	G	583	CYS
2	H	95	GLN
2	H	569	CYS
9	K	18	VAL
10	L	75	GLU
3	N	11	CYS
6	Q	28	ASN
6	Q	141	SER
8	S	14	MET
1	a	583	CYS
2	b	85	ARG
2	b	569	CYS
3	c	11	CYS
4	d	113	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
2	B	34	HIS
2	B	111	ASN
2	B	133	GLN
2	B	275	HIS
2	B	363	HIS
2	B	373	HIS
2	B	705	GLN
5	E	47	ASN
6	F	28	ASN
1	G	54	ASN
1	G	109	HIS
1	G	218	HIS
2	H	34	HIS
2	H	95	GLN
2	H	133	GLN
2	H	158	GLN
2	H	205	GLN
2	H	275	HIS
2	H	361	GLN
2	H	363	HIS
2	H	705	GLN
10	L	122	GLN
10	L	157	ASN
4	P	7	GLN
10	U	36	ASN
10	U	122	GLN
1	a	54	ASN
1	a	93	HIS
2	b	14	GLN
2	b	34	HIS
2	b	158	GLN
2	b	275	HIS
2	b	361	GLN
2	b	363	HIS
2	b	631	GLN
2	b	705	GLN
4	d	115	GLN
7	i	33	HIS
9	k	80	ASN
10	l	9	GLN

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Mol	Chain	Res	Type
10	l	122	GLN
10	l	144	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 436 ligands modelled in this entry, 7 are monoatomic - leaving 429 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	A	825	22	69,73,73	0.98	5 (7%)	82,113,113	0.95	2 (2%)
14	CLA	b	822	22	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
18	LMG	H	851	-	36,36,55	0.59	0	44,44,63	0.72	0
14	CLA	H	822	2	50,54,73	1.15	4 (8%)	59,90,113	0.91	2 (3%)
14	CLA	B	828	2	69,73,73	0.99	5 (7%)	82,113,113	0.92	4 (4%)
14	CLA	A	829	1	69,73,73	0.99	5 (7%)	82,113,113	1.00	5 (6%)
14	CLA	B	831	2	69,73,73	0.97	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	a	808	1	69,73,73	0.98	4 (5%)	82,113,113	0.92	4 (4%)
14	CLA	a	817	22	50,54,73	1.17	4 (8%)	59,90,113	1.06	3 (5%)
14	CLA	A	803	22	69,73,73	0.98	4 (5%)	82,113,113	0.90	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	813	2	69,73,73	0.97	3 (4%)	82,113,113	0.94	3 (3%)
14	CLA	a	811	1	49,53,73	1.16	4 (8%)	58,89,113	1.03	2 (3%)
14	CLA	A	843	22	69,73,73	0.97	5 (7%)	82,113,113	0.93	3 (3%)
14	CLA	H	840	22	69,73,73	0.96	4 (5%)	82,113,113	0.92	5 (6%)
14	CLA	G	838	1	69,73,73	0.95	3 (4%)	82,113,113	0.99	5 (6%)
14	CLA	H	835	22	49,53,73	1.17	5 (10%)	58,89,113	1.03	5 (8%)
14	CLA	A	805	1	69,73,73	0.97	4 (5%)	82,113,113	1.02	5 (6%)
14	CLA	k	101	9	49,53,73	1.18	4 (8%)	58,89,113	0.96	2 (3%)
14	CLA	A	807	1	69,73,73	0.97	3 (4%)	82,113,113	0.94	5 (6%)
14	CLA	b	801	22	69,73,73	0.97	3 (4%)	82,113,113	0.97	3 (3%)
18	LMG	G	852	-	46,46,55	0.55	0	54,54,63	0.65	0
14	CLA	H	810	2	69,73,73	0.97	5 (7%)	82,113,113	0.92	4 (4%)
14	CLA	B	816	2	69,73,73	0.97	4 (5%)	82,113,113	0.92	3 (3%)
17	BCR	b	851	-	41,41,41	0.30	0	56,56,56	0.70	0
14	CLA	B	824	2	49,53,73	1.16	5 (10%)	58,89,113	1.01	2 (3%)
17	BCR	J	1104	-	41,41,41	0.29	0	56,56,56	0.55	0
14	CLA	b	826	2	57,61,73	1.09	5 (8%)	67,98,113	0.92	1 (1%)
14	CLA	H	841	2	69,73,73	0.96	3 (4%)	82,113,113	1.05	6 (7%)
14	CLA	G	818	1	69,73,73	0.96	4 (5%)	82,113,113	1.06	6 (7%)
14	CLA	G	826	22	69,73,73	0.98	4 (5%)	82,113,113	1.03	4 (4%)
17	BCR	K	104	-	41,41,41	0.29	0	56,56,56	0.46	0
14	CLA	B	811	2	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
12	LHG	M	104	-	41,41,48	0.55	0	44,47,54	0.50	0
17	BCR	b	846	-	41,41,41	0.30	0	56,56,56	0.56	0
17	BCR	a	849	-	41,41,41	0.29	0	56,56,56	0.57	0
14	CLA	H	809	2	69,73,73	0.97	3 (4%)	82,113,113	1.00	6 (7%)
14	CLA	b	837	22	49,53,73	1.14	3 (6%)	58,89,113	0.98	2 (3%)
14	CLA	A	831	1	69,73,73	0.98	5 (7%)	82,113,113	0.91	4 (4%)
14	CLA	B	836	22	49,53,73	1.17	3 (6%)	58,89,113	0.97	3 (5%)
14	CLA	a	819	1	69,73,73	0.97	5 (7%)	82,113,113	1.01	4 (4%)
18	LMG	A	855	-	42,42,55	0.54	0	50,50,63	0.62	0
14	CLA	b	838	-	50,54,73	1.15	4 (8%)	59,90,113	0.94	2 (3%)
15	PQN	b	845	-	34,34,34	0.43	0	43,45,45	0.68	1 (2%)
14	CLA	B	821	22	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
14	CLA	S	1102	8	49,53,73	1.17	4 (8%)	58,89,113	0.98	2 (3%)
17	BCR	A	848	-	41,41,41	0.29	0	56,56,56	0.56	0
17	BCR	A	851	-	41,41,41	0.31	0	56,56,56	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	826	22	69,73,73	0.99	4 (5%)	82,113,113	0.95	2 (2%)
14	CLA	H	811	2	69,73,73	0.97	4 (5%)	82,113,113	0.98	2 (2%)
19	LMT	J	1106	-	36,36,36	0.55	0	47,47,47	0.67	0
14	CLA	G	808	1	69,73,73	0.98	4 (5%)	82,113,113	0.91	2 (2%)
14	CLA	a	832	1	69,73,73	0.97	4 (5%)	82,113,113	0.96	5 (6%)
14	CLA	a	814	1	69,73,73	0.98	5 (7%)	82,113,113	0.93	3 (3%)
17	BCR	H	847	-	30,30,41	0.43	0	39,39,56	0.72	0
14	CLA	H	825	22	69,73,73	0.99	5 (7%)	82,113,113	1.13	5 (6%)
16	SF4	N	101	-	0,12,12	-	-	-		
14	CLA	A	819	1	69,73,73	0.97	5 (7%)	82,113,113	1.08	5 (6%)
12	LHG	G	856	-	24,24,48	0.68	0	27,30,54	0.65	0
14	CLA	A	817	1	69,73,73	0.97	4 (5%)	82,113,113	0.90	2 (2%)
14	CLA	B	827	22	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
14	CLA	B	835	22	59,63,73	1.04	4 (6%)	70,101,113	1.00	5 (7%)
14	CLA	b	844	12	50,54,73	1.13	3 (6%)	59,90,113	0.97	3 (5%)
18	LMG	U	201	-	38,38,55	0.60	0	46,46,63	0.70	0
14	CLA	A	841	22	69,73,73	0.97	4 (5%)	82,113,113	0.93	4 (4%)
14	CLA	G	812	1	69,73,73	0.96	3 (4%)	82,113,113	0.94	2 (2%)
14	CLA	A	821	22	69,73,73	0.98	4 (5%)	82,113,113	0.91	3 (3%)
14	CLA	G	843	22	69,73,73	0.97	5 (7%)	82,113,113	0.92	2 (2%)
21	ECH	V	102	-	42,42,42	0.36	0	55,58,58	0.66	0
14	CLA	A	840	1	69,73,73	0.97	4 (5%)	82,113,113	0.98	4 (4%)
14	CLA	b	811	2	69,73,73	0.96	3 (4%)	82,113,113	0.99	4 (4%)
14	CLA	b	814	2	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
19	LMT	A	853	-	36,36,36	0.59	0	47,47,47	0.65	0
14	CLA	b	834	2	59,63,73	1.06	5 (8%)	70,101,113	1.01	4 (5%)
14	CLA	a	804	1	69,73,73	0.97	4 (5%)	82,113,113	0.89	3 (3%)
18	LMG	B	852	-	38,38,55	0.58	0	46,46,63	0.61	0
14	CLA	B	830	-	69,73,73	0.97	5 (7%)	82,113,113	1.01	5 (6%)
14	CLA	U	204	10	69,73,73	0.97	4 (5%)	82,113,113	0.90	3 (3%)
17	BCR	b	847	-	41,41,41	0.31	0	56,56,56	0.70	0
17	BCR	j	103	-	41,41,41	0.30	0	56,56,56	0.57	0
14	CLA	a	838	1	55,59,73	1.09	4 (7%)	64,96,113	0.99	3 (4%)
16	SF4	N	102	-	0,12,12	-	-	-		
14	CLA	A	804	1,14	69,73,73	0.98	4 (5%)	82,113,113	0.90	2 (2%)
14	CLA	b	812	2	69,73,73	0.96	4 (5%)	82,113,113	0.94	4 (4%)
19	LMT	B	855	-	36,36,36	0.55	0	47,47,47	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	G	850	-	41,41,41	0.29	0	56,56,56	0.66	1 (1%)
17	BCR	a	848	-	41,41,41	0.29	0	56,56,56	0.49	0
17	BCR	f	206	-	41,41,41	0.28	0	56,56,56	0.54	0
17	BCR	a	851	-	41,41,41	0.30	0	56,56,56	0.69	2 (3%)
14	CLA	G	805	1	69,73,73	0.98	4 (5%)	82,113,113	0.94	2 (2%)
14	CLA	G	815	1	69,73,73	0.98	4 (5%)	82,113,113	0.93	3 (3%)
19	LMT	f	207	-	36,36,36	0.54	0	47,47,47	0.70	0
14	CLA	A	836	1	69,73,73	0.98	4 (5%)	82,113,113	0.90	3 (3%)
14	CLA	B	810	2	69,73,73	0.97	3 (4%)	82,113,113	0.98	6 (7%)
14	CLA	H	804	-	69,73,73	0.97	5 (7%)	82,113,113	0.99	2 (2%)
14	CLA	H	842	12	50,54,73	1.14	3 (6%)	59,90,113	0.96	3 (5%)
17	BCR	A	849	-	41,41,41	0.29	0	56,56,56	0.46	0
14	CLA	H	837	2	54,58,73	1.09	4 (7%)	64,95,113	0.97	3 (4%)
14	CLA	a	806	1	69,73,73	0.98	4 (5%)	82,113,113	1.06	7 (8%)
14	CLA	A	814	1	51,55,73	1.12	4 (7%)	60,91,113	1.01	3 (5%)
14	CLA	a	812	1	69,73,73	0.97	3 (4%)	82,113,113	0.91	2 (2%)
14	CLA	k	103	22	69,73,73	0.98	3 (4%)	82,113,113	1.04	7 (8%)
21	ECH	m	101	-	42,42,42	0.36	0	55,58,58	0.87	2 (3%)
14	CLA	G	811	1	49,53,73	1.15	5 (10%)	58,89,113	1.11	2 (3%)
15	PQN	B	844	-	34,34,34	0.44	0	43,45,45	0.70	1 (2%)
12	LHG	H	850	14	37,37,48	0.58	0	40,43,54	0.57	0
17	BCR	G	848	-	41,41,41	0.29	0	56,56,56	0.52	0
17	BCR	G	858	-	41,41,41	0.31	0	56,56,56	0.74	1 (1%)
18	LMG	H	801	-	50,50,55	0.56	0	58,58,63	0.65	0
14	CLA	G	827	22	64,68,73	1.01	4 (6%)	76,107,113	0.97	4 (5%)
14	CLA	a	845	12	50,54,73	1.12	3 (6%)	59,90,113	0.99	3 (5%)
17	BCR	R	101	-	41,41,41	0.33	0	56,56,56	0.76	1 (1%)
14	CLA	A	818	1	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
14	CLA	B	832	2	69,73,73	0.98	4 (5%)	82,113,113	0.87	2 (2%)
14	CLA	H	807	2	69,73,73	0.98	4 (5%)	82,113,113	0.96	4 (4%)
14	CLA	a	842	22	69,73,73	0.98	4 (5%)	82,113,113	0.90	3 (3%)
14	CLA	b	843	2	69,73,73	0.96	3 (4%)	82,113,113	0.98	4 (4%)
14	CLA	A	839	1	69,73,73	0.96	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	b	805	2	69,73,73	0.98	4 (5%)	82,113,113	0.98	2 (2%)
14	CLA	b	840	2	69,73,73	0.96	3 (4%)	82,113,113	0.92	2 (2%)
14	CLA	a	810	1	55,59,73	1.10	4 (7%)	64,96,113	1.02	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LMT	L	1505	-	36,36,36	0.56	0	47,47,47	0.87	2 (4%)
14	CLA	B	825	2	57,61,73	1.07	4 (7%)	67,98,113	1.06	4 (5%)
14	CLA	B	819	2	69,73,73	0.96	4 (5%)	82,113,113	0.96	5 (6%)
14	CLA	G	806	1	69,73,73	0.97	3 (4%)	82,113,113	1.05	5 (6%)
19	LMT	A	857	-	36,36,36	0.56	0	47,47,47	0.63	0
13	CL0	G	801	1	69,73,73	0.98	5 (7%)	82,113,113	0.99	4 (4%)
14	CLA	A	844	12	50,54,73	1.12	3 (6%)	59,90,113	0.97	3 (5%)
14	CLA	A	808	1	69,73,73	0.96	5 (7%)	82,113,113	1.09	4 (4%)
17	BCR	S	1105	-	41,41,41	0.29	0	56,56,56	0.62	0
21	ECH	B	847	-	42,42,42	0.34	0	55,58,58	0.68	0
17	BCR	H	844	-	41,41,41	0.29	0	56,56,56	0.57	0
14	CLA	H	817	2	69,73,73	0.97	5 (7%)	82,113,113	0.97	5 (6%)
17	BCR	H	848	-	41,41,41	0.30	0	56,56,56	0.72	0
17	BCR	a	850	-	41,41,41	0.28	0	56,56,56	0.45	0
14	CLA	l	5006	-	69,73,73	0.97	5 (7%)	82,113,113	0.99	4 (4%)
14	CLA	b	825	2	49,53,73	1.15	4 (8%)	58,89,113	1.02	2 (3%)
12	LHG	M	102	-	39,39,48	0.55	0	42,45,54	0.56	0
14	CLA	G	823	1	54,58,73	1.09	3 (5%)	64,95,113	0.98	2 (3%)
14	CLA	a	833	1	64,68,73	1.00	4 (6%)	76,107,113	1.04	5 (6%)
14	CLA	b	817	2	69,73,73	0.96	5 (7%)	82,113,113	0.94	4 (4%)
14	CLA	B	837	-	50,54,73	1.15	4 (8%)	59,90,113	0.97	2 (3%)
12	LHG	G	854	-	47,47,48	0.51	0	50,53,54	0.54	0
14	CLA	G	802	22	69,73,73	0.97	3 (4%)	82,113,113	0.98	4 (4%)
16	SF4	G	846	2,1	0,12,12	-	-	-		
14	CLA	H	827	2	69,73,73	0.98	4 (5%)	82,113,113	0.93	4 (4%)
14	CLA	H	813	2	69,73,73	0.96	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	H	826	22	69,73,73	0.97	5 (7%)	82,113,113	0.99	2 (2%)
17	BCR	S	1104	-	41,41,41	0.29	0	56,56,56	0.56	0
14	CLA	a	828	1	69,73,73	0.97	4 (5%)	82,113,113	0.96	3 (3%)
14	CLA	H	808	2	69,73,73	0.98	4 (5%)	82,113,113	1.12	6 (7%)
14	CLA	G	809	1	69,73,73	0.97	4 (5%)	82,113,113	1.15	5 (6%)
14	CLA	a	827	22	64,68,73	1.01	4 (6%)	76,107,113	0.94	2 (2%)
14	CLA	b	806	-	69,73,73	0.97	5 (7%)	82,113,113	1.02	3 (3%)
19	LMT	b	855	-	36,36,36	0.55	0	47,47,47	0.63	0
14	CLA	B	833	2	59,63,73	1.05	4 (6%)	70,101,113	0.99	4 (5%)
14	CLA	A	842	1	69,73,73	0.99	5 (7%)	82,113,113	0.93	5 (6%)
17	BCR	U	203	-	41,41,41	0.29	0	56,56,56	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	827	22	69,73,73	1.00	4 (5%)	82,113,113	1.11	4 (4%)
12	LHG	L	1510	-	32,32,48	0.61	0	35,38,54	0.63	0
14	CLA	A	806	1	69,73,73	1.00	4 (5%)	82,113,113	0.94	3 (3%)
12	LHG	V	101	-	39,39,48	0.57	0	42,45,54	0.53	0
14	CLA	a	844	22	69,73,73	0.97	5 (7%)	82,113,113	0.93	3 (3%)
17	BCR	A	860	-	41,41,41	0.30	0	56,56,56	0.74	1 (1%)
14	CLA	T	103	22	69,73,73	0.98	5 (7%)	82,113,113	0.95	3 (3%)
18	LMG	b	803	-	50,50,55	0.55	0	58,58,63	0.63	0
14	CLA	A	837	1	55,59,73	1.10	3 (5%)	64,96,113	0.99	5 (7%)
14	CLA	G	820	1	69,73,73	0.97	4 (5%)	82,113,113	1.10	5 (6%)
14	CLA	Q	202	2	69,73,73	0.98	4 (5%)	82,113,113	0.96	3 (3%)
14	CLA	A	813	1	69,73,73	0.98	4 (5%)	82,113,113	0.96	3 (3%)
19	LMT	a	854	-	36,36,36	0.60	0	47,47,47	0.64	0
14	CLA	B	840	2	69,73,73	0.98	5 (7%)	82,113,113	0.93	3 (3%)
16	SF4	C	101	-	0,12,12	-	-	-		
14	CLA	G	839	1	69,73,73	0.97	3 (4%)	82,113,113	1.01	5 (6%)
16	SF4	C	102	-	0,12,12	-	-	-		
19	LMT	G	857	-	36,36,36	0.53	0	47,47,47	0.62	0
14	CLA	Q	204	22	49,53,73	1.17	3 (6%)	58,89,113	1.03	3 (5%)
19	LMT	U	207	-	36,36,36	0.56	0	47,47,47	0.65	0
14	CLA	B	817	2	64,68,73	1.02	3 (4%)	76,107,113	0.99	5 (6%)
14	CLA	B	834	2	69,73,73	0.97	4 (5%)	82,113,113	0.95	3 (3%)
14	CLA	f	205	6	50,54,73	1.15	4 (8%)	59,90,113	0.93	2 (3%)
14	CLA	G	844	12	50,54,73	1.13	3 (6%)	59,90,113	0.96	1 (1%)
17	BCR	b	849	-	30,30,41	0.44	0	39,39,56	0.62	0
17	BCR	H	849	-	41,41,41	0.30	0	56,56,56	0.69	0
14	CLA	A	830	1	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
14	CLA	a	841	1	69,73,73	0.97	4 (5%)	82,113,113	0.95	3 (3%)
17	BCR	l	5007	-	41,41,41	0.31	0	56,56,56	0.47	0
19	LMT	H	853	-	36,36,36	0.56	0	47,47,47	0.63	0
14	CLA	H	832	2	59,63,73	1.05	3 (5%)	70,101,113	1.03	5 (7%)
14	CLA	B	841	22	69,73,73	0.97	4 (5%)	82,113,113	0.93	5 (6%)
14	CLA	H	814	2	69,73,73	0.97	4 (5%)	82,113,113	0.96	4 (4%)
17	BCR	G	847	-	41,41,41	0.29	0	56,56,56	0.48	0
14	CLA	A	833	1	69,73,73	0.98	5 (7%)	82,113,113	1.02	3 (3%)
14	CLA	B	826	22	69,73,73	0.99	4 (5%)	82,113,113	1.10	4 (4%)
19	LMT	H	852	-	36,36,36	0.53	0	47,47,47	0.82	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	H	818	2	69,73,73	0.97	3 (4%)	82,113,113	0.91	4 (4%)
17	BCR	b	850	-	41,41,41	0.29	0	56,56,56	0.75	0
14	CLA	a	815	1	69,73,73	0.99	4 (5%)	82,113,113	0.94	5 (6%)
14	CLA	G	829	1	69,73,73	0.99	5 (7%)	82,113,113	0.98	5 (6%)
14	CLA	k	102	9	49,53,73	1.19	4 (8%)	58,89,113	0.98	2 (3%)
14	CLA	b	802	-	69,73,73	0.96	5 (7%)	82,113,113	0.98	4 (4%)
14	CLA	A	828	1	69,73,73	0.98	5 (7%)	82,113,113	1.02	4 (4%)
14	CLA	B	842	2	69,73,73	0.97	3 (4%)	82,113,113	1.01	4 (4%)
14	CLA	K	103	22	69,73,73	0.98	4 (5%)	82,113,113	0.93	3 (3%)
21	ECH	b	848	-	42,42,42	0.35	0	55,58,58	0.60	0
14	CLA	A	827	1	69,73,73	0.98	4 (5%)	82,113,113	0.93	4 (4%)
14	CLA	b	841	2	69,73,73	0.98	4 (5%)	82,113,113	0.92	4 (4%)
14	CLA	H	839	2	69,73,73	0.98	4 (5%)	82,113,113	0.96	5 (6%)
14	CLA	a	843	1	69,73,73	0.96	5 (7%)	82,113,113	0.94	5 (6%)
14	CLA	H	812	2	69,73,73	0.97	4 (5%)	82,113,113	0.90	2 (2%)
14	CLA	A	834	1	69,73,73	0.96	4 (5%)	82,113,113	0.98	5 (6%)
17	BCR	J	1105	-	41,41,41	0.30	0	56,56,56	0.69	0
14	CLA	A	822	1	54,58,73	1.09	4 (7%)	64,95,113	0.98	2 (3%)
18	LMG	a	853	-	46,46,55	0.53	0	54,54,63	0.67	0
14	CLA	a	813	1	58,62,73	1.06	4 (6%)	68,99,113	0.95	3 (4%)
14	CLA	L	1501	10	69,73,73	0.97	4 (5%)	82,113,113	1.03	1 (1%)
17	BCR	B	846	-	41,41,41	0.31	0	56,56,56	0.66	0
17	BCR	k	104	-	41,41,41	0.30	0	56,56,56	0.49	0
14	CLA	B	818	2	69,73,73	0.98	5 (7%)	82,113,113	0.95	4 (4%)
14	CLA	G	807	1	69,73,73	0.99	4 (5%)	82,113,113	0.97	5 (6%)
12	LHG	a	801	-	47,47,48	0.51	0	50,53,54	0.56	0
17	BCR	l	5003	-	41,41,41	0.29	0	56,56,56	0.61	1 (1%)
14	CLA	H	820	22	69,73,73	0.96	4 (5%)	82,113,113	0.95	3 (3%)
14	CLA	b	829	2	69,73,73	0.98	4 (5%)	82,113,113	0.93	4 (4%)
14	CLA	G	813	1	58,62,73	1.05	4 (6%)	68,99,113	1.00	3 (4%)
14	CLA	b	808	2	69,73,73	0.96	4 (5%)	82,113,113	0.99	4 (4%)
14	CLA	b	839	2	54,58,73	1.09	4 (7%)	64,95,113	1.04	4 (6%)
14	CLA	J	1102	8	49,53,73	1.16	4 (8%)	58,89,113	0.95	2 (3%)
17	BCR	b	856	-	41,41,41	0.29	0	56,56,56	0.48	0
19	LMT	B	854	-	36,36,36	0.55	0	47,47,47	0.63	0
18	LMG	K	105	-	35,35,55	0.57	0	43,43,63	0.70	0
14	CLA	G	816	1	49,53,73	1.15	3 (6%)	58,89,113	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	U	205	10	69,73,73	0.96	4 (5%)	82,113,113	0.94	2 (2%)
14	CLA	a	839	1	69,73,73	0.96	4 (5%)	82,113,113	0.94	4 (4%)
16	SF4	c	101	-	0,12,12	-	-	-		
12	LHG	A	801	-	47,47,48	0.52	0	50,53,54	0.54	0
17	BCR	A	850	-	41,41,41	0.29	0	56,56,56	0.69	1 (1%)
21	ECH	i	102	-	42,42,42	0.35	0	55,58,58	0.61	0
18	LMG	A	852	-	46,46,55	0.53	0	54,54,63	0.69	0
14	CLA	G	828	1	69,73,73	0.96	4 (5%)	82,113,113	0.94	4 (4%)
14	CLA	A	815	1	49,53,73	1.16	3 (6%)	58,89,113	1.06	3 (5%)
14	CLA	A	826	22	64,68,73	1.01	4 (6%)	76,107,113	0.96	3 (3%)
14	CLA	B	808	2	69,73,73	0.97	4 (5%)	82,113,113	0.92	3 (3%)
14	CLA	b	810	2	69,73,73	0.99	4 (5%)	82,113,113	1.10	6 (7%)
14	CLA	S	1103	8	54,58,73	1.11	4 (7%)	64,95,113	1.04	6 (9%)
19	LMT	b	854	-	36,36,36	0.56	0	47,47,47	0.64	0
14	CLA	G	831	1	69,73,73	0.97	3 (4%)	82,113,113	0.94	2 (2%)
17	BCR	F	202	-	41,41,41	0.32	0	56,56,56	0.91	1 (1%)
21	ECH	R	102	-	42,42,42	0.37	0	55,58,58	0.59	0
14	CLA	A	823	1	55,59,73	1.08	4 (7%)	64,96,113	1.01	4 (6%)
14	CLA	B	812	2	69,73,73	0.96	4 (5%)	82,113,113	1.01	3 (3%)
15	PQN	A	845	-	34,34,34	0.40	0	43,45,45	0.66	1 (2%)
21	ECH	I	102	-	42,42,42	0.37	0	55,58,58	0.56	0
14	CLA	G	821	1	69,73,73	0.98	4 (5%)	82,113,113	0.91	4 (4%)
12	LHG	a	855	14	48,48,48	0.54	0	51,54,54	0.49	0
14	CLA	b	830	2	69,73,73	0.97	4 (5%)	82,113,113	0.96	5 (6%)
14	CLA	a	818	1	69,73,73	0.98	4 (5%)	82,113,113	1.03	5 (6%)
14	CLA	b	832	2	69,73,73	0.96	4 (5%)	82,113,113	0.92	3 (3%)
17	BCR	a	858	-	41,41,41	0.31	0	56,56,56	0.74	1 (1%)
14	CLA	G	824	1	55,59,73	1.07	3 (5%)	64,96,113	1.04	3 (4%)
14	CLA	H	833	2	69,73,73	0.98	5 (7%)	82,113,113	0.94	3 (3%)
16	SF4	c	102	-	0,12,12	-	-	-		
18	LMG	B	853	-	49,49,55	0.56	0	57,57,63	0.71	2 (3%)
19	LMT	a	856	-	36,36,36	0.56	0	47,47,47	0.92	2 (4%)
14	CLA	f	201	2	69,73,73	0.97	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	a	836	1	69,73,73	0.96	4 (5%)	82,113,113	0.93	4 (4%)
14	CLA	b	807	2	69,73,73	0.97	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	A	858	-	69,73,73	0.97	5 (7%)	82,113,113	1.02	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	809	1	69,73,73	0.97	3 (4%)	82,113,113	1.13	5 (6%)
14	CLA	b	831	-	69,73,73	0.97	5 (7%)	82,113,113	1.00	4 (4%)
14	CLA	G	835	1	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)
19	LMT	a	857	-	36,36,36	0.55	0	47,47,47	0.67	0
14	CLA	G	841	22	69,73,73	0.98	3 (4%)	82,113,113	0.92	2 (2%)
14	CLA	B	815	2	69,73,73	0.99	5 (7%)	82,113,113	0.88	3 (3%)
14	CLA	G	825	1	69,73,73	0.99	3 (4%)	82,113,113	0.99	3 (3%)
14	CLA	a	805	1	69,73,73	0.98	4 (5%)	82,113,113	0.94	3 (3%)
17	BCR	B	849	-	41,41,41	0.29	0	56,56,56	0.72	0
14	CLA	b	813	2	69,73,73	0.97	4 (5%)	82,113,113	0.96	2 (2%)
21	ECH	M	103	-	42,42,42	0.35	0	55,58,58	0.64	0
17	BCR	F	205	-	41,41,41	0.28	0	56,56,56	0.53	0
14	CLA	H	821	2	49,53,73	1.16	4 (8%)	58,89,113	1.04	1 (1%)
14	CLA	G	836	1	69,73,73	0.97	4 (5%)	82,113,113	0.88	2 (2%)
14	CLA	B	843	12	50,54,73	1.14	4 (8%)	59,90,113	1.01	5 (8%)
14	CLA	Q	205	6	50,54,73	1.14	3 (6%)	59,90,113	0.94	0
14	CLA	H	834	22	59,63,73	1.05	4 (6%)	70,101,113	1.00	5 (7%)
14	CLA	b	821	2	69,73,73	0.97	4 (5%)	82,113,113	0.95	2 (2%)
14	CLA	a	824	1	55,59,73	1.08	4 (7%)	64,96,113	1.01	5 (7%)
17	BCR	Q	206	-	41,41,41	0.28	0	56,56,56	0.55	0
14	CLA	a	835	1	69,73,73	0.97	3 (4%)	82,113,113	0.97	7 (8%)
14	CLA	B	823	2	69,73,73	1.00	4 (5%)	82,113,113	0.92	3 (3%)
14	CLA	K	102	9	49,53,73	1.19	4 (8%)	58,89,113	1.07	4 (6%)
14	CLA	G	830	1	69,73,73	0.99	5 (7%)	82,113,113	1.01	5 (6%)
14	CLA	G	803	-	69,73,73	0.95	5 (7%)	82,113,113	0.98	4 (4%)
14	CLA	H	806	2	69,73,73	0.95	3 (4%)	82,113,113	0.99	5 (6%)
14	CLA	H	824	2	57,61,73	1.08	5 (8%)	67,98,113	0.99	4 (5%)
17	BCR	H	854	-	41,41,41	0.28	0	56,56,56	0.47	0
14	CLA	a	823	1	69,73,73	0.99	3 (4%)	82,113,113	0.90	3 (3%)
14	CLA	G	804	22	69,73,73	0.97	4 (5%)	82,113,113	0.93	4 (4%)
15	PQN	H	843	-	34,34,34	0.43	0	43,45,45	0.68	1 (2%)
14	CLA	B	809	2	69,73,73	0.98	5 (7%)	82,113,113	1.15	6 (7%)
14	CLA	J	1103	8	54,58,73	1.12	5 (9%)	64,95,113	1.07	5 (7%)
14	CLA	F	204	6	50,54,73	1.13	4 (8%)	59,90,113	0.96	2 (3%)
14	CLA	H	838	2	69,73,73	0.97	4 (5%)	82,113,113	0.90	3 (3%)
14	CLA	b	818	2	69,73,73	0.98	5 (7%)	82,113,113	0.97	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	B	850	-	41,41,41	0.30	0	56,56,56	0.71	0
14	CLA	b	828	22	69,73,73	0.97	5 (7%)	82,113,113	0.96	3 (3%)
14	CLA	A	812	1	58,62,73	1.06	4 (6%)	68,99,113	0.90	1 (1%)
17	BCR	L	1504	-	41,41,41	0.30	0	56,56,56	0.48	0
14	CLA	b	835	2	69,73,73	0.96	5 (7%)	82,113,113	0.97	4 (4%)
14	CLA	A	832	1	64,68,73	0.99	4 (6%)	76,107,113	1.00	4 (5%)
17	BCR	f	202	-	41,41,41	0.30	0	56,56,56	0.87	2 (3%)
14	CLA	B	805	2	69,73,73	0.97	3 (4%)	82,113,113	0.91	3 (3%)
14	CLA	L	1502	10	69,73,73	0.96	4 (5%)	82,113,113	0.94	3 (3%)
14	CLA	H	836	-	50,54,73	1.16	4 (8%)	59,90,113	0.94	1 (1%)
18	LMG	b	853	-	42,42,55	0.64	0	50,50,63	0.65	0
14	CLA	b	819	2	69,73,73	0.97	4 (5%)	82,113,113	0.97	4 (4%)
14	CLA	G	810	1	55,59,73	1.10	5 (9%)	64,96,113	0.98	0
14	CLA	b	836	22	59,63,73	1.04	3 (5%)	70,101,113	1.02	5 (7%)
14	CLA	K	101	9	49,53,73	1.18	4 (8%)	58,89,113	0.93	2 (3%)
19	LMT	Q	201	-	36,36,36	0.57	0	47,47,47	0.88	3 (6%)
17	BCR	H	845	-	41,41,41	0.31	0	56,56,56	0.65	0
19	LMT	A	856	-	36,36,36	0.56	0	47,47,47	0.81	0
14	CLA	a	807	1	69,73,73	0.99	4 (5%)	82,113,113	0.94	3 (3%)
14	CLA	a	834	1	69,73,73	0.98	5 (7%)	82,113,113	0.93	4 (4%)
17	BCR	B	848	-	30,30,41	0.43	0	39,39,56	0.61	0
17	BCR	j	104	-	41,41,41	0.29	0	56,56,56	0.64	0
14	CLA	H	805	2	69,73,73	0.97	4 (5%)	82,113,113	0.91	2 (2%)
14	CLA	H	815	2	69,73,73	0.97	4 (5%)	82,113,113	0.91	3 (3%)
21	ECH	L	1506	-	42,42,42	0.35	0	55,58,58	0.77	1 (1%)
14	CLA	F	203	22	49,53,73	1.15	3 (6%)	58,89,113	0.97	3 (5%)
14	CLA	b	823	2	69,73,73	0.98	4 (5%)	82,113,113	0.86	3 (3%)
14	CLA	H	823	2	49,53,73	1.15	4 (8%)	58,89,113	1.00	2 (3%)
18	LMG	l	5001	-	38,38,55	0.59	0	46,46,63	0.70	0
13	CL0	a	802	1	69,73,73	0.99	4 (5%)	82,113,113	0.98	4 (4%)
17	BCR	a	852	-	41,41,41	0.30	0	56,56,56	0.57	0
14	CLA	b	842	22	69,73,73	0.97	4 (5%)	82,113,113	0.91	4 (4%)
14	CLA	H	829	-	69,73,73	0.96	4 (5%)	82,113,113	0.93	4 (4%)
14	CLA	G	819	1	69,73,73	0.97	4 (5%)	82,113,113	0.94	2 (2%)
14	CLA	B	806	2	69,73,73	0.97	4 (5%)	82,113,113	0.89	2 (2%)
14	CLA	b	809	2	69,73,73	0.98	4 (5%)	82,113,113	0.92	3 (3%)
12	LHG	L	1509	-	39,39,48	0.56	0	42,45,54	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	810	1	49,53,73	1.15	4 (8%)	58,89,113	1.07	3 (5%)
14	CLA	l	5004	10	69,73,73	0.98	3 (4%)	82,113,113	0.93	1 (1%)
14	CLA	H	831	2	69,73,73	0.98	4 (5%)	82,113,113	0.91	4 (4%)
17	BCR	T	104	-	41,41,41	0.28	0	56,56,56	0.47	0
14	CLA	A	820	1	69,73,73	0.98	3 (4%)	82,113,113	0.93	2 (2%)
14	CLA	b	815	2	59,63,73	1.05	4 (6%)	70,101,113	0.97	4 (5%)
14	CLA	a	825	1	69,73,73	0.98	5 (7%)	82,113,113	0.99	4 (4%)
14	CLA	L	1503	-	69,73,73	0.97	4 (5%)	82,113,113	0.88	4 (4%)
21	ECH	H	846	-	42,42,42	0.36	0	55,58,58	0.64	0
13	CL0	A	802	1	69,73,73	0.97	5 (7%)	82,113,113	0.99	5 (6%)
19	LMT	G	853	-	36,36,36	0.59	0	47,47,47	0.64	0
14	CLA	a	829	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	5 (6%)
14	CLA	B	801	22	69,73,73	0.97	3 (4%)	82,113,113	0.96	3 (3%)
18	LMG	B	803	-	50,50,55	0.54	0	58,58,63	0.63	0
14	CLA	G	837	1	55,59,73	1.10	3 (5%)	64,96,113	1.02	5 (7%)
14	CLA	j	101	8	49,53,73	1.16	5 (10%)	58,89,113	0.98	2 (3%)
14	CLA	B	802	-	69,73,73	0.97	5 (7%)	82,113,113	0.90	1 (1%)
18	LMG	L	1508	-	38,38,55	0.60	0	46,46,63	0.68	0
17	BCR	G	849	-	41,41,41	0.30	0	56,56,56	0.47	0
14	CLA	A	835	1	69,73,73	0.98	4 (5%)	82,113,113	0.91	3 (3%)
19	LMT	f	203	-	36,36,36	0.53	0	47,47,47	0.82	1 (2%)
14	CLA	U	206	-	69,73,73	0.97	5 (7%)	82,113,113	0.91	3 (3%)
17	BCR	B	845	-	41,41,41	0.30	0	56,56,56	0.48	0
17	BCR	I	101	-	41,41,41	0.34	0	56,56,56	0.82	1 (1%)
14	CLA	B	838	2	69,73,73	0.97	5 (7%)	82,113,113	0.99	4 (4%)
14	CLA	B	814	2	69,73,73	0.96	3 (4%)	82,113,113	0.95	4 (4%)
14	CLA	J	1101	1	69,73,73	0.97	3 (4%)	82,113,113	0.97	3 (3%)
14	CLA	b	816	2	69,73,73	0.99	4 (5%)	82,113,113	0.88	3 (3%)
19	LMT	Q	207	-	36,36,36	0.54	0	47,47,47	0.69	0
14	CLA	G	833	1	64,68,73	1.00	4 (6%)	76,107,113	0.99	4 (5%)
17	BCR	R	103	-	41,41,41	0.30	0	56,56,56	0.49	0
14	CLA	F	201	2	69,73,73	0.97	3 (4%)	82,113,113	1.03	2 (2%)
14	CLA	A	809	1	55,59,73	1.10	5 (9%)	64,96,113	1.03	2 (3%)
14	CLA	T	101	9	49,53,73	1.17	5 (10%)	58,89,113	1.06	4 (6%)
14	CLA	b	824	2	50,54,73	1.14	4 (8%)	59,90,113	0.92	2 (3%)
14	CLA	G	822	22	69,73,73	0.98	4 (5%)	82,113,113	0.92	2 (2%)
19	LMT	l	5008	-	36,36,36	0.56	0	47,47,47	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	j	102	8	50,54,73	1.14	4 (8%)	59,90,113	1.00	2 (3%)
14	CLA	B	829	2	69,73,73	0.97	4 (5%)	82,113,113	0.98	4 (4%)
14	CLA	a	831	1	69,73,73	0.97	4 (5%)	82,113,113	0.96	3 (3%)
14	CLA	U	202	1	69,73,73	0.96	4 (5%)	82,113,113	0.98	6 (7%)
14	CLA	l	5005	10	69,73,73	0.96	4 (5%)	82,113,113	0.96	2 (2%)
12	LHG	A	854	14	48,48,48	0.53	0	51,54,54	0.51	0
14	CLA	G	832	1	69,73,73	0.98	5 (7%)	82,113,113	0.94	4 (4%)
14	CLA	B	820	2	69,73,73	0.96	4 (5%)	82,113,113	0.94	2 (2%)
14	CLA	G	814	1	69,73,73	0.98	3 (4%)	82,113,113	0.92	4 (4%)
14	CLA	a	821	1	69,73,73	0.98	3 (4%)	82,113,113	0.93	3 (3%)
16	SF4	A	846	2,1	0,12,12	-	-	-		
14	CLA	f	204	22	49,53,73	1.14	3 (6%)	58,89,113	1.00	3 (5%)
14	CLA	H	803	2	69,73,73	0.98	3 (4%)	82,113,113	0.92	4 (4%)
19	LMT	A	859	-	36,36,36	0.60	0	47,47,47	0.69	0
14	CLA	G	840	1	69,73,73	0.97	4 (5%)	82,113,113	0.97	3 (3%)
14	CLA	B	839	2	69,73,73	0.97	3 (4%)	82,113,113	0.87	2 (2%)
14	CLA	a	820	1	69,73,73	0.97	4 (5%)	82,113,113	1.11	6 (7%)
14	CLA	a	816	1	49,53,73	1.15	3 (6%)	58,89,113	1.01	2 (3%)
14	CLA	a	830	1	69,73,73	0.99	5 (7%)	82,113,113	1.02	6 (7%)
14	CLA	B	822	2	49,53,73	1.16	5 (10%)	58,89,113	0.99	2 (3%)
14	CLA	a	803	22	69,73,73	0.98	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	G	817	22	50,54,73	1.16	4 (8%)	59,90,113	1.03	2 (3%)
15	PQN	a	846	-	34,34,34	0.38	0	43,45,45	0.63	1 (2%)
14	CLA	G	834	1	69,73,73	0.97	5 (7%)	82,113,113	0.94	4 (4%)
15	PQN	G	845	-	34,34,34	0.40	0	43,45,45	0.67	1 (2%)
14	CLA	A	811	1,14	69,73,73	0.98	4 (5%)	82,113,113	0.95	1 (1%)
14	CLA	b	833	2	69,73,73	0.97	4 (5%)	82,113,113	0.96	3 (3%)
17	BCR	i	101	-	41,41,41	0.34	0	56,56,56	0.78	1 (1%)
14	CLA	T	102	9	49,53,73	1.18	5 (10%)	58,89,113	1.04	5 (8%)
14	CLA	B	807	2	69,73,73	0.95	3 (4%)	82,113,113	1.02	5 (6%)
17	BCR	G	851	-	41,41,41	0.30	0	56,56,56	0.57	0
17	BCR	Q	203	-	41,41,41	0.31	0	56,56,56	0.88	1 (1%)
17	BCR	A	847	-	41,41,41	0.29	0	56,56,56	0.45	0
14	CLA	a	837	1	69,73,73	0.97	5 (7%)	82,113,113	0.96	4 (4%)
14	CLA	H	830	2	69,73,73	0.97	5 (7%)	82,113,113	0.96	5 (6%)
14	CLA	A	816	22	50,54,73	1.16	3 (6%)	59,90,113	0.99	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	H	828	2	69,73,73	0.97	4 (5%)	82,113,113	1.02	5 (6%)
14	CLA	G	842	1	69,73,73	0.98	4 (5%)	82,113,113	0.95	5 (6%)
14	CLA	a	822	22	69,73,73	0.97	4 (5%)	82,113,113	0.91	4 (4%)
12	LHG	M	101	-	37,37,48	0.57	0	40,43,54	0.55	0
17	BCR	B	856	-	41,41,41	0.28	0	56,56,56	0.47	0
12	LHG	b	852	14	37,37,48	0.58	0	40,43,54	0.58	0
14	CLA	A	838	1	69,73,73	0.97	3 (4%)	82,113,113	0.95	4 (4%)
16	SF4	a	847	2,1	0,12,12	-	-	-		
14	CLA	A	824	1	69,73,73	0.98	4 (5%)	82,113,113	1.06	6 (7%)
12	LHG	G	855	14	48,48,48	0.53	0	51,54,54	0.51	0
12	LHG	B	851	14	37,37,48	0.57	0	40,43,54	0.56	0
14	CLA	b	820	2	69,73,73	0.98	4 (5%)	82,113,113	0.90	3 (3%)
14	CLA	H	816	2	69,73,73	0.96	3 (4%)	82,113,113	0.95	5 (6%)
14	CLA	a	840	1	69,73,73	0.96	5 (7%)	82,113,113	0.96	4 (4%)
14	CLA	S	1101	1	69,73,73	0.98	3 (4%)	82,113,113	0.88	3 (3%)
14	CLA	H	819	2	69,73,73	0.95	4 (5%)	82,113,113	0.96	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	825	22	-	20/39/115/115	-
14	CLA	b	822	22	-	9/39/115/115	-
18	LMG	H	851	-	-	10/31/51/70	0/1/1/1
14	CLA	H	822	2	-	4/17/93/115	-
14	CLA	B	828	2	-	8/39/115/115	-
14	CLA	A	829	1	-	7/39/115/115	-
14	CLA	B	831	2	-	10/39/115/115	-
14	CLA	a	808	1	-	10/39/115/115	-
14	CLA	a	817	22	-	6/17/93/115	-
14	CLA	A	803	22	-	8/39/115/115	-
14	CLA	B	813	2	-	8/39/115/115	-
14	CLA	a	811	1	-	1/15/91/115	-
14	CLA	A	843	22	-	14/39/115/115	-
14	CLA	H	840	22	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	838	1	-	6/39/115/115	-
14	CLA	H	835	22	-	5/15/91/115	-
14	CLA	A	805	1	-	10/39/115/115	-
14	CLA	k	101	9	-	4/15/91/115	-
14	CLA	A	807	1	-	6/39/115/115	-
14	CLA	b	801	22	-	6/39/115/115	-
18	LMG	G	852	-	-	14/41/61/70	0/1/1/1
14	CLA	H	810	2	-	8/39/115/115	-
14	CLA	B	816	2	-	9/39/115/115	-
17	BCR	b	851	-	-	0/29/63/63	0/2/2/2
14	CLA	B	824	2	-	2/15/91/115	-
17	BCR	J	1104	-	-	3/29/63/63	0/2/2/2
14	CLA	b	826	2	-	6/25/101/115	-
14	CLA	H	841	2	-	13/39/115/115	-
14	CLA	G	818	1	-	10/39/115/115	-
14	CLA	G	826	22	-	16/39/115/115	-
17	BCR	K	104	-	-	2/29/63/63	0/2/2/2
14	CLA	B	811	2	-	8/39/115/115	-
12	LHG	M	104	-	-	7/46/46/53	-
17	BCR	b	846	-	-	6/29/63/63	0/2/2/2
17	BCR	a	849	-	-	6/29/63/63	0/2/2/2
14	CLA	H	809	2	-	7/39/115/115	-
14	CLA	b	837	22	-	2/15/91/115	-
14	CLA	A	831	1	-	9/39/115/115	-
14	CLA	B	836	22	-	0/15/91/115	-
14	CLA	a	819	1	-	9/39/115/115	-
18	LMG	A	855	-	-	13/37/57/70	0/1/1/1
14	CLA	b	838	-	-	3/17/93/115	-
15	PQN	b	845	-	-	4/23/43/43	0/2/2/2
14	CLA	B	821	22	-	8/39/115/115	-
14	CLA	S	1102	8	-	6/15/91/115	-
17	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	BCR	A	851	-	-	10/29/63/63	0/2/2/2
14	CLA	a	826	22	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	811	2	-	8/39/115/115	-
19	LMT	J	1106	-	-	7/21/61/61	0/2/2/2
14	CLA	G	808	1	-	7/39/115/115	-
14	CLA	a	832	1	-	6/39/115/115	-
14	CLA	a	814	1	-	8/39/115/115	-
17	BCR	H	847	-	-	2/24/41/63	0/1/1/2
14	CLA	H	825	22	-	14/39/115/115	-
16	SF4	N	101	-	-	-	0/6/5/5
14	CLA	A	819	1	-	6/39/115/115	-
12	LHG	G	856	-	-	10/29/29/53	-
14	CLA	A	817	1	-	8/39/115/115	-
14	CLA	B	827	22	-	8/39/115/115	-
14	CLA	B	835	22	-	4/27/103/115	-
14	CLA	b	844	12	-	1/17/93/115	-
18	LMG	U	201	-	-	9/33/53/70	0/1/1/1
14	CLA	A	841	22	-	11/39/115/115	-
14	CLA	G	812	1	-	12/39/115/115	-
14	CLA	A	821	22	-	4/39/115/115	-
14	CLA	G	843	22	-	14/39/115/115	-
21	ECH	V	102	-	-	9/29/66/66	0/2/2/2
14	CLA	A	840	1	-	6/39/115/115	-
14	CLA	b	811	2	-	8/39/115/115	-
14	CLA	b	814	2	-	10/39/115/115	-
19	LMT	A	853	-	-	6/21/61/61	0/2/2/2
14	CLA	b	834	2	-	6/27/103/115	-
14	CLA	a	804	1	-	2/39/115/115	-
18	LMG	B	852	-	-	11/33/53/70	0/1/1/1
14	CLA	B	830	-	-	6/39/115/115	-
14	CLA	U	204	10	-	3/39/115/115	-
17	BCR	b	847	-	-	5/29/63/63	0/2/2/2
17	BCR	j	103	-	-	5/29/63/63	0/2/2/2
14	CLA	a	838	1	-	2/23/99/115	-
16	SF4	N	102	-	-	-	0/6/5/5
14	CLA	A	804	1,14	-	11/39/115/115	-
14	CLA	b	812	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LMT	B	855	-	-	5/21/61/61	0/2/2/2
17	BCR	G	850	-	-	7/29/63/63	0/2/2/2
17	BCR	a	848	-	-	1/29/63/63	0/2/2/2
17	BCR	f	206	-	-	2/29/63/63	0/2/2/2
17	BCR	a	851	-	-	7/29/63/63	0/2/2/2
14	CLA	G	805	1	-	15/39/115/115	-
14	CLA	G	815	1	-	10/39/115/115	-
19	LMT	f	207	-	-	7/21/61/61	0/2/2/2
14	CLA	A	836	1	-	13/39/115/115	-
14	CLA	B	810	2	-	8/39/115/115	-
14	CLA	H	804	-	-	6/39/115/115	-
14	CLA	H	842	12	-	3/17/93/115	-
17	BCR	A	849	-	-	5/29/63/63	0/2/2/2
14	CLA	H	837	2	-	2/21/97/115	-
14	CLA	a	806	1	-	10/39/115/115	-
14	CLA	A	814	1	-	5/18/94/115	-
14	CLA	a	812	1	-	11/39/115/115	-
14	CLA	k	103	22	-	11/39/115/115	-
21	ECH	m	101	-	-	10/29/66/66	0/2/2/2
14	CLA	G	811	1	-	4/15/91/115	-
15	PQN	B	844	-	-	5/23/43/43	0/2/2/2
12	LHG	H	850	14	-	8/42/42/53	-
17	BCR	G	848	-	-	6/29/63/63	0/2/2/2
17	BCR	G	858	-	-	5/29/63/63	0/2/2/2
18	LMG	H	801	-	-	11/45/65/70	0/1/1/1
14	CLA	G	827	22	-	2/33/109/115	-
14	CLA	a	845	12	-	7/17/93/115	-
17	BCR	R	101	-	-	5/29/63/63	0/2/2/2
14	CLA	A	818	1	-	10/39/115/115	-
14	CLA	B	832	2	-	7/39/115/115	-
14	CLA	H	807	2	-	7/39/115/115	-
14	CLA	a	842	22	-	9/39/115/115	-
14	CLA	b	843	2	-	10/39/115/115	-
14	CLA	A	839	1	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	805	2	-	2/39/115/115	-
14	CLA	b	840	2	-	12/39/115/115	-
14	CLA	a	810	1	-	6/23/99/115	-
19	LMT	L	1505	-	-	6/21/61/61	0/2/2/2
14	CLA	B	825	2	-	6/25/101/115	-
14	CLA	B	819	2	-	8/39/115/115	-
14	CLA	G	806	1	-	13/39/115/115	-
19	LMT	A	857	-	-	5/21/61/61	0/2/2/2
13	CL0	G	801	1	-	4/39/115/115	-
14	CLA	A	844	12	-	10/17/93/115	-
14	CLA	A	808	1	-	5/39/115/115	-
17	BCR	S	1105	-	-	7/29/63/63	0/2/2/2
21	ECH	B	847	-	-	11/29/66/66	0/2/2/2
17	BCR	H	844	-	-	6/29/63/63	0/2/2/2
14	CLA	H	817	2	-	12/39/115/115	-
17	BCR	H	848	-	-	4/29/63/63	0/2/2/2
17	BCR	a	850	-	-	5/29/63/63	0/2/2/2
14	CLA	l	5006	-	-	14/39/115/115	-
14	CLA	b	825	2	-	5/15/91/115	-
12	LHG	M	102	-	-	9/44/44/53	-
14	CLA	G	823	1	-	4/21/97/115	-
14	CLA	a	833	1	-	4/33/109/115	-
14	CLA	b	817	2	-	10/39/115/115	-
14	CLA	B	837	-	-	4/17/93/115	-
12	LHG	G	854	-	-	17/52/52/53	-
14	CLA	G	802	22	-	9/39/115/115	-
16	SF4	G	846	2,1	-	-	0/6/5/5
14	CLA	H	827	2	-	6/39/115/115	-
14	CLA	H	813	2	-	8/39/115/115	-
14	CLA	H	826	22	-	10/39/115/115	-
17	BCR	S	1104	-	-	6/29/63/63	0/2/2/2
14	CLA	a	828	1	-	9/39/115/115	-
14	CLA	H	808	2	-	4/39/115/115	-
14	CLA	G	809	1	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	827	22	-	2/33/109/115	-
14	CLA	b	806	-	-	7/39/115/115	-
19	LMT	b	855	-	-	3/21/61/61	0/2/2/2
14	CLA	B	833	2	-	3/27/103/115	-
14	CLA	A	842	1	-	7/39/115/115	-
17	BCR	U	203	-	-	5/29/63/63	0/2/2/2
14	CLA	b	827	22	-	17/39/115/115	-
12	LHG	L	1510	-	-	13/37/37/53	-
14	CLA	A	806	1	-	14/39/115/115	-
12	LHG	V	101	-	-	8/44/44/53	-
14	CLA	a	844	22	-	14/39/115/115	-
17	BCR	A	860	-	-	5/29/63/63	0/2/2/2
14	CLA	T	103	22	-	14/39/115/115	-
18	LMG	b	803	-	-	12/45/65/70	0/1/1/1
14	CLA	A	837	1	-	2/23/99/115	-
14	CLA	G	820	1	-	4/39/115/115	-
14	CLA	Q	202	2	-	8/39/115/115	-
14	CLA	A	813	1	-	7/39/115/115	-
19	LMT	a	854	-	-	4/21/61/61	0/2/2/2
14	CLA	B	840	2	-	10/39/115/115	-
16	SF4	C	101	-	-	-	0/6/5/5
14	CLA	G	839	1	-	8/39/115/115	-
16	SF4	C	102	-	-	-	0/6/5/5
19	LMT	G	857	-	-	4/21/61/61	0/2/2/2
14	CLA	Q	204	22	-	6/15/91/115	-
19	LMT	U	207	-	-	5/21/61/61	0/2/2/2
14	CLA	B	817	2	-	12/33/109/115	-
14	CLA	B	834	2	-	9/39/115/115	-
14	CLA	f	205	6	-	7/17/93/115	-
14	CLA	G	844	12	-	6/17/93/115	-
17	BCR	b	849	-	-	0/24/41/63	0/1/1/2
17	BCR	H	849	-	-	0/29/63/63	0/2/2/2
14	CLA	A	830	1	-	11/39/115/115	-
14	CLA	a	841	1	-	6/39/115/115	-
17	BCR	l	5007	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LMT	H	853	-	-	3/21/61/61	0/2/2/2
14	CLA	H	832	2	-	3/27/103/115	-
14	CLA	B	841	22	-	4/39/115/115	-
14	CLA	H	814	2	-	8/39/115/115	-
17	BCR	G	847	-	-	3/29/63/63	0/2/2/2
14	CLA	A	833	1	-	6/39/115/115	-
14	CLA	B	826	22	-	14/39/115/115	-
19	LMT	H	852	-	-	6/21/61/61	0/2/2/2
14	CLA	H	818	2	-	9/39/115/115	-
17	BCR	b	850	-	-	4/29/63/63	0/2/2/2
14	CLA	a	815	1	-	9/39/115/115	-
14	CLA	G	829	1	-	14/39/115/115	-
14	CLA	k	102	9	-	6/15/91/115	-
14	CLA	b	802	-	-	4/39/115/115	-
14	CLA	A	828	1	-	13/39/115/115	-
14	CLA	B	842	2	-	11/39/115/115	-
14	CLA	K	103	22	-	13/39/115/115	-
21	ECH	b	848	-	-	10/29/66/66	0/2/2/2
14	CLA	A	827	1	-	4/39/115/115	-
14	CLA	b	841	2	-	8/39/115/115	-
14	CLA	H	839	2	-	9/39/115/115	-
14	CLA	a	843	1	-	6/39/115/115	-
14	CLA	H	812	2	-	11/39/115/115	-
14	CLA	A	834	1	-	8/39/115/115	-
17	BCR	J	1105	-	-	8/29/63/63	0/2/2/2
14	CLA	A	822	1	-	6/21/97/115	-
18	LMG	a	853	-	-	15/41/61/70	0/1/1/1
14	CLA	a	813	1	-	5/26/102/115	-
14	CLA	L	1501	10	-	9/39/115/115	-
17	BCR	B	846	-	-	4/29/63/63	0/2/2/2
17	BCR	k	104	-	-	4/29/63/63	0/2/2/2
14	CLA	B	818	2	-	6/39/115/115	-
14	CLA	G	807	1	-	15/39/115/115	-
12	LHG	a	801	-	-	10/52/52/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	l	5003	-	-	6/29/63/63	0/2/2/2
14	CLA	H	820	22	-	10/39/115/115	-
14	CLA	b	829	2	-	6/39/115/115	-
14	CLA	G	813	1	-	6/26/102/115	-
14	CLA	b	808	2	-	14/39/115/115	-
14	CLA	b	839	2	-	4/21/97/115	-
14	CLA	J	1102	8	-	4/15/91/115	-
17	BCR	b	856	-	-	6/29/63/63	0/2/2/2
19	LMT	B	854	-	-	3/21/61/61	0/2/2/2
18	LMG	K	105	-	-	8/30/50/70	0/1/1/1
14	CLA	G	816	1	-	3/15/91/115	-
14	CLA	U	205	10	-	6/39/115/115	-
14	CLA	a	839	1	-	4/39/115/115	-
16	SF4	c	101	-	-	-	0/6/5/5
12	LHG	A	801	-	-	19/52/52/53	-
17	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	ECH	i	102	-	-	7/29/66/66	0/2/2/2
18	LMG	A	852	-	-	8/41/61/70	0/1/1/1
14	CLA	G	828	1	-	8/39/115/115	-
14	CLA	A	815	1	-	1/15/91/115	-
14	CLA	A	826	22	-	2/33/109/115	-
14	CLA	B	808	2	-	4/39/115/115	-
14	CLA	b	810	2	-	7/39/115/115	-
14	CLA	S	1103	8	-	7/21/97/115	-
19	LMT	b	854	-	-	6/21/61/61	0/2/2/2
14	CLA	G	831	1	-	8/39/115/115	-
17	BCR	F	202	-	-	6/29/63/63	0/2/2/2
21	ECH	R	102	-	-	9/29/66/66	0/2/2/2
14	CLA	A	823	1	-	4/23/99/115	-
14	CLA	B	812	2	-	5/39/115/115	-
15	PQN	A	845	-	-	0/23/43/43	0/2/2/2
21	ECH	I	102	-	-	7/29/66/66	0/2/2/2
14	CLA	G	821	1	-	7/39/115/115	-
12	LHG	a	855	14	-	10/53/53/53	-
14	CLA	b	830	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	818	1	-	9/39/115/115	-
14	CLA	b	832	2	-	10/39/115/115	-
17	BCR	a	858	-	-	6/29/63/63	0/2/2/2
14	CLA	G	824	1	-	4/23/99/115	-
14	CLA	H	833	2	-	6/39/115/115	-
16	SF4	c	102	-	-	-	0/6/5/5
18	LMG	B	853	-	-	7/44/64/70	0/1/1/1
19	LMT	a	856	-	-	5/21/61/61	0/2/2/2
14	CLA	f	201	2	-	8/39/115/115	-
14	CLA	a	836	1	-	4/39/115/115	-
14	CLA	b	807	2	-	5/39/115/115	-
14	CLA	A	858	-	-	6/39/115/115	-
14	CLA	a	809	1	-	6/39/115/115	-
14	CLA	b	831	-	-	6/39/115/115	-
14	CLA	G	835	1	-	8/39/115/115	-
19	LMT	a	857	-	-	3/21/61/61	0/2/2/2
14	CLA	G	841	22	-	8/39/115/115	-
14	CLA	B	815	2	-	9/39/115/115	-
14	CLA	G	825	1	-	13/39/115/115	-
14	CLA	a	805	1	-	15/39/115/115	-
17	BCR	B	849	-	-	4/29/63/63	0/2/2/2
14	CLA	b	813	2	-	5/39/115/115	-
21	ECH	M	103	-	-	8/29/66/66	0/2/2/2
17	BCR	F	205	-	-	2/29/63/63	0/2/2/2
14	CLA	H	821	2	-	7/15/91/115	-
14	CLA	G	836	1	-	11/39/115/115	-
14	CLA	B	843	12	-	3/17/93/115	-
14	CLA	Q	205	6	-	7/17/93/115	-
14	CLA	H	834	22	-	7/27/103/115	-
14	CLA	b	821	2	-	8/39/115/115	-
14	CLA	a	824	1	-	4/23/99/115	-
17	BCR	Q	206	-	-	2/29/63/63	0/2/2/2
14	CLA	a	835	1	-	6/39/115/115	-
14	CLA	B	823	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	K	102	9	-	9/15/91/115	-
14	CLA	G	830	1	-	7/39/115/115	-
14	CLA	G	803	-	-	4/39/115/115	-
14	CLA	H	806	2	-	13/39/115/115	-
14	CLA	H	824	2	-	5/25/101/115	-
17	BCR	H	854	-	-	6/29/63/63	0/2/2/2
14	CLA	a	823	1	-	12/39/115/115	-
14	CLA	G	804	22	-	7/39/115/115	-
15	PQN	H	843	-	-	4/23/43/43	0/2/2/2
14	CLA	B	809	2	-	6/39/115/115	-
14	CLA	J	1103	8	-	8/21/97/115	-
14	CLA	F	204	6	-	6/17/93/115	-
14	CLA	H	838	2	-	7/39/115/115	-
14	CLA	b	818	2	-	13/39/115/115	-
17	BCR	B	850	-	-	0/29/63/63	0/2/2/2
14	CLA	b	828	22	-	11/39/115/115	-
14	CLA	A	812	1	-	2/26/102/115	-
17	BCR	L	1504	-	-	6/29/63/63	0/2/2/2
14	CLA	b	835	2	-	6/39/115/115	-
14	CLA	A	832	1	-	3/33/109/115	-
17	BCR	f	202	-	-	6/29/63/63	0/2/2/2
14	CLA	B	805	2	-	3/39/115/115	-
14	CLA	L	1502	10	-	7/39/115/115	-
14	CLA	H	836	-	-	4/17/93/115	-
18	LMG	b	853	-	-	9/37/57/70	0/1/1/1
14	CLA	b	819	2	-	10/39/115/115	-
14	CLA	G	810	1	-	6/23/99/115	-
14	CLA	b	836	22	-	3/27/103/115	-
14	CLA	K	101	9	-	4/15/91/115	-
19	LMT	Q	201	-	-	8/21/61/61	0/2/2/2
17	BCR	H	845	-	-	4/29/63/63	0/2/2/2
19	LMT	A	856	-	-	6/21/61/61	0/2/2/2
14	CLA	a	807	1	-	11/39/115/115	-
14	CLA	a	834	1	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	B	848	-	-	3/24/41/63	0/1/1/2
17	BCR	j	104	-	-	5/29/63/63	0/2/2/2
14	CLA	H	805	2	-	7/39/115/115	-
14	CLA	H	815	2	-	14/39/115/115	-
21	ECH	L	1506	-	-	6/29/66/66	0/2/2/2
14	CLA	F	203	22	-	7/15/91/115	-
14	CLA	b	823	2	-	18/39/115/115	-
14	CLA	H	823	2	-	4/15/91/115	-
18	LMG	l	5001	-	-	8/33/53/70	0/1/1/1
13	CL0	a	802	1	-	6/39/115/115	-
17	BCR	a	852	-	-	11/29/63/63	0/2/2/2
14	CLA	b	842	22	-	5/39/115/115	-
14	CLA	H	829	-	-	4/39/115/115	-
14	CLA	G	819	1	-	9/39/115/115	-
14	CLA	B	806	2	-	5/39/115/115	-
14	CLA	b	809	2	-	5/39/115/115	-
12	LHG	L	1509	-	-	12/44/44/53	-
14	CLA	A	810	1	-	4/15/91/115	-
14	CLA	l	5004	10	-	9/39/115/115	-
14	CLA	H	831	2	-	6/39/115/115	-
17	BCR	T	104	-	-	0/29/63/63	0/2/2/2
14	CLA	A	820	1	-	6/39/115/115	-
14	CLA	b	815	2	-	5/27/103/115	-
14	CLA	a	825	1	-	11/39/115/115	-
14	CLA	L	1503	-	-	11/39/115/115	-
21	ECH	H	846	-	-	10/29/66/66	0/2/2/2
13	CL0	A	802	1	-	5/39/115/115	-
19	LMT	G	853	-	-	6/21/61/61	0/2/2/2
14	CLA	a	829	1	-	12/39/115/115	-
14	CLA	B	801	22	-	7/39/115/115	-
18	LMG	B	803	-	-	10/45/65/70	0/1/1/1
14	CLA	G	837	1	-	2/23/99/115	-
14	CLA	j	101	8	-	4/15/91/115	-
14	CLA	B	802	-	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMG	L	1508	-	-	9/33/53/70	0/1/1/1
17	BCR	G	849	-	-	5/29/63/63	0/2/2/2
14	CLA	A	835	1	-	5/39/115/115	-
19	LMT	f	203	-	-	2/21/61/61	0/2/2/2
14	CLA	U	206	-	-	4/39/115/115	-
17	BCR	B	845	-	-	4/29/63/63	0/2/2/2
17	BCR	I	101	-	-	5/29/63/63	0/2/2/2
14	CLA	B	838	2	-	9/39/115/115	-
14	CLA	B	814	2	-	10/39/115/115	-
14	CLA	J	1101	1	-	4/39/115/115	-
14	CLA	b	816	2	-	9/39/115/115	-
19	LMT	Q	207	-	-	8/21/61/61	0/2/2/2
14	CLA	G	833	1	-	2/33/109/115	-
17	BCR	R	103	-	-	7/29/63/63	0/2/2/2
14	CLA	F	201	2	-	9/39/115/115	-
14	CLA	A	809	1	-	8/23/99/115	-
14	CLA	T	101	9	-	6/15/91/115	-
14	CLA	b	824	2	-	2/17/93/115	-
14	CLA	G	822	22	-	10/39/115/115	-
19	LMT	l	5008	-	-	2/21/61/61	0/2/2/2
14	CLA	j	102	8	-	8/17/93/115	-
14	CLA	B	829	2	-	9/39/115/115	-
14	CLA	a	831	1	-	11/39/115/115	-
14	CLA	U	202	1	-	11/39/115/115	-
14	CLA	l	5005	10	-	5/39/115/115	-
12	LHG	A	854	14	-	6/53/53/53	-
14	CLA	G	832	1	-	4/39/115/115	-
14	CLA	B	820	2	-	10/39/115/115	-
14	CLA	G	814	1	-	10/39/115/115	-
14	CLA	a	821	1	-	6/39/115/115	-
16	SF4	A	846	2,1	-	-	0/6/5/5
14	CLA	f	204	22	-	5/15/91/115	-
14	CLA	H	803	2	-	4/39/115/115	-
19	LMT	A	859	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	840	1	-	8/39/115/115	-
14	CLA	B	839	2	-	10/39/115/115	-
14	CLA	a	820	1	-	12/39/115/115	-
14	CLA	a	816	1	-	5/15/91/115	-
14	CLA	a	830	1	-	7/39/115/115	-
14	CLA	B	822	2	-	5/15/91/115	-
14	CLA	a	803	22	-	7/39/115/115	-
14	CLA	G	817	22	-	5/17/93/115	-
15	PQN	a	846	-	-	0/23/43/43	0/2/2/2
14	CLA	G	834	1	-	7/39/115/115	-
15	PQN	G	845	-	-	0/23/43/43	0/2/2/2
14	CLA	A	811	1,14	-	18/39/115/115	-
14	CLA	b	833	2	-	6/39/115/115	-
17	BCR	i	101	-	-	5/29/63/63	0/2/2/2
14	CLA	T	102	9	-	6/15/91/115	-
14	CLA	B	807	2	-	12/39/115/115	-
17	BCR	G	851	-	-	10/29/63/63	0/2/2/2
17	BCR	Q	203	-	-	6/29/63/63	0/2/2/2
17	BCR	A	847	-	-	2/29/63/63	0/2/2/2
14	CLA	a	837	1	-	9/39/115/115	-
14	CLA	H	830	2	-	11/39/115/115	-
14	CLA	A	816	22	-	5/17/93/115	-
14	CLA	H	828	2	-	8/39/115/115	-
14	CLA	G	842	1	-	6/39/115/115	-
14	CLA	a	822	22	-	7/39/115/115	-
12	LHG	M	101	-	-	14/42/42/53	-
17	BCR	B	856	-	-	4/29/63/63	0/2/2/2
12	LHG	b	852	14	-	5/42/42/53	-
14	CLA	A	838	1	-	5/39/115/115	-
16	SF4	a	847	2,1	-	-	0/6/5/5
14	CLA	A	824	1	-	17/39/115/115	-
12	LHG	G	855	14	-	8/53/53/53	-
12	LHG	B	851	14	-	4/42/42/53	-
14	CLA	b	820	2	-	7/39/115/115	-
14	CLA	H	816	2	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	840	1	-	6/39/115/115	-
14	CLA	S	1101	1	-	5/39/115/115	-
14	CLA	H	819	2	-	13/39/115/115	-

All (1168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	836	CLA	C1D-ND	3.60	1.42	1.37
14	k	101	CLA	C1D-ND	3.49	1.42	1.37
14	A	816	CLA	C1D-ND	3.44	1.42	1.37
14	Q	204	CLA	C1D-ND	3.43	1.42	1.37
14	k	102	CLA	C1D-ND	3.43	1.42	1.37
14	S	1102	CLA	C1D-ND	3.42	1.42	1.37
14	B	823	CLA	C1D-ND	3.42	1.42	1.37
14	K	101	CLA	C1D-ND	3.42	1.42	1.37
14	A	836	CLA	C1D-ND	3.41	1.42	1.37
14	b	838	CLA	C1D-ND	3.39	1.42	1.37
14	J	1103	CLA	C1D-ND	3.38	1.42	1.37
14	K	102	CLA	C1D-ND	3.38	1.42	1.37
14	a	808	CLA	C1D-ND	3.37	1.42	1.37
14	H	809	CLA	C1D-ND	3.36	1.42	1.37
14	S	1103	CLA	C1D-ND	3.36	1.42	1.37
14	B	806	CLA	C1D-ND	3.35	1.42	1.37
14	Q	205	CLA	C1D-ND	3.35	1.42	1.37
14	A	806	CLA	C1D-ND	3.34	1.42	1.37
14	H	842	CLA	C1D-ND	3.34	1.42	1.37
14	A	811	CLA	C1D-ND	3.34	1.42	1.37
14	b	816	CLA	C1D-ND	3.33	1.42	1.37
14	a	823	CLA	C1D-ND	3.33	1.42	1.37
14	A	812	CLA	C1D-ND	3.32	1.42	1.37
14	B	843	CLA	C1D-ND	3.32	1.42	1.37
14	H	822	CLA	C1D-ND	3.32	1.42	1.37
14	B	837	CLA	C1D-ND	3.32	1.42	1.37
14	B	817	CLA	C1D-ND	3.32	1.42	1.37
14	a	815	CLA	C1D-ND	3.30	1.42	1.37
14	b	809	CLA	C1D-ND	3.30	1.42	1.37
14	G	841	CLA	C1D-ND	3.30	1.42	1.37
14	B	836	CLA	C1D-ND	3.30	1.42	1.37
14	b	822	CLA	C1D-ND	3.30	1.42	1.37
14	G	837	CLA	C1D-ND	3.30	1.42	1.37
14	S	1101	CLA	C1D-ND	3.30	1.42	1.37
14	G	836	CLA	C1D-ND	3.30	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	820	CLA	C1D-ND	3.30	1.42	1.37
14	f	205	CLA	C1D-ND	3.30	1.42	1.37
14	b	829	CLA	C1D-ND	3.29	1.42	1.37
14	A	814	CLA	C1D-ND	3.29	1.42	1.37
14	G	817	CLA	C1D-ND	3.28	1.42	1.37
14	H	805	CLA	C1D-ND	3.27	1.42	1.37
14	G	844	CLA	C1D-ND	3.26	1.42	1.37
14	a	811	CLA	C1D-ND	3.26	1.42	1.37
14	G	822	CLA	C1D-ND	3.26	1.42	1.37
14	a	842	CLA	C1D-ND	3.26	1.42	1.37
14	a	826	CLA	C1D-ND	3.25	1.42	1.37
14	G	805	CLA	C1D-ND	3.25	1.42	1.37
14	b	823	CLA	C1D-ND	3.25	1.42	1.37
14	J	1102	CLA	C1D-ND	3.25	1.42	1.37
14	a	812	CLA	C1D-ND	3.25	1.42	1.37
14	b	821	CLA	C1D-ND	3.25	1.42	1.37
14	F	204	CLA	C1D-ND	3.24	1.42	1.37
14	H	808	CLA	C1D-ND	3.24	1.42	1.37
14	G	808	CLA	C1D-ND	3.24	1.42	1.37
14	a	835	CLA	C1D-ND	3.24	1.42	1.37
14	b	813	CLA	C1D-ND	3.24	1.42	1.37
14	G	812	CLA	C1D-ND	3.24	1.42	1.37
14	G	825	CLA	C1D-ND	3.24	1.42	1.37
14	H	828	CLA	C1D-ND	3.24	1.42	1.37
14	A	822	CLA	C1D-ND	3.23	1.42	1.37
14	F	203	CLA	C1D-ND	3.23	1.42	1.37
14	G	807	CLA	C1D-ND	3.23	1.42	1.37
14	b	824	CLA	C1D-ND	3.23	1.42	1.37
14	a	816	CLA	C1D-ND	3.23	1.42	1.37
14	Q	202	CLA	C1D-ND	3.23	1.42	1.37
14	a	841	CLA	C1D-ND	3.23	1.42	1.37
14	a	813	CLA	C1D-ND	3.22	1.42	1.37
14	b	810	CLA	C1D-ND	3.22	1.42	1.37
14	k	103	CLA	C1D-ND	3.22	1.42	1.37
14	B	809	CLA	C1D-ND	3.22	1.42	1.37
14	H	835	CLA	C1D-ND	3.22	1.42	1.37
14	a	821	CLA	C1D-ND	3.22	1.42	1.37
14	b	807	CLA	C1D-ND	3.22	1.42	1.37
14	b	818	CLA	C1D-ND	3.21	1.42	1.37
14	G	814	CLA	C1D-ND	3.21	1.42	1.37
14	G	815	CLA	C1D-ND	3.21	1.42	1.37
14	A	844	CLA	C1D-ND	3.21	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	815	CLA	C1D-ND	3.21	1.42	1.37
14	A	837	CLA	C1D-ND	3.21	1.42	1.37
14	b	840	CLA	C1D-ND	3.21	1.42	1.37
14	A	828	CLA	C1D-ND	3.21	1.42	1.37
14	H	834	CLA	C1D-ND	3.21	1.42	1.37
14	G	809	CLA	C1D-ND	3.21	1.42	1.37
14	J	1101	CLA	C1D-ND	3.21	1.42	1.37
14	a	828	CLA	C1D-ND	3.20	1.42	1.37
14	G	829	CLA	C1D-ND	3.20	1.42	1.37
14	b	811	CLA	C1D-ND	3.20	1.42	1.37
14	B	832	CLA	C1D-ND	3.20	1.42	1.37
14	H	831	CLA	C1D-ND	3.20	1.42	1.37
14	a	845	CLA	C1D-ND	3.20	1.42	1.37
14	H	821	CLA	C1D-ND	3.20	1.42	1.37
14	G	821	CLA	C1D-ND	3.20	1.42	1.37
14	H	838	CLA	C1D-ND	3.20	1.42	1.37
14	A	827	CLA	C1D-ND	3.19	1.42	1.37
14	b	844	CLA	C1D-ND	3.19	1.42	1.37
14	B	828	CLA	C1D-ND	3.19	1.42	1.37
14	B	818	CLA	C1D-ND	3.18	1.42	1.37
14	B	827	CLA	C1D-ND	3.18	1.42	1.37
14	A	825	CLA	C1D-ND	3.18	1.42	1.37
14	G	823	CLA	C1D-ND	3.18	1.42	1.37
14	a	822	CLA	C1D-ND	3.18	1.42	1.37
14	B	825	CLA	C1D-ND	3.18	1.42	1.37
14	B	829	CLA	C1D-ND	3.18	1.42	1.37
14	A	807	CLA	C1D-ND	3.18	1.42	1.37
14	A	805	CLA	C1D-ND	3.18	1.42	1.37
14	b	805	CLA	C1D-ND	3.17	1.42	1.37
14	G	842	CLA	C1D-ND	3.17	1.42	1.37
14	j	102	CLA	C1D-ND	3.17	1.42	1.37
14	A	821	CLA	C1D-ND	3.17	1.42	1.37
14	H	815	CLA	C1D-ND	3.17	1.42	1.37
14	a	817	CLA	C1D-ND	3.17	1.42	1.37
14	H	837	CLA	C1D-ND	3.17	1.42	1.37
14	b	834	CLA	C1D-ND	3.17	1.42	1.37
14	j	101	CLA	C1D-ND	3.17	1.42	1.37
14	G	820	CLA	C1D-ND	3.17	1.42	1.37
14	H	819	CLA	C1D-ND	3.17	1.42	1.37
14	K	103	CLA	C1D-ND	3.16	1.42	1.37
14	a	820	CLA	C1D-ND	3.16	1.42	1.37
14	a	827	CLA	C1D-ND	3.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	840	CLA	C1D-ND	3.16	1.42	1.37
14	B	810	CLA	C1D-ND	3.16	1.42	1.37
14	G	826	CLA	C1D-ND	3.16	1.42	1.37
14	b	837	CLA	C1D-ND	3.16	1.42	1.37
14	B	840	CLA	C1D-ND	3.16	1.42	1.37
14	B	807	CLA	C1D-ND	3.15	1.42	1.37
14	G	827	CLA	C1D-ND	3.15	1.42	1.37
14	a	814	CLA	C1D-ND	3.15	1.42	1.37
14	a	807	CLA	C1D-ND	3.15	1.42	1.37
14	a	824	CLA	C1D-ND	3.15	1.42	1.37
14	H	803	CLA	C1D-ND	3.15	1.42	1.37
14	a	806	CLA	C1D-ND	3.15	1.42	1.37
14	b	836	CLA	C1D-ND	3.15	1.42	1.37
14	U	202	CLA	C1D-ND	3.15	1.42	1.37
14	A	839	CLA	C1D-ND	3.14	1.42	1.37
14	G	804	CLA	C1D-ND	3.14	1.42	1.37
14	G	816	CLA	C1D-ND	3.14	1.42	1.37
14	H	807	CLA	C1D-ND	3.14	1.42	1.37
14	U	204	CLA	C1D-ND	3.14	1.42	1.37
14	b	801	CLA	C1D-ND	3.14	1.42	1.37
14	a	810	CLA	C1D-ND	3.14	1.42	1.37
14	H	811	CLA	C1D-ND	3.14	1.42	1.37
14	G	811	CLA	C1D-ND	3.14	1.42	1.37
14	H	818	CLA	C1D-ND	3.14	1.42	1.37
14	b	814	CLA	C1D-ND	3.14	1.42	1.37
14	H	832	CLA	C1D-ND	3.13	1.42	1.37
14	B	812	CLA	C1D-ND	3.13	1.42	1.37
14	A	803	CLA	C1D-ND	3.13	1.42	1.37
14	a	809	CLA	C1D-ND	3.13	1.42	1.37
14	b	830	CLA	C1D-ND	3.13	1.42	1.37
14	B	821	CLA	C1D-ND	3.13	1.42	1.37
14	B	841	CLA	C1D-ND	3.13	1.42	1.37
14	H	804	CLA	C1D-ND	3.13	1.42	1.37
14	a	805	CLA	C1D-ND	3.13	1.42	1.37
14	A	842	CLA	C1D-ND	3.13	1.42	1.37
14	b	820	CLA	C1D-ND	3.13	1.42	1.37
14	T	102	CLA	C1D-ND	3.13	1.42	1.37
14	a	829	CLA	C1D-ND	3.13	1.42	1.37
14	A	815	CLA	C1D-ND	3.12	1.42	1.37
14	A	838	CLA	C1D-ND	3.12	1.42	1.37
14	B	839	CLA	C1D-ND	3.12	1.42	1.37
14	G	828	CLA	C1D-ND	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	816	CLA	C1D-ND	3.11	1.42	1.37
14	l	5004	CLA	C1D-ND	3.11	1.42	1.37
14	f	204	CLA	C1D-ND	3.11	1.41	1.37
14	B	824	CLA	C1D-ND	3.11	1.41	1.37
14	a	830	CLA	C1D-ND	3.11	1.41	1.37
14	A	858	CLA	C1D-ND	3.11	1.41	1.37
14	f	201	CLA	C1D-ND	3.11	1.41	1.37
14	B	814	CLA	C1D-ND	3.11	1.41	1.37
14	a	803	CLA	C1D-ND	3.11	1.41	1.37
14	B	833	CLA	C1D-ND	3.11	1.41	1.37
14	G	802	CLA	C1D-ND	3.11	1.41	1.37
14	H	813	CLA	C1D-ND	3.11	1.41	1.37
14	b	825	CLA	C1D-ND	3.11	1.41	1.37
14	G	840	CLA	C1D-ND	3.10	1.41	1.37
13	a	802	CL0	C1D-ND	3.10	1.41	1.37
14	A	804	CLA	C1D-ND	3.10	1.41	1.37
14	B	820	CLA	C1D-ND	3.10	1.41	1.37
14	A	824	CLA	C1D-ND	3.10	1.41	1.37
14	T	101	CLA	C1D-ND	3.10	1.41	1.37
14	H	816	CLA	C1D-ND	3.10	1.41	1.37
14	T	103	CLA	C1D-ND	3.10	1.41	1.37
14	L	1503	CLA	C1D-ND	3.09	1.41	1.37
14	H	810	CLA	C1D-ND	3.09	1.41	1.37
14	b	842	CLA	C1D-ND	3.09	1.41	1.37
14	b	819	CLA	C1D-ND	3.09	1.41	1.37
14	b	806	CLA	C1D-ND	3.09	1.41	1.37
14	F	201	CLA	C1D-ND	3.09	1.41	1.37
14	G	838	CLA	C1D-ND	3.09	1.41	1.37
14	a	844	CLA	C1D-ND	3.09	1.41	1.37
14	H	824	CLA	C1D-ND	3.09	1.41	1.37
14	G	813	CLA	C1D-ND	3.09	1.41	1.37
14	H	820	CLA	C1D-ND	3.08	1.41	1.37
14	b	815	CLA	C1D-ND	3.08	1.41	1.37
14	B	813	CLA	C1D-ND	3.08	1.41	1.37
14	B	822	CLA	C1D-ND	3.08	1.41	1.37
14	a	831	CLA	C1D-ND	3.08	1.41	1.37
14	A	835	CLA	C1D-ND	3.07	1.41	1.37
14	H	823	CLA	C1D-ND	3.07	1.41	1.37
14	a	825	CLA	C1D-ND	3.07	1.41	1.37
14	B	801	CLA	C1D-ND	3.07	1.41	1.37
14	B	831	CLA	C1D-ND	3.07	1.41	1.37
14	B	835	CLA	C1D-ND	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	806	CLA	C1D-ND	3.07	1.41	1.37
14	G	831	CLA	C1D-ND	3.07	1.41	1.37
14	a	818	CLA	C1D-ND	3.07	1.41	1.37
14	A	841	CLA	C1D-ND	3.07	1.41	1.37
14	b	808	CLA	C1D-ND	3.07	1.41	1.37
14	G	810	CLA	C1D-ND	3.06	1.41	1.37
14	H	826	CLA	C1D-ND	3.06	1.41	1.37
14	G	824	CLA	C1D-ND	3.06	1.41	1.37
14	G	819	CLA	C1D-ND	3.06	1.41	1.37
14	H	812	CLA	C1D-ND	3.06	1.41	1.37
14	H	817	CLA	C1D-ND	3.06	1.41	1.37
14	H	840	CLA	C1D-ND	3.06	1.41	1.37
14	B	819	CLA	C1D-ND	3.06	1.41	1.37
14	G	843	CLA	C1D-ND	3.06	1.41	1.37
14	H	830	CLA	C1D-ND	3.06	1.41	1.37
14	b	839	CLA	C1D-ND	3.06	1.41	1.37
14	U	206	CLA	C1D-ND	3.06	1.41	1.37
14	b	832	CLA	C1D-ND	3.06	1.41	1.37
14	H	839	CLA	C1D-ND	3.06	1.41	1.37
14	A	809	CLA	C1D-ND	3.05	1.41	1.37
14	a	838	CLA	C1D-ND	3.05	1.41	1.37
14	A	830	CLA	C1D-ND	3.05	1.41	1.37
14	a	804	CLA	C1D-ND	3.05	1.41	1.37
14	A	808	CLA	C1D-ND	3.05	1.41	1.37
14	a	837	CLA	C1D-ND	3.05	1.41	1.37
14	B	808	CLA	C1D-ND	3.05	1.41	1.37
14	H	833	CLA	C1D-ND	3.05	1.41	1.37
14	a	834	CLA	C1D-ND	3.05	1.41	1.37
14	A	834	CLA	C1D-ND	3.04	1.41	1.37
14	B	842	CLA	C1D-ND	3.04	1.41	1.37
14	L	1501	CLA	C1D-ND	3.04	1.41	1.37
14	b	828	CLA	C1D-ND	3.04	1.41	1.37
14	B	811	CLA	C1D-ND	3.04	1.41	1.37
14	G	833	CLA	C1D-ND	3.04	1.41	1.37
14	a	833	CLA	C1D-ND	3.04	1.41	1.37
14	A	813	CLA	C1D-ND	3.04	1.41	1.37
13	A	802	CL0	C1D-ND	3.04	1.41	1.37
14	A	810	CLA	C1D-ND	3.03	1.41	1.37
14	A	843	CLA	C1D-ND	3.03	1.41	1.37
14	G	835	CLA	C1D-ND	3.03	1.41	1.37
14	b	843	CLA	C1D-ND	3.03	1.41	1.37
14	A	823	CLA	C1D-ND	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	829	CLA	C1D-ND	3.03	1.41	1.37
14	A	818	CLA	C1D-ND	3.03	1.41	1.37
14	b	841	CLA	C1D-ND	3.03	1.41	1.37
14	b	812	CLA	C1D-ND	3.03	1.41	1.37
14	G	839	CLA	C1D-ND	3.03	1.41	1.37
14	B	830	CLA	C1D-ND	3.03	1.41	1.37
14	H	827	CLA	C1D-ND	3.03	1.41	1.37
14	B	805	CLA	C1D-ND	3.02	1.41	1.37
14	a	843	CLA	C1D-ND	3.02	1.41	1.37
14	A	826	CLA	C1D-ND	3.02	1.41	1.37
14	b	833	CLA	C1D-ND	3.02	1.41	1.37
14	G	830	CLA	C1D-ND	3.02	1.41	1.37
14	b	826	CLA	C1D-ND	3.02	1.41	1.37
14	a	840	CLA	C1D-ND	3.01	1.41	1.37
14	B	834	CLA	C1D-ND	3.01	1.41	1.37
14	A	819	CLA	C1D-ND	3.01	1.41	1.37
14	B	826	CLA	C1D-ND	3.01	1.41	1.37
14	H	841	CLA	C1D-ND	3.01	1.41	1.37
14	H	814	CLA	C1D-ND	3.01	1.41	1.37
14	a	819	CLA	C1D-ND	3.00	1.41	1.37
14	b	817	CLA	C1D-ND	3.00	1.41	1.37
14	l	5005	CLA	C1D-ND	3.00	1.41	1.37
14	G	834	CLA	C1D-ND	3.00	1.41	1.37
14	A	817	CLA	C1D-ND	3.00	1.41	1.37
14	A	833	CLA	C1D-ND	2.99	1.41	1.37
13	G	801	CL0	C1D-ND	2.98	1.41	1.37
14	L	1502	CLA	C1D-ND	2.98	1.41	1.37
14	H	829	CLA	C1D-ND	2.97	1.41	1.37
14	b	827	CLA	C1D-ND	2.96	1.41	1.37
14	H	825	CLA	C1D-ND	2.96	1.41	1.37
14	A	832	CLA	C1D-ND	2.95	1.41	1.37
14	U	205	CLA	C1D-ND	2.95	1.41	1.37
14	a	839	CLA	C1D-ND	2.94	1.41	1.37
14	b	831	CLA	C1D-ND	2.94	1.41	1.37
14	b	835	CLA	C1D-ND	2.93	1.41	1.37
14	B	838	CLA	C1D-ND	2.93	1.41	1.37
14	H	806	CLA	C1D-ND	2.93	1.41	1.37
14	a	832	CLA	C1D-ND	2.93	1.41	1.37
14	G	832	CLA	C1D-ND	2.93	1.41	1.37
14	a	836	CLA	C1D-ND	2.91	1.41	1.37
14	G	818	CLA	C1D-ND	2.91	1.41	1.37
14	A	831	CLA	C1D-ND	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	802	CLA	C1D-ND	2.85	1.41	1.37
14	G	803	CLA	C1D-ND	2.84	1.41	1.37
14	l	5006	CLA	C1D-ND	2.82	1.41	1.37
14	b	802	CLA	C1D-ND	2.78	1.41	1.37
14	a	817	CLA	C1B-C2B	2.67	1.49	1.43
13	G	801	CL0	C1B-C2B	2.65	1.49	1.43
14	k	102	CLA	C1B-C2B	2.63	1.49	1.43
14	K	102	CLA	C1B-C2B	2.62	1.49	1.43
14	G	817	CLA	C1B-C2B	2.61	1.49	1.43
14	A	816	CLA	C1B-C2B	2.60	1.49	1.43
14	H	835	CLA	C1B-C2B	2.60	1.49	1.43
13	a	802	CL0	C1B-C2B	2.59	1.49	1.43
14	A	838	CLA	C1B-C2B	2.59	1.49	1.43
14	k	103	CLA	C1B-C2B	2.59	1.49	1.43
13	A	802	CL0	C1B-C2B	2.59	1.49	1.43
14	T	101	CLA	C1B-C2B	2.58	1.49	1.43
14	H	834	CLA	C1B-C2B	2.57	1.49	1.43
14	b	844	CLA	C1B-C2B	2.57	1.49	1.43
14	B	824	CLA	C1B-C2B	2.56	1.49	1.43
14	B	823	CLA	C1B-C2B	2.55	1.49	1.43
14	b	825	CLA	C1B-C2B	2.55	1.49	1.43
14	J	1103	CLA	C1B-C2B	2.55	1.49	1.43
14	J	1101	CLA	C1B-C2B	2.54	1.49	1.43
14	T	102	CLA	C1B-C2B	2.53	1.49	1.43
14	H	822	CLA	C1B-C2B	2.53	1.49	1.43
14	A	817	CLA	C1B-C2B	2.53	1.49	1.43
14	k	101	CLA	C1B-C2B	2.53	1.49	1.43
14	H	842	CLA	C1B-C2B	2.52	1.49	1.43
14	G	824	CLA	C1B-C2B	2.52	1.49	1.43
14	S	1101	CLA	C1B-C2B	2.52	1.49	1.43
14	K	101	CLA	C1B-C2B	2.52	1.49	1.43
14	H	836	CLA	C1B-C2B	2.51	1.49	1.43
14	a	839	CLA	C1B-C2B	2.51	1.49	1.43
14	H	823	CLA	C1B-C2B	2.50	1.49	1.43
14	G	818	CLA	C1B-C2B	2.50	1.49	1.43
14	b	824	CLA	C1B-C2B	2.50	1.49	1.43
14	j	102	CLA	C1B-C2B	2.50	1.49	1.43
14	K	103	CLA	C1B-C2B	2.50	1.49	1.43
14	B	801	CLA	C1B-C2B	2.50	1.49	1.43
14	B	843	CLA	C1B-C2B	2.50	1.49	1.43
14	J	1102	CLA	C1B-C2B	2.50	1.49	1.43
14	A	815	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	C1B-C2B	2.50	1.49	1.43
14	S	1103	CLA	C1B-C2B	2.49	1.49	1.43
14	B	817	CLA	C1B-C2B	2.49	1.49	1.43
14	b	815	CLA	C1B-C2B	2.49	1.49	1.43
14	F	203	CLA	C1B-C2B	2.49	1.49	1.43
14	A	823	CLA	C1B-C2B	2.49	1.49	1.43
14	a	804	CLA	C1B-C2B	2.48	1.49	1.43
14	a	813	CLA	C3B-C4B	2.48	1.50	1.42
14	A	804	CLA	C1B-C2B	2.48	1.49	1.43
14	H	828	CLA	C1B-C2B	2.48	1.49	1.43
14	b	805	CLA	C1B-C2B	2.48	1.48	1.43
14	G	821	CLA	C1B-C2B	2.48	1.48	1.43
14	a	824	CLA	C1B-C2B	2.48	1.48	1.43
14	B	819	CLA	C1B-C2B	2.48	1.48	1.43
14	B	839	CLA	C1B-C2B	2.48	1.48	1.43
14	a	812	CLA	C1B-C2B	2.48	1.48	1.43
14	H	816	CLA	C1B-C2B	2.48	1.48	1.43
14	G	816	CLA	C1B-C2B	2.47	1.48	1.43
14	a	815	CLA	C1B-C2B	2.47	1.48	1.43
14	B	822	CLA	C1B-C2B	2.47	1.48	1.43
14	T	103	CLA	C1B-C2B	2.47	1.48	1.43
14	H	824	CLA	C1B-C2B	2.47	1.48	1.43
14	H	832	CLA	C1B-C2B	2.47	1.48	1.43
14	G	838	CLA	C1B-C2B	2.47	1.48	1.43
14	a	806	CLA	C1B-C2B	2.47	1.48	1.43
14	a	829	CLA	C1B-C2B	2.47	1.48	1.43
14	A	832	CLA	C1B-C2B	2.47	1.48	1.43
14	B	810	CLA	C1B-C2B	2.46	1.48	1.43
14	A	824	CLA	C1B-C2B	2.46	1.48	1.43
14	B	834	CLA	C1B-C2B	2.46	1.48	1.43
14	A	820	CLA	C1B-C2B	2.46	1.48	1.43
14	G	825	CLA	C1B-C2B	2.46	1.48	1.43
14	S	1103	CLA	C3B-C4B	2.46	1.49	1.42
14	a	838	CLA	C1B-C2B	2.46	1.48	1.43
14	Q	204	CLA	C1B-C2B	2.46	1.48	1.43
14	a	808	CLA	C1B-C2B	2.46	1.48	1.43
14	b	835	CLA	C1B-C2B	2.46	1.48	1.43
14	l	5004	CLA	C1B-C2B	2.46	1.48	1.43
14	A	810	CLA	C1B-C2B	2.46	1.48	1.43
14	j	101	CLA	C1B-C2B	2.46	1.48	1.43
14	H	827	CLA	C1B-C2B	2.46	1.48	1.43
14	a	814	CLA	C1B-C2B	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	832	CLA	C1B-C2B	2.45	1.48	1.43
14	a	821	CLA	C1B-C2B	2.45	1.48	1.43
14	a	845	CLA	C1B-C2B	2.45	1.48	1.43
14	a	811	CLA	C1B-C2B	2.45	1.48	1.43
14	A	812	CLA	C3B-C4B	2.45	1.49	1.42
14	G	815	CLA	C1B-C2B	2.45	1.48	1.43
14	A	808	CLA	C1B-C2B	2.45	1.48	1.43
14	G	813	CLA	C3B-C4B	2.45	1.49	1.42
14	A	811	CLA	C1B-C2B	2.45	1.48	1.43
14	G	829	CLA	C1B-C2B	2.45	1.48	1.43
14	b	809	CLA	C1B-C2B	2.45	1.48	1.43
14	H	811	CLA	C1B-C2B	2.45	1.48	1.43
14	A	807	CLA	C1B-C2B	2.45	1.48	1.43
14	H	817	CLA	C1B-C2B	2.44	1.48	1.43
14	H	833	CLA	C1B-C2B	2.44	1.48	1.43
14	B	812	CLA	C1B-C2B	2.44	1.48	1.43
14	A	830	CLA	C1B-C2B	2.44	1.48	1.43
14	B	837	CLA	C1B-C2B	2.44	1.48	1.43
14	H	838	CLA	C1B-C2B	2.44	1.48	1.43
14	F	201	CLA	C1B-C2B	2.44	1.48	1.43
14	G	802	CLA	C1B-C2B	2.44	1.48	1.43
14	H	826	CLA	C1B-C2B	2.44	1.48	1.43
14	b	818	CLA	C1B-C2B	2.44	1.48	1.43
14	Q	202	CLA	C1B-C2B	2.44	1.48	1.43
14	b	834	CLA	C1B-C2B	2.44	1.48	1.43
14	G	831	CLA	C1B-C2B	2.44	1.48	1.43
14	B	805	CLA	C1B-C2B	2.43	1.48	1.43
14	b	813	CLA	C1B-C2B	2.43	1.48	1.43
14	B	828	CLA	C1B-C2B	2.43	1.48	1.43
14	a	841	CLA	C1B-C2B	2.43	1.48	1.43
14	b	810	CLA	C1B-C2B	2.43	1.48	1.43
14	H	803	CLA	C1B-C2B	2.43	1.48	1.43
14	L	1502	CLA	C1B-C2B	2.43	1.48	1.43
14	G	826	CLA	C1B-C2B	2.43	1.48	1.43
14	G	814	CLA	C1B-C2B	2.43	1.48	1.43
14	G	812	CLA	C1B-C2B	2.43	1.48	1.43
14	b	833	CLA	C1B-C2B	2.43	1.48	1.43
14	b	837	CLA	C1B-C2B	2.43	1.48	1.43
14	G	805	CLA	C1B-C2B	2.43	1.48	1.43
14	H	815	CLA	C1B-C2B	2.43	1.48	1.43
14	S	1102	CLA	C1B-C2B	2.43	1.48	1.43
14	B	816	CLA	C1B-C2B	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	843	CLA	C1B-C2B	2.43	1.48	1.43
14	B	808	CLA	C1B-C2B	2.42	1.48	1.43
14	B	806	CLA	C1B-C2B	2.42	1.48	1.43
14	U	205	CLA	C1B-C2B	2.42	1.48	1.43
14	a	831	CLA	C1B-C2B	2.42	1.48	1.43
14	f	201	CLA	C1B-C2B	2.42	1.48	1.43
14	H	807	CLA	C1B-C2B	2.42	1.48	1.43
14	j	102	CLA	C3B-C4B	2.42	1.49	1.42
14	b	829	CLA	C1B-C2B	2.42	1.48	1.43
14	B	815	CLA	C1B-C2B	2.42	1.48	1.43
14	H	804	CLA	C1B-C2B	2.42	1.48	1.43
14	A	844	CLA	C1B-C2B	2.42	1.48	1.43
14	f	205	CLA	C3B-C4B	2.42	1.49	1.42
14	G	820	CLA	C3B-C4B	2.42	1.49	1.42
14	b	828	CLA	C1B-C2B	2.42	1.48	1.43
14	H	831	CLA	C1B-C2B	2.42	1.48	1.43
14	A	827	CLA	C1B-C2B	2.42	1.48	1.43
14	H	806	CLA	C1B-C2B	2.41	1.48	1.43
14	A	822	CLA	C1B-C2B	2.41	1.48	1.43
14	H	813	CLA	C1B-C2B	2.41	1.48	1.43
14	B	825	CLA	C1B-C2B	2.41	1.48	1.43
14	H	821	CLA	C1B-C2B	2.41	1.48	1.43
14	Q	205	CLA	C1B-C2B	2.41	1.48	1.43
14	A	826	CLA	C1B-C2B	2.41	1.48	1.43
14	b	806	CLA	C1B-C2B	2.41	1.48	1.43
14	a	826	CLA	C1B-C2B	2.41	1.48	1.43
14	b	819	CLA	C1B-C2B	2.41	1.48	1.43
14	b	820	CLA	C1B-C2B	2.41	1.48	1.43
14	B	814	CLA	C1B-C2B	2.41	1.48	1.43
14	B	835	CLA	C1B-C2B	2.41	1.48	1.43
14	a	809	CLA	C1B-C2B	2.41	1.48	1.43
14	A	839	CLA	C3B-C4B	2.41	1.49	1.42
14	G	835	CLA	C3B-C4B	2.41	1.49	1.42
14	B	833	CLA	C1B-C2B	2.41	1.48	1.43
14	B	841	CLA	C1B-C2B	2.41	1.48	1.43
14	B	842	CLA	C1B-C2B	2.41	1.48	1.43
14	G	808	CLA	C1B-C2B	2.41	1.48	1.43
14	H	809	CLA	C1B-C2B	2.41	1.48	1.43
14	Q	205	CLA	C3B-C4B	2.41	1.49	1.42
14	b	814	CLA	C1B-C2B	2.41	1.48	1.43
14	a	803	CLA	C1B-C2B	2.41	1.48	1.43
14	b	831	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	835	CLA	C3B-C4B	2.41	1.49	1.42
14	a	805	CLA	C1B-C2B	2.40	1.48	1.43
14	a	828	CLA	C1B-C2B	2.40	1.48	1.43
14	b	836	CLA	C1B-C2B	2.40	1.48	1.43
14	H	841	CLA	C1B-C2B	2.40	1.48	1.43
14	G	842	CLA	C3B-C4B	2.40	1.49	1.42
14	A	842	CLA	C3B-C4B	2.40	1.49	1.42
14	S	1102	CLA	C3B-C4B	2.40	1.49	1.42
14	f	205	CLA	C1B-C2B	2.40	1.48	1.43
14	J	1103	CLA	C3B-C4B	2.40	1.49	1.42
14	A	825	CLA	C1B-C2B	2.40	1.48	1.43
14	a	820	CLA	C3B-C4B	2.40	1.49	1.42
14	A	841	CLA	C3B-C4B	2.40	1.49	1.42
14	A	813	CLA	C1B-C2B	2.40	1.48	1.43
14	G	823	CLA	C1B-C2B	2.40	1.48	1.43
14	b	826	CLA	C1B-C2B	2.39	1.48	1.43
14	B	837	CLA	C3B-C4B	2.39	1.49	1.42
14	b	823	CLA	C3B-C4B	2.39	1.49	1.42
14	B	818	CLA	C1B-C2B	2.39	1.48	1.43
14	U	206	CLA	C1B-C2B	2.39	1.48	1.43
14	G	809	CLA	C1B-C2B	2.39	1.48	1.43
14	G	830	CLA	C1B-C2B	2.39	1.48	1.43
14	B	807	CLA	C1B-C2B	2.39	1.48	1.43
14	B	809	CLA	C1B-C2B	2.39	1.48	1.43
14	b	817	CLA	C1B-C2B	2.39	1.48	1.43
14	b	838	CLA	C3B-C4B	2.39	1.49	1.42
14	A	814	CLA	C1B-C2B	2.39	1.48	1.43
14	b	816	CLA	C1B-C2B	2.39	1.48	1.43
14	B	821	CLA	C1B-C2B	2.39	1.48	1.43
14	a	816	CLA	C1B-C2B	2.39	1.48	1.43
14	G	827	CLA	C1B-C2B	2.39	1.48	1.43
14	G	844	CLA	C1B-C2B	2.39	1.48	1.43
14	b	801	CLA	C1B-C2B	2.39	1.48	1.43
14	b	839	CLA	C1B-C2B	2.39	1.48	1.43
14	b	823	CLA	C1B-C2B	2.38	1.48	1.43
14	A	858	CLA	C1B-C2B	2.38	1.48	1.43
14	a	837	CLA	C3B-C4B	2.38	1.49	1.42
14	A	833	CLA	C1B-C2B	2.38	1.48	1.43
14	B	829	CLA	C1B-C2B	2.38	1.48	1.43
14	F	204	CLA	C3B-C4B	2.38	1.49	1.42
14	b	811	CLA	C1B-C2B	2.38	1.48	1.43
14	A	836	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	839	CLA	C3B-C4B	2.38	1.49	1.42
14	G	833	CLA	C1B-C2B	2.38	1.48	1.43
14	a	830	CLA	C1B-C2B	2.38	1.48	1.43
14	G	836	CLA	C3B-C4B	2.38	1.49	1.42
14	A	804	CLA	C3B-C4B	2.38	1.49	1.42
14	A	812	CLA	C1B-C2B	2.38	1.48	1.43
14	l	5006	CLA	C1B-C2B	2.38	1.48	1.43
14	G	805	CLA	C3B-C4B	2.38	1.49	1.42
14	G	828	CLA	C1B-C2B	2.38	1.48	1.43
14	H	836	CLA	C3B-C4B	2.38	1.49	1.42
14	b	807	CLA	C1B-C2B	2.37	1.48	1.43
14	H	839	CLA	C1B-C2B	2.37	1.48	1.43
14	j	101	CLA	C3B-C4B	2.37	1.49	1.42
14	a	843	CLA	C3B-C4B	2.37	1.49	1.42
14	B	838	CLA	C1B-C2B	2.37	1.48	1.43
14	B	827	CLA	C1B-C2B	2.37	1.48	1.43
14	a	833	CLA	C1B-C2B	2.37	1.48	1.43
14	B	842	CLA	C3B-C4B	2.37	1.49	1.42
14	a	823	CLA	C1B-C2B	2.37	1.48	1.43
14	b	840	CLA	C1B-C2B	2.37	1.48	1.43
14	H	812	CLA	C1B-C2B	2.37	1.48	1.43
14	U	202	CLA	C1B-C2B	2.37	1.48	1.43
14	G	834	CLA	C1B-C2B	2.37	1.48	1.43
14	A	829	CLA	C1B-C2B	2.37	1.48	1.43
14	A	809	CLA	C3B-C4B	2.37	1.49	1.42
14	f	204	CLA	C1B-C2B	2.36	1.48	1.43
14	A	828	CLA	C1B-C2B	2.36	1.48	1.43
14	B	830	CLA	C1B-C2B	2.36	1.48	1.43
14	b	842	CLA	C1B-C2B	2.36	1.48	1.43
14	L	1501	CLA	C1B-C2B	2.36	1.48	1.43
14	a	834	CLA	C1B-C2B	2.36	1.48	1.43
14	G	839	CLA	C1B-C2B	2.36	1.48	1.43
14	a	840	CLA	C3B-C4B	2.36	1.49	1.42
14	b	839	CLA	C3B-C4B	2.36	1.49	1.42
14	B	831	CLA	C1B-C2B	2.36	1.48	1.43
14	A	803	CLA	C1B-C2B	2.36	1.48	1.43
14	G	837	CLA	C1B-C2B	2.36	1.48	1.43
14	H	814	CLA	C1B-C2B	2.36	1.48	1.43
14	G	840	CLA	C1B-C2B	2.36	1.48	1.43
14	L	1503	CLA	C1B-C2B	2.36	1.48	1.43
14	k	102	CLA	C3B-C4B	2.36	1.49	1.42
14	a	805	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	813	CLA	C1B-C2B	2.36	1.48	1.43
14	b	808	CLA	C1B-C2B	2.36	1.48	1.43
14	a	829	CLA	C3B-C4B	2.36	1.49	1.42
14	U	204	CLA	C1B-C2B	2.36	1.48	1.43
14	A	819	CLA	C3B-C4B	2.36	1.49	1.42
14	A	840	CLA	C1B-C2B	2.35	1.48	1.43
14	H	829	CLA	C1B-C2B	2.35	1.48	1.43
14	G	807	CLA	C1B-C2B	2.35	1.48	1.43
14	A	821	CLA	C1B-C2B	2.35	1.48	1.43
14	a	842	CLA	C1B-C2B	2.35	1.48	1.43
14	b	822	CLA	C3B-C4B	2.35	1.49	1.42
14	K	101	CLA	C3B-C4B	2.35	1.49	1.42
14	H	818	CLA	C1B-C2B	2.35	1.48	1.43
14	b	842	CLA	C3B-C4B	2.35	1.49	1.42
14	G	811	CLA	C1B-C2B	2.35	1.48	1.43
14	H	837	CLA	C3B-C4B	2.35	1.49	1.42
14	b	802	CLA	C3B-C4B	2.35	1.49	1.42
14	G	813	CLA	C1B-C2B	2.35	1.48	1.43
14	H	820	CLA	C3B-C4B	2.34	1.49	1.42
14	a	827	CLA	C1B-C2B	2.34	1.48	1.43
14	b	841	CLA	C3B-C4B	2.34	1.49	1.42
14	a	842	CLA	C3B-C4B	2.34	1.49	1.42
14	G	819	CLA	C1B-C2B	2.34	1.48	1.43
14	a	818	CLA	C1B-C2B	2.34	1.48	1.43
14	H	808	CLA	C1B-C2B	2.34	1.48	1.43
14	G	841	CLA	C1B-C2B	2.34	1.48	1.43
14	H	819	CLA	C1B-C2B	2.34	1.48	1.43
14	G	829	CLA	C3B-C4B	2.34	1.49	1.42
14	G	840	CLA	C3B-C4B	2.34	1.49	1.42
14	B	813	CLA	C3B-C4B	2.34	1.49	1.42
14	J	1102	CLA	C3B-C4B	2.34	1.49	1.42
14	A	842	CLA	C1B-C2B	2.33	1.48	1.43
14	B	806	CLA	C3B-C4B	2.33	1.49	1.42
14	B	838	CLA	C3B-C4B	2.33	1.49	1.42
14	G	841	CLA	C3B-C4B	2.33	1.49	1.42
14	a	819	CLA	C1B-C2B	2.33	1.48	1.43
14	A	837	CLA	C1B-C2B	2.33	1.48	1.43
14	b	814	CLA	C3B-C4B	2.33	1.49	1.42
14	T	101	CLA	C3B-C4B	2.33	1.49	1.42
14	l	5005	CLA	C1B-C2B	2.33	1.48	1.43
14	A	843	CLA	C1B-C2B	2.33	1.48	1.43
14	A	806	CLA	C1B-C2B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	828	CLA	C3B-C4B	2.33	1.49	1.42
14	B	802	CLA	C1B-C2B	2.33	1.48	1.43
14	A	827	CLA	C3B-C4B	2.32	1.49	1.42
14	B	821	CLA	C3B-C4B	2.32	1.49	1.42
14	A	841	CLA	C1B-C2B	2.32	1.48	1.43
14	B	802	CLA	C3B-C4B	2.32	1.49	1.42
14	F	204	CLA	C1B-C2B	2.32	1.48	1.43
14	A	834	CLA	C3B-C4B	2.32	1.49	1.42
14	B	841	CLA	C3B-C4B	2.32	1.49	1.42
14	a	835	CLA	C1B-C2B	2.32	1.48	1.43
14	a	814	CLA	C3B-C4B	2.32	1.49	1.42
14	b	807	CLA	C3B-C4B	2.32	1.49	1.42
14	H	840	CLA	C3B-C4B	2.32	1.49	1.42
14	b	830	CLA	C1B-C2B	2.32	1.48	1.43
14	G	842	CLA	C1B-C2B	2.32	1.48	1.43
14	b	838	CLA	C1B-C2B	2.32	1.48	1.43
14	b	832	CLA	C1B-C2B	2.31	1.48	1.43
14	A	805	CLA	C3B-C4B	2.31	1.49	1.42
14	G	806	CLA	C1B-C2B	2.31	1.48	1.43
14	B	840	CLA	C1B-C2B	2.31	1.48	1.43
14	a	807	CLA	C1B-C2B	2.31	1.48	1.43
14	b	808	CLA	C3B-C4B	2.31	1.49	1.42
14	a	825	CLA	C1B-C2B	2.31	1.48	1.43
14	A	835	CLA	C1B-C2B	2.31	1.48	1.43
14	H	825	CLA	C3B-C4B	2.31	1.49	1.42
14	H	840	CLA	C1B-C2B	2.31	1.48	1.43
14	K	102	CLA	C3B-C4B	2.31	1.49	1.42
14	G	804	CLA	C1B-C2B	2.31	1.48	1.43
14	H	827	CLA	C3B-C4B	2.31	1.49	1.42
14	b	841	CLA	C1B-C2B	2.30	1.48	1.43
14	A	837	CLA	C3B-C4B	2.30	1.49	1.42
14	a	820	CLA	C1B-C2B	2.30	1.48	1.43
14	B	831	CLA	C3B-C4B	2.30	1.49	1.42
14	G	811	CLA	C3B-C4B	2.30	1.49	1.42
14	T	102	CLA	C3B-C4B	2.30	1.49	1.42
14	A	834	CLA	C1B-C2B	2.30	1.48	1.43
14	G	832	CLA	C1B-C2B	2.30	1.48	1.43
14	A	843	CLA	C3B-C4B	2.30	1.49	1.42
14	G	810	CLA	C3B-C4B	2.30	1.49	1.42
14	b	843	CLA	C3B-C4B	2.30	1.49	1.42
14	H	830	CLA	C1B-C2B	2.30	1.48	1.43
14	a	841	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	5006	CLA	C3B-C4B	2.30	1.49	1.42
14	B	822	CLA	C3B-C4B	2.30	1.49	1.42
14	H	841	CLA	C3B-C4B	2.30	1.49	1.42
14	B	840	CLA	C3B-C4B	2.30	1.49	1.42
14	G	836	CLA	C1B-C2B	2.30	1.48	1.43
14	H	809	CLA	C3B-C4B	2.30	1.49	1.42
14	a	818	CLA	C3B-C4B	2.30	1.49	1.42
14	a	810	CLA	C1B-C2B	2.30	1.48	1.43
14	G	816	CLA	C3B-C4B	2.30	1.49	1.42
14	a	811	CLA	C3B-C4B	2.30	1.49	1.42
14	a	822	CLA	C3B-C4B	2.29	1.49	1.42
14	b	816	CLA	C3B-C4B	2.29	1.49	1.42
14	a	844	CLA	C1B-C2B	2.29	1.48	1.43
14	H	810	CLA	C3B-C4B	2.29	1.49	1.42
14	a	815	CLA	C3B-C4B	2.29	1.49	1.42
14	a	836	CLA	C1B-C2B	2.29	1.48	1.43
14	L	1503	CLA	C3B-C4B	2.29	1.49	1.42
14	a	813	CLA	C1B-C2B	2.29	1.48	1.43
14	F	201	CLA	C3B-C4B	2.29	1.49	1.42
14	a	822	CLA	C1B-C2B	2.29	1.48	1.43
14	B	816	CLA	C3B-C4B	2.29	1.49	1.42
14	B	826	CLA	C3B-C4B	2.29	1.49	1.42
14	b	826	CLA	C3B-C4B	2.29	1.49	1.42
14	H	837	CLA	C1B-C2B	2.29	1.48	1.43
14	G	822	CLA	C1B-C2B	2.29	1.48	1.43
14	b	821	CLA	C1B-C2B	2.29	1.48	1.43
14	b	827	CLA	C3B-C4B	2.29	1.49	1.42
14	T	103	CLA	C3B-C4B	2.29	1.49	1.42
14	G	828	CLA	C3B-C4B	2.29	1.49	1.42
14	H	805	CLA	C1B-C2B	2.29	1.48	1.43
14	A	805	CLA	C1B-C2B	2.29	1.48	1.43
14	H	820	CLA	C1B-C2B	2.29	1.48	1.43
14	B	827	CLA	C3B-C4B	2.29	1.49	1.42
14	A	831	CLA	C1B-C2B	2.29	1.48	1.43
14	H	839	CLA	C3B-C4B	2.28	1.49	1.42
14	G	822	CLA	C3B-C4B	2.28	1.49	1.42
14	A	814	CLA	C3B-C4B	2.28	1.49	1.42
14	l	5005	CLA	C3B-C4B	2.28	1.49	1.42
14	G	843	CLA	C1B-C2B	2.28	1.48	1.43
14	A	809	CLA	C1B-C2B	2.28	1.48	1.43
14	G	803	CLA	C3B-C4B	2.28	1.49	1.42
14	a	807	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	101	CLA	C3B-C4B	2.28	1.49	1.42
14	b	812	CLA	C1B-C2B	2.28	1.48	1.43
14	H	825	CLA	C1B-C2B	2.28	1.48	1.43
14	H	830	CLA	C3B-C4B	2.28	1.49	1.42
14	A	840	CLA	C3B-C4B	2.28	1.49	1.42
14	G	808	CLA	C3B-C4B	2.28	1.49	1.42
14	b	811	CLA	C3B-C4B	2.28	1.49	1.42
14	a	810	CLA	C3B-C4B	2.28	1.49	1.42
14	f	201	CLA	C3B-C4B	2.28	1.49	1.42
14	A	803	CLA	C3B-C4B	2.28	1.49	1.42
14	B	818	CLA	C3B-C4B	2.28	1.49	1.42
14	H	805	CLA	C3B-C4B	2.28	1.49	1.42
14	B	817	CLA	C3B-C4B	2.28	1.49	1.42
14	H	821	CLA	C3B-C4B	2.28	1.49	1.42
14	H	811	CLA	C3B-C4B	2.28	1.49	1.42
14	G	814	CLA	C3B-C4B	2.27	1.49	1.42
14	A	839	CLA	C1B-C2B	2.27	1.48	1.43
14	K	103	CLA	C3B-C4B	2.27	1.49	1.42
14	a	840	CLA	C1B-C2B	2.27	1.48	1.43
14	b	822	CLA	C1B-C2B	2.27	1.48	1.43
14	U	202	CLA	C3B-C4B	2.27	1.49	1.42
14	G	810	CLA	C1B-C2B	2.27	1.48	1.43
14	b	828	CLA	C3B-C4B	2.27	1.49	1.42
14	a	821	CLA	C3B-C4B	2.27	1.49	1.42
14	a	827	CLA	C3B-C4B	2.27	1.49	1.42
14	a	836	CLA	C3B-C4B	2.27	1.49	1.42
14	A	813	CLA	C3B-C4B	2.27	1.49	1.42
14	H	812	CLA	C3B-C4B	2.27	1.49	1.42
14	G	837	CLA	C3B-C4B	2.27	1.49	1.42
14	B	814	CLA	C3B-C4B	2.27	1.49	1.42
14	B	829	CLA	C3B-C4B	2.27	1.49	1.42
14	b	834	CLA	C3B-C4B	2.27	1.49	1.42
14	Q	202	CLA	C3B-C4B	2.27	1.49	1.42
14	B	820	CLA	C1B-C2B	2.27	1.48	1.43
14	H	804	CLA	C3B-C4B	2.26	1.49	1.42
14	a	816	CLA	C3B-C4B	2.26	1.49	1.42
14	G	834	CLA	C3B-C4B	2.26	1.49	1.42
14	U	206	CLA	C3B-C4B	2.26	1.49	1.42
14	B	811	CLA	C3B-C4B	2.26	1.49	1.42
14	B	833	CLA	C3B-C4B	2.26	1.49	1.42
14	G	815	CLA	C3B-C4B	2.26	1.49	1.42
14	b	830	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	802	CLA	C1B-C2B	2.26	1.48	1.43
14	B	825	CLA	C3B-C4B	2.26	1.49	1.42
14	l	5004	CLA	C3B-C4B	2.26	1.49	1.42
14	G	803	CLA	C1B-C2B	2.26	1.48	1.43
14	H	833	CLA	C3B-C4B	2.26	1.49	1.42
14	A	818	CLA	C1B-C2B	2.26	1.48	1.43
14	Q	204	CLA	C3B-C4B	2.26	1.49	1.42
14	A	858	CLA	C3B-C4B	2.26	1.49	1.42
14	b	801	CLA	C3B-C4B	2.26	1.49	1.42
14	B	835	CLA	C3B-C4B	2.25	1.49	1.42
14	b	836	CLA	C3B-C4B	2.25	1.49	1.42
14	B	826	CLA	C1B-C2B	2.25	1.48	1.43
14	b	832	CLA	C3B-C4B	2.25	1.49	1.42
14	B	810	CLA	C3B-C4B	2.25	1.49	1.42
14	a	834	CLA	C3B-C4B	2.25	1.49	1.42
14	H	814	CLA	C3B-C4B	2.25	1.49	1.42
14	a	828	CLA	C3B-C4B	2.25	1.49	1.42
14	G	829	CLA	CHC-C1C	2.25	1.43	1.38
14	A	810	CLA	C3B-C4B	2.25	1.49	1.42
14	B	815	CLA	C3B-C4B	2.25	1.49	1.42
14	A	819	CLA	C1B-C2B	2.25	1.48	1.43
14	H	822	CLA	C3B-C4B	2.25	1.49	1.42
14	A	836	CLA	C1B-C2B	2.25	1.48	1.43
14	a	843	CLA	C1B-C2B	2.25	1.48	1.43
14	H	813	CLA	C3B-C4B	2.25	1.49	1.42
14	G	820	CLA	C1B-C2B	2.25	1.48	1.43
14	H	838	CLA	C3B-C4B	2.25	1.49	1.42
14	a	844	CLA	C3B-C4B	2.25	1.49	1.42
14	A	808	CLA	C3B-C4B	2.24	1.49	1.42
14	B	843	CLA	C3B-C4B	2.24	1.49	1.42
14	f	204	CLA	C3B-C4B	2.24	1.49	1.42
14	B	823	CLA	C3B-C4B	2.24	1.49	1.42
14	B	811	CLA	C1B-C2B	2.24	1.48	1.43
14	a	806	CLA	C3B-C4B	2.24	1.49	1.42
14	A	806	CLA	C3B-C4B	2.24	1.49	1.42
14	G	821	CLA	C3B-C4B	2.24	1.49	1.42
14	F	203	CLA	C3B-C4B	2.24	1.49	1.42
14	b	815	CLA	C3B-C4B	2.24	1.49	1.42
14	A	820	CLA	C3B-C4B	2.24	1.49	1.42
14	a	826	CLA	C3B-C4B	2.24	1.49	1.42
14	G	826	CLA	C3B-C4B	2.24	1.49	1.42
14	a	809	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	807	CLA	C3B-C4B	2.24	1.49	1.42
14	B	834	CLA	C3B-C4B	2.24	1.49	1.42
14	b	812	CLA	C3B-C4B	2.24	1.49	1.42
14	A	829	CLA	C3B-C4B	2.24	1.49	1.42
14	b	819	CLA	C3B-C4B	2.24	1.49	1.42
14	B	812	CLA	C3B-C4B	2.24	1.49	1.42
14	a	808	CLA	C3B-C4B	2.24	1.49	1.42
14	b	824	CLA	C3B-C4B	2.24	1.49	1.42
14	G	843	CLA	C3B-C4B	2.24	1.49	1.42
14	b	813	CLA	C3B-C4B	2.24	1.49	1.42
14	b	805	CLA	C3B-C4B	2.23	1.49	1.42
14	G	806	CLA	C3B-C4B	2.23	1.49	1.42
14	a	830	CLA	C3B-C4B	2.23	1.49	1.42
14	b	821	CLA	C3B-C4B	2.23	1.49	1.42
14	A	822	CLA	C3B-C4B	2.23	1.49	1.42
14	B	807	CLA	C3B-C4B	2.23	1.49	1.42
14	L	1502	CLA	C3B-C4B	2.23	1.49	1.42
14	A	832	CLA	C3B-C4B	2.23	1.49	1.42
14	B	839	CLA	C3B-C4B	2.23	1.49	1.42
14	a	831	CLA	C3B-C4B	2.23	1.49	1.42
14	b	840	CLA	C3B-C4B	2.23	1.49	1.42
14	U	205	CLA	C3B-C4B	2.23	1.49	1.42
14	a	804	CLA	C3B-C4B	2.23	1.49	1.42
14	A	825	CLA	C3B-C4B	2.23	1.49	1.42
14	H	815	CLA	C3B-C4B	2.22	1.49	1.42
14	b	827	CLA	C1B-C2B	2.22	1.48	1.43
14	B	828	CLA	C3B-C4B	2.22	1.49	1.42
14	U	204	CLA	C3B-C4B	2.22	1.49	1.42
14	a	835	CLA	C3B-C4B	2.22	1.49	1.42
14	A	815	CLA	C3B-C4B	2.22	1.49	1.42
14	G	823	CLA	C3B-C4B	2.22	1.49	1.42
14	b	818	CLA	C3B-C4B	2.22	1.49	1.42
14	G	830	CLA	C3B-C4B	2.22	1.49	1.42
14	a	832	CLA	MG-ND	-2.22	2.01	2.05
14	H	832	CLA	C3B-C4B	2.22	1.49	1.42
14	G	807	CLA	C3B-C4B	2.22	1.49	1.42
14	G	812	CLA	C3B-C4B	2.22	1.49	1.42
14	a	832	CLA	C1B-C2B	2.22	1.48	1.43
14	G	827	CLA	C3B-C4B	2.22	1.49	1.42
14	G	833	CLA	C3B-C4B	2.22	1.49	1.42
14	H	808	CLA	C3B-C4B	2.22	1.49	1.42
14	a	833	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	819	CLA	C3B-C4B	2.21	1.49	1.42
14	G	809	CLA	C3B-C4B	2.21	1.49	1.42
14	G	835	CLA	C1B-C2B	2.21	1.48	1.43
14	B	830	CLA	C3B-C4B	2.21	1.49	1.42
14	a	837	CLA	C1B-C2B	2.21	1.48	1.43
14	G	832	CLA	MG-ND	-2.21	2.01	2.05
14	H	834	CLA	C3B-C4B	2.21	1.49	1.42
14	a	819	CLA	C3B-C4B	2.21	1.49	1.42
14	a	823	CLA	C3B-C4B	2.21	1.49	1.42
14	b	817	CLA	C3B-C4B	2.21	1.49	1.42
14	A	811	CLA	C3B-C4B	2.21	1.49	1.42
14	A	818	CLA	C3B-C4B	2.21	1.49	1.42
14	B	820	CLA	C3B-C4B	2.21	1.49	1.42
14	b	809	CLA	C3B-C4B	2.21	1.49	1.42
14	S	1101	CLA	C3B-C4B	2.20	1.49	1.42
14	b	806	CLA	C3B-C4B	2.20	1.49	1.42
14	A	831	CLA	C3B-C4B	2.20	1.49	1.42
14	H	810	CLA	C1B-C2B	2.20	1.48	1.43
14	H	824	CLA	C3B-C4B	2.20	1.49	1.42
14	b	837	CLA	C3B-C4B	2.20	1.49	1.42
14	H	842	CLA	C3B-C4B	2.20	1.49	1.42
14	b	825	CLA	C3B-C4B	2.20	1.49	1.42
14	H	829	CLA	C3B-C4B	2.20	1.49	1.42
14	L	1501	CLA	C3B-C4B	2.20	1.49	1.42
14	B	824	CLA	C3B-C4B	2.20	1.49	1.42
14	G	831	CLA	C3B-C4B	2.19	1.49	1.42
14	H	823	CLA	C3B-C4B	2.19	1.49	1.42
14	a	812	CLA	C3B-C4B	2.19	1.49	1.42
14	G	832	CLA	C3B-C4B	2.19	1.49	1.42
14	B	809	CLA	C3B-C4B	2.19	1.49	1.42
14	H	831	CLA	C3B-C4B	2.19	1.49	1.42
14	A	833	CLA	C3B-C4B	2.19	1.49	1.42
14	G	804	CLA	C3B-C4B	2.18	1.49	1.42
14	H	806	CLA	C3B-C4B	2.18	1.49	1.42
14	G	802	CLA	C3B-C4B	2.18	1.49	1.42
14	a	825	CLA	C3B-C4B	2.18	1.49	1.42
14	A	821	CLA	C3B-C4B	2.18	1.49	1.42
14	A	842	CLA	CHC-C1C	2.18	1.42	1.38
14	b	822	CLA	CHC-C1C	2.18	1.42	1.38
14	b	829	CLA	C3B-C4B	2.18	1.49	1.42
14	B	805	CLA	C3B-C4B	2.18	1.49	1.42
14	G	819	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	826	CLA	C3B-C4B	2.18	1.49	1.42
14	A	828	CLA	CHC-C1C	2.18	1.42	1.38
14	A	831	CLA	MG-ND	-2.18	2.01	2.05
14	H	816	CLA	C3B-C4B	2.17	1.49	1.42
14	b	835	CLA	C3B-C4B	2.17	1.49	1.42
14	A	826	CLA	C3B-C4B	2.17	1.49	1.42
14	H	817	CLA	C3B-C4B	2.17	1.49	1.42
14	H	828	CLA	C3B-C4B	2.17	1.49	1.42
14	B	801	CLA	C3B-C4B	2.17	1.49	1.42
14	H	818	CLA	C3B-C4B	2.16	1.49	1.42
14	b	833	CLA	C3B-C4B	2.16	1.49	1.42
13	A	802	CL0	CHC-C1C	2.16	1.42	1.38
14	k	102	CLA	CHC-C1C	2.16	1.42	1.38
14	a	805	CLA	CHC-C1C	2.16	1.42	1.38
14	a	803	CLA	C3B-C4B	2.16	1.49	1.42
14	A	836	CLA	CHC-C1C	2.16	1.42	1.38
14	b	810	CLA	MG-ND	-2.16	2.01	2.05
14	A	824	CLA	C3B-C4B	2.16	1.49	1.42
14	B	808	CLA	C3B-C4B	2.16	1.49	1.42
14	k	103	CLA	C3B-C4B	2.16	1.49	1.42
14	B	832	CLA	C3B-C4B	2.16	1.49	1.42
14	A	829	CLA	MG-ND	-2.16	2.01	2.05
14	G	844	CLA	C3B-C4B	2.16	1.49	1.42
14	a	824	CLA	C3B-C4B	2.16	1.49	1.42
14	a	813	CLA	CHC-C1C	2.16	1.42	1.38
13	A	802	CL0	C3B-C4B	2.16	1.49	1.42
14	S	1103	CLA	CHC-C1C	2.15	1.42	1.38
14	A	823	CLA	C3B-C4B	2.15	1.49	1.42
13	a	802	CL0	C3B-C4B	2.15	1.49	1.42
14	b	830	CLA	CHC-C1C	2.15	1.42	1.38
14	B	826	CLA	CHC-C1C	2.15	1.42	1.38
14	a	838	CLA	C3B-C4B	2.15	1.49	1.42
14	G	825	CLA	C3B-C4B	2.15	1.49	1.42
14	b	844	CLA	C3B-C4B	2.15	1.49	1.42
14	G	818	CLA	C3B-C4B	2.15	1.49	1.42
14	A	809	CLA	MG-ND	-2.15	2.01	2.05
14	b	831	CLA	C3B-C4B	2.15	1.49	1.42
14	b	826	CLA	CHC-C1C	2.15	1.42	1.38
14	H	803	CLA	C3B-C4B	2.15	1.49	1.42
14	B	819	CLA	C3B-C4B	2.14	1.49	1.42
14	J	1101	CLA	C3B-C4B	2.14	1.49	1.42
14	a	832	CLA	C3B-C4B	2.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	C3B-C4B	2.14	1.49	1.42
14	B	822	CLA	MG-ND	-2.14	2.01	2.05
14	B	802	CLA	CHC-C1C	2.14	1.42	1.38
14	G	842	CLA	CHC-C1C	2.14	1.42	1.38
14	G	824	CLA	C3B-C4B	2.13	1.49	1.42
14	B	821	CLA	CHC-C1C	2.13	1.42	1.38
14	l	5006	CLA	MG-ND	-2.13	2.01	2.05
14	A	830	CLA	C3B-C4B	2.13	1.49	1.42
14	F	204	CLA	CHC-C1C	2.13	1.42	1.38
14	A	809	CLA	CHC-C1C	2.13	1.42	1.38
14	b	834	CLA	CHC-C1C	2.13	1.42	1.38
14	b	820	CLA	C3B-C4B	2.13	1.48	1.42
13	G	801	CL0	C3B-C4B	2.13	1.48	1.42
14	H	804	CLA	MG-ND	-2.13	2.01	2.05
14	H	807	CLA	C3B-C4B	2.13	1.48	1.42
14	T	102	CLA	CHC-C1C	2.13	1.42	1.38
14	a	844	CLA	MG-ND	-2.13	2.01	2.05
14	a	817	CLA	MG-ND	-2.12	2.01	2.05
14	A	806	CLA	MG-ND	-2.12	2.01	2.05
14	G	834	CLA	CHC-C1C	2.12	1.42	1.38
14	H	820	CLA	CHC-C1C	2.12	1.42	1.38
14	a	830	CLA	CHC-C1C	2.12	1.42	1.38
14	G	805	CLA	CHC-C1C	2.12	1.42	1.38
14	b	841	CLA	CHC-C1C	2.12	1.42	1.38
14	B	809	CLA	MG-ND	-2.12	2.01	2.05
14	b	826	CLA	MG-ND	-2.12	2.01	2.05
14	a	837	CLA	CHC-C1C	2.12	1.42	1.38
14	a	843	CLA	CHC-C1C	2.12	1.42	1.38
14	A	858	CLA	MG-ND	-2.12	2.01	2.05
14	a	834	CLA	CHC-C1C	2.12	1.42	1.38
14	j	102	CLA	CHC-C1C	2.12	1.42	1.38
14	a	829	CLA	MG-ND	-2.12	2.01	2.05
14	G	813	CLA	CHC-C1C	2.12	1.42	1.38
14	A	828	CLA	MG-ND	-2.12	2.01	2.05
14	A	804	CLA	CHC-C1C	2.11	1.42	1.38
14	G	815	CLA	CHC-C1C	2.11	1.42	1.38
13	G	801	CL0	CHC-C1C	2.11	1.42	1.38
14	a	845	CLA	C3B-C4B	2.11	1.48	1.42
14	b	810	CLA	C3B-C4B	2.11	1.48	1.42
14	G	809	CLA	CHC-C1C	2.11	1.42	1.38
14	B	824	CLA	MG-ND	-2.11	2.01	2.05
14	a	815	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	808	CLA	MG-ND	-2.11	2.01	2.05
14	B	816	CLA	CHC-C1C	2.11	1.42	1.38
14	J	1103	CLA	CHC-C1C	2.11	1.42	1.38
14	b	806	CLA	CHC-C1C	2.11	1.42	1.38
14	H	833	CLA	MG-ND	-2.11	2.01	2.05
14	b	802	CLA	MG-ND	-2.11	2.01	2.05
14	A	817	CLA	C3B-C4B	2.11	1.48	1.42
14	S	1102	CLA	CHC-C1C	2.10	1.42	1.38
14	a	830	CLA	MG-ND	-2.10	2.01	2.05
14	b	825	CLA	MG-ND	-2.10	2.01	2.05
13	a	802	CL0	CHC-C1C	2.10	1.42	1.38
14	A	812	CLA	CHC-C1C	2.10	1.42	1.38
14	A	858	CLA	CHC-C1C	2.10	1.42	1.38
14	H	837	CLA	CHC-C1C	2.10	1.42	1.38
14	b	802	CLA	CHC-C1C	2.10	1.42	1.38
14	H	835	CLA	C3B-C4B	2.10	1.48	1.42
14	a	807	CLA	MG-ND	-2.10	2.01	2.05
14	A	841	CLA	CHC-C1C	2.10	1.42	1.38
14	H	817	CLA	MG-ND	-2.10	2.01	2.05
14	b	835	CLA	MG-ND	-2.10	2.01	2.05
14	B	830	CLA	MG-ND	-2.09	2.01	2.05
14	G	803	CLA	MG-ND	-2.09	2.01	2.05
14	G	810	CLA	CHC-C1C	2.09	1.42	1.38
14	G	807	CLA	MG-ND	-2.09	2.01	2.05
14	G	818	CLA	MG-ND	-2.09	2.01	2.05
14	B	802	CLA	MG-ND	-2.09	2.01	2.05
14	b	838	CLA	CHC-C1C	2.09	1.42	1.38
14	A	844	CLA	C3B-C4B	2.09	1.48	1.42
14	G	811	CLA	CHC-C1C	2.09	1.42	1.38
14	K	102	CLA	CHC-C1C	2.09	1.42	1.38
14	G	836	CLA	CHC-C1C	2.09	1.42	1.38
14	A	808	CLA	CHC-C1C	2.09	1.42	1.38
14	B	818	CLA	CHC-C1C	2.09	1.42	1.38
14	G	835	CLA	CHC-C1C	2.09	1.42	1.38
14	G	817	CLA	MG-ND	-2.09	2.01	2.05
14	A	840	CLA	CHC-C1C	2.09	1.42	1.38
14	H	805	CLA	CHC-C1C	2.08	1.42	1.38
14	H	815	CLA	CHC-C1C	2.08	1.42	1.38
14	A	833	CLA	MG-ND	-2.08	2.01	2.05
14	A	833	CLA	CHC-C1C	2.08	1.42	1.38
14	A	823	CLA	MG-ND	-2.08	2.01	2.05
14	U	205	CLA	MG-ND	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	838	CLA	CHC-C1C	2.08	1.42	1.38
14	L	1502	CLA	MG-ND	-2.08	2.01	2.05
14	b	806	CLA	MG-ND	-2.08	2.01	2.05
14	b	819	CLA	MG-ND	-2.08	2.01	2.05
14	G	828	CLA	CHC-C1C	2.08	1.42	1.38
14	G	843	CLA	MG-ND	-2.08	2.01	2.05
14	b	834	CLA	MG-ND	-2.08	2.01	2.05
14	B	828	CLA	MG-ND	-2.08	2.01	2.05
14	B	840	CLA	CHC-C1C	2.07	1.42	1.38
14	b	832	CLA	CHC-C1C	2.07	1.42	1.38
14	a	817	CLA	C3B-C4B	2.07	1.48	1.42
14	a	808	CLA	CHC-C1C	2.07	1.42	1.38
14	A	817	CLA	MG-ND	-2.07	2.01	2.05
14	B	837	CLA	CHC-C1C	2.07	1.42	1.38
14	b	839	CLA	CHC-C1C	2.07	1.42	1.38
14	f	205	CLA	CHC-C1C	2.07	1.42	1.38
14	a	829	CLA	CHC-C1C	2.07	1.42	1.38
14	A	821	CLA	CHC-C1C	2.07	1.42	1.38
14	a	810	CLA	CHC-C1C	2.07	1.42	1.38
14	B	834	CLA	MG-ND	-2.07	2.01	2.05
14	G	829	CLA	MG-ND	-2.07	2.01	2.05
14	H	836	CLA	CHC-C1C	2.07	1.42	1.38
14	G	830	CLA	CHC-C1C	2.07	1.42	1.38
14	a	833	CLA	CHC-C1C	2.07	1.42	1.38
14	G	830	CLA	MG-ND	-2.07	2.01	2.05
14	T	101	CLA	MG-ND	-2.07	2.01	2.05
14	a	824	CLA	MG-ND	-2.07	2.01	2.05
14	A	843	CLA	CHC-C1C	2.07	1.42	1.38
14	A	818	CLA	CHC-C1C	2.07	1.42	1.38
14	G	832	CLA	CHC-C1C	2.06	1.42	1.38
14	U	202	CLA	CHC-C1C	2.06	1.42	1.38
13	G	801	CL0	MG-NB	-2.06	2.01	2.05
14	A	810	CLA	CHC-C1C	2.06	1.42	1.38
14	T	103	CLA	CHC-C1C	2.06	1.42	1.38
14	a	842	CLA	CHC-C1C	2.06	1.42	1.38
14	G	833	CLA	MG-ND	-2.06	2.01	2.05
14	H	839	CLA	MG-ND	-2.06	2.01	2.05
14	b	831	CLA	CHC-C1C	2.06	1.42	1.38
14	G	827	CLA	CHC-C1C	2.06	1.42	1.38
14	B	818	CLA	MG-ND	-2.06	2.01	2.05
14	B	829	CLA	MG-ND	-2.06	2.01	2.05
14	A	842	CLA	MG-ND	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	835	CLA	CHC-C1C	2.06	1.42	1.38
14	a	841	CLA	CHC-C1C	2.06	1.42	1.38
14	G	821	CLA	MG-ND	-2.06	2.01	2.05
14	G	826	CLA	MG-ND	-2.06	2.01	2.05
14	a	803	CLA	CHC-C1C	2.06	1.42	1.38
14	H	823	CLA	MG-ND	-2.05	2.01	2.05
14	a	819	CLA	CHC-C1C	2.05	1.42	1.38
14	b	829	CLA	MG-ND	-2.05	2.01	2.05
14	B	831	CLA	CHC-C1C	2.05	1.42	1.38
14	H	804	CLA	CHC-C1C	2.05	1.42	1.38
14	f	201	CLA	CHC-C1C	2.05	1.42	1.38
14	K	103	CLA	CHC-C1C	2.05	1.42	1.38
14	b	807	CLA	CHC-C1C	2.05	1.42	1.38
14	B	820	CLA	MG-ND	-2.05	2.01	2.05
14	A	826	CLA	MG-ND	-2.05	2.01	2.05
14	H	835	CLA	MG-ND	-2.05	2.01	2.05
14	L	1501	CLA	MG-ND	-2.05	2.01	2.05
14	T	101	CLA	CHC-C1C	2.05	1.42	1.38
14	A	819	CLA	CHC-C1C	2.05	1.42	1.38
14	H	807	CLA	MG-ND	-2.05	2.01	2.05
14	H	828	CLA	MG-ND	-2.05	2.01	2.05
14	b	809	CLA	MG-ND	-2.05	2.01	2.05
14	B	833	CLA	CHC-C1C	2.05	1.42	1.38
14	b	823	CLA	CHC-C1C	2.05	1.42	1.38
14	A	830	CLA	MG-ND	-2.05	2.01	2.05
14	B	835	CLA	CHC-C1C	2.05	1.42	1.38
14	G	843	CLA	CHC-C1C	2.05	1.42	1.38
14	a	827	CLA	CHC-C1C	2.05	1.42	1.38
14	H	819	CLA	MG-ND	-2.05	2.01	2.05
14	a	814	CLA	CHC-C1C	2.05	1.42	1.38
14	B	808	CLA	MG-ND	-2.05	2.01	2.05
14	G	810	CLA	MG-ND	-2.05	2.01	2.05
14	A	814	CLA	CHC-C1C	2.05	1.42	1.38
14	A	825	CLA	MG-ND	-2.05	2.01	2.05
14	a	806	CLA	MG-ND	-2.05	2.01	2.05
14	a	825	CLA	MG-ND	-2.05	2.01	2.05
14	b	833	CLA	MG-ND	-2.04	2.01	2.05
14	G	817	CLA	C3B-C4B	2.04	1.48	1.42
14	a	828	CLA	CHC-C1C	2.04	1.42	1.38
14	b	816	CLA	CHC-C1C	2.04	1.42	1.38
14	H	810	CLA	MG-ND	-2.04	2.01	2.05
14	a	836	CLA	MG-ND	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	839	CLA	MG-ND	-2.04	2.01	2.05
14	A	803	CLA	MG-ND	-2.04	2.01	2.05
14	L	1503	CLA	CHC-C1C	2.04	1.42	1.38
14	U	206	CLA	CHC-C1C	2.04	1.42	1.38
14	b	815	CLA	MG-ND	-2.04	2.01	2.05
14	B	822	CLA	CHC-C1C	2.04	1.42	1.38
14	a	844	CLA	CHC-C1C	2.04	1.42	1.38
14	b	808	CLA	CHC-C1C	2.04	1.42	1.38
14	H	830	CLA	CHC-C1C	2.04	1.42	1.38
14	G	819	CLA	MG-ND	-2.04	2.01	2.05
14	U	206	CLA	MG-ND	-2.04	2.01	2.05
14	a	826	CLA	MG-ND	-2.04	2.01	2.05
14	a	822	CLA	CHC-C1C	2.04	1.42	1.38
14	b	824	CLA	CHC-C1C	2.03	1.42	1.38
14	a	819	CLA	MG-ND	-2.03	2.01	2.05
14	a	834	CLA	MG-ND	-2.03	2.01	2.05
14	G	820	CLA	CHC-C1C	2.03	1.42	1.38
14	b	818	CLA	MG-ND	-2.03	2.01	2.05
14	B	827	CLA	CHC-C1C	2.03	1.42	1.38
14	b	842	CLA	CHC-C1C	2.03	1.42	1.38
14	G	804	CLA	CHC-C1C	2.03	1.42	1.38
14	j	101	CLA	CHC-C1C	2.03	1.42	1.38
14	B	811	CLA	CHC-C1C	2.03	1.42	1.38
14	B	828	CLA	CHC-C1C	2.03	1.42	1.38
14	K	101	CLA	CHC-C1C	2.03	1.42	1.38
14	A	827	CLA	CHC-C1C	2.03	1.42	1.38
14	B	806	CLA	CHC-C1C	2.03	1.42	1.38
14	H	829	CLA	MG-ND	-2.03	2.01	2.05
14	T	102	CLA	MG-ND	-2.03	2.01	2.05
14	B	809	CLA	CHC-C1C	2.03	1.42	1.38
14	A	824	CLA	MG-ND	-2.03	2.01	2.05
14	B	840	CLA	MG-ND	-2.03	2.01	2.05
14	b	813	CLA	MG-ND	-2.03	2.01	2.05
14	T	103	CLA	MG-ND	-2.03	2.01	2.05
14	b	817	CLA	MG-ND	-2.03	2.01	2.05
14	A	835	CLA	CHC-C1C	2.03	1.42	1.38
14	J	1102	CLA	CHC-C1C	2.03	1.42	1.38
14	A	816	CLA	C3B-C4B	2.03	1.48	1.42
14	B	824	CLA	CHC-C1C	2.03	1.42	1.38
14	A	831	CLA	CHC-C1C	2.03	1.42	1.38
14	H	817	CLA	CHC-C1C	2.03	1.42	1.38
14	B	832	CLA	MG-ND	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	826	CLA	MG-ND	-2.03	2.01	2.05
14	H	810	CLA	CHC-C1C	2.03	1.42	1.38
14	A	839	CLA	CHC-C1C	2.03	1.42	1.38
14	H	825	CLA	CHC-C1C	2.03	1.42	1.38
14	j	101	CLA	MG-ND	-2.02	2.01	2.05
14	b	814	CLA	CHC-C1C	2.02	1.42	1.38
14	H	827	CLA	MG-ND	-2.02	2.01	2.05
14	A	838	CLA	C3B-C4B	2.02	1.48	1.42
14	U	204	CLA	CHC-C1C	2.02	1.42	1.38
14	G	834	CLA	MG-ND	-2.02	2.01	2.05
14	a	838	CLA	MG-ND	-2.02	2.01	2.05
14	G	808	CLA	CHC-C1C	2.02	1.42	1.38
14	A	825	CLA	CHC-C1C	2.02	1.42	1.38
14	G	803	CLA	CHC-C1C	2.02	1.42	1.38
14	H	824	CLA	MG-ND	-2.02	2.01	2.05
14	A	834	CLA	CHC-C1C	2.02	1.42	1.38
14	B	823	CLA	CHC-C1C	2.02	1.42	1.38
14	H	831	CLA	CHC-C1C	2.02	1.42	1.38
14	H	833	CLA	CHC-C1C	2.02	1.42	1.38
14	b	821	CLA	CHC-C1C	2.02	1.42	1.38
14	a	804	CLA	MG-ND	-2.02	2.01	2.05
14	H	840	CLA	CHC-C1C	2.02	1.42	1.38
14	b	812	CLA	CHC-C1C	2.02	1.42	1.38
14	b	805	CLA	CHC-C1C	2.02	1.42	1.38
14	a	814	CLA	MG-ND	-2.02	2.01	2.05
14	l	5006	CLA	CHC-C1C	2.02	1.42	1.38
14	B	812	CLA	MG-ND	-2.02	2.01	2.05
14	G	840	CLA	MG-ND	-2.02	2.01	2.05
14	H	830	CLA	MG-ND	-2.02	2.01	2.05
14	A	822	CLA	CHC-C1C	2.02	1.42	1.38
14	b	828	CLA	CHC-C1C	2.02	1.42	1.38
14	b	835	CLA	CHC-C1C	2.02	1.42	1.38
14	a	818	CLA	CHC-C1C	2.02	1.42	1.38
14	B	815	CLA	MG-ND	-2.02	2.01	2.05
14	B	819	CLA	MG-ND	-2.02	2.01	2.05
14	A	843	CLA	MG-ND	-2.02	2.01	2.05
14	H	825	CLA	MG-ND	-2.02	2.01	2.05
14	b	831	CLA	MG-ND	-2.02	2.01	2.05
14	H	822	CLA	CHC-C1C	2.02	1.42	1.38
14	b	818	CLA	CHC-C1C	2.02	1.42	1.38
14	a	840	CLA	MG-ND	-2.02	2.01	2.05
14	A	805	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	826	CLA	CHC-C1C	2.01	1.42	1.38
14	a	811	CLA	CHC-C1C	2.01	1.42	1.38
14	B	815	CLA	CHC-C1C	2.01	1.42	1.38
14	a	820	CLA	CHC-C1C	2.01	1.42	1.38
14	a	837	CLA	MG-ND	-2.01	2.01	2.05
14	B	825	CLA	CHC-C1C	2.01	1.42	1.38
14	H	814	CLA	CHC-C1C	2.01	1.42	1.38
13	A	802	CL0	MG-NB	-2.01	2.01	2.05
14	A	829	CLA	CHC-C1C	2.01	1.42	1.38
14	a	839	CLA	C3B-C4B	2.01	1.48	1.42
14	A	808	CLA	MG-ND	-2.01	2.01	2.05
14	A	819	CLA	MG-ND	-2.01	2.01	2.05
14	A	832	CLA	CHC-C1C	2.01	1.42	1.38
14	A	811	CLA	CHC-C1C	2.01	1.42	1.38
14	G	838	CLA	C3B-C4B	2.01	1.48	1.42
14	a	831	CLA	CHC-C1C	2.01	1.42	1.38
14	A	813	CLA	MG-ND	-2.01	2.01	2.05
14	b	817	CLA	CHC-C1C	2.01	1.42	1.38
14	G	822	CLA	CHC-C1C	2.01	1.42	1.38
14	H	813	CLA	MG-ND	-2.01	2.01	2.05
14	Q	202	CLA	CHC-C1C	2.01	1.42	1.38
14	a	825	CLA	CHC-C1C	2.01	1.42	1.38
14	B	838	CLA	MG-ND	-2.00	2.01	2.05
14	H	834	CLA	CHC-C1C	2.00	1.42	1.38
14	l	5005	CLA	CHC-C1C	2.00	1.42	1.38
14	G	811	CLA	MG-ND	-2.00	2.01	2.05
14	H	821	CLA	CHC-C1C	2.00	1.42	1.38
14	B	830	CLA	CHC-C1C	2.00	1.42	1.38
14	B	843	CLA	MG-ND	-2.00	2.01	2.05
14	a	840	CLA	CHC-C1C	2.00	1.42	1.38
14	b	827	CLA	CHC-C1C	2.00	1.42	1.38
14	H	838	CLA	MG-ND	-2.00	2.01	2.05
14	H	824	CLA	CHC-C1C	2.00	1.42	1.38
14	b	828	CLA	MG-ND	-2.00	2.01	2.05
14	B	841	CLA	CHC-C1C	2.00	1.42	1.38
14	H	811	CLA	MG-ND	-2.00	2.01	2.05
14	J	1103	CLA	MG-ND	-2.00	2.01	2.05
14	a	843	CLA	MG-ND	-2.00	2.01	2.05
14	b	820	CLA	MG-ND	-2.00	2.01	2.05
14	k	101	CLA	MG-ND	-2.00	2.01	2.05
14	H	812	CLA	CHC-C1C	2.00	1.42	1.38

All (1042) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	809	CLA	C4A-NA-C1A	6.00	109.42	106.68
14	a	809	CLA	C4A-NA-C1A	5.49	109.18	106.68
14	H	825	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	B	826	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	b	827	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	A	808	CLA	C4A-NA-C1A	4.79	108.86	106.68
14	L	1501	CLA	C4A-NA-C1A	4.62	108.79	106.68
14	b	806	CLA	C4A-NA-C1A	4.60	108.78	106.68
14	B	825	CLA	C4A-NA-C1A	4.58	108.77	106.68
14	G	826	CLA	C4A-NA-C1A	4.55	108.75	106.68
14	b	805	CLA	C4A-NA-C1A	4.55	108.75	106.68
14	F	201	CLA	C4A-NA-C1A	4.41	108.69	106.68
14	B	809	CLA	C4A-NA-C1A	4.38	108.68	106.68
14	B	812	CLA	C4A-NA-C1A	4.21	108.60	106.68
14	H	808	CLA	C4A-NA-C1A	4.04	108.52	106.68
14	G	820	CLA	C1-C2-C3	-3.95	119.72	126.20
14	G	839	CLA	C4A-NA-C1A	3.91	108.46	106.68
14	b	831	CLA	C4A-NA-C1A	3.87	108.44	106.68
14	H	828	CLA	C4A-NA-C1A	3.86	108.44	106.68
14	b	811	CLA	C4A-NA-C1A	3.82	108.42	106.68
14	A	819	CLA	C1-C2-C3	-3.80	119.97	126.20
14	b	818	CLA	C4A-NA-C1A	3.79	108.41	106.68
14	G	811	CLA	C4A-NA-C1A	3.76	108.40	106.68
14	b	810	CLA	C4A-NA-C1A	3.73	108.38	106.68
14	H	811	CLA	C4A-NA-C1A	3.71	108.37	106.68
14	A	833	CLA	C4A-NA-C1A	3.67	108.35	106.68
14	a	820	CLA	C1-C2-C3	-3.66	120.20	126.20
14	B	807	CLA	C4A-NA-C1A	3.65	108.34	106.68
14	H	841	CLA	C4A-NA-C1A	3.64	108.34	106.68
13	a	802	CL0	C4A-NA-C1A	3.48	108.27	106.68
14	K	102	CLA	C4A-NA-C1A	3.48	108.27	106.68
14	Q	202	CLA	C4A-NA-C1A	3.46	108.26	106.68
14	G	818	CLA	C4A-NA-C1A	3.43	108.25	106.68
14	H	804	CLA	C4A-NA-C1A	3.40	108.23	106.68
14	H	809	CLA	C4A-NA-C1A	3.33	108.20	106.68
14	B	817	CLA	C4A-NA-C1A	3.31	108.19	106.68
14	G	840	CLA	C1-C2-C3	-3.28	120.82	126.20
14	A	858	CLA	C4A-NA-C1A	3.28	108.18	106.68
14	H	803	CLA	C4A-NA-C1A	3.27	108.17	106.68
13	G	801	CL0	C4A-NA-C1A	3.27	108.17	106.68
14	B	830	CLA	C4A-NA-C1A	3.25	108.16	106.68
14	a	817	CLA	C3B-C4B-NB	-3.25	107.63	110.53
14	k	103	CLA	C1-C2-C3	-3.23	120.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	803	CLA	C4A-NA-C1A	3.22	108.15	106.68
19	L	1505	LMT	C1B-O1B-C4'	3.19	125.53	117.98
14	B	829	CLA	C4A-NA-C1A	3.17	108.12	106.68
14	Q	204	CLA	C4A-NA-C1A	3.17	108.12	106.68
14	a	833	CLA	C4A-NA-C1A	3.14	108.11	106.68
14	B	810	CLA	C4A-NA-C1A	3.14	108.11	106.68
14	a	829	CLA	C4A-NA-C1A	3.13	108.11	106.68
14	G	807	CLA	C4A-NA-C1A	3.13	108.11	106.68
14	G	815	CLA	C4A-NA-C1A	3.13	108.11	106.68
14	K	103	CLA	C1-C2-C3	-3.12	121.08	126.20
14	a	807	CLA	C4A-NA-C1A	3.12	108.10	106.68
14	H	832	CLA	C3B-C2B-C1B	-3.12	103.49	107.17
14	b	813	CLA	C4A-NA-C1A	3.11	108.10	106.68
15	B	844	PQN	C11-C3-C4	-3.10	115.31	118.58
14	B	842	CLA	C4A-NA-C1A	3.08	108.08	106.68
14	H	821	CLA	C4A-NA-C1A	3.08	108.08	106.68
14	B	813	CLA	C4A-NA-C1A	3.08	108.08	106.68
14	A	840	CLA	C1-C2-C3	-3.05	121.20	126.20
14	J	1101	CLA	C4A-NA-C1A	3.04	108.06	106.68
14	b	815	CLA	C4A-NA-C1A	3.03	108.06	106.68
14	A	824	CLA	C4A-NA-C1A	3.00	108.05	106.68
15	A	845	PQN	C11-C3-C4	-2.99	115.42	118.58
14	T	102	CLA	C4A-NA-C1A	2.99	108.04	106.68
14	a	819	CLA	C3B-C4B-NB	-2.99	107.86	110.53
17	R	101	BCR	C24-C23-C22	-2.99	121.82	126.23
14	T	103	CLA	C1-C2-C3	-2.99	121.31	126.20
14	a	811	CLA	C4A-NA-C1A	2.98	108.04	106.68
14	a	841	CLA	C1-C2-C3	-2.97	121.32	126.20
14	b	836	CLA	C1-C2-C3	-2.97	121.33	126.20
15	H	843	PQN	C11-C3-C4	-2.97	115.45	118.58
14	H	839	CLA	C4A-NA-C1A	2.97	108.03	106.68
14	B	809	CLA	C2A-C1A-CHA	2.96	129.01	123.87
17	i	101	BCR	C24-C23-C22	-2.94	121.89	126.23
15	G	845	PQN	C11-C3-C4	-2.93	115.49	118.58
14	a	833	CLA	C3B-C4B-NB	-2.93	107.92	110.53
21	m	101	ECH	C12-C13-C14	-2.92	114.41	119.01
14	a	825	CLA	C3B-C2B-C1B	-2.92	103.73	107.17
14	b	833	CLA	C4A-NA-C1A	2.89	108.00	106.68
14	G	816	CLA	C3B-C2B-C1B	-2.89	103.77	107.17
14	H	824	CLA	C4A-NA-C1A	2.86	107.99	106.68
13	A	802	CL0	C4A-NA-C1A	2.86	107.98	106.68
14	a	818	CLA	C4A-NA-C1A	2.86	107.98	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	845	PQN	C11-C3-C4	-2.86	115.57	118.58
14	B	805	CLA	C4A-NA-C1A	2.85	107.98	106.68
14	G	825	CLA	C3B-C2B-C1B	-2.84	103.82	107.17
14	a	840	CLA	CHD-C1D-ND	-2.83	120.82	124.80
14	b	810	CLA	C2A-C1A-CHA	2.82	128.77	123.87
14	B	809	CLA	C1-C2-C3	-2.81	121.59	126.20
14	A	814	CLA	C4A-NA-C1A	2.81	107.96	106.68
14	F	203	CLA	CHD-C1D-ND	-2.80	120.86	124.80
14	a	806	CLA	C4A-NA-C1A	2.80	107.96	106.68
14	A	824	CLA	C3B-C2B-C1B	-2.80	103.87	107.17
14	H	808	CLA	C1-C2-C3	-2.79	121.63	126.20
14	G	838	CLA	C4A-NA-C1A	2.79	107.95	106.68
14	b	834	CLA	C3B-C2B-C1B	-2.78	103.89	107.17
14	B	814	CLA	C4A-NA-C1A	2.77	107.94	106.68
14	H	825	CLA	CHD-C1D-ND	-2.77	120.91	124.80
14	B	835	CLA	C1-C2-C3	-2.76	121.67	126.20
14	l	5006	CLA	C4-C3-C5	2.76	120.02	115.23
14	H	808	CLA	C2A-C1A-CHA	2.75	128.65	123.87
14	a	815	CLA	C4A-NA-C1A	2.75	107.93	106.68
14	B	816	CLA	CHD-C1D-ND	-2.75	120.93	124.80
14	A	811	CLA	C3B-C2B-C1B	-2.75	103.93	107.17
14	H	814	CLA	C4A-NA-C1A	2.74	107.93	106.68
14	T	101	CLA	CHD-C1D-ND	-2.74	120.95	124.80
14	a	825	CLA	C3B-C4B-NB	-2.73	108.09	110.53
14	S	1103	CLA	C4A-NA-C1A	2.73	107.92	106.68
14	H	813	CLA	C3B-C2B-C1B	-2.72	103.97	107.17
17	A	850	BCR	C24-C23-C22	-2.72	122.22	126.23
14	G	823	CLA	C1-C2-C3	-2.71	122.38	126.76
14	A	805	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
14	G	830	CLA	C4A-NA-C1A	2.69	107.91	106.68
14	G	838	CLA	C3B-C2B-C1B	-2.68	104.00	107.17
14	G	832	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
14	G	812	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
14	B	830	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
14	b	810	CLA	C1-C2-C3	-2.68	121.81	126.20
14	B	818	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
14	B	843	CLA	C4A-NA-C1A	2.67	107.90	106.68
14	a	816	CLA	C3B-C2B-C1B	-2.67	104.02	107.17
14	H	833	CLA	CHD-C1D-ND	-2.67	121.04	124.80
14	G	806	CLA	C4A-NA-C1A	2.67	107.90	106.68
14	a	837	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	A	815	CLA	C3B-C2B-C1B	-2.66	104.03	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	829	CLA	C3B-C2B-C1B	-2.66	104.04	107.17
14	G	806	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
14	A	843	CLA	CHD-C1D-ND	-2.65	121.07	124.80
14	b	835	CLA	CHD-C1D-ND	-2.65	121.07	124.80
14	B	840	CLA	C3B-C2B-C1B	-2.65	104.05	107.17
14	B	818	CLA	CHD-C1D-ND	-2.65	121.08	124.80
14	H	817	CLA	CHD-C1D-ND	-2.64	121.08	124.80
14	b	819	CLA	CHD-C1D-ND	-2.64	121.09	124.80
14	G	809	CLA	CHA-C1A-NA	-2.63	120.43	126.39
14	f	204	CLA	CHD-C1D-ND	-2.63	121.11	124.80
14	A	858	CLA	CHD-C1D-ND	-2.62	121.11	124.80
14	b	831	CLA	C3B-C2B-C1B	-2.62	104.08	107.17
14	A	826	CLA	CHD-C1D-ND	-2.62	121.12	124.80
14	a	809	CLA	CHA-C1A-NA	-2.62	120.47	126.39
14	T	102	CLA	CHD-C1D-ND	-2.61	121.13	124.80
14	B	811	CLA	CHD-C1D-ND	-2.61	121.14	124.80
14	H	841	CLA	C3B-C2B-C1B	-2.60	104.10	107.17
14	F	203	CLA	C3B-C2B-C1B	-2.60	104.11	107.17
14	a	806	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
14	a	827	CLA	C3B-C2B-C1B	-2.59	104.12	107.17
14	b	817	CLA	CHD-C1D-ND	-2.59	121.16	124.80
14	U	206	CLA	C1-C2-C3	-2.58	121.97	126.20
14	A	810	CLA	CHD-C1D-ND	-2.58	121.17	124.80
14	A	823	CLA	C3B-C2B-C1B	-2.57	104.13	107.17
14	A	815	CLA	C4A-NA-C1A	2.57	107.85	106.68
14	A	817	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
14	A	827	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
14	G	807	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
13	G	801	CL0	C3B-C4B-NB	-2.57	108.24	110.53
14	B	833	CLA	C3B-C2B-C1B	-2.56	104.15	107.17
15	a	846	PQN	C11-C3-C4	-2.56	115.88	118.58
14	a	820	CLA	CHD-C1D-ND	-2.56	121.20	124.80
14	H	826	CLA	CHD-C1D-ND	-2.56	121.20	124.80
14	a	832	CLA	CHD-C1D-ND	-2.56	121.20	124.80
14	H	806	CLA	C4-C3-C5	2.56	119.66	115.23
14	G	827	CLA	C3B-C2B-C1B	-2.55	104.16	107.17
14	b	807	CLA	CHD-C1D-ND	-2.55	121.22	124.80
14	A	815	CLA	CHD-C1D-ND	-2.55	121.22	124.80
14	b	830	CLA	C3B-C2B-C1B	-2.55	104.17	107.17
14	H	829	CLA	C4A-NA-C1A	2.54	107.84	106.68
18	B	853	LMG	C1-C2-C3	-2.54	104.67	110.01
14	b	808	CLA	C4-C3-C5	2.54	119.63	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	807	CLA	C3B-C2B-C1B	-2.54	104.18	107.17
14	A	808	CLA	CHA-C1A-NA	-2.54	120.65	126.39
14	a	832	CLA	C4A-NA-C1A	2.54	107.84	106.68
14	B	838	CLA	CHD-C1D-ND	-2.54	121.23	124.80
14	G	817	CLA	CMB-C2B-C1B	2.54	129.28	125.42
14	b	843	CLA	CMB-C2B-C1B	2.54	129.28	125.42
14	A	816	CLA	CMB-C2B-C1B	2.53	129.27	125.42
14	H	807	CLA	C4A-NA-C1A	2.53	107.83	106.68
14	U	202	CLA	CHA-C1A-NA	-2.53	120.67	126.39
14	G	841	CLA	C3B-C2B-C1B	-2.52	104.19	107.17
14	a	806	CLA	CHD-C1D-ND	-2.52	121.25	124.80
14	Q	204	CLA	CHD-C1D-ND	-2.52	121.26	124.80
14	F	201	CLA	CHD-C1D-ND	-2.52	121.26	124.80
14	B	801	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
14	b	801	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
14	H	834	CLA	C1-C2-C3	-2.51	122.08	126.20
14	G	833	CLA	C4A-NA-C1A	2.51	107.82	106.68
14	A	832	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
14	a	819	CLA	CHD-C1D-ND	-2.50	121.28	124.80
14	G	830	CLA	C1-C2-C3	-2.50	122.09	126.20
14	f	201	CLA	CHA-C1A-NA	-2.50	120.72	126.39
14	a	835	CLA	CHA-C1A-NA	-2.50	120.72	126.39
14	A	806	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
14	G	815	CLA	CHD-C1D-ND	-2.50	121.29	124.80
14	H	805	CLA	CHD-C1D-ND	-2.50	121.29	124.80
14	A	828	CLA	CHA-C1A-NA	-2.50	120.73	126.39
14	a	818	CLA	C1-C2-C3	-2.50	122.11	126.20
14	b	816	CLA	C3B-C2B-C1B	-2.50	104.23	107.17
14	A	839	CLA	CHD-C1D-ND	-2.50	121.29	124.80
14	A	834	CLA	CHA-C1A-NA	-2.50	120.74	126.39
14	A	826	CLA	C3B-C2B-C1B	-2.49	104.23	107.17
14	b	812	CLA	CHD-C1D-ND	-2.49	121.30	124.80
14	b	819	CLA	C3B-C2B-C1B	-2.49	104.23	107.17
17	I	101	BCR	C24-C23-C22	-2.49	122.55	126.23
14	G	802	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
21	L	1506	ECH	C7-C8-C9	-2.49	122.56	126.23
14	J	1103	CLA	C1-C2-C3	-2.49	122.74	126.76
14	a	833	CLA	C3B-C2B-C1B	-2.48	104.25	107.17
14	A	832	CLA	CHD-C1D-ND	-2.48	121.31	124.80
14	G	836	CLA	C3B-C4B-NB	-2.48	108.32	110.53
14	b	839	CLA	C4A-NA-C1A	2.48	107.81	106.68
14	b	805	CLA	CHD-C1D-ND	-2.48	121.32	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	807	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
14	b	828	CLA	CHD-C1D-ND	-2.47	121.32	124.80
14	f	204	CLA	C4A-NA-C1A	2.47	107.81	106.68
14	B	840	CLA	CHD-C1D-ND	-2.47	121.32	124.80
14	b	834	CLA	CHD-C1D-ND	-2.47	121.32	124.80
14	a	838	CLA	CHD-C1D-ND	-2.47	121.33	124.80
14	a	814	CLA	CHD-C1D-ND	-2.47	121.33	124.80
14	b	841	CLA	CHD-C1D-ND	-2.46	121.33	124.80
14	A	825	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
14	a	844	CLA	CHD-C1D-ND	-2.46	121.34	124.80
14	H	828	CLA	CHD-C1D-ND	-2.46	121.34	124.80
14	a	843	CLA	CHD-C1D-ND	-2.46	121.34	124.80
14	A	834	CLA	C1-C2-C3	-2.46	122.17	126.20
14	A	830	CLA	C4A-NA-C1A	2.46	107.80	106.68
14	H	812	CLA	CHD-C1D-ND	-2.46	121.35	124.80
14	a	830	CLA	CHD-C1D-ND	-2.46	121.35	124.80
14	H	816	CLA	C1-C2-C3	-2.45	122.18	126.20
19	Q	201	LMT	O1B-C4'-C3'	2.45	113.47	107.23
14	A	822	CLA	C1-C2-C3	-2.45	122.80	126.76
14	B	832	CLA	CHD-C1D-ND	-2.45	121.36	124.80
14	G	832	CLA	CHD-C1D-ND	-2.45	121.36	124.80
14	A	831	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
14	Q	204	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
14	B	810	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
14	a	831	CLA	O2A-CGA-O1A	-2.44	117.51	123.63
14	A	829	CLA	C1-C2-C3	-2.44	122.19	126.20
14	B	817	CLA	C1-C2-C3	-2.44	122.20	126.20
14	A	840	CLA	CHD-C1D-ND	-2.44	121.37	124.80
14	B	835	CLA	CHD-C1D-ND	-2.43	121.38	124.80
14	b	827	CLA	CHD-C1D-ND	-2.43	121.38	124.80
14	a	803	CLA	CHD-C1D-ND	-2.43	121.38	124.80
14	G	832	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	b	839	CLA	CHD-C1D-ND	-2.43	121.38	124.80
14	H	820	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	f	201	CLA	CHD-C1D-ND	-2.43	121.39	124.80
14	b	808	CLA	CHD-C1D-ND	-2.43	121.39	124.80
14	G	826	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
14	A	836	CLA	C3B-C4B-NB	-2.42	108.37	110.53
14	b	841	CLA	C3B-C2B-C1B	-2.42	104.31	107.17
14	A	836	CLA	CHD-C1D-ND	-2.42	121.40	124.80
14	A	839	CLA	C3B-C2B-C1B	-2.42	104.32	107.17
14	G	834	CLA	CHD-C1D-ND	-2.42	121.40	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	818	CLA	CHA-C1A-NA	-2.42	120.92	126.39
14	b	810	CLA	CHD-C1D-ND	-2.42	121.40	124.80
14	H	807	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
14	G	813	CLA	C4A-NA-C1A	2.42	107.78	106.68
14	a	821	CLA	CHD-C1D-ND	-2.41	121.41	124.80
14	A	810	CLA	C4A-NA-C1A	2.41	107.78	106.68
14	G	804	CLA	CHD-C1D-ND	-2.41	121.41	124.80
14	G	806	CLA	CHD-C1D-ND	-2.41	121.41	124.80
14	b	829	CLA	C3B-C2B-C1B	-2.41	104.33	107.17
14	b	809	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
14	A	813	CLA	CHD-C1D-ND	-2.40	121.42	124.80
14	A	805	CLA	C3B-C2B-C1B	-2.40	104.33	107.17
14	A	805	CLA	CHD-C1D-ND	-2.40	121.42	124.80
14	G	807	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
14	a	839	CLA	C4A-NA-C1A	2.40	107.78	106.68
14	A	803	CLA	CHD-C1D-ND	-2.40	121.42	124.80
14	B	823	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	a	818	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
14	A	806	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
14	G	839	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
14	T	101	CLA	C3B-C4B-NB	-2.40	108.39	110.53
14	G	835	CLA	CHD-C1D-ND	-2.40	121.43	124.80
14	A	813	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
14	a	824	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
14	A	833	CLA	CHD-C1D-ND	-2.40	121.43	124.80
14	J	1103	CLA	C4A-NA-C1A	2.39	107.77	106.68
14	H	816	CLA	CHD-C1D-ND	-2.39	121.44	124.80
14	a	818	CLA	C2A-C1A-CHA	2.39	128.02	123.87
14	F	204	CLA	CHD-C1D-ND	-2.39	121.44	124.80
14	b	830	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	H	852	LMT	O1B-C4'-C3'	2.39	113.30	107.23
14	a	819	CLA	C3B-C2B-C1B	-2.39	104.36	107.17
14	G	802	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	G	834	CLA	CMB-C2B-C1B	2.39	129.05	125.42
14	a	828	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
14	b	811	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
14	B	808	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
14	a	826	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
14	J	1101	CLA	CHD-C1D-ND	-2.38	121.45	124.80
14	b	835	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
14	B	842	CLA	CMB-C2B-C1B	2.38	129.04	125.42
14	b	840	CLA	C3B-C2B-C1B	-2.38	104.36	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	842	CLA	C5-C3-C2	2.38	126.51	121.17
14	B	832	CLA	C3B-C2B-C1B	-2.38	104.37	107.17
14	H	809	CLA	C1-C2-C3	-2.38	122.31	126.20
14	H	815	CLA	C1-C2-C3	-2.37	122.31	126.20
14	A	818	CLA	CHD-C1D-ND	-2.37	121.46	124.80
14	A	830	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
14	B	834	CLA	CHD-C1D-ND	-2.37	121.46	124.80
14	B	807	CLA	C4-C3-C5	2.37	119.34	115.23
14	a	845	CLA	CHB-C4A-NA	2.37	127.82	124.40
14	A	842	CLA	C4A-NA-C1A	2.37	107.76	106.68
14	H	830	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
14	l	5006	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
14	B	839	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	a	828	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	A	832	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
14	a	821	CLA	C4A-NA-C1A	2.37	107.76	106.68
14	G	808	CLA	CHD-C1D-ND	-2.36	121.47	124.80
14	A	819	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
14	G	824	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
14	G	817	CLA	C3B-C4B-NB	-2.36	108.42	110.53
14	a	829	CLA	C2A-C1A-CHA	2.36	127.97	123.87
17	l	5003	BCR	C7-C8-C9	-2.36	122.74	126.23
14	a	830	CLA	C4A-NA-C1A	2.36	107.76	106.68
14	G	804	CLA	C3B-C4B-NB	-2.36	108.42	110.53
13	G	801	CL0	CHD-C1D-ND	-2.36	121.48	124.80
14	G	843	CLA	CHD-C1D-ND	-2.36	121.48	124.80
17	F	202	BCR	C12-C13-C14	-2.36	115.30	119.01
14	b	830	CLA	C3B-C4B-NB	-2.36	108.42	110.53
14	H	834	CLA	CHD-C1D-ND	-2.36	121.48	124.80
14	G	820	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
14	A	820	CLA	C4A-NA-C1A	2.36	107.75	106.68
14	H	828	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
14	H	809	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
14	G	842	CLA	CHD-C1D-ND	-2.36	121.49	124.80
13	A	802	CL0	CHD-C1D-ND	-2.35	121.49	124.80
14	A	828	CLA	C4A-NA-C1A	2.35	107.75	106.68
14	b	831	CLA	CHD-C1D-ND	-2.35	121.49	124.80
14	b	827	CLA	C5-C3-C2	2.35	126.45	121.17
14	H	841	CLA	CHD-C1D-ND	-2.35	121.49	124.80
14	f	204	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
14	H	806	CLA	CHD-C1D-ND	-2.35	121.49	124.80
14	G	835	CLA	C3B-C4B-NB	-2.35	108.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	203	BCR	C12-C13-C14	-2.35	115.31	119.01
14	H	804	CLA	CHD-C1D-ND	-2.35	121.50	124.80
14	G	819	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
14	a	812	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
14	B	806	CLA	CHD-C1D-ND	-2.35	121.50	124.80
14	B	833	CLA	CHD-C1D-ND	-2.35	121.50	124.80
14	H	827	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
14	j	102	CLA	CHD-C1D-ND	-2.35	121.50	124.80
14	b	807	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
14	G	820	CLA	CHD-C1D-ND	-2.34	121.50	124.80
14	A	834	CLA	C4A-NA-C1A	2.34	107.75	106.68
14	a	820	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	U	202	CLA	CHD-C1D-ND	-2.34	121.51	124.80
14	b	833	CLA	CHD-C1D-ND	-2.34	121.51	124.80
14	H	842	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	k	103	CLA	CHD-C1D-ND	-2.34	121.51	124.80
14	H	807	CLA	C3B-C2B-C1B	-2.34	104.41	107.17
14	H	831	CLA	C3B-C2B-C1B	-2.34	104.41	107.17
14	H	819	CLA	CHD-C1D-ND	-2.34	121.51	124.80
14	H	838	CLA	C4A-NA-C1A	2.34	107.75	106.68
14	B	810	CLA	CMB-C2B-C1B	2.34	128.98	125.42
14	A	831	CLA	CHD-C1D-ND	-2.34	121.52	124.80
14	k	103	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
14	B	831	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	G	805	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	U	202	CLA	C1-C2-C3	-2.33	122.37	126.20
14	G	824	CLA	C1-C2-C3	-2.33	122.38	126.20
14	A	807	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	B	836	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	A	839	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	a	827	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
14	B	810	CLA	C1-C2-C3	-2.33	122.38	126.20
14	B	829	CLA	C3B-C2B-C1B	-2.33	104.42	107.17
14	B	805	CLA	CMB-C2B-C1B	2.33	128.97	125.42
14	H	827	CLA	C1-C2-C3	-2.33	122.38	126.20
14	b	821	CLA	CHD-C1D-ND	-2.33	121.53	124.80
14	B	806	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
14	a	808	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	a	805	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	a	833	CLA	CHD-C1D-ND	-2.33	121.53	124.80
14	b	806	CLA	CHD-C1D-ND	-2.33	121.53	124.80
14	G	831	CLA	O2A-CGA-O1A	-2.33	117.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	830	CLA	CHA-C1A-NA	-2.32	121.13	126.39
14	a	832	CLA	C3B-C2B-C1B	-2.32	104.43	107.17
14	b	836	CLA	C4A-NA-C1A	2.32	107.74	106.68
14	A	831	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	a	819	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
14	B	829	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
14	B	841	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	b	833	CLA	C3B-C2B-C1B	-2.32	104.43	107.17
14	G	836	CLA	CHD-C1D-ND	-2.32	121.54	124.80
14	b	826	CLA	CHD-C1D-ND	-2.32	121.54	124.80
14	a	836	CLA	CHD-C1D-ND	-2.32	121.54	124.80
14	b	829	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	b	819	CLA	C1-C2-C3	-2.31	122.41	126.20
14	H	830	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
14	H	823	CLA	CHD-C1D-ND	-2.31	121.55	124.80
14	B	826	CLA	CHD-C1D-ND	-2.31	121.55	124.80
14	H	842	CLA	C3B-C2B-C1B	-2.31	104.44	107.17
14	S	1103	CLA	C3B-C2B-C1B	-2.31	104.44	107.17
14	G	837	CLA	C4A-NA-C1A	2.31	107.73	106.68
14	B	831	CLA	CHA-C1A-NA	-2.31	121.16	126.39
14	A	804	CLA	CHD-C1D-ND	-2.31	121.56	124.80
14	G	825	CLA	CHD-C1D-ND	-2.31	121.56	124.80
14	A	838	CLA	C4A-NA-C1A	2.31	107.73	106.68
14	a	809	CLA	CHD-C1D-ND	-2.30	121.56	124.80
14	H	815	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
14	H	834	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
14	B	840	CLA	C3B-C4B-NB	-2.30	108.47	110.53
14	H	835	CLA	C3B-C4B-NB	-2.30	108.47	110.53
14	H	805	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
14	G	842	CLA	C3B-C2B-C1B	-2.30	104.46	107.17
14	b	837	CLA	CHD-C1D-ND	-2.30	121.56	124.80
14	H	808	CLA	CHD-C1D-ND	-2.30	121.56	124.80
14	G	822	CLA	C3B-C2B-C1B	-2.30	104.46	107.17
14	B	810	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	b	811	CLA	C1-C2-C3	-2.30	122.43	126.20
14	G	834	CLA	C4A-NA-C1A	2.29	107.72	106.68
14	b	802	CLA	C4A-NA-C1A	2.29	107.72	106.68
14	A	818	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	b	825	CLA	C3B-C4B-NB	-2.29	108.48	110.53
14	B	835	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
17	U	203	BCR	C7-C8-C9	-2.29	122.85	126.23
14	a	808	CLA	CHD-C1D-ND	-2.29	121.58	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	818	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
14	A	835	CLA	CHD-C1D-ND	-2.29	121.58	124.80
14	b	820	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	G	843	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
14	b	825	CLA	CHD-C1D-ND	-2.28	121.59	124.80
14	A	841	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
14	A	819	CLA	CHB-C4A-NA	2.28	127.70	124.40
14	a	804	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
14	H	831	CLA	CHD-C1D-ND	-2.28	121.59	124.80
14	B	808	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
14	K	102	CLA	CHD-C1D-ND	-2.28	121.60	124.80
17	a	858	BCR	C24-C23-C22	-2.28	122.86	126.23
14	B	835	CLA	C3B-C4B-NB	-2.28	108.50	110.53
14	H	810	CLA	CHD-C1D-ND	-2.28	121.60	124.80
14	a	810	CLA	C4A-NA-C1A	2.28	107.72	106.68
14	G	844	CLA	CHD-C1D-ND	-2.27	121.60	124.80
14	A	809	CLA	CHD-C1D-ND	-2.27	121.60	124.80
14	H	833	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
14	l	5005	CLA	CHD-C1D-ND	-2.27	121.61	124.80
14	A	842	CLA	CHD-C1D-ND	-2.27	121.61	124.80
14	G	840	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
14	G	811	CLA	CHD-C1D-ND	-2.27	121.61	124.80
14	a	805	CLA	CHD-C1D-ND	-2.27	121.61	124.80
14	G	833	CLA	C3B-C2B-C1B	-2.27	104.50	107.17
14	H	817	CLA	C3B-C2B-C1B	-2.27	104.50	107.17
14	k	103	CLA	C3B-C2B-C1B	-2.27	104.50	107.17
14	B	809	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
14	K	101	CLA	C3B-C4B-NB	-2.27	108.51	110.53
14	H	828	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
14	H	808	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	G	806	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
14	A	843	CLA	CMB-C2B-C1B	2.26	128.86	125.42
14	A	828	CLA	C2A-C1A-CHA	2.26	127.79	123.87
14	B	831	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	a	825	CLA	CHD-C1D-ND	-2.26	121.62	124.80
14	a	825	CLA	C4A-NA-C1A	2.26	107.71	106.68
19	H	852	LMT	C1B-O1B-C4'	2.26	123.33	117.98
14	G	827	CLA	CHD-C1D-ND	-2.26	121.62	124.80
14	G	815	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
14	a	845	CLA	CHD-C1D-ND	-2.26	121.63	124.80
17	G	858	BCR	C24-C23-C22	-2.26	122.90	126.23
14	a	844	CLA	O2A-CGA-O1A	-2.25	117.99	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	837	CLA	CHD-C1D-ND	-2.25	121.63	124.80
14	b	836	CLA	CHD-C1D-ND	-2.25	121.63	124.80
14	G	835	CLA	C3B-C2B-C1B	-2.25	104.51	107.17
14	G	818	CLA	C1-C2-C3	-2.25	122.50	126.20
14	B	827	CLA	CMB-C2B-C1B	2.25	128.85	125.42
14	B	820	CLA	CHD-C1D-ND	-2.25	121.63	124.80
14	A	826	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
14	H	806	CLA	C4A-NA-C1A	2.25	107.71	106.68
14	U	202	CLA	C4A-NA-C1A	2.25	107.71	106.68
14	G	822	CLA	CHD-C1D-ND	-2.25	121.64	124.80
14	H	814	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
14	a	814	CLA	C3B-C2B-C1B	-2.25	104.52	107.17
14	b	802	CLA	C3B-C4B-NB	-2.25	108.52	110.53
14	B	814	CLA	C3B-C2B-C1B	-2.25	104.52	107.17
14	B	830	CLA	CHD-C1D-ND	-2.25	121.64	124.80
14	A	803	CLA	C3B-C4B-NB	-2.24	108.53	110.53
14	b	810	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
14	b	809	CLA	CHD-C1D-ND	-2.24	121.64	124.80
14	a	823	CLA	C1-C2-C3	-2.24	122.52	126.20
14	A	819	CLA	CHD-C1D-ND	-2.24	121.64	124.80
14	B	834	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	B	841	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
14	A	834	CLA	CHD-C1D-ND	-2.24	121.65	124.80
14	T	103	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	B	805	CLA	CHD-C1D-ND	-2.24	121.65	124.80
14	G	827	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	U	205	CLA	CHD-C1D-ND	-2.24	121.65	124.80
14	A	843	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
14	A	827	CLA	C3B-C4B-NB	-2.24	108.53	110.53
14	A	838	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
14	G	807	CLA	C1-C2-C3	-2.24	122.53	126.20
14	H	840	CLA	CHD-C1D-ND	-2.23	121.66	124.80
14	a	829	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
14	A	829	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
14	G	813	CLA	CHD-C1D-ND	-2.23	121.66	124.80
14	A	824	CLA	C3B-C4B-NB	-2.23	108.54	110.53
14	a	839	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
14	b	832	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	T	101	CLA	C4A-NA-C1A	2.23	107.70	106.68
14	b	844	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	a	856	LMT	O1B-C4'-C3'	2.23	112.90	107.23
14	H	840	CLA	C3B-C4B-NB	-2.23	108.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	824	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	A	833	CLA	C3B-C4B-NB	-2.23	108.54	110.53
14	L	1502	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
14	H	838	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	A	841	CLA	CHB-C4A-NA	2.23	127.61	124.40
14	B	836	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
14	U	205	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
14	H	835	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	U	206	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	B	812	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	G	821	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	G	833	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	b	818	CLA	C3B-C2B-C1B	-2.22	104.55	107.17
19	f	203	LMT	C1B-O1B-C4'	2.22	123.25	117.98
14	A	840	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
14	A	832	CLA	C3B-C4B-NB	-2.22	108.55	110.53
14	G	805	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
14	a	830	CLA	C1-C2-C3	-2.22	122.55	126.20
14	B	809	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	G	840	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	G	814	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	A	844	CLA	CHB-C4A-NA	2.22	127.61	124.40
14	H	822	CLA	CHB-C4A-NA	2.22	127.60	124.40
14	G	829	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	a	834	CLA	CHD-C1D-ND	-2.22	121.68	124.80
14	G	818	CLA	C3B-C2B-C1B	-2.22	104.55	107.17
14	A	828	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	G	814	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
14	B	843	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
14	K	103	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	H	835	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
14	b	836	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	T	101	CLA	CHA-C1A-NA	-2.22	121.38	126.39
14	B	801	CLA	CHB-C4A-NA	2.21	127.60	124.40
14	a	815	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	B	814	CLA	C1-C2-C3	-2.21	122.57	126.20
14	a	841	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	G	813	CLA	CHA-C1A-NA	-2.21	121.38	126.39
14	b	808	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
19	L	1505	LMT	O1B-C4'-C5'	2.21	115.28	109.48
14	B	802	CLA	C3B-C4B-NB	-2.21	108.56	110.53
14	B	815	CLA	O2A-CGA-O1A	-2.21	118.10	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	826	CLA	C5-C3-C2	2.21	126.13	121.17
14	S	1103	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
14	B	839	CLA	C3B-C2B-C1B	-2.21	104.57	107.17
14	b	830	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	H	825	CLA	C5-C3-C2	2.21	126.12	121.17
14	l	5005	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	a	823	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
14	a	835	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
14	a	833	CLA	C1-C2-C3	-2.20	122.59	126.20
14	H	832	CLA	C3B-C4B-NB	-2.20	108.56	110.53
14	b	842	CLA	C3B-C4B-NB	-2.20	108.56	110.53
14	b	830	CLA	C4A-NA-C1A	2.20	107.68	106.68
14	A	825	CLA	CHD-C1D-ND	-2.20	121.71	124.80
14	f	205	CLA	CHD-C1D-ND	-2.20	121.71	124.80
14	B	824	CLA	C3B-C4B-NB	-2.20	108.57	110.53
14	b	844	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
14	a	811	CLA	CHD-C1D-ND	-2.20	121.71	124.80
14	A	807	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
14	A	837	CLA	CHD-C1D-ND	-2.20	121.71	124.80
14	b	814	CLA	CHD-C1D-ND	-2.20	121.71	124.80
14	G	831	CLA	CHA-C1A-NA	-2.20	121.42	126.39
14	S	1102	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
14	B	818	CLA	C1-C2-C3	-2.19	122.60	126.20
14	H	814	CLA	C3B-C2B-C1B	-2.19	104.58	107.17
14	B	821	CLA	CHD-C1D-ND	-2.19	121.72	124.80
14	G	837	CLA	C3B-C2B-C1B	-2.19	104.58	107.17
14	A	858	CLA	C3B-C4B-NB	-2.19	108.57	110.53
14	H	841	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
14	a	829	CLA	CHA-C1A-NA	-2.19	121.43	126.39
14	A	808	CLA	CHD-C1D-ND	-2.19	121.72	124.80
14	b	838	CLA	C3B-C2B-C1B	-2.19	104.59	107.17
14	J	1103	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
14	H	820	CLA	CHD-C1D-ND	-2.19	121.72	124.80
14	a	835	CLA	C1-C2-C3	-2.19	122.61	126.20
14	b	817	CLA	C1-C2-C3	-2.19	122.61	126.20
14	H	832	CLA	CHB-C4A-NA	2.19	127.56	124.40
14	b	815	CLA	C1-C2-C3	-2.19	122.61	126.20
14	T	103	CLA	CHD-C1D-ND	-2.19	121.72	124.80
14	G	839	CLA	C3B-C4B-NB	-2.19	108.58	110.53
14	G	842	CLA	C3B-C4B-NB	-2.19	108.58	110.53
14	k	101	CLA	C3B-C4B-NB	-2.19	108.58	110.53
14	Q	202	CLA	CHD-C1D-ND	-2.19	121.73	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	807	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	a	808	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	B	833	CLA	CHB-C4A-NA	2.18	127.55	124.40
17	G	850	BCR	C24-C23-C22	-2.18	123.00	126.23
14	a	841	CLA	CHD-C1D-ND	-2.18	121.73	124.80
14	G	841	CLA	C3B-C4B-NB	-2.18	108.58	110.53
14	G	842	CLA	C4A-NA-C1A	2.18	107.67	106.68
14	G	838	CLA	CHD-C1D-ND	-2.18	121.73	124.80
14	G	829	CLA	C2A-C1A-CHA	2.18	127.65	123.87
14	b	816	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	A	819	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
14	B	829	CLA	CHD-C1D-ND	-2.18	121.74	124.80
14	b	823	CLA	CHD-C1D-ND	-2.18	121.74	124.80
14	k	102	CLA	CHD-C1D-ND	-2.18	121.74	124.80
14	H	806	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	G	812	CLA	CHD-C1D-ND	-2.18	121.74	124.80
14	G	839	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	H	834	CLA	C4A-NA-C1A	2.18	107.67	106.68
14	G	838	CLA	C3B-C4B-NB	-2.18	108.59	110.53
14	H	803	CLA	CMB-C2B-C1B	2.18	128.73	125.42
14	A	814	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
14	H	829	CLA	C3B-C4B-NB	-2.18	108.59	110.53
14	a	830	CLA	C3B-C4B-NB	-2.18	108.59	110.53
14	k	103	CLA	C4A-NA-C1A	2.17	107.67	106.68
14	B	817	CLA	CHD-C1D-ND	-2.17	121.74	124.80
14	b	822	CLA	CHD-C1D-ND	-2.17	121.74	124.80
14	A	821	CLA	C3B-C4B-NB	-2.17	108.59	110.53
14	b	817	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
14	A	824	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	a	817	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	B	807	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	a	804	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	G	837	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
14	H	823	CLA	CMB-C2B-C1B	2.17	128.72	125.42
14	B	841	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	b	842	CLA	CHB-C4A-NA	2.17	127.53	124.40
17	A	860	BCR	C24-C23-C22	-2.17	123.03	126.23
14	b	829	CLA	C1-C2-C3	-2.17	122.64	126.20
14	G	819	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	H	832	CLA	CHD-C1D-ND	-2.17	121.75	124.80
14	J	1103	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
14	a	806	CLA	C3B-C2B-C1B	-2.17	104.61	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	835	CLA	C3B-C4B-NB	-2.17	108.59	110.53
14	A	806	CLA	C4A-NA-C1A	2.17	107.67	106.68
14	a	815	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
21	m	101	ECH	C15-C14-C13	2.16	130.31	127.28
14	J	1103	CLA	C3B-C4B-NB	-2.16	108.60	110.53
14	G	806	CLA	C1-O2A-CGA	2.16	121.88	116.65
14	B	813	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	B	834	CLA	CHA-C1A-NA	-2.16	121.50	126.39
14	a	838	CLA	C1-C2-C3	-2.16	122.66	126.20
14	b	821	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	a	834	CLA	C4A-NA-C1A	2.16	107.66	106.68
14	a	834	CLA	C3B-C4B-NB	-2.16	108.60	110.53
14	k	103	CLA	C3B-C4B-NB	-2.16	108.60	110.53
14	A	830	CLA	CHA-C1A-NA	-2.16	121.50	126.39
14	a	828	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	B	824	CLA	CHD-C1D-ND	-2.16	121.77	124.80
14	A	821	CLA	CHD-C1D-ND	-2.16	121.77	124.80
14	b	829	CLA	CHD-C1D-ND	-2.16	121.77	124.80
14	H	841	CLA	CMB-C2B-C1B	2.16	128.70	125.42
14	B	841	CLA	CHB-C4A-NA	2.16	127.51	124.40
13	A	802	CL0	C3B-C4B-NB	-2.16	108.61	110.53
14	B	833	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	a	809	CLA	C3B-C2B-C1B	-2.16	104.63	107.17
14	G	830	CLA	CHD-C1D-ND	-2.16	121.77	124.80
14	H	803	CLA	CHD-C1D-ND	-2.15	121.77	124.80
14	a	832	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
14	a	843	CLA	C4A-NA-C1A	2.15	107.66	106.68
14	G	837	CLA	C1-C2-C3	-2.15	122.67	126.20
14	a	803	CLA	CHB-C4A-NA	2.15	127.51	124.40
14	B	819	CLA	C3B-C4B-NB	-2.15	108.61	110.53
17	f	202	BCR	C12-C13-C14	-2.15	115.62	119.01
14	l	5004	CLA	CHD-C1D-ND	-2.15	121.77	124.80
14	G	821	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
14	S	1103	CLA	C1-C2-C3	-2.15	123.28	126.76
14	H	815	CLA	CHD-C1D-ND	-2.15	121.77	124.80
14	B	841	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	b	836	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	a	831	CLA	CHA-C1A-NA	-2.15	121.52	126.39
14	B	828	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	b	840	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	B	823	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	G	825	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	830	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	a	822	CLA	C3B-C2B-C1B	-2.15	104.64	107.17
14	B	817	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
14	a	839	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	b	843	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	G	828	CLA	CHD-C1D-ND	-2.14	121.78	124.80
14	G	802	CLA	CHD-C1D-ND	-2.14	121.78	124.80
14	A	839	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	a	830	CLA	C3B-C2B-C1B	-2.14	104.64	107.17
14	H	813	CLA	CHD-C1D-ND	-2.14	121.79	124.80
14	j	101	CLA	CHD-C1D-ND	-2.14	121.79	124.80
14	B	819	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	a	814	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	G	816	CLA	CHD-C1D-ND	-2.14	121.79	124.80
14	B	816	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	S	1103	CLA	C3B-C4B-NB	-2.14	108.62	110.53
14	B	819	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	H	809	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	A	820	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	a	806	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	a	842	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	A	842	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
14	b	822	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	H	827	CLA	C3B-C4B-NB	-2.14	108.62	110.53
14	a	843	CLA	C3B-C4B-NB	-2.14	108.62	110.53
14	A	822	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	b	820	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	G	826	CLA	CHA-C1A-NA	-2.14	121.55	126.39
14	B	837	CLA	CHD-C1D-ND	-2.14	121.80	124.80
14	B	817	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
14	B	819	CLA	CHD-C1D-ND	-2.14	121.80	124.80
14	B	825	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	A	802	CL0	C3B-C2B-C1B	-2.14	104.65	107.17
14	G	828	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
14	G	827	CLA	C3B-C4B-NB	-2.14	108.62	110.53
14	B	836	CLA	O2A-CGA-O1A	-2.13	117.84	123.33
14	b	820	CLA	C3B-C2B-C1B	-2.13	104.65	107.17
14	G	820	CLA	CHB-C4A-NA	2.13	127.48	124.40
14	A	823	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	G	809	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	G	828	CLA	C3B-C4B-NB	-2.13	108.62	110.53
14	a	815	CLA	CHD-C1D-ND	-2.13	121.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	832	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
14	J	1101	CLA	C1-C2-C3	-2.13	122.70	126.20
14	A	841	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	B	822	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	a	822	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	A	805	CLA	C1-O2A-CGA	2.13	121.81	116.65
14	b	839	CLA	CMB-C2B-C1B	2.13	128.66	125.42
14	G	839	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	b	814	CLA	C4A-NA-C1A	2.13	107.65	106.68
14	H	809	CLA	CMB-C2B-C1B	2.13	128.66	125.42
14	A	837	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
14	b	809	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
14	b	810	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
14	A	814	CLA	CHD-C1D-ND	-2.13	121.81	124.80
14	H	837	CLA	CHD-C1D-ND	-2.13	121.81	124.80
14	A	844	CLA	CMB-C2B-C1B	2.13	128.66	125.42
14	B	828	CLA	CMB-C2B-C1B	2.13	128.66	125.42
14	H	834	CLA	C3B-C4B-NB	-2.13	108.63	110.53
14	a	842	CLA	CHD-C1D-ND	-2.13	121.81	124.80
14	F	204	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
14	a	820	CLA	C3A-C2A-C1A	-2.13	98.15	101.34
14	G	828	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
14	G	842	CLA	C1-C2-C3	-2.13	122.72	126.20
14	a	820	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
14	b	827	CLA	C4-C3-C2	-2.12	118.17	123.63
14	b	819	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
14	H	836	CLA	C3B-C4B-NB	-2.12	108.64	110.53
19	Q	201	LMT	O3'-C3'-C2'	-2.12	105.37	110.38
14	S	1102	CLA	CHD-C1D-ND	-2.12	121.82	124.80
14	G	814	CLA	C1-C2-C3	-2.12	122.72	126.20
14	H	829	CLA	CHD-C1D-ND	-2.12	121.82	124.80
14	B	828	CLA	C1-C2-C3	-2.12	122.72	126.20
14	H	835	CLA	O2A-CGA-O1A	-2.12	117.88	123.33
14	H	808	CLA	CMB-C2B-C1B	2.12	128.65	125.42
14	a	824	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	b	814	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	a	826	CLA	C4A-NA-C1A	2.12	107.65	106.68
14	a	840	CLA	C3B-C4B-NB	-2.12	108.64	110.53
14	k	102	CLA	C3B-C4B-NB	-2.12	108.64	110.53
14	A	838	CLA	CHD-C1D-ND	-2.12	121.82	124.80
14	A	824	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	B	826	CLA	C4-C3-C2	-2.12	118.19	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	k	103	CLA	CMB-C2B-C3B	-2.12	121.57	126.55
14	U	204	CLA	CHD-C1D-ND	-2.12	121.82	124.80
14	b	842	CLA	CHD-C1D-ND	-2.12	121.82	124.80
14	H	828	CLA	CHA-C1A-NA	-2.12	121.60	126.39
14	A	835	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	a	837	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	B	825	CLA	CHD-C1D-ND	-2.11	121.83	124.80
14	a	803	CLA	C3B-C4B-NB	-2.11	108.64	110.53
14	b	835	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
14	H	822	CLA	CHD-C1D-ND	-2.11	121.83	124.80
14	A	824	CLA	CHB-C4A-NA	2.11	127.45	124.40
14	B	811	CLA	C3B-C4B-NB	-2.11	108.64	110.53
14	A	817	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	K	102	CLA	CMB-C2B-C1B	2.11	128.63	125.42
14	H	820	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	B	825	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
14	a	836	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	b	834	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
17	a	851	BCR	C30-C25-C26	-2.11	119.76	122.64
14	B	842	CLA	CHD-C1D-ND	-2.11	121.84	124.80
14	b	844	CLA	C4A-NA-C1A	2.11	107.64	106.68
14	H	816	CLA	CHB-C4A-NA	2.11	127.44	124.40
14	a	832	CLA	C3B-C4B-NB	-2.10	108.65	110.53
14	b	839	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
14	b	843	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
14	B	843	CLA	CHB-C4A-NA	2.10	127.44	124.40
14	B	843	CLA	CHA-C1A-NA	-2.10	121.63	126.39
14	B	814	CLA	CHD-C1D-ND	-2.10	121.84	124.80
14	a	824	CLA	CHA-C1A-NA	-2.10	121.63	126.39
14	A	823	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	H	817	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	H	840	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	H	842	CLA	CHD-C1D-ND	-2.10	121.84	124.80
14	B	838	CLA	CMB-C2B-C1B	2.10	128.62	125.42
14	l	5006	CLA	CHD-C1D-ND	-2.10	121.85	124.80
14	H	816	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	G	829	CLA	CHA-C1A-NA	-2.10	121.64	126.39
14	B	815	CLA	C3B-C2B-C1B	-2.10	104.70	107.17
14	a	821	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	a	802	CL0	C3B-C4B-NB	-2.10	108.66	110.53
14	H	814	CLA	CHD-C1D-ND	-2.10	121.85	124.80
14	b	812	CLA	C3B-C2B-C1B	-2.10	104.70	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	830	CLA	C3B-C4B-NB	-2.10	108.66	110.53
14	b	824	CLA	CHB-C4A-NA	2.10	127.42	124.40
14	H	818	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	G	807	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	A	837	CLA	C1-C2-C3	-2.09	122.77	126.20
14	a	835	CLA	C3B-C4B-NB	-2.09	108.66	110.53
14	H	839	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	B	838	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	H	827	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	A	808	CLA	C1-C2-C3	-2.09	122.77	126.20
14	B	822	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	B	809	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
14	G	830	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
14	a	840	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	b	815	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
14	A	803	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	a	802	CL0	C3B-C2B-C1B	-2.09	104.71	107.17
14	B	816	CLA	C1-C2-C3	-2.09	122.77	126.20
14	b	824	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	G	833	CLA	C1-C2-C3	-2.09	122.78	126.20
14	A	829	CLA	C3B-C4B-NB	-2.09	108.67	110.53
14	H	816	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
14	B	815	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	H	809	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	a	812	CLA	CHD-C1D-ND	-2.09	121.86	124.80
18	B	853	LMG	O1-C7-C8	-2.09	105.74	110.82
14	G	829	CLA	CHB-C4A-NA	2.09	127.41	124.40
14	H	839	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
14	H	838	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
13	a	802	CL0	CHD-C1D-ND	-2.09	121.87	124.80
14	A	829	CLA	CHD-C1D-ND	-2.09	121.87	124.80
14	b	831	CLA	C3B-C4B-NB	-2.08	108.67	110.53
14	b	816	CLA	CHD-C1D-ND	-2.08	121.87	124.80
13	G	801	CL0	C3B-C2B-C1B	-2.08	104.71	107.17
14	G	814	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	b	828	CLA	C3B-C4B-NB	-2.08	108.67	110.53
14	a	834	CLA	CMB-C2B-C1B	2.08	128.59	125.42
14	a	805	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	B	827	CLA	CHD-C1D-ND	-2.08	121.87	124.80
14	a	835	CLA	C4A-NA-C1A	2.08	107.63	106.68
14	G	809	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
14	b	842	CLA	O2A-CGA-O1A	-2.08	118.42	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	831	CLA	C1-C2-C3	-2.08	122.79	126.20
14	H	817	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
14	G	808	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	a	838	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	a	842	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
14	F	203	CLA	C3B-C4B-NB	-2.08	108.68	110.53
14	H	819	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	B	801	CLA	CHD-C1D-ND	-2.08	121.88	124.80
14	G	804	CLA	CHB-C4A-NA	2.08	127.40	124.40
14	H	839	CLA	CHD-C1D-ND	-2.08	121.88	124.80
14	b	802	CLA	CHD-C1D-ND	-2.08	121.88	124.80
14	G	837	CLA	CHD-C1D-ND	-2.07	121.88	124.80
14	A	837	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
14	G	835	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
14	A	823	CLA	C4A-NA-C1A	2.07	107.62	106.68
14	f	201	CLA	C4A-NA-C1A	2.07	107.62	106.68
14	a	840	CLA	C3B-C2B-C1B	-2.07	104.72	107.17
14	S	1101	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	a	815	CLA	C1C-C2C-C3C	-2.07	104.80	106.98
14	H	840	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
14	H	839	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	A	804	CLA	C3B-C4B-NB	-2.07	108.68	110.53
14	b	832	CLA	CHA-C1A-NA	-2.07	121.70	126.39
19	a	856	LMT	C1-O1'-C1'	2.07	117.22	113.68
14	A	812	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	A	807	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	a	813	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	G	834	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	B	843	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	B	820	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	b	818	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	A	835	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
14	H	811	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	U	204	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	K	101	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	a	835	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	a	803	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	b	802	CLA	CHB-C4A-NA	2.07	127.38	124.40
14	A	840	CLA	C3B-C4B-NB	-2.07	108.69	110.53
14	H	824	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	B	819	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
14	a	843	CLA	C1-C2-C3	-2.07	122.81	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	1503	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
14	B	837	CLA	C3B-C4B-NB	-2.07	108.69	110.53
14	Q	202	CLA	C3B-C4B-NB	-2.07	108.69	110.53
14	L	1503	CLA	CHD-C1D-ND	-2.07	121.90	124.80
14	B	821	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	L	1503	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	H	806	CLA	C3B-C2B-C1B	-2.06	104.73	107.17
14	L	1502	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	A	827	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
14	B	813	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
19	Q	201	LMT	C1B-O1B-C4'	2.06	122.87	117.98
14	K	103	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	a	816	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	H	837	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
14	a	836	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	a	818	CLA	CHA-C1A-NA	-2.06	121.72	126.39
14	b	801	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	H	833	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	S	1103	CLA	CHD-C1D-ND	-2.06	121.91	124.80
14	G	829	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	G	803	CLA	CHB-C4A-NA	2.06	127.37	124.40
14	b	823	CLA	C1-C2-C3	-2.06	122.82	126.20
14	b	801	CLA	CHB-C4A-NA	2.06	127.37	124.40
14	G	826	CLA	CHD-C1D-ND	-2.06	121.91	124.80
14	b	812	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	a	822	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	a	844	CLA	C4A-NA-C1A	2.06	107.62	106.68
14	b	818	CLA	CHD-C1D-ND	-2.06	121.91	124.80
14	H	825	CLA	CHA-C1A-NA	-2.06	121.74	126.39
14	G	830	CLA	C2A-C1A-CHA	2.05	127.43	123.87
14	b	843	CLA	C4-C3-C2	-2.05	118.35	123.63
14	A	844	CLA	CHD-C1D-ND	-2.05	121.91	124.80
14	H	841	CLA	C3B-C4B-NB	-2.05	108.70	110.53
14	b	838	CLA	CHD-C1D-ND	-2.05	121.91	124.80
14	A	841	CLA	C1-C2-C3	-2.05	122.83	126.20
14	A	834	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
14	b	841	CLA	C3B-C4B-NB	-2.05	108.70	110.53
14	S	1101	CLA	C1-C2-C3	-2.05	122.84	126.20
14	l	5006	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
14	B	808	CLA	CHD-C1D-ND	-2.05	121.92	124.80
14	a	817	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
14	L	1503	CLA	C1C-C2C-C3C	-2.05	104.83	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	k	101	CLA	CHD-C1D-ND	-2.05	121.92	124.80
14	b	818	CLA	C1-C2-C3	-2.05	122.84	126.20
14	b	837	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
14	A	858	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	B	818	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	A	805	CLA	C4A-NA-C1A	2.04	107.61	106.68
14	G	838	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	A	842	CLA	C1-C2-C3	-2.04	122.85	126.20
14	A	813	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	H	807	CLA	CHD-C1D-ND	-2.04	121.93	124.80
14	B	823	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	U	204	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
14	U	206	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	G	803	CLA	CHD-C1D-ND	-2.04	121.93	124.80
14	a	831	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
14	a	810	CLA	CHD-C1D-ND	-2.04	121.93	124.80
14	b	813	CLA	CHD-C1D-ND	-2.04	121.93	124.80
14	A	827	CLA	CHD-C1D-ND	-2.04	121.94	124.80
14	G	823	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	U	202	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
14	a	830	CLA	C2A-C1A-CHA	2.04	127.40	123.87
14	H	826	CLA	CHA-C1A-NA	-2.04	121.78	126.39
14	a	824	CLA	CHD-C1D-ND	-2.04	121.94	124.80
14	A	829	CLA	C2A-C1A-CHA	2.04	127.40	123.87
14	A	842	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	a	813	CLA	CHD-C1D-ND	-2.03	121.94	124.80
14	b	832	CLA	CHD-C1D-ND	-2.03	121.94	124.80
14	H	824	CLA	C3B-C4B-NB	-2.03	108.71	110.53
14	G	809	CLA	C1-C2-C3	-2.03	122.86	126.20
14	a	809	CLA	C1-C2-C3	-2.03	122.86	126.20
14	T	102	CLA	CMB-C2B-C1B	2.03	128.51	125.42
14	H	813	CLA	CHA-C1A-NA	-2.03	121.79	126.39
14	b	808	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
14	H	831	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
14	a	836	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
14	G	820	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
14	L	1502	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
14	H	825	CLA	C3B-C4B-NB	-2.03	108.72	110.53
14	U	202	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
14	H	835	CLA	CHA-C1A-NA	-2.03	121.80	126.39
14	A	831	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
14	b	828	CLA	CHA-C1A-NA	-2.03	121.80	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	813	CLA	C1-C2-C3	-2.03	122.88	126.20
14	b	817	CLA	C1C-C2C-C3C	-2.03	104.85	106.98
14	A	807	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
14	j	102	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
14	b	815	CLA	CHD-C1D-ND	-2.03	121.95	124.80
14	H	810	CLA	CHA-C1A-NA	-2.03	121.80	126.39
14	B	810	CLA	CHD-C1D-ND	-2.03	121.95	124.80
14	H	813	CLA	C1-C2-C3	-2.03	122.88	126.20
14	H	840	CLA	CHB-C4A-NA	2.02	127.32	124.40
14	H	810	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
14	b	823	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
14	a	806	CLA	C7-C6-C5	-2.02	107.87	113.26
14	A	809	CLA	C1-C2-C3	-2.02	122.88	126.20
14	G	803	CLA	C3B-C4B-NB	-2.02	108.72	110.53
14	b	834	CLA	C3B-C4B-NB	-2.02	108.72	110.53
14	K	102	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
14	G	804	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	a	839	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	a	824	CLA	C1-C2-C3	-2.02	122.89	126.20
14	H	810	CLA	C3B-C4B-NB	-2.02	108.73	110.53
14	B	830	CLA	CHB-C4A-NA	2.02	127.32	124.40
14	b	841	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	T	102	CLA	C3B-C4B-NB	-2.02	108.73	110.53
14	T	102	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
14	a	806	CLA	C1-O2A-CGA	2.02	121.54	116.65
14	b	811	CLA	CHD-C1D-ND	-2.02	121.96	124.80
14	j	101	CLA	CHA-C1A-NA	-2.02	121.82	126.39
14	f	205	CLA	CHB-C4A-NA	2.02	127.31	124.40
14	A	836	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
14	A	807	CLA	C3B-C4B-NB	-2.02	108.73	110.53
14	a	843	CLA	C3B-C2B-C1B	-2.02	104.79	107.17
14	a	804	CLA	C1-C2-C3	-2.02	122.89	126.20
14	B	835	CLA	C4A-NA-C1A	2.02	107.60	106.68
14	S	1101	CLA	C3B-C2B-C1B	-2.01	104.79	107.17
14	b	807	CLA	C4A-NA-C1A	2.01	107.60	106.68
14	G	818	CLA	CHD-C1D-ND	-2.01	121.97	124.80
14	H	817	CLA	C1-C2-C3	-2.01	122.90	126.20
17	f	202	BCR	C16-C15-C14	-2.01	119.40	123.52
14	J	1102	CLA	CHD-C1D-ND	-2.01	121.97	124.80
14	A	838	CLA	C1-C2-C3	-2.01	122.90	126.20
14	G	832	CLA	CHD-C1D-C2D	2.01	129.67	125.49
14	b	806	CLA	O2A-CGA-O1A	-2.01	118.59	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	818	CLA	CHB-C4A-NA	2.01	127.30	124.40
14	G	821	CLA	CHA-C1A-NA	-2.01	121.83	126.39
14	A	821	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	b	812	CLA	C3B-C4B-NB	-2.01	108.73	110.53
14	a	810	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	H	803	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	H	812	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	G	821	CLA	C4A-NA-C1A	2.01	107.60	106.68
14	a	820	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	B	807	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	B	828	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	H	830	CLA	C3B-C4B-NB	-2.01	108.74	110.53
14	a	837	CLA	CHB-C4A-NA	2.01	127.30	124.40
14	B	838	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	G	802	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	H	818	CLA	CHD-C1D-ND	-2.01	121.98	124.80
14	B	812	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	a	829	CLA	C3B-C4B-NB	-2.01	108.74	110.53
14	A	816	CLA	CHD-C1D-ND	-2.01	121.98	124.80
14	a	823	CLA	C4A-NA-C1A	2.01	107.59	106.68
14	a	808	CLA	CHB-C4A-NA	2.01	127.29	124.40
14	a	835	CLA	C1C-C2C-C3C	-2.01	104.87	106.98
14	A	837	CLA	CHA-C1A-NA	-2.00	121.85	126.39
14	a	845	CLA	CMB-C2B-C1B	2.00	128.47	125.42
14	H	837	CLA	C1-C2-C3	-2.00	123.52	126.76
14	G	818	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
13	A	802	CL0	O2A-CGA-O1A	-2.00	118.62	123.63
14	A	810	CLA	C3B-C2B-C1B	-2.00	104.81	107.17
14	H	824	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	J	1102	CLA	CHA-C1A-NA	-2.00	121.86	126.39
17	a	851	BCR	C40-C30-C25	2.00	113.38	110.24
14	a	810	CLA	CHB-C4A-NA	2.00	127.29	124.40
14	a	822	CLA	C7-C6-C5	-2.00	107.93	113.26

There are no chirality outliers.

All (2988) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	LHG	C3-O3-P-O5
12	A	801	LHG	C4-O6-P-O5
12	A	801	LHG	O9-C7-O7-C5
12	A	854	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
12	B	851	LHG	C3-O3-P-O6
12	G	854	LHG	C3-O3-P-O5
12	G	854	LHG	C4-O6-P-O3
12	G	854	LHG	C4-O6-P-O5
12	G	854	LHG	O9-C7-O7-C5
12	G	855	LHG	C3-O3-P-O5
12	G	856	LHG	C3-O3-P-O6
12	G	856	LHG	C4-O6-P-O3
12	G	856	LHG	C8-C7-O7-C5
12	H	850	LHG	C3-O3-P-O4
12	H	850	LHG	C3-O3-P-O5
12	H	850	LHG	C3-O3-P-O6
12	L	1509	LHG	C2-C3-O3-P
12	L	1509	LHG	O9-C7-O7-C5
12	L	1509	LHG	C8-C7-O7-C5
12	L	1510	LHG	C2-C3-O3-P
12	L	1510	LHG	C3-O3-P-O4
12	L	1510	LHG	C3-O3-P-O5
12	L	1510	LHG	C3-O3-P-O6
12	L	1510	LHG	C8-C7-O7-C5
12	M	101	LHG	C2-C3-O3-P
12	M	101	LHG	C3-O3-P-O4
12	M	102	LHG	C2-C3-O3-P
12	M	102	LHG	O9-C7-O7-C5
12	M	104	LHG	C2-C3-O3-P
12	V	101	LHG	C2-C3-O3-P
12	V	101	LHG	O9-C7-O7-C5
12	a	801	LHG	O9-C7-O7-C5
12	a	855	LHG	C3-O3-P-O5
12	b	852	LHG	C3-O3-P-O6
13	A	802	CL0	C2-C3-C5-C6
13	A	802	CL0	C4-C3-C5-C6
13	G	801	CL0	C4-C3-C5-C6
13	a	802	CL0	C4-C3-C5-C6
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	CHA-CBD-CGD-O1D
14	A	806	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	808	CLA	CHA-CBD-CGD-O1D
14	A	808	CLA	CHA-CBD-CGD-O2D
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	C2-C3-C5-C6
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	810	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	CHA-CBD-CGD-O1D
14	A	811	CLA	CHA-CBD-CGD-O2D
14	A	818	CLA	C1A-C2A-CAA-CBA
14	A	818	CLA	C3A-C2A-CAA-CBA
14	A	818	CLA	C2B-C3B-CAB-CBB
14	A	818	CLA	C4B-C3B-CAB-CBB
14	A	822	CLA	C1A-C2A-CAA-CBA
14	A	822	CLA	C3A-C2A-CAA-CBA
14	A	822	CLA	CHA-CBD-CGD-O2D
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	824	CLA	C4B-C3B-CAB-CBB
14	A	825	CLA	CHA-CBD-CGD-O1D
14	A	825	CLA	CHA-CBD-CGD-O2D
14	A	829	CLA	C1A-C2A-CAA-CBA
14	A	830	CLA	CHA-CBD-CGD-O1D
14	A	830	CLA	CHA-CBD-CGD-O2D
14	A	833	CLA	C2B-C3B-CAB-CBB
14	A	833	CLA	C4B-C3B-CAB-CBB
14	A	834	CLA	CHA-CBD-CGD-O1D
14	A	834	CLA	CHA-CBD-CGD-O2D
14	A	841	CLA	C1A-C2A-CAA-CBA
14	A	844	CLA	CBA-CGA-O2A-C1
14	B	807	CLA	C1A-C2A-CAA-CBA
14	B	809	CLA	C1A-C2A-CAA-CBA
14	B	810	CLA	CHA-CBD-CGD-O1D
14	B	810	CLA	CHA-CBD-CGD-O2D
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	813	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	CHA-CBD-CGD-O1D
14	B	817	CLA	CHA-CBD-CGD-O2D
14	B	820	CLA	C1A-C2A-CAA-CBA
14	B	820	CLA	C3A-C2A-CAA-CBA
14	B	826	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	B	826	CLA	CHA-CBD-CGD-O2D
14	B	827	CLA	CHA-CBD-CGD-O1D
14	B	827	CLA	CHA-CBD-CGD-O2D
14	B	837	CLA	CBA-CGA-O2A-C1
14	F	201	CLA	C1A-C2A-CAA-CBA
14	F	203	CLA	C1A-C2A-CAA-CBA
14	F	203	CLA	C3A-C2A-CAA-CBA
14	F	204	CLA	C4B-C3B-CAB-CBB
14	F	204	CLA	CBD-CGD-O2D-CED
14	G	806	CLA	C1A-C2A-CAA-CBA
14	G	807	CLA	C1A-C2A-CAA-CBA
14	G	807	CLA	CHA-CBD-CGD-O2D
14	G	809	CLA	CHA-CBD-CGD-O1D
14	G	809	CLA	CHA-CBD-CGD-O2D
14	G	810	CLA	C1A-C2A-CAA-CBA
14	G	810	CLA	C3A-C2A-CAA-CBA
14	G	812	CLA	CHA-CBD-CGD-O1D
14	G	812	CLA	CHA-CBD-CGD-O2D
14	G	813	CLA	C1A-C2A-CAA-CBA
14	G	815	CLA	CHA-CBD-CGD-O1D
14	G	815	CLA	CHA-CBD-CGD-O2D
14	G	818	CLA	C1A-C2A-CAA-CBA
14	G	819	CLA	C1A-C2A-CAA-CBA
14	G	819	CLA	C3A-C2A-CAA-CBA
14	G	819	CLA	C2B-C3B-CAB-CBB
14	G	819	CLA	C4B-C3B-CAB-CBB
14	G	823	CLA	C1A-C2A-CAA-CBA
14	G	824	CLA	C1A-C2A-CAA-CBA
14	G	826	CLA	CHA-CBD-CGD-O1D
14	G	826	CLA	CHA-CBD-CGD-O2D
14	G	830	CLA	C1A-C2A-CAA-CBA
14	G	831	CLA	CHA-CBD-CGD-O1D
14	G	831	CLA	CHA-CBD-CGD-O2D
14	G	834	CLA	C4B-C3B-CAB-CBB
14	G	835	CLA	C11-C10-C8-C9
14	G	843	CLA	C4B-C3B-CAB-CBB
14	H	806	CLA	C1A-C2A-CAA-CBA
14	H	806	CLA	C2-C3-C5-C6
14	H	806	CLA	C4-C3-C5-C6
14	H	808	CLA	C1A-C2A-CAA-CBA
14	H	809	CLA	C4B-C3B-CAB-CBB
14	H	809	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	H	809	CLA	CHA-CBD-CGD-O2D
14	H	812	CLA	C1A-C2A-CAA-CBA
14	H	812	CLA	C3A-C2A-CAA-CBA
14	H	813	CLA	C1A-C2A-CAA-CBA
14	H	819	CLA	C1A-C2A-CAA-CBA
14	H	819	CLA	C3A-C2A-CAA-CBA
14	H	825	CLA	CHA-CBD-CGD-O1D
14	H	825	CLA	CHA-CBD-CGD-O2D
14	H	826	CLA	CHA-CBD-CGD-O1D
14	H	826	CLA	CHA-CBD-CGD-O2D
14	H	830	CLA	C1A-C2A-CAA-CBA
14	J	1103	CLA	C1A-C2A-CAA-CBA
14	J	1103	CLA	C3A-C2A-CAA-CBA
14	K	102	CLA	CHA-CBD-CGD-O2D
14	K	102	CLA	CBD-CGD-O2D-CED
14	K	103	CLA	C3A-C2A-CAA-CBA
14	L	1501	CLA	C1A-C2A-CAA-CBA
14	Q	202	CLA	C1A-C2A-CAA-CBA
14	Q	205	CLA	CHA-CBD-CGD-O1D
14	Q	205	CLA	CHA-CBD-CGD-O2D
14	S	1103	CLA	C1A-C2A-CAA-CBA
14	S	1103	CLA	C3A-C2A-CAA-CBA
14	S	1103	CLA	CBD-CGD-O2D-CED
14	T	101	CLA	CHA-CBD-CGD-O2D
14	T	102	CLA	CHA-CBD-CGD-O1D
14	T	102	CLA	CHA-CBD-CGD-O2D
14	T	102	CLA	CBD-CGD-O2D-CED
14	U	202	CLA	CHA-CBD-CGD-O1D
14	U	202	CLA	CHA-CBD-CGD-O2D
14	U	204	CLA	C1A-C2A-CAA-CBA
14	U	204	CLA	C3A-C2A-CAA-CBA
14	a	805	CLA	CHA-CBD-CGD-O1D
14	a	805	CLA	CHA-CBD-CGD-O2D
14	a	806	CLA	C1A-C2A-CAA-CBA
14	a	806	CLA	C3A-C2A-CAA-CBA
14	a	807	CLA	C1A-C2A-CAA-CBA
14	a	809	CLA	CHA-CBD-CGD-O1D
14	a	809	CLA	CHA-CBD-CGD-O2D
14	a	810	CLA	C1A-C2A-CAA-CBA
14	a	810	CLA	C3A-C2A-CAA-CBA
14	a	812	CLA	CHA-CBD-CGD-O1D
14	a	812	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	a	817	CLA	C4B-C3B-CAB-CBB
14	a	818	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	C4B-C3B-CAB-CBB
14	a	823	CLA	C1A-C2A-CAA-CBA
14	a	823	CLA	CHA-CBD-CGD-O1D
14	a	823	CLA	CHA-CBD-CGD-O2D
14	a	824	CLA	C1A-C2A-CAA-CBA
14	a	825	CLA	C4B-C3B-CAB-CBB
14	a	826	CLA	CHA-CBD-CGD-O1D
14	a	826	CLA	CHA-CBD-CGD-O2D
14	a	830	CLA	C1A-C2A-CAA-CBA
14	a	831	CLA	CHA-CBD-CGD-O1D
14	a	831	CLA	CHA-CBD-CGD-O2D
14	a	834	CLA	C2B-C3B-CAB-CBB
14	a	834	CLA	C4B-C3B-CAB-CBB
14	a	835	CLA	CHA-CBD-CGD-O1D
14	a	835	CLA	CHA-CBD-CGD-O2D
14	a	844	CLA	C4B-C3B-CAB-CBB
14	a	845	CLA	CBA-CGA-O2A-C1
14	a	845	CLA	O1A-CGA-O2A-C1
14	b	808	CLA	C1A-C2A-CAA-CBA
14	b	808	CLA	C4-C3-C5-C6
14	b	810	CLA	C1A-C2A-CAA-CBA
14	b	811	CLA	CHA-CBD-CGD-O1D
14	b	811	CLA	CHA-CBD-CGD-O2D
14	b	814	CLA	C1A-C2A-CAA-CBA
14	b	814	CLA	C3A-C2A-CAA-CBA
14	b	815	CLA	C1A-C2A-CAA-CBA
14	b	815	CLA	C3A-C2A-CAA-CBA
14	b	818	CLA	CHA-CBD-CGD-O1D
14	b	818	CLA	CHA-CBD-CGD-O2D
14	b	821	CLA	C1A-C2A-CAA-CBA
14	b	821	CLA	C3A-C2A-CAA-CBA
14	b	827	CLA	CHA-CBD-CGD-O1D
14	b	827	CLA	CHA-CBD-CGD-O2D
14	b	828	CLA	CHA-CBD-CGD-O1D
14	b	828	CLA	CHA-CBD-CGD-O2D
14	b	832	CLA	C1A-C2A-CAA-CBA
14	b	832	CLA	C14-C13-C15-C16
14	b	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	835	CLA	C3A-C2A-CAA-CBA
14	b	842	CLA	C14-C13-C15-C16
14	f	201	CLA	C1A-C2A-CAA-CBA
14	f	204	CLA	C1A-C2A-CAA-CBA
14	f	204	CLA	C3A-C2A-CAA-CBA
14	f	205	CLA	CHA-CBD-CGD-O1D
14	f	205	CLA	CHA-CBD-CGD-O2D
14	j	102	CLA	C3A-C2A-CAA-CBA
14	j	102	CLA	CBD-CGD-O2D-CED
14	k	101	CLA	CHA-CBD-CGD-O1D
14	k	101	CLA	CHA-CBD-CGD-O2D
14	k	102	CLA	CBD-CGD-O2D-CED
14	l	5004	CLA	C1A-C2A-CAA-CBA
14	l	5004	CLA	C3A-C2A-CAA-CBA
17	A	848	BCR	C7-C8-C9-C10
17	A	850	BCR	C23-C24-C25-C30
17	A	851	BCR	C17-C18-C19-C20
17	A	851	BCR	C23-C24-C25-C26
17	B	845	BCR	C21-C22-C23-C24
17	B	845	BCR	C37-C22-C23-C24
17	B	845	BCR	C23-C24-C25-C26
17	B	846	BCR	C11-C12-C13-C14
17	B	849	BCR	C7-C8-C9-C10
17	B	856	BCR	C23-C24-C25-C26
17	F	202	BCR	C11-C12-C13-C14
17	F	202	BCR	C17-C18-C19-C20
17	F	202	BCR	C21-C22-C23-C24
17	F	202	BCR	C37-C22-C23-C24
17	G	849	BCR	C21-C22-C23-C24
17	G	849	BCR	C37-C22-C23-C24
17	G	850	BCR	C17-C18-C19-C20
17	G	850	BCR	C23-C24-C25-C26
17	G	850	BCR	C23-C24-C25-C30
17	G	851	BCR	C17-C18-C19-C20
17	G	851	BCR	C21-C22-C23-C24
17	G	851	BCR	C23-C24-C25-C26
17	H	844	BCR	C23-C24-C25-C26
17	H	848	BCR	C7-C8-C9-C10
17	H	854	BCR	C23-C24-C25-C26
17	I	101	BCR	C21-C22-C23-C24
17	I	101	BCR	C37-C22-C23-C24
17	I	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
17	J	1104	BCR	C11-C12-C13-C14
17	J	1104	BCR	C11-C12-C13-C35
17	J	1105	BCR	C17-C18-C19-C20
17	J	1105	BCR	C36-C18-C19-C20
17	J	1105	BCR	C21-C22-C23-C24
17	L	1504	BCR	C21-C22-C23-C24
17	L	1504	BCR	C37-C22-C23-C24
17	L	1504	BCR	C23-C24-C25-C30
17	Q	203	BCR	C11-C12-C13-C14
17	Q	203	BCR	C17-C18-C19-C20
17	R	101	BCR	C17-C18-C19-C20
17	R	103	BCR	C21-C22-C23-C24
17	R	103	BCR	C37-C22-C23-C24
17	R	103	BCR	C23-C24-C25-C30
17	S	1104	BCR	C7-C8-C9-C10
17	S	1104	BCR	C11-C12-C13-C14
17	S	1104	BCR	C11-C12-C13-C35
17	S	1105	BCR	C11-C12-C13-C14
17	S	1105	BCR	C17-C18-C19-C20
17	S	1105	BCR	C36-C18-C19-C20
17	S	1105	BCR	C21-C22-C23-C24
17	U	203	BCR	C1-C6-C7-C8
17	a	849	BCR	C5-C6-C7-C8
17	a	849	BCR	C7-C8-C9-C10
17	a	849	BCR	C7-C8-C9-C34
17	a	851	BCR	C23-C24-C25-C26
17	a	852	BCR	C17-C18-C19-C20
17	a	852	BCR	C36-C18-C19-C20
17	a	852	BCR	C23-C24-C25-C26
17	a	852	BCR	C23-C24-C25-C30
17	b	846	BCR	C23-C24-C25-C26
17	b	856	BCR	C7-C8-C9-C10
17	b	856	BCR	C23-C24-C25-C26
17	f	202	BCR	C11-C12-C13-C14
17	f	202	BCR	C17-C18-C19-C20
17	f	202	BCR	C36-C18-C19-C20
17	f	202	BCR	C21-C22-C23-C24
17	f	202	BCR	C37-C22-C23-C24
17	i	101	BCR	C17-C18-C19-C20
17	j	103	BCR	C11-C12-C13-C14
17	j	103	BCR	C11-C12-C13-C35
17	j	104	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
17	k	104	BCR	C23-C24-C25-C26
17	l	5003	BCR	C1-C6-C7-C8
17	l	5007	BCR	C21-C22-C23-C24
17	l	5007	BCR	C37-C22-C23-C24
17	l	5007	BCR	C23-C24-C25-C30
18	B	852	LMG	C11-C10-O7-C8
18	G	852	LMG	O9-C10-O7-C8
18	H	851	LMG	C2-C1-O1-C7
18	H	851	LMG	O6-C1-O1-C7
18	H	851	LMG	C11-C10-O7-C8
18	K	105	LMG	O9-C10-O7-C8
18	K	105	LMG	C11-C10-O7-C8
18	a	853	LMG	O9-C10-O7-C8
18	l	5001	LMG	O9-C10-O7-C8
18	l	5001	LMG	C11-C10-O7-C8
19	L	1505	LMT	O5'-C1'-O1'-C1
19	L	1505	LMT	C2-C1-O1'-C1'
19	a	856	LMT	C3'-C4'-O1B-C1B
19	a	856	LMT	O5'-C1'-O1'-C1
21	B	847	ECH	C7-C8-C9-C10
21	B	847	ECH	C7-C8-C9-C34
21	H	846	ECH	C7-C8-C9-C10
21	H	846	ECH	C7-C8-C9-C34
21	L	1506	ECH	C1-C6-C7-C8
21	M	103	ECH	C9-C10-C11-C12
21	M	103	ECH	C11-C12-C13-C35
21	V	102	ECH	C9-C10-C11-C12
21	V	102	ECH	C23-C24-C25-C26
21	V	102	ECH	C23-C24-C25-C30
21	b	848	ECH	C7-C8-C9-C10
21	b	848	ECH	C7-C8-C9-C34
21	m	101	ECH	C5-C6-C7-C8
21	m	101	ECH	C11-C12-C13-C14
21	m	101	ECH	C11-C12-C13-C35
21	m	101	ECH	C23-C24-C25-C26
19	L	1505	LMT	C5'-C4'-O1B-C1B
19	f	203	LMT	C3'-C4'-O1B-C1B
14	K	102	CLA	C4C-C3C-CAC-CBC
14	J	1103	CLA	O1D-CGD-O2D-CED
19	A	856	LMT	C3'-C4'-O1B-C1B
19	H	852	LMT	C3'-C4'-O1B-C1B
19	Q	201	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
14	A	806	CLA	O1D-CGD-O2D-CED
14	G	807	CLA	O1D-CGD-O2D-CED
14	K	102	CLA	O1D-CGD-O2D-CED
14	S	1103	CLA	O1D-CGD-O2D-CED
14	T	102	CLA	O1D-CGD-O2D-CED
14	j	102	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	CBD-CGD-O2D-CED
14	A	810	CLA	CBD-CGD-O2D-CED
14	B	842	CLA	CBD-CGD-O2D-CED
14	G	807	CLA	CBD-CGD-O2D-CED
14	G	811	CLA	CBD-CGD-O2D-CED
14	H	841	CLA	CBD-CGD-O2D-CED
14	J	1103	CLA	CBD-CGD-O2D-CED
14	Q	205	CLA	CBD-CGD-O2D-CED
14	f	205	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	O1A-CGA-O2A-C1
14	B	817	CLA	O1A-CGA-O2A-C1
14	a	821	CLA	O1A-CGA-O2A-C1
18	L	1508	LMG	O10-C28-O8-C9
18	U	201	LMG	O10-C28-O8-C9
14	A	844	CLA	O1A-CGA-O2A-C1
14	T	102	CLA	C4C-C3C-CAC-CBC
14	F	204	CLA	CBA-CGA-O2A-C1
14	f	205	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
14	G	821	CLA	CBA-CGA-O2A-C1
14	a	821	CLA	CBA-CGA-O2A-C1
18	L	1508	LMG	C29-C28-O8-C9
18	U	201	LMG	C29-C28-O8-C9
18	l	5001	LMG	C29-C28-O8-C9
14	F	203	CLA	CBD-CGD-O2D-CED
14	T	101	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	O1A-CGA-O2A-C1
14	B	831	CLA	O1A-CGA-O2A-C1
14	F	201	CLA	O1A-CGA-O2A-C1
14	G	806	CLA	O1A-CGA-O2A-C1
14	G	812	CLA	O1A-CGA-O2A-C1
14	G	821	CLA	O1A-CGA-O2A-C1
14	G	825	CLA	O1A-CGA-O2A-C1
14	G	831	CLA	O1A-CGA-O2A-C1
14	H	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	H	832	CLA	O1A-CGA-O2A-C1
14	Q	202	CLA	O1A-CGA-O2A-C1
14	a	806	CLA	O1A-CGA-O2A-C1
14	a	826	CLA	O1A-CGA-O2A-C1
14	a	831	CLA	O1A-CGA-O2A-C1
14	b	832	CLA	O1A-CGA-O2A-C1
14	b	834	CLA	O1A-CGA-O2A-C1
14	f	201	CLA	O1A-CGA-O2A-C1
18	A	855	LMG	O10-C28-O8-C9
18	B	852	LMG	O10-C28-O8-C9
18	H	851	LMG	O10-C28-O8-C9
18	l	5001	LMG	O10-C28-O8-C9
14	B	837	CLA	O1A-CGA-O2A-C1
14	f	205	CLA	O1A-CGA-O2A-C1
14	k	102	CLA	C4C-C3C-CAC-CBC
14	k	102	CLA	O1D-CGD-O2D-CED
14	a	812	CLA	O1A-CGA-O2A-C1
12	L	1510	LHG	O9-C7-O7-C5
18	B	852	LMG	O9-C10-O7-C8
18	H	851	LMG	O9-C10-O7-C8
14	A	816	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	C3-C5-C6-C7
14	A	831	CLA	C3-C5-C6-C7
14	A	843	CLA	C3-C5-C6-C7
14	B	815	CLA	C3-C5-C6-C7
14	B	827	CLA	C3-C5-C6-C7
14	B	840	CLA	C3-C5-C6-C7
14	G	813	CLA	C3-C5-C6-C7
14	G	831	CLA	C3-C5-C6-C7
14	G	836	CLA	C3-C5-C6-C7
14	H	826	CLA	C3-C5-C6-C7
14	H	839	CLA	C3-C5-C6-C7
14	H	841	CLA	C3-C5-C6-C7
14	a	815	CLA	C3-C5-C6-C7
14	b	821	CLA	C3-C5-C6-C7
14	b	828	CLA	C3-C5-C6-C7
14	b	841	CLA	C3-C5-C6-C7
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	830	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	CBA-CGA-O2A-C1
14	F	201	CLA	CBA-CGA-O2A-C1
14	G	806	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	G	815	CLA	CBA-CGA-O2A-C1
14	G	825	CLA	CBA-CGA-O2A-C1
14	G	827	CLA	CBA-CGA-O2A-C1
14	G	830	CLA	CBA-CGA-O2A-C1
14	Q	202	CLA	CBA-CGA-O2A-C1
14	a	806	CLA	CBA-CGA-O2A-C1
14	a	815	CLA	CBA-CGA-O2A-C1
14	a	827	CLA	CBA-CGA-O2A-C1
14	a	832	CLA	CBA-CGA-O2A-C1
14	b	834	CLA	CBA-CGA-O2A-C1
14	b	841	CLA	CBA-CGA-O2A-C1
14	b	843	CLA	CBA-CGA-O2A-C1
14	f	201	CLA	CBA-CGA-O2A-C1
18	B	852	LMG	C29-C28-O8-C9
18	H	851	LMG	C29-C28-O8-C9
18	K	105	LMG	C29-C28-O8-C9
14	A	809	CLA	CBD-CGD-O2D-CED
14	G	821	CLA	CBD-CGD-O2D-CED
14	S	1102	CLA	CBD-CGD-O2D-CED
14	b	843	CLA	CBD-CGD-O2D-CED
14	f	204	CLA	CBD-CGD-O2D-CED
12	A	801	LHG	C8-C7-O7-C5
12	G	854	LHG	C8-C7-O7-C5
12	M	102	LHG	C8-C7-O7-C5
12	V	101	LHG	C8-C7-O7-C5
12	a	801	LHG	C8-C7-O7-C5
18	G	852	LMG	C11-C10-O7-C8
18	a	853	LMG	C11-C10-O7-C8
14	F	204	CLA	O1D-CGD-O2D-CED
14	H	816	CLA	O1A-CGA-O2A-C1
19	l	5008	LMT	C3'-C4'-O1B-C1B
14	B	807	CLA	C4-C3-C5-C6
14	B	813	CLA	C4-C3-C5-C6
14	b	814	CLA	C4-C3-C5-C6
14	l	5006	CLA	C4-C3-C5-C6
13	G	801	CL0	C2-C3-C5-C6
13	a	802	CL0	C2-C3-C5-C6
14	B	807	CLA	C2-C3-C5-C6
14	B	813	CLA	C2-C3-C5-C6
14	b	808	CLA	C2-C3-C5-C6
14	b	814	CLA	C2-C3-C5-C6
14	l	5006	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	H	836	CLA	CBA-CGA-O2A-C1
14	Q	205	CLA	CBA-CGA-O2A-C1
14	A	844	CLA	CBD-CGD-O2D-CED
14	G	810	CLA	CBD-CGD-O2D-CED
14	H	842	CLA	C2A-CAA-CBA-CGA
14	J	1103	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	C3-C5-C6-C7
14	B	826	CLA	C3-C5-C6-C7
14	G	815	CLA	C3-C5-C6-C7
14	H	819	CLA	C3-C5-C6-C7
14	H	825	CLA	C3-C5-C6-C7
14	U	204	CLA	C3-C5-C6-C7
14	b	827	CLA	C3-C5-C6-C7
12	V	101	LHG	C24-C23-O8-C6
14	A	811	CLA	CBA-CGA-O2A-C1
14	A	814	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	821	CLA	CBA-CGA-O2A-C1
14	B	831	CLA	CBA-CGA-O2A-C1
14	B	840	CLA	CBA-CGA-O2A-C1
14	G	805	CLA	CBA-CGA-O2A-C1
14	G	812	CLA	CBA-CGA-O2A-C1
14	G	831	CLA	CBA-CGA-O2A-C1
14	H	814	CLA	CBA-CGA-O2A-C1
14	H	820	CLA	CBA-CGA-O2A-C1
14	H	830	CLA	CBA-CGA-O2A-C1
14	H	832	CLA	CBA-CGA-O2A-C1
14	H	839	CLA	CBA-CGA-O2A-C1
14	H	841	CLA	CBA-CGA-O2A-C1
14	J	1103	CLA	CBA-CGA-O2A-C1
14	a	812	CLA	CBA-CGA-O2A-C1
14	a	813	CLA	CBA-CGA-O2A-C1
14	a	826	CLA	CBA-CGA-O2A-C1
14	a	830	CLA	CBA-CGA-O2A-C1
14	a	831	CLA	CBA-CGA-O2A-C1
14	b	816	CLA	CBA-CGA-O2A-C1
14	b	818	CLA	CBA-CGA-O2A-C1
14	b	822	CLA	CBA-CGA-O2A-C1
14	b	832	CLA	CBA-CGA-O2A-C1
14	l	5005	CLA	CBA-CGA-O2A-C1
18	A	855	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
14	H	836	CLA	O1A-CGA-O2A-C1
17	J	1105	BCR	C19-C20-C21-C22
14	A	826	CLA	O1A-CGA-O2A-C1
14	A	830	CLA	O1A-CGA-O2A-C1
14	G	827	CLA	O1A-CGA-O2A-C1
14	G	830	CLA	O1A-CGA-O2A-C1
14	H	841	CLA	O1A-CGA-O2A-C1
14	a	813	CLA	O1A-CGA-O2A-C1
14	a	815	CLA	O1A-CGA-O2A-C1
14	a	827	CLA	O1A-CGA-O2A-C1
14	b	816	CLA	O1A-CGA-O2A-C1
14	b	818	CLA	O1A-CGA-O2A-C1
14	b	841	CLA	O1A-CGA-O2A-C1
12	G	856	LHG	O9-C7-O7-C5
14	Q	205	CLA	O1D-CGD-O2D-CED
14	A	816	CLA	CBA-CGA-O2A-C1
14	F	204	CLA	O1A-CGA-O2A-C1
14	A	825	CLA	C3-C5-C6-C7
14	B	813	CLA	C3-C5-C6-C7
14	G	826	CLA	C3-C5-C6-C7
14	H	810	CLA	C3-C5-C6-C7
14	H	816	CLA	C3-C5-C6-C7
14	a	812	CLA	C3-C5-C6-C7
14	a	826	CLA	C3-C5-C6-C7
14	a	831	CLA	C3-C5-C6-C7
14	f	205	CLA	O1D-CGD-O2D-CED
12	M	102	LHG	C24-C23-O8-C6
14	A	828	CLA	CBA-CGA-O2A-C1
14	A	831	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	B	811	CLA	CBA-CGA-O2A-C1
14	H	810	CLA	CBA-CGA-O2A-C1
14	H	816	CLA	CBA-CGA-O2A-C1
14	L	1502	CLA	CBA-CGA-O2A-C1
14	S	1103	CLA	CBA-CGA-O2A-C1
14	U	205	CLA	CBA-CGA-O2A-C1
14	a	805	CLA	CBA-CGA-O2A-C1
14	a	829	CLA	CBA-CGA-O2A-C1
14	b	812	CLA	CBA-CGA-O2A-C1
14	b	823	CLA	CBA-CGA-O2A-C1
14	A	831	CLA	O1A-CGA-O2A-C1
14	B	833	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	G	815	CLA	O1A-CGA-O2A-C1
14	H	820	CLA	O1A-CGA-O2A-C1
14	a	832	CLA	O1A-CGA-O2A-C1
14	b	843	CLA	O1A-CGA-O2A-C1
14	l	5005	CLA	O1A-CGA-O2A-C1
18	K	105	LMG	O10-C28-O8-C9
18	B	803	LMG	C10-C11-C12-C13
14	G	829	CLA	CBD-CGD-O2D-CED
14	a	837	CLA	CBD-CGD-O2D-CED
18	L	1508	LMG	C11-C10-O7-C8
18	U	201	LMG	C11-C10-O7-C8
14	b	824	CLA	CBA-CGA-O2A-C1
14	A	811	CLA	O1A-CGA-O2A-C1
14	A	828	CLA	O1A-CGA-O2A-C1
14	B	811	CLA	O1A-CGA-O2A-C1
14	B	821	CLA	O1A-CGA-O2A-C1
14	H	814	CLA	O1A-CGA-O2A-C1
14	b	812	CLA	O1A-CGA-O2A-C1
14	b	823	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	O1D-CGD-O2D-CED
19	b	855	LMT	O1'-C1-C2-C3
14	A	830	CLA	C3-C5-C6-C7
14	B	838	CLA	C3-C5-C6-C7
14	G	812	CLA	C3-C5-C6-C7
14	b	818	CLA	C3-C5-C6-C7
18	H	801	LMG	C10-C11-C12-C13
14	H	841	CLA	O1D-CGD-O2D-CED
12	L	1510	LHG	C24-C23-O8-C6
14	B	833	CLA	CBA-CGA-O2A-C1
14	B	838	CLA	C4-C3-C5-C6
14	H	812	CLA	C4-C3-C5-C6
12	M	102	LHG	O10-C23-O8-C6
12	V	101	LHG	O10-C23-O8-C6
14	A	814	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	O1A-CGA-O2A-C1
14	A	832	CLA	O1A-CGA-O2A-C1
14	B	840	CLA	O1A-CGA-O2A-C1
14	G	805	CLA	O1A-CGA-O2A-C1
14	H	839	CLA	O1A-CGA-O2A-C1
14	L	1502	CLA	O1A-CGA-O2A-C1
14	S	1103	CLA	O1A-CGA-O2A-C1
14	b	822	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	817	CLA	CBA-CGA-O2A-C1
14	a	817	CLA	C2C-C3C-CAC-CBC
14	b	830	CLA	CBD-CGD-O2D-CED
14	G	842	CLA	C2A-CAA-CBA-CGA
12	L	1510	LHG	O10-C23-O8-C6
14	a	805	CLA	O1A-CGA-O2A-C1
14	a	829	CLA	O1A-CGA-O2A-C1
14	a	830	CLA	O1A-CGA-O2A-C1
18	B	852	LMG	O6-C1-O1-C7
14	B	842	CLA	O1D-CGD-O2D-CED
14	G	811	CLA	O1D-CGD-O2D-CED
14	T	101	CLA	O1D-CGD-O2D-CED
14	B	815	CLA	CBA-CGA-O2A-C1
14	G	807	CLA	CBA-CGA-O2A-C1
14	G	818	CLA	CBA-CGA-O2A-C1
14	G	826	CLA	CBA-CGA-O2A-C1
14	G	829	CLA	CBA-CGA-O2A-C1
14	B	806	CLA	CBD-CGD-O2D-CED
14	B	825	CLA	CBD-CGD-O2D-CED
14	B	831	CLA	CBD-CGD-O2D-CED
14	H	805	CLA	CBD-CGD-O2D-CED
14	H	819	CLA	CBD-CGD-O2D-CED
14	H	821	CLA	CBD-CGD-O2D-CED
14	a	819	CLA	CBD-CGD-O2D-CED
18	b	803	LMG	C10-C11-C12-C13
14	Q	205	CLA	O1A-CGA-O2A-C1
14	H	810	CLA	O1A-CGA-O2A-C1
14	U	205	CLA	O1A-CGA-O2A-C1
14	F	203	CLA	O1D-CGD-O2D-CED
14	a	810	CLA	O1D-CGD-O2D-CED
14	A	824	CLA	CBD-CGD-O2D-CED
14	b	814	CLA	CBD-CGD-O2D-CED
14	b	834	CLA	CBD-CGD-O2D-CED
14	l	5004	CLA	CBD-CGD-O2D-CED
14	G	818	CLA	O1A-CGA-O2A-C1
14	G	829	CLA	O1A-CGA-O2A-C1
18	L	1508	LMG	O9-C10-O7-C8
18	U	201	LMG	O9-C10-O7-C8
12	L	1509	LHG	C24-C23-O8-C6
14	B	813	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	CBA-CGA-O2A-C1
14	B	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	829	CLA	CBA-CGA-O2A-C1
14	B	832	CLA	CBA-CGA-O2A-C1
14	B	842	CLA	CBA-CGA-O2A-C1
14	G	833	CLA	CBA-CGA-O2A-C1
14	H	812	CLA	CBA-CGA-O2A-C1
14	H	818	CLA	CBA-CGA-O2A-C1
14	H	828	CLA	CBA-CGA-O2A-C1
14	H	831	CLA	CBA-CGA-O2A-C1
14	L	1503	CLA	CBA-CGA-O2A-C1
14	U	206	CLA	CBA-CGA-O2A-C1
14	a	833	CLA	CBA-CGA-O2A-C1
14	a	837	CLA	CBA-CGA-O2A-C1
14	b	814	CLA	CBA-CGA-O2A-C1
14	b	820	CLA	CBA-CGA-O2A-C1
14	b	830	CLA	CBA-CGA-O2A-C1
14	b	833	CLA	CBA-CGA-O2A-C1
14	b	835	CLA	CBA-CGA-O2A-C1
14	l	5006	CLA	CBA-CGA-O2A-C1
18	G	852	LMG	C29-C28-O8-C9
18	a	853	LMG	C29-C28-O8-C9
14	b	826	CLA	CBD-CGD-O2D-CED
14	b	840	CLA	C4-C3-C5-C6
14	B	838	CLA	C2-C3-C5-C6
14	b	840	CLA	C2-C3-C5-C6
14	a	844	CLA	C3-C5-C6-C7
14	A	804	CLA	C11-C12-C13-C14
14	A	805	CLA	C6-C7-C8-C9
14	A	824	CLA	C11-C12-C13-C14
14	B	823	CLA	C11-C10-C8-C9
14	B	831	CLA	C11-C10-C8-C9
14	B	831	CLA	C14-C13-C15-C16
14	B	840	CLA	C11-C10-C8-C9
14	B	841	CLA	C14-C13-C15-C16
14	G	805	CLA	C11-C12-C13-C14
14	G	806	CLA	C6-C7-C8-C9
14	G	835	CLA	C11-C12-C13-C14
14	G	836	CLA	C11-C12-C13-C14
14	H	815	CLA	C14-C13-C15-C16
14	H	819	CLA	C6-C7-C8-C9
14	H	839	CLA	C11-C10-C8-C9
14	H	840	CLA	C14-C13-C15-C16
14	a	805	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	a	806	CLA	C6-C7-C8-C9
14	a	825	CLA	C11-C12-C13-C14
14	b	823	CLA	C14-C13-C15-C16
19	a	856	LMT	C2'-C1'-O1'-C1
14	G	817	CLA	CBA-CGA-O2A-C1
14	B	842	CLA	O1A-CGA-O2A-C1
14	G	833	CLA	O1A-CGA-O2A-C1
14	H	831	CLA	O1A-CGA-O2A-C1
17	A	848	BCR	C7-C8-C9-C34
17	A	851	BCR	C36-C18-C19-C20
17	A	851	BCR	C37-C22-C23-C24
17	A	860	BCR	C37-C22-C23-C24
17	B	846	BCR	C11-C12-C13-C35
17	B	846	BCR	C37-C22-C23-C24
17	B	849	BCR	C7-C8-C9-C34
17	B	856	BCR	C7-C8-C9-C34
17	F	202	BCR	C11-C12-C13-C35
17	F	202	BCR	C36-C18-C19-C20
17	G	848	BCR	C7-C8-C9-C34
17	G	849	BCR	C36-C18-C19-C20
17	G	850	BCR	C36-C18-C19-C20
17	G	850	BCR	C37-C22-C23-C24
17	G	851	BCR	C36-C18-C19-C20
17	G	851	BCR	C37-C22-C23-C24
17	G	858	BCR	C37-C22-C23-C24
17	H	844	BCR	C37-C22-C23-C24
17	H	848	BCR	C7-C8-C9-C34
17	H	854	BCR	C7-C8-C9-C34
17	H	854	BCR	C11-C12-C13-C35
17	J	1105	BCR	C37-C22-C23-C24
17	Q	203	BCR	C11-C12-C13-C35
17	Q	203	BCR	C36-C18-C19-C20
17	Q	203	BCR	C37-C22-C23-C24
17	R	101	BCR	C36-C18-C19-C20
17	S	1104	BCR	C7-C8-C9-C34
17	S	1105	BCR	C11-C12-C13-C35
17	S	1105	BCR	C37-C22-C23-C24
17	U	203	BCR	C7-C8-C9-C34
17	a	851	BCR	C36-C18-C19-C20
17	a	852	BCR	C37-C22-C23-C24
17	a	858	BCR	C37-C22-C23-C24
17	b	846	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
17	b	846	BCR	C37-C22-C23-C24
17	b	847	BCR	C11-C12-C13-C35
17	b	856	BCR	C7-C8-C9-C34
17	b	856	BCR	C11-C12-C13-C35
17	f	202	BCR	C11-C12-C13-C35
17	i	101	BCR	C36-C18-C19-C20
17	j	104	BCR	C36-C18-C19-C20
17	k	104	BCR	C36-C18-C19-C20
17	l	5003	BCR	C7-C8-C9-C34
21	B	847	ECH	C37-C22-C23-C24
21	L	1506	ECH	C7-C8-C9-C34
21	V	102	ECH	C11-C12-C13-C35
17	A	860	BCR	C21-C22-C23-C24
17	G	850	BCR	C21-C22-C23-C24
17	G	858	BCR	C21-C22-C23-C24
17	H	844	BCR	C21-C22-C23-C24
17	Q	203	BCR	C21-C22-C23-C24
17	U	203	BCR	C7-C8-C9-C10
17	a	858	BCR	C21-C22-C23-C24
17	b	846	BCR	C21-C22-C23-C24
17	l	5003	BCR	C7-C8-C9-C10
21	L	1506	ECH	C7-C8-C9-C10
21	M	103	ECH	C11-C12-C13-C14
21	V	102	ECH	C11-C12-C13-C14
12	M	101	LHG	C7-C8-C9-C10
14	B	823	CLA	O1A-CGA-O2A-C1
14	H	812	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	O1A-CGA-O2A-C1
14	a	833	CLA	O1A-CGA-O2A-C1
14	b	833	CLA	O1A-CGA-O2A-C1
14	b	835	CLA	O1A-CGA-O2A-C1
14	l	5006	CLA	O1A-CGA-O2A-C1
18	G	852	LMG	O10-C28-O8-C9
14	A	820	CLA	C3-C5-C6-C7
19	f	207	LMT	O5B-C1B-O1B-C4'
14	G	821	CLA	O1D-CGD-O2D-CED
14	b	843	CLA	O1D-CGD-O2D-CED
14	G	844	CLA	CBD-CGD-O2D-CED
14	B	807	CLA	C5-C6-C7-C8
14	G	809	CLA	C13-C15-C16-C17
14	H	806	CLA	C5-C6-C7-C8
14	b	808	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	f	204	CLA	O1D-CGD-O2D-CED
14	B	842	CLA	C3-C5-C6-C7
14	G	821	CLA	C3-C5-C6-C7
14	G	843	CLA	C3-C5-C6-C7
14	l	5004	CLA	C3-C5-C6-C7
14	b	824	CLA	O1A-CGA-O2A-C1
14	B	829	CLA	O1A-CGA-O2A-C1
14	H	824	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	C6-C7-C8-C10
17	S	1105	BCR	C19-C20-C21-C22
14	S	1102	CLA	O1D-CGD-O2D-CED
12	L	1510	LHG	C7-C8-C9-C10
12	L	1509	LHG	O10-C23-O8-C6
14	B	813	CLA	O1A-CGA-O2A-C1
14	B	819	CLA	O1A-CGA-O2A-C1
14	H	818	CLA	O1A-CGA-O2A-C1
14	a	837	CLA	O1A-CGA-O2A-C1
14	G	816	CLA	CBD-CGD-O2D-CED
14	H	817	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	C10-C11-C12-C13
14	H	804	CLA	C8-C10-C11-C12
14	a	832	CLA	C5-C6-C7-C8
14	b	806	CLA	C8-C10-C11-C12
14	A	842	CLA	C2A-CAA-CBA-CGA
14	B	841	CLA	C2A-CAA-CBA-CGA
14	H	840	CLA	C2A-CAA-CBA-CGA
14	a	843	CLA	C2A-CAA-CBA-CGA
14	b	842	CLA	C2A-CAA-CBA-CGA
14	b	844	CLA	C2A-CAA-CBA-CGA
14	A	803	CLA	C15-C16-C17-C18
14	A	808	CLA	C13-C15-C16-C17
14	A	858	CLA	C8-C10-C11-C12
14	B	816	CLA	C15-C16-C17-C18
14	G	804	CLA	C15-C16-C17-C18
14	H	814	CLA	C8-C10-C11-C12
14	H	816	CLA	C8-C10-C11-C12
14	a	809	CLA	C13-C15-C16-C17
14	a	812	CLA	C5-C6-C7-C8
14	a	823	CLA	C8-C10-C11-C12
14	b	802	CLA	C13-C15-C16-C17
15	H	843	PQN	C25-C26-C27-C28
14	A	809	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	832	CLA	O1A-CGA-O2A-C1
14	H	828	CLA	O1A-CGA-O2A-C1
14	b	820	CLA	O1A-CGA-O2A-C1
14	b	830	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	C15-C16-C17-C18
14	B	826	CLA	C10-C11-C12-C13
14	G	803	CLA	C13-C15-C16-C17
14	L	1503	CLA	C8-C10-C11-C12
14	a	803	CLA	C15-C16-C17-C18
14	b	817	CLA	C15-C16-C17-C18
14	b	818	CLA	C5-C6-C7-C8
14	b	836	CLA	C5-C6-C7-C8
14	l	5006	CLA	C5-C6-C7-C8
14	A	825	CLA	CBA-CGA-O2A-C1
14	B	815	CLA	O1A-CGA-O2A-C1
14	G	807	CLA	O1A-CGA-O2A-C1
14	b	814	CLA	O1A-CGA-O2A-C1
18	a	853	LMG	O10-C28-O8-C9
14	B	815	CLA	C10-C11-C12-C13
14	b	827	CLA	C10-C11-C12-C13
19	G	857	LMT	O1'-C1-C2-C3
14	G	810	CLA	O1D-CGD-O2D-CED
14	j	102	CLA	CBA-CGA-O2A-C1
14	H	812	CLA	C3-C5-C6-C7
14	A	844	CLA	O1D-CGD-O2D-CED
14	B	815	CLA	C8-C10-C11-C12
14	b	802	CLA	C8-C10-C11-C12
14	b	821	CLA	C8-C10-C11-C12
14	K	102	CLA	C2C-C3C-CAC-CBC
14	G	826	CLA	O1A-CGA-O2A-C1
14	U	206	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	C15-C16-C17-C18
14	B	808	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	CBA-CGA-O2A-C1
14	G	837	CLA	CBA-CGA-O2A-C1
14	H	806	CLA	CBA-CGA-O2A-C1
14	b	815	CLA	CBA-CGA-O2A-C1
14	b	840	CLA	CBA-CGA-O2A-C1
19	b	854	LMT	C1-C2-C3-C4
14	G	826	CLA	CBD-CGD-O2D-CED
14	a	817	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	G	822	CLA	C3-C5-C6-C7
14	b	835	CLA	C3-C5-C6-C7
14	H	842	CLA	CBD-CGD-O2D-CED
15	b	845	PQN	C25-C26-C27-C28
14	G	810	CLA	C2A-CAA-CBA-CGA
14	f	204	CLA	C2A-CAA-CBA-CGA
12	M	101	LHG	C24-C23-O8-C6
14	A	835	CLA	CBA-CGA-O2A-C1
14	A	837	CLA	CBA-CGA-O2A-C1
14	B	807	CLA	CBA-CGA-O2A-C1
14	a	807	CLA	CBA-CGA-O2A-C1
14	a	836	CLA	CBA-CGA-O2A-C1
14	b	808	CLA	CBA-CGA-O2A-C1
14	b	831	CLA	CBA-CGA-O2A-C1
13	a	802	CL0	C5-C6-C7-C8
14	A	806	CLA	C5-C6-C7-C8
14	A	834	CLA	C15-C16-C17-C18
14	B	802	CLA	C13-C15-C16-C17
14	B	820	CLA	C8-C10-C11-C12
14	G	803	CLA	C8-C10-C11-C12
14	G	832	CLA	C5-C6-C7-C8
14	G	836	CLA	C10-C11-C12-C13
14	H	825	CLA	C15-C16-C17-C18
14	H	830	CLA	C8-C10-C11-C12
14	H	830	CLA	C10-C11-C12-C13
14	U	202	CLA	C15-C16-C17-C18
14	a	805	CLA	C5-C6-C7-C8
14	a	818	CLA	C5-C6-C7-C8
14	b	815	CLA	C5-C6-C7-C8
14	b	819	CLA	C8-C10-C11-C12
14	L	1501	CLA	CBD-CGD-O2D-CED
13	G	801	CL0	C5-C6-C7-C8
14	B	832	CLA	C15-C16-C17-C18
14	G	805	CLA	C5-C6-C7-C8
14	H	831	CLA	C15-C16-C17-C18
14	k	103	CLA	C13-C15-C16-C17
15	B	844	PQN	C25-C26-C27-C28
15	b	845	PQN	C23-C25-C26-C27
14	a	837	CLA	O1D-CGD-O2D-CED
13	A	802	CL0	C5-C6-C7-C8
14	B	818	CLA	C8-C10-C11-C12
14	G	812	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	b	833	CLA	C15-C16-C17-C18
14	G	832	CLA	CBA-CGA-O2A-C1
14	H	825	CLA	CBA-CGA-O2A-C1
14	b	827	CLA	CBA-CGA-O2A-C1
14	a	829	CLA	C4-C3-C5-C6
14	a	835	CLA	C15-C16-C17-C18
14	b	827	CLA	CBD-CGD-O2D-CED
14	A	839	CLA	C11-C12-C13-C14
14	G	829	CLA	O1D-CGD-O2D-CED
19	L	1505	LMT	C2'-C1'-O1'-C1
14	A	807	CLA	CBA-CGA-O2A-C1
14	B	816	CLA	CBA-CGA-O2A-C1
14	G	808	CLA	CBA-CGA-O2A-C1
14	G	843	CLA	CBA-CGA-O2A-C1
14	a	808	CLA	CBA-CGA-O2A-C1
14	B	810	CLA	C16-C17-C18-C19
14	b	807	CLA	C16-C17-C18-C20
14	b	811	CLA	C16-C17-C18-C19
14	H	825	CLA	C10-C11-C12-C13
14	a	821	CLA	C3-C5-C6-C7
14	A	816	CLA	C2C-C3C-CAC-CBC
17	A	848	BCR	C36-C18-C19-C20
17	A	850	BCR	C37-C22-C23-C24
17	B	848	BCR	C37-C22-C23-C24
17	H	845	BCR	C11-C12-C13-C35
17	H	845	BCR	C37-C22-C23-C24
17	J	1105	BCR	C11-C12-C13-C35
17	K	104	BCR	C36-C18-C19-C20
17	R	101	BCR	C37-C22-C23-C24
17	a	849	BCR	C36-C18-C19-C20
17	a	851	BCR	C37-C22-C23-C24
17	b	850	BCR	C7-C8-C9-C34
17	i	101	BCR	C37-C22-C23-C24
17	j	103	BCR	C7-C8-C9-C34
17	j	104	BCR	C37-C22-C23-C24
17	l	5007	BCR	C7-C8-C9-C34
21	H	846	ECH	C37-C22-C23-C24
21	R	102	ECH	C37-C22-C23-C24
21	i	102	ECH	C7-C8-C9-C34
17	A	850	BCR	C21-C22-C23-C24
17	B	846	BCR	C21-C22-C23-C24
17	G	848	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
17	G	849	BCR	C17-C18-C19-C20
17	R	101	BCR	C21-C22-C23-C24
17	a	851	BCR	C21-C22-C23-C24
17	b	846	BCR	C17-C18-C19-C20
17	b	856	BCR	C11-C12-C13-C14
17	i	101	BCR	C21-C22-C23-C24
17	k	104	BCR	C17-C18-C19-C20
14	B	807	CLA	O1A-CGA-O2A-C1
14	b	831	CLA	O1A-CGA-O2A-C1
14	A	808	CLA	C2A-CAA-CBA-CGA
14	A	809	CLA	C2A-CAA-CBA-CGA
14	F	203	CLA	C2A-CAA-CBA-CGA
14	H	818	CLA	C2A-CAA-CBA-CGA
14	a	809	CLA	C2A-CAA-CBA-CGA
14	b	820	CLA	C2A-CAA-CBA-CGA
14	b	838	CLA	CBA-CGA-O2A-C1
19	J	1106	LMT	O5B-C1B-O1B-C4'
14	B	806	CLA	C16-C17-C18-C20
14	B	840	CLA	C16-C17-C18-C19
14	H	839	CLA	C16-C17-C18-C20
14	b	812	CLA	C16-C17-C18-C19
14	A	825	CLA	O1A-CGA-O2A-C1
14	H	806	CLA	O1A-CGA-O2A-C1
14	b	815	CLA	O1A-CGA-O2A-C1
14	F	201	CLA	C3-C5-C6-C7
14	H	834	CLA	C3-C5-C6-C7
14	b	809	CLA	C3-C5-C6-C7
14	b	843	CLA	C3-C5-C6-C7
14	f	201	CLA	C3-C5-C6-C7
19	Q	207	LMT	O5B-C1B-O1B-C4'
14	H	822	CLA	CBA-CGA-O2A-C1
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	843	CLA	CBA-CGA-O2A-C1
14	B	801	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	CBA-CGA-O2A-C1
14	G	814	CLA	CBA-CGA-O2A-C1
14	b	801	CLA	CBA-CGA-O2A-C1
14	b	809	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	C5-C6-C7-C8
14	B	802	CLA	C8-C10-C11-C12
14	a	825	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	H	820	CLA	CBD-CGD-O2D-CED
14	l	5006	CLA	C3-C5-C6-C7
14	H	805	CLA	O1D-CGD-O2D-CED
14	b	830	CLA	O1D-CGD-O2D-CED
14	b	841	CLA	C2-C1-O2A-CGA
14	A	836	CLA	C16-C17-C18-C20
14	B	806	CLA	C16-C17-C18-C19
14	B	811	CLA	C16-C17-C18-C19
14	B	840	CLA	C16-C17-C18-C20
14	H	805	CLA	C16-C17-C18-C20
14	H	810	CLA	C16-C17-C18-C19
14	a	844	CLA	C16-C17-C18-C20
14	b	811	CLA	C16-C17-C18-C20
12	M	101	LHG	O10-C23-O8-C6
14	A	835	CLA	O1A-CGA-O2A-C1
14	B	826	CLA	O1A-CGA-O2A-C1
14	G	837	CLA	O1A-CGA-O2A-C1
14	a	836	CLA	O1A-CGA-O2A-C1
14	b	840	CLA	O1A-CGA-O2A-C1
14	G	826	CLA	C5-C6-C7-C8
14	H	809	CLA	C13-C15-C16-C17
18	A	855	LMG	C31-C32-C33-C34
14	B	831	CLA	O1D-CGD-O2D-CED
14	H	819	CLA	O1D-CGD-O2D-CED
14	A	813	CLA	CBA-CGA-O2A-C1
14	a	828	CLA	CBA-CGA-O2A-C1
12	a	855	LHG	C10-C11-C12-C13
12	G	854	LHG	C16-C17-C18-C19
14	A	840	CLA	C4B-C3B-CAB-CBB
14	A	836	CLA	C16-C17-C18-C19
14	B	810	CLA	C16-C17-C18-C20
14	B	811	CLA	C16-C17-C18-C20
14	F	201	CLA	C16-C17-C18-C19
14	F	201	CLA	C16-C17-C18-C20
14	H	810	CLA	C16-C17-C18-C20
14	H	839	CLA	C16-C17-C18-C19
14	Q	202	CLA	C16-C17-C18-C19
14	Q	202	CLA	C16-C17-C18-C20
14	a	844	CLA	C16-C17-C18-C19
14	b	807	CLA	C16-C17-C18-C19
14	b	823	CLA	C16-C17-C18-C19
14	b	823	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	b	841	CLA	C16-C17-C18-C19
14	b	841	CLA	C16-C17-C18-C20
14	f	201	CLA	C16-C17-C18-C19
14	B	825	CLA	O1D-CGD-O2D-CED
14	a	819	CLA	O1D-CGD-O2D-CED
14	b	808	CLA	O1A-CGA-O2A-C1
14	H	816	CLA	C2A-CAA-CBA-CGA
14	A	804	CLA	C5-C6-C7-C8
14	G	825	CLA	C13-C15-C16-C17
14	a	844	CLA	C5-C6-C7-C8
15	H	843	PQN	C23-C25-C26-C27
14	A	831	CLA	C11-C12-C13-C15
14	b	840	CLA	C12-C13-C15-C16
12	L	1509	LHG	C30-C31-C32-C33
18	G	852	LMG	C13-C14-C15-C16
14	A	827	CLA	CBA-CGA-O2A-C1
14	a	839	CLA	C8-C10-C11-C12
12	a	855	LHG	C27-C28-C29-C30
18	H	801	LMG	C14-C15-C16-C17
14	A	837	CLA	O1A-CGA-O2A-C1
14	B	808	CLA	O1A-CGA-O2A-C1
14	b	827	CLA	O1A-CGA-O2A-C1
14	Q	202	CLA	C3-C5-C6-C7
19	B	855	LMT	O5B-C1B-O1B-C4'
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	C3A-C2A-CAA-CBA
14	A	841	CLA	C3A-C2A-CAA-CBA
14	B	807	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	C3A-C2A-CAA-CBA
14	B	826	CLA	C3A-C2A-CAA-CBA
14	F	201	CLA	C3A-C2A-CAA-CBA
14	G	806	CLA	C3A-C2A-CAA-CBA
14	G	811	CLA	C3A-C2A-CAA-CBA
14	G	813	CLA	C3A-C2A-CAA-CBA
14	G	818	CLA	C3A-C2A-CAA-CBA
14	G	823	CLA	C3A-C2A-CAA-CBA
14	G	824	CLA	C3A-C2A-CAA-CBA
14	G	841	CLA	C3A-C2A-CAA-CBA
14	H	806	CLA	C3A-C2A-CAA-CBA
14	H	825	CLA	C3A-C2A-CAA-CBA
14	J	1101	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	L	1501	CLA	C3A-C2A-CAA-CBA
14	Q	202	CLA	C3A-C2A-CAA-CBA
14	Q	204	CLA	C3A-C2A-CAA-CBA
14	S	1101	CLA	C3A-C2A-CAA-CBA
14	T	103	CLA	C3A-C2A-CAA-CBA
14	a	804	CLA	C3A-C2A-CAA-CBA
14	a	824	CLA	C3A-C2A-CAA-CBA
14	a	826	CLA	C3A-C2A-CAA-CBA
14	a	842	CLA	C3A-C2A-CAA-CBA
14	b	808	CLA	C3A-C2A-CAA-CBA
14	b	827	CLA	C3A-C2A-CAA-CBA
14	k	103	CLA	C3A-C2A-CAA-CBA
14	B	806	CLA	O1D-CGD-O2D-CED
14	H	812	CLA	C2-C3-C5-C6
18	U	201	LMG	C11-C12-C13-C14
18	l	5001	LMG	C11-C12-C13-C14
14	A	843	CLA	C5-C6-C7-C8
14	G	818	CLA	C5-C6-C7-C8
14	G	819	CLA	C15-C16-C17-C18
14	H	819	CLA	C8-C10-C11-C12
14	b	818	CLA	C15-C16-C17-C18
14	H	805	CLA	C16-C17-C18-C19
14	b	812	CLA	C16-C17-C18-C20
14	f	201	CLA	C16-C17-C18-C20
14	A	807	CLA	O1A-CGA-O2A-C1
14	G	832	CLA	O1A-CGA-O2A-C1
14	H	825	CLA	O1A-CGA-O2A-C1
18	B	853	LMG	C14-C15-C16-C17
14	a	820	CLA	C5-C6-C7-C8
14	a	823	CLA	CBD-CGD-O2D-CED
14	b	832	CLA	CBD-CGD-O2D-CED
19	A	853	LMT	C7-C8-C9-C10
14	H	821	CLA	O1D-CGD-O2D-CED
14	G	813	CLA	CBA-CGA-O2A-C1
14	G	828	CLA	CBA-CGA-O2A-C1
14	H	807	CLA	CBA-CGA-O2A-C1
14	a	838	CLA	CBA-CGA-O2A-C1
14	a	844	CLA	CBA-CGA-O2A-C1
18	B	803	LMG	C40-C41-C42-C43
14	B	814	CLA	O1A-CGA-O2A-C1
14	G	808	CLA	O1A-CGA-O2A-C1
14	G	843	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	807	CLA	O1A-CGA-O2A-C1
14	a	808	CLA	O1A-CGA-O2A-C1
19	b	854	LMT	O1'-C1-C2-C3
19	A	856	LMT	C3-C4-C5-C6
18	B	852	LMG	C11-C12-C13-C14
19	G	853	LMT	C7-C8-C9-C10
19	A	857	LMT	C2-C3-C4-C5
18	B	852	LMG	C10-C11-C12-C13
14	A	804	CLA	O1A-CGA-O2A-C1
14	A	843	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	O1A-CGA-O2A-C1
14	B	830	CLA	O1A-CGA-O2A-C1
14	G	834	CLA	C2B-C3B-CAB-CBB
14	a	825	CLA	C2B-C3B-CAB-CBB
17	A	848	BCR	C1-C6-C7-C8
17	A	848	BCR	C5-C6-C7-C8
17	A	849	BCR	C23-C24-C25-C30
17	A	850	BCR	C23-C24-C25-C26
17	A	851	BCR	C23-C24-C25-C30
17	B	845	BCR	C23-C24-C25-C30
17	B	856	BCR	C23-C24-C25-C30
17	G	848	BCR	C1-C6-C7-C8
17	G	848	BCR	C5-C6-C7-C8
17	G	851	BCR	C23-C24-C25-C30
17	H	844	BCR	C23-C24-C25-C30
17	H	854	BCR	C23-C24-C25-C30
17	I	101	BCR	C23-C24-C25-C26
17	J	1105	BCR	C23-C24-C25-C26
17	L	1504	BCR	C23-C24-C25-C26
17	R	103	BCR	C23-C24-C25-C26
17	U	203	BCR	C5-C6-C7-C8
17	a	849	BCR	C1-C6-C7-C8
17	a	851	BCR	C23-C24-C25-C30
17	a	858	BCR	C23-C24-C25-C30
17	b	846	BCR	C23-C24-C25-C30
17	b	856	BCR	C23-C24-C25-C30
17	i	101	BCR	C23-C24-C25-C30
17	k	104	BCR	C23-C24-C25-C30
17	l	5003	BCR	C5-C6-C7-C8
17	l	5007	BCR	C23-C24-C25-C26
21	L	1506	ECH	C5-C6-C7-C8
21	M	103	ECH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	M	103	ECH	C23-C24-C25-C30
21	m	101	ECH	C1-C6-C7-C8
21	m	101	ECH	C23-C24-C25-C30
18	a	853	LMG	C13-C14-C15-C16
19	A	857	LMT	C5-C6-C7-C8
14	G	825	CLA	CBD-CGD-O2D-CED
14	G	817	CLA	O1A-CGA-O2A-C1
14	G	802	CLA	CBA-CGA-O2A-C1
14	G	822	CLA	CBA-CGA-O2A-C1
18	H	851	LMG	C29-C30-C31-C32
19	G	853	LMT	C1-C2-C3-C4
14	B	819	CLA	C2A-CAA-CBA-CGA
14	a	810	CLA	C2A-CAA-CBA-CGA
12	M	104	LHG	C11-C12-C13-C14
14	A	813	CLA	O1A-CGA-O2A-C1
14	A	827	CLA	O1A-CGA-O2A-C1
14	B	801	CLA	O1A-CGA-O2A-C1
14	G	814	CLA	O1A-CGA-O2A-C1
14	a	828	CLA	O1A-CGA-O2A-C1
14	a	838	CLA	O1A-CGA-O2A-C1
14	a	844	CLA	O1A-CGA-O2A-C1
14	b	801	CLA	O1A-CGA-O2A-C1
14	b	809	CLA	O1A-CGA-O2A-C1
19	B	855	LMT	O1'-C1-C2-C3
18	H	801	LMG	C17-C18-C19-C20
18	L	1508	LMG	C11-C12-C13-C14
14	A	828	CLA	C4-C3-C5-C6
14	H	826	CLA	C4-C3-C5-C6
14	A	817	CLA	C5-C6-C7-C8
14	a	815	CLA	C5-C6-C7-C8
14	a	829	CLA	C2-C3-C5-C6
14	l	5006	CLA	C16-C17-C18-C20
18	A	855	LMG	C16-C17-C18-C19
18	B	852	LMG	C29-C30-C31-C32
14	A	842	CLA	CBA-CGA-O2A-C1
14	H	815	CLA	CBA-CGA-O2A-C1
14	G	828	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	C14-C13-C15-C16
14	A	838	CLA	C11-C12-C13-C14
14	G	825	CLA	C11-C12-C13-C14
14	a	840	CLA	C11-C12-C13-C14
14	b	817	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	b	832	CLA	C11-C10-C8-C9
14	b	841	CLA	C11-C10-C8-C9
14	a	820	CLA	C15-C16-C17-C18
18	K	105	LMG	C29-C30-C31-C32
19	a	857	LMT	C7-C8-C9-C10
14	A	824	CLA	O1D-CGD-O2D-CED
19	A	856	LMT	O5B-C1B-O1B-C4'
18	b	803	LMG	C40-C41-C42-C43
14	b	819	CLA	C15-C16-C17-C18
14	A	806	CLA	CBA-CGA-O2A-C1
14	H	829	CLA	CBA-CGA-O2A-C1
14	a	814	CLA	CBA-CGA-O2A-C1
21	m	101	ECH	C13-C14-C15-C16
12	M	101	LHG	C8-C7-O7-C5
18	B	853	LMG	C11-C10-O7-C8
12	A	801	LHG	C23-C24-C25-C26
12	M	101	LHG	O9-C7-O7-C5
18	A	855	LMG	C12-C13-C14-C15
17	G	848	BCR	C36-C18-C19-C20
17	H	848	BCR	C36-C18-C19-C20
17	a	850	BCR	C37-C22-C23-C24
21	m	101	ECH	C7-C8-C9-C34
12	a	801	LHG	C16-C17-C18-C19
17	H	854	BCR	C11-C12-C13-C14
17	a	850	BCR	C21-C22-C23-C24
17	a	851	BCR	C17-C18-C19-C20
21	B	847	ECH	C21-C22-C23-C24
14	b	834	CLA	O1D-CGD-O2D-CED
18	a	853	LMG	C8-C7-O1-C1
14	B	823	CLA	C2A-CAA-CBA-CGA
14	G	809	CLA	C2A-CAA-CBA-CGA
14	b	807	CLA	C2A-CAA-CBA-CGA
14	G	807	CLA	C16-C17-C18-C20
14	G	835	CLA	C16-C17-C18-C19
14	a	823	CLA	C16-C17-C18-C19
12	G	855	LHG	C27-C28-C29-C30
14	H	834	CLA	C4-C3-C5-C6
14	a	831	CLA	C4-C3-C5-C6
14	b	828	CLA	C4-C3-C5-C6
19	Q	207	LMT	C1-C2-C3-C4
14	G	813	CLA	O1A-CGA-O2A-C1
14	a	812	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	a	837	CLA	C13-C15-C16-C17
12	A	801	LHG	C16-C17-C18-C19
14	L	1501	CLA	C3-C5-C6-C7
14	a	807	CLA	C5-C6-C7-C8
14	B	826	CLA	C15-C16-C17-C18
14	a	807	CLA	C16-C17-C18-C20
14	a	823	CLA	C16-C17-C18-C20
14	l	5006	CLA	C16-C17-C18-C19
14	H	807	CLA	O1A-CGA-O2A-C1
19	G	857	LMT	C5-C6-C7-C8
14	A	819	CLA	C5-C6-C7-C8
19	B	854	LMT	C6-C7-C8-C9
18	G	852	LMG	O6-C5-C6-O5
18	K	105	LMG	O6-C5-C6-O5
14	B	808	CLA	C3-C5-C6-C7
18	U	201	LMG	O7-C8-C9-O8
18	b	853	LMG	O7-C8-C9-O8
14	l	5004	CLA	O1D-CGD-O2D-CED
14	b	817	CLA	CBA-CGA-O2A-C1
12	G	854	LHG	C11-C10-C9-C8
14	a	839	CLA	C13-C15-C16-C17
12	a	801	LHG	C11-C10-C9-C8
14	A	806	CLA	C16-C17-C18-C20
14	A	824	CLA	C13-C15-C16-C17
19	Q	201	LMT	C7-C8-C9-C10
14	H	815	CLA	C2-C3-C5-C6
14	H	834	CLA	C2-C3-C5-C6
18	B	853	LMG	O9-C10-O7-C8
14	A	813	CLA	C2A-CAA-CBA-CGA
14	H	805	CLA	C2A-CAA-CBA-CGA
14	a	813	CLA	C2A-CAA-CBA-CGA
14	A	833	CLA	CBD-CGD-O2D-CED
14	b	814	CLA	O1D-CGD-O2D-CED
14	B	818	CLA	C15-C16-C17-C18
14	G	838	CLA	C8-C10-C11-C12
14	G	843	CLA	C5-C6-C7-C8
14	A	843	CLA	C16-C17-C18-C20
14	b	826	CLA	O1D-CGD-O2D-CED
14	A	842	CLA	O1A-CGA-O2A-C1
14	G	802	CLA	O1A-CGA-O2A-C1
18	b	853	LMG	C16-C17-C18-C19
14	A	832	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	836	CLA	C1A-C2A-CAA-CBA
14	B	822	CLA	C1A-C2A-CAA-CBA
14	B	824	CLA	C1A-C2A-CAA-CBA
14	B	826	CLA	C1A-C2A-CAA-CBA
14	B	829	CLA	C1A-C2A-CAA-CBA
14	B	831	CLA	C1A-C2A-CAA-CBA
14	B	833	CLA	C1A-C2A-CAA-CBA
14	B	834	CLA	C1A-C2A-CAA-CBA
14	B	842	CLA	C1A-C2A-CAA-CBA
14	G	811	CLA	C1A-C2A-CAA-CBA
14	G	812	CLA	C1A-C2A-CAA-CBA
14	G	841	CLA	C1A-C2A-CAA-CBA
14	H	817	CLA	C1A-C2A-CAA-CBA
14	H	821	CLA	C1A-C2A-CAA-CBA
14	H	823	CLA	C1A-C2A-CAA-CBA
14	H	825	CLA	C1A-C2A-CAA-CBA
14	H	841	CLA	C1A-C2A-CAA-CBA
14	J	1102	CLA	C1A-C2A-CAA-CBA
14	K	103	CLA	C1A-C2A-CAA-CBA
14	Q	204	CLA	C1A-C2A-CAA-CBA
14	S	1102	CLA	C1A-C2A-CAA-CBA
14	T	103	CLA	C1A-C2A-CAA-CBA
14	a	804	CLA	C1A-C2A-CAA-CBA
14	a	812	CLA	C1A-C2A-CAA-CBA
14	a	842	CLA	C1A-C2A-CAA-CBA
14	b	825	CLA	C1A-C2A-CAA-CBA
14	b	827	CLA	C1A-C2A-CAA-CBA
14	b	843	CLA	C1A-C2A-CAA-CBA
14	j	101	CLA	C1A-C2A-CAA-CBA
14	j	102	CLA	C1A-C2A-CAA-CBA
14	k	103	CLA	C1A-C2A-CAA-CBA
14	G	822	CLA	O1A-CGA-O2A-C1
15	B	844	PQN	C23-C25-C26-C27
18	b	803	LMG	C14-C15-C16-C17
14	A	804	CLA	C11-C10-C8-C7
14	A	811	CLA	C6-C7-C8-C10
14	A	830	CLA	C6-C7-C8-C10
14	B	802	CLA	C11-C12-C13-C15
14	B	831	CLA	C12-C13-C15-C16
14	G	803	CLA	C11-C12-C13-C15
14	G	820	CLA	C11-C12-C13-C15
14	G	822	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	G	829	CLA	C11-C12-C13-C15
14	G	835	CLA	C11-C12-C13-C15
14	G	839	CLA	C11-C10-C8-C7
14	G	843	CLA	C12-C13-C15-C16
14	H	820	CLA	C6-C7-C8-C10
14	H	826	CLA	C6-C7-C8-C10
14	H	827	CLA	C11-C12-C13-C15
14	H	830	CLA	C6-C7-C8-C10
14	K	103	CLA	C11-C12-C13-C15
14	L	1502	CLA	C11-C10-C8-C7
14	T	103	CLA	C11-C12-C13-C15
14	a	803	CLA	C12-C13-C15-C16
14	a	808	CLA	C12-C13-C15-C16
14	a	829	CLA	C11-C12-C13-C15
14	a	831	CLA	C6-C7-C8-C10
14	a	841	CLA	C11-C10-C8-C7
14	b	802	CLA	C11-C12-C13-C15
14	b	832	CLA	C12-C13-C15-C16
14	H	815	CLA	O1A-CGA-O2A-C1
14	a	822	CLA	C4-C3-C5-C6
12	A	801	LHG	C11-C10-C9-C8
14	a	814	CLA	O1A-CGA-O2A-C1
18	U	201	LMG	O6-C5-C6-O5
18	a	853	LMG	O6-C5-C6-O5
14	A	829	CLA	C2A-CAA-CBA-CGA
14	B	801	CLA	C2A-CAA-CBA-CGA
14	G	814	CLA	C2A-CAA-CBA-CGA
14	b	801	CLA	C2A-CAA-CBA-CGA
14	A	804	CLA	C11-C10-C8-C9
14	A	811	CLA	C6-C7-C8-C9
14	A	811	CLA	C14-C13-C15-C16
14	A	830	CLA	C6-C7-C8-C9
14	A	831	CLA	C11-C12-C13-C14
14	A	840	CLA	C11-C10-C8-C9
14	A	843	CLA	C14-C13-C15-C16
14	B	814	CLA	C11-C10-C8-C9
14	G	808	CLA	C11-C12-C13-C14
14	G	825	CLA	C11-C10-C8-C9
14	G	831	CLA	C11-C10-C8-C9
14	H	810	CLA	C11-C10-C8-C9
14	H	827	CLA	C11-C12-C13-C14
14	H	830	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	K	103	CLA	C11-C12-C13-C14
14	T	103	CLA	C11-C12-C13-C14
14	a	803	CLA	C14-C13-C15-C16
14	a	808	CLA	C14-C13-C15-C16
14	a	822	CLA	C6-C7-C8-C9
14	a	825	CLA	C11-C10-C8-C9
14	a	829	CLA	C11-C12-C13-C14
14	a	844	CLA	C14-C13-C15-C16
15	B	844	PQN	C24-C23-C25-C26
19	L	1505	LMT	C7-C8-C9-C10
14	G	835	CLA	CBA-CGA-O2A-C1
14	G	836	CLA	CBA-CGA-O2A-C1
14	G	842	CLA	CBA-CGA-O2A-C1
14	a	842	CLA	CBA-CGA-O2A-C1
14	G	820	CLA	C5-C6-C7-C8
14	k	102	CLA	C2C-C3C-CAC-CBC
18	H	851	LMG	O6-C5-C6-O5
19	a	854	LMT	O5B-C5B-C6B-O6B
19	a	857	LMT	O5B-C5B-C6B-O6B
12	a	801	LHG	C10-C11-C12-C13
18	A	852	LMG	O6-C5-C6-O5
12	G	854	LHG	C23-C24-C25-C26
14	G	844	CLA	O1D-CGD-O2D-CED
18	A	855	LMG	O6-C5-C6-O5
14	b	821	CLA	CBD-CGD-O2D-CED
14	a	806	CLA	C8-C10-C11-C12
14	b	827	CLA	C15-C16-C17-C18
18	L	1508	LMG	O6-C5-C6-O5
19	G	857	LMT	O5B-C5B-C6B-O6B
19	Q	201	LMT	O5B-C5B-C6B-O6B
19	a	856	LMT	O5B-C5B-C6B-O6B
14	A	843	CLA	C16-C17-C18-C19
19	Q	207	LMT	C3-C4-C5-C6
18	K	105	LMG	C8-C9-O8-C28
19	H	852	LMT	O5B-C5B-C6B-O6B
14	H	817	CLA	O1D-CGD-O2D-CED
14	H	824	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	C8-C10-C11-C12
12	G	854	LHG	C14-C15-C16-C17
14	H	829	CLA	O1A-CGA-O2A-C1
14	H	815	CLA	C4-C3-C5-C6
14	B	809	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	H	824	CLA	C2-C3-C5-C6
14	a	822	CLA	C2-C3-C5-C6
14	A	830	CLA	C5-C6-C7-C8
14	G	807	CLA	C10-C11-C12-C13
14	G	812	CLA	C15-C16-C17-C18
18	B	803	LMG	C14-C15-C16-C17
14	L	1503	CLA	C16-C17-C18-C20
19	A	853	LMT	O5B-C5B-C6B-O6B
19	A	857	LMT	O5B-C5B-C6B-O6B
19	G	853	LMT	O5B-C5B-C6B-O6B
17	H	845	BCR	C11-C12-C13-C14
17	H	854	BCR	C7-C8-C9-C10
17	b	847	BCR	C11-C12-C13-C14
14	G	842	CLA	O1A-CGA-O2A-C1
14	b	817	CLA	O1A-CGA-O2A-C1
14	A	840	CLA	C8-C10-C11-C12
14	G	812	CLA	C13-C15-C16-C17
14	A	844	CLA	C2A-CAA-CBA-CGA
14	B	806	CLA	C2A-CAA-CBA-CGA
14	B	843	CLA	C2A-CAA-CBA-CGA
14	G	802	CLA	C2A-CAA-CBA-CGA
14	j	102	CLA	O1A-CGA-O2A-C1
18	l	5001	LMG	O6-C5-C6-O5
14	A	807	CLA	C10-C11-C12-C13
19	b	855	LMT	C2-C3-C4-C5
19	f	207	LMT	C11-C10-C9-C8
14	H	803	CLA	CBA-CGA-O2A-C1
14	H	817	CLA	CBA-CGA-O2A-C1
14	H	833	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	O2A-C1-C2-C3
14	G	806	CLA	O2A-C1-C2-C3
14	L	1503	CLA	O2A-C1-C2-C3
14	a	806	CLA	O2A-C1-C2-C3
12	a	855	LHG	C29-C30-C31-C32
17	H	847	BCR	C19-C20-C21-C22
17	l	5003	BCR	C19-C20-C21-C22
14	G	836	CLA	O1A-CGA-O2A-C1
12	A	854	LHG	C28-C29-C30-C31
14	a	807	CLA	C10-C11-C12-C13
14	a	843	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	O1A-CGA-O2A-C1
14	a	842	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	854	LMT	C4-C5-C6-C7
19	G	853	LMT	C6-C7-C8-C9
14	G	815	CLA	C5-C6-C7-C8
14	G	829	CLA	C4-C3-C5-C6
14	B	818	CLA	C2-C3-C5-C6
14	B	825	CLA	C2-C3-C5-C6
14	G	822	CLA	C2-C3-C5-C6
14	H	826	CLA	C2-C3-C5-C6
14	b	819	CLA	C2-C3-C5-C6
14	B	820	CLA	CBD-CGD-O2D-CED
18	H	801	LMG	C40-C41-C42-C43
12	G	854	LHG	C34-C35-C36-C37
19	A	853	LMT	C9-C10-C11-C12
18	b	853	LMG	C29-C28-O8-C9
14	G	816	CLA	O1D-CGD-O2D-CED
14	H	807	CLA	C3-C5-C6-C7
14	G	835	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	C10-C11-C12-C13
14	A	822	CLA	CBA-CGA-O2A-C1
14	B	834	CLA	CBA-CGA-O2A-C1
14	H	813	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	C2C-C3C-CAC-CBC
12	M	101	LHG	C13-C14-C15-C16
18	H	801	LMG	C36-C37-C38-C39
14	A	836	CLA	O1D-CGD-O2D-CED
18	a	853	LMG	C37-C38-C39-C40
19	G	853	LMT	C9-C10-C11-C12
14	a	831	CLA	C5-C6-C7-C8
14	G	843	CLA	C16-C17-C18-C20
14	a	820	CLA	CBD-CGD-O2D-CED
14	B	809	CLA	C4-C3-C5-C6
14	B	816	CLA	C4-C3-C5-C6
14	G	822	CLA	C4-C3-C5-C6
14	H	824	CLA	C4-C3-C5-C6
14	a	841	CLA	C4-C3-C5-C6
14	A	858	CLA	C15-C16-C17-C18
12	A	854	LHG	C26-C27-C28-C29
12	A	854	LHG	C27-C28-C29-C30
19	J	1106	LMT	C2-C1-O1'-C1'
19	Q	207	LMT	C2-C1-O1'-C1'
19	U	207	LMT	C2-C1-O1'-C1'
19	f	207	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
14	H	822	CLA	O1A-CGA-O2A-C1
14	b	838	CLA	O1A-CGA-O2A-C1
14	A	803	CLA	C14-C13-C15-C16
14	A	824	CLA	C11-C10-C8-C9
14	A	828	CLA	C11-C12-C13-C14
14	A	835	CLA	C11-C10-C8-C9
14	A	839	CLA	C11-C10-C8-C9
14	B	802	CLA	C11-C12-C13-C14
14	B	811	CLA	C11-C10-C8-C9
14	B	816	CLA	C14-C13-C15-C16
14	G	803	CLA	C11-C12-C13-C14
14	G	804	CLA	C14-C13-C15-C16
14	G	808	CLA	C14-C13-C15-C16
14	G	822	CLA	C6-C7-C8-C9
14	G	839	CLA	C11-C10-C8-C9
14	G	839	CLA	C11-C12-C13-C14
14	G	843	CLA	C14-C13-C15-C16
14	H	813	CLA	C11-C10-C8-C9
14	H	819	CLA	C11-C12-C13-C14
14	H	820	CLA	C6-C7-C8-C9
14	H	826	CLA	C6-C7-C8-C9
14	K	103	CLA	C11-C10-C8-C9
14	L	1502	CLA	C11-C10-C8-C9
14	T	103	CLA	C11-C10-C8-C9
14	a	823	CLA	C11-C10-C8-C9
14	a	831	CLA	C6-C7-C8-C9
14	a	841	CLA	C11-C10-C8-C9
14	b	802	CLA	C11-C12-C13-C14
14	b	812	CLA	C11-C10-C8-C9
14	b	840	CLA	C14-C13-C15-C16
14	H	842	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	C15-C16-C17-C18
14	B	840	CLA	C13-C15-C16-C17
14	A	816	CLA	C4B-C3B-CAB-CBB
14	A	842	CLA	C4B-C3B-CAB-CBB
14	B	821	CLA	C4B-C3B-CAB-CBB
14	B	822	CLA	C4B-C3B-CAB-CBB
14	G	825	CLA	C4B-C3B-CAB-CBB
14	H	821	CLA	C4B-C3B-CAB-CBB
14	K	102	CLA	C4B-C3B-CAB-CBB
14	T	103	CLA	C4B-C3B-CAB-CBB
14	a	841	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	811	CLA	C4B-C3B-CAB-CBB
18	B	853	LMG	C21-C22-C23-C24
19	A	853	LMT	C1-C2-C3-C4
14	b	806	CLA	C15-C16-C17-C18
14	H	822	CLA	CBD-CGD-O2D-CED
19	a	854	LMT	C9-C10-C11-C12
12	A	854	LHG	C13-C14-C15-C16
12	a	801	LHG	C34-C35-C36-C37
14	A	811	CLA	C12-C13-C15-C16
14	A	824	CLA	C11-C10-C8-C7
14	A	828	CLA	C11-C12-C13-C15
14	A	839	CLA	C11-C10-C8-C7
14	A	840	CLA	C11-C10-C8-C7
14	A	843	CLA	C6-C7-C8-C10
14	A	843	CLA	C12-C13-C15-C16
14	B	811	CLA	C11-C10-C8-C7
14	B	814	CLA	C11-C10-C8-C7
14	B	839	CLA	C11-C10-C8-C7
14	B	839	CLA	C12-C13-C15-C16
14	G	804	CLA	C12-C13-C15-C16
14	G	808	CLA	C11-C12-C13-C15
14	G	808	CLA	C12-C13-C15-C16
14	G	825	CLA	C11-C10-C8-C7
14	G	831	CLA	C11-C10-C8-C7
14	G	835	CLA	C11-C10-C8-C7
14	G	839	CLA	C12-C13-C15-C16
14	G	843	CLA	C6-C7-C8-C10
14	H	810	CLA	C11-C10-C8-C7
14	H	811	CLA	C12-C13-C15-C16
14	H	813	CLA	C11-C10-C8-C7
14	H	819	CLA	C11-C12-C13-C15
14	H	831	CLA	C6-C7-C8-C10
14	K	103	CLA	C11-C10-C8-C7
14	T	103	CLA	C11-C10-C8-C7
14	a	822	CLA	C6-C7-C8-C10
14	a	823	CLA	C11-C10-C8-C7
14	a	825	CLA	C11-C10-C8-C7
14	a	825	CLA	C12-C13-C15-C16
14	a	844	CLA	C12-C13-C15-C16
14	b	812	CLA	C11-C10-C8-C7
14	b	823	CLA	C12-C13-C15-C16
14	b	829	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	b	830	CLA	C12-C13-C15-C16
15	B	844	PQN	C22-C23-C25-C26
15	b	845	PQN	C22-C23-C25-C26
14	A	825	CLA	C13-C15-C16-C17
14	A	825	CLA	CBD-CGD-O2D-CED
19	l	5008	LMT	C5'-C4'-O1B-C1B
14	A	806	CLA	C3A-C2A-CAA-CBA
14	B	825	CLA	C4-C3-C5-C6
14	B	829	CLA	C3A-C2A-CAA-CBA
14	G	807	CLA	C3A-C2A-CAA-CBA
14	G	830	CLA	C3A-C2A-CAA-CBA
14	H	813	CLA	C3A-C2A-CAA-CBA
14	H	828	CLA	C3A-C2A-CAA-CBA
14	K	102	CLA	C3A-C2A-CAA-CBA
14	T	103	CLA	C4-C3-C5-C6
14	a	807	CLA	C3A-C2A-CAA-CBA
14	a	823	CLA	C3A-C2A-CAA-CBA
14	b	830	CLA	C3A-C2A-CAA-CBA
14	G	838	CLA	C13-C15-C16-C17
14	L	1501	CLA	O1D-CGD-O2D-CED
14	a	831	CLA	C2-C3-C5-C6
14	T	102	CLA	C2C-C3C-CAC-CBC
18	a	853	LMG	C32-C33-C34-C35
14	B	838	CLA	CBA-CGA-O2A-C1
14	H	826	CLA	CBA-CGA-O2A-C1
17	G	849	BCR	C19-C20-C21-C22
17	G	850	BCR	C19-C20-C21-C22
17	j	104	BCR	C19-C20-C21-C22
21	L	1506	ECH	C19-C20-C21-C22
14	L	1503	CLA	C16-C17-C18-C19
17	a	858	BCR	C36-C18-C19-C20
21	I	102	ECH	C37-C22-C23-C24
14	A	809	CLA	C4-C3-C5-C6
14	H	803	CLA	O1A-CGA-O2A-C1
14	H	817	CLA	O1A-CGA-O2A-C1
14	A	824	CLA	C15-C16-C17-C18
14	G	829	CLA	C13-C15-C16-C17
17	A	851	BCR	C21-C22-C23-C24
17	B	856	BCR	C7-C8-C9-C10
17	a	852	BCR	C21-C22-C23-C24
12	V	101	LHG	C29-C30-C31-C32
18	b	853	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
14	k	103	CLA	C16-C17-C18-C19
14	a	812	CLA	C13-C15-C16-C17
14	a	841	CLA	C8-C10-C11-C12
14	a	826	CLA	C13-C15-C16-C17
14	A	830	CLA	C4-C3-C5-C6
14	B	818	CLA	C4-C3-C5-C6
14	G	840	CLA	C4-C3-C5-C6
14	b	810	CLA	C4-C3-C5-C6
14	b	819	CLA	C4-C3-C5-C6
14	b	826	CLA	C4-C3-C5-C6
14	G	840	CLA	C2-C3-C5-C6
14	b	826	CLA	C2-C3-C5-C6
14	G	826	CLA	O1D-CGD-O2D-CED
14	b	827	CLA	O1D-CGD-O2D-CED
14	b	819	CLA	CBD-CGD-O2D-CED
14	G	843	CLA	C16-C17-C18-C19
14	H	809	CLA	C16-C17-C18-C19
12	G	856	LHG	O6-C4-C5-O7
12	L	1510	LHG	O6-C4-C5-O7
12	a	801	LHG	O6-C4-C5-O7
14	H	833	CLA	O1A-CGA-O2A-C1
14	H	820	CLA	O1D-CGD-O2D-CED
17	G	858	BCR	C23-C24-C25-C30
17	R	101	BCR	C23-C24-C25-C30
17	a	850	BCR	C23-C24-C25-C30
14	G	805	CLA	C15-C16-C17-C18
14	A	836	CLA	C3-C5-C6-C7
18	b	853	LMG	C33-C34-C35-C36
19	A	853	LMT	C6-C7-C8-C9
14	H	804	CLA	C15-C16-C17-C18
14	H	818	CLA	C15-C16-C17-C18
14	a	805	CLA	C15-C16-C17-C18
14	a	825	CLA	C15-C16-C17-C18
14	A	842	CLA	CBD-CGD-O2D-CED
18	B	803	LMG	C36-C37-C38-C39
14	B	830	CLA	C16-C17-C18-C20
14	A	818	CLA	CAA-CBA-CGA-O2A
14	G	817	CLA	C2C-C3C-CAC-CBC
14	A	858	CLA	C10-C11-C12-C13
14	B	835	CLA	C5-C6-C7-C8
18	l	5001	LMG	O7-C8-C9-O8
19	Q	201	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
18	b	853	LMG	C10-C11-C12-C13
14	a	843	CLA	O1A-CGA-O2A-C1
14	G	828	CLA	C4-C3-C5-C6
14	a	839	CLA	C4-C3-C5-C6
14	A	831	CLA	C13-C15-C16-C17
14	B	816	CLA	C2-C3-C5-C6
14	T	103	CLA	C2-C3-C5-C6
14	a	841	CLA	C2-C3-C5-C6
19	H	852	LMT	C6-C7-C8-C9
14	H	809	CLA	C16-C17-C18-C20
14	k	103	CLA	C16-C17-C18-C20
14	b	832	CLA	O1D-CGD-O2D-CED
19	H	853	LMT	C7-C8-C9-C10
14	B	826	CLA	C14-C13-C15-C16
14	B	839	CLA	C11-C10-C8-C9
14	G	829	CLA	C11-C12-C13-C14
14	H	838	CLA	C11-C10-C8-C9
14	L	1503	CLA	C14-C13-C15-C16
14	b	811	CLA	C14-C13-C15-C16
14	b	830	CLA	C14-C13-C15-C16
15	b	845	PQN	C24-C23-C25-C26
14	B	815	CLA	C4C-C3C-CAC-CBC
14	G	825	CLA	O1D-CGD-O2D-CED
14	a	823	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	C16-C17-C18-C19
14	b	814	CLA	C3-C5-C6-C7
19	Q	201	LMT	C1-C2-C3-C4
19	f	203	LMT	C1-C2-C3-C4
19	A	859	LMT	C2-C3-C4-C5
14	a	839	CLA	C2-C3-C5-C6
14	b	810	CLA	C2-C3-C5-C6
14	B	830	CLA	C16-C17-C18-C19
18	A	852	LMG	C11-C10-O7-C8
14	A	807	CLA	C13-C15-C16-C17
14	B	823	CLA	C8-C10-C11-C12
14	G	843	CLA	C13-C15-C16-C17
18	L	1508	LMG	C34-C35-C36-C37
14	G	834	CLA	CBA-CGA-O2A-C1
14	b	828	CLA	CBA-CGA-O2A-C1
12	a	801	LHG	O6-C4-C5-C6
14	a	805	CLA	C13-C15-C16-C17
14	a	830	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	A	849	BCR	C37-C22-C23-C24
17	R	103	BCR	C7-C8-C9-C34
17	b	847	BCR	C37-C22-C23-C24
14	A	803	CLA	C12-C13-C15-C16
14	A	825	CLA	C11-C12-C13-C15
14	A	858	CLA	C11-C12-C13-C15
14	B	810	CLA	C12-C13-C15-C16
14	B	823	CLA	C11-C10-C8-C7
14	B	829	CLA	C12-C13-C15-C16
14	B	842	CLA	C11-C12-C13-C15
14	G	805	CLA	C11-C10-C8-C7
14	G	807	CLA	C6-C7-C8-C10
14	G	828	CLA	C11-C12-C13-C15
14	H	804	CLA	C11-C12-C13-C15
14	H	815	CLA	C11-C12-C13-C15
14	H	816	CLA	C12-C13-C15-C16
14	H	828	CLA	C12-C13-C15-C16
14	H	838	CLA	C11-C10-C8-C7
14	H	838	CLA	C12-C13-C15-C16
14	H	841	CLA	C11-C12-C13-C15
14	L	1501	CLA	C6-C7-C8-C10
14	L	1503	CLA	C12-C13-C15-C16
14	U	205	CLA	C11-C10-C8-C7
14	a	805	CLA	C11-C10-C8-C7
14	a	812	CLA	C12-C13-C15-C16
14	a	828	CLA	C11-C12-C13-C15
14	a	840	CLA	C11-C10-C8-C7
14	a	844	CLA	C6-C7-C8-C10
14	b	806	CLA	C11-C12-C13-C15
14	b	811	CLA	C12-C13-C15-C16
14	b	813	CLA	C12-C13-C15-C16
14	k	103	CLA	C11-C10-C8-C7
14	l	5004	CLA	C6-C7-C8-C10
15	H	843	PQN	C22-C23-C25-C26
14	G	831	CLA	C5-C6-C7-C8
14	b	806	CLA	C10-C11-C12-C13
17	A	848	BCR	C17-C18-C19-C20
17	A	849	BCR	C21-C22-C23-C24
17	B	848	BCR	C21-C22-C23-C24
17	G	848	BCR	C17-C18-C19-C20
17	H	845	BCR	C21-C22-C23-C24
17	J	1105	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	K	104	BCR	C17-C18-C19-C20
17	a	849	BCR	C17-C18-C19-C20
17	b	850	BCR	C7-C8-C9-C10
17	j	104	BCR	C21-C22-C23-C24
17	l	5007	BCR	C7-C8-C9-C10
21	i	102	ECH	C7-C8-C9-C10
21	m	101	ECH	C7-C8-C9-C10
12	A	801	LHG	C24-C23-O8-C6
14	L	1501	CLA	CBA-CGA-O2A-C1
14	B	834	CLA	O1A-CGA-O2A-C1
14	B	838	CLA	O1A-CGA-O2A-C1
14	H	813	CLA	O1A-CGA-O2A-C1
18	b	853	LMG	O10-C28-O8-C9
18	G	852	LMG	C8-C7-O1-C1
14	B	817	CLA	C2A-CAA-CBA-CGA
14	G	804	CLA	C2A-CAA-CBA-CGA
14	a	830	CLA	C2A-CAA-CBA-CGA
14	b	816	CLA	C4C-C3C-CAC-CBC
14	G	807	CLA	C16-C17-C18-C19
14	G	835	CLA	C16-C17-C18-C20
14	B	814	CLA	CBD-CGD-O2D-CED
14	b	817	CLA	C4-C3-C5-C6
13	A	802	CL0	CAA-CBA-CGA-O2A
14	G	828	CLA	C2-C3-C5-C6
14	b	828	CLA	C2-C3-C5-C6
12	a	855	LHG	C11-C10-C9-C8
14	H	838	CLA	CBA-CGA-O2A-C1
12	M	102	LHG	C6-C5-O7-C7
12	V	101	LHG	C6-C5-O7-C7
18	A	852	LMG	C9-C8-O7-C10
14	A	822	CLA	O1A-CGA-O2A-C1
14	H	814	CLA	C4C-C3C-CAC-CBC
14	a	807	CLA	C16-C17-C18-C19
14	H	826	CLA	O1A-CGA-O2A-C1
19	J	1106	LMT	C3-C4-C5-C6
14	A	812	CLA	C6-C7-C8-C9
14	B	828	CLA	C16-C17-C18-C20
14	a	828	CLA	C4-C3-C5-C6
14	A	803	CLA	C2A-CAA-CBA-CGA
14	A	828	CLA	C2-C3-C5-C6
14	b	817	CLA	C2-C3-C5-C6
14	A	843	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	G	825	CLA	C15-C16-C17-C18
18	G	852	LMG	O1-C7-C8-O7
18	H	851	LMG	O1-C7-C8-O7
18	L	1508	LMG	O7-C8-C9-O8
14	a	821	CLA	C5-C6-C7-C8
14	A	858	CLA	C11-C12-C13-C14
14	B	801	CLA	C11-C12-C13-C14
14	B	821	CLA	C6-C7-C8-C9
14	B	842	CLA	C11-C12-C13-C14
14	G	839	CLA	C14-C13-C15-C16
14	H	804	CLA	C11-C12-C13-C14
14	H	816	CLA	C14-C13-C15-C16
14	H	825	CLA	C14-C13-C15-C16
14	H	830	CLA	C14-C13-C15-C16
14	H	841	CLA	C11-C12-C13-C14
14	L	1501	CLA	C6-C7-C8-C9
14	U	205	CLA	C11-C10-C8-C9
14	a	805	CLA	C11-C10-C8-C9
14	a	836	CLA	C11-C10-C8-C9
14	a	840	CLA	C11-C10-C8-C9
14	a	844	CLA	C6-C7-C8-C9
14	b	827	CLA	C14-C13-C15-C16
14	k	103	CLA	C11-C10-C8-C9
15	H	843	PQN	C24-C23-C25-C26
14	b	829	CLA	C16-C17-C18-C20
19	Q	207	LMT	C2-C3-C4-C5
19	b	854	LMT	C2-C3-C4-C5
14	L	1501	CLA	O1A-CGA-O2A-C1
14	b	828	CLA	O1A-CGA-O2A-C1
19	A	859	LMT	C4-C5-C6-C7
14	A	841	CLA	C13-C15-C16-C17
14	a	845	CLA	CBD-CGD-O2D-CED
18	A	852	LMG	C32-C33-C34-C35
18	a	853	LMG	C14-C15-C16-C17
14	L	1503	CLA	C10-C11-C12-C13
14	B	840	CLA	C2-C1-O2A-CGA
14	B	805	CLA	CBA-CGA-O2A-C1
14	G	841	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	C5-C6-C7-C8
14	B	810	CLA	C13-C15-C16-C17
14	H	814	CLA	C3-C5-C6-C7
18	A	852	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
12	a	855	LHG	C9-C10-C11-C12
14	a	840	CLA	C16-C17-C18-C19
12	M	104	LHG	C23-C24-C25-C26
14	G	834	CLA	O1A-CGA-O2A-C1
14	H	838	CLA	O1A-CGA-O2A-C1
14	b	823	CLA	C3-C5-C6-C7
18	G	852	LMG	C37-C38-C39-C40
19	H	853	LMT	O1'-C1-C2-C3
14	B	832	CLA	C3-C5-C6-C7
14	b	832	CLA	C10-C11-C12-C13
17	B	849	BCR	C36-C18-C19-C20
21	I	102	ECH	C7-C8-C9-C34
18	A	852	LMG	C13-C14-C15-C16
19	b	854	LMT	C3-C4-C5-C6
14	A	843	CLA	C4B-C3B-CAB-CBB
14	B	810	CLA	C4B-C3B-CAB-CBB
14	B	837	CLA	C4B-C3B-CAB-CBB
14	B	842	CLA	C4B-C3B-CAB-CBB
14	G	813	CLA	C4B-C3B-CAB-CBB
14	G	817	CLA	C1A-C2A-CAA-CBA
14	G	842	CLA	C4B-C3B-CAB-CBB
14	H	820	CLA	C4B-C3B-CAB-CBB
14	H	828	CLA	C1A-C2A-CAA-CBA
14	H	836	CLA	C4B-C3B-CAB-CBB
14	H	840	CLA	C4B-C3B-CAB-CBB
14	J	1101	CLA	C1A-C2A-CAA-CBA
14	J	1102	CLA	C4B-C3B-CAB-CBB
14	J	1103	CLA	C4B-C3B-CAB-CBB
14	Q	205	CLA	C4B-C3B-CAB-CBB
14	S	1101	CLA	C1A-C2A-CAA-CBA
14	S	1102	CLA	C4B-C3B-CAB-CBB
14	S	1103	CLA	C4B-C3B-CAB-CBB
14	a	826	CLA	C1A-C2A-CAA-CBA
14	a	837	CLA	C4B-C3B-CAB-CBB
14	a	843	CLA	C4B-C3B-CAB-CBB
14	b	816	CLA	C1A-C2A-CAA-CBA
14	b	822	CLA	C4B-C3B-CAB-CBB
14	b	823	CLA	C4B-C3B-CAB-CBB
14	b	830	CLA	C1A-C2A-CAA-CBA
14	b	838	CLA	C4B-C3B-CAB-CBB
14	b	842	CLA	C4B-C3B-CAB-CBB
14	f	205	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	j	101	CLA	C4B-C3B-CAB-CBB
14	j	102	CLA	C4B-C3B-CAB-CBB
14	k	101	CLA	C4B-C3B-CAB-CBB
14	A	833	CLA	O1D-CGD-O2D-CED
14	b	821	CLA	O1D-CGD-O2D-CED
17	a	858	BCR	C17-C18-C19-C20
17	j	103	BCR	C7-C8-C9-C10
21	R	102	ECH	C21-C22-C23-C24
12	L	1509	LHG	C24-C25-C26-C27
14	a	842	CLA	C2A-CAA-CBA-CGA
18	b	853	LMG	C13-C14-C15-C16
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	823	CLA	C2-C3-C5-C6
14	G	824	CLA	C2-C3-C5-C6
14	a	824	CLA	C2-C3-C5-C6
14	a	808	CLA	C10-C11-C12-C13
19	A	853	LMT	O1'-C1-C2-C3
14	B	820	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	C11-C12-C13-C15
14	A	821	CLA	C6-C7-C8-C10
14	A	824	CLA	C12-C13-C15-C16
14	B	807	CLA	C11-C12-C13-C15
14	B	821	CLA	C6-C7-C8-C10
14	B	828	CLA	C12-C13-C15-C16
14	B	832	CLA	C6-C7-C8-C10
14	G	812	CLA	C12-C13-C15-C16
14	G	814	CLA	C6-C7-C8-C10
14	G	819	CLA	C11-C12-C13-C15
14	G	826	CLA	C11-C12-C13-C15
14	G	826	CLA	C12-C13-C15-C16
14	G	840	CLA	C11-C12-C13-C15
14	H	819	CLA	C6-C7-C8-C10
14	H	827	CLA	C12-C13-C15-C16
14	K	103	CLA	C12-C13-C15-C16
14	T	103	CLA	C12-C13-C15-C16
14	a	814	CLA	C6-C7-C8-C10
14	a	826	CLA	C11-C12-C13-C15
14	b	828	CLA	C12-C13-C15-C16
14	b	833	CLA	C6-C7-C8-C10
14	b	840	CLA	C6-C7-C8-C10
14	k	103	CLA	C11-C12-C13-C15
14	l	5005	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	H	815	CLA	C16-C17-C18-C20
14	b	816	CLA	C16-C17-C18-C20
18	b	853	LMG	C12-C13-C14-C15
19	a	854	LMT	C7-C8-C9-C10
14	a	819	CLA	C15-C16-C17-C18
12	M	102	LHG	C29-C30-C31-C32
14	B	805	CLA	O1A-CGA-O2A-C1
12	M	104	LHG	C11-C10-C9-C8
14	A	821	CLA	C4-C3-C5-C6
14	H	829	CLA	C4-C3-C5-C6
14	L	1503	CLA	C4-C3-C5-C6
14	b	816	CLA	C3A-C2A-CAA-CBA
14	G	826	CLA	C16-C17-C18-C19
14	G	826	CLA	C16-C17-C18-C20
14	a	803	CLA	C13-C15-C16-C17
14	a	844	CLA	C13-C15-C16-C17
14	A	843	CLA	C6-C7-C8-C9
14	B	810	CLA	C14-C13-C15-C16
14	B	829	CLA	C14-C13-C15-C16
14	B	839	CLA	C14-C13-C15-C16
14	G	805	CLA	C11-C10-C8-C9
14	G	820	CLA	C11-C12-C13-C14
14	G	828	CLA	C11-C12-C13-C14
14	G	843	CLA	C6-C7-C8-C9
14	H	811	CLA	C14-C13-C15-C16
14	H	828	CLA	C14-C13-C15-C16
14	H	838	CLA	C14-C13-C15-C16
14	a	812	CLA	C14-C13-C15-C16
14	a	828	CLA	C11-C12-C13-C14
14	b	806	CLA	C11-C12-C13-C14
14	b	813	CLA	C14-C13-C15-C16
14	b	829	CLA	C14-C13-C15-C16
14	l	5004	CLA	C6-C7-C8-C9
12	A	801	LHG	O10-C23-O8-C6
14	G	841	CLA	O1A-CGA-O2A-C1
14	b	814	CLA	CAA-CBA-CGA-O2A
14	a	814	CLA	C13-C15-C16-C17
14	H	834	CLA	C6-C7-C8-C10
14	a	807	CLA	CBD-CGD-O2D-CED
14	H	822	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C13-C15-C16-C17
14	H	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	H	811	CLA	C15-C16-C17-C18
14	b	812	CLA	C8-C10-C11-C12
14	A	814	CLA	C2-C1-O2A-CGA
14	H	838	CLA	C3-C5-C6-C7
12	H	850	LHG	O7-C5-C6-O8
18	A	855	LMG	O1-C7-C8-O7
19	G	853	LMT	O1'-C1-C2-C3
14	B	814	CLA	O1D-CGD-O2D-CED
14	G	804	CLA	C13-C15-C16-C17
12	A	801	LHG	C4-C5-C6-O8
12	G	854	LHG	C4-C5-C6-O8
18	A	855	LMG	O1-C7-C8-C9
14	G	819	CLA	CAA-CBA-CGA-O2A
14	A	805	CLA	CAD-CBD-CGD-O2D
14	A	844	CLA	CAD-CBD-CGD-O2D
14	B	801	CLA	CAD-CBD-CGD-O2D
14	B	807	CLA	CAD-CBD-CGD-O2D
14	G	802	CLA	CAD-CBD-CGD-O2D
14	G	806	CLA	CAD-CBD-CGD-O2D
14	G	844	CLA	CAD-CBD-CGD-O2D
14	H	806	CLA	CAD-CBD-CGD-O2D
14	a	806	CLA	CAD-CBD-CGD-O2D
14	a	845	CLA	CAD-CBD-CGD-O2D
14	b	801	CLA	CAD-CBD-CGD-O2D
14	b	819	CLA	O1D-CGD-O2D-CED
14	B	815	CLA	C16-C17-C18-C20
19	f	207	LMT	C6-C7-C8-C9
14	G	808	CLA	C3-C5-C6-C7
14	G	830	CLA	C2A-CAA-CBA-CGA
14	a	803	CLA	C2A-CAA-CBA-CGA
12	a	855	LHG	C13-C14-C15-C16
18	G	852	LMG	C36-C37-C38-C39
12	A	801	LHG	C4-O6-P-O3
12	A	801	LHG	C4-O6-P-O4
12	B	851	LHG	C3-O3-P-O5
12	G	854	LHG	C4-O6-P-O4
12	G	855	LHG	C4-O6-P-O5
12	G	856	LHG	C3-O3-P-O5
12	G	856	LHG	C4-O6-P-O4
12	M	101	LHG	C3-O3-P-O5
12	M	101	LHG	C3-O3-P-O6
12	a	801	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
12	b	852	LHG	C3-O3-P-O5
14	A	805	CLA	CAD-CBD-CGD-O1D
14	A	814	CLA	CHA-CBD-CGD-O1D
14	A	814	CLA	CHA-CBD-CGD-O2D
14	A	822	CLA	CHA-CBD-CGD-O1D
14	A	844	CLA	CAD-CBD-CGD-O1D
14	B	801	CLA	CAD-CBD-CGD-O1D
14	B	807	CLA	CAD-CBD-CGD-O1D
14	B	834	CLA	CHA-CBD-CGD-O1D
14	B	834	CLA	CHA-CBD-CGD-O2D
14	G	802	CLA	CAD-CBD-CGD-O1D
14	G	805	CLA	CHA-CBD-CGD-O1D
14	G	805	CLA	CHA-CBD-CGD-O2D
14	G	806	CLA	CAD-CBD-CGD-O1D
14	G	807	CLA	CHA-CBD-CGD-O1D
14	G	823	CLA	CHA-CBD-CGD-O1D
14	G	823	CLA	CHA-CBD-CGD-O2D
14	G	844	CLA	CAD-CBD-CGD-O1D
14	H	806	CLA	CAD-CBD-CGD-O1D
14	H	816	CLA	CAD-CBD-CGD-O1D
14	K	102	CLA	CHA-CBD-CGD-O1D
14	T	101	CLA	CHA-CBD-CGD-O1D
14	a	806	CLA	CAD-CBD-CGD-O1D
14	a	808	CLA	CHA-CBD-CGD-O1D
14	a	816	CLA	CAD-CBD-CGD-O1D
14	a	845	CLA	CAD-CBD-CGD-O1D
14	b	801	CLA	CAD-CBD-CGD-O1D
14	b	823	CLA	CHA-CBD-CGD-O1D
14	b	823	CLA	CHA-CBD-CGD-O2D
17	A	849	BCR	C19-C20-C21-C22
17	S	1104	BCR	C9-C10-C11-C12
17	a	851	BCR	C19-C20-C21-C22
17	a	852	BCR	C19-C20-C21-C22
21	m	101	ECH	C15-C16-C17-C18
14	B	831	CLA	C10-C11-C12-C13
14	A	836	CLA	C4-C3-C5-C6
14	A	824	CLA	C2B-C3B-CAB-CBB
14	F	204	CLA	C2B-C3B-CAB-CBB
14	G	843	CLA	C2B-C3B-CAB-CBB
14	a	810	CLA	C2B-C3B-CAB-CBB
14	a	819	CLA	C2B-C3B-CAB-CBB
18	A	852	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
14	a	828	CLA	C2-C3-C5-C6
14	H	818	CLA	C13-C15-C16-C17
12	G	856	LHG	C2-C3-O3-P
17	G	847	BCR	C37-C22-C23-C24
21	R	102	ECH	C7-C8-C9-C34
21	R	102	ECH	C36-C18-C19-C20
21	b	848	ECH	C37-C22-C23-C24
14	A	825	CLA	C16-C17-C18-C19
14	a	826	CLA	C16-C17-C18-C19
12	M	101	LHG	C12-C13-C14-C15
14	B	817	CLA	C3-C5-C6-C7
12	H	850	LHG	C7-C8-C9-C10
19	B	854	LMT	C2-C3-C4-C5
12	L	1510	LHG	C6-C5-O7-C7
14	A	825	CLA	O1D-CGD-O2D-CED
18	B	853	LMG	C34-C35-C36-C37
19	U	207	LMT	C2-C3-C4-C5
14	j	102	CLA	CAA-CBA-CGA-O2A
14	A	830	CLA	C2-C3-C5-C6
14	H	829	CLA	C2-C3-C5-C6
19	A	859	LMT	C6-C7-C8-C9
19	U	207	LMT	C7-C8-C9-C10
19	a	854	LMT	C6-C7-C8-C9
19	A	859	LMT	O1'-C1-C2-C3
17	a	858	BCR	C19-C20-C21-C22
12	G	856	LHG	O6-C4-C5-C6
12	L	1510	LHG	O6-C4-C5-C6
12	M	101	LHG	O6-C4-C5-C6
14	a	829	CLA	C13-C15-C16-C17
14	A	819	CLA	C11-C12-C13-C14
14	A	825	CLA	C11-C12-C13-C14
14	B	817	CLA	C11-C10-C8-C9
14	B	820	CLA	C11-C12-C13-C14
14	B	821	CLA	C14-C13-C15-C16
14	B	834	CLA	C11-C10-C8-C9
14	G	814	CLA	C6-C7-C8-C9
14	H	831	CLA	C6-C7-C8-C9
14	a	825	CLA	C14-C13-C15-C16
14	b	801	CLA	C11-C12-C13-C14
14	b	817	CLA	C6-C7-C8-C9
14	b	822	CLA	C14-C13-C15-C16
14	b	823	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	840	CLA	C6-C7-C8-C9
14	l	5006	CLA	C11-C10-C8-C9
14	A	819	CLA	C11-C12-C13-C15
14	A	836	CLA	C11-C12-C13-C15
14	B	812	CLA	C12-C13-C15-C16
14	B	820	CLA	C11-C12-C13-C15
14	B	834	CLA	C11-C10-C8-C7
14	G	825	CLA	C12-C13-C15-C16
14	b	817	CLA	C6-C7-C8-C10
14	b	822	CLA	C12-C13-C15-C16
14	b	823	CLA	C6-C7-C8-C10
14	A	825	CLA	C16-C17-C18-C20
14	H	815	CLA	C16-C17-C18-C19
14	H	834	CLA	C6-C7-C8-C9
14	B	823	CLA	C13-C15-C16-C17
14	H	834	CLA	C5-C6-C7-C8
14	A	824	CLA	C8-C10-C11-C12
14	H	807	CLA	C10-C11-C12-C13
14	a	805	CLA	C4-C3-C5-C6
14	G	829	CLA	C2-C3-C5-C6
14	A	833	CLA	C16-C17-C18-C20
14	a	840	CLA	C16-C17-C18-C20
19	H	852	LMT	C7-C8-C9-C10
12	G	855	LHG	C13-C14-C15-C16
14	B	817	CLA	C10-C11-C12-C13
12	A	801	LHG	O7-C5-C6-O8
12	G	854	LHG	O7-C5-C6-O8
18	a	853	LMG	O1-C7-C8-O7
14	H	812	CLA	CAA-CBA-CGA-O2A
14	A	841	CLA	CBA-CGA-O2A-C1
12	L	1509	LHG	C31-C32-C33-C34
14	G	834	CLA	C16-C17-C18-C20
14	a	820	CLA	C16-C17-C18-C20
14	a	826	CLA	C16-C17-C18-C20
14	b	827	CLA	C16-C17-C18-C20
14	A	817	CLA	O1D-CGD-O2D-CED
18	H	801	LMG	C11-C10-O7-C8
13	a	802	CL0	CAA-CBA-CGA-O2A
14	b	818	CLA	C2A-CAA-CBA-CGA
14	H	825	CLA	C5-C6-C7-C8
14	H	817	CLA	C3-C5-C6-C7
19	A	859	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	G	815	CLA	C4-C3-C5-C6
14	A	827	CLA	C16-C17-C18-C19
14	G	839	CLA	C16-C17-C18-C19
13	G	801	CL0	CAA-CBA-CGA-O2A
14	a	819	CLA	CAA-CBA-CGA-O2A
14	A	821	CLA	C2-C3-C5-C6
18	G	852	LMG	O1-C7-C8-C9
18	U	201	LMG	C7-C8-C9-O8
14	A	842	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	C8-C10-C11-C12
14	b	823	CLA	C10-C11-C12-C13
19	f	207	LMT	C5'-C4'-O1B-C1B
14	a	845	CLA	O1D-CGD-O2D-CED
14	B	813	CLA	CAA-CBA-CGA-O2A
14	G	814	CLA	C13-C15-C16-C17
17	A	860	BCR	C36-C18-C19-C20
14	H	817	CLA	C10-C11-C12-C13
17	R	103	BCR	C7-C8-C9-C10
21	H	846	ECH	C21-C22-C23-C24
18	K	105	LMG	C8-C7-O1-C1
14	A	841	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	O1D-CGD-O2D-CED
17	B	848	BCR	C19-C20-C21-C22
14	a	828	CLA	C16-C17-C18-C19
14	H	817	CLA	C4-C3-C5-C6
14	H	819	CLA	C4-C3-C5-C6
14	G	806	CLA	C2C-C3C-CAC-CBC
12	H	850	LHG	C16-C17-C18-C19
19	G	857	LMT	C2-C1-O1'-C1'
13	a	802	CL0	C16-C17-C18-C19
14	A	821	CLA	C6-C7-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	B	816	CLA	C6-C7-C8-C9
14	B	827	CLA	C6-C7-C8-C9
14	B	828	CLA	C14-C13-C15-C16
14	G	826	CLA	C11-C12-C13-C14
14	G	826	CLA	C14-C13-C15-C16
14	G	840	CLA	C11-C12-C13-C14
14	H	805	CLA	C11-C10-C8-C9
14	H	827	CLA	C14-C13-C15-C16
14	a	814	CLA	C6-C7-C8-C9
14	a	832	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	b	808	CLA	C6-C7-C8-C9
14	b	828	CLA	C6-C7-C8-C9
14	b	840	CLA	C11-C10-C8-C9
14	k	103	CLA	C11-C12-C13-C14
14	l	5005	CLA	C14-C13-C15-C16
14	l	5006	CLA	C14-C13-C15-C16
14	H	837	CLA	CBA-CGA-O2A-C1
18	A	852	LMG	C33-C34-C35-C36
14	A	836	CLA	C4B-C3B-CAB-CBB
14	G	809	CLA	C4B-C3B-CAB-CBB
14	G	836	CLA	C4B-C3B-CAB-CBB
14	H	815	CLA	C4B-C3B-CAB-CBB
14	H	841	CLA	C4B-C3B-CAB-CBB
14	K	101	CLA	C4B-C3B-CAB-CBB
14	T	101	CLA	C4B-C3B-CAB-CBB
19	A	856	LMT	C5-C6-C7-C8
12	b	852	LHG	C7-C8-C9-C10
14	A	839	CLA	C16-C17-C18-C19
14	B	835	CLA	C6-C7-C8-C10
14	T	103	CLA	C16-C17-C18-C19
14	a	834	CLA	C16-C17-C18-C20
14	G	807	CLA	C5-C6-C7-C8
14	Q	202	CLA	C13-C15-C16-C17
14	A	840	CLA	C4-C3-C5-C6
14	A	836	CLA	C2-C3-C5-C6
14	G	815	CLA	C2-C3-C5-C6
14	H	817	CLA	C2-C3-C5-C6
12	G	854	LHG	C10-C11-C12-C13
14	B	827	CLA	CBD-CGD-O2D-CED
14	a	842	CLA	C13-C15-C16-C17
14	A	833	CLA	C11-C12-C13-C15
14	A	841	CLA	C6-C7-C8-C10
14	B	816	CLA	C6-C7-C8-C10
14	B	817	CLA	C11-C10-C8-C7
14	a	820	CLA	C11-C12-C13-C15
14	a	832	CLA	C11-C12-C13-C15
14	b	808	CLA	C6-C7-C8-C10
14	b	822	CLA	C6-C7-C8-C10
14	H	810	CLA	C8-C10-C11-C12
19	A	856	LMT	C7-C8-C9-C10
14	A	827	CLA	C16-C17-C18-C20
14	a	820	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	a	828	CLA	C16-C17-C18-C20
14	b	827	CLA	C16-C17-C18-C19
12	G	855	LHG	C26-C27-C28-C29
12	B	851	LHG	C16-C17-C18-C19
14	A	828	CLA	C3A-C2A-CAA-CBA
14	A	829	CLA	C3A-C2A-CAA-CBA
14	G	829	CLA	C3A-C2A-CAA-CBA
14	H	835	CLA	C3A-C2A-CAA-CBA
14	a	815	CLA	C4-C3-C5-C6
14	a	829	CLA	C3A-C2A-CAA-CBA
14	a	830	CLA	C3A-C2A-CAA-CBA
14	f	201	CLA	C3A-C2A-CAA-CBA
17	A	851	BCR	C11-C10-C9-C34
17	A	851	BCR	C16-C17-C18-C36
17	F	205	BCR	C35-C13-C14-C15
17	G	851	BCR	C11-C10-C9-C34
17	G	851	BCR	C16-C17-C18-C36
17	Q	206	BCR	C35-C13-C14-C15
17	a	852	BCR	C11-C10-C9-C34
17	a	852	BCR	C16-C17-C18-C36
17	f	206	BCR	C35-C13-C14-C15
21	B	847	ECH	C11-C10-C9-C34
21	B	847	ECH	C20-C21-C22-C37
21	H	846	ECH	C11-C10-C9-C34
21	H	846	ECH	C20-C21-C22-C37
21	I	102	ECH	C11-C10-C9-C34
21	M	103	ECH	C11-C10-C9-C34
21	R	102	ECH	C11-C10-C9-C34
21	V	102	ECH	C11-C10-C9-C34
21	b	848	ECH	C11-C10-C9-C34
21	b	848	ECH	C20-C21-C22-C37
21	i	102	ECH	C11-C10-C9-C34
14	a	822	CLA	C3-C5-C6-C7
18	A	855	LMG	C13-C14-C15-C16
14	b	811	CLA	C13-C15-C16-C17
19	a	857	LMT	C3-C4-C5-C6
18	b	803	LMG	C30-C31-C32-C33
14	A	811	CLA	C2-C1-O2A-CGA
14	H	839	CLA	C2-C1-O2A-CGA
14	a	832	CLA	C2-C1-O2A-CGA
14	b	843	CLA	C2-C1-O2A-CGA
17	G	858	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
21	V	102	ECH	C13-C14-C15-C16
19	Q	201	LMT	O5B-C1B-O1B-C4'
14	A	841	CLA	C8-C10-C11-C12
14	G	830	CLA	C5-C6-C7-C8
14	G	840	CLA	C8-C10-C11-C12
17	L	1504	BCR	C7-C8-C9-C34
21	i	102	ECH	C36-C18-C19-C20
14	A	823	CLA	C4-C3-C5-C6
14	G	824	CLA	C4-C3-C5-C6
14	a	824	CLA	C4-C3-C5-C6
14	A	811	CLA	C13-C15-C16-C17
14	b	809	CLA	C10-C11-C12-C13
12	A	801	LHG	C14-C15-C16-C17
14	a	807	CLA	O1D-CGD-O2D-CED
14	J	1102	CLA	CAA-CBA-CGA-O2A
14	a	825	CLA	C8-C10-C11-C12
17	H	848	BCR	C17-C18-C19-C20
14	G	805	CLA	C4-C3-C5-C6
14	L	1503	CLA	C2-C3-C5-C6
14	G	839	CLA	C16-C17-C18-C20
14	K	103	CLA	C16-C17-C18-C19
14	a	818	CLA	C16-C17-C18-C20
19	Q	207	LMT	C5'-C4'-O1B-C1B
14	Q	204	CLA	CAA-CBA-CGA-O1A
14	G	802	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	C14-C13-C15-C16
14	A	828	CLA	C6-C7-C8-C9
14	A	836	CLA	C6-C7-C8-C9
14	A	841	CLA	C6-C7-C8-C9
14	B	812	CLA	C11-C12-C13-C14
14	B	832	CLA	C6-C7-C8-C9
14	B	841	CLA	C6-C7-C8-C9
14	G	802	CLA	C11-C12-C13-C14
14	G	819	CLA	C14-C13-C15-C16
14	G	829	CLA	C6-C7-C8-C9
14	G	829	CLA	C11-C10-C8-C9
14	G	838	CLA	C11-C12-C13-C14
14	G	840	CLA	C11-C10-C8-C9
14	H	812	CLA	C11-C10-C8-C9
14	H	820	CLA	C11-C12-C13-C14
14	H	833	CLA	C11-C10-C8-C9
14	H	839	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	U	202	CLA	C14-C13-C15-C16
14	a	808	CLA	C6-C7-C8-C9
14	a	820	CLA	C11-C12-C13-C14
14	a	820	CLA	C14-C13-C15-C16
14	a	829	CLA	C6-C7-C8-C9
14	a	835	CLA	C14-C13-C15-C16
14	a	836	CLA	C11-C12-C13-C14
14	a	837	CLA	C11-C12-C13-C14
14	b	822	CLA	C6-C7-C8-C9
14	b	833	CLA	C6-C7-C8-C9
14	b	842	CLA	C6-C7-C8-C9
18	B	852	LMG	C28-C29-C30-C31
14	A	828	CLA	C16-C17-C18-C19
14	G	828	CLA	C16-C17-C18-C19
14	b	840	CLA	C13-C15-C16-C17
14	H	830	CLA	CBD-CGD-O2D-CED
12	V	101	LHG	C24-C25-C26-C27
12	L	1509	LHG	C4-C5-O7-C7
12	L	1509	LHG	C6-C5-O7-C7
14	b	819	CLA	O2A-C1-C2-C3
18	A	855	LMG	C7-C8-O7-C10
14	G	802	CLA	CBD-CGD-O2D-CED
14	H	812	CLA	C13-C15-C16-C17
17	b	847	BCR	C19-C20-C21-C22
18	B	803	LMG	C13-C14-C15-C16
14	B	828	CLA	C16-C17-C18-C19
14	a	817	CLA	C4C-C3C-CAC-CBC
14	a	815	CLA	C2-C3-C5-C6
14	H	837	CLA	O1A-CGA-O2A-C1
14	H	821	CLA	CAA-CBA-CGA-O1A
14	Q	204	CLA	CAA-CBA-CGA-O2A
14	a	814	CLA	C2A-CAA-CBA-CGA
19	f	207	LMT	C3'-C4'-O1B-C1B
14	A	815	CLA	C1A-C2A-CAA-CBA
14	A	828	CLA	C1A-C2A-CAA-CBA
14	B	815	CLA	C1A-C2A-CAA-CBA
14	B	828	CLA	C1A-C2A-CAA-CBA
14	G	804	CLA	C1A-C2A-CAA-CBA
14	G	836	CLA	C1A-C2A-CAA-CBA
14	G	844	CLA	C1A-C2A-CAA-CBA
14	H	814	CLA	C1A-C2A-CAA-CBA
14	H	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	835	CLA	C1A-C2A-CAA-CBA
14	K	102	CLA	C1A-C2A-CAA-CBA
14	U	202	CLA	C1A-C2A-CAA-CBA
14	a	803	CLA	C1A-C2A-CAA-CBA
14	b	819	CLA	C1A-C2A-CAA-CBA
17	A	851	BCR	C11-C10-C9-C8
17	A	851	BCR	C16-C17-C18-C19
17	F	205	BCR	C12-C13-C14-C15
17	G	851	BCR	C11-C10-C9-C8
17	G	851	BCR	C16-C17-C18-C19
17	Q	206	BCR	C12-C13-C14-C15
17	a	852	BCR	C11-C10-C9-C8
17	a	852	BCR	C16-C17-C18-C19
17	f	206	BCR	C12-C13-C14-C15
21	B	847	ECH	C11-C10-C9-C8
21	B	847	ECH	C20-C21-C22-C23
21	H	846	ECH	C11-C10-C9-C8
21	H	846	ECH	C20-C21-C22-C23
21	I	102	ECH	C11-C10-C9-C8
21	M	103	ECH	C11-C10-C9-C8
21	R	102	ECH	C11-C10-C9-C8
21	V	102	ECH	C11-C10-C9-C8
21	b	848	ECH	C11-C10-C9-C8
21	b	848	ECH	C20-C21-C22-C23
21	i	102	ECH	C11-C10-C9-C8
12	a	801	LHG	C26-C27-C28-C29
14	a	829	CLA	C16-C17-C18-C19
18	b	803	LMG	C36-C37-C38-C39
14	A	809	CLA	C2B-C3B-CAB-CBB
14	G	810	CLA	C2B-C3B-CAB-CBB
14	G	822	CLA	C2B-C3B-CAB-CBB
14	H	823	CLA	C2B-C3B-CAB-CBB
14	a	818	CLA	C2B-C3B-CAB-CBB
14	a	844	CLA	C2B-C3B-CAB-CBB
14	b	833	CLA	C2B-C3B-CAB-CBB
14	b	837	CLA	C2B-C3B-CAB-CBB
17	A	847	BCR	C1-C6-C7-C8
17	A	847	BCR	C5-C6-C7-C8
17	G	847	BCR	C5-C6-C7-C8
17	J	1104	BCR	C5-C6-C7-C8
17	S	1104	BCR	C5-C6-C7-C8
17	a	848	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	a	850	BCR	C23-C24-C25-C26
17	j	103	BCR	C5-C6-C7-C8
21	B	847	ECH	C5-C6-C7-C8
21	B	847	ECH	C23-C24-C25-C26
12	L	1509	LHG	C29-C30-C31-C32
14	J	1102	CLA	CAA-CBA-CGA-O1A
19	Q	201	LMT	C2B-C1B-O1B-C4'
14	B	827	CLA	O1D-CGD-O2D-CED
14	A	840	CLA	C2-C3-C5-C6
14	S	1102	CLA	CAA-CBA-CGA-O2A
14	A	825	CLA	C12-C13-C15-C16
14	A	834	CLA	C11-C12-C13-C15
14	B	812	CLA	C11-C12-C13-C15
14	B	821	CLA	C12-C13-C15-C16
14	B	827	CLA	C6-C7-C8-C10
14	B	827	CLA	C12-C13-C15-C16
14	G	806	CLA	C6-C7-C8-C10
14	G	815	CLA	C11-C12-C13-C15
14	H	805	CLA	C11-C10-C8-C7
14	H	825	CLA	C11-C10-C8-C7
14	H	833	CLA	C11-C10-C8-C7
14	H	840	CLA	C12-C13-C15-C16
14	H	841	CLA	C11-C10-C8-C7
14	U	202	CLA	C11-C12-C13-C15
14	U	205	CLA	C12-C13-C15-C16
14	a	815	CLA	C11-C12-C13-C15
14	a	820	CLA	C12-C13-C15-C16
14	b	808	CLA	C11-C12-C13-C15
14	b	816	CLA	C11-C10-C8-C7
14	b	818	CLA	C12-C13-C15-C16
14	b	828	CLA	C6-C7-C8-C10
14	b	840	CLA	C11-C10-C8-C7
14	b	843	CLA	C11-C12-C13-C15
14	k	103	CLA	C12-C13-C15-C16
14	l	5006	CLA	C12-C13-C15-C16
14	G	829	CLA	C16-C17-C18-C19
12	H	850	LHG	C23-C24-C25-C26
19	J	1106	LMT	C2-C3-C4-C5
12	M	104	LHG	C27-C28-C29-C30
14	b	819	CLA	C3-C5-C6-C7
14	B	835	CLA	C6-C7-C8-C9
14	l	5005	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	M	102	LHG	C30-C31-C32-C33
17	H	844	BCR	C36-C18-C19-C20
17	a	850	BCR	C36-C18-C19-C20
17	b	850	BCR	C36-C18-C19-C20
18	B	853	LMG	C15-C16-C17-C18
14	a	816	CLA	CAA-CBA-CGA-O2A
14	a	826	CLA	C4-C3-C5-C6
19	U	207	LMT	C1-C2-C3-C4
14	H	818	CLA	C2-C1-O2A-CGA
14	H	832	CLA	C2-C1-O2A-CGA
14	b	808	CLA	C2-C1-O2A-CGA
14	b	820	CLA	C2-C1-O2A-CGA
14	A	806	CLA	C15-C16-C17-C18
14	A	820	CLA	C13-C15-C16-C17
14	G	821	CLA	C5-C6-C7-C8
14	K	103	CLA	C13-C15-C16-C17
14	a	818	CLA	C8-C10-C11-C12
14	k	102	CLA	CAA-CBA-CGA-O2A
17	b	847	BCR	C21-C22-C23-C24
14	a	833	CLA	C11-C12-C13-C15
14	b	829	CLA	C16-C17-C18-C19
14	H	811	CLA	C3-C5-C6-C7
14	A	835	CLA	C11-C12-C13-C14
14	B	828	CLA	C11-C12-C13-C14
14	G	805	CLA	C13-C15-C16-C17
14	H	815	CLA	C10-C11-C12-C13
18	H	801	LMG	O9-C10-O7-C8
17	A	860	BCR	C19-C20-C21-C22
17	l	5003	BCR	C9-C10-C11-C12
14	B	808	CLA	C10-C11-C12-C13
14	S	1102	CLA	CAA-CBA-CGA-O1A
14	a	840	CLA	C13-C15-C16-C17
18	B	853	LMG	C16-C17-C18-C19
19	A	856	LMT	C2B-C1B-O1B-C4'
14	H	830	CLA	O1D-CGD-O2D-CED
14	G	821	CLA	C4-C3-C5-C6
14	H	814	CLA	C4-C3-C5-C6
14	b	822	CLA	C4-C3-C5-C6
14	A	817	CLA	C8-C10-C11-C12
12	G	856	LHG	C5-C4-O6-P
14	A	836	CLA	C10-C11-C12-C13
14	G	806	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	H	827	CLA	C15-C16-C17-C18
14	T	103	CLA	C16-C17-C18-C20
18	G	852	LMG	C32-C33-C34-C35
14	G	836	CLA	CBD-CGD-O2D-CED
14	G	825	CLA	C8-C10-C11-C12
14	a	814	CLA	C10-C11-C12-C13
14	G	836	CLA	O1D-CGD-O2D-CED
14	H	834	CLA	CAA-CBA-CGA-O2A
18	H	851	LMG	O1-C7-C8-C9
18	L	1508	LMG	O1-C7-C8-C9
12	A	801	LHG	C26-C27-C28-C29
19	f	207	LMT	C4-C5-C6-C7
14	H	835	CLA	CAA-CBA-CGA-O2A
14	Q	204	CLA	C2A-CAA-CBA-CGA
13	a	802	CL0	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C20
19	b	854	LMT	C6-C7-C8-C9
14	j	101	CLA	CAA-CBA-CGA-O2A
12	G	855	LHG	C10-C11-C12-C13
19	J	1106	LMT	C5'-C4'-O1B-C1B
14	A	820	CLA	C4-C3-C5-C6
14	U	202	CLA	C4-C3-C5-C6
14	a	821	CLA	C4-C3-C5-C6
14	H	803	CLA	CAA-CBA-CGA-O2A
19	A	857	LMT	C6-C7-C8-C9
14	B	834	CLA	C16-C17-C18-C19
14	G	828	CLA	C16-C17-C18-C20
14	G	818	CLA	C8-C10-C11-C12
14	b	820	CLA	C10-C11-C12-C13
14	A	811	CLA	C4B-C3B-CAB-CBB
14	A	841	CLA	C4B-C3B-CAB-CBB
14	B	809	CLA	C4B-C3B-CAB-CBB
14	B	816	CLA	C4B-C3B-CAB-CBB
14	B	835	CLA	C4B-C3B-CAB-CBB
14	G	817	CLA	C4B-C3B-CAB-CBB
14	b	810	CLA	C4B-C3B-CAB-CBB
14	b	825	CLA	C4B-C3B-CAB-CBB
14	H	835	CLA	CAA-CBA-CGA-O1A
19	B	855	LMT	C5'-C4'-O1B-C1B
14	A	824	CLA	C16-C17-C18-C19
14	K	103	CLA	C16-C17-C18-C20
14	a	818	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	b	827	CLA	C5-C6-C7-C8
14	G	814	CLA	C10-C11-C12-C13
14	f	201	CLA	C10-C11-C12-C13
18	b	803	LMG	C16-C17-C18-C19
14	A	835	CLA	C16-C17-C18-C20
14	B	821	CLA	C4-C3-C5-C6
12	A	801	LHG	C10-C11-C12-C13
14	H	821	CLA	CAA-CBA-CGA-O2A
14	a	816	CLA	CAA-CBA-CGA-O1A
14	F	201	CLA	C13-C15-C16-C17
14	A	817	CLA	C12-C13-C15-C16
14	a	837	CLA	C11-C12-C13-C15
19	B	855	LMT	C2B-C1B-O1B-C4'
19	U	207	LMT	C11-C10-C9-C8
17	R	103	BCR	C13-C14-C15-C16
21	L	1506	ECH	C15-C16-C17-C18
21	M	103	ECH	C13-C14-C15-C16
14	H	833	CLA	C3-C5-C6-C7
19	Q	201	LMT	C5-C6-C7-C8
14	A	838	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	C11-C10-C8-C9
14	A	831	CLA	C6-C7-C8-C9
14	A	841	CLA	C11-C12-C13-C14
14	B	801	CLA	C11-C10-C8-C9
14	B	818	CLA	C14-C13-C15-C16
14	B	838	CLA	C11-C10-C8-C9
14	G	807	CLA	C6-C7-C8-C9
14	G	812	CLA	C14-C13-C15-C16
14	G	818	CLA	C14-C13-C15-C16
14	G	838	CLA	C11-C10-C8-C9
14	G	841	CLA	C11-C12-C13-C14
14	H	815	CLA	C6-C7-C8-C9
14	K	103	CLA	C14-C13-C15-C16
14	T	103	CLA	C14-C13-C15-C16
14	a	842	CLA	C6-C7-C8-C9
14	b	821	CLA	C11-C12-C13-C14
14	b	829	CLA	C11-C12-C13-C14
14	a	818	CLA	CAA-CBA-CGA-O2A
14	B	819	CLA	C2-C1-O2A-CGA
14	G	805	CLA	C2-C1-O2A-CGA
14	H	806	CLA	C2-C1-O2A-CGA
14	H	841	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	b	818	CLA	C2-C1-O2A-CGA
18	B	803	LMG	C16-C17-C18-C19
14	B	815	CLA	C3A-C2A-CAA-CBA
14	G	804	CLA	C3A-C2A-CAA-CBA
14	G	844	CLA	C3A-C2A-CAA-CBA
14	H	814	CLA	C3A-C2A-CAA-CBA
14	H	816	CLA	C3A-C2A-CAA-CBA
14	K	103	CLA	C4-C3-C5-C6
14	U	206	CLA	C4-C3-C5-C6
14	b	816	CLA	C4-C3-C5-C6
14	b	837	CLA	C3A-C2A-CAA-CBA
14	l	5004	CLA	C4-C3-C5-C6
14	A	838	CLA	CBD-CGD-O2D-CED
12	M	101	LHG	C25-C26-C27-C28
14	H	817	CLA	C5-C6-C7-C8
14	k	102	CLA	CAA-CBA-CGA-O1A
14	G	843	CLA	CAA-CBA-CGA-O2A
14	a	813	CLA	O2A-C1-C2-C3
18	B	852	LMG	C9-C8-O7-C10
19	Q	207	LMT	C3'-C4'-O1B-C1B
19	b	854	LMT	C7-C8-C9-C10
14	A	806	CLA	CAA-CBA-CGA-O2A
14	G	826	CLA	C13-C15-C16-C17
12	M	104	LHG	C12-C13-C14-C15
14	j	101	CLA	CAA-CBA-CGA-O1A
12	B	851	LHG	C17-C18-C19-C20
14	G	834	CLA	C5-C6-C7-C8
14	a	842	CLA	C8-C10-C11-C12
14	B	822	CLA	CAA-CBA-CGA-O1A
14	F	203	CLA	CAA-CBA-CGA-O2A
14	U	202	CLA	C2-C3-C5-C6
14	H	812	CLA	C16-C17-C18-C20
14	B	818	CLA	C3-C5-C6-C7
14	b	808	CLA	O1D-CGD-O2D-CED
12	L	1510	LHG	C11-C10-C9-C8
14	B	819	CLA	C15-C16-C17-C18
14	b	808	CLA	CBD-CGD-O2D-CED
12	L	1509	LHG	C7-C8-C9-C10
14	G	802	CLA	C13-C15-C16-C17
15	B	844	PQN	C26-C27-C28-C29
14	A	818	CLA	CAA-CBA-CGA-O1A
14	H	808	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	b	826	CLA	C5-C6-C7-C8
12	G	854	LHG	O8-C23-C24-C25
17	U	203	BCR	C19-C20-C21-C22
21	H	846	ECH	C19-C20-C21-C22
12	M	102	LHG	C24-C25-C26-C27
14	H	820	CLA	C3-C5-C6-C7
14	b	816	CLA	C5-C6-C7-C8
19	b	855	LMT	C1-C2-C3-C4
14	F	203	CLA	CAA-CBA-CGA-O1A
14	A	824	CLA	C14-C13-C15-C16
14	B	820	CLA	C6-C7-C8-C9
14	B	839	CLA	C6-C7-C8-C9
14	G	819	CLA	C11-C12-C13-C14
14	H	820	CLA	C14-C13-C15-C16
14	H	840	CLA	C6-C7-C8-C9
14	H	841	CLA	C14-C13-C15-C16
14	J	1101	CLA	C11-C10-C8-C9
14	a	822	CLA	C11-C10-C8-C9
14	a	826	CLA	C11-C12-C13-C14
14	a	829	CLA	C11-C10-C8-C9
14	b	828	CLA	C14-C13-C15-C16
14	b	835	CLA	C11-C12-C13-C14
14	G	820	CLA	C16-C17-C18-C20
14	B	819	CLA	CAA-CBA-CGA-O2A
14	H	811	CLA	CAA-CBA-CGA-O2A
14	b	820	CLA	CAA-CBA-CGA-O2A
14	b	827	CLA	CAA-CBA-CGA-O2A
18	b	803	LMG	O10-C28-O8-C9
14	H	831	CLA	C3-C5-C6-C7
14	H	816	CLA	CAA-CBA-CGA-O2A
14	G	841	CLA	C16-C17-C18-C20
14	A	807	CLA	C11-C12-C13-C15
14	A	841	CLA	C11-C12-C13-C15
14	B	809	CLA	C12-C13-C15-C16
14	B	828	CLA	C11-C12-C13-C15
14	B	838	CLA	C11-C10-C8-C7
14	B	839	CLA	C6-C7-C8-C10
14	B	840	CLA	C11-C10-C8-C7
14	G	809	CLA	C12-C13-C15-C16
14	G	818	CLA	C12-C13-C15-C16
14	G	834	CLA	C12-C13-C15-C16
14	G	836	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	G	840	CLA	C11-C10-C8-C7
14	G	841	CLA	C11-C12-C13-C15
14	H	806	CLA	C11-C12-C13-C15
14	H	815	CLA	C6-C7-C8-C10
14	H	826	CLA	C12-C13-C15-C16
14	H	839	CLA	C11-C10-C8-C7
14	J	1101	CLA	C12-C13-C15-C16
14	L	1502	CLA	C12-C13-C15-C16
14	S	1101	CLA	C12-C13-C15-C16
14	a	809	CLA	C12-C13-C15-C16
14	a	823	CLA	C11-C12-C13-C15
14	a	826	CLA	C12-C13-C15-C16
14	a	842	CLA	C6-C7-C8-C10
14	b	841	CLA	C11-C10-C8-C7
14	l	5004	CLA	C12-C13-C15-C16
14	A	803	CLA	C2B-C3B-CAB-CBB
14	A	825	CLA	C2B-C3B-CAB-CBB
14	A	838	CLA	C2B-C3B-CAB-CBB
14	A	844	CLA	C2B-C3B-CAB-CBB
14	B	832	CLA	C2B-C3B-CAB-CBB
14	G	838	CLA	C2B-C3B-CAB-CBB
14	G	840	CLA	C2B-C3B-CAB-CBB
14	a	817	CLA	C2B-C3B-CAB-CBB
14	a	845	CLA	C2B-C3B-CAB-CBB
17	H	847	BCR	C23-C24-C25-C26
21	B	847	ECH	C23-C24-C25-C30
21	H	846	ECH	C5-C6-C7-C8
21	I	102	ECH	C1-C6-C7-C8
21	R	102	ECH	C1-C6-C7-C8
21	V	102	ECH	C5-C6-C7-C8
21	b	848	ECH	C23-C24-C25-C26
21	b	848	ECH	C23-C24-C25-C30
21	i	102	ECH	C1-C6-C7-C8
14	A	825	CLA	C2-C1-O2A-CGA
14	G	818	CLA	C2-C1-O2A-CGA
14	H	816	CLA	C2-C1-O2A-CGA
14	a	805	CLA	C2-C1-O2A-CGA
14	B	817	CLA	C11-C12-C13-C15
14	B	826	CLA	C16-C17-C18-C20
14	B	829	CLA	CBD-CGD-O2D-CED
19	L	1505	LMT	C1-C2-C3-C4
19	Q	207	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
14	B	839	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	CAA-CBA-CGA-O2A
14	b	818	CLA	CAA-CBA-CGA-O2A
14	b	825	CLA	CAA-CBA-CGA-O2A
14	b	839	CLA	CBA-CGA-O2A-C1
14	A	824	CLA	C16-C17-C18-C20
14	T	103	CLA	C13-C15-C16-C17
14	A	819	CLA	C4-C3-C5-C6
14	a	834	CLA	CBD-CGD-O2D-CED
14	H	818	CLA	CAA-CBA-CGA-O2A
14	H	825	CLA	CAA-CBA-CGA-O2A
14	A	819	CLA	C2-C3-C5-C6
14	B	830	CLA	C2-C3-C5-C6
14	H	808	CLA	C2-C3-C5-C6
14	H	819	CLA	C2-C3-C5-C6
14	K	103	CLA	C2-C3-C5-C6
14	U	206	CLA	C2-C3-C5-C6
14	a	820	CLA	C2-C3-C5-C6
14	b	836	CLA	C2-C3-C5-C6
14	G	822	CLA	O1D-CGD-O2D-CED
14	B	811	CLA	C8-C10-C11-C12
18	B	803	LMG	C11-C10-O7-C8
18	b	803	LMG	C11-C10-O7-C8
14	A	820	CLA	C5-C6-C7-C8
14	B	817	CLA	CAA-CBA-CGA-O2A
14	a	805	CLA	CAA-CBA-CGA-O2A
14	B	834	CLA	C16-C17-C18-C20
19	H	852	LMT	C1-C2-C3-C4
14	b	807	CLA	O1D-CGD-O2D-CED
12	a	855	LHG	O7-C7-C8-C9
14	B	843	CLA	CAA-CBA-CGA-O2A
18	b	803	LMG	O9-C10-O7-C8
14	b	839	CLA	O1A-CGA-O2A-C1
14	B	822	CLA	CAA-CBA-CGA-O2A
14	B	830	CLA	C4-C3-C5-C6
14	b	836	CLA	C4-C3-C5-C6
14	B	826	CLA	CAA-CBA-CGA-O2A
18	A	855	LMG	O7-C10-C11-C12
14	G	805	CLA	C2-C3-C5-C6
14	a	805	CLA	C2-C3-C5-C6
12	b	852	LHG	C14-C15-C16-C17
18	B	852	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	b	803	LMG	C29-C28-O8-C9
14	A	834	CLA	CBD-CGD-O2D-CED
14	a	835	CLA	CBD-CGD-O2D-CED
14	a	814	CLA	C8-C10-C11-C12
14	A	858	CLA	C2A-CAA-CBA-CGA
14	B	829	CLA	C2A-CAA-CBA-CGA
14	b	806	CLA	C2A-CAA-CBA-CGA
14	H	823	CLA	CAA-CBA-CGA-O2A
18	b	803	LMG	O7-C10-C11-C12
18	A	855	LMG	C17-C18-C19-C20
14	H	811	CLA	O1D-CGD-O2D-CED
14	A	825	CLA	C14-C13-C15-C16
14	G	815	CLA	C11-C12-C13-C14
14	G	825	CLA	C14-C13-C15-C16
14	H	815	CLA	C11-C12-C13-C14
14	H	816	CLA	C6-C7-C8-C9
14	H	841	CLA	C11-C10-C8-C9
14	S	1101	CLA	C11-C10-C8-C9
14	a	815	CLA	C11-C12-C13-C14
14	b	819	CLA	C11-C12-C13-C14
14	b	843	CLA	C11-C12-C13-C14
14	k	103	CLA	C14-C13-C15-C16
14	B	829	CLA	O1D-CGD-O2D-CED
14	b	823	CLA	C13-C15-C16-C17
17	A	849	BCR	C36-C18-C19-C20
14	A	825	CLA	CAA-CBA-CGA-O2A
14	a	843	CLA	CAA-CBA-CGA-O2A
19	J	1106	LMT	C3'-C4'-O1B-C1B
18	a	853	LMG	O1-C7-C8-C9
19	A	857	LMT	C9-C10-C11-C12
14	B	819	CLA	C10-C11-C12-C13
14	A	803	CLA	C1A-C2A-CAA-CBA
14	A	812	CLA	C4B-C3B-CAB-CBB
14	A	813	CLA	C1A-C2A-CAA-CBA
14	B	825	CLA	C4B-C3B-CAB-CBB
14	B	838	CLA	C1A-C2A-CAA-CBA
14	G	814	CLA	C1A-C2A-CAA-CBA
14	G	829	CLA	C1A-C2A-CAA-CBA
14	G	841	CLA	C4B-C3B-CAB-CBB
14	H	807	CLA	C4B-C3B-CAB-CBB
14	H	833	CLA	C1A-C2A-CAA-CBA
14	H	835	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	a	813	CLA	C4B-C3B-CAB-CBB
14	a	837	CLA	C1A-C2A-CAA-CBA
14	b	826	CLA	C4B-C3B-CAB-CBB
14	b	834	CLA	C1A-C2A-CAA-CBA
14	b	839	CLA	C1A-C2A-CAA-CBA
14	b	843	CLA	C4B-C3B-CAB-CBB
14	a	835	CLA	O1D-CGD-O2D-CED
14	Q	204	CLA	C4C-C3C-CAC-CBC
19	B	855	LMT	C3'-C4'-O1B-C1B
14	H	811	CLA	CBD-CGD-O2D-CED
14	a	820	CLA	C4-C3-C5-C6
14	a	808	CLA	C13-C15-C16-C17
14	l	5006	CLA	CAA-CBA-CGA-O2A
18	a	853	LMG	O7-C10-C11-C12
12	M	101	LHG	O7-C5-C6-O8
12	b	852	LHG	O7-C5-C6-O8
17	A	860	BCR	C17-C18-C19-C20
17	B	849	BCR	C17-C18-C19-C20
17	G	847	BCR	C21-C22-C23-C24
17	H	844	BCR	C17-C18-C19-C20
17	I	101	BCR	C17-C18-C19-C20
17	L	1504	BCR	C7-C8-C9-C10
17	b	850	BCR	C17-C18-C19-C20
21	I	102	ECH	C7-C8-C9-C10
21	I	102	ECH	C21-C22-C23-C24
21	R	102	ECH	C17-C18-C19-C20
21	b	848	ECH	C21-C22-C23-C24
21	i	102	ECH	C17-C18-C19-C20
14	G	822	CLA	CBD-CGD-O2D-CED
14	H	816	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C16-C17-C18-C20
14	H	817	CLA	C16-C17-C18-C20
14	a	833	CLA	C11-C12-C13-C14
14	H	828	CLA	C3-C5-C6-C7
14	A	844	CLA	CAA-CBA-CGA-O2A
14	G	805	CLA	CAA-CBA-CGA-O2A
14	G	842	CLA	CAA-CBA-CGA-O2A
18	B	803	LMG	O7-C10-C11-C12
18	G	852	LMG	O7-C10-C11-C12
18	H	801	LMG	O7-C10-C11-C12
14	a	825	CLA	C4C-C3C-CAC-CBC
14	A	817	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	H	804	CLA	C2A-CAA-CBA-CGA
14	H	828	CLA	C2A-CAA-CBA-CGA
14	b	830	CLA	C2A-CAA-CBA-CGA
18	H	801	LMG	C38-C39-C40-C41
14	A	817	CLA	C16-C17-C18-C20
14	B	820	CLA	C16-C17-C18-C20
14	H	816	CLA	C16-C17-C18-C20
14	a	822	CLA	C16-C17-C18-C20
14	b	831	CLA	C16-C17-C18-C19
14	B	823	CLA	CAA-CBA-CGA-O2A
14	b	823	CLA	CAA-CBA-CGA-O2A
14	a	834	CLA	O1D-CGD-O2D-CED
14	b	806	CLA	O1D-CGD-O2D-CED
14	G	836	CLA	C8-C10-C11-C12
14	b	840	CLA	C8-C10-C11-C12
19	H	853	LMT	C5'-C4'-O1B-C1B
14	B	807	CLA	C2-C1-O2A-CGA
14	b	834	CLA	C2-C1-O2A-CGA
14	l	5006	CLA	C2-C1-O2A-CGA
14	A	811	CLA	CAA-CBA-CGA-O2A
14	B	812	CLA	CAA-CBA-CGA-O2A
14	b	813	CLA	CAA-CBA-CGA-O2A
12	H	850	LHG	C17-C18-C19-C20
14	A	808	CLA	C12-C13-C15-C16
14	A	818	CLA	C11-C12-C13-C15
14	A	818	CLA	C12-C13-C15-C16
14	A	824	CLA	C11-C12-C13-C15
14	A	825	CLA	C11-C10-C8-C7
14	A	828	CLA	C12-C13-C15-C16
14	B	814	CLA	C12-C13-C15-C16
14	B	841	CLA	C12-C13-C15-C16
14	B	842	CLA	C11-C10-C8-C7
14	G	812	CLA	C11-C10-C8-C7
14	G	826	CLA	C11-C10-C8-C7
14	G	838	CLA	C11-C10-C8-C7
14	H	807	CLA	C11-C10-C8-C7
14	H	817	CLA	C12-C13-C15-C16
14	a	808	CLA	C11-C12-C13-C15
14	a	818	CLA	C11-C10-C8-C7
14	a	819	CLA	C11-C12-C13-C15
14	a	831	CLA	C11-C10-C8-C7
14	a	834	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	b	809	CLA	C11-C10-C8-C7
14	b	810	CLA	C12-C13-C15-C16
14	b	817	CLA	C12-C13-C15-C16
14	b	821	CLA	C11-C12-C13-C15
14	b	823	CLA	C11-C10-C8-C7
14	b	842	CLA	C12-C13-C15-C16
14	B	839	CLA	CBA-CGA-O2A-C1
14	a	826	CLA	C2-C3-C5-C6
14	b	831	CLA	C2-C3-C5-C6
14	A	813	CLA	C16-C17-C18-C19
14	b	817	CLA	C16-C17-C18-C20
12	M	104	LHG	C13-C14-C15-C16
12	A	801	LHG	C4-C5-O7-C7
14	F	201	CLA	C10-C11-C12-C13
14	G	814	CLA	C8-C10-C11-C12
14	a	830	CLA	C13-C15-C16-C17
14	A	834	CLA	O1D-CGD-O2D-CED
14	K	101	CLA	CAA-CBA-CGA-O1A
14	H	813	CLA	CAA-CBA-CGA-O2A
14	H	809	CLA	C15-C16-C17-C18
13	A	802	CL0	CAA-CBA-CGA-O1A
18	B	803	LMG	O9-C10-O7-C8
14	A	807	CLA	C16-C17-C18-C20
14	G	832	CLA	C16-C17-C18-C19
14	b	831	CLA	C16-C17-C18-C20
19	J	1106	LMT	C2B-C1B-O1B-C4'
18	U	201	LMG	C33-C34-C35-C36
14	b	805	CLA	C8-C10-C11-C12
14	H	825	CLA	CAA-CBA-CGA-O1A
14	U	202	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C3A-C2A-CAA-CBA
14	A	813	CLA	C3A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
14	B	809	CLA	C3A-C2A-CAA-CBA
14	B	824	CLA	C3A-C2A-CAA-CBA
14	B	825	CLA	C3A-C2A-CAA-CBA
14	B	828	CLA	C3A-C2A-CAA-CBA
14	B	831	CLA	C3A-C2A-CAA-CBA
14	B	838	CLA	C3A-C2A-CAA-CBA
14	G	814	CLA	C3A-C2A-CAA-CBA
14	H	808	CLA	C3A-C2A-CAA-CBA
14	H	824	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	830	CLA	C3A-C2A-CAA-CBA
14	a	803	CLA	C3A-C2A-CAA-CBA
14	a	811	CLA	C3A-C2A-CAA-CBA
14	b	810	CLA	C3A-C2A-CAA-CBA
14	b	825	CLA	C3A-C2A-CAA-CBA
14	b	832	CLA	C3A-C2A-CAA-CBA
14	b	839	CLA	C3A-C2A-CAA-CBA
14	b	818	CLA	CAA-CBA-CGA-O1A
14	H	818	CLA	C10-C11-C12-C13
14	a	807	CLA	C15-C16-C17-C18
14	b	810	CLA	C16-C17-C18-C20
14	G	816	CLA	CAA-CBA-CGA-O2A
14	b	825	CLA	CAA-CBA-CGA-O1A
14	H	818	CLA	CAA-CBA-CGA-O1A
14	b	827	CLA	CAA-CBA-CGA-O1A
14	a	805	CLA	CAA-CBA-CGA-O1A
14	b	820	CLA	CAA-CBA-CGA-O1A
14	H	827	CLA	C16-C17-C18-C20
14	B	839	CLA	C3-C5-C6-C7
14	A	824	CLA	CBA-CGA-O2A-C1
14	A	834	CLA	C11-C12-C13-C14
14	A	836	CLA	C11-C12-C13-C14
14	B	807	CLA	C11-C12-C13-C14
14	B	811	CLA	C6-C7-C8-C9
14	B	812	CLA	C14-C13-C15-C16
14	B	842	CLA	C11-C10-C8-C9
14	H	806	CLA	C11-C12-C13-C14
14	L	1502	CLA	C14-C13-C15-C16
14	S	1101	CLA	C14-C13-C15-C16
14	U	202	CLA	C11-C12-C13-C14
14	U	205	CLA	C14-C13-C15-C16
14	a	808	CLA	C11-C12-C13-C14
14	a	818	CLA	C11-C10-C8-C9
14	a	826	CLA	C14-C13-C15-C16
14	b	813	CLA	C11-C12-C13-C14
14	b	818	CLA	C14-C13-C15-C16
14	b	823	CLA	C11-C10-C8-C9
14	B	819	CLA	CAA-CBA-CGA-O1A
14	a	843	CLA	CAA-CBA-CGA-O1A
18	B	803	LMG	O9-C10-C11-C12
14	G	830	CLA	C13-C15-C16-C17
14	B	826	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	B	839	CLA	C16-C17-C18-C20
14	b	831	CLA	C4-C3-C5-C6
12	a	855	LHG	O9-C7-C8-C9
14	B	843	CLA	CAA-CBA-CGA-O1A
14	H	813	CLA	CAA-CBA-CGA-O1A
18	a	853	LMG	O9-C10-C11-C12
18	b	803	LMG	O9-C10-C11-C12
12	G	854	LHG	C24-C23-O8-C6
12	A	801	LHG	O8-C23-C24-C25
14	H	816	CLA	CAA-CBA-CGA-O1A
14	B	814	CLA	C8-C10-C11-C12
19	H	852	LMT	C4-C5-C6-C7
14	b	807	CLA	CBD-CGD-O2D-CED
17	G	858	BCR	C11-C12-C13-C14
21	R	102	ECH	C7-C8-C9-C10
14	A	816	CLA	C4C-C3C-CAC-CBC
14	L	1502	CLA	C2C-C3C-CAC-CBC
14	a	821	CLA	C13-C15-C16-C17
14	B	817	CLA	CAA-CBA-CGA-O1A
14	H	811	CLA	CAA-CBA-CGA-O1A
14	b	823	CLA	CAA-CBA-CGA-O1A
18	A	855	LMG	O9-C10-C11-C12
12	G	855	LHG	O7-C7-C8-C9
14	H	807	CLA	CAA-CBA-CGA-O2A
14	a	806	CLA	CAA-CBA-CGA-O2A
14	a	816	CLA	CBD-CGD-O2D-CED
19	a	856	LMT	C1-C2-C3-C4
18	l	5001	LMG	C7-C8-C9-O8
14	H	823	CLA	CAA-CBA-CGA-O1A
14	K	101	CLA	CAA-CBA-CGA-O2A
12	G	854	LHG	O10-C23-C24-C25
14	B	823	CLA	CAA-CBA-CGA-O1A
18	G	852	LMG	O9-C10-C11-C12
14	H	815	CLA	C8-C10-C11-C12
14	H	819	CLA	C5-C6-C7-C8
14	A	843	CLA	CAA-CBA-CGA-O2A
14	G	807	CLA	CAA-CBA-CGA-O2A
14	H	806	CLA	CAA-CBA-CGA-O2A
14	J	1103	CLA	CAA-CBA-CGA-O2A
14	A	829	CLA	C13-C15-C16-C17
14	G	805	CLA	CAA-CBA-CGA-O1A
14	a	829	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	B	822	CLA	CAD-CBD-CGD-O2D
14	H	816	CLA	CAD-CBD-CGD-O2D
14	H	821	CLA	CAD-CBD-CGD-O2D
14	K	101	CLA	CAD-CBD-CGD-O2D
14	a	809	CLA	CAD-CBD-CGD-O2D
14	a	815	CLA	CAD-CBD-CGD-O2D
14	a	828	CLA	CAD-CBD-CGD-O2D
12	a	855	LHG	C11-C12-C13-C14
12	A	854	LHG	O7-C7-C8-C9
14	A	842	CLA	CAA-CBA-CGA-O2A
14	A	811	CLA	CAA-CBA-CGA-O1A
14	A	825	CLA	CAA-CBA-CGA-O1A
14	B	826	CLA	CAA-CBA-CGA-O1A
14	b	813	CLA	CAA-CBA-CGA-O1A
18	H	801	LMG	O9-C10-C11-C12
12	G	855	LHG	C28-C29-C30-C31
14	A	824	CLA	O1A-CGA-O2A-C1
14	H	803	CLA	C8-C10-C11-C12
14	G	806	CLA	CAA-CBA-CGA-O1A
14	l	5006	CLA	CAA-CBA-CGA-O1A
14	a	816	CLA	O1D-CGD-O2D-CED
14	b	808	CLA	CAA-CBA-CGA-O2A
14	A	828	CLA	C16-C17-C18-C20
14	G	839	CLA	C3-C5-C6-C7
14	A	811	CLA	C2A-CAA-CBA-CGA
14	T	101	CLA	CAA-CBA-CGA-O2A
14	k	101	CLA	CAA-CBA-CGA-O2A
14	U	202	CLA	CBD-CGD-O2D-CED
12	A	801	LHG	O10-C23-C24-C25
14	A	844	CLA	CAA-CBA-CGA-O1A
14	G	842	CLA	CAA-CBA-CGA-O1A
14	A	830	CLA	C11-C10-C8-C7
14	b	829	CLA	C11-C12-C13-C15
14	B	837	CLA	CAA-CBA-CGA-O2A
14	B	840	CLA	CAA-CBA-CGA-O2A
14	G	806	CLA	CAA-CBA-CGA-O2A
14	G	818	CLA	CAA-CBA-CGA-O2A
14	a	844	CLA	CAA-CBA-CGA-O2A
14	b	805	CLA	CAA-CBA-CGA-O2A
18	a	853	LMG	O8-C28-C29-C30
14	A	813	CLA	C16-C17-C18-C20
14	b	822	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	H	836	CLA	CAA-CBA-CGA-O2A
18	H	801	LMG	C39-C40-C41-C42

There are no ring outliers.

152 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	822	CLA	2	0
14	B	828	CLA	1	0
14	A	803	CLA	2	0
14	A	805	CLA	1	0
14	b	801	CLA	2	0
17	J	1104	BCR	2	0
14	B	811	CLA	1	0
17	a	849	BCR	1	0
14	H	809	CLA	1	0
14	A	831	CLA	2	0
17	A	851	BCR	3	0
14	a	826	CLA	2	0
14	H	811	CLA	2	0
14	a	832	CLA	2	0
14	H	825	CLA	2	0
14	A	819	CLA	1	0
14	G	812	CLA	1	0
21	V	102	ECH	1	0
14	B	830	CLA	2	0
17	j	103	BCR	1	0
14	A	804	CLA	1	0
14	b	812	CLA	1	0
17	G	850	BCR	1	0
17	f	206	BCR	2	0
14	G	805	CLA	1	0
14	A	836	CLA	1	0
14	a	806	CLA	1	0
14	a	812	CLA	1	0
14	k	103	CLA	2	0
21	m	101	ECH	1	0
17	G	848	BCR	1	0
17	G	858	BCR	2	0
14	H	807	CLA	1	0
14	b	843	CLA	1	0
14	b	805	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	840	CLA	1	0
14	B	819	CLA	1	0
19	A	857	LMT	1	0
13	G	801	CL0	6	0
14	A	844	CLA	1	0
14	a	833	CLA	1	0
14	b	817	CLA	1	0
14	G	802	CLA	1	0
16	G	846	SF4	1	0
14	H	827	CLA	1	0
14	H	813	CLA	3	0
14	H	826	CLA	1	0
14	a	828	CLA	1	0
14	H	808	CLA	1	0
17	U	203	BCR	1	0
14	b	827	CLA	3	0
14	A	806	CLA	1	0
17	A	860	BCR	2	0
18	b	803	LMG	1	0
14	Q	202	CLA	2	0
14	A	813	CLA	2	0
14	B	840	CLA	3	0
14	B	817	CLA	1	0
17	l	5007	BCR	1	0
14	B	841	CLA	1	0
14	H	814	CLA	1	0
14	H	818	CLA	2	0
14	G	829	CLA	2	0
14	k	102	CLA	1	0
14	b	802	CLA	3	0
14	A	828	CLA	1	0
14	B	842	CLA	1	0
14	A	827	CLA	1	0
14	H	839	CLA	1	0
17	J	1105	BCR	1	0
14	L	1501	CLA	1	0
17	B	846	BCR	3	0
14	G	807	CLA	1	0
17	l	5003	BCR	3	0
14	H	820	CLA	1	0
17	b	856	BCR	2	0
18	K	105	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	816	CLA	1	0
14	U	205	CLA	1	0
17	A	850	BCR	2	0
14	G	828	CLA	1	0
14	A	815	CLA	1	0
17	F	202	BCR	1	0
14	A	823	CLA	2	0
14	B	812	CLA	2	0
14	G	821	CLA	1	0
14	b	830	CLA	1	0
17	a	858	BCR	1	0
14	b	807	CLA	1	0
14	A	858	CLA	1	0
14	b	831	CLA	1	0
14	G	825	CLA	2	0
14	b	813	CLA	1	0
21	M	103	ECH	4	0
14	G	836	CLA	1	0
14	B	823	CLA	1	0
14	G	803	CLA	1	0
14	G	804	CLA	1	0
14	H	838	CLA	1	0
14	b	818	CLA	2	0
17	B	850	BCR	2	0
17	L	1504	BCR	1	0
14	A	832	CLA	1	0
14	L	1502	CLA	1	0
17	H	845	BCR	3	0
14	a	807	CLA	1	0
14	H	805	CLA	1	0
21	L	1506	ECH	1	0
13	a	802	CL0	7	0
17	a	852	BCR	4	0
14	H	829	CLA	1	0
14	B	806	CLA	2	0
14	l	5004	CLA	1	0
14	H	831	CLA	1	0
14	a	825	CLA	3	0
21	H	846	ECH	1	0
13	A	802	CL0	4	0
14	a	829	CLA	2	0
14	B	801	CLA	1	0

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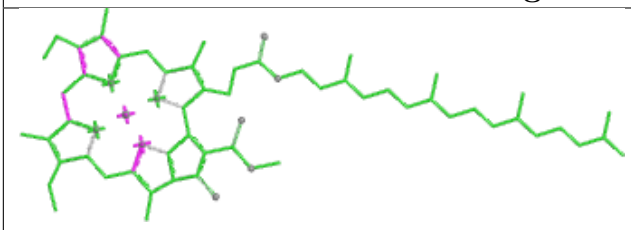
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	803	LMG	1	0
14	B	802	CLA	1	0
17	I	101	BCR	2	0
14	B	838	CLA	3	0
14	B	814	CLA	3	0
14	J	1101	CLA	1	0
14	b	816	CLA	2	0
14	F	201	CLA	3	0
14	A	809	CLA	2	0
14	G	832	CLA	1	0
14	B	820	CLA	1	0
14	G	814	CLA	1	0
16	A	846	SF4	1	0
14	f	204	CLA	1	0
14	G	840	CLA	1	0
14	B	839	CLA	1	0
14	a	820	CLA	2	0
14	a	816	CLA	1	0
14	a	830	CLA	1	0
14	a	803	CLA	1	0
14	G	834	CLA	1	0
17	i	101	BCR	1	0
14	T	102	CLA	1	0
14	B	807	CLA	1	0
17	G	851	BCR	2	0
14	H	830	CLA	1	0
14	a	822	CLA	2	0
17	B	856	BCR	1	0
14	A	824	CLA	2	0
12	G	855	LHG	1	0
14	b	820	CLA	1	0
14	H	816	CLA	1	0
14	a	840	CLA	1	0

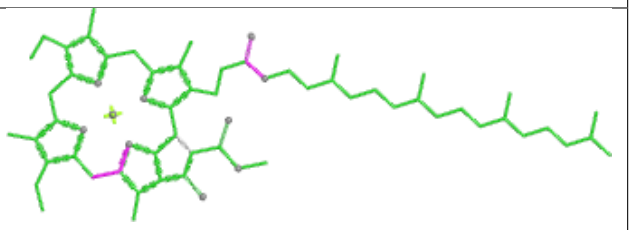
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

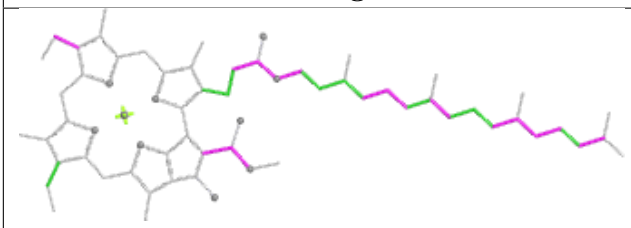
Ligand CLA A 825



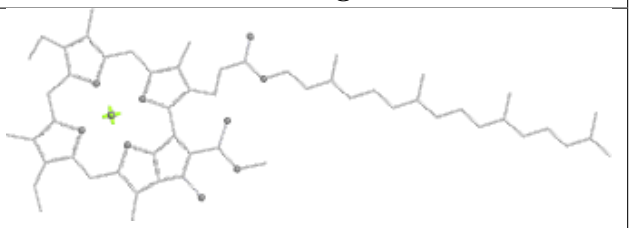
Bond lengths



Bond angles

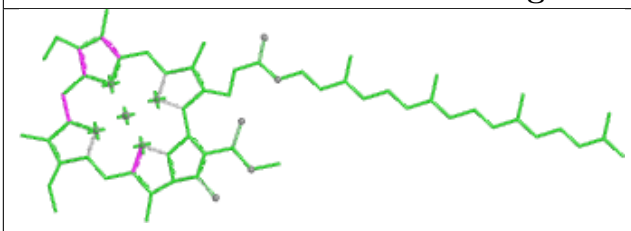


Torsions

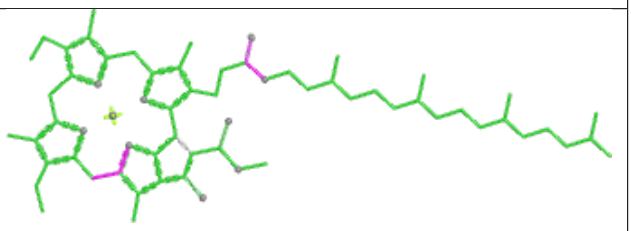


Rings

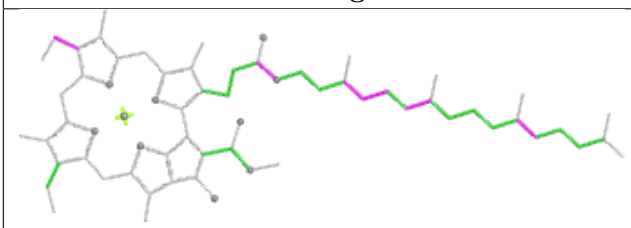
Ligand CLA b 822



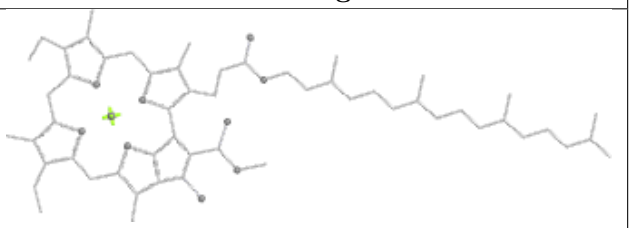
Bond lengths



Bond angles

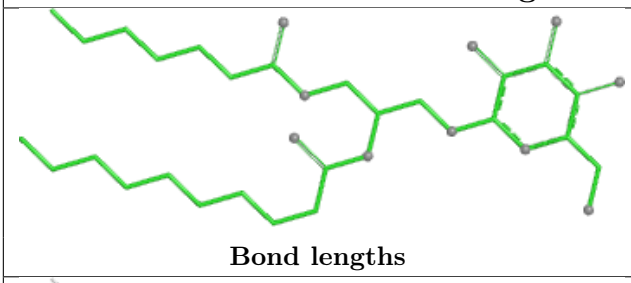


Torsions

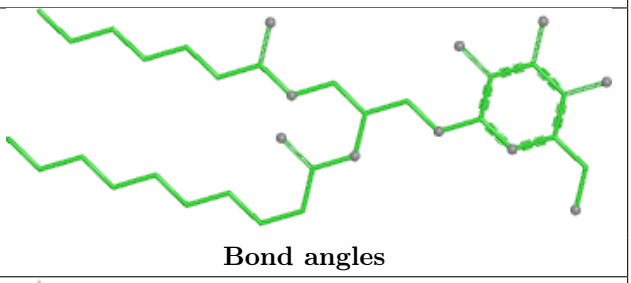


Rings

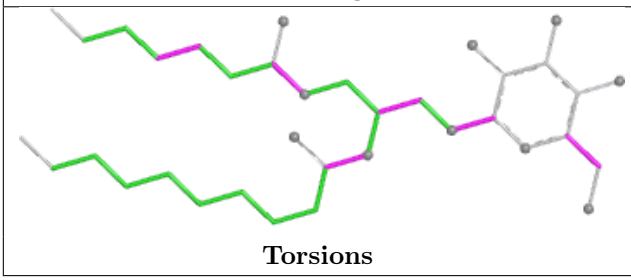
Ligand LMG H 851



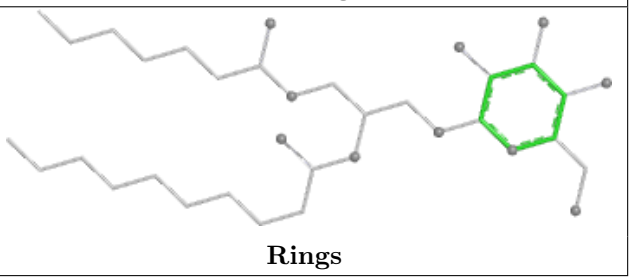
Bond lengths



Bond angles

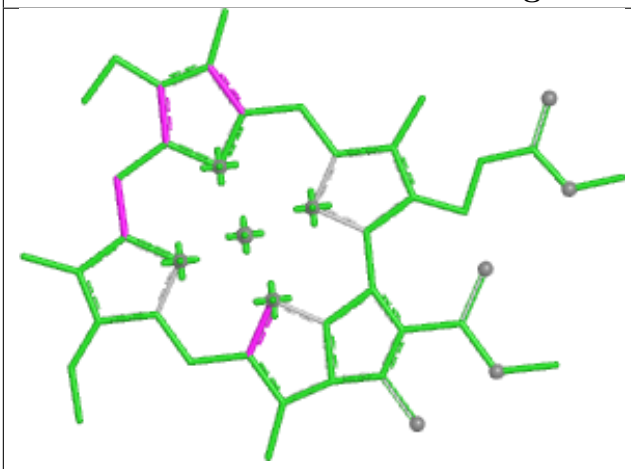


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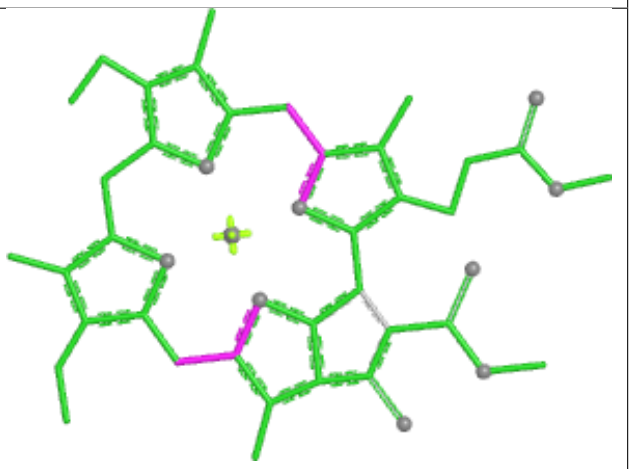


Rings

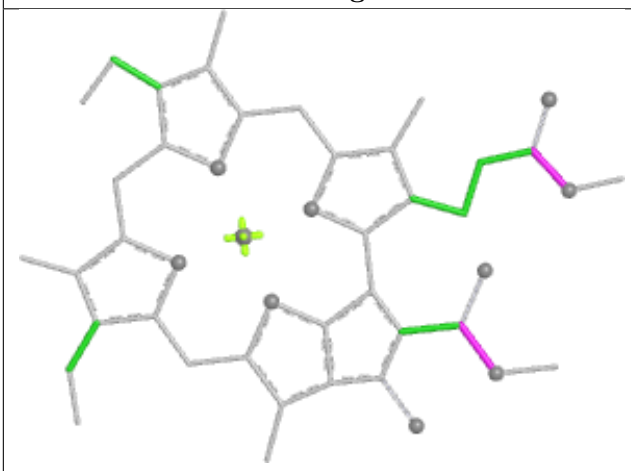
Ligand CLA H 822



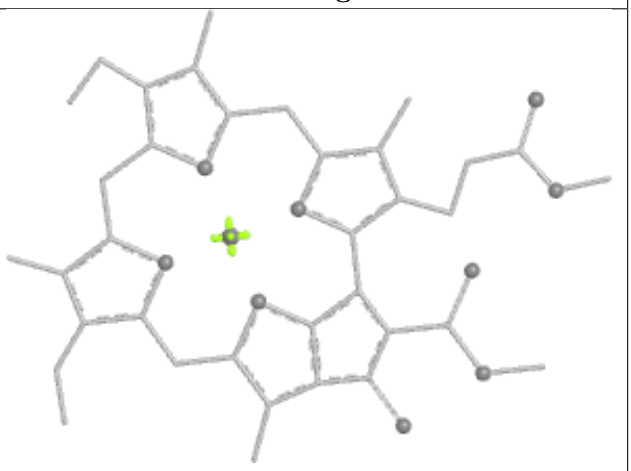
Bond lengths



Bond angles

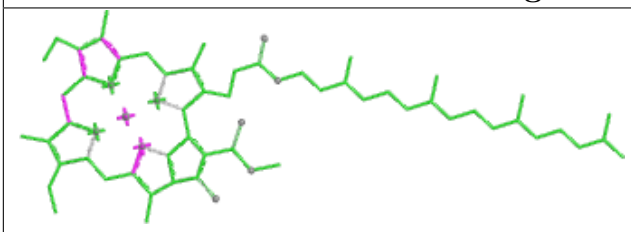


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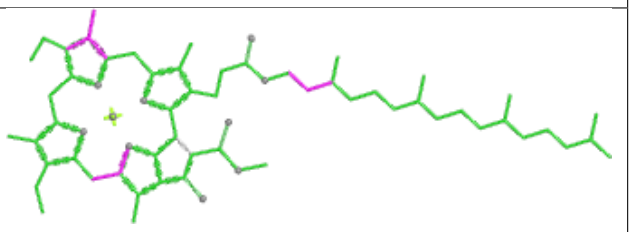


Rings

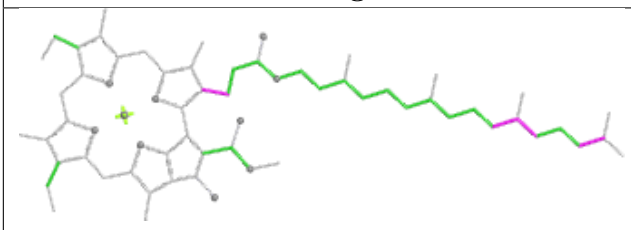
Ligand CLA B 828



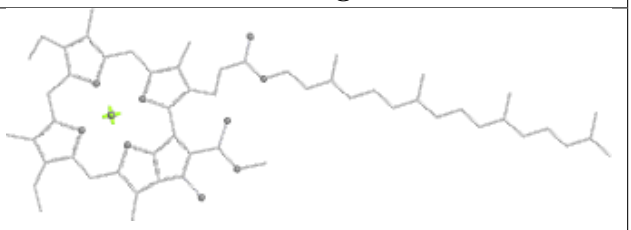
Bond lengths



Bond angles

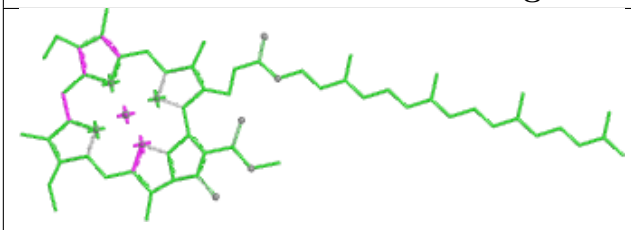


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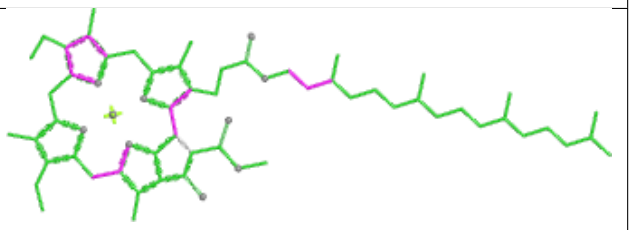


Rings

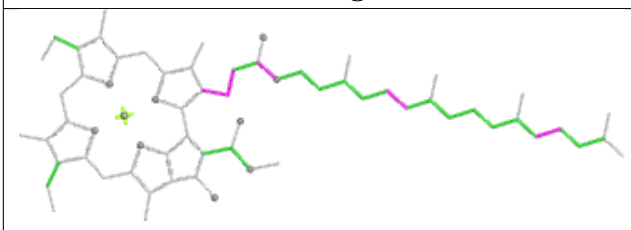
Ligand CLA A 829



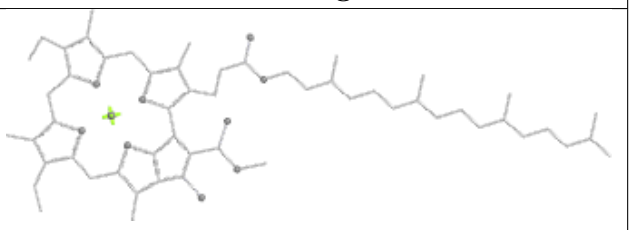
Bond lengths



Bond angles

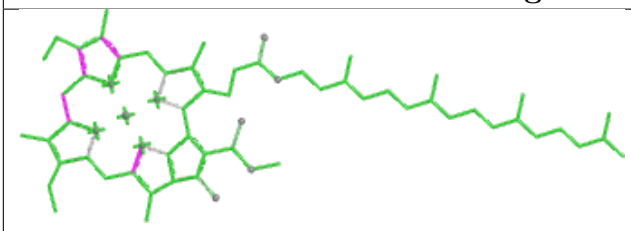


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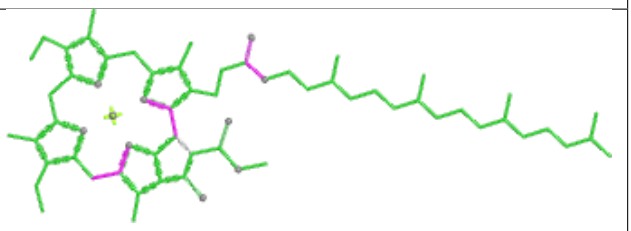


Rings

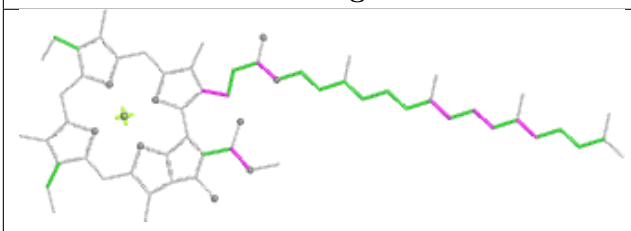
Ligand CLA B 831



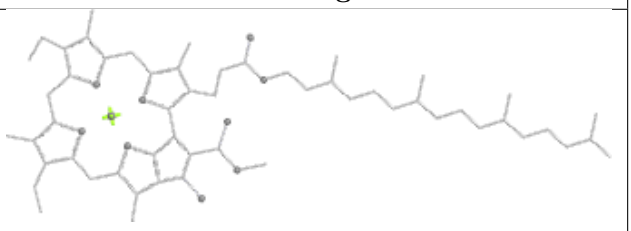
Bond lengths



Bond angles

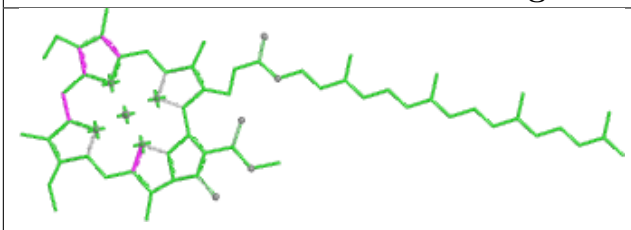


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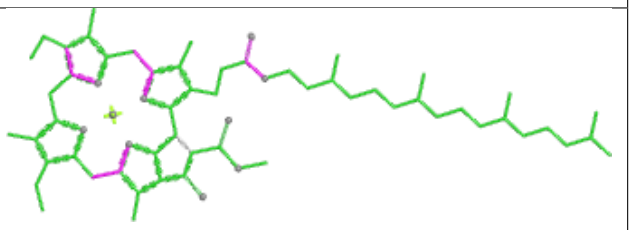


Rings

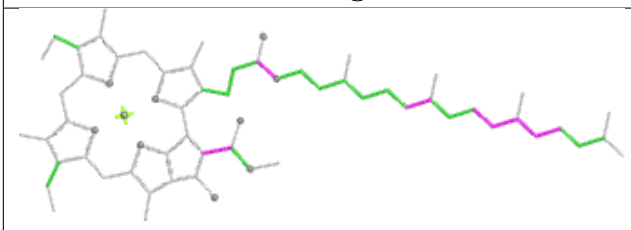
Ligand CLA a 808



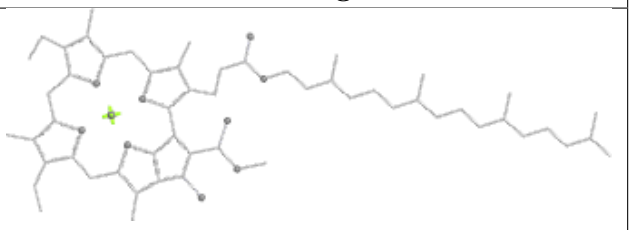
Bond lengths



Bond angles

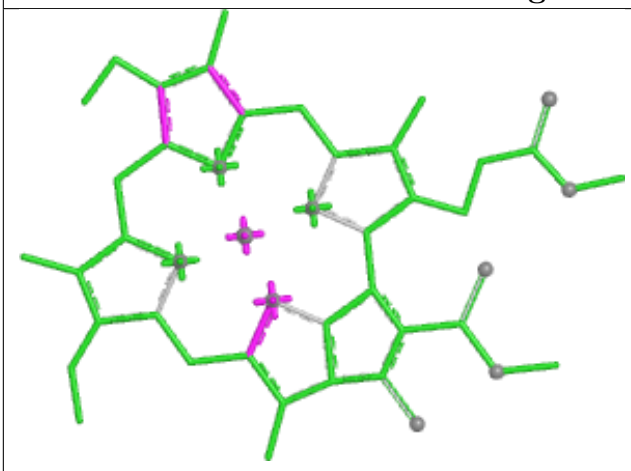


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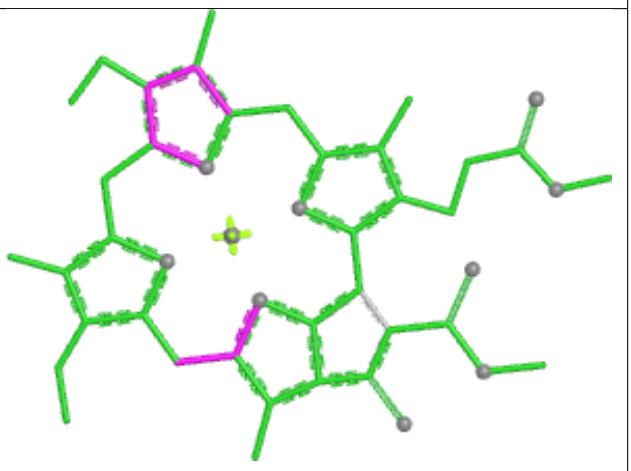


Rings

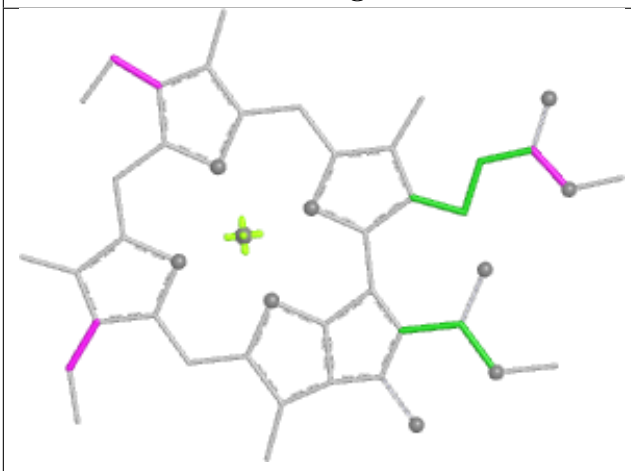
Ligand CLA a 817



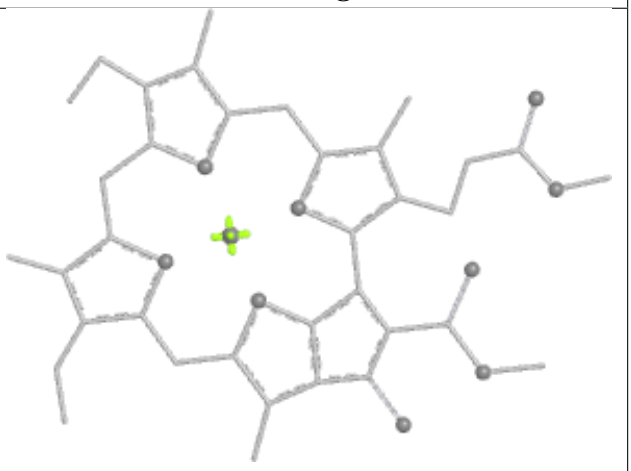
Bond lengths



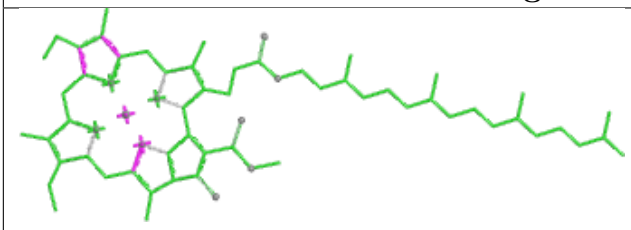
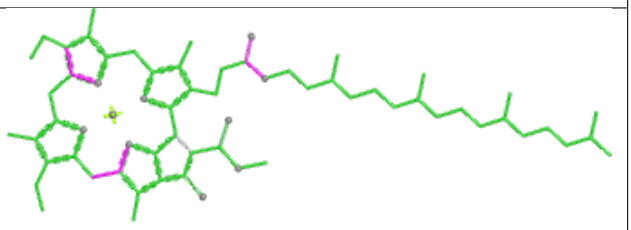
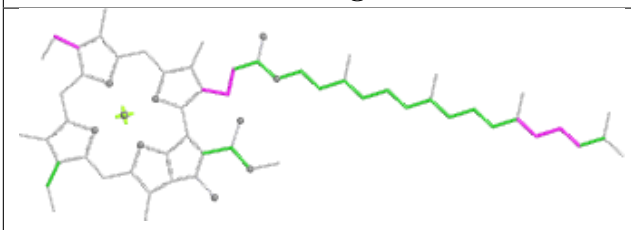
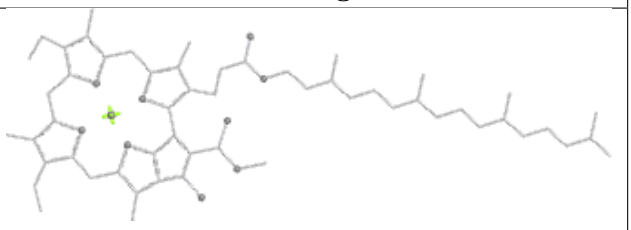
Bond angles

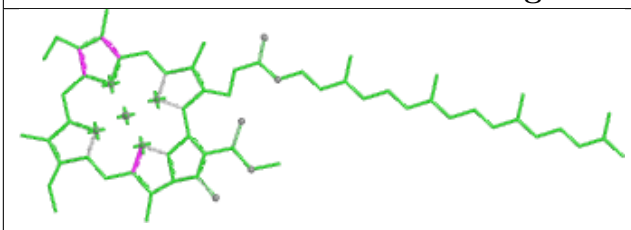
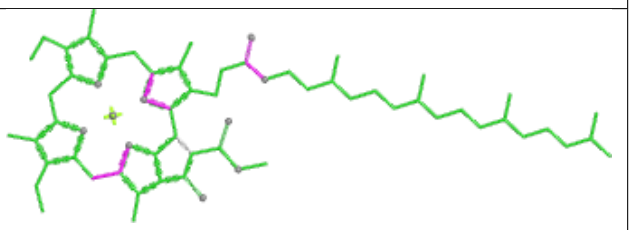
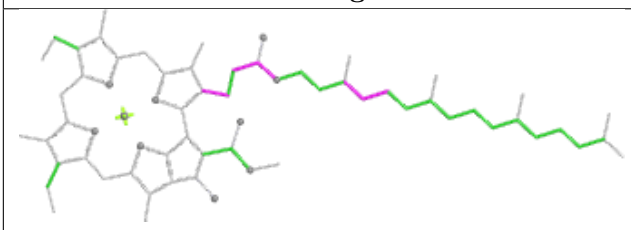
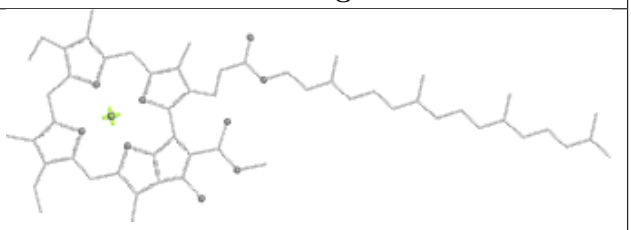


Torsions

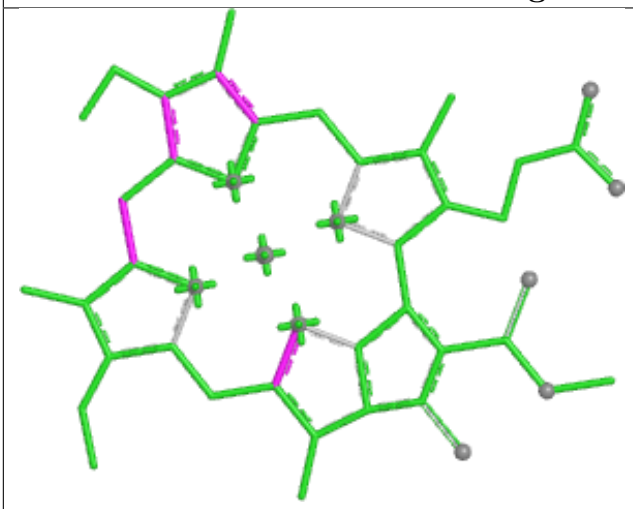


Rings

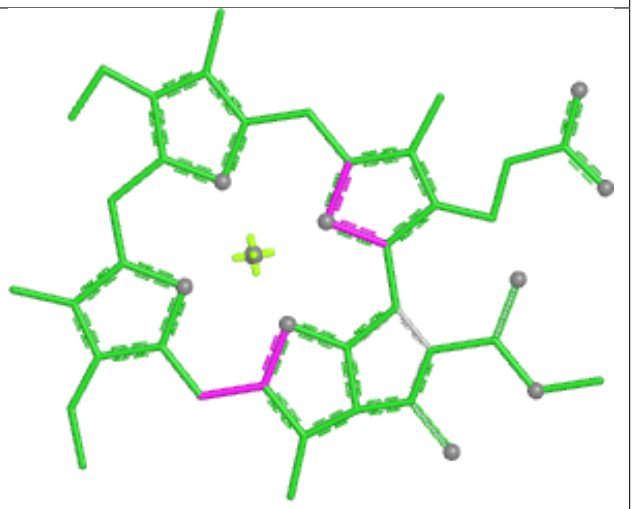
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

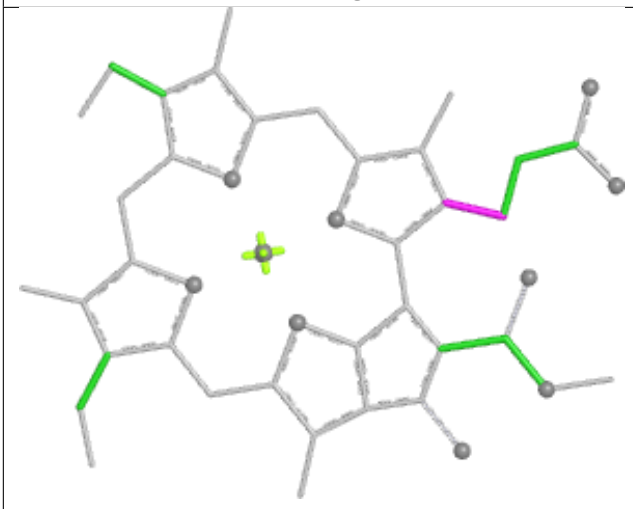
Ligand CLA a 811



Bond lengths



Bond angles

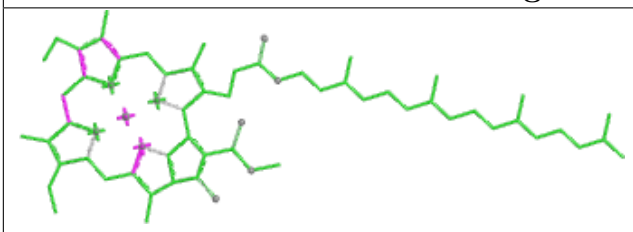


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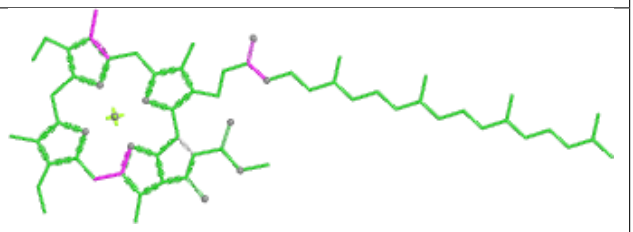


Rings

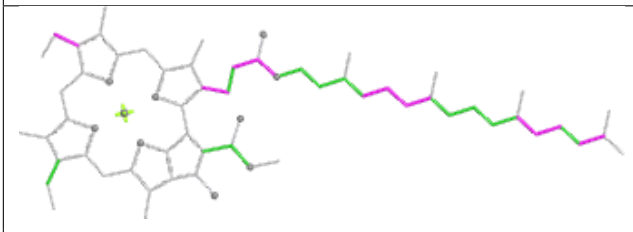
Ligand CLA A 843



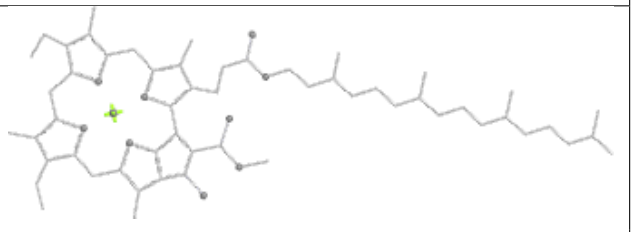
Bond lengths



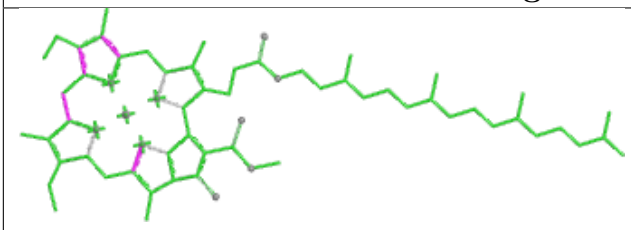
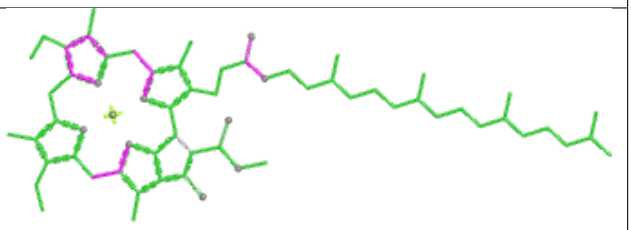
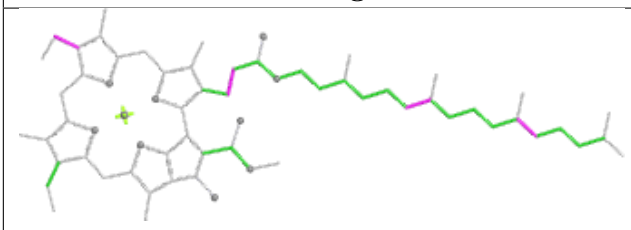
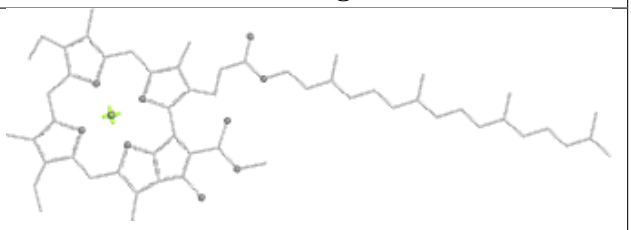
Bond angles

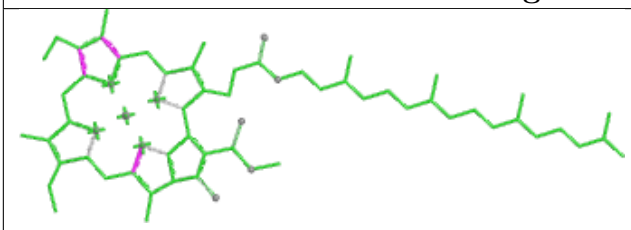
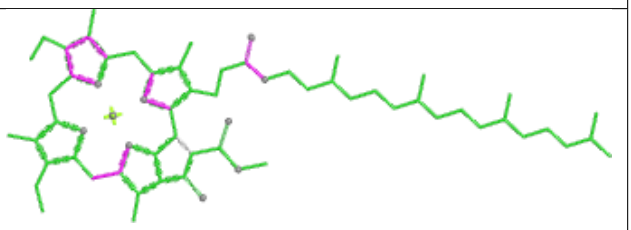
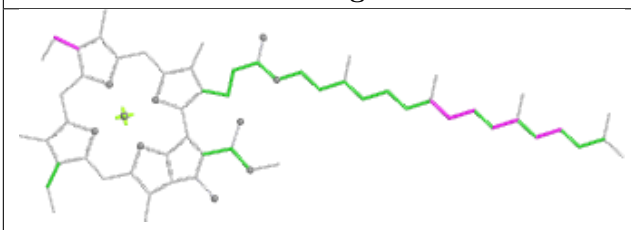
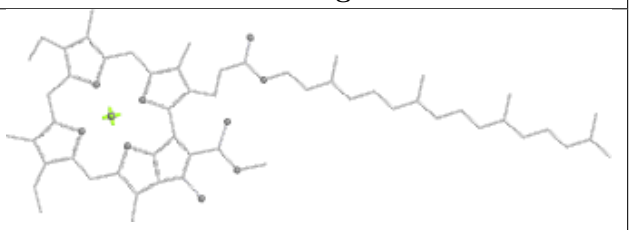


Torsions

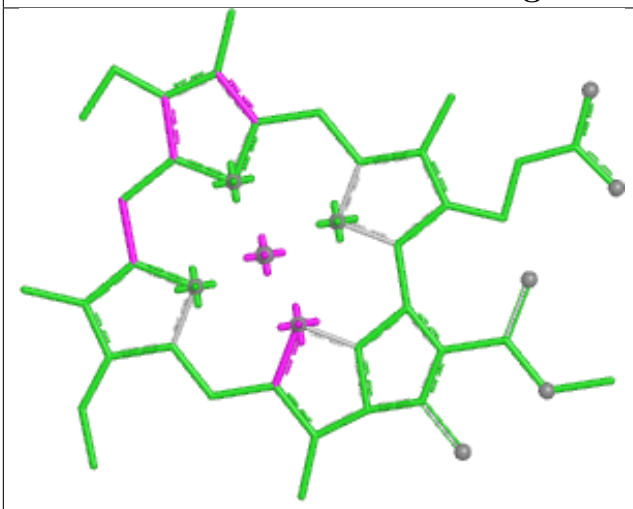


Rings

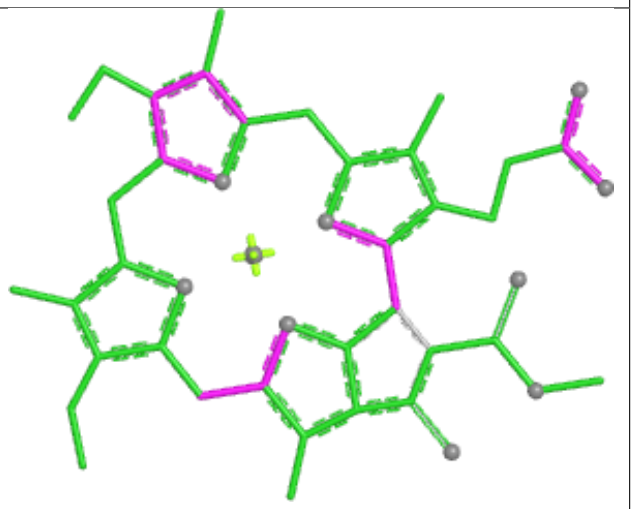
Ligand CLA H 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

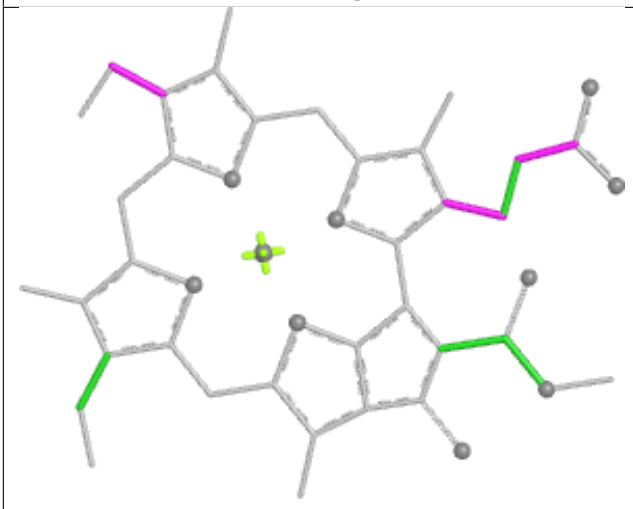
Ligand CLA H 835



Bond lengths



Bond angles

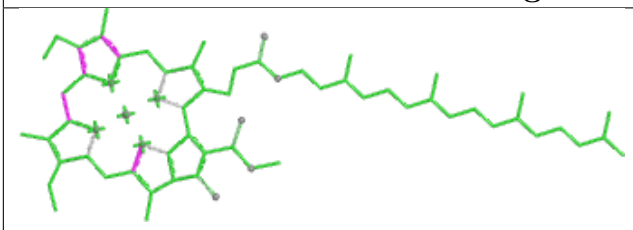


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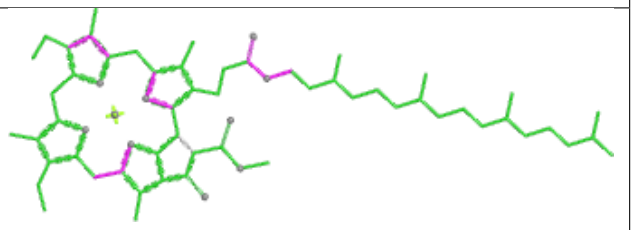


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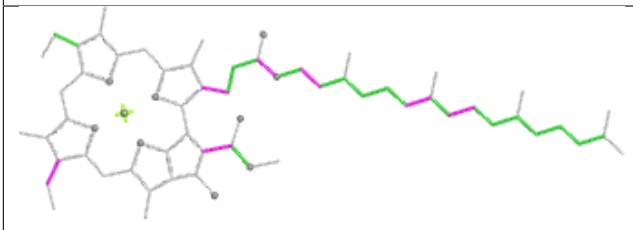
Ligand CLA A 805



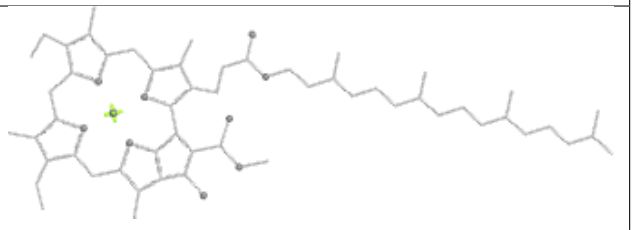
Bond lengths



Bond angles

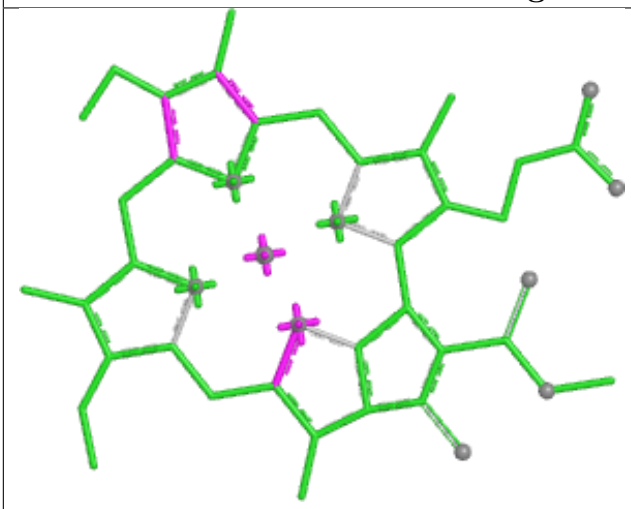


Torsions

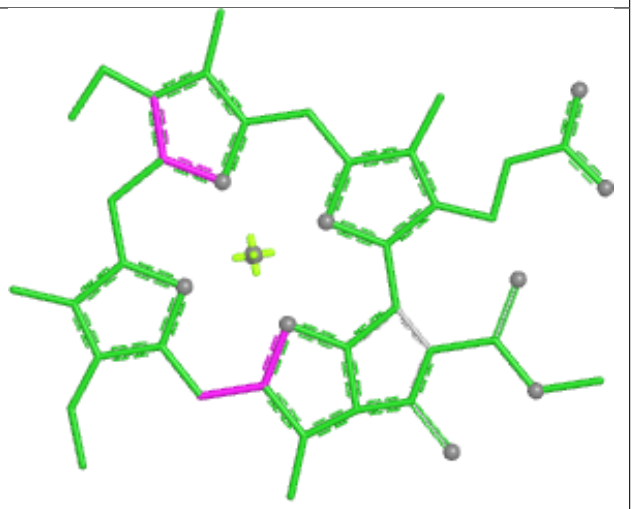


Rings

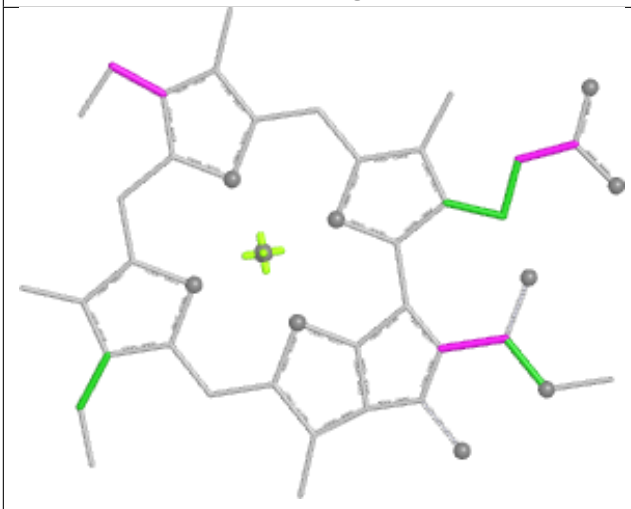
Ligand CLA k 101



Bond lengths



Bond angles

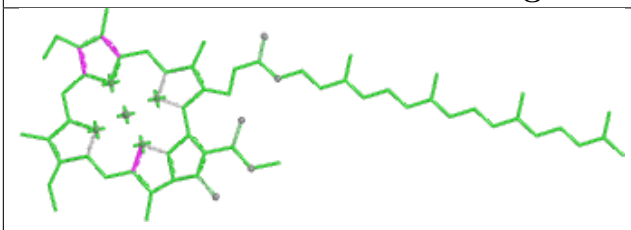


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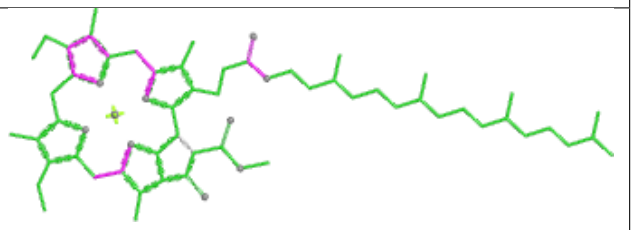


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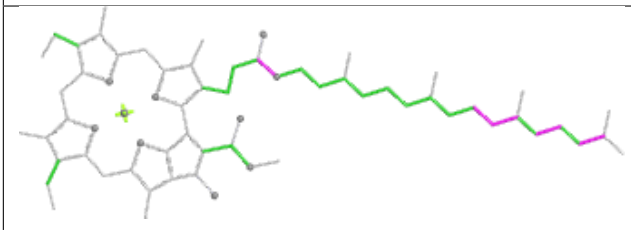
Ligand CLA A 807



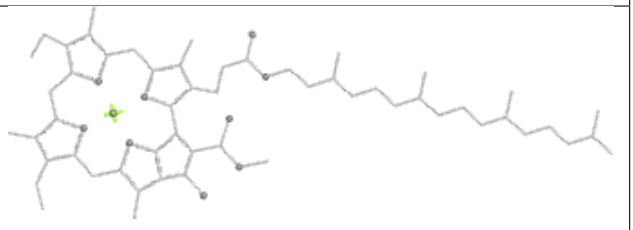
Bond lengths



Bond angles

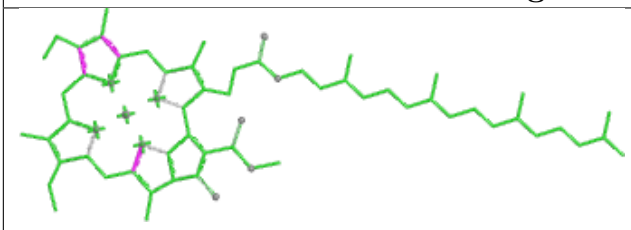


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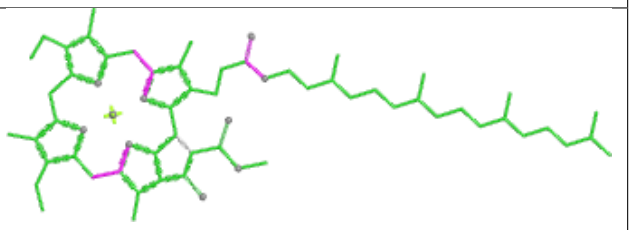


Rings

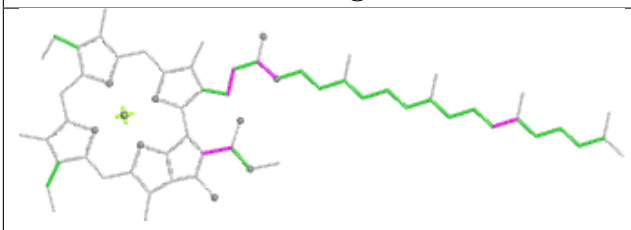
Ligand CLA b 801



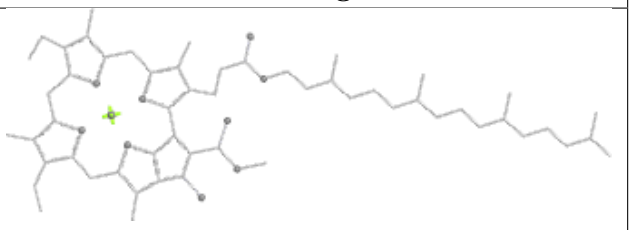
Bond lengths



Bond angles

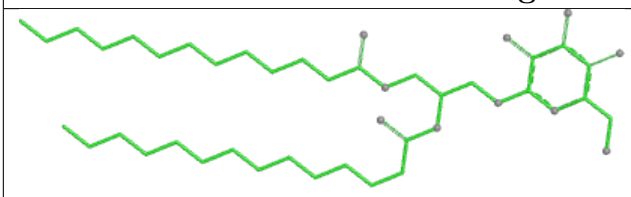


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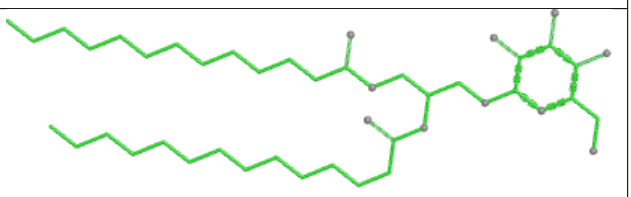


Rings

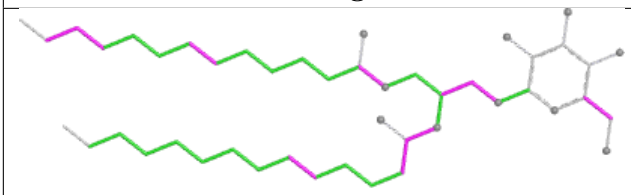
Ligand LMG G 852



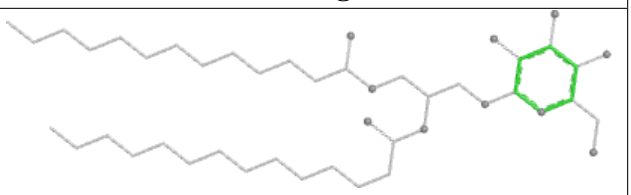
Bond lengths



Bond angles

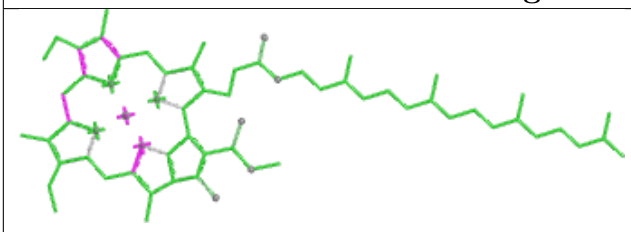


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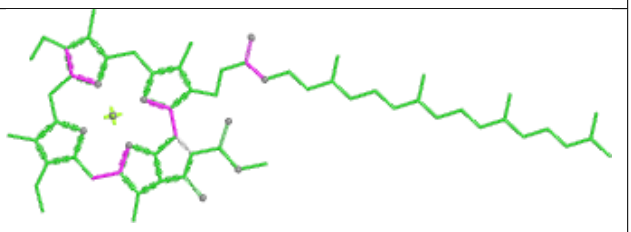


Rings

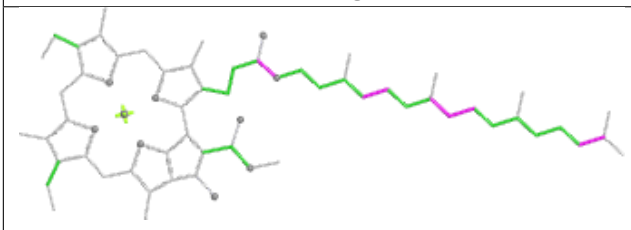
Ligand CLA H 810



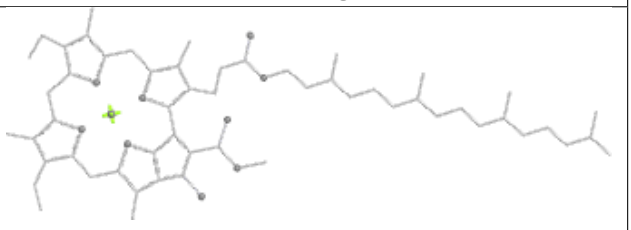
Bond lengths



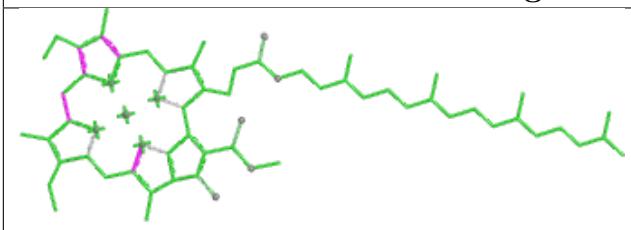
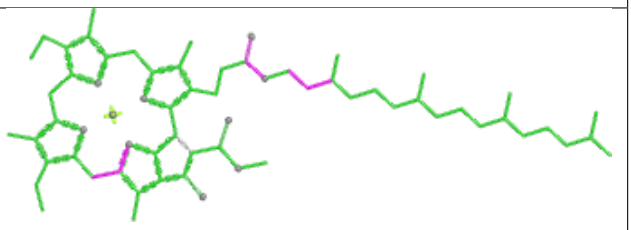
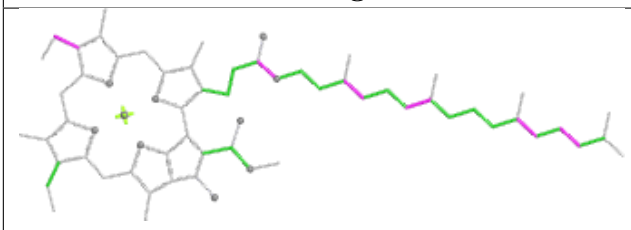
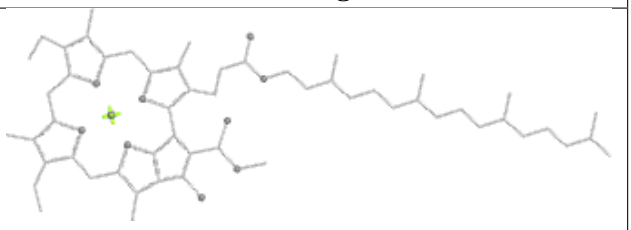
Bond angles

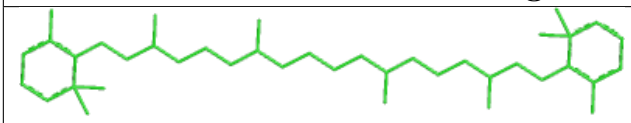
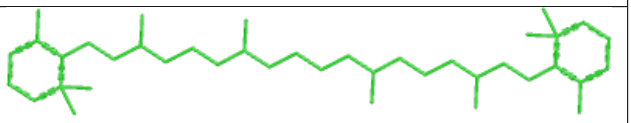
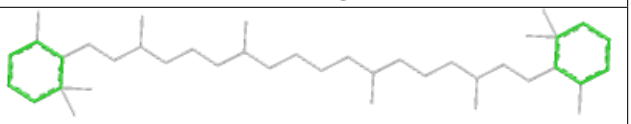


Torsions

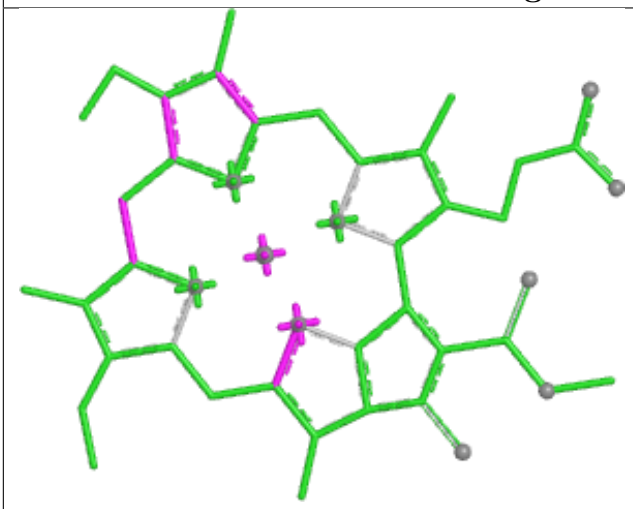


Rings

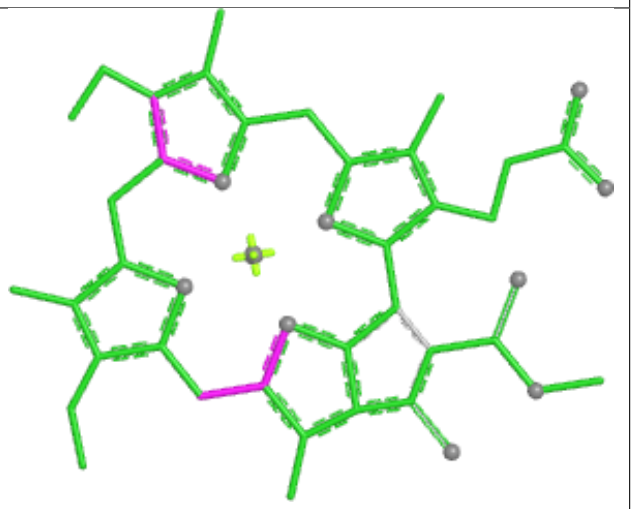
Ligand CLA B 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

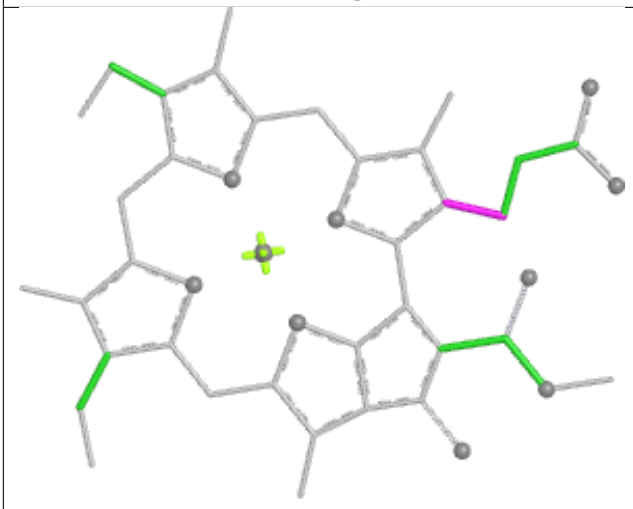
Ligand CLA B 824



Bond lengths



Bond angles

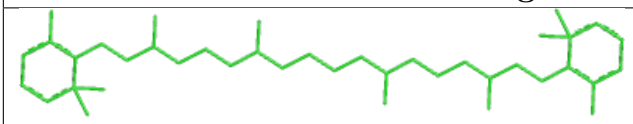


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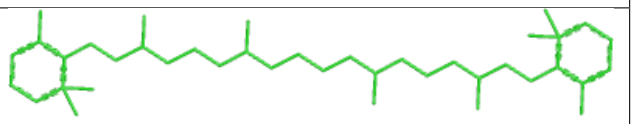


Rings

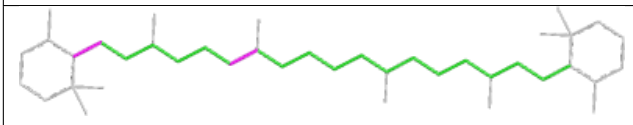
Ligand BCR J 1104



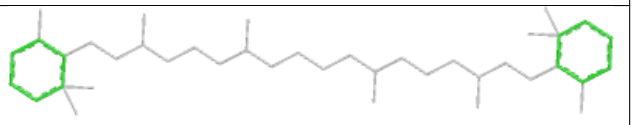
Bond lengths



Bond angles

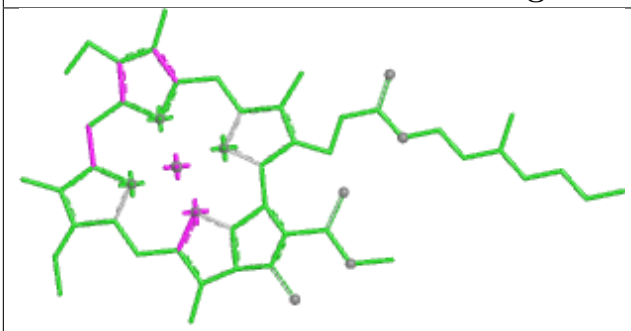


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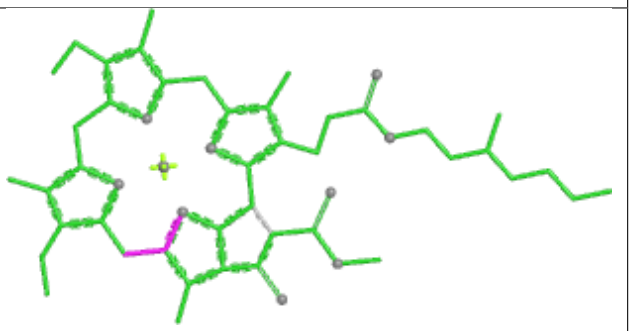


Rings

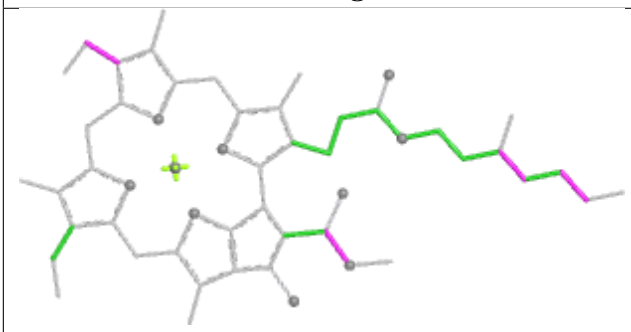
Ligand CLA b 826



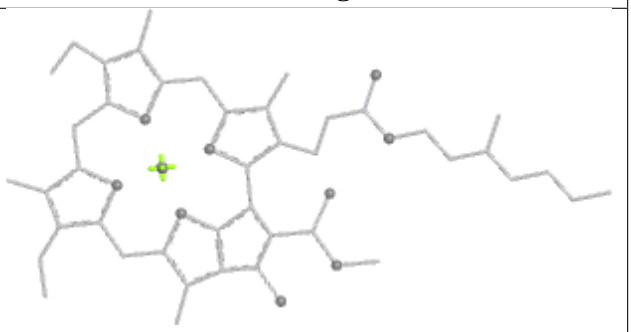
Bond lengths



Bond angles

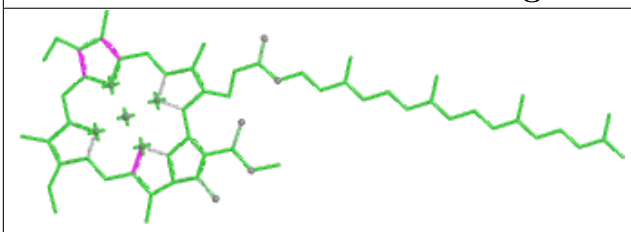


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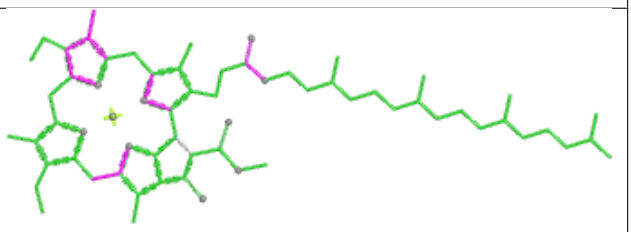


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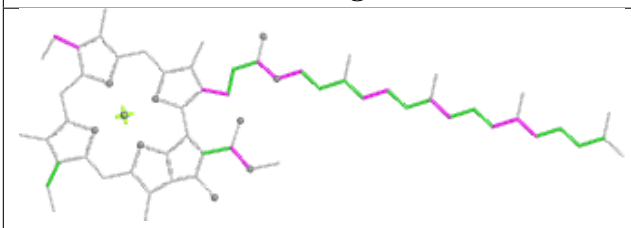
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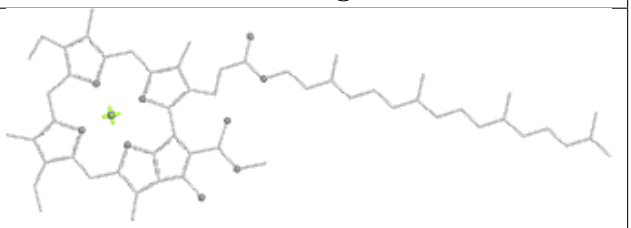
Bond lengths



Bond angles

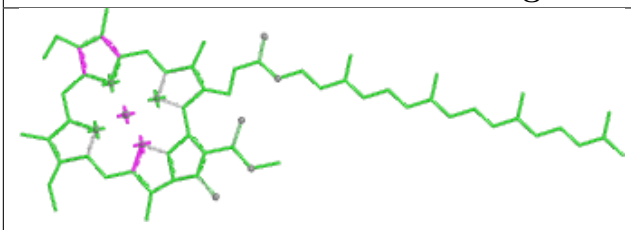


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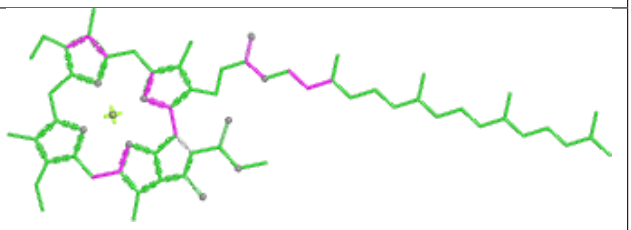


Rings

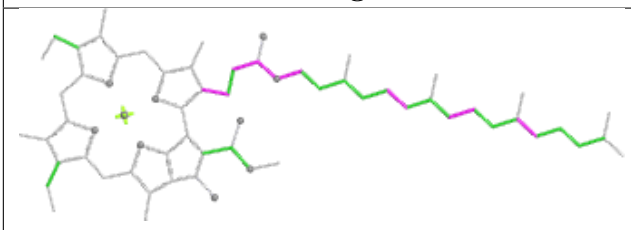
Ligand CLA G 818



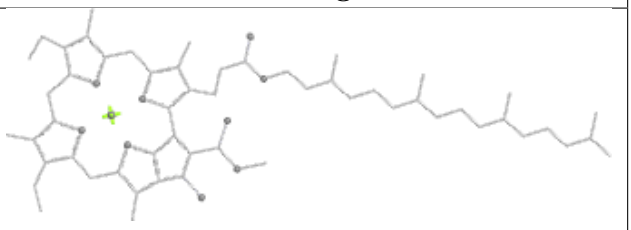
Bond lengths



Bond angles

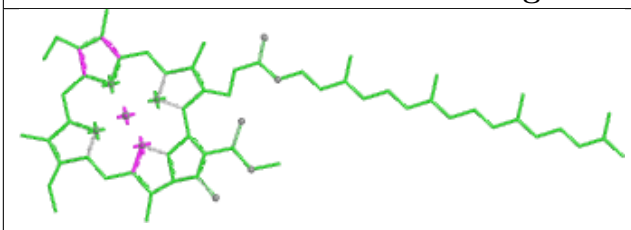


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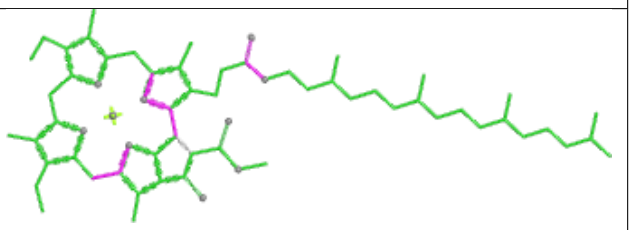


Rings

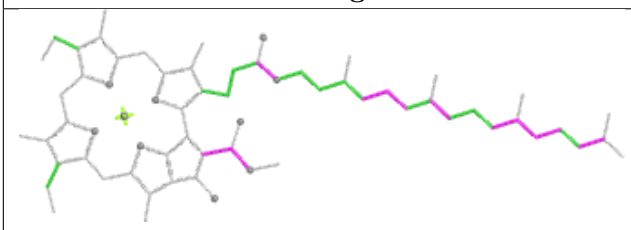
Ligand CLA G 826



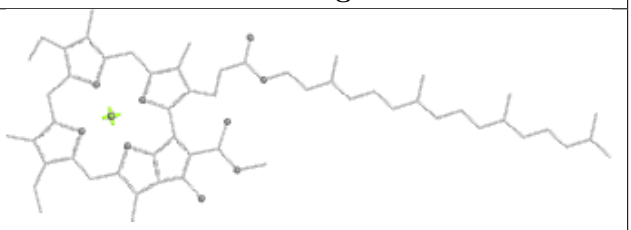
Bond lengths



Bond angles



Torsions



Rings

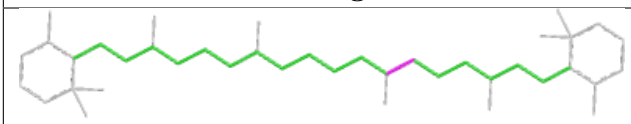
Ligand BCR K 104



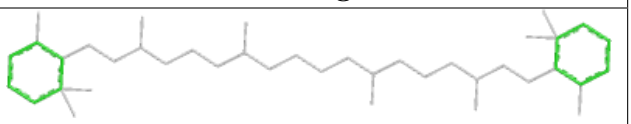
Bond lengths



Bond angles

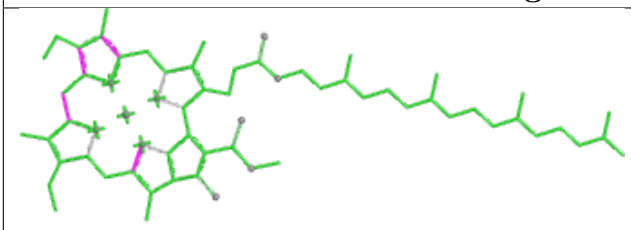


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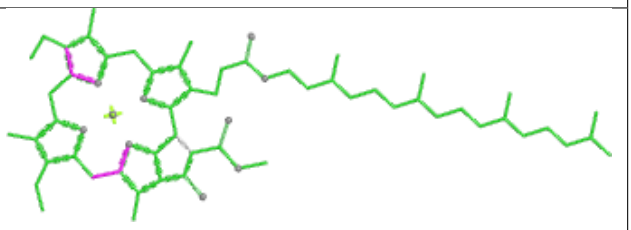


Rings

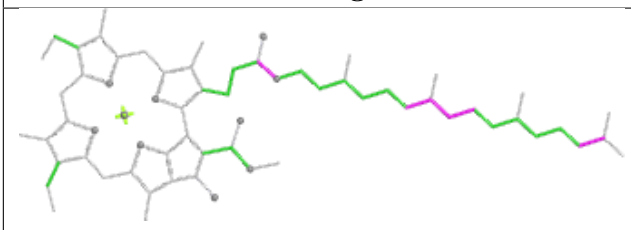
Ligand CLA B 811



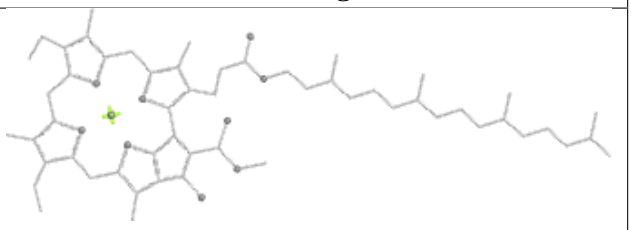
Bond lengths



Bond angles

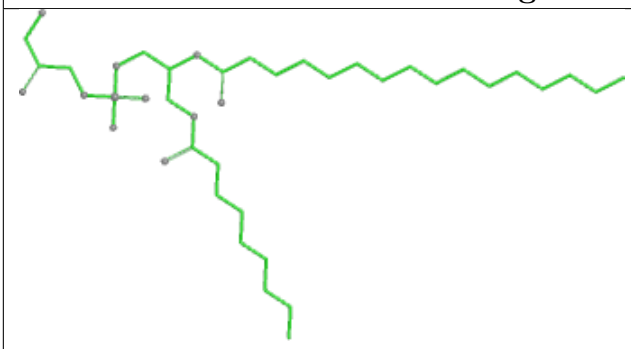


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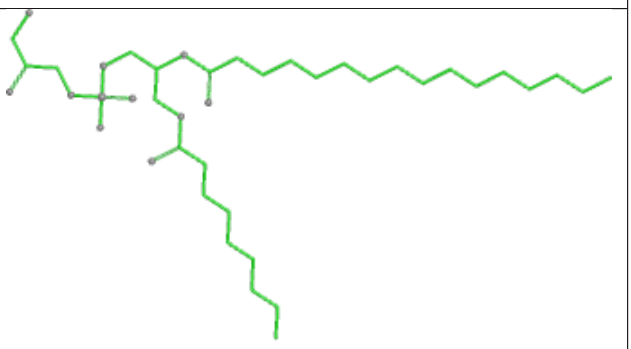


Rings

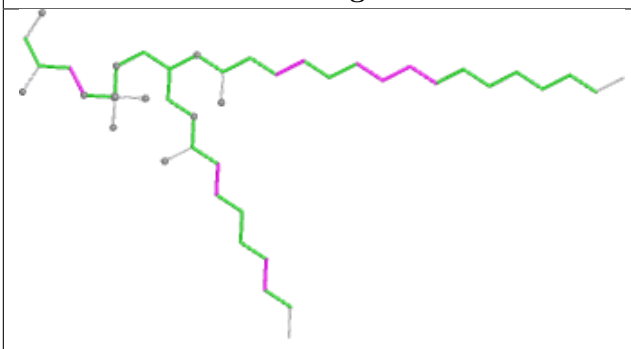
Ligand LHG M 104



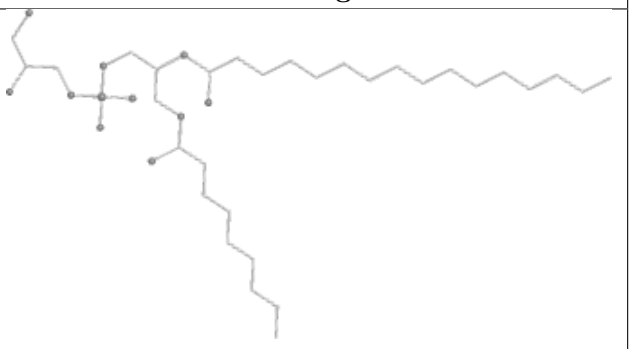
Bond lengths



Bond angles

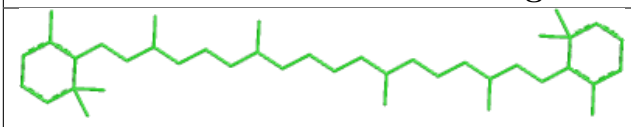


Torsions

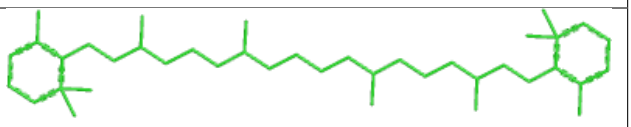


Rings

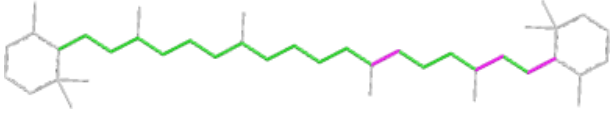
Ligand BCR b 846



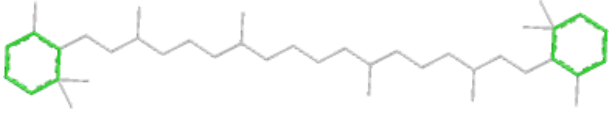
Bond lengths



Bond angles

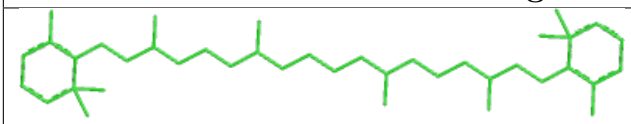


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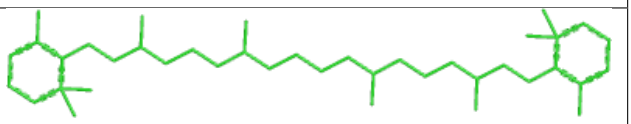


Rings

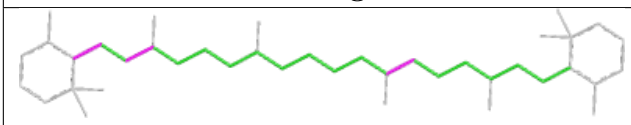
Ligand BCR a 849



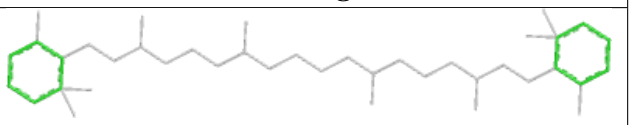
Bond lengths



Bond angles

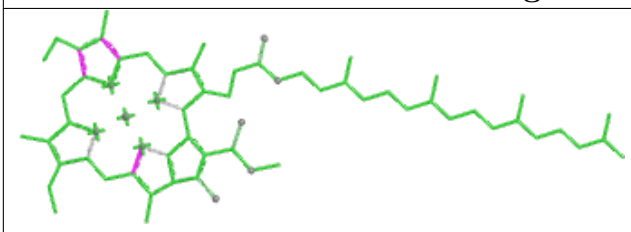


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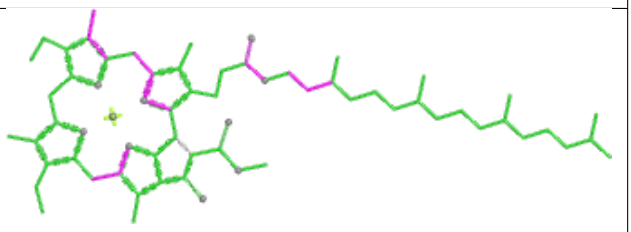


Rings

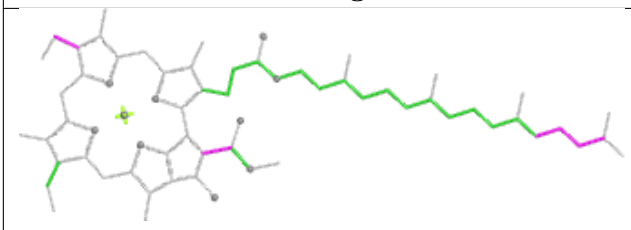
Ligand CLA H 809



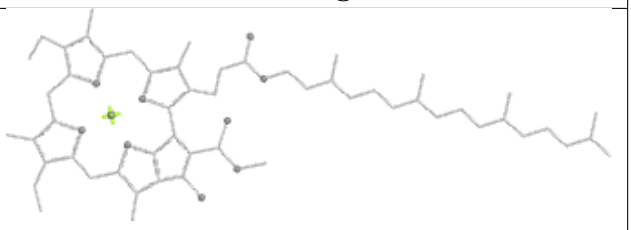
Bond lengths



Bond angles

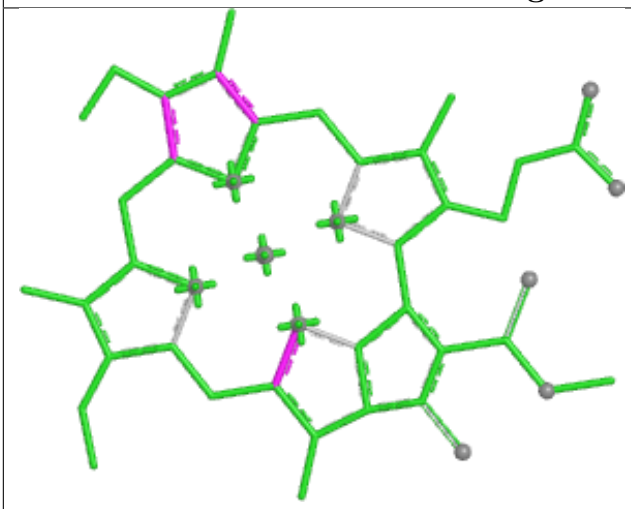


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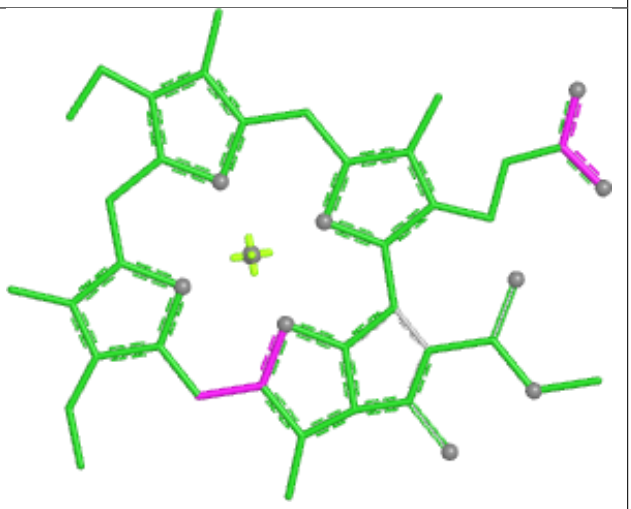


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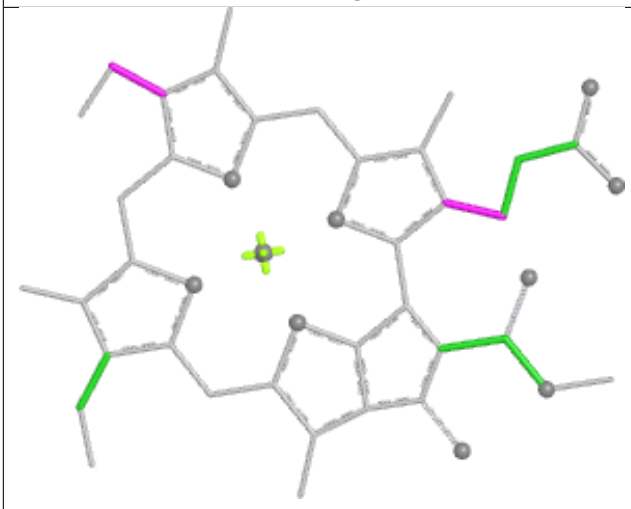
Ligand CLA b 837



Bond lengths



Bond angles

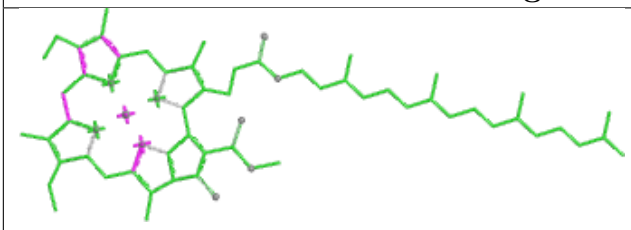


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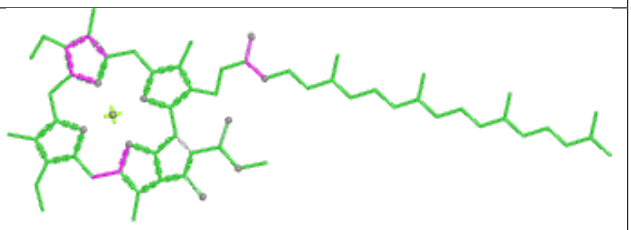


Rings

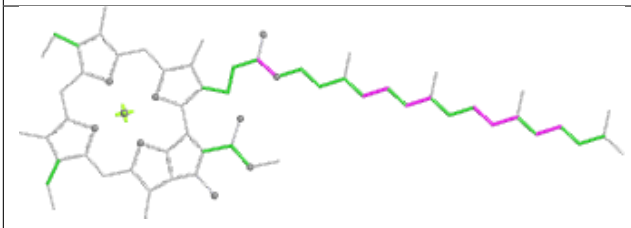
Ligand CLA A 831



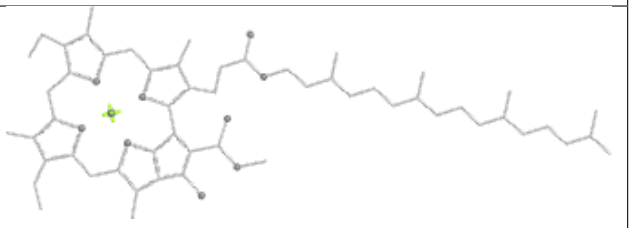
Bond lengths



Bond angles

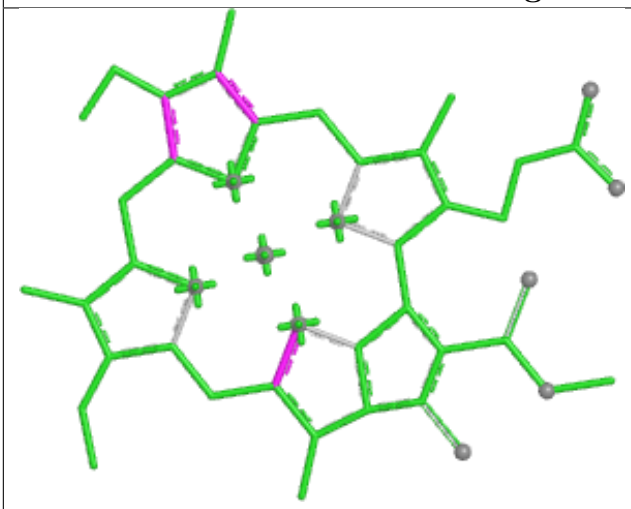


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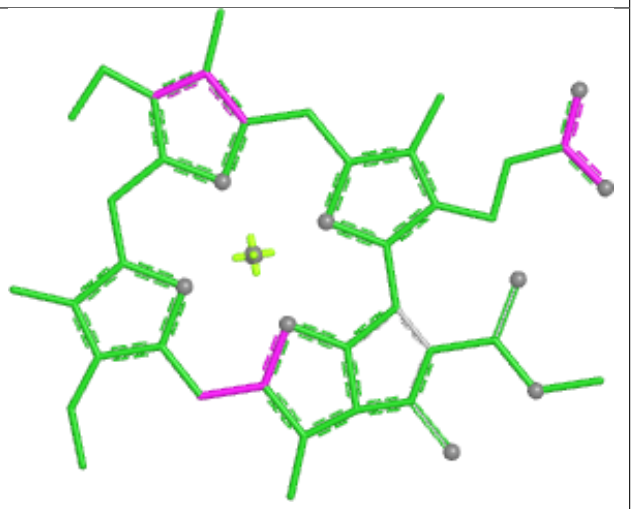


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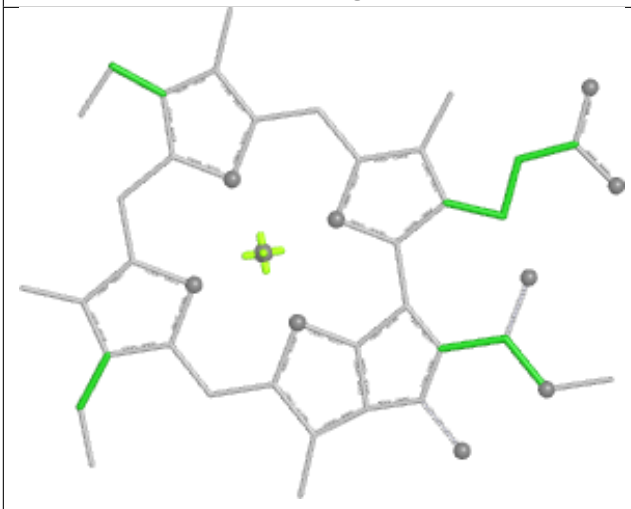
Ligand CLA B 836



Bond lengths



Bond angles

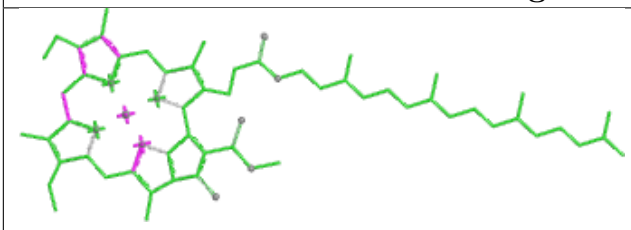


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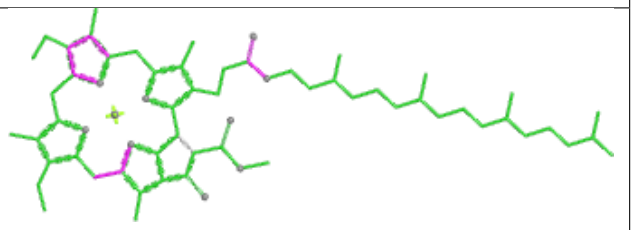


Rings

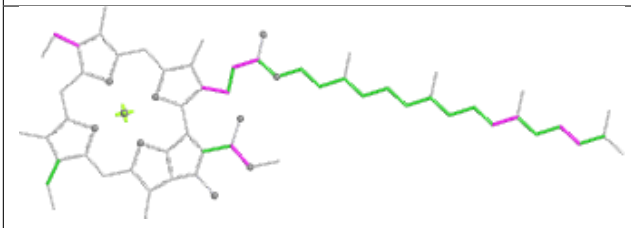
Ligand CLA a 819



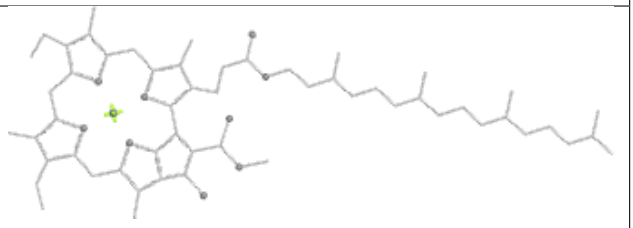
Bond lengths



Bond angles

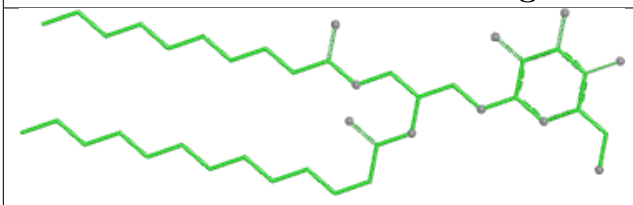


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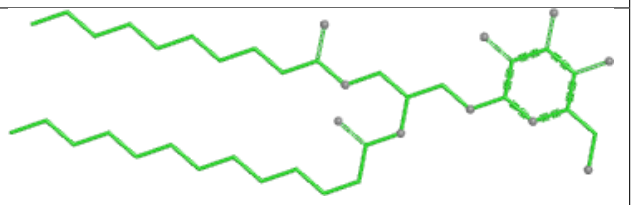


Rings

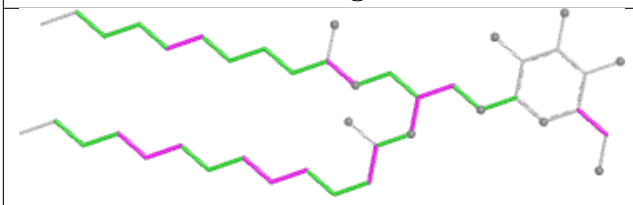
Ligand LMG A 855



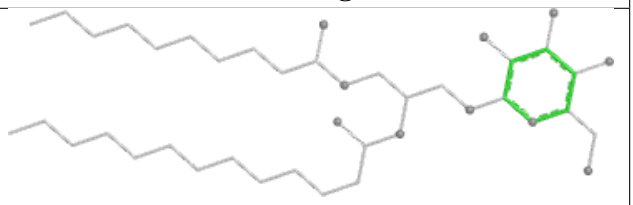
Bond lengths



Bond angles

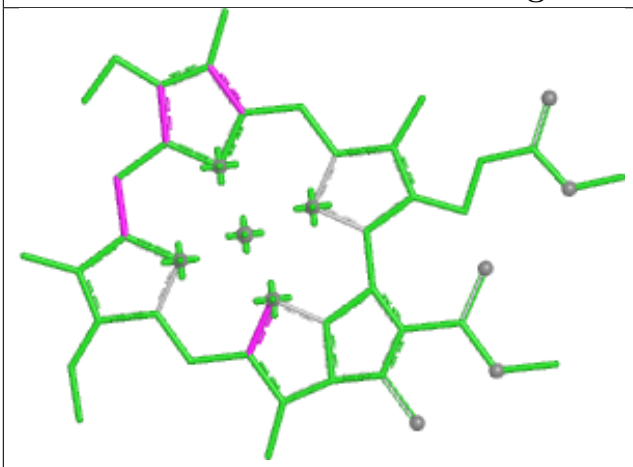


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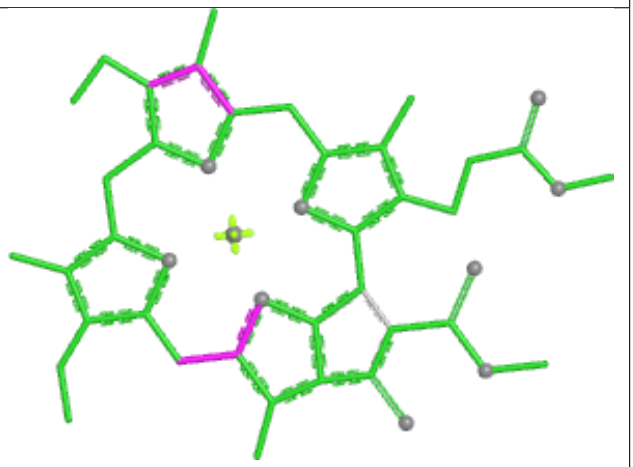


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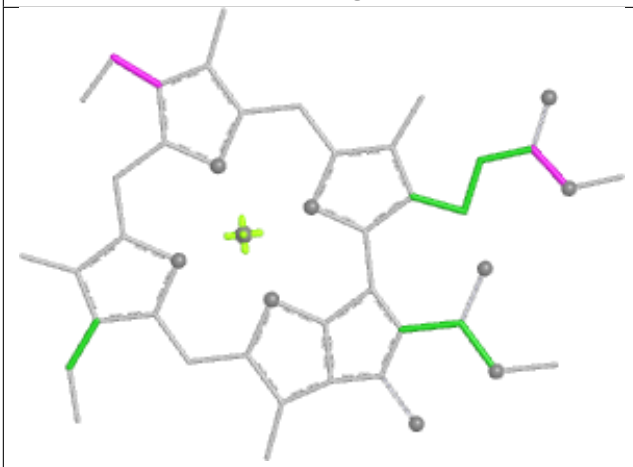
Ligand CLA b 838



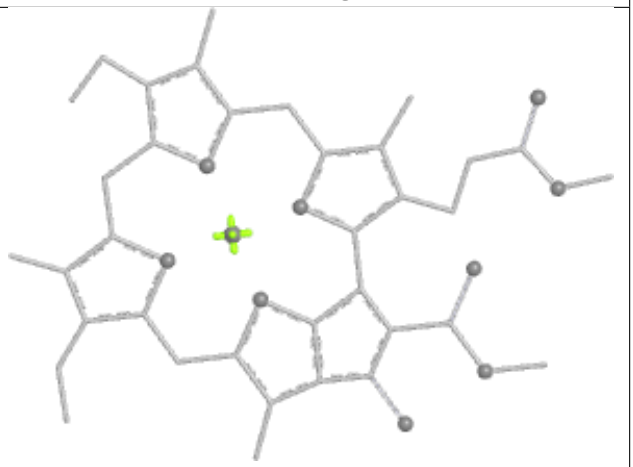
Bond lengths



Bond angles

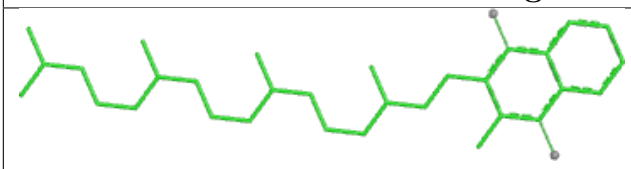


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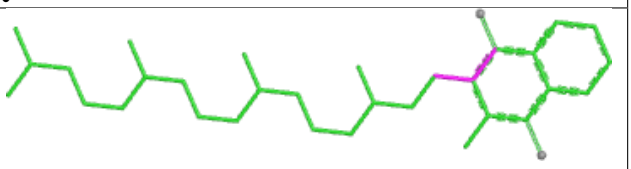


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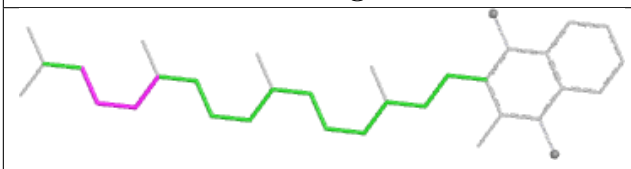
Ligand PQN b 845



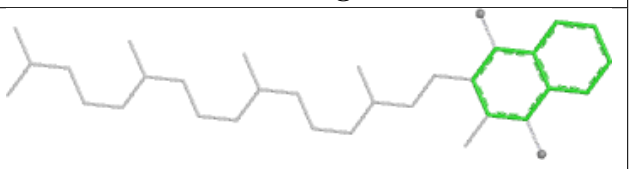
Bond lengths



Bond angles

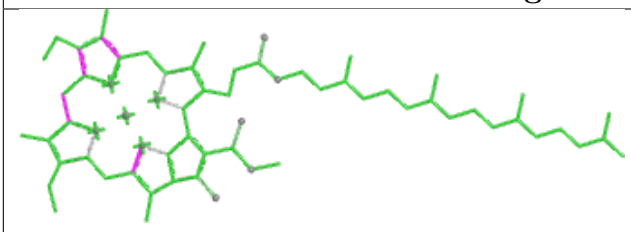


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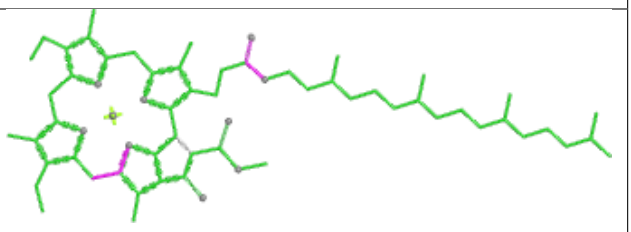


Rings

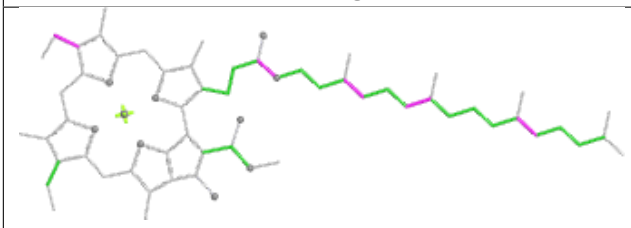
Ligand CLA B 821



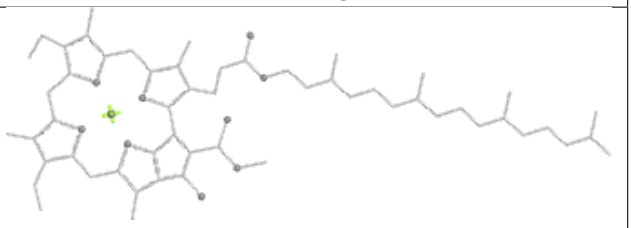
Bond lengths



Bond angles

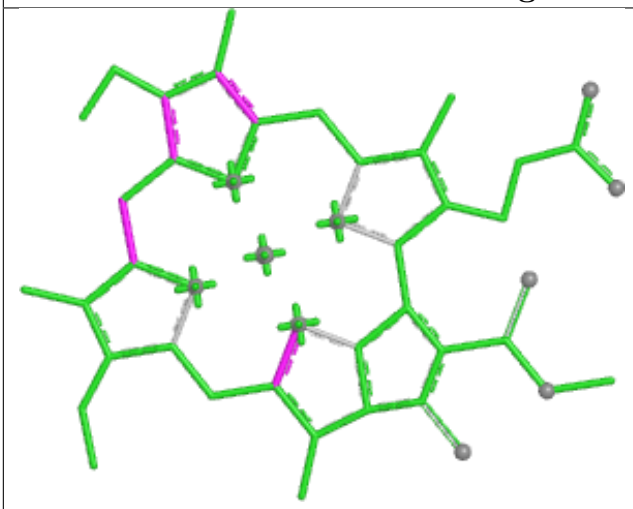


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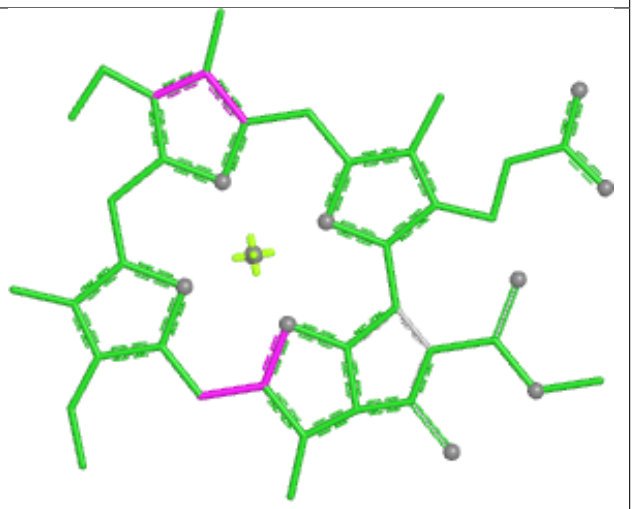


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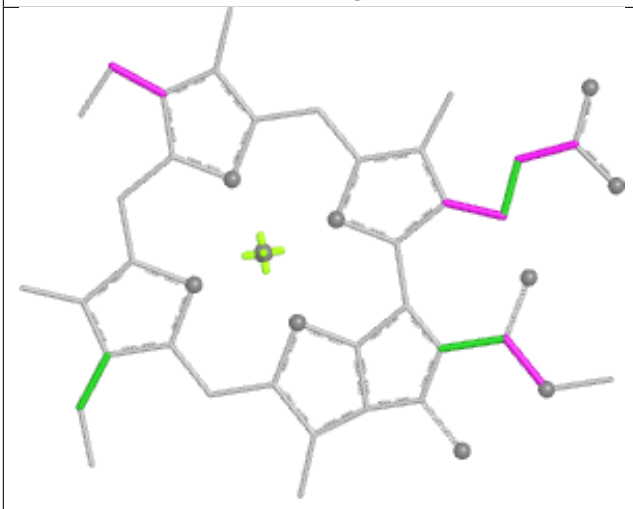
Ligand CLA S 1102



Bond lengths



Bond angles

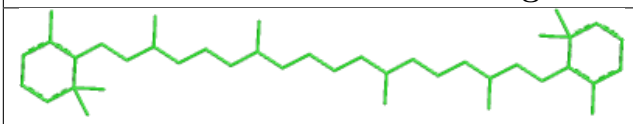


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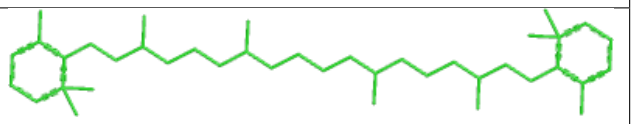


Rings

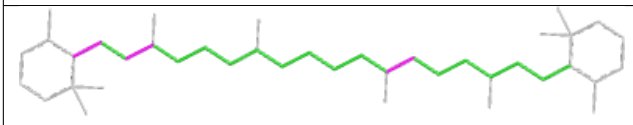
Ligand BCR A 848



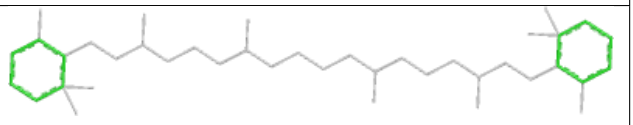
Bond lengths



Bond angles

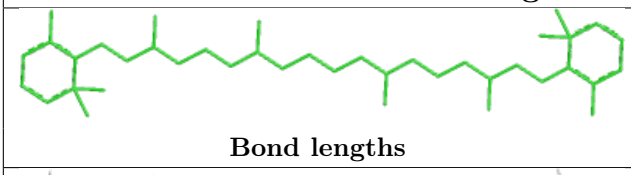


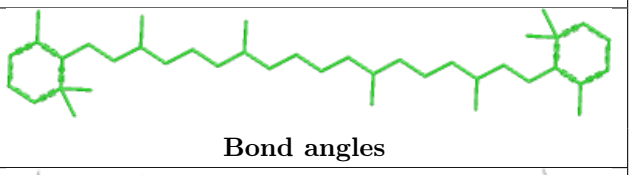
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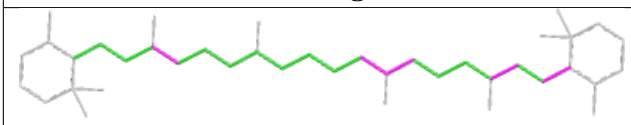


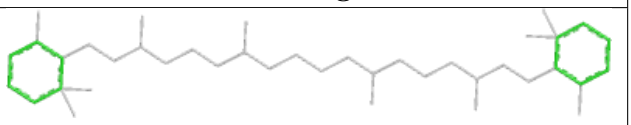
Rings

Ligand BCR A 851

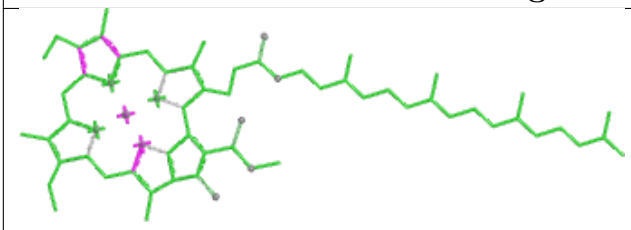

Bond lengths

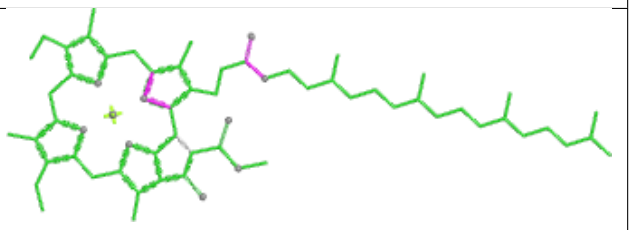

Bond angles

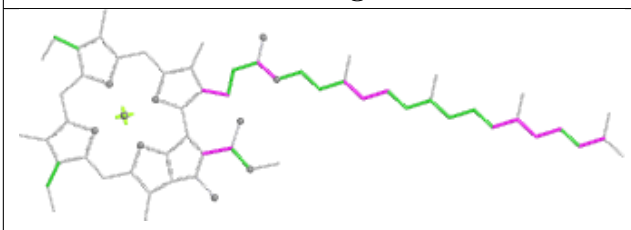

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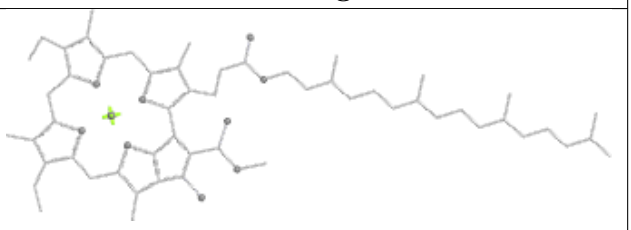

Rings

Ligand CLA a 826

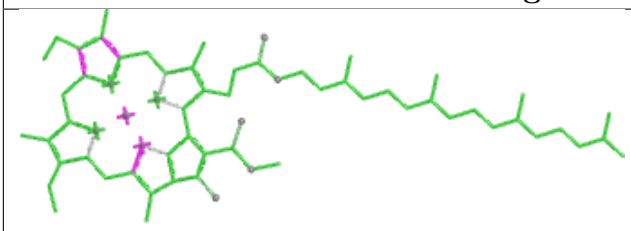

Bond lengths

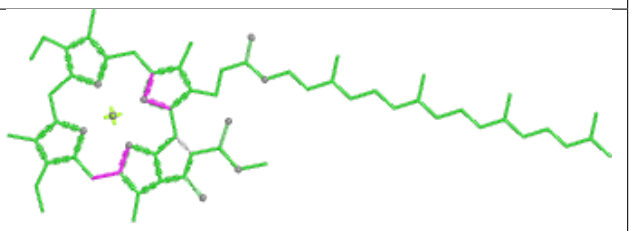

Bond angles

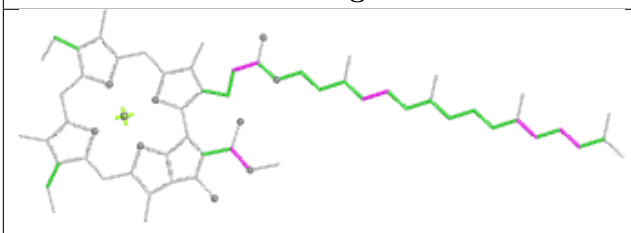

Torsions

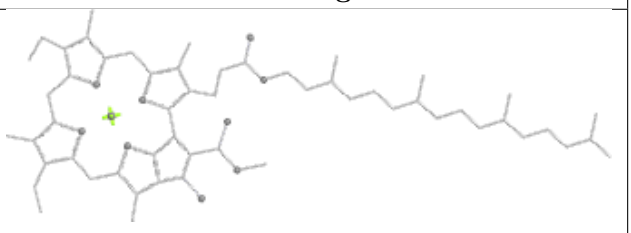

Rings

Ligand CLA H 811

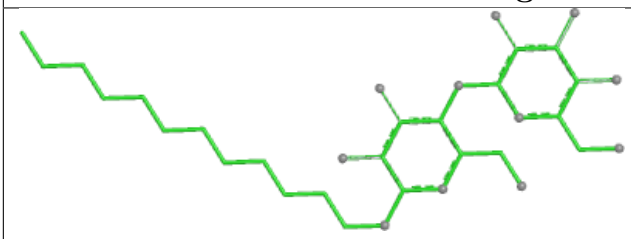

Bond lengths

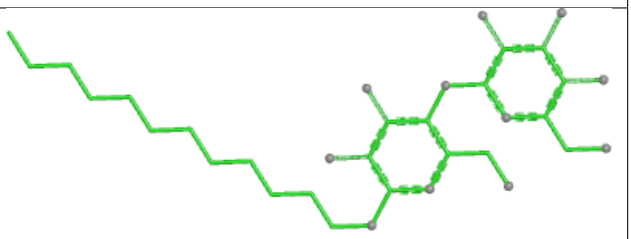

Bond angles

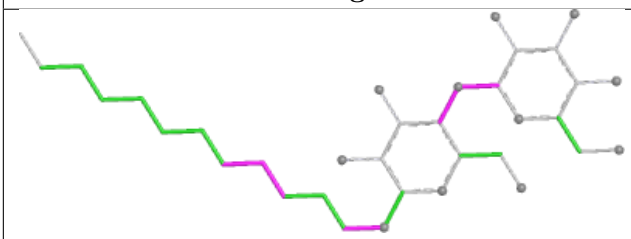

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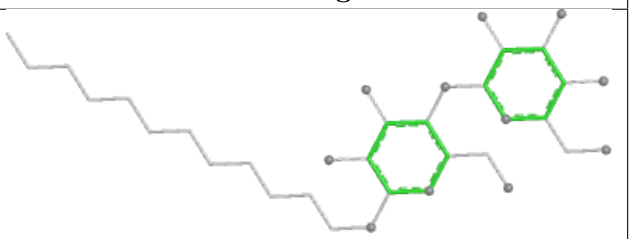

Rings

Ligand LMT J 1106

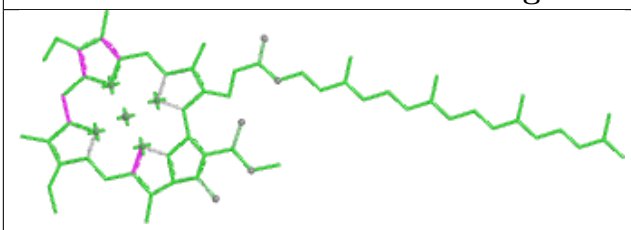

Bond lengths

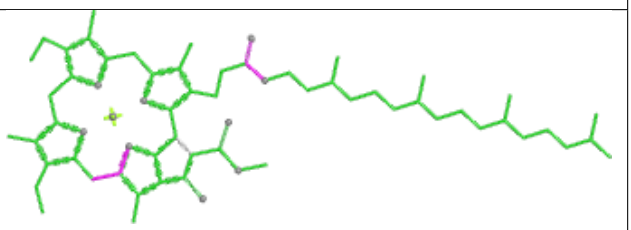

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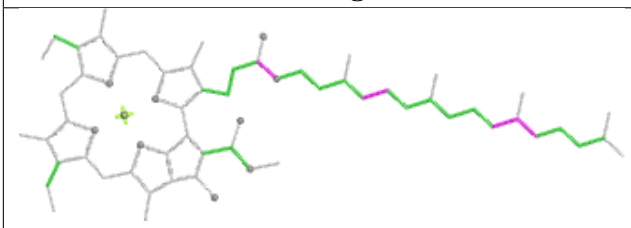

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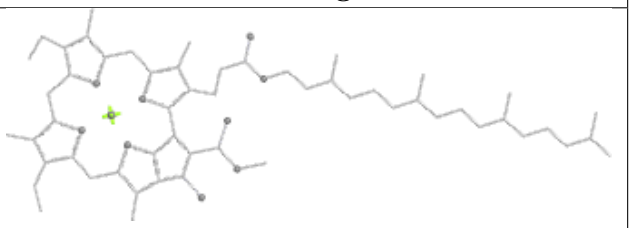

Rings

Ligand CLA G 808

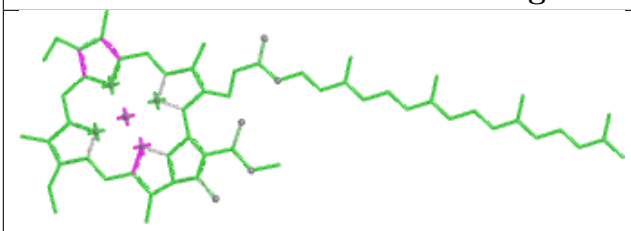

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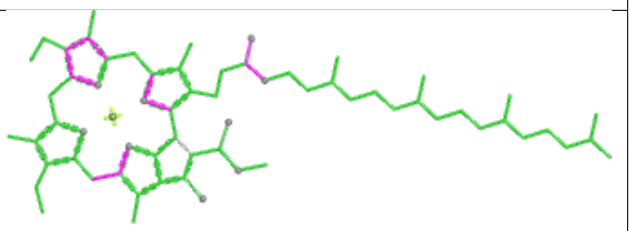

Bond angles

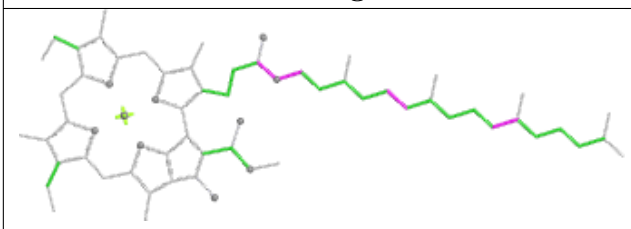

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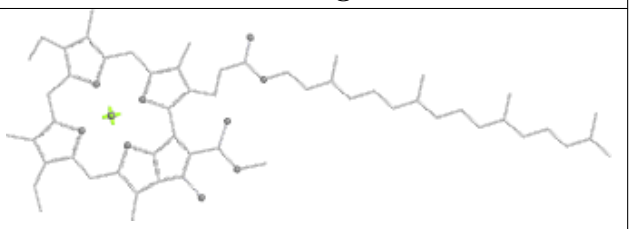

Rings

Ligand CLA a 832

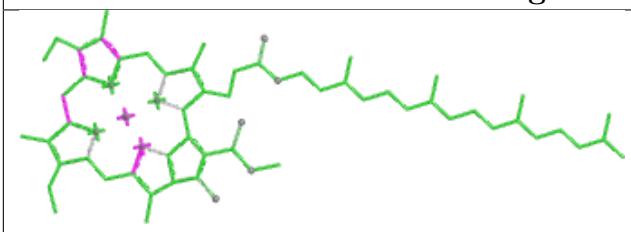

Bond lengths


Bond angles

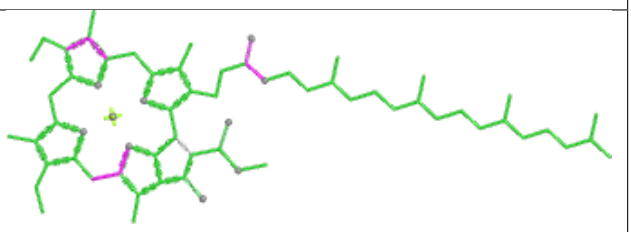

Torsions


Rings

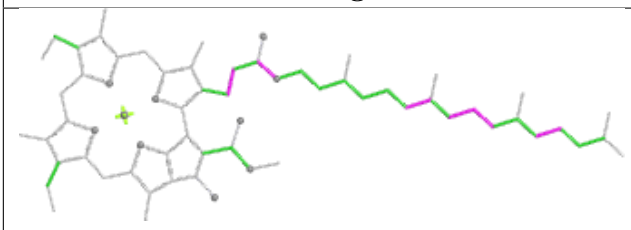
Ligand CLA a 814



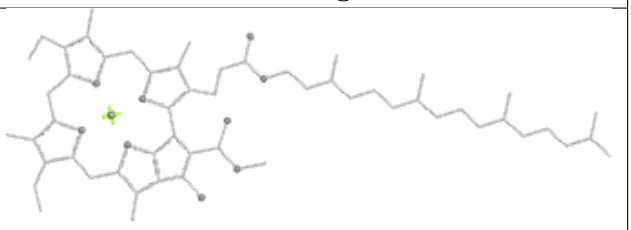
Bond lengths



Bond angles

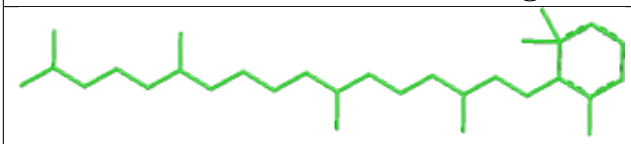


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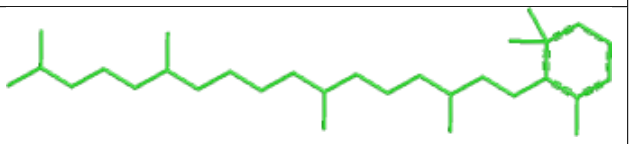


Rings

Ligand BCR H 847



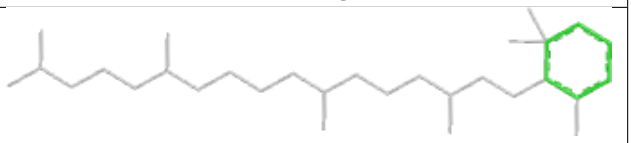
Bond lengths



Bond angles

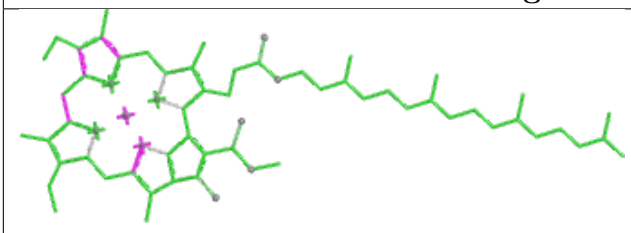


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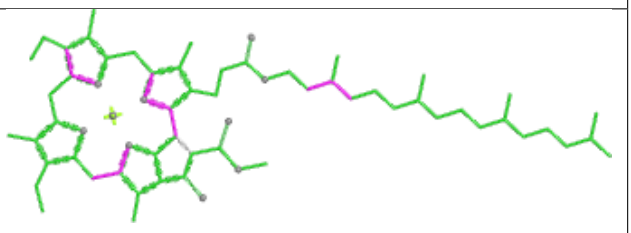


Rings

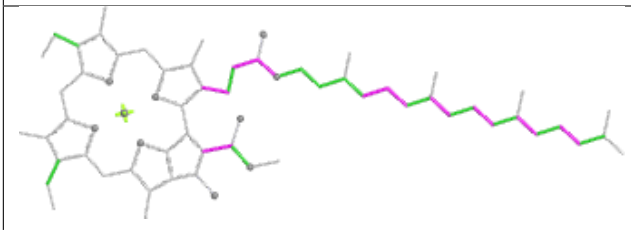
Ligand CLA H 825



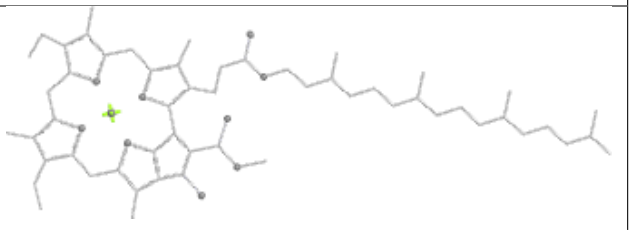
Bond lengths



Bond angles

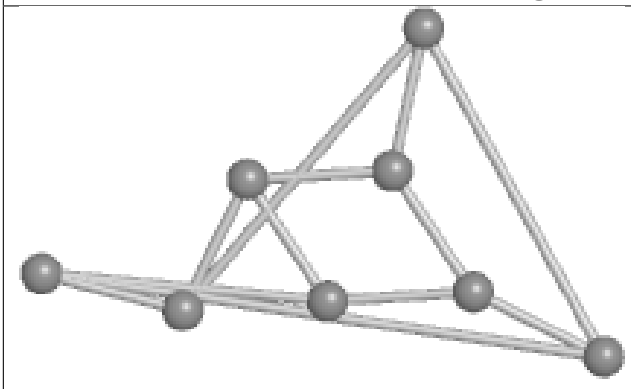


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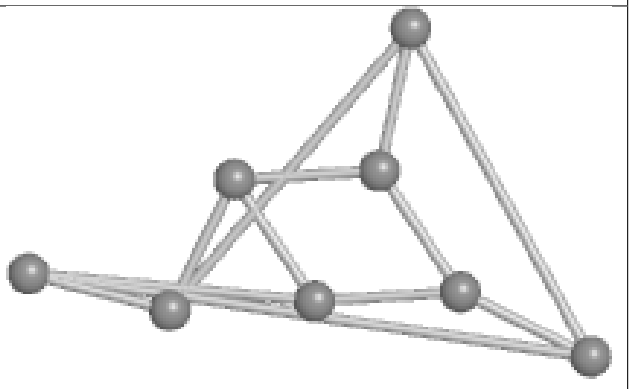


Rings

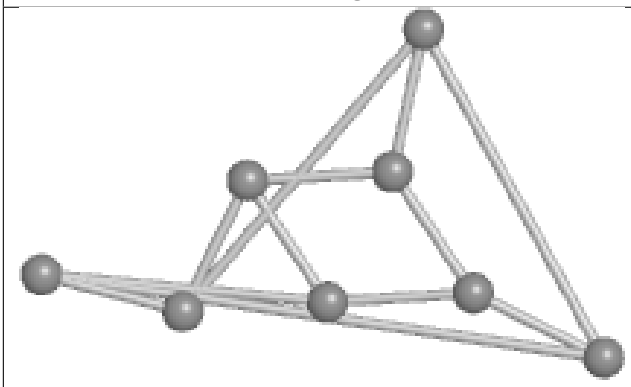
Ligand SF4 N 101



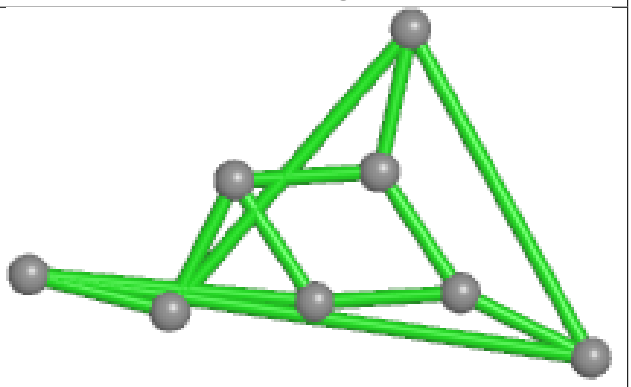
Bond lengths



Bond angles

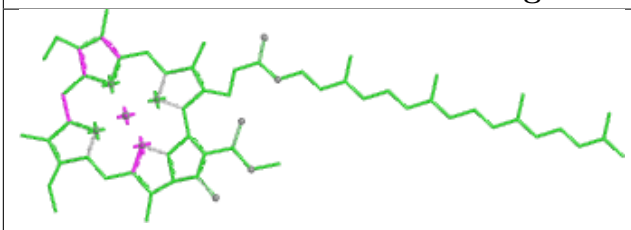


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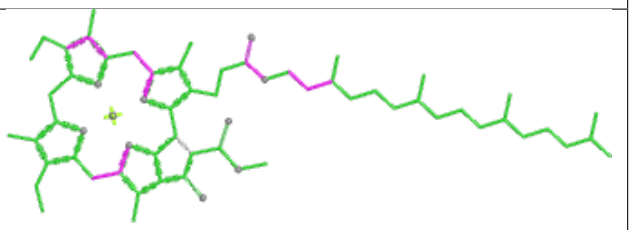


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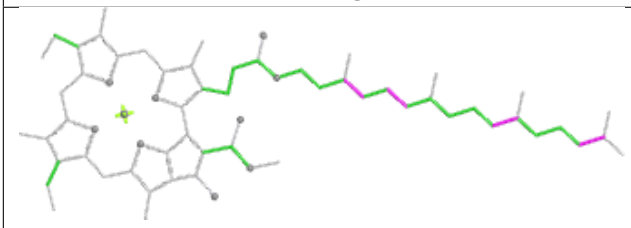
Ligand CLA A 819



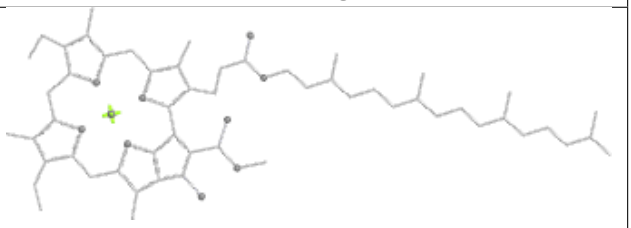
Bond lengths



Bond angles

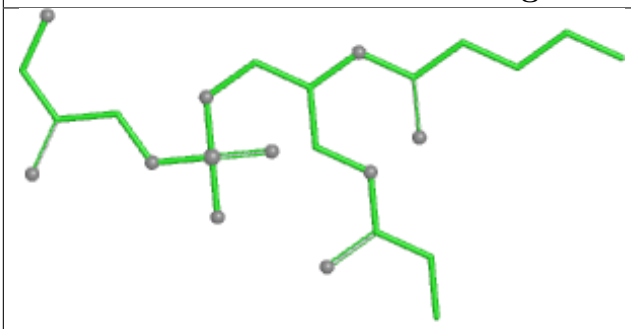


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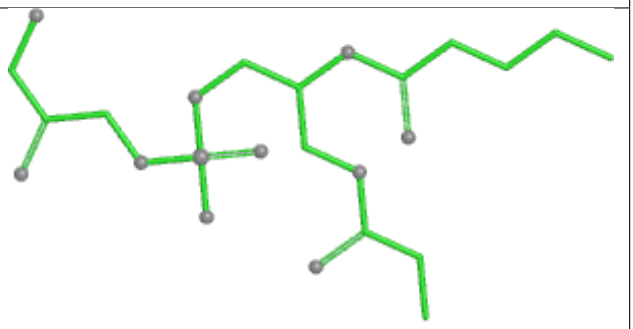


Rings

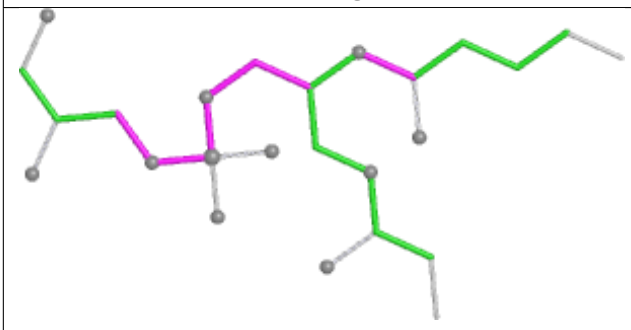
Ligand LHG G 856



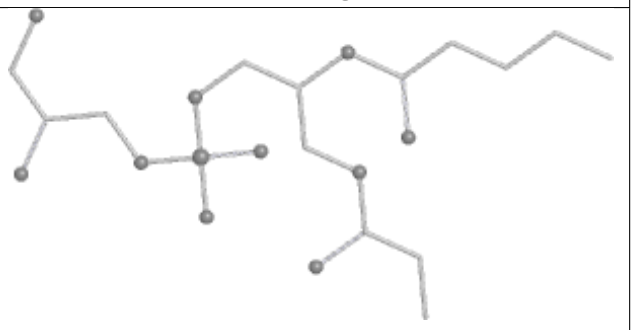
Bond lengths



Bond angles

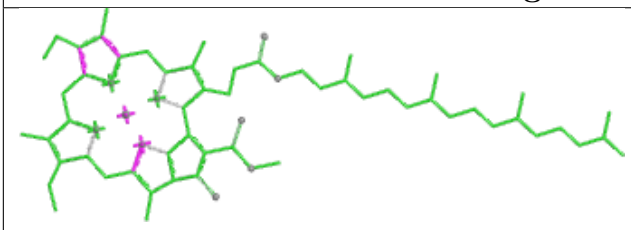


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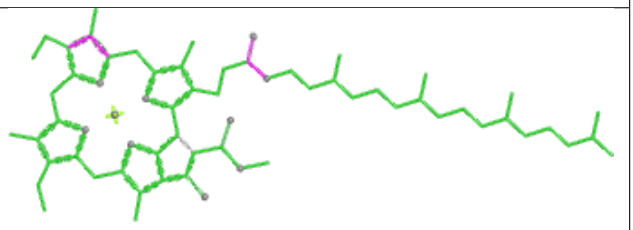


Rings

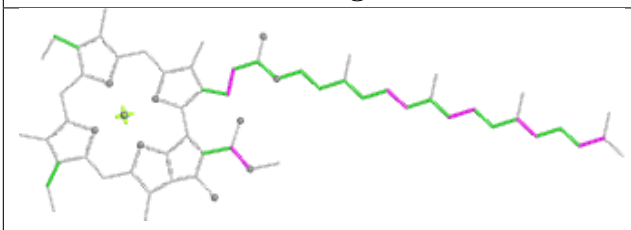
Ligand CLA A 817



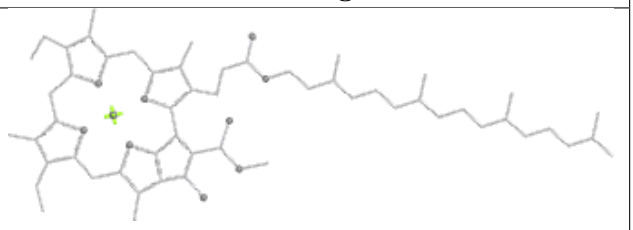
Bond lengths



Bond angles

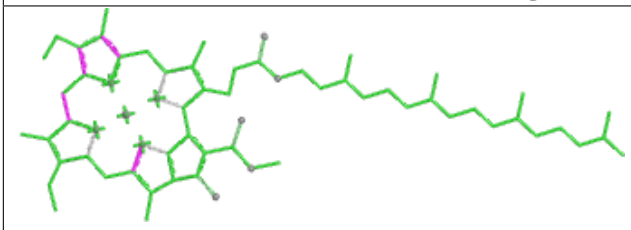


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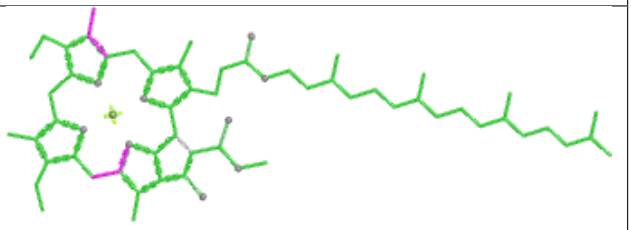


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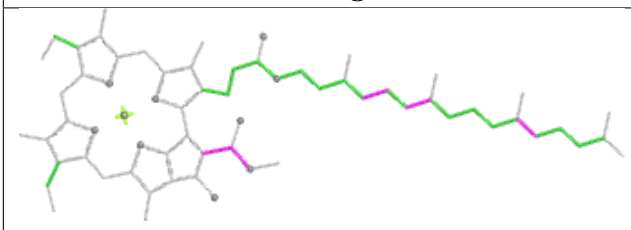
Ligand CLA B 827



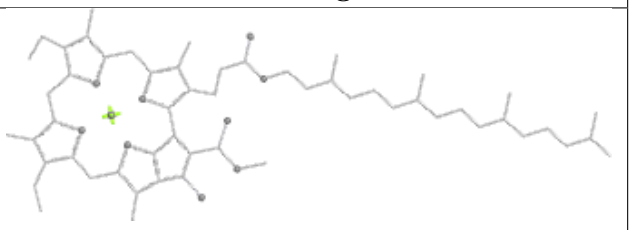
Bond lengths



Bond angles

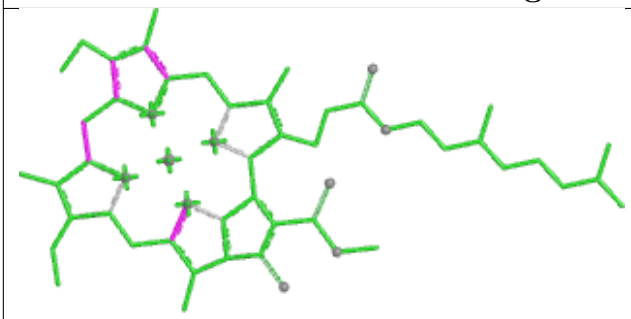


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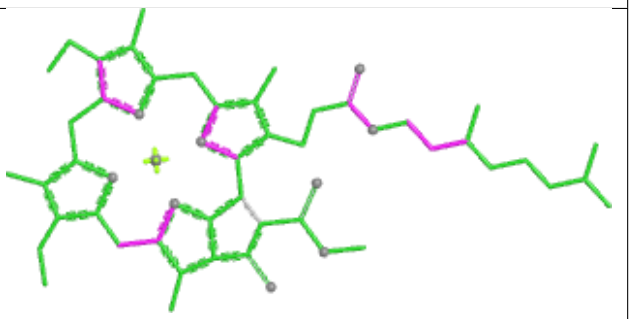


Rings

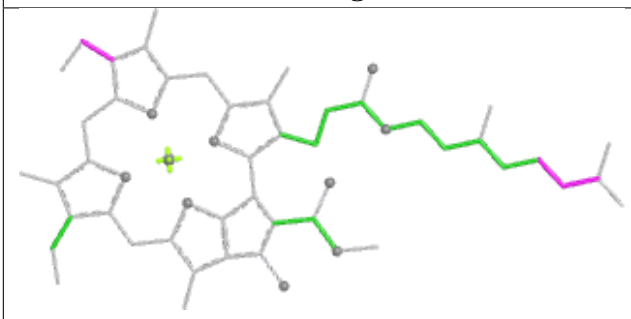
Ligand CLA B 835



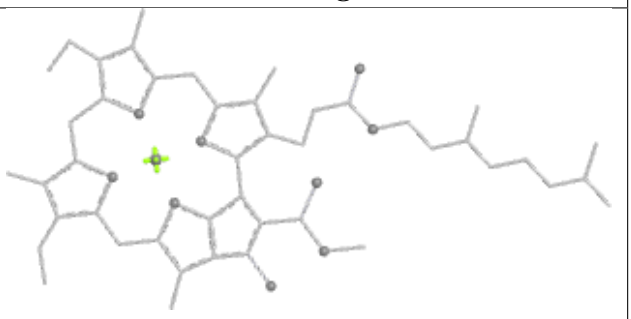
Bond lengths



Bond angles

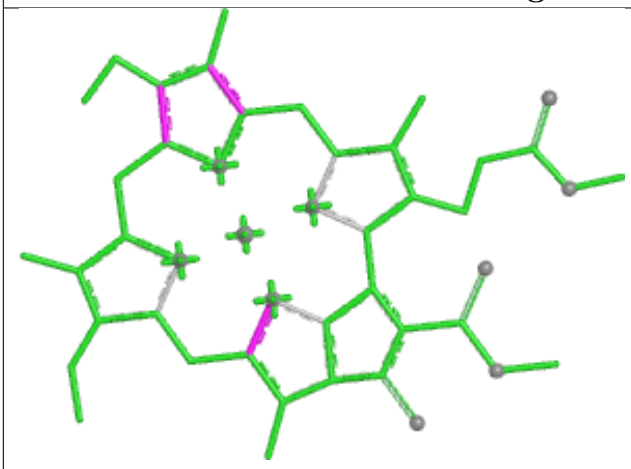


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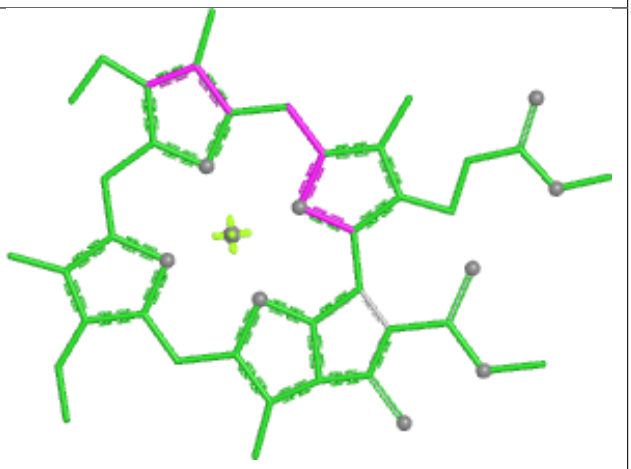


Rings

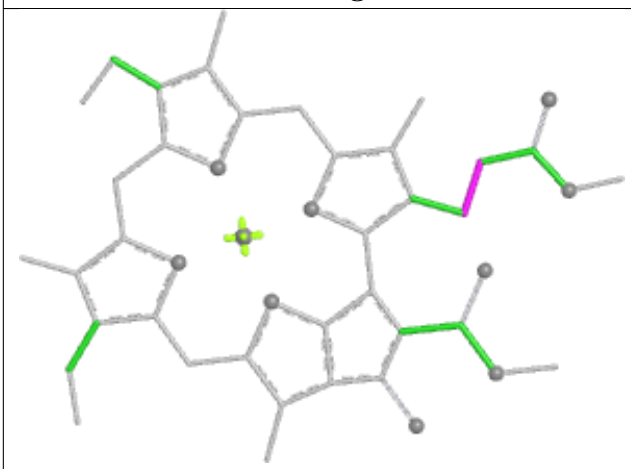
Ligand CLA b 844



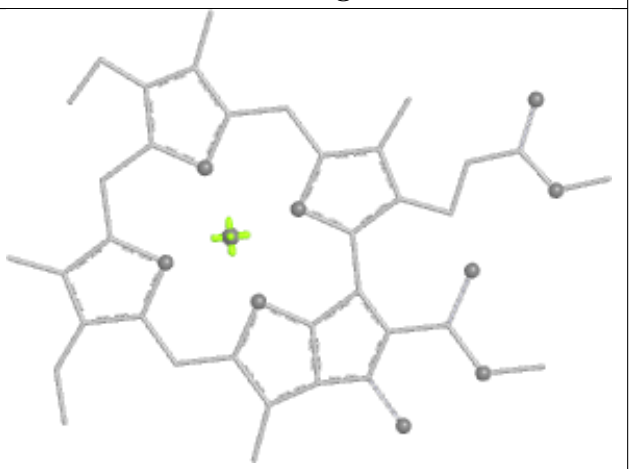
Bond lengths



Bond angles

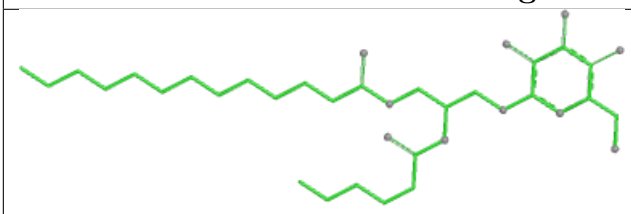


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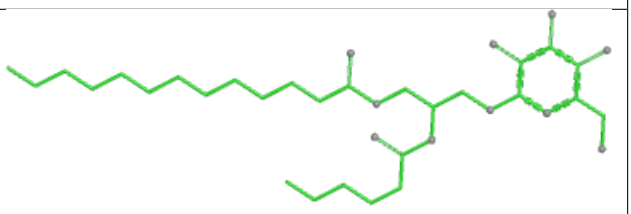


Rings

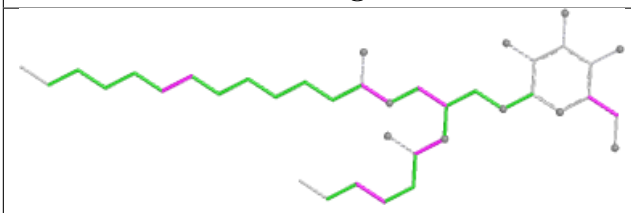
Ligand LMG U 201



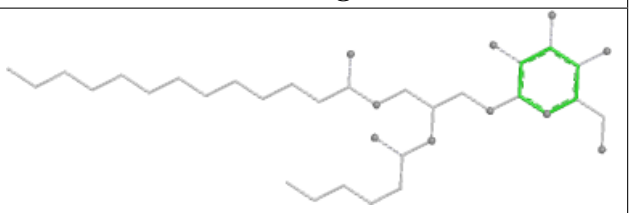
Bond lengths



Bond angles

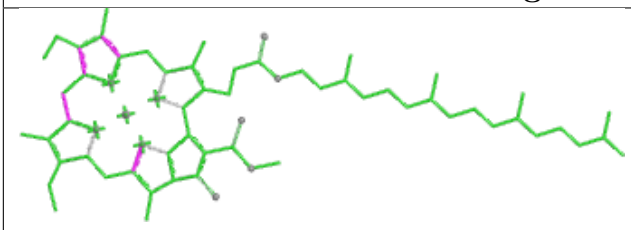


Torsions

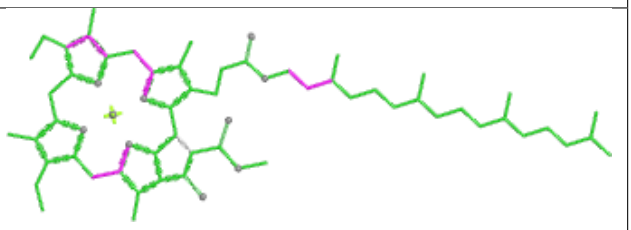


Rings

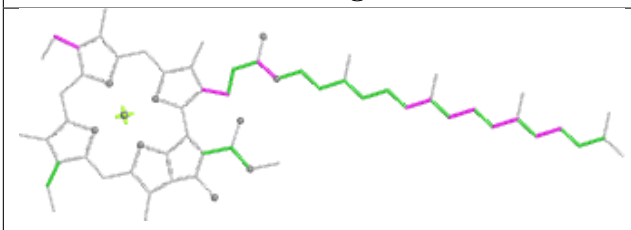
Ligand CLA A 841



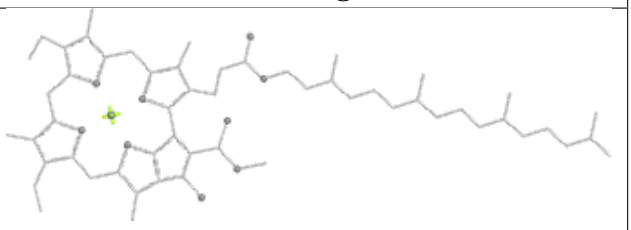
Bond lengths



Bond angles

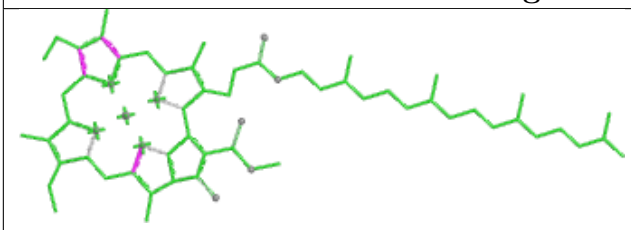


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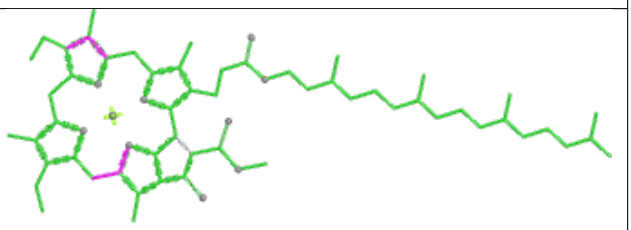


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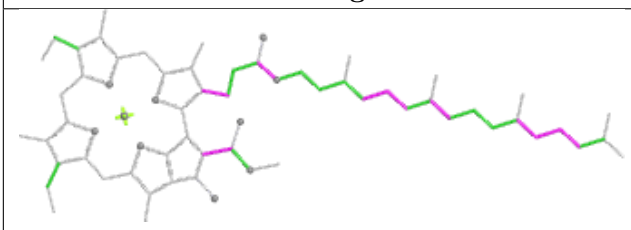
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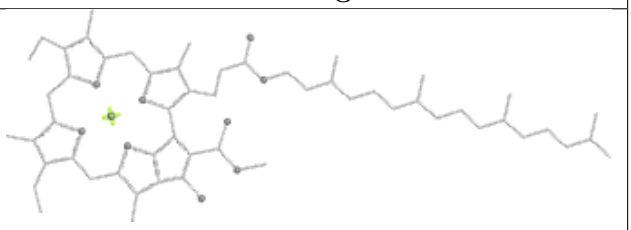
Bond lengths



Bond angles

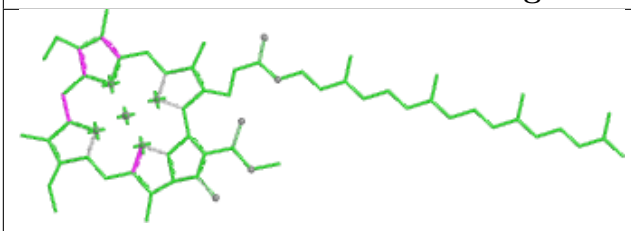


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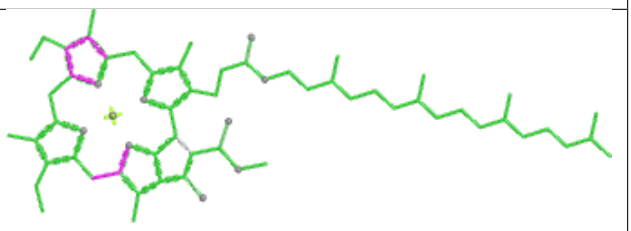


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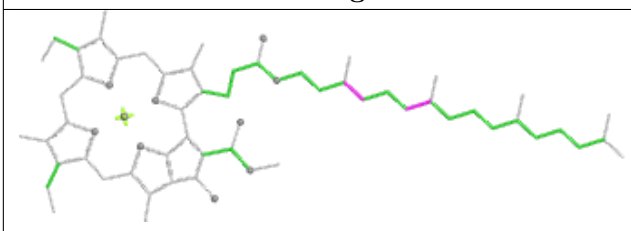
Ligand CLA A 821



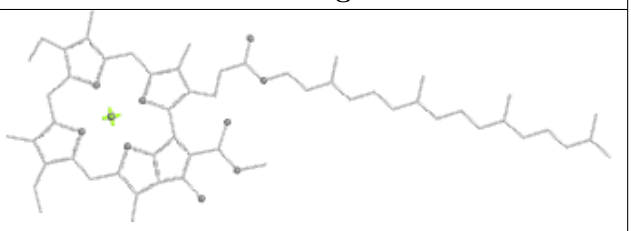
Bond lengths



Bond angles

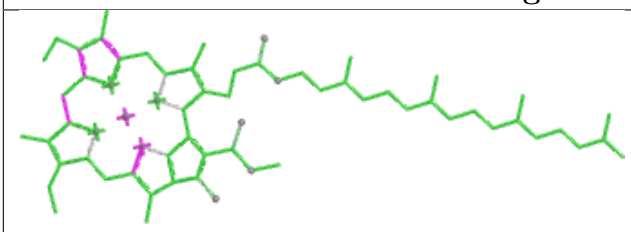


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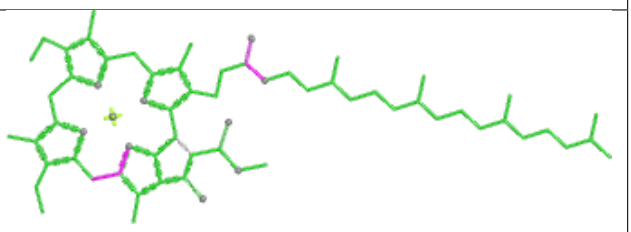


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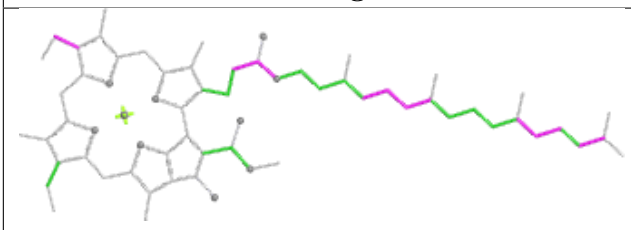
Ligand CLA G 843



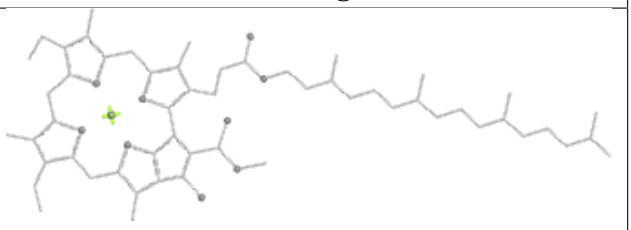
Bond lengths



Bond angles

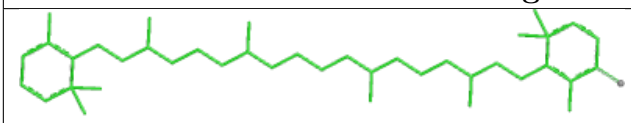


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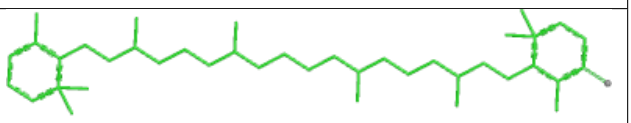


Rings

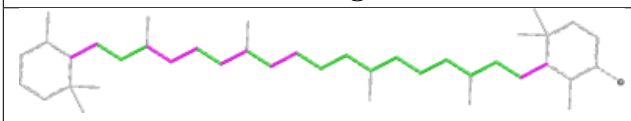
Ligand ECH V 102



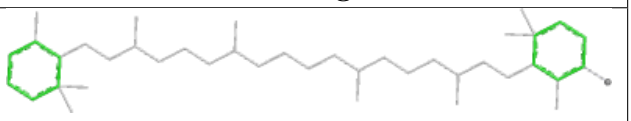
Bond lengths



Bond angles

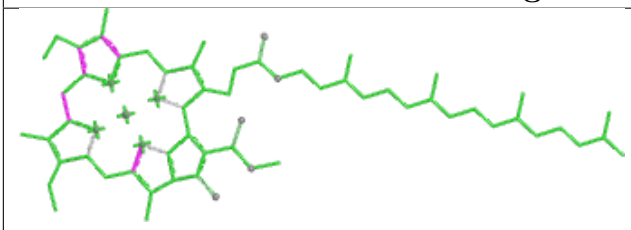


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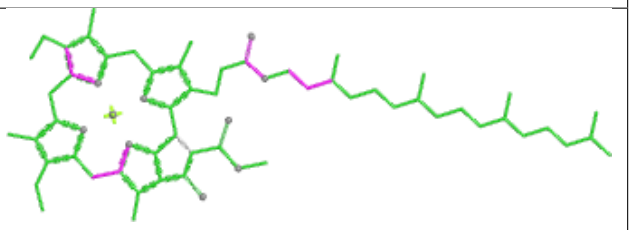


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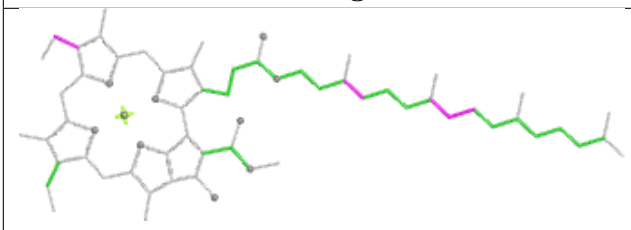
Ligand CLA A 840



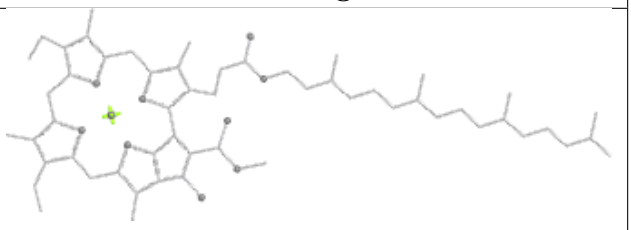
Bond lengths



Bond angles

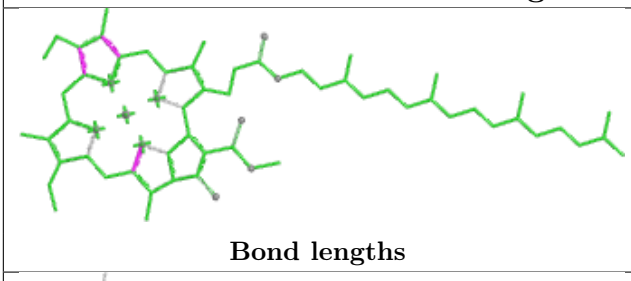


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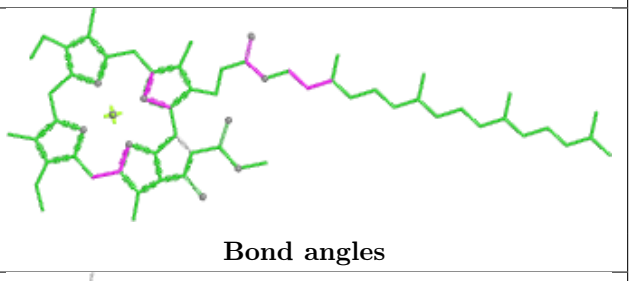


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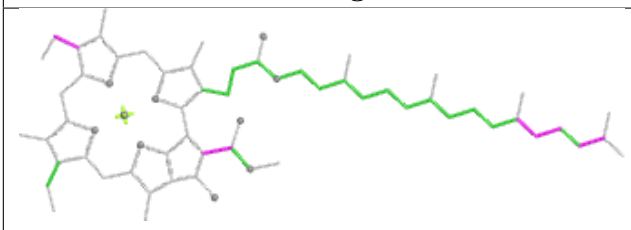
Ligand CLA b 811



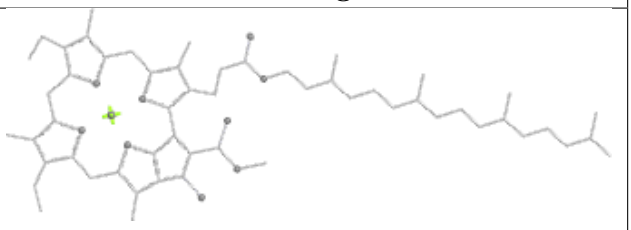
Bond lengths



Bond angles

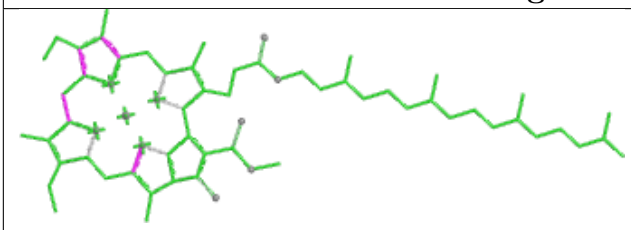


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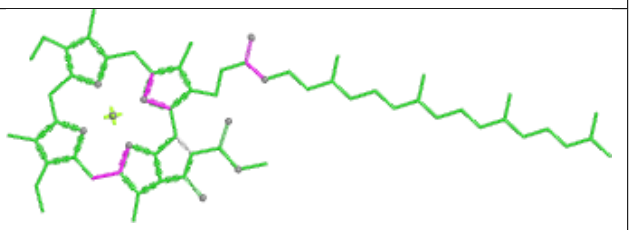


Rings

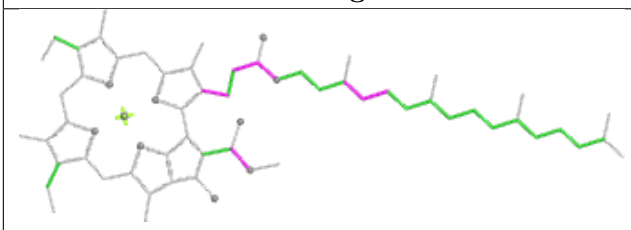
Ligand CLA b 814



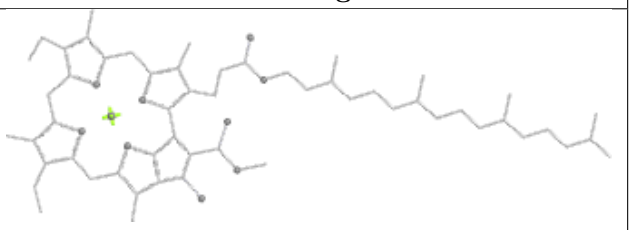
Bond lengths



Bond angles

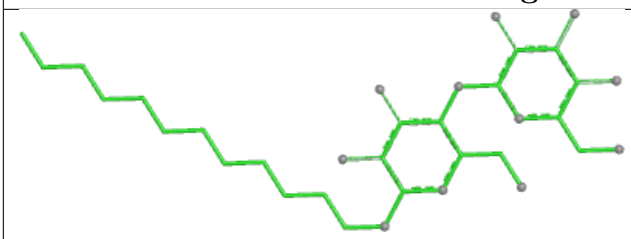


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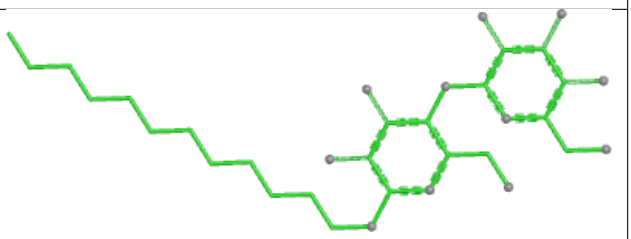


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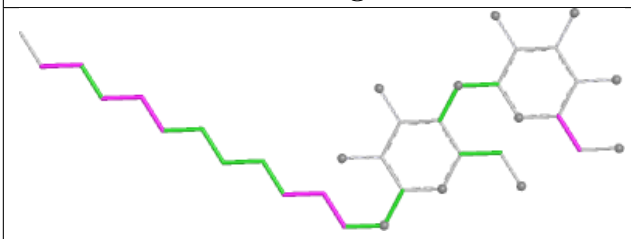
Ligand LMT A 853



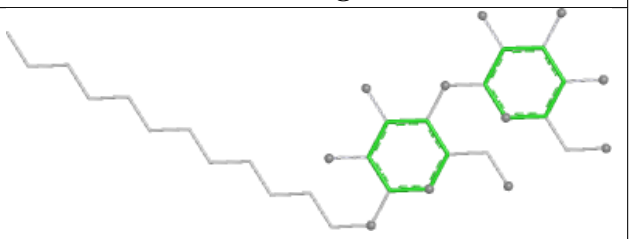
Bond lengths



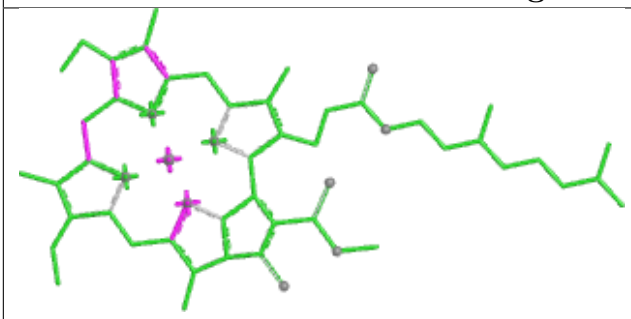
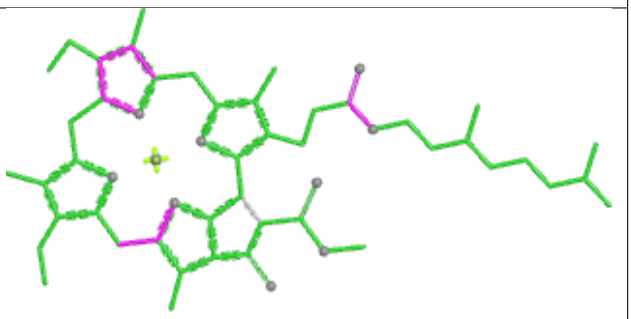
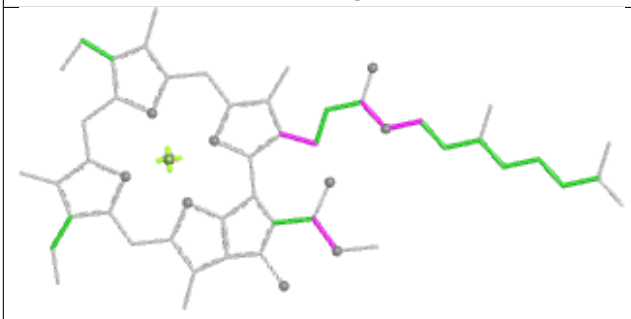
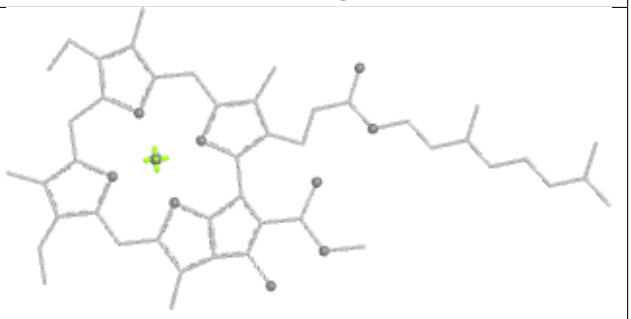
Bond angles

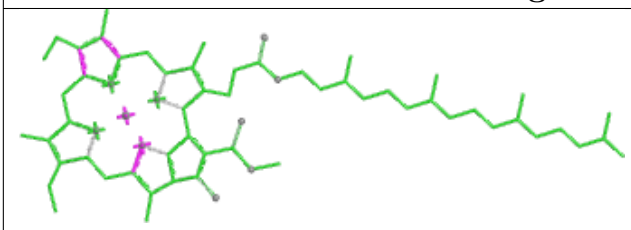
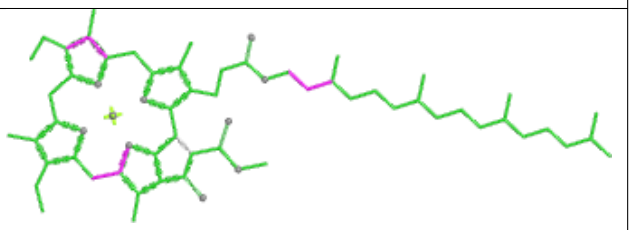
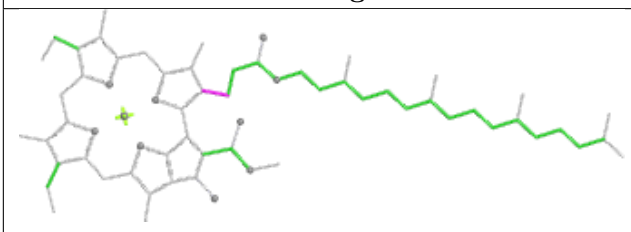
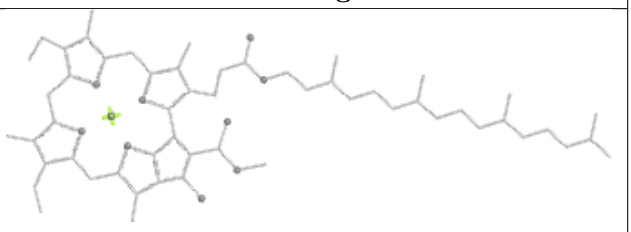


Torsions

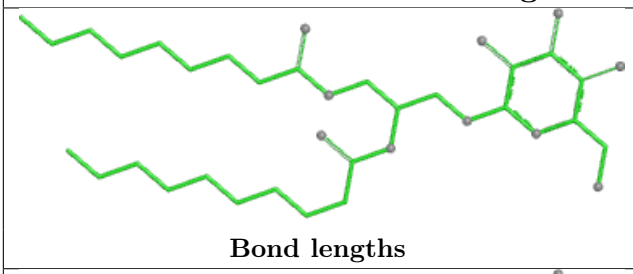


Rings

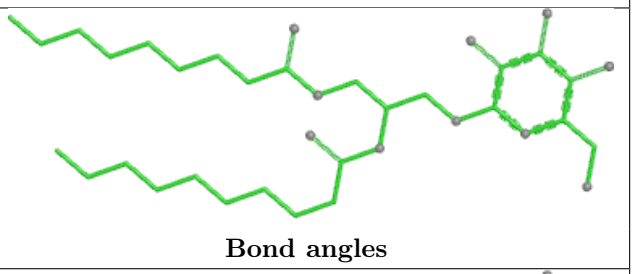
Ligand CLA b 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

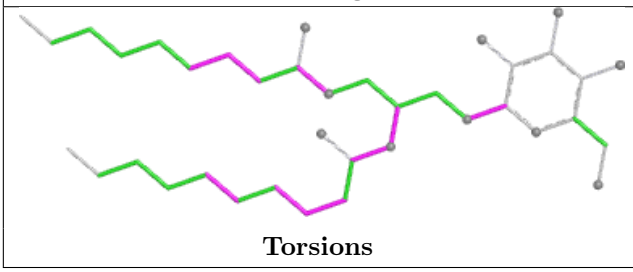
Ligand LMG B 852



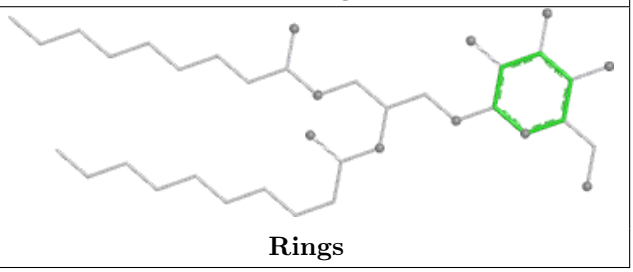
Bond lengths



Bond angles

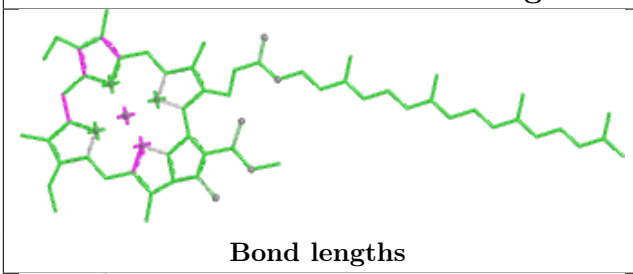


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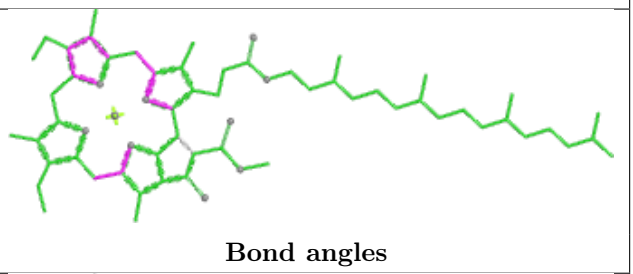


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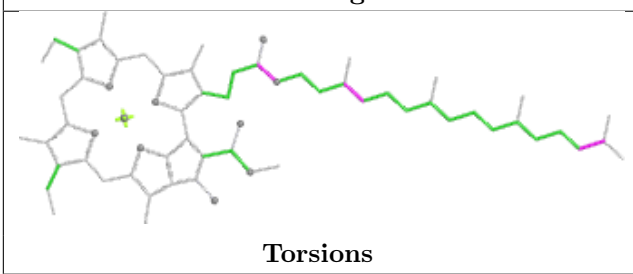
Ligand CLA B 830



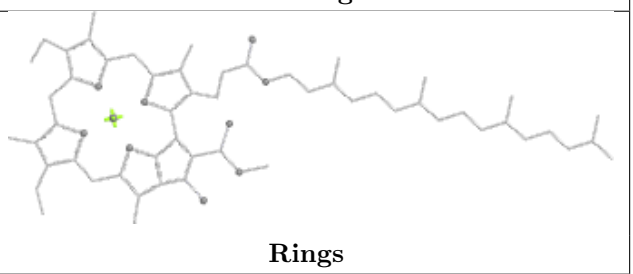
Bond lengths



Bond angles

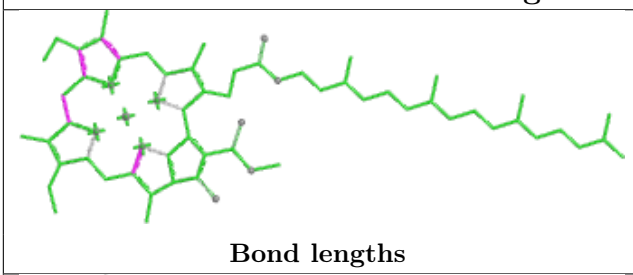


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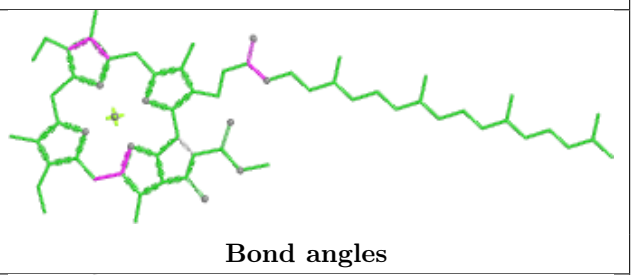


Rings

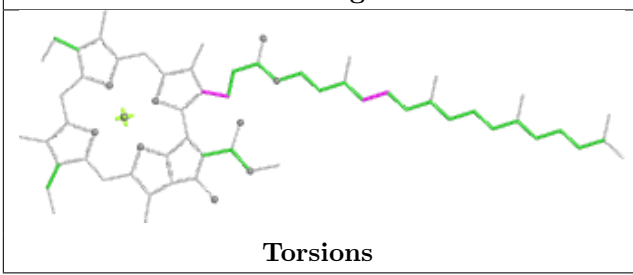
Ligand CLA U 204



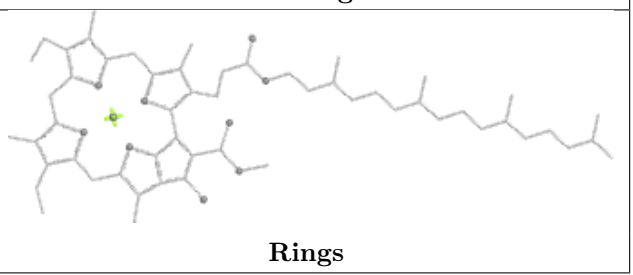
Bond lengths



Bond angles

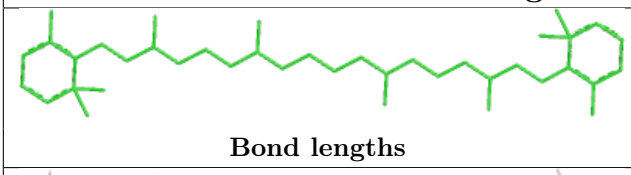


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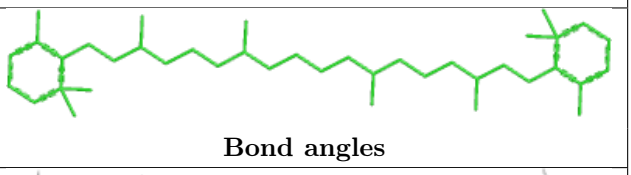


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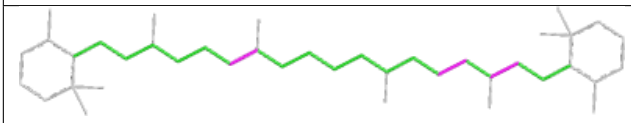
Ligand BCR b 847



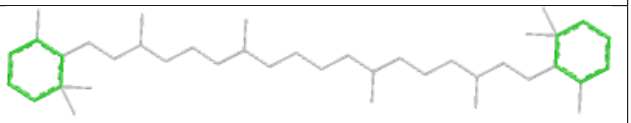
Bond lengths



Bond angles



Torsions

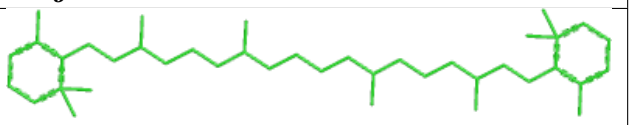


Rings

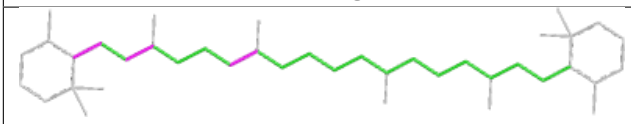
Ligand BCR j 103



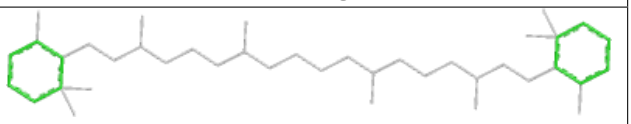
Bond lengths



Bond angles

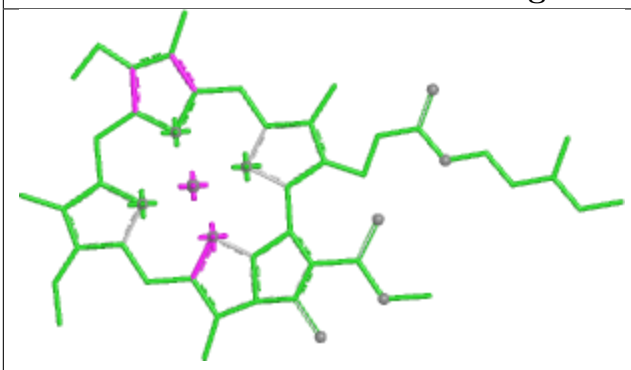


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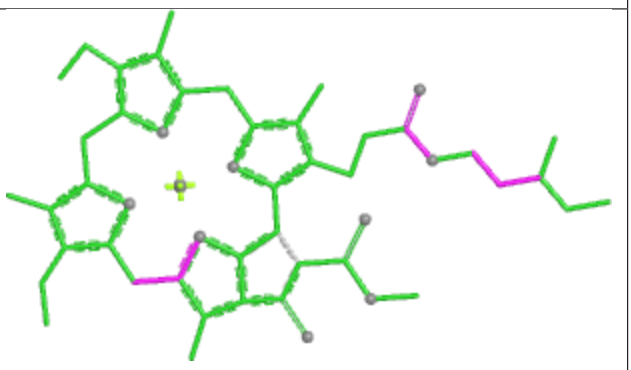


Rings

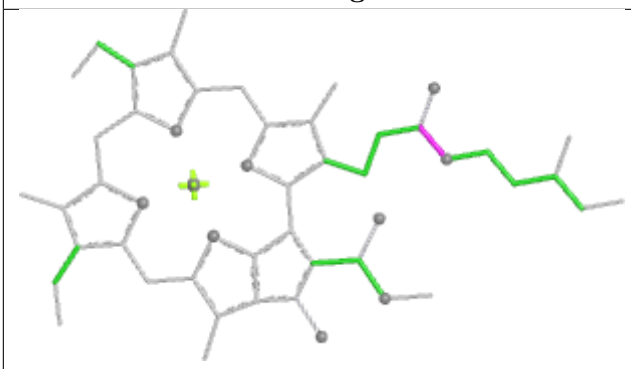
Ligand CLA a 838



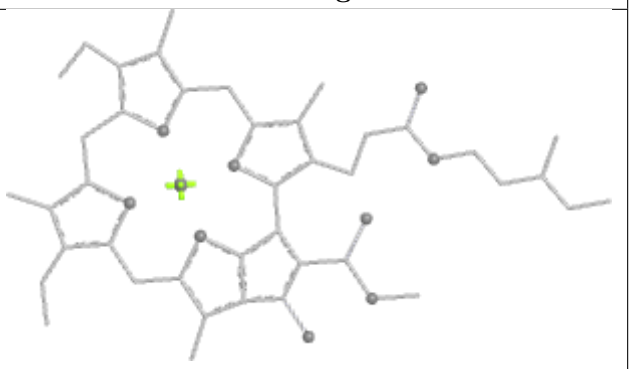
Bond lengths



Bond angles

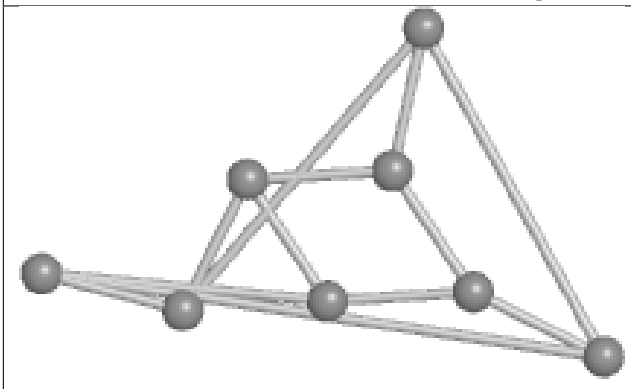


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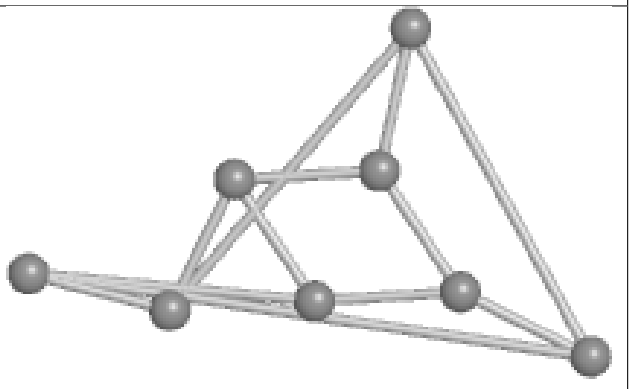


Rings

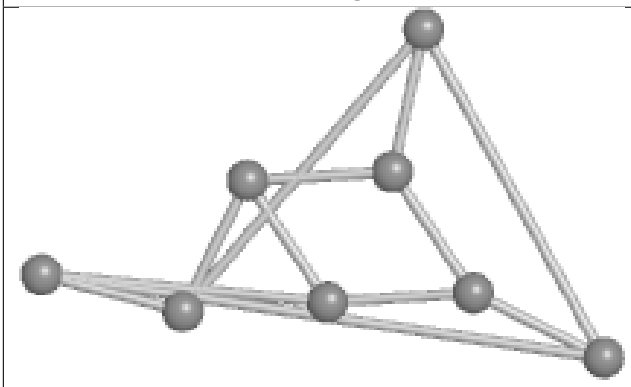
Ligand SF4 N 102



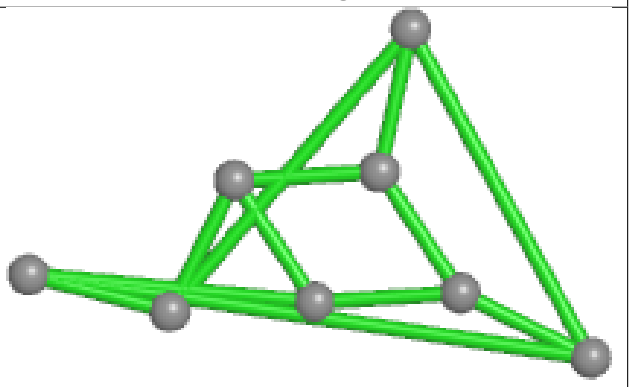
Bond lengths



Bond angles

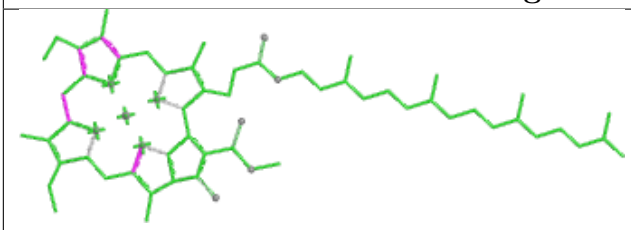


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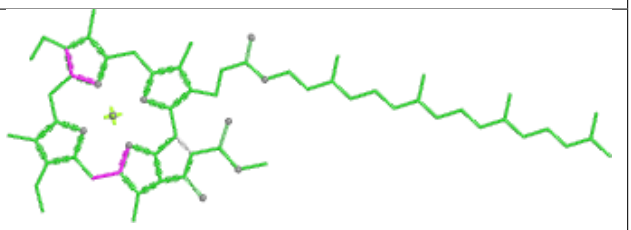


Rings

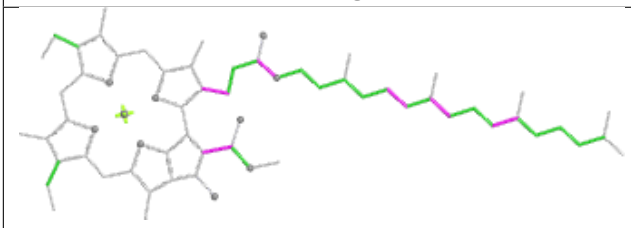
Ligand CLA A 804



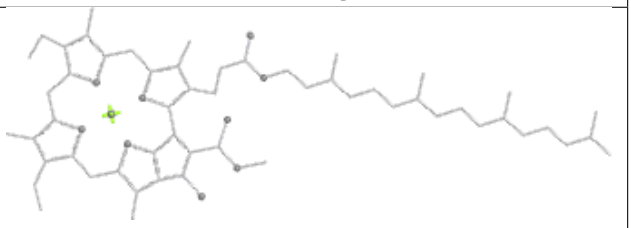
Bond lengths



Bond angles

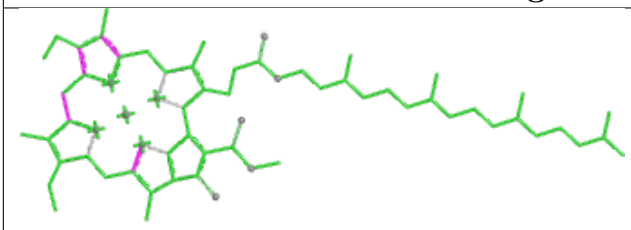


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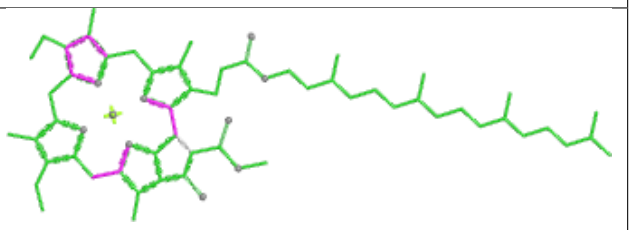


Rings

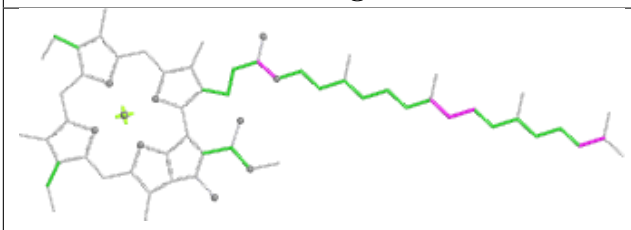
Ligand CLA b 812



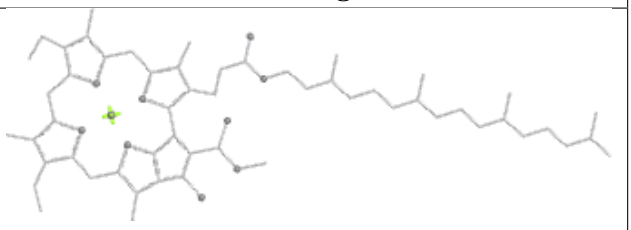
Bond lengths



Bond angles

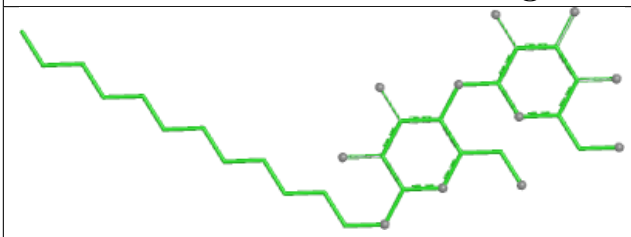


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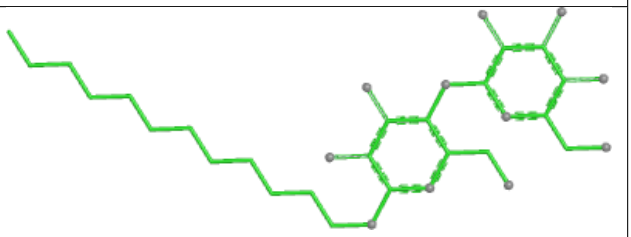


Rings

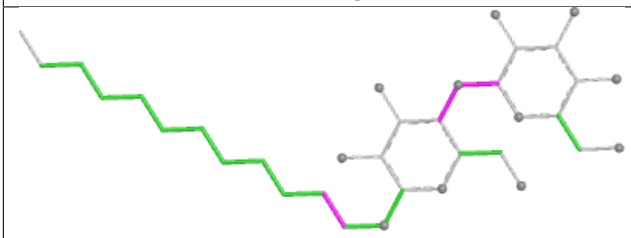
Ligand LMT B 855



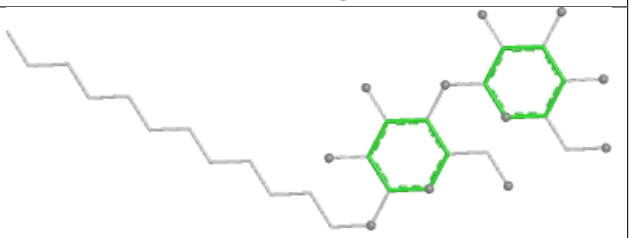
Bond lengths



Bond angles



Torsions

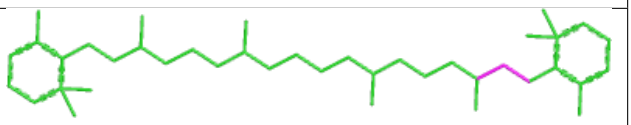


Rings

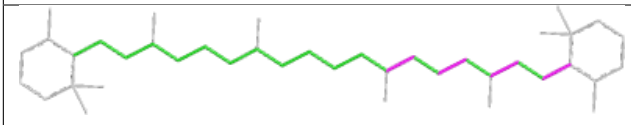
Ligand BCR G 850



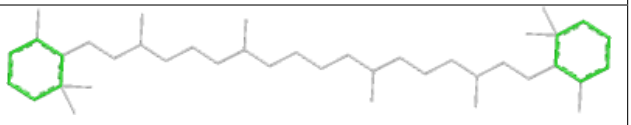
Bond lengths



Bond angles

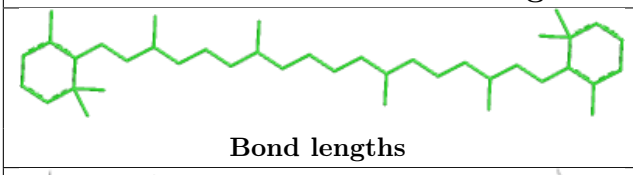


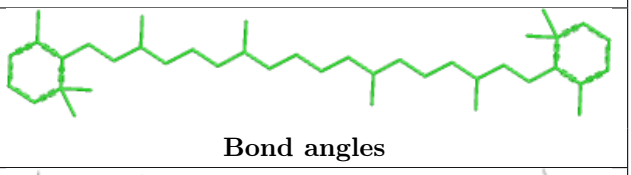
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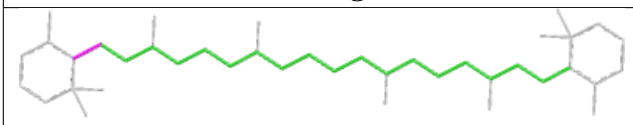


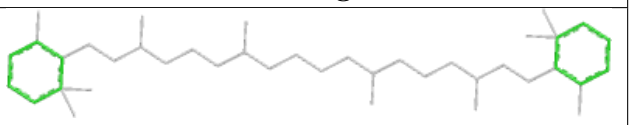
Rings

Ligand BCR a 848


Bond lengths

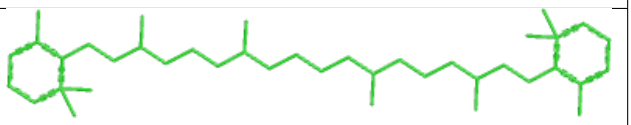

Bond angles

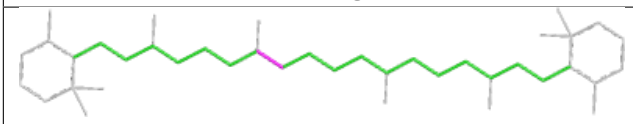

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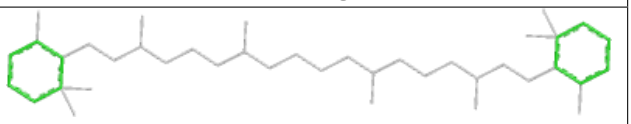

Rings

Ligand BCR f 206

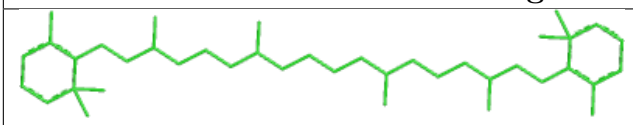

Bond lengths

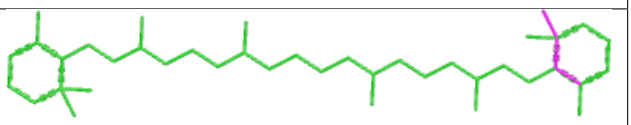

Bond angles

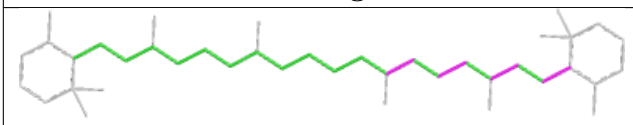

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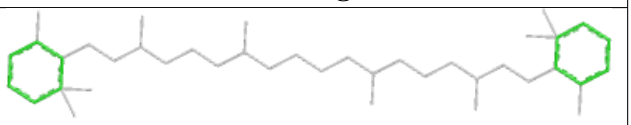

Rings

Ligand BCR a 851

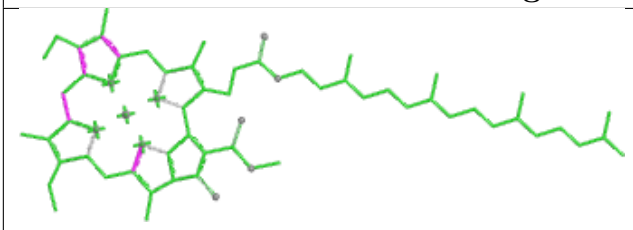

Bond lengths

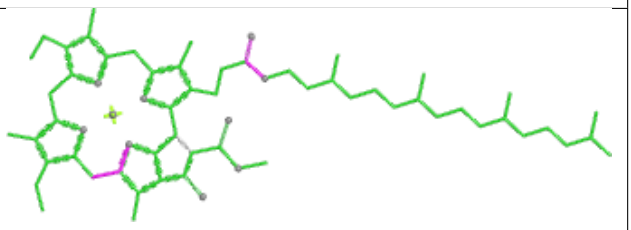

Bond angles

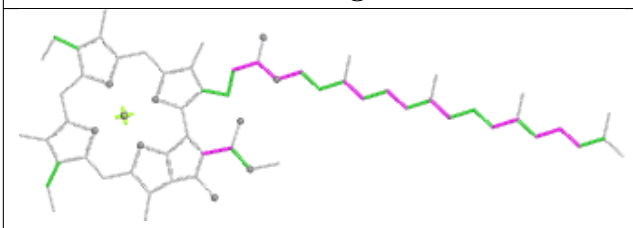

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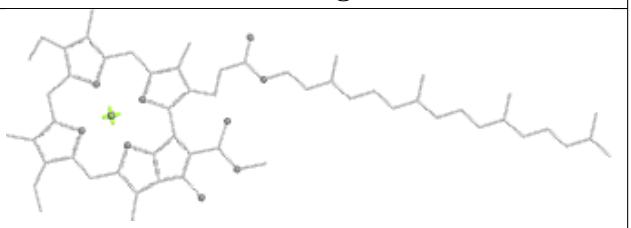

Rings

Ligand CLA G 805

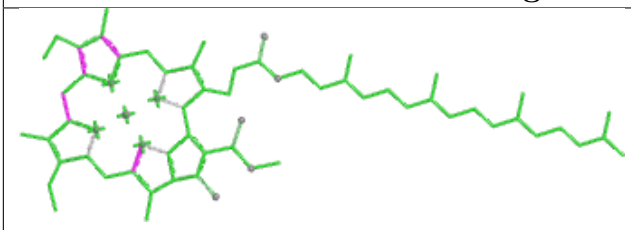

Bond lengths


Bond angles

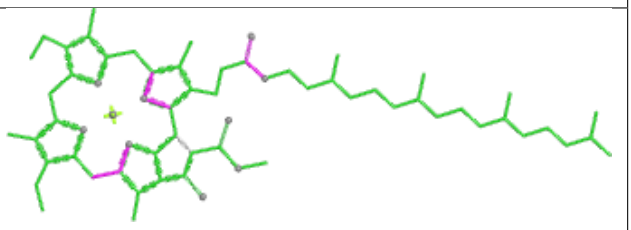

Torsions


Rings

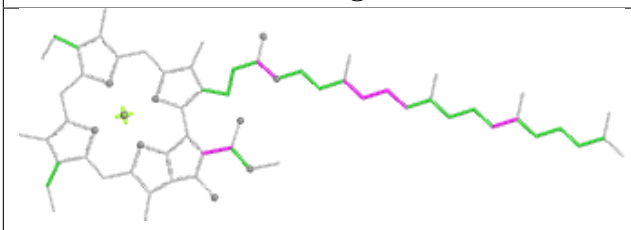
Ligand CLA G 815



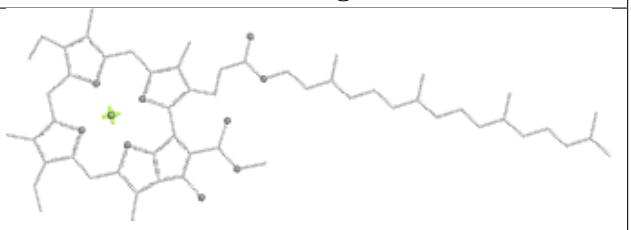
Bond lengths



Bond angles

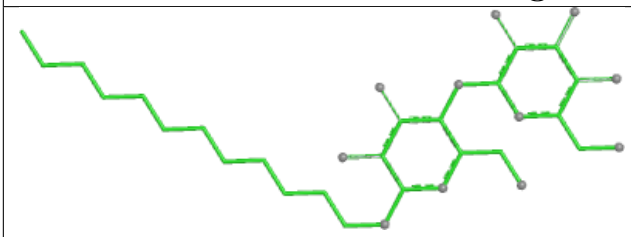


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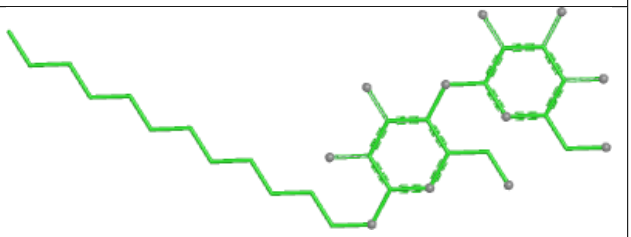


Rings

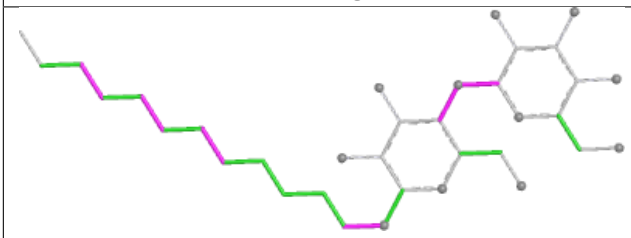
Ligand LMT f 207



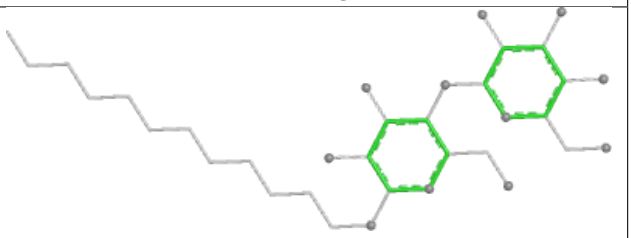
Bond lengths



Bond angles

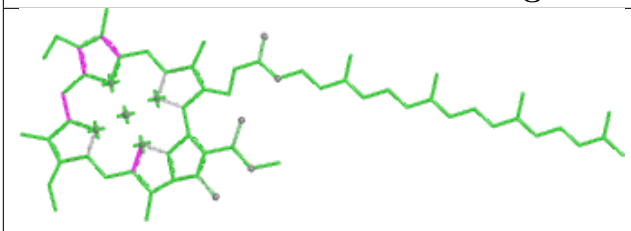


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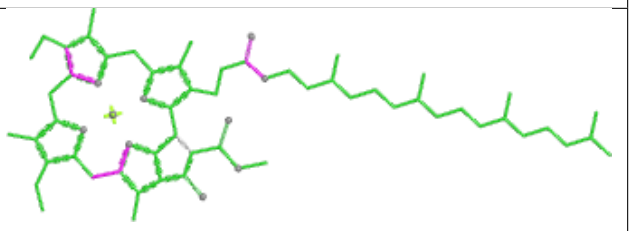


Rings

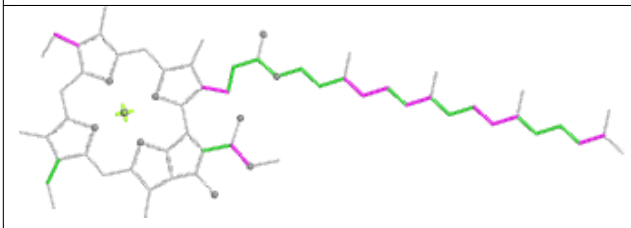
Ligand CLA A 836



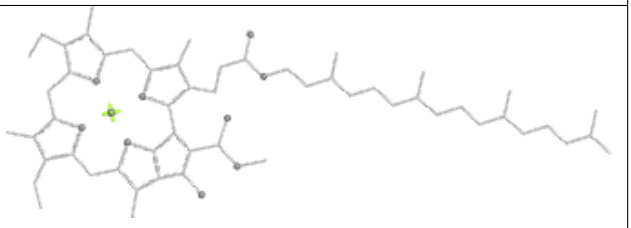
Bond lengths



Bond angles

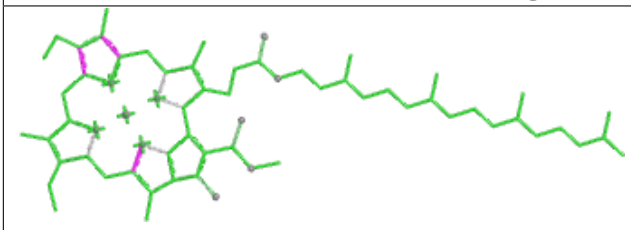


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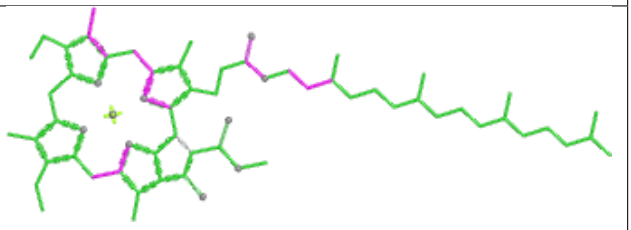


Rings

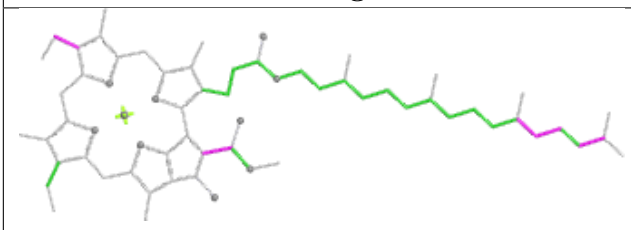
Ligand CLA B 810



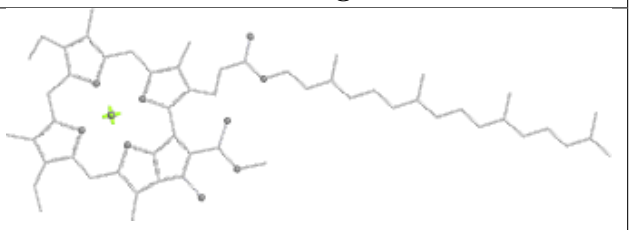
Bond lengths



Bond angles

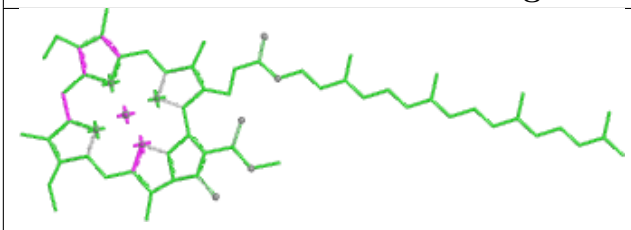


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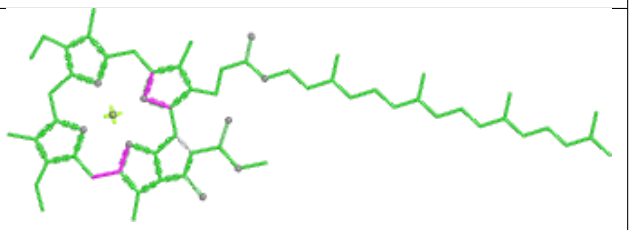


Rings

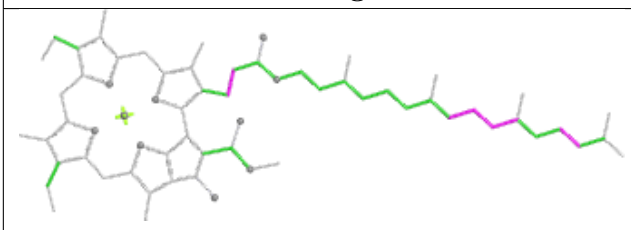
Ligand CLA H 804



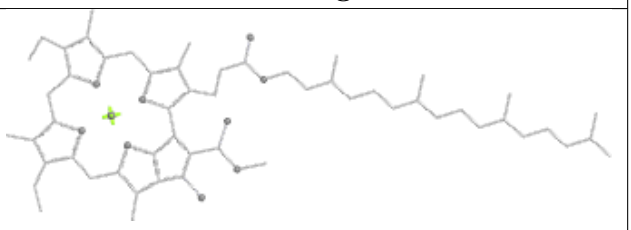
Bond lengths



Bond angles

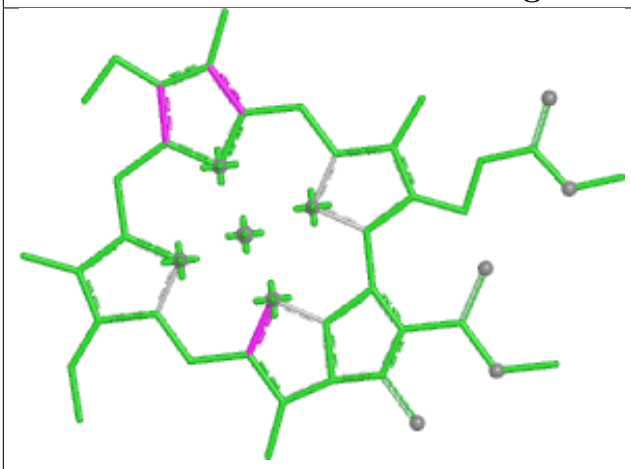


Torsions

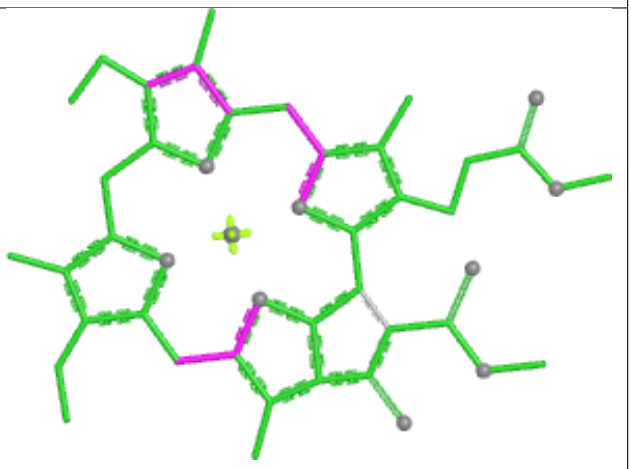


Rings

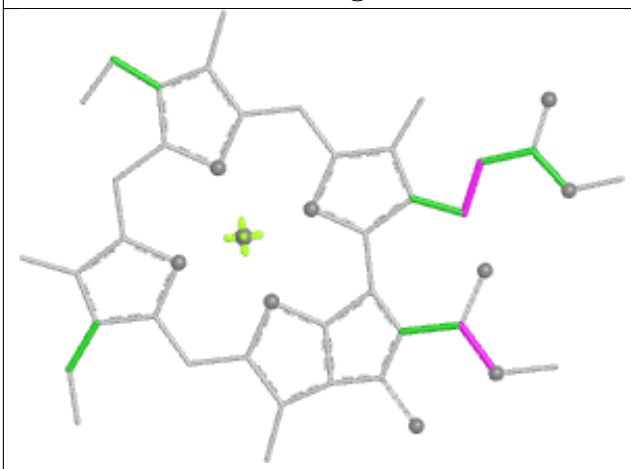
Ligand CLA H 842



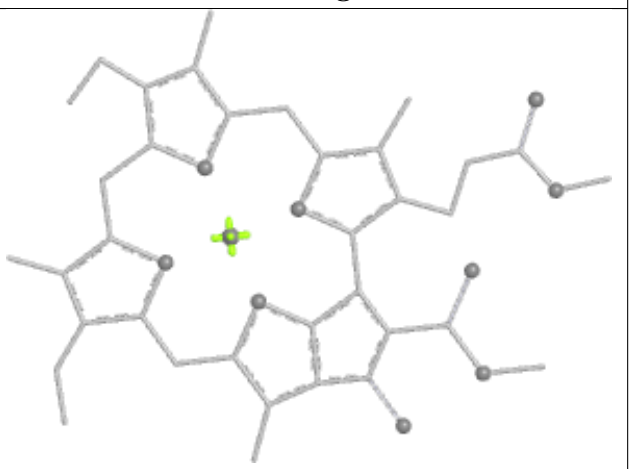
Bond lengths



Bond angles



Torsions



Rings

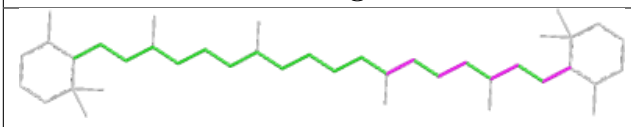
Ligand BCR A 849



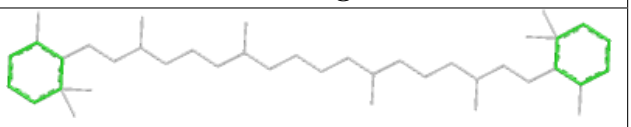
Bond lengths



Bond angles

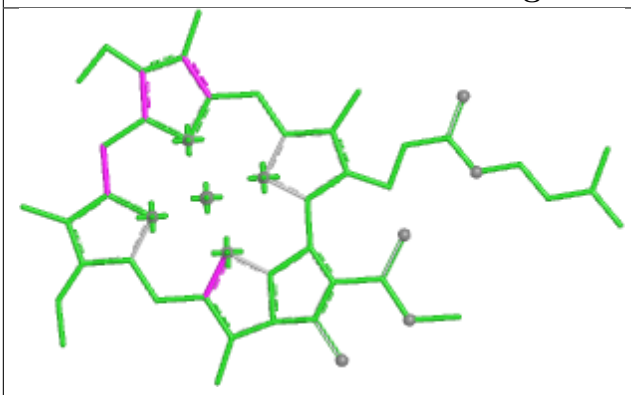


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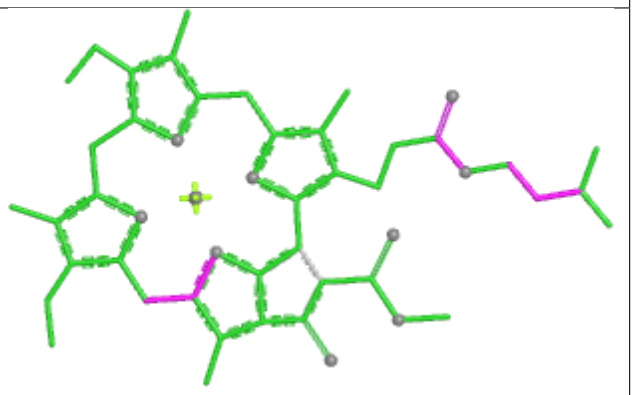


Rings

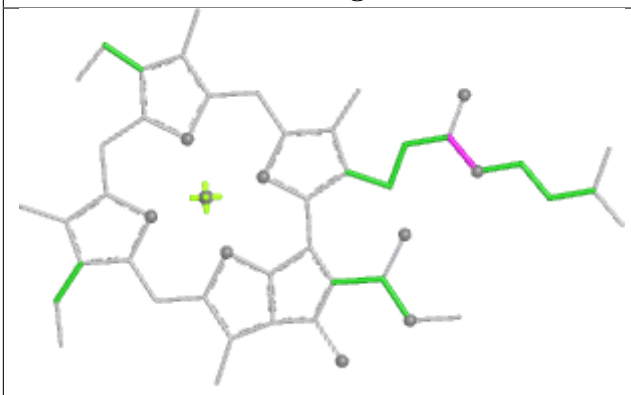
Ligand CLA H 837



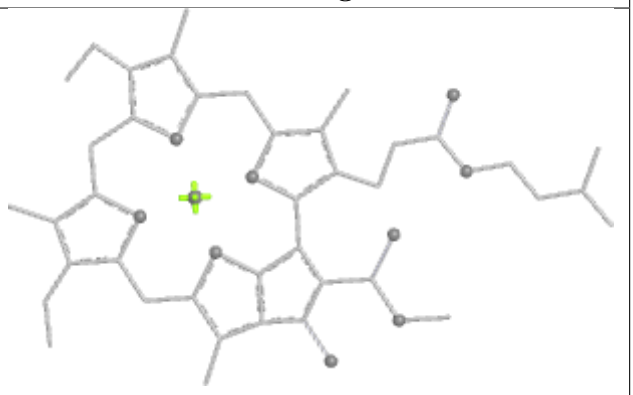
Bond lengths



Bond angles

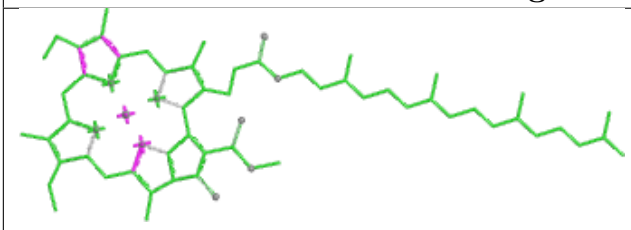


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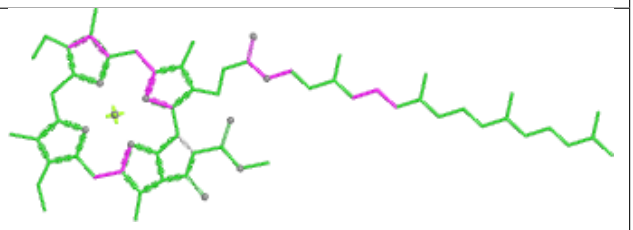


Rings

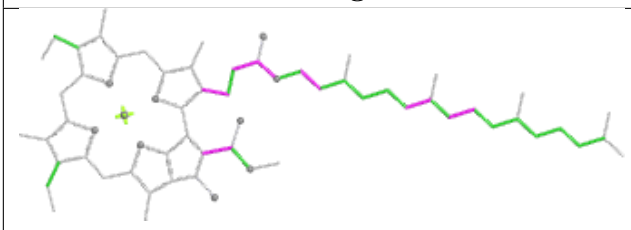
Ligand CLA a 806



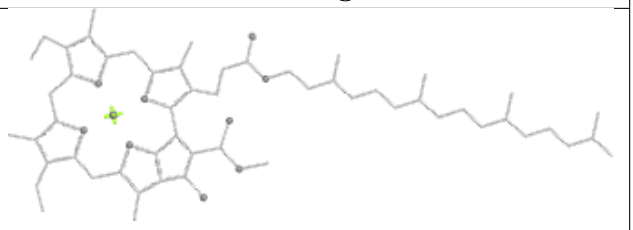
Bond lengths



Bond angles

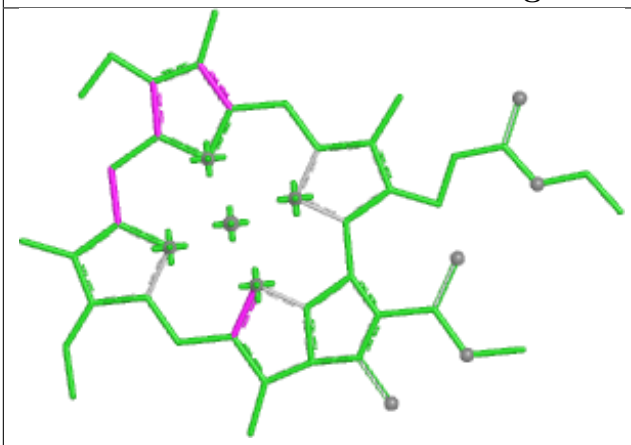


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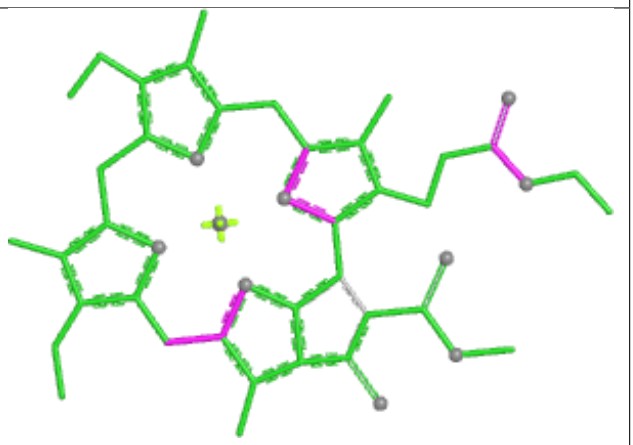


Rings

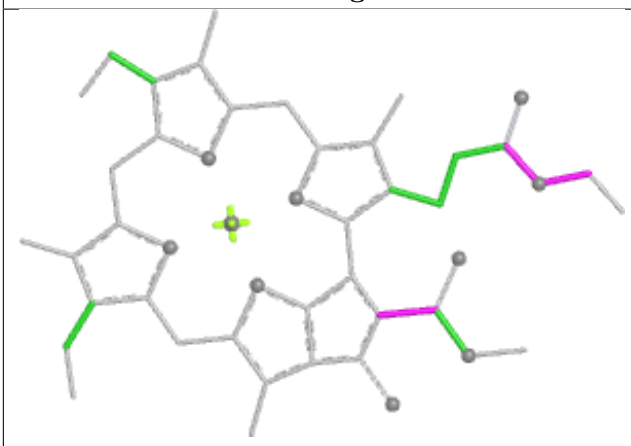
Ligand CLA A 814



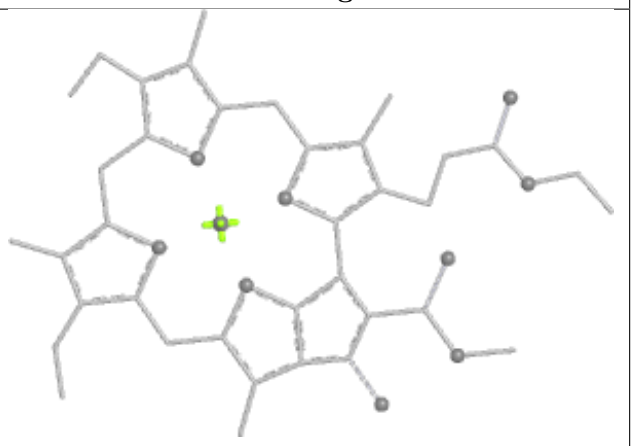
Bond lengths



Bond angles

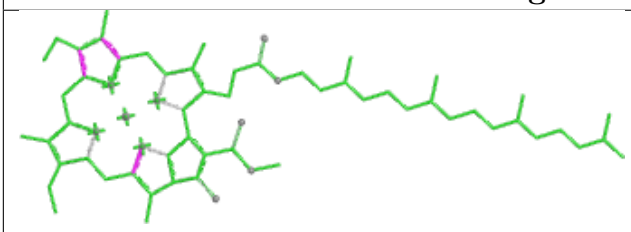


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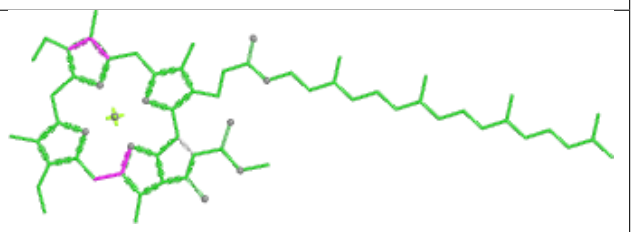


Rings

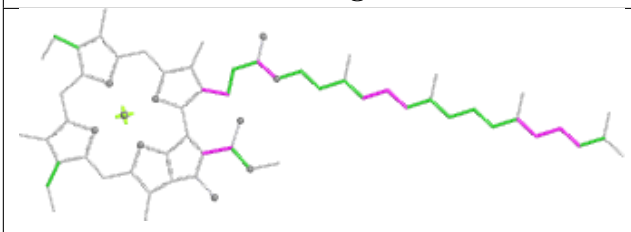
Ligand CLA a 812



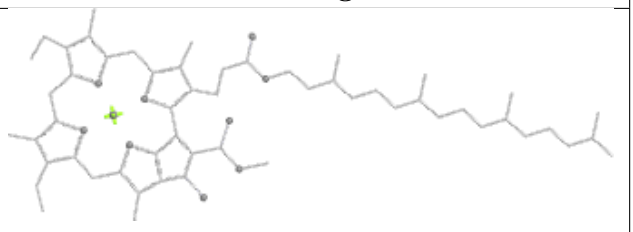
Bond lengths



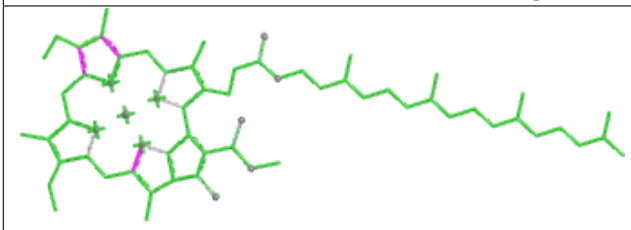
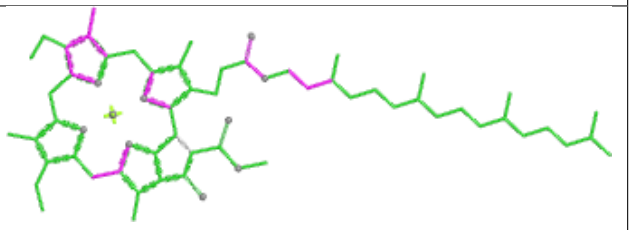
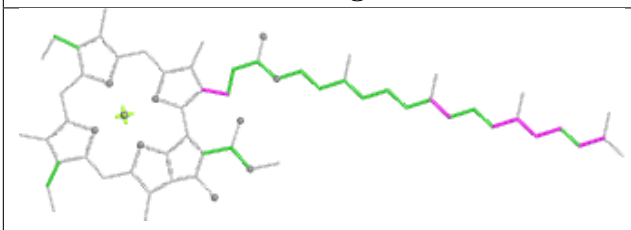
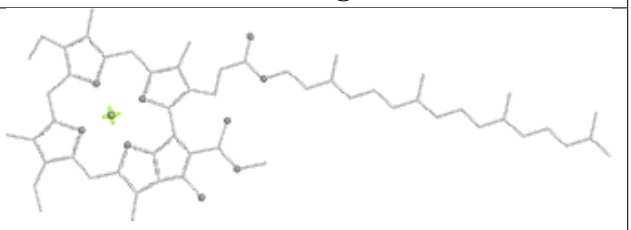
Bond angles

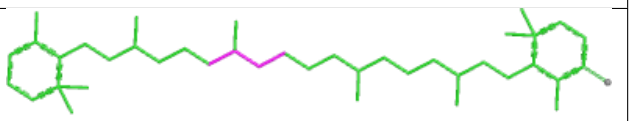
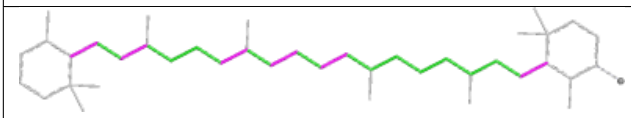
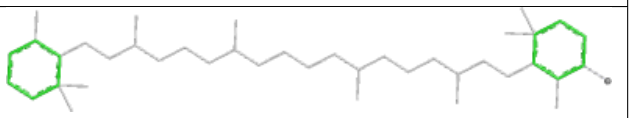


Torsions

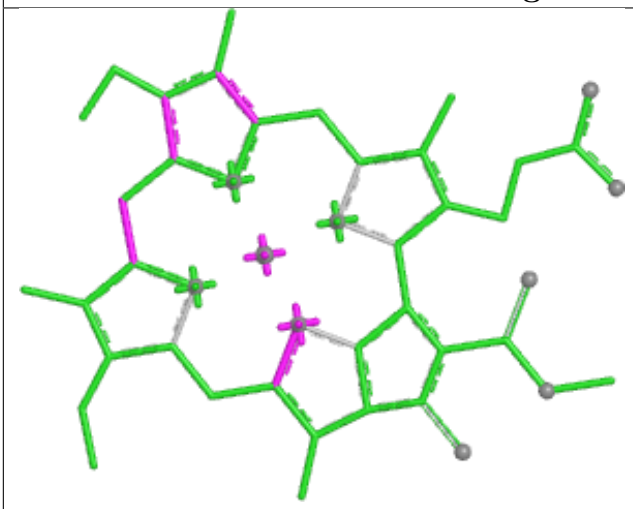


Rings

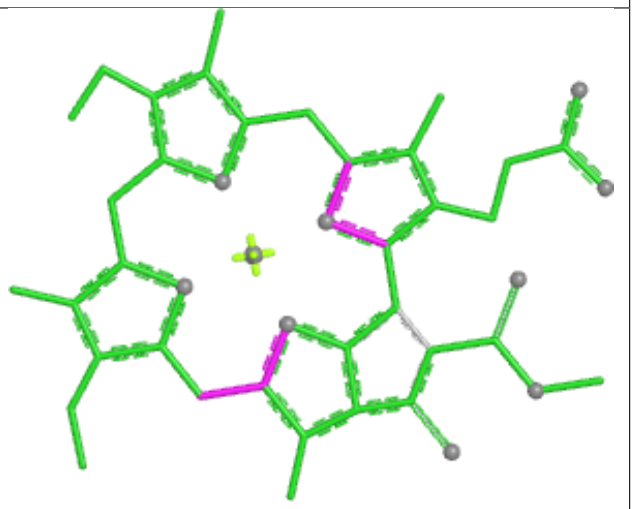
Ligand CLA k 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ECH m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

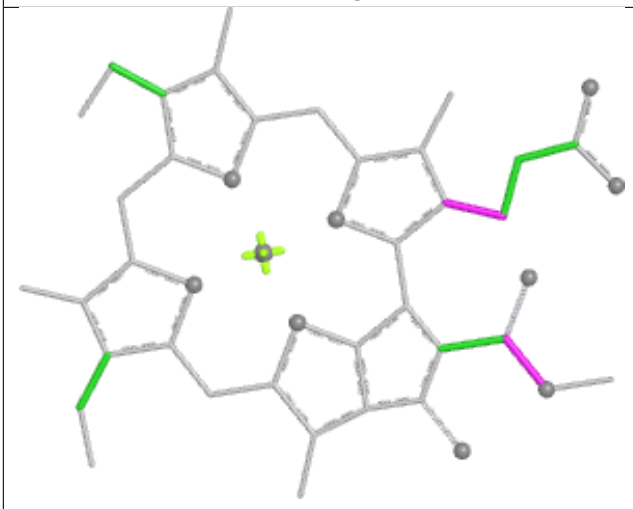
Ligand CLA G 811



Bond lengths



Bond angles

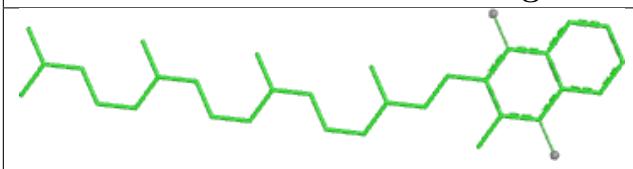


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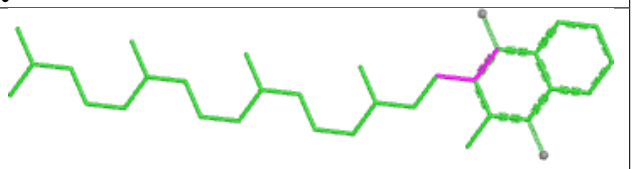


Rings

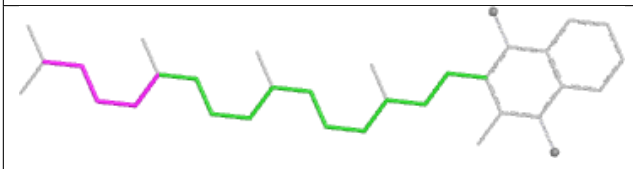
Ligand PQN B 844



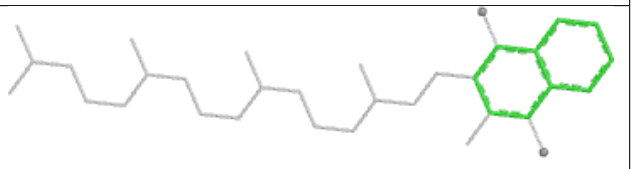
Bond lengths



Bond angles

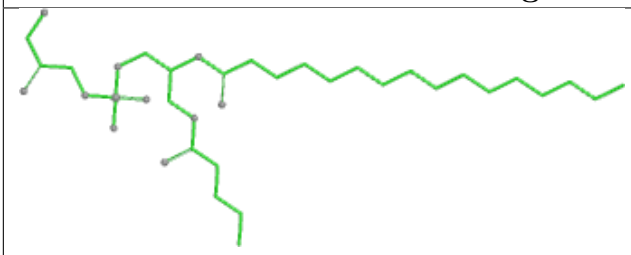


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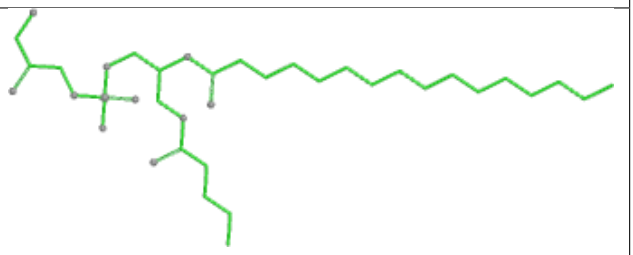


Rings

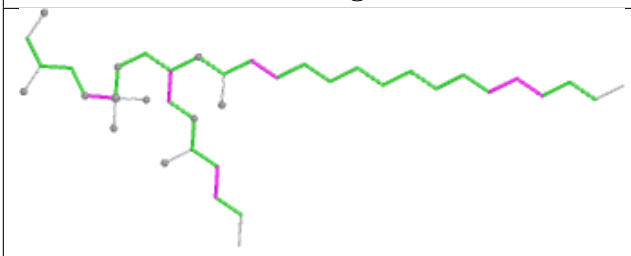
Ligand LHG H 850



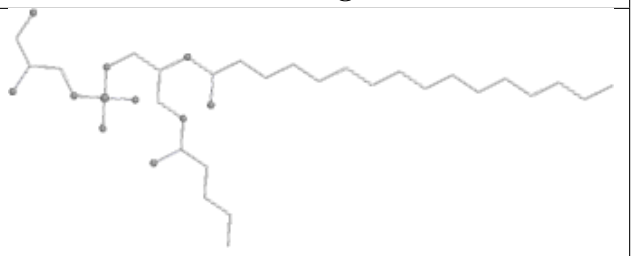
Bond lengths



Bond angles



Torsions



Rings

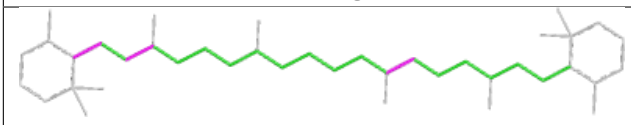
Ligand BCR G 848



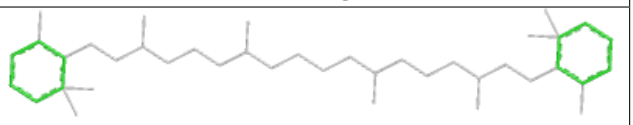
Bond lengths



Bond angles

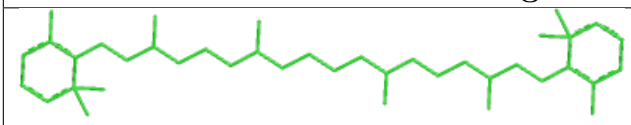


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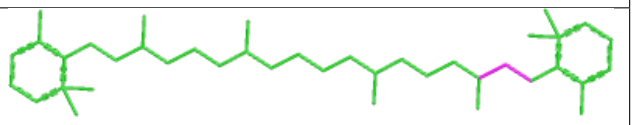


Rings

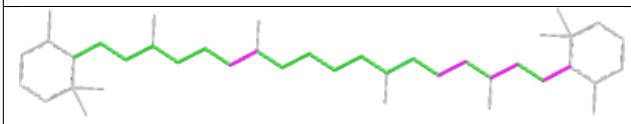
Ligand BCR G 858



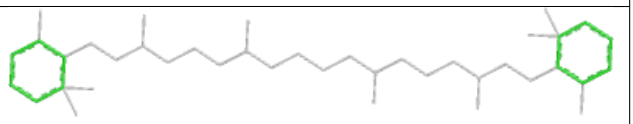
Bond lengths



Bond angles

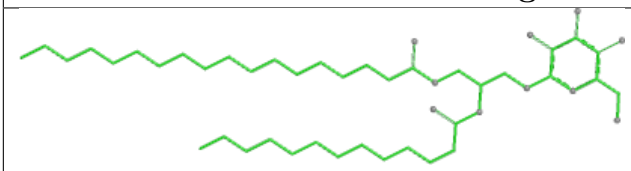


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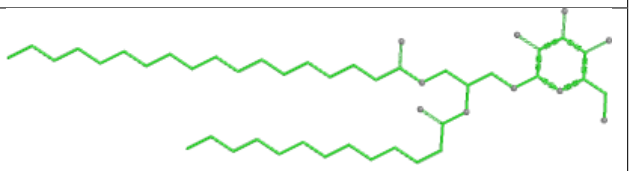


Rings

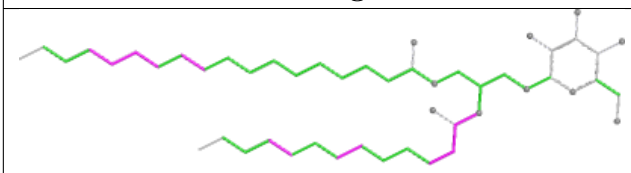
Ligand LMG H 801



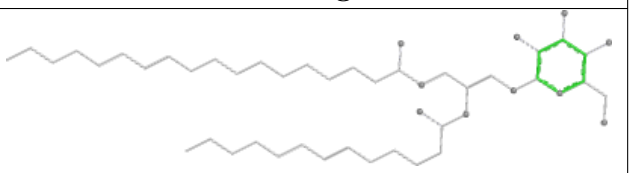
Bond lengths



Bond angles

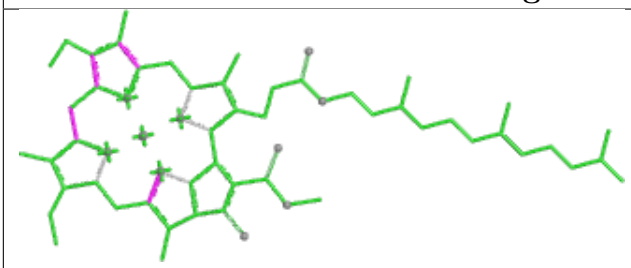


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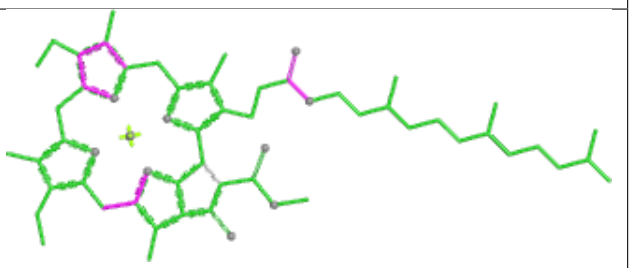


Rings

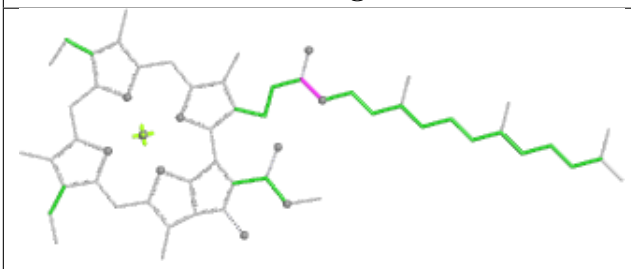
Ligand CLA G 827



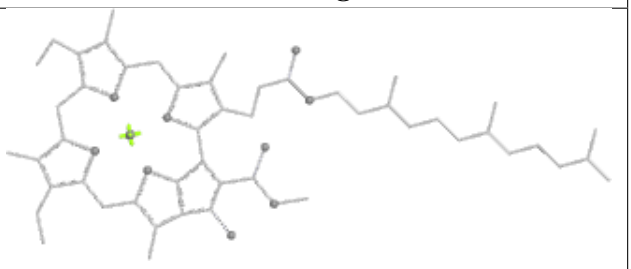
Bond lengths



Bond angles

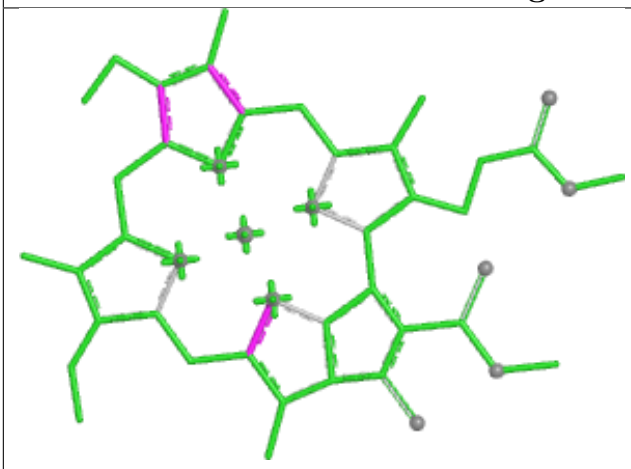


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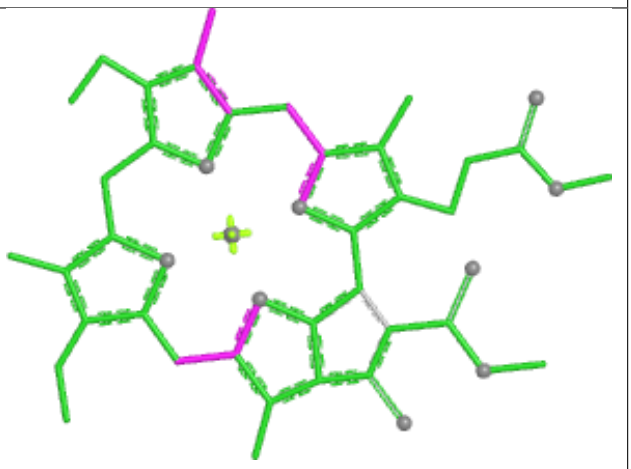


Rings

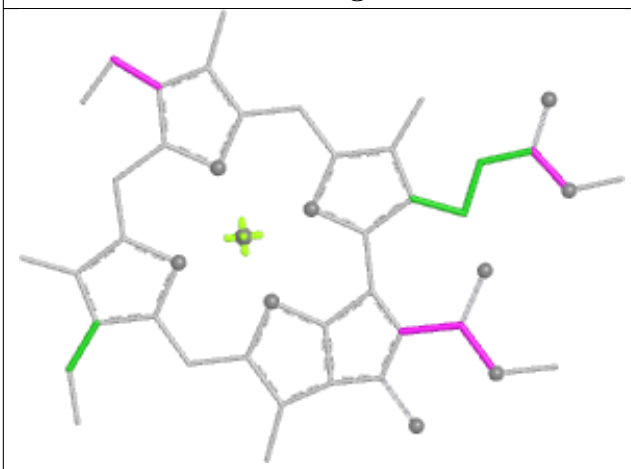
Ligand CLA a 845



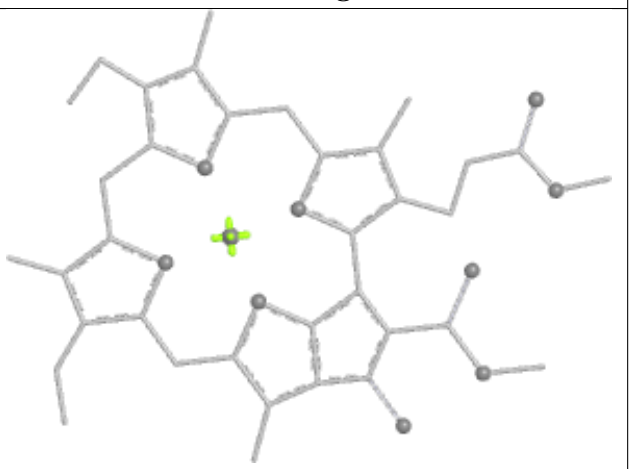
Bond lengths



Bond angles



Torsions



Rings

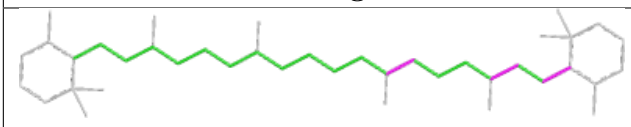
Ligand BCR R 101



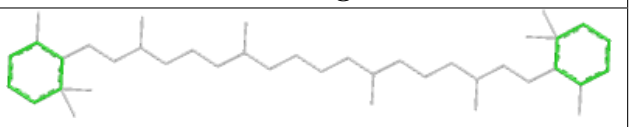
Bond lengths



Bond angles

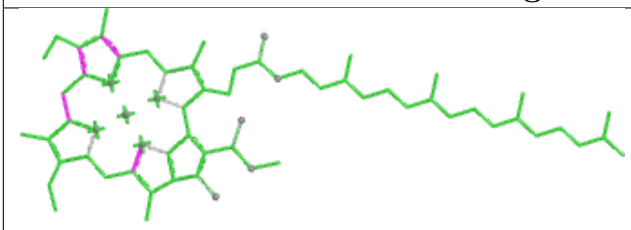


Torsions

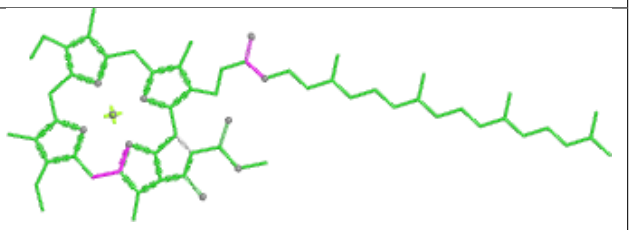


Rings

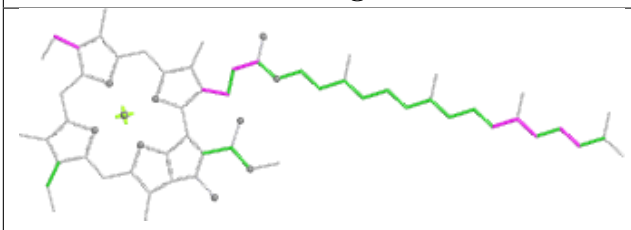
Ligand CLA A 818



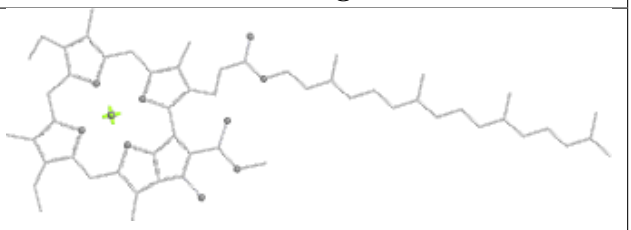
Bond lengths



Bond angles

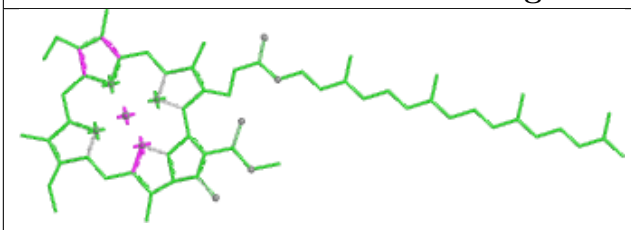


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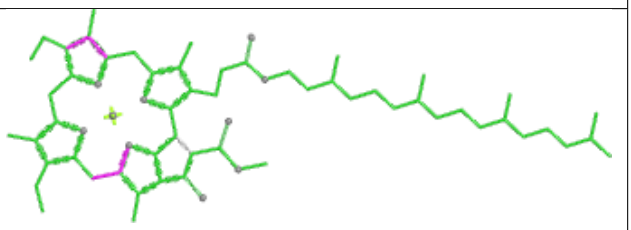


Rings

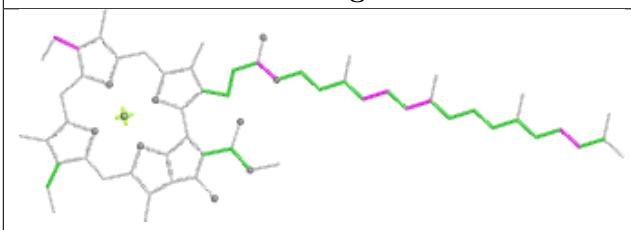
Ligand CLA B 832



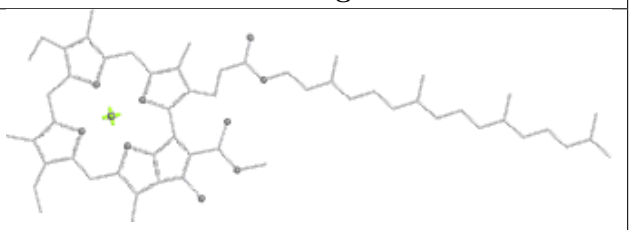
Bond lengths



Bond angles

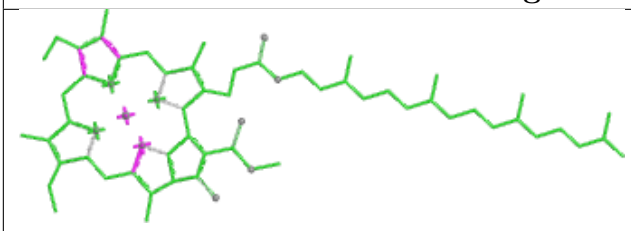


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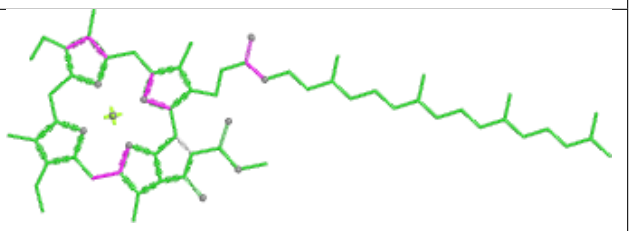


Rings

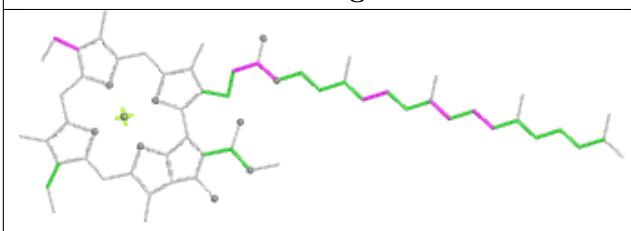
Ligand CLA H 807



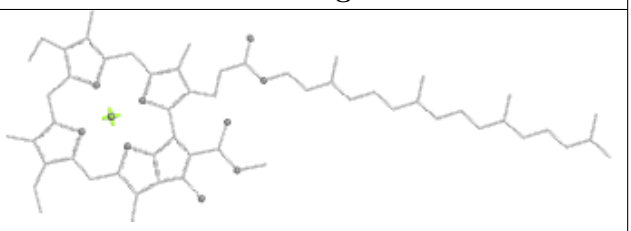
Bond lengths



Bond angles

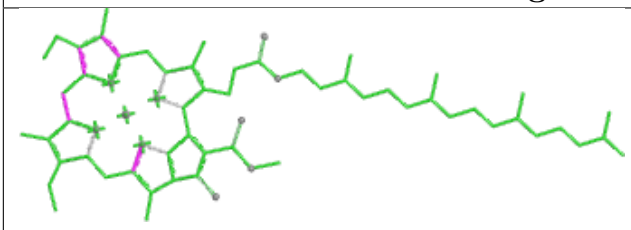


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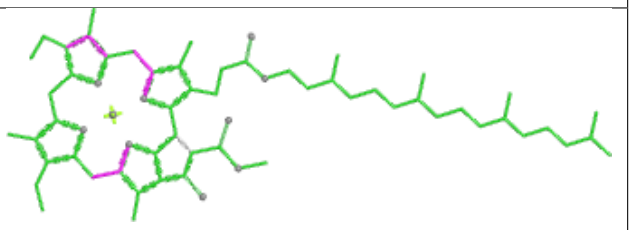


Rings

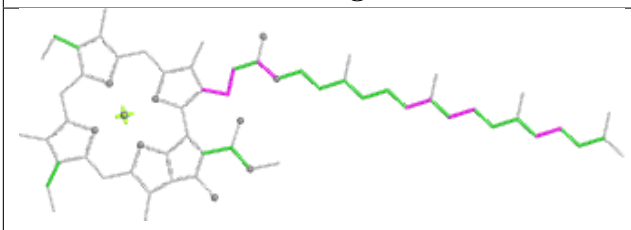
Ligand CLA a 842



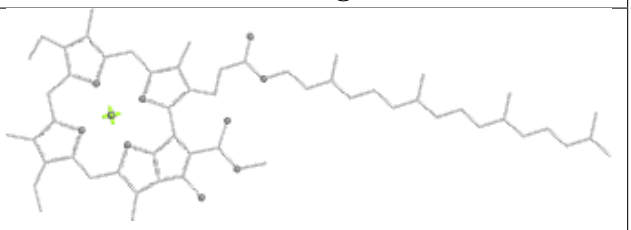
Bond lengths



Bond angles

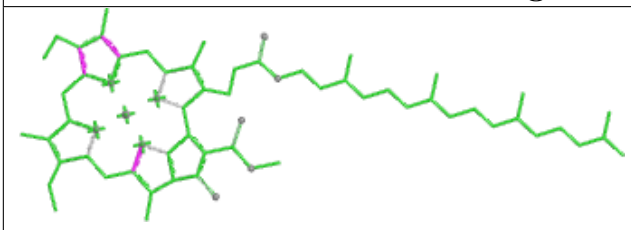


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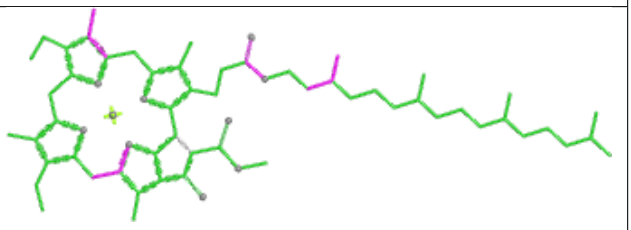


Rings

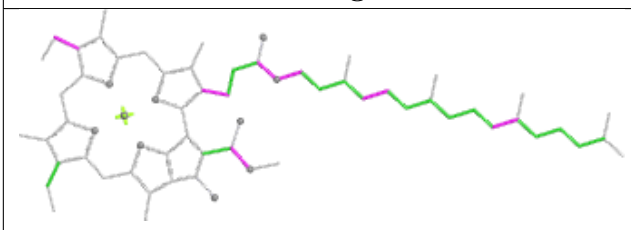
Ligand CLA b 843



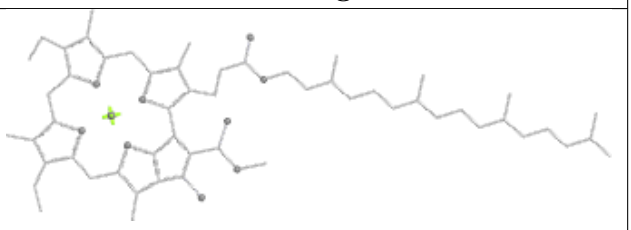
Bond lengths



Bond angles

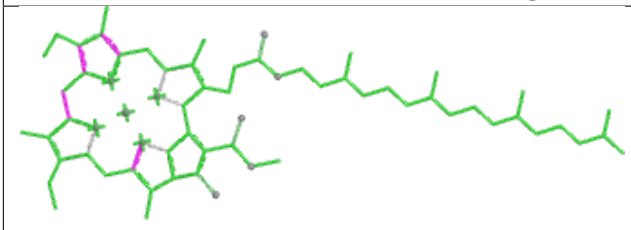


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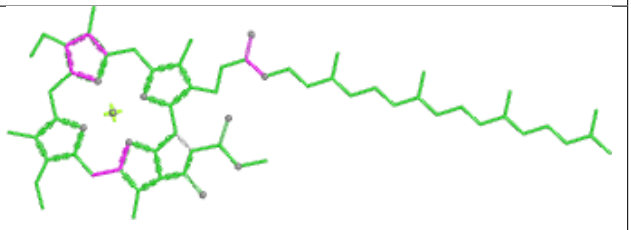


Rings

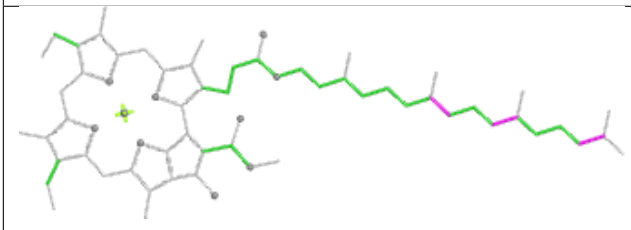
Ligand CLA A 839



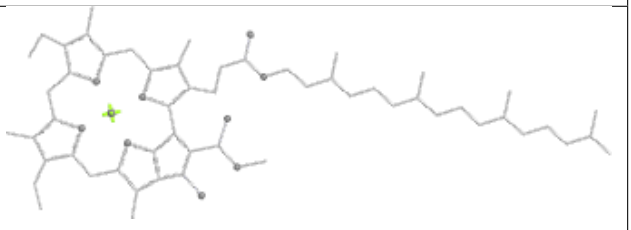
Bond lengths



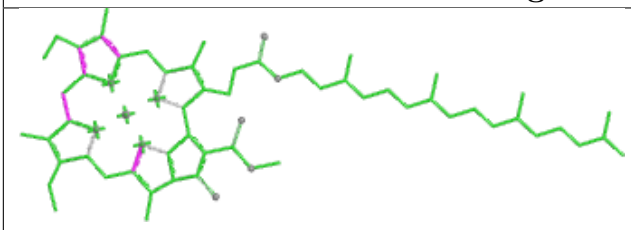
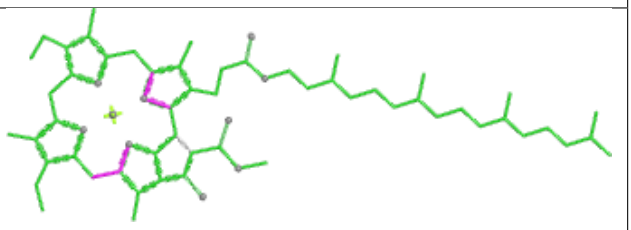
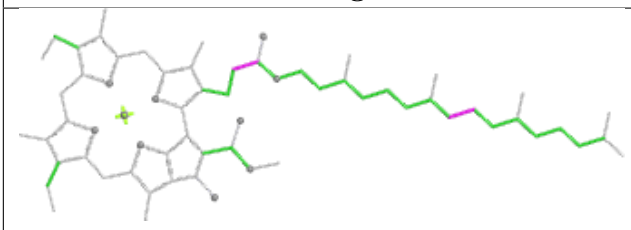
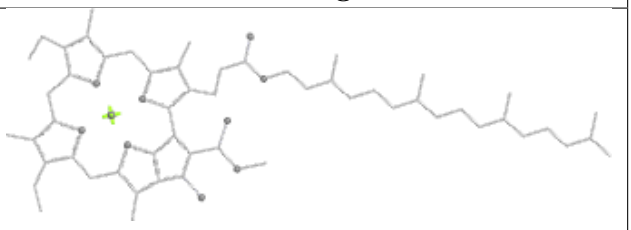
Bond angles

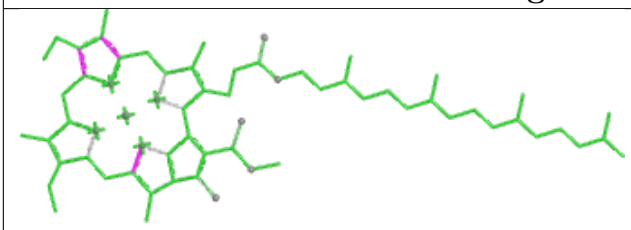
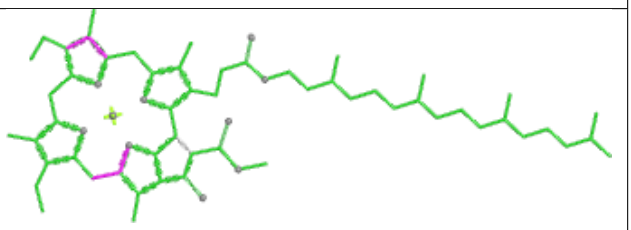
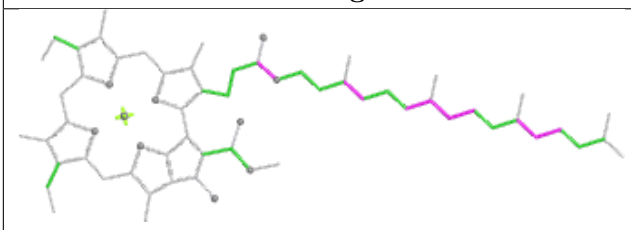
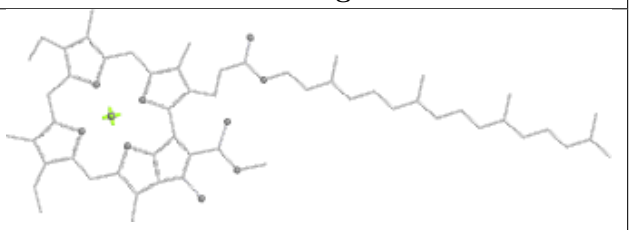


Torsions

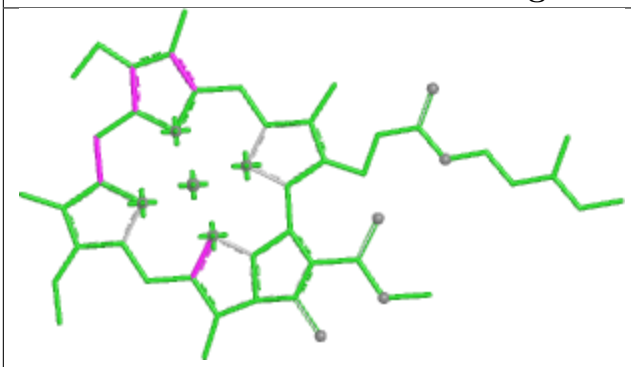


Rings

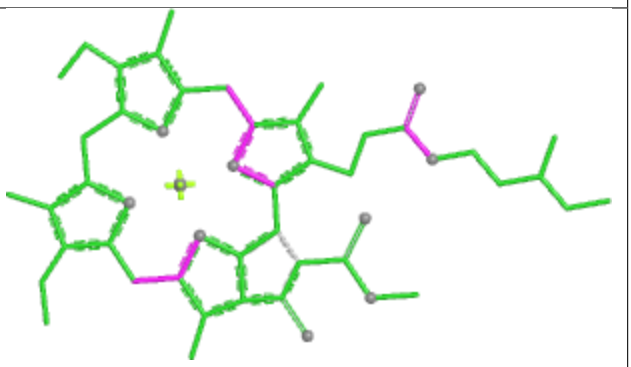
Ligand CLA b 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

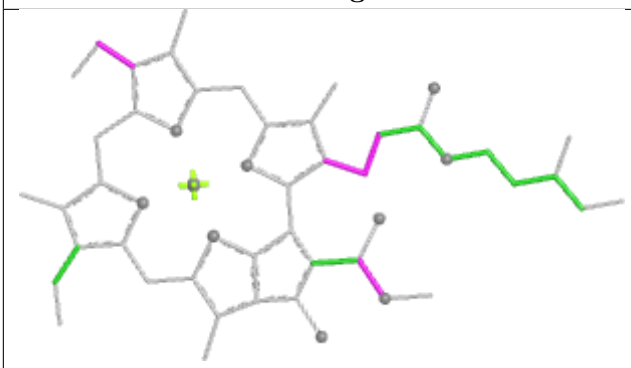
Ligand CLA a 810



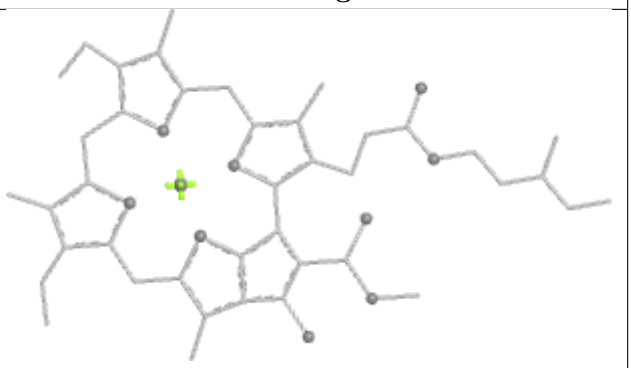
Bond lengths



Bond angles

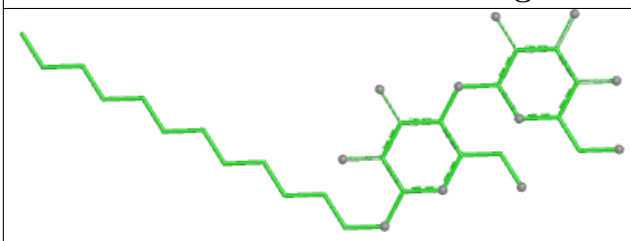


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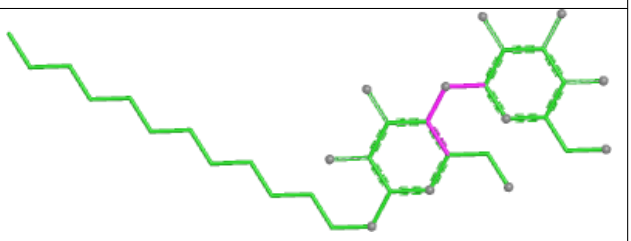


Rings

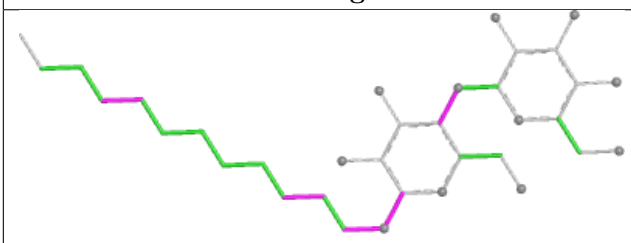
Ligand LMT L 1505



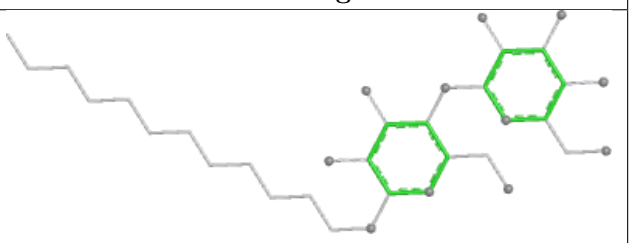
Bond lengths



Bond angles

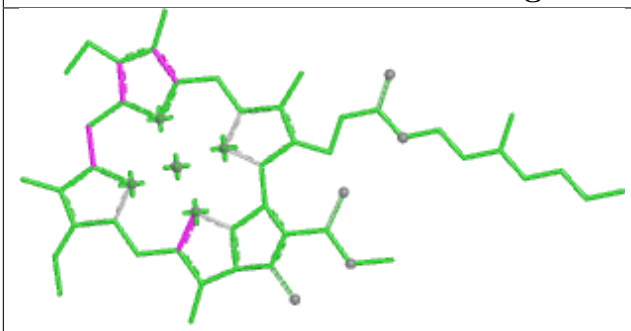


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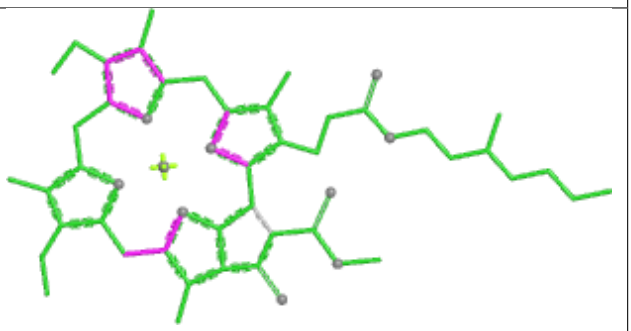


Rings

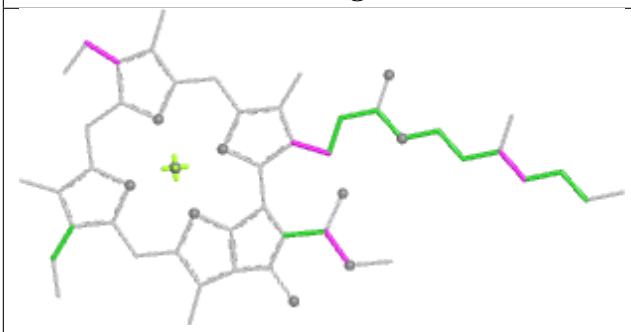
Ligand CLA B 825



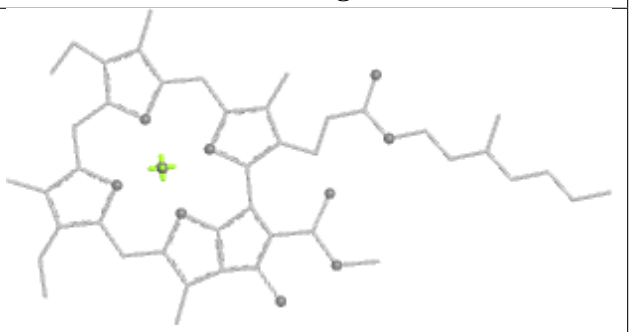
Bond lengths



Bond angles

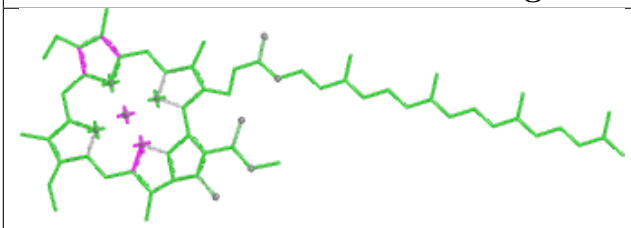


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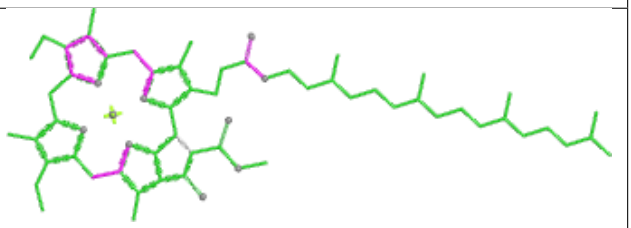


Rings

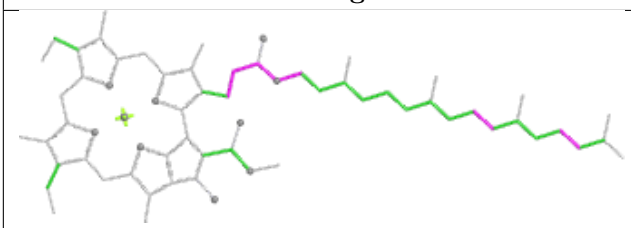
Ligand CLA B 819



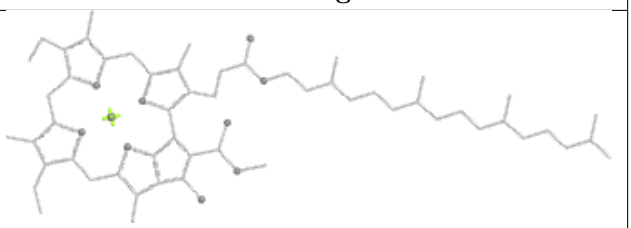
Bond lengths



Bond angles

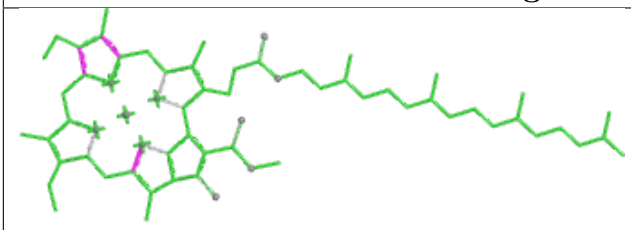


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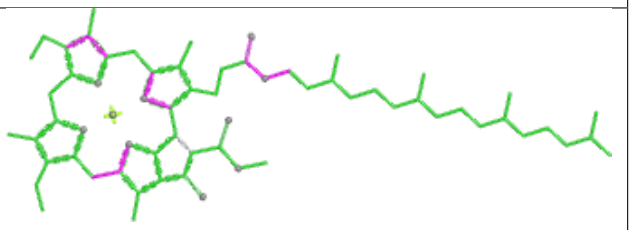


Rings

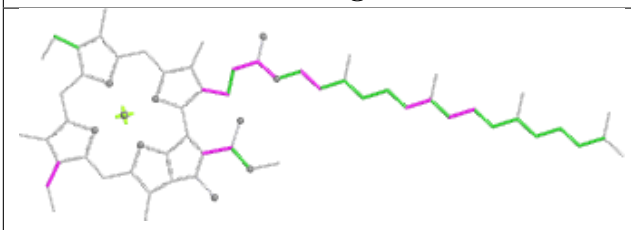
Ligand CLA G 806



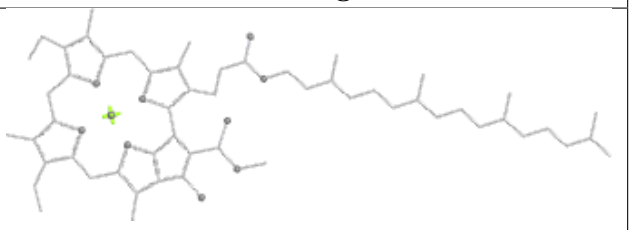
Bond lengths



Bond angles

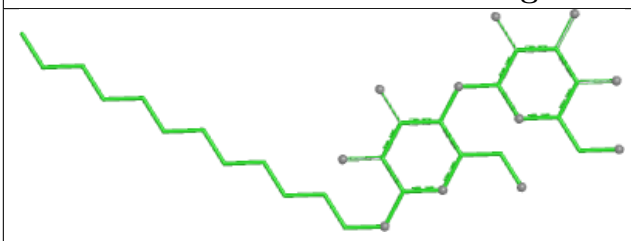


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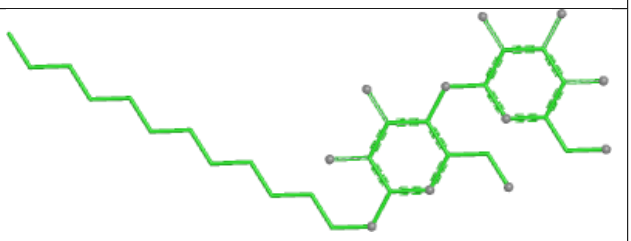


Rings

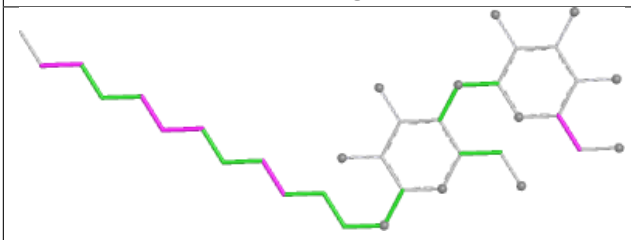
Ligand LMT A 857



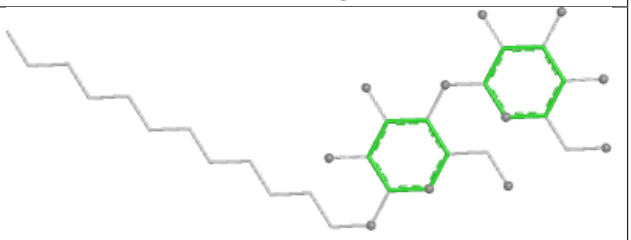
Bond lengths



Bond angles

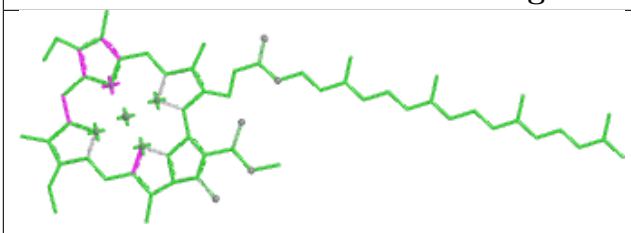


Torsions

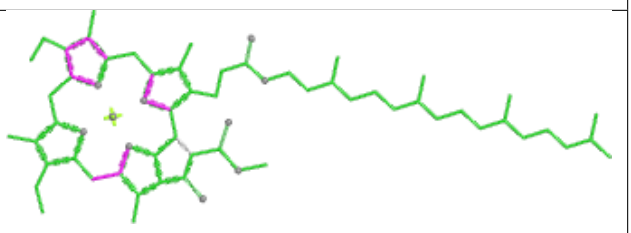


Rings

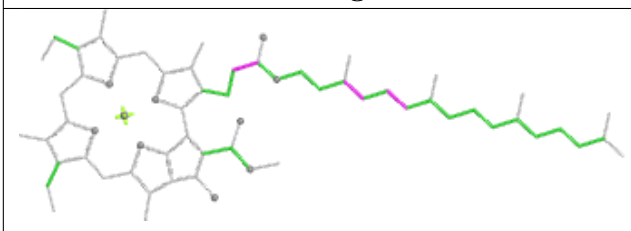
Ligand CL0 G 801



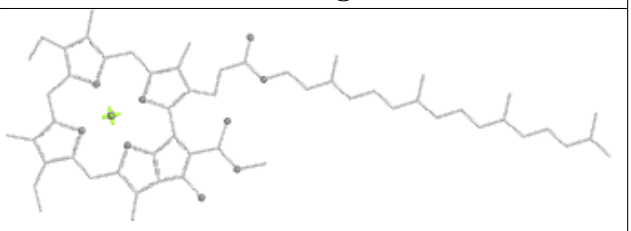
Bond lengths



Bond angles

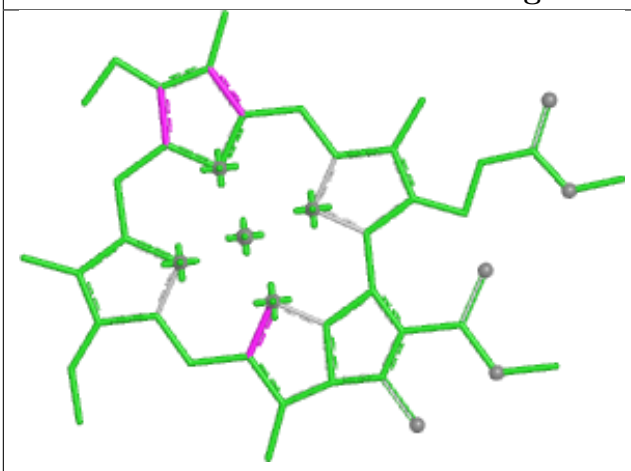


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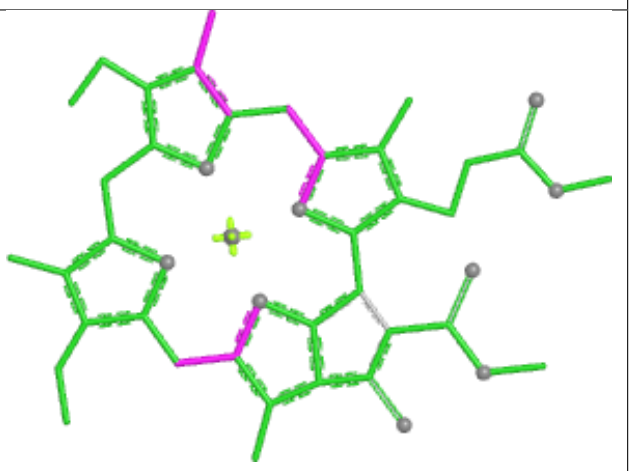


Rings

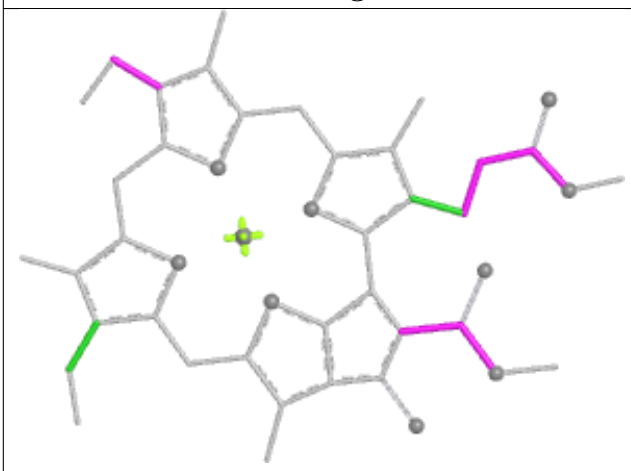
Ligand CLA A 844



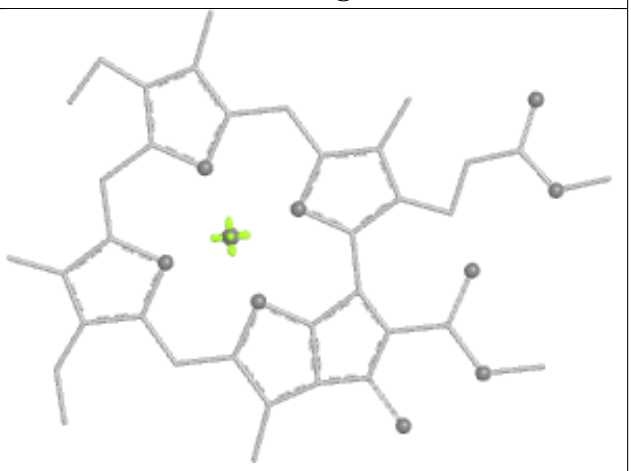
Bond lengths



Bond angles

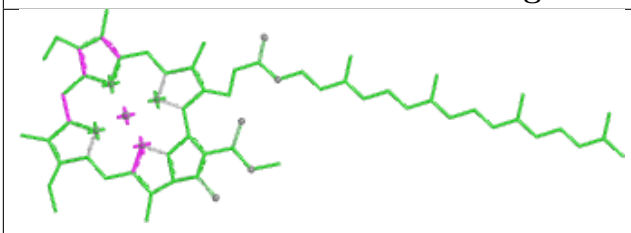


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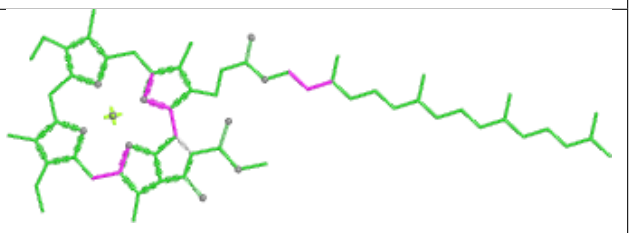


Rings

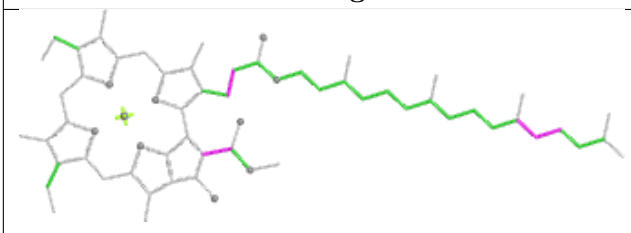
Ligand CLA A 808



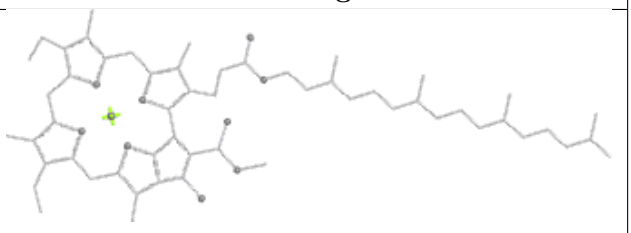
Bond lengths



Bond angles

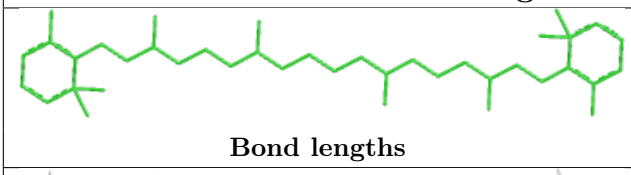


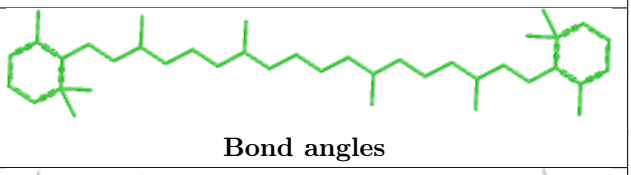
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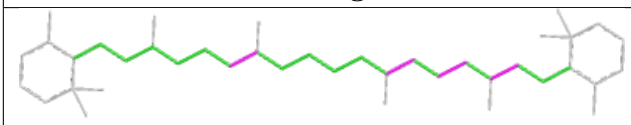


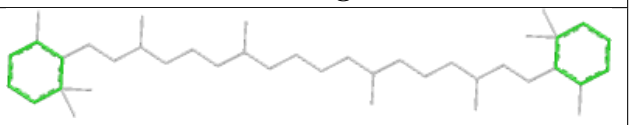
Rings

Ligand BCR S 1105


Bond lengths


Bond angles

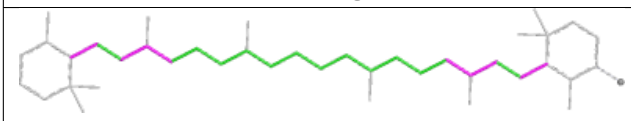

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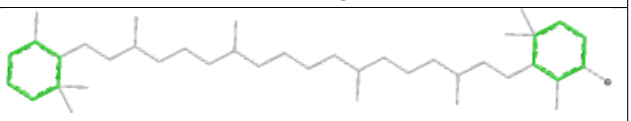

Rings

Ligand ECH B 847

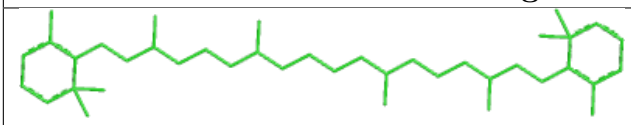

Bond lengths

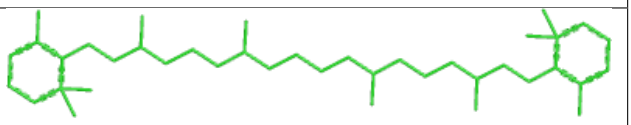

Bond angles

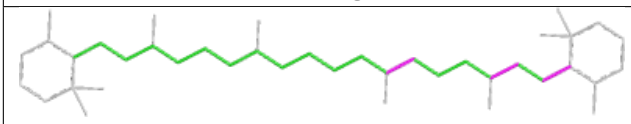

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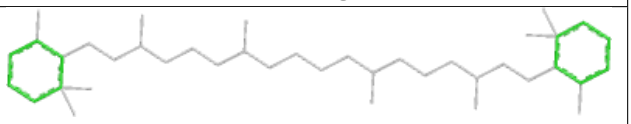

Rings

Ligand BCR H 844

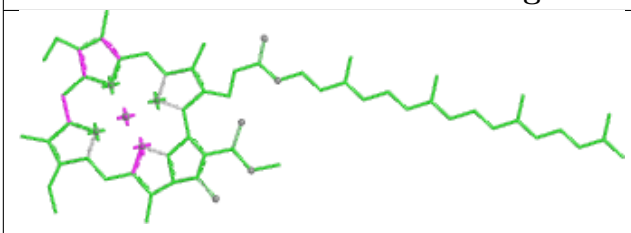

Bond lengths

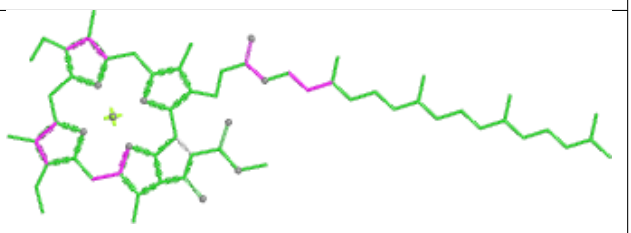

Bond angles

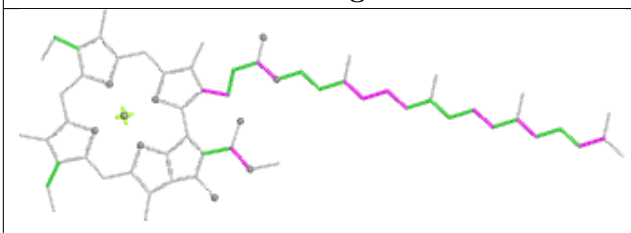

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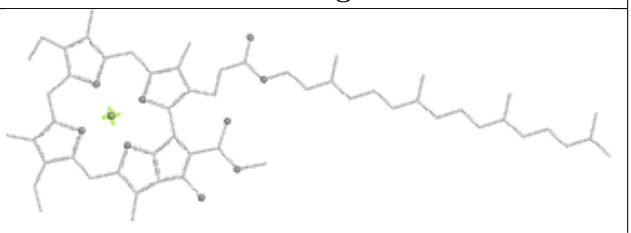

Rings

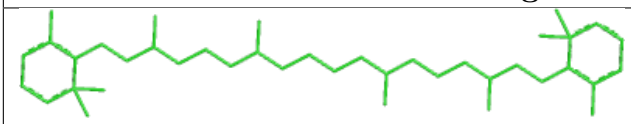
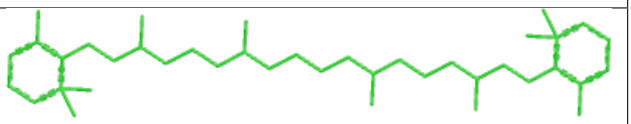
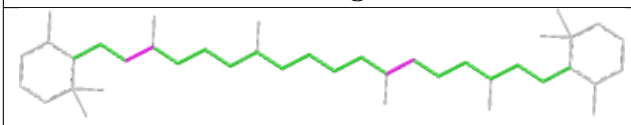
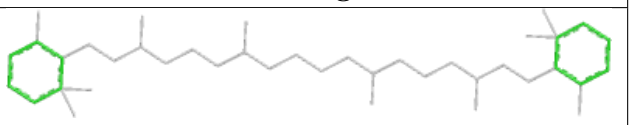
Ligand CLA H 817

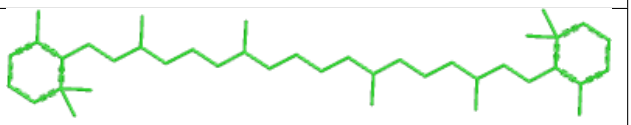
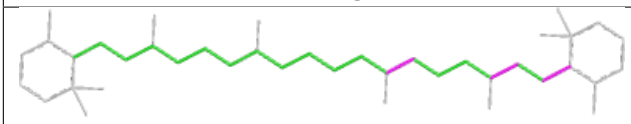
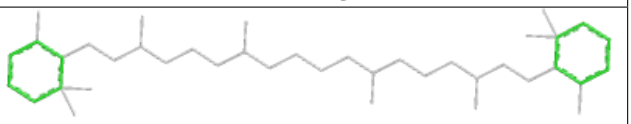

Bond lengths

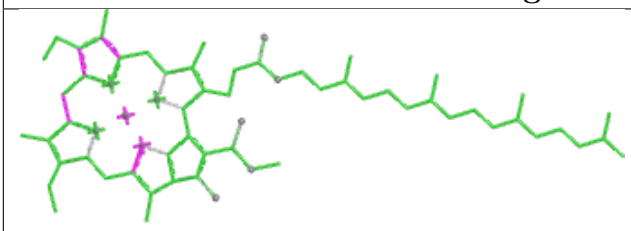
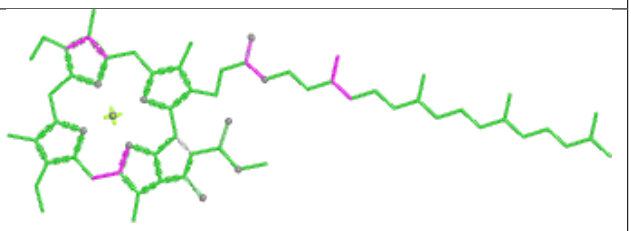
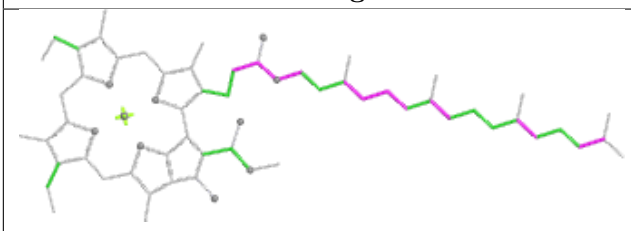
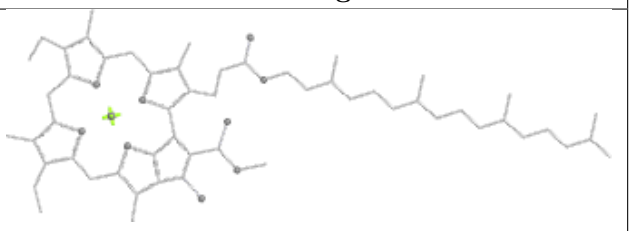

Bond angles


Torsions

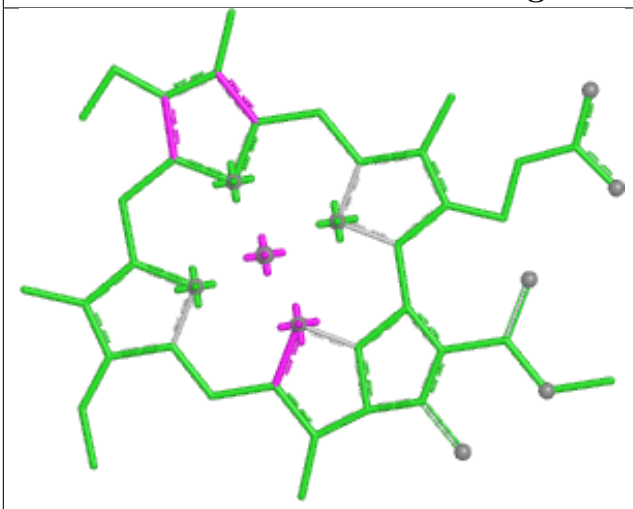

Rings

Ligand BCR H 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

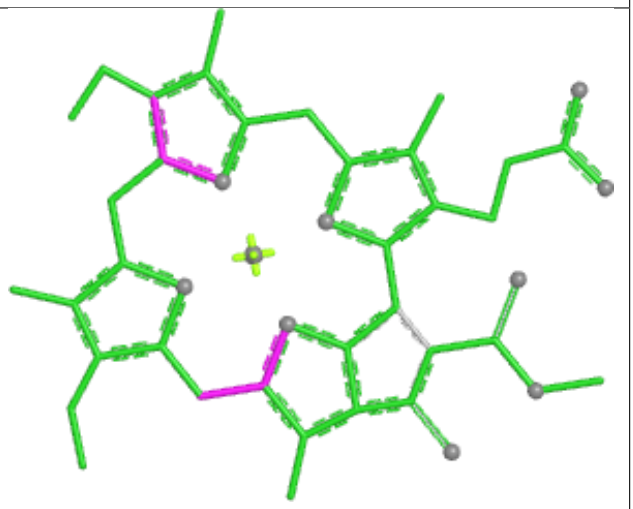
Ligand BCR a 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA l 5006	
 Bond lengths	 Bond angles
 Torsions	 Rings

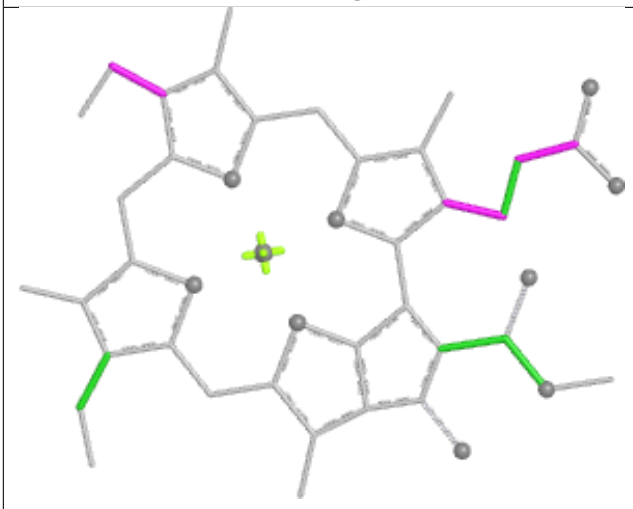
Ligand CLA b 825



Bond lengths



Bond angles

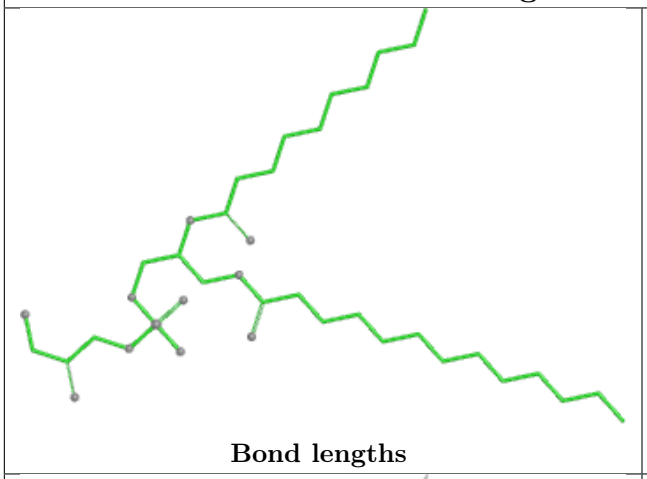


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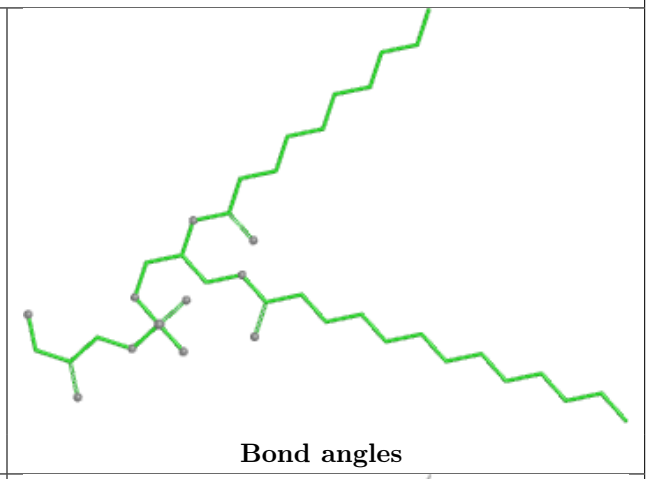


Rings

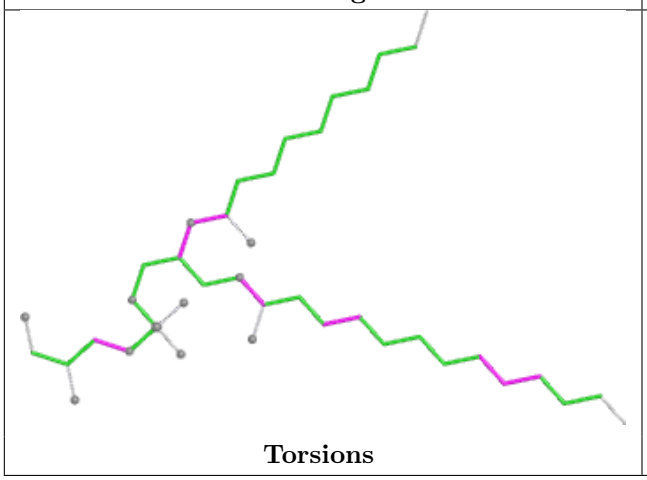
Ligand LHG M 102



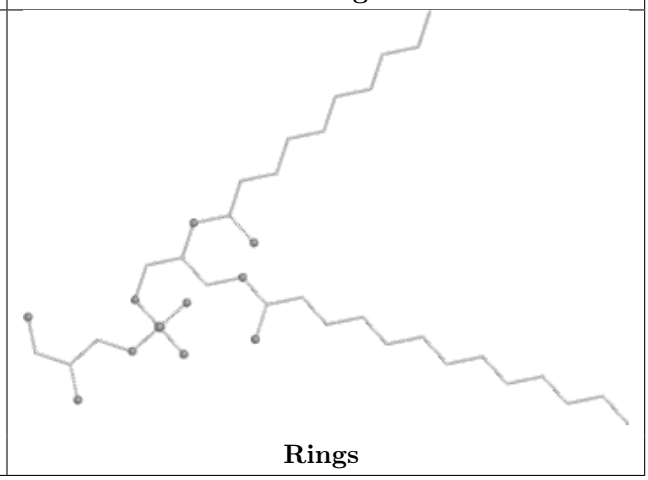
Bond lengths



Bond angles

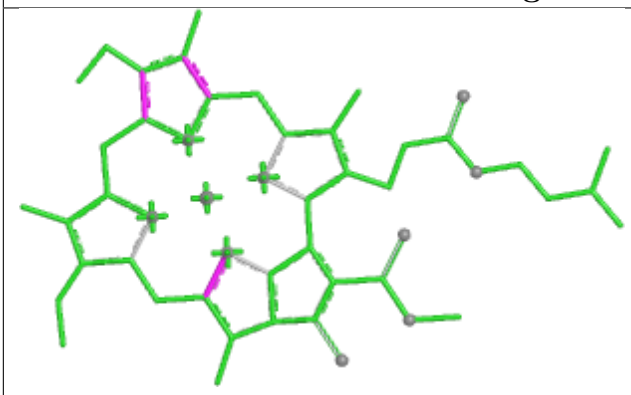


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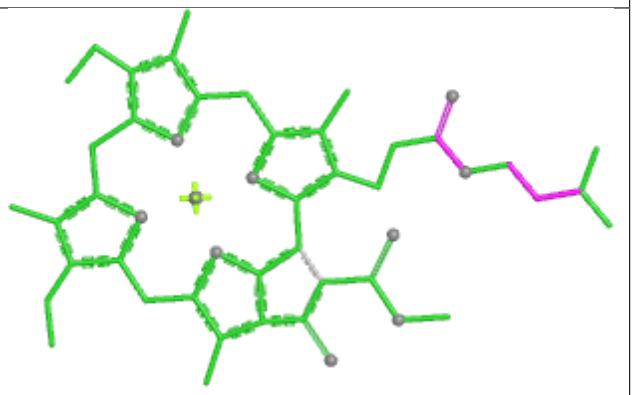


Rings

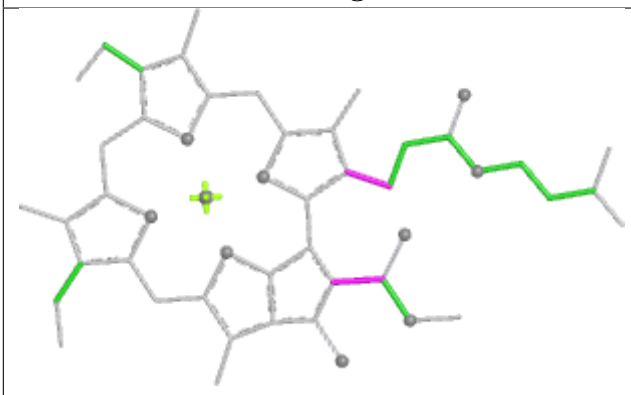
Ligand CLA G 823



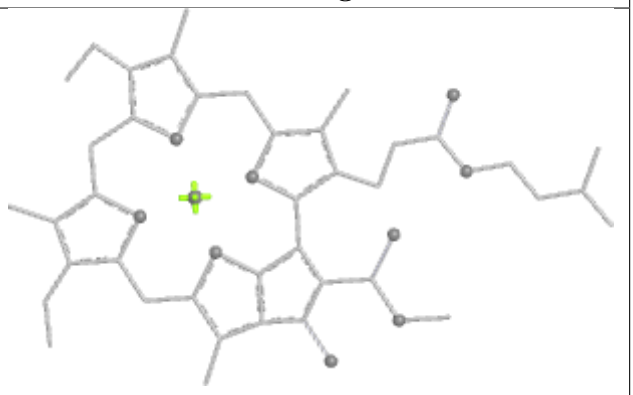
Bond lengths



Bond angles

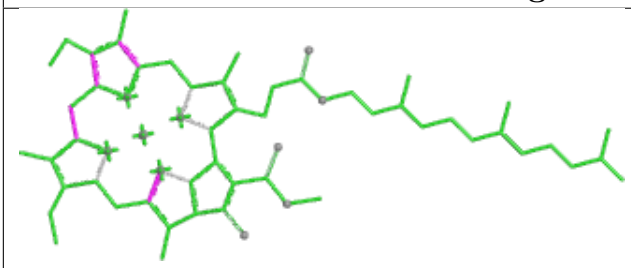


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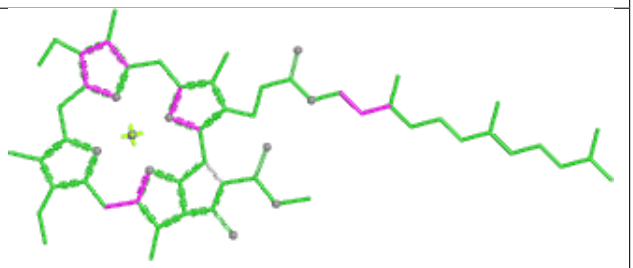


Rings

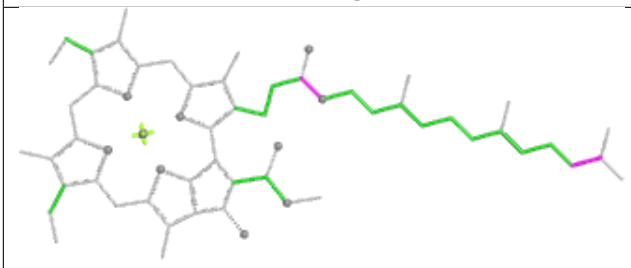
Ligand CLA a 833



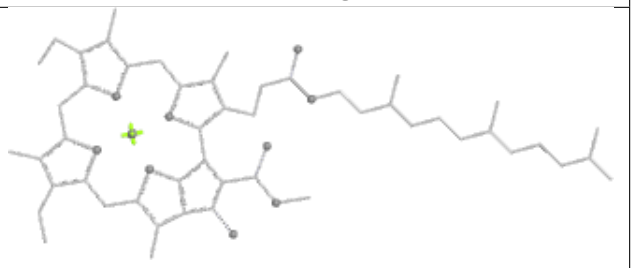
Bond lengths



Bond angles

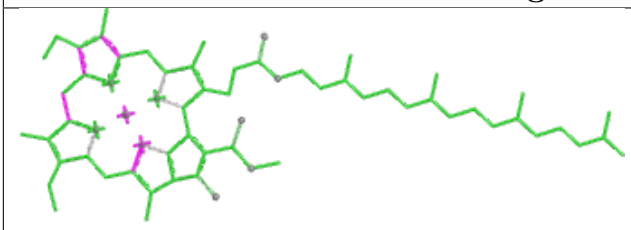


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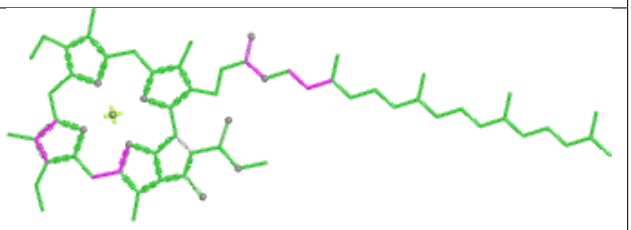


Rings

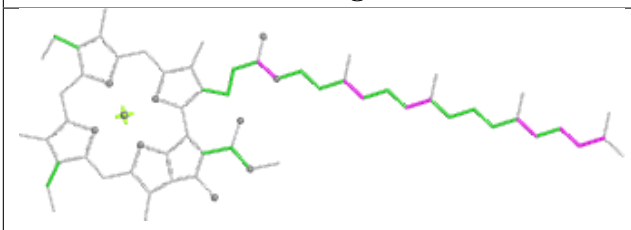
Ligand CLA b 817



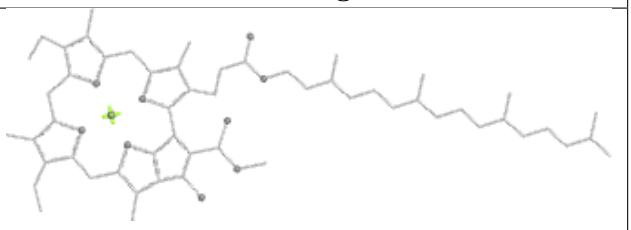
Bond lengths



Bond angles

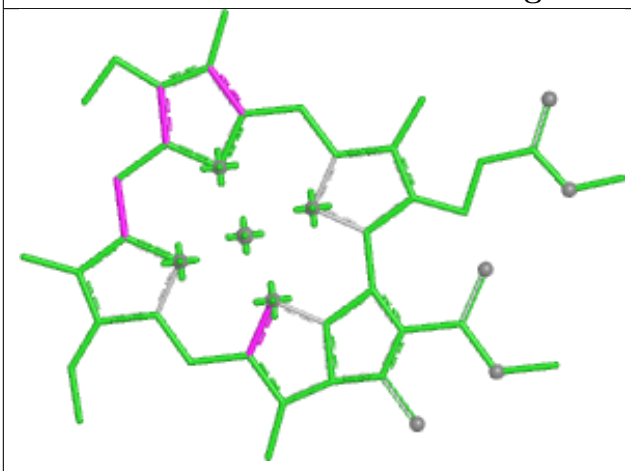


Torsions

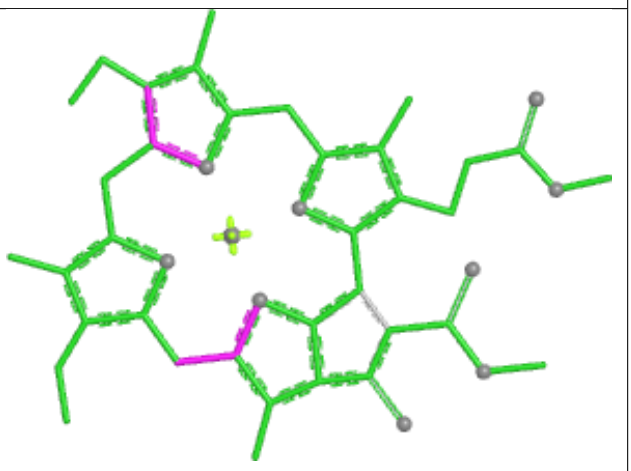


Rings

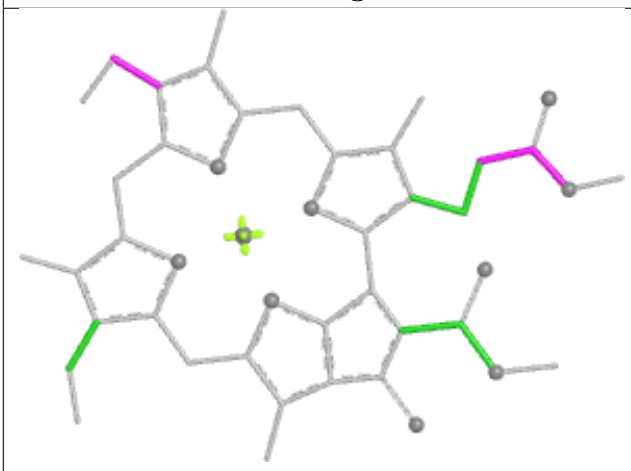
Ligand CLA B 837



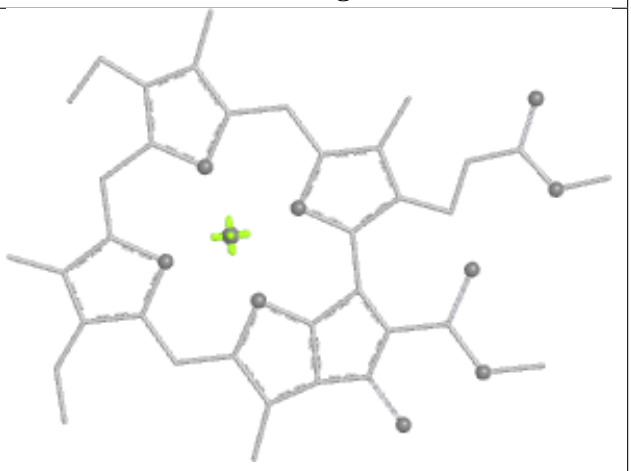
Bond lengths



Bond angles

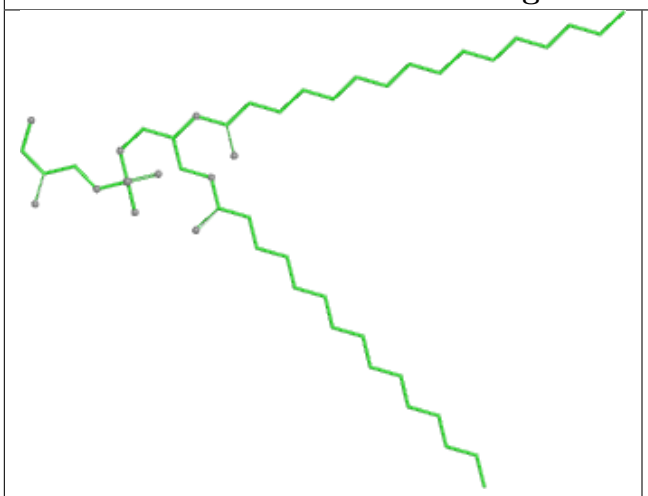


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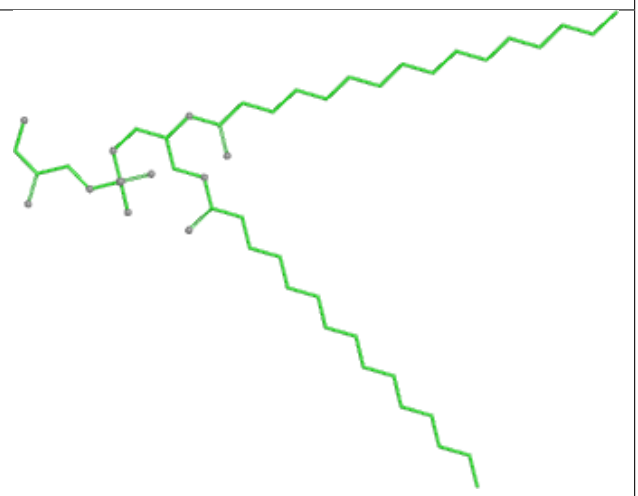


Rings

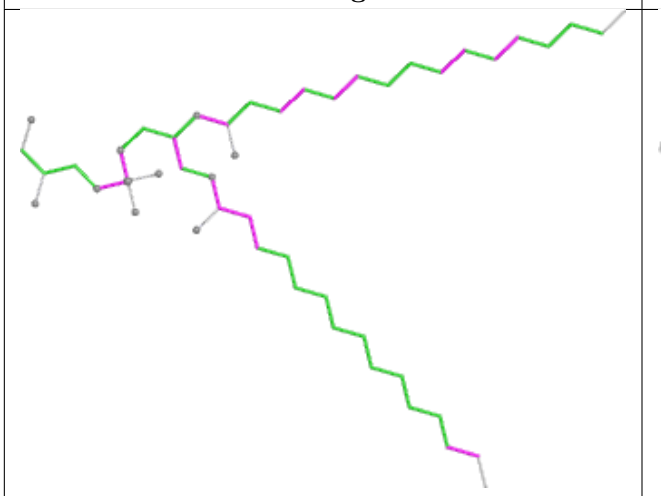
Ligand LHG G 854



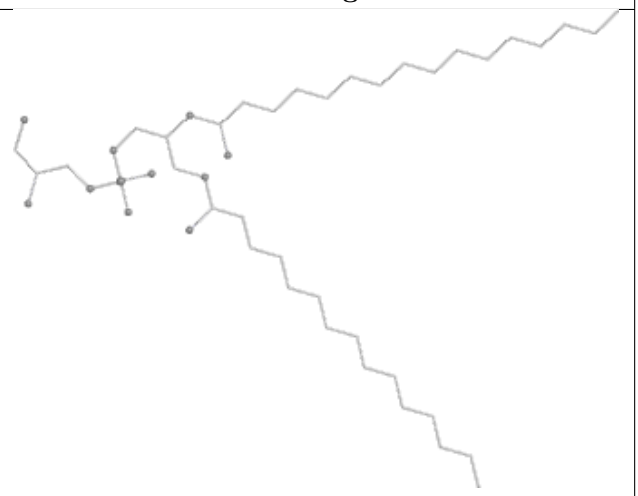
Bond lengths



Bond angles

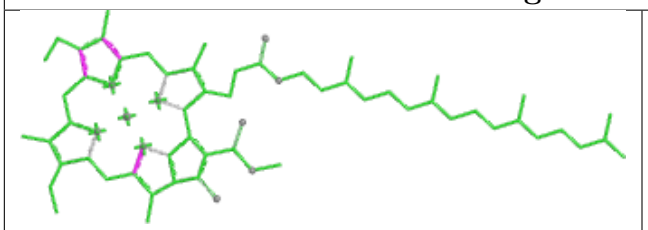


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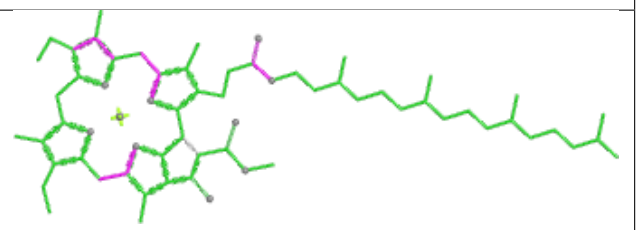


Rings

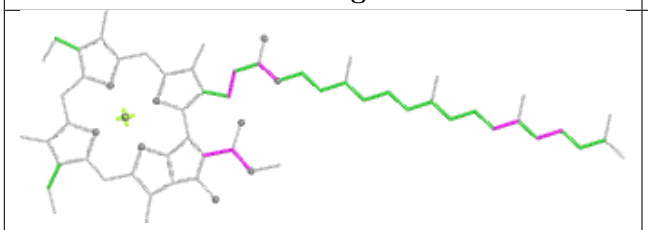
Ligand CLA G 802



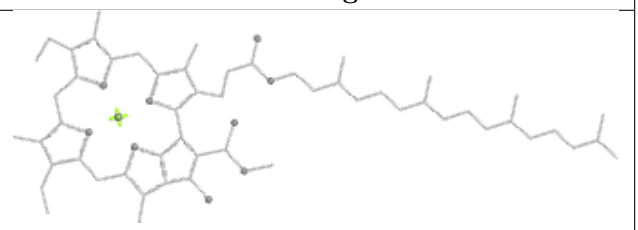
Bond lengths



Bond angles

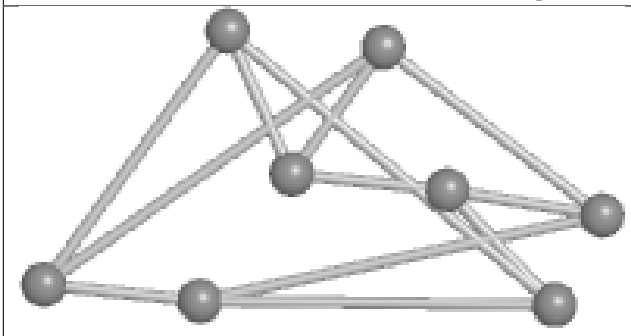


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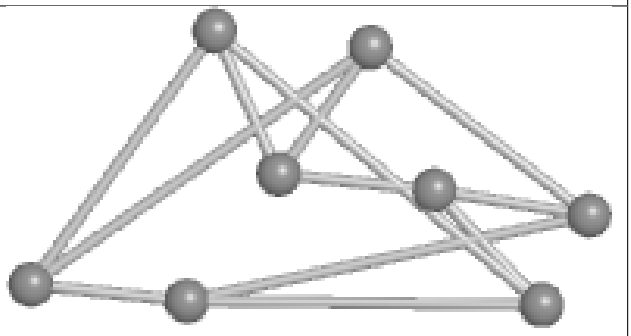


Rings

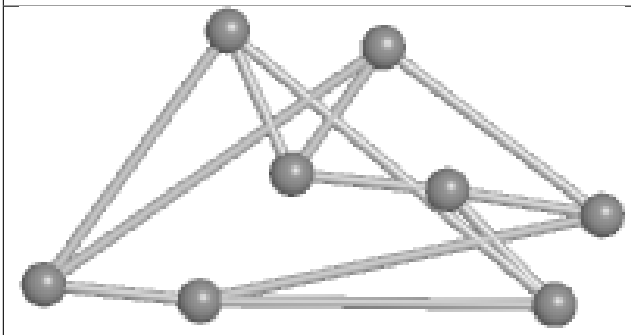
Ligand SF4 G 846



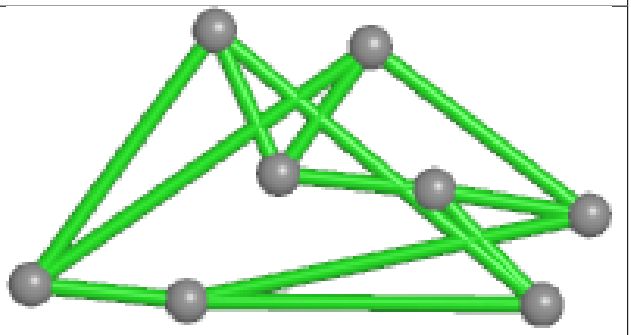
Bond lengths



Bond angles

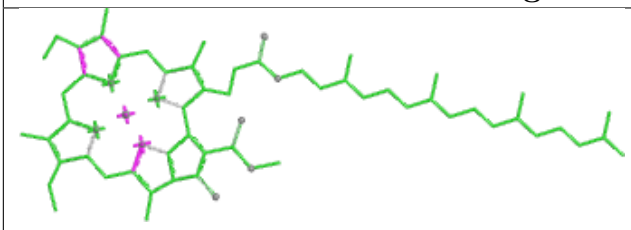


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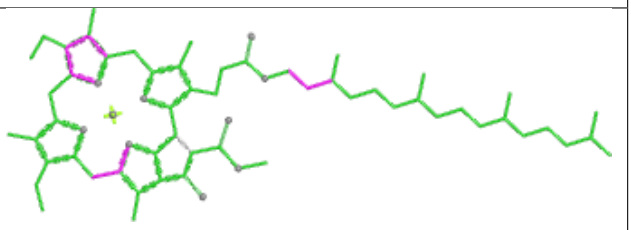


Rings

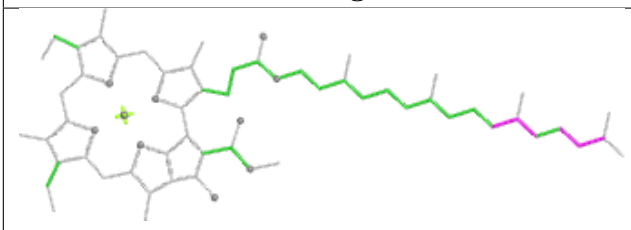
Ligand CLA H 827



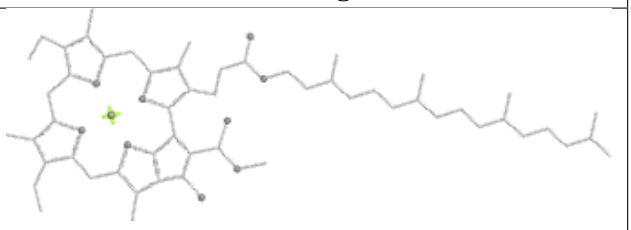
Bond lengths



Bond angles

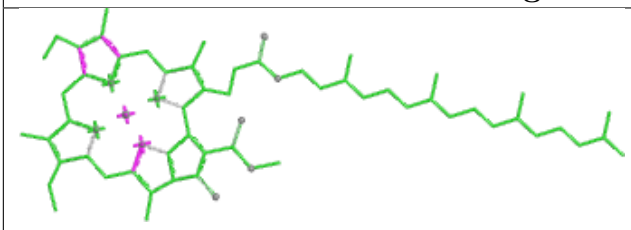


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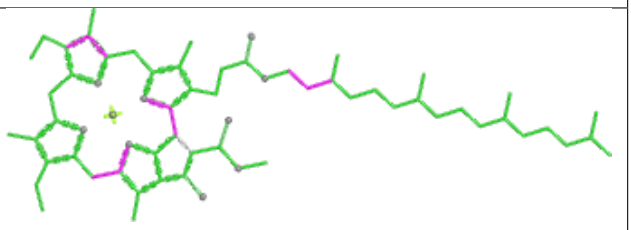


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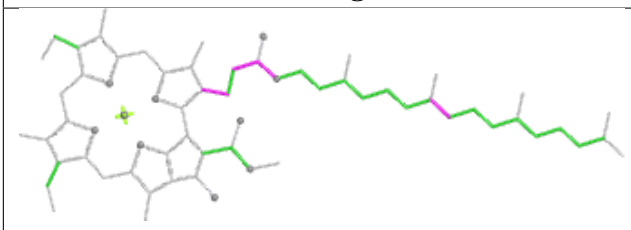
Ligand CLA H 813



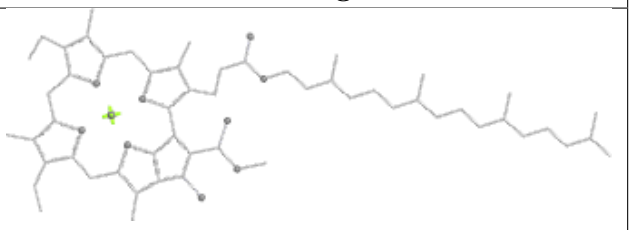
Bond lengths



Bond angles

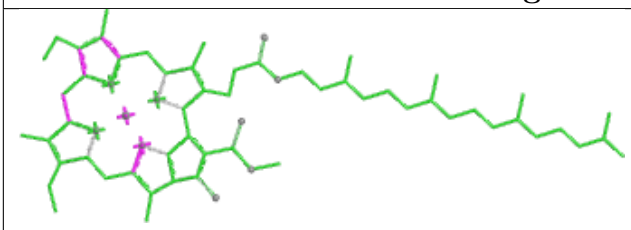


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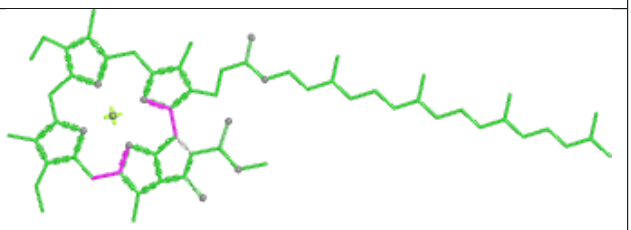


Rings

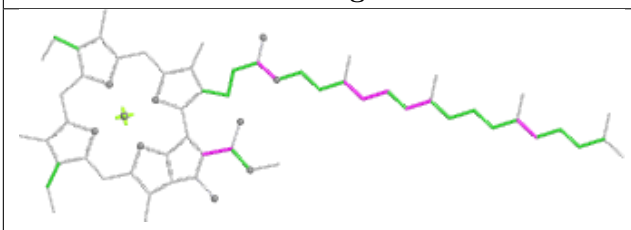
Ligand CLA H 826



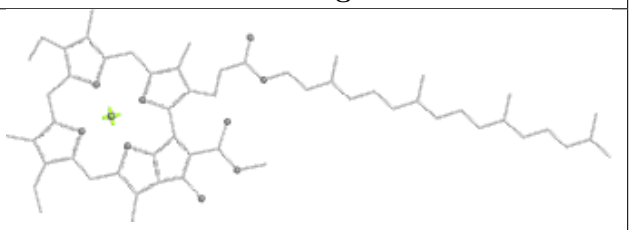
Bond lengths



Bond angles



Torsions



Rings

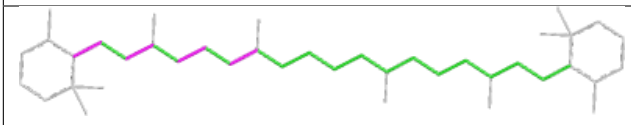
Ligand BCR S 1104



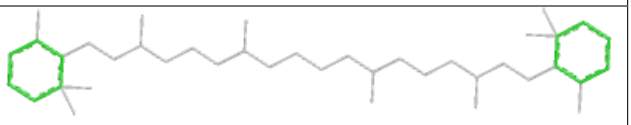
Bond lengths



Bond angles

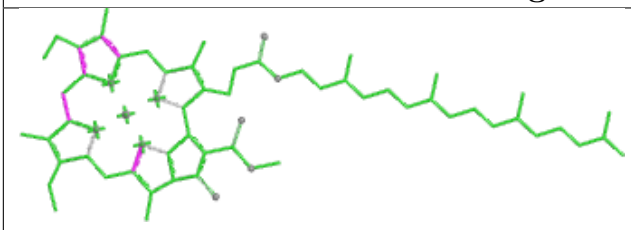


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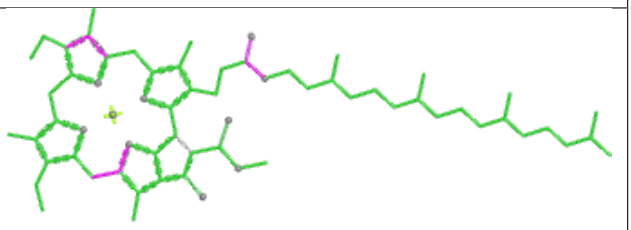


Rings

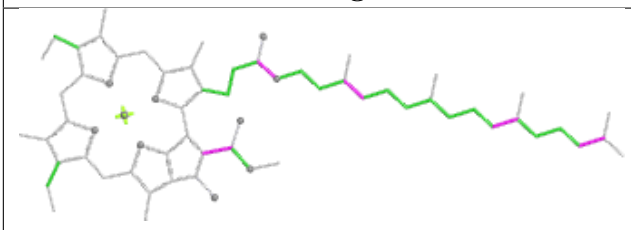
Ligand CLA a 828



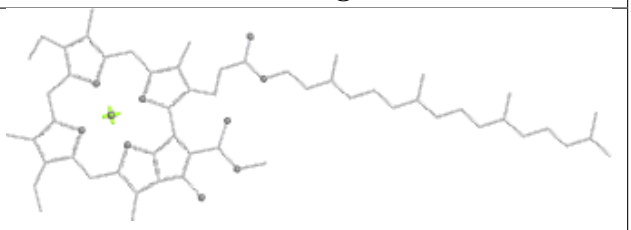
Bond lengths



Bond angles

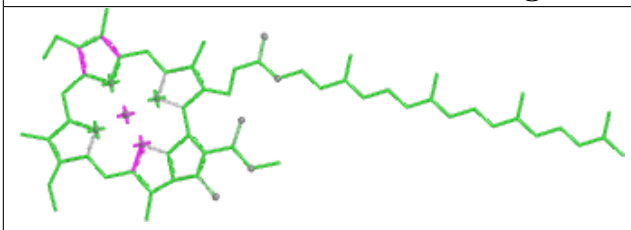


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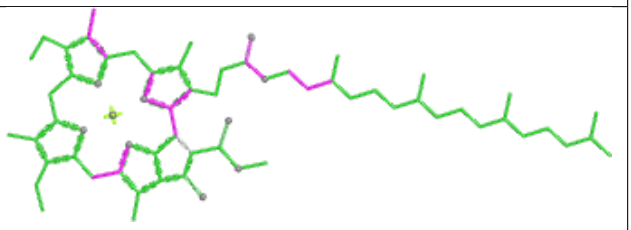


Rings

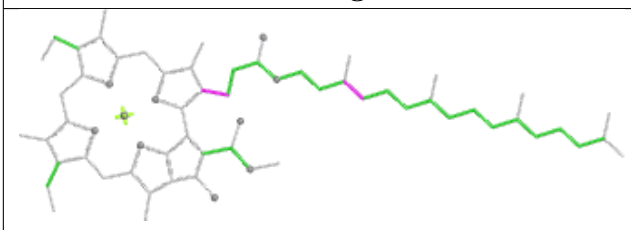
Ligand CLA H 808



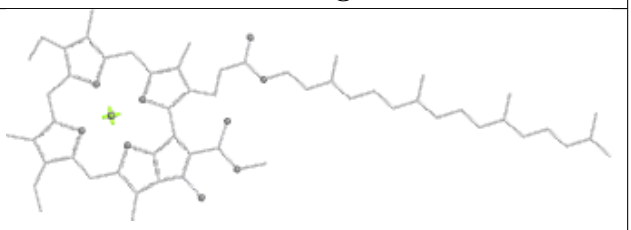
Bond lengths



Bond angles

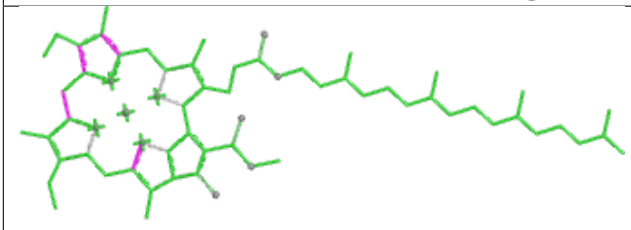


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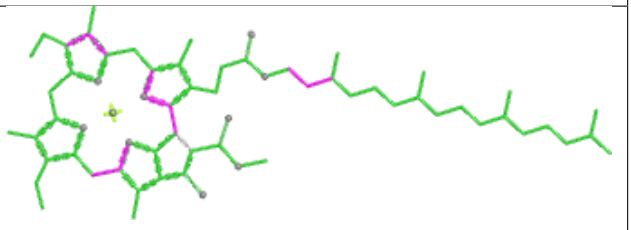


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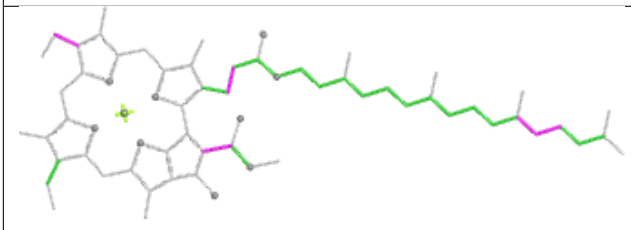
Ligand CLA G 809



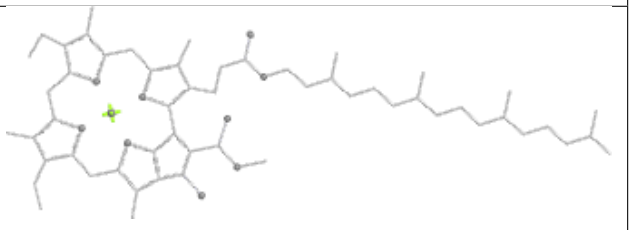
Bond lengths



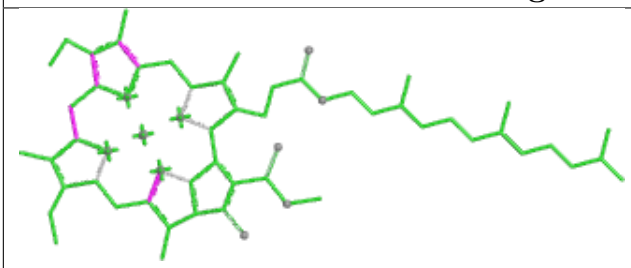
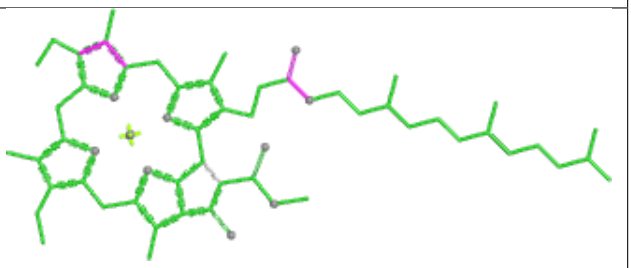
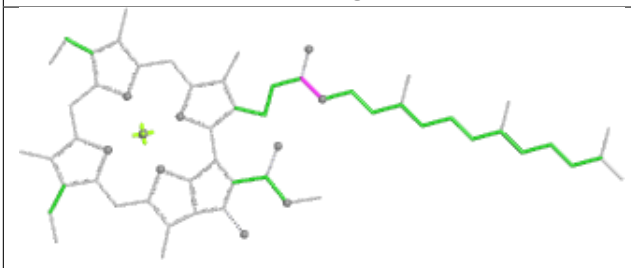
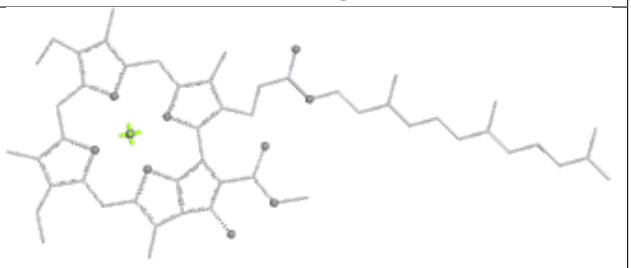
Bond angles

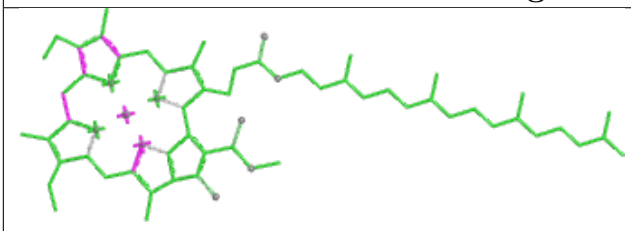
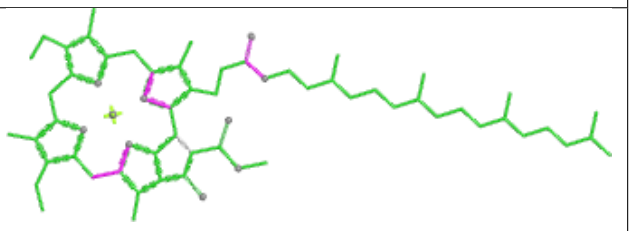
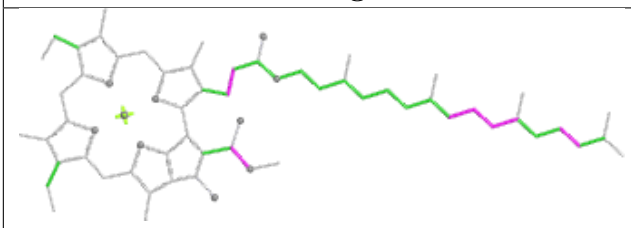
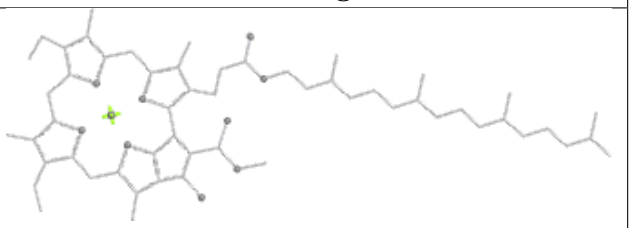


Torsions

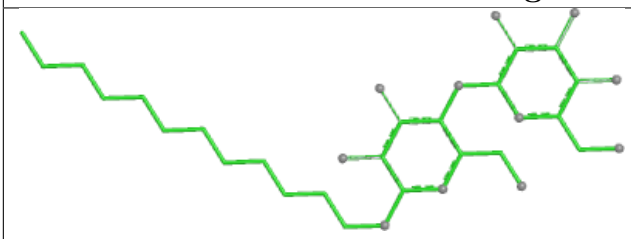


Rings

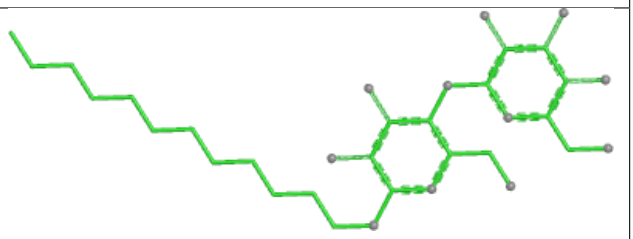
Ligand CLA a 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

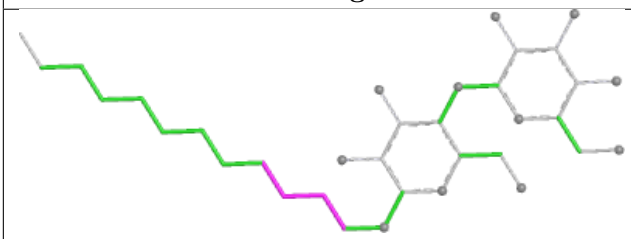
Ligand LMT b 855



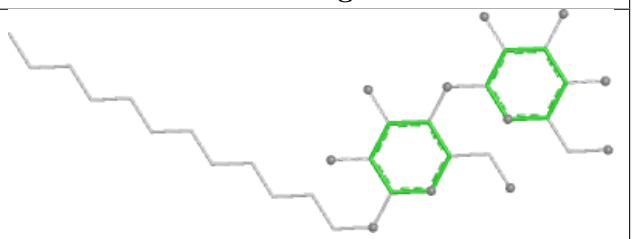
Bond lengths



Bond angles

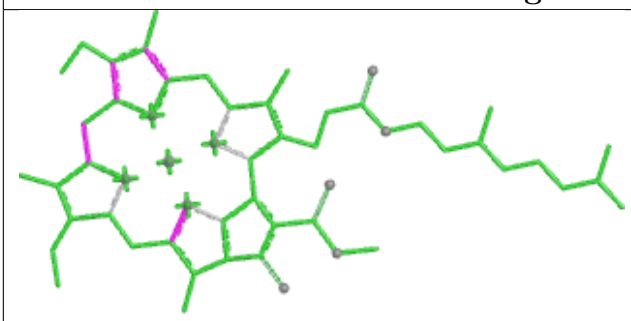


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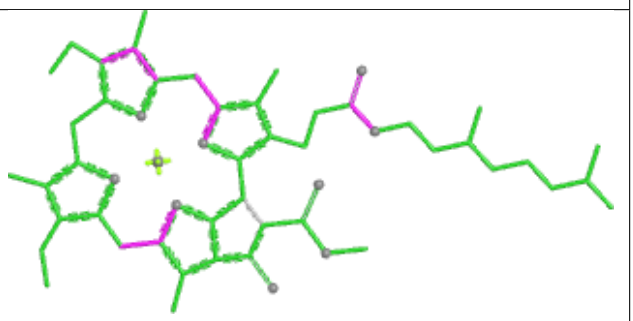


Rings

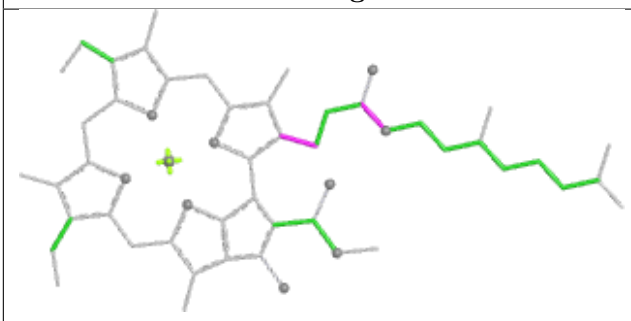
Ligand CLA B 833



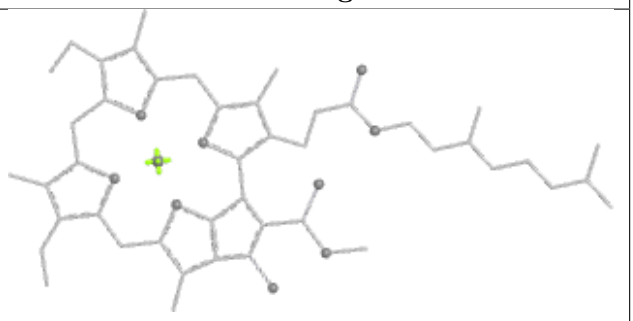
Bond lengths



Bond angles

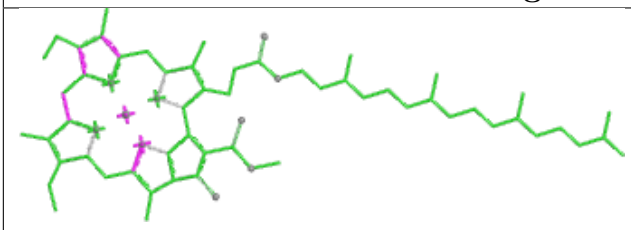


Torsions

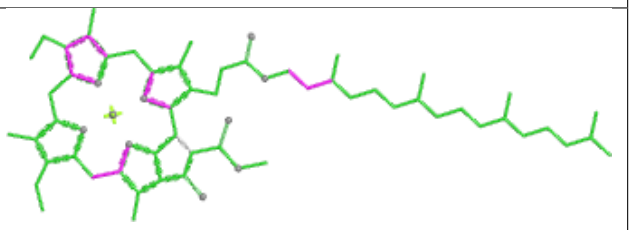


Rings

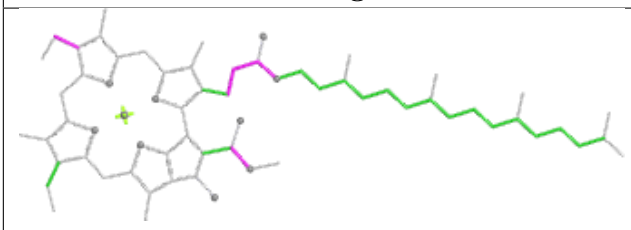
Ligand CLA A 842



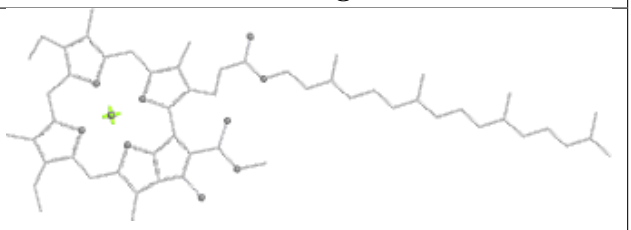
Bond lengths



Bond angles

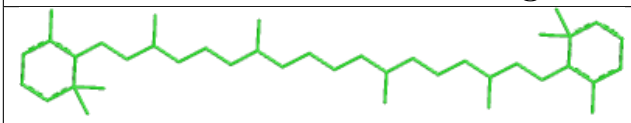


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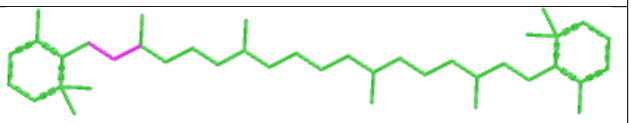


Rings

Ligand BCR U 203



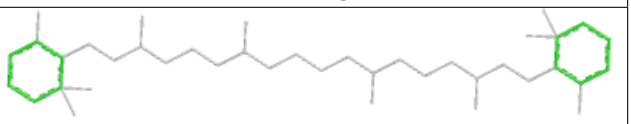
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Bond angles

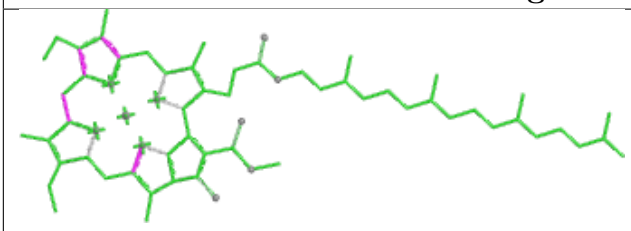


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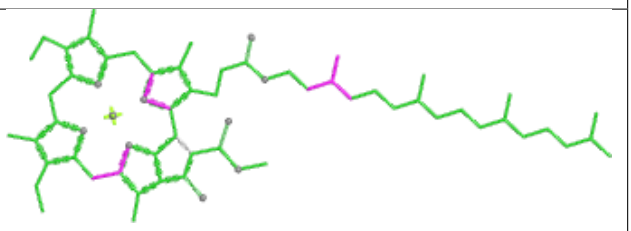


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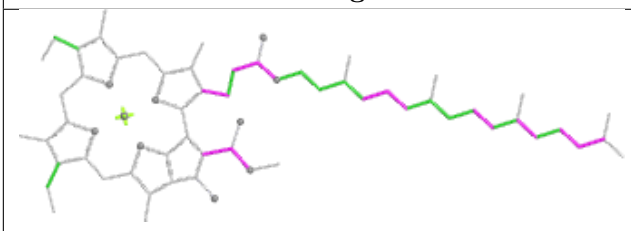
Ligand CLA b 827



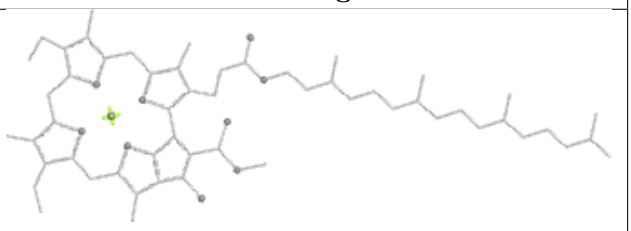
Bond lengths



Bond angles

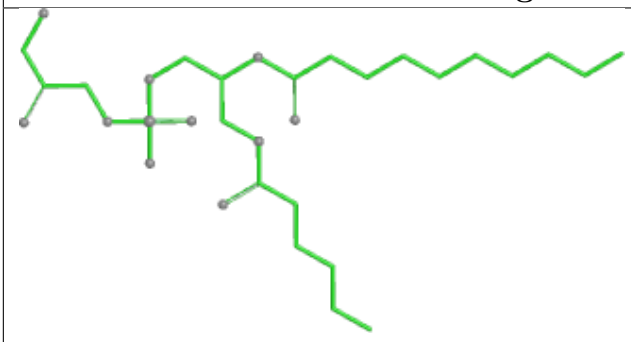


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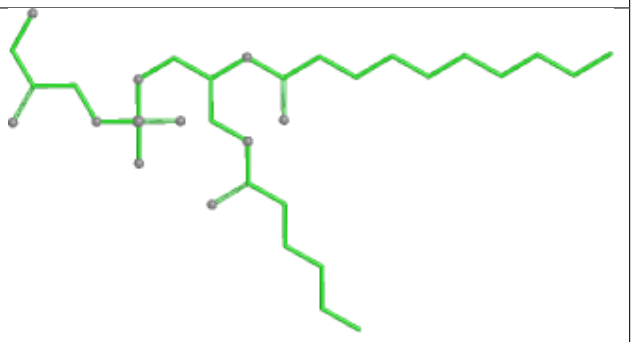


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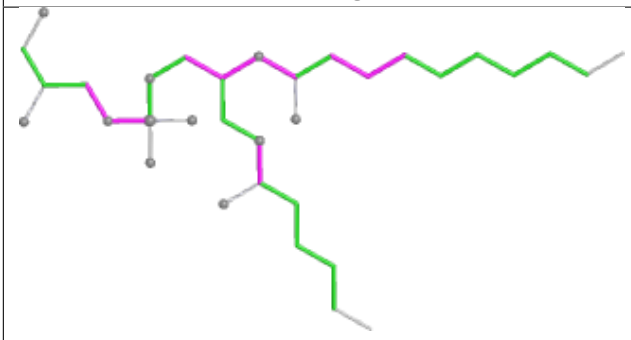
Ligand LHG L 1510



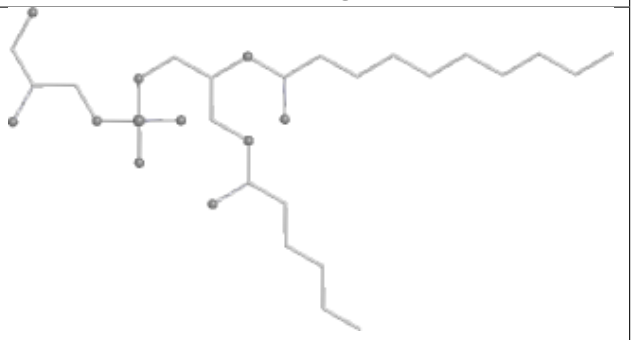
Bond lengths



Bond angles

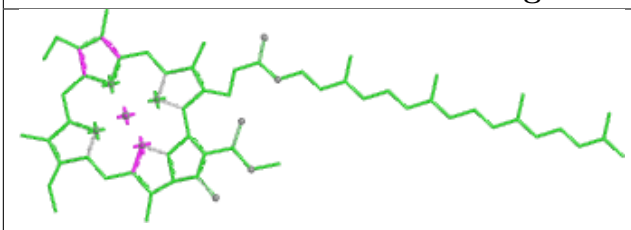


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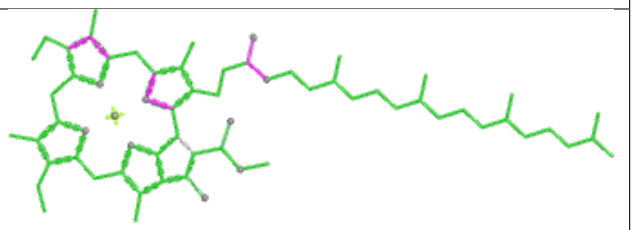


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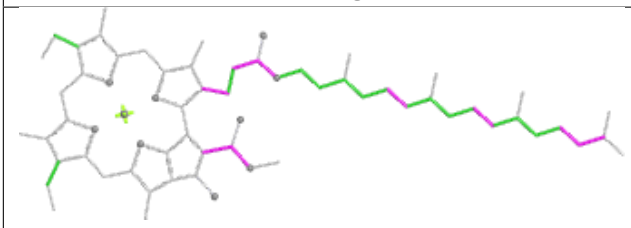
Ligand CLA A 806



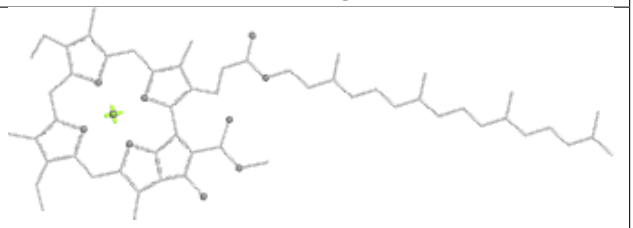
Bond lengths



Bond angles

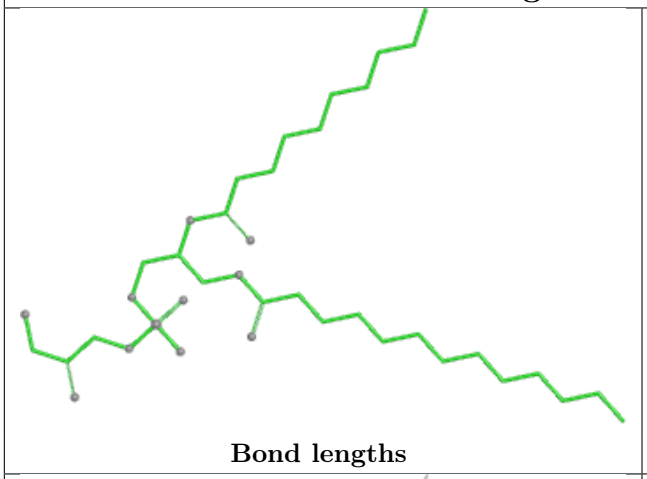


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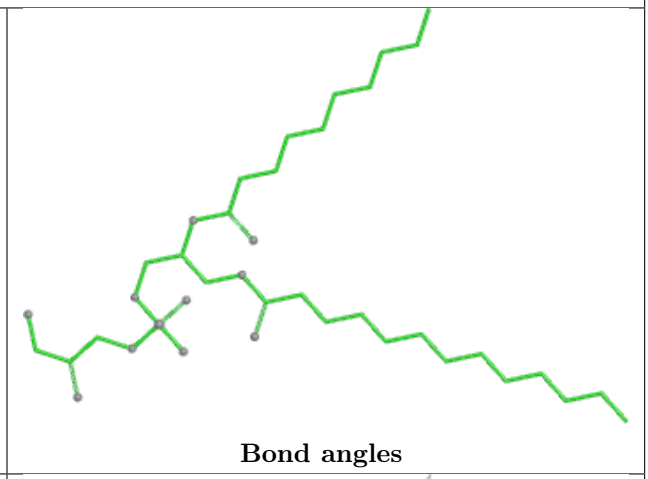


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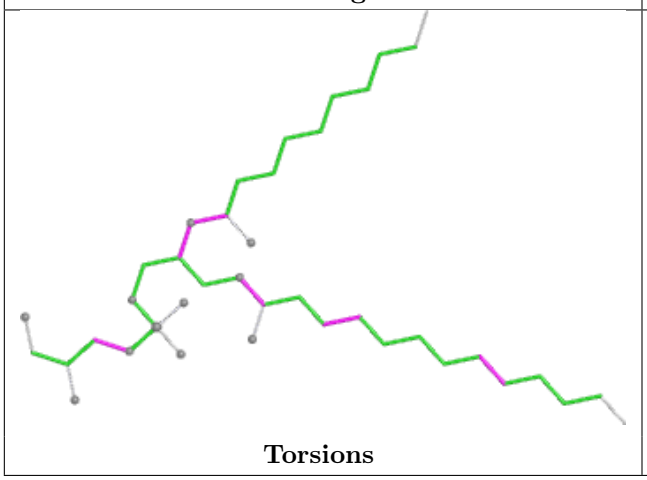
Ligand LHG V 101



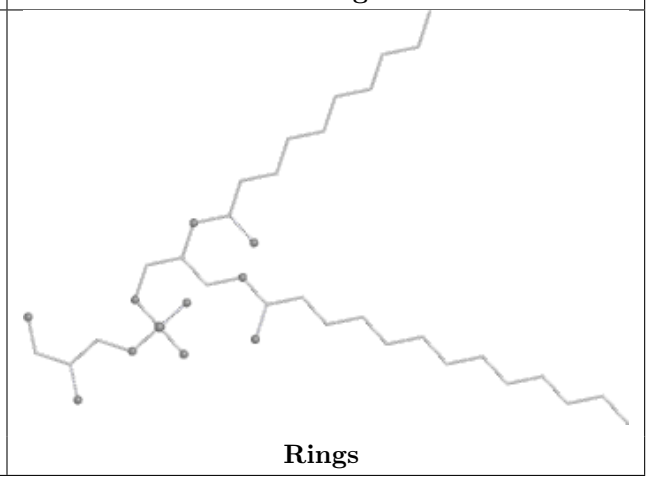
Bond lengths



Bond angles

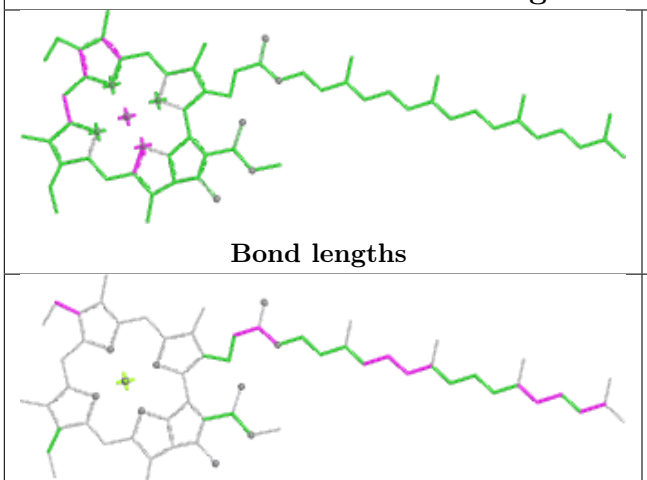


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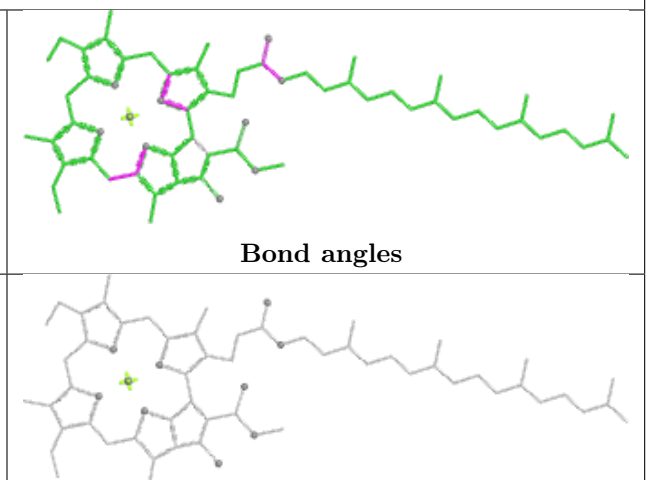


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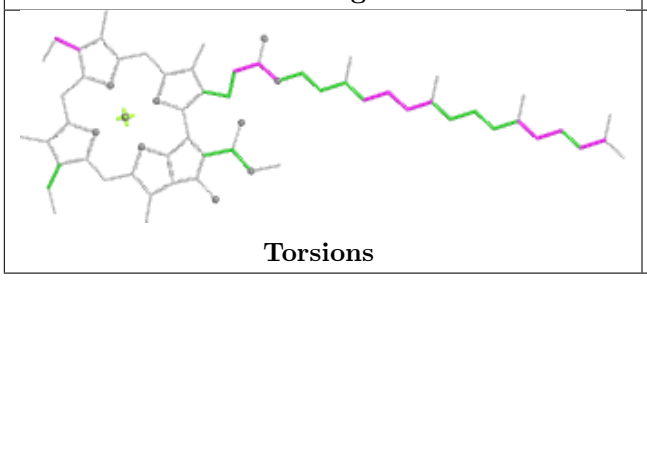
Ligand CLA a 844



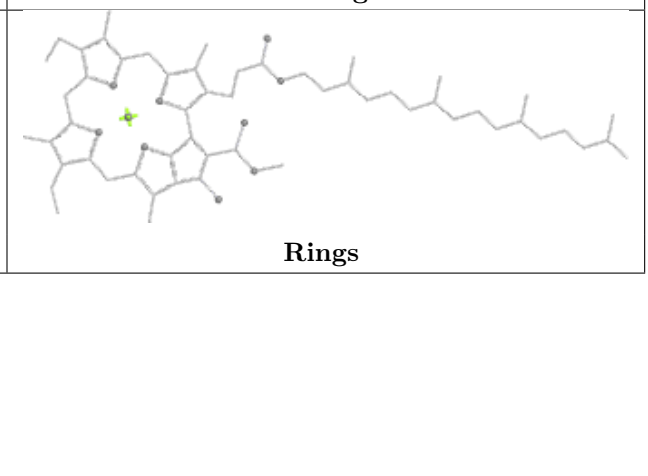
Bond lengths



Bond angles

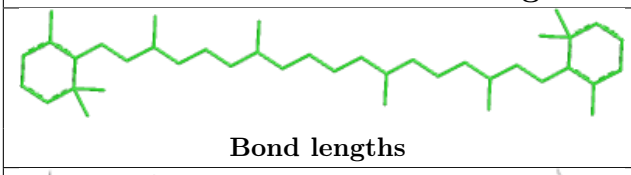


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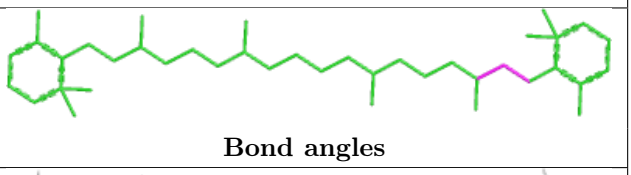


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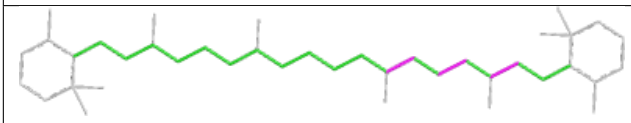
Ligand BCR A 860



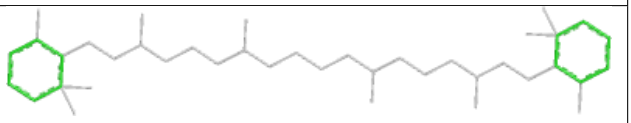
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Bond angles

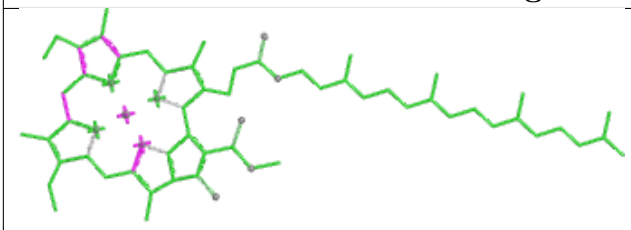


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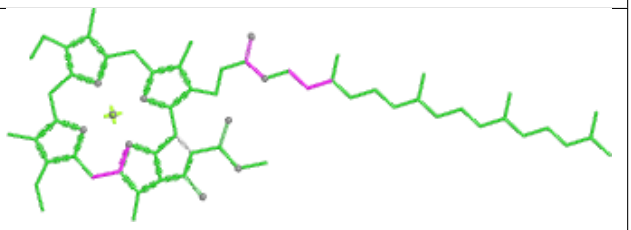


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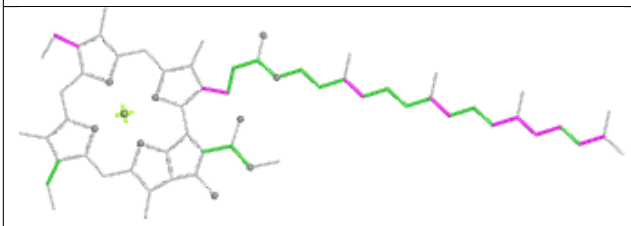
Ligand CLA T 103



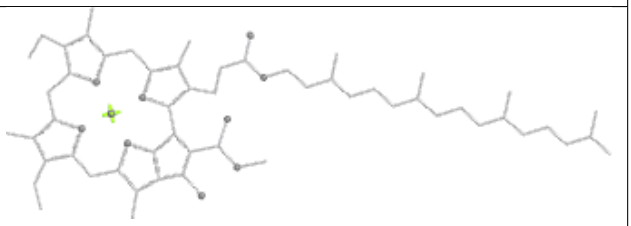
Bond lengths



Bond angles

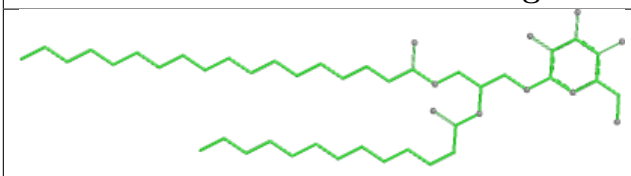


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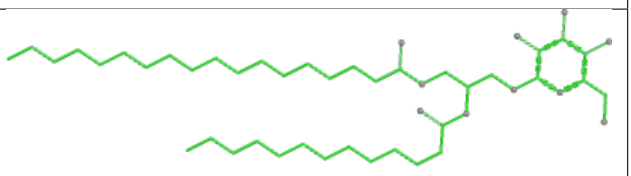


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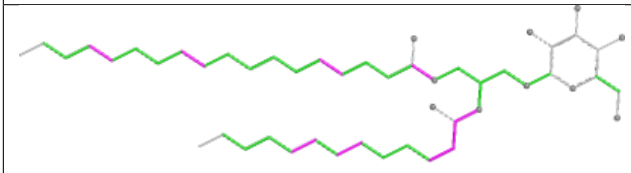
Ligand LMG b 803



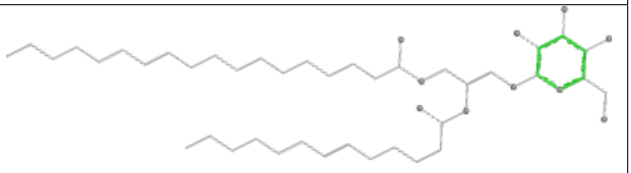
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Bond angles

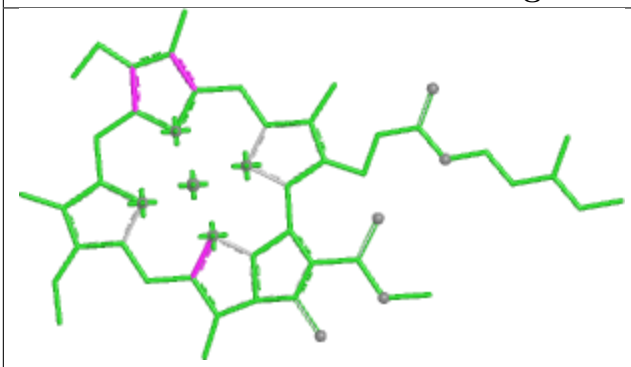


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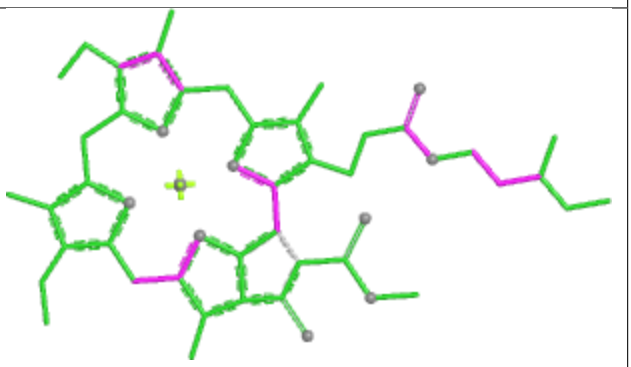


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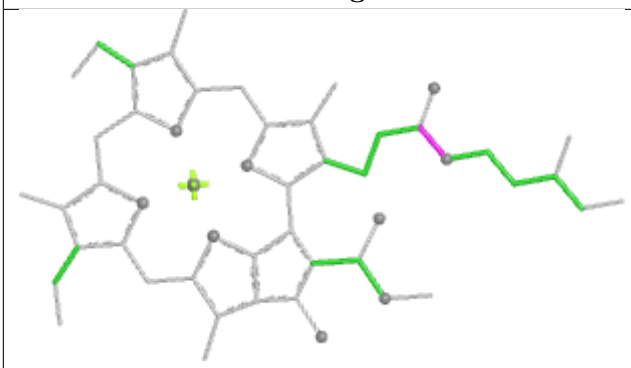
Ligand CLA A 837



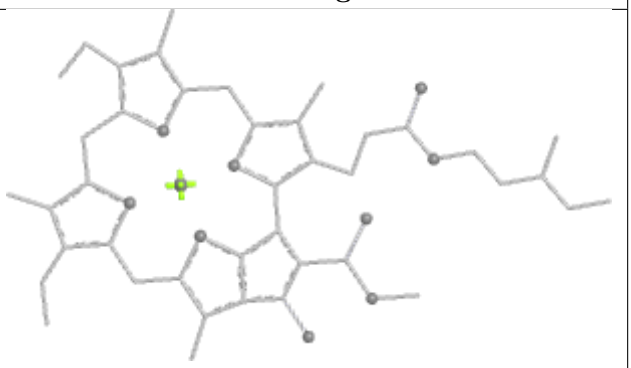
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Bond angles

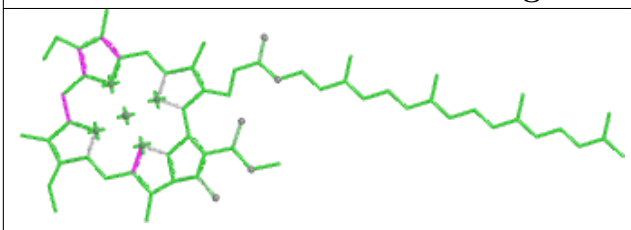


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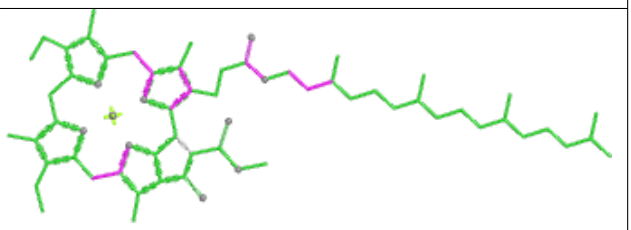


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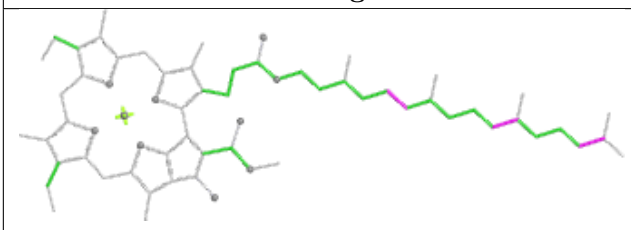
Ligand CLA G 820



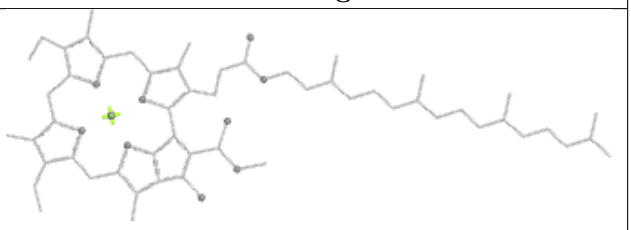
Bond lengths



Bond angles

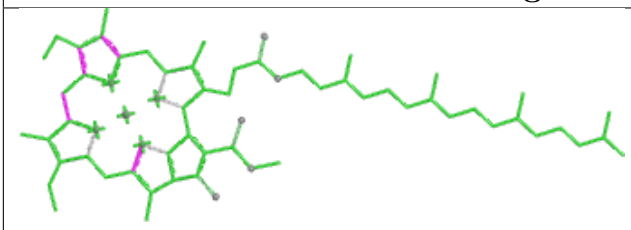


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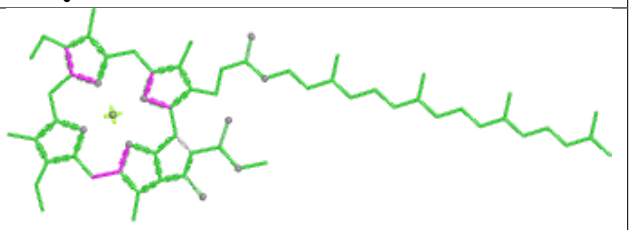


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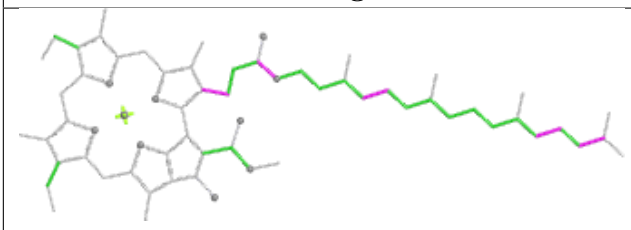
Ligand CLA Q 202



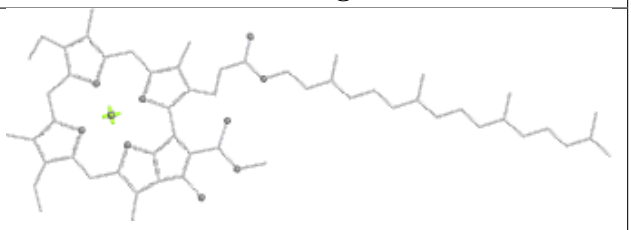
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Bond angles

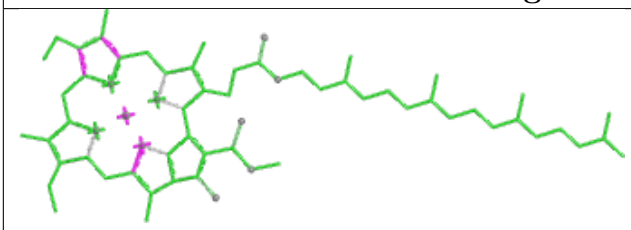


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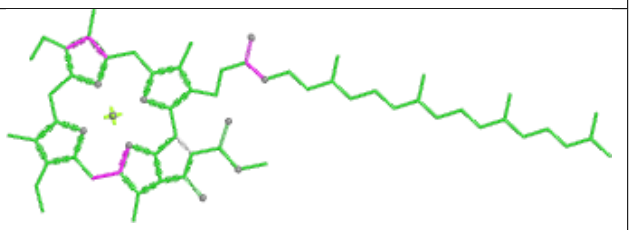


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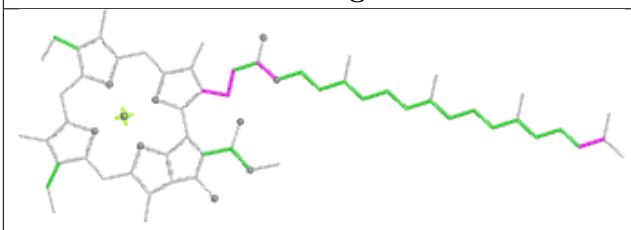
Ligand CLA A 813



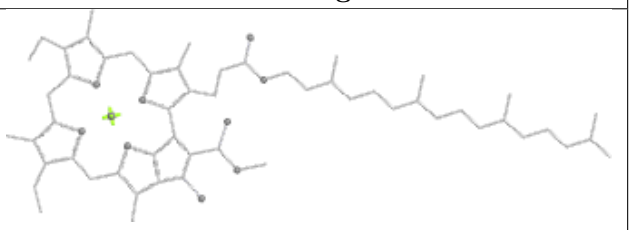
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Bond angles

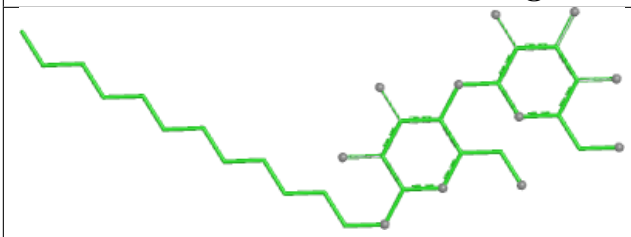


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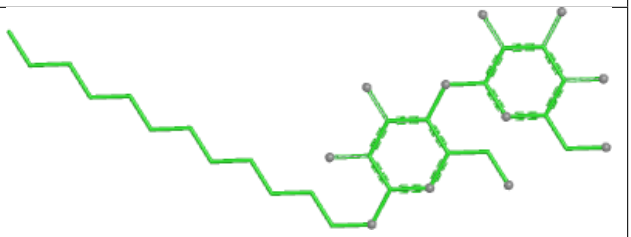


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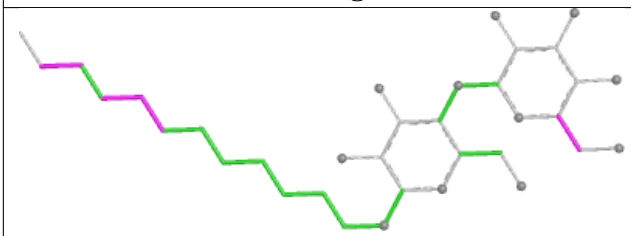
Ligand LMT a 854



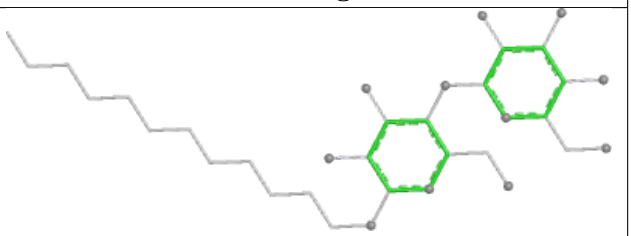
Bond lengths



Bond angles

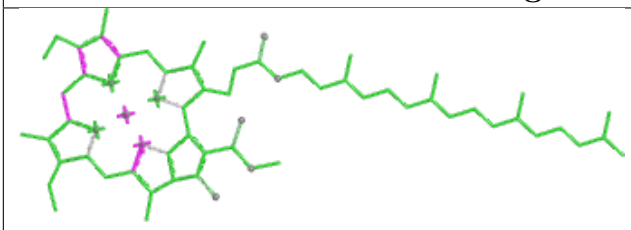


Torsions

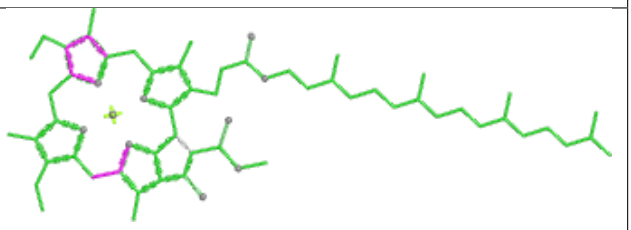


Rings

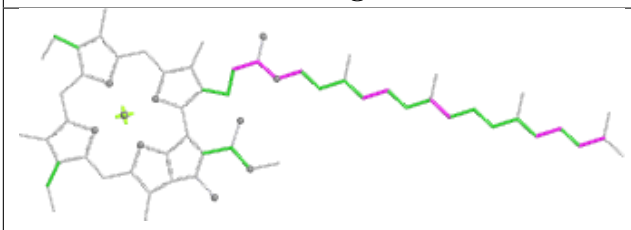
Ligand CLA B 840



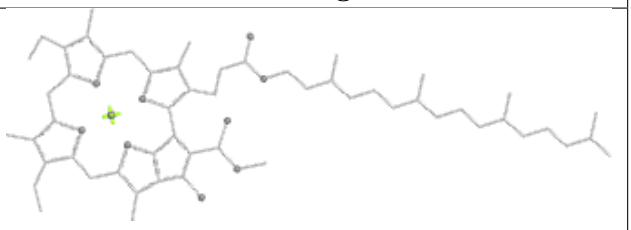
Bond lengths



Bond angles

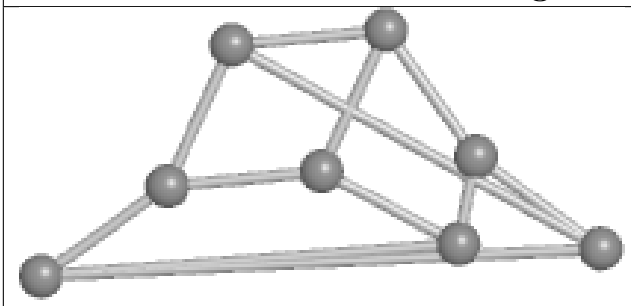


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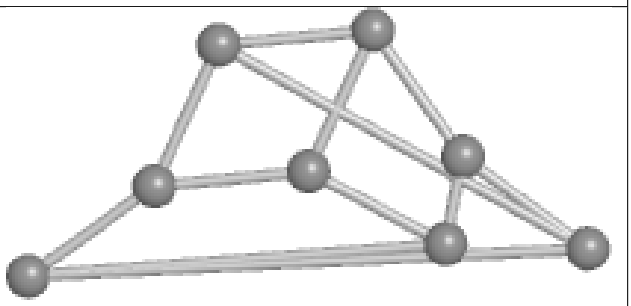


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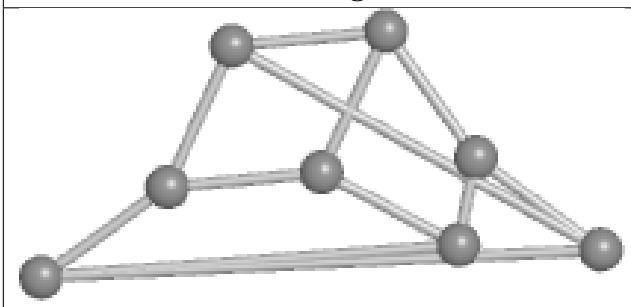
Ligand SF4 C 101



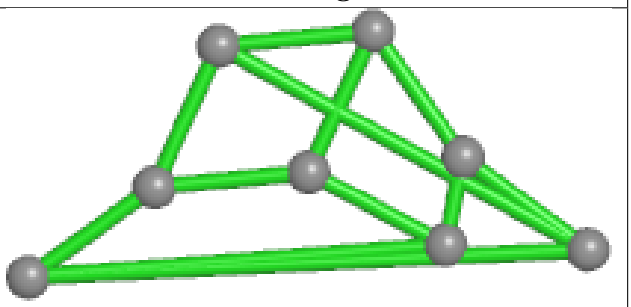
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Bond angles

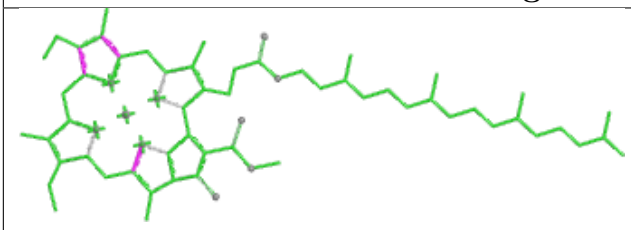


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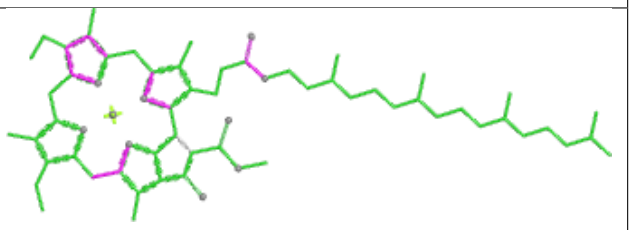


Rings

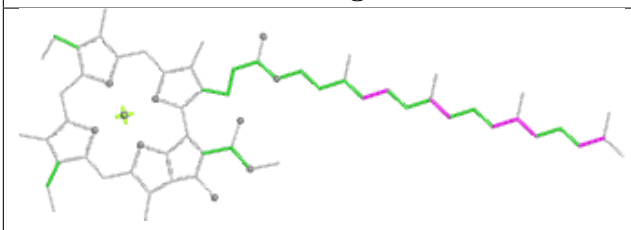
Ligand CLA G 839



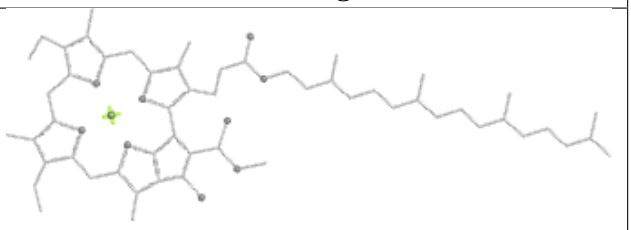
Bond lengths



Bond angles

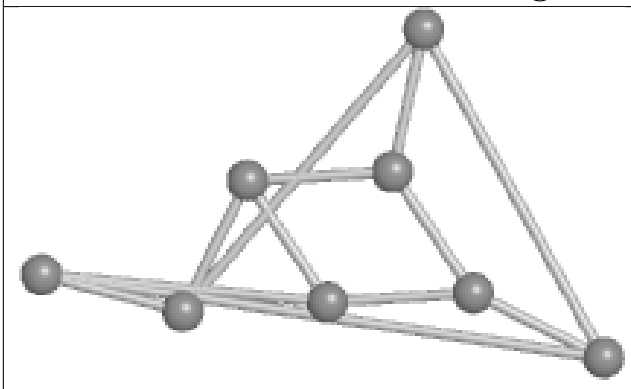


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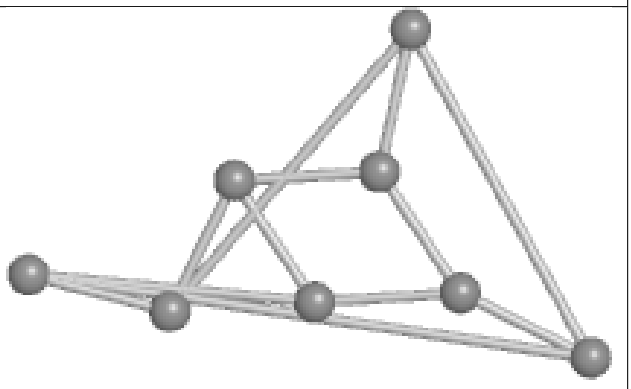


Rings

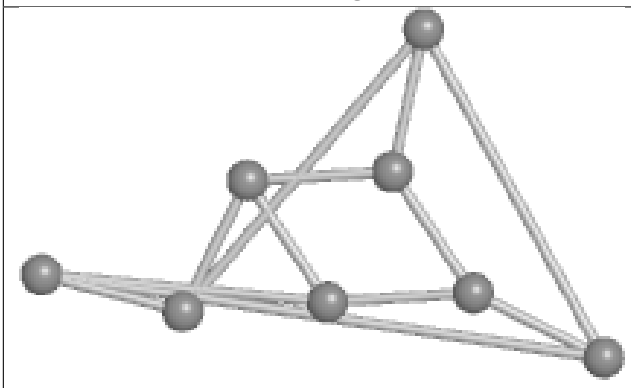
Ligand SF4 C 102



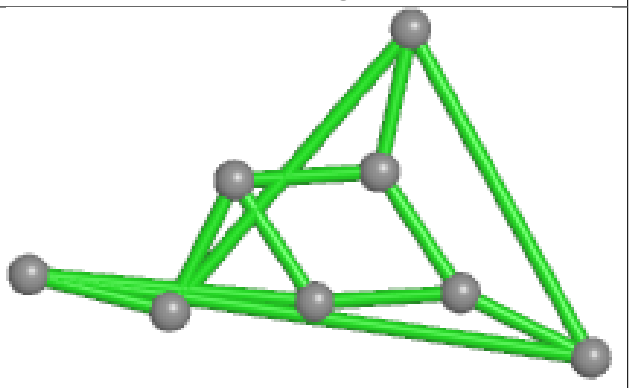
Bond lengths



Bond angles

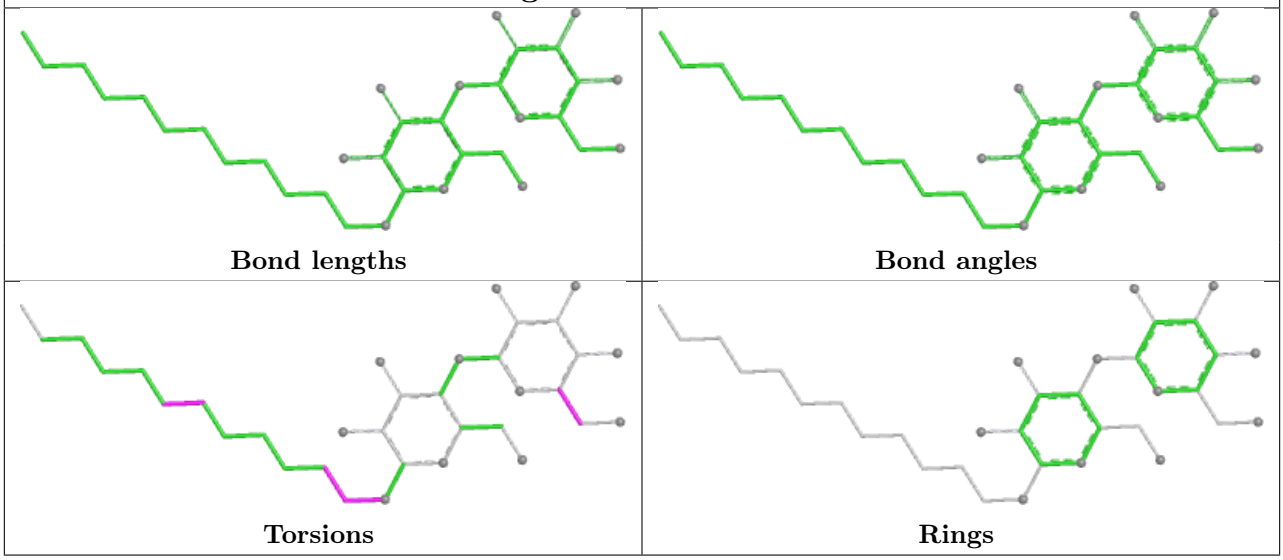


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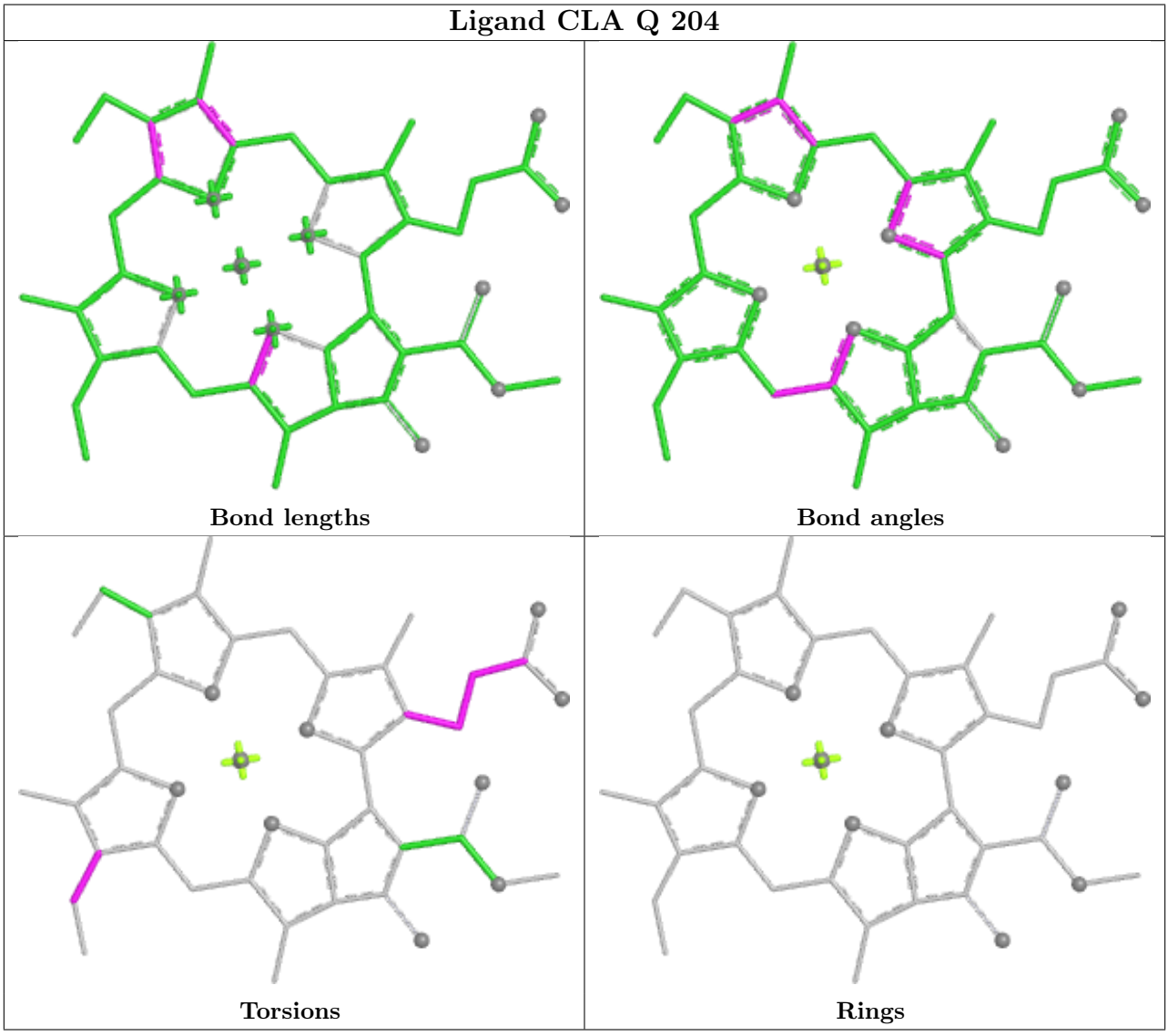


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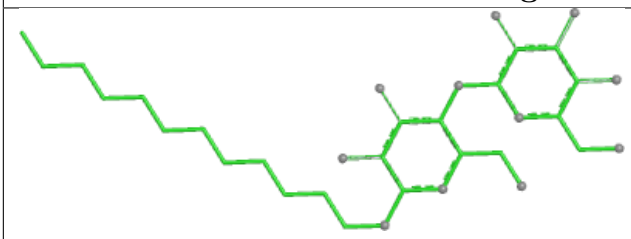
Ligand LMT G 857



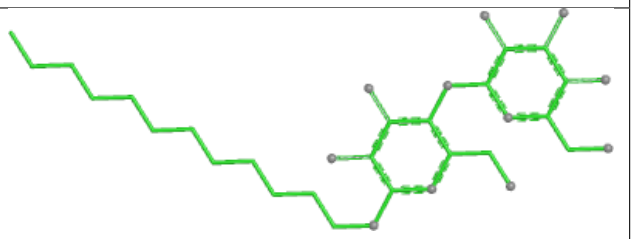
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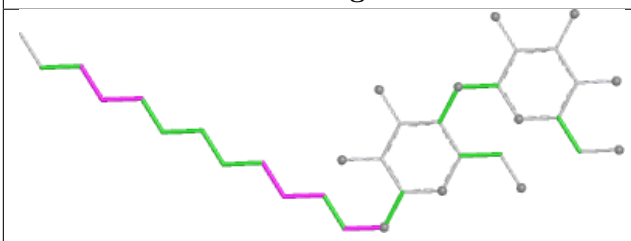
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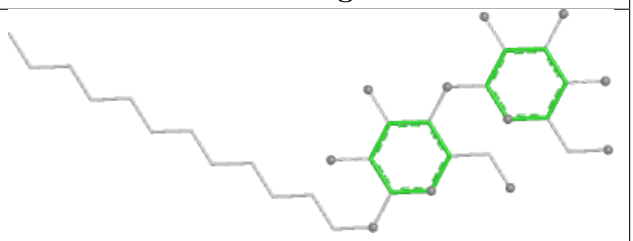
Bond lengths



Bond angles

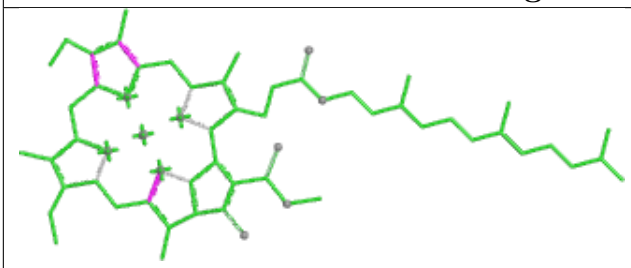


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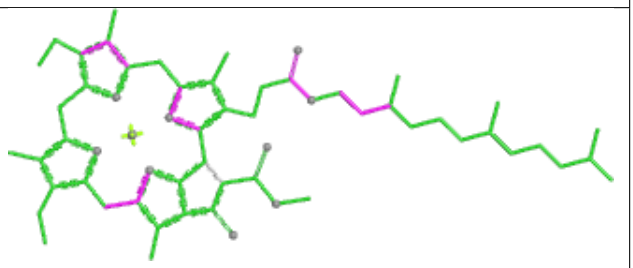


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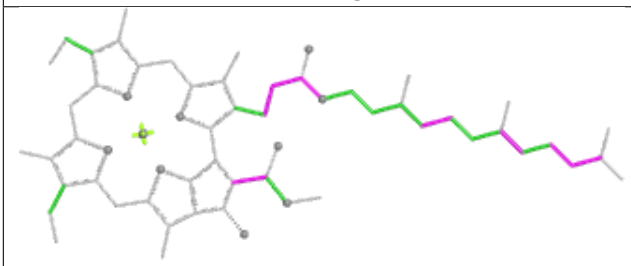
Ligand CLA B 817



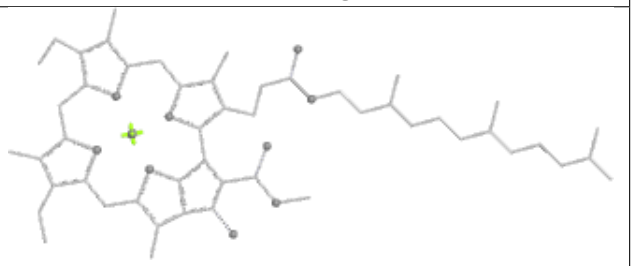
Bond lengths



Bond angles

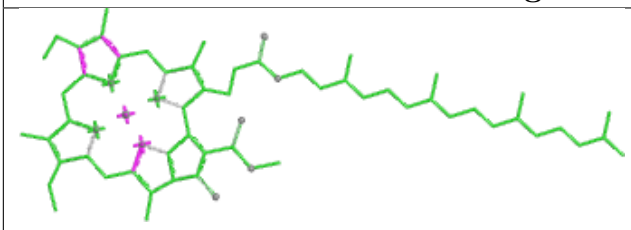


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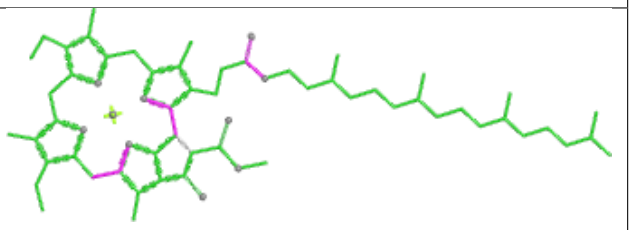


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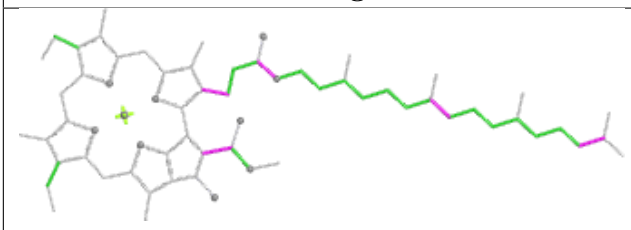
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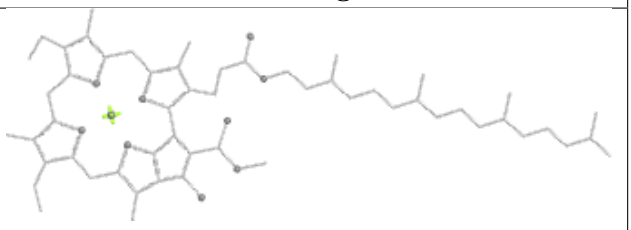
Bond lengths



Bond angles

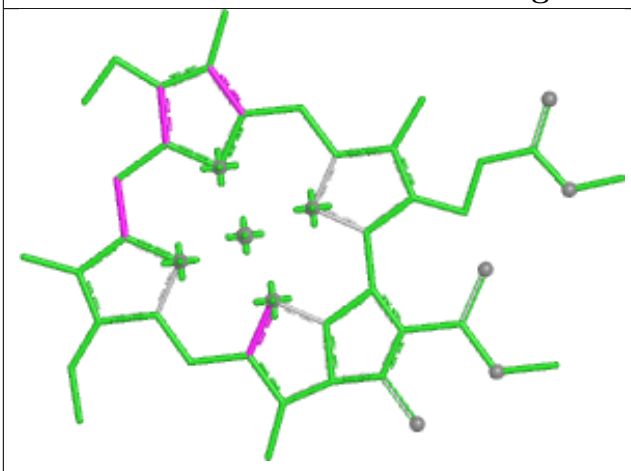


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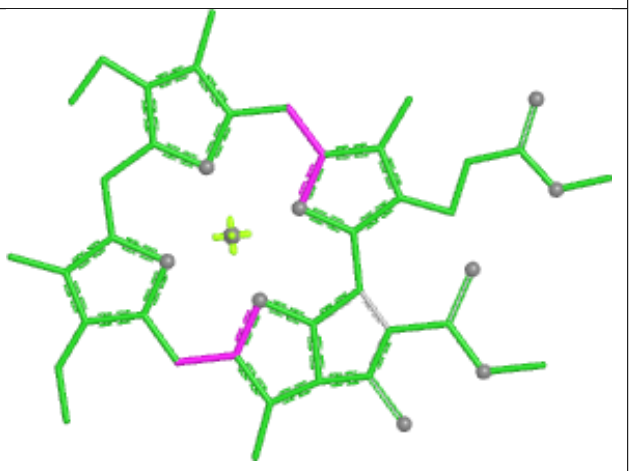


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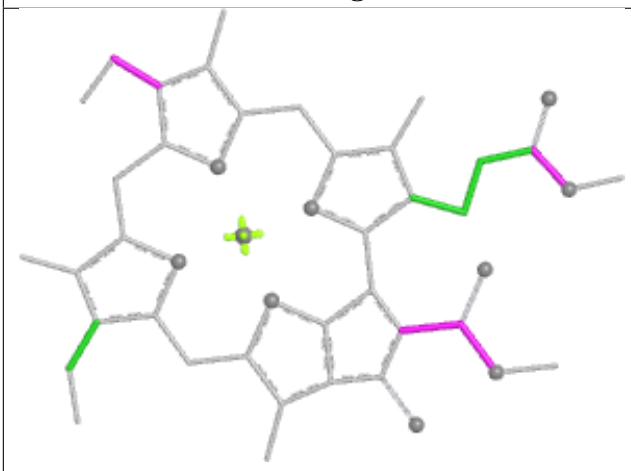
Ligand CLA f 205



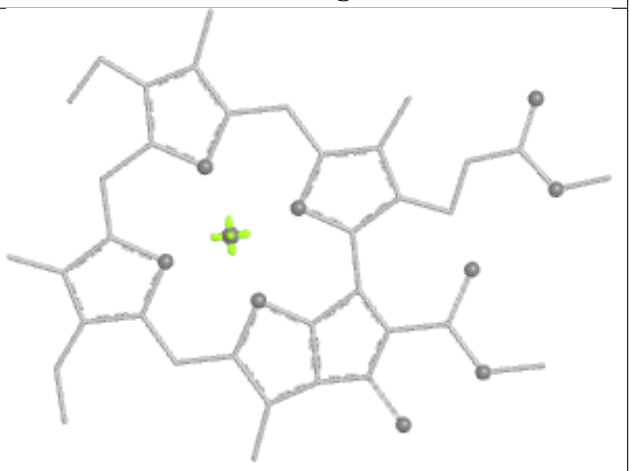
Bond lengths



Bond angles

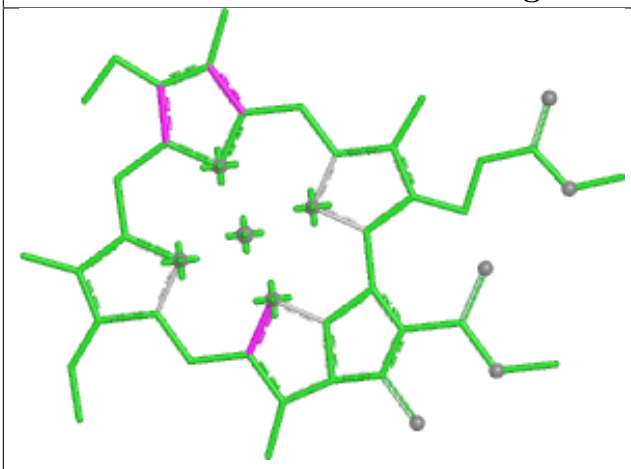


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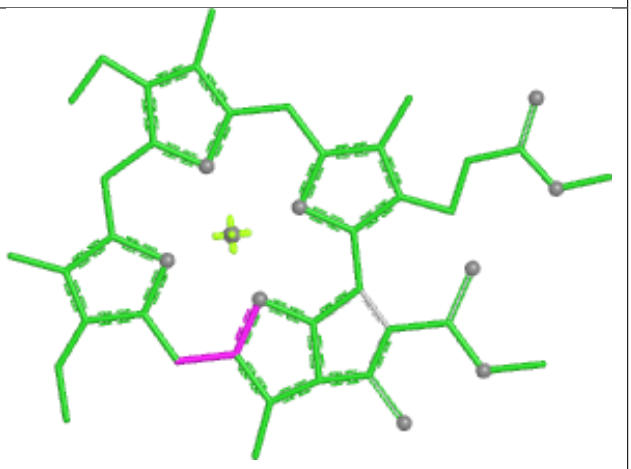


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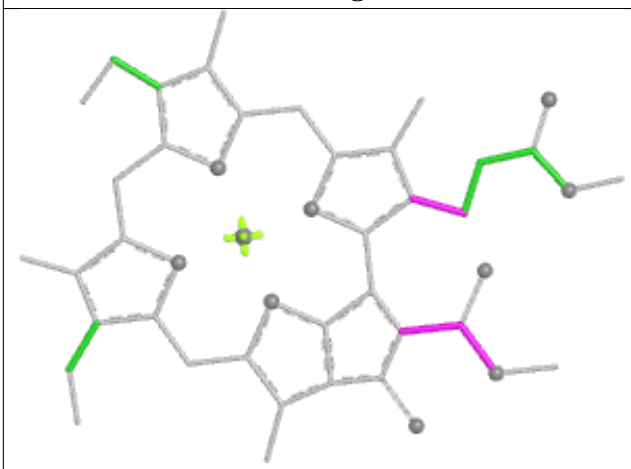
Ligand CLA G 844



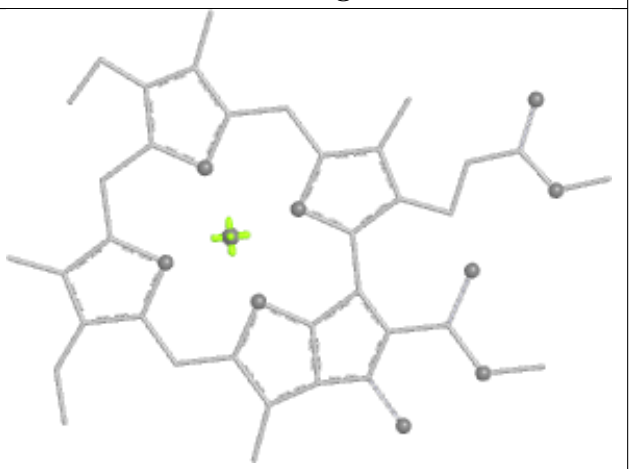
Bond lengths



Bond angles



Torsions

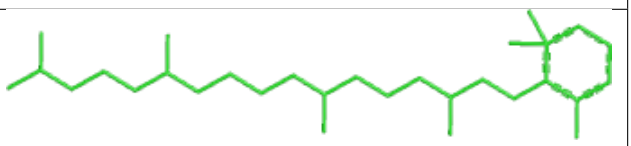


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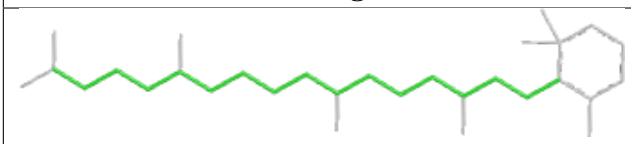
Ligand BCR b 849



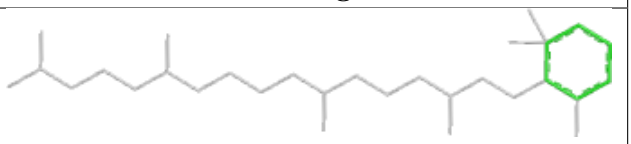
Bond lengths



Bond angles

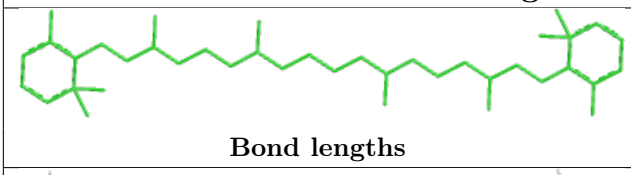


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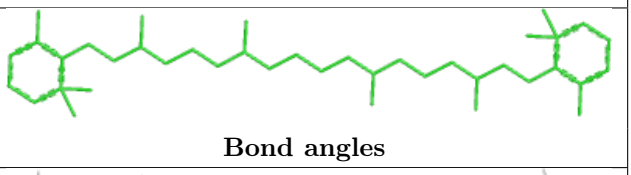


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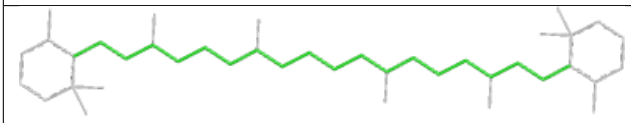
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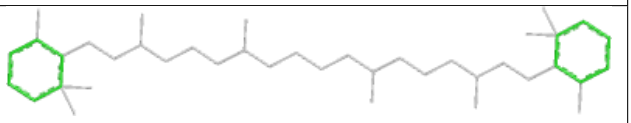
Bond lengths



Bond angles

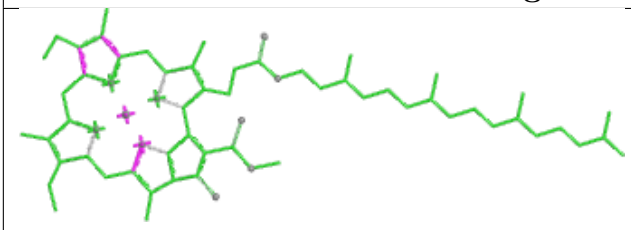


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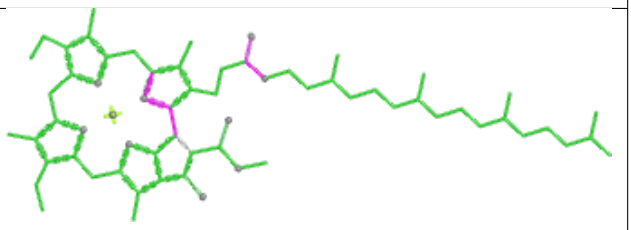


Rings

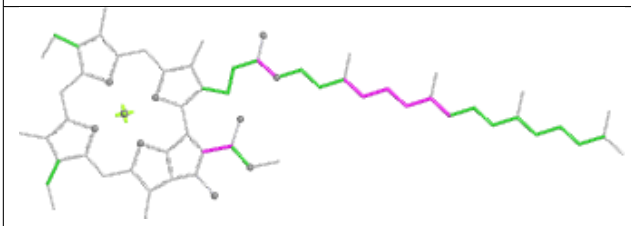
Ligand CLA A 830



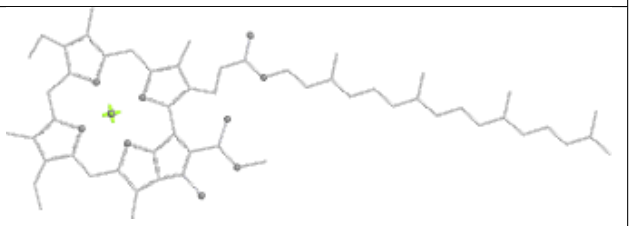
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Bond angles

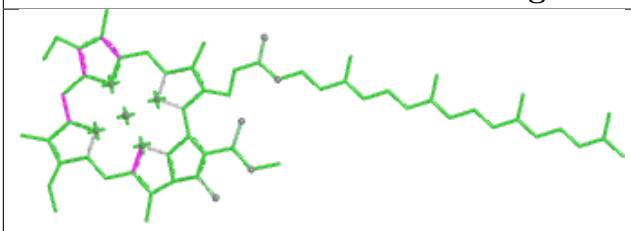


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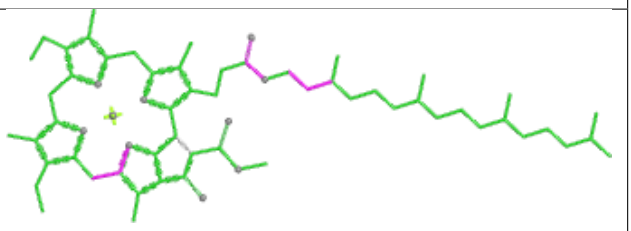


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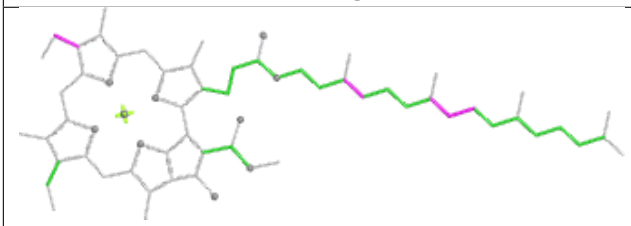
Ligand CLA a 841



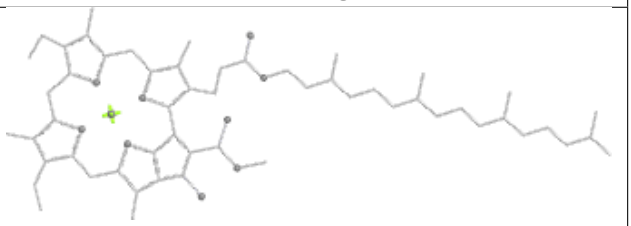
Bond lengths



Bond angles

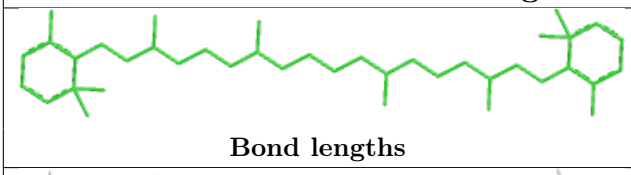


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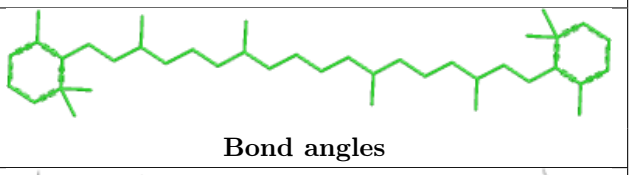


Rings

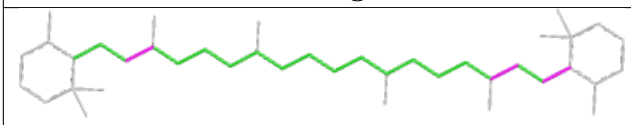
Ligand BCR l 5007



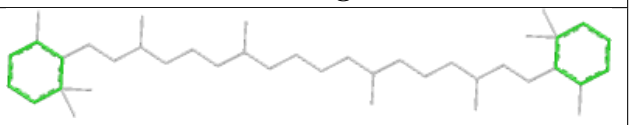
Bond lengths



Bond angles

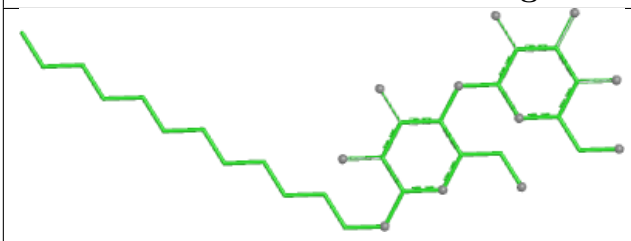


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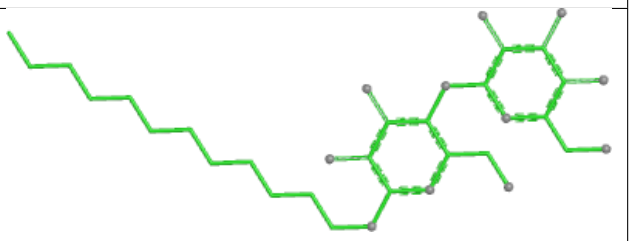


Rings

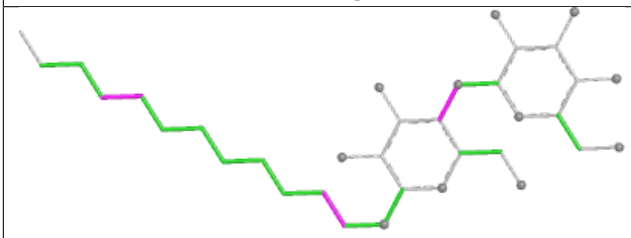
Ligand LMT H 853



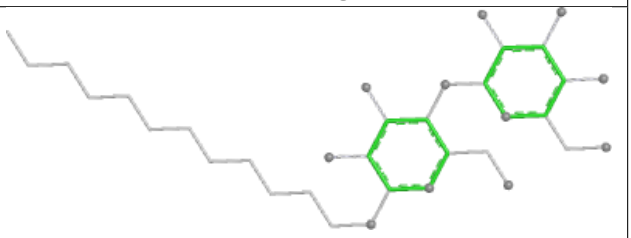
Bond lengths



Bond angles

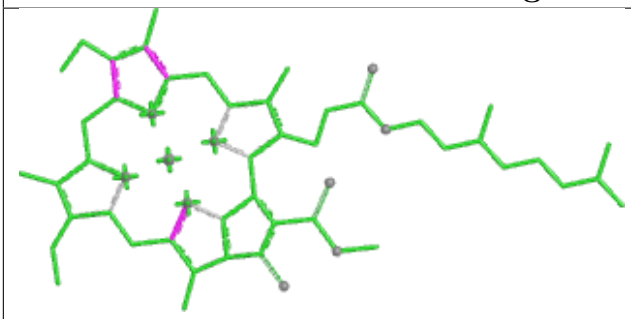


Torsions

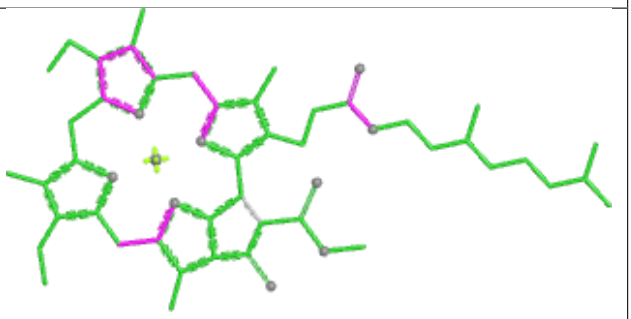


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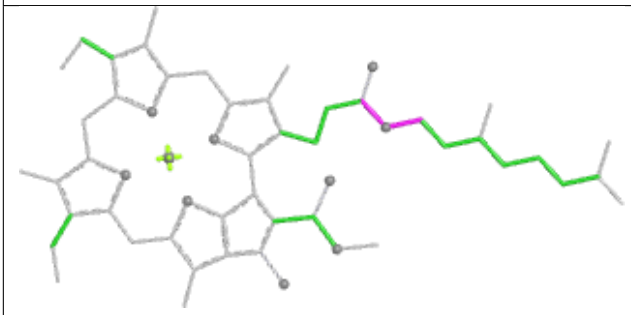
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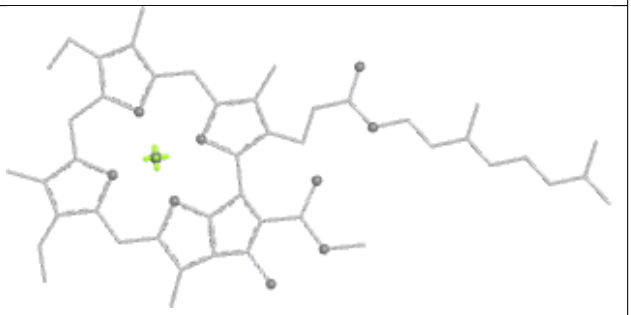
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Bond angles

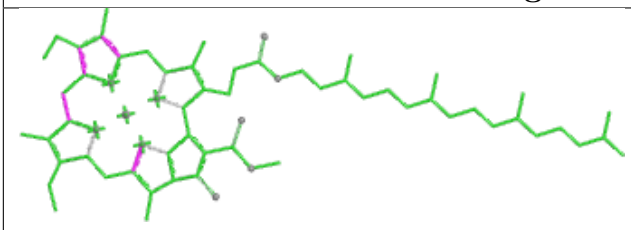


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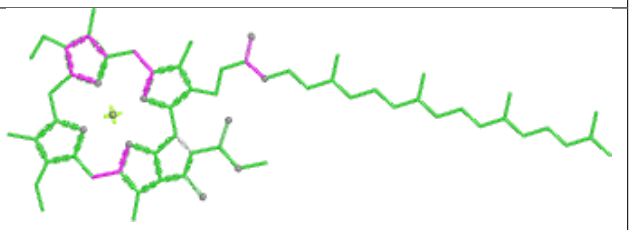


Rings

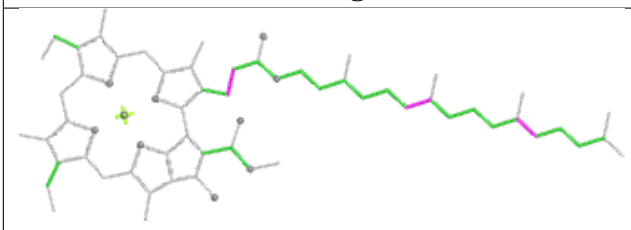
Ligand CLA B 841



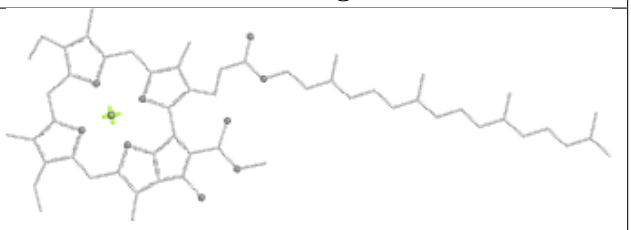
Bond lengths



Bond angles

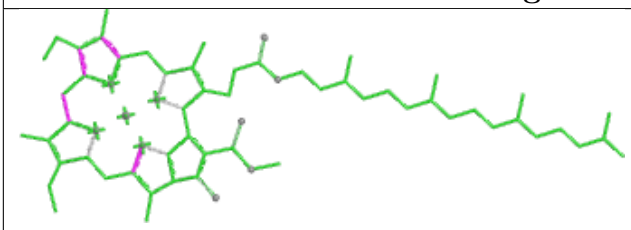


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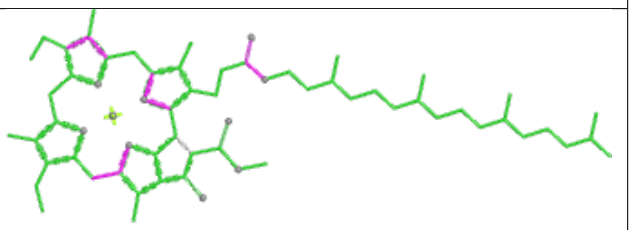


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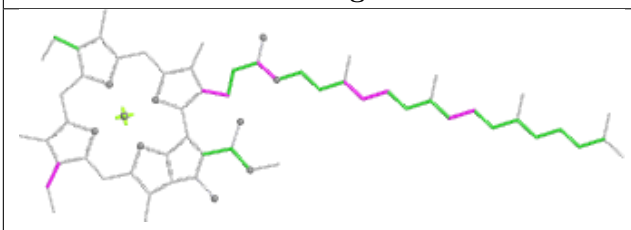
Ligand CLA H 814



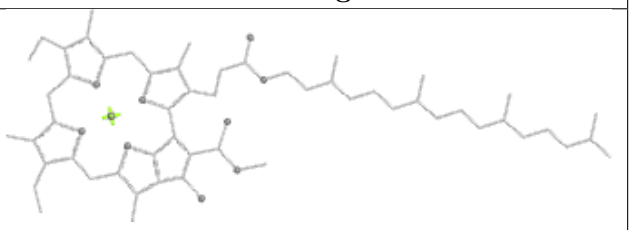
Bond lengths



Bond angles



Torsions



Rings

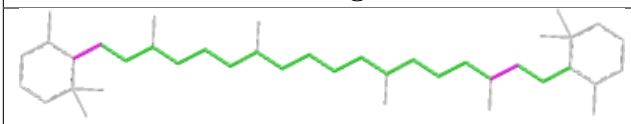
Ligand BCR G 847



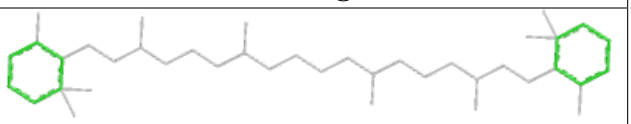
Bond lengths



Bond angles

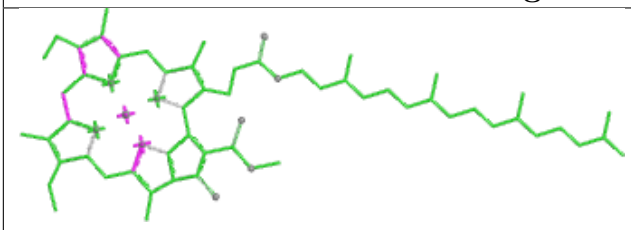


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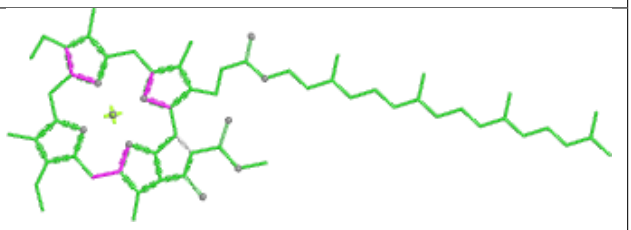


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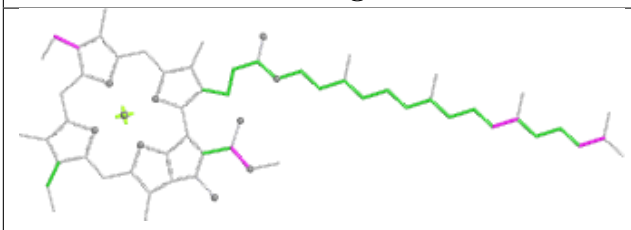
Ligand CLA A 833



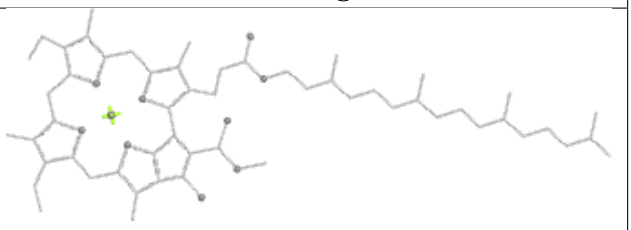
Bond lengths



Bond angles

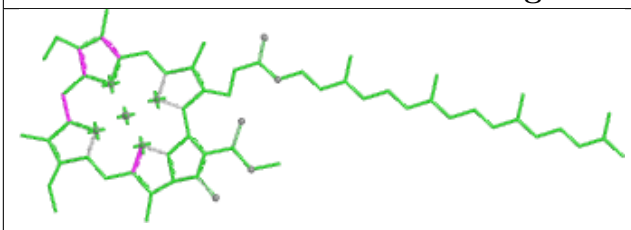


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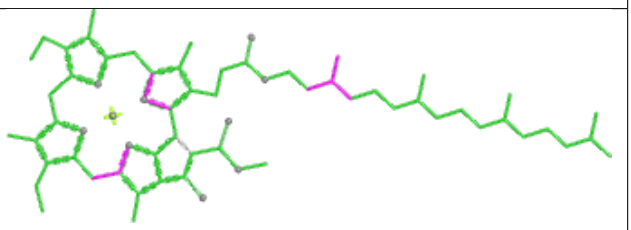


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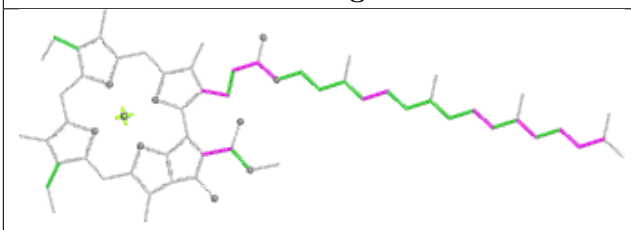
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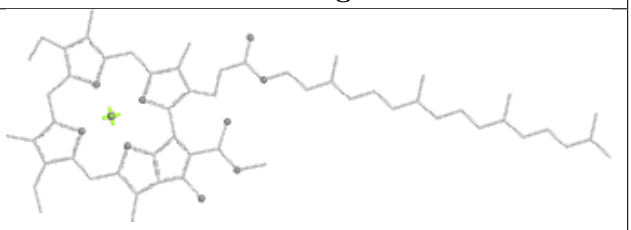
Bond lengths



Bond angles

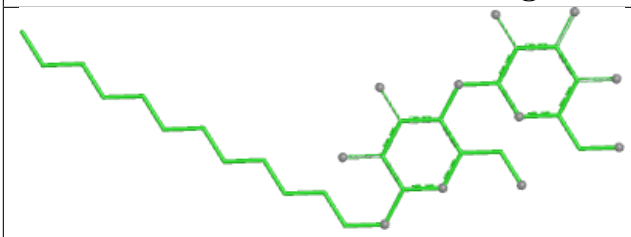


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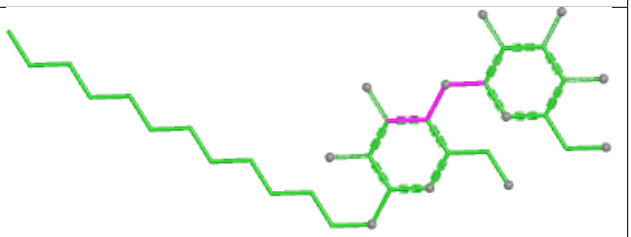


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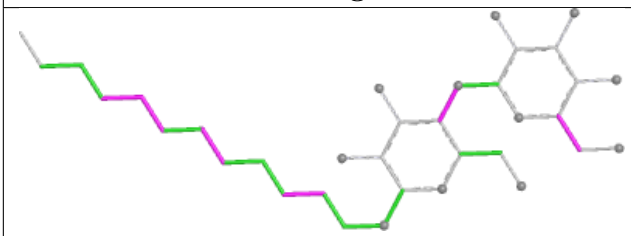
Ligand LMT H 852



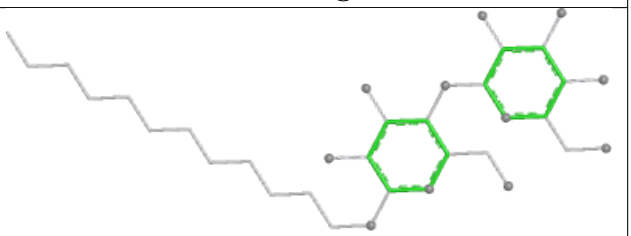
Bond lengths



Bond angles

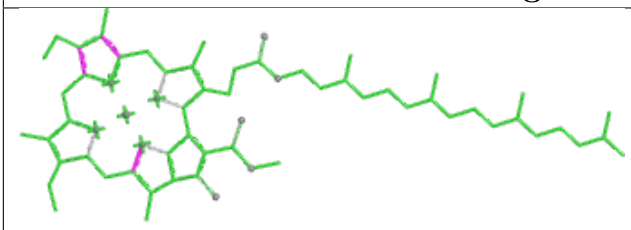


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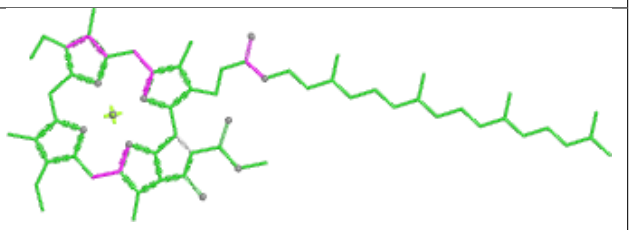


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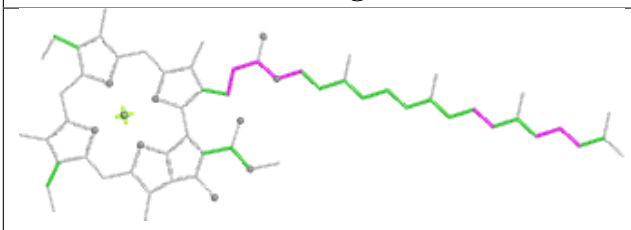
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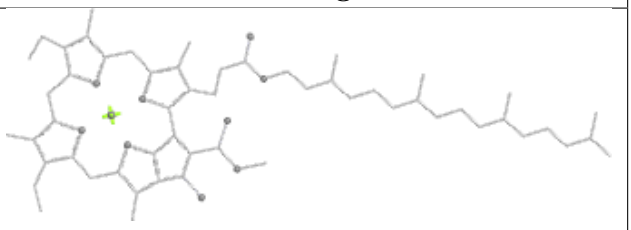
Bond lengths



Bond angles

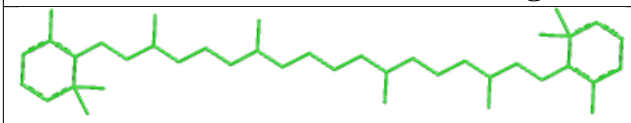


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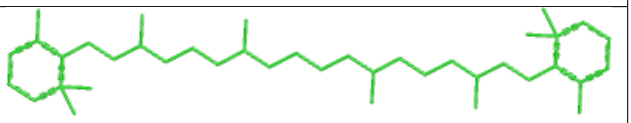


Rings

Ligand BCR b 850



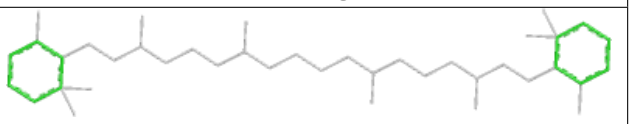
Bond lengths



Bond angles

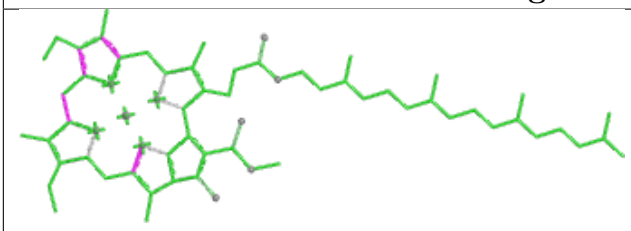


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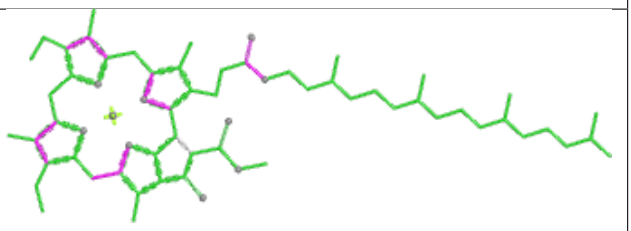


Rings

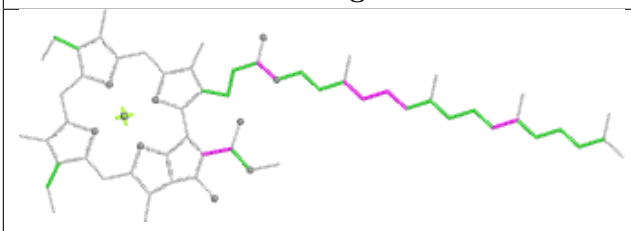
Ligand CLA a 815



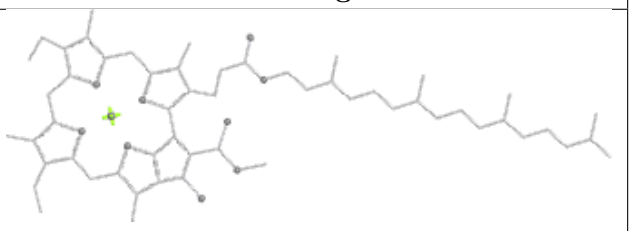
Bond lengths



Bond angles

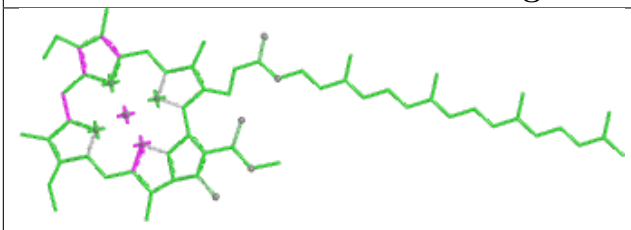


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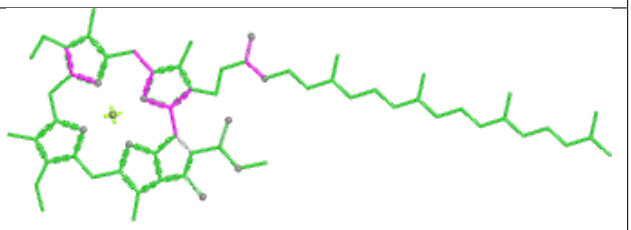


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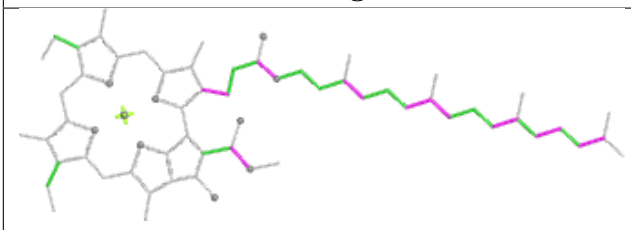
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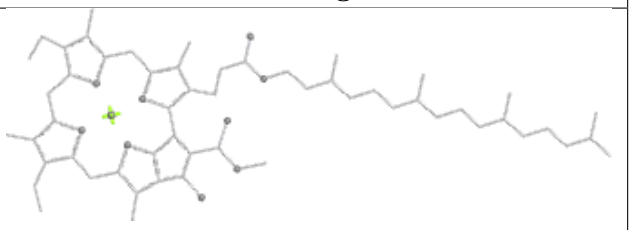
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Bond angles

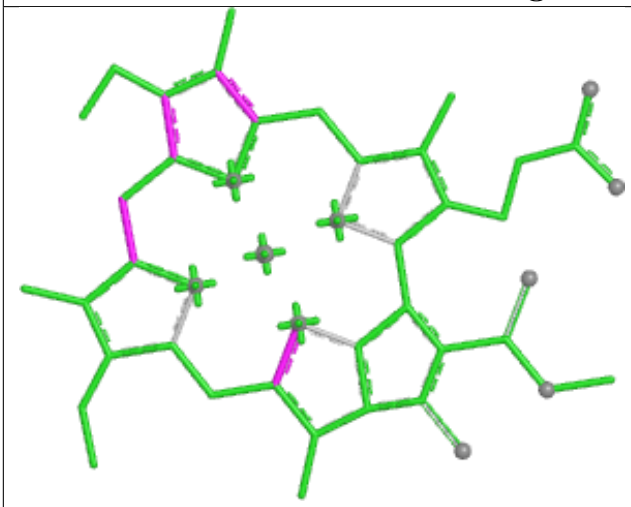


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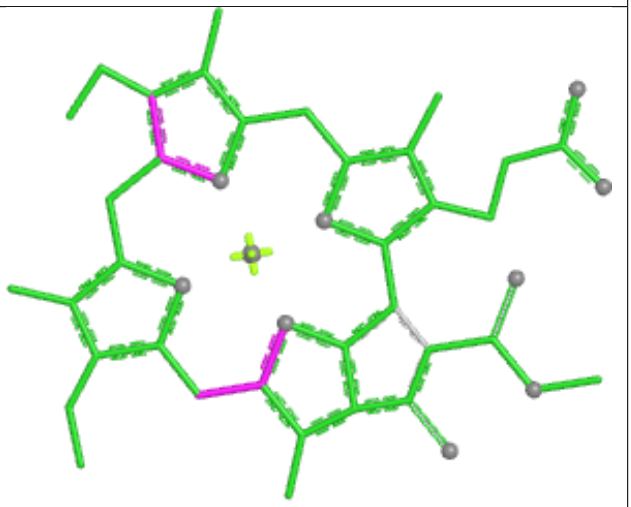


Rings

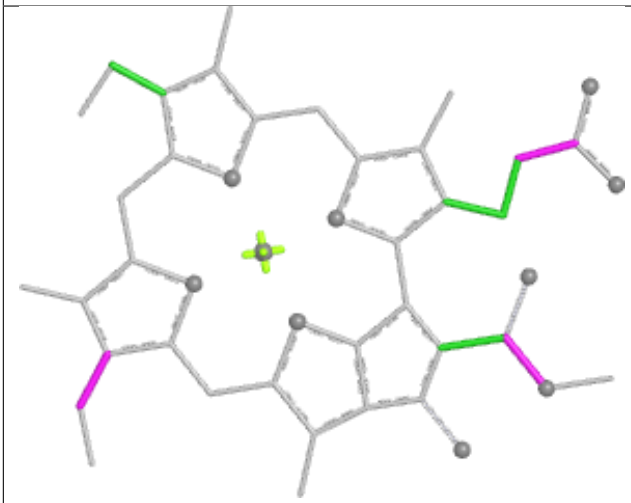
Ligand CLA k 102



Bond lengths



Bond angles

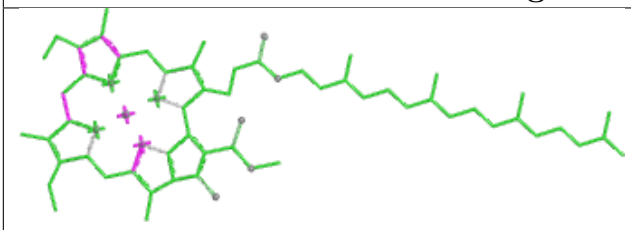


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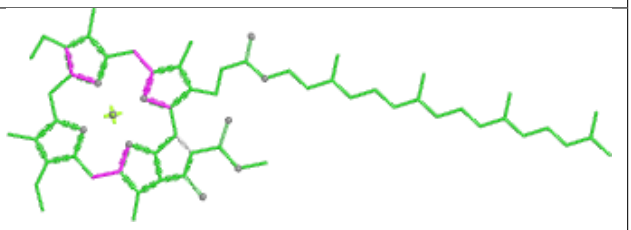


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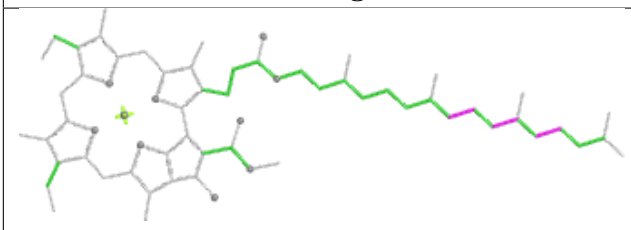
Ligand CLA b 802



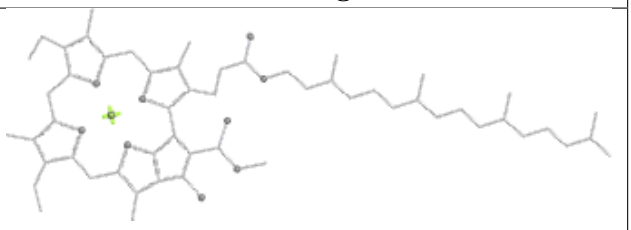
Bond lengths



Bond angles

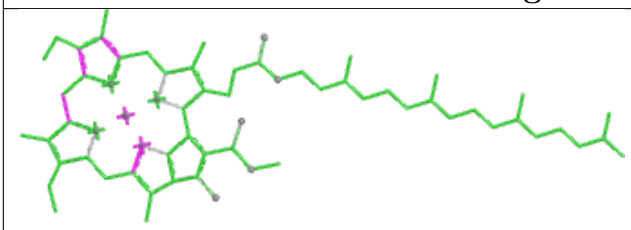


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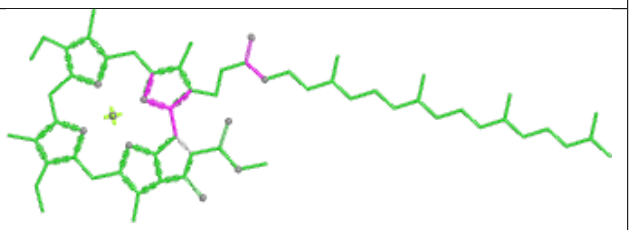


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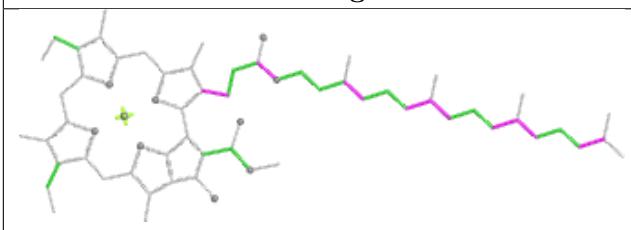
Ligand CLA A 828



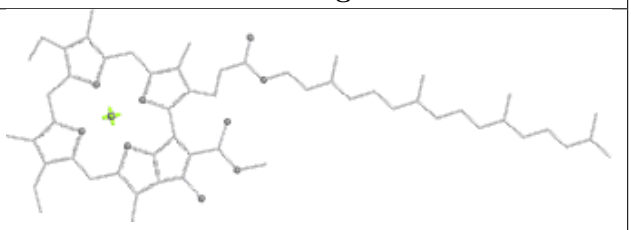
Bond lengths



Bond angles

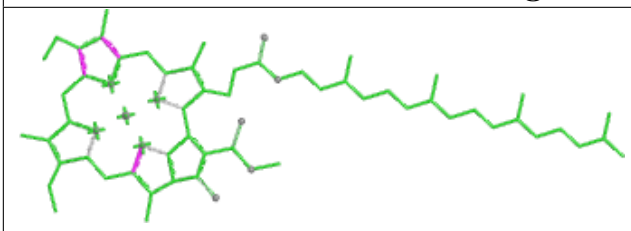


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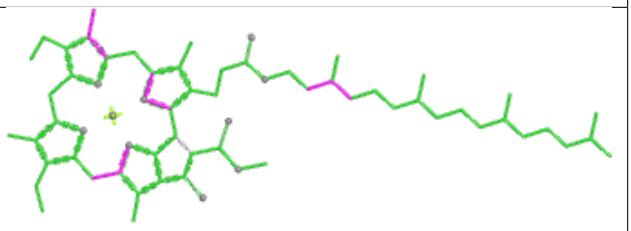


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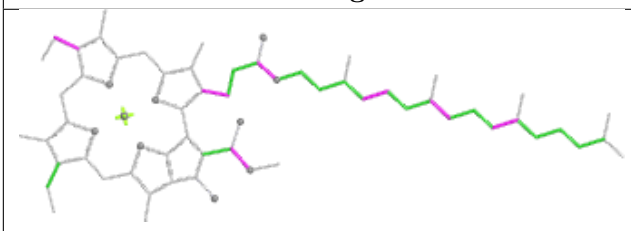
Ligand CLA B 842



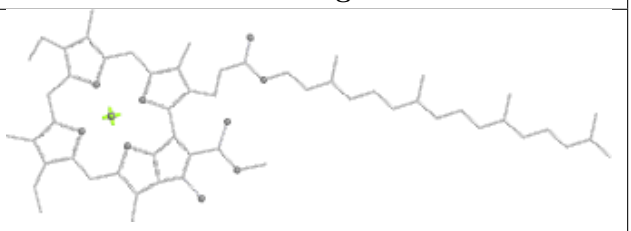
Bond lengths



Bond angles

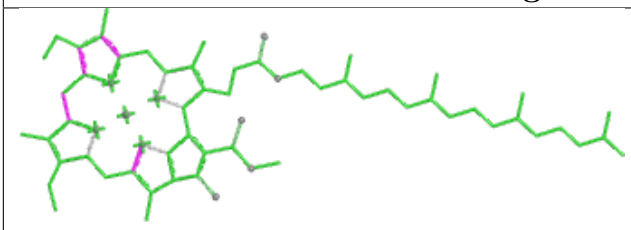


Torsions

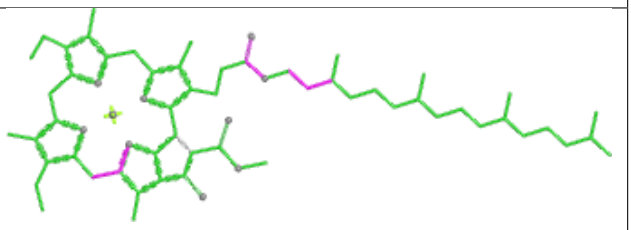


Rings

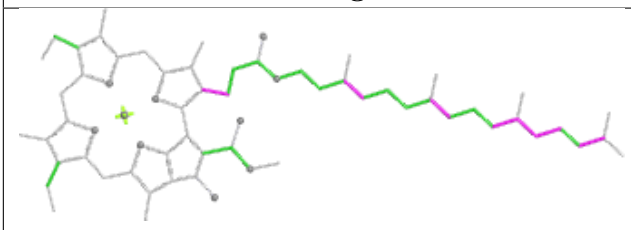
Ligand CLA K 103



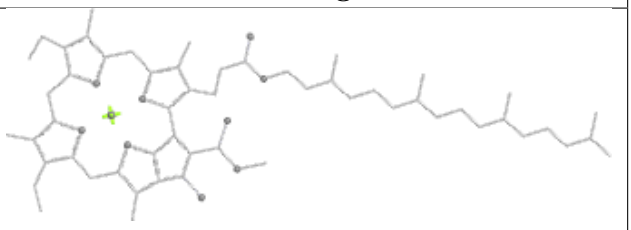
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Bond angles

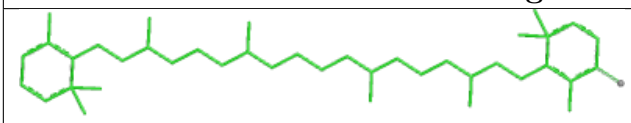


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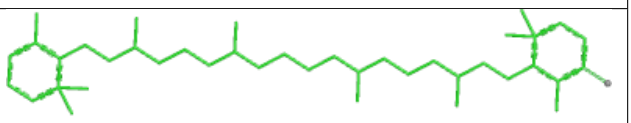


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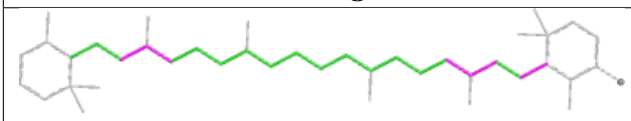
Ligand ECH b 848



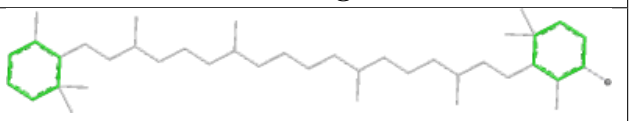
Bond lengths



Bond angles

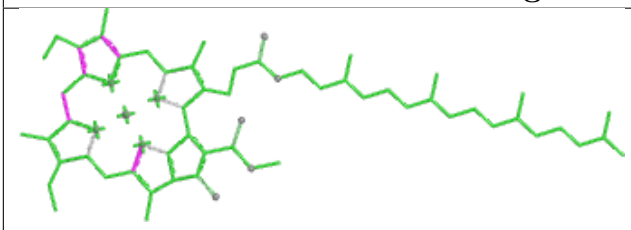


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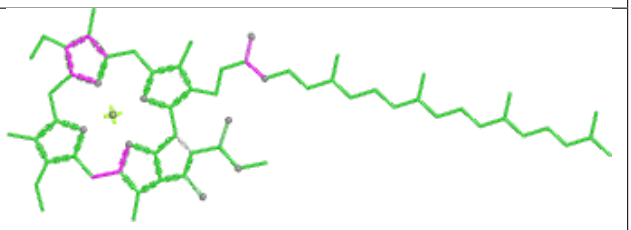


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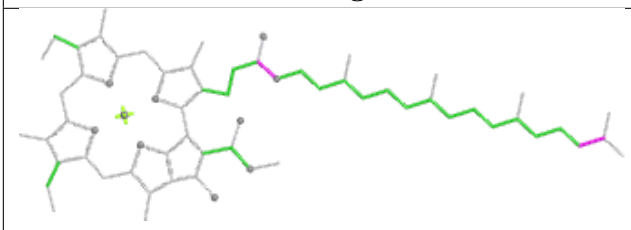
Ligand CLA A 827



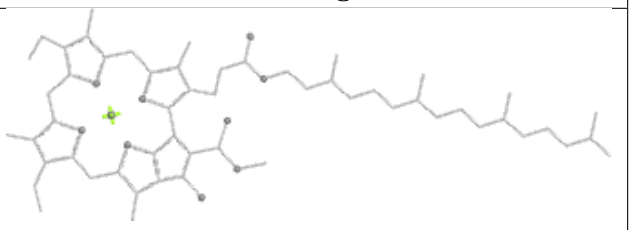
Bond lengths



Bond angles

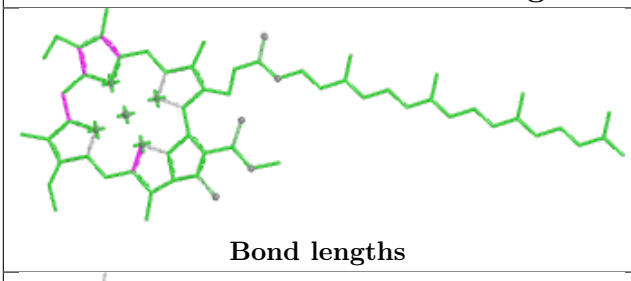


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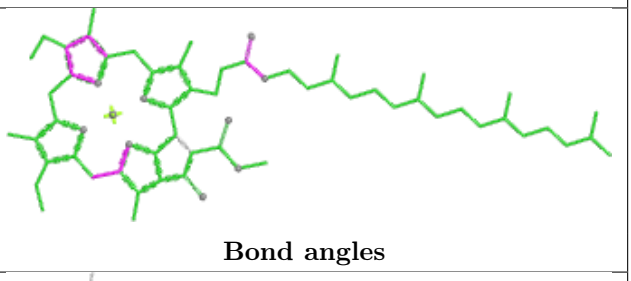


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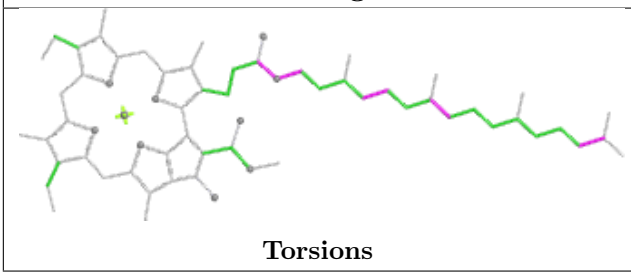
Ligand CLA b 841



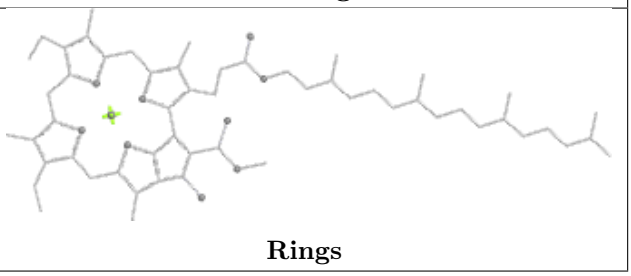
Bond lengths



Bond angles

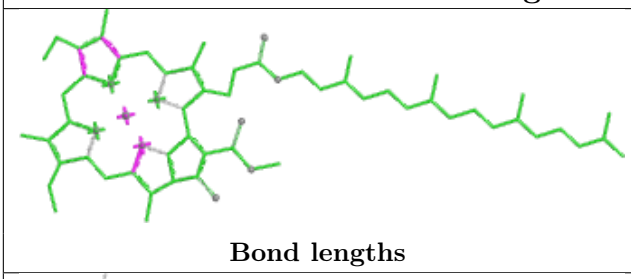


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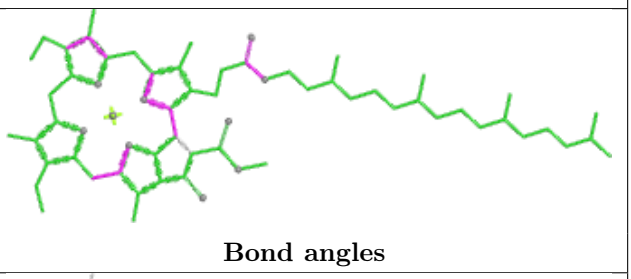


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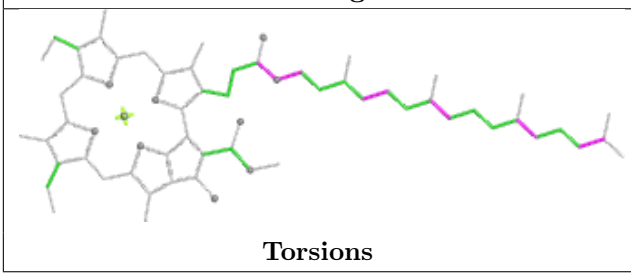
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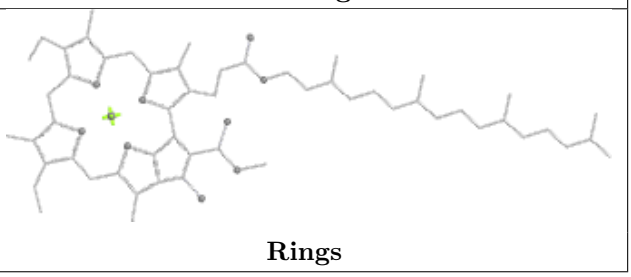
Bond lengths



Bond angles

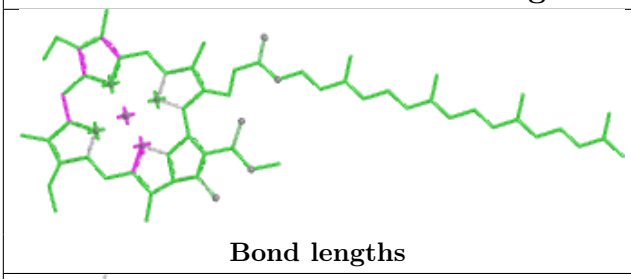


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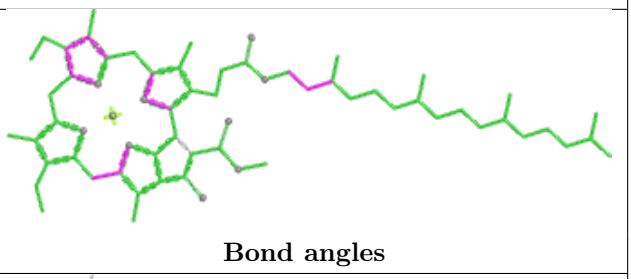


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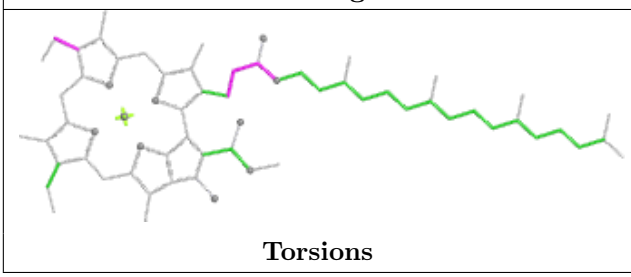
Ligand CLA a 843



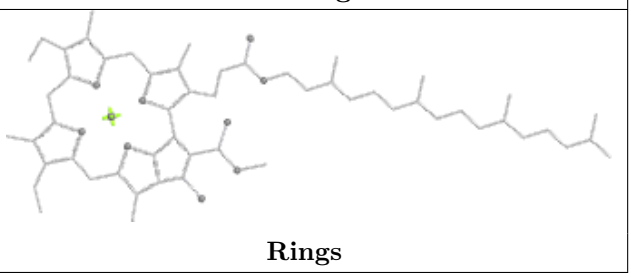
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Bond angles

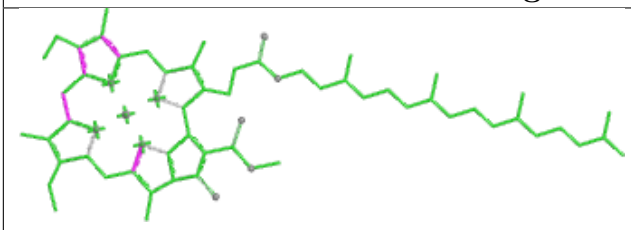


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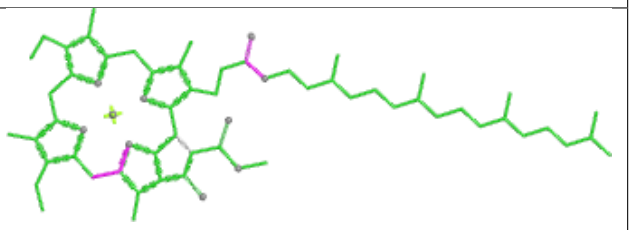


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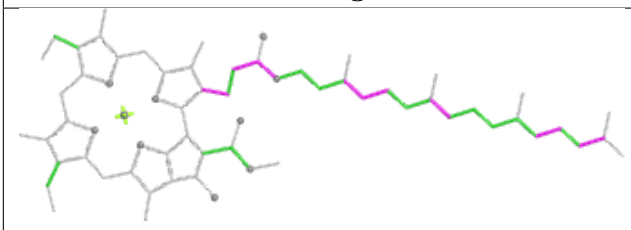
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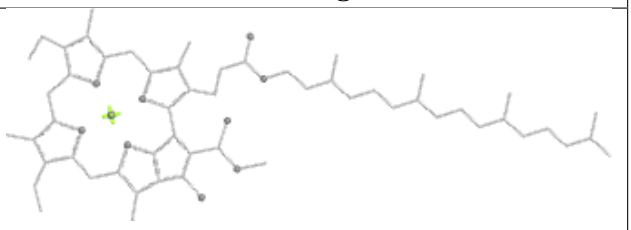
Bond lengths



Bond angles

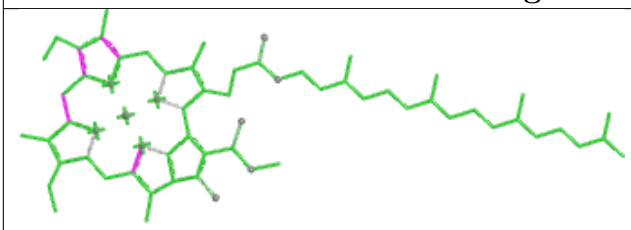


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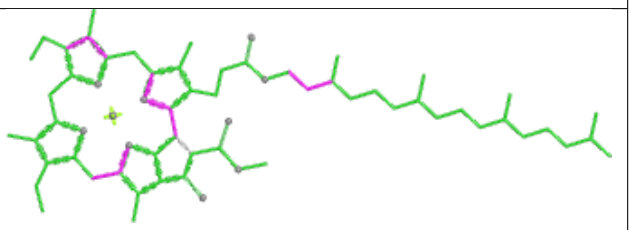


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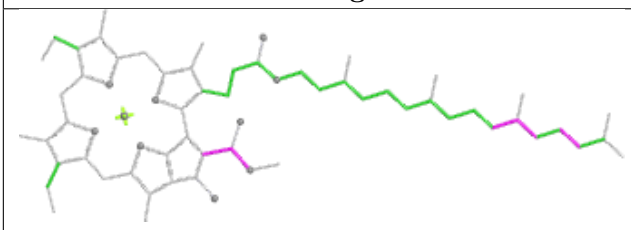
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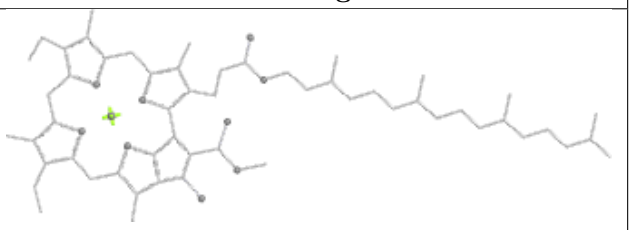
Bond lengths



Bond angles



Torsions



Rings

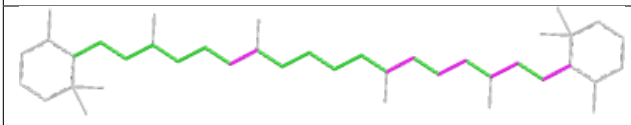
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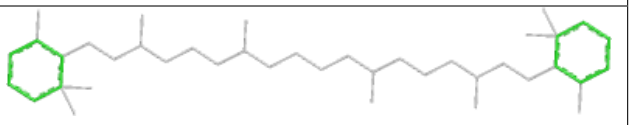
Bond lengths



Bond angles

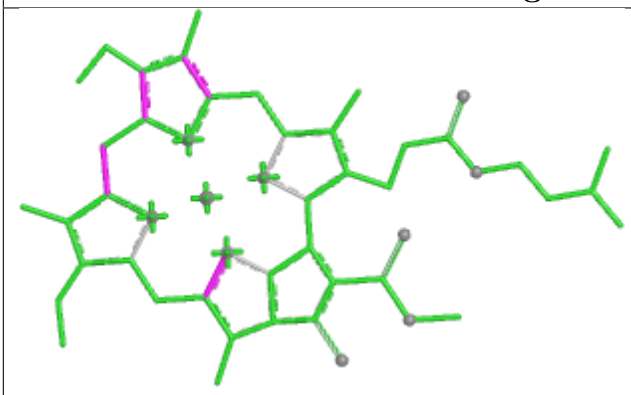


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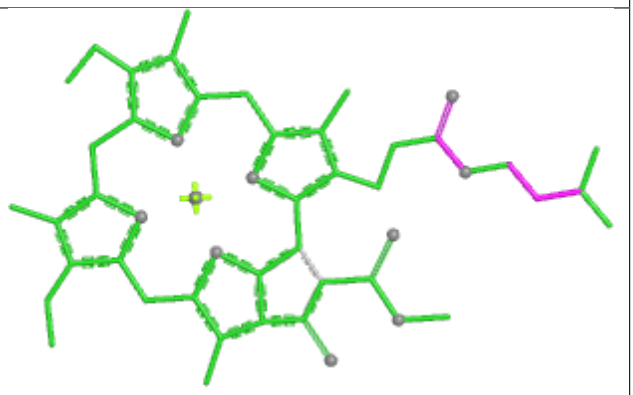


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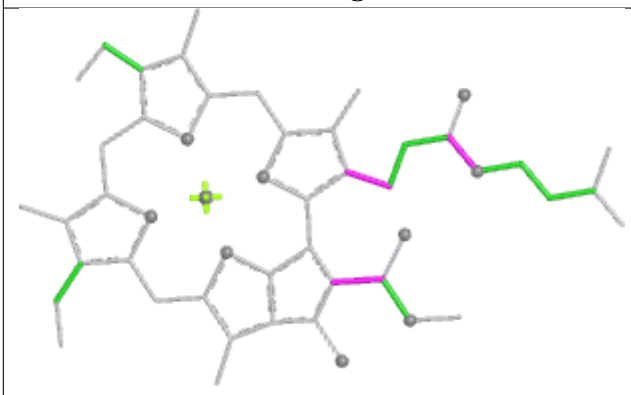
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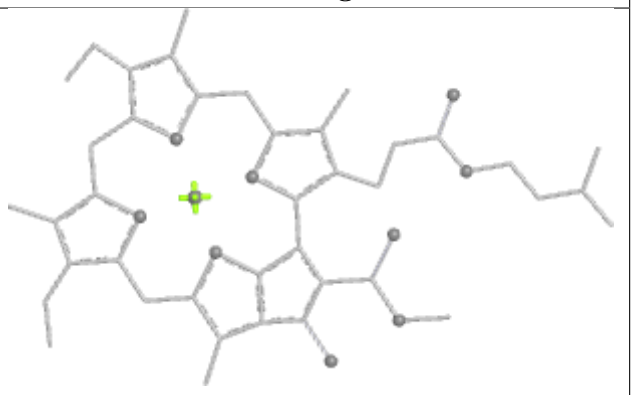
Bond lengths



Bond angles

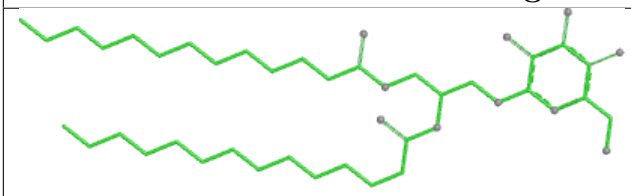


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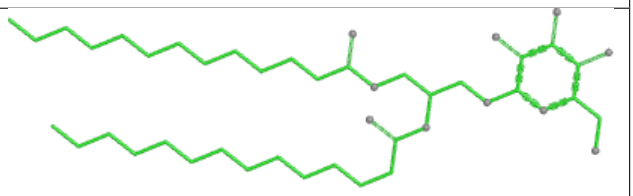


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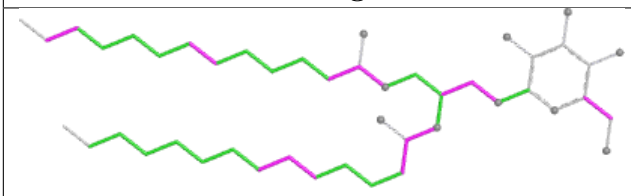
Ligand LMG a 853



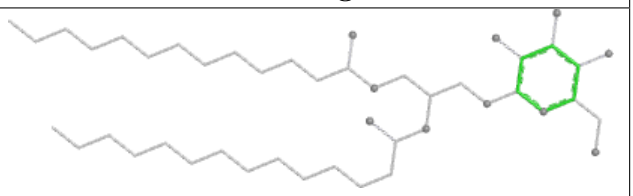
Bond lengths



Bond angles

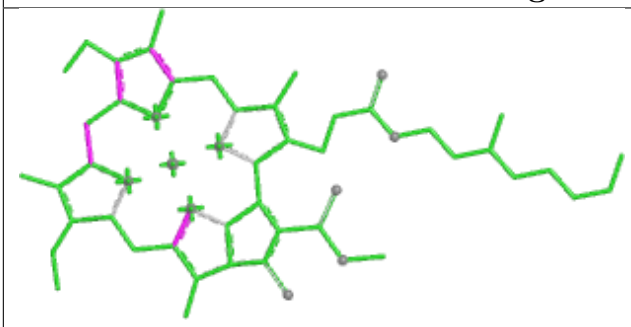


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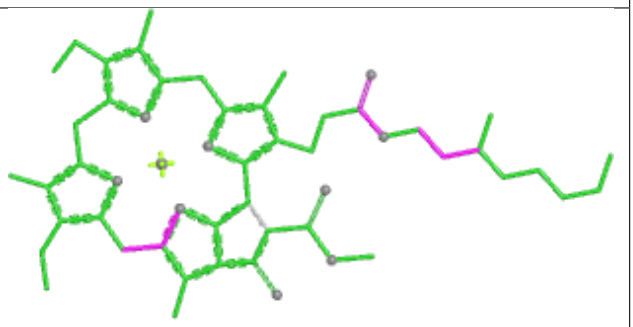


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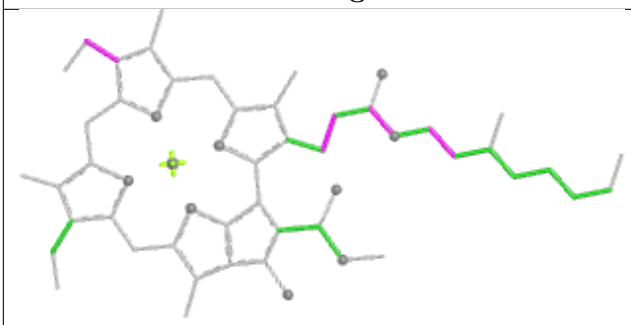
Ligand CLA a 813



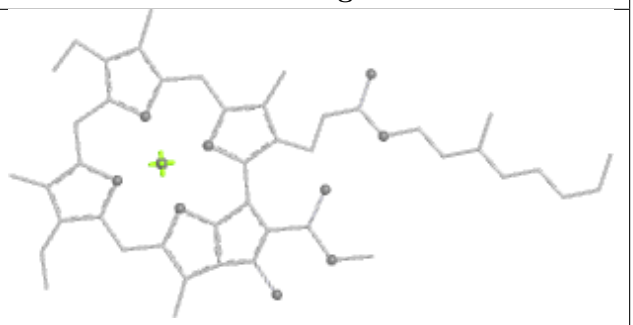
Bond lengths



Bond angles

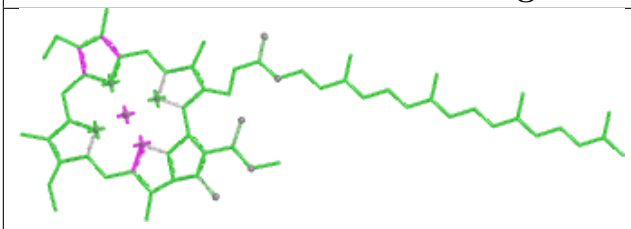


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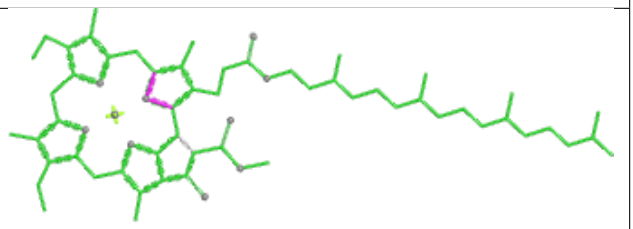


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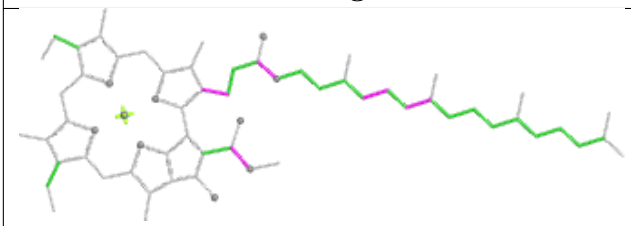
Ligand CLA L 1501



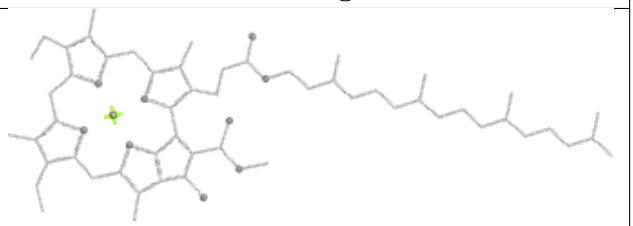
Bond lengths



Bond angles

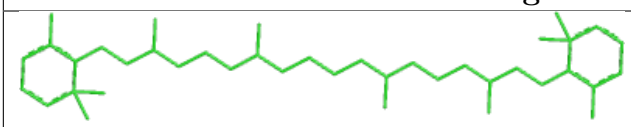


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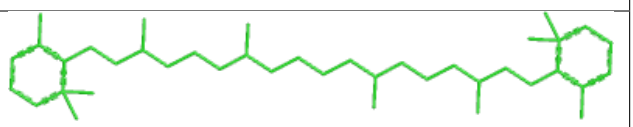


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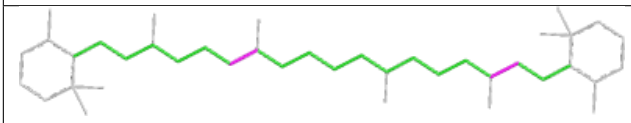
Ligand BCR B 846



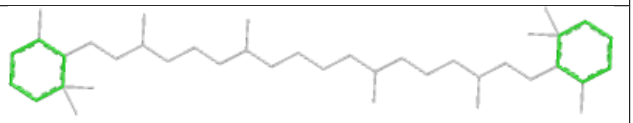
Bond lengths



Bond angles

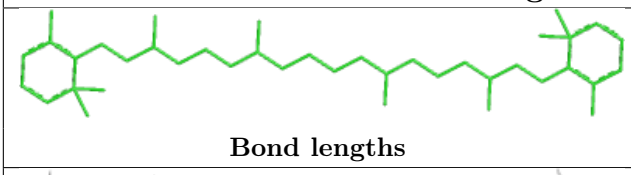


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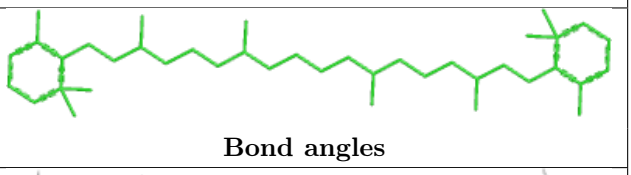


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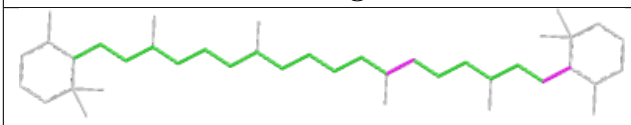
Ligand BCR k 104



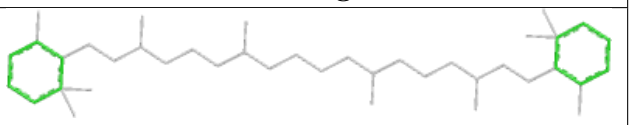
Bond lengths



Bond angles

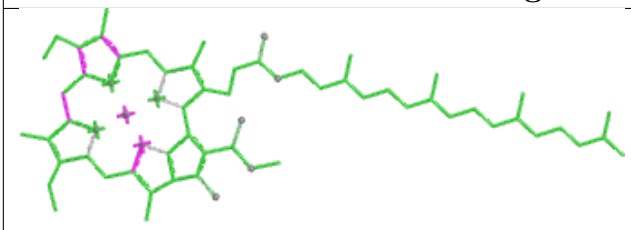


Torsions

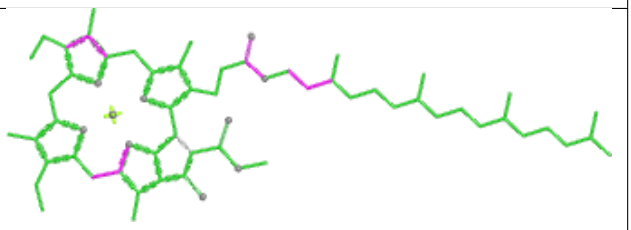


Rings

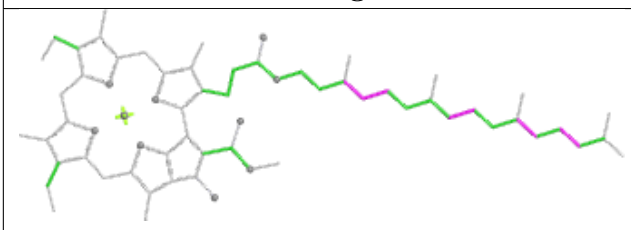
Ligand CLA B 818



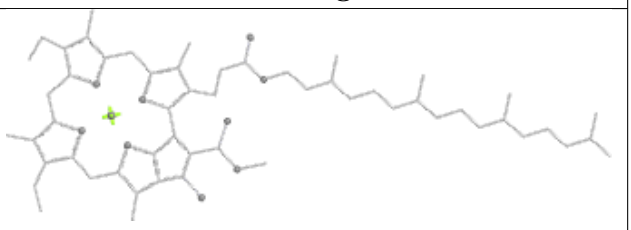
Bond lengths



Bond angles

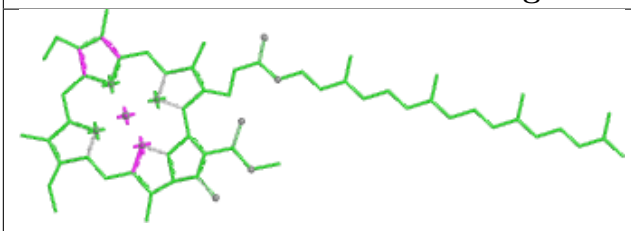


Torsions

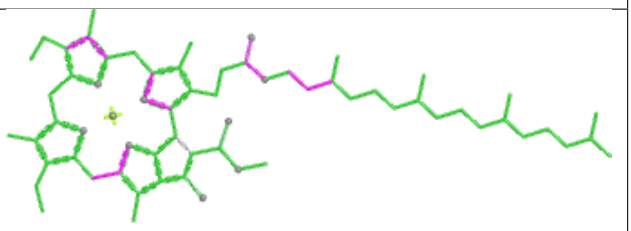


Rings

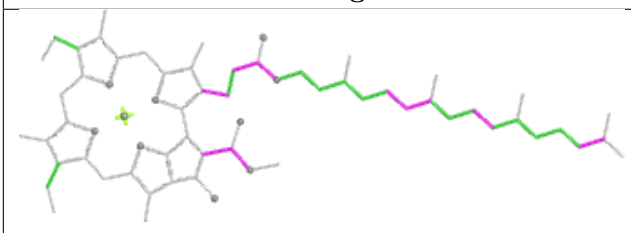
Ligand CLA G 807



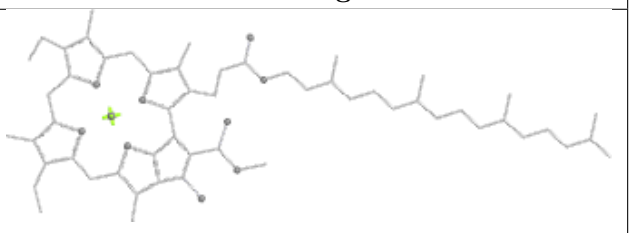
Bond lengths



Bond angles

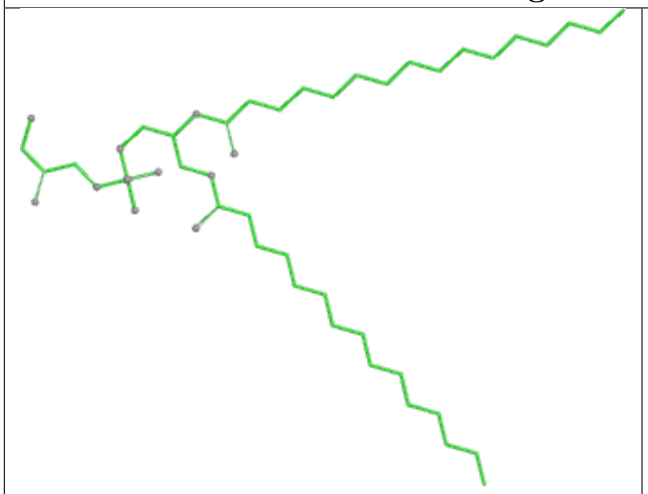


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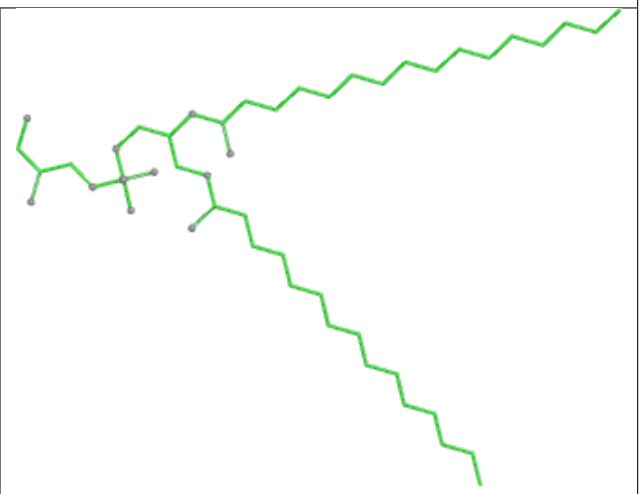


Rings

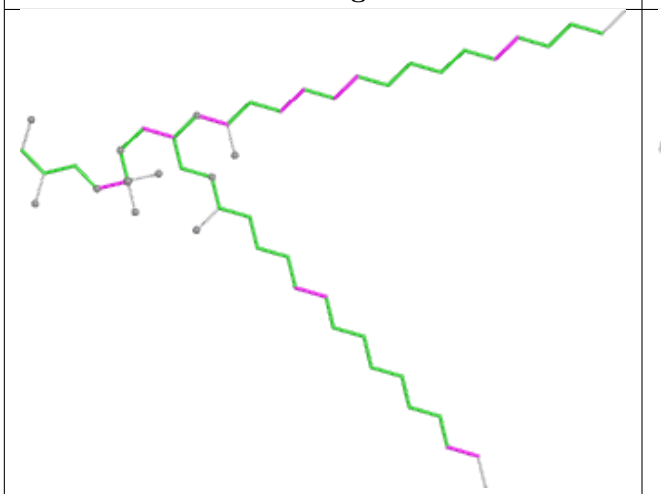
Ligand LHG a 801



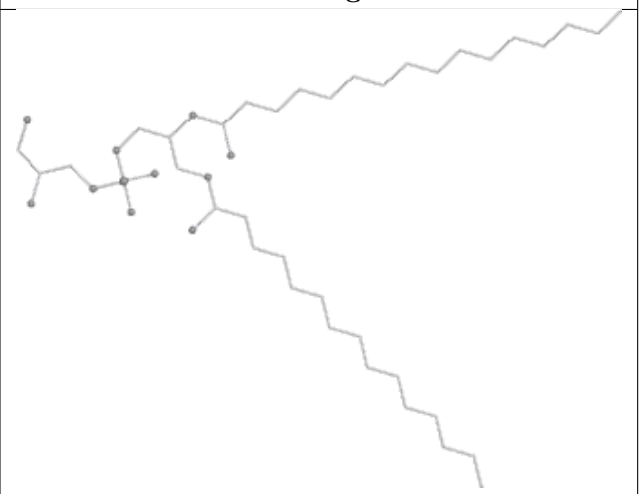
Bond lengths



Bond angles



Torsions



Rings

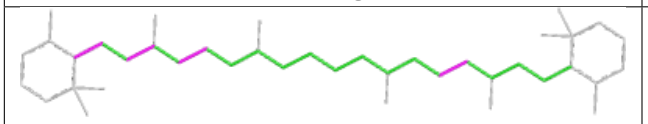
Ligand BCR l 5003



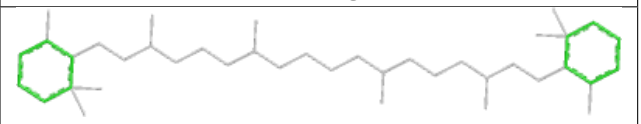
Bond lengths



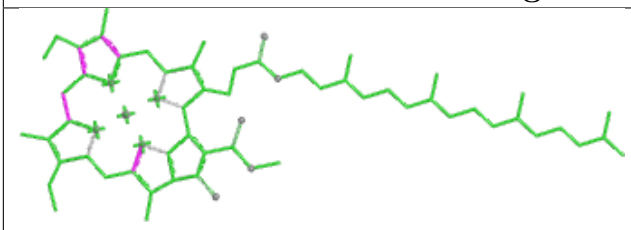
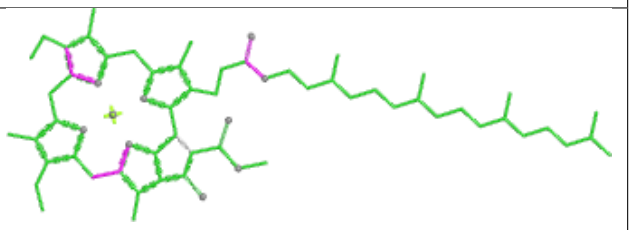
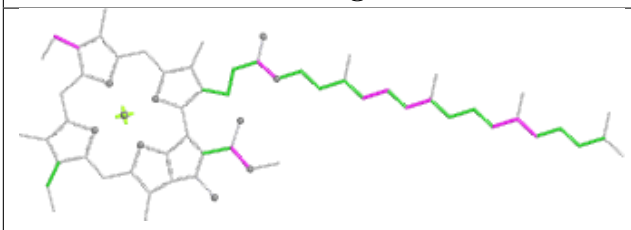
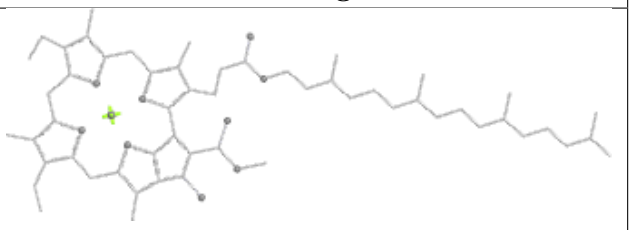
Bond angles

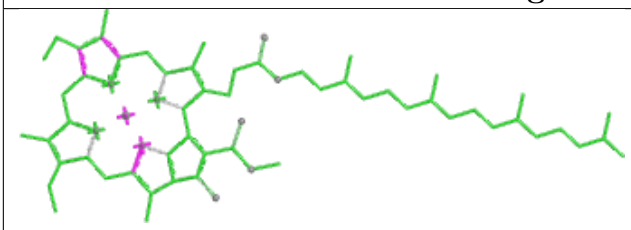
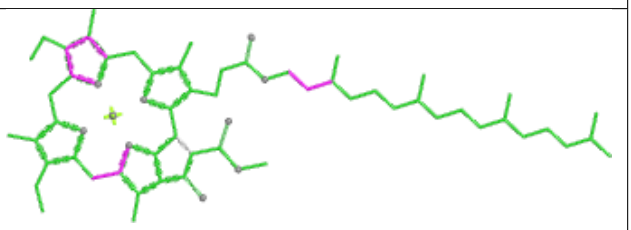
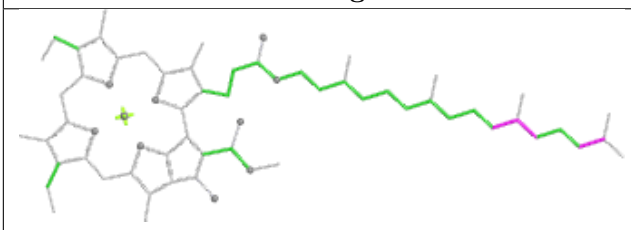
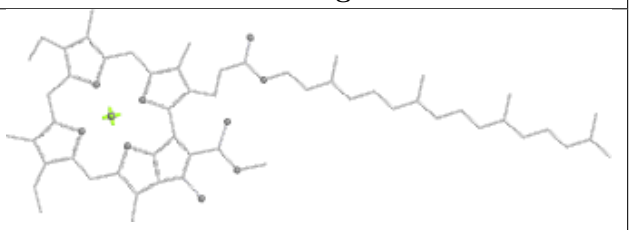


Torsions

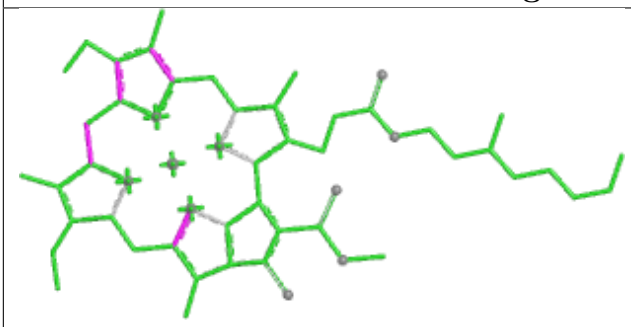


Rings

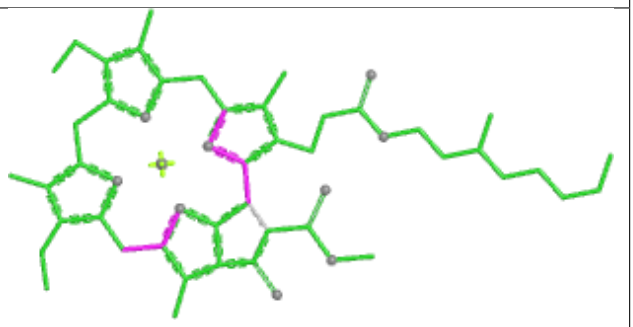
Ligand CLA H 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

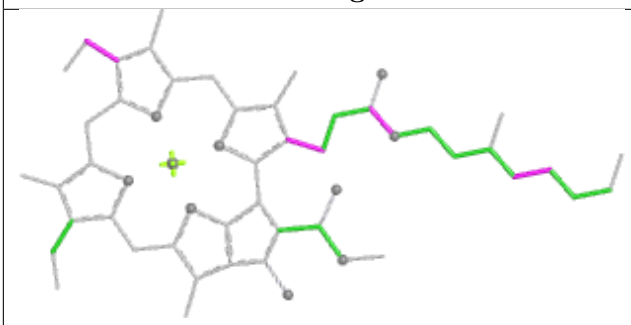
Ligand CLA G 813



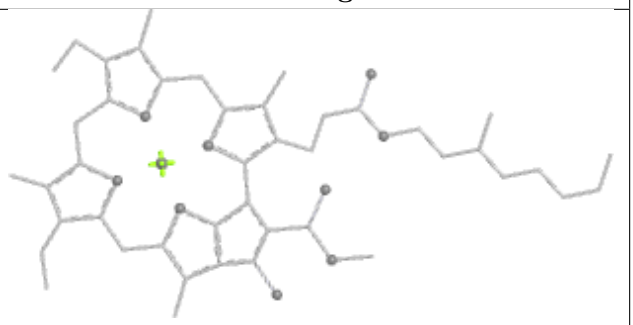
Bond lengths



Bond angles

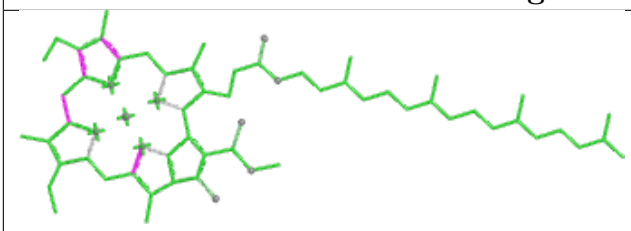


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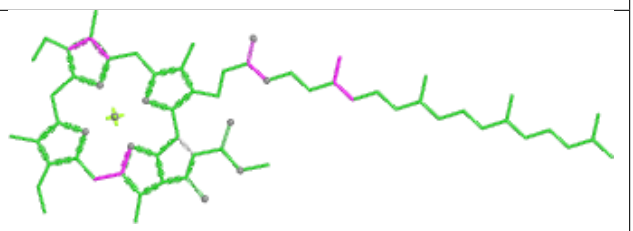


Rings

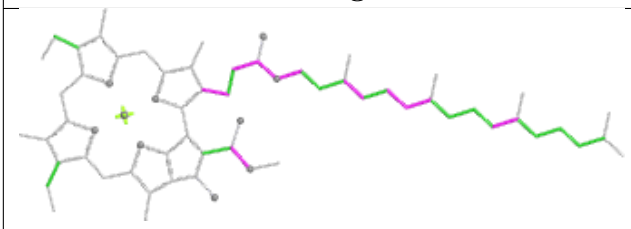
Ligand CLA b 808



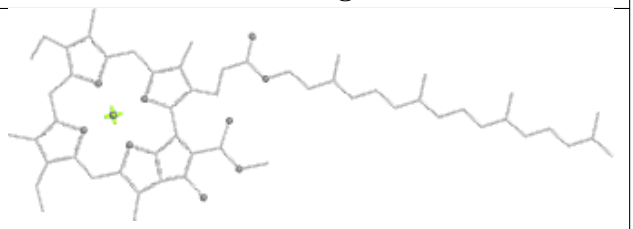
Bond lengths



Bond angles

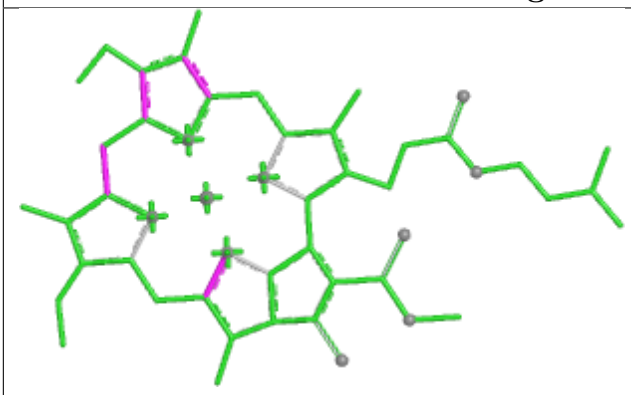


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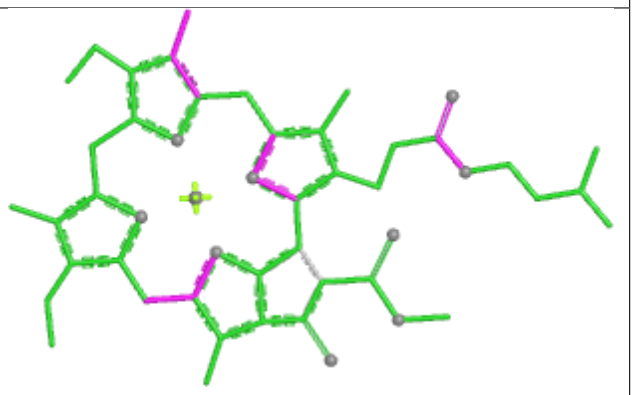


Rings

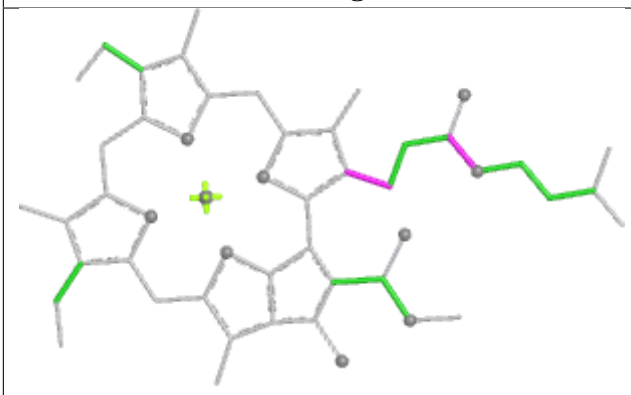
Ligand CLA b 839



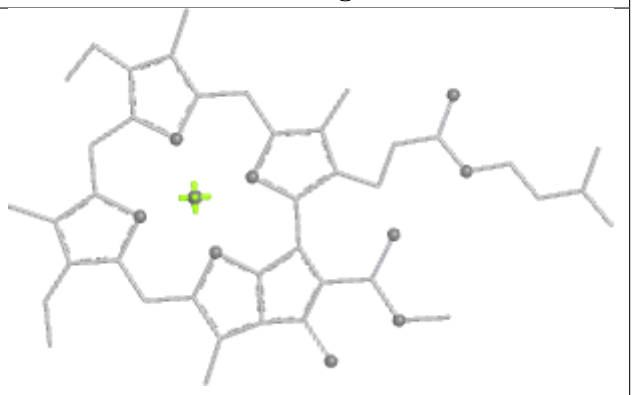
Bond lengths



Bond angles

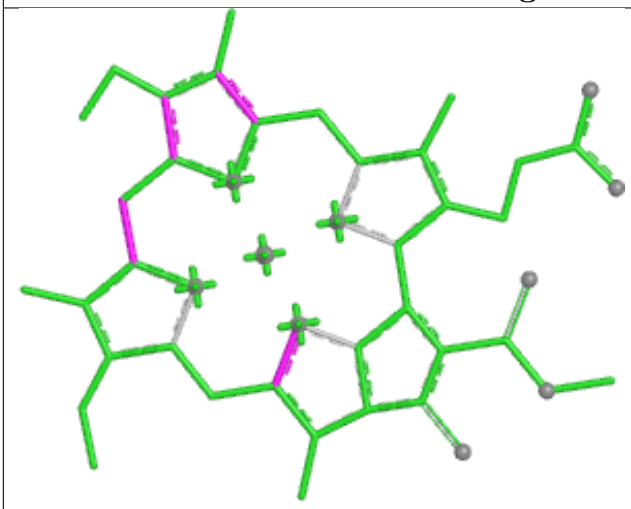


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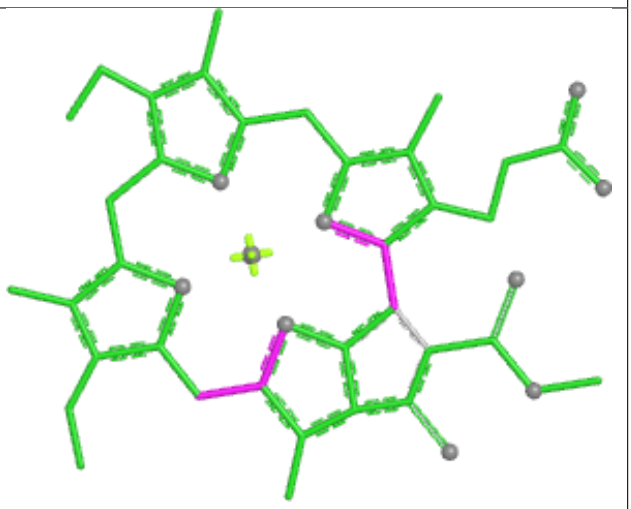


Rings

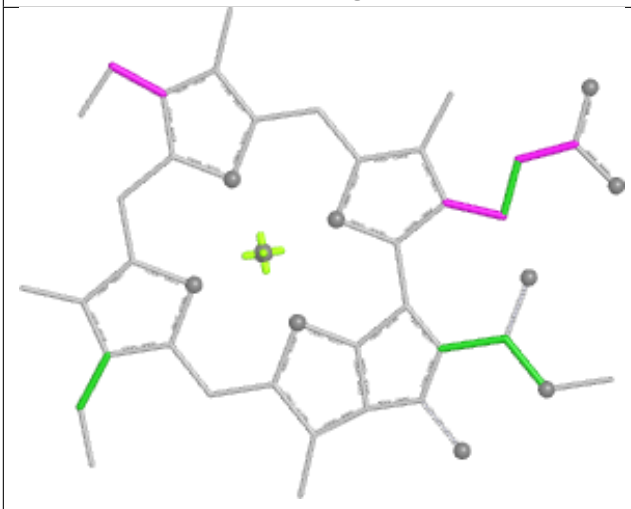
Ligand CLA J 1102



Bond lengths



Bond angles

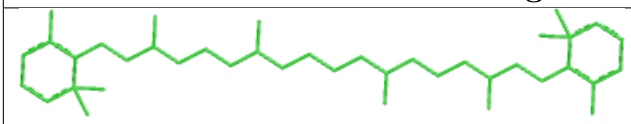


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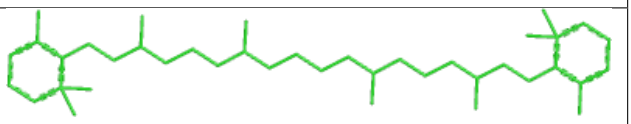


Rings

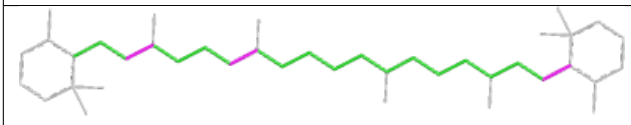
Ligand BCR b 856



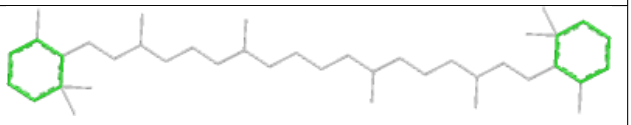
Bond lengths



Bond angles

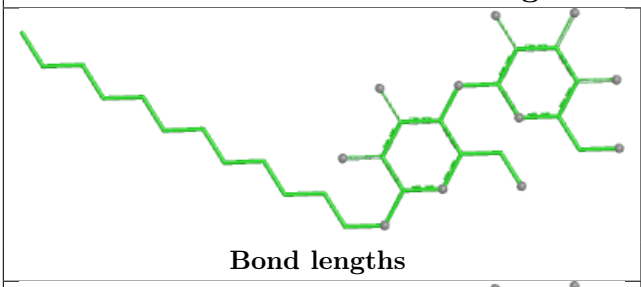


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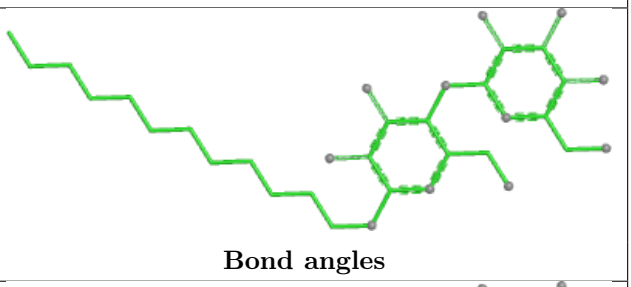


Rings

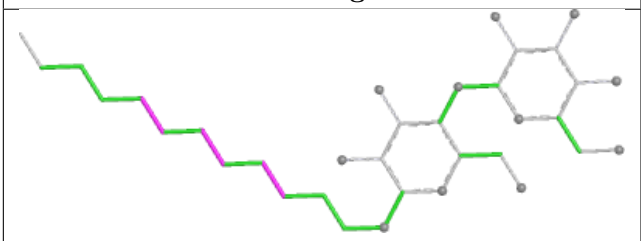
Ligand LMT B 854



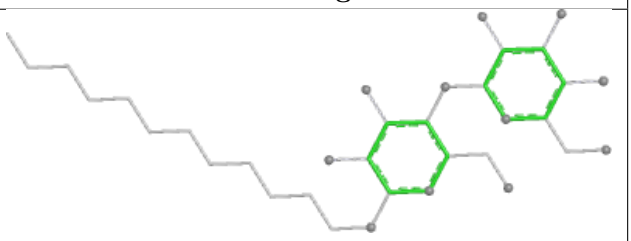
Bond lengths



Bond angles

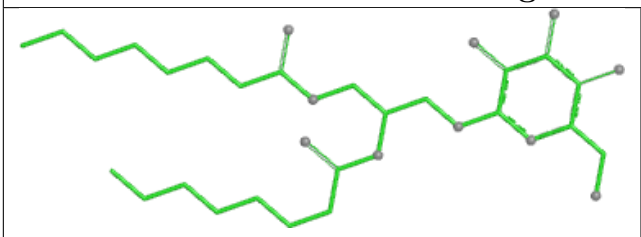


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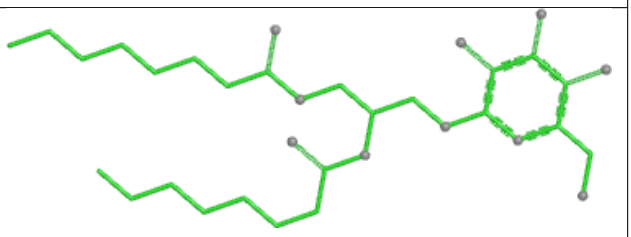


Rings

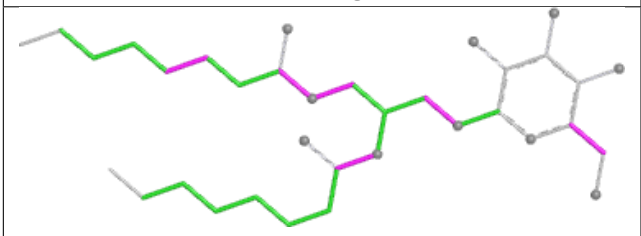
Ligand LMG K 105



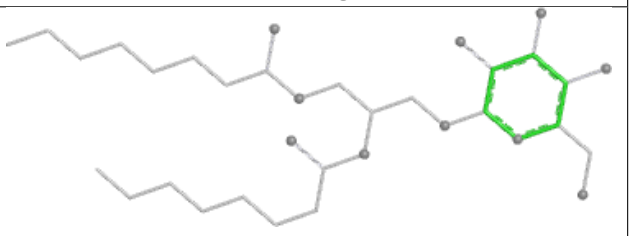
Bond lengths



Bond angles

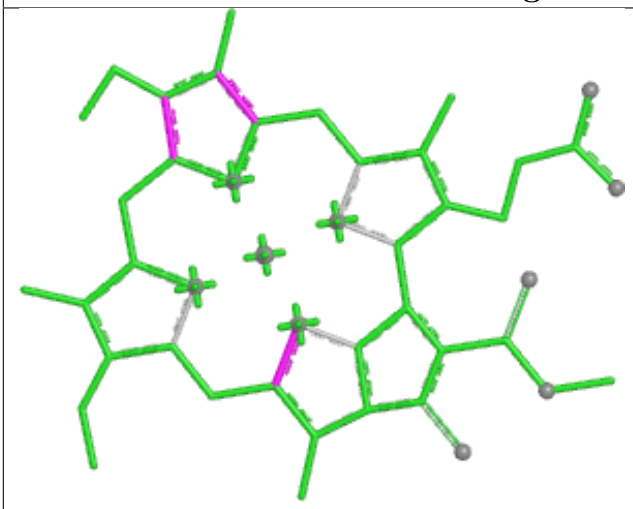


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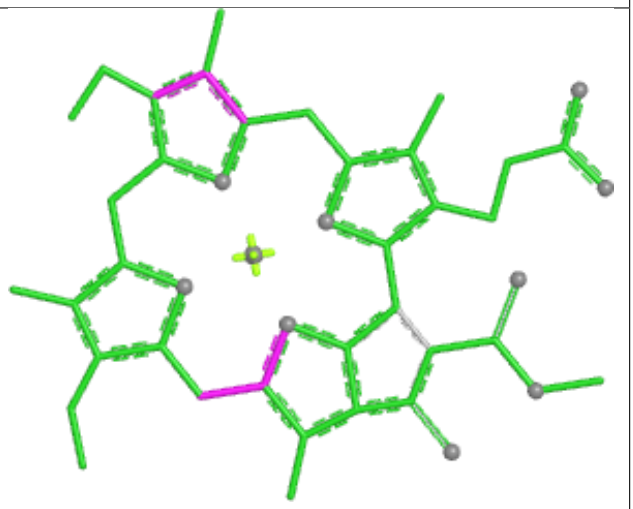


Rings

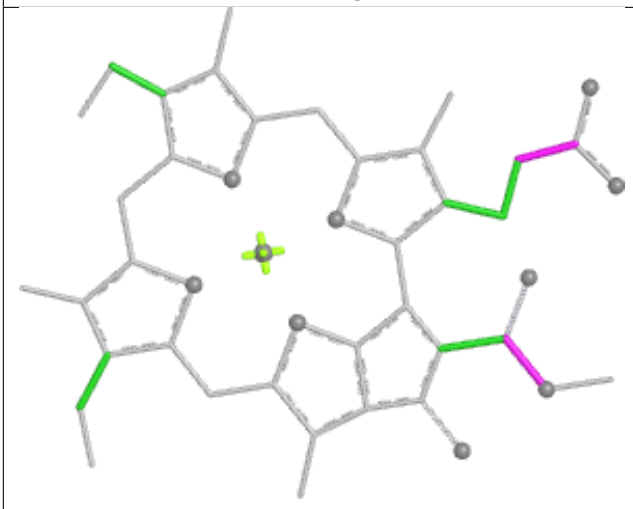
Ligand CLA G 816



Bond lengths



Bond angles

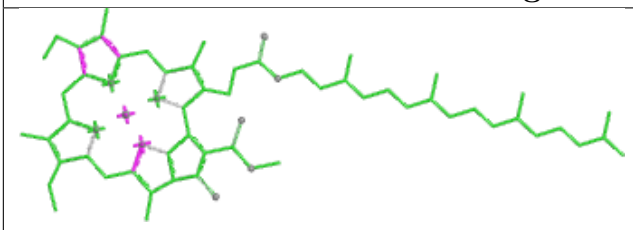


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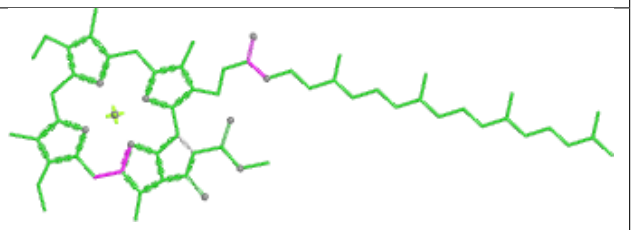


Rings

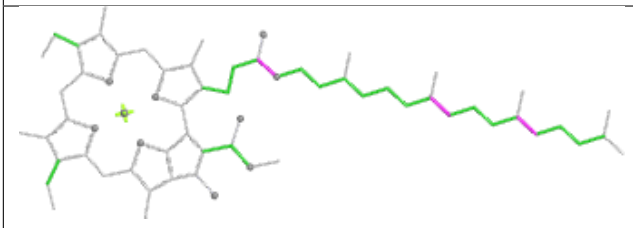
Ligand CLA U 205



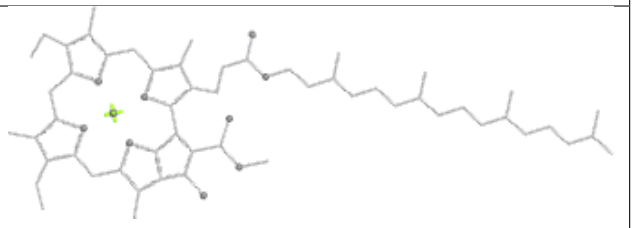
Bond lengths



Bond angles

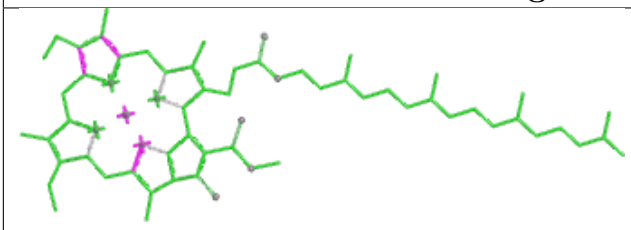


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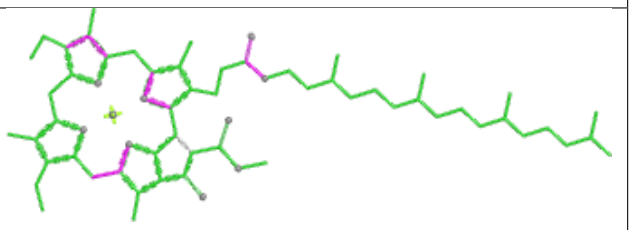


Rings

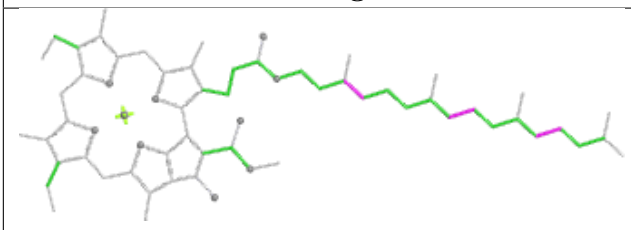
Ligand CLA a 839



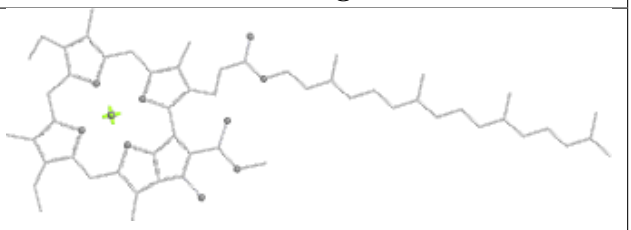
Bond lengths



Bond angles

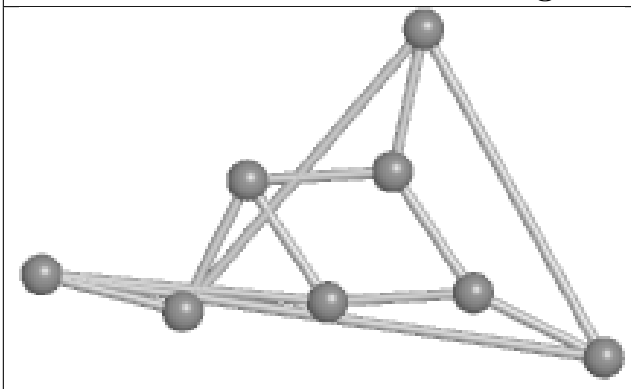


Torsions

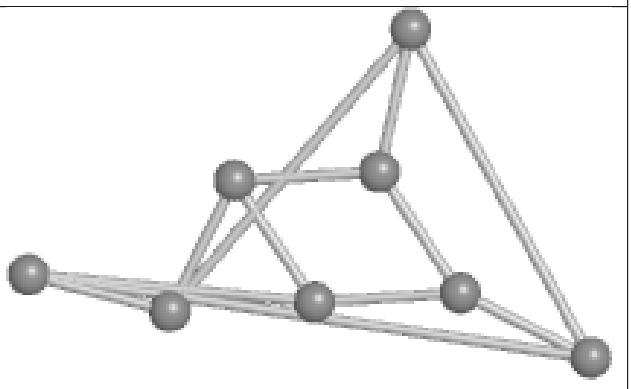


Rings

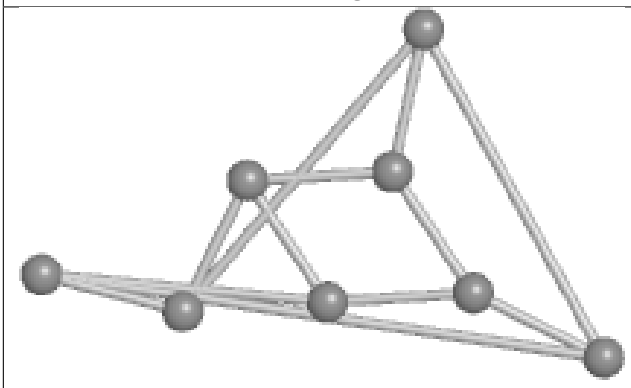
Ligand SF4 c 101



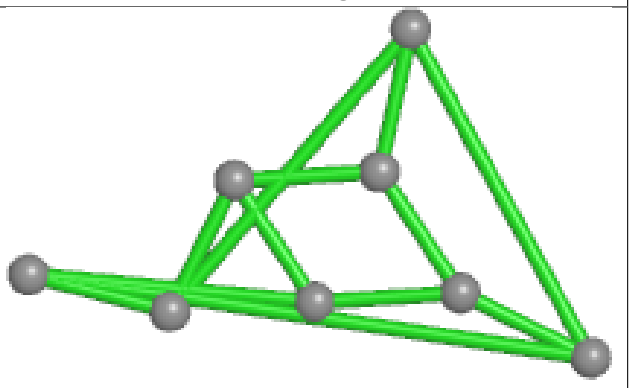
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Bond angles

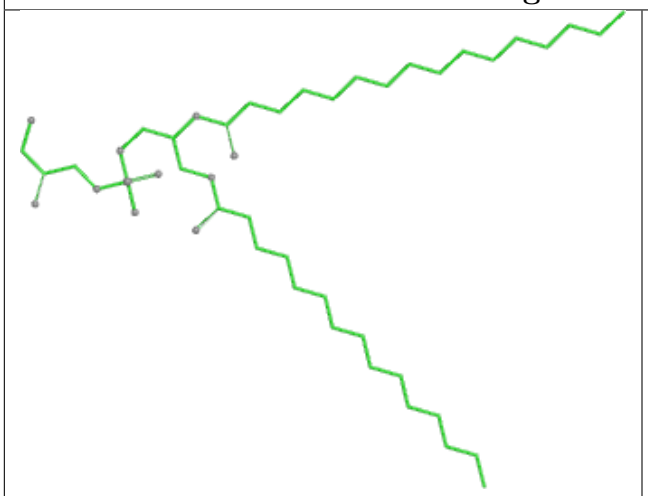


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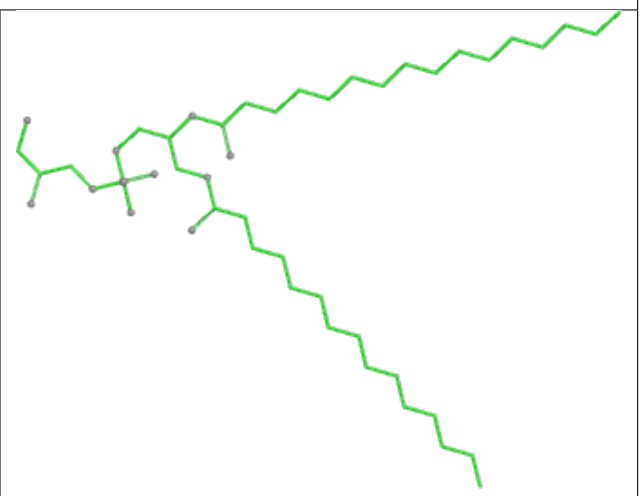


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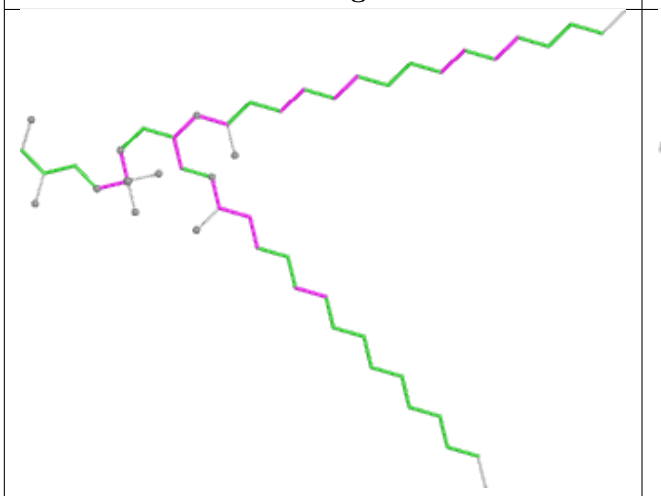
Ligand LHG A 801



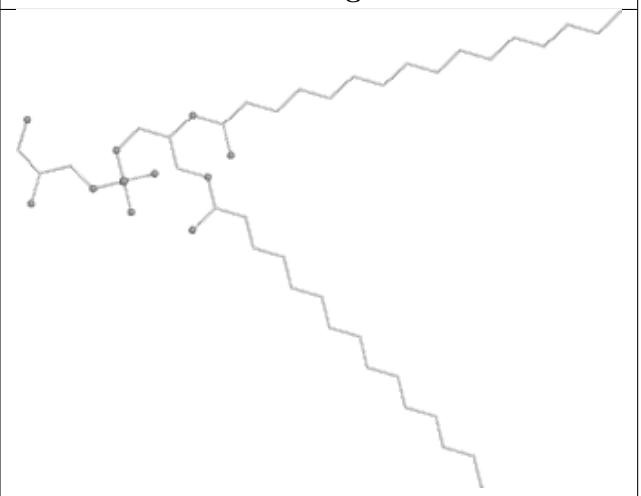
Bond lengths



Bond angles

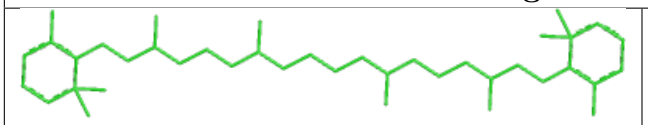


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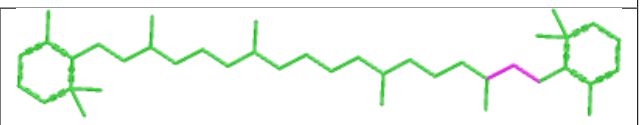


Rings

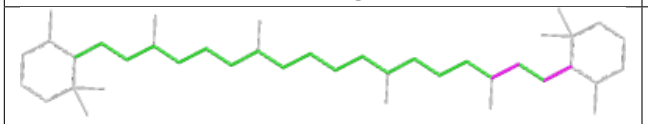
Ligand BCR A 850



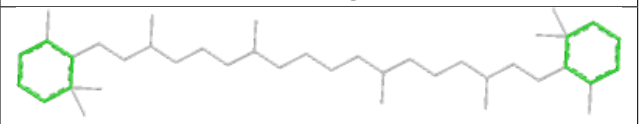
Bond lengths



Bond angles

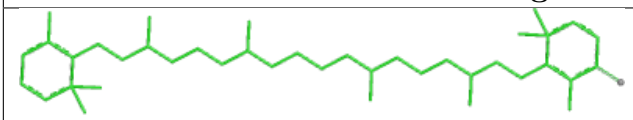


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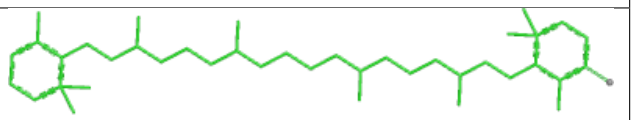


Rings

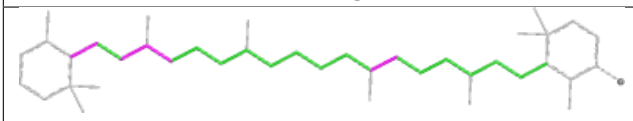
Ligand ECH i 102



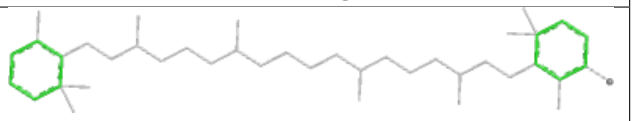
Bond lengths



Bond angles

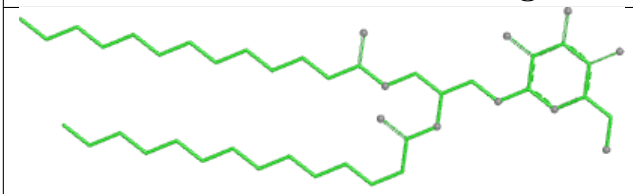


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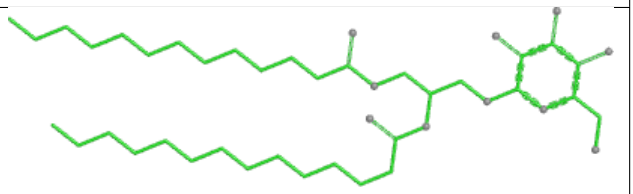


Rings

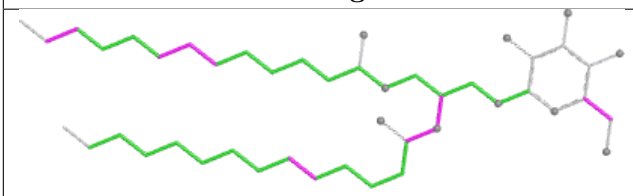
Ligand LMG A 852



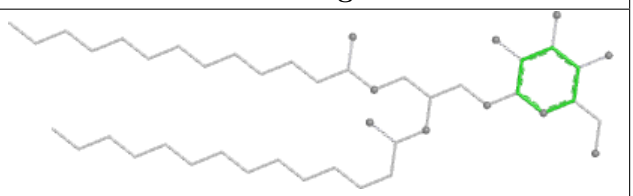
Bond lengths



Bond angles

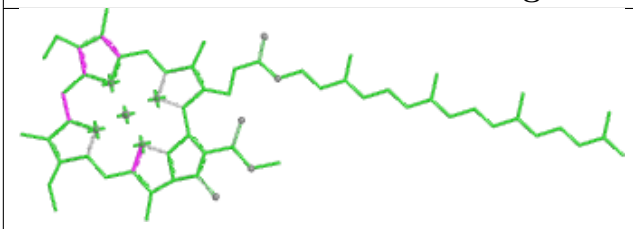


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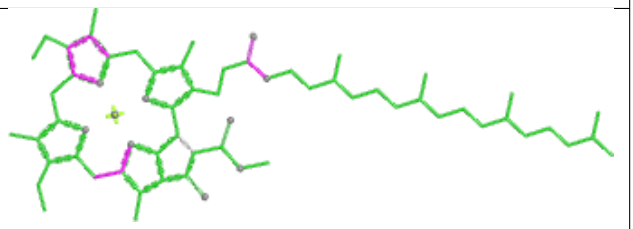


Rings

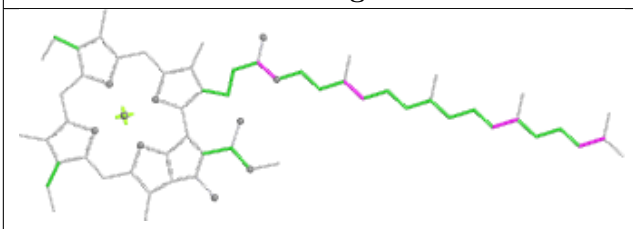
Ligand CLA G 828



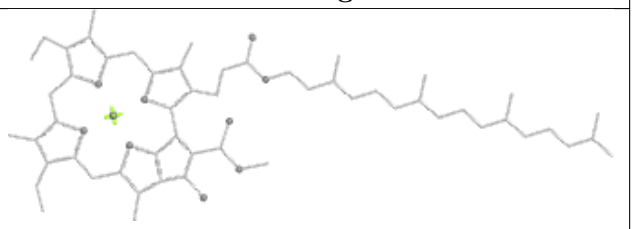
Bond lengths



Bond angles

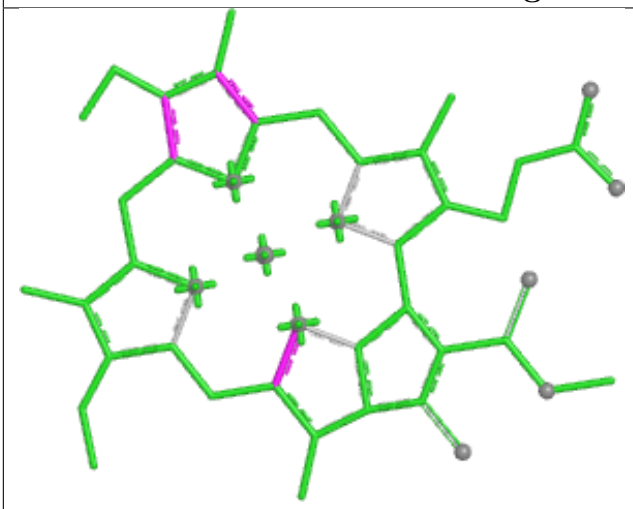


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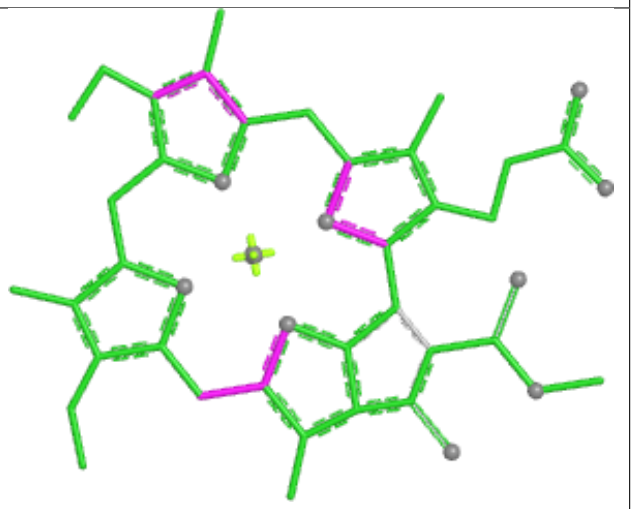


Rings

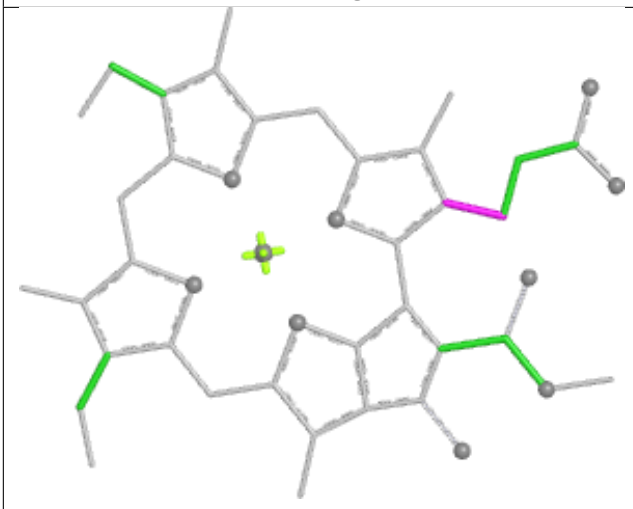
Ligand CLA A 815



Bond lengths



Bond angles

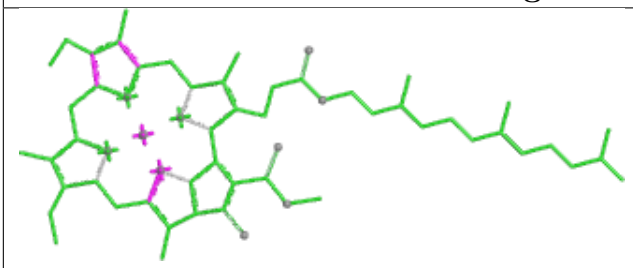


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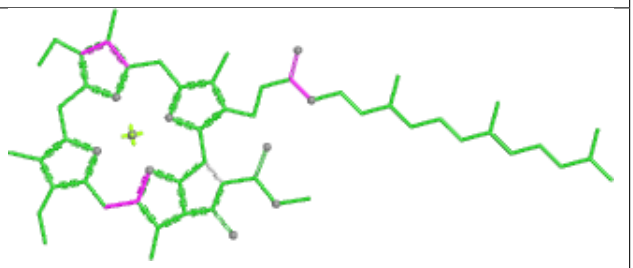


Rings

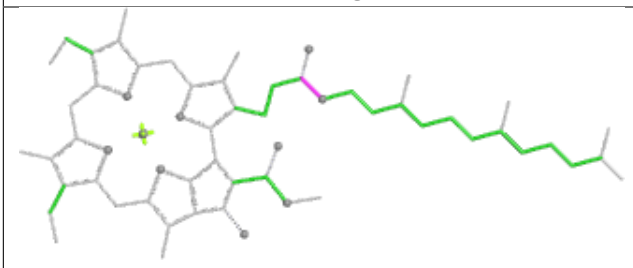
Ligand CLA A 826



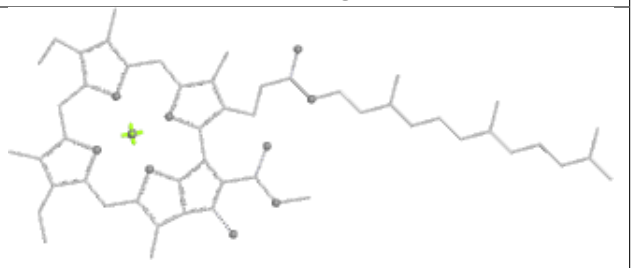
Bond lengths



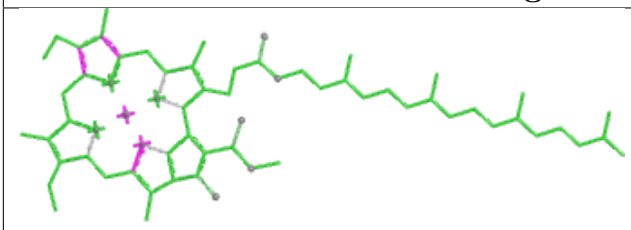
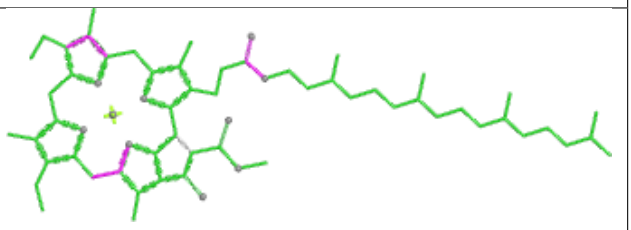
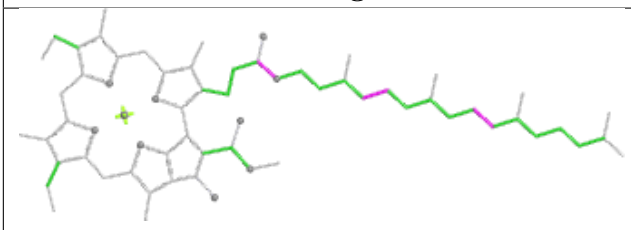
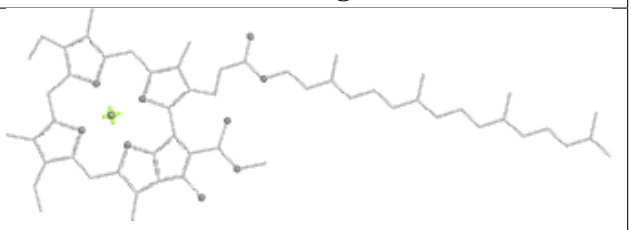
Bond angles

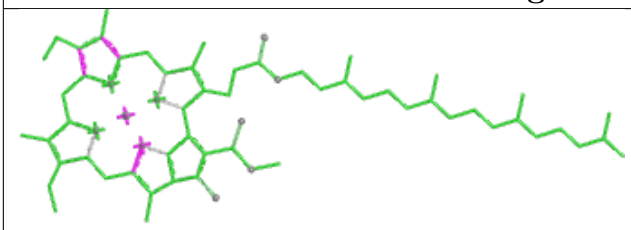
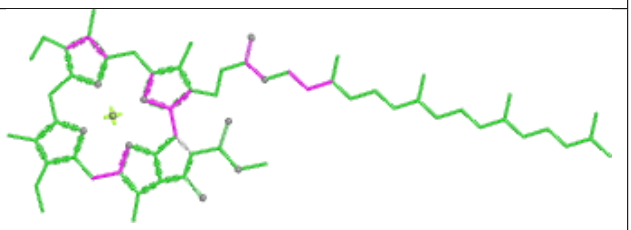
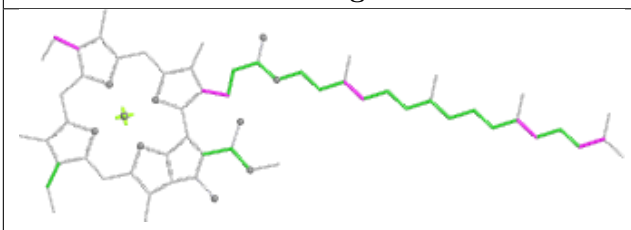
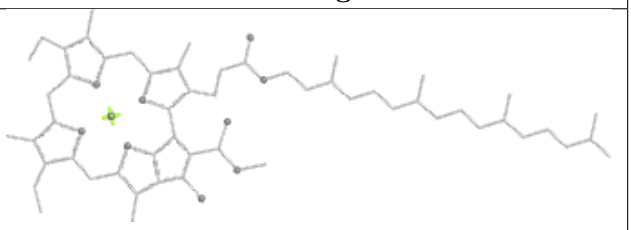


Torsions

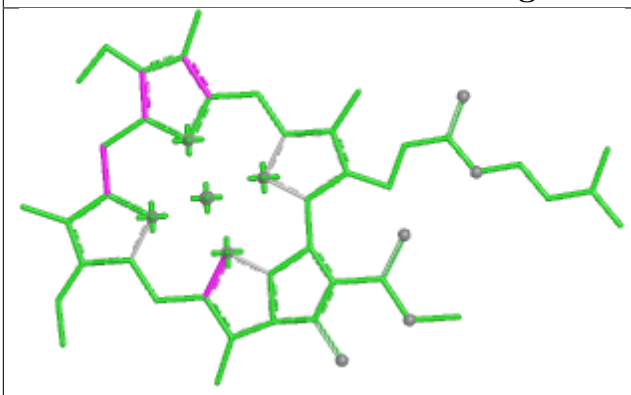


Rings

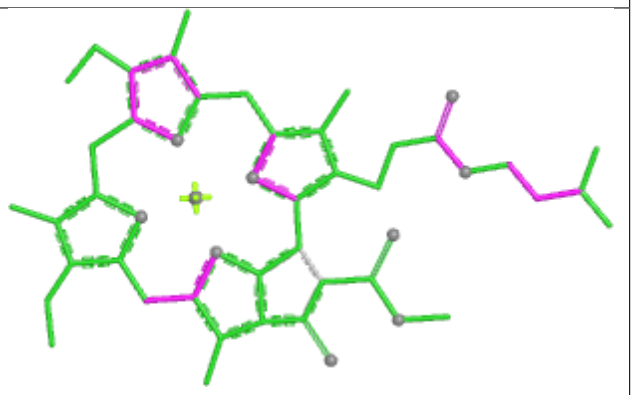
Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

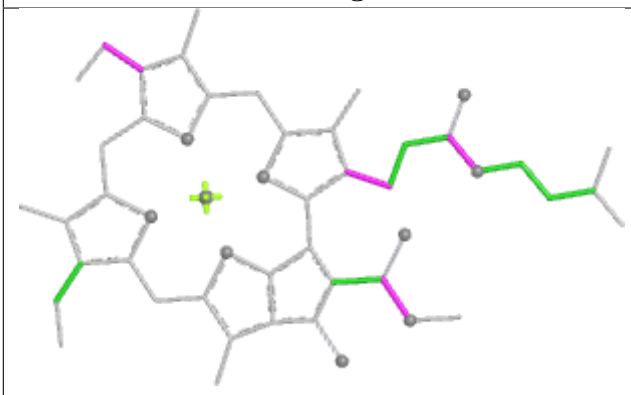
Ligand CLA S 1103



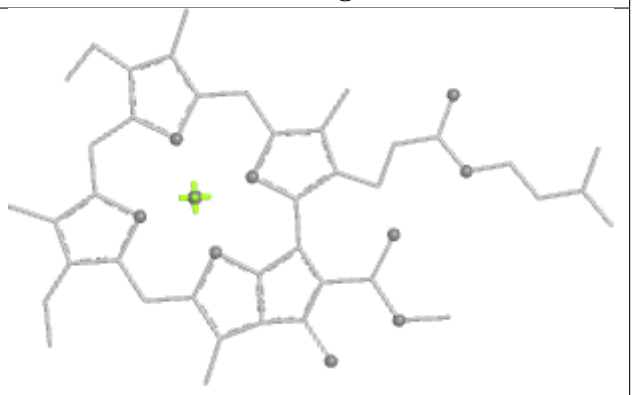
Bond lengths



Bond angles

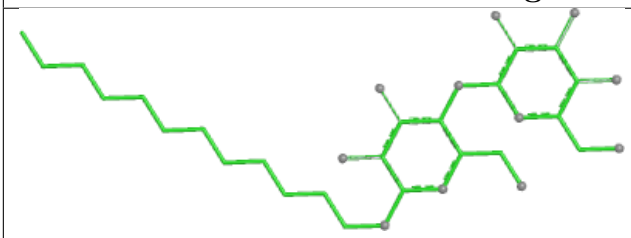


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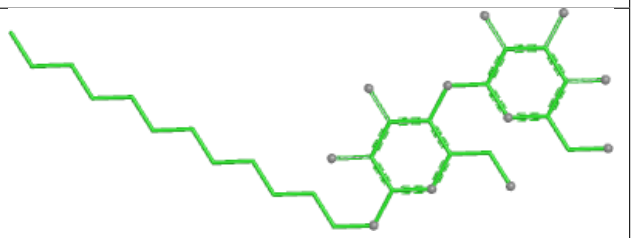


Rings

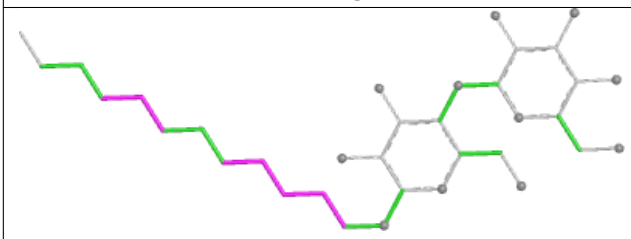
Ligand LMT b 854



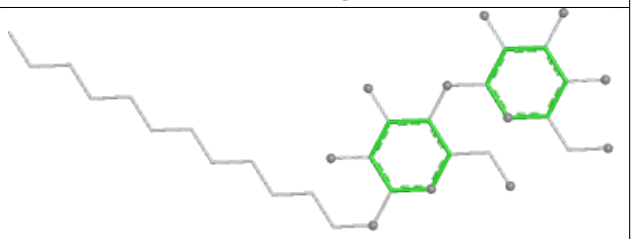
Bond lengths



Bond angles

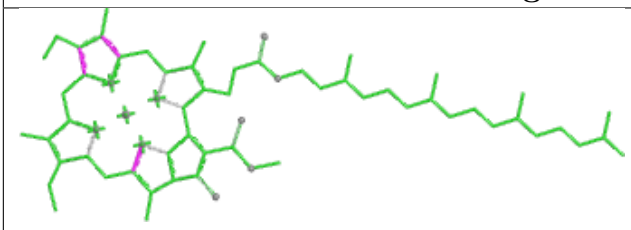


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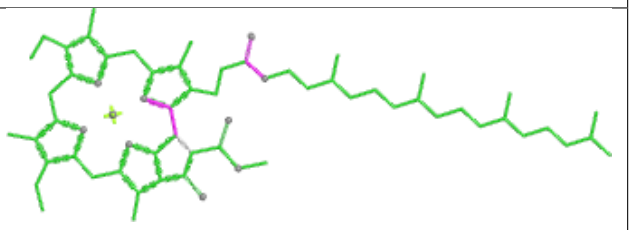


Rings

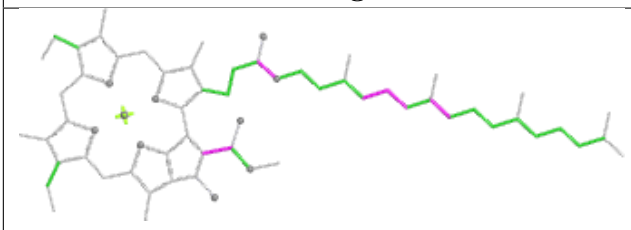
Ligand CLA G 831



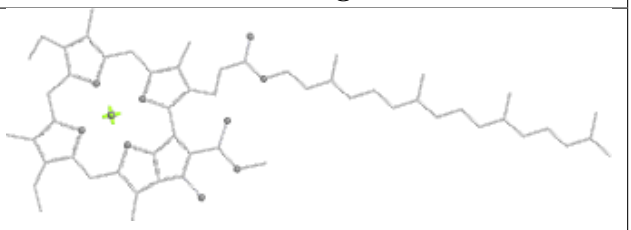
Bond lengths



Bond angles

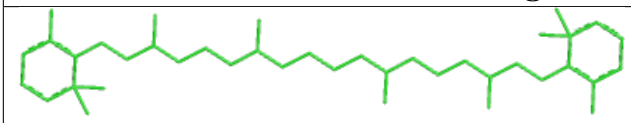


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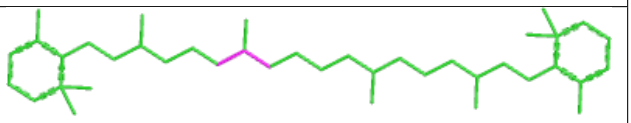


Rings

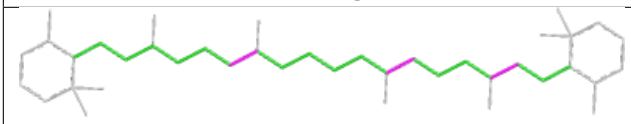
Ligand BCR F 202



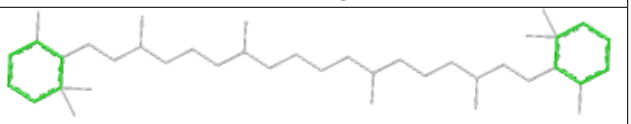
Bond lengths



Bond angles

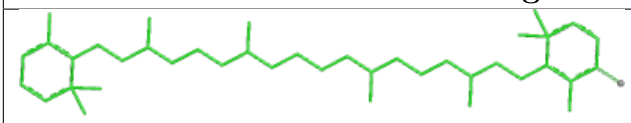


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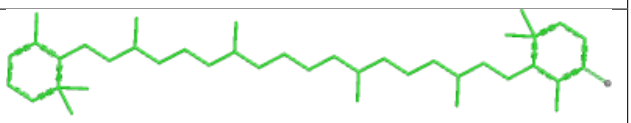


Rings

Ligand ECH R 102



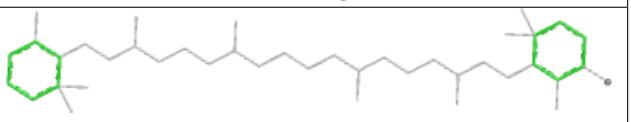
Bond lengths



Bond angles

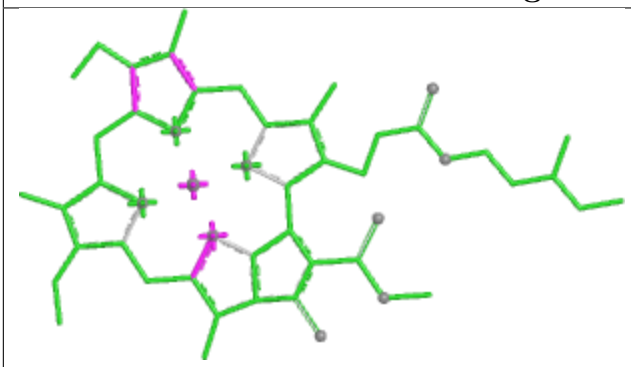


Torsions

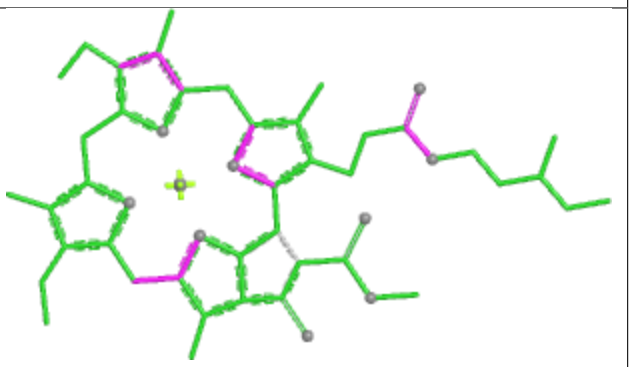


Rings

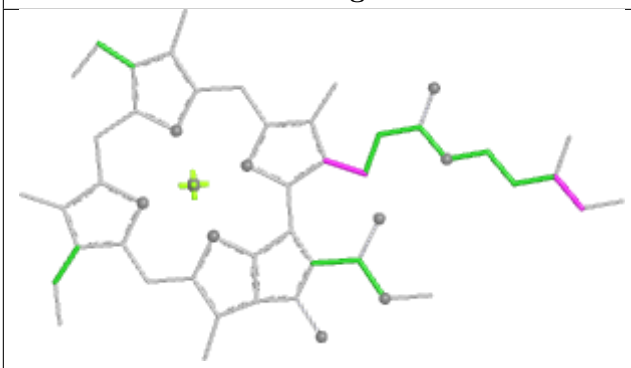
Ligand CLA A 823



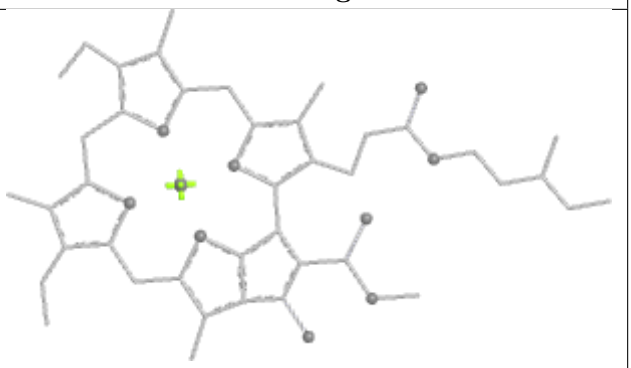
Bond lengths



Bond angles

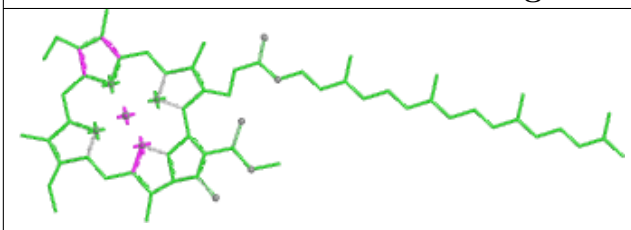


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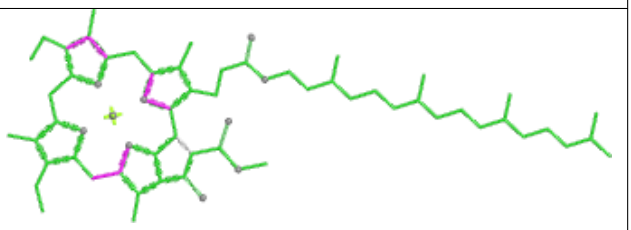


Rings

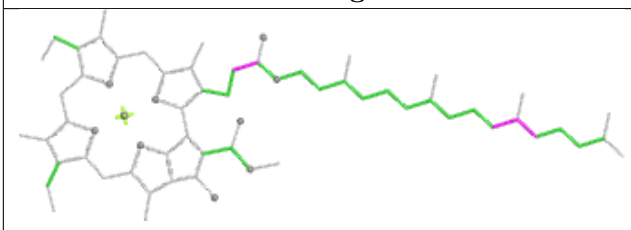
Ligand CLA B 812



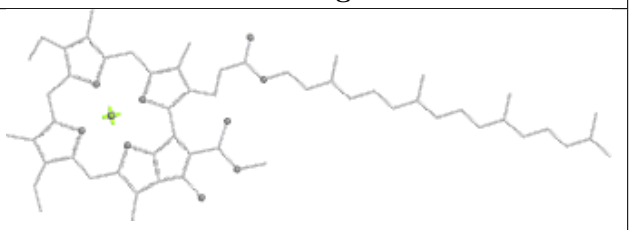
Bond lengths



Bond angles

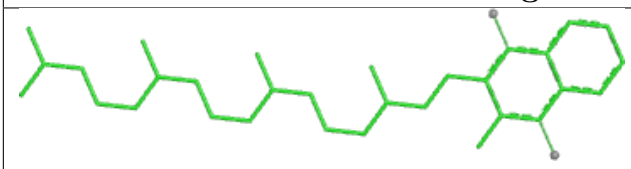


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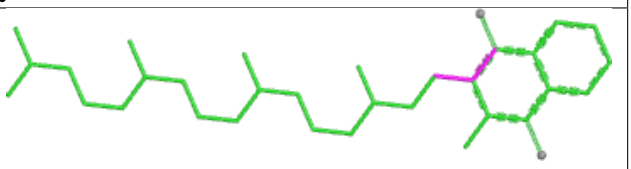


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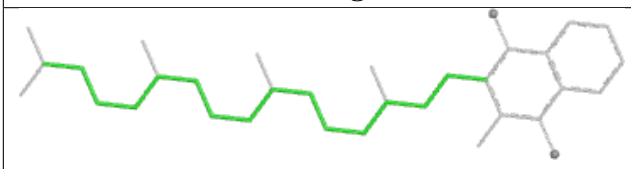
Ligand PQN A 845



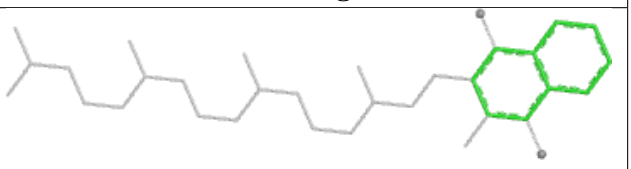
Bond lengths



Bond angles

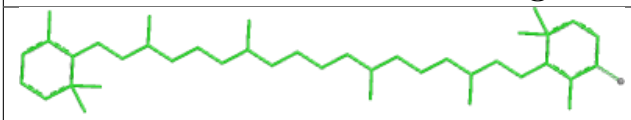


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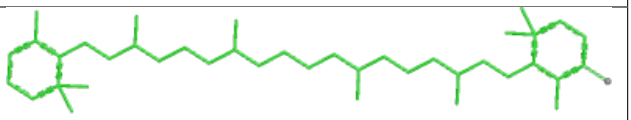


Rings

Ligand ECH I 102



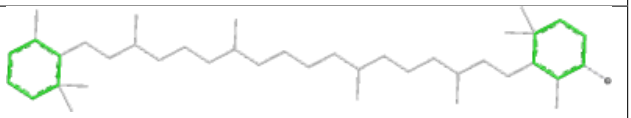
Bond lengths



Bond angles

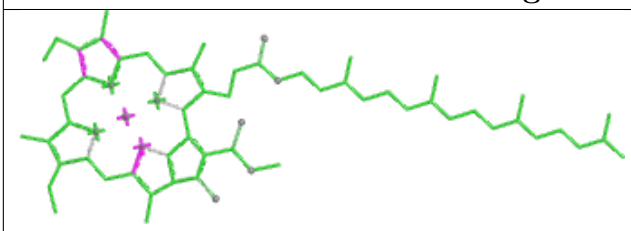


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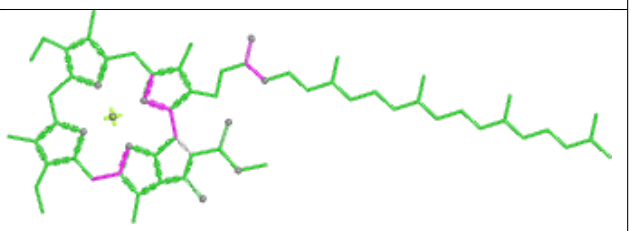


Rings

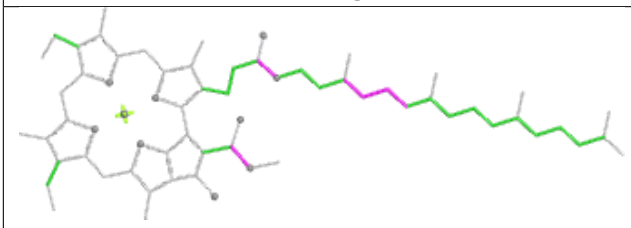
Ligand CLA G 821



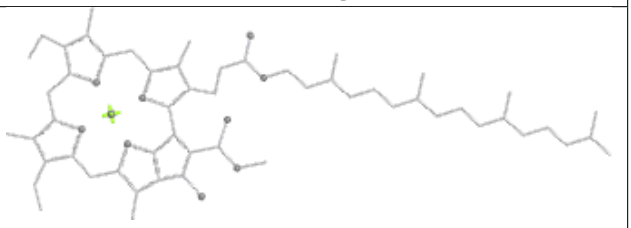
Bond lengths



Bond angles

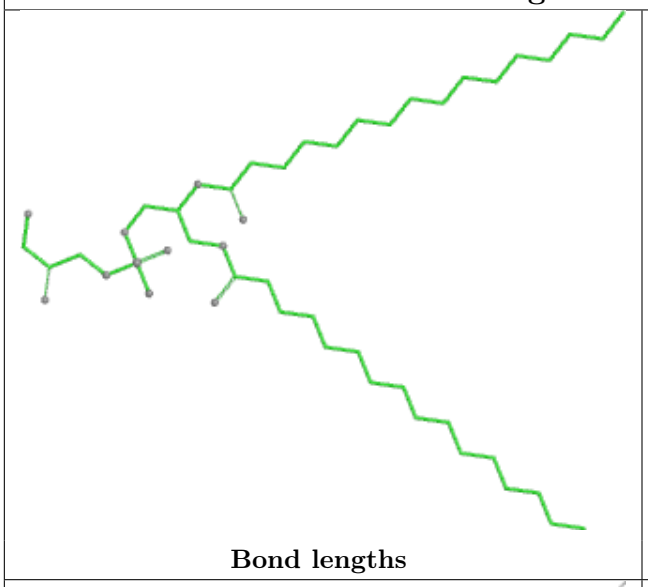


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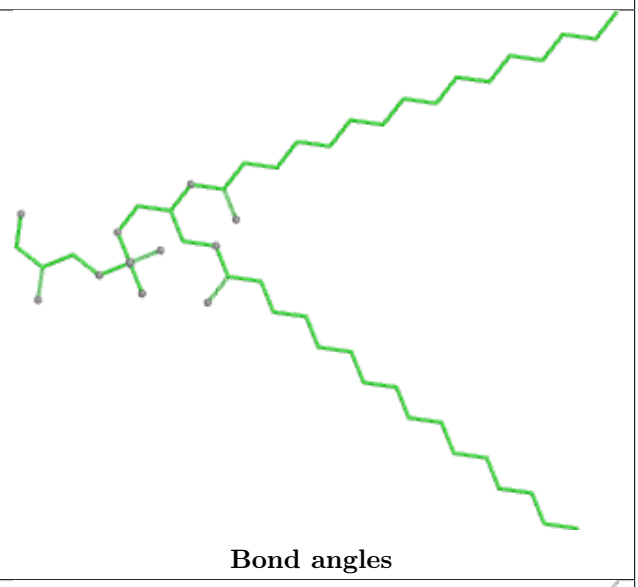


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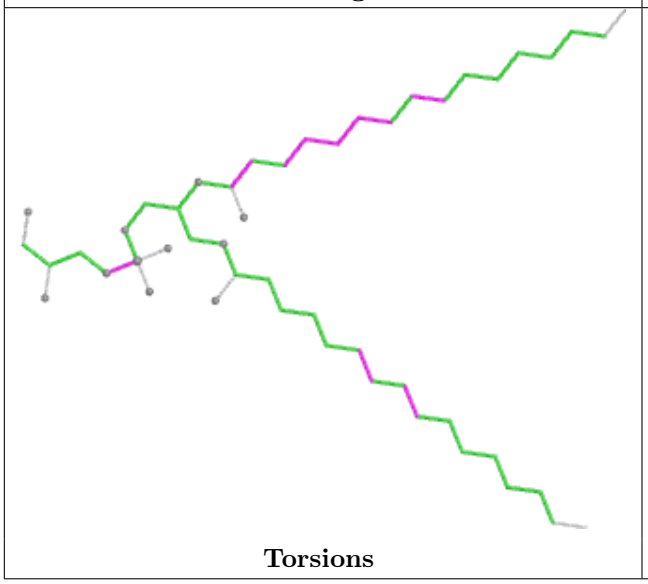
Ligand LHG a 855



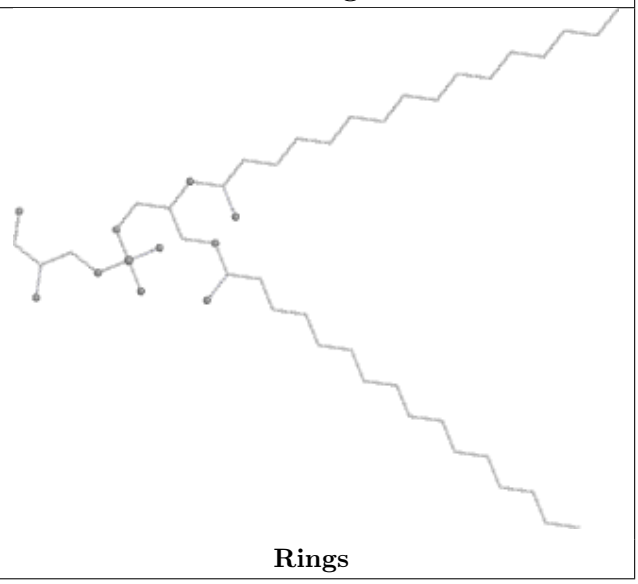
Bond lengths



Bond angles

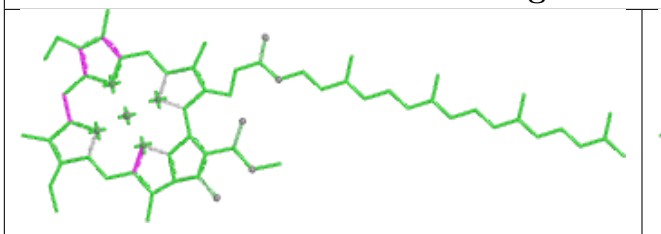


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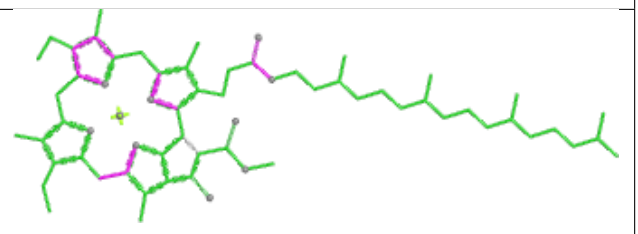


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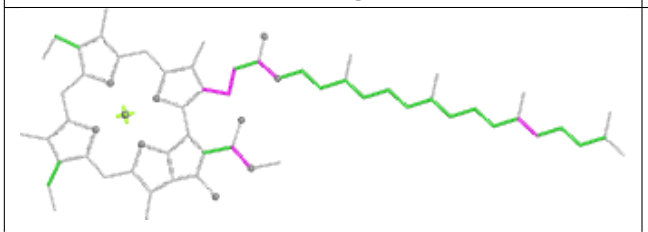
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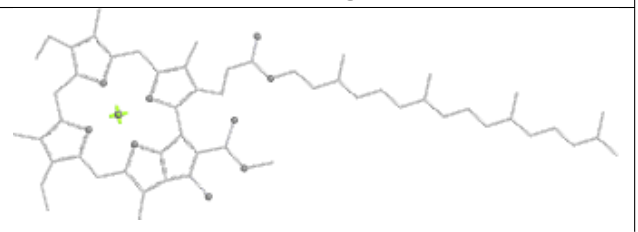
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Bond angles

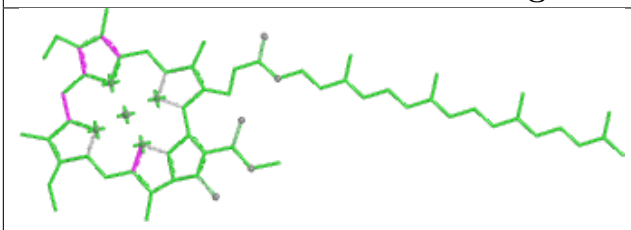


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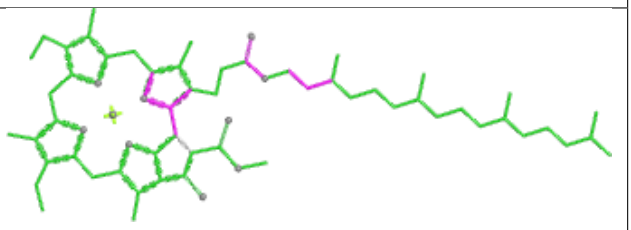


Rings

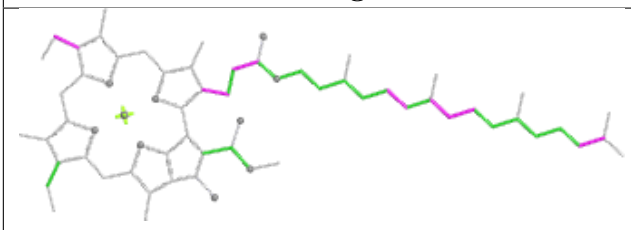
Ligand CLA a 818



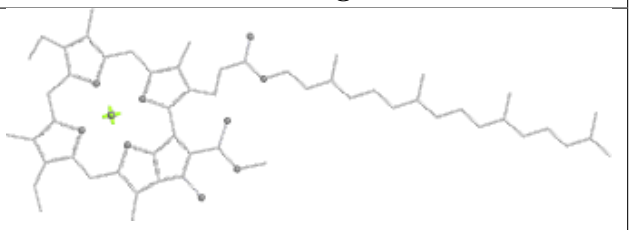
Bond lengths



Bond angles

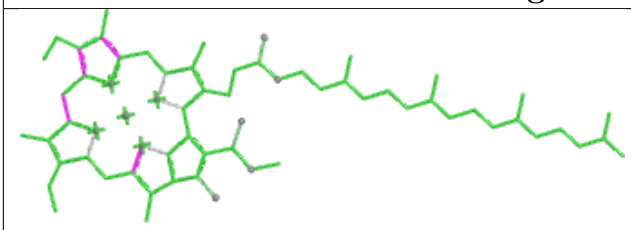


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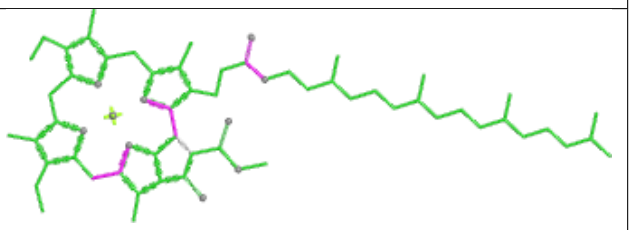


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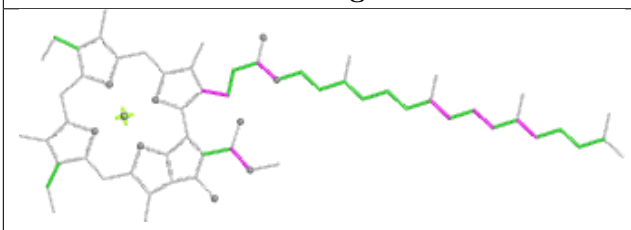
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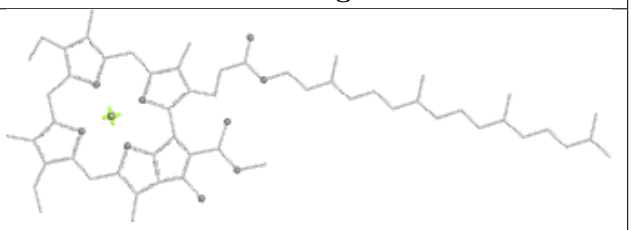
Bond lengths



Bond angles



Torsions



Rings

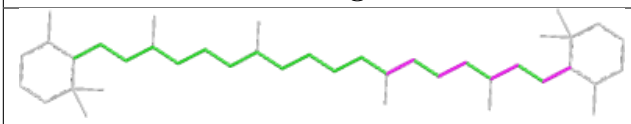
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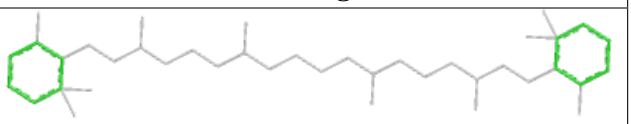
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Bond angles

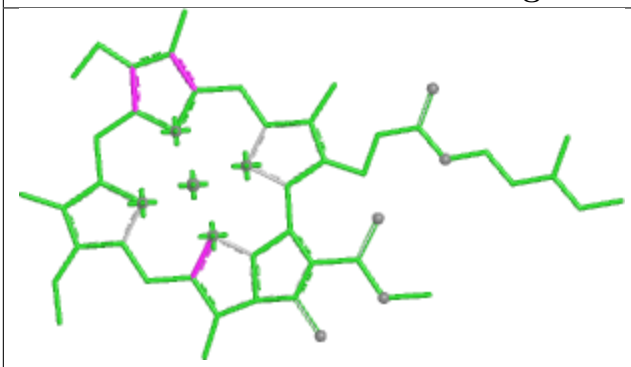


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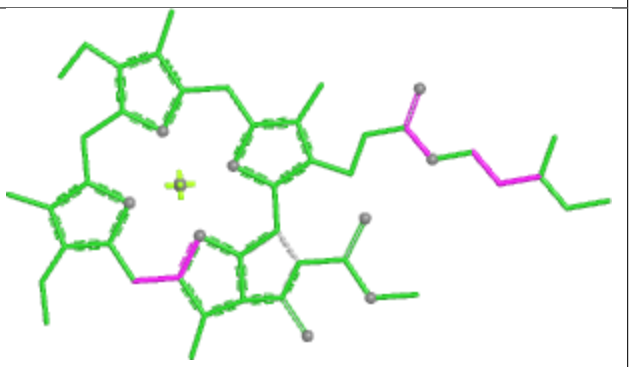


Rings

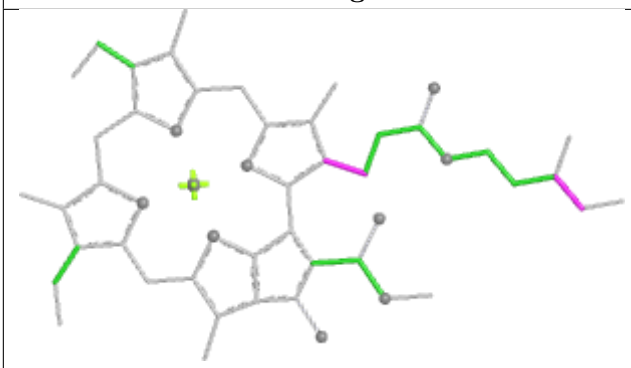
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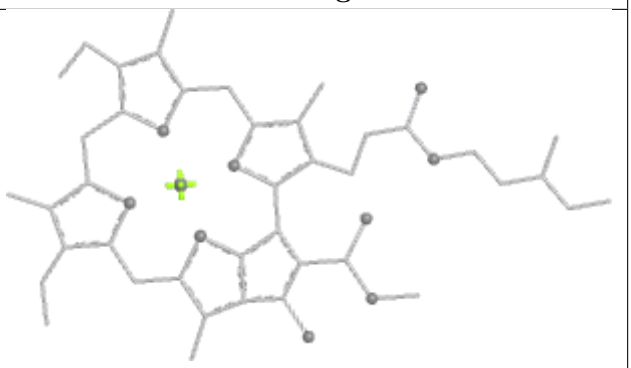
Bond lengths



Bond angles

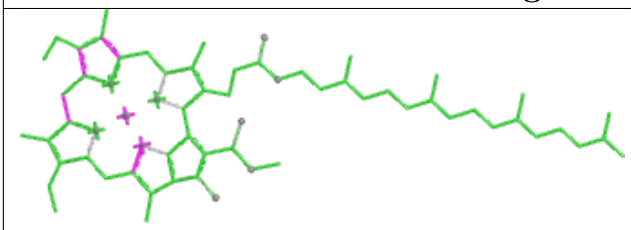


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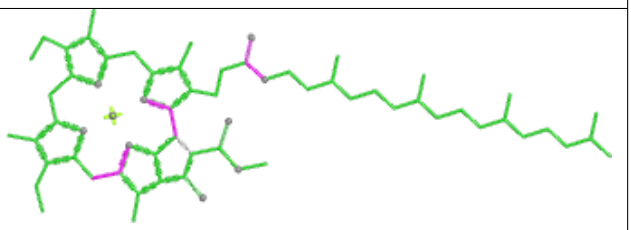


Rings

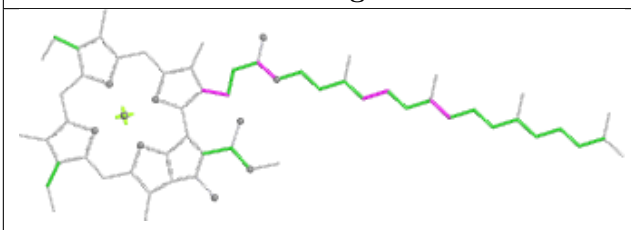
Ligand CLA H 833



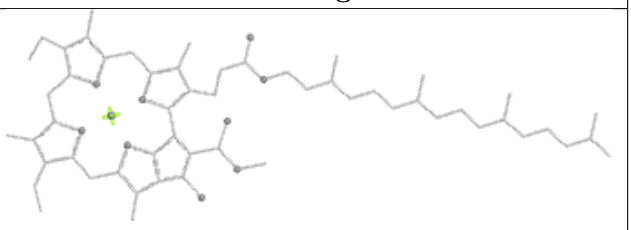
Bond lengths



Bond angles

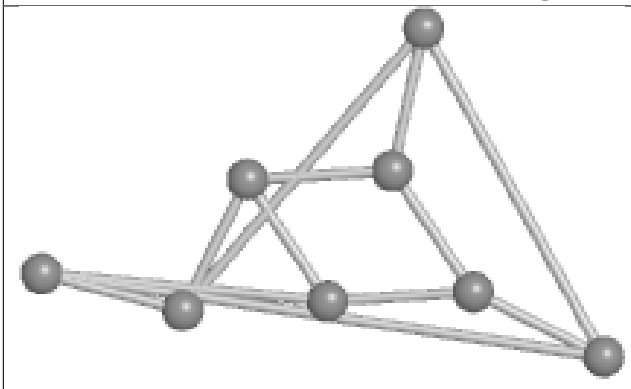


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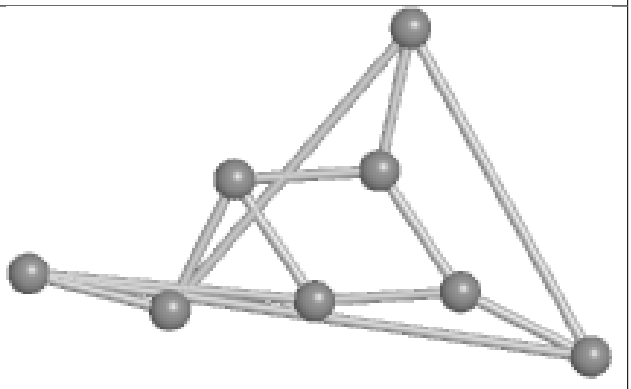


Rings

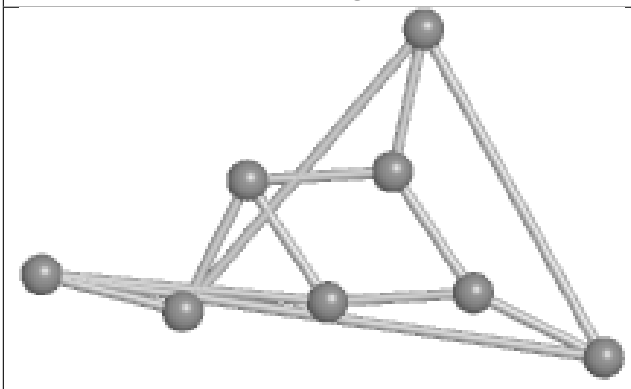
Ligand SF4 c 102



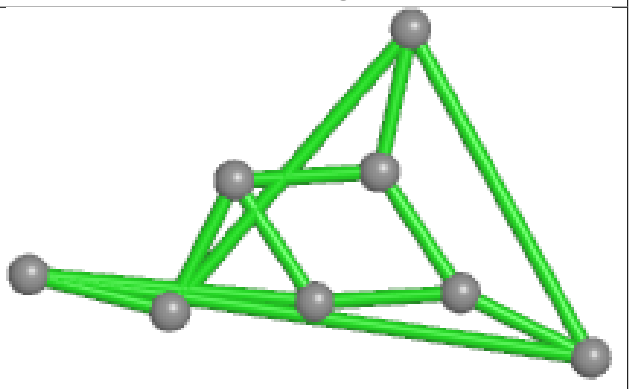
Bond lengths



Bond angles

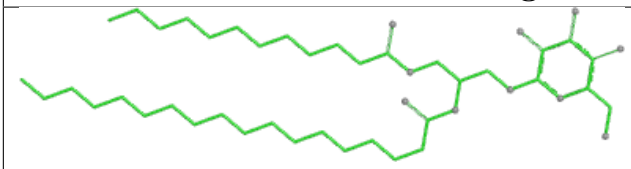


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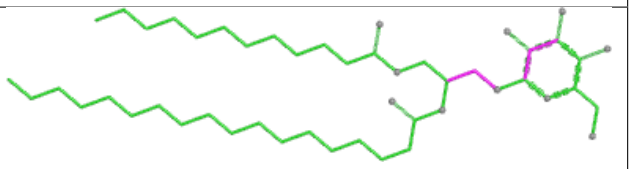


Rings

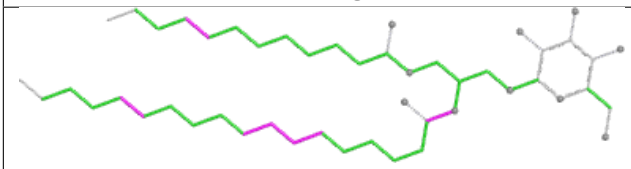
Ligand LMG B 853



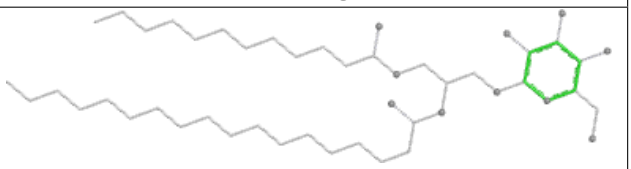
Bond lengths



Bond angles

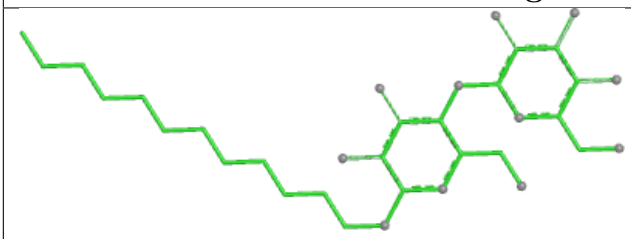


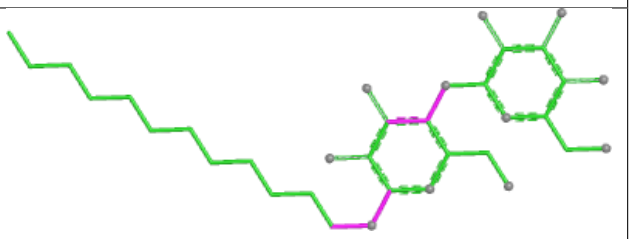
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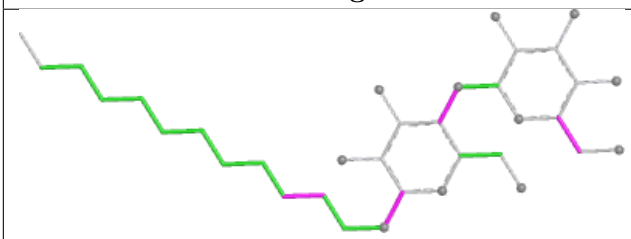


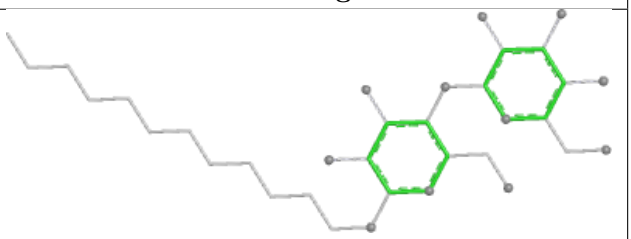
Rings

Ligand LMT a 856

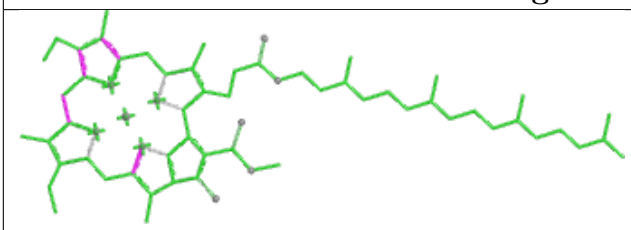

Bond lengths

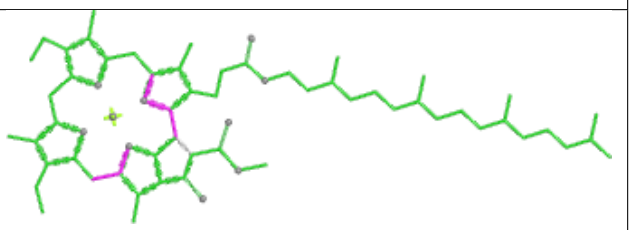

Bond angles

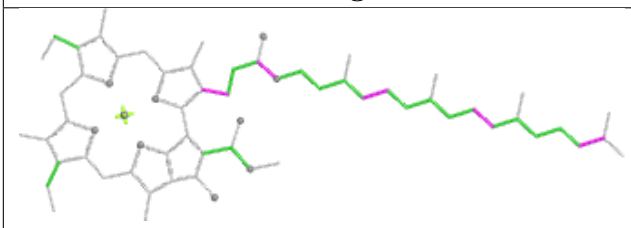

Torsions

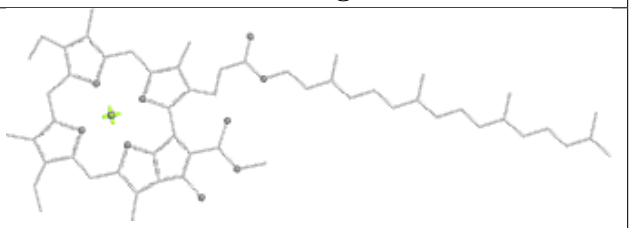

Rings

Ligand CLA f 201

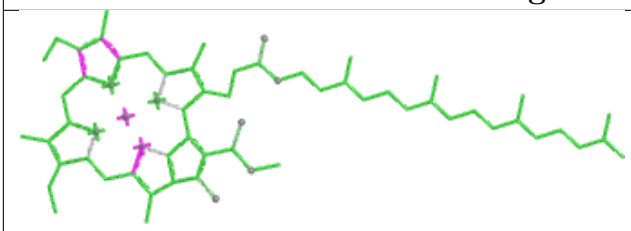

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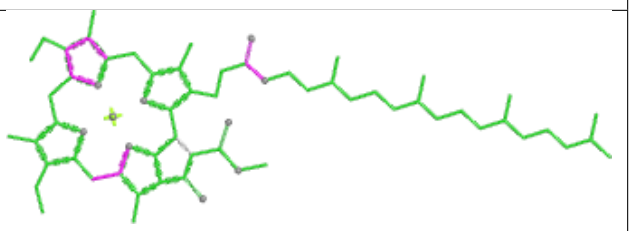

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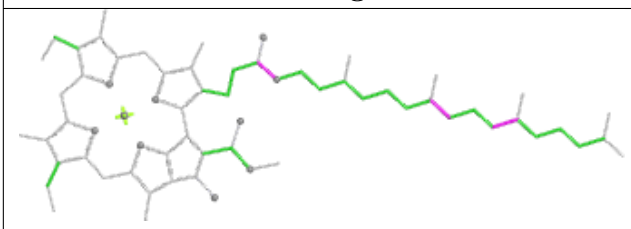

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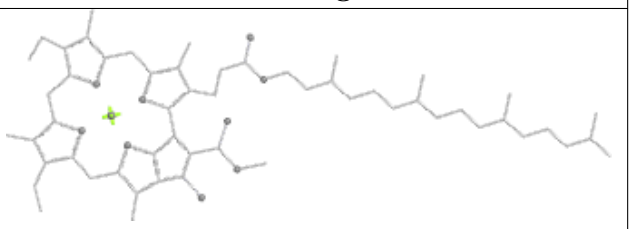

Rings

Ligand CLA a 836

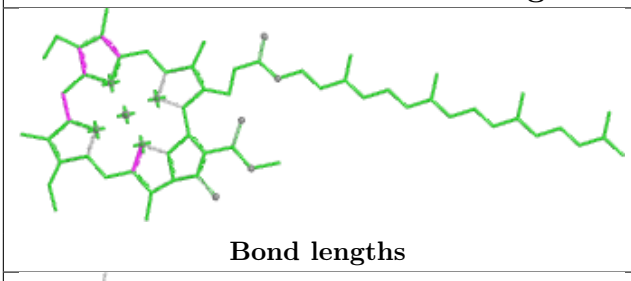

Bond lengths


Bond angles

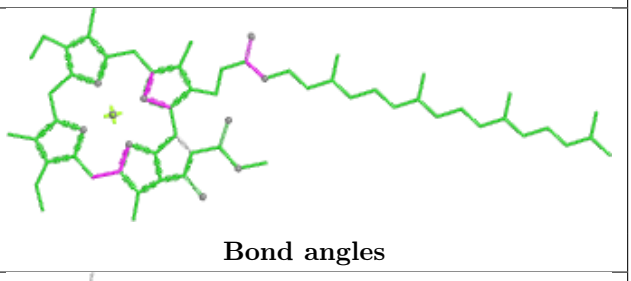

Torsions


Rings

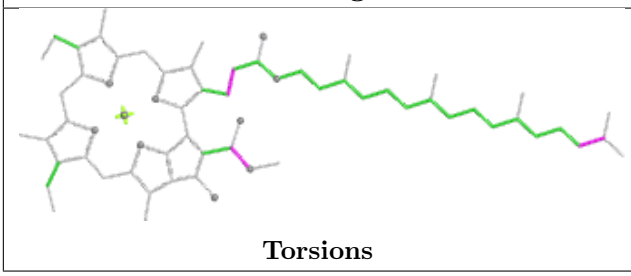
Ligand CLA b 807



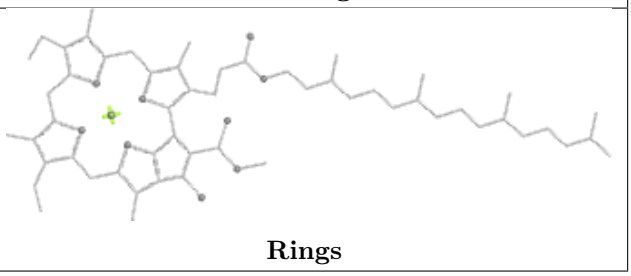
Bond lengths



Bond angles

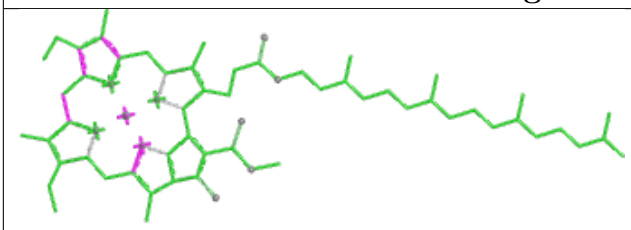


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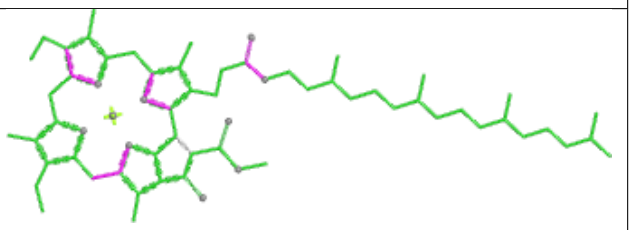


Rings

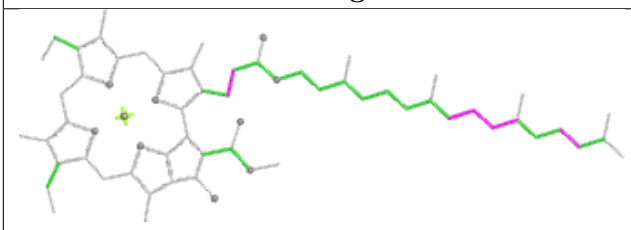
Ligand CLA A 858



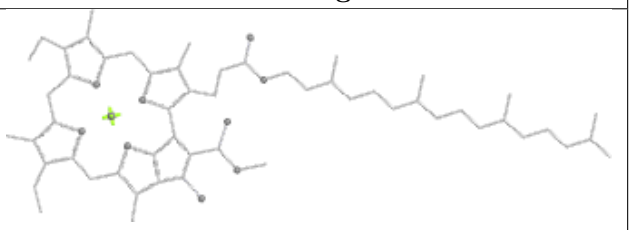
Bond lengths



Bond angles

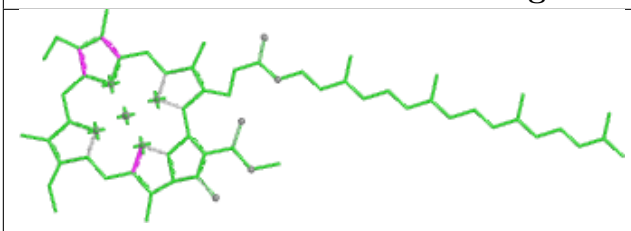


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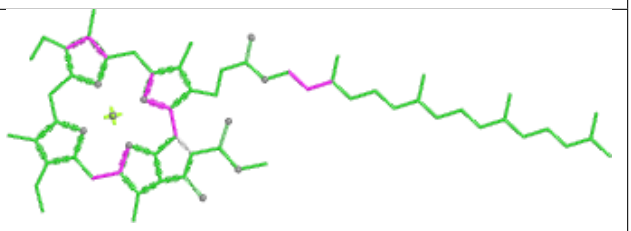


Rings

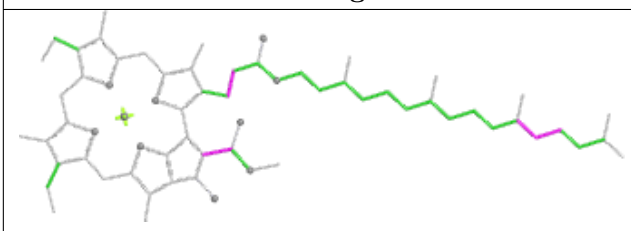
Ligand CLA a 809



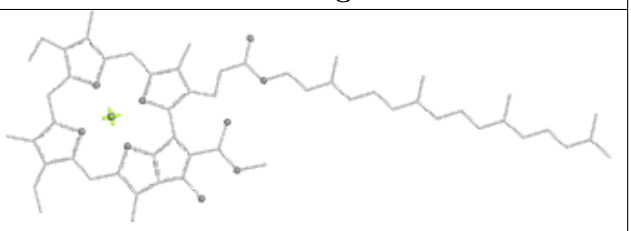
Bond lengths



Bond angles

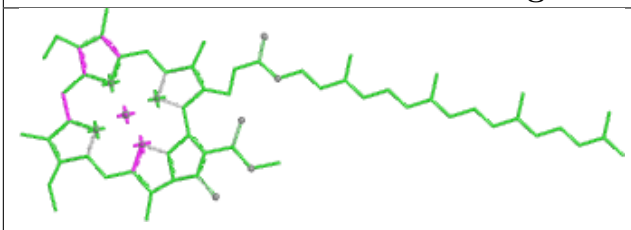


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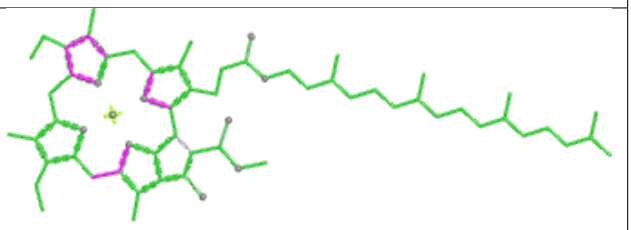


Rings

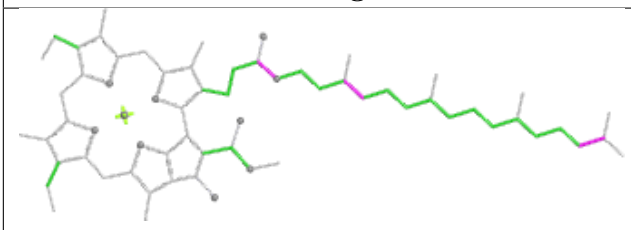
Ligand CLA b 831



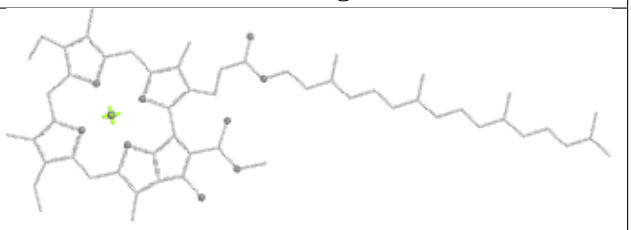
Bond lengths



Bond angles

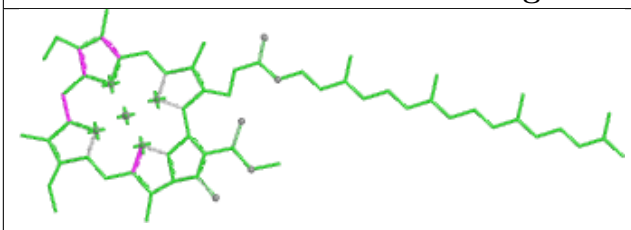


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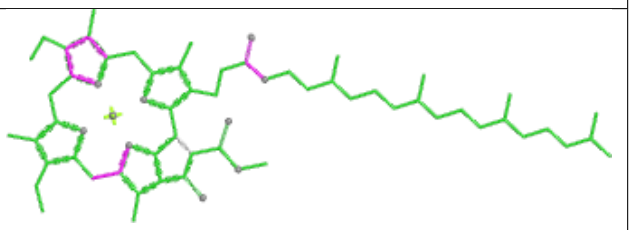


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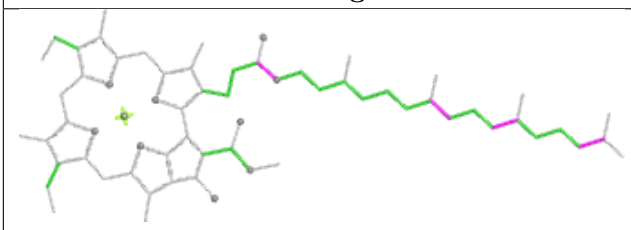
Ligand CLA G 835



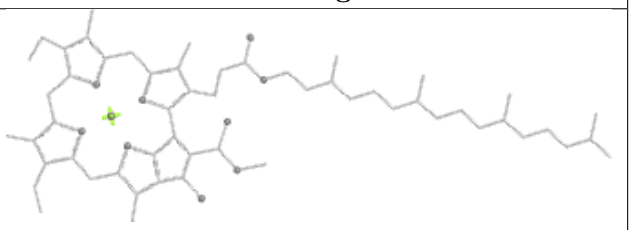
Bond lengths



Bond angles

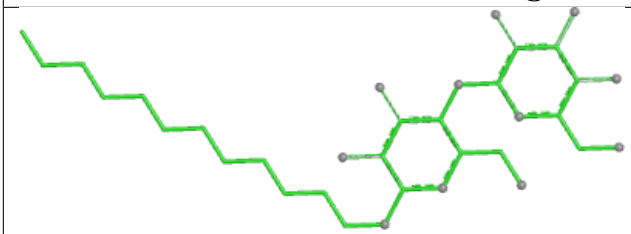


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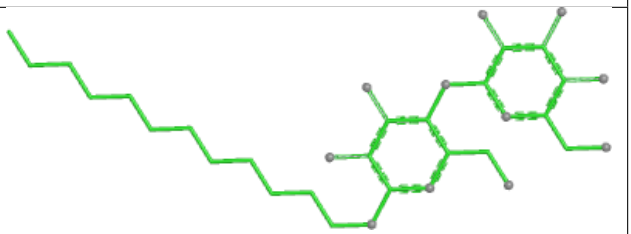


Rings

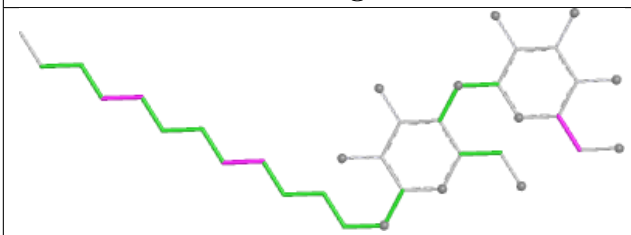
Ligand LMT a 857



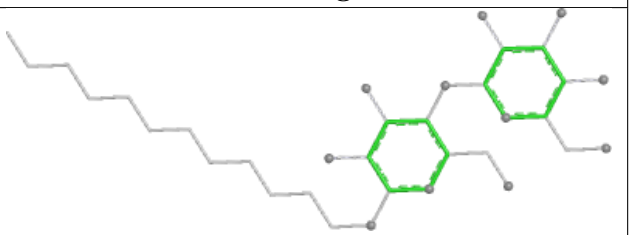
Bond lengths



Bond angles

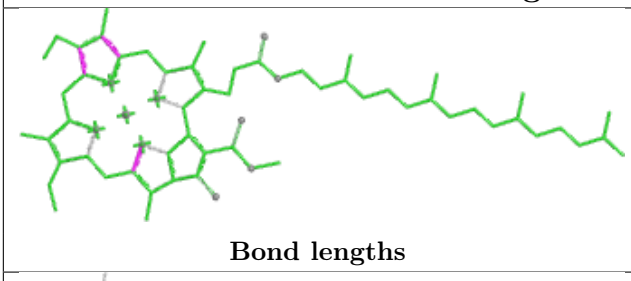


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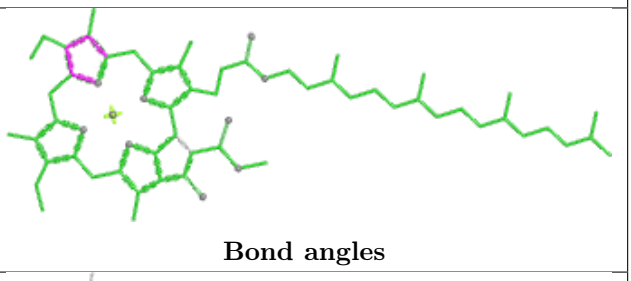


Rings

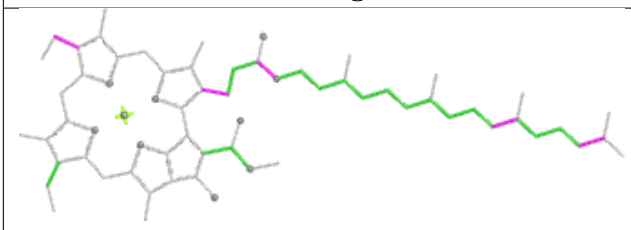
Ligand CLA G 841



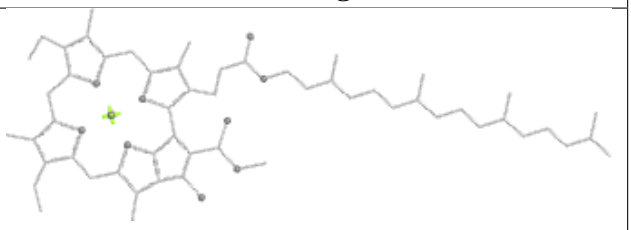
Bond lengths



Bond angles

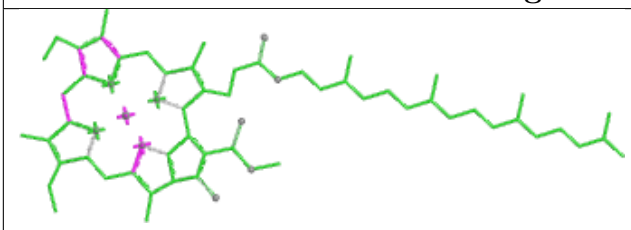


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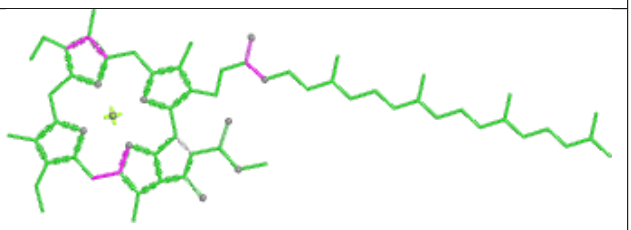


Rings

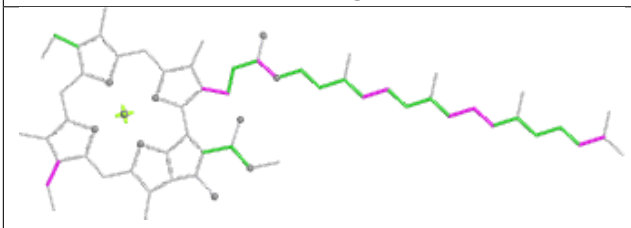
Ligand CLA B 815



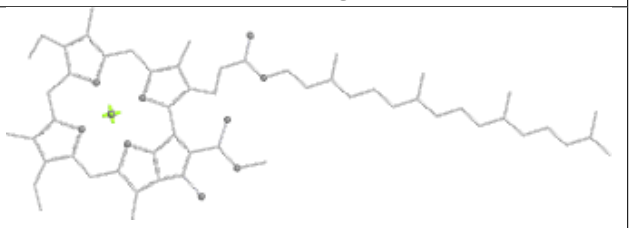
Bond lengths



Bond angles

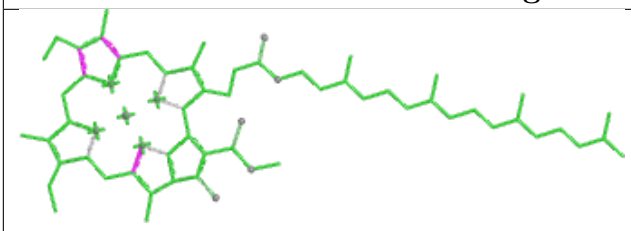


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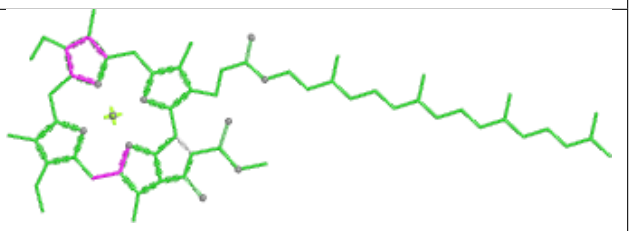


Rings

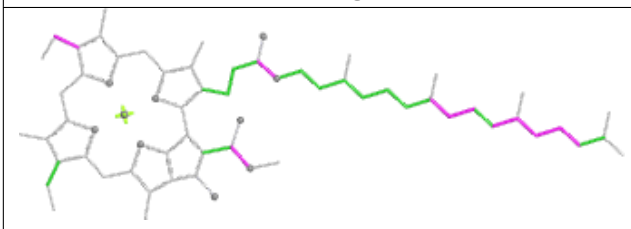
Ligand CLA G 825



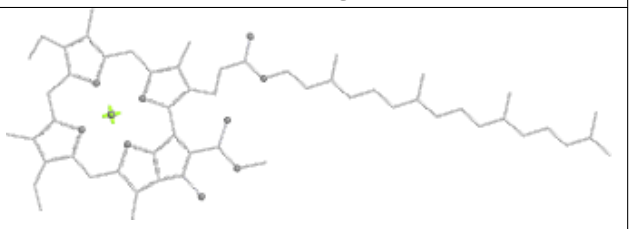
Bond lengths



Bond angles

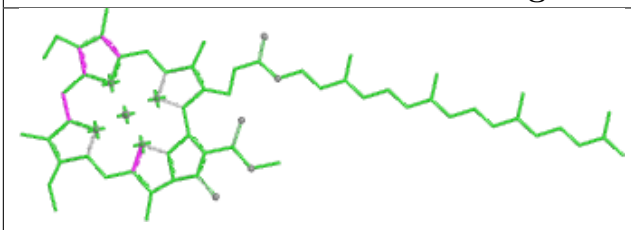


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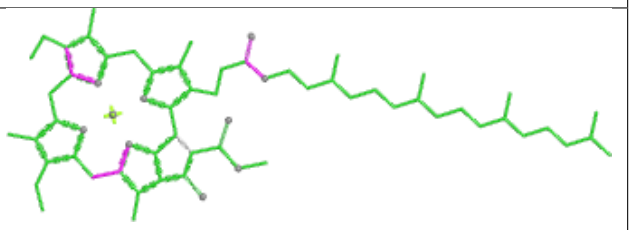


Rings

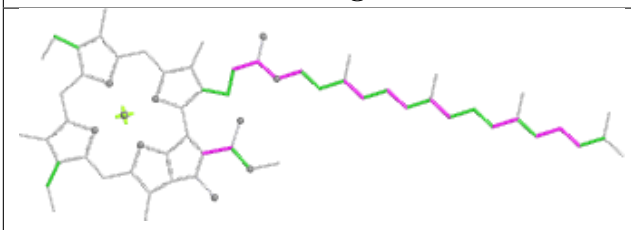
Ligand CLA a 805



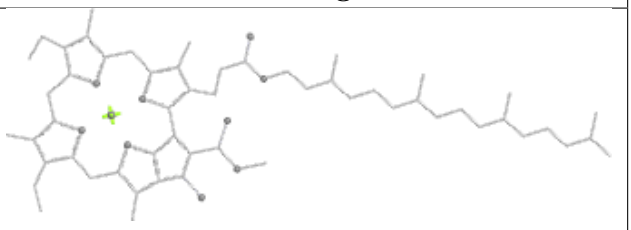
Bond lengths



Bond angles

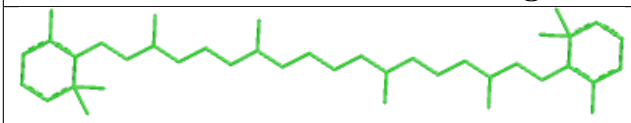


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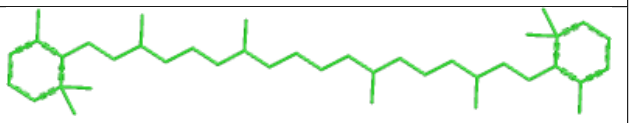


Rings

Ligand BCR B 849



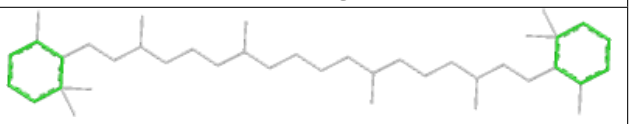
Bond lengths



Bond angles

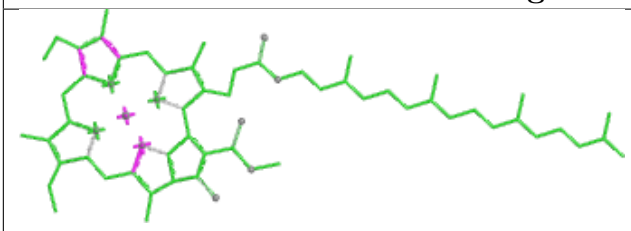


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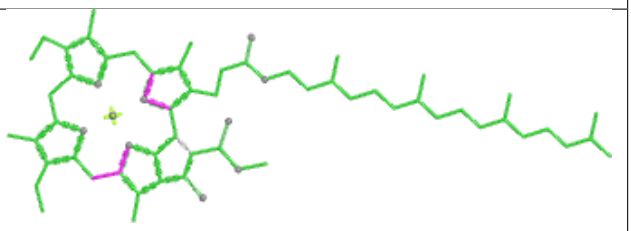


Rings

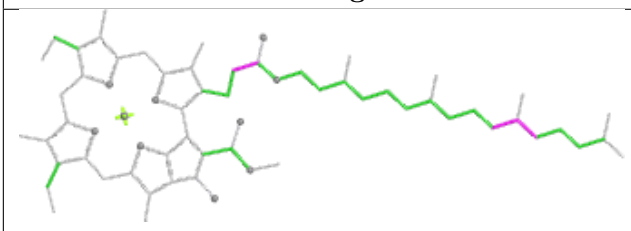
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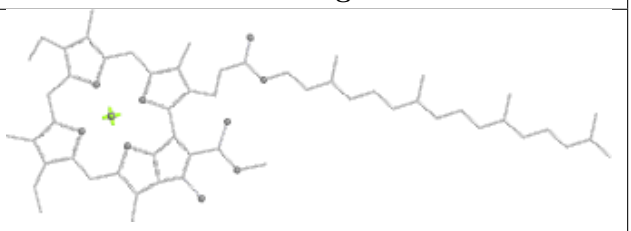
Bond lengths



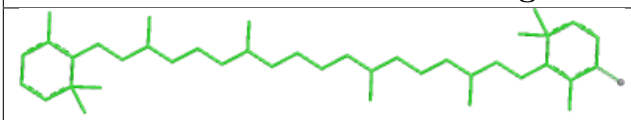
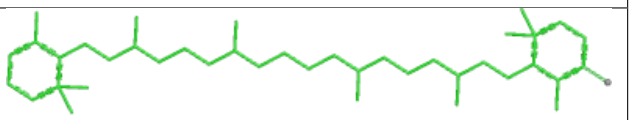
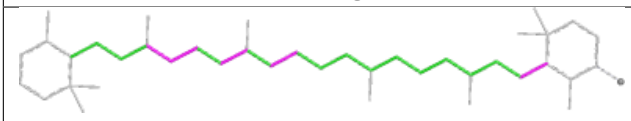
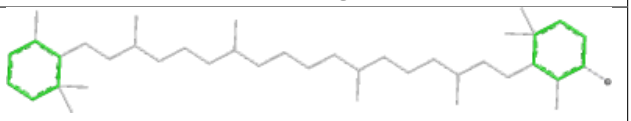
Bond angles

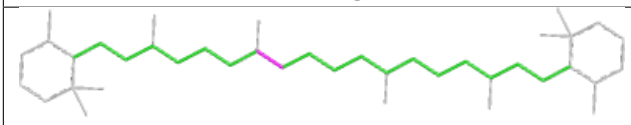
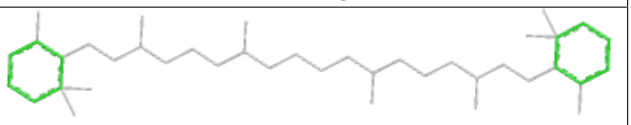


Torsions

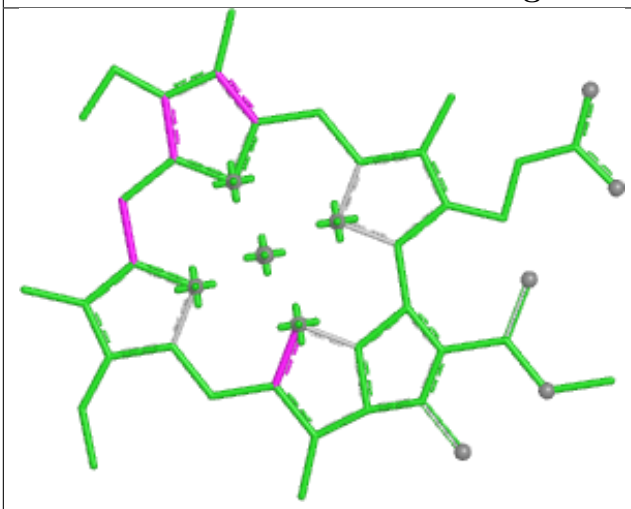


Rings

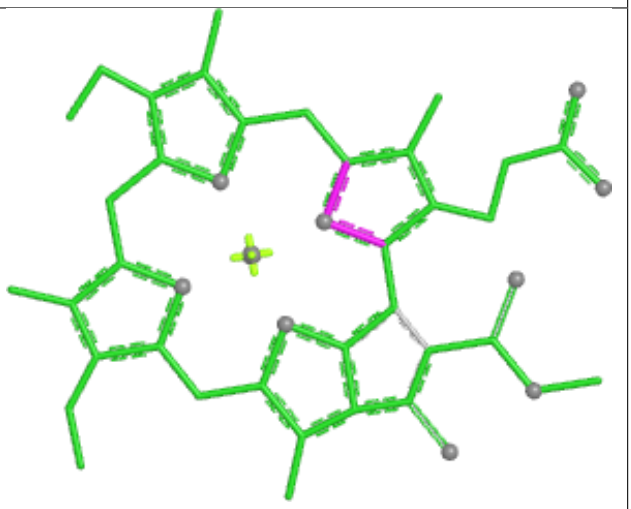
Ligand ECH M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

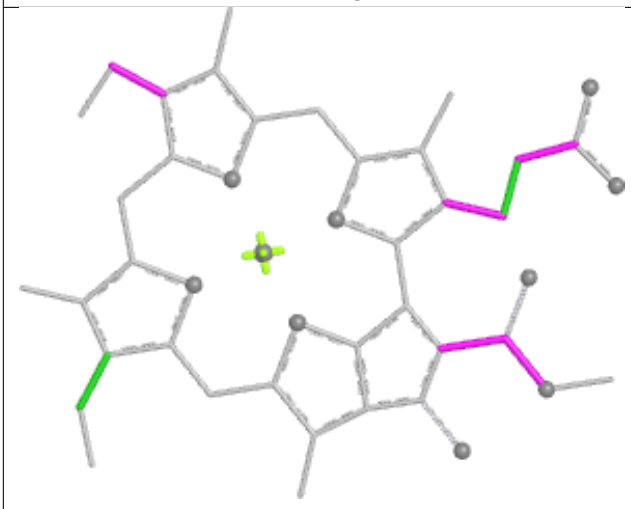
Ligand CLA H 821



Bond lengths



Bond angles

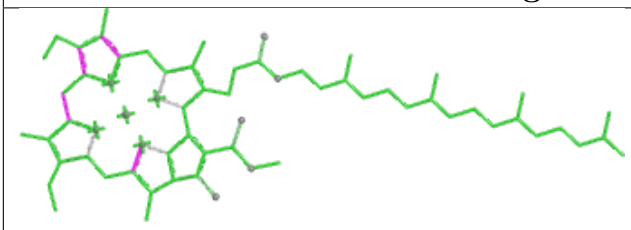


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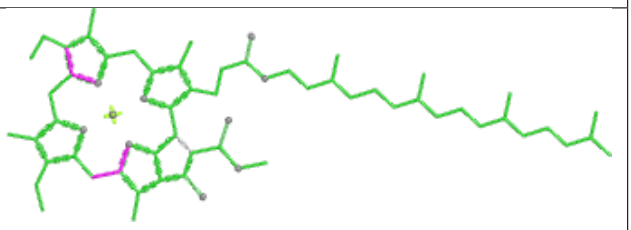


Rings

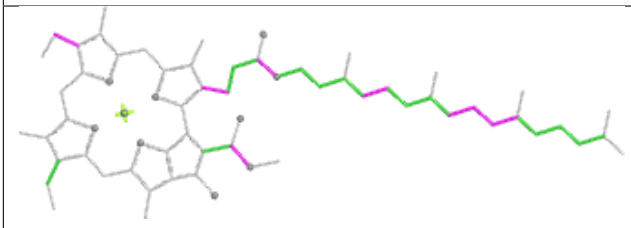
Ligand CLA G 836



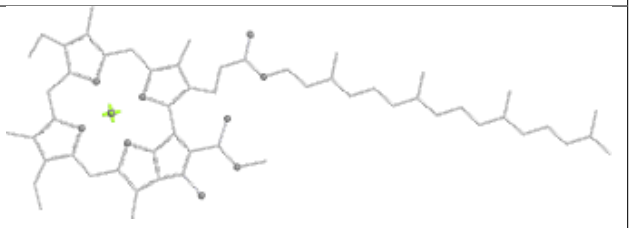
Bond lengths



Bond angles

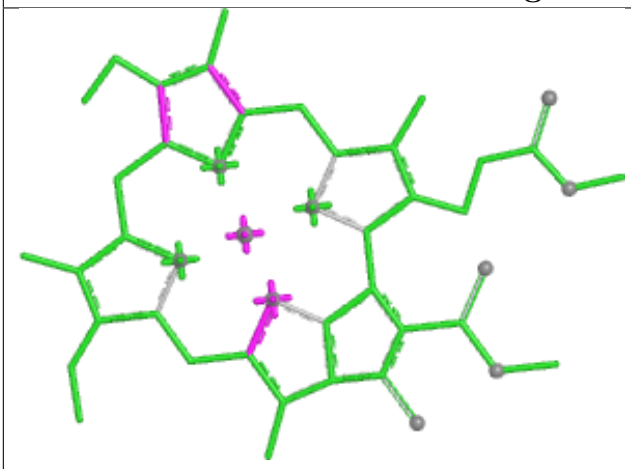


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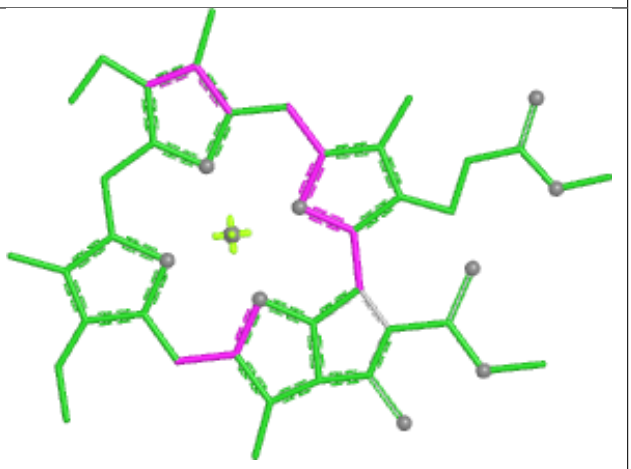


Rings

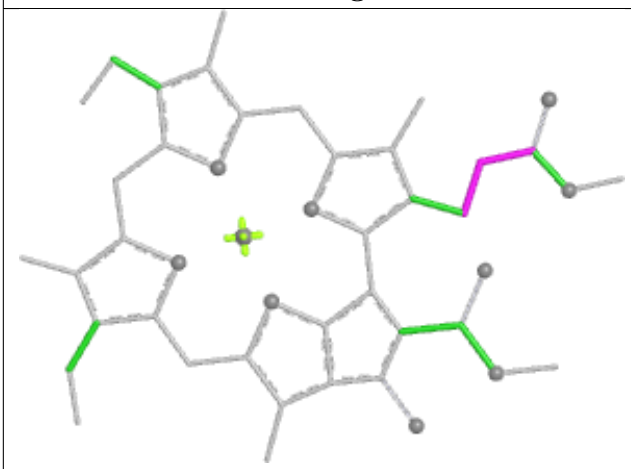
Ligand CLA B 843



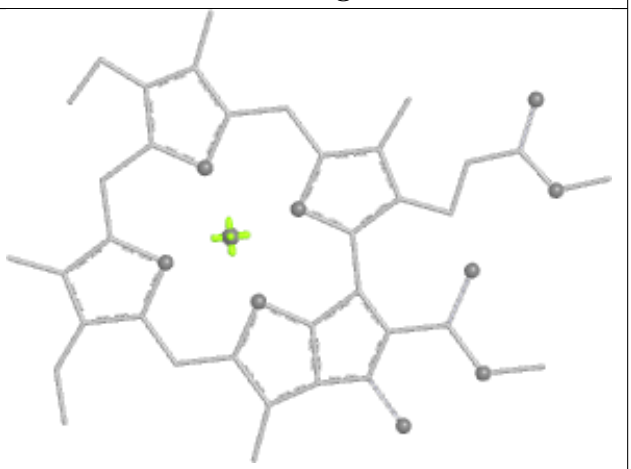
Bond lengths



Bond angles

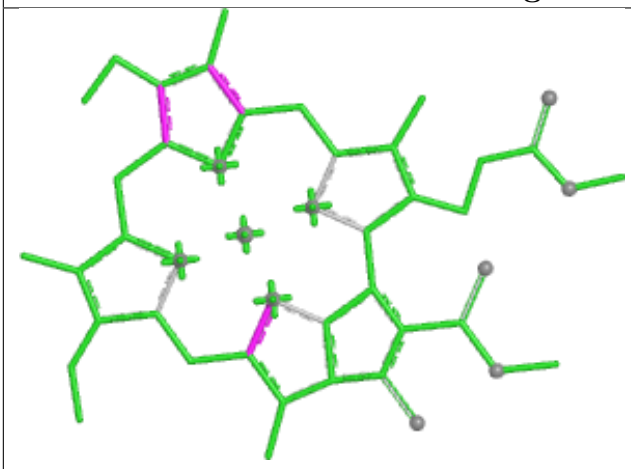


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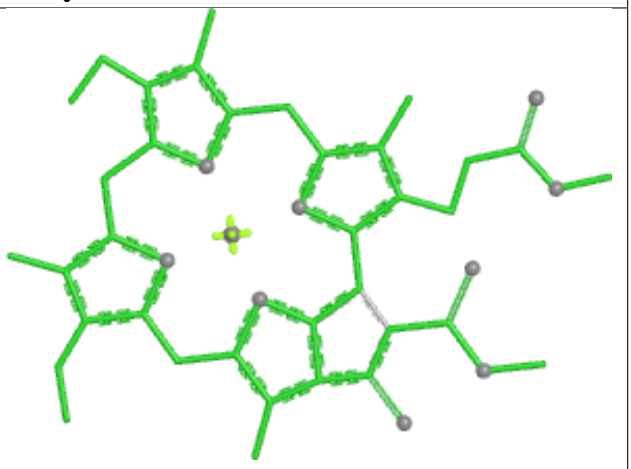


Rings

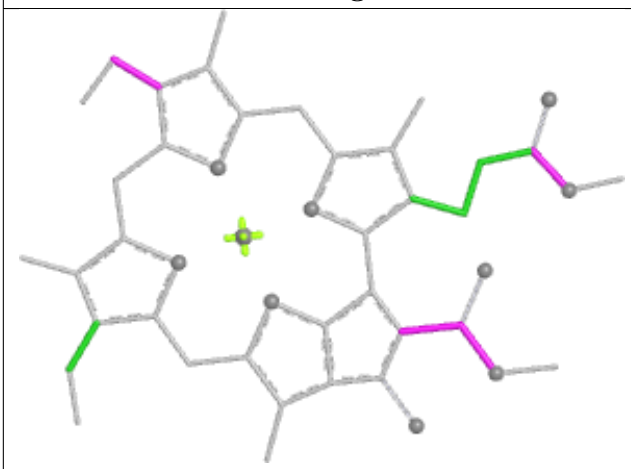
Ligand CLA Q 205



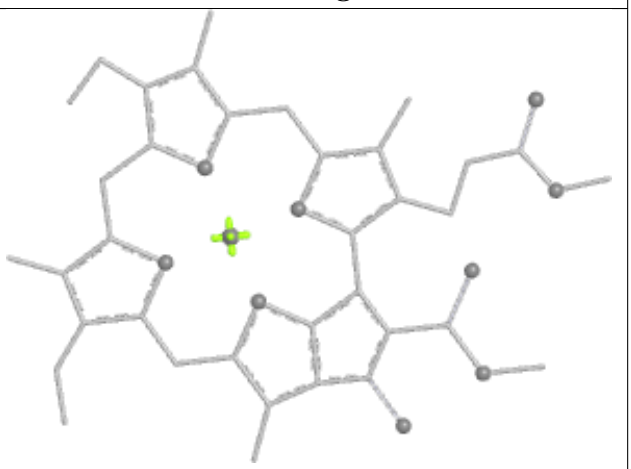
Bond lengths



Bond angles

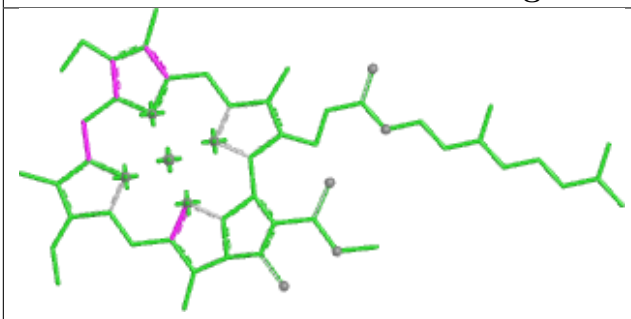


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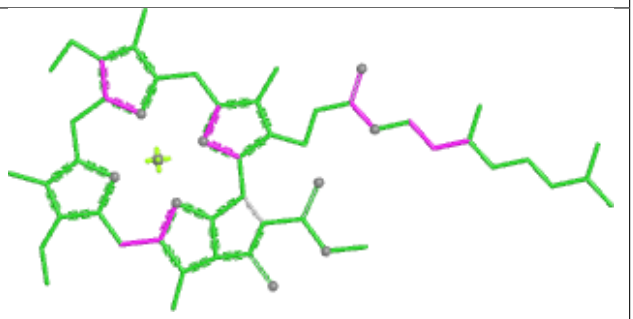


Rings

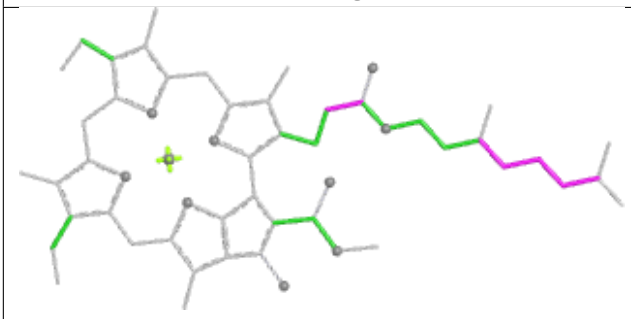
Ligand CLA H 834



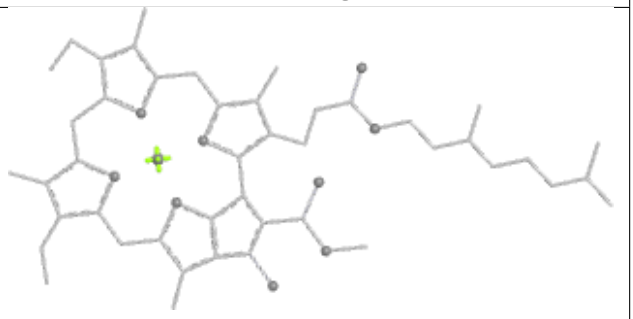
Bond lengths



Bond angles

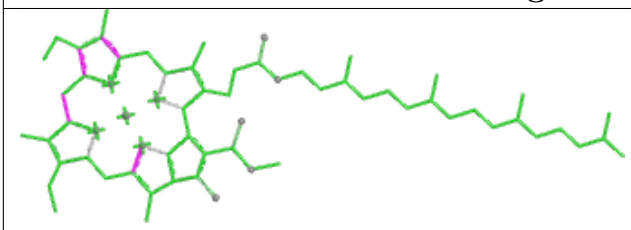


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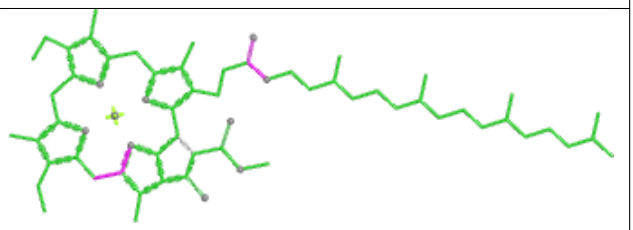


Rings

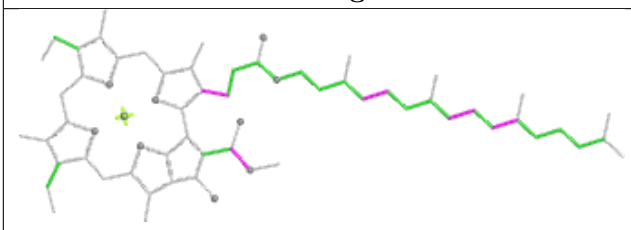
Ligand CLA b 821



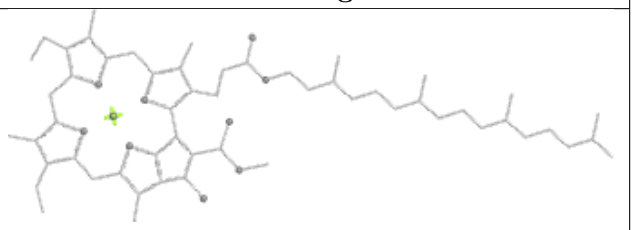
Bond lengths



Bond angles

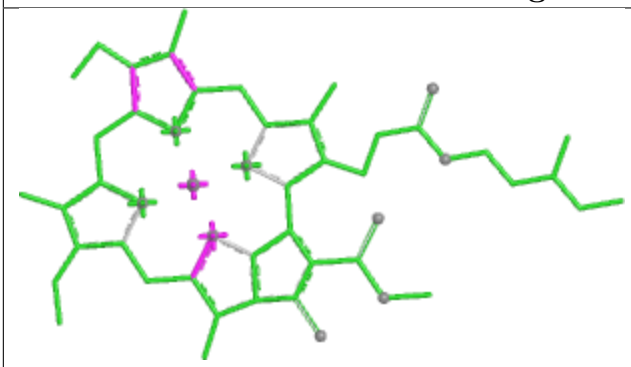


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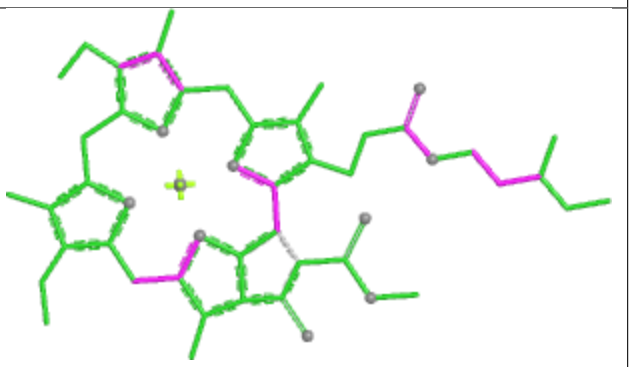


Rings

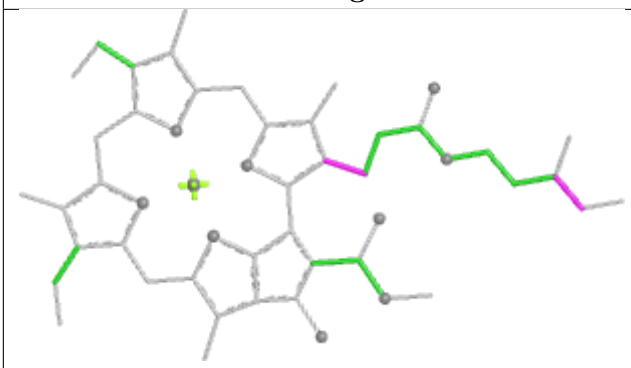
Ligand CLA a 824



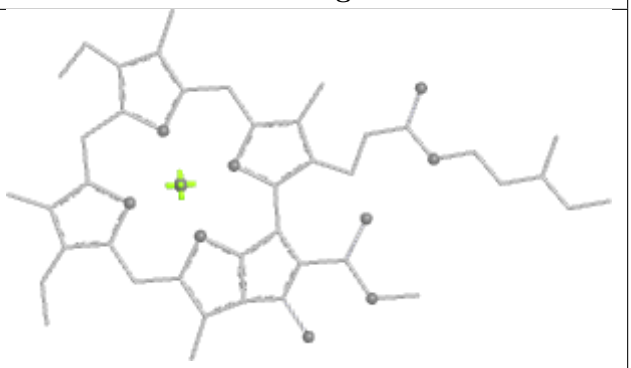
Bond lengths



Bond angles

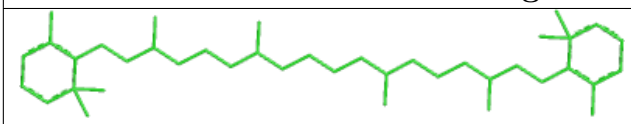


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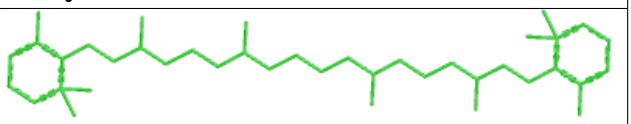


Rings

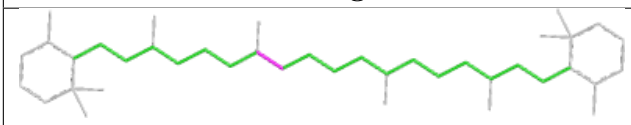
Ligand BCR Q 206



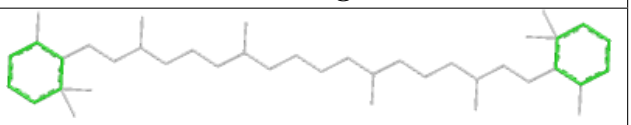
Bond lengths



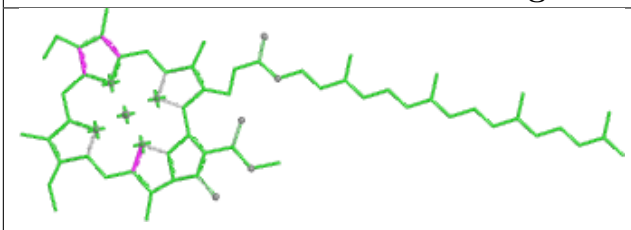
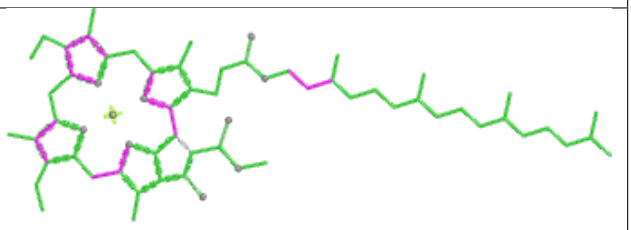
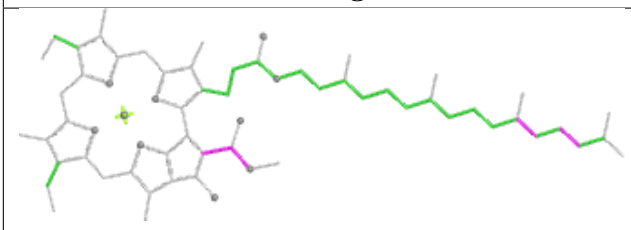
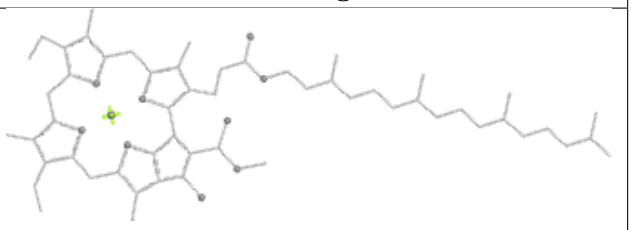
Bond angles

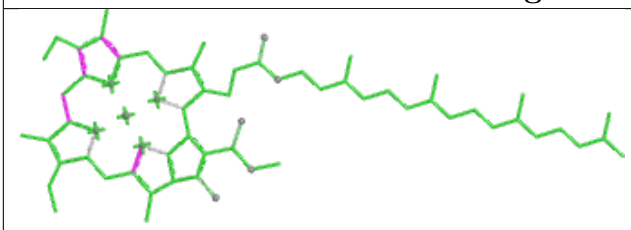
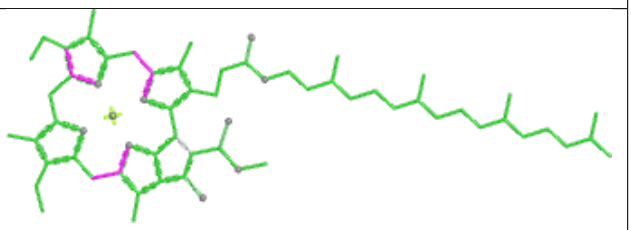
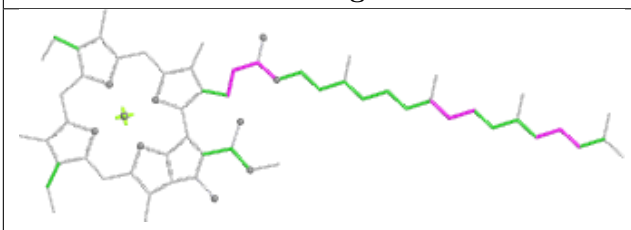
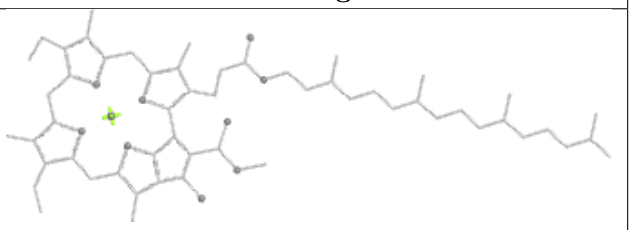


Torsions

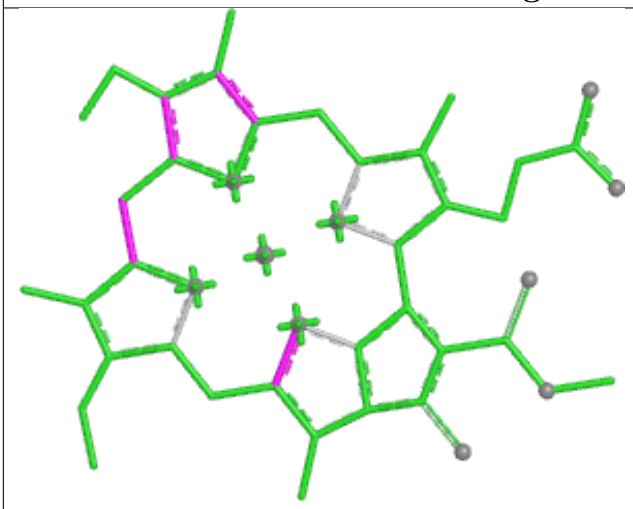


Rings

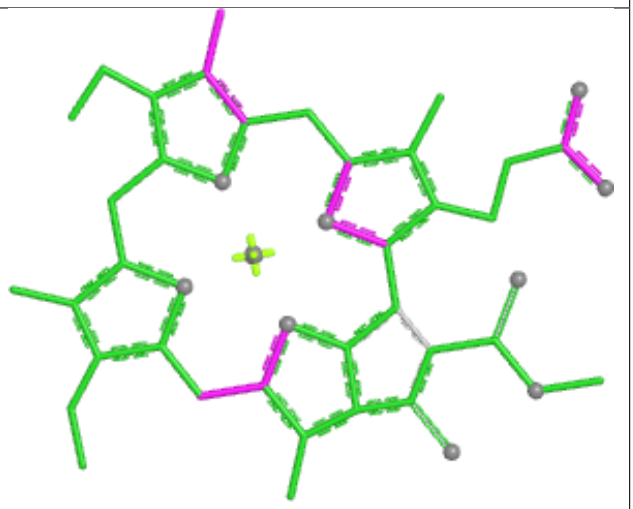
Ligand CLA a 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

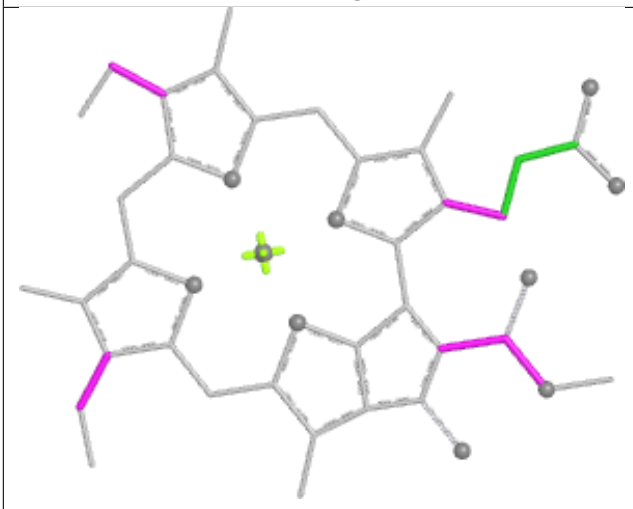
Ligand CLA K 102



Bond lengths



Bond angles

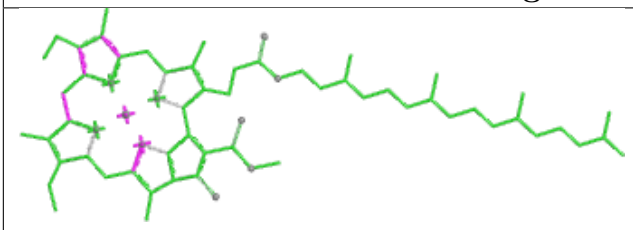


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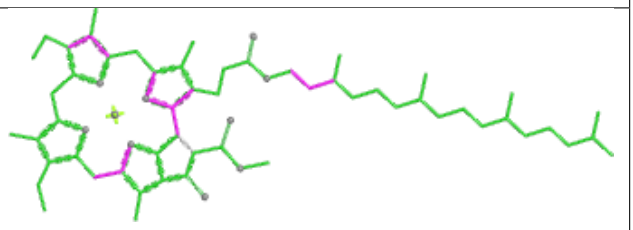


Rings

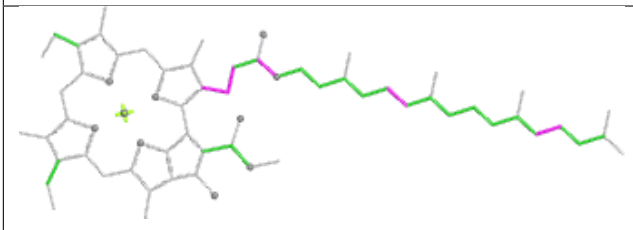
Ligand CLA G 830



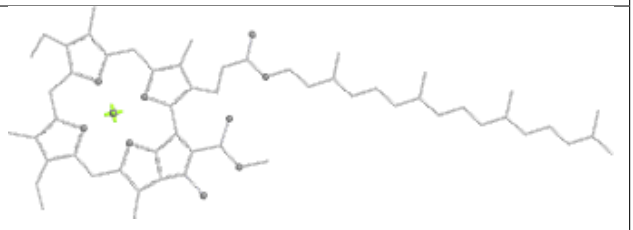
Bond lengths



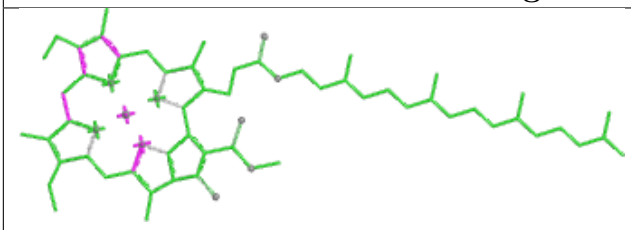
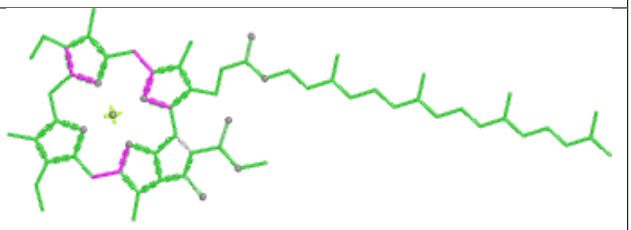
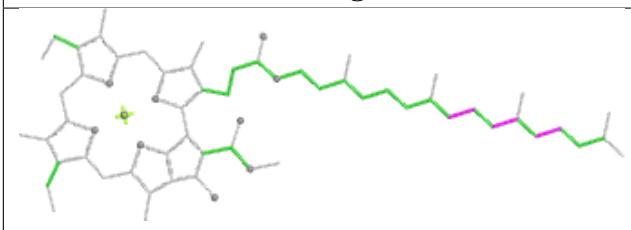
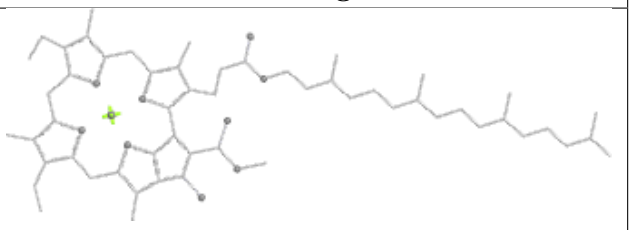
Bond angles

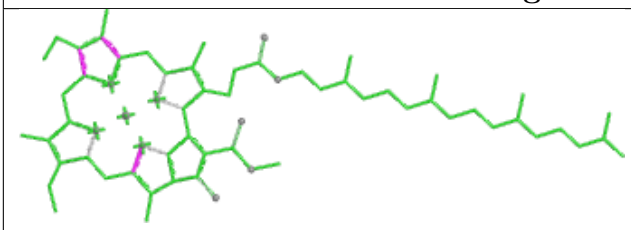
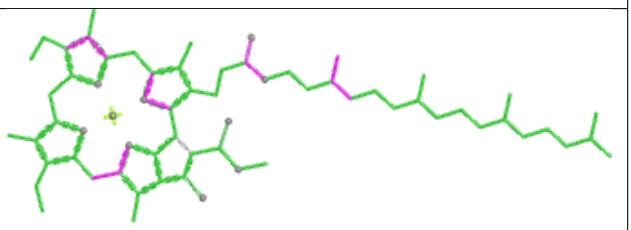
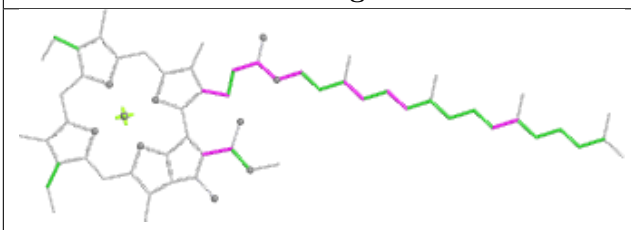
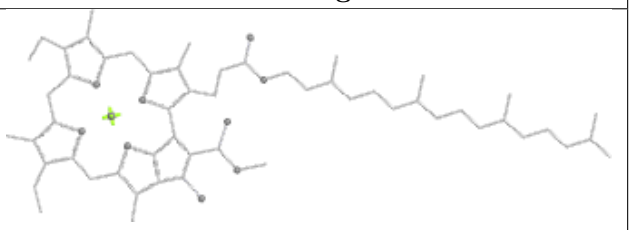


Torsions

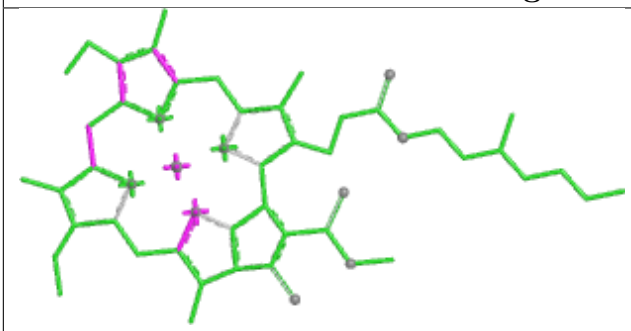


Rings

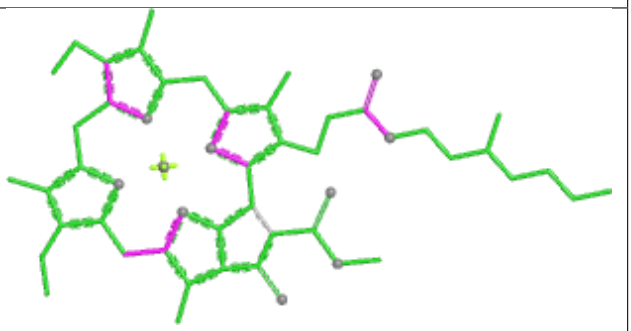
Ligand CLA G 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

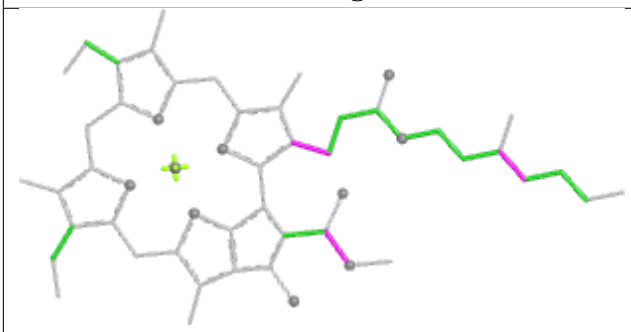
Ligand CLA H 824



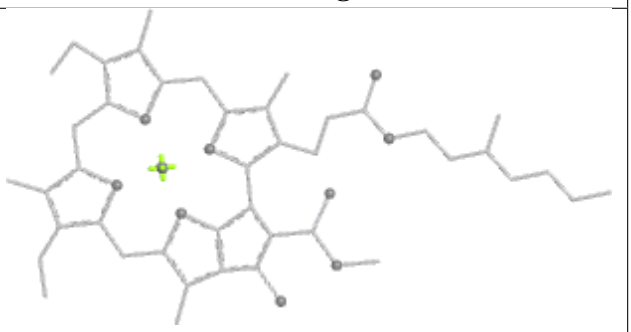
Bond lengths



Bond angles



Torsions

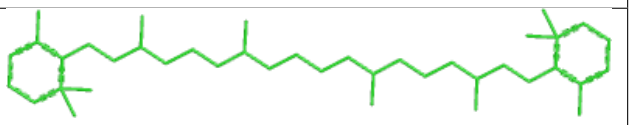


Rings

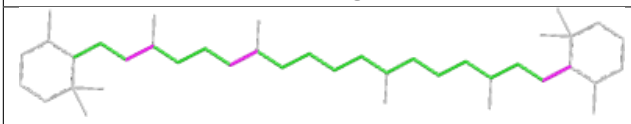
Ligand BCR H 854



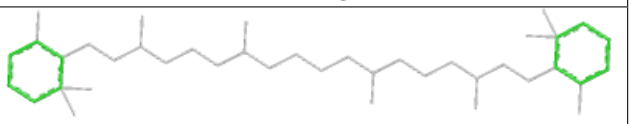
Bond lengths



Bond angles

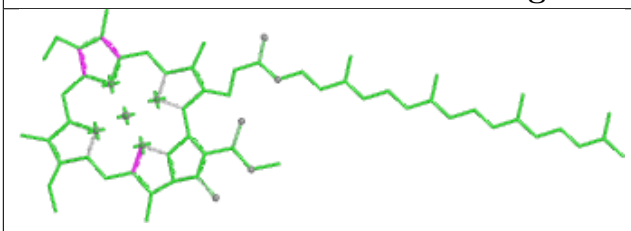


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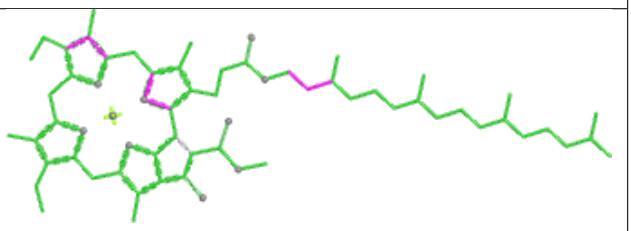


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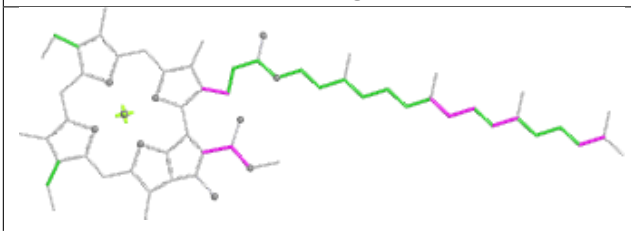
Ligand CLA a 823



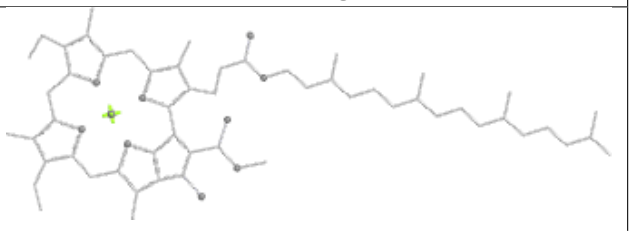
Bond lengths



Bond angles

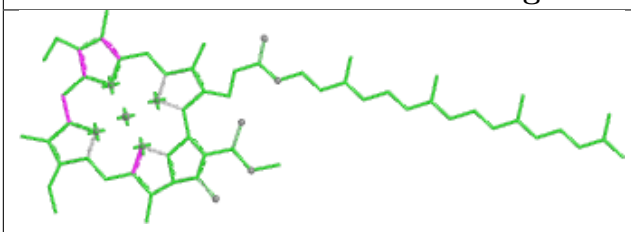


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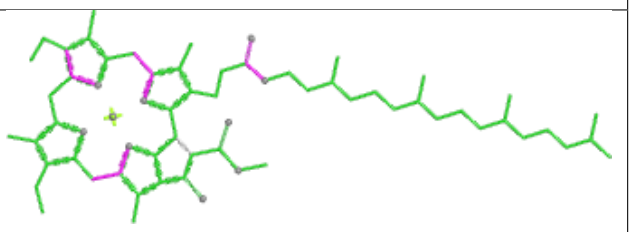


Rings

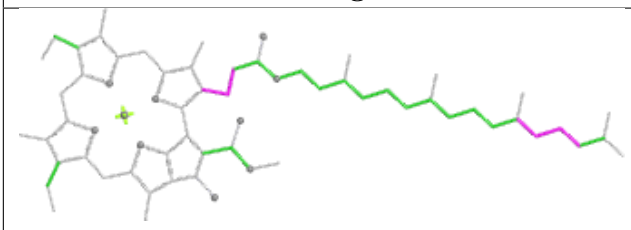
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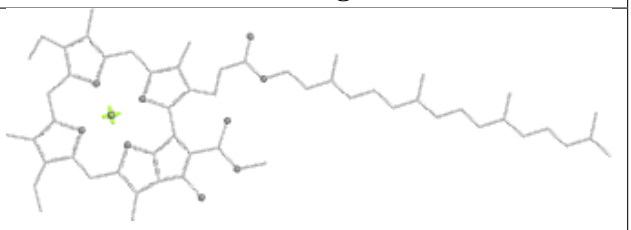
Bond lengths



Bond angles

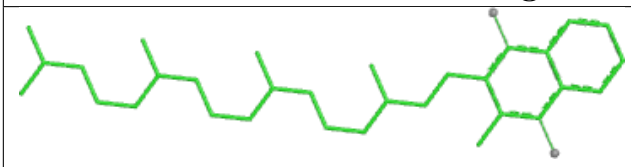


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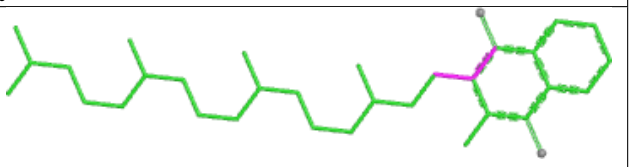


Rings

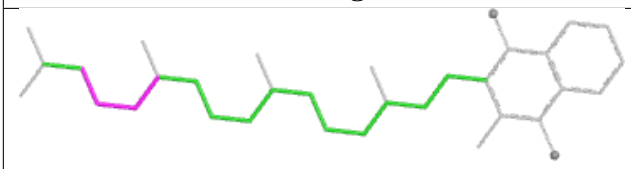
Ligand PQN H 843



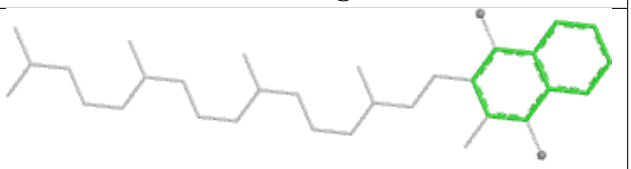
Bond lengths



Bond angles

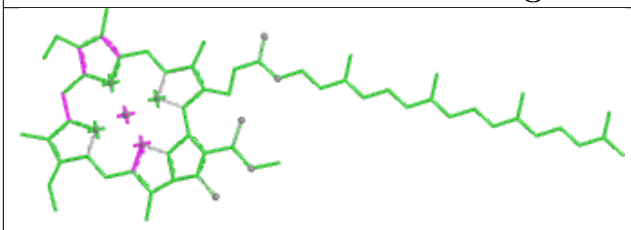


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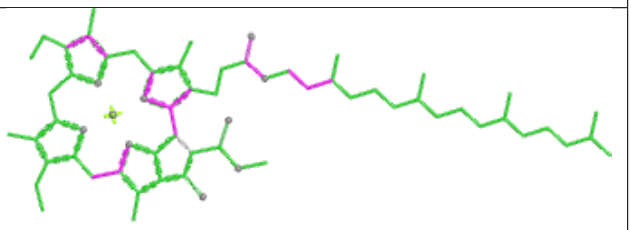


Rings

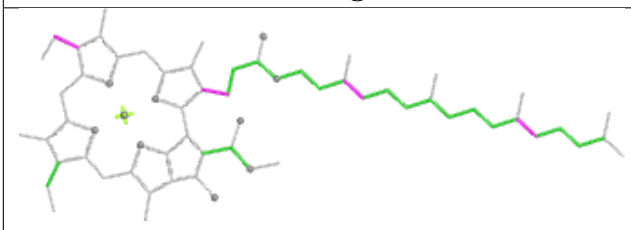
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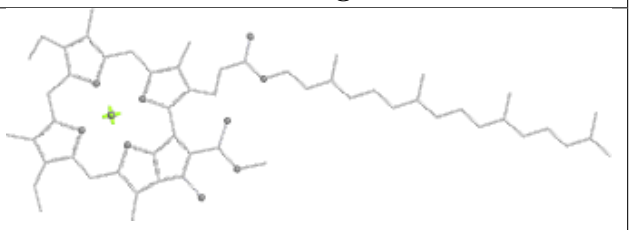
Bond lengths



Bond angles

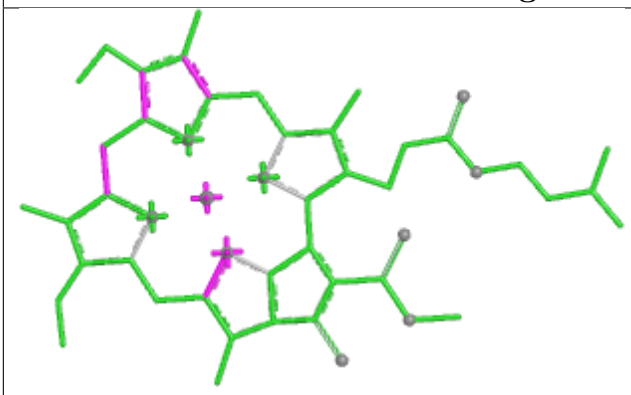


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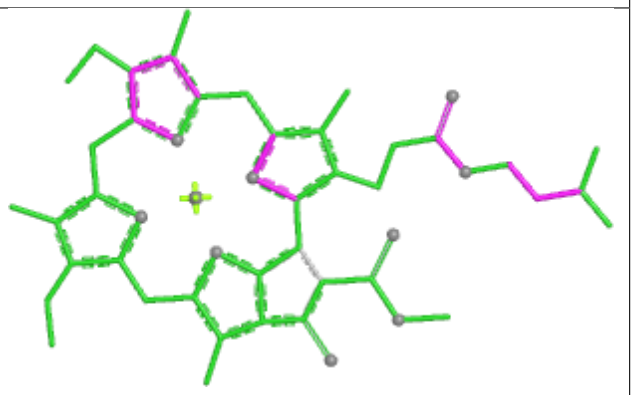


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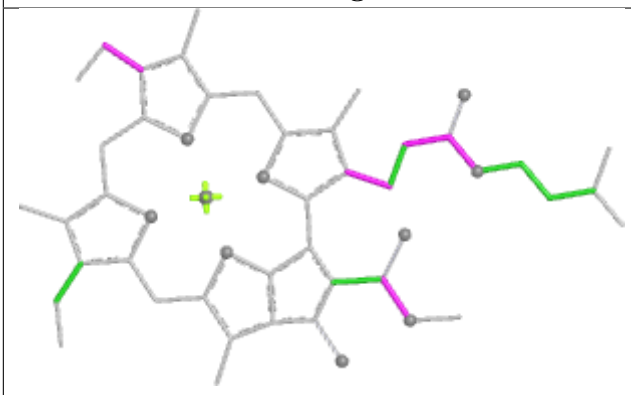
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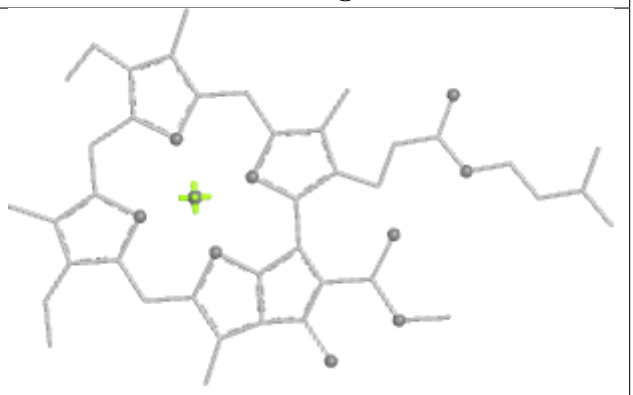
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Bond angles

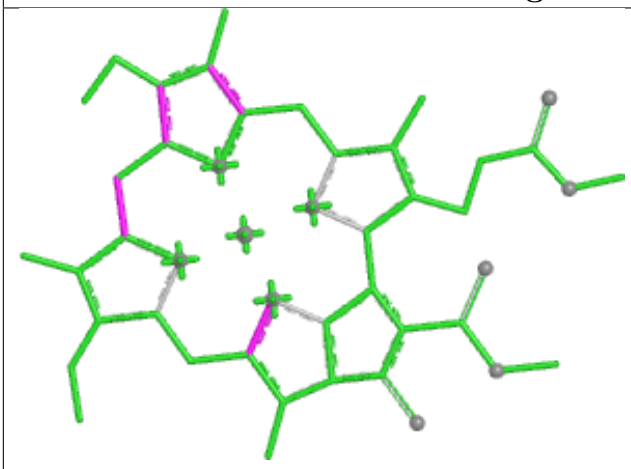


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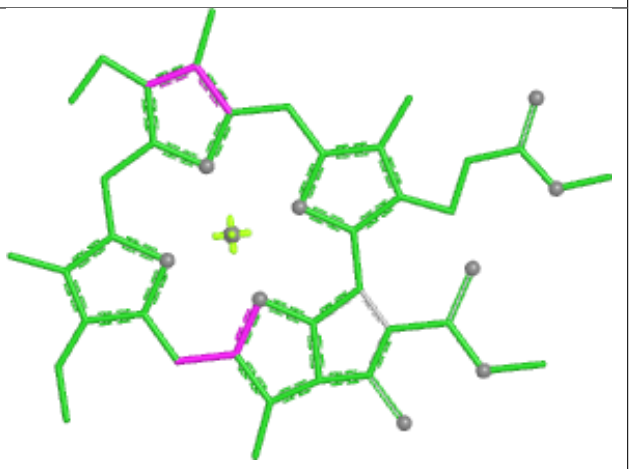


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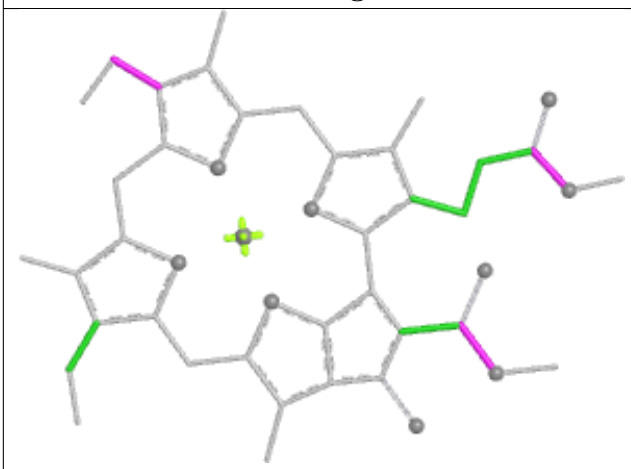
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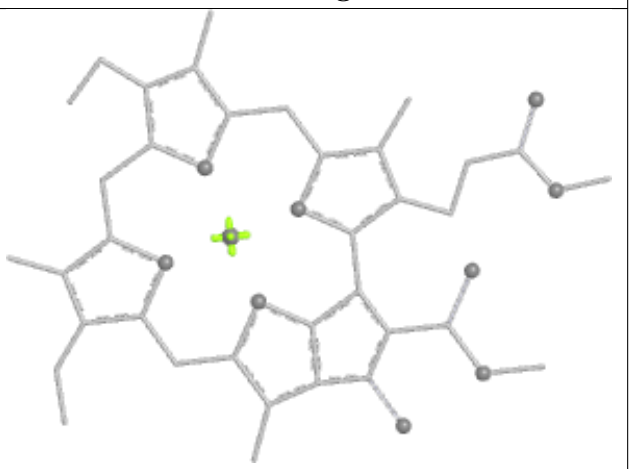
Bond lengths



Bond angles

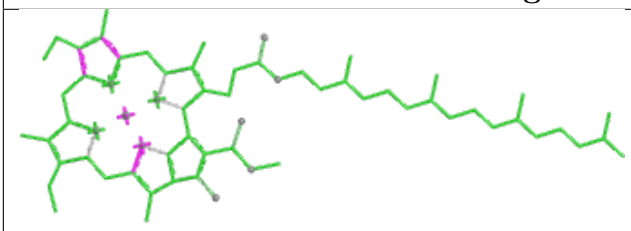


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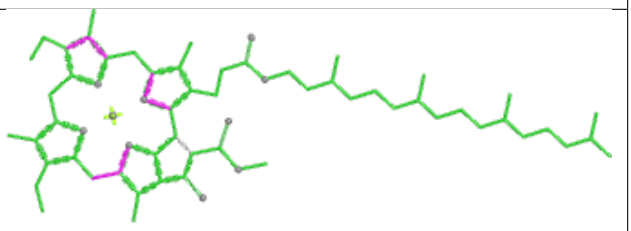


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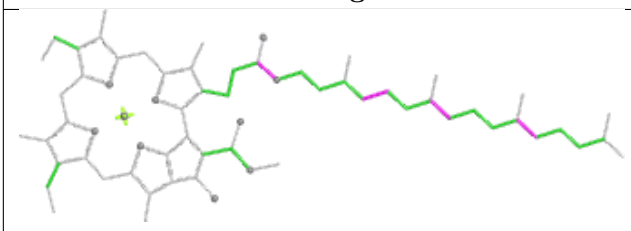
Ligand CLA H 838



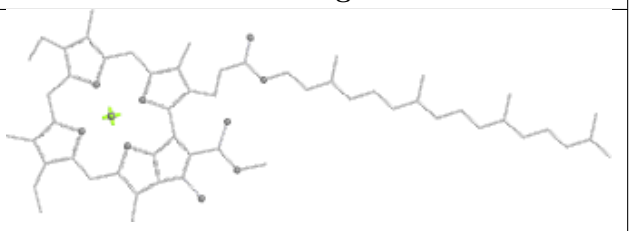
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Bond angles

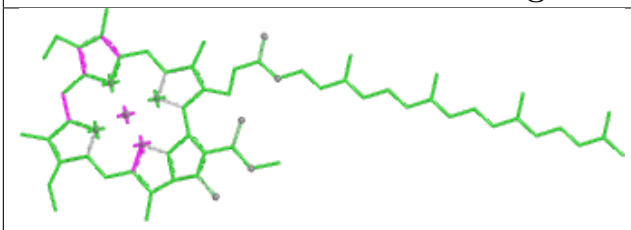


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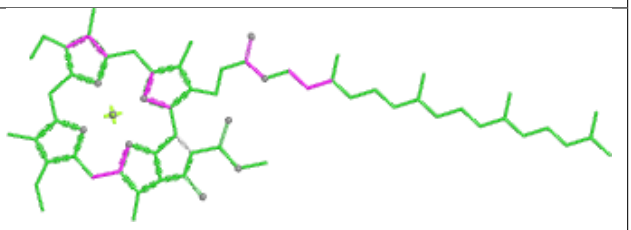


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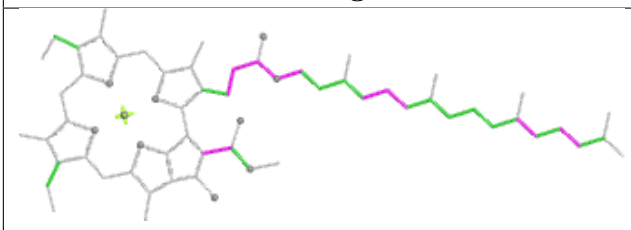
Ligand CLA b 818



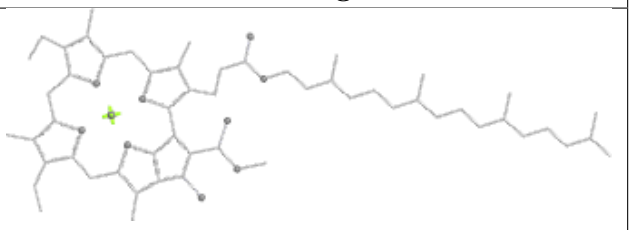
Bond lengths



Bond angles

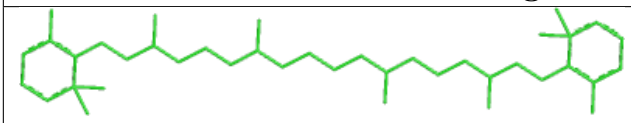


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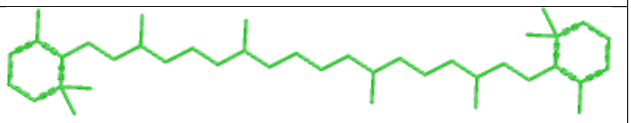


Rings

Ligand BCR B 850



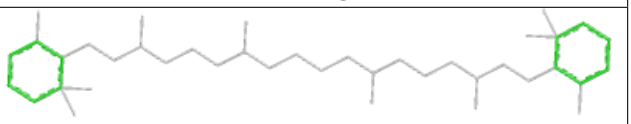
Bond lengths



Bond angles

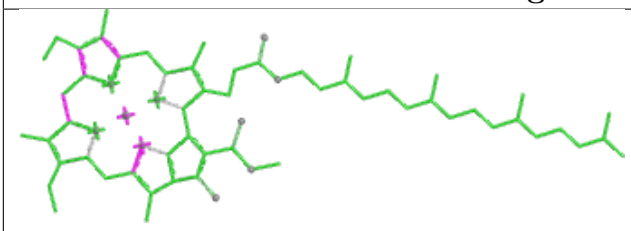


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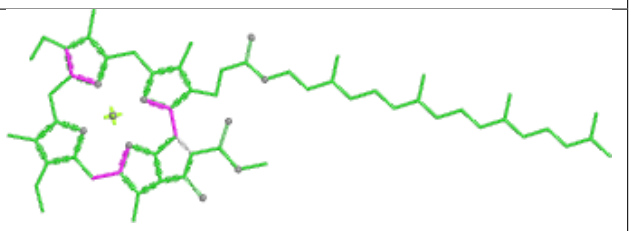


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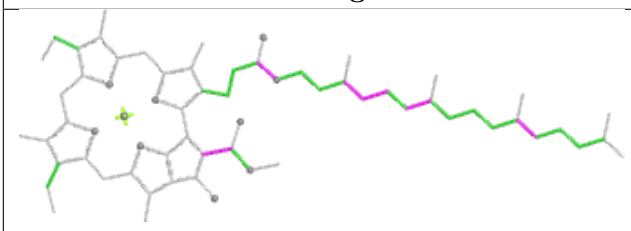
Ligand CLA b 828



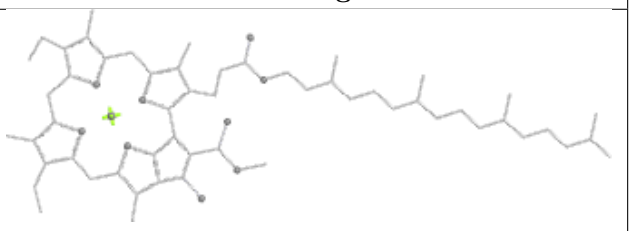
Bond lengths



Bond angles

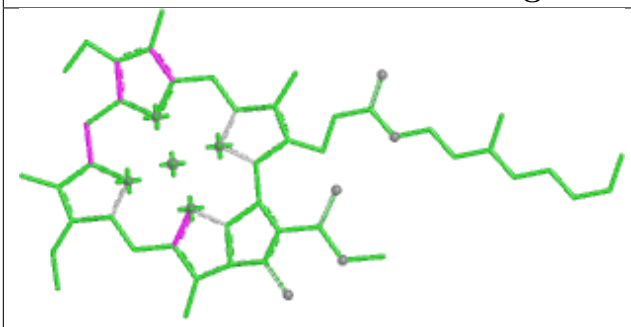


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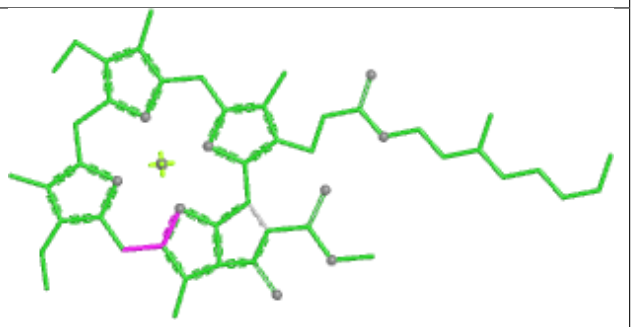


Rings

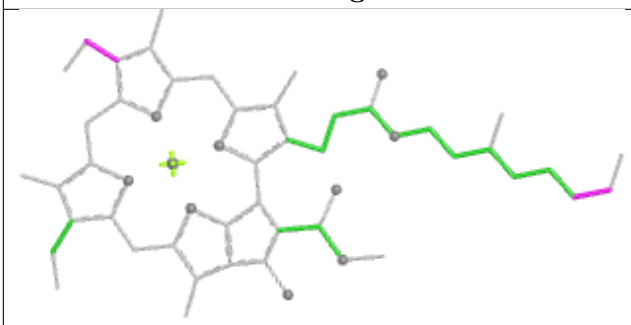
Ligand CLA A 812



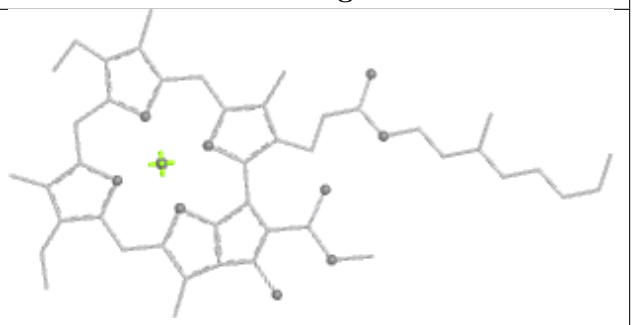
Bond lengths



Bond angles



Torsions



Rings

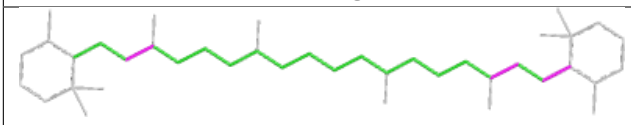
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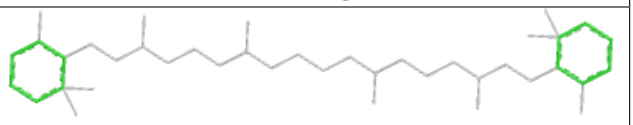
Bond lengths



Bond angles

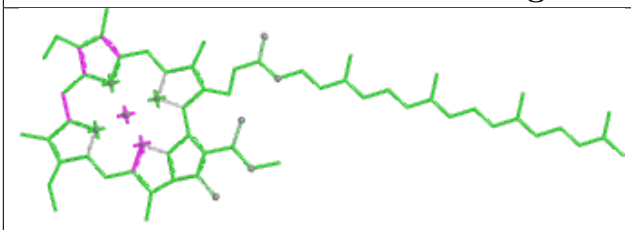


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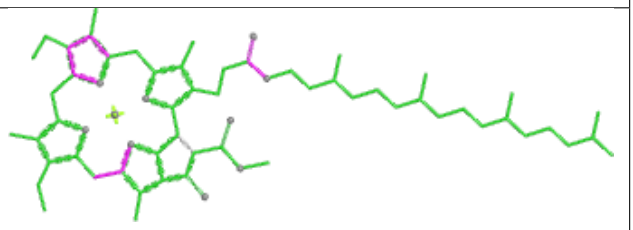


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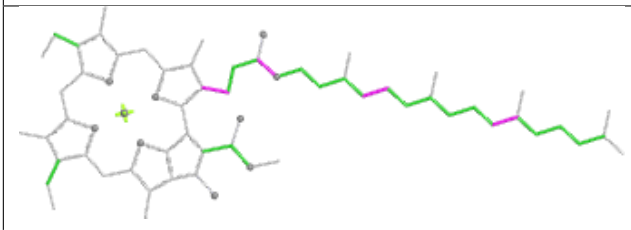
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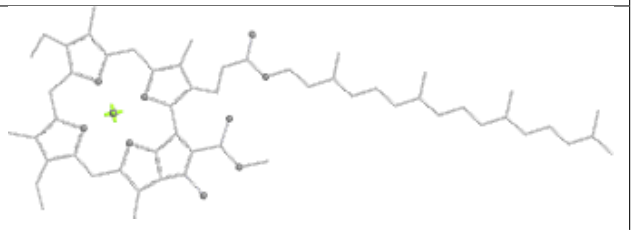
Bond lengths



Bond angles

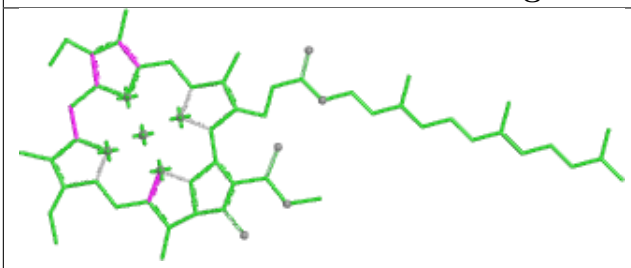


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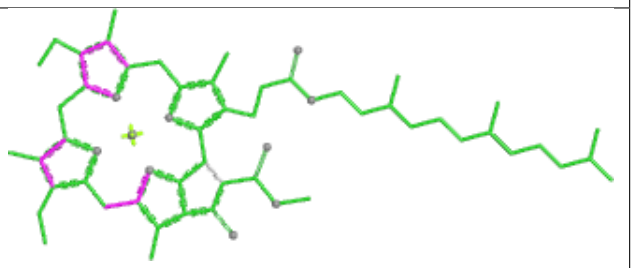


Rings

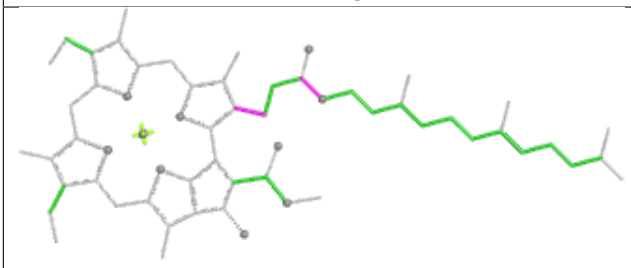
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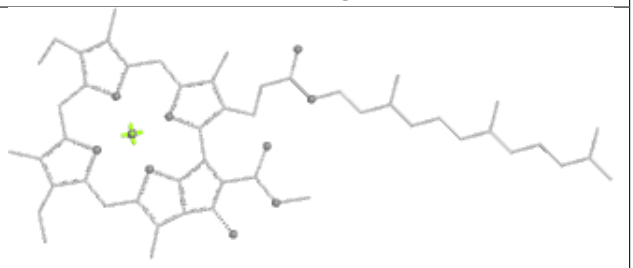
Bond lengths



Bond angles

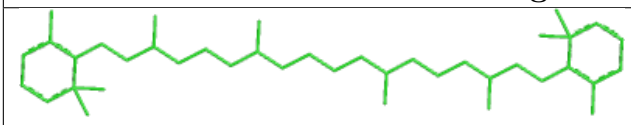


Torsions

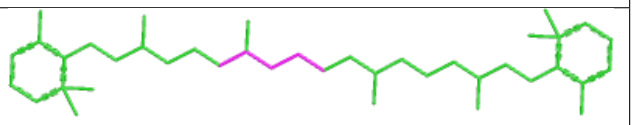


Rings

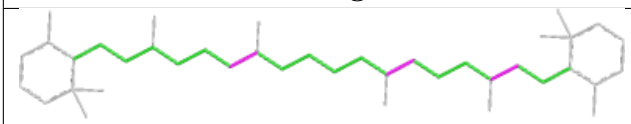
Ligand BCR f 202



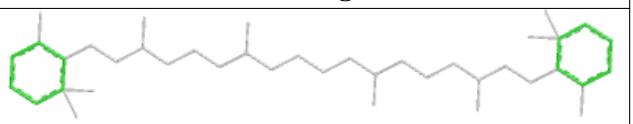
Bond lengths



Bond angles

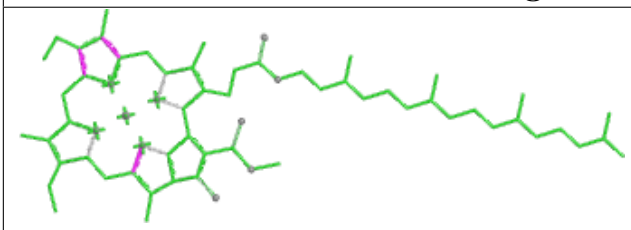


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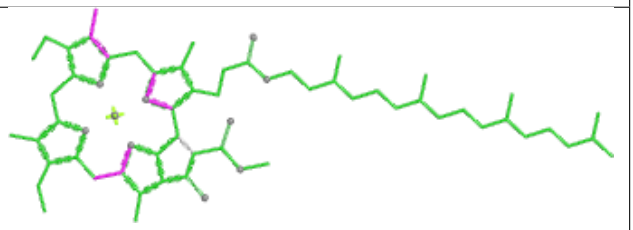


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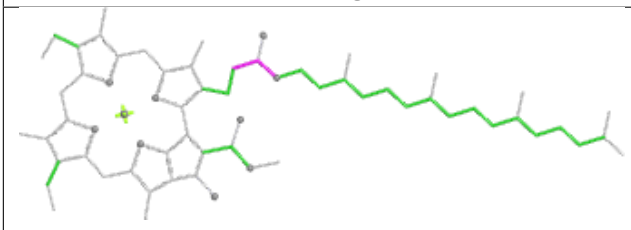
Ligand CLA B 805



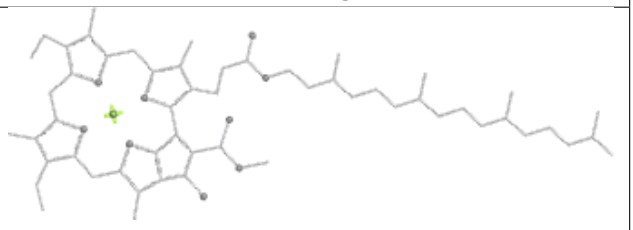
Bond lengths



Bond angles

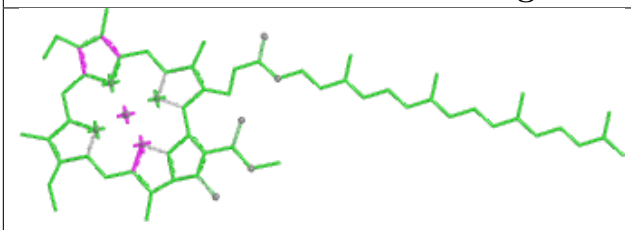


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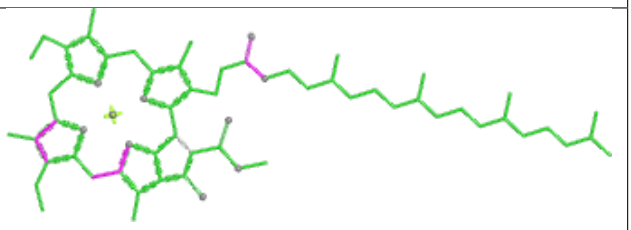


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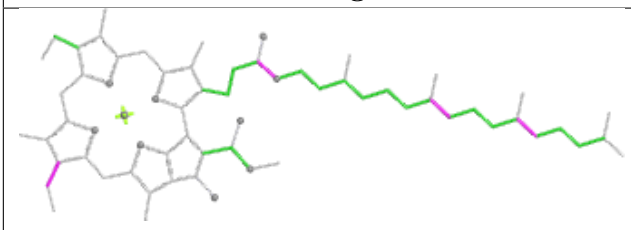
Ligand CLA L 1502



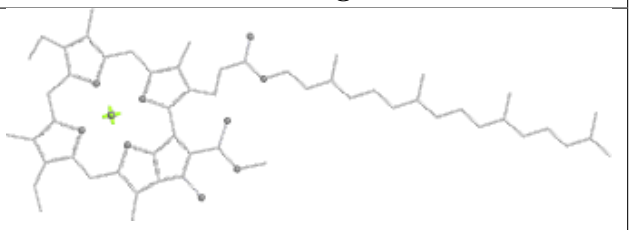
Bond lengths



Bond angles

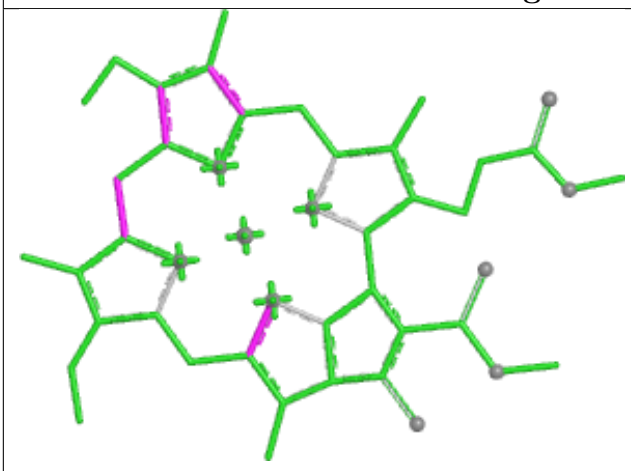


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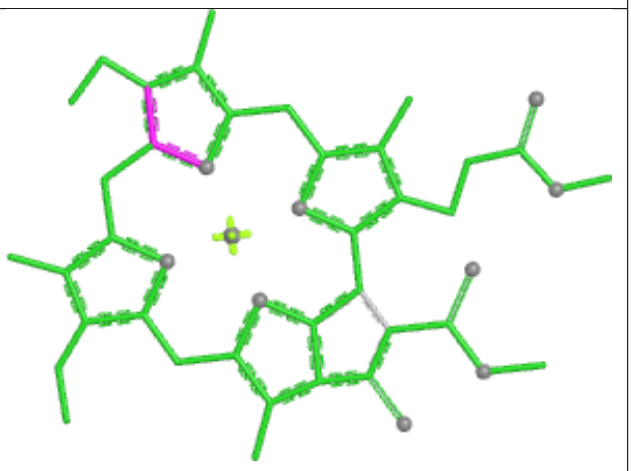


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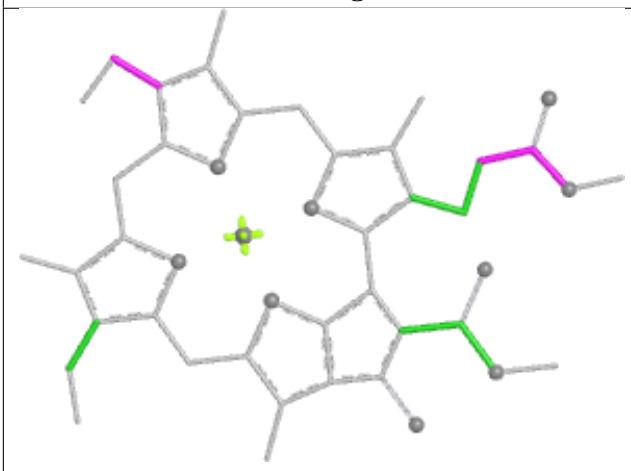
Ligand CLA H 836



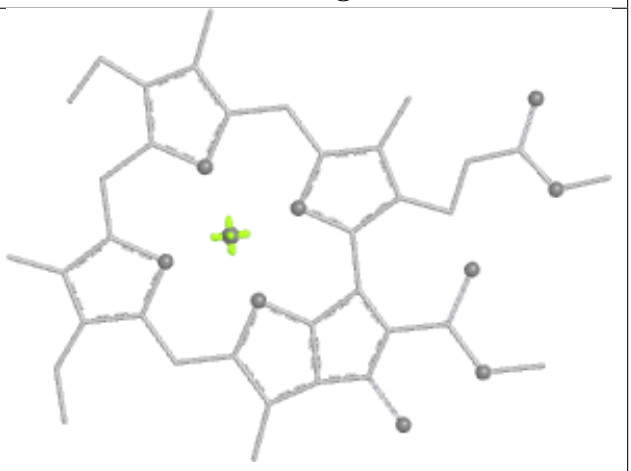
Bond lengths



Bond angles

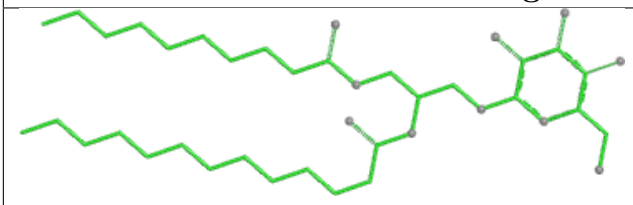


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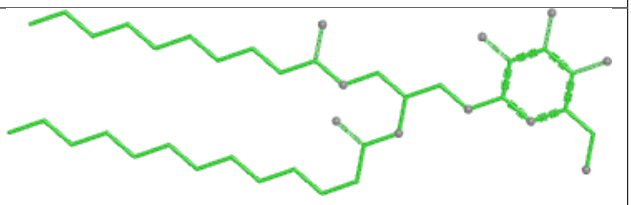


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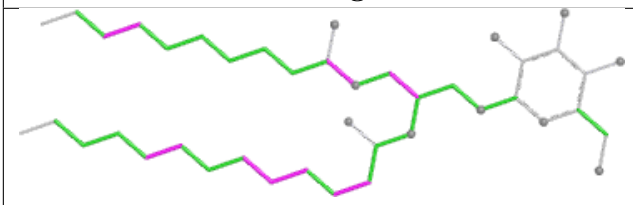
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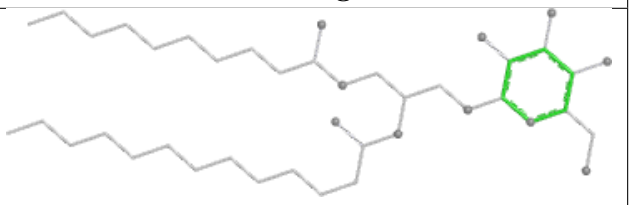
Bond lengths



Bond angles

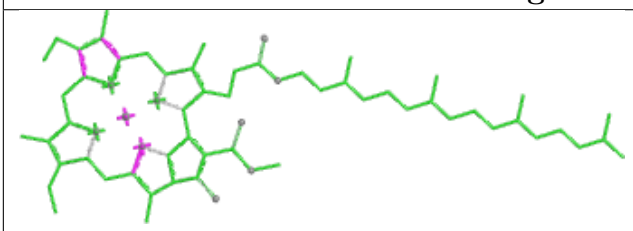


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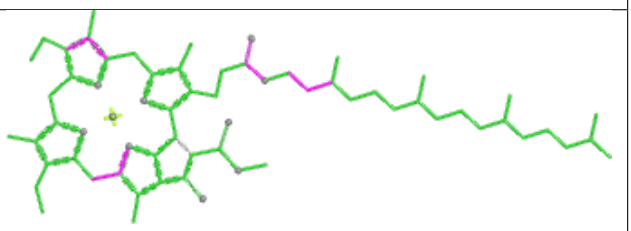


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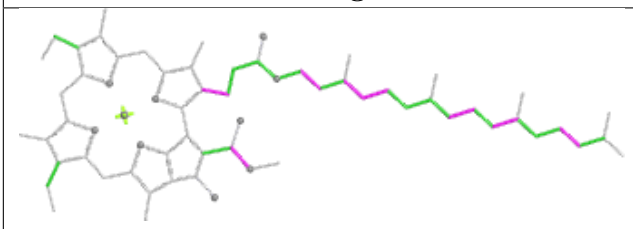
Ligand CLA b 819



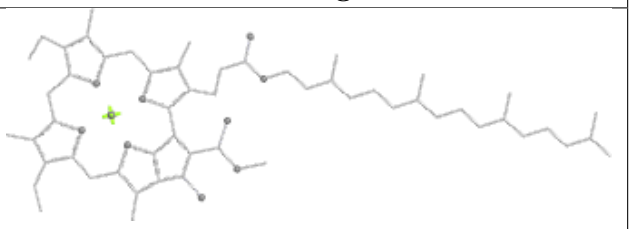
Bond lengths



Bond angles

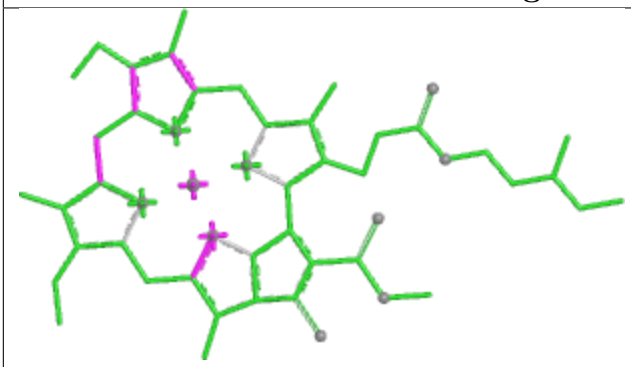


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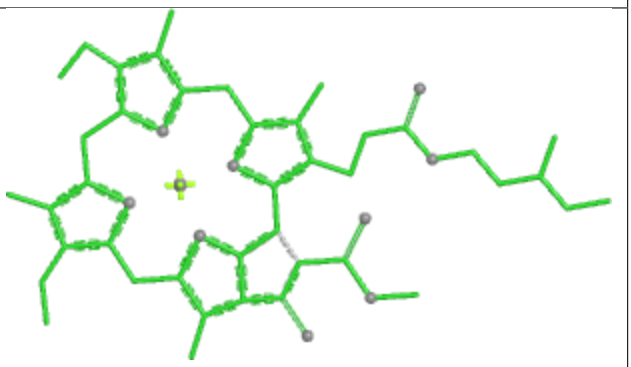


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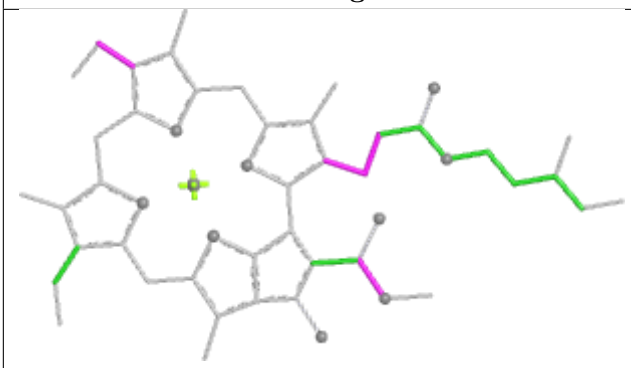
Ligand CLA G 810



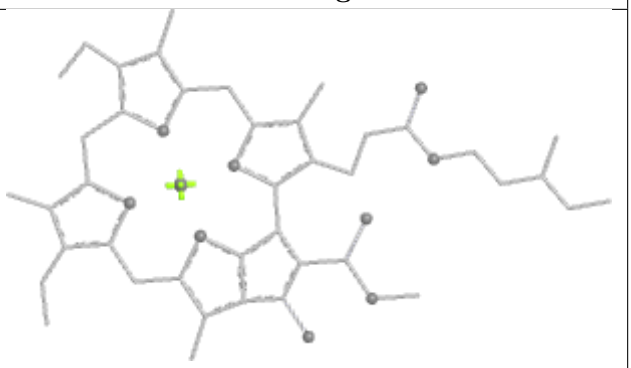
Bond lengths



Bond angles

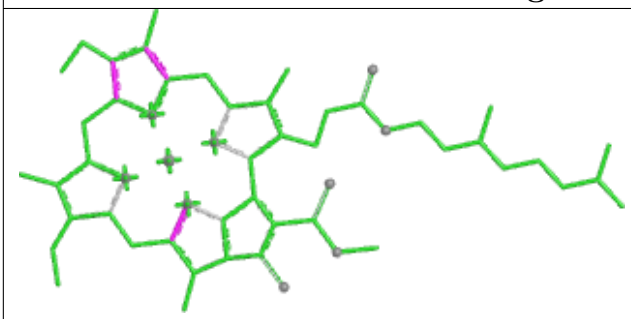


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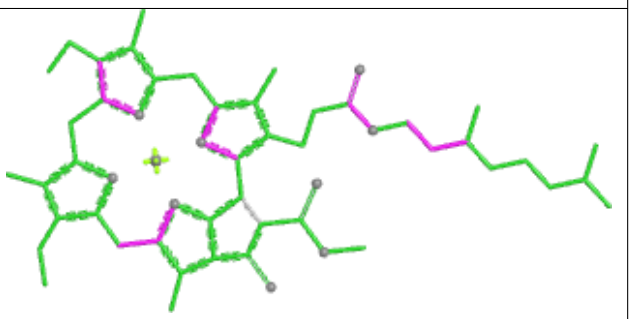


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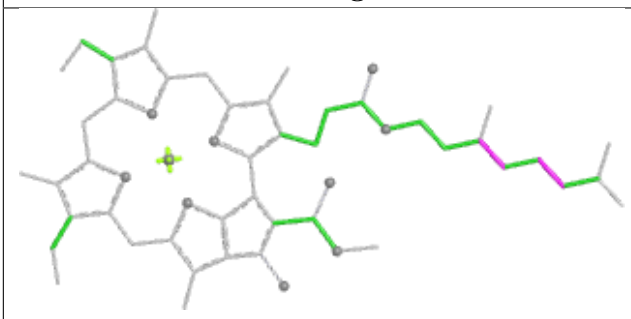
Ligand CLA b 836



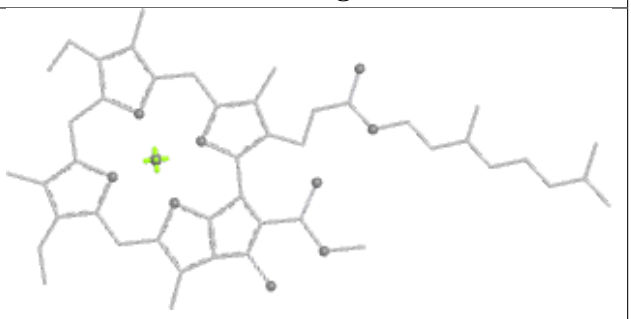
Bond lengths



Bond angles

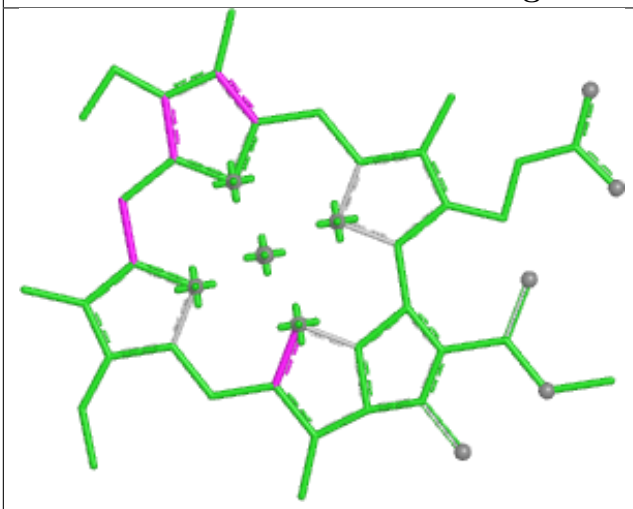


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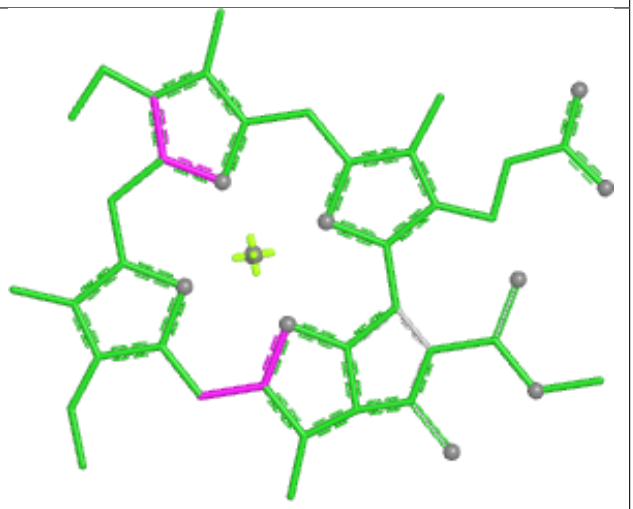


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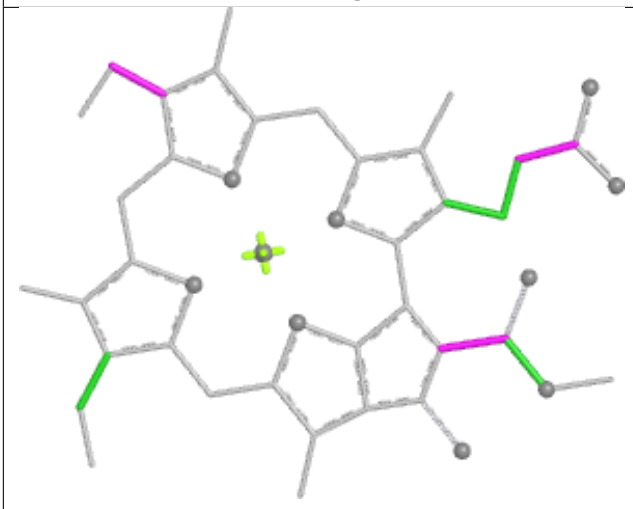
Ligand CLA K 101



Bond lengths



Bond angles

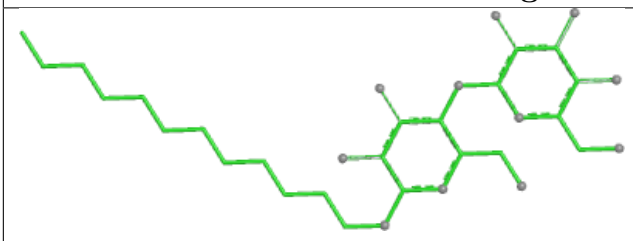


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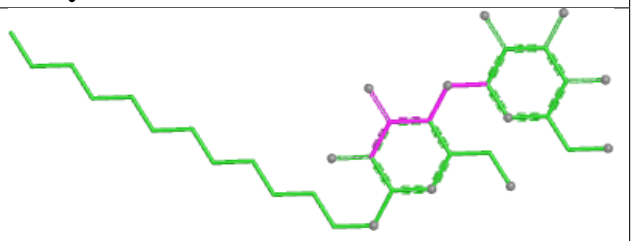


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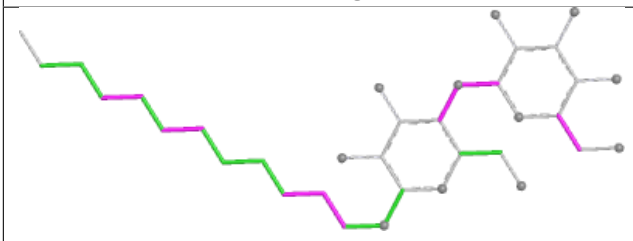
Ligand LMT Q 201



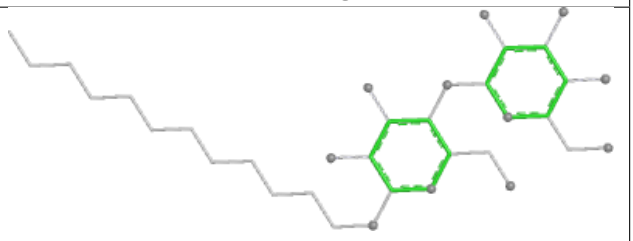
Bond lengths



Bond angles

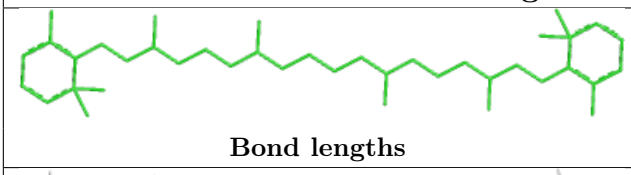


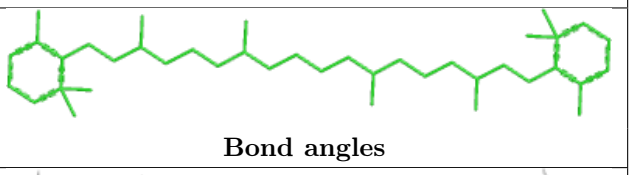
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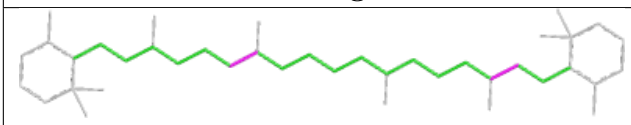


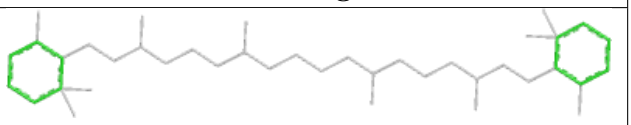
Rings

Ligand BCR H 845

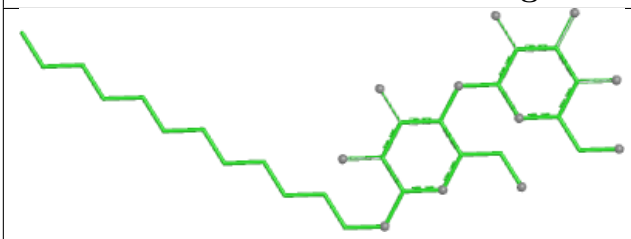

Bond lengths

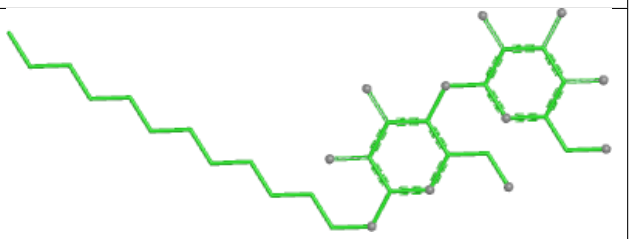

Bond angles

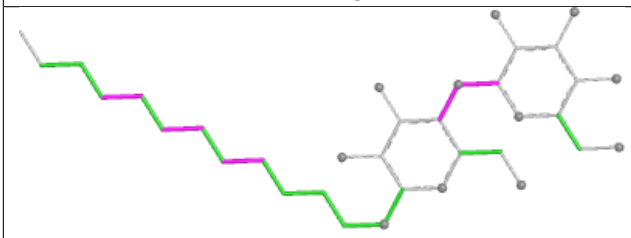

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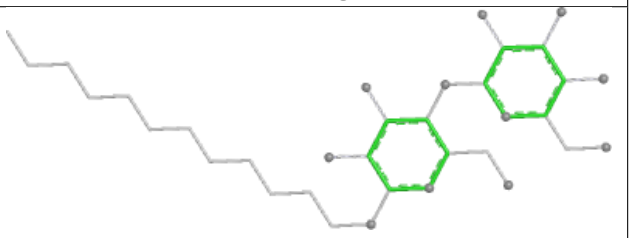

Rings

Ligand LMT A 856

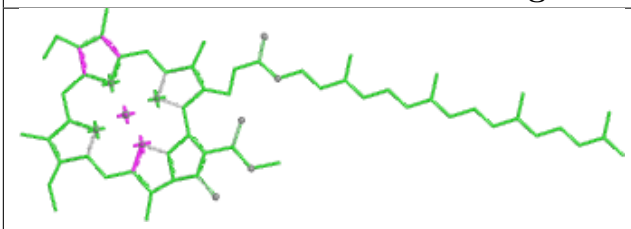

Bond lengths

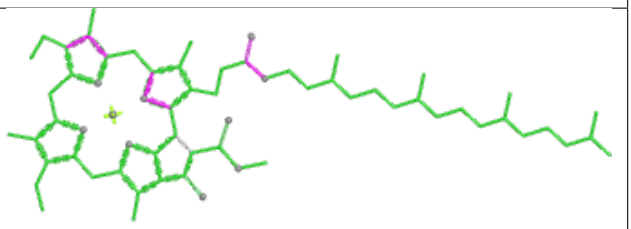

Bond angles

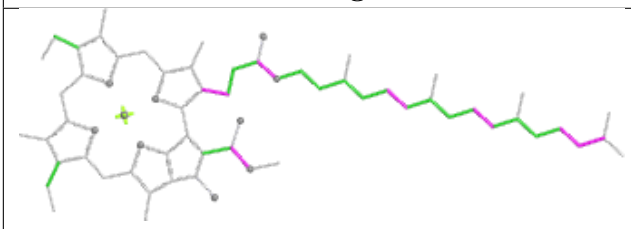

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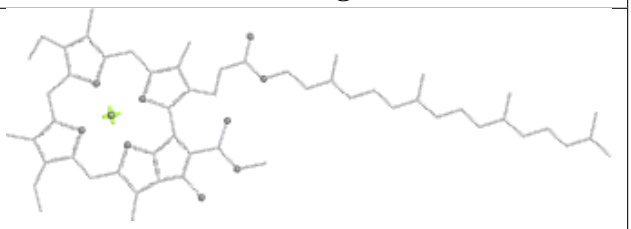

Rings

Ligand CLA a 807

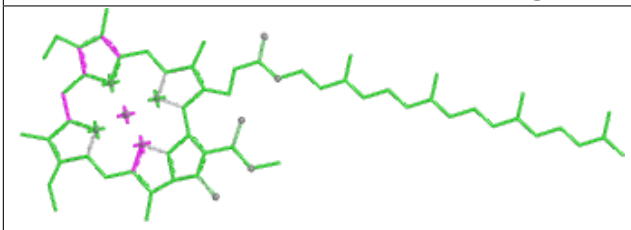

Bond lengths


Bond angles

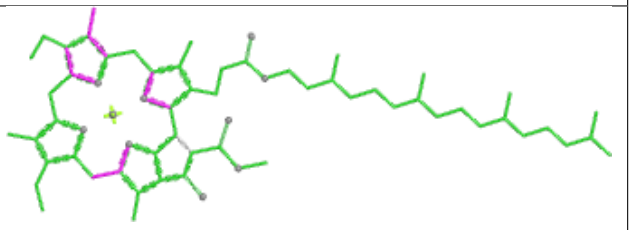

Torsions


Rings

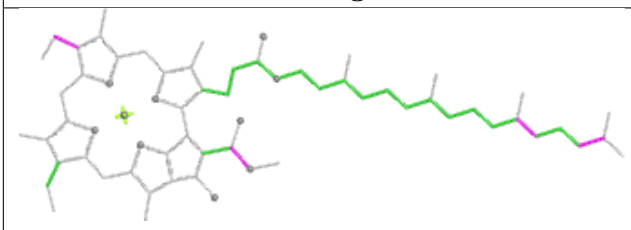
Ligand CLA a 834



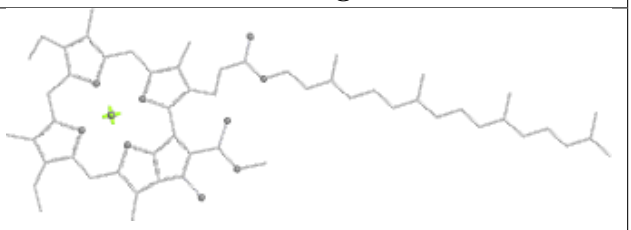
Bond lengths



Bond angles



Torsions

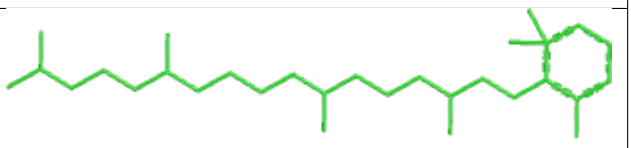


Rings

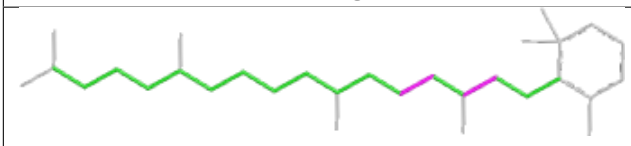
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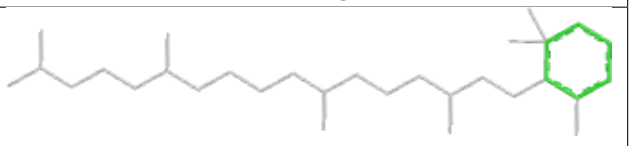
Bond lengths



Bond angles

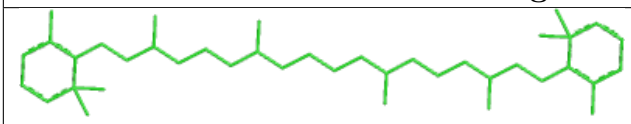


Torsions

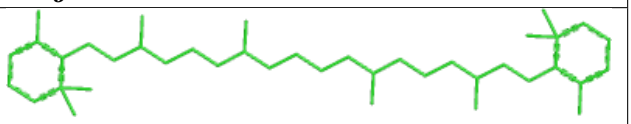


Rings

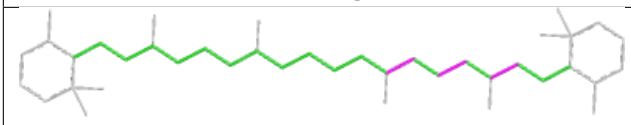
Ligand BCR j 104



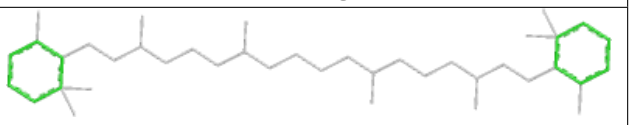
Bond lengths



Bond angles

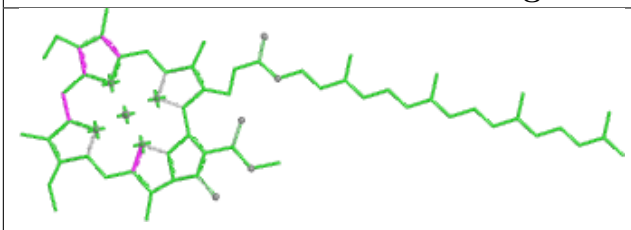


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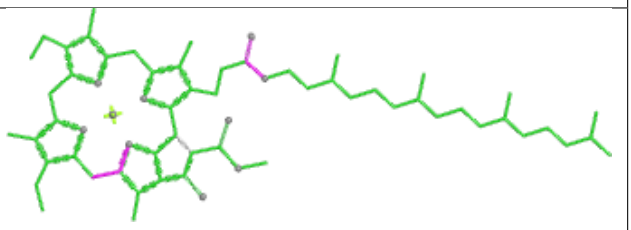


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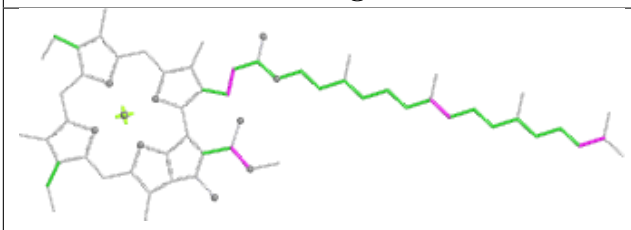
Ligand CLA H 805



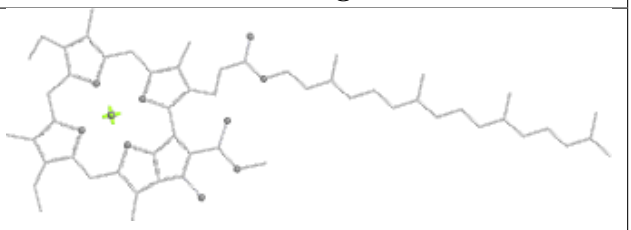
Bond lengths



Bond angles

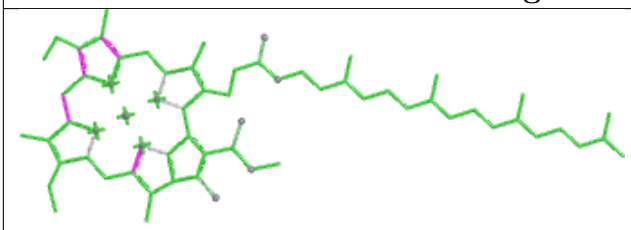


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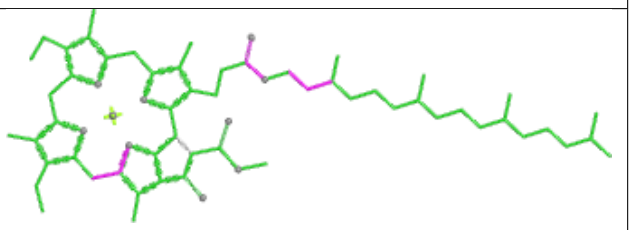


Rings

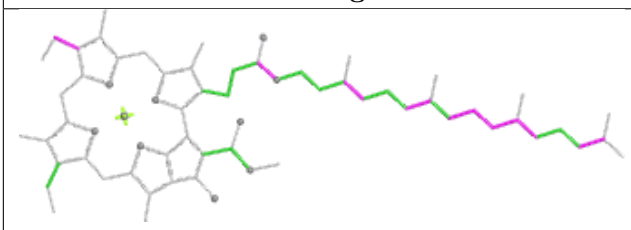
Ligand CLA H 815



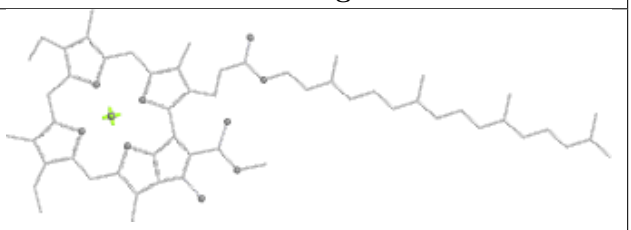
Bond lengths



Bond angles



Torsions



Rings

Ligand ECH L 1506



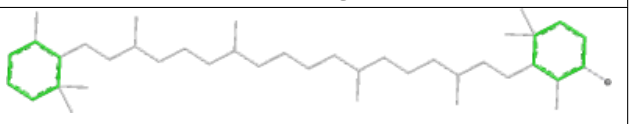
Bond lengths



Bond angles

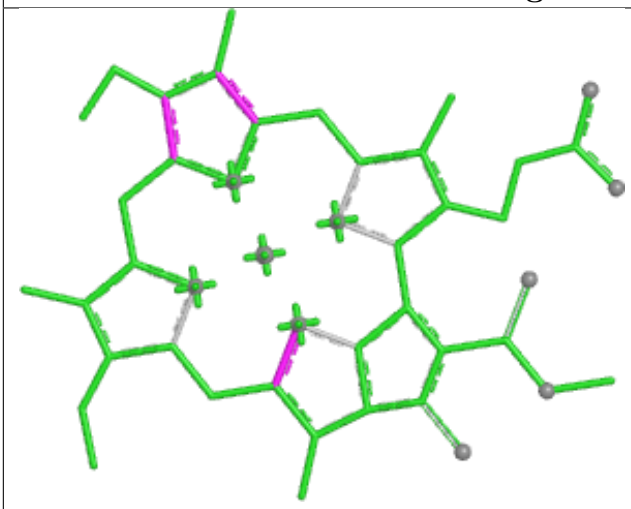


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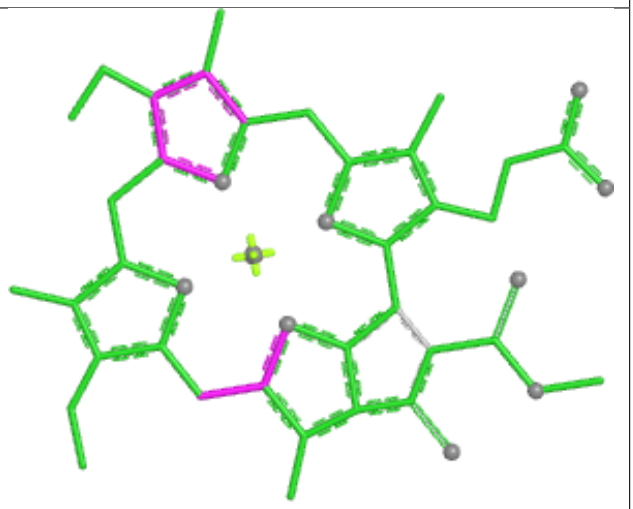


Rings

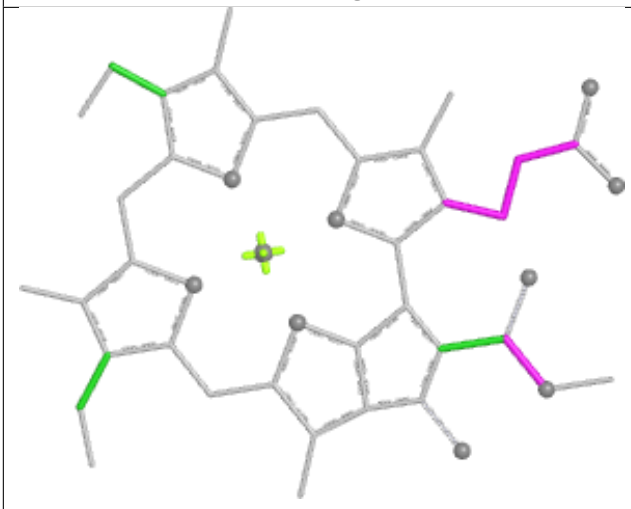
Ligand CLA F 203



Bond lengths



Bond angles

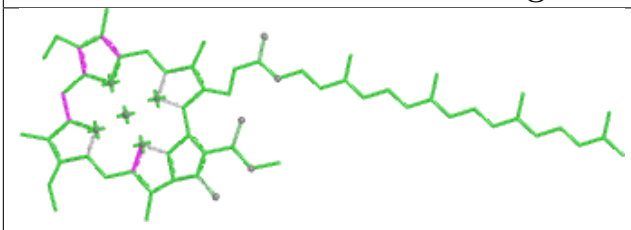


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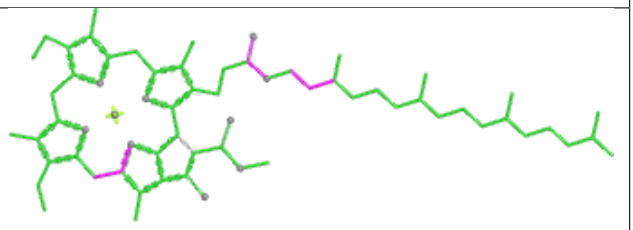


Rings

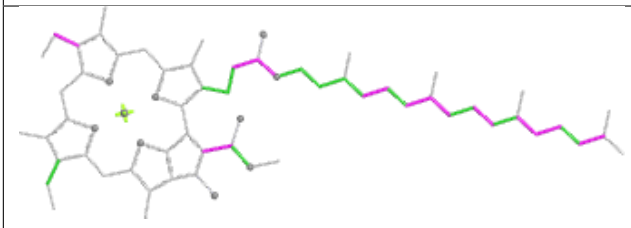
Ligand CLA b 823



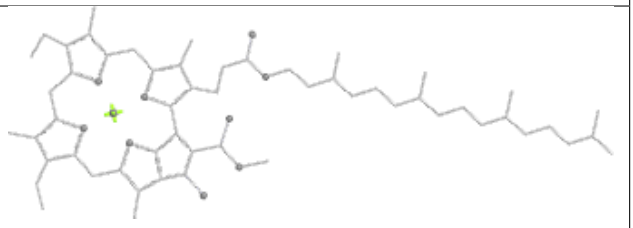
Bond lengths



Bond angles

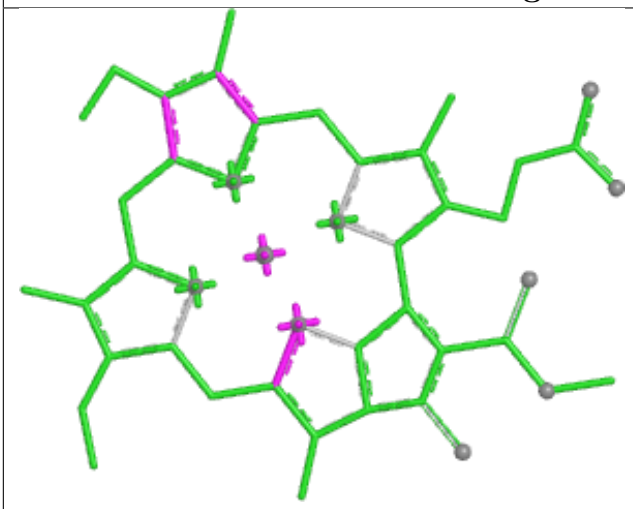


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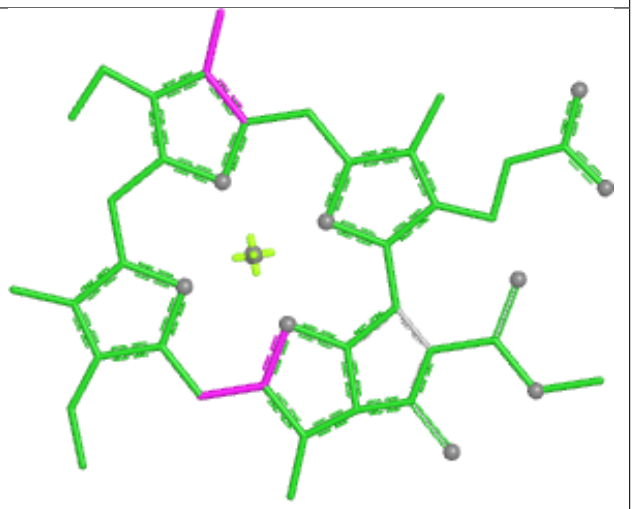


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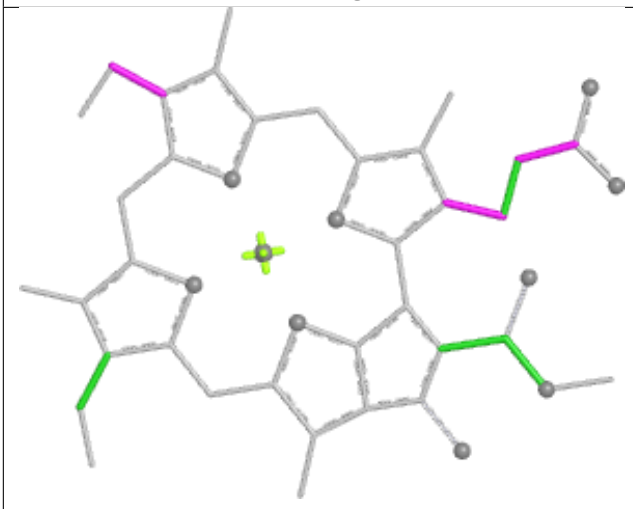
Ligand CLA H 823



Bond lengths



Bond angles

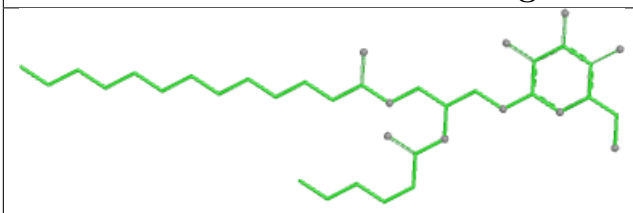


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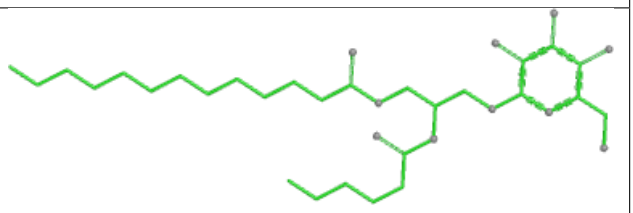


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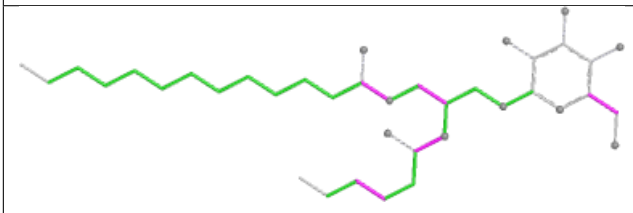
Ligand LMG l 5001



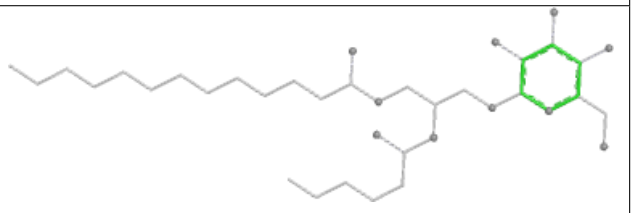
Bond lengths



Bond angles

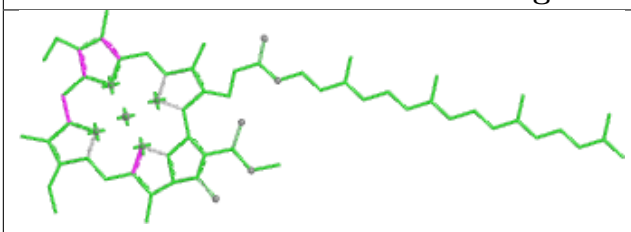


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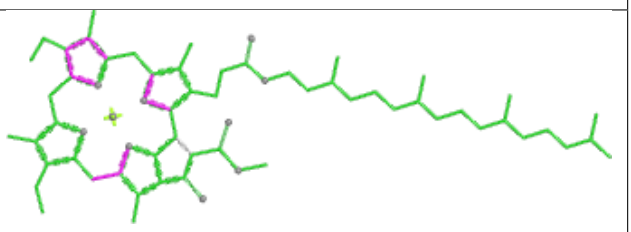


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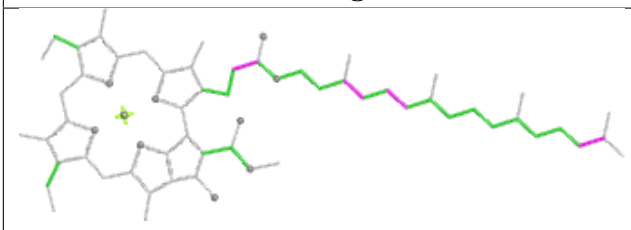
Ligand CL0 a 802



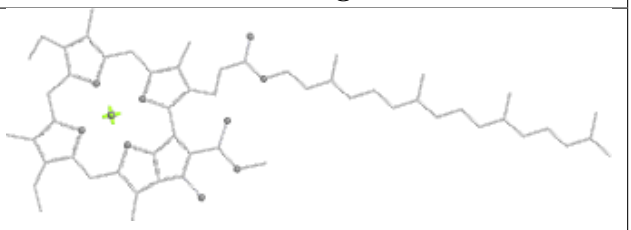
Bond lengths



Bond angles

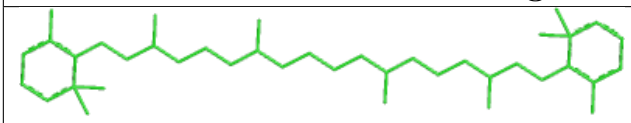


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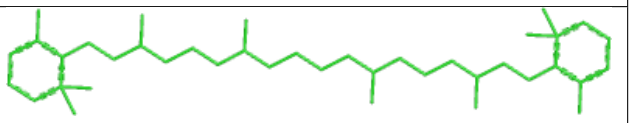


Rings

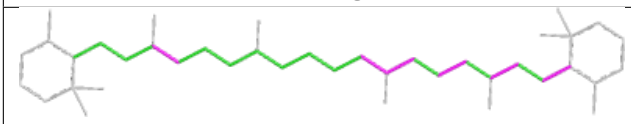
Ligand BCR a 852



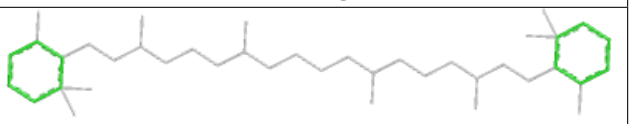
Bond lengths



Bond angles

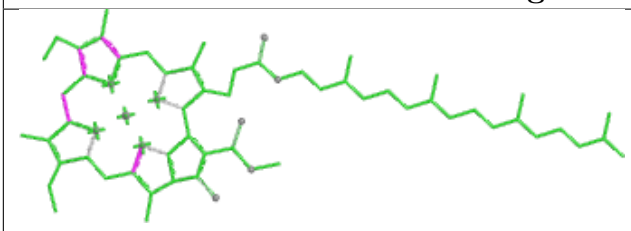


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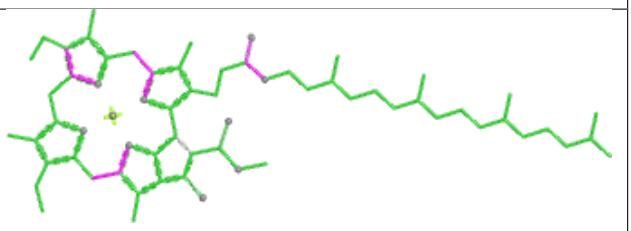


Rings

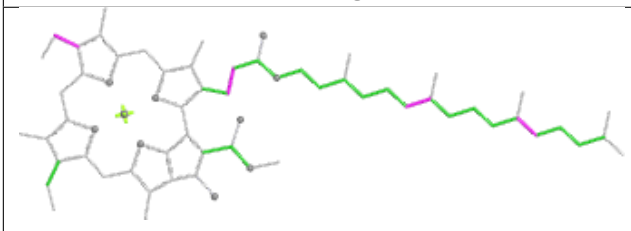
Ligand CLA b 842



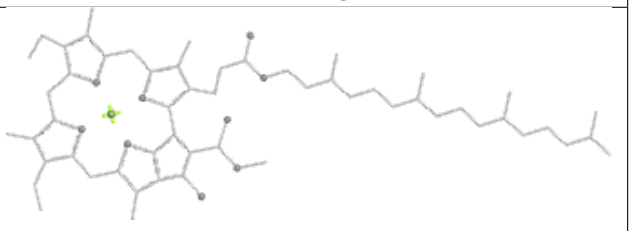
Bond lengths



Bond angles

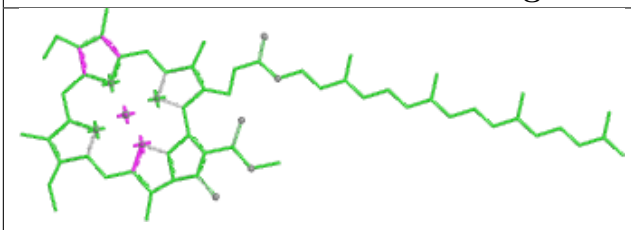


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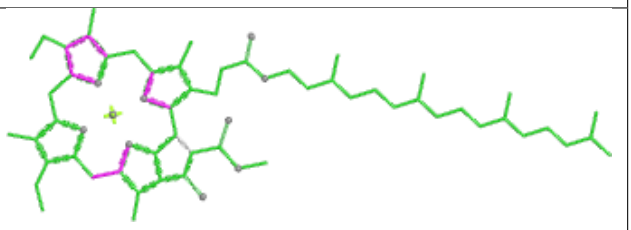


Rings

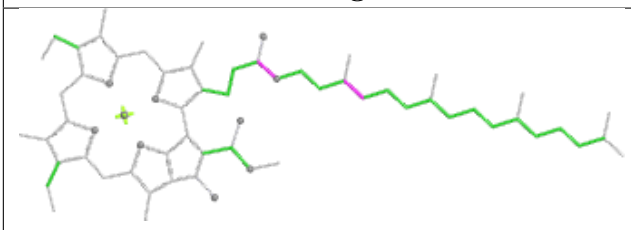
Ligand CLA H 829



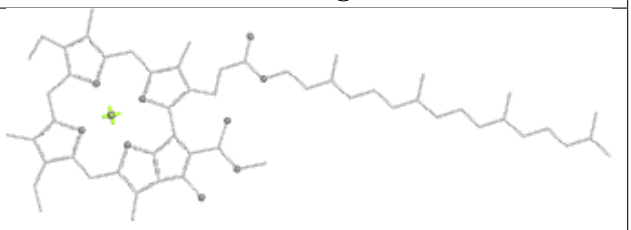
Bond lengths



Bond angles

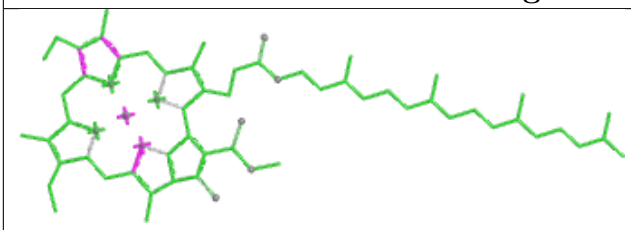


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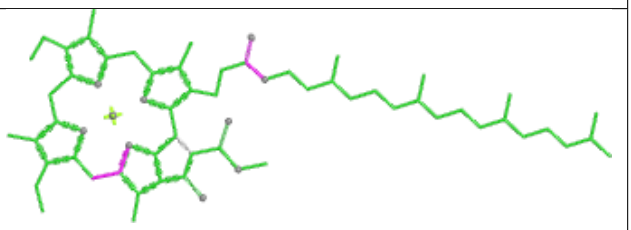


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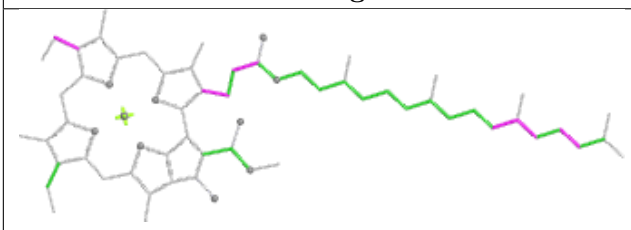
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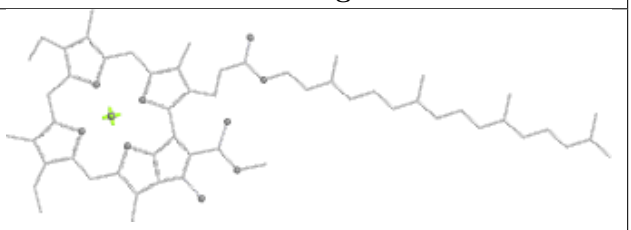
Bond lengths



Bond angles

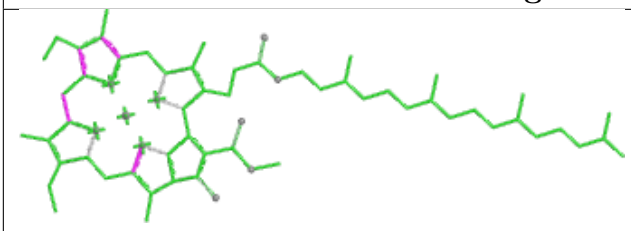


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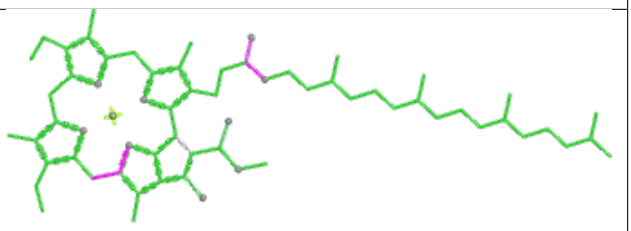


Rings

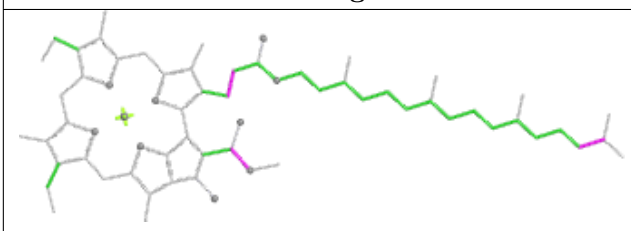
Ligand CLA B 806



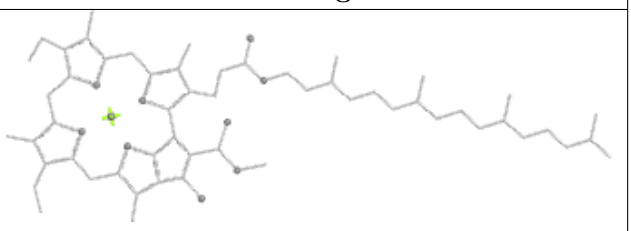
Bond lengths



Bond angles

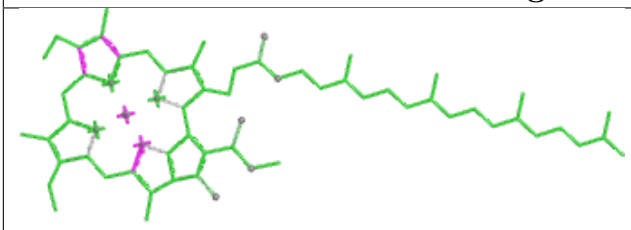


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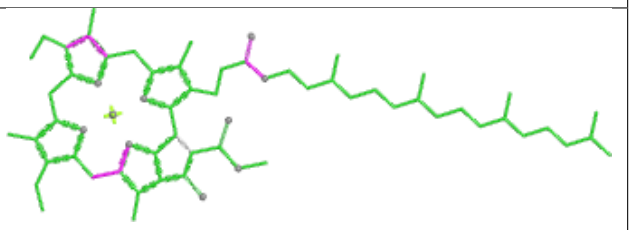


Rings

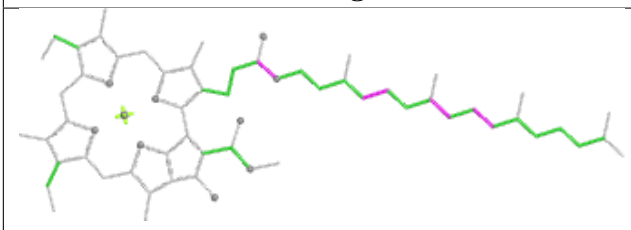
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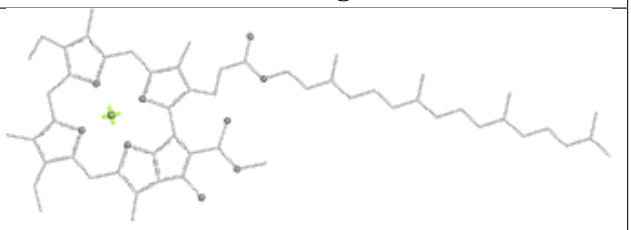
Bond lengths



Bond angles

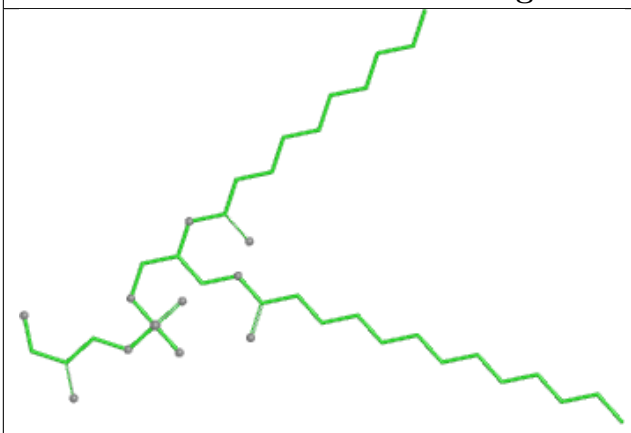


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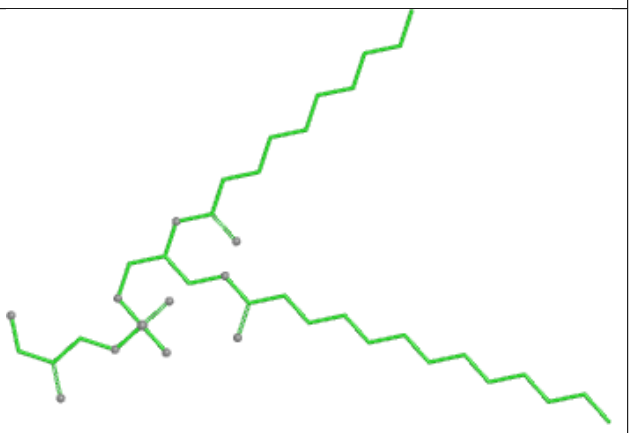


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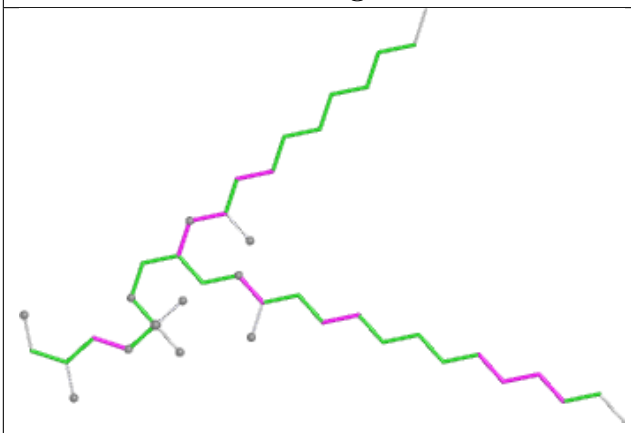
Ligand LHG L 1509



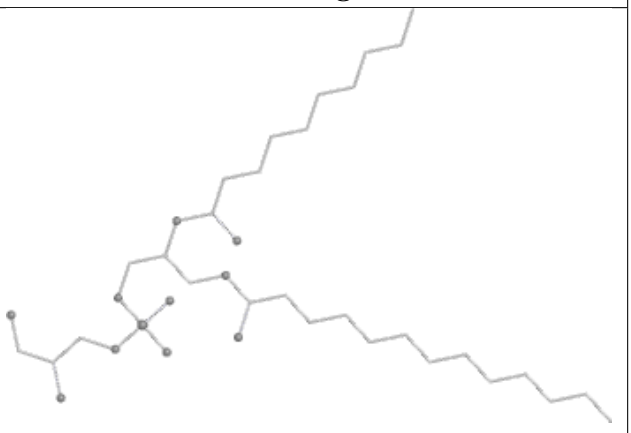
Bond lengths



Bond angles

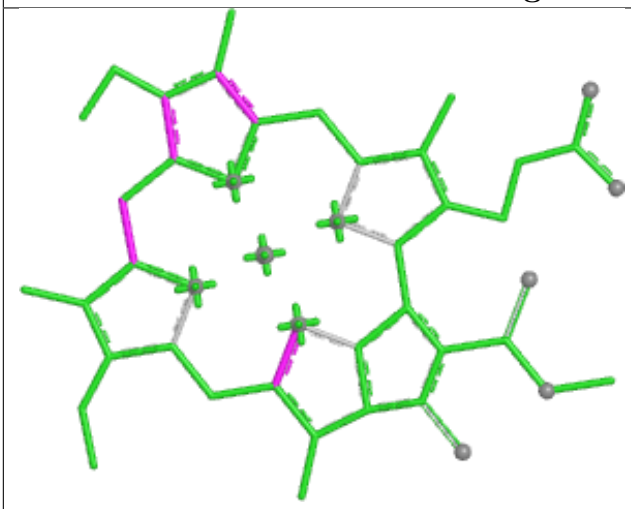


Torsions

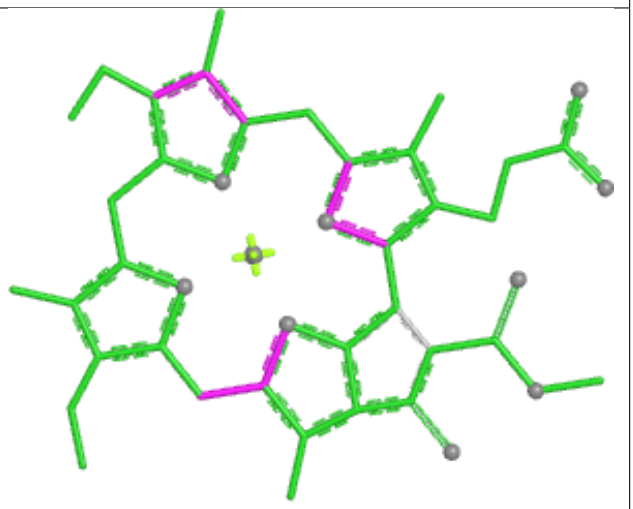


Rings

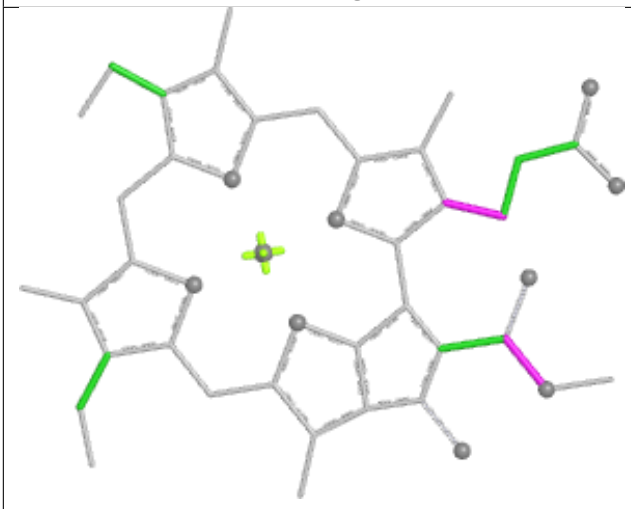
Ligand CLA A 810



Bond lengths



Bond angles

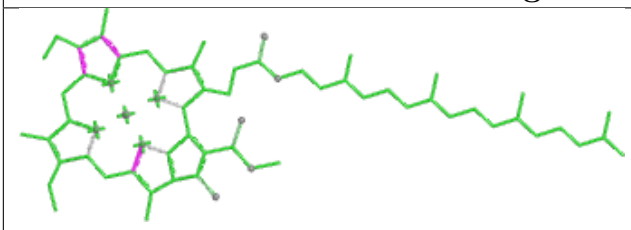


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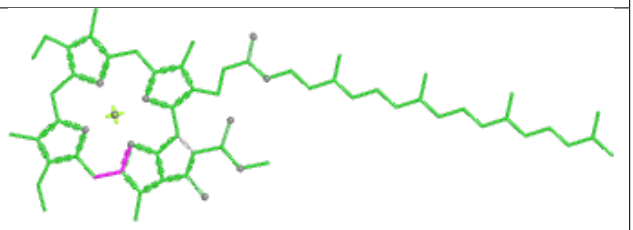


Rings

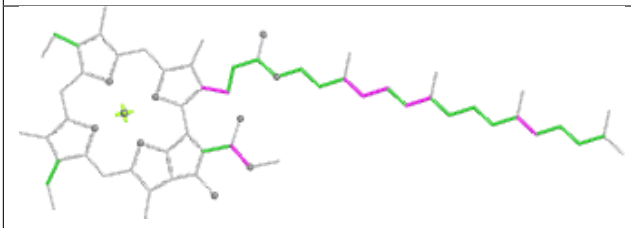
Ligand CLA l 5004



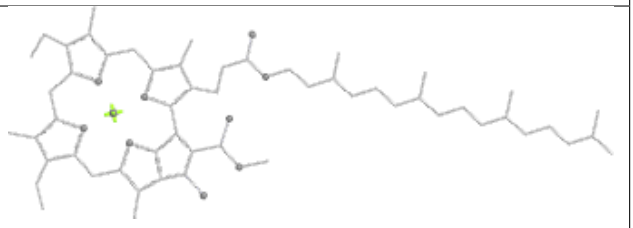
Bond lengths



Bond angles

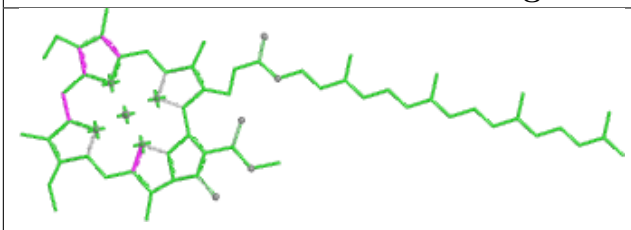


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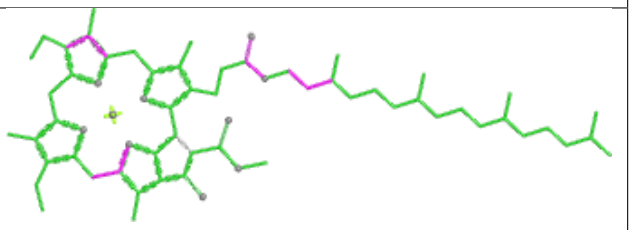


Rings

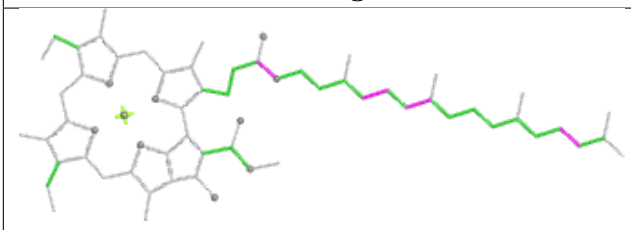
Ligand CLA H 831



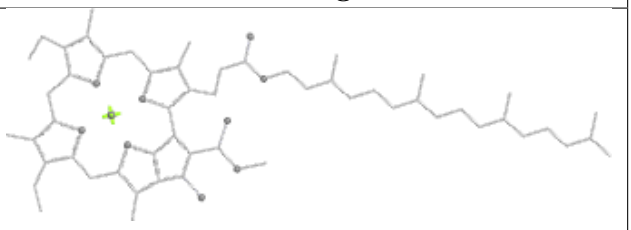
Bond lengths



Bond angles

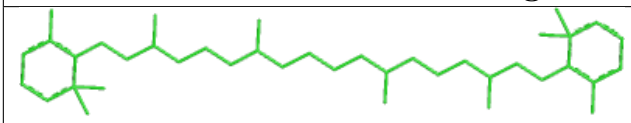


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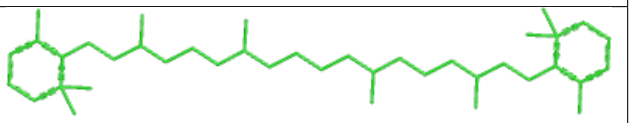


Rings

Ligand BCR T 104



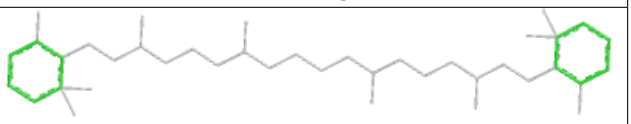
Bond lengths



Bond angles

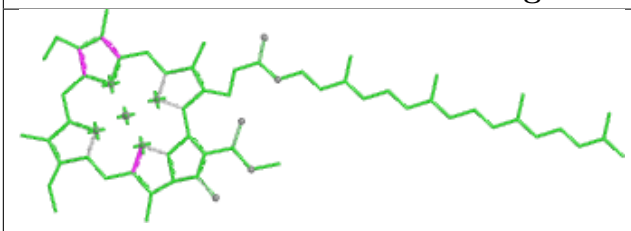


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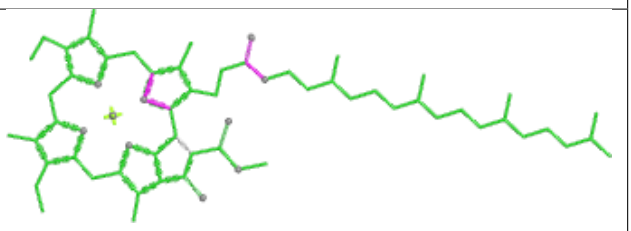


Rings

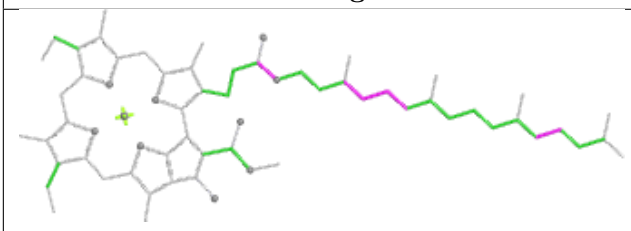
Ligand CLA A 820



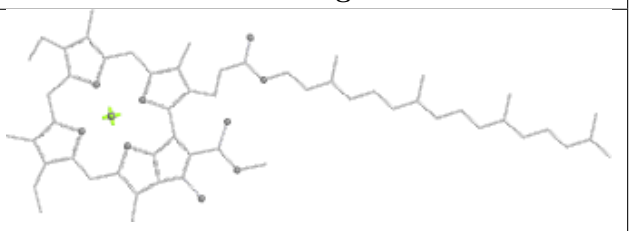
Bond lengths



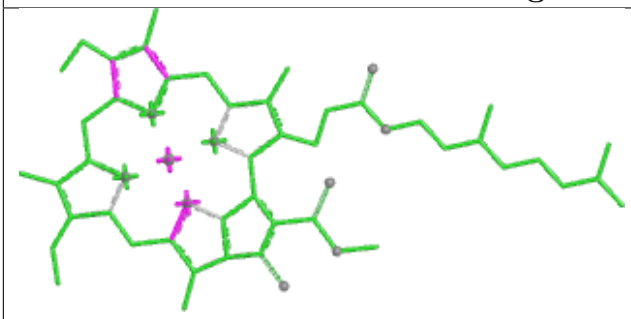
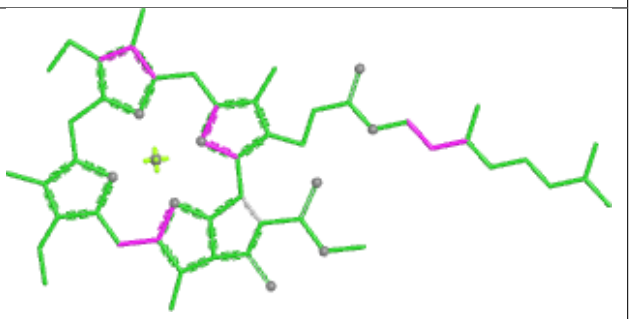
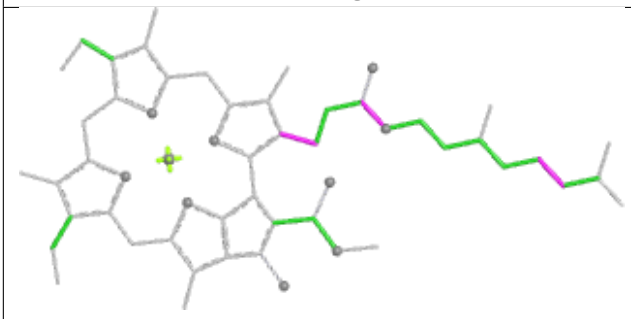
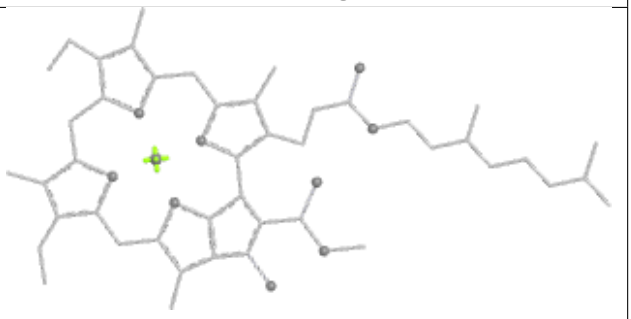
Bond angles

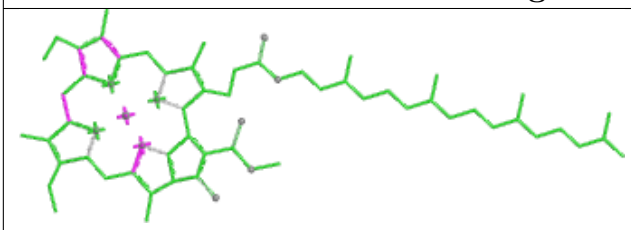
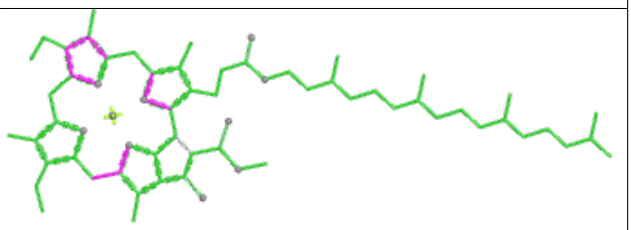
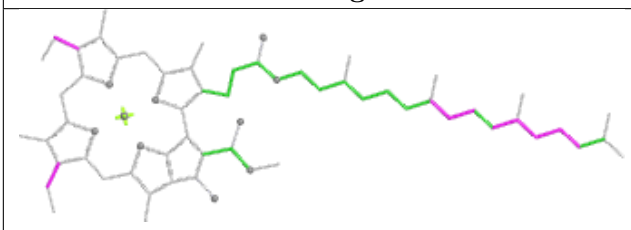
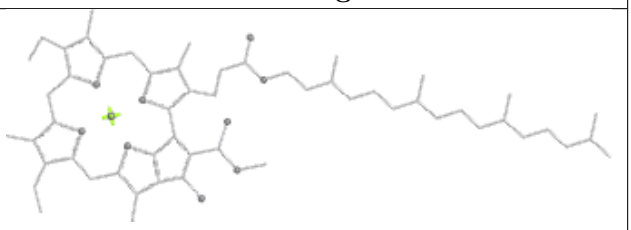


Torsions

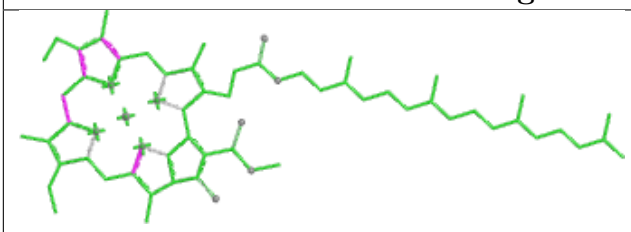


Rings

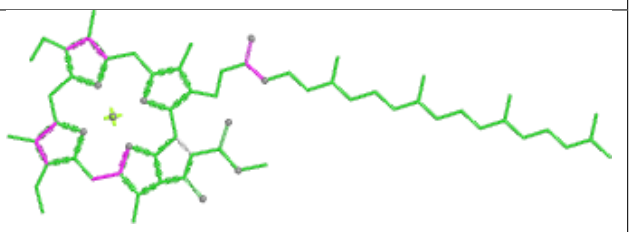
Ligand CLA b 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

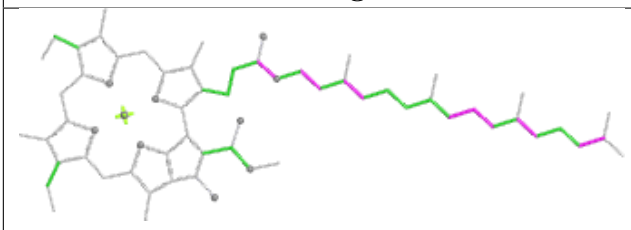
Ligand CLA L 1503



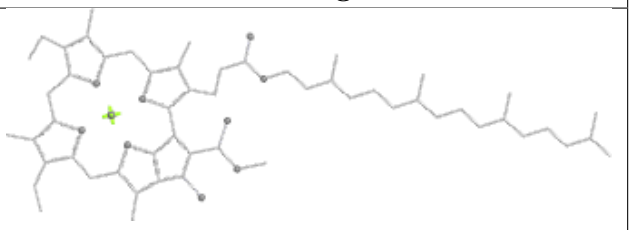
Bond lengths



Bond angles

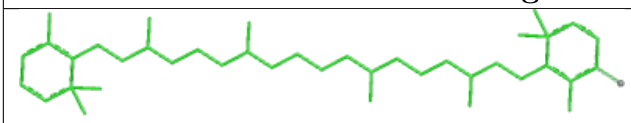


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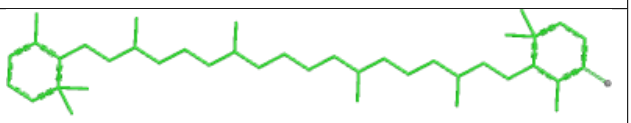


Rings

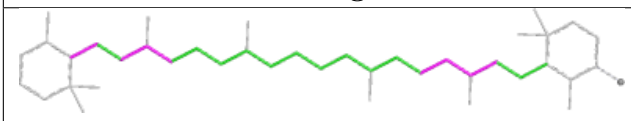
Ligand ECH H 846



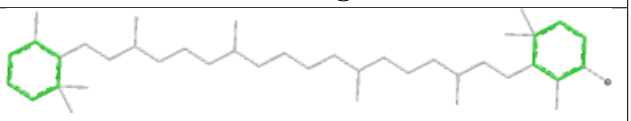
Bond lengths



Bond angles

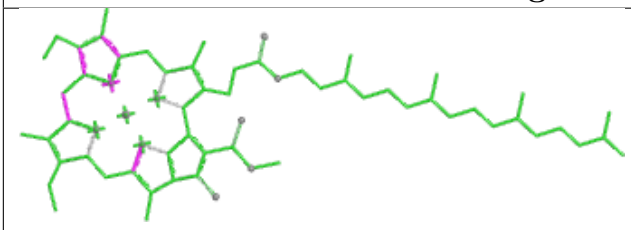


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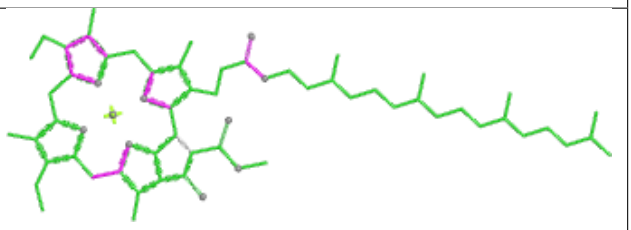


Rings

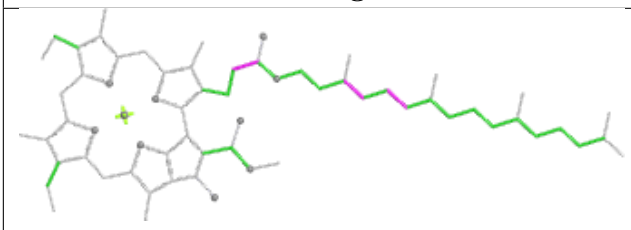
Ligand CL0 A 802



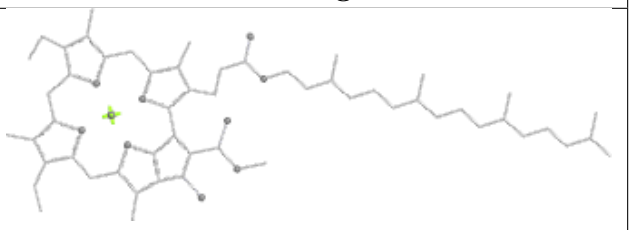
Bond lengths



Bond angles

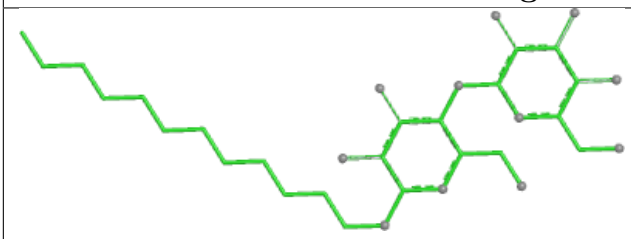


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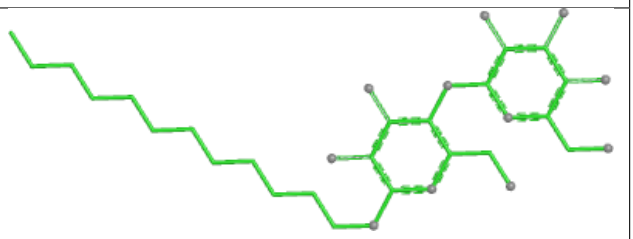


Rings

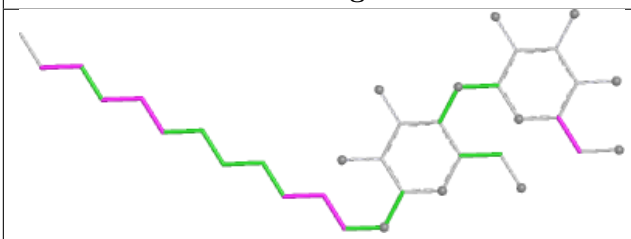
Ligand LMT G 853



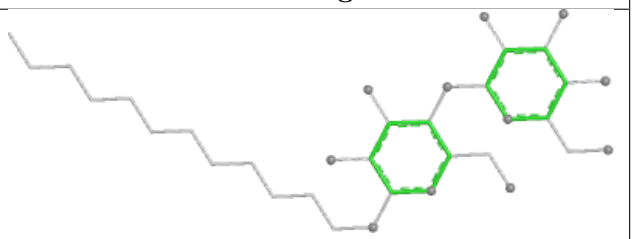
Bond lengths



Bond angles

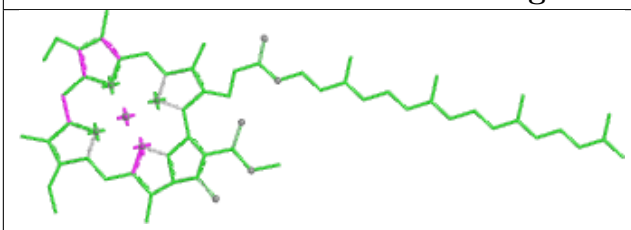


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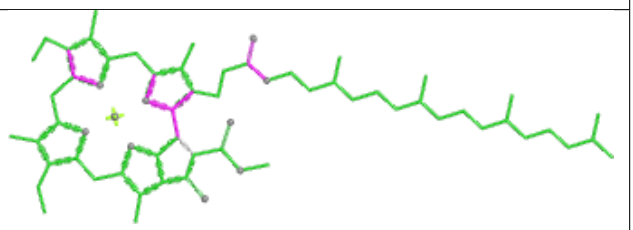


Rings

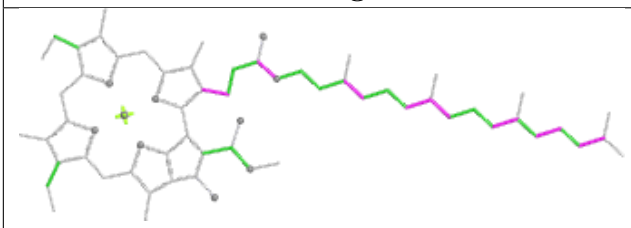
Ligand CLA a 829



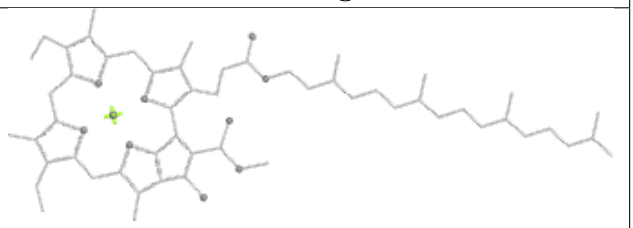
Bond lengths



Bond angles

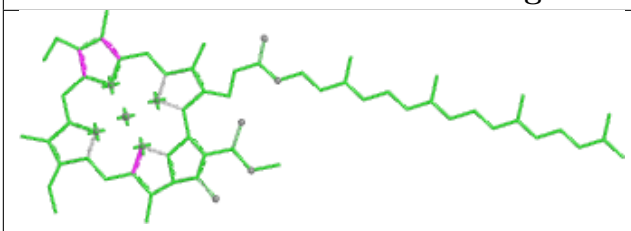


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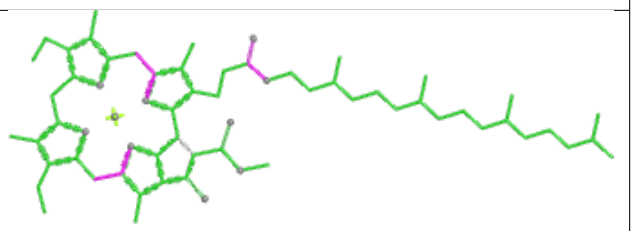


Rings

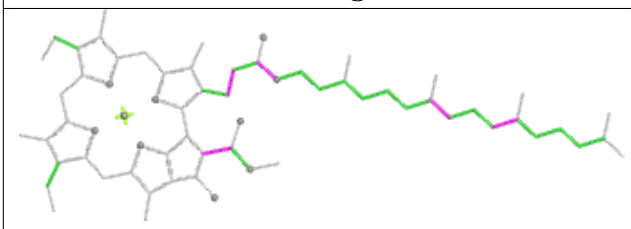
Ligand CLA B 801



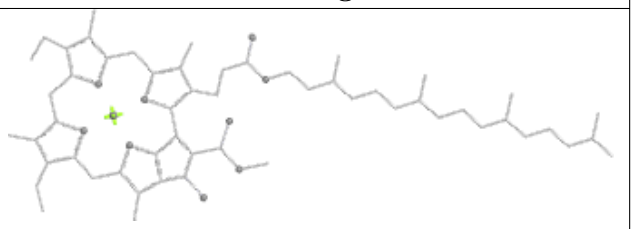
Bond lengths



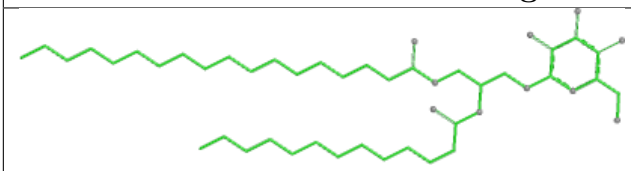
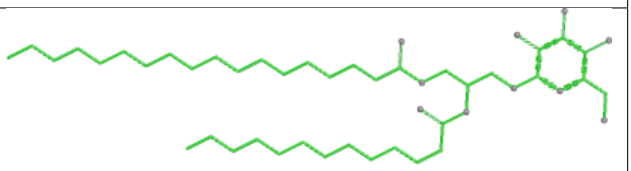
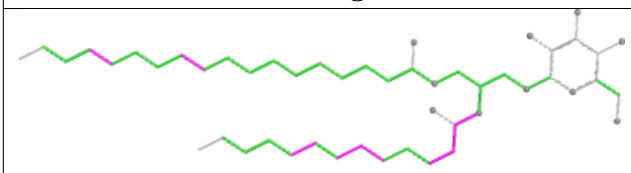
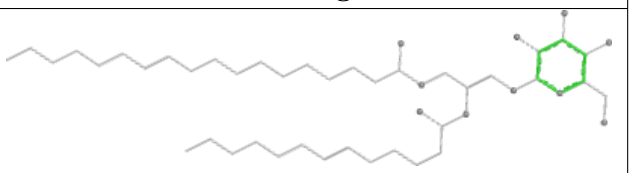
Bond angles

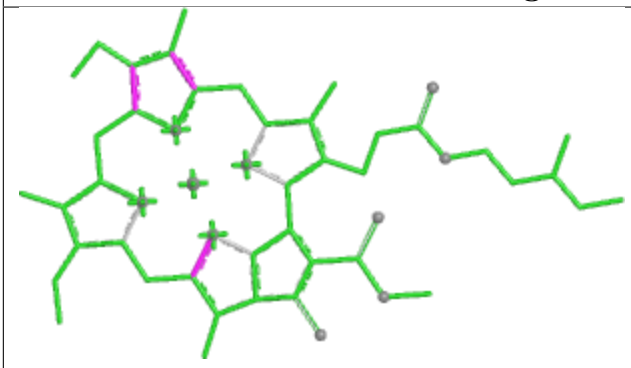
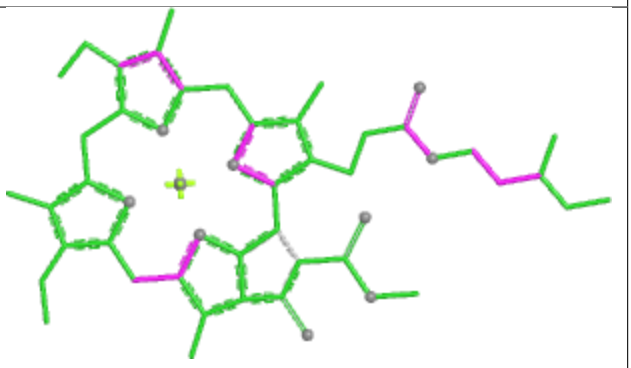
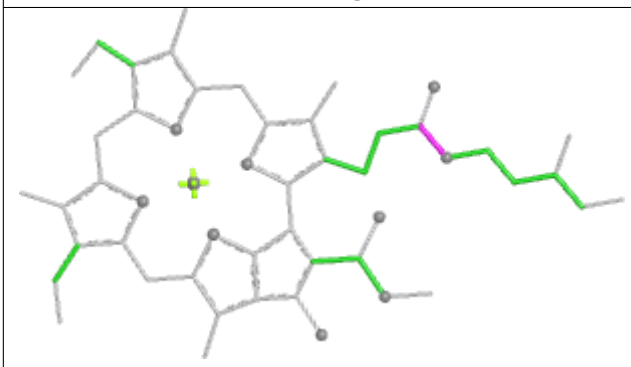
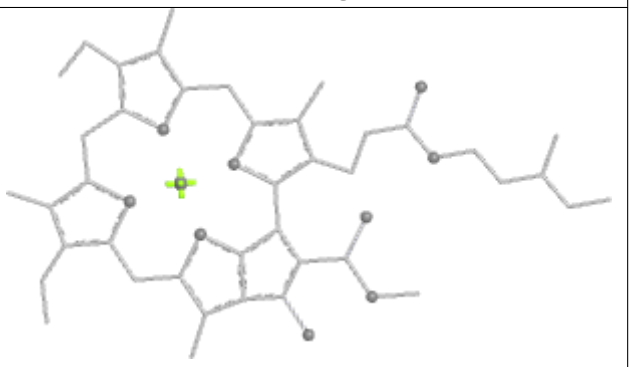


Torsions

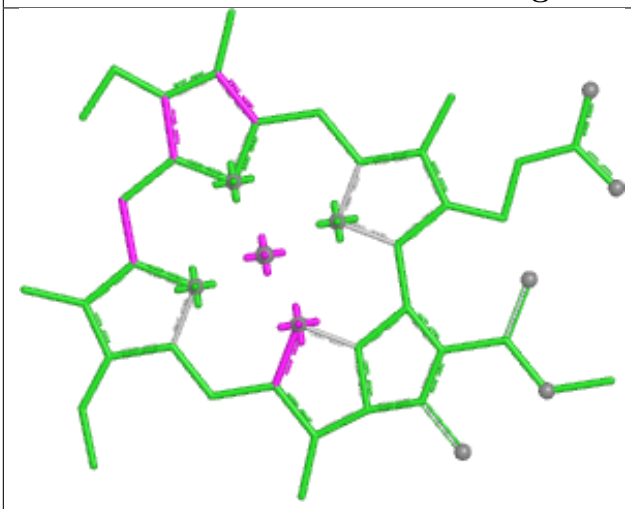


Rings

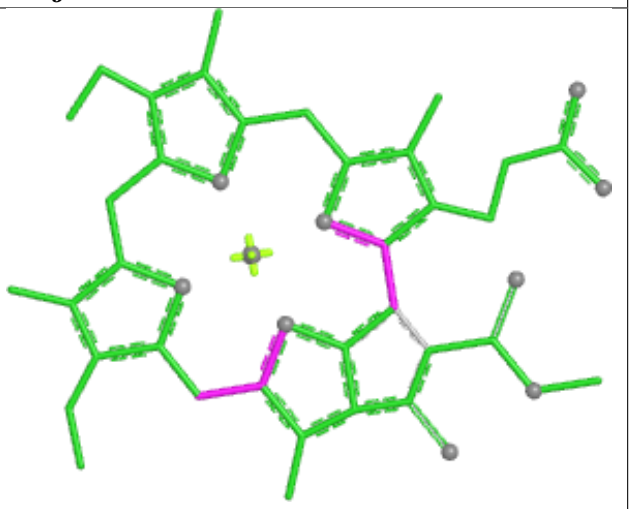
Ligand LMG B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

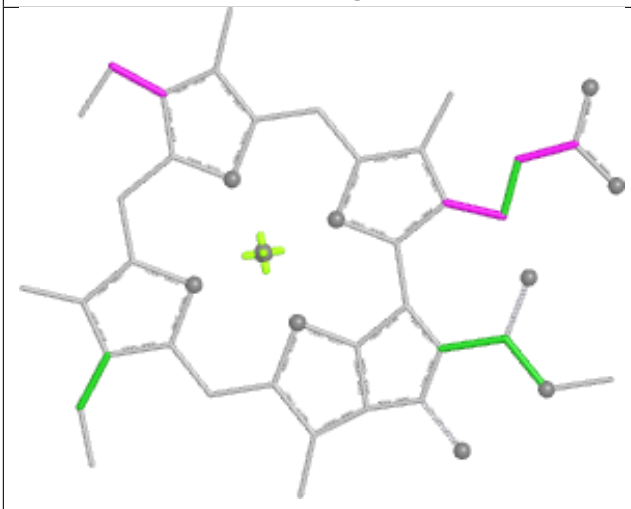
Ligand CLA j 101



Bond lengths



Bond angles

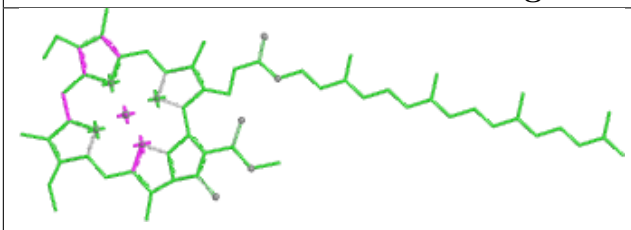


Torsions

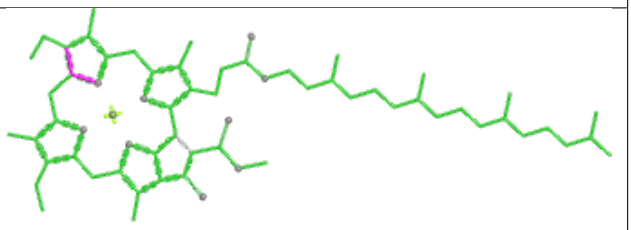


Rings

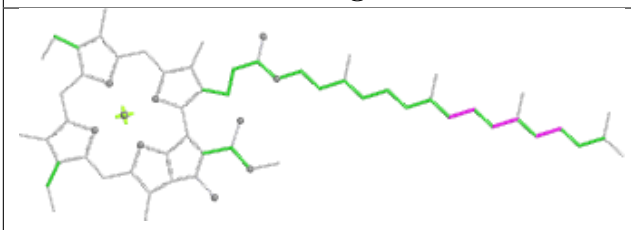
Ligand CLA B 802



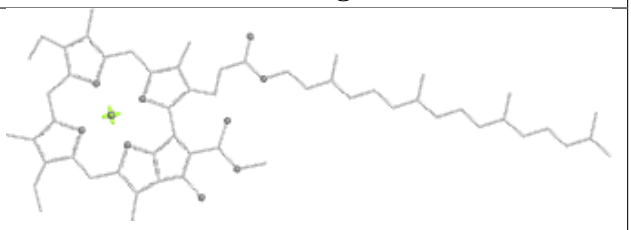
Bond lengths



Bond angles

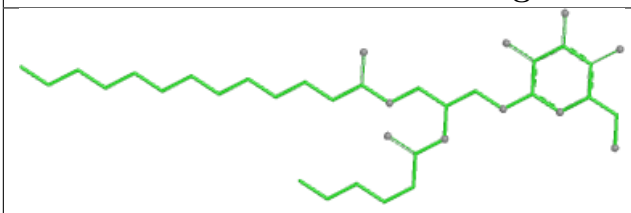


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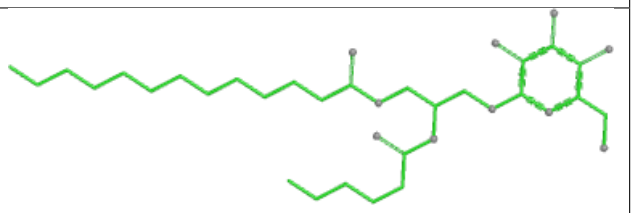


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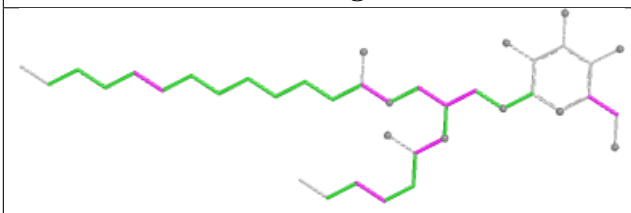
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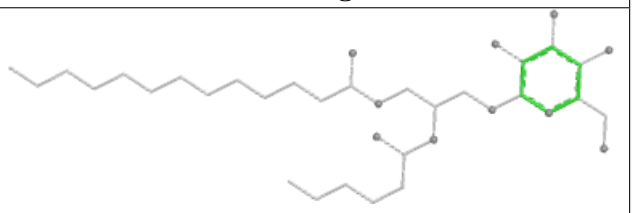
Bond lengths



Bond angles



Torsions



Rings

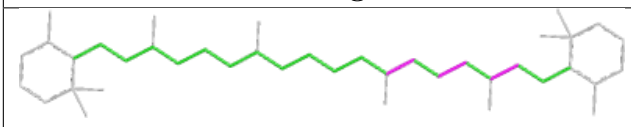
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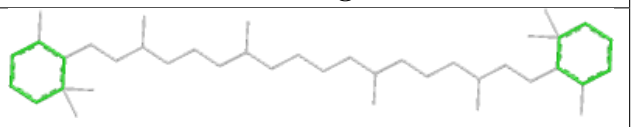
Bond lengths



Bond angles

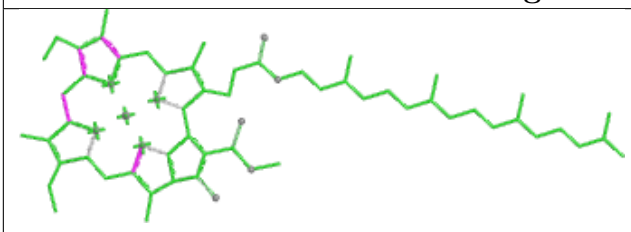


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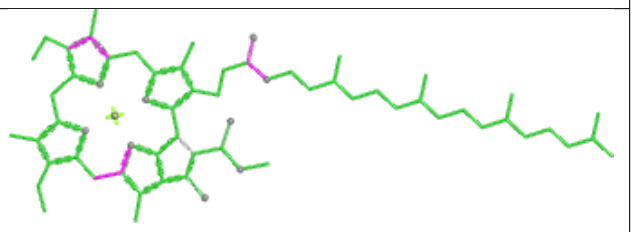


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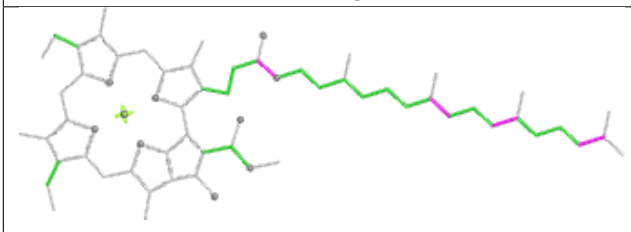
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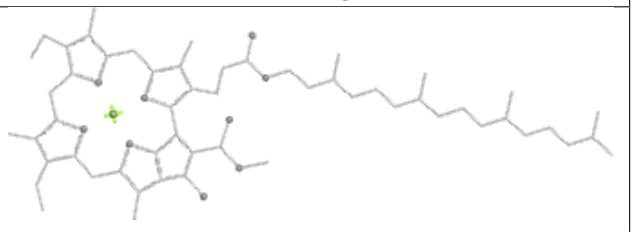
Bond lengths



Bond angles

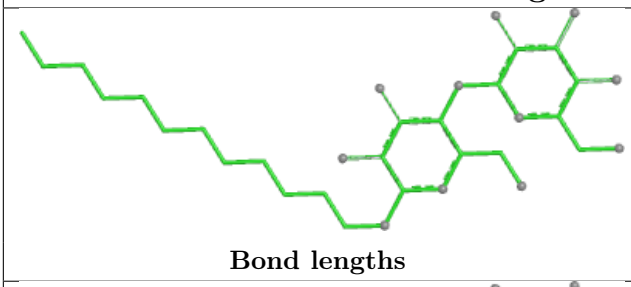


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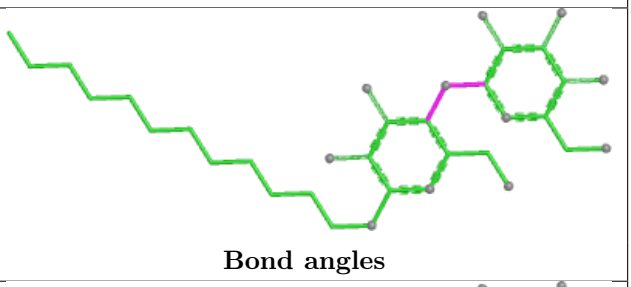


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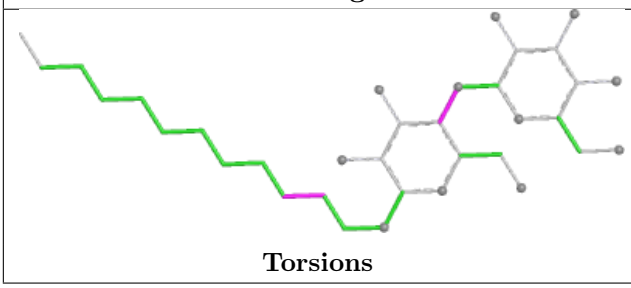
Ligand LMT f 203



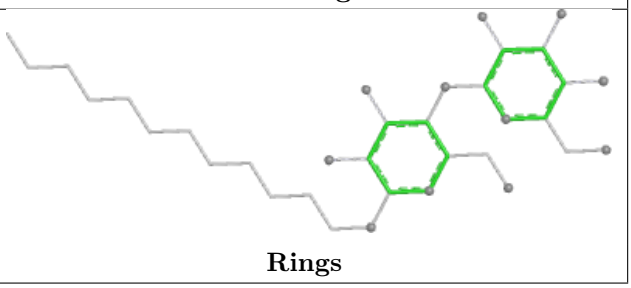
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Bond angles

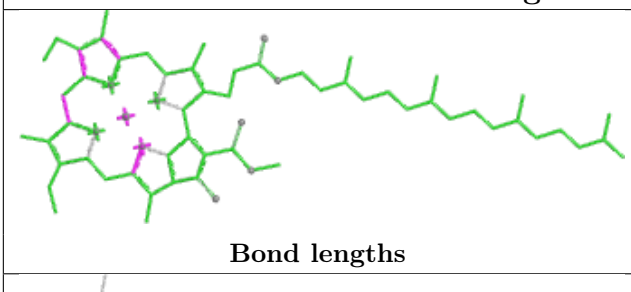


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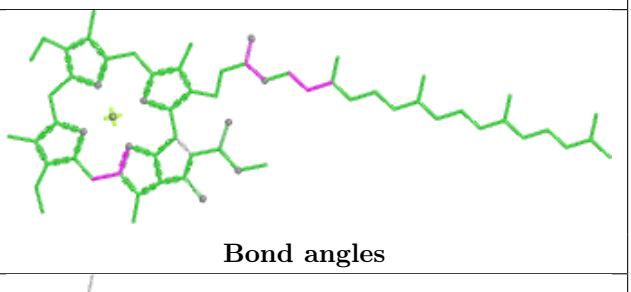


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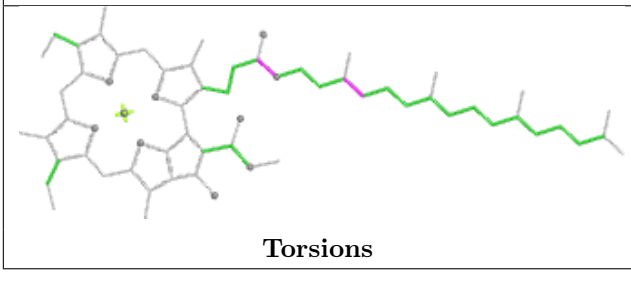
Ligand CLA U 206



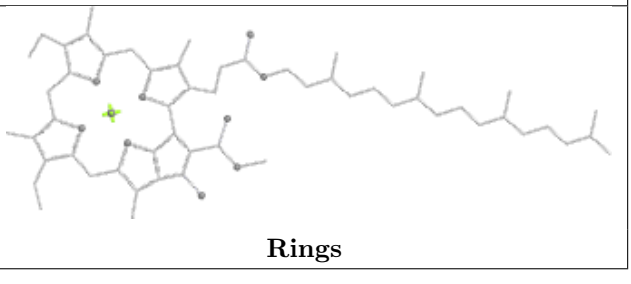
Bond lengths



Bond angles



Torsions

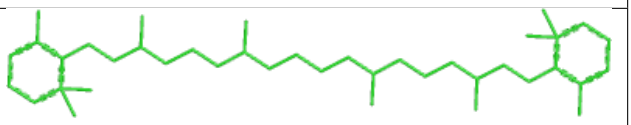


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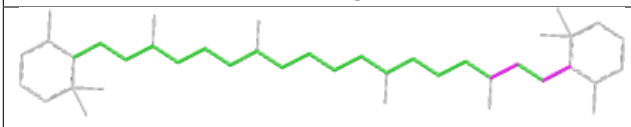
Ligand BCR B 845



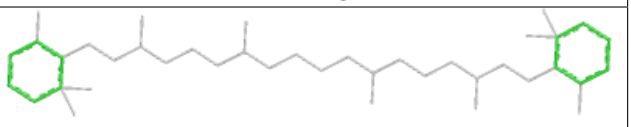
Bond lengths



Bond angles

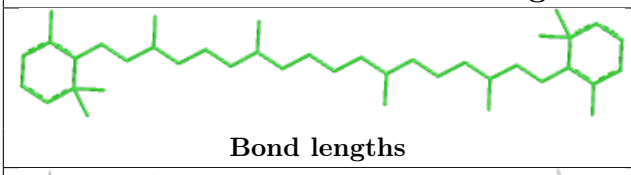


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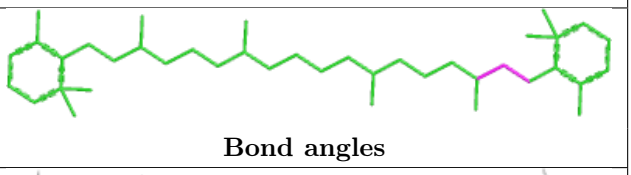


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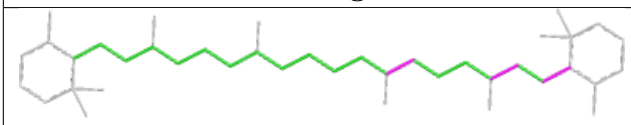
Ligand BCR I 101



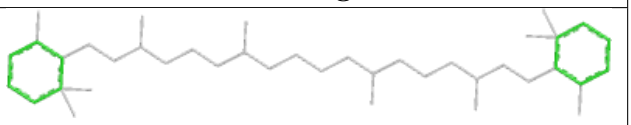
Bond lengths



Bond angles

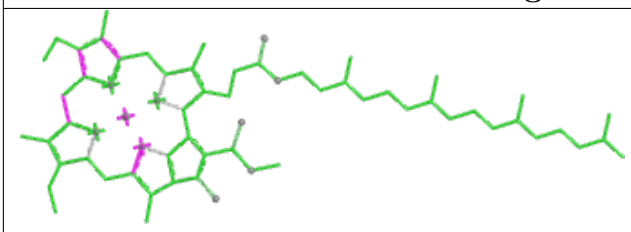


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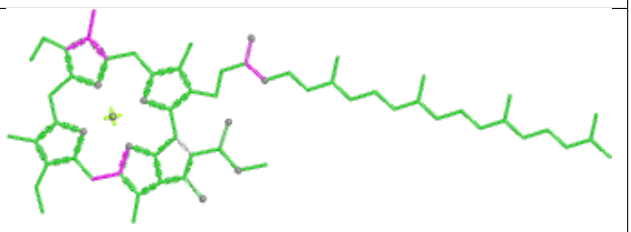


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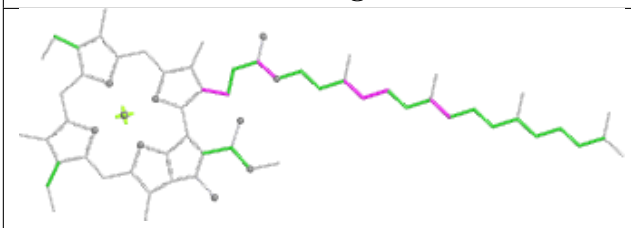
Ligand CLA B 838



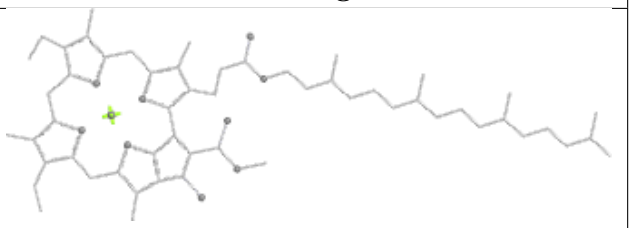
Bond lengths



Bond angles

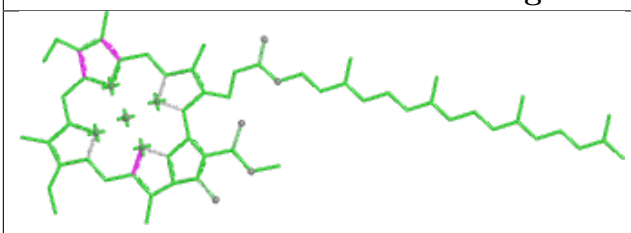


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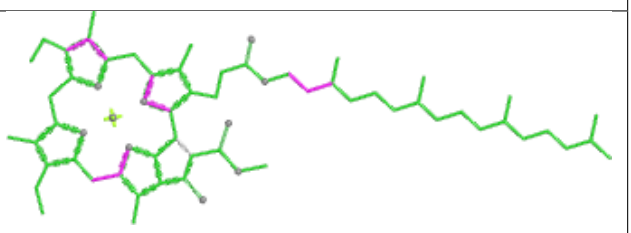


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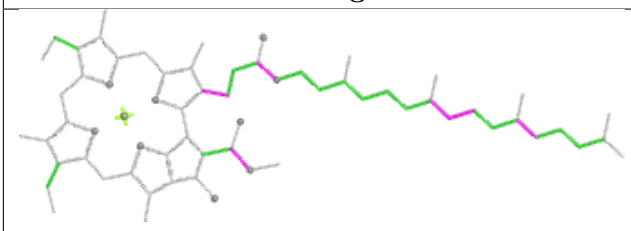
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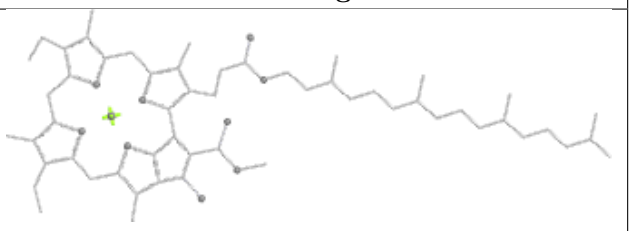
Bond lengths



Bond angles

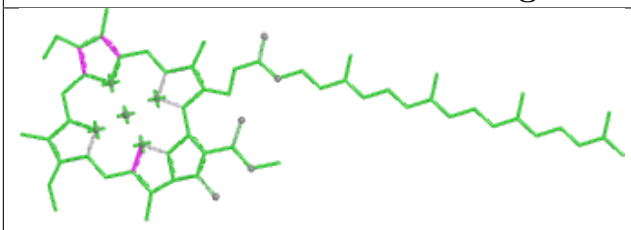


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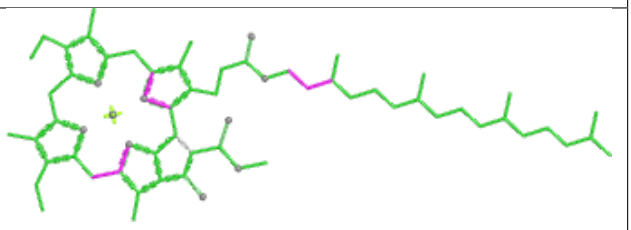


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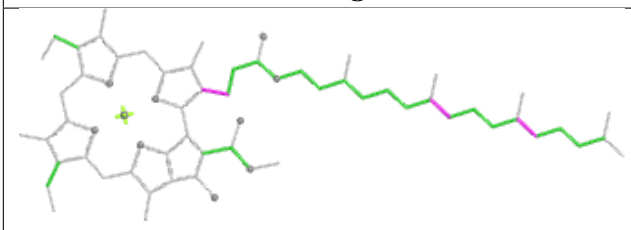
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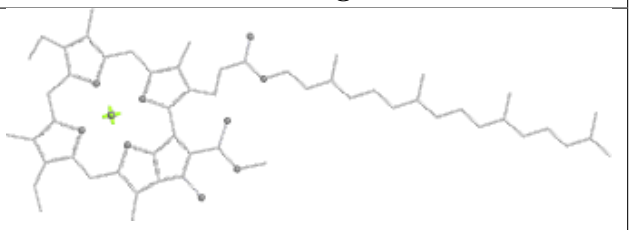
Bond lengths



Bond angles

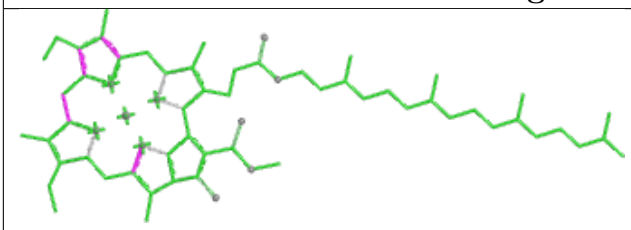


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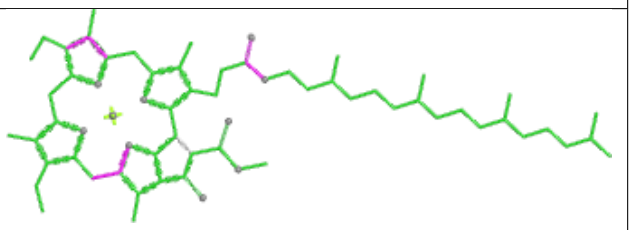


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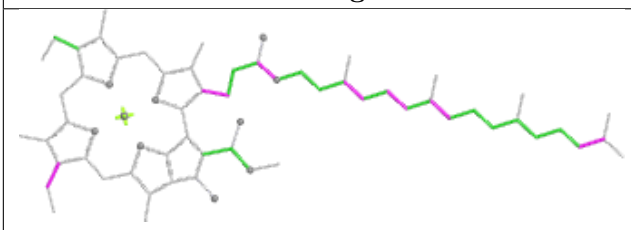
Ligand CLA b 816



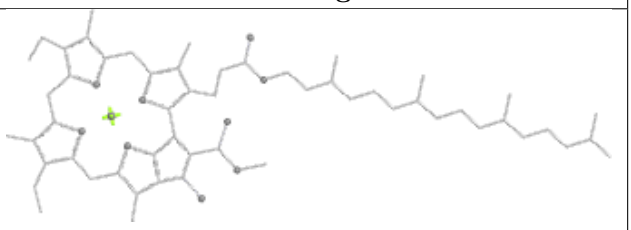
Bond lengths



Bond angles

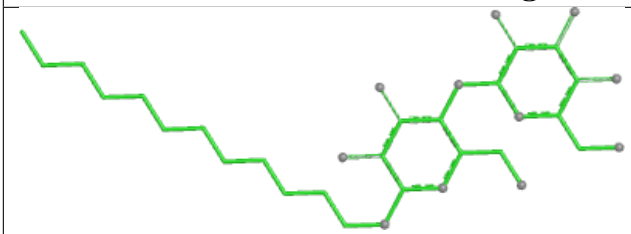


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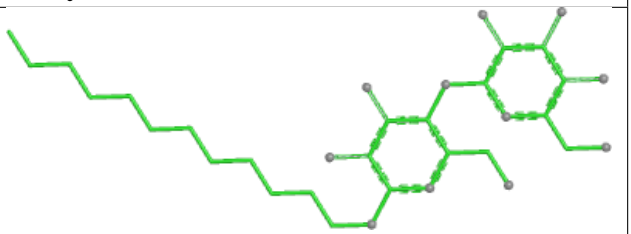


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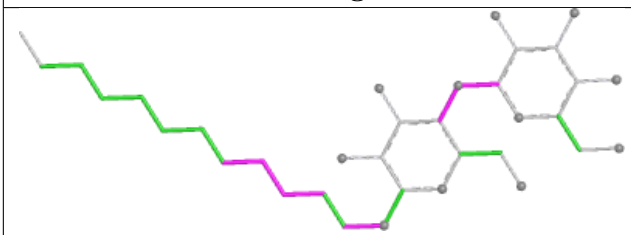
Ligand LMT Q 207



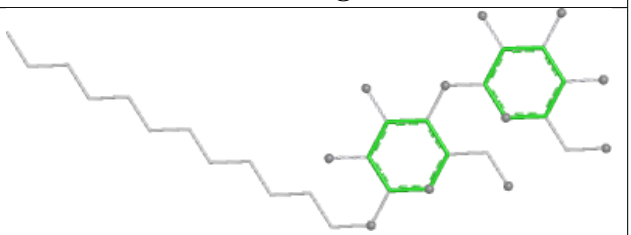
Bond lengths



Bond angles

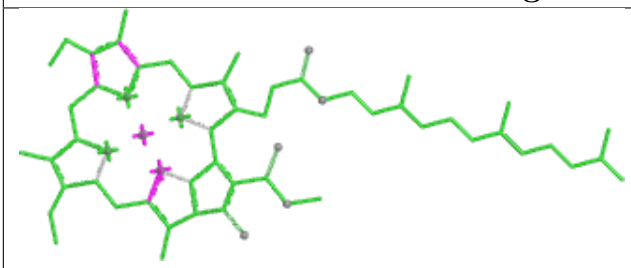


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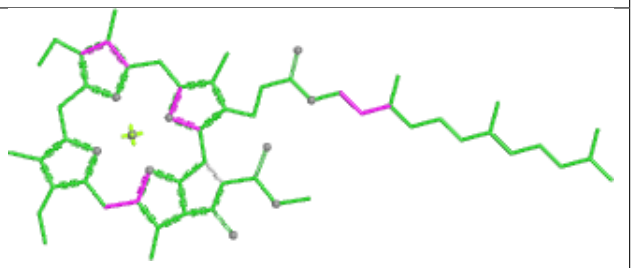


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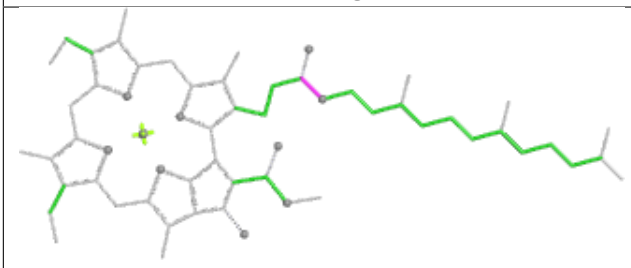
Ligand CLA G 833



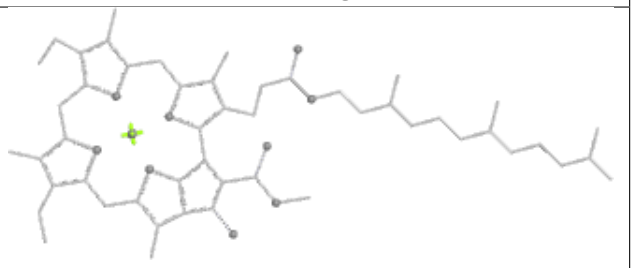
Bond lengths



Bond angles

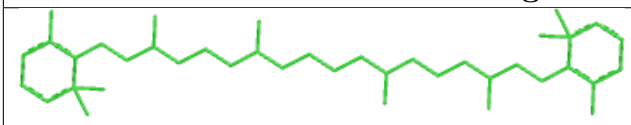


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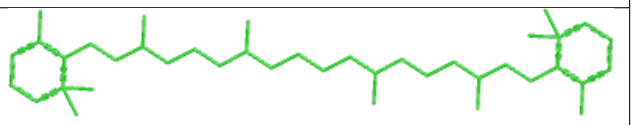


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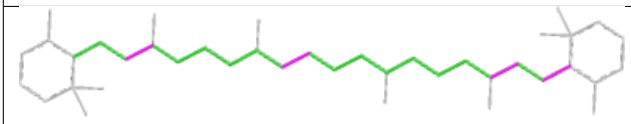
Ligand BCR R 103



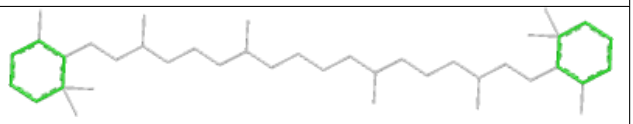
Bond lengths



Bond angles

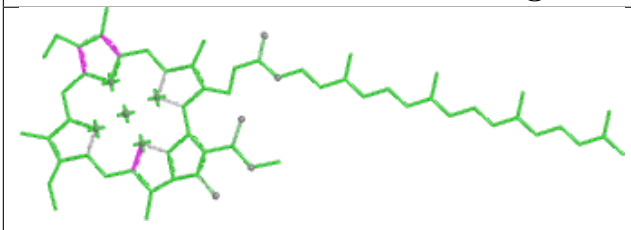


Torsions

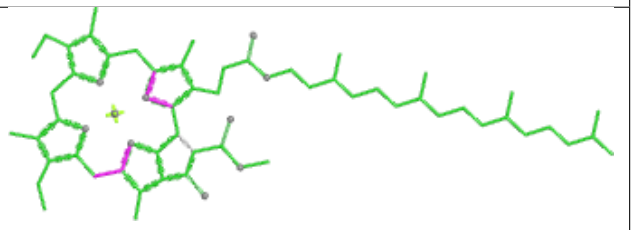


Rings

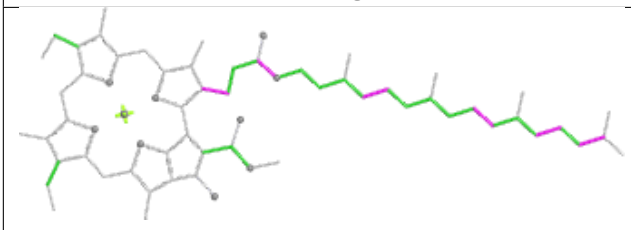
Ligand CLA F 201



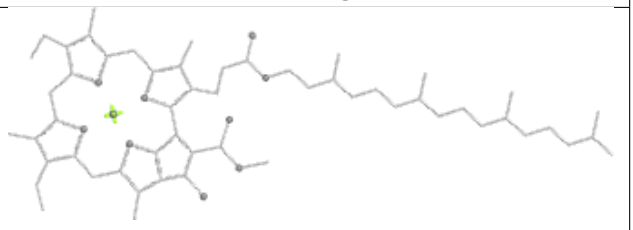
Bond lengths



Bond angles

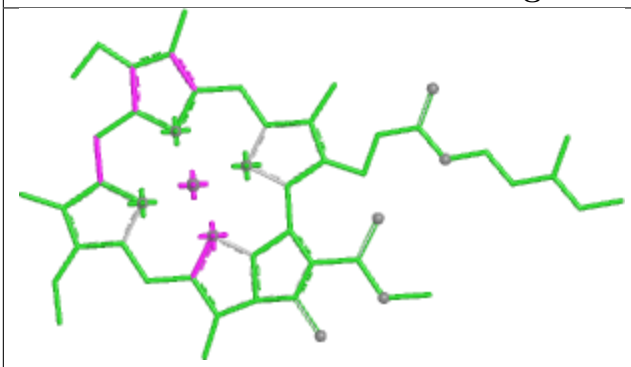


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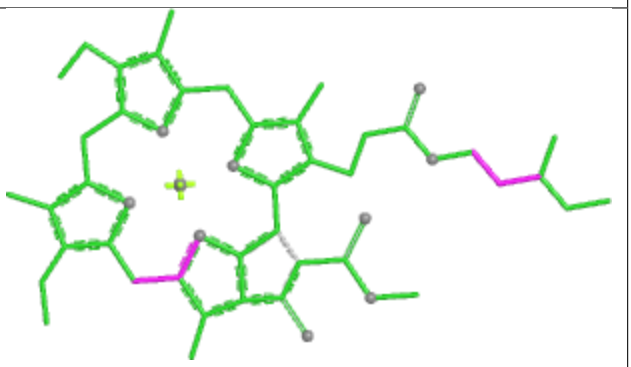


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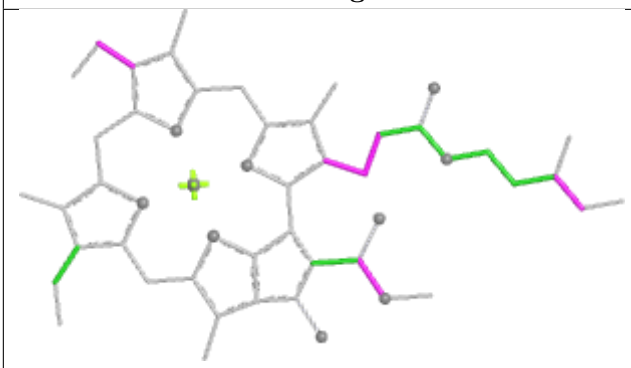
Ligand CLA A 809



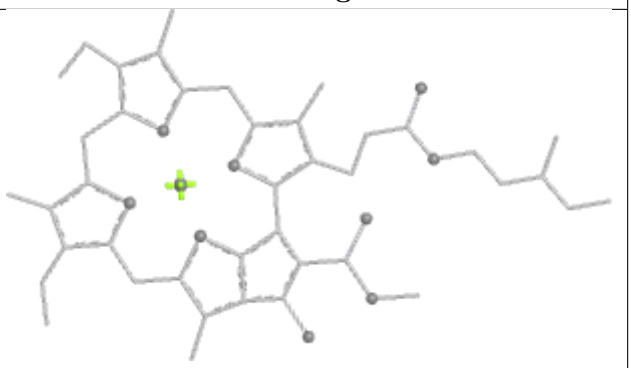
Bond lengths



Bond angles

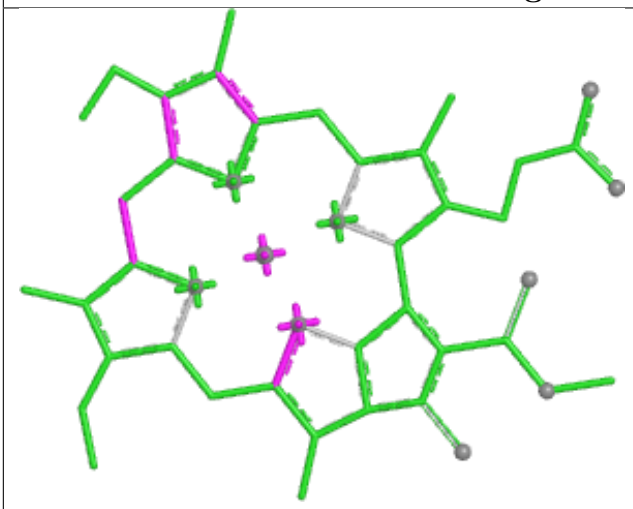


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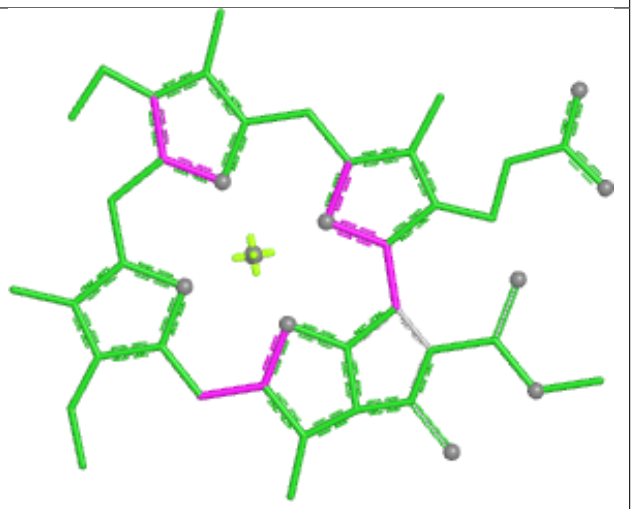


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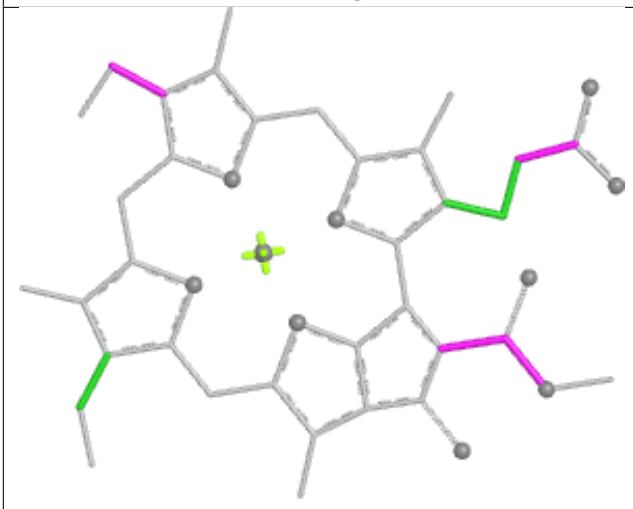
Ligand CLA T 101



Bond lengths



Bond angles

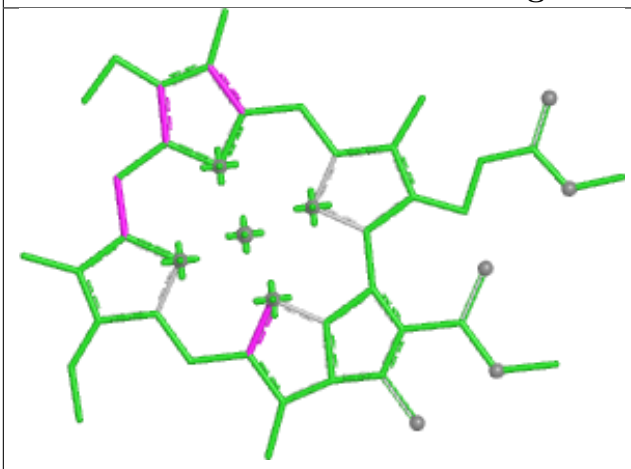


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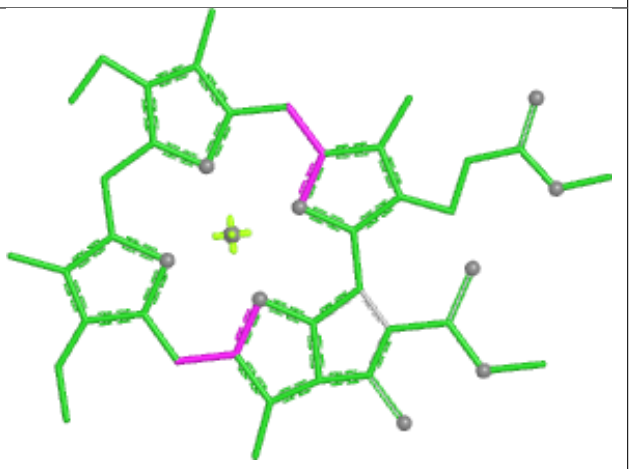


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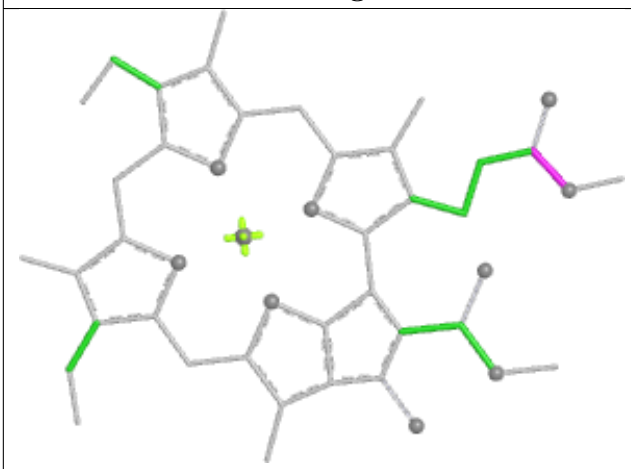
Ligand CLA b 824



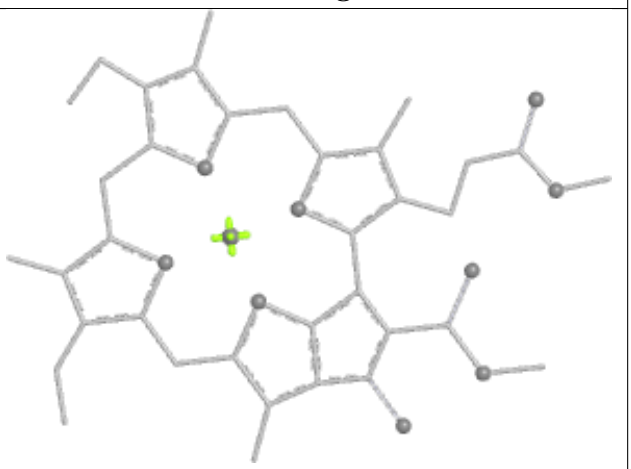
Bond lengths



Bond angles

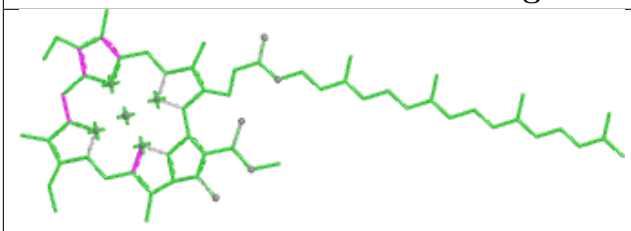


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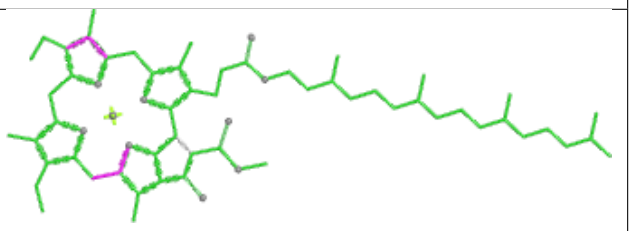


Rings

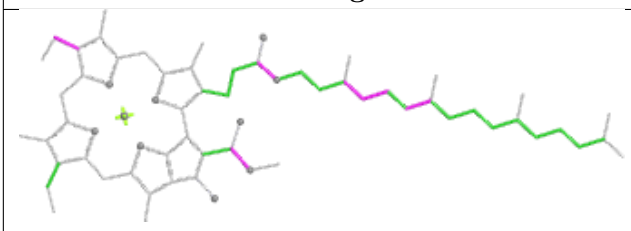
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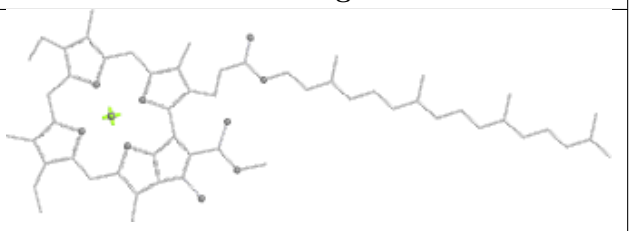
Bond lengths



Bond angles

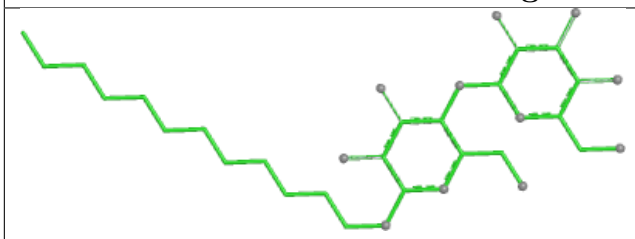


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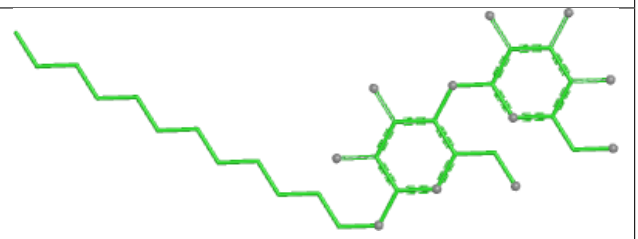


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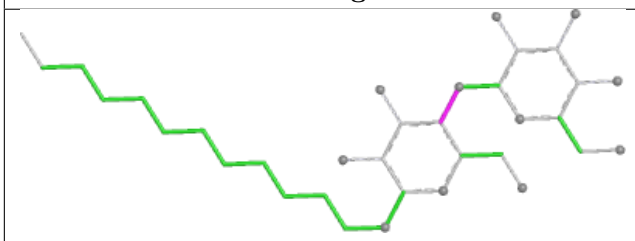
Ligand LMT l 5008



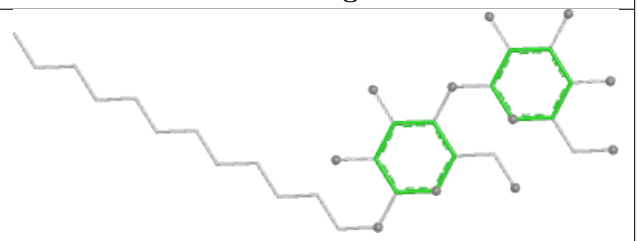
Bond lengths



Bond angles

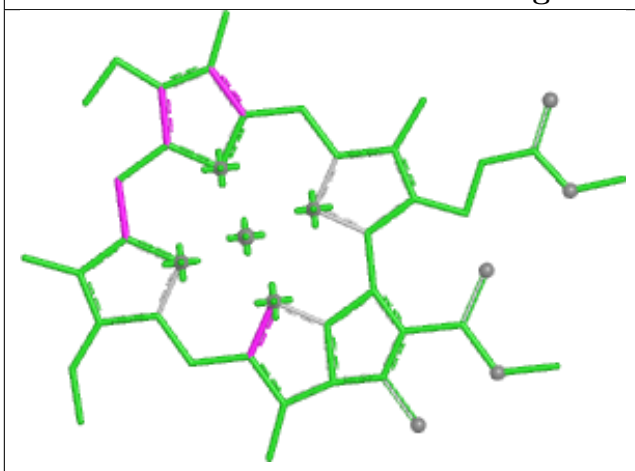


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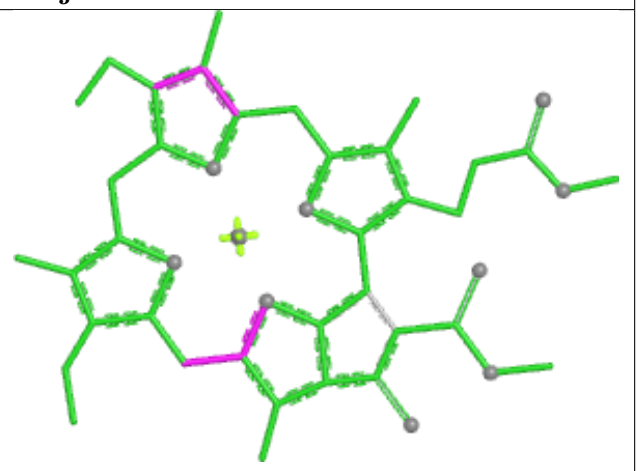


Rings

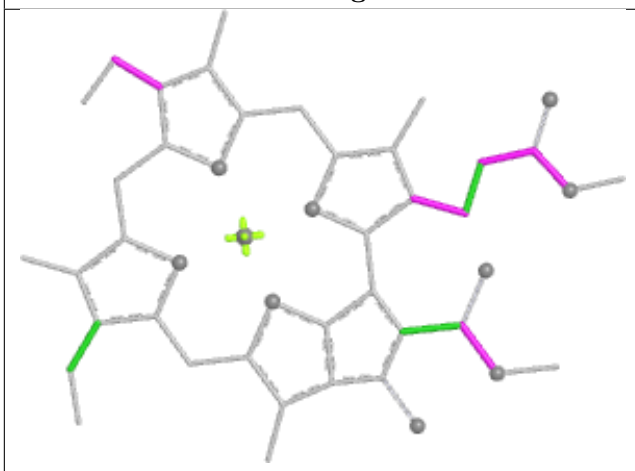
Ligand CLA j 102



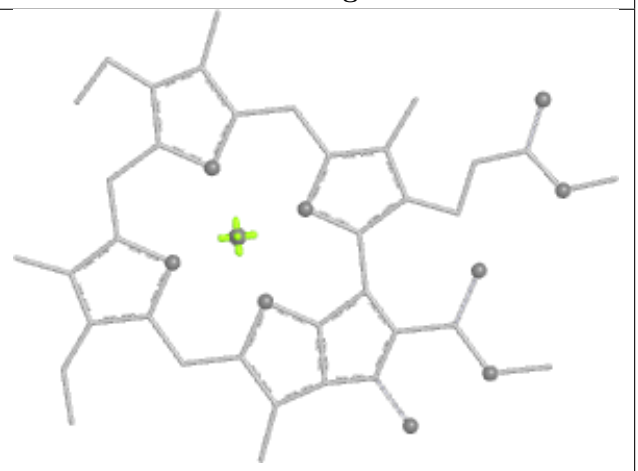
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Bond angles

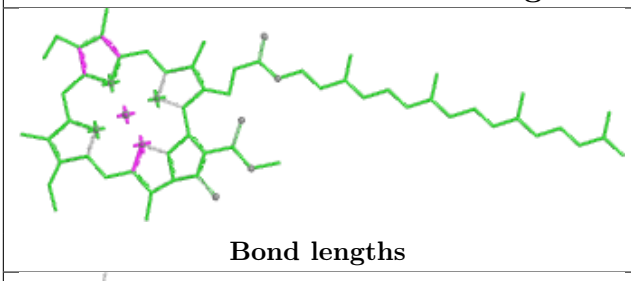


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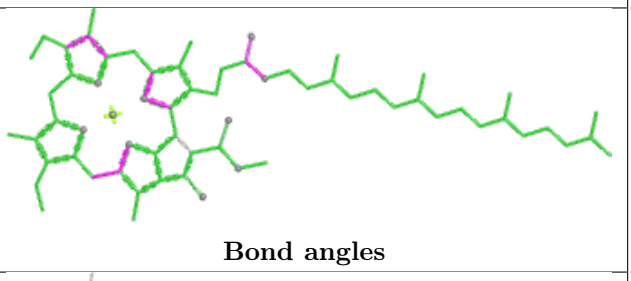


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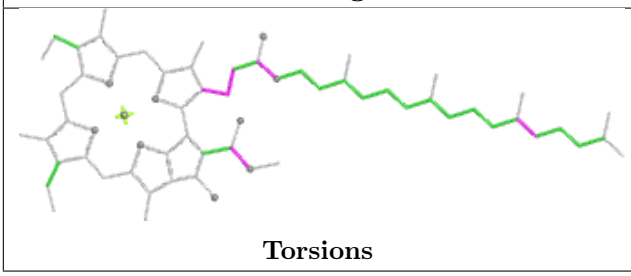
Ligand CLA B 829



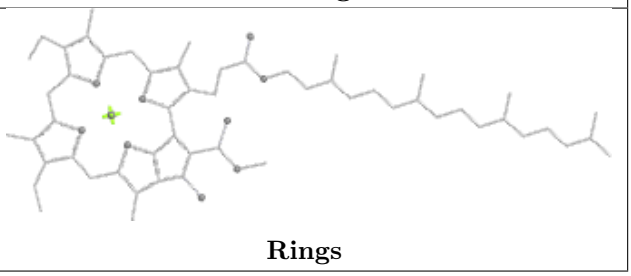
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Bond angles

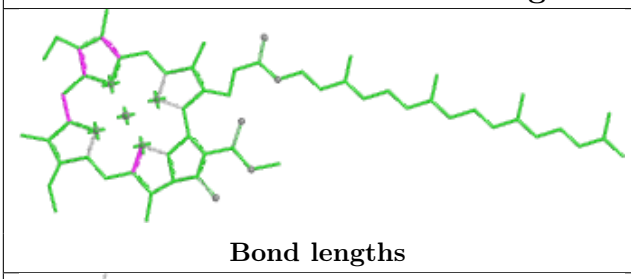


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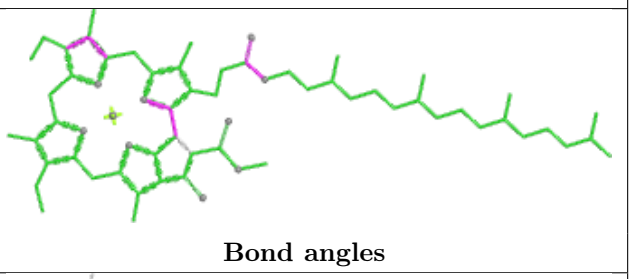


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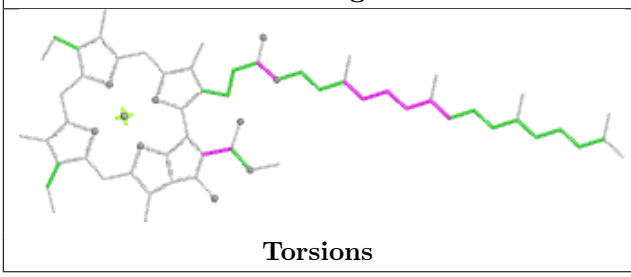
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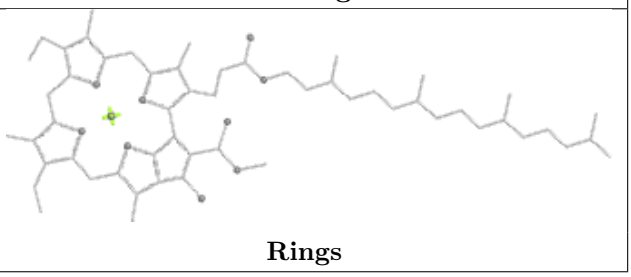
Bond lengths



Bond angles

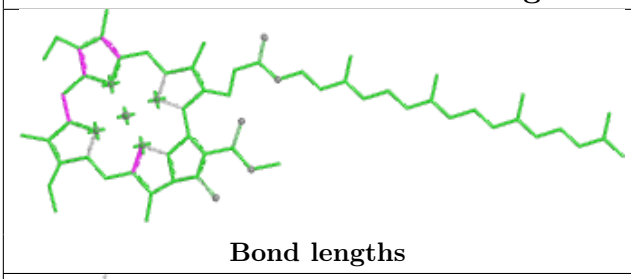


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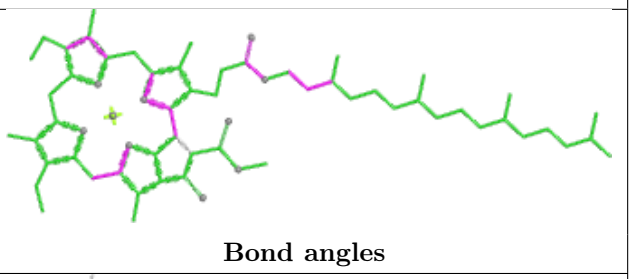


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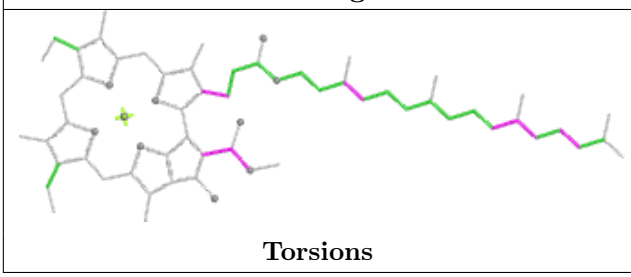
Ligand CLA U 202



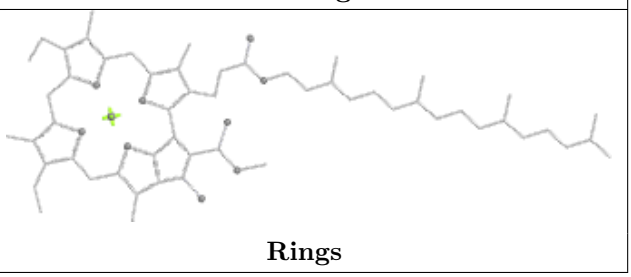
Bond lengths



Bond angles

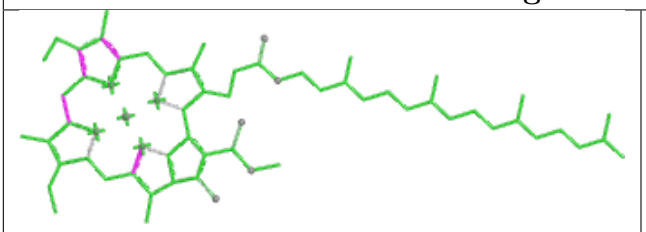


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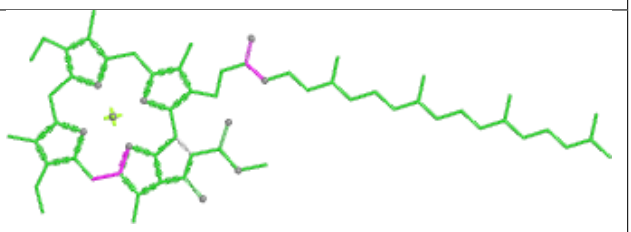


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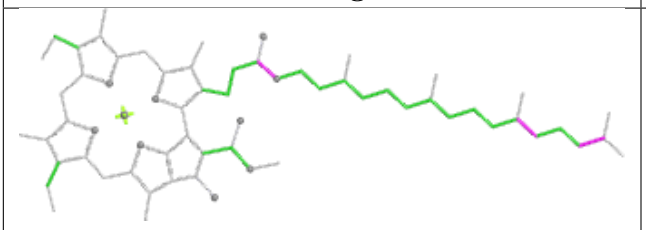
Ligand CLA l 5005



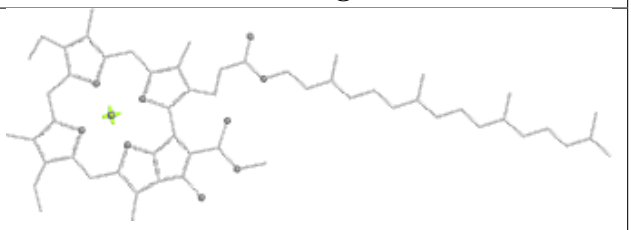
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Bond angles

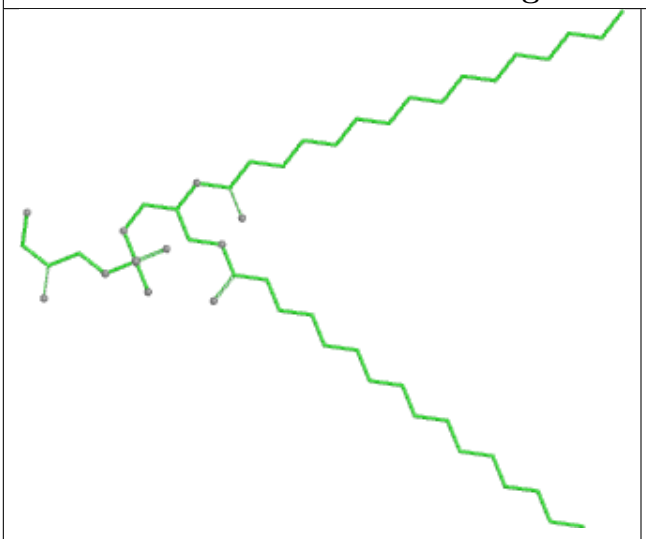


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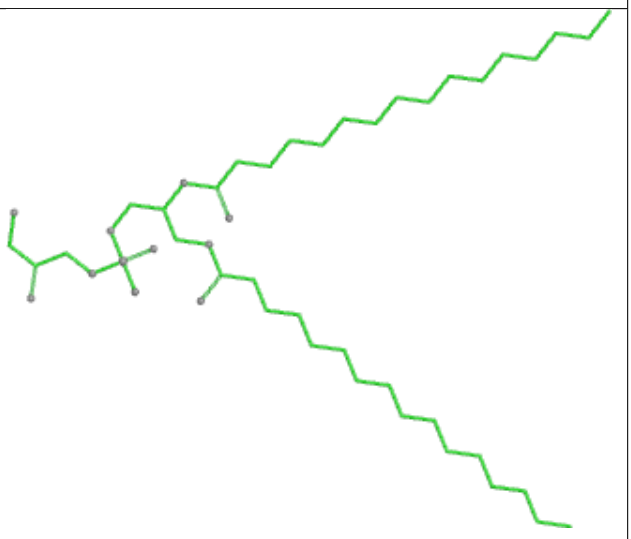


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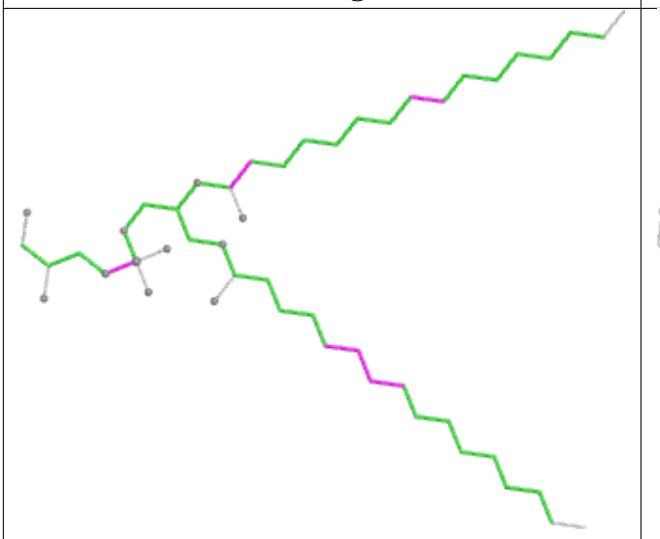
Ligand LHG A 854



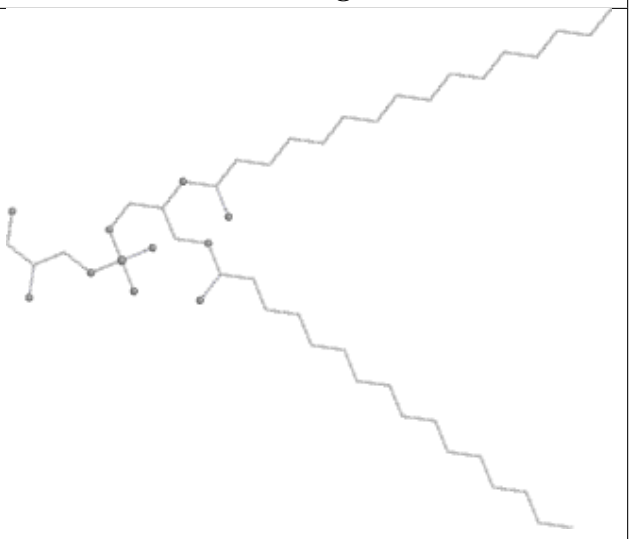
Bond lengths



Bond angles

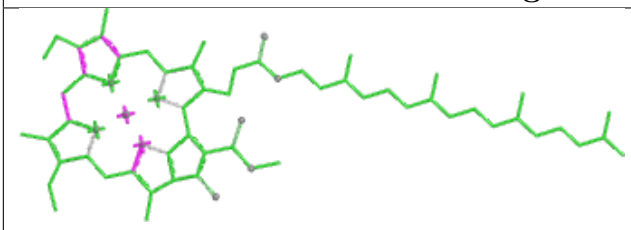


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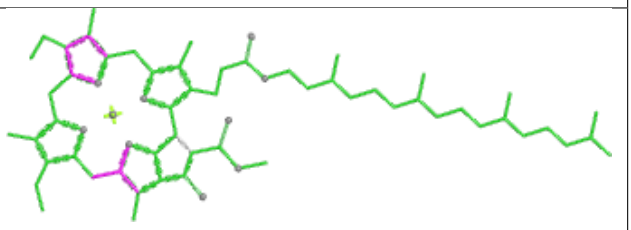


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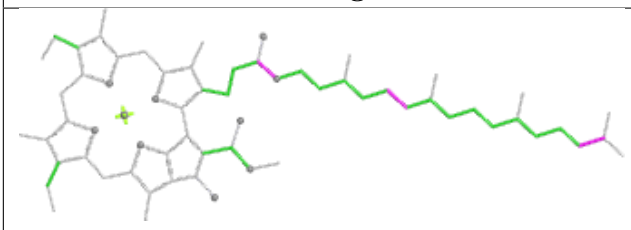
Ligand CLA G 832



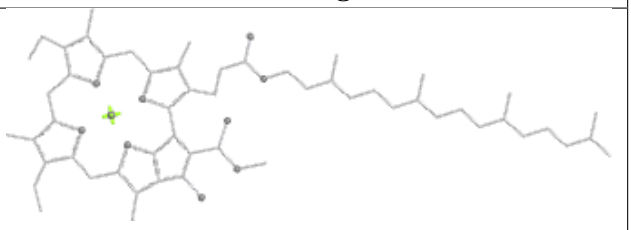
Bond lengths



Bond angles

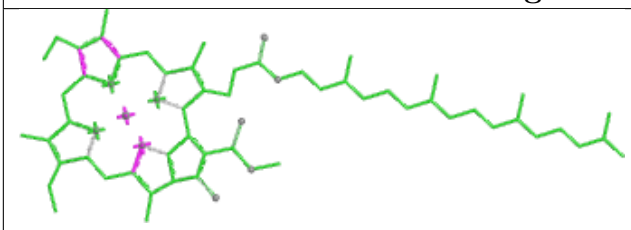


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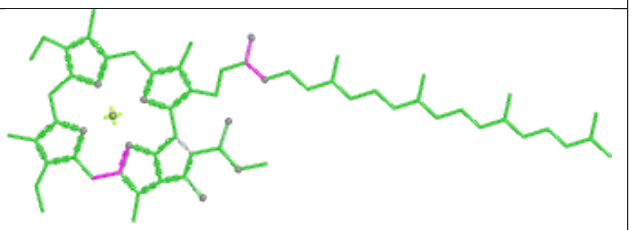


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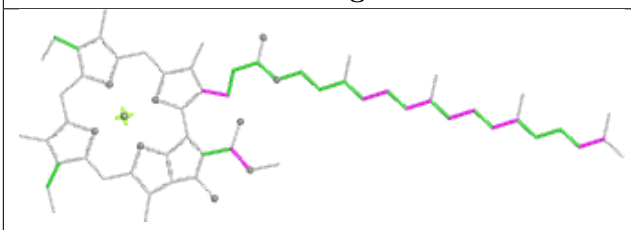
Ligand CLA B 820



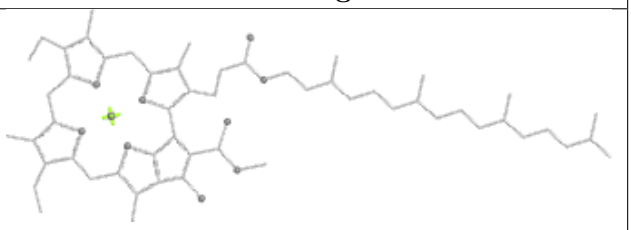
Bond lengths



Bond angles

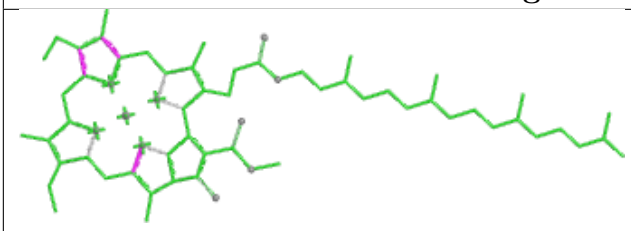


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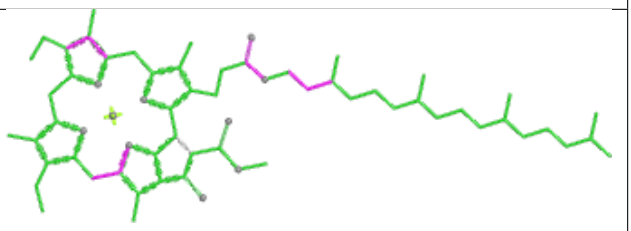


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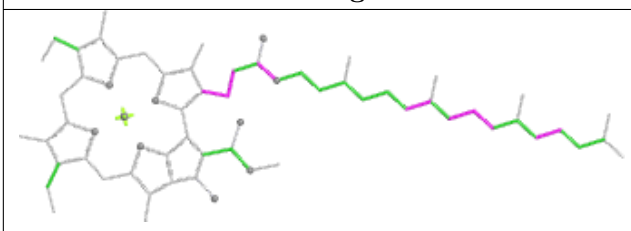
Ligand CLA G 814



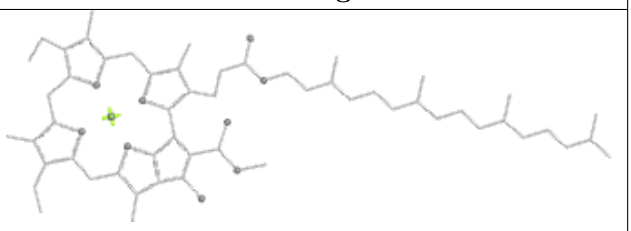
Bond lengths



Bond angles

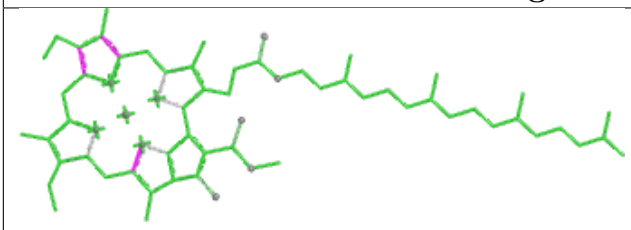


Torsions

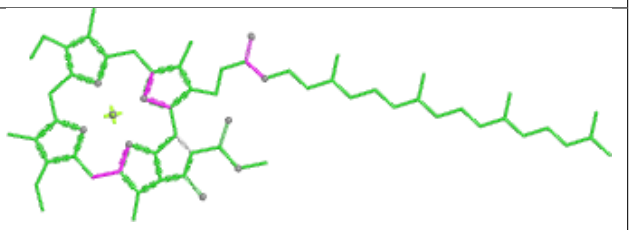


Rings

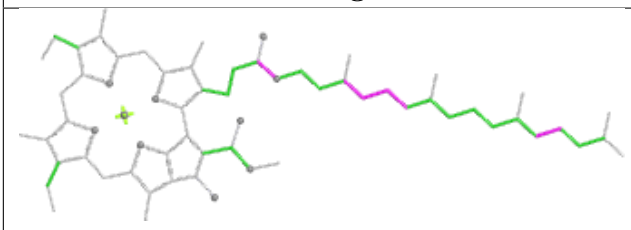
Ligand CLA a 821



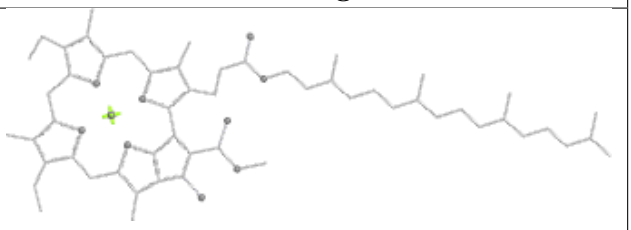
Bond lengths



Bond angles

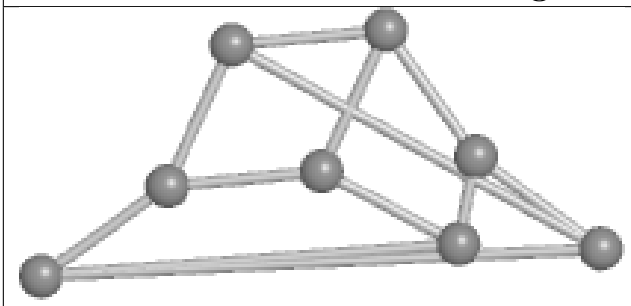


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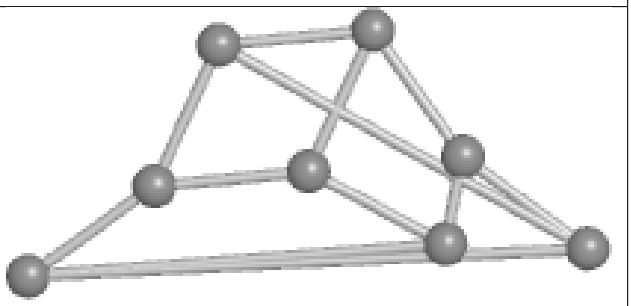


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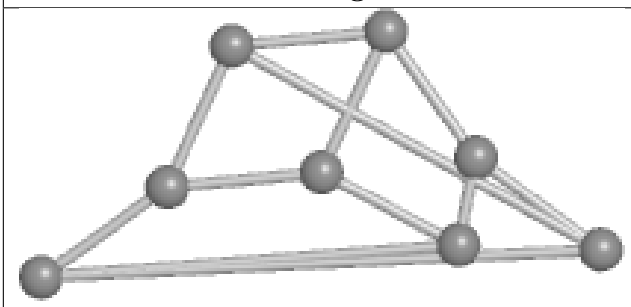
Ligand SF4 A 846



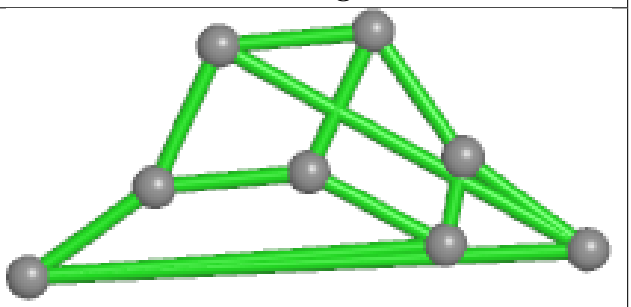
Bond lengths



Bond angles

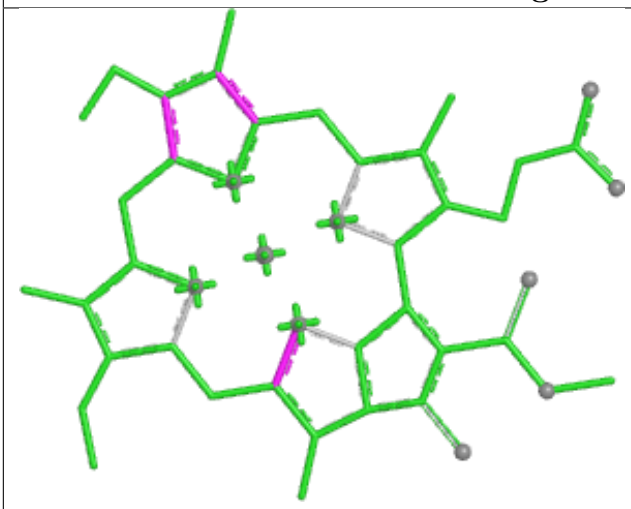


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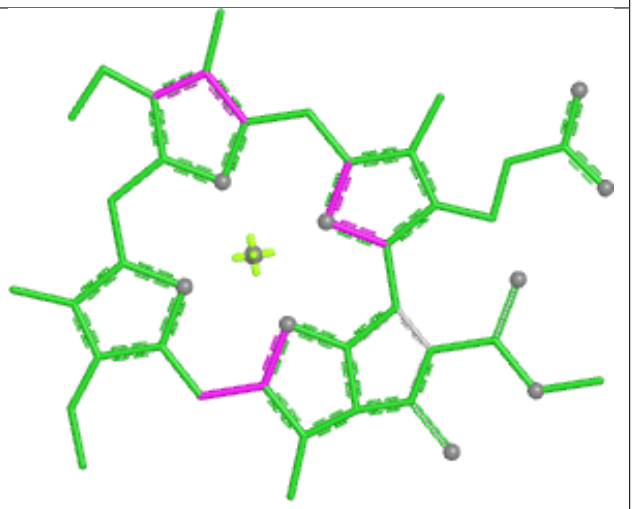


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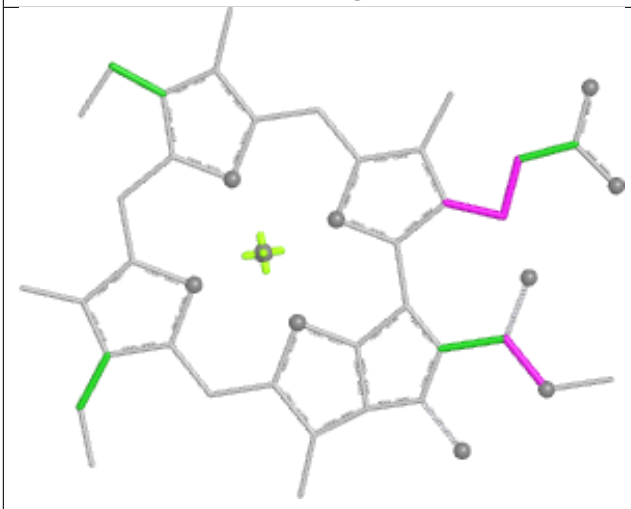
Ligand CLA f 204



Bond lengths



Bond angles

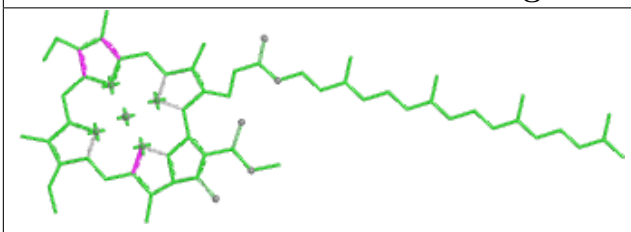


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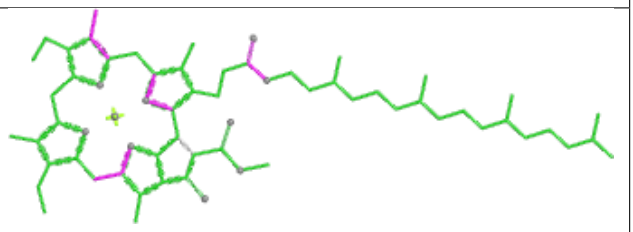


Rings

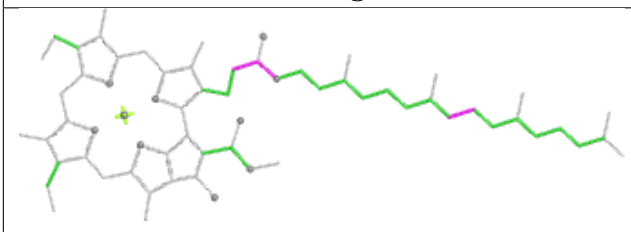
Ligand CLA H 803



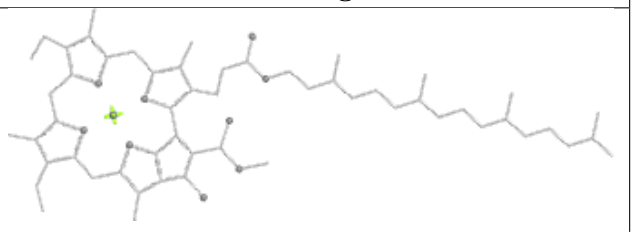
Bond lengths



Bond angles

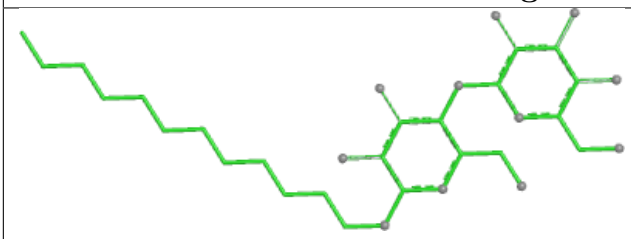


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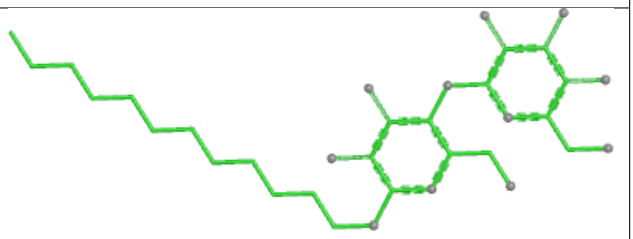


Rings

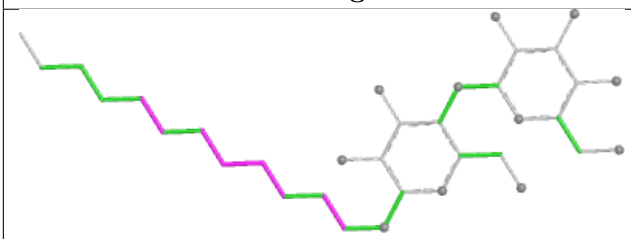
Ligand LMT A 859



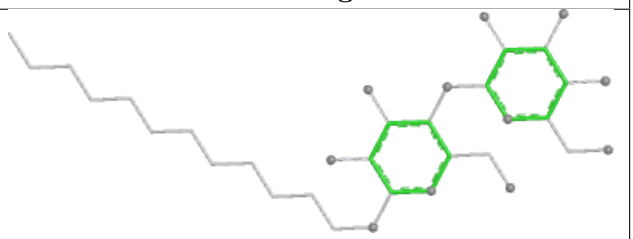
Bond lengths



Bond angles

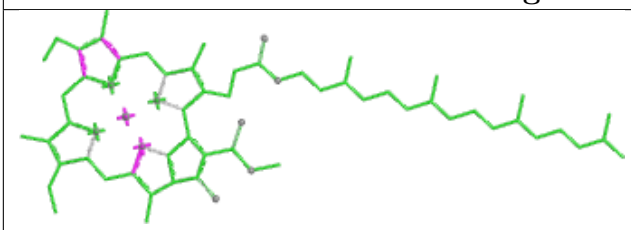


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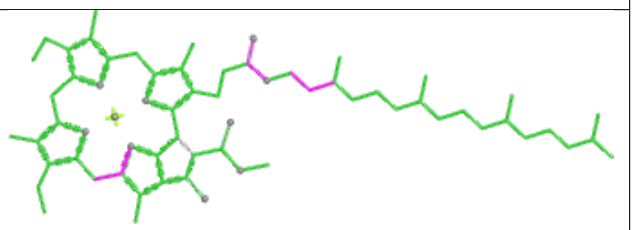


Rings

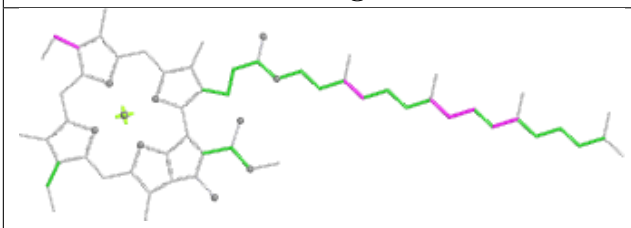
Ligand CLA G 840



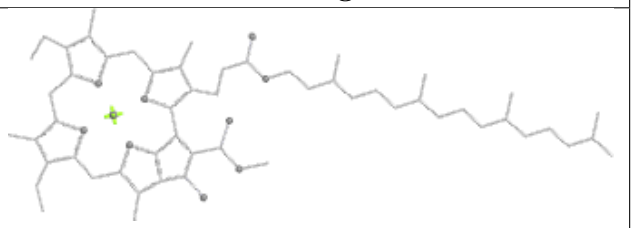
Bond lengths



Bond angles

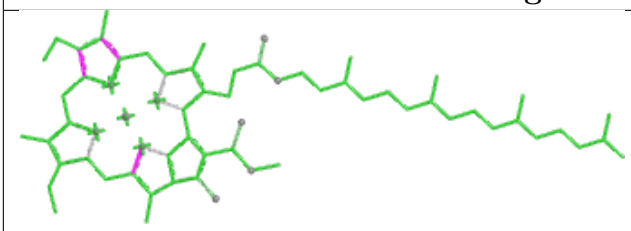


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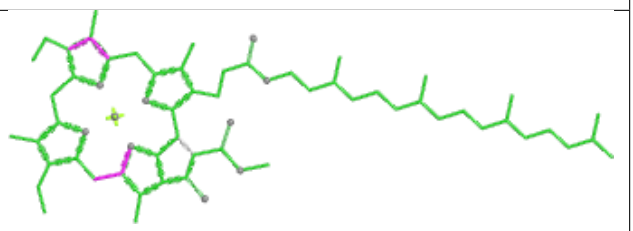


Rings

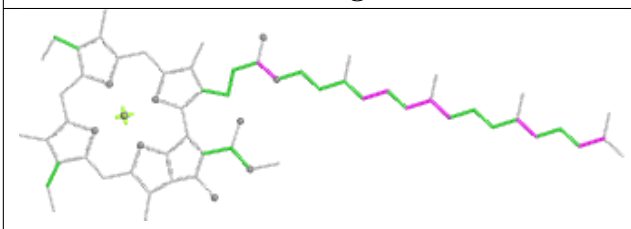
Ligand CLA B 839



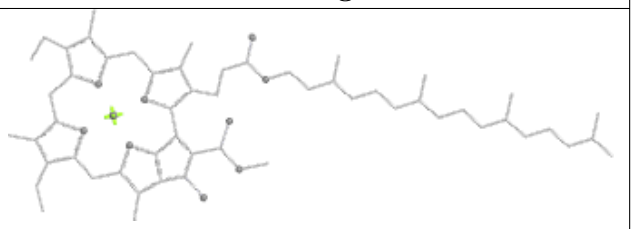
Bond lengths



Bond angles

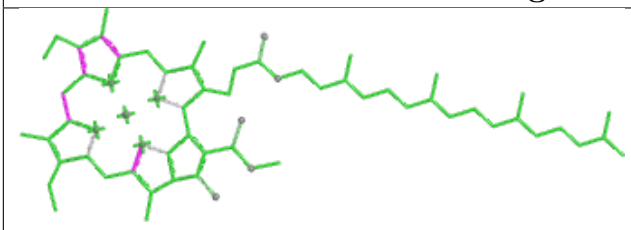


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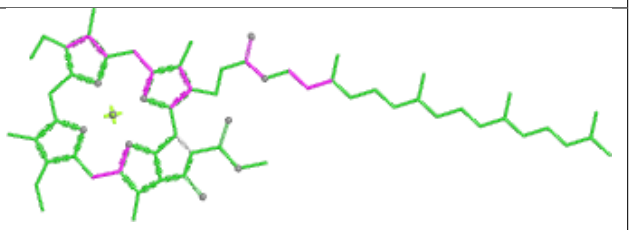


Rings

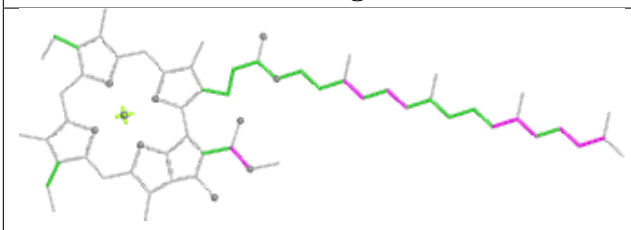
Ligand CLA a 820



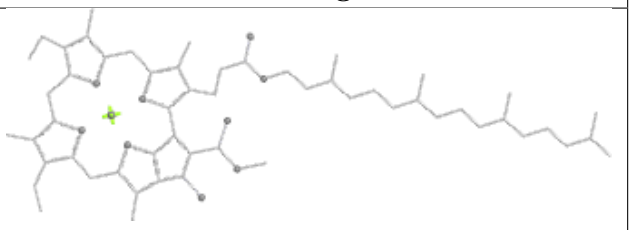
Bond lengths



Bond angles

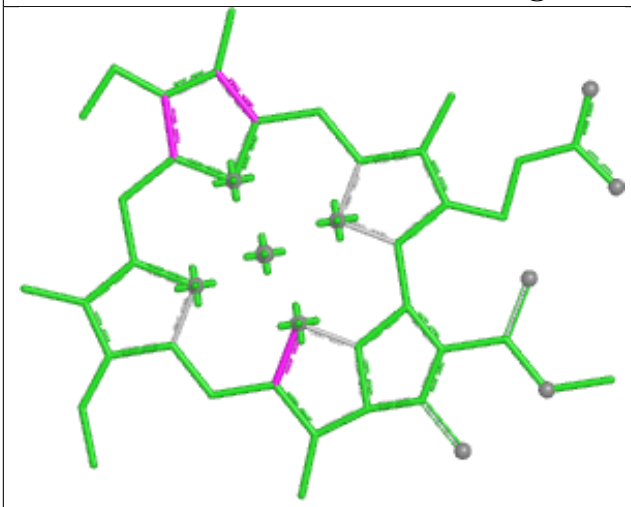


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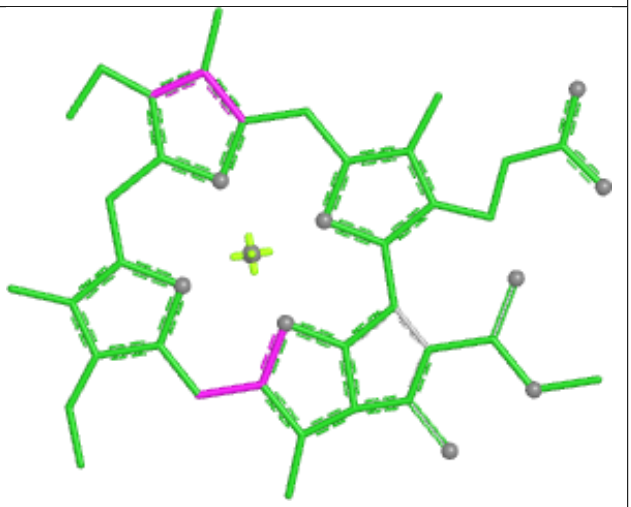


Rings

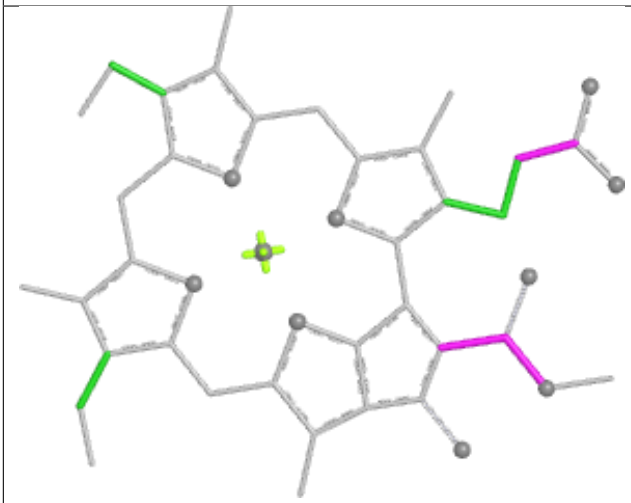
Ligand CLA a 816



Bond lengths



Bond angles

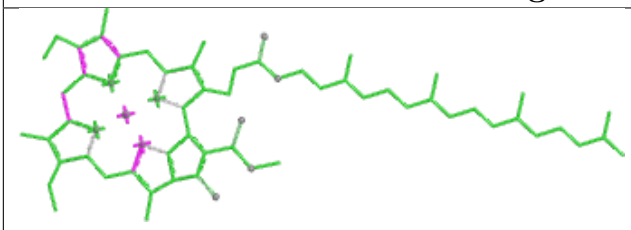


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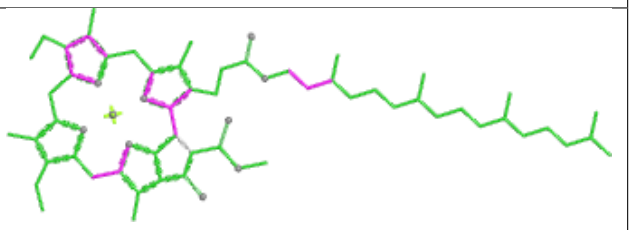


Rings

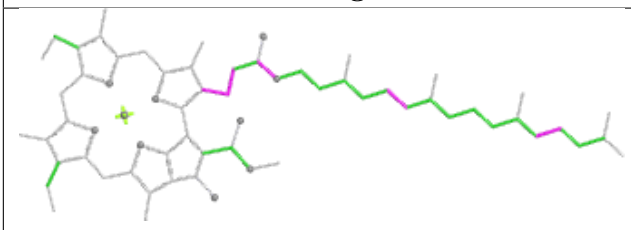
Ligand CLA a 830



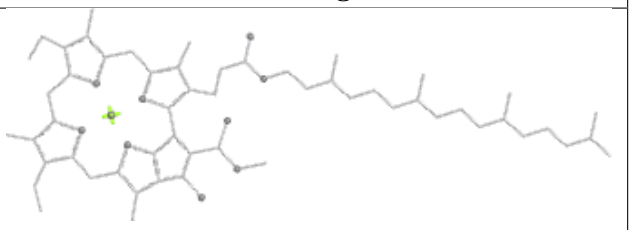
Bond lengths



Bond angles

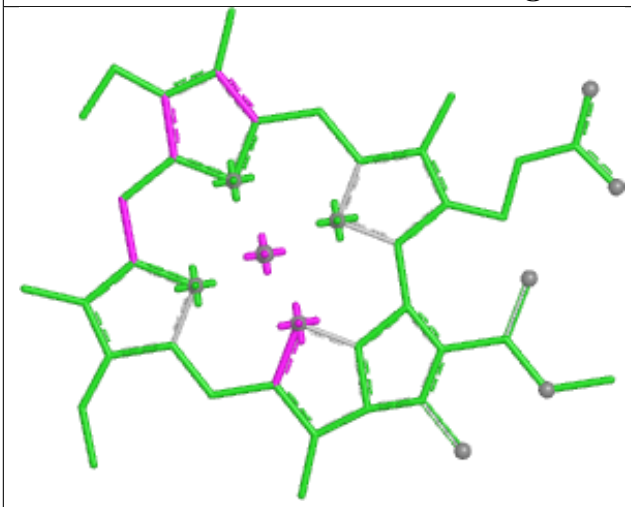


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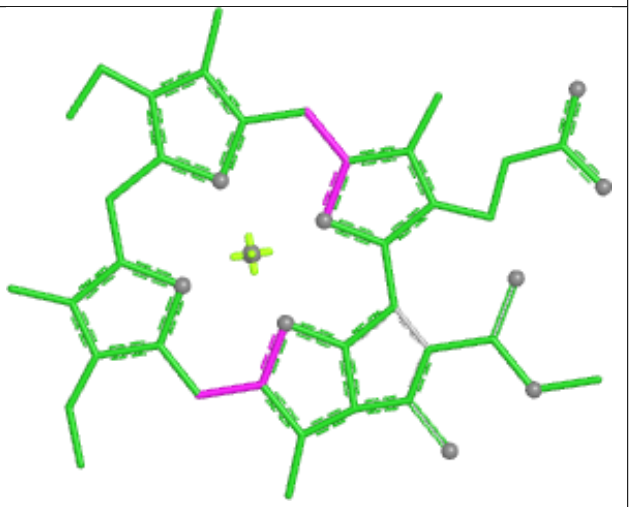


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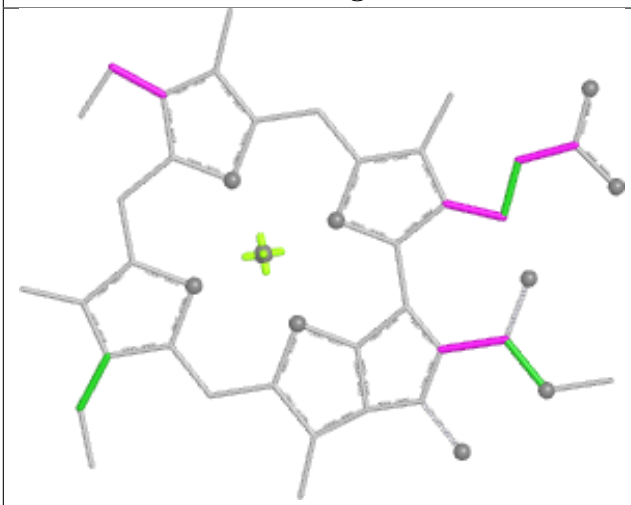
Ligand CLA B 822



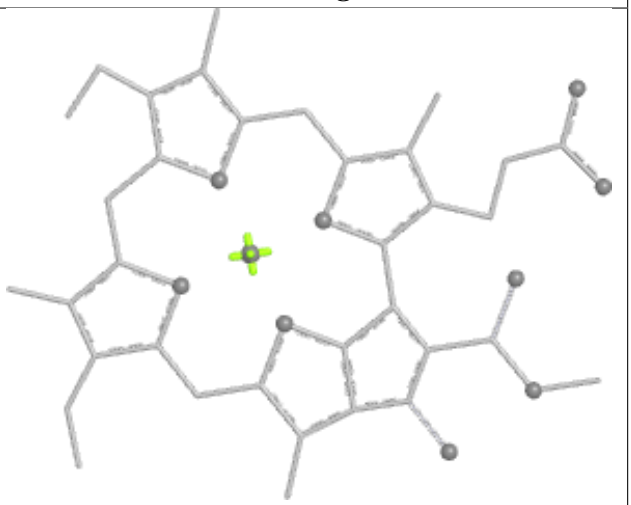
Bond lengths



Bond angles

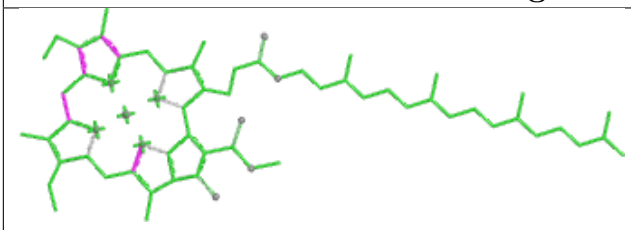


Torsions

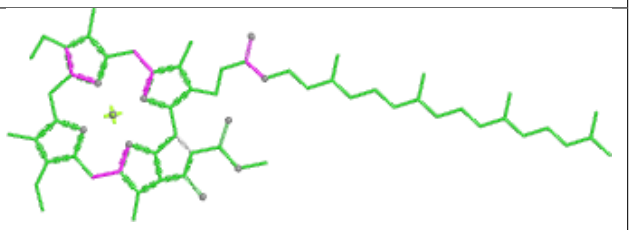


Rings

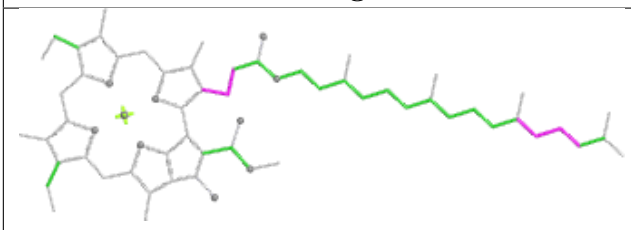
Ligand CLA a 803



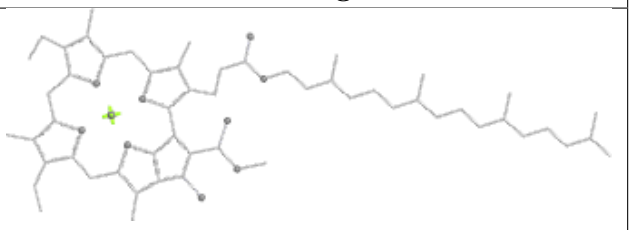
Bond lengths



Bond angles

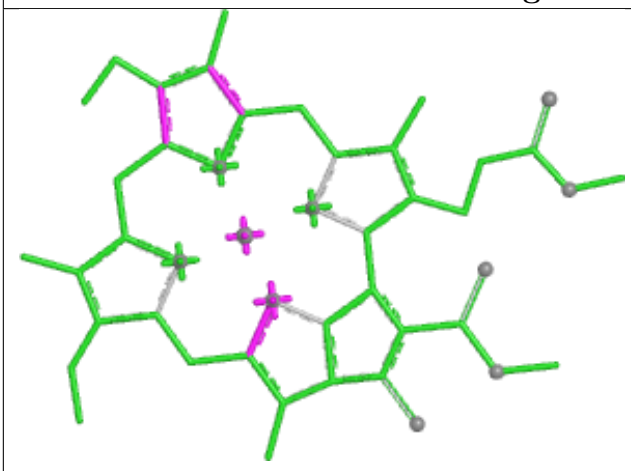


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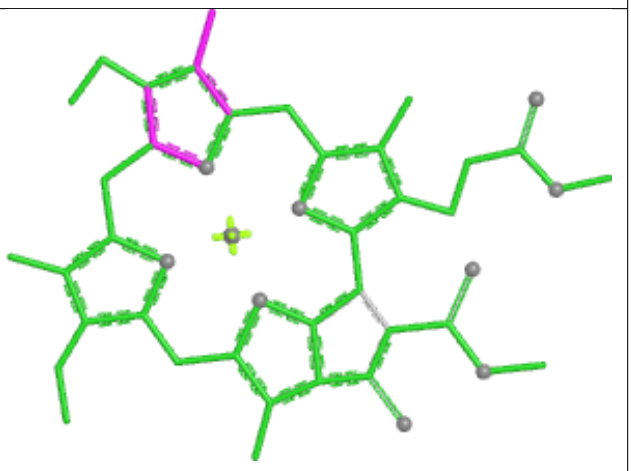


Rings

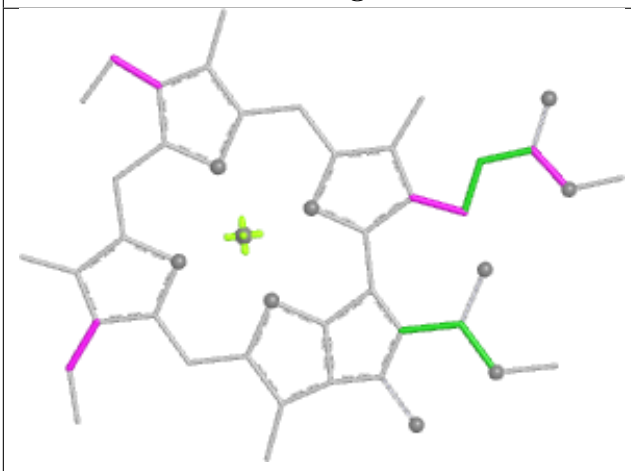
Ligand CLA G 817



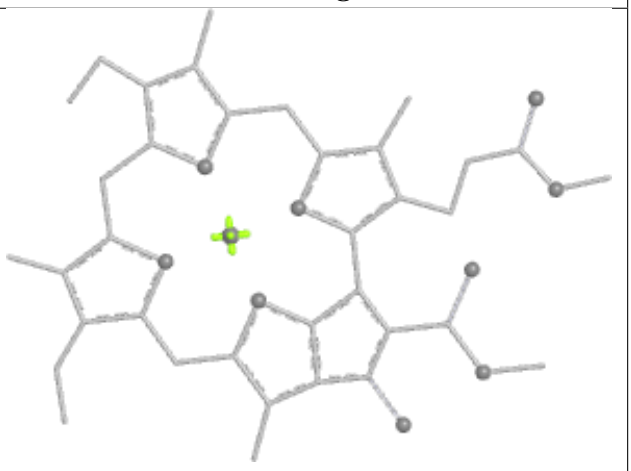
Bond lengths



Bond angles

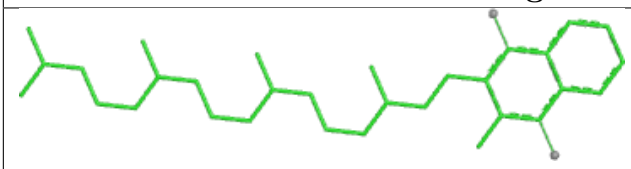


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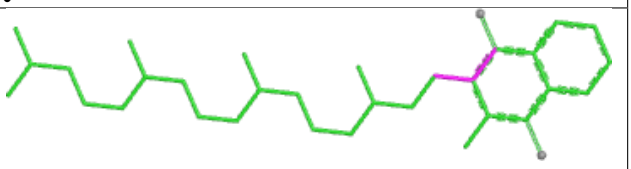


Rings

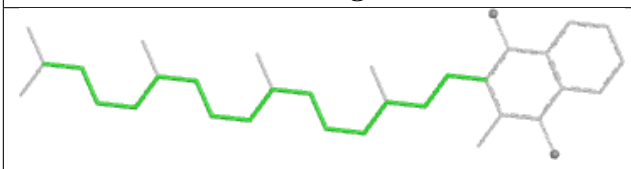
Ligand PQN a 846



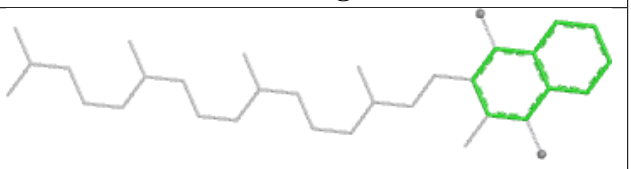
Bond lengths



Bond angles

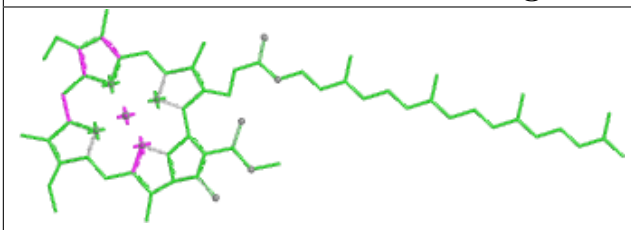


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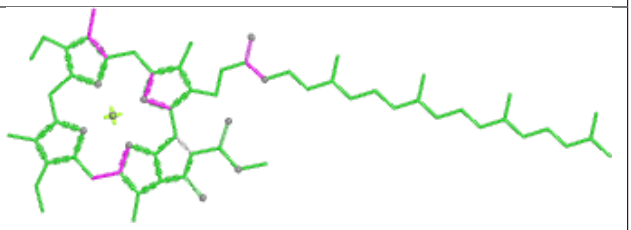


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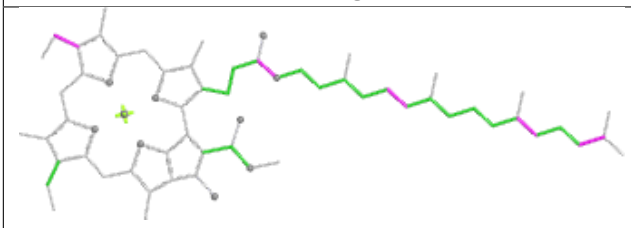
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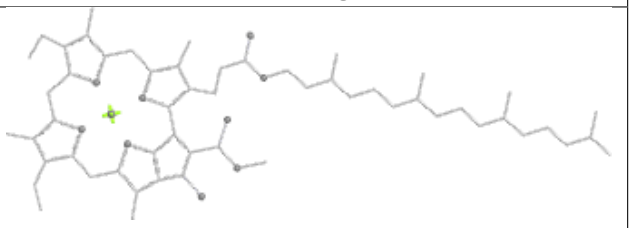
Bond lengths



Bond angles

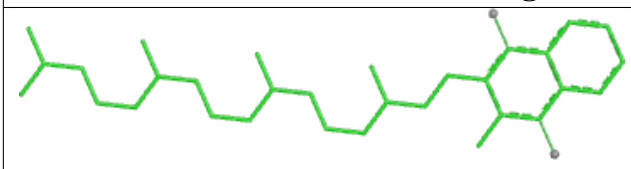


Torsions

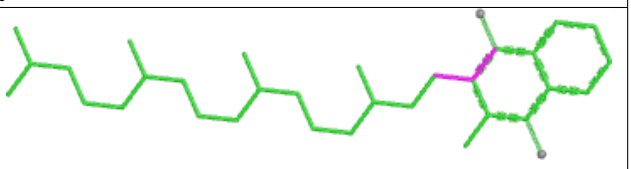


Rings

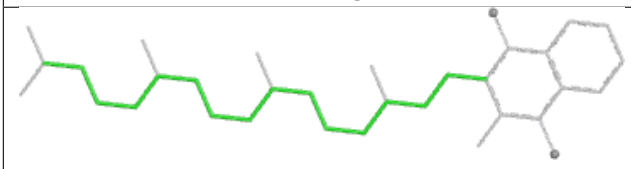
Ligand PQN G 845



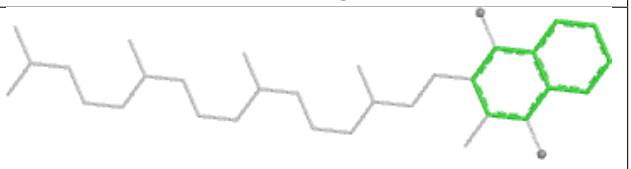
Bond lengths



Bond angles

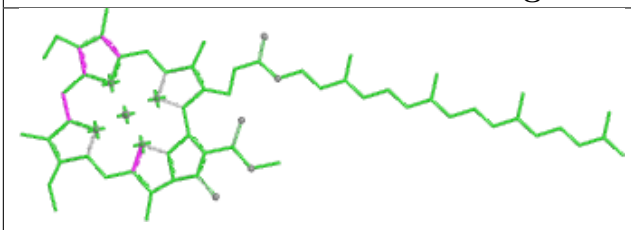


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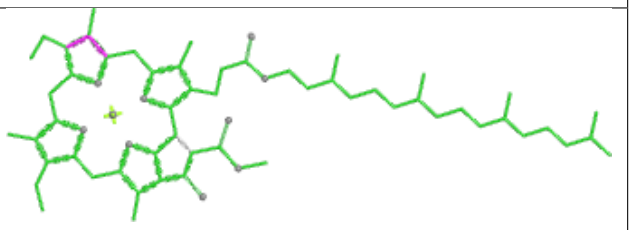


Rings

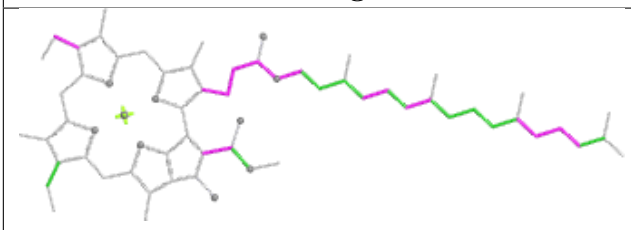
Ligand CLA A 811



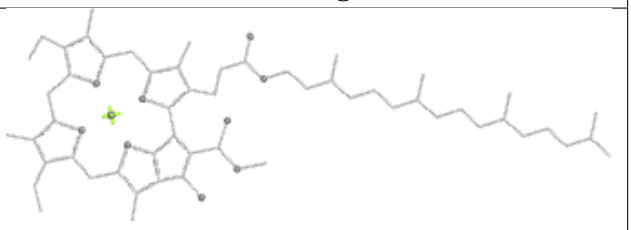
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Bond angles

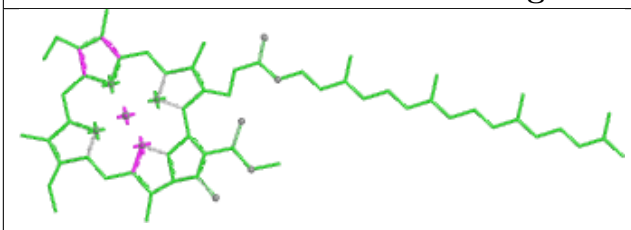


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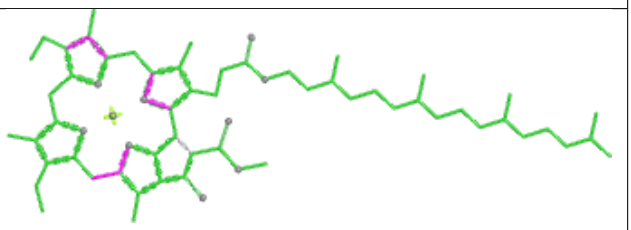


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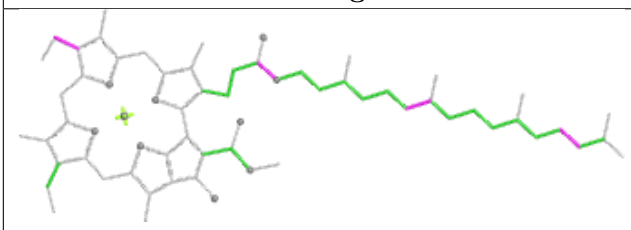
Ligand CLA b 833



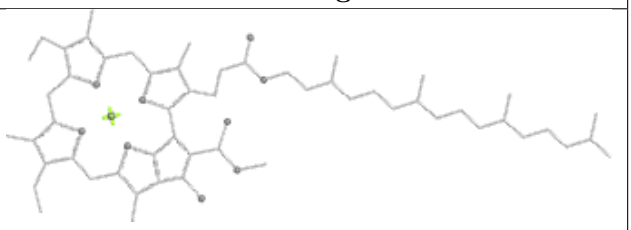
Bond lengths



Bond angles



Torsions



Rings

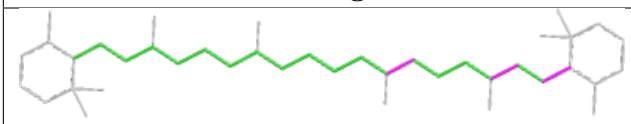
Ligand BCR i 101



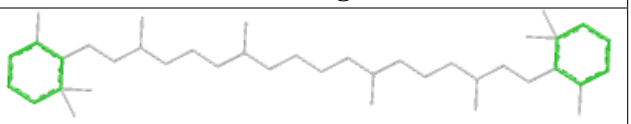
Bond lengths



Bond angles

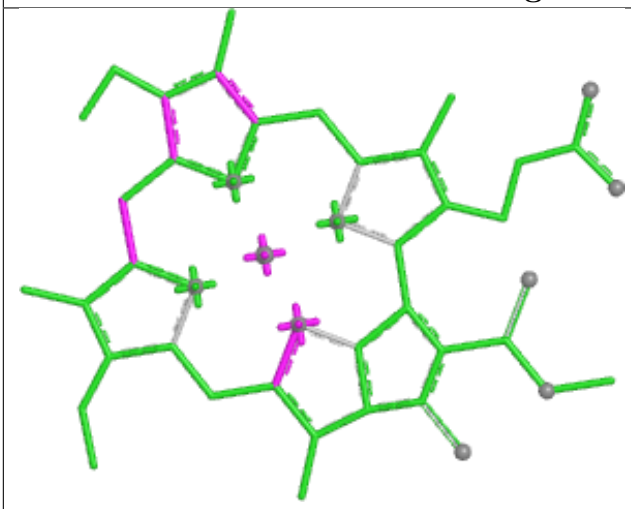


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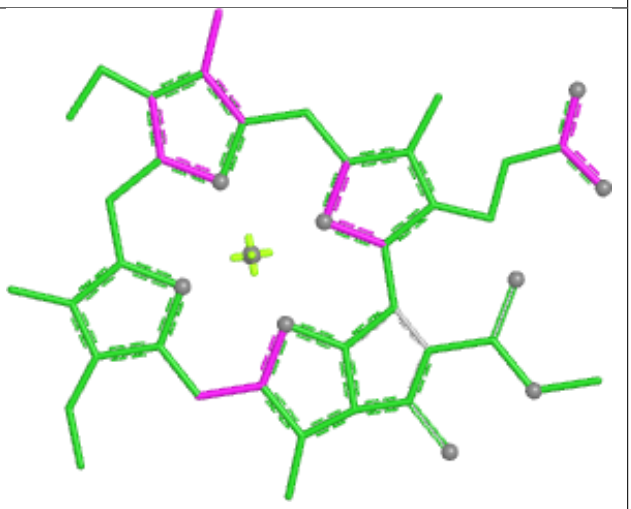


Rings

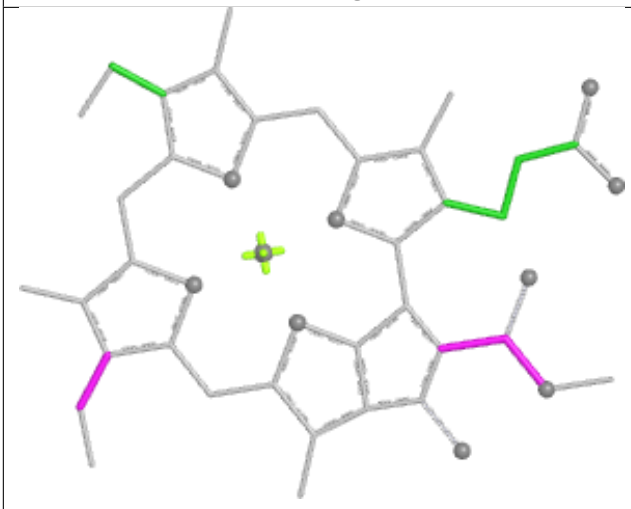
Ligand CLA T 102



Bond lengths



Bond angles

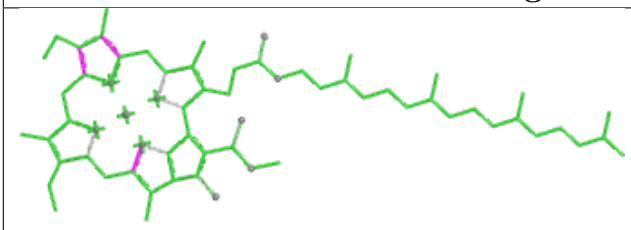


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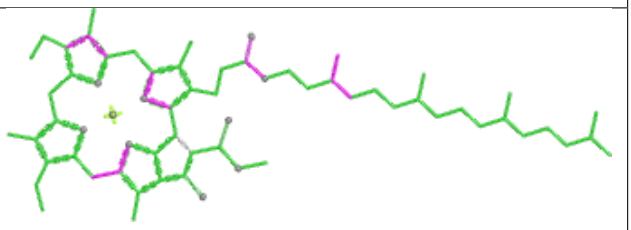


Rings

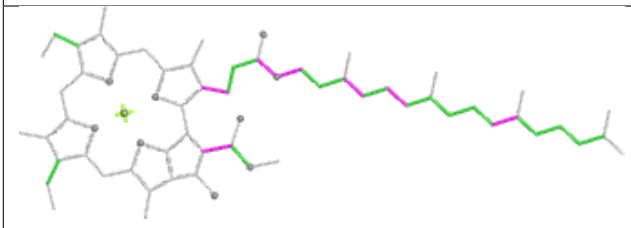
Ligand CLA B 807



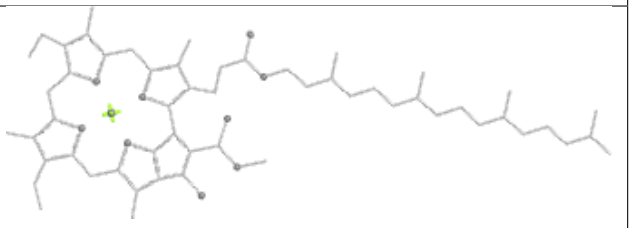
Bond lengths



Bond angles

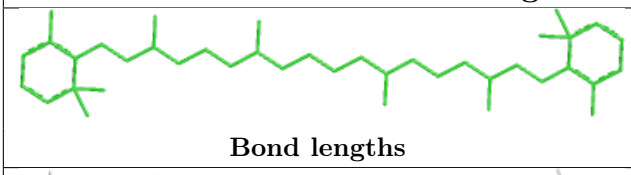


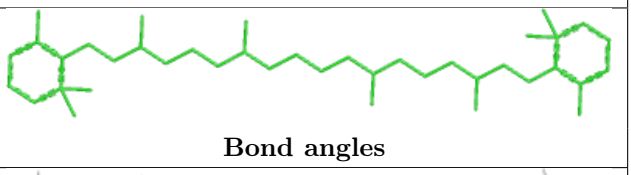
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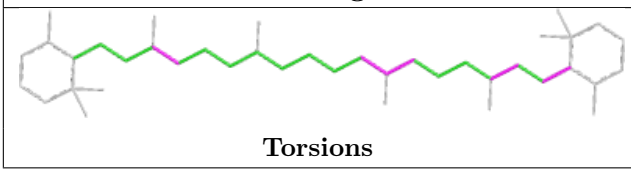


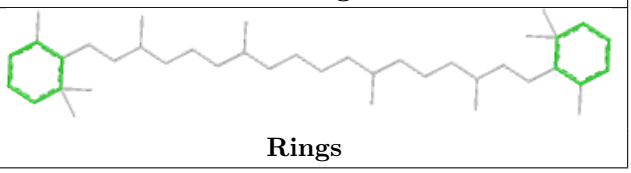
Rings

Ligand BCR G 851

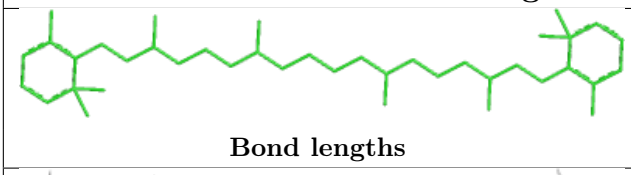

Bond lengths

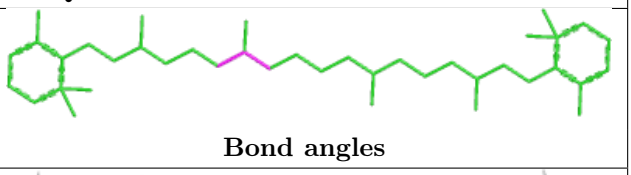

Bond angles

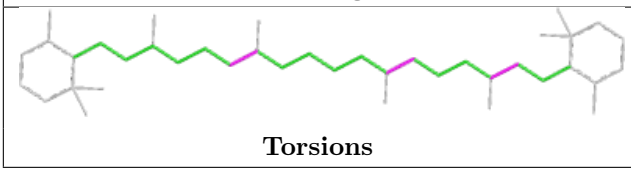

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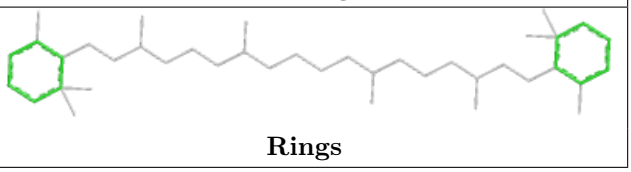

Rings

Ligand BCR Q 203

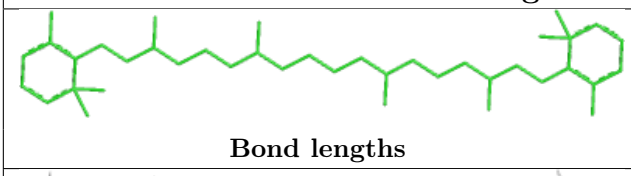

Bond lengths

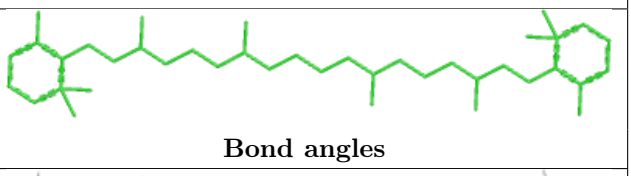

Bond angles

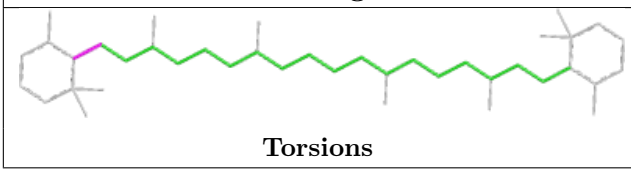

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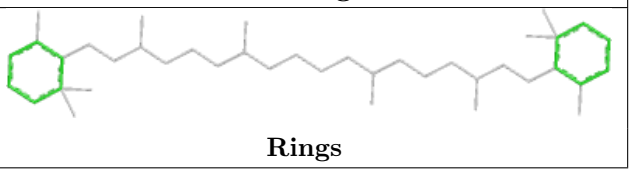

Rings

Ligand BCR A 847

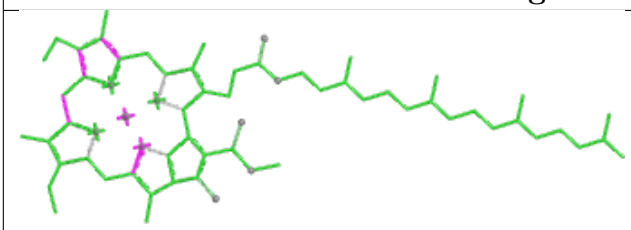

Bond lengths

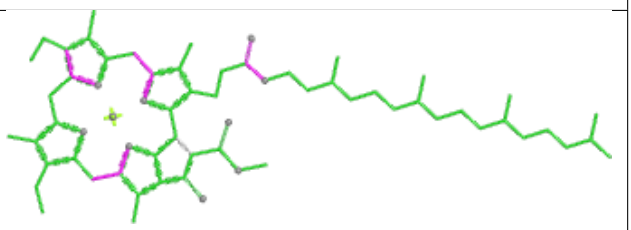

Bond angles

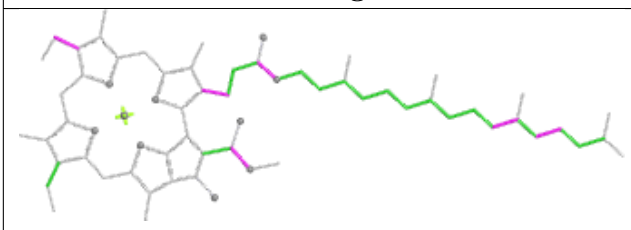

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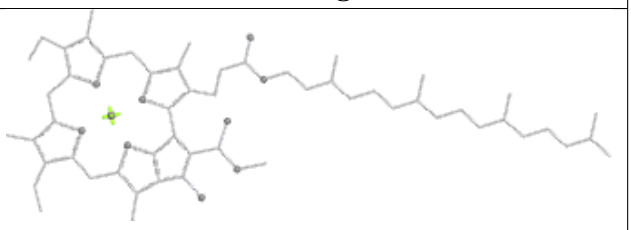

Rings

Ligand CLA a 837

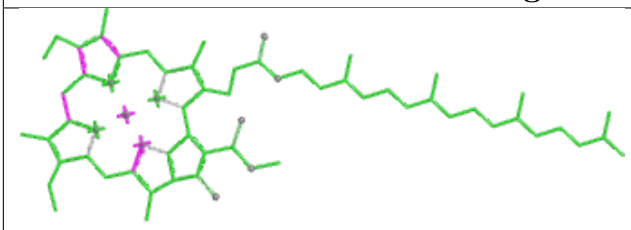

Bond lengths


Bond angles

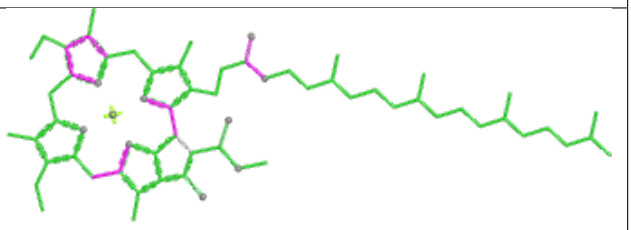

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Rings

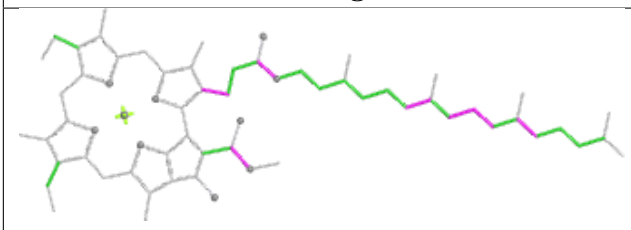
Ligand CLA H 830



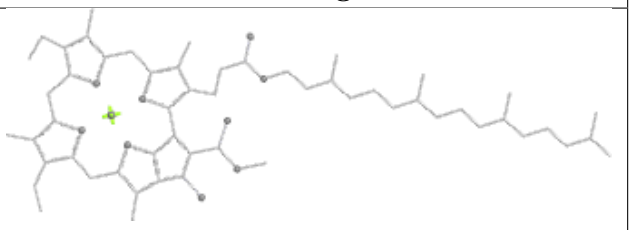
Bond lengths



Bond angles

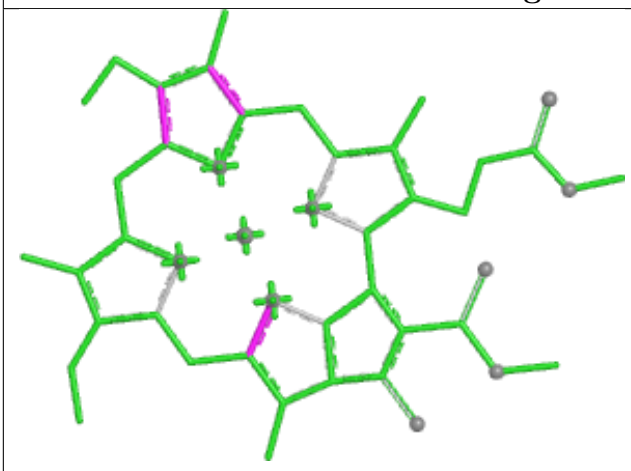


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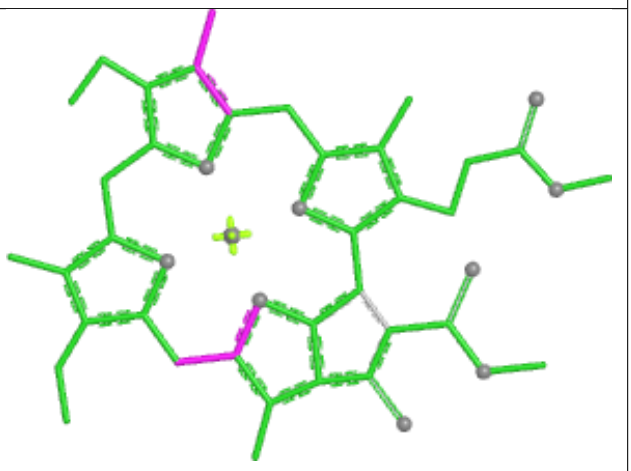


Rings

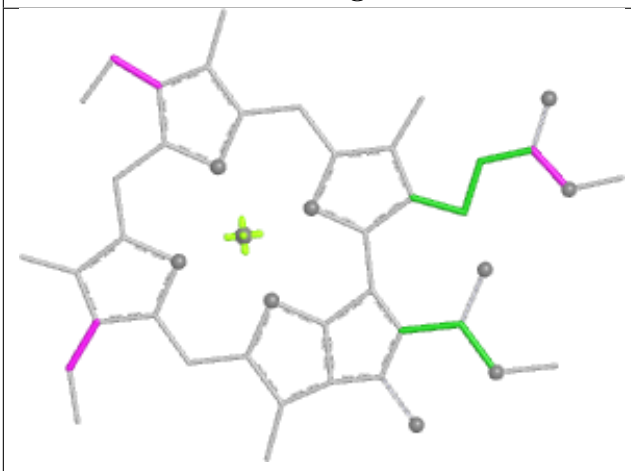
Ligand CLA A 816



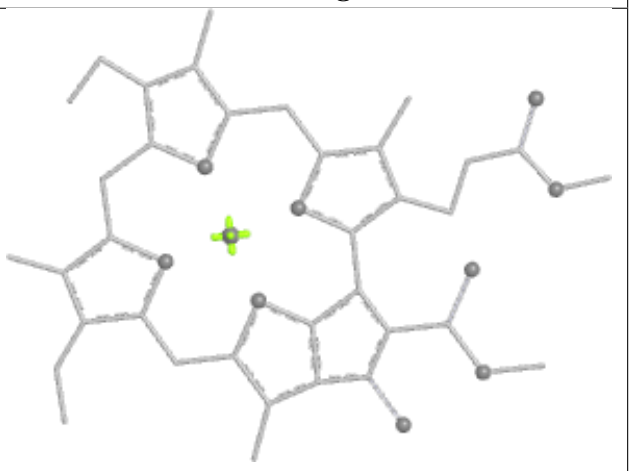
Bond lengths



Bond angles

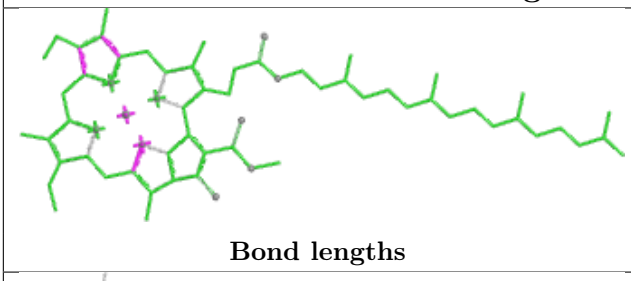


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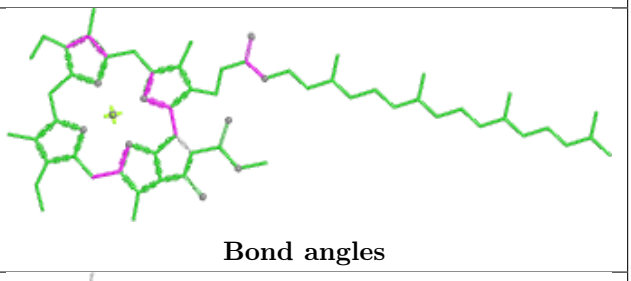


Rings

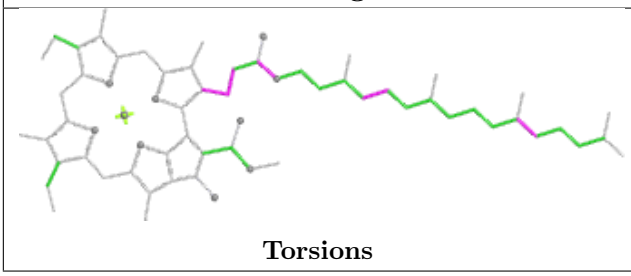
Ligand CLA H 828



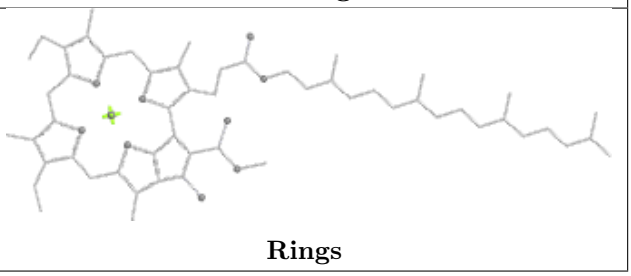
Bond lengths



Bond angles

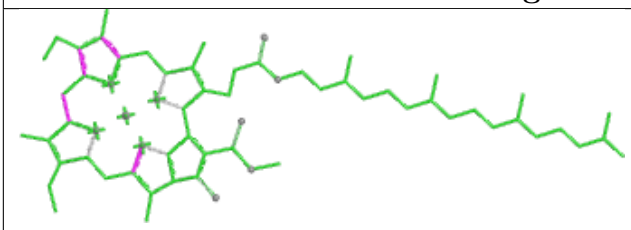


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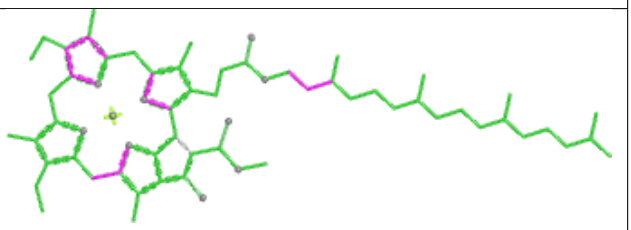


Rings

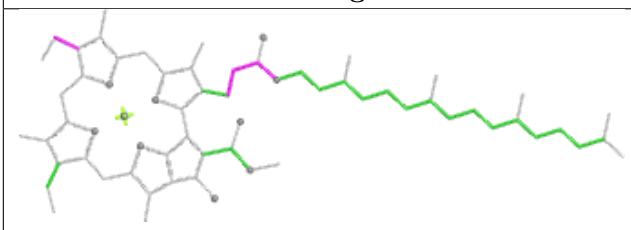
Ligand CLA G 842



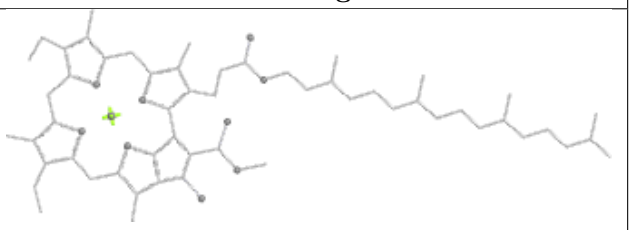
Bond lengths



Bond angles

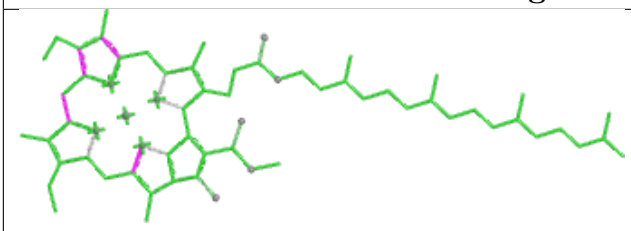


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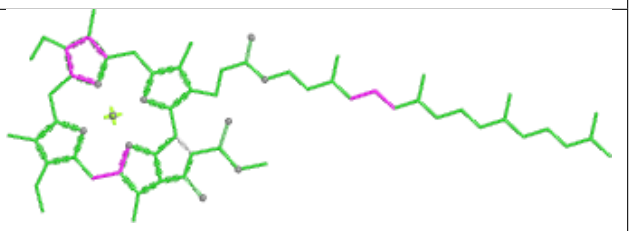


Rings

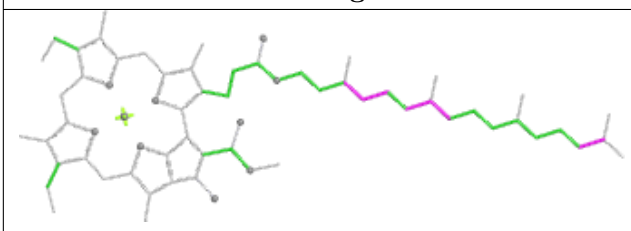
Ligand CLA a 822



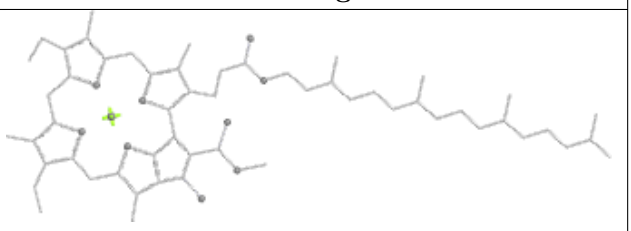
Bond lengths



Bond angles

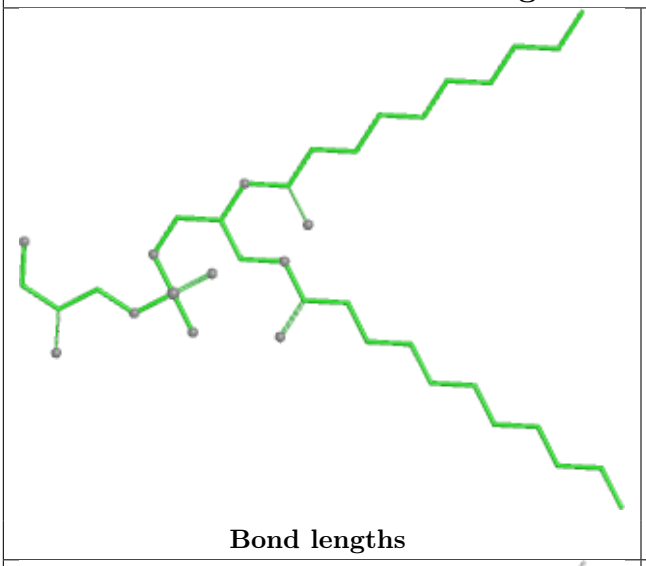


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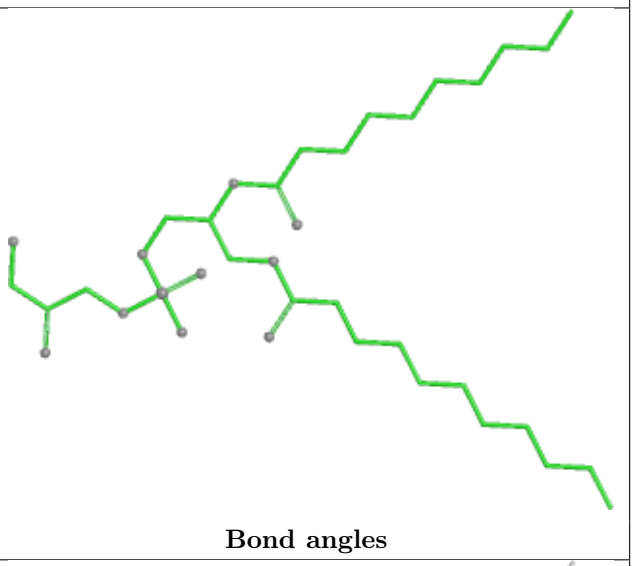


Rings

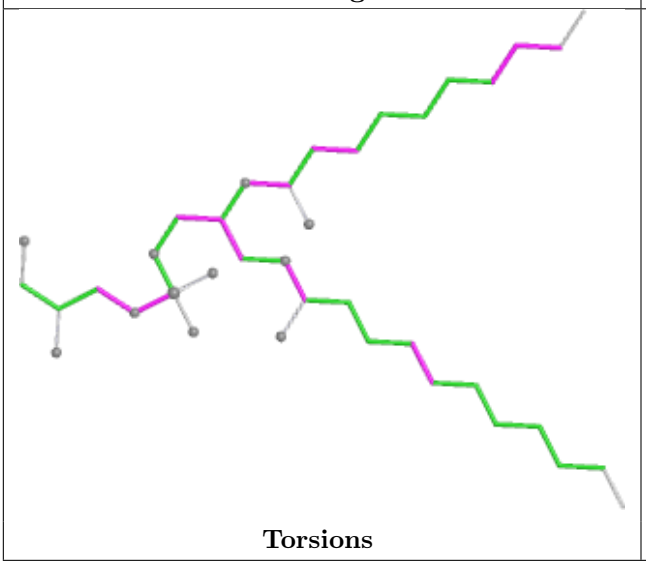
Ligand LHG M 101



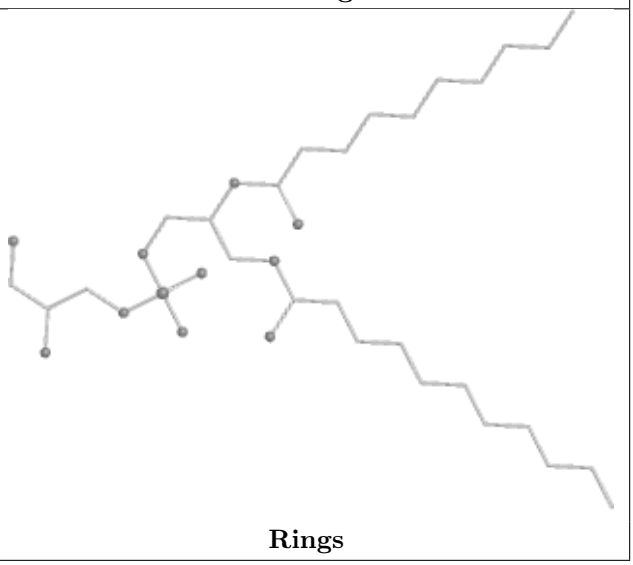
Bond lengths



Bond angles

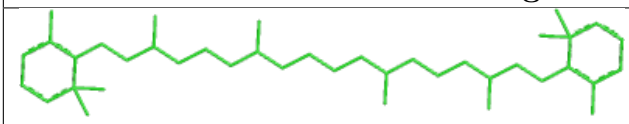


Torsions

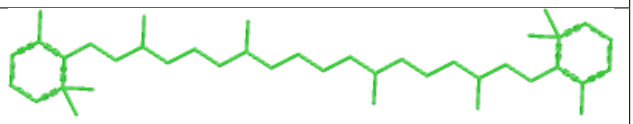


Rings

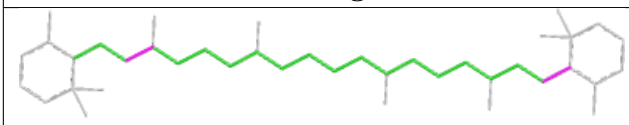
Ligand BCR B 856



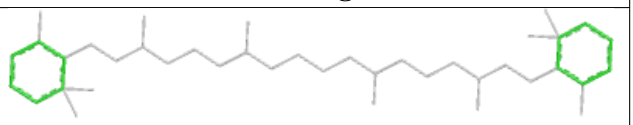
Bond lengths



Bond angles

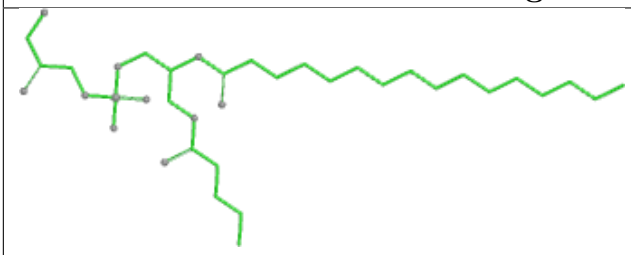


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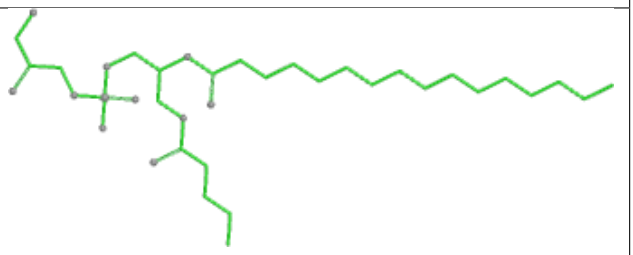


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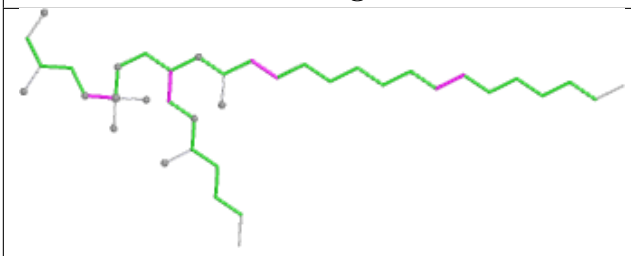
Ligand LHG b 852



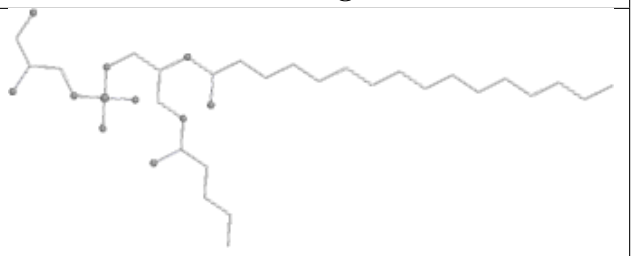
Bond lengths



Bond angles

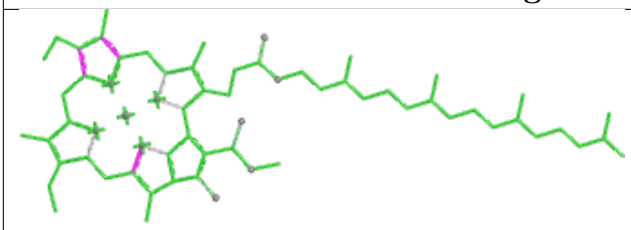


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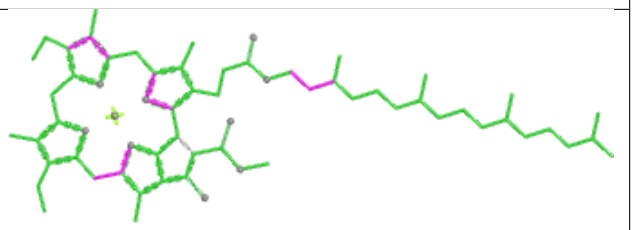


Rings

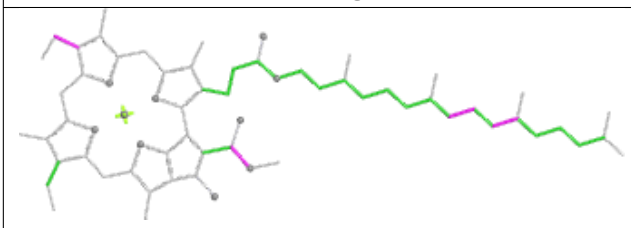
Ligand CLA A 838



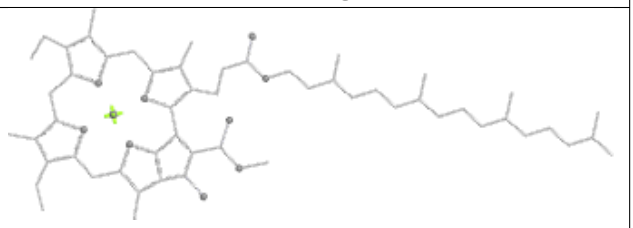
Bond lengths



Bond angles

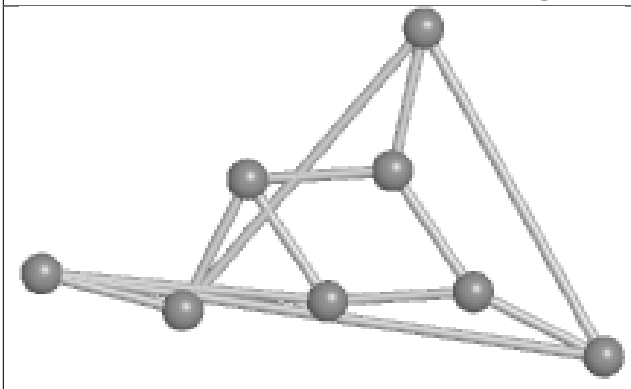


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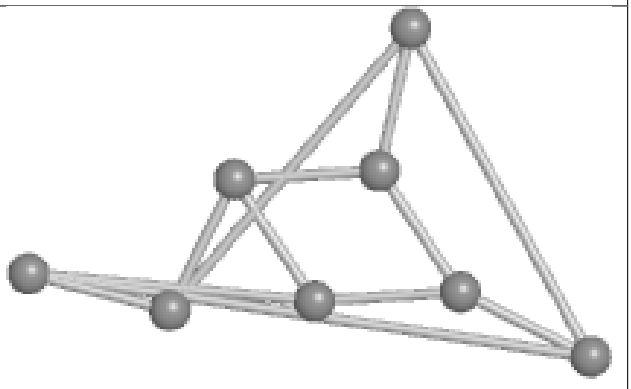


Rings

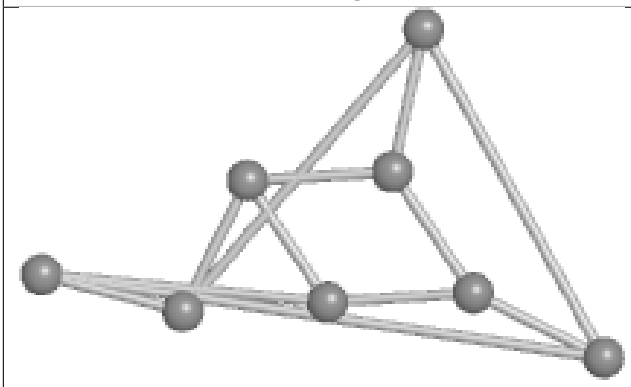
Ligand SF4 a 847



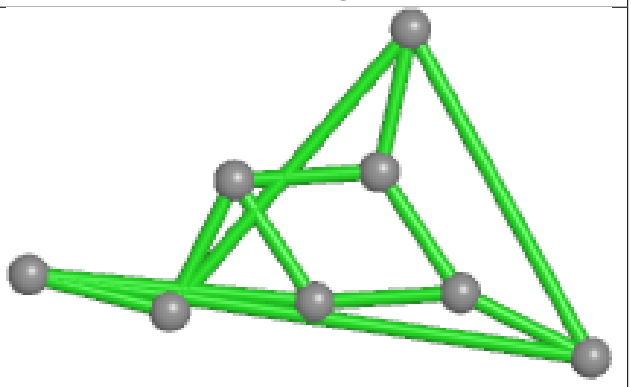
Bond lengths



Bond angles

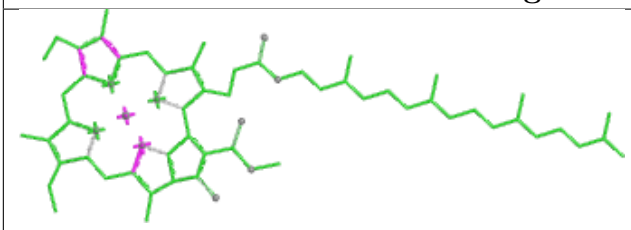


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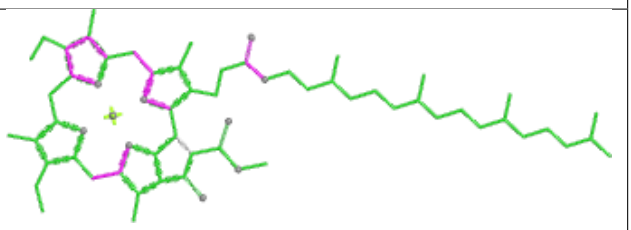


Rings

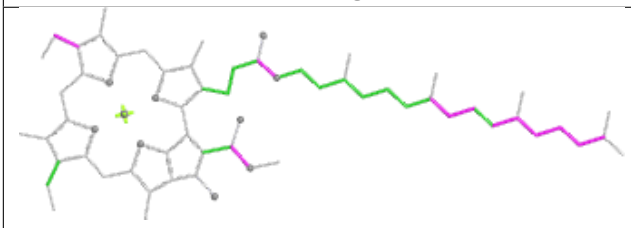
Ligand CLA A 824



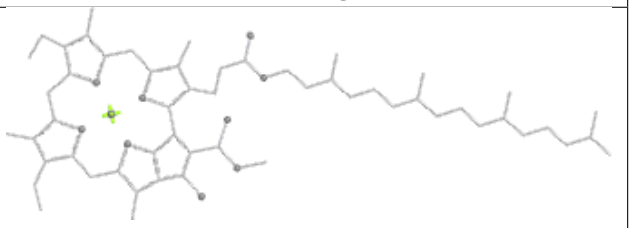
Bond lengths



Bond angles

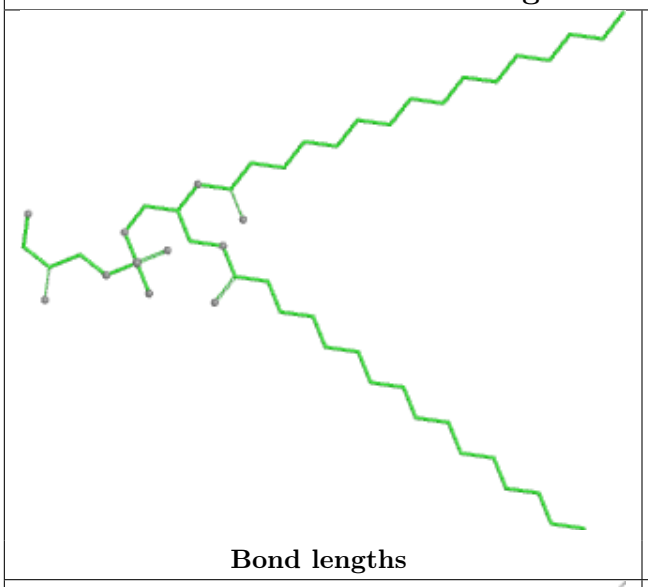


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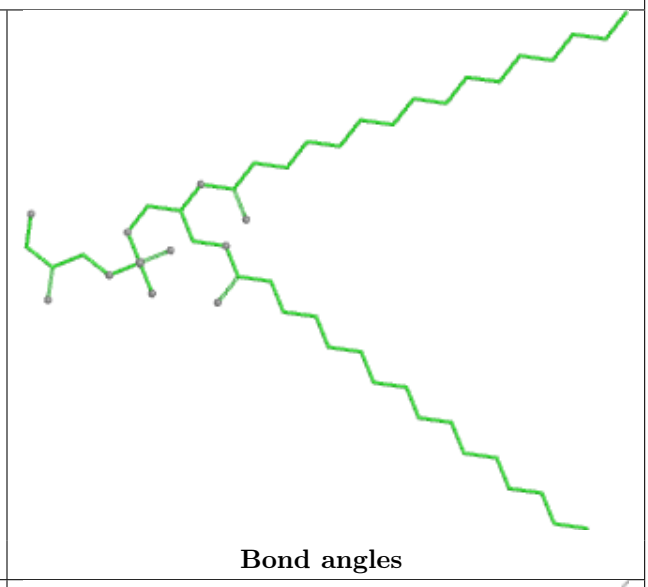


Rings

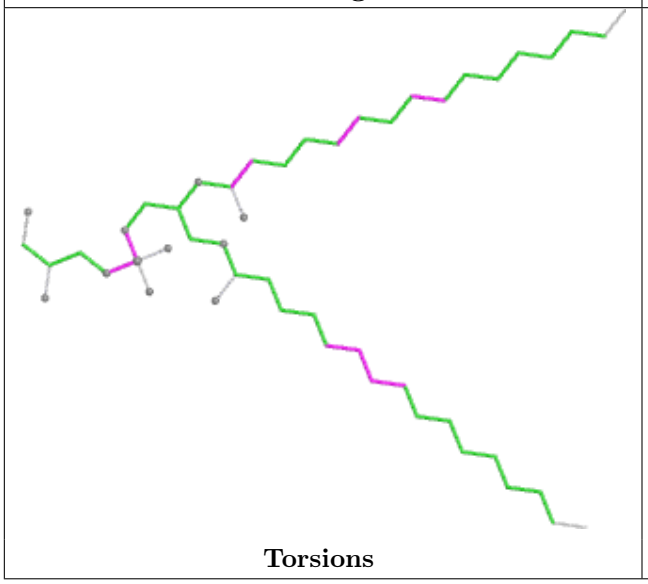
Ligand LHG G 855



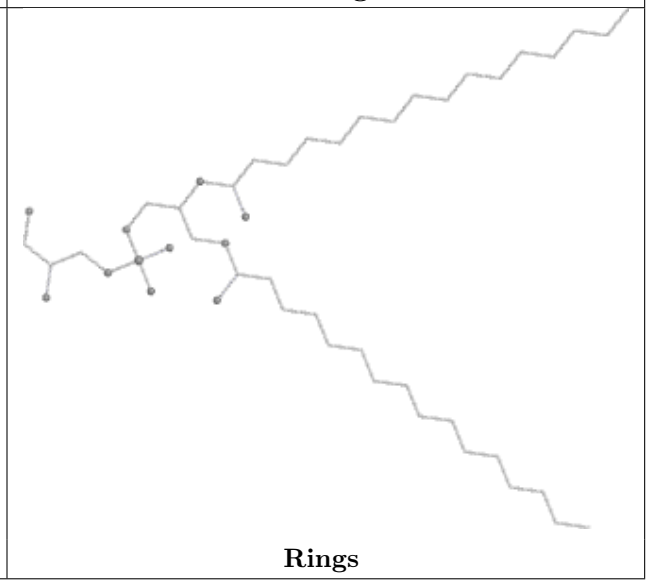
Bond lengths



Bond angles

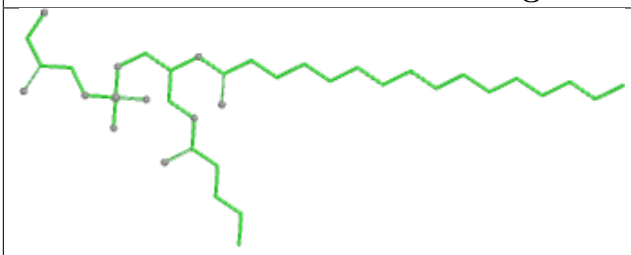


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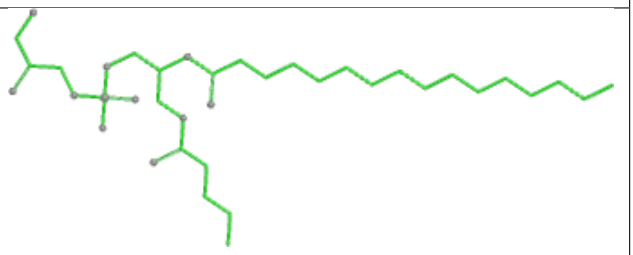


Rings

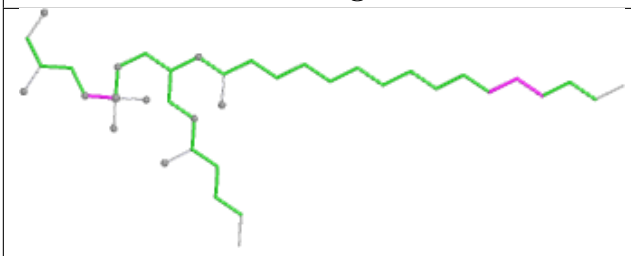
Ligand LHG B 851



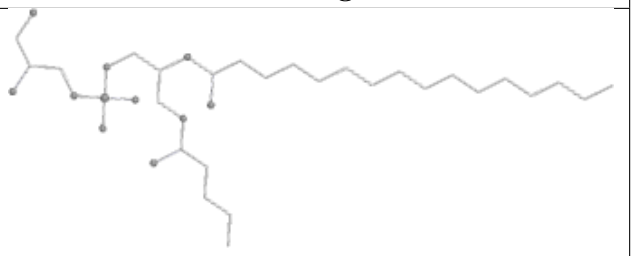
Bond lengths



Bond angles

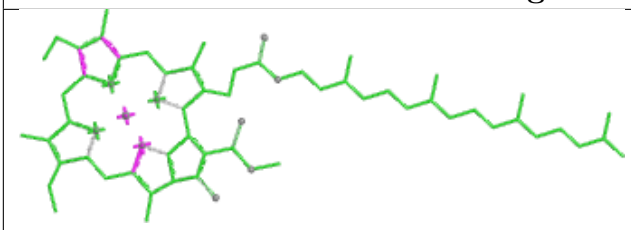


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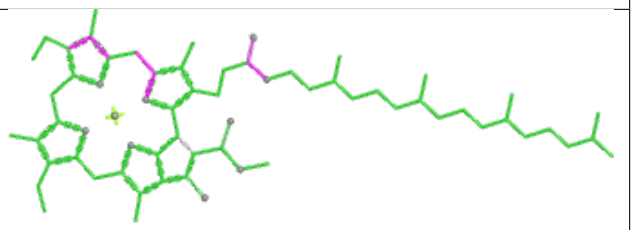


Rings

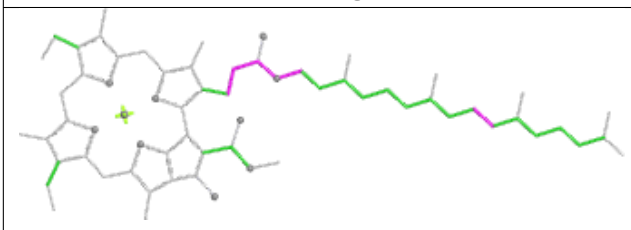
Ligand CLA b 820



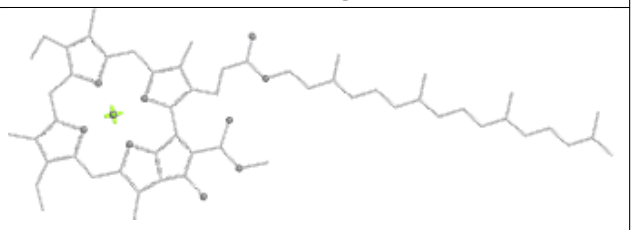
Bond lengths



Bond angles

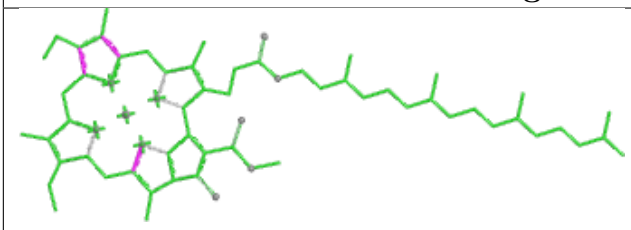


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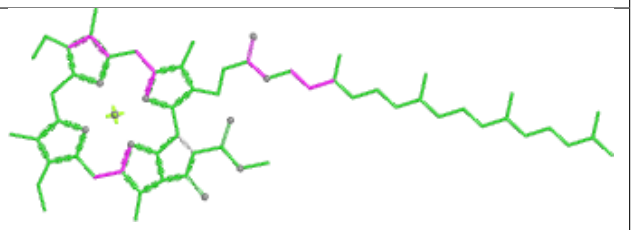


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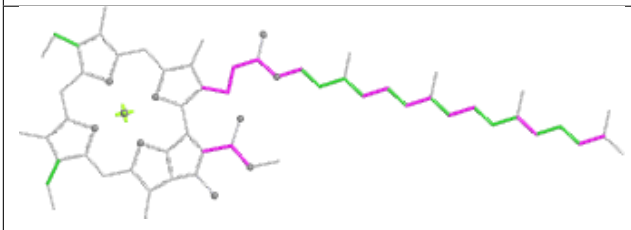
Ligand CLA H 816



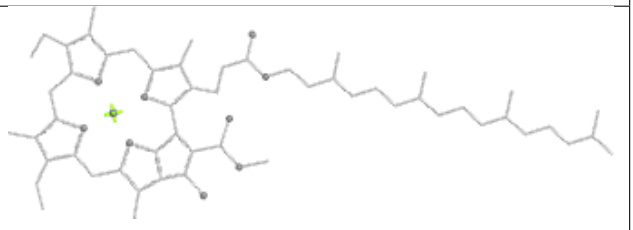
Bond lengths



Bond angles

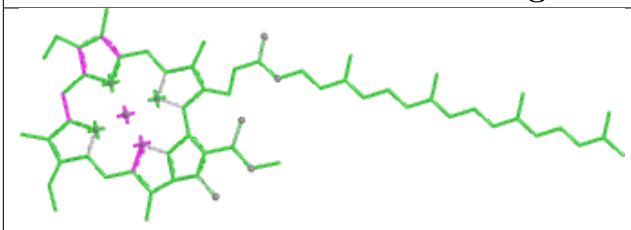


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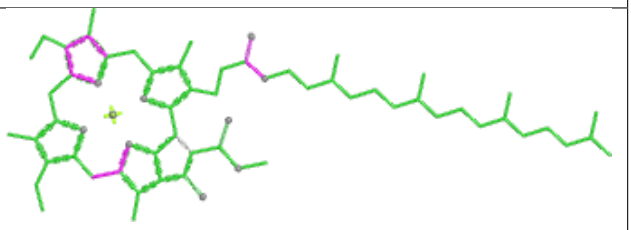


Rings

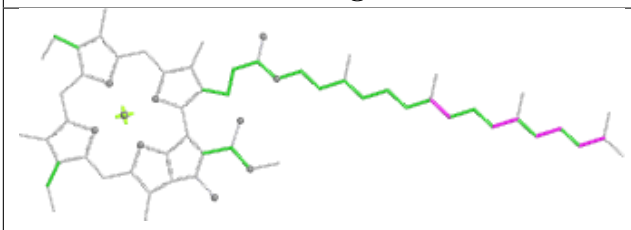
Ligand CLA a 840



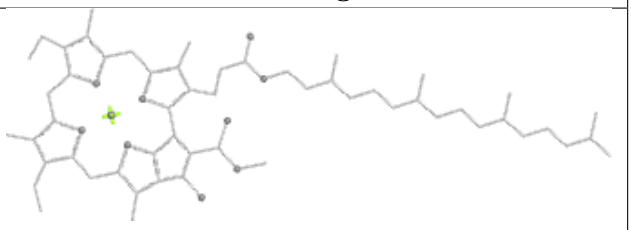
Bond lengths



Bond angles

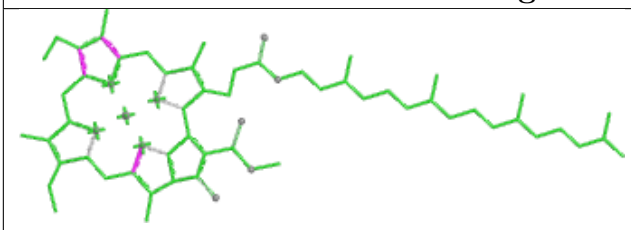


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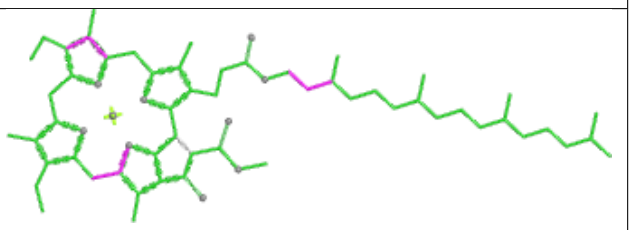


Rings

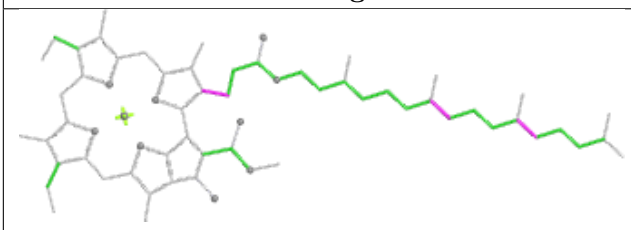
Ligand CLA S 1101



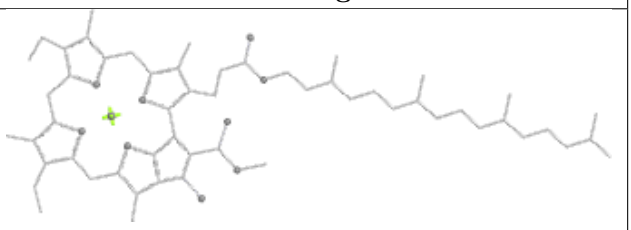
Bond lengths



Bond angles

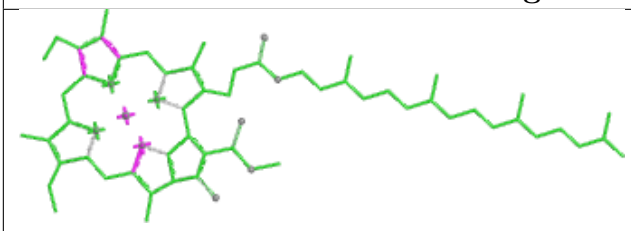


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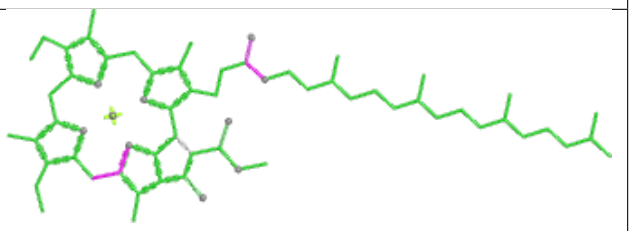


Rings

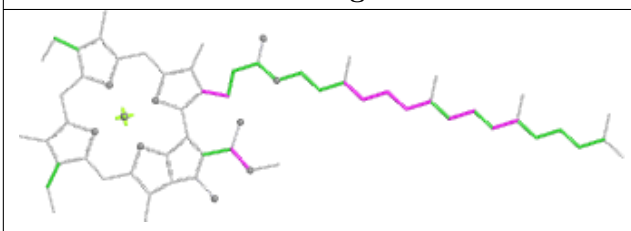
Ligand CLA H 819



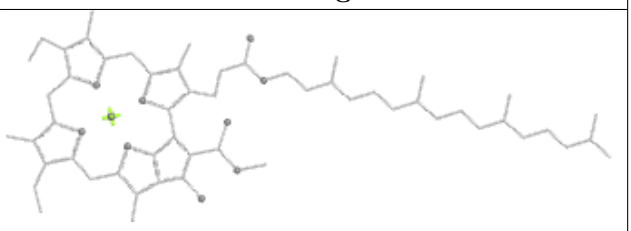
Bond lengths



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.

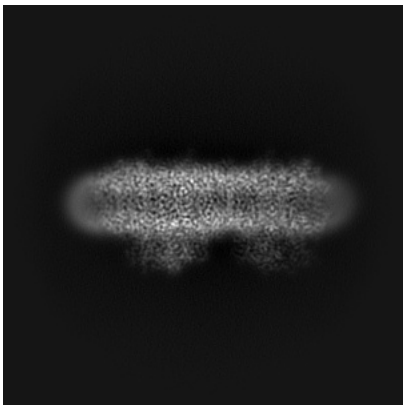
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71048. These allow visual inspection of the internal detail of the map and identification of artifacts.

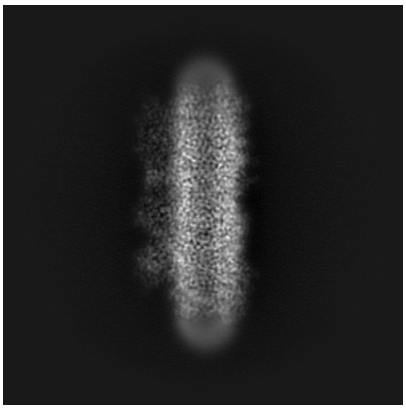
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

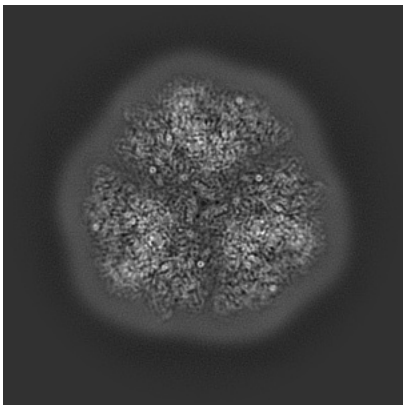
6.1.1 Primary map



X

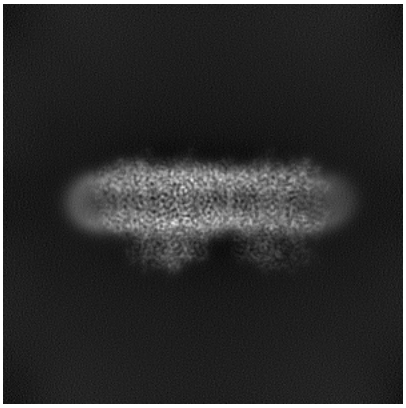


Y

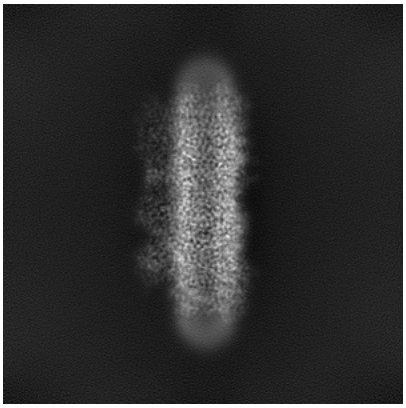


Z

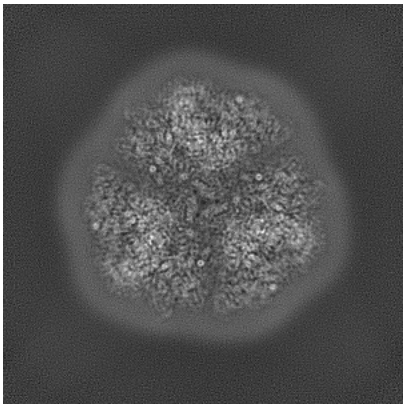
6.1.2 Raw map



X



Y

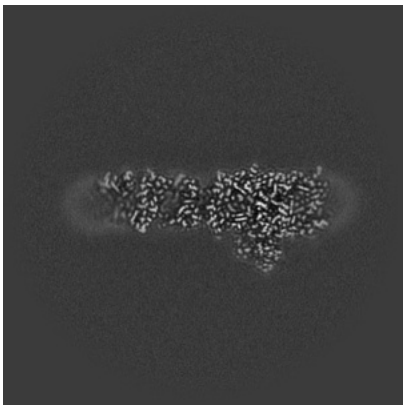


Z

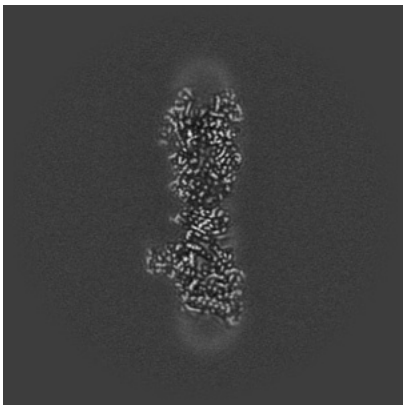
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

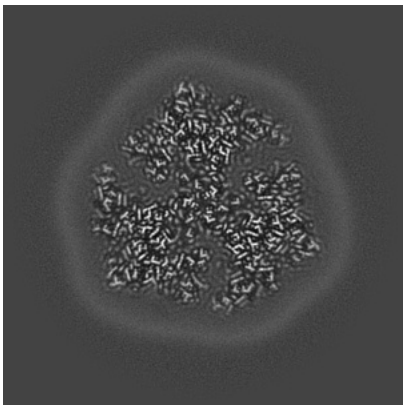
6.2.1 Primary map



X Index: 220

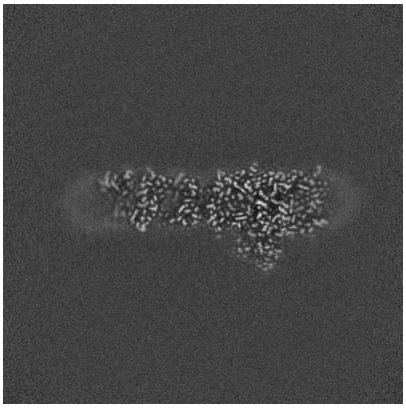


Y Index: 220

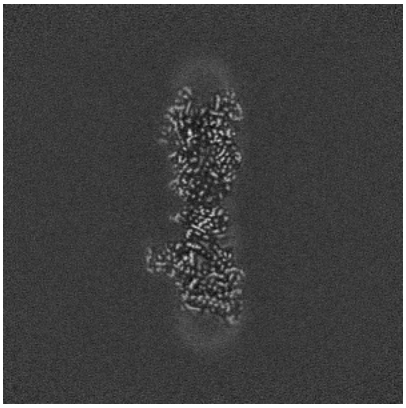


Z Index: 220

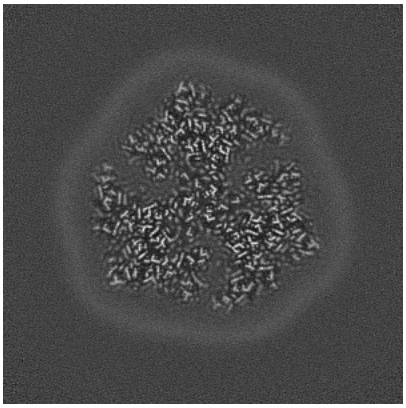
6.2.2 Raw map



X Index: 220



Y Index: 220

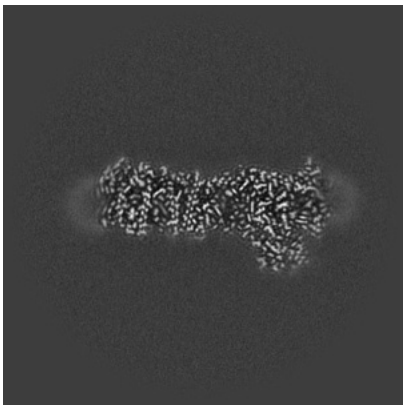


Z Index: 220

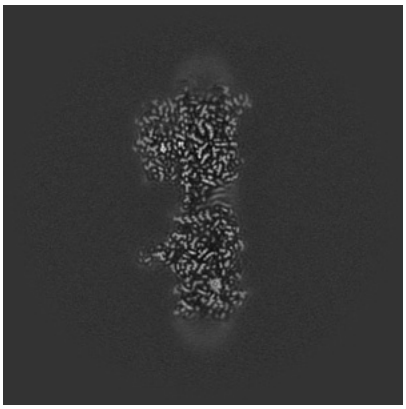
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

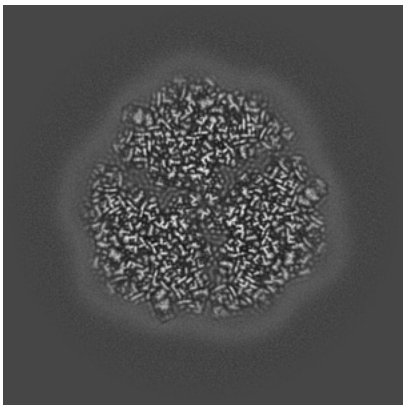
6.3.1 Primary map



X Index: 205

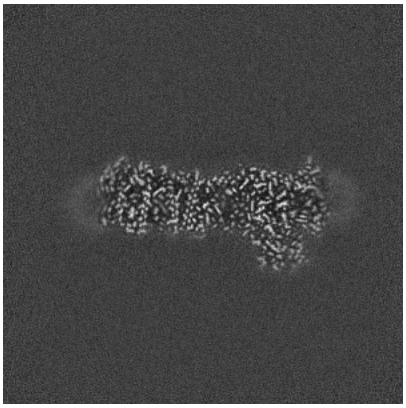


Y Index: 190

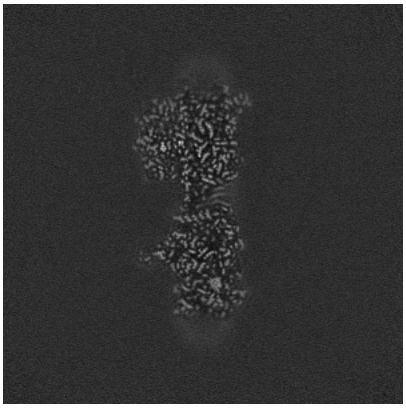


Z Index: 238

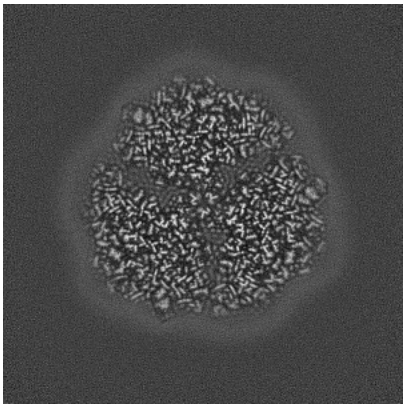
6.3.2 Raw map



X Index: 205



Y Index: 190

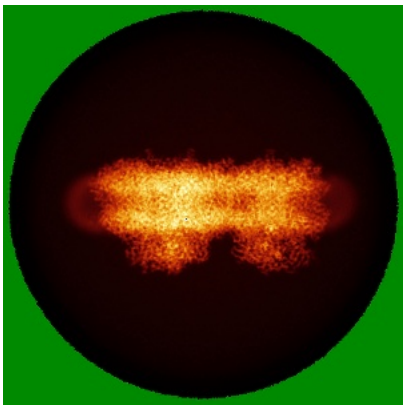


Z Index: 238

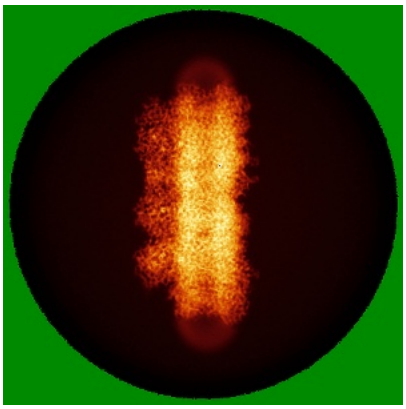
The images above show the largest variance slices of the map in three orthogonal directions.

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

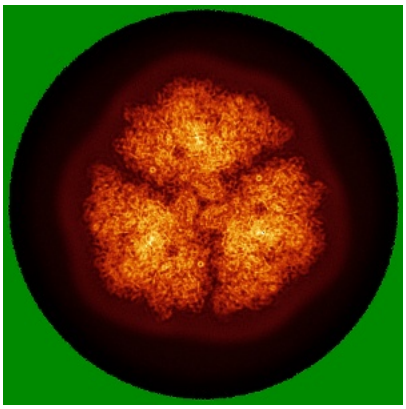
6.4.1 Primary map



X

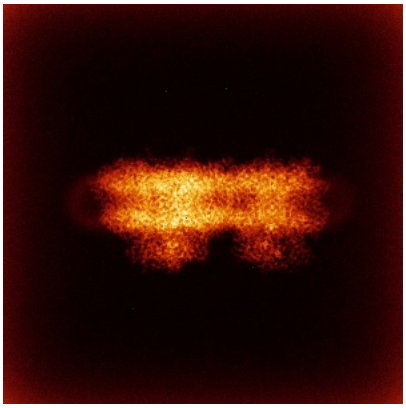


Y

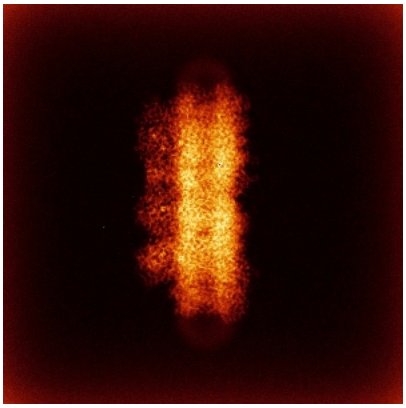


Z

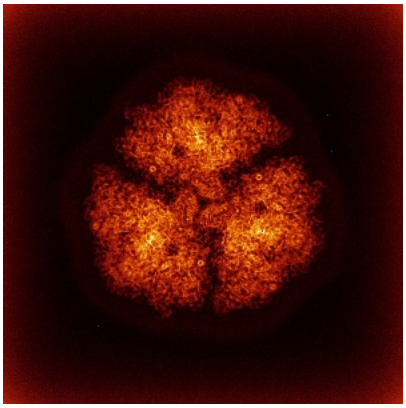
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

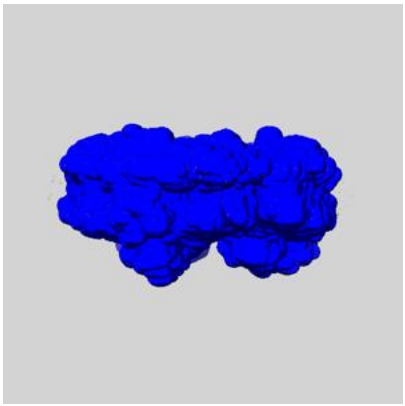
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

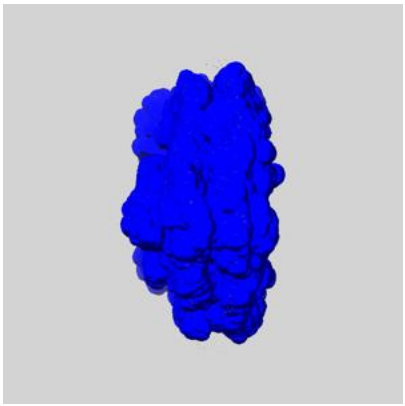
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

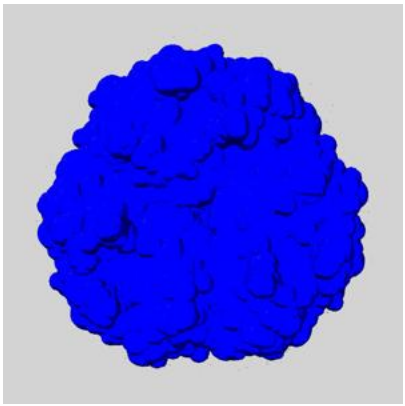
6.6.1 emd_71048_msk_1.map



X



Y

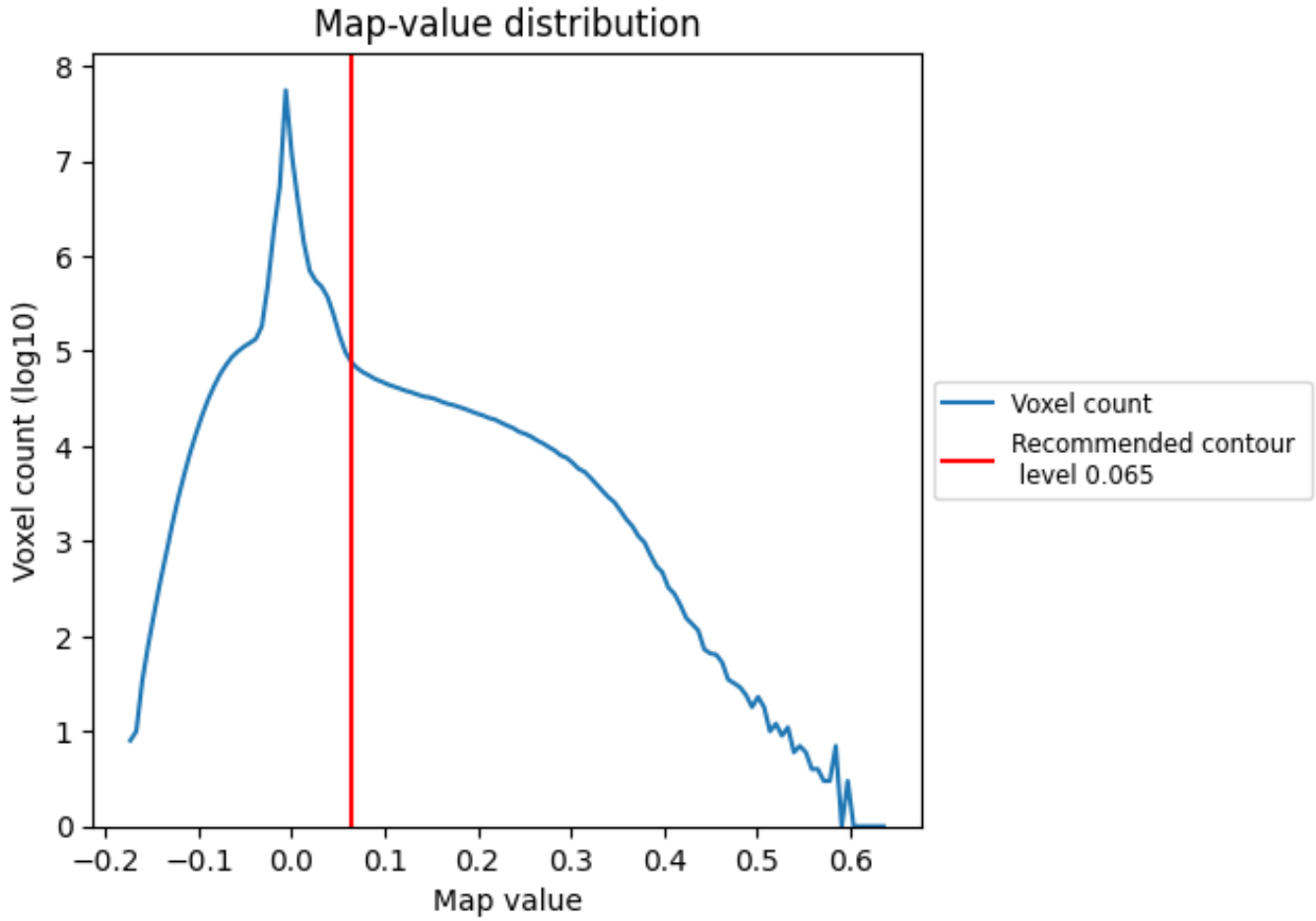


Z

7 Map analysis

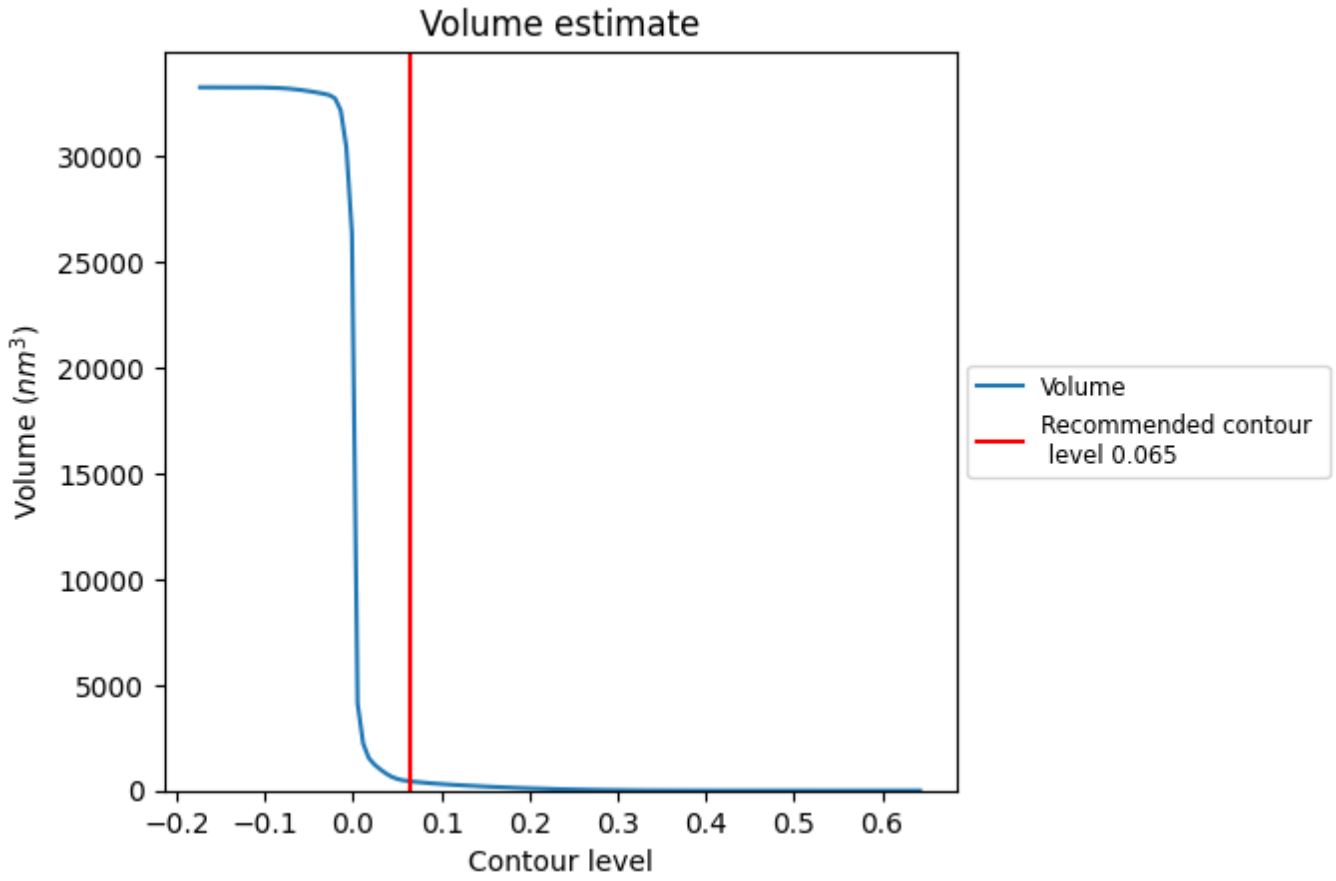
This section contains the results of statistical analysis of the map.

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.

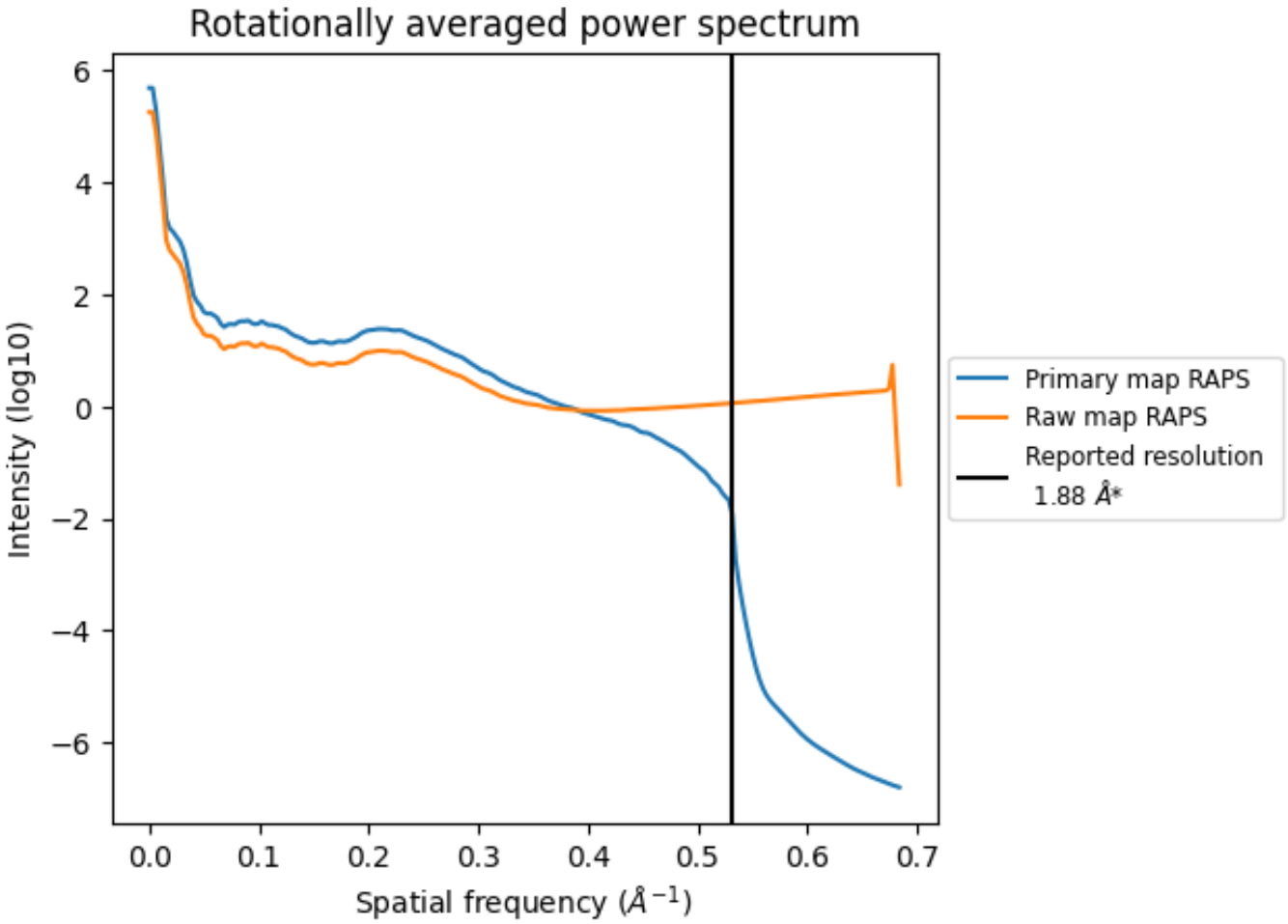
7.2 Volume estimate



The volume at the recommended contour level is 436 nm^3; this corresponds to an approximate mass of 394 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)

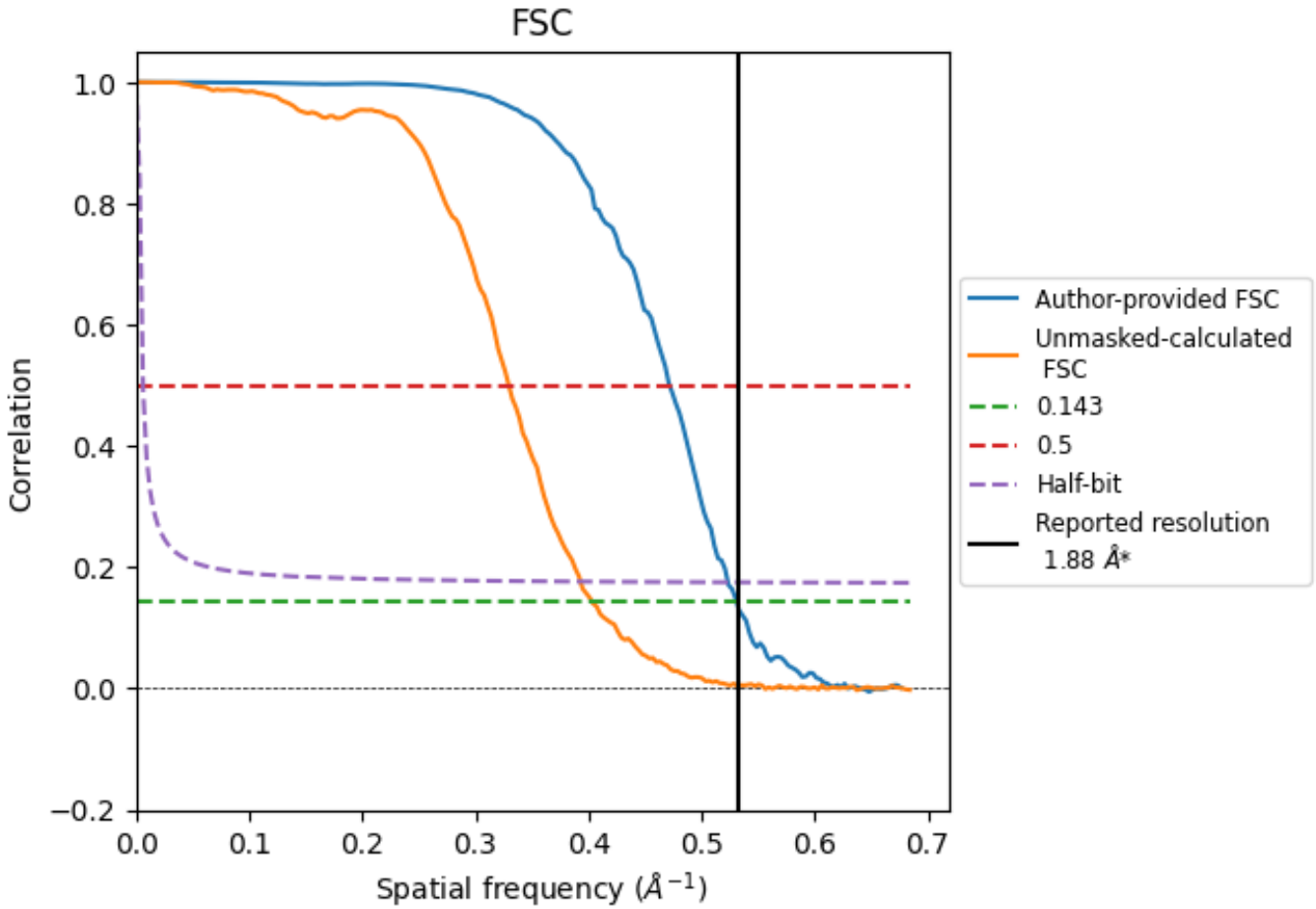


*Reported resolution corresponds to spatial frequency of 0.532 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.532 Å^{-1}

8.2 Resolution estimates (i)

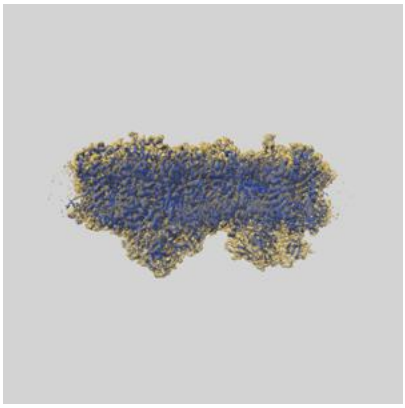
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.88	-	-
Author-provided FSC curve	1.88	2.12	1.91
Unmasked-calculated*	2.48	3.03	2.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.48 differs from the reported value 1.88 by more than 10 %

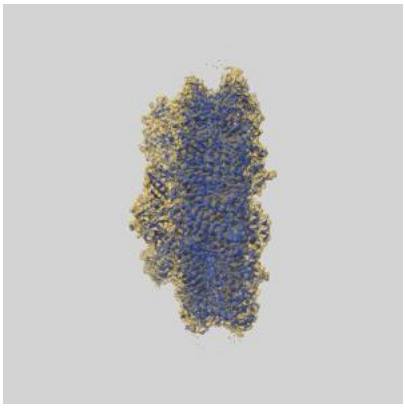
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71048 and PDB model 9OZ3. Per-residue inclusion information can be found in section 3 on page 36.

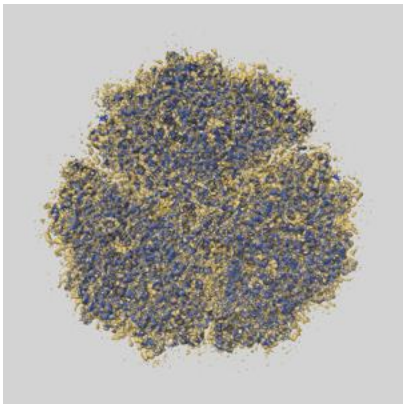
9.1 Map-model overlay



X



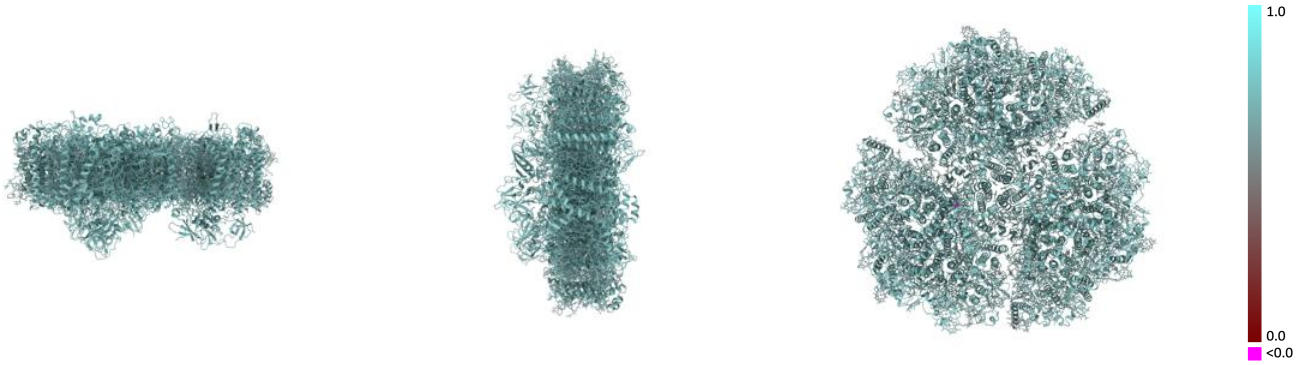
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

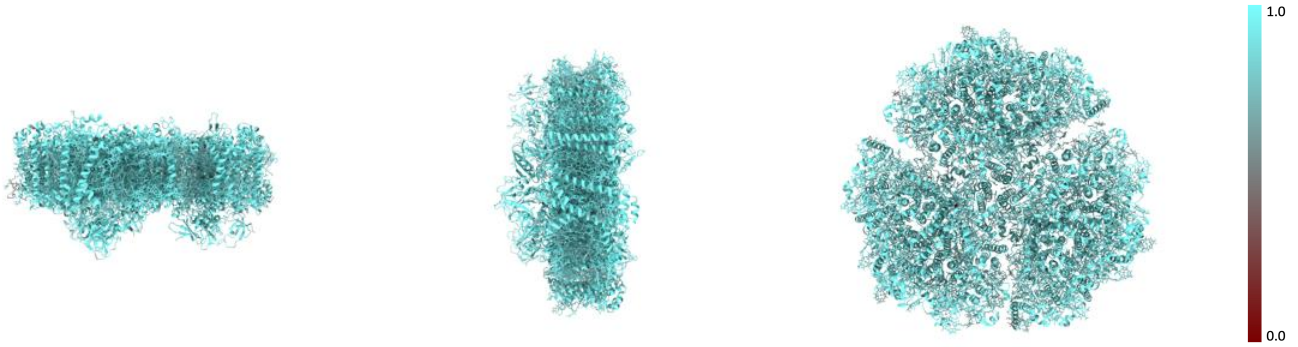
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

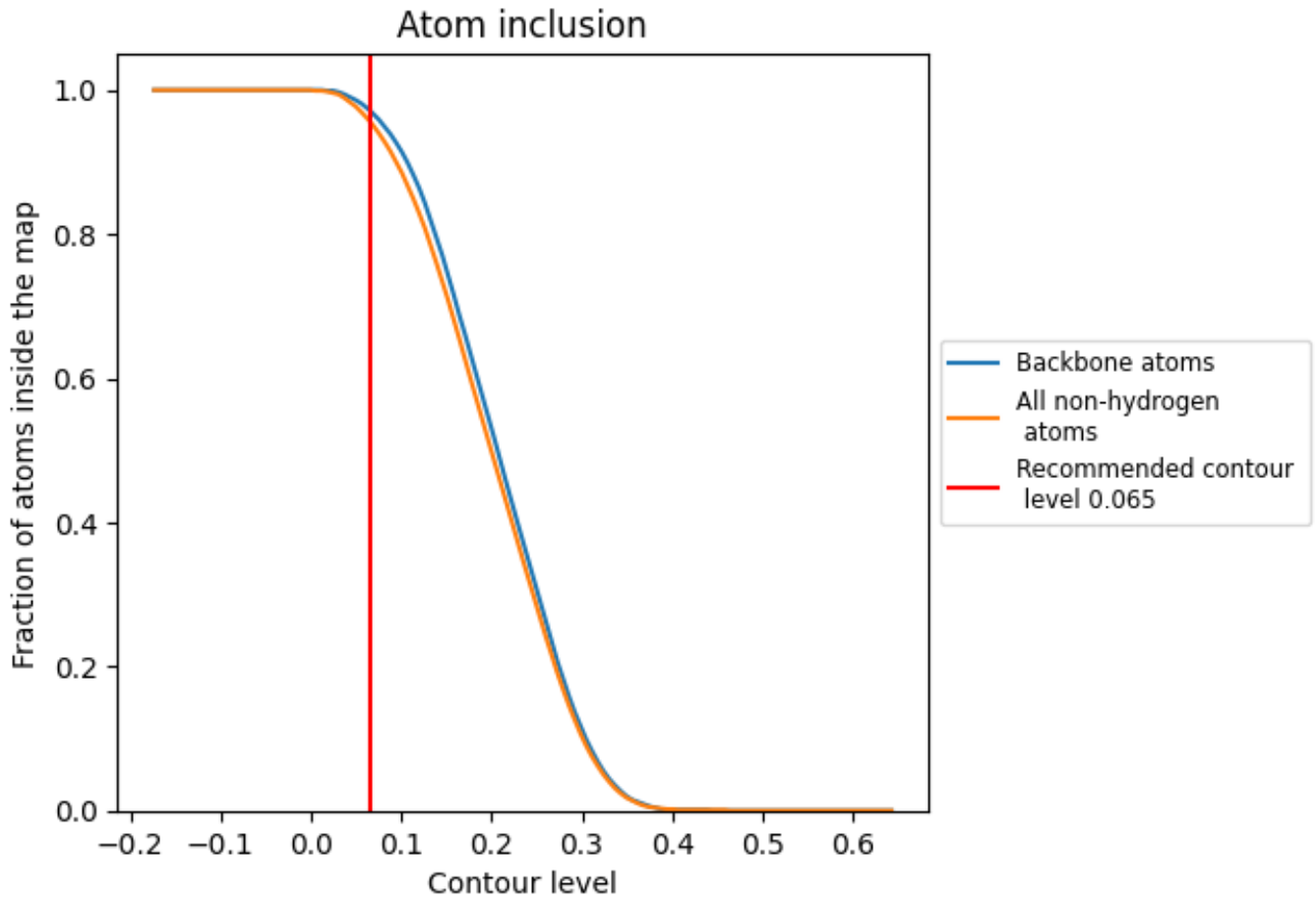
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.6990
A	0.9630	0.7050
B	0.9550	0.7030
C	0.9830	0.7150
D	0.9590	0.6970
E	0.9300	0.6780
F	0.9450	0.6750
G	0.9610	0.7020
H	0.9610	0.7040
I	0.9870	0.7210
J	0.9200	0.6660
K	0.8900	0.6490
L	0.9530	0.7080
M	0.9120	0.6730
N	0.9900	0.7150
O	0.9300	0.6750
P	0.9600	0.6950
Q	0.9340	0.6710
R	0.9930	0.7240
S	0.9390	0.6700
T	0.8890	0.6430
U	0.9670	0.7140
V	0.9620	0.7040
a	0.9630	0.7030
b	0.9610	0.7060
c	0.9880	0.7130
d	0.9620	0.7010
e	0.9290	0.6720
f	0.9300	0.6630
i	0.9920	0.7240
j	0.9310	0.6580
k	0.8250	0.6210
l	0.9660	0.7140
m	0.9710	0.7150

