wwPDB EM Validation Summary Report (i)

Oct 1, 2026 – 12:33 AM JST

PDB ID	:	7F4V / pdb_00007f4v
EMDB ID	:	EMD-31455
Title	:	Cryo-EM structure of a primordial cyanobacterial photosystem I
Authors	:	Kato, K.; Hamaguchi, T.; Nagao, R.; Kawakami, K.; Yonekura, K.; Shen, J.R.
Deposited on	:	2021-06-21
Resolution	:	2.04 Å(reported)

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

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

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

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

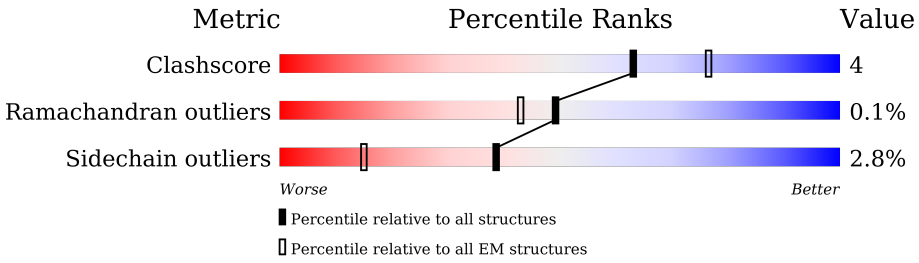
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

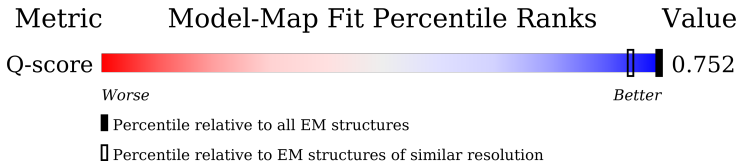
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.04 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	1810 (1.55 - 2.54)

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

Mol	Chain	Length	Quality of chain
1	aA	783	7% 90% 8%
1	bA	783	7% 90% 8%
1	cA	783	7% 90% 8%
2	aB	872	77% 6% 17%

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Mol	Chain	Length	Quality of chain
2	bB	872	77% 6% 17%
2	cB	872	77% 6% 17%
3	aC	81	88% 10%
3	bC	81	89% 9%
3	cC	81	90% 6%
4	aD	144	19% 76% 17% 8%
4	bD	144	19% 75% 17% 8%
4	cD	144	20% 76% 16% 8%
5	aE	65	28% 82% 14% 5%
5	bE	65	34% 82% 14% 5%
5	cE	65	31% 82% 14% 5%
6	aF	181	30% 69% 12% 17%
6	bF	181	34% 68% 13% 17%
6	cF	181	30% 70% 11% 17%
7	aI	35	80% 9% 11%
7	bI	35	83% 6% 11%
7	cI	35	74% 14% 11%
8	aJ	33	18% 97%
8	bJ	33	18% 97%
8	cJ	33	15% 97%
9	aL	147	9% 77% 10% 12%
9	bL	147	9% 77% 10% 12%
9	cL	147	10% 77% 10% 12%
10	aM	34	82% 15%
10	bM	34	82% 15%

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Mol	Chain	Length	Quality of chain
10	cM	34	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 67641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	772	Total	C	N	O	S	0	0
			6038	3957	1031	1025	25		
1	bA	772	Total	C	N	O	S	0	0
			6038	3957	1031	1025	25		
1	cA	772	Total	C	N	O	S	0	0
			6038	3957	1031	1025	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	725	Total	C	N	O	S	0	0
			5701	3761	954	968	18		
2	bB	725	Total	C	N	O	S	0	0
			5701	3761	954	968	18		
2	cB	725	Total	C	N	O	S	0	0
			5701	3761	954	968	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			599	368	103	118	10		
3	bC	80	Total	C	N	O	S	0	0
			599	368	103	118	10		
3	cC	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		
4	cD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	62	Total	C	N	O	0	0
			507	321	87	99		
5	bE	62	Total	C	N	O	0	0
			507	321	87	99		
5	cE	62	Total	C	N	O	0	0
			507	321	87	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		
6	bF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		
6	cF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		
7	bI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		
7	cI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		

- Molecule 8 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	33	Total	C	N	O	0	0
			164	98	33	33		
8	bJ	33	Total	C	N	O	0	0
			164	98	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	cJ	33	Total	C	N	O	0	0
			164	98	33	33		

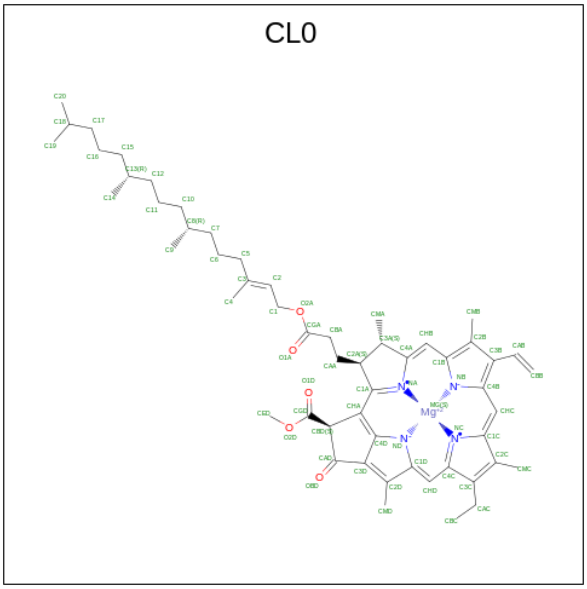
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aL	129	Total	C	N	O	S	0	0
			974	641	162	169	2		
9	bL	129	Total	C	N	O	S	0	0
			974	641	162	169	2		
9	cL	129	Total	C	N	O	S	0	0
			974	641	162	169	2		

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

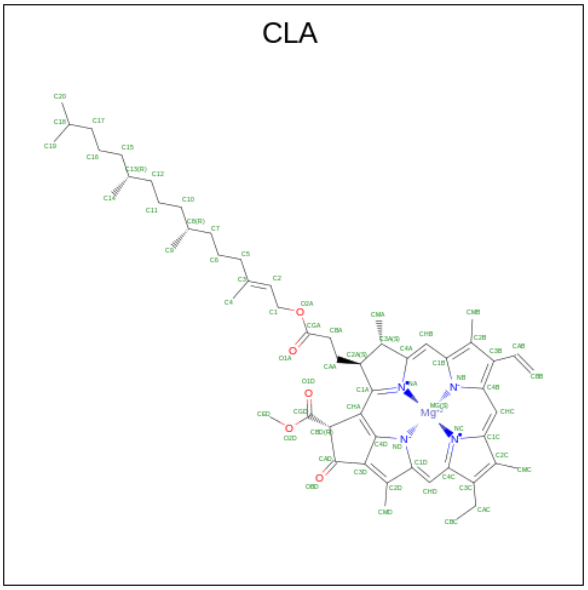
Mol	Chain	Residues	Atoms				AltConf	Trace
10	aM	29	Total	C	N	O	0	0
			190	127	30	33		
10	bM	29	Total	C	N	O	0	0
			190	127	30	33		
10	cM	29	Total	C	N	O	0	0
			190	127	30	33		

- Molecule 11 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aL	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	aL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bL	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	bL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	cF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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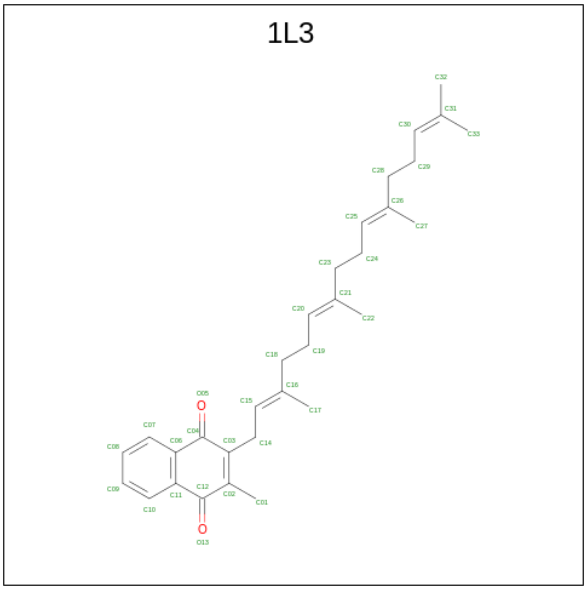
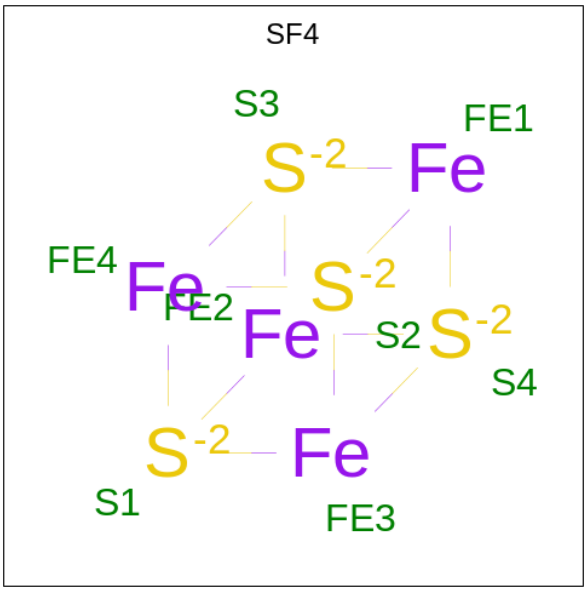
Mol	Chain	Residues	Atoms					AltConf
12	cL	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	cL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 13 is Menaquinone-4 (CCD ID: 1L3) (formula: $C_{31}H_{40}O_2$).



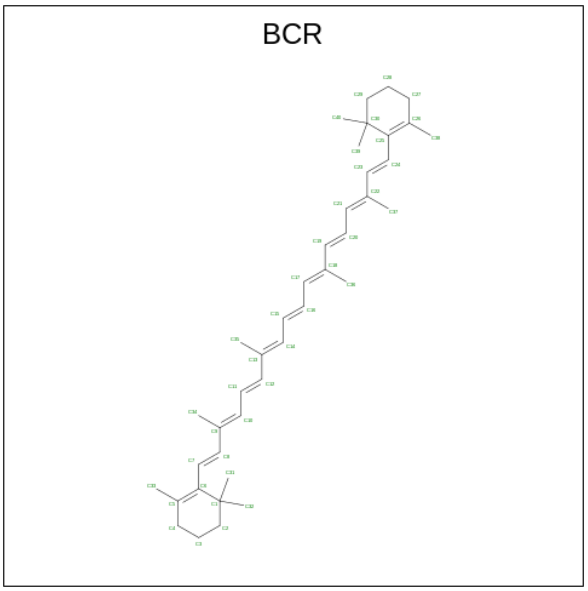
Mol	Chain	Residues	Atoms			AltConf
13	aA	1	Total	C	O	0
			33	31	2	
13	aB	1	Total	C	O	0
			33	31	2	
13	bA	1	Total	C	O	0
			33	31	2	
13	bB	1	Total	C	O	0
			33	31	2	
13	cA	1	Total	C	O	0
			33	31	2	
13	cB	1	Total	C	O	0
			33	31	2	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
14	aA	1	Total Fe S 8 4 4	0
14	aC	1	Total Fe S 8 4 4	0
14	aC	1	Total Fe S 8 4 4	0
14	bA	1	Total Fe S 8 4 4	0
14	bC	1	Total Fe S 8 4 4	0
14	bC	1	Total Fe S 8 4 4	0
14	cA	1	Total Fe S 8 4 4	0
14	cC	1	Total Fe S 8 4 4	0
14	cC	1	Total Fe S 8 4 4	0

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aF	1	Total C 40 40	0
15	aF	1	Total C 40 40	0
15	aF	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	aI	1	Total C 40 40	0
15	aJ	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aM	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bF	1	Total C 40 40	0
15	bF	1	Total C 40 40	0
15	bF	1	Total C 40 40	0
15	bI	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	bJ	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bM	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cF	1	Total C 40 40	0
15	cF	1	Total C 40 40	0
15	cF	1	Total C 40 40	0
15	cI	1	Total C 40 40	0
15	cJ	1	Total C 40 40	0

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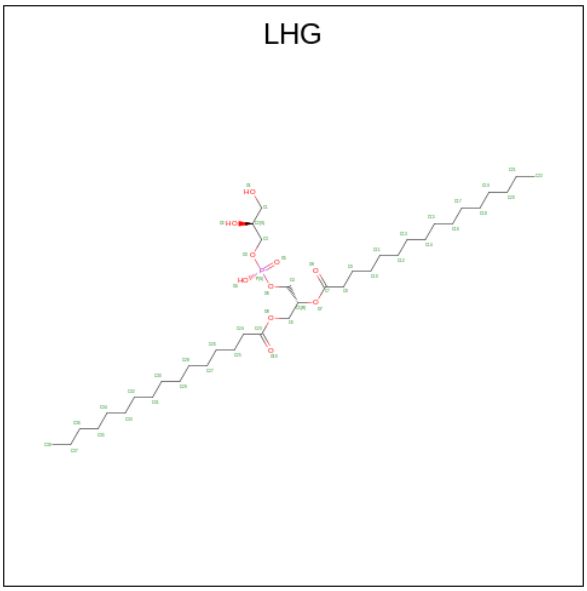
Mol	Chain	Residues	Atoms	AltConf
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cM	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
16	aA	1	Total C O P 49 38 10 1	0
16	aA	1	Total C O P 27 16 10 1	0
16	aB	1	Total C O P 23 12 10 1	0
16	bA	1	Total C O P 49 38 10 1	0
16	bA	1	Total C O P 27 16 10 1	0
16	bB	1	Total C O P 23 12 10 1	0
16	cA	1	Total C O P 49 38 10 1	0

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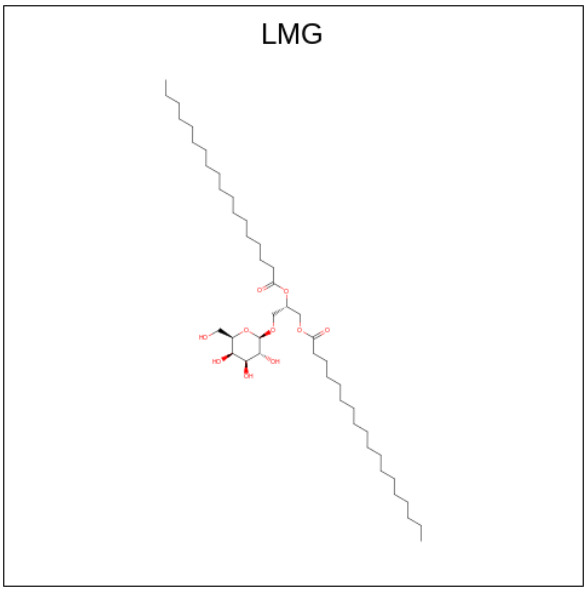
Mol	Chain	Residues	Atoms				AltConf
16	cA	1	Total	C	O	P	0
			27	16	10	1	
16	cB	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
17	aB	1	Total	C	O	0
			43	33	10	
17	bB	1	Total	C	O	0
			43	33	10	
17	cB	1	Total	C	O	0
			43	33	10	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	aA	45	Total	O	0
			45	45	
18	aB	67	Total	O	0
			67	67	
18	aC	14	Total	O	0
			14	14	
18	aD	2	Total	O	0
			2	2	

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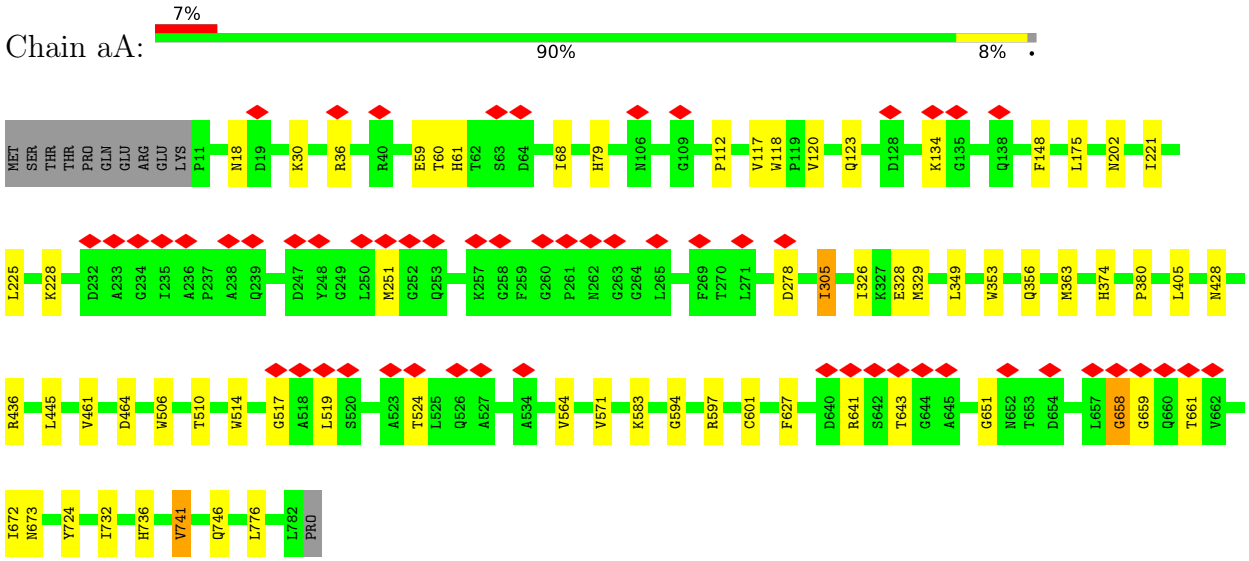
Mol	Chain	Residues	Atoms	AltConf
18	aE	3	Total O 3 3	0
18	aF	1	Total O 1 1	0
18	aJ	1	Total O 1 1	0
18	aL	1	Total O 1 1	0
18	bA	45	Total O 45 45	0
18	bB	67	Total O 67 67	0
18	bC	14	Total O 14 14	0
18	bD	2	Total O 2 2	0
18	bE	3	Total O 3 3	0
18	bF	1	Total O 1 1	0
18	bJ	1	Total O 1 1	0
18	bL	1	Total O 1 1	0
18	cA	45	Total O 45 45	0
18	cB	67	Total O 67 67	0
18	cC	14	Total O 14 14	0
18	cD	2	Total O 2 2	0
18	cE	3	Total O 3 3	0
18	cF	1	Total O 1 1	0
18	cJ	1	Total O 1 1	0
18	cL	1	Total O 1 1	0

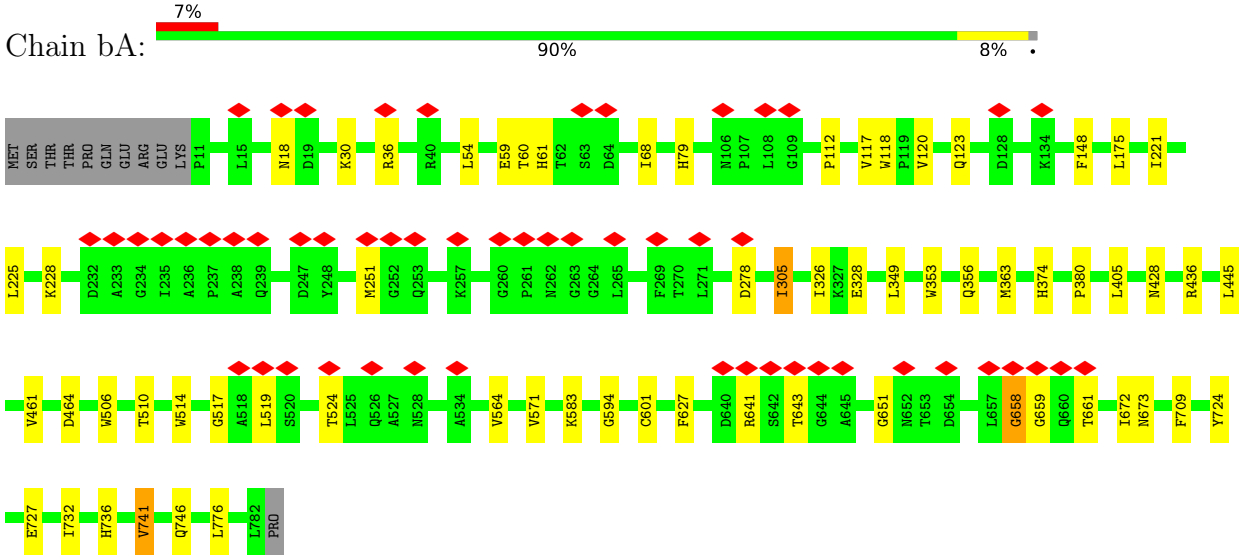
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

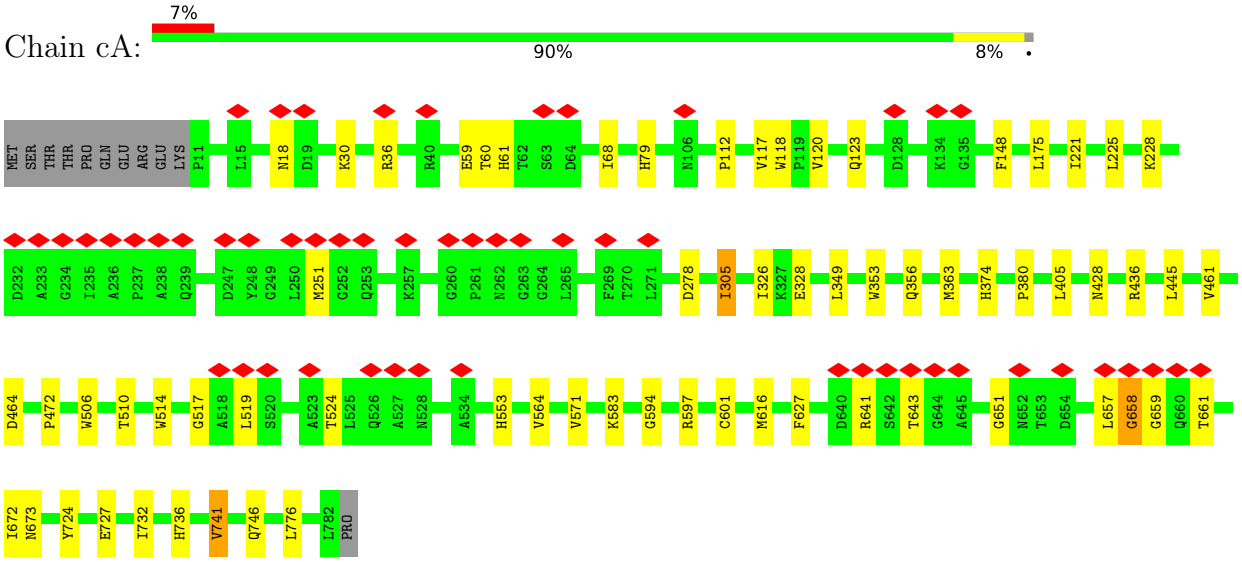


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



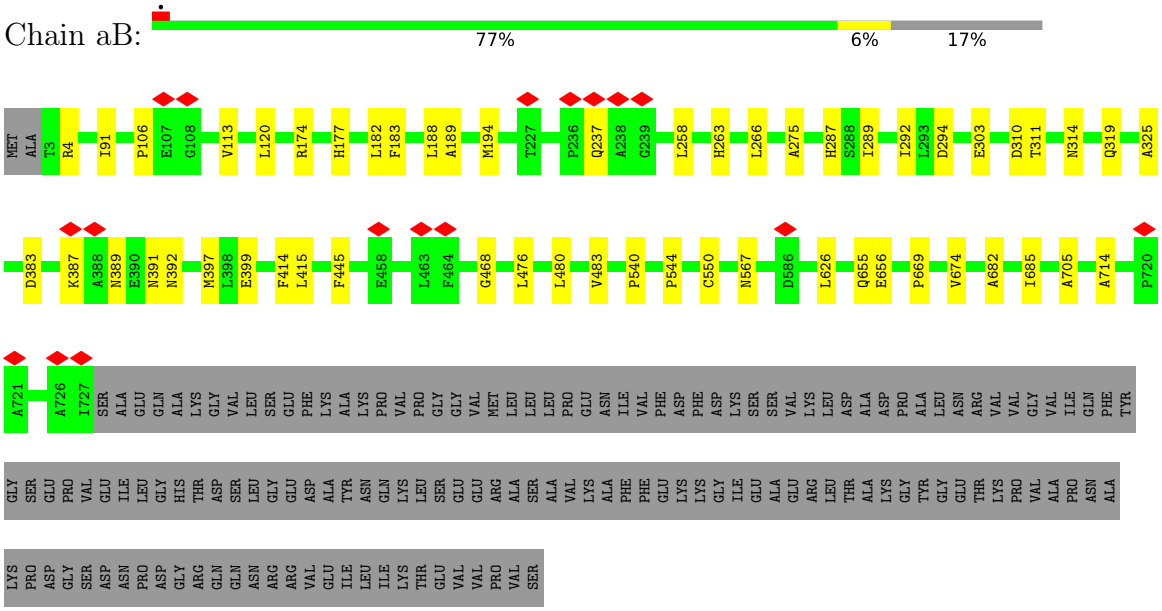
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:



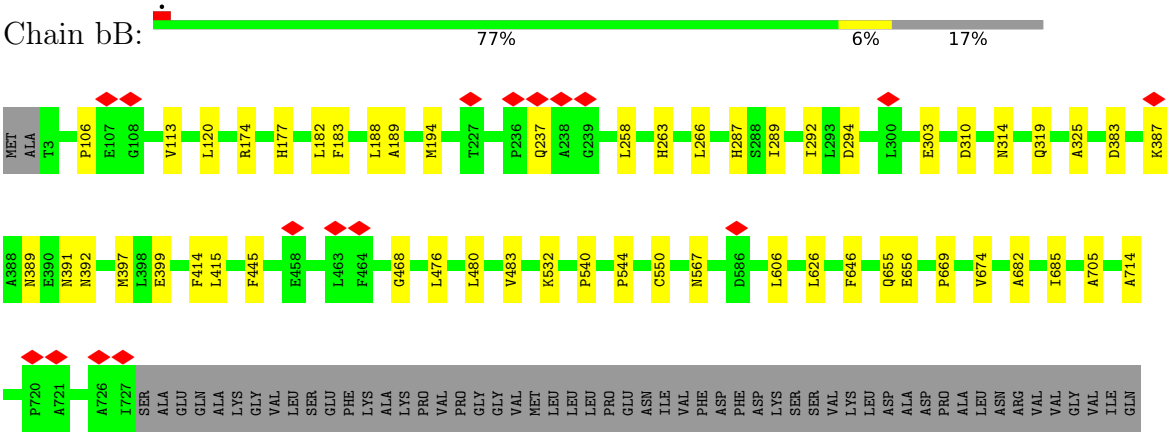
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

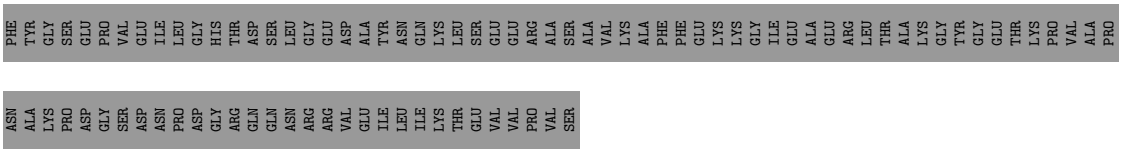
Chain aB:



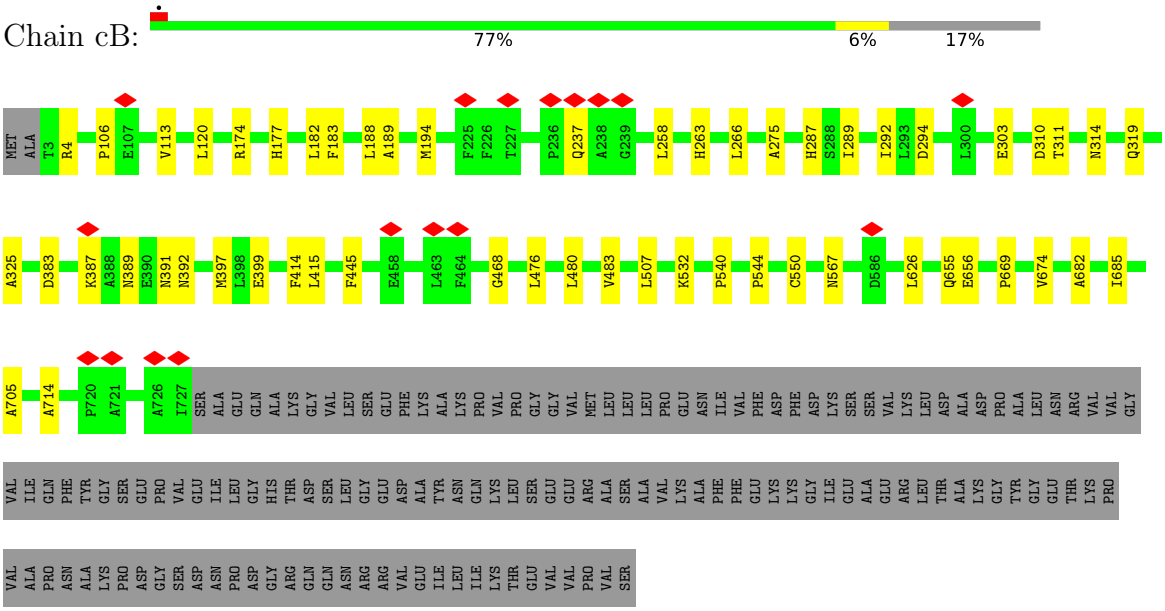
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:

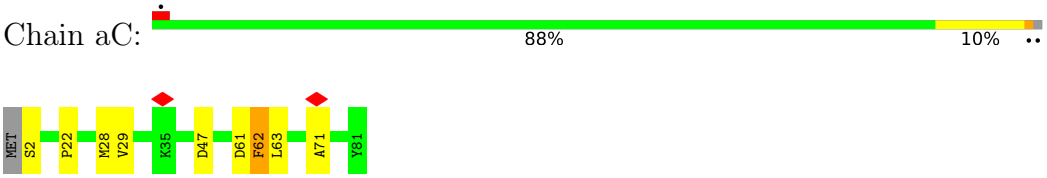




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 3: Photosystem I iron-sulfur center



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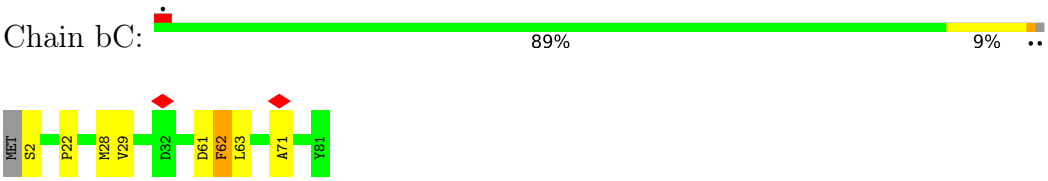

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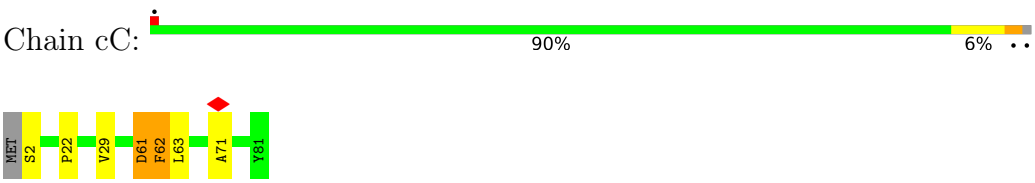
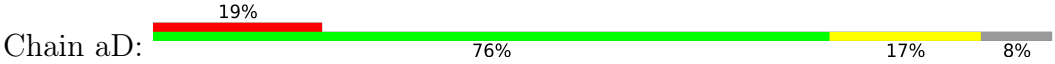
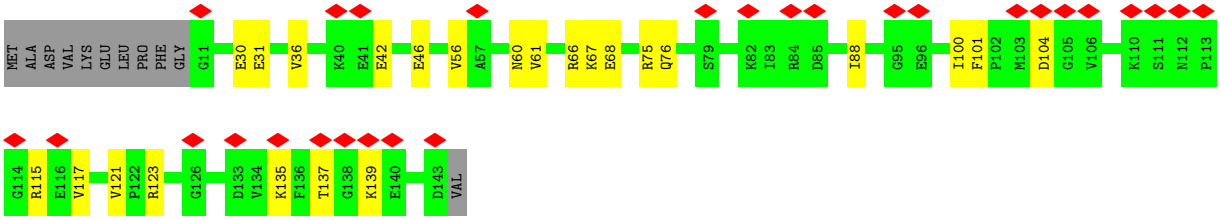
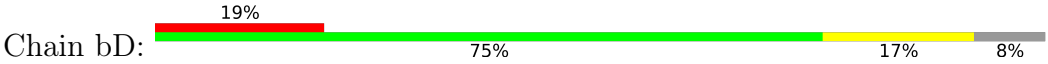


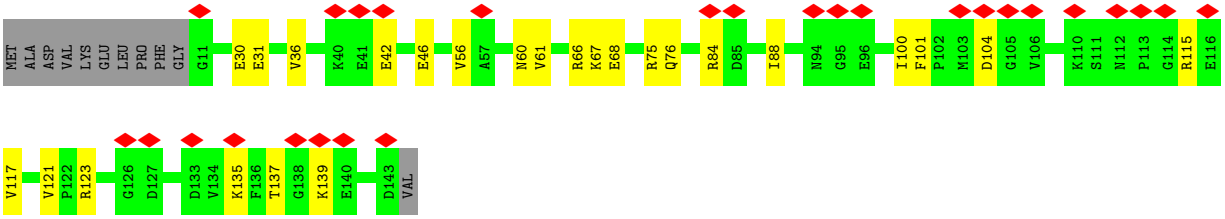
• Molecule 4: Photosystem I reaction center subunit II



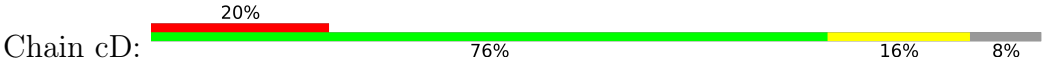


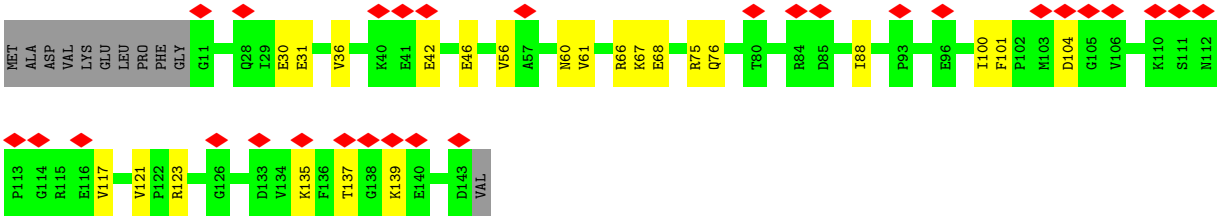
• Molecule 4: Photosystem I reaction center subunit II



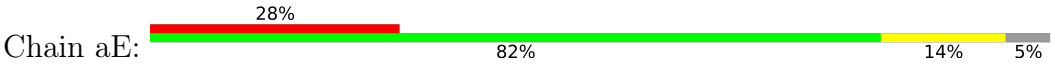


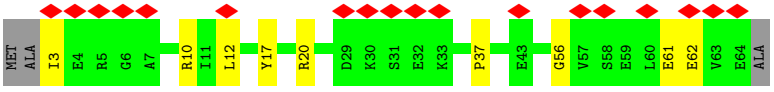
• Molecule 4: Photosystem I reaction center subunit II



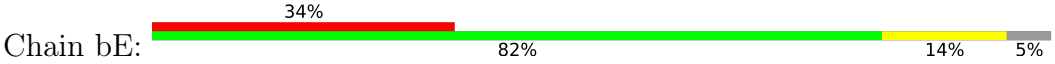


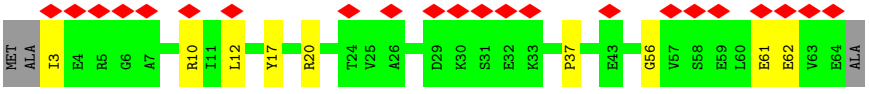
• Molecule 5: Photosystem I reaction center subunit IV



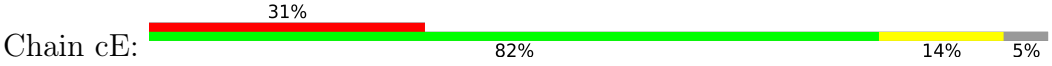


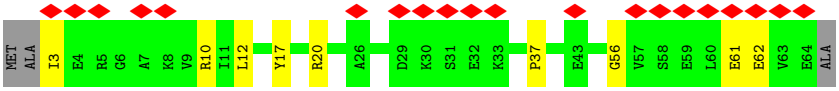
• Molecule 5: Photosystem I reaction center subunit IV





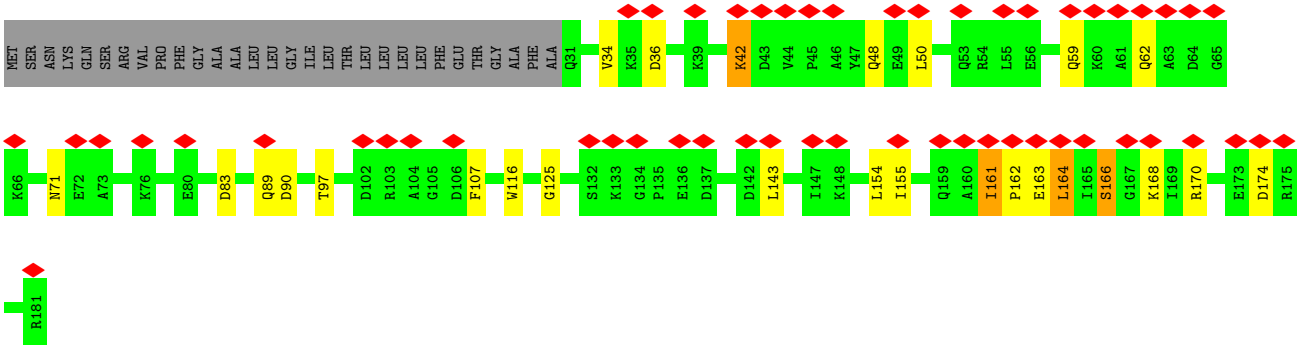
• Molecule 5: Photosystem I reaction center subunit IV





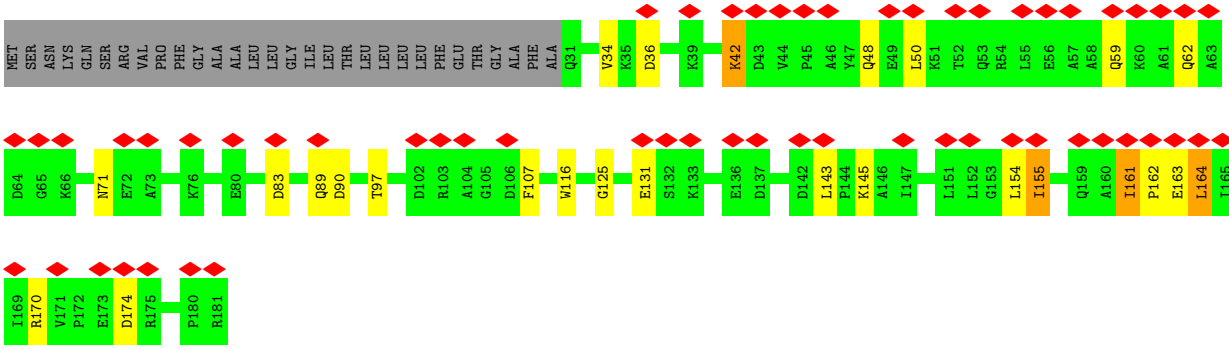
• Molecule 6: Photosystem I reaction center subunit III





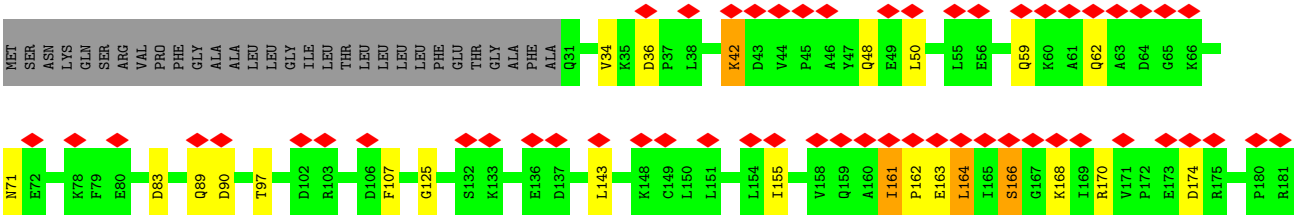
• Molecule 6: Photosystem I reaction center subunit III



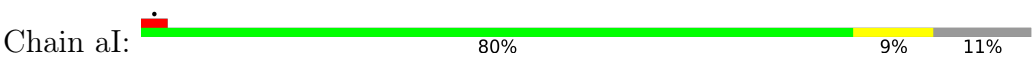


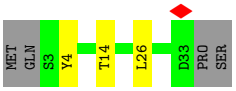
• Molecule 6: Photosystem I reaction center subunit III





• Molecule 7: Photosystem I reaction center subunit Z

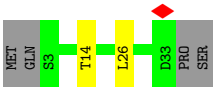




• Molecule 7: Photosystem I reaction center subunit Z

Chain bI:

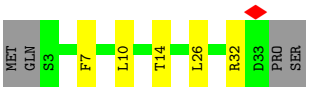




• Molecule 7: Photosystem I reaction center subunit Z

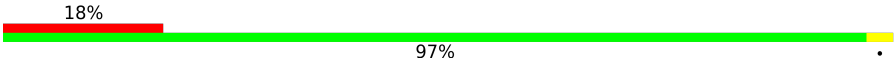
Chain cI:

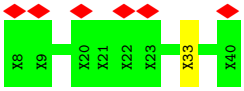




• Molecule 8: Unknown protein

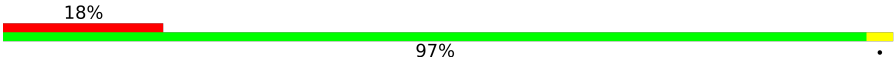
Chain aJ:

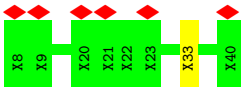




• Molecule 8: Unknown protein

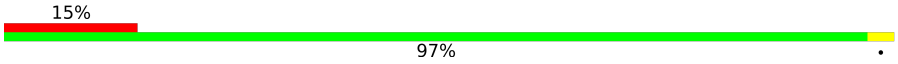
Chain bJ:

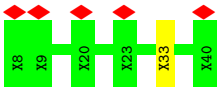




• Molecule 8: Unknown protein

Chain cJ:

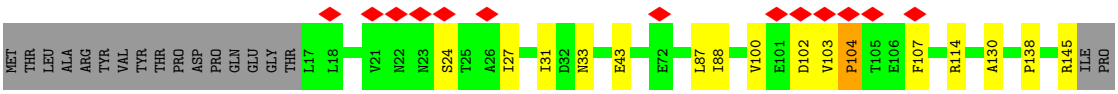




• Molecule 9: Photosystem I reaction center subunit XI

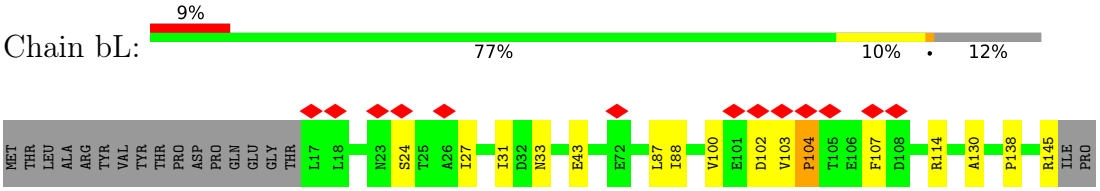
Chain aL:





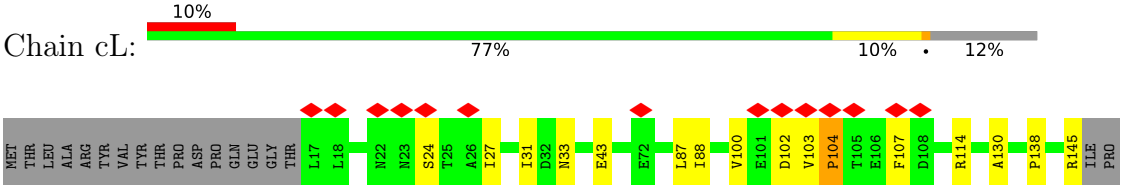
• Molecule 9: Photosystem I reaction center subunit XI

Chain bL:



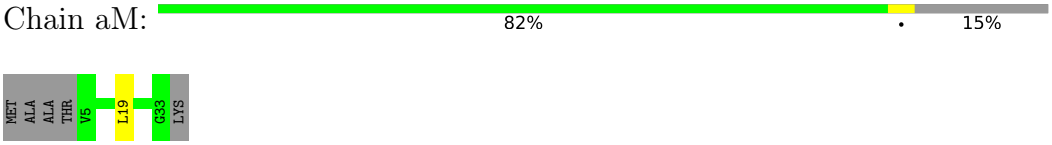
• Molecule 9: Photosystem I reaction center subunit XI

Chain cL:



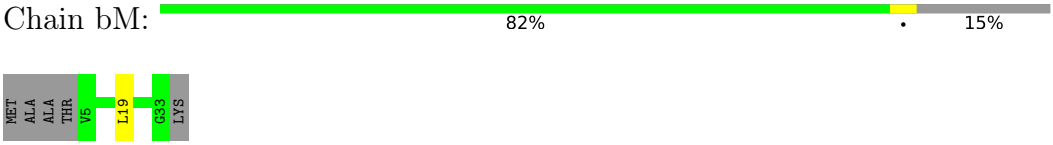
• Molecule 10: Photosystem I reaction center subunit XII

Chain aM:



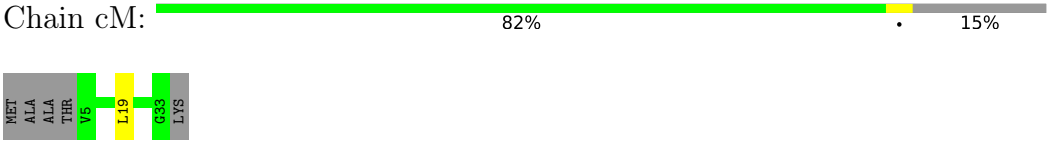
• Molecule 10: Photosystem I reaction center subunit XII

Chain bM:



• Molecule 10: Photosystem I reaction center subunit XII

Chain cM:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	261743	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70.22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.465	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	329.2, 329.2, 329.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.823, 0.823, 0.823	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SF4, 1L3, BCR, LMG, CL0, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	aA	0.31	0/6244	0.54	4/8520 (0.0%)
1	bA	0.31	0/6244	0.54	4/8520 (0.0%)
1	cA	0.31	0/6244	0.54	4/8520 (0.0%)
2	aB	0.32	0/5911	0.51	2/8084 (0.0%)
2	bB	0.32	0/5911	0.51	2/8084 (0.0%)
2	cB	0.32	0/5911	0.51	2/8084 (0.0%)
3	aC	0.30	0/609	0.61	2/825 (0.2%)
3	bC	0.31	0/609	0.61	2/825 (0.2%)
3	cC	0.30	0/609	0.61	2/825 (0.2%)
4	aD	0.26	0/1061	0.46	0/1434
4	bD	0.26	0/1061	0.46	0/1434
4	cD	0.26	0/1061	0.46	0/1434
5	aE	0.25	0/515	0.53	0/694
5	bE	0.26	0/515	0.53	0/694
5	cE	0.25	0/515	0.53	0/694
6	aF	0.26	0/1208	0.54	0/1638
6	bF	0.26	0/1208	0.53	0/1638
6	cF	0.26	0/1208	0.54	0/1638
7	aI	0.31	0/245	0.58	0/336
7	bI	0.32	0/245	0.58	0/336
7	cI	0.32	0/245	0.58	0/336
9	aL	0.32	0/997	0.63	0/1357
9	bL	0.32	0/997	0.63	0/1357
9	cL	0.32	0/997	0.63	0/1357
10	aM	0.29	0/190	0.43	0/260
10	bM	0.29	0/190	0.43	0/260
10	cM	0.28	0/190	0.44	0/260
All	All	0.31	0/50940	0.53	24/69444 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	aC	0	1
3	bC	0	1
3	cC	0	1
8	aJ	0	1
8	bJ	0	1
8	cJ	0	1
9	aL	0	1
9	bL	0	1
9	cL	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	aA	517	GLY	CA-C-N	9.84	139.41	121.70
1	aA	517	GLY	C-N-CA	9.84	139.41	121.70
1	cA	517	GLY	CA-C-N	9.83	139.39	121.70
1	cA	517	GLY	C-N-CA	9.83	139.39	121.70
1	bA	517	GLY	CA-C-N	9.82	139.38	121.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	aC	61	ASP	Peptide
8	aJ	33	UNK	Peptide
9	aL	104	PRO	Peptide
3	bC	61	ASP	Peptide
8	bJ	33	UNK	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	6038	0	5897	35	0
1	bA	6038	0	5897	34	0
1	cA	6038	0	5897	36	0
2	aB	5701	0	5519	38	0
2	bB	5701	0	5519	37	0
2	cB	5701	0	5519	39	0
3	aC	599	0	579	5	0
3	bC	599	0	579	4	0
3	cC	599	0	579	4	0
4	aD	1038	0	1039	15	0
4	bD	1038	0	1039	14	0
4	cD	1038	0	1039	14	0
5	aE	507	0	504	4	0
5	bE	507	0	504	4	0
5	cE	507	0	504	5	0
6	aF	1182	0	1207	11	0
6	bF	1182	0	1207	13	0
6	cF	1182	0	1207	10	0
7	aI	240	0	255	3	0
7	bI	240	0	255	2	0
7	cI	240	0	255	4	0
8	aJ	164	0	35	0	0
8	bJ	164	0	35	0	0
8	cJ	164	0	35	0	0
9	aL	974	0	998	9	0
9	bL	974	0	998	9	0
9	cL	974	0	998	9	0
10	aM	190	0	215	0	0
10	bM	190	0	215	0	0
10	cM	190	0	215	0	0
11	aA	65	0	72	0	0
11	bA	65	0	72	0	0
11	cA	65	0	72	0	0
12	aA	2396	0	2199	54	0
12	aB	2144	0	1874	46	0
12	aF	45	0	33	0	0
12	aL	143	0	111	3	0
12	bA	2351	0	2166	55	0
12	bB	2144	0	1874	44	0
12	bF	45	0	33	0	0
12	bL	143	0	111	3	0
12	cA	2351	0	2166	61	0
12	cB	2099	0	1841	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	cF	45	0	33	0	0
12	cL	143	0	111	3	0
13	aA	33	0	0	0	0
13	aB	33	0	0	0	0
13	bA	33	0	0	0	0
13	bB	33	0	0	1	0
13	cA	33	0	0	0	0
13	cB	33	0	0	0	0
14	aA	8	0	0	0	0
14	aC	16	0	0	0	0
14	bA	8	0	0	0	0
14	bC	16	0	0	0	0
14	cA	8	0	0	0	0
14	cC	16	0	0	0	0
15	aA	200	0	280	8	0
15	aB	240	0	336	11	0
15	aF	120	0	168	7	0
15	aI	40	0	56	2	0
15	aJ	40	0	56	1	0
15	aL	120	0	168	4	0
15	aM	40	0	55	0	0
15	bA	200	0	280	10	0
15	bB	240	0	336	12	0
15	bF	120	0	168	5	0
15	bI	40	0	56	2	0
15	bJ	40	0	56	1	0
15	bL	120	0	168	4	0
15	bM	40	0	55	0	0
15	cA	200	0	280	12	0
15	cB	240	0	336	9	0
15	cF	120	0	168	7	0
15	cI	40	0	56	1	0
15	cJ	40	0	56	0	0
15	cL	120	0	168	6	0
15	cM	40	0	55	0	0
16	aA	76	0	98	1	0
16	aB	23	0	16	0	0
16	bA	76	0	98	2	0
16	bB	23	0	16	0	0
16	cA	76	0	98	2	0
16	cB	23	0	16	0	0
17	aB	43	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bB	43	0	56	0	0
17	cB	43	0	56	0	0
18	aA	45	0	0	1	0
18	aB	67	0	0	1	0
18	aC	14	0	0	0	0
18	aD	2	0	0	0	0
18	aE	3	0	0	0	0
18	aF	1	0	0	0	0
18	aJ	1	0	0	0	0
18	aL	1	0	0	0	0
18	bA	45	0	0	1	0
18	bB	67	0	0	1	0
18	bC	14	0	0	0	0
18	bD	2	0	0	0	0
18	bE	3	0	0	0	0
18	bF	1	0	0	0	0
18	bJ	1	0	0	0	0
18	bL	1	0	0	0	0
18	cA	45	0	0	1	0
18	cB	67	0	0	1	0
18	cC	14	0	0	0	0
18	cD	2	0	0	0	0
18	cE	3	0	0	0	0
18	cF	1	0	0	0	0
18	cJ	1	0	0	0	0
18	cL	1	0	0	0	0
All	All	67641	0	65379	561	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 4.

The worst 5 of 561 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)
12:cA:809:CLA:HBB2	12:cA:828:CLA:H171	1.71	0.72
12:bA:809:CLA:HBB2	12:bA:828:CLA:H171	1.71	0.72
12:aA:809:CLA:HBB2	12:aA:828:CLA:H171	1.71	0.71
12:bA:818:CLA:HBA2	12:bA:827:CLA:HBB2	1.73	0.71
12:aA:818:CLA:HBA2	12:aA:827:CLA:HBB2	1.73	0.69

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
1	bA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
1	cA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
2	aB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
2	bB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
2	cB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
3	aC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	3
3	bC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	3
3	cC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	3
4	aD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
4	bD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
4	cD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
5	aE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
5	bE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
5	cE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
6	aF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
6	bF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
6	cF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
7	aI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	bI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	cI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
9	aL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	16	9
9	bL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	16	9
9	cL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	16	9
10	aM	27/34 (79%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	bM	27/34 (79%)	27 (100%)	0	0	100 100
10	cM	27/34 (79%)	27 (100%)	0	0	100 100
All	All	6282/7026 (89%)	6087 (97%)	189 (3%)	6 (0%)	49 43

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	aL	104	PRO
9	bL	104	PRO
9	cL	104	PRO
3	aC	62	PHE
3	bC	62	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	aA	612/623 (98%)	592 (97%)	20 (3%)	33 28
1	bA	612/623 (98%)	592 (97%)	20 (3%)	33 28
1	cA	612/623 (98%)	592 (97%)	20 (3%)	33 28
2	aB	573/694 (83%)	569 (99%)	4 (1%)	76 80
2	bB	573/694 (83%)	569 (99%)	4 (1%)	76 80
2	cB	573/694 (83%)	569 (99%)	4 (1%)	76 80
3	aC	68/69 (99%)	67 (98%)	1 (2%)	57 58
3	bC	68/69 (99%)	67 (98%)	1 (2%)	57 58
3	cC	68/69 (99%)	67 (98%)	1 (2%)	57 58
4	aD	113/122 (93%)	110 (97%)	3 (3%)	39 36
4	bD	113/122 (93%)	110 (97%)	3 (3%)	39 36
4	cD	113/122 (93%)	110 (97%)	3 (3%)	39 36
5	aE	56/57 (98%)	53 (95%)	3 (5%)	20 12
5	bE	56/57 (98%)	53 (95%)	3 (5%)	20 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	cE	56/57 (98%)	53 (95%)	3 (5%)	20 12
6	aF	125/148 (84%)	113 (90%)	12 (10%)	8 3
6	bF	125/148 (84%)	113 (90%)	12 (10%)	8 3
6	cF	125/148 (84%)	113 (90%)	12 (10%)	8 3
7	aI	26/30 (87%)	25 (96%)	1 (4%)	29 24
7	bI	26/30 (87%)	25 (96%)	1 (4%)	29 24
7	cI	26/30 (87%)	25 (96%)	1 (4%)	29 24
9	aL	100/116 (86%)	98 (98%)	2 (2%)	48 48
9	bL	100/116 (86%)	98 (98%)	2 (2%)	48 48
9	cL	100/116 (86%)	98 (98%)	2 (2%)	48 48
10	aM	18/21 (86%)	17 (94%)	1 (6%)	19 12
10	bM	18/21 (86%)	17 (94%)	1 (6%)	19 12
10	cM	18/21 (86%)	17 (94%)	1 (6%)	19 12
All	All	5073/5640 (90%)	4932 (97%)	141 (3%)	38 34

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	cB	294	ASP
4	cD	42	GLU
6	cF	83	ASP
1	bA	30	LYS
1	bA	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	bB	349	GLN
6	cF	62	GLN
6	bF	62	GLN
4	cD	76	GLN
2	cB	389	ASN

5.3.3 RNA

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)

354 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	bA	828	1	69,73,73	1.97	20 (28%)	83,113,113	2.80	30 (36%)
15	BCR	bL	206	-	41,41,41	1.03	1 (2%)	56,56,56	1.19	5 (8%)
15	BCR	bA	848	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
12	CLA	aA	835	1	49,53,73	2.33	19 (38%)	59,89,113	3.01	27 (45%)
12	CLA	aB	917	2	59,63,73	2.09	19 (32%)	71,101,113	2.92	30 (42%)
12	CLA	aB	903	2	55,59,73	2.18	20 (36%)	66,96,113	3.09	30 (45%)
15	BCR	aF	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	7 (12%)
15	BCR	cA	848	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
12	CLA	cA	825	18	69,73,73	2.01	20 (28%)	83,113,113	2.77	31 (37%)
12	CLA	bA	841	18	55,59,73	2.23	21 (38%)	66,96,113	3.07	26 (39%)
12	CLA	bA	802	18	69,73,73	1.92	18 (26%)	83,113,113	2.75	28 (33%)
15	BCR	bF	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	7 (12%)
12	CLA	aA	814	1	49,53,73	2.32	19 (38%)	59,89,113	3.11	27 (45%)
15	BCR	aA	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.39	6 (10%)
12	CLA	bA	810	1	49,53,73	2.35	19 (38%)	59,89,113	3.31	28 (47%)
12	CLA	bB	905	2	69,73,73	1.94	20 (28%)	83,113,113	2.75	29 (34%)
12	CLA	cA	805	1	57,61,73	2.18	22 (38%)	68,98,113	3.13	28 (41%)
12	CLA	aA	844	16	49,53,73	2.33	20 (40%)	59,89,113	3.02	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cA	827	1	50,54,73	2.26	20 (40%)	60,90,113	3.24	27 (45%)
12	CLA	cB	913	2	60,64,73	2.09	20 (33%)	72,102,113	2.95	32 (44%)
12	CLA	bB	932	2	49,53,73	2.33	18 (36%)	59,89,113	3.29	29 (49%)
12	CLA	bA	805	1	57,61,73	2.18	22 (38%)	68,98,113	3.13	28 (41%)
12	CLA	bA	824	1	51,55,73	2.30	21 (41%)	61,91,113	3.09	28 (45%)
12	CLA	aA	842	1	69,73,73	1.96	19 (27%)	83,113,113	2.79	30 (36%)
12	CLA	aB	932	2	49,53,73	2.33	18 (36%)	59,89,113	3.31	29 (49%)
12	CLA	cB	924	18	50,54,73	2.29	21 (42%)	60,90,113	3.24	27 (45%)
12	CLA	cB	904	2	69,73,73	1.96	21 (30%)	83,113,113	2.92	33 (39%)
12	CLA	cA	834	1	69,73,73	1.96	20 (28%)	83,113,113	2.89	30 (36%)
15	BCR	aF	204	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	9 (16%)
12	CLA	bA	842	1	69,73,73	1.95	19 (27%)	83,113,113	2.79	30 (36%)
12	CLA	cB	909	2	59,63,73	2.09	20 (33%)	71,101,113	2.83	32 (45%)
17	LMG	bB	947	-	43,43,55	0.95	1 (2%)	51,51,63	1.25	6 (11%)
12	CLA	aA	832	1	59,63,73	2.14	20 (33%)	71,101,113	3.00	32 (45%)
12	CLA	aA	840	1	69,73,73	1.99	19 (27%)	83,113,113	2.67	30 (36%)
14	SF4	cA	845	1,2	0,12,12	-	-	-		
12	CLA	bB	921	2	59,63,73	2.17	20 (33%)	71,101,113	3.04	27 (38%)
12	CLA	cA	816	1	49,53,73	2.35	21 (42%)	59,89,113	3.17	25 (42%)
12	CLA	cA	843	18	69,73,73	1.93	20 (28%)	83,113,113	2.82	34 (40%)
12	CLA	bA	835	1	49,53,73	2.34	20 (40%)	59,89,113	3.01	27 (45%)
12	CLA	bA	853	18	60,64,73	2.04	20 (33%)	72,102,113	3.05	29 (40%)
12	CLA	bB	918	18	50,54,73	2.32	19 (38%)	60,90,113	2.98	27 (45%)
16	LHG	aB	948	12	22,22,48	1.05	1 (4%)	25,28,54	1.10	1 (4%)
12	CLA	aA	824	1	51,55,73	2.29	21 (41%)	61,91,113	3.09	30 (49%)
15	BCR	cL	201	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	4 (7%)
12	CLA	aA	839	1	49,53,73	2.28	20 (40%)	59,89,113	3.25	27 (45%)
12	CLA	bA	806	1	69,73,73	1.93	20 (28%)	83,113,113	2.89	28 (33%)
12	CLA	cB	918	18	50,54,73	2.33	19 (38%)	60,90,113	2.99	26 (43%)
12	CLA	bB	922	2	49,53,73	2.30	20 (40%)	59,89,113	3.09	28 (47%)
12	CLA	cA	821	18	54,58,73	2.23	18 (33%)	65,95,113	2.92	28 (43%)
12	CLA	cB	921	2	59,63,73	2.17	20 (33%)	71,101,113	3.04	27 (38%)
12	CLA	aB	950	16	49,53,73	2.33	20 (40%)	59,89,113	3.01	23 (38%)
12	CLA	bA	815	1	49,53,73	2.39	19 (38%)	59,89,113	3.20	26 (44%)
12	CLA	cA	840	1	69,73,73	1.98	19 (27%)	83,113,113	2.67	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cA	842	1	69,73,73	1.96	19 (27%)	83,113,113	2.80	30 (36%)
14	SF4	bC	101	3	0,12,12	-	-	-		
12	CLA	cB	936	2	63,67,73	2.05	21 (33%)	75,105,113	2.94	32 (42%)
12	CLA	bB	912	2	69,73,73	1.90	21 (30%)	83,113,113	2.68	29 (34%)
12	CLA	cA	833	1	55,59,73	2.14	18 (32%)	66,96,113	3.05	33 (50%)
12	CLA	bA	813	1	49,53,73	2.42	21 (42%)	59,89,113	3.09	26 (44%)
12	CLA	aB	937	2	51,55,73	2.27	22 (43%)	61,91,113	3.24	27 (44%)
12	CLA	cA	836	1	49,53,73	2.39	19 (38%)	59,89,113	3.09	29 (49%)
12	CLA	cB	912	2	69,73,73	1.91	21 (30%)	83,113,113	2.68	29 (34%)
12	CLA	bB	917	2	59,63,73	2.09	19 (32%)	71,101,113	2.92	30 (42%)
12	CLA	cA	807	1	69,73,73	1.97	20 (28%)	83,113,113	2.82	34 (40%)
12	CLA	aA	818	1	58,62,73	2.11	19 (32%)	69,99,113	3.01	29 (42%)
12	CLA	aB	927	2	69,73,73	1.97	19 (27%)	83,113,113	2.46	25 (30%)
12	CLA	aB	939	2	49,53,73	2.26	18 (36%)	59,89,113	3.28	27 (45%)
12	CLA	bB	929	2	49,53,73	2.33	20 (40%)	59,89,113	3.33	27 (45%)
12	CLA	bA	820	1	60,64,73	2.13	21 (35%)	72,102,113	2.93	31 (43%)
12	CLA	bA	811	1	49,53,73	2.37	19 (38%)	59,89,113	3.17	27 (45%)
14	SF4	cC	101	3	0,12,12	-	-	-		
16	LHG	cA	851	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
12	CLA	bA	823	1	55,59,73	2.20	20 (36%)	66,96,113	3.11	30 (45%)
15	BCR	cA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	8 (14%)
14	SF4	aC	101	3	0,12,12	-	-	-		
14	SF4	aA	846	1,2	0,12,12	-	-	-		
12	CLA	cA	809	1	49,53,73	2.32	20 (40%)	59,89,113	3.28	29 (49%)
12	CLA	aA	828	1	69,73,73	1.98	20 (28%)	83,113,113	2.80	30 (36%)
15	BCR	cB	944	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	7 (12%)
13	1L3	cA	844	-	34,34,34	2.31	9 (26%)	42,45,45	1.62	9 (21%)
12	CLA	aA	836	1	49,53,73	2.38	19 (38%)	59,89,113	3.08	29 (49%)
12	CLA	aB	923	18	58,62,73	2.07	19 (32%)	69,99,113	2.97	27 (39%)
12	CLA	bB	907	2	56,60,73	2.13	19 (33%)	67,97,113	3.01	31 (46%)
12	CLA	aA	838	1	69,73,73	1.94	19 (27%)	83,113,113	2.80	28 (33%)
12	CLA	aA	826	18	59,63,73	2.10	20 (33%)	71,101,113	3.07	28 (39%)
15	BCR	cA	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	7 (12%)
12	CLA	bB	935	2	54,58,73	2.21	20 (37%)	65,95,113	3.14	31 (47%)
12	CLA	aA	803	-	69,73,73	1.92	20 (28%)	83,113,113	2.77	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CL0	aA	801	1	69,73,73	1.93	20 (28%)	83,113,113	2.65	35 (42%)
12	CLA	bA	839	1	49,53,73	2.28	20 (40%)	59,89,113	3.25	27 (45%)
12	CLA	bB	909	2	59,63,73	2.09	21 (35%)	71,101,113	2.83	32 (45%)
12	CLA	aL	203	9	49,53,73	2.32	21 (42%)	59,89,113	3.27	25 (42%)
16	LHG	bB	948	12	22,22,48	1.06	1 (4%)	25,28,54	1.10	1 (4%)
12	CLA	bA	840	1	69,73,73	1.99	19 (27%)	83,113,113	2.68	29 (34%)
15	BCR	aL	206	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
12	CLA	cB	917	2	59,63,73	2.08	19 (32%)	71,101,113	2.92	30 (42%)
12	CLA	cF	202	6	49,53,73	2.37	21 (42%)	59,89,113	3.22	28 (47%)
12	CLA	aA	816	1	49,53,73	2.36	21 (42%)	59,89,113	3.17	25 (42%)
12	CLA	aB	925	2	59,63,73	2.08	18 (30%)	71,101,113	3.12	32 (45%)
12	CLA	cL	204	18	49,53,73	2.36	21 (42%)	59,89,113	3.24	26 (44%)
12	CLA	bA	829	1	64,68,73	2.00	19 (29%)	77,107,113	2.77	30 (38%)
16	LHG	cA	852	12	26,26,48	0.94	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	cA	812	1	69,73,73	1.94	20 (28%)	83,113,113	2.77	32 (38%)
15	BCR	cB	945	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	7 (12%)
12	CLA	aB	908	2	52,56,73	2.23	17 (32%)	62,92,113	2.80	27 (43%)
12	CLA	aB	901	2	69,73,73	1.89	18 (26%)	83,113,113	2.79	31 (37%)
15	BCR	bB	943	-	41,41,41	1.07	2 (4%)	56,56,56	1.16	4 (7%)
12	CLA	bA	834	1	69,73,73	1.95	20 (28%)	83,113,113	2.89	32 (38%)
12	CLA	bB	927	2	69,73,73	1.97	20 (28%)	83,113,113	2.46	25 (30%)
12	CLA	bA	830	1	69,73,73	1.93	19 (27%)	83,113,113	2.66	28 (33%)
12	CLA	cB	937	2	51,55,73	2.27	22 (43%)	61,91,113	3.25	27 (44%)
12	CLA	bB	914	2	49,53,73	2.32	20 (40%)	59,89,113	3.35	26 (44%)
12	CLA	cA	819	1	64,68,73	2.04	19 (29%)	77,107,113	3.01	35 (45%)
12	CLA	bB	930	2	53,57,73	2.27	20 (37%)	62,93,113	3.17	29 (46%)
12	CLA	aB	921	2	59,63,73	2.17	20 (33%)	71,101,113	3.04	27 (38%)
15	BCR	cL	206	-	41,41,41	1.03	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	cA	835	1	49,53,73	2.34	20 (40%)	59,89,113	3.01	27 (45%)
12	CLA	bA	808	1	55,59,73	2.25	21 (38%)	66,96,113	3.07	31 (46%)
12	CLA	aB	913	2	60,64,73	2.08	20 (33%)	72,102,113	2.95	31 (43%)
12	CLA	cA	818	1	58,62,73	2.10	19 (32%)	69,99,113	3.02	30 (43%)
12	CLA	aA	831	1	54,58,73	2.20	19 (35%)	65,95,113	3.04	34 (52%)
15	BCR	aJ	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	aB	912	2	69,73,73	1.91	21 (30%)	83,113,113	2.68	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aB	922	2	49,53,73	2.31	19 (38%)	59,89,113	3.10	28 (47%)
12	CLA	aB	926	2	69,73,73	1.91	20 (28%)	83,113,113	2.71	31 (37%)
12	CLA	bA	818	1	58,62,73	2.10	19 (32%)	69,99,113	3.01	30 (43%)
12	CLA	bA	832	1	59,63,73	2.13	20 (33%)	71,101,113	3.00	32 (45%)
12	CLA	cA	815	1	49,53,73	2.38	20 (40%)	59,89,113	3.19	26 (44%)
12	CLA	cB	922	2	49,53,73	2.31	19 (38%)	59,89,113	3.09	29 (49%)
12	CLA	bB	916	2	63,67,73	2.05	18 (28%)	75,105,113	2.97	30 (40%)
12	CLA	aB	929	2	49,53,73	2.34	20 (40%)	59,89,113	3.33	27 (45%)
12	CLA	bB	913	2	60,64,73	2.08	20 (33%)	72,102,113	2.94	31 (43%)
12	CLA	bA	817	1	58,62,73	2.19	19 (32%)	69,99,113	3.10	27 (39%)
15	BCR	cL	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
15	BCR	aA	851	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	8 (14%)
15	BCR	aL	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
15	BCR	bB	946	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
16	LHG	bA	851	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
12	CLA	aA	827	1	50,54,73	2.26	19 (38%)	60,90,113	3.23	27 (45%)
12	CLA	bB	910	2	49,53,73	2.36	19 (38%)	59,89,113	3.15	28 (47%)
15	BCR	cI	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
12	CLA	aL	202	9	57,61,73	2.17	21 (36%)	68,98,113	3.11	29 (42%)
12	CLA	bB	906	2	59,63,73	2.13	21 (35%)	71,101,113	2.96	30 (42%)
12	CLA	cL	203	9	49,53,73	2.32	22 (44%)	59,89,113	3.27	25 (42%)
13	1L3	bA	844	-	34,34,34	2.31	9 (26%)	42,45,45	1.61	9 (21%)
15	BCR	cA	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.51	13 (23%)
15	BCR	aB	943	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
12	CLA	aB	911	2	49,53,73	2.34	19 (38%)	59,89,113	3.16	29 (49%)
17	LMG	aB	947	-	43,43,55	0.95	1 (2%)	51,51,63	1.25	6 (11%)
15	BCR	cB	941	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	5 (8%)
12	CLA	bA	838	1	69,73,73	1.93	19 (27%)	83,113,113	2.80	28 (33%)
12	CLA	bA	803	-	69,73,73	1.93	20 (28%)	83,113,113	2.78	33 (39%)
12	CLA	aB	930	2	53,57,73	2.27	20 (37%)	62,93,113	3.18	29 (46%)
12	CLA	bA	822	1	53,57,73	2.29	20 (37%)	62,93,113	3.30	26 (41%)
12	CLA	aB	924	18	50,54,73	2.28	21 (42%)	60,90,113	3.23	27 (45%)
12	CLA	bA	812	1	69,73,73	1.95	21 (30%)	83,113,113	2.77	32 (38%)
12	CLA	bB	919	2	51,55,73	2.26	19 (37%)	61,91,113	3.16	28 (45%)
12	CLA	aB	915	2	56,60,73	2.20	19 (33%)	67,97,113	3.17	27 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aB	931	2	69,73,73	1.94	19 (27%)	83,113,113	2.98	32 (38%)
12	CLA	aB	910	2	49,53,73	2.35	19 (38%)	59,89,113	3.13	28 (47%)
12	CLA	cB	925	2	59,63,73	2.08	19 (32%)	71,101,113	3.11	32 (45%)
11	CL0	bA	801	1	69,73,73	1.93	20 (28%)	83,113,113	2.65	34 (40%)
12	CLA	cB	919	2	51,55,73	2.26	18 (35%)	61,91,113	3.17	28 (45%)
12	CLA	cB	923	18	58,62,73	2.07	19 (32%)	69,99,113	2.97	27 (39%)
15	BCR	cF	201	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
12	CLA	cB	901	2	69,73,73	1.88	18 (26%)	83,113,113	2.80	31 (37%)
12	CLA	cA	839	1	49,53,73	2.28	20 (40%)	59,89,113	3.26	27 (45%)
12	CLA	aB	909	2	59,63,73	2.09	20 (33%)	71,101,113	2.83	32 (45%)
12	CLA	aB	933	18	49,53,73	2.27	19 (38%)	59,89,113	3.06	27 (45%)
12	CLA	cB	905	2	69,73,73	1.94	20 (28%)	83,113,113	2.75	29 (34%)
12	CLA	cB	934	2	49,53,73	2.46	19 (38%)	59,89,113	3.04	25 (42%)
12	CLA	cL	202	9	57,61,73	2.18	21 (36%)	68,98,113	3.11	29 (42%)
15	BCR	aM	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.16	6 (10%)
12	CLA	bA	816	1	49,53,73	2.36	21 (42%)	59,89,113	3.17	25 (42%)
12	CLA	cA	828	1	69,73,73	1.97	20 (28%)	83,113,113	2.80	30 (36%)
15	BCR	bB	942	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	3 (5%)
16	LHG	aA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
14	SF4	bC	102	3	0,12,12	-	-	-		
12	CLA	bL	203	9	49,53,73	2.32	20 (40%)	59,89,113	3.26	24 (40%)
12	CLA	cB	939	2	49,53,73	2.26	18 (36%)	59,89,113	3.26	27 (45%)
12	CLA	bB	936	2	63,67,73	2.05	21 (33%)	75,105,113	2.93	31 (41%)
15	BCR	bA	846	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	cA	826	18	59,63,73	2.09	20 (33%)	71,101,113	3.07	28 (39%)
15	BCR	bF	204	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	9 (16%)
12	CLA	bB	925	2	59,63,73	2.09	18 (30%)	71,101,113	3.11	32 (45%)
12	CLA	bA	825	18	69,73,73	2.01	20 (28%)	83,113,113	2.78	31 (37%)
15	BCR	aA	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.51	13 (23%)
12	CLA	aB	935	2	54,58,73	2.21	20 (37%)	65,95,113	3.15	31 (47%)
12	CLA	cB	907	2	56,60,73	2.14	19 (33%)	67,97,113	3.01	31 (46%)
12	CLA	cA	829	1	64,68,73	2.00	19 (29%)	77,107,113	2.77	31 (40%)
12	CLA	aB	918	18	50,54,73	2.33	19 (38%)	60,90,113	2.99	26 (43%)
12	CLA	bA	804	1	60,64,73	2.09	19 (31%)	72,102,113	2.94	29 (40%)
12	CLA	aF	202	6	49,53,73	2.37	20 (40%)	59,89,113	3.22	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	bB	950	16	49,53,73	2.33	20 (40%)	59,89,113	3.02	23 (38%)
12	CLA	cB	916	2	63,67,73	2.04	18 (28%)	75,105,113	2.97	30 (40%)
12	CLA	bB	928	2	54,58,73	2.22	20 (37%)	65,95,113	2.91	30 (46%)
12	CLA	bA	807	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	34 (40%)
15	BCR	cF	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	aL	204	18	49,53,73	2.35	21 (42%)	59,89,113	3.23	26 (44%)
12	CLA	cA	831	1	54,58,73	2.20	19 (35%)	65,95,113	3.03	34 (52%)
12	CLA	bA	837	1	55,59,73	2.18	20 (36%)	66,96,113	3.07	29 (43%)
15	BCR	bA	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.51	13 (23%)
12	CLA	aA	812	1	69,73,73	1.94	21 (30%)	83,113,113	2.78	32 (38%)
12	CLA	bA	831	1	54,58,73	2.21	19 (35%)	65,95,113	3.04	34 (52%)
12	CLA	aA	810	1	49,53,73	2.35	20 (40%)	59,89,113	3.31	28 (47%)
12	CLA	cB	906	2	59,63,73	2.13	21 (35%)	71,101,113	2.95	30 (42%)
12	CLA	aA	837	1	55,59,73	2.19	20 (36%)	66,96,113	3.08	28 (42%)
12	CLA	cB	932	2	49,53,73	2.33	18 (36%)	59,89,113	3.30	29 (49%)
12	CLA	bB	938	18	55,59,73	2.20	19 (34%)	66,96,113	2.95	30 (45%)
15	BCR	bI	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	9 (16%)
15	BCR	aI	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.39	9 (16%)
12	CLA	aB	916	2	63,67,73	2.05	18 (28%)	75,105,113	2.97	30 (40%)
12	CLA	bA	814	1	49,53,73	2.32	19 (38%)	59,89,113	3.10	27 (45%)
15	BCR	bJ	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	bB	902	-	65,69,73	1.95	20 (30%)	78,108,113	2.82	26 (33%)
15	BCR	aA	849	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
12	CLA	cA	823	1	55,59,73	2.19	20 (36%)	66,96,113	3.11	30 (45%)
12	CLA	aA	841	18	55,59,73	2.22	21 (38%)	66,96,113	3.07	26 (39%)
12	CLA	bL	204	18	49,53,73	2.36	21 (42%)	59,89,113	3.24	26 (44%)
15	BCR	aB	946	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
12	CLA	aA	813	1	49,53,73	2.41	21 (42%)	59,89,113	3.10	26 (44%)
15	BCR	bA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	8 (14%)
13	1L3	aA	845	-	34,34,34	2.31	9 (26%)	42,45,45	1.61	10 (23%)
12	CLA	aB	919	2	51,55,73	2.26	19 (37%)	61,91,113	3.16	28 (45%)
12	CLA	aA	829	1	64,68,73	2.00	19 (29%)	77,107,113	2.77	30 (38%)
12	CLA	aA	807	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	34 (40%)
12	CLA	aB	906	2	59,63,73	2.13	20 (33%)	71,101,113	2.95	30 (42%)
15	BCR	bF	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aA	833	1	55,59,73	2.14	18 (32%)	66,96,113	3.06	33 (50%)
15	BCR	aA	847	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	cB	910	2	49,53,73	2.36	18 (36%)	59,89,113	3.14	28 (47%)
12	CLA	cB	908	2	52,56,73	2.22	17 (32%)	62,92,113	2.80	27 (43%)
15	BCR	cF	204	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	9 (16%)
12	CLA	bB	933	18	49,53,73	2.28	19 (38%)	59,89,113	3.07	27 (45%)
15	BCR	bB	941	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	5 (8%)
12	CLA	bB	911	2	49,53,73	2.34	19 (38%)	59,89,113	3.16	29 (49%)
14	SF4	aC	102	3	0,12,12	-	-	-		
12	CLA	cB	938	18	55,59,73	2.20	19 (34%)	66,96,113	2.94	30 (45%)
12	CLA	cA	820	1	60,64,73	2.13	21 (35%)	72,102,113	2.93	31 (43%)
16	LHG	cB	948	12	22,22,48	1.05	1 (4%)	25,28,54	1.10	1 (4%)
12	CLA	aA	815	1	49,53,73	2.39	19 (38%)	59,89,113	3.20	26 (44%)
12	CLA	cA	830	1	69,73,73	1.93	19 (27%)	83,113,113	2.66	28 (33%)
15	BCR	bM	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	6 (10%)
13	1L3	cB	940	-	34,34,34	2.30	9 (26%)	42,45,45	1.44	7 (16%)
12	CLA	cA	838	1	69,73,73	1.94	19 (27%)	83,113,113	2.80	28 (33%)
12	CLA	bB	924	18	50,54,73	2.29	21 (42%)	60,90,113	3.23	27 (45%)
12	CLA	bB	939	2	49,53,73	2.26	18 (36%)	59,89,113	3.27	27 (45%)
12	CLA	bB	931	2	69,73,73	1.94	19 (27%)	83,113,113	2.97	32 (38%)
12	CLA	cA	803	-	69,73,73	1.93	20 (28%)	83,113,113	2.78	33 (39%)
12	CLA	aA	822	1	53,57,73	2.29	20 (37%)	62,93,113	3.31	27 (43%)
12	CLA	cA	841	18	55,59,73	2.22	21 (38%)	66,96,113	3.07	26 (39%)
12	CLA	cA	813	1	49,53,73	2.41	21 (42%)	59,89,113	3.10	26 (44%)
12	CLA	cB	935	2	54,58,73	2.21	20 (37%)	65,95,113	3.15	31 (47%)
12	CLA	aB	938	18	55,59,73	2.20	19 (34%)	66,96,113	2.96	30 (45%)
12	CLA	aA	820	1	60,64,73	2.13	21 (35%)	72,102,113	2.94	31 (43%)
15	BCR	aB	942	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	3 (5%)
12	CLA	bB	904	2	69,73,73	1.96	21 (30%)	83,113,113	2.92	33 (39%)
16	LHG	bA	852	12	26,26,48	0.94	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	aB	902	-	65,69,73	1.96	19 (29%)	78,108,113	2.82	26 (33%)
12	CLA	cA	832	1	59,63,73	2.14	20 (33%)	71,101,113	3.00	31 (43%)
12	CLA	cB	902	-	65,69,73	1.95	19 (29%)	78,108,113	2.82	26 (33%)
12	CLA	cA	817	1	58,62,73	2.19	19 (32%)	69,99,113	3.12	27 (39%)
12	CLA	aB	920	2	49,53,73	2.35	19 (38%)	59,89,113	3.33	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	bB	926	2	69,73,73	1.90	20 (28%)	83,113,113	2.71	32 (38%)
14	SF4	cC	102	3	0,12,12	-	-	-		
13	1L3	aB	940	-	34,34,34	2.31	9 (26%)	42,45,45	1.43	6 (14%)
12	CLA	bA	836	1	49,53,73	2.38	19 (38%)	59,89,113	3.08	29 (49%)
12	CLA	aA	809	1	49,53,73	2.32	20 (40%)	59,89,113	3.28	29 (49%)
11	CL0	cA	801	1	69,73,73	1.92	20 (28%)	83,113,113	2.64	35 (42%)
12	CLA	aB	928	2	54,58,73	2.22	20 (37%)	65,95,113	2.91	29 (44%)
12	CLA	bB	903	2	55,59,73	2.19	20 (36%)	66,96,113	3.08	30 (45%)
12	CLA	cB	903	2	55,59,73	2.19	20 (36%)	66,96,113	3.08	30 (45%)
12	CLA	bB	920	2	49,53,73	2.35	19 (38%)	59,89,113	3.33	25 (42%)
12	CLA	bL	202	9	57,61,73	2.17	21 (36%)	68,98,113	3.10	29 (42%)
15	BCR	aB	945	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	7 (12%)
15	BCR	bL	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	6 (10%)
15	BCR	cB	946	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
12	CLA	aB	936	2	63,67,73	2.05	21 (33%)	75,105,113	2.93	32 (42%)
15	BCR	cA	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.39	6 (10%)
12	CLA	aA	805	1	57,61,73	2.18	22 (38%)	68,98,113	3.13	29 (42%)
12	CLA	cB	930	2	53,57,73	2.27	20 (37%)	62,93,113	3.18	29 (46%)
14	SF4	bA	845	1,2	0,12,12	-	-	-		
15	BCR	aB	941	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	5 (8%)
15	BCR	bA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	6 (10%)
12	CLA	bF	202	6	49,53,73	2.37	20 (40%)	59,89,113	3.22	28 (47%)
12	CLA	cB	915	2	56,60,73	2.19	19 (33%)	67,97,113	3.16	27 (40%)
12	CLA	cA	814	1	49,53,73	2.32	20 (40%)	59,89,113	3.10	27 (45%)
15	BCR	bB	944	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	7 (12%)
12	CLA	aB	905	2	69,73,73	1.94	20 (28%)	83,113,113	2.75	29 (34%)
12	CLA	aB	934	2	49,53,73	2.46	19 (38%)	59,89,113	3.05	25 (42%)
13	1L3	bB	940	-	34,34,34	2.31	9 (26%)	42,45,45	1.43	7 (16%)
12	CLA	cA	806	1	69,73,73	1.93	20 (28%)	83,113,113	2.89	28 (33%)
12	CLA	aA	834	1	69,73,73	1.96	20 (28%)	83,113,113	2.89	31 (37%)
12	CLA	bA	833	1	55,59,73	2.14	18 (32%)	66,96,113	3.06	33 (50%)
12	CLA	bB	937	2	51,55,73	2.28	22 (43%)	61,91,113	3.25	27 (44%)
12	CLA	cA	853	18	60,64,73	2.04	20 (33%)	72,102,113	3.04	29 (40%)
12	CLA	aA	854	18	60,64,73	2.04	20 (33%)	72,102,113	3.05	29 (40%)
12	CLA	aA	830	1	69,73,73	1.92	19 (27%)	83,113,113	2.66	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aA	843	18	69,73,73	1.93	20 (28%)	83,113,113	2.82	34 (40%)
12	CLA	aA	804	1	60,64,73	2.09	19 (31%)	72,102,113	2.94	29 (40%)
12	CLA	aB	949	16	45,49,73	2.50	18 (40%)	54,84,113	3.48	29 (53%)
12	CLA	bB	949	16	45,49,73	2.50	19 (42%)	54,84,113	3.50	29 (53%)
12	CLA	cA	822	1	53,57,73	2.29	20 (37%)	62,93,113	3.29	27 (43%)
12	CLA	aB	904	2	69,73,73	1.96	21 (30%)	83,113,113	2.92	33 (39%)
15	BCR	bL	201	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	4 (7%)
15	BCR	cM	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	6 (10%)
12	CLA	aA	821	18	54,58,73	2.22	19 (35%)	65,95,113	2.92	28 (43%)
12	CLA	cB	926	2	69,73,73	1.91	20 (28%)	83,113,113	2.71	32 (38%)
15	BCR	aL	201	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	4 (7%)
12	CLA	aA	802	18	69,73,73	1.93	19 (27%)	83,113,113	2.76	28 (33%)
12	CLA	bA	826	18	59,63,73	2.09	20 (33%)	71,101,113	3.07	28 (39%)
12	CLA	aB	914	2	49,53,73	2.32	20 (40%)	59,89,113	3.33	26 (44%)
12	CLA	bA	827	1	50,54,73	2.26	20 (40%)	60,90,113	3.22	27 (45%)
12	CLA	cA	810	1	49,53,73	2.35	20 (40%)	59,89,113	3.30	28 (47%)
12	CLA	cA	804	1	60,64,73	2.10	20 (33%)	72,102,113	2.94	29 (40%)
12	CLA	aA	817	1	58,62,73	2.19	19 (32%)	69,99,113	3.10	27 (39%)
12	CLA	aA	825	18	69,73,73	2.01	20 (28%)	83,113,113	2.77	31 (37%)
12	CLA	cA	837	1	55,59,73	2.18	20 (36%)	66,96,113	3.08	29 (43%)
12	CLA	cB	928	2	54,58,73	2.22	20 (37%)	65,95,113	2.91	30 (46%)
12	CLA	cB	927	2	69,73,73	1.97	20 (28%)	83,113,113	2.46	25 (30%)
12	CLA	aA	808	1	55,59,73	2.25	21 (38%)	66,96,113	3.06	31 (46%)
12	CLA	aB	907	2	56,60,73	2.13	19 (33%)	67,97,113	3.00	31 (46%)
16	LHG	aA	853	12	26,26,48	0.94	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	bA	821	18	54,58,73	2.22	18 (33%)	65,95,113	2.91	28 (43%)
12	CLA	bA	809	1	49,53,73	2.32	20 (40%)	59,89,113	3.28	29 (49%)
12	CLA	cB	911	2	49,53,73	2.34	19 (38%)	59,89,113	3.16	29 (49%)
15	BCR	cB	943	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	4 (7%)
12	CLA	bB	908	2	52,56,73	2.22	17 (32%)	62,92,113	2.80	27 (43%)
12	CLA	cB	931	2	69,73,73	1.94	19 (27%)	83,113,113	2.97	32 (38%)
12	CLA	bB	915	2	56,60,73	2.20	19 (33%)	67,97,113	3.16	27 (40%)
12	CLA	bB	901	2	69,73,73	1.88	18 (26%)	83,113,113	2.80	31 (37%)
12	CLA	cB	933	18	49,53,73	2.27	20 (40%)	59,89,113	3.05	27 (45%)
12	CLA	bA	819	1	64,68,73	2.03	19 (29%)	77,107,113	3.02	34 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cB	949	16	45,49,73	2.50	18 (40%)	54,84,113	3.48	29 (53%)
15	BCR	bB	945	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	7 (12%)
12	CLA	aA	806	1	69,73,73	1.93	20 (28%)	83,113,113	2.90	28 (33%)
12	CLA	aA	819	1	64,68,73	2.04	19 (29%)	77,107,113	3.01	35 (45%)
12	CLA	cA	811	1	49,53,73	2.37	19 (38%)	59,89,113	3.17	27 (45%)
12	CLA	cA	824	1	51,55,73	2.29	21 (41%)	61,91,113	3.10	30 (49%)
12	CLA	bB	934	2	49,53,73	2.46	19 (38%)	59,89,113	3.04	25 (42%)
15	BCR	aF	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	8 (14%)
15	BCR	cB	942	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	4 (7%)
17	LMG	cB	947	-	43,43,55	0.95	2 (4%)	51,51,63	1.25	6 (11%)
12	CLA	cA	808	1	55,59,73	2.25	21 (38%)	66,96,113	3.07	31 (46%)
15	BCR	aB	944	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	7 (12%)
12	CLA	bA	843	18	69,73,73	1.93	20 (28%)	83,113,113	2.81	34 (40%)
12	CLA	cB	929	2	49,53,73	2.34	20 (40%)	59,89,113	3.33	28 (47%)
15	BCR	cJ	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	cA	802	18	69,73,73	1.93	19 (27%)	83,113,113	2.76	28 (33%)
12	CLA	aA	823	1	55,59,73	2.19	19 (34%)	66,96,113	3.12	31 (46%)
12	CLA	bB	923	18	58,62,73	2.07	19 (32%)	69,99,113	2.97	27 (39%)
12	CLA	aA	811	1	49,53,73	2.37	19 (38%)	59,89,113	3.16	27 (45%)
12	CLA	cB	914	2	49,53,73	2.32	20 (40%)	59,89,113	3.34	26 (44%)
12	CLA	cB	920	2	49,53,73	2.35	19 (38%)	59,89,113	3.32	25 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bA	828	1	-	3/39/115/115	-
15	BCR	bL	206	-	-	6/29/63/63	0/2/2/2
15	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	835	1	-	2/15/91/115	-
12	CLA	aB	917	2	-	10/27/103/115	-
12	CLA	aB	903	2	-	5/23/99/115	-
15	BCR	aF	201	-	-	9/29/63/63	0/2/2/2
15	BCR	cA	848	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cA	825	18	-	12/39/115/115	-
12	CLA	bA	841	18	-	5/23/99/115	-
12	CLA	bA	802	18	-	5/39/115/115	-
15	BCR	bF	203	-	-	15/29/63/63	0/2/2/2
12	CLA	aA	814	1	-	8/15/91/115	-
15	BCR	aA	850	-	-	10/29/63/63	0/2/2/2
12	CLA	bA	810	1	-	7/15/91/115	-
12	CLA	bB	905	2	-	15/39/115/115	-
12	CLA	cA	805	1	-	6/25/101/115	-
12	CLA	aA	844	16	-	6/15/91/115	-
12	CLA	cA	827	1	-	6/17/93/115	-
12	CLA	cB	913	2	-	6/29/105/115	-
12	CLA	bB	932	2	-	4/15/91/115	-
12	CLA	bA	805	1	-	6/25/101/115	-
12	CLA	bA	824	1	-	7/18/94/115	-
12	CLA	aA	842	1	-	14/39/115/115	-
12	CLA	aB	932	2	-	4/15/91/115	-
12	CLA	cB	924	18	-	2/17/93/115	-
12	CLA	cB	904	2	-	12/39/115/115	-
12	CLA	cA	834	1	-	14/39/115/115	-
15	BCR	aF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	bA	842	1	-	14/39/115/115	-
12	CLA	cB	909	2	-	9/27/103/115	-
17	LMG	bB	947	-	-	12/38/58/70	0/1/1/1
12	CLA	aA	832	1	-	10/27/103/115	-
12	CLA	aA	840	1	-	11/39/115/115	-
14	SF4	cA	845	1,2	-	-	0/6/5/5
12	CLA	bB	921	2	-	8/27/103/115	-
12	CLA	cA	816	1	-	6/15/91/115	-
12	CLA	cA	843	18	-	11/39/115/115	-
12	CLA	bA	835	1	-	2/15/91/115	-
12	CLA	bA	853	18	-	6/29/105/115	-
12	CLA	bB	918	18	-	3/17/93/115	-
16	LHG	aB	948	12	-	8/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	824	1	-	7/18/94/115	-
15	BCR	cL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	aA	839	1	-	7/15/91/115	-
12	CLA	bA	806	1	-	11/39/115/115	-
12	CLA	cB	918	18	-	3/17/93/115	-
12	CLA	bB	922	2	-	7/15/91/115	-
12	CLA	cA	821	18	-	4/21/97/115	-
12	CLA	cB	921	2	-	8/27/103/115	-
12	CLA	aB	950	16	-	7/15/91/115	-
12	CLA	bA	815	1	-	6/15/91/115	-
12	CLA	cA	840	1	-	11/39/115/115	-
12	CLA	cA	842	1	-	14/39/115/115	-
14	SF4	bC	101	3	-	-	0/6/5/5
12	CLA	cB	936	2	-	9/32/108/115	-
12	CLA	bB	912	2	-	17/39/115/115	-
12	CLA	cA	833	1	-	5/23/99/115	-
12	CLA	bA	813	1	-	3/15/91/115	-
12	CLA	aB	937	2	-	3/18/94/115	-
12	CLA	cA	836	1	-	5/15/91/115	-
12	CLA	cB	912	2	-	17/39/115/115	-
12	CLA	bB	917	2	-	10/27/103/115	-
12	CLA	cA	807	1	-	13/39/115/115	-
12	CLA	aA	818	1	-	12/26/102/115	-
12	CLA	aB	927	2	-	12/39/115/115	-
12	CLA	aB	939	2	-	5/15/91/115	-
12	CLA	bB	929	2	-	7/15/91/115	-
12	CLA	bA	820	1	-	13/29/105/115	-
12	CLA	bA	811	1	-	6/15/91/115	-
14	SF4	cC	101	3	-	-	0/6/5/5
16	LHG	cA	851	-	-	22/53/53/53	-
12	CLA	bA	823	1	-	8/23/99/115	-
15	BCR	cA	850	-	-	10/29/63/63	0/2/2/2
14	SF4	aC	101	3	-	-	0/6/5/5
14	SF4	aA	846	1,2	-	-	0/6/5/5
12	CLA	cA	809	1	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	828	1	-	3/39/115/115	-
15	BCR	cB	944	-	-	16/29/63/63	0/2/2/2
13	1L3	cA	844	-	-	3/23/43/43	0/2/2/2
12	CLA	aA	836	1	-	5/15/91/115	-
12	CLA	aB	923	18	-	12/26/102/115	-
12	CLA	bB	907	2	-	8/24/100/115	-
12	CLA	aA	838	1	-	8/39/115/115	-
12	CLA	aA	826	18	-	8/27/103/115	-
15	BCR	cA	846	-	-	11/29/63/63	0/2/2/2
12	CLA	bB	935	2	-	7/21/97/115	-
12	CLA	aA	803	-	-	7/39/115/115	-
11	CL0	aA	801	1	-	7/39/115/115	-
12	CLA	bA	839	1	-	7/15/91/115	-
12	CLA	bB	909	2	-	9/27/103/115	-
12	CLA	aL	203	9	-	6/15/91/115	-
16	LHG	bB	948	12	-	8/26/26/53	-
12	CLA	bA	840	1	-	11/39/115/115	-
15	BCR	aL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	cB	917	2	-	10/27/103/115	-
12	CLA	cF	202	6	-	9/15/91/115	-
12	CLA	aA	816	1	-	6/15/91/115	-
12	CLA	aB	925	2	-	5/27/103/115	-
12	CLA	cL	204	18	-	0/15/91/115	-
12	CLA	bA	829	1	-	6/33/109/115	-
16	LHG	cA	852	12	-	11/31/31/53	-
12	CLA	cA	812	1	-	10/39/115/115	-
15	BCR	cB	945	-	-	9/29/63/63	0/2/2/2
12	CLA	aB	908	2	-	10/19/95/115	-
12	CLA	aB	901	2	-	8/39/115/115	-
15	BCR	bB	943	-	-	9/29/63/63	0/2/2/2
12	CLA	bA	834	1	-	14/39/115/115	-
12	CLA	bB	927	2	-	12/39/115/115	-
12	CLA	bA	830	1	-	11/39/115/115	-
12	CLA	cB	937	2	-	2/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bB	914	2	-	7/15/91/115	-
12	CLA	cA	819	1	-	6/33/109/115	-
12	CLA	bB	930	2	-	4/20/96/115	-
12	CLA	aB	921	2	-	8/27/103/115	-
15	BCR	cL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	cA	835	1	-	2/15/91/115	-
12	CLA	bA	808	1	-	7/23/99/115	-
12	CLA	aB	913	2	-	6/29/105/115	-
12	CLA	cA	818	1	-	12/26/102/115	-
12	CLA	aA	831	1	-	6/21/97/115	-
15	BCR	aJ	101	-	-	13/29/63/63	0/2/2/2
12	CLA	aB	912	2	-	17/39/115/115	-
12	CLA	aB	922	2	-	7/15/91/115	-
12	CLA	aB	926	2	-	23/39/115/115	-
12	CLA	bA	818	1	-	12/26/102/115	-
12	CLA	bA	832	1	-	10/27/103/115	-
12	CLA	cA	815	1	-	6/15/91/115	-
12	CLA	cB	922	2	-	7/15/91/115	-
12	CLA	bB	916	2	-	9/32/108/115	-
12	CLA	aB	929	2	-	7/15/91/115	-
12	CLA	bB	913	2	-	6/29/105/115	-
12	CLA	bA	817	1	-	9/26/102/115	-
15	BCR	cL	205	-	-	10/29/63/63	0/2/2/2
15	BCR	aA	851	-	-	10/29/63/63	0/2/2/2
15	BCR	aL	205	-	-	10/29/63/63	0/2/2/2
15	BCR	bB	946	-	-	4/29/63/63	0/2/2/2
16	LHG	bA	851	-	-	23/53/53/53	-
12	CLA	aA	827	1	-	6/17/93/115	-
12	CLA	bB	910	2	-	4/15/91/115	-
15	BCR	cI	101	-	-	10/29/63/63	0/2/2/2
12	CLA	aL	202	9	-	2/25/101/115	-
12	CLA	bB	906	2	-	2/27/103/115	-
12	CLA	cL	203	9	-	6/15/91/115	-
13	1L3	bA	844	-	-	3/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	cA	847	-	-	7/29/63/63	0/2/2/2
15	BCR	aB	943	-	-	9/29/63/63	0/2/2/2
12	CLA	aB	911	2	-	0/15/91/115	-
17	LMG	aB	947	-	-	12/38/58/70	0/1/1/1
15	BCR	cB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	bA	838	1	-	8/39/115/115	-
12	CLA	bA	803	-	-	7/39/115/115	-
12	CLA	aB	930	2	-	4/20/96/115	-
12	CLA	bA	822	1	-	8/20/96/115	-
12	CLA	aB	924	18	-	2/17/93/115	-
12	CLA	bA	812	1	-	10/39/115/115	-
12	CLA	bB	919	2	-	7/18/94/115	-
12	CLA	aB	915	2	-	11/24/100/115	-
12	CLA	aB	931	2	-	12/39/115/115	-
12	CLA	aB	910	2	-	4/15/91/115	-
12	CLA	cB	925	2	-	5/27/103/115	-
11	CL0	bA	801	1	-	7/39/115/115	-
12	CLA	cB	919	2	-	7/18/94/115	-
12	CLA	cB	923	18	-	12/26/102/115	-
15	BCR	cF	201	-	-	9/29/63/63	0/2/2/2
12	CLA	cB	901	2	-	8/39/115/115	-
12	CLA	cA	839	1	-	7/15/91/115	-
12	CLA	aB	909	2	-	9/27/103/115	-
12	CLA	aB	933	18	-	3/15/91/115	-
12	CLA	cB	905	2	-	15/39/115/115	-
12	CLA	cB	934	2	-	4/15/91/115	-
12	CLA	cL	202	9	-	2/25/101/115	-
15	BCR	aM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	bA	816	1	-	7/15/91/115	-
12	CLA	cA	828	1	-	3/39/115/115	-
15	BCR	bB	942	-	-	9/29/63/63	0/2/2/2
16	LHG	aA	852	-	-	22/53/53/53	-
14	SF4	bC	102	3	-	-	0/6/5/5
12	CLA	bL	203	9	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cB	939	2	-	5/15/91/115	-
12	CLA	bB	936	2	-	9/32/108/115	-
15	BCR	bA	846	-	-	11/29/63/63	0/2/2/2
12	CLA	cA	826	18	-	8/27/103/115	-
15	BCR	bF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	bB	925	2	-	5/27/103/115	-
12	CLA	bA	825	18	-	12/39/115/115	-
15	BCR	aA	848	-	-	7/29/63/63	0/2/2/2
12	CLA	aB	935	2	-	7/21/97/115	-
12	CLA	cB	907	2	-	7/24/100/115	-
12	CLA	cA	829	1	-	6/33/109/115	-
12	CLA	aB	918	18	-	3/17/93/115	-
12	CLA	bA	804	1	-	7/29/105/115	-
12	CLA	aF	202	6	-	9/15/91/115	-
12	CLA	bB	950	16	-	6/15/91/115	-
12	CLA	cB	916	2	-	9/32/108/115	-
12	CLA	bB	928	2	-	4/21/97/115	-
12	CLA	bA	807	1	-	13/39/115/115	-
15	BCR	cF	203	-	-	15/29/63/63	0/2/2/2
12	CLA	aL	204	18	-	0/15/91/115	-
12	CLA	cA	831	1	-	6/21/97/115	-
12	CLA	bA	837	1	-	7/23/99/115	-
15	BCR	bA	847	-	-	7/29/63/63	0/2/2/2
12	CLA	aA	812	1	-	10/39/115/115	-
12	CLA	bA	831	1	-	6/21/97/115	-
12	CLA	aA	810	1	-	7/15/91/115	-
12	CLA	cB	906	2	-	2/27/103/115	-
12	CLA	aA	837	1	-	7/23/99/115	-
12	CLA	cB	932	2	-	4/15/91/115	-
12	CLA	bB	938	18	-	1/23/99/115	-
15	BCR	bI	101	-	-	10/29/63/63	0/2/2/2
15	BCR	aI	101	-	-	10/29/63/63	0/2/2/2
12	CLA	aB	916	2	-	9/32/108/115	-
12	CLA	bA	814	1	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	bJ	101	-	-	13/29/63/63	0/2/2/2
12	CLA	bB	902	-	-	9/35/111/115	-
15	BCR	aA	849	-	-	10/29/63/63	0/2/2/2
12	CLA	cA	823	1	-	8/23/99/115	-
12	CLA	aA	841	18	-	5/23/99/115	-
12	CLA	bL	204	18	-	0/15/91/115	-
15	BCR	aB	946	-	-	4/29/63/63	0/2/2/2
12	CLA	aA	813	1	-	3/15/91/115	-
15	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
13	1L3	aA	845	-	-	3/23/43/43	0/2/2/2
12	CLA	aB	919	2	-	7/18/94/115	-
12	CLA	aA	829	1	-	6/33/109/115	-
12	CLA	aA	807	1	-	13/39/115/115	-
12	CLA	aB	906	2	-	2/27/103/115	-
15	BCR	bF	201	-	-	9/29/63/63	0/2/2/2
12	CLA	aA	833	1	-	5/23/99/115	-
15	BCR	aA	847	-	-	11/29/63/63	0/2/2/2
12	CLA	cB	910	2	-	4/15/91/115	-
12	CLA	cB	908	2	-	10/19/95/115	-
15	BCR	cF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	bB	933	18	-	3/15/91/115	-
15	BCR	bB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	911	2	-	0/15/91/115	-
14	SF4	aC	102	3	-	-	0/6/5/5
12	CLA	cB	938	18	-	1/23/99/115	-
12	CLA	cA	820	1	-	13/29/105/115	-
16	LHG	cB	948	12	-	8/26/26/53	-
12	CLA	aA	815	1	-	6/15/91/115	-
12	CLA	cA	830	1	-	11/39/115/115	-
15	BCR	bM	101	-	-	18/29/63/63	0/2/2/2
13	1L3	cB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	cA	838	1	-	8/39/115/115	-
12	CLA	bB	924	18	-	2/17/93/115	-
12	CLA	bB	939	2	-	5/15/91/115	-
12	CLA	bB	931	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cA	803	-	-	7/39/115/115	-
12	CLA	aA	822	1	-	8/20/96/115	-
12	CLA	cA	841	18	-	5/23/99/115	-
12	CLA	cA	813	1	-	3/15/91/115	-
12	CLA	cB	935	2	-	7/21/97/115	-
12	CLA	aB	938	18	-	1/23/99/115	-
12	CLA	aA	820	1	-	13/29/105/115	-
15	BCR	aB	942	-	-	9/29/63/63	0/2/2/2
12	CLA	bB	904	2	-	12/39/115/115	-
16	LHG	bA	852	12	-	11/31/31/53	-
12	CLA	aB	902	-	-	9/35/111/115	-
12	CLA	cA	832	1	-	10/27/103/115	-
12	CLA	cB	902	-	-	9/35/111/115	-
12	CLA	cA	817	1	-	9/26/102/115	-
12	CLA	aB	920	2	-	3/15/91/115	-
12	CLA	bB	926	2	-	23/39/115/115	-
14	SF4	cC	102	3	-	-	0/6/5/5
13	1L3	aB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	bA	836	1	-	5/15/91/115	-
12	CLA	aA	809	1	-	7/15/91/115	-
11	CL0	cA	801	1	-	7/39/115/115	-
12	CLA	aB	928	2	-	4/21/97/115	-
12	CLA	bB	903	2	-	5/23/99/115	-
12	CLA	cB	903	2	-	5/23/99/115	-
12	CLA	bB	920	2	-	3/15/91/115	-
12	CLA	bL	202	9	-	2/25/101/115	-
15	BCR	aB	945	-	-	9/29/63/63	0/2/2/2
15	BCR	bL	205	-	-	10/29/63/63	0/2/2/2
15	BCR	cB	946	-	-	4/29/63/63	0/2/2/2
12	CLA	aB	936	2	-	9/32/108/115	-
15	BCR	cA	849	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	805	1	-	6/25/101/115	-
12	CLA	cB	930	2	-	4/20/96/115	-
14	SF4	bA	845	1,2	-	-	0/6/5/5
15	BCR	aB	941	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
12	CLA	bF	202	6	-	9/15/91/115	-
12	CLA	cB	915	2	-	11/24/100/115	-
12	CLA	cA	814	1	-	8/15/91/115	-
15	BCR	bB	944	-	-	16/29/63/63	0/2/2/2
12	CLA	aB	905	2	-	15/39/115/115	-
12	CLA	aB	934	2	-	4/15/91/115	-
13	1L3	bB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	cA	806	1	-	11/39/115/115	-
12	CLA	aA	834	1	-	14/39/115/115	-
12	CLA	bA	833	1	-	5/23/99/115	-
12	CLA	bB	937	2	-	3/18/94/115	-
12	CLA	cA	853	18	-	6/29/105/115	-
12	CLA	aA	854	18	-	6/29/105/115	-
12	CLA	aA	830	1	-	11/39/115/115	-
12	CLA	aA	843	18	-	11/39/115/115	-
12	CLA	aA	804	1	-	7/29/105/115	-
12	CLA	aB	949	16	-	3/10/86/115	-
12	CLA	bB	949	16	-	3/10/86/115	-
12	CLA	cA	822	1	-	8/20/96/115	-
12	CLA	aB	904	2	-	12/39/115/115	-
15	BCR	bL	201	-	-	7/29/63/63	0/2/2/2
15	BCR	cM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	aA	821	18	-	4/21/97/115	-
12	CLA	cB	926	2	-	23/39/115/115	-
15	BCR	aL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	aA	802	18	-	5/39/115/115	-
12	CLA	bA	826	18	-	8/27/103/115	-
12	CLA	aB	914	2	-	7/15/91/115	-
12	CLA	bA	827	1	-	6/17/93/115	-
12	CLA	cA	810	1	-	7/15/91/115	-
12	CLA	cA	804	1	-	7/29/105/115	-
12	CLA	aA	817	1	-	9/26/102/115	-
12	CLA	aA	825	18	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cA	837	1	-	7/23/99/115	-
12	CLA	cB	928	2	-	4/21/97/115	-
12	CLA	cB	927	2	-	12/39/115/115	-
12	CLA	aA	808	1	-	7/23/99/115	-
12	CLA	aB	907	2	-	7/24/100/115	-
16	LHG	aA	853	12	-	11/31/31/53	-
12	CLA	bA	821	18	-	4/21/97/115	-
12	CLA	bA	809	1	-	7/15/91/115	-
12	CLA	cB	911	2	-	0/15/91/115	-
15	BCR	cB	943	-	-	9/29/63/63	0/2/2/2
12	CLA	bB	908	2	-	10/19/95/115	-
12	CLA	cB	931	2	-	12/39/115/115	-
12	CLA	bB	915	2	-	11/24/100/115	-
12	CLA	bB	901	2	-	8/39/115/115	-
12	CLA	cB	933	18	-	3/15/91/115	-
12	CLA	bA	819	1	-	6/33/109/115	-
12	CLA	cB	949	16	-	3/10/86/115	-
15	BCR	bB	945	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	806	1	-	11/39/115/115	-
12	CLA	aA	819	1	-	6/33/109/115	-
12	CLA	cA	811	1	-	6/15/91/115	-
12	CLA	cA	824	1	-	7/18/94/115	-
12	CLA	bB	934	2	-	3/15/91/115	-
15	BCR	aF	203	-	-	15/29/63/63	0/2/2/2
15	BCR	cB	942	-	-	9/29/63/63	0/2/2/2
17	LMG	cB	947	-	-	12/38/58/70	0/1/1/1
12	CLA	cA	808	1	-	7/23/99/115	-
15	BCR	aB	944	-	-	16/29/63/63	0/2/2/2
12	CLA	bA	843	18	-	11/39/115/115	-
12	CLA	cB	929	2	-	7/15/91/115	-
15	BCR	cJ	101	-	-	13/29/63/63	0/2/2/2
12	CLA	cA	802	18	-	5/39/115/115	-
12	CLA	aA	823	1	-	8/23/99/115	-
12	CLA	bB	923	18	-	12/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	811	1	-	6/15/91/115	-
12	CLA	cB	914	2	-	7/15/91/115	-
12	CLA	cB	920	2	-	3/15/91/115	-

The worst 5 of 5449 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bB	940	1L3	C03-C02	7.88	1.49	1.35
13	aB	940	1L3	C03-C02	7.85	1.49	1.35
13	cB	940	1L3	C03-C02	7.83	1.49	1.35
13	bA	844	1L3	C03-C02	7.76	1.49	1.35
13	cA	844	1L3	C03-C02	7.74	1.49	1.35

The worst 5 of 8212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	931	CLA	C1D-ND-C4D	-10.64	98.77	106.33
12	cB	931	CLA	C1D-ND-C4D	-10.60	98.81	106.33
12	bB	931	CLA	C1D-ND-C4D	-10.58	98.82	106.33
12	aB	931	CLA	C2D-C1D-ND	10.15	117.58	110.10
12	cB	931	CLA	C2D-C1D-ND	10.10	117.55	110.10

There are no chirality outliers.

5 of 2727 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	aA	804	CLA	C1A-C2A-CAA-CBA
12	aA	804	CLA	C3A-C2A-CAA-CBA
12	aA	807	CLA	C1A-C2A-CAA-CBA
12	aA	808	CLA	C2A-CAA-CBA-CGA
12	aA	808	CLA	C2-C3-C5-C6

There are no ring outliers.

235 monomers are involved in 370 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	bA	828	CLA	1	0
15	bA	848	BCR	2	0
12	aB	917	CLA	1	0
15	aF	201	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	848	BCR	2	0
12	cA	825	CLA	6	0
12	bA	841	CLA	2	0
12	bA	802	CLA	2	0
15	bF	203	BCR	1	0
12	aA	814	CLA	1	0
15	aA	850	BCR	3	0
12	bA	810	CLA	2	0
12	bB	905	CLA	1	0
12	cA	805	CLA	1	0
12	cA	827	CLA	2	0
12	cB	913	CLA	1	0
12	aA	842	CLA	3	0
12	cB	924	CLA	1	0
12	cA	834	CLA	3	0
15	aF	204	BCR	3	0
12	bA	842	CLA	4	0
12	cB	909	CLA	1	0
12	aA	832	CLA	2	0
12	aA	840	CLA	4	0
12	bB	921	CLA	1	0
12	cA	843	CLA	4	0
12	bA	853	CLA	2	0
15	cL	201	BCR	3	0
12	bA	806	CLA	4	0
12	cB	918	CLA	1	0
12	bB	922	CLA	1	0
12	cA	821	CLA	2	0
12	cA	840	CLA	4	0
12	cA	842	CLA	4	0
12	cB	936	CLA	2	0
12	bB	912	CLA	4	0
12	cA	836	CLA	1	0
12	cB	912	CLA	5	0
12	bB	917	CLA	1	0
12	cA	807	CLA	2	0
12	aA	818	CLA	2	0
12	aB	927	CLA	3	0
12	bB	929	CLA	2	0
12	bA	820	CLA	1	0
16	cA	851	LHG	1	0
15	cA	850	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	cA	809	CLA	3	0
12	aA	828	CLA	1	0
15	cB	944	BCR	2	0
12	aA	836	CLA	1	0
12	aB	923	CLA	3	0
12	aA	838	CLA	1	0
12	aA	826	CLA	1	0
15	cA	846	BCR	1	0
12	bB	935	CLA	1	0
12	aA	803	CLA	1	0
12	bB	909	CLA	2	0
12	bA	840	CLA	4	0
15	aL	206	BCR	1	0
12	cB	917	CLA	1	0
12	aB	925	CLA	2	0
12	cL	204	CLA	1	0
12	bA	829	CLA	1	0
16	cA	852	LHG	1	0
12	cA	812	CLA	1	0
15	cB	945	BCR	3	0
15	bB	943	BCR	3	0
12	bA	834	CLA	2	0
12	bB	927	CLA	2	0
12	bA	830	CLA	2	0
12	bB	914	CLA	1	0
12	cA	819	CLA	3	0
12	bB	930	CLA	1	0
15	cL	206	BCR	1	0
12	bA	808	CLA	1	0
12	cA	818	CLA	3	0
15	aJ	101	BCR	1	0
12	aB	912	CLA	5	0
12	aB	922	CLA	2	0
12	aB	926	CLA	2	0
12	bA	818	CLA	3	0
12	bA	832	CLA	2	0
12	cB	922	CLA	2	0
12	bB	916	CLA	2	0
12	aB	929	CLA	2	0
12	bA	817	CLA	1	0
15	cL	205	BCR	2	0
15	aA	851	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aL	205	BCR	2	0
15	bB	946	BCR	2	0
16	bA	851	LHG	1	0
12	aA	827	CLA	2	0
15	cI	101	BCR	1	0
12	aL	202	CLA	2	0
12	bB	906	CLA	1	0
15	cA	847	BCR	3	0
15	aB	943	BCR	3	0
12	aB	911	CLA	1	0
15	cB	941	BCR	1	0
12	bA	838	CLA	1	0
12	bA	803	CLA	1	0
12	aB	930	CLA	1	0
12	bA	822	CLA	1	0
12	bA	812	CLA	1	0
12	bB	919	CLA	1	0
12	aB	915	CLA	2	0
12	aB	931	CLA	6	0
12	cB	925	CLA	3	0
12	cB	919	CLA	1	0
12	cB	923	CLA	3	0
15	cF	201	BCR	2	0
12	aB	909	CLA	2	0
12	aB	933	CLA	1	0
12	cB	905	CLA	2	0
12	cL	202	CLA	2	0
12	cA	828	CLA	1	0
15	bB	942	BCR	1	0
12	bB	936	CLA	2	0
12	cA	826	CLA	1	0
15	bF	204	BCR	3	0
12	bB	925	CLA	2	0
12	bA	825	CLA	6	0
15	aA	848	BCR	2	0
12	aB	935	CLA	1	0
12	cA	829	CLA	1	0
12	aB	918	CLA	1	0
12	bA	804	CLA	2	0
12	cB	916	CLA	2	0
12	bA	807	CLA	1	0
15	cF	203	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	aL	204	CLA	1	0
12	bA	837	CLA	1	0
15	bA	847	BCR	3	0
12	aA	812	CLA	1	0
12	aA	810	CLA	2	0
12	cB	906	CLA	1	0
12	aA	837	CLA	2	0
15	bI	101	BCR	2	0
15	aI	101	BCR	2	0
12	aB	916	CLA	2	0
12	bA	814	CLA	1	0
15	bJ	101	BCR	1	0
12	bB	902	CLA	1	0
15	aA	849	BCR	1	0
12	aA	841	CLA	2	0
12	bL	204	CLA	1	0
15	aB	946	BCR	2	0
15	bA	850	BCR	3	0
12	aB	919	CLA	1	0
12	aA	829	CLA	1	0
12	aA	807	CLA	1	0
12	aB	906	CLA	1	0
15	bF	201	BCR	1	0
12	aA	833	CLA	1	0
15	cF	204	BCR	3	0
12	bB	933	CLA	1	0
15	bB	941	BCR	1	0
12	bB	911	CLA	1	0
12	cA	820	CLA	1	0
12	cA	830	CLA	2	0
12	cA	838	CLA	2	0
12	bB	931	CLA	5	0
12	cA	803	CLA	1	0
12	cA	841	CLA	2	0
12	cB	935	CLA	1	0
12	aA	820	CLA	1	0
12	bB	904	CLA	2	0
16	bA	852	LHG	1	0
12	aB	902	CLA	1	0
12	cA	832	CLA	2	0
12	cA	817	CLA	1	0
12	bB	926	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	bA	836	CLA	1	0
12	aA	809	CLA	4	0
12	bL	202	CLA	2	0
15	aB	945	BCR	1	0
15	bL	205	BCR	2	0
15	cB	946	BCR	1	0
12	aB	936	CLA	2	0
15	cA	849	BCR	4	0
12	cB	930	CLA	1	0
15	aB	941	BCR	2	0
15	bA	849	BCR	2	0
12	cB	915	CLA	2	0
12	cA	814	CLA	1	0
15	bB	944	BCR	3	0
12	aB	905	CLA	2	0
13	bB	940	1L3	1	0
12	cA	806	CLA	5	0
12	aA	834	CLA	2	0
12	cA	853	CLA	3	0
12	aA	854	CLA	2	0
12	aA	830	CLA	2	0
12	aA	843	CLA	4	0
12	aA	804	CLA	2	0
12	aB	949	CLA	1	0
12	bB	949	CLA	1	0
12	cA	822	CLA	1	0
12	aB	904	CLA	1	0
15	bL	201	BCR	2	0
12	aA	821	CLA	2	0
12	cB	926	CLA	3	0
15	aL	201	BCR	1	0
12	aA	802	CLA	2	0
12	bA	826	CLA	1	0
12	aB	914	CLA	1	0
12	bA	827	CLA	2	0
12	cA	810	CLA	2	0
12	cA	804	CLA	2	0
12	aA	817	CLA	1	0
12	aA	825	CLA	5	0
12	cA	837	CLA	1	0
12	cB	927	CLA	3	0
12	aA	808	CLA	1	0

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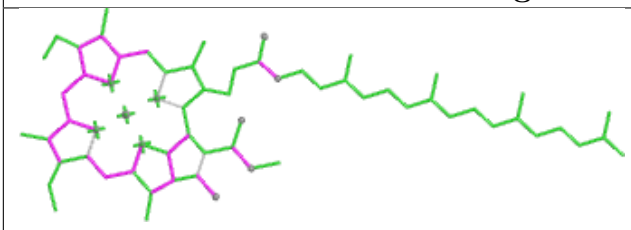
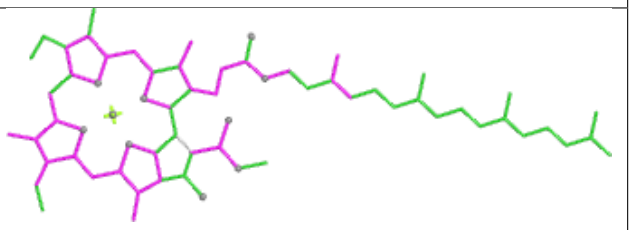
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	aA	853	LHG	1	0
12	bA	821	CLA	2	0
12	bA	809	CLA	3	0
12	cB	911	CLA	1	0
15	cB	943	BCR	2	0
12	cB	931	CLA	4	0
12	bB	915	CLA	2	0
12	bB	901	CLA	1	0
12	cB	933	CLA	1	0
12	bA	819	CLA	3	0
15	bB	945	BCR	2	0
12	aA	806	CLA	3	0
12	aA	819	CLA	3	0
15	aF	203	BCR	2	0
12	cA	808	CLA	1	0
15	aB	944	BCR	3	0
12	bA	843	CLA	3	0
12	cB	929	CLA	2	0
12	cA	802	CLA	1	0
12	bB	923	CLA	2	0
12	cB	914	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.

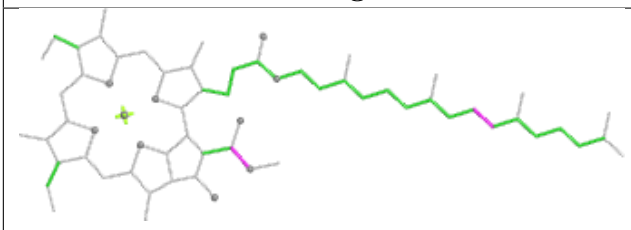
Ligand CLA bA 828



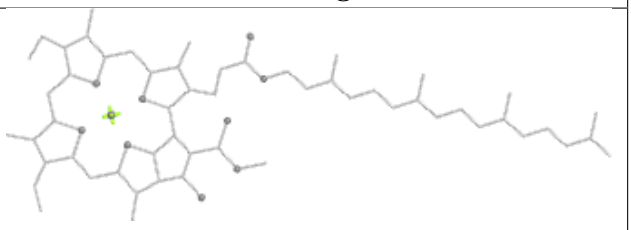
Bond lengths



Bond angles

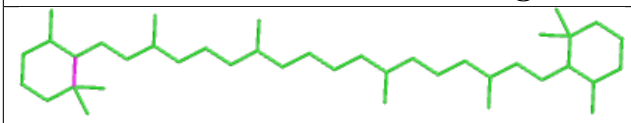


Torsions



Rings

Ligand BCR bL 206



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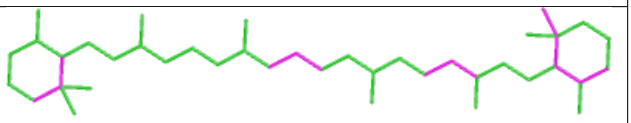
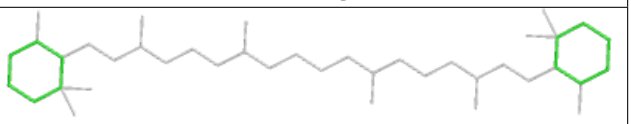


Bond angles

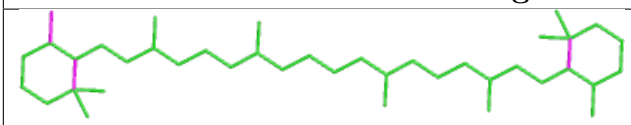


Torsions

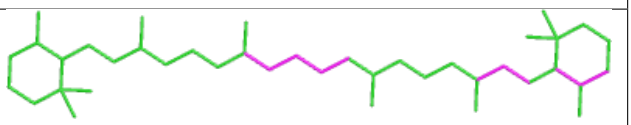


Rings

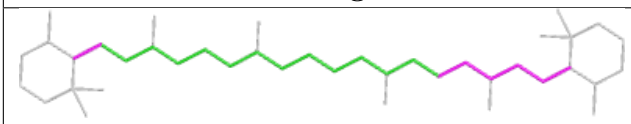
Ligand BCR bA 848



Bond lengths



Bond angles



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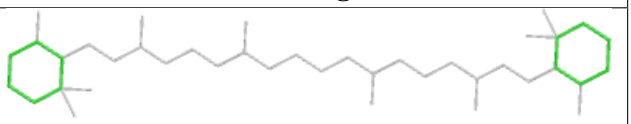
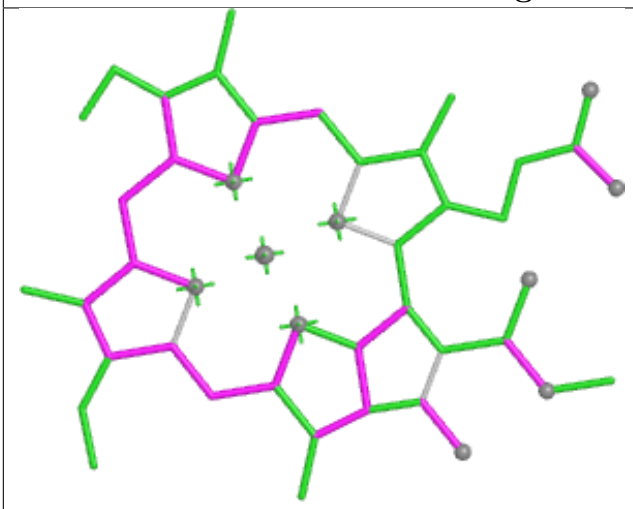


Rings

Ligand CLA aA 835



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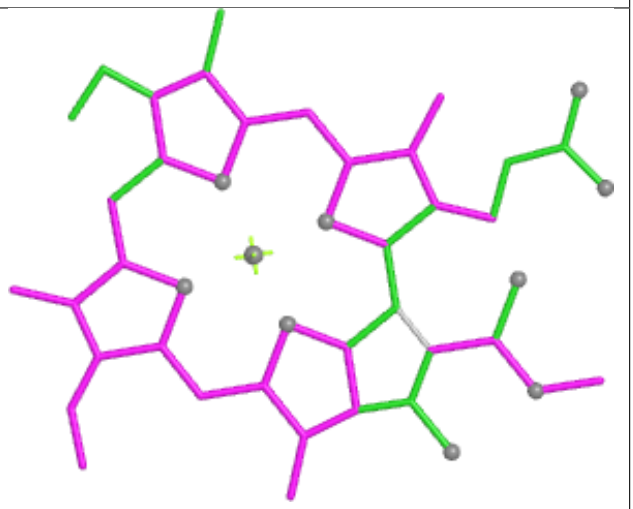
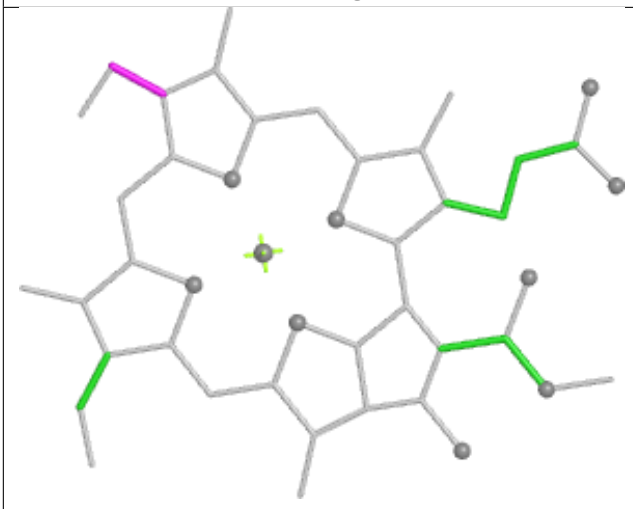


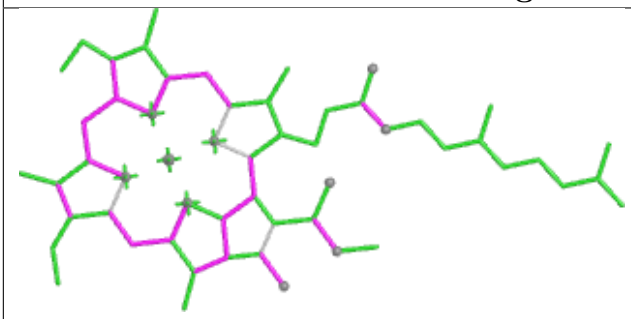
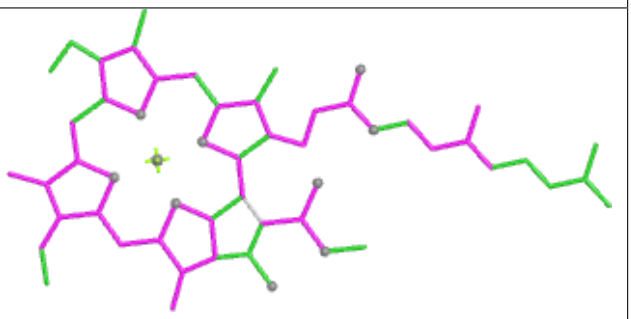
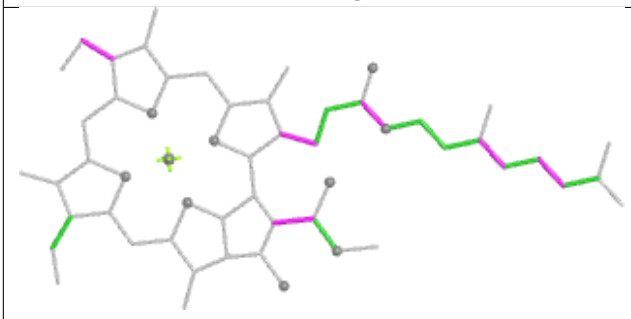
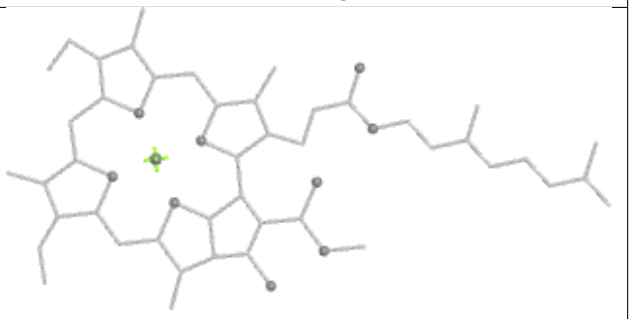
Bond angles



Torsions



Rings

Ligand CLA aB 917	
	
Bond lengths	Bond angles
	
Torsions	Rings

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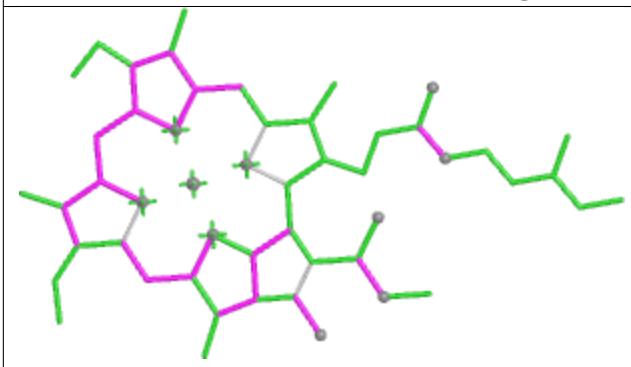
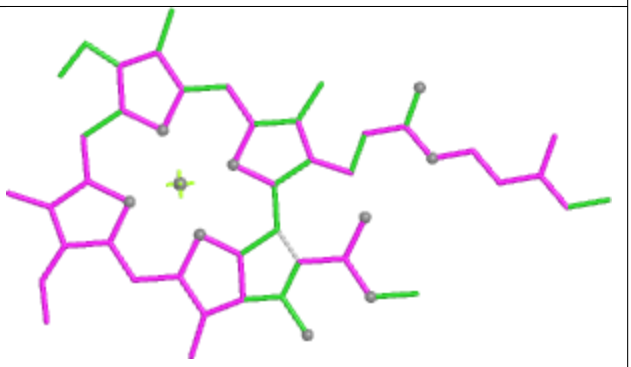
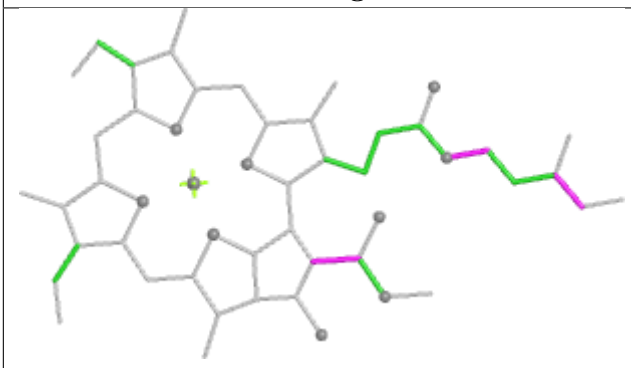
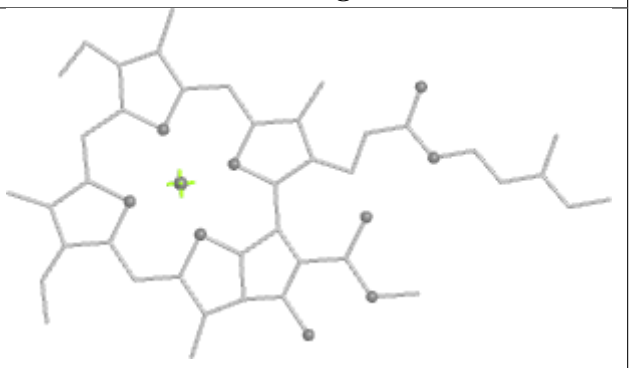
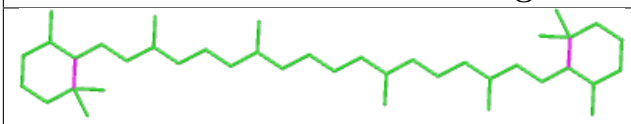
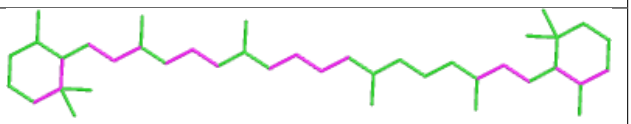
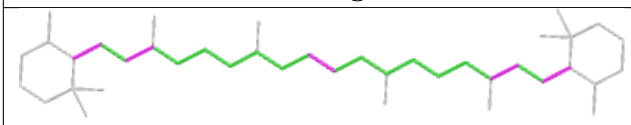
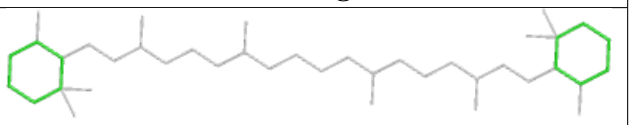
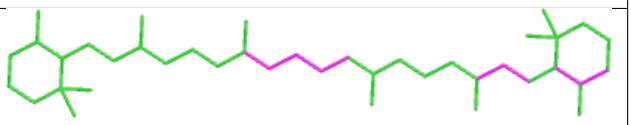
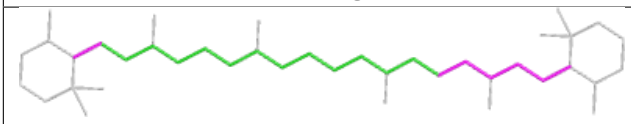
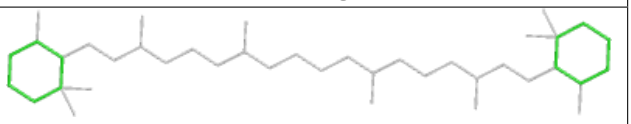
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aF 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR cA 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

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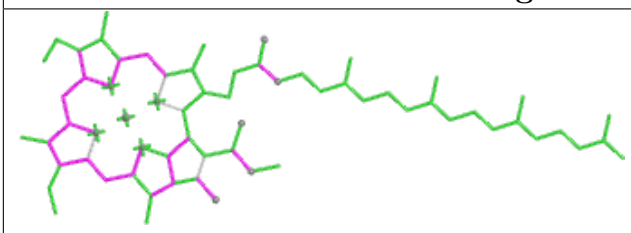
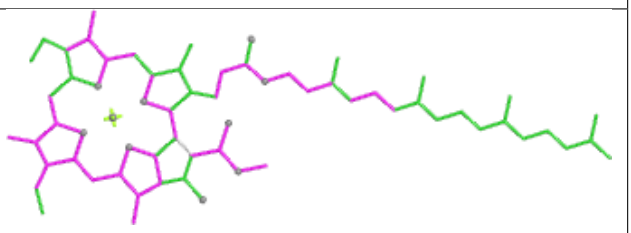
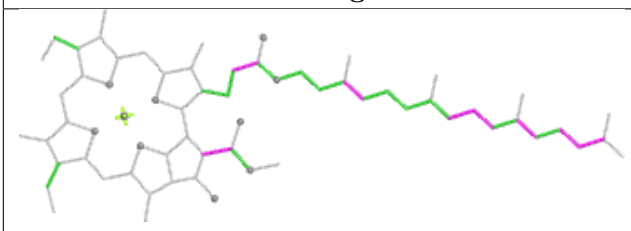
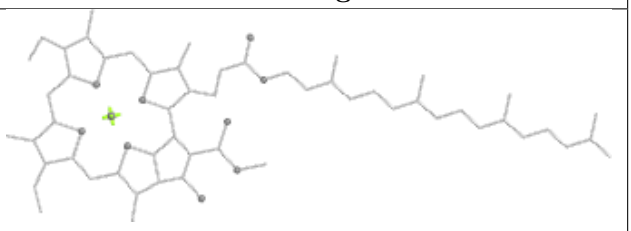
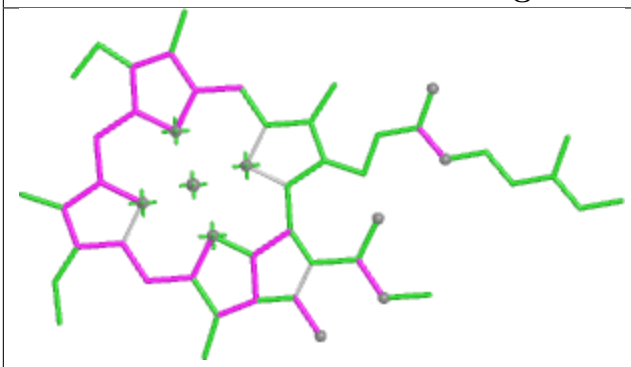
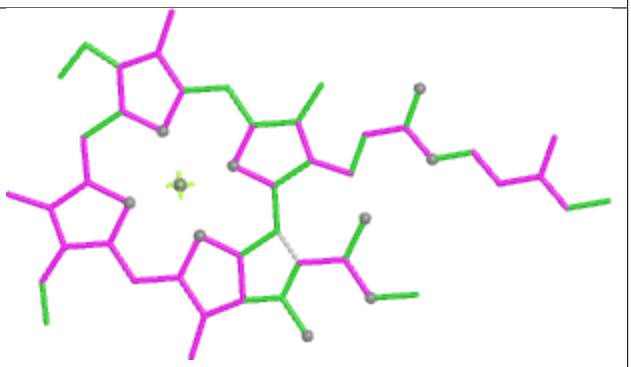
 Bond lengths	 Bond angles
 Torsions	 Rings

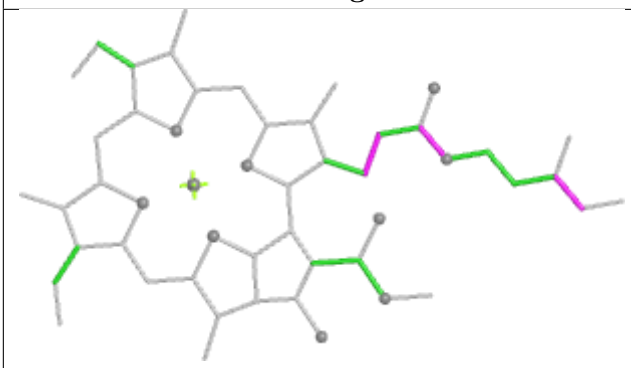
Ligand CLA bA 841



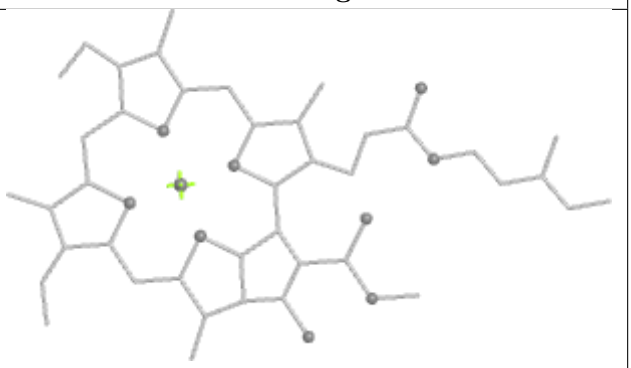
Bond lengths



Bond angles

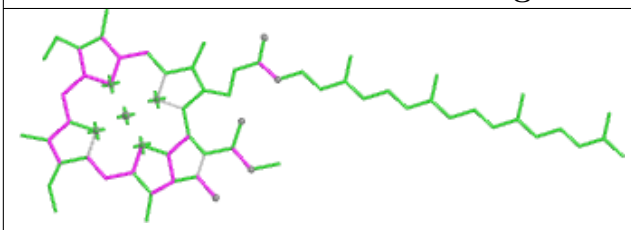


Torsions



Rings

Ligand CLA bA 802



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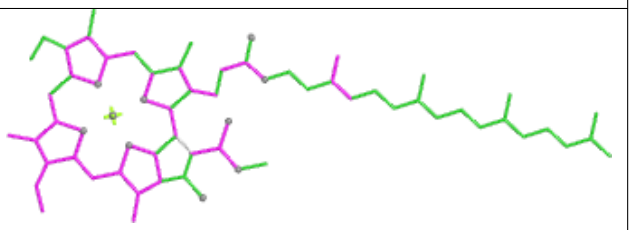

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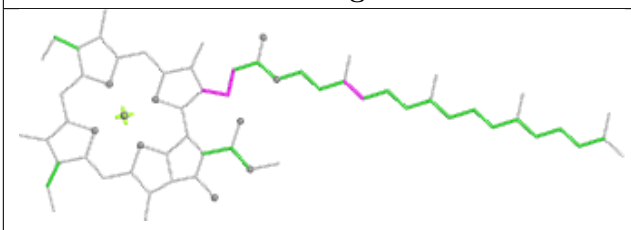

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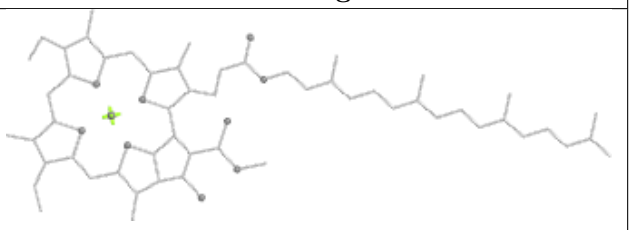
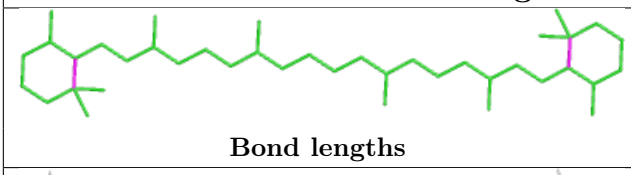


Rings

Ligand BCR bF 203



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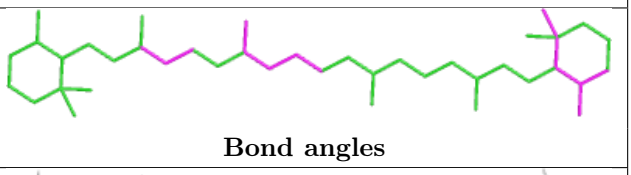
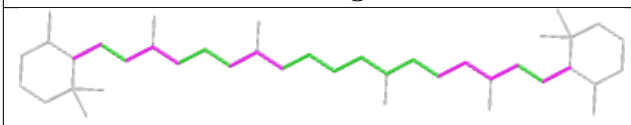


Bond angles



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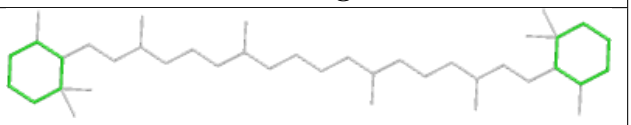
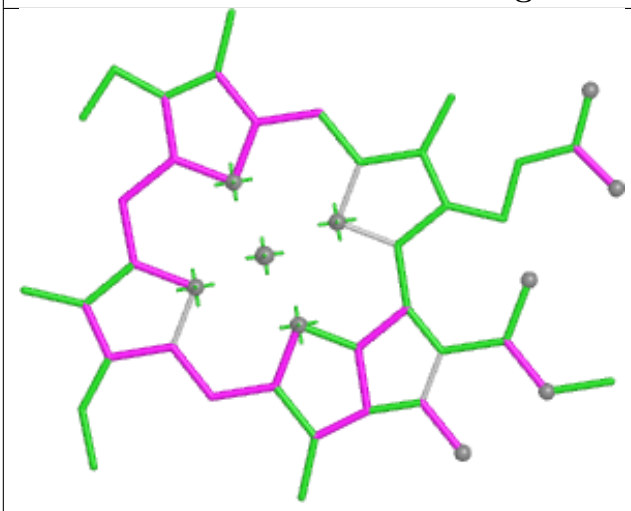
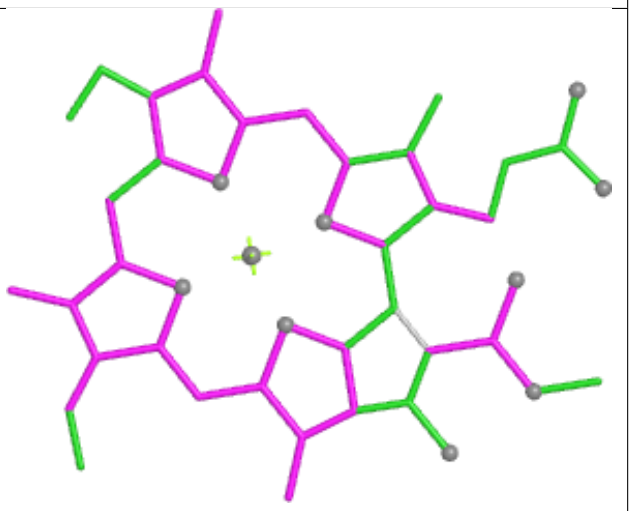


Rings

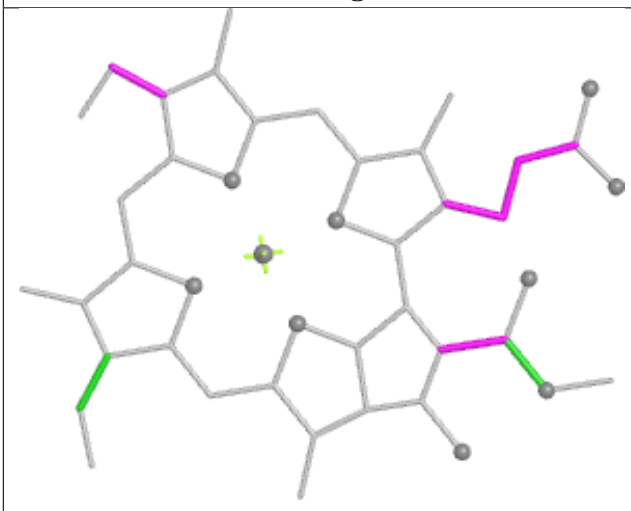
Ligand CLA aA 814



Bond lengths



Bond angles



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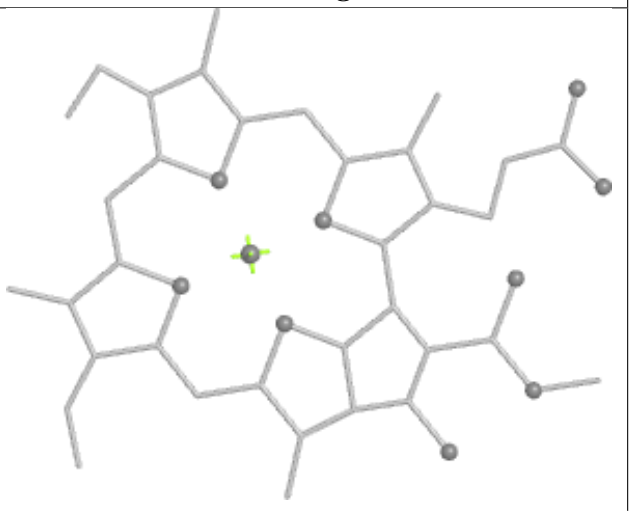
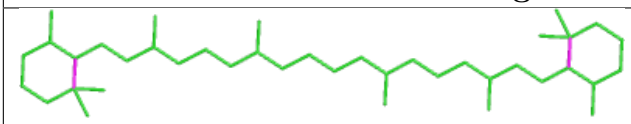
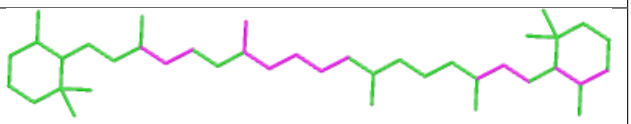


Rings

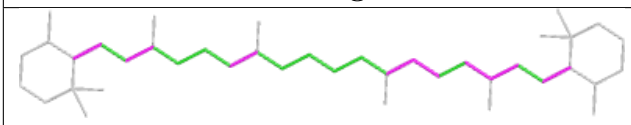
Ligand BCR aA 850



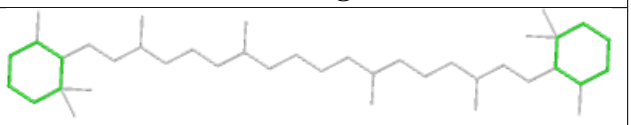
Bond lengths



Bond angles

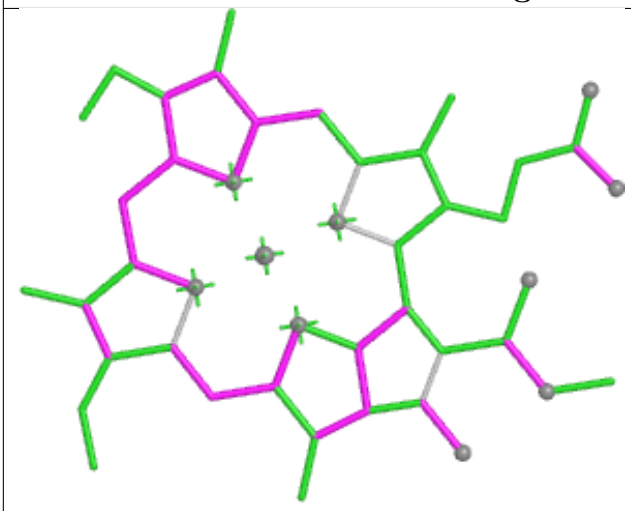


Torsions



Rings

Ligand CLA bA 810



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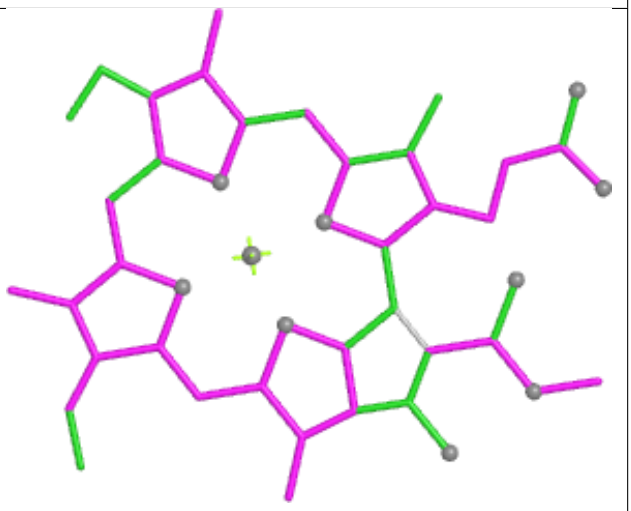

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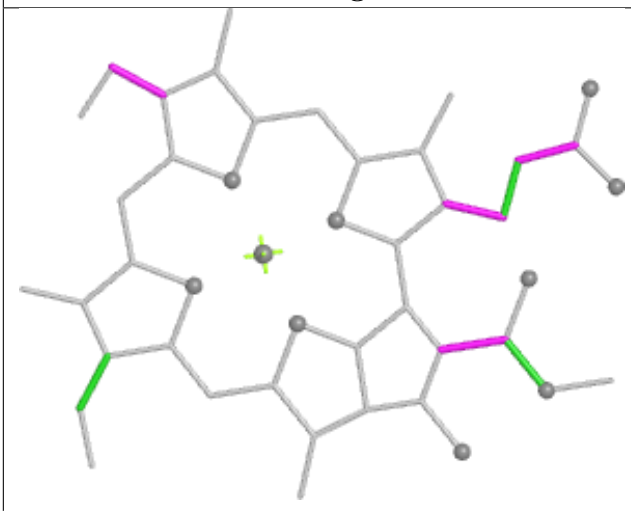

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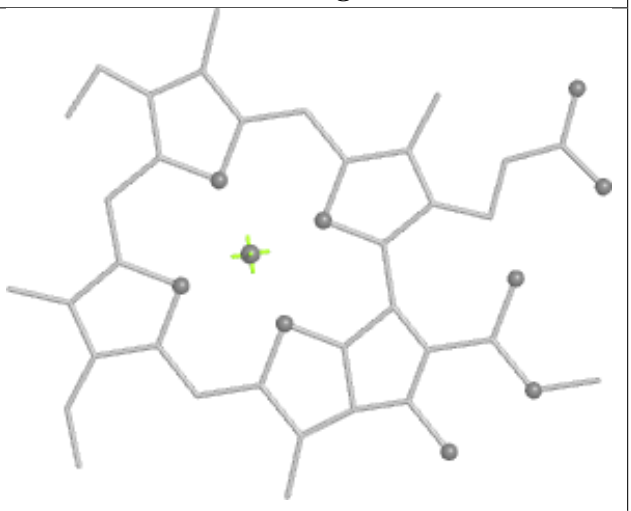
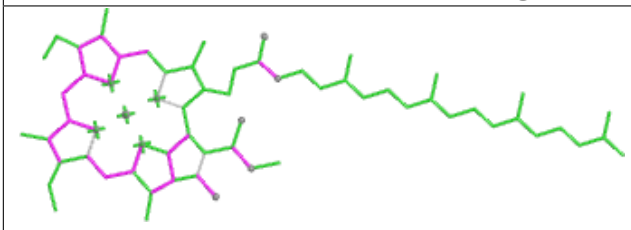


Rings

Ligand CLA bB 905



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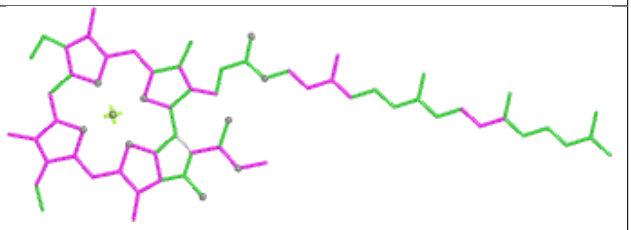
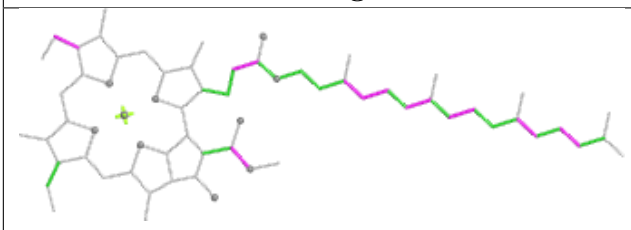


Bond angles



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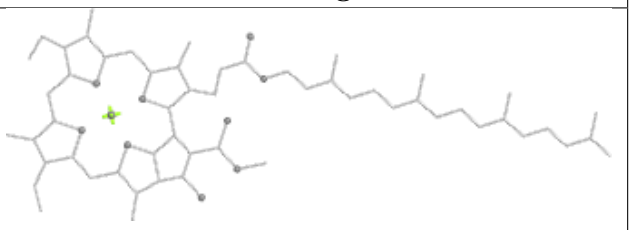
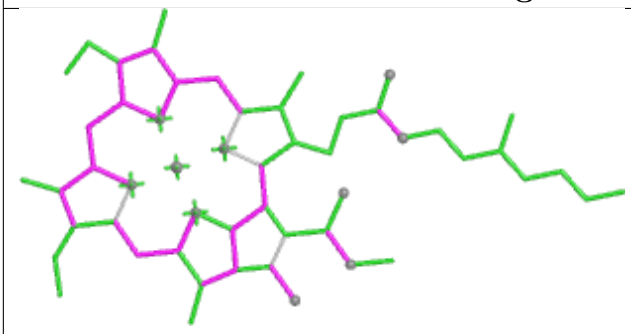


Rings

Ligand CLA cA 805



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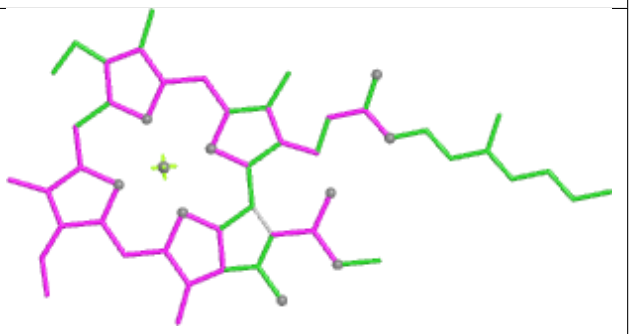
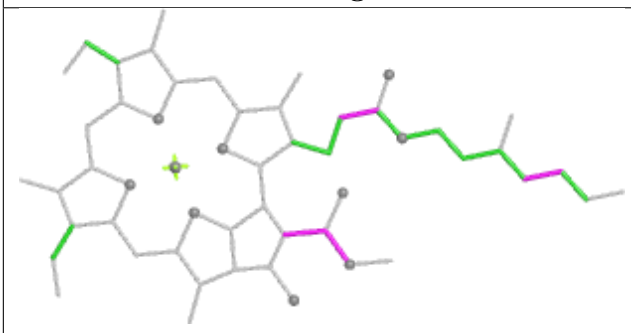


Bond angles



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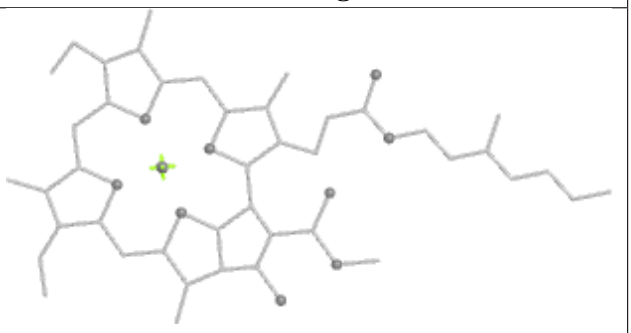
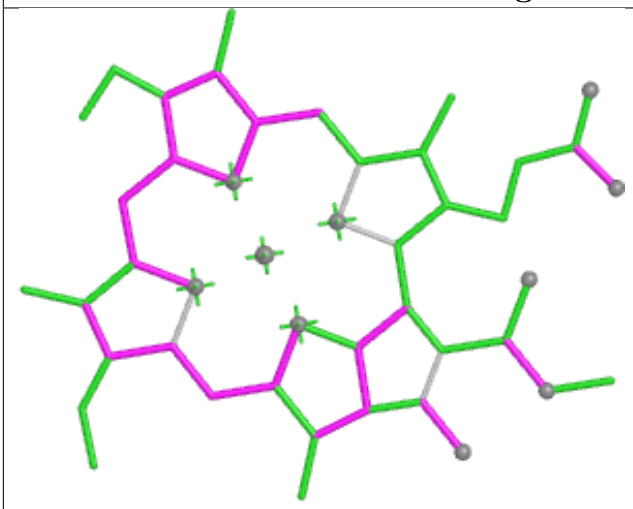


Rings

Ligand CLA aA 844



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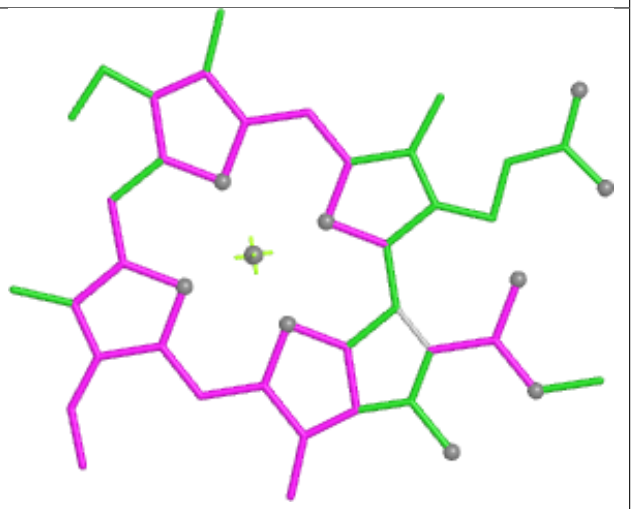
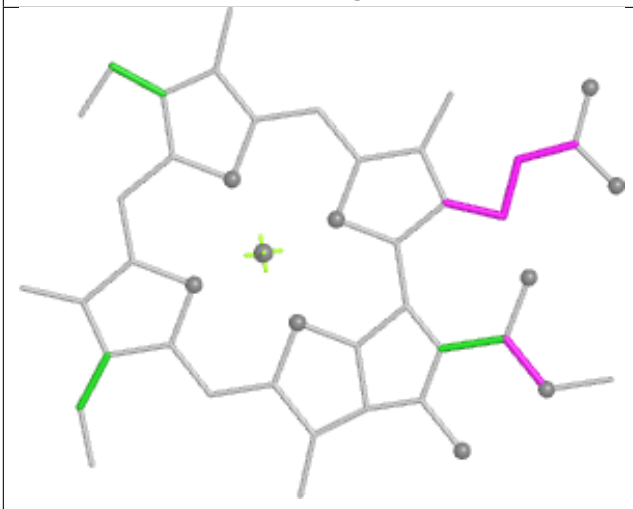


Bond angles

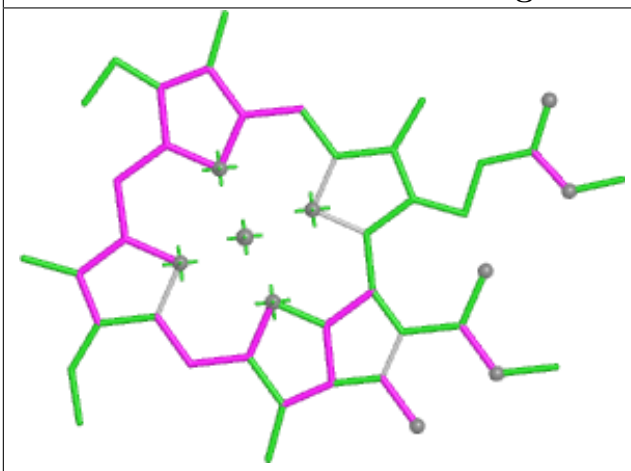


Torsions



Rings

Ligand CLA cA 827



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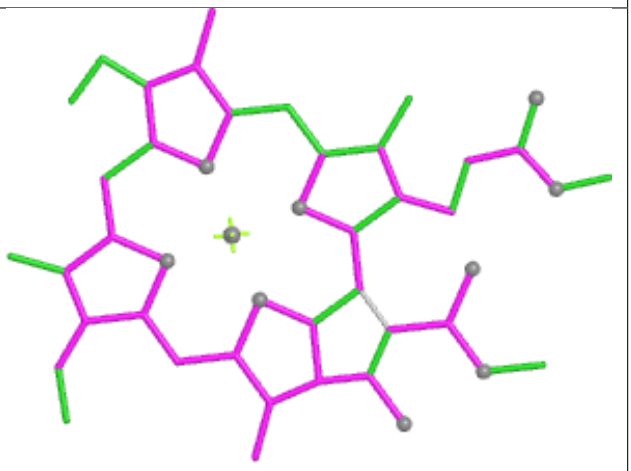

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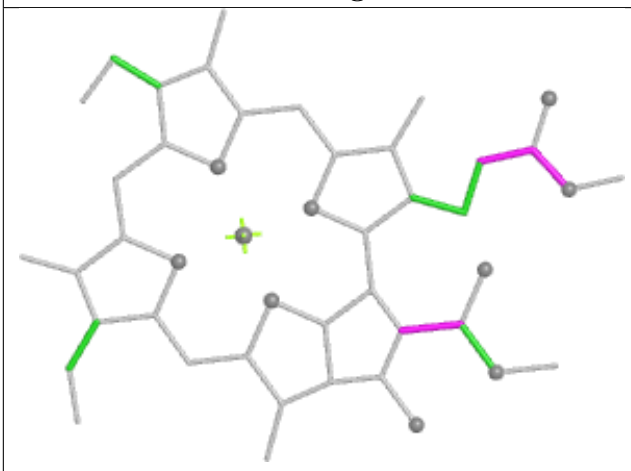

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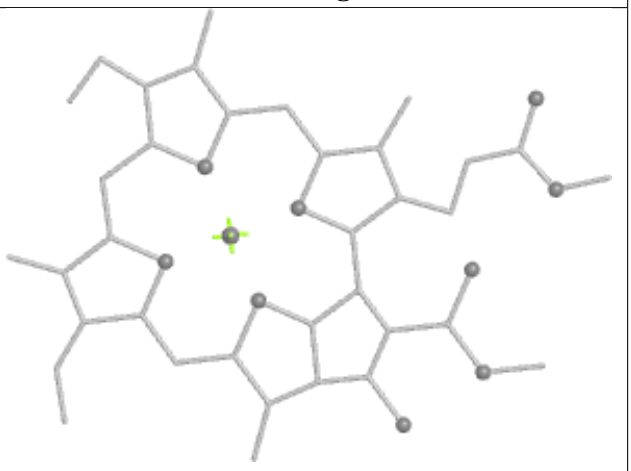
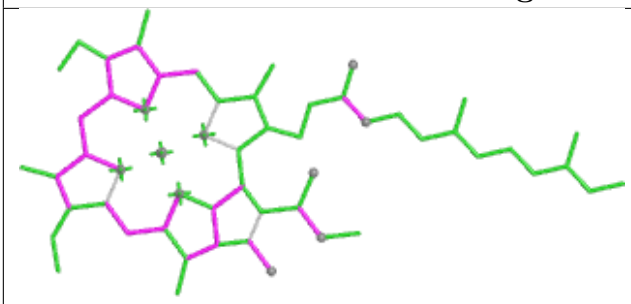


Rings

Ligand CLA cB 913



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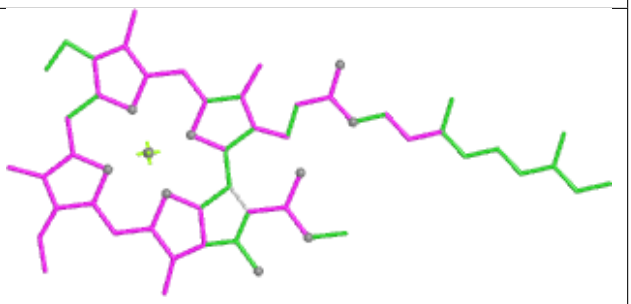

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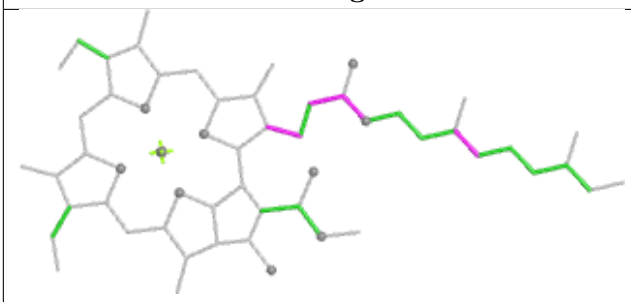

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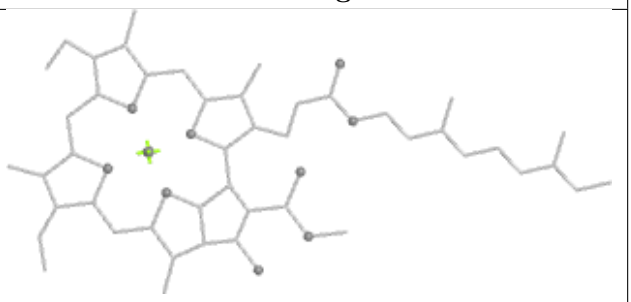
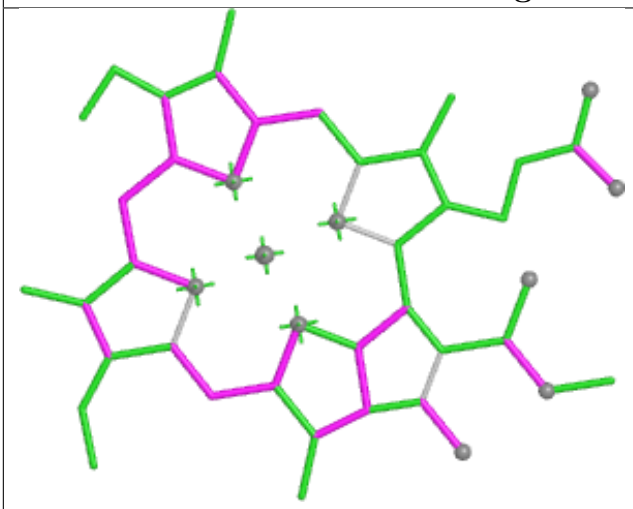


Rings

Ligand CLA bB 932



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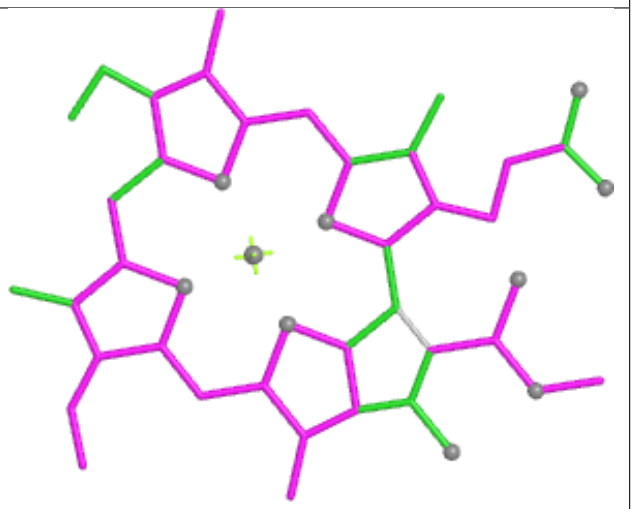
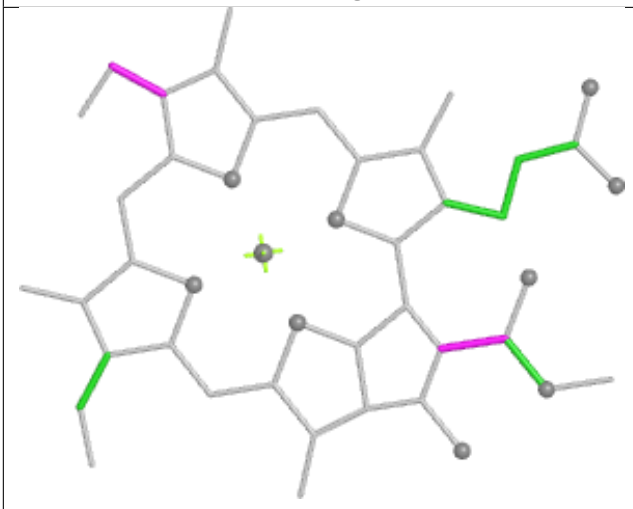


Bond angles

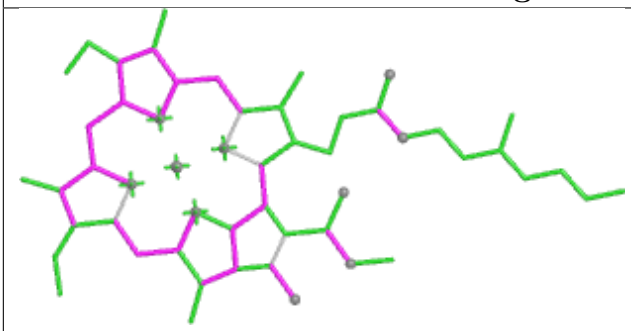


Torsions



Rings

Ligand CLA bA 805



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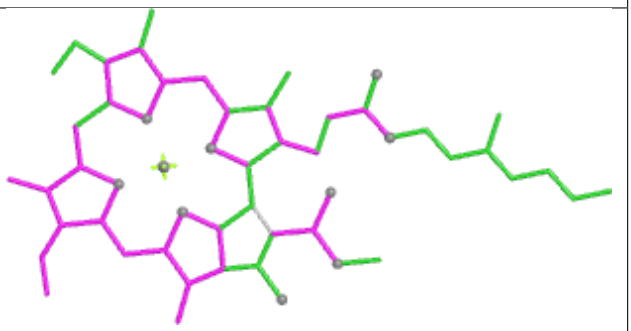
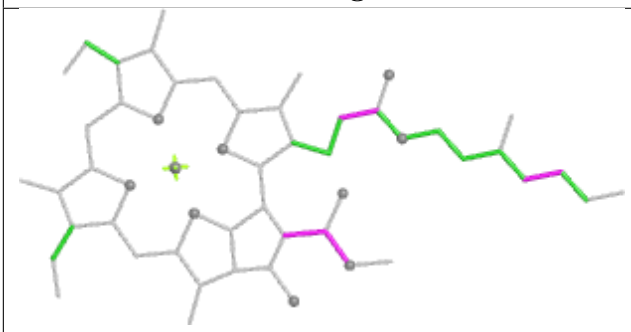


Bond angles



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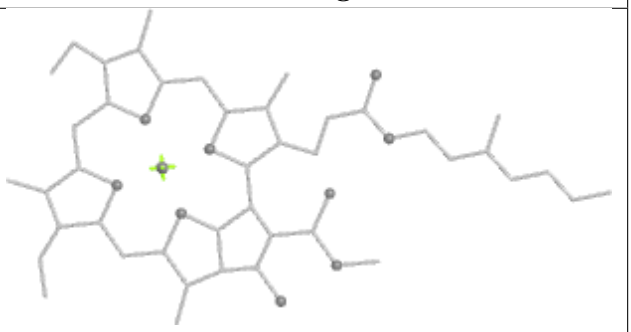
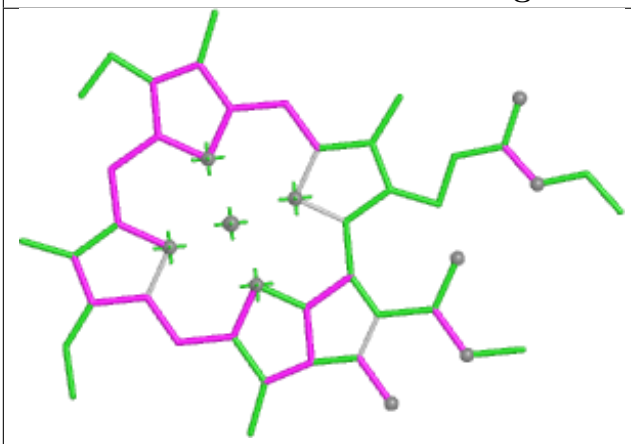


Rings

Ligand CLA bA 824



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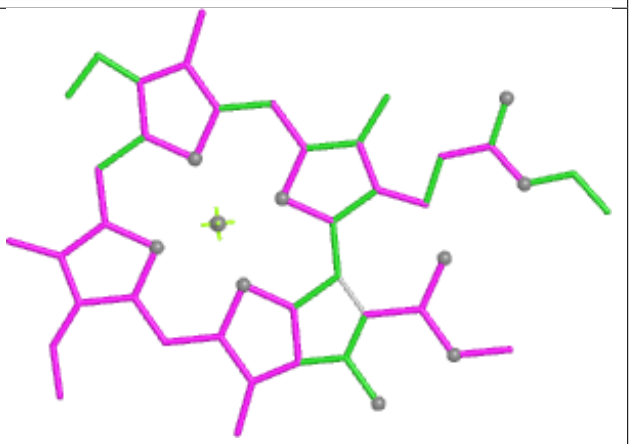
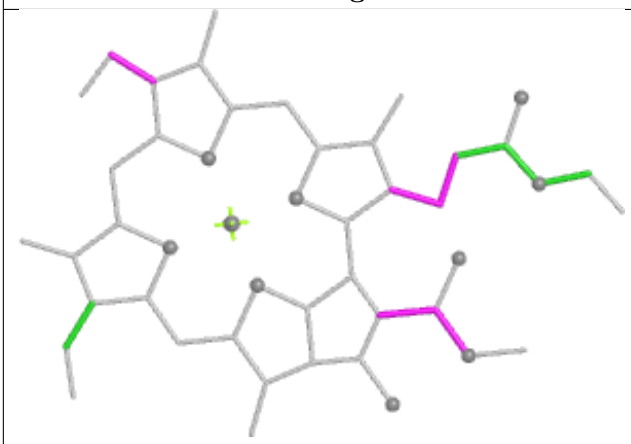


Bond angles



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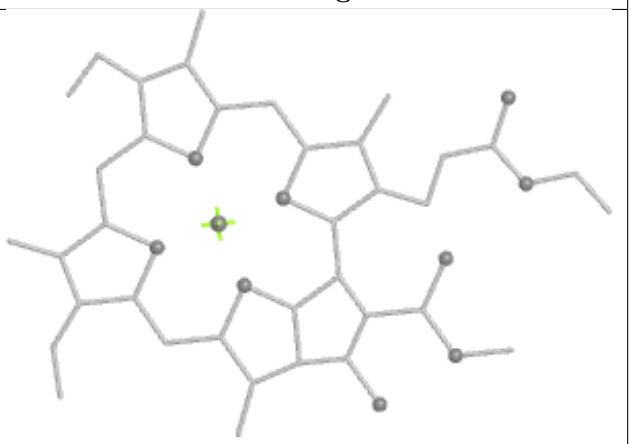
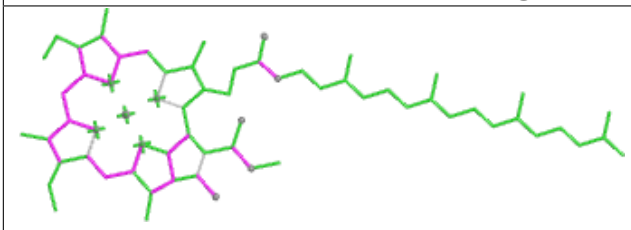


Rings

Ligand CLA aA 842



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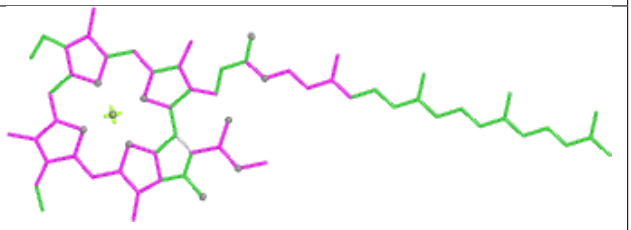

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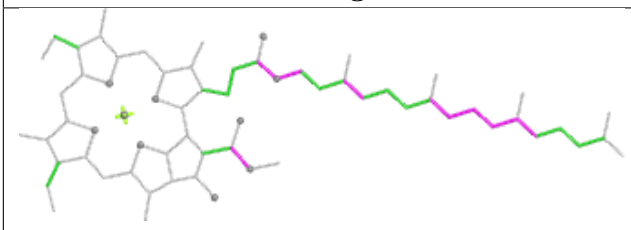

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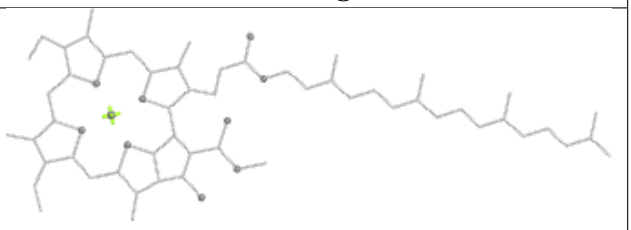
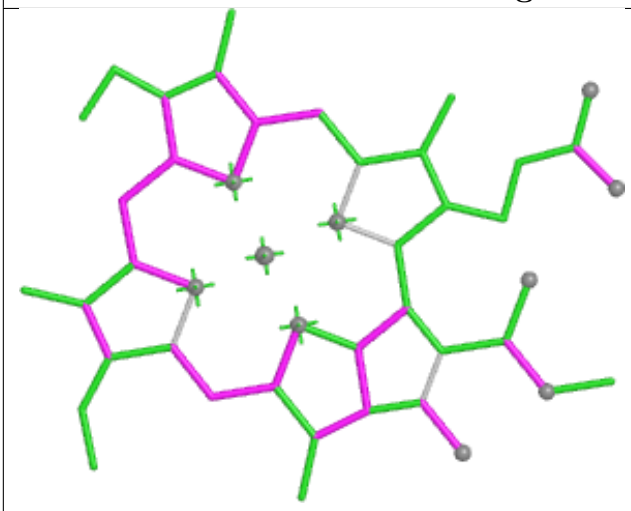


Rings

Ligand CLA aB 932



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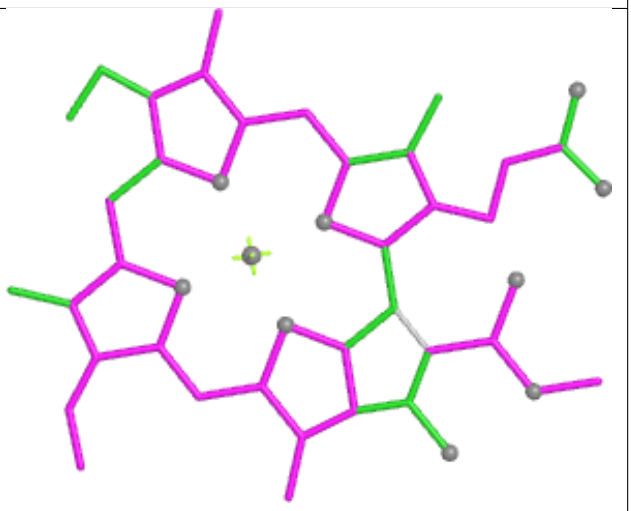
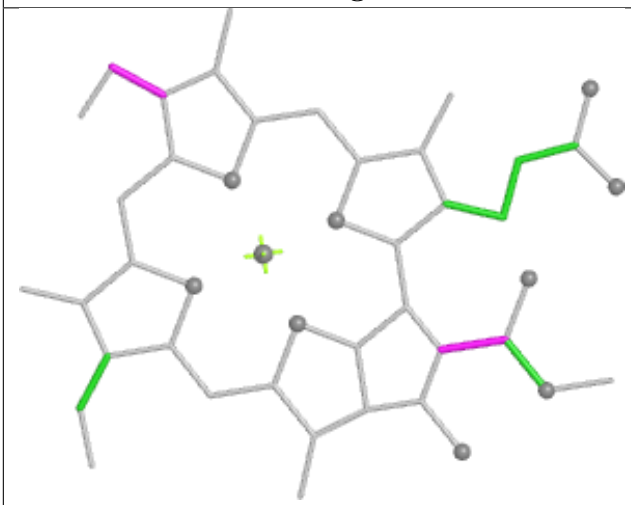


Bond angles



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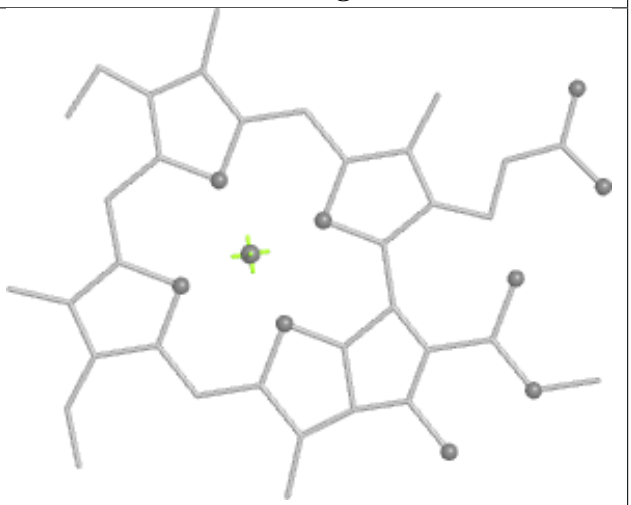
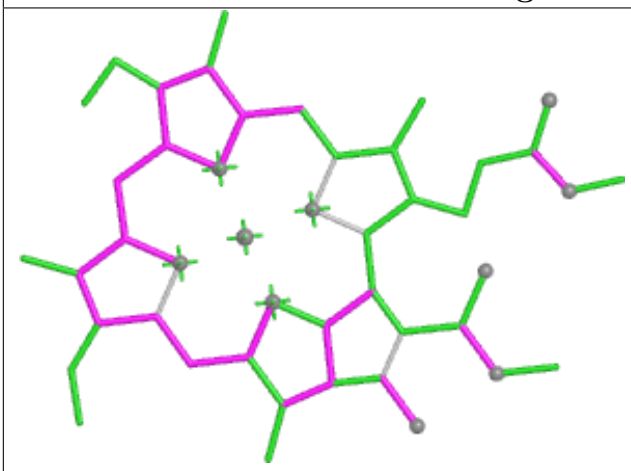


Rings

Ligand CLA cB 924



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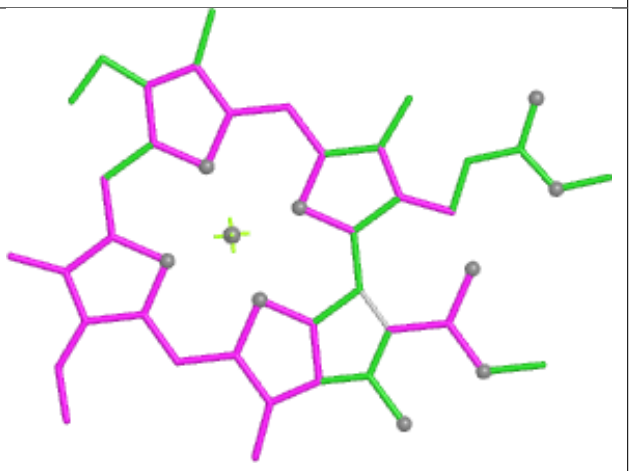
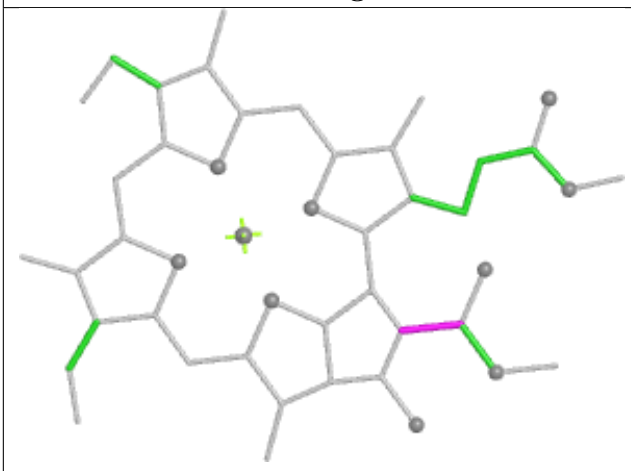


Bond angles



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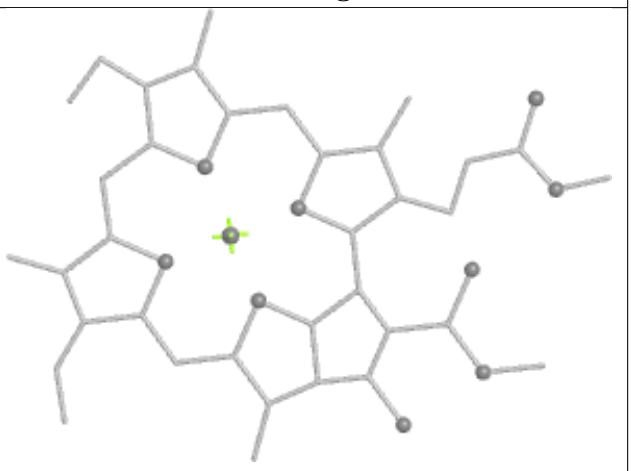
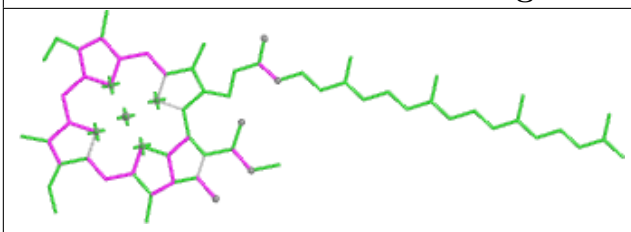


Rings

Ligand CLA cB 904



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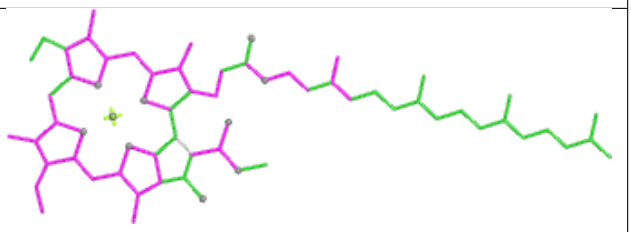
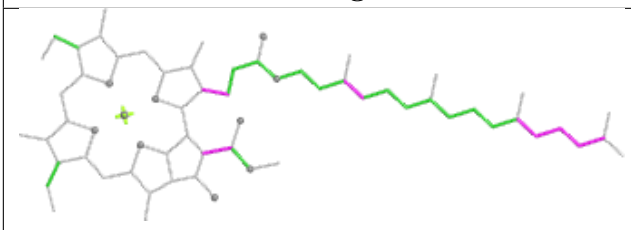
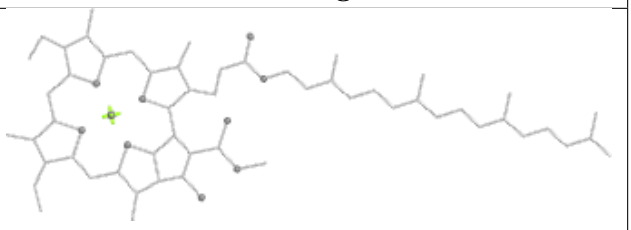


Bond angles

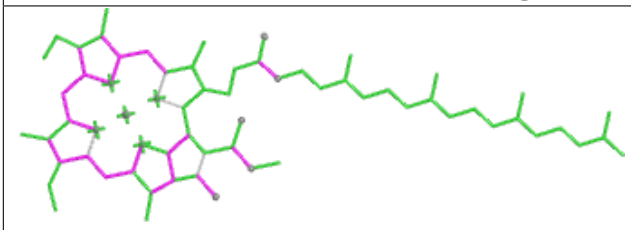


Torsions



Rings

Ligand CLA cA 834



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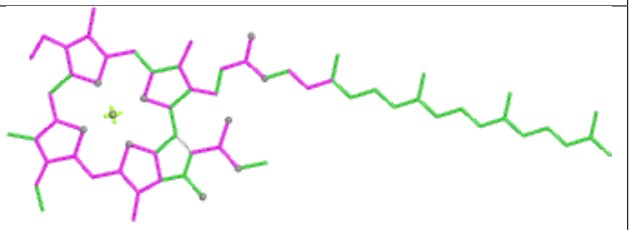
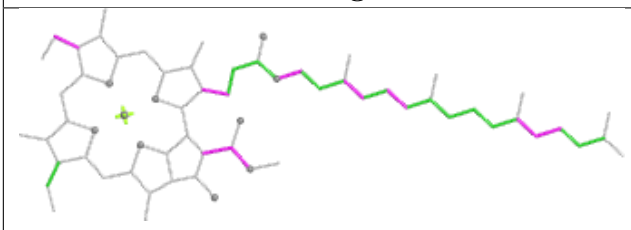
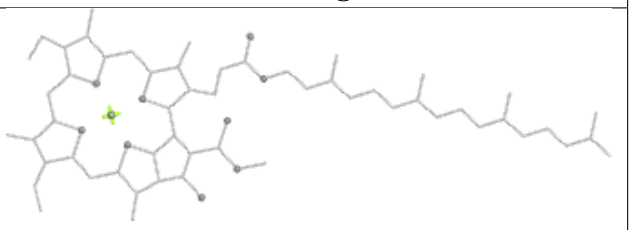


Bond angles



Torsions

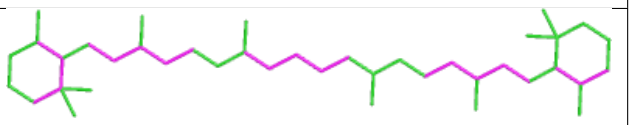


Rings

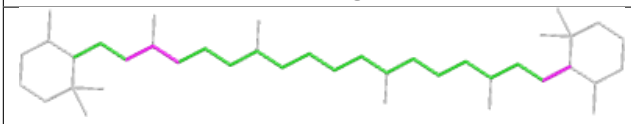
Ligand BCR aF 204



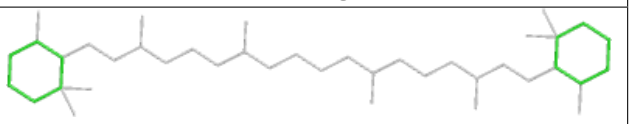
Bond lengths



Bond angles

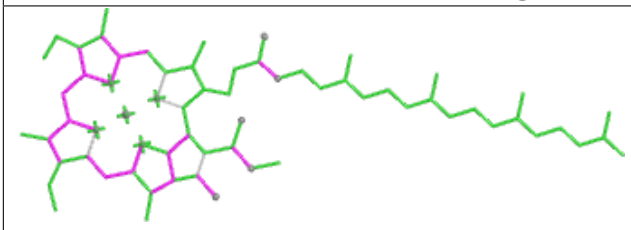


Torsions

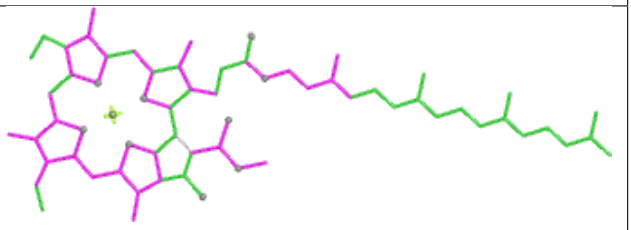


Rings

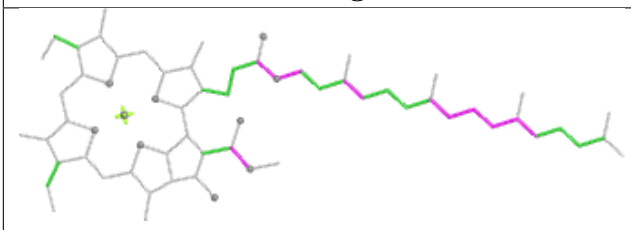
Ligand CLA bA 842



Bond lengths



Bond angles



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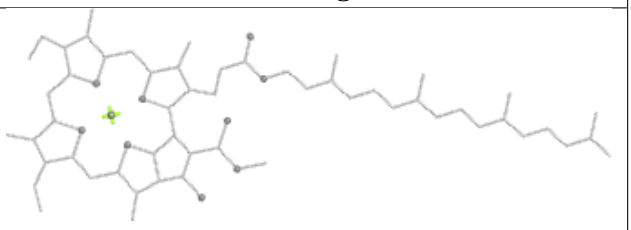
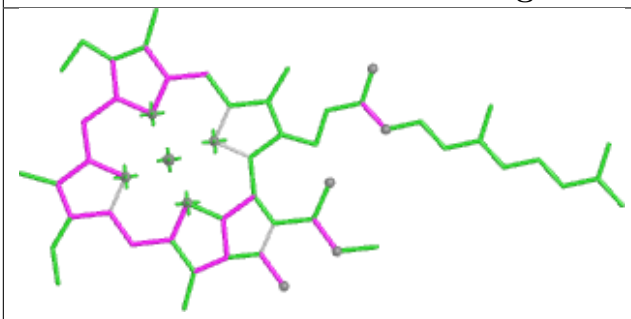
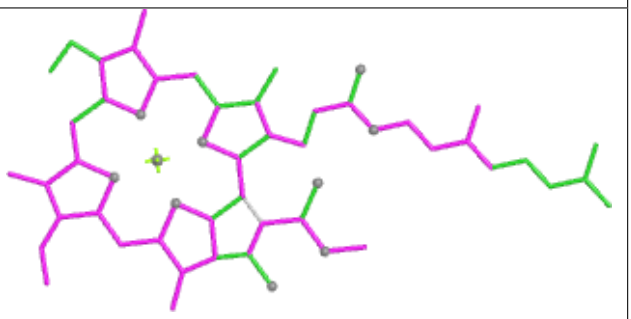


Rings

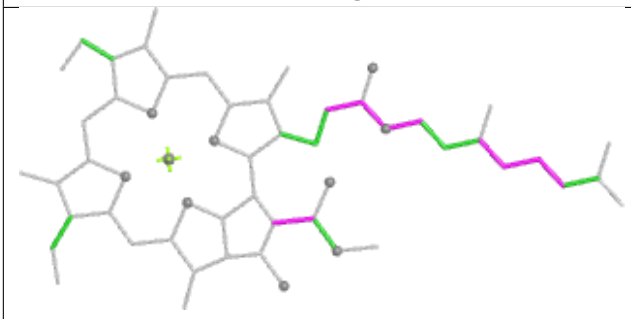
Ligand CLA cB 909



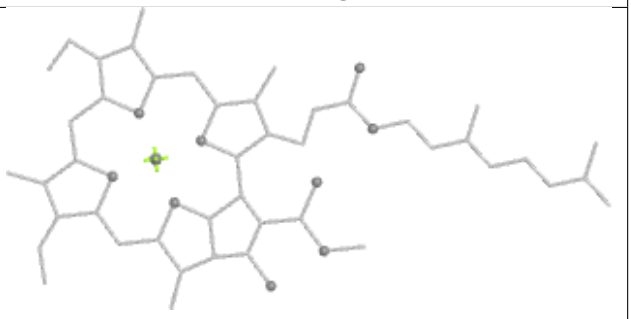
Bond lengths



Bond angles

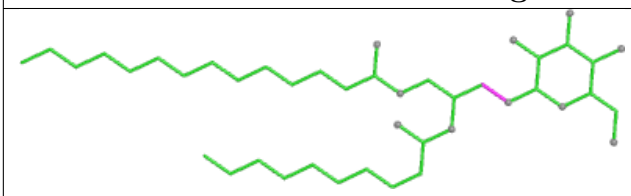


Torsions



Rings

Ligand LMG bB 947



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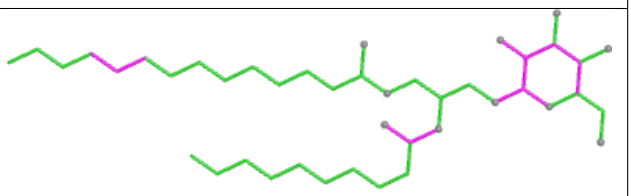
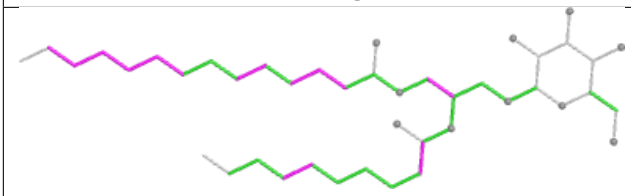
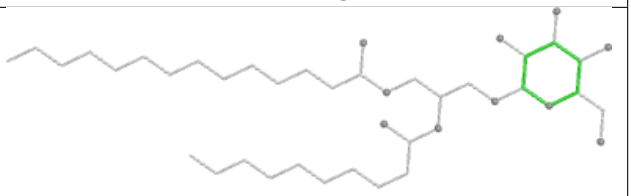


Bond angles

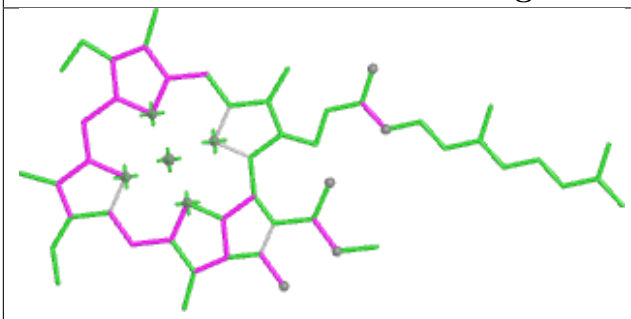


Torsions



Rings

Ligand CLA aA 832



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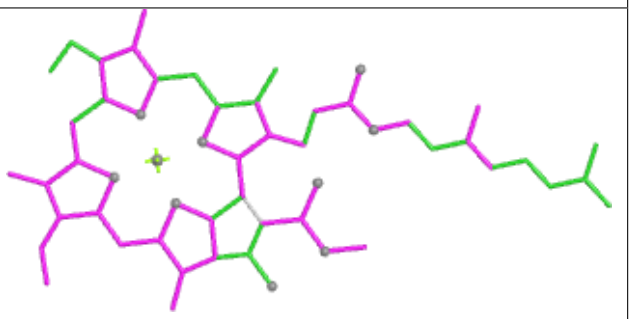
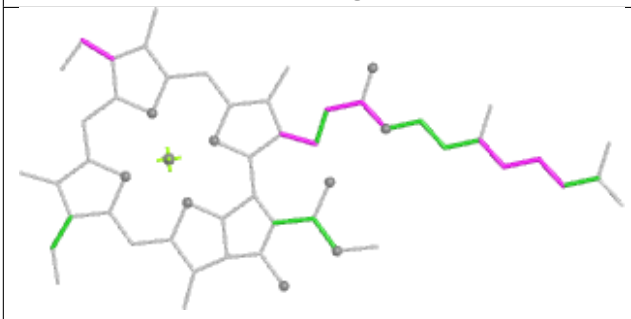


Bond angles



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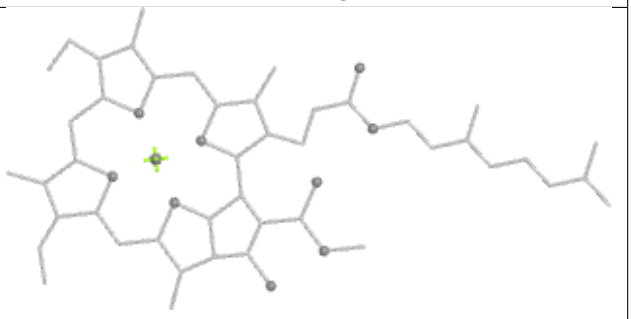
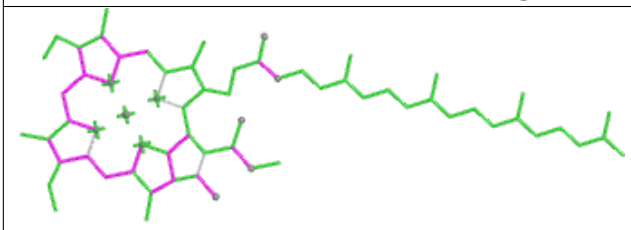


Rings

Ligand CLA aA 840



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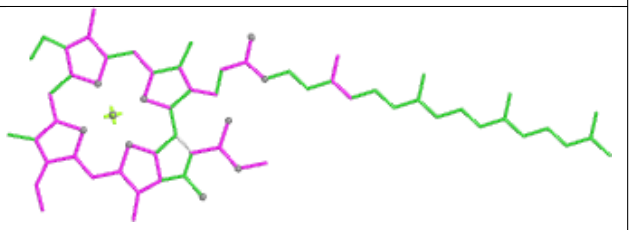
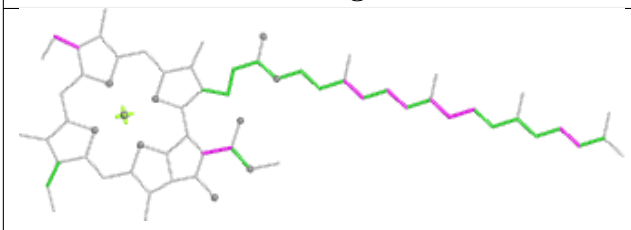


Bond angles



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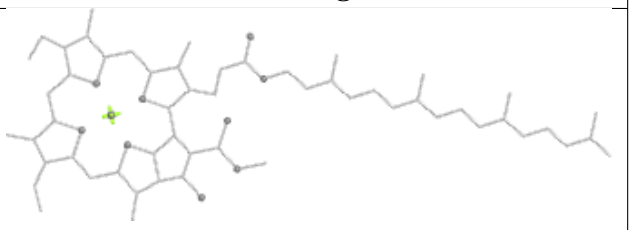
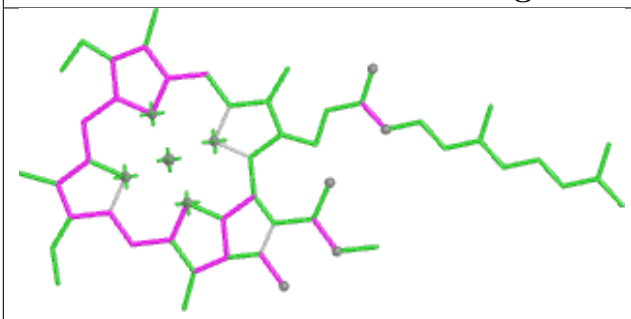


Rings

Ligand CLA bB 921



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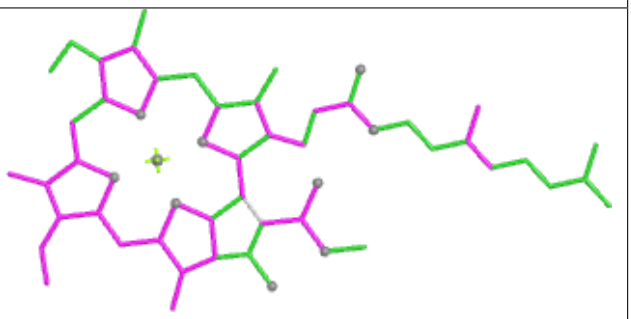
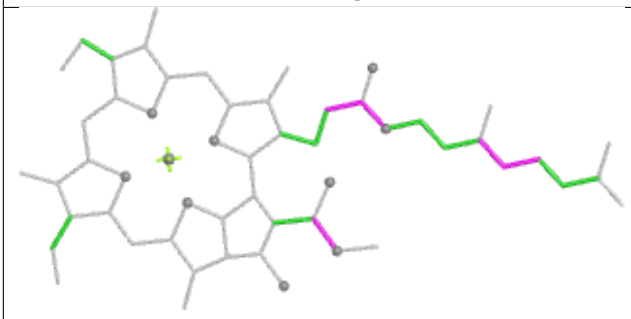


Bond angles



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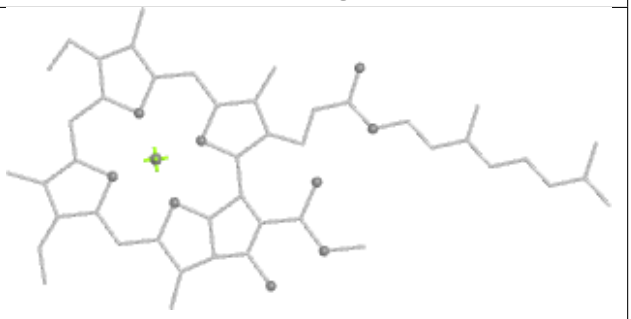
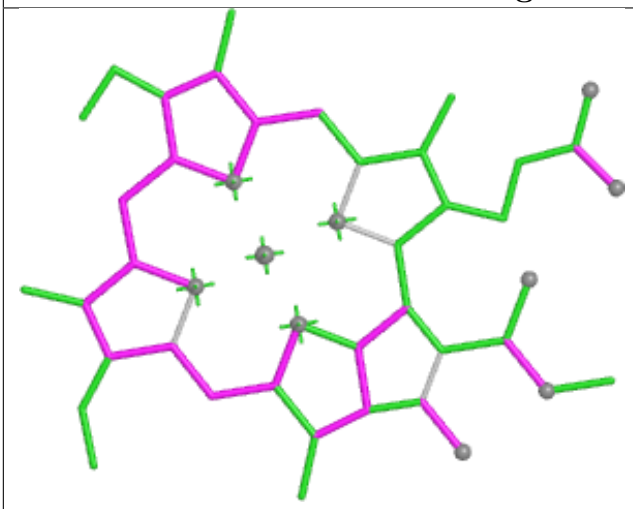


Rings

Ligand CLA cA 816



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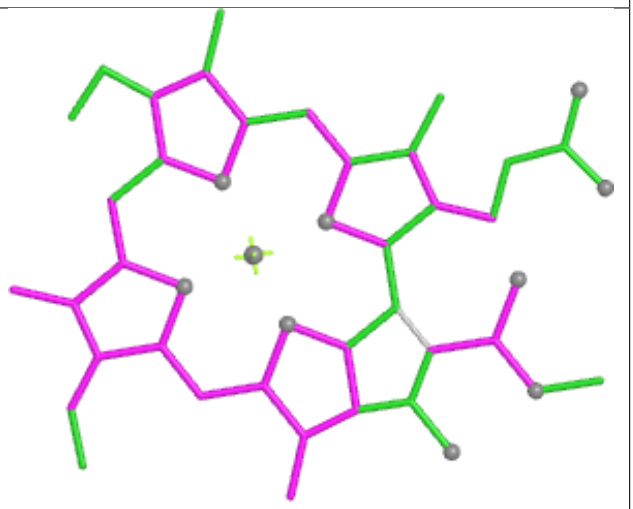
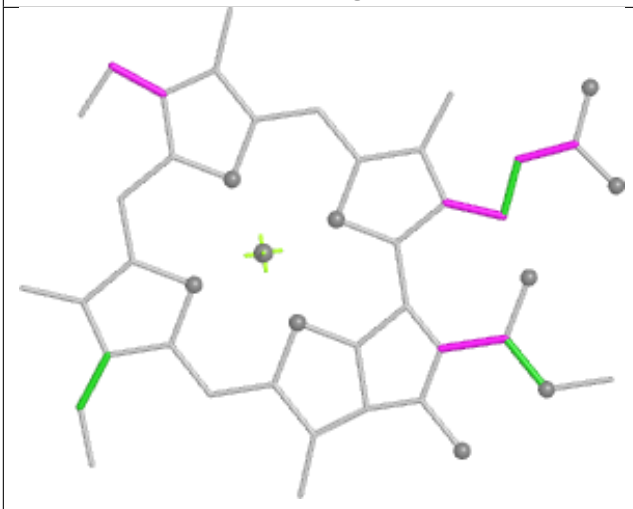


Bond angles

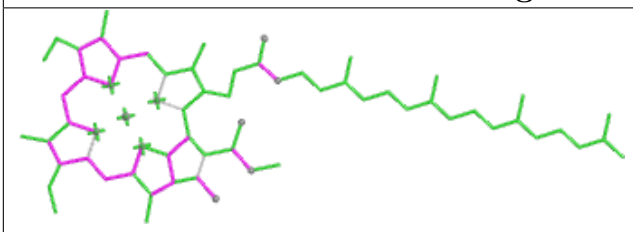


Torsions



Rings

Ligand CLA cA 843



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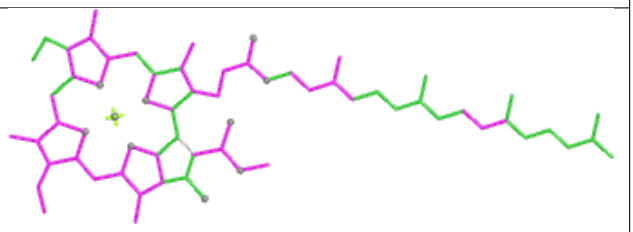
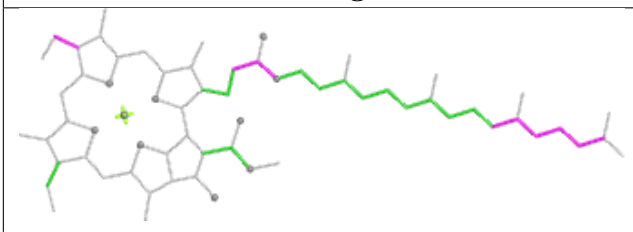
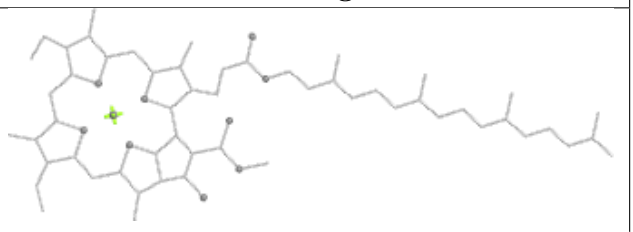


Bond angles

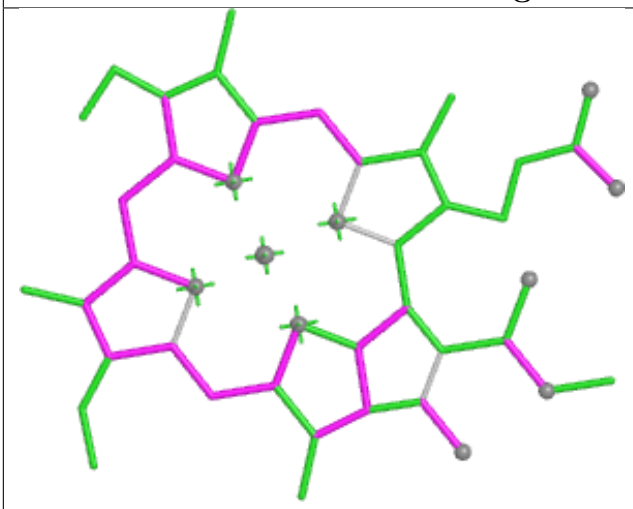


Torsions



Rings

Ligand CLA bA 835



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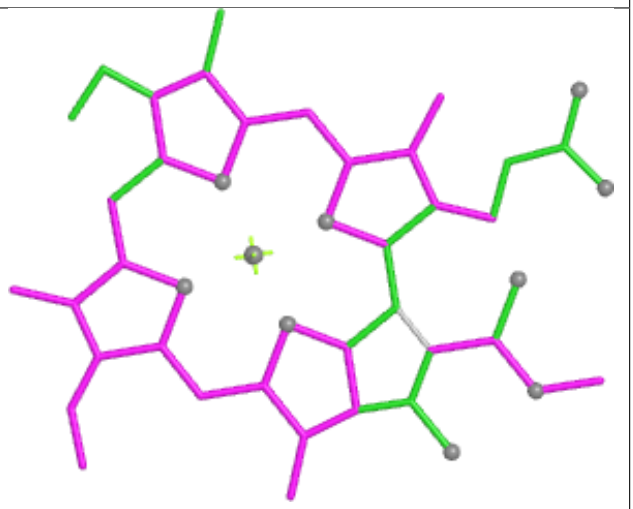
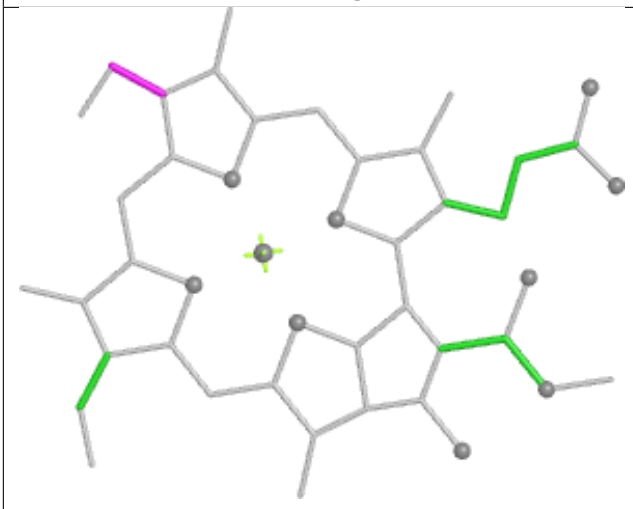


Bond angles

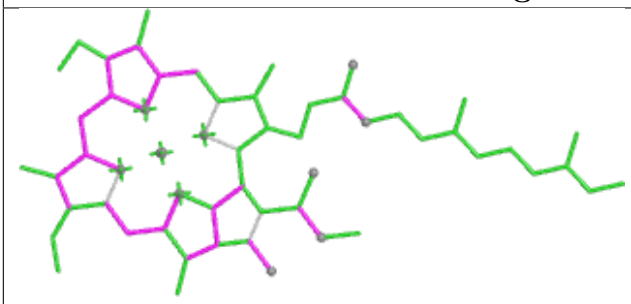


Torsions



Rings

Ligand CLA bA 853



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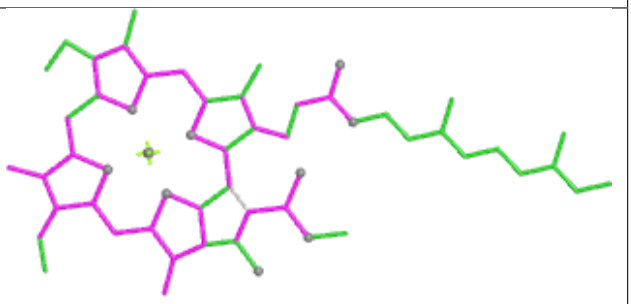
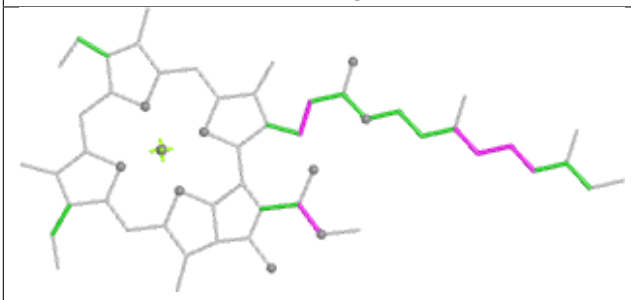
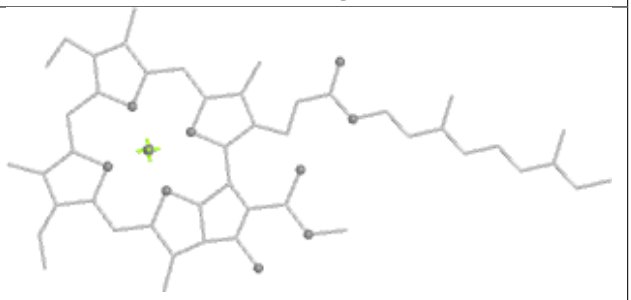


Bond angles

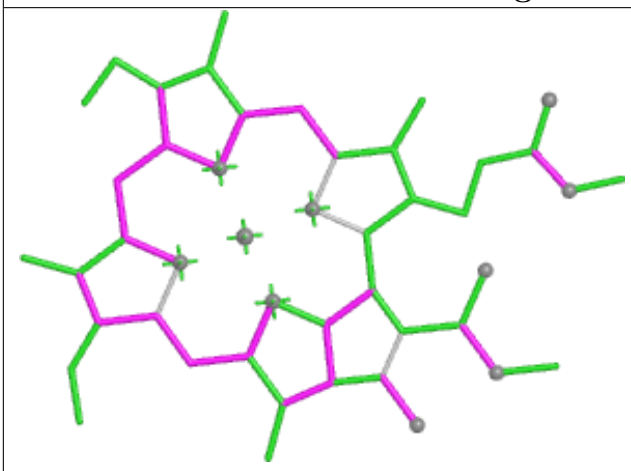


Torsions



Rings

Ligand CLA bB 918



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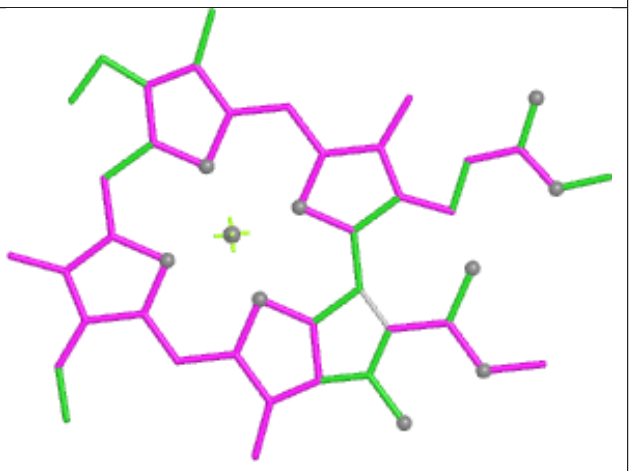
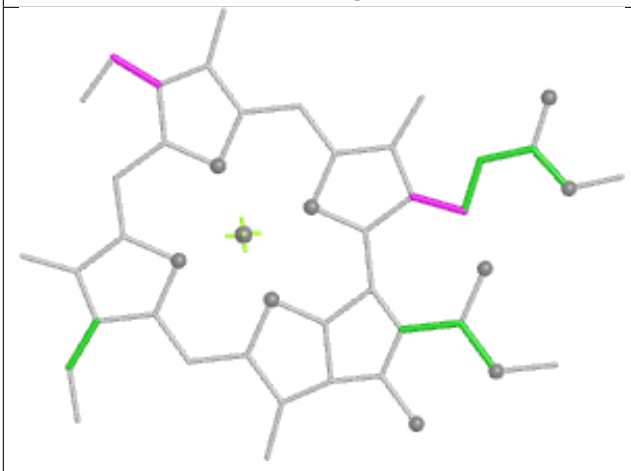


Bond angles

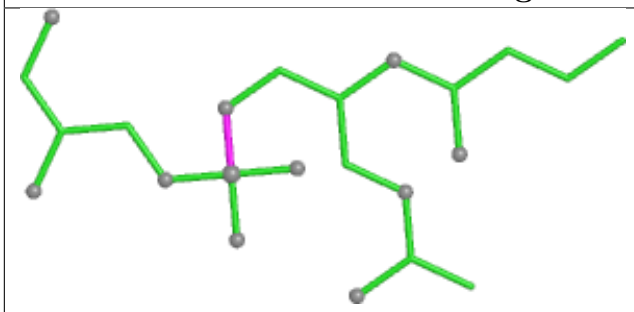


Torsions



Rings

Ligand LHG aB 948



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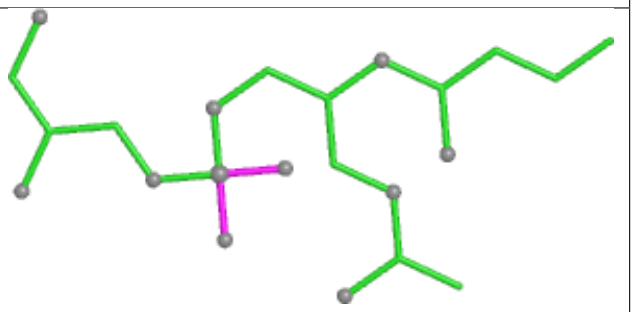
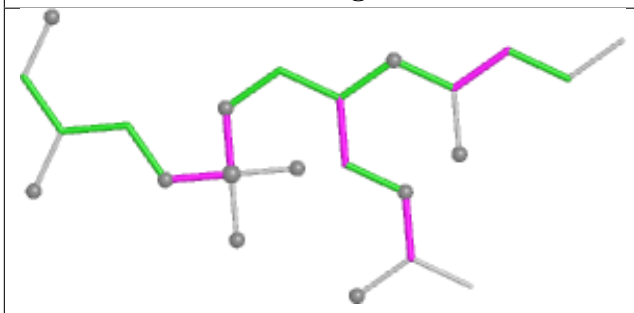
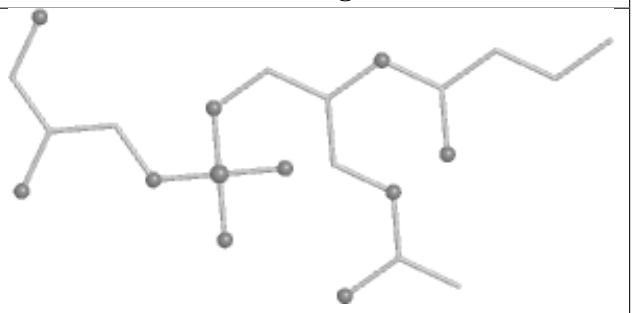


Bond angles

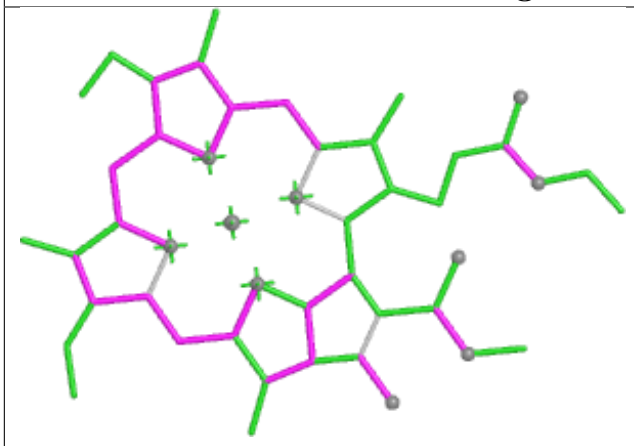


Torsions



Rings

Ligand CLA aA 824



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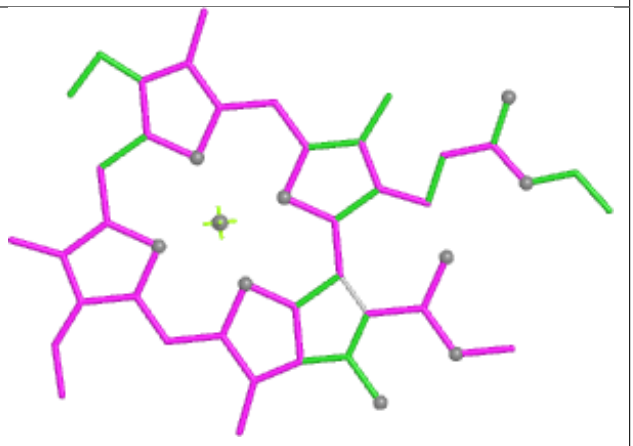
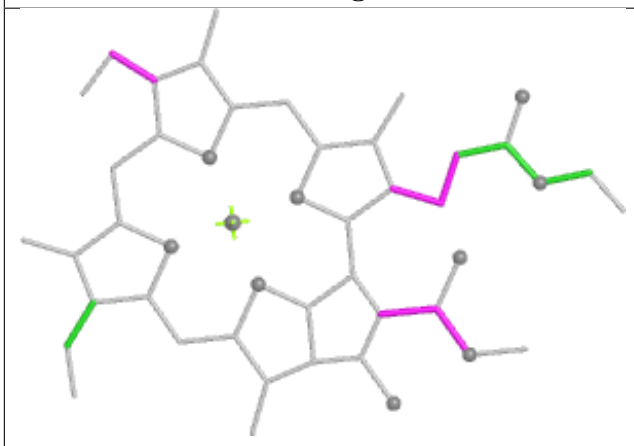
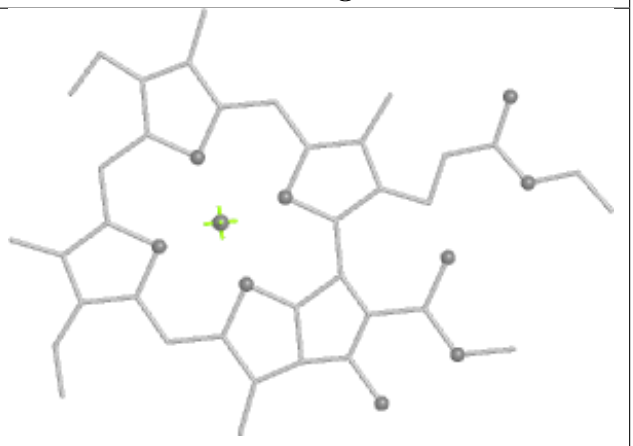


Bond angles

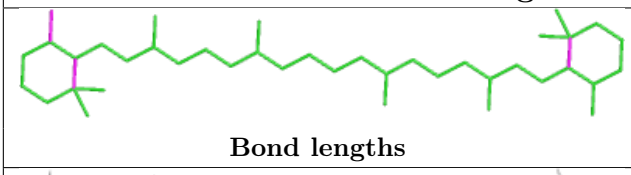


Torsions

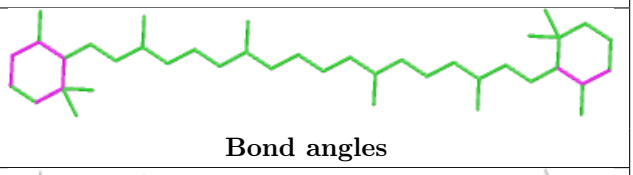


Rings

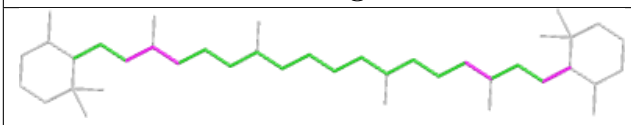
Ligand BCR cL 201



Bond lengths



Bond angles



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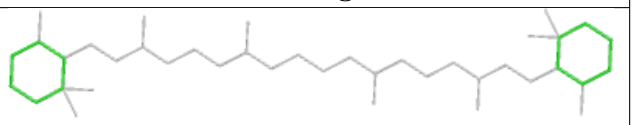
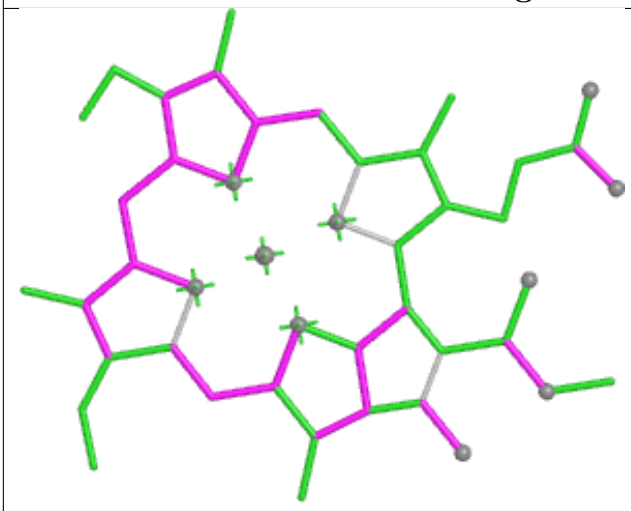


Rings

Ligand CLA aA 839



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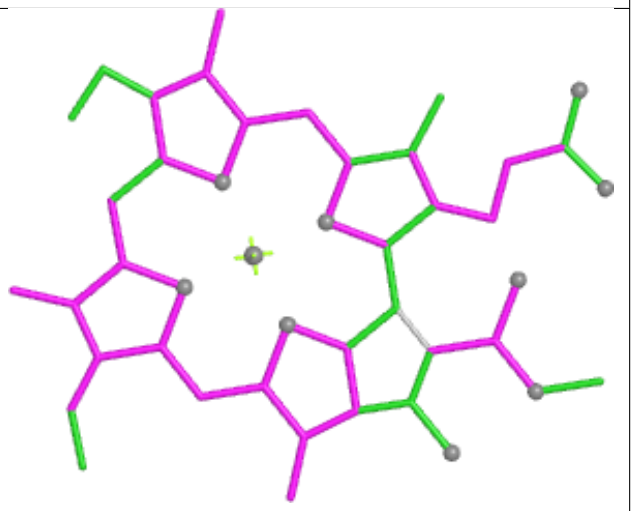
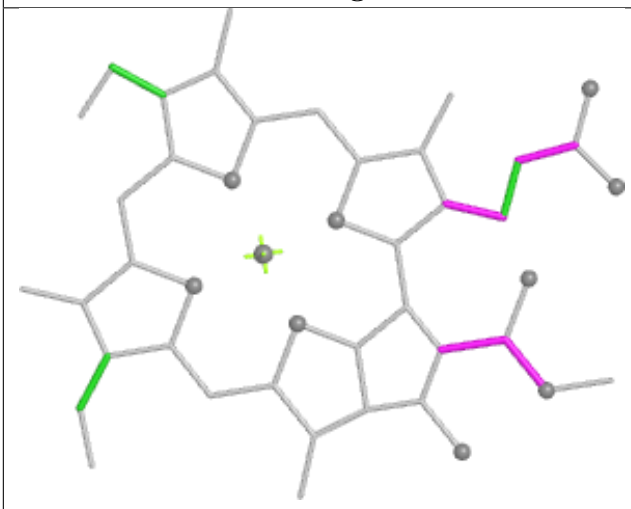
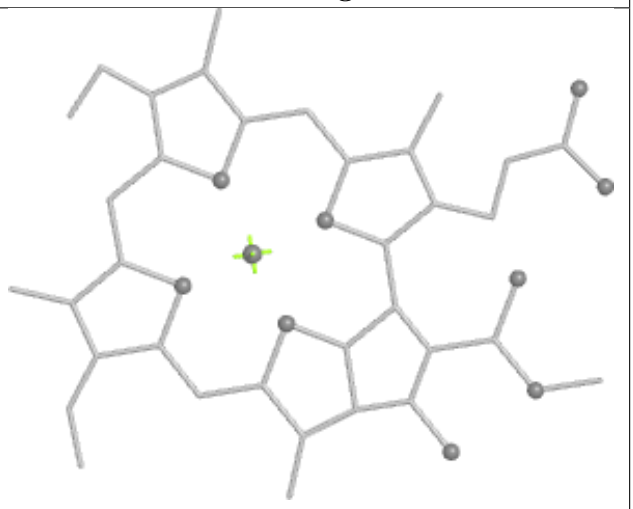


Bond angles

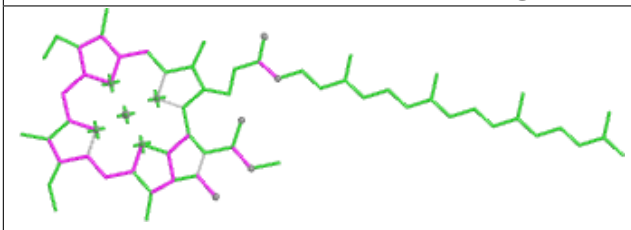


Torsions

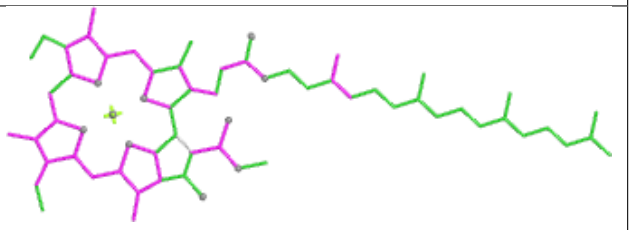


Rings

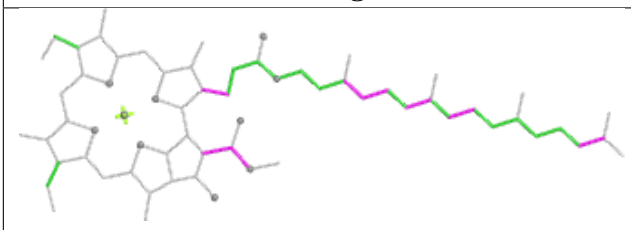
Ligand CLA bA 806



Bond lengths



Bond angles



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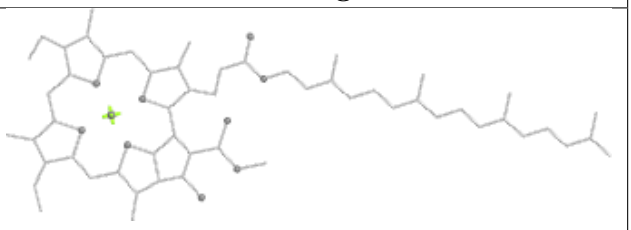
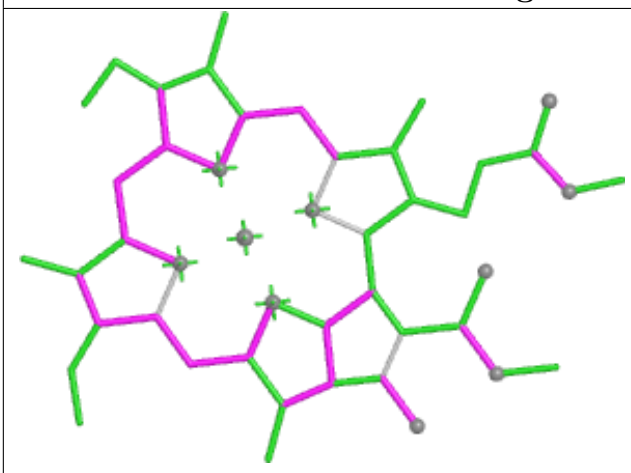


Rings

Ligand CLA cB 918



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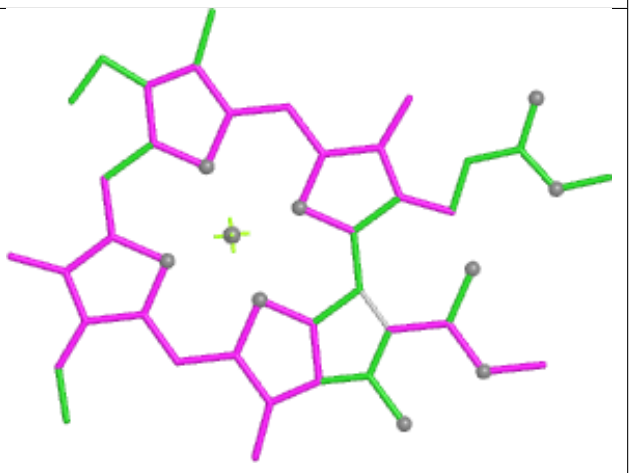
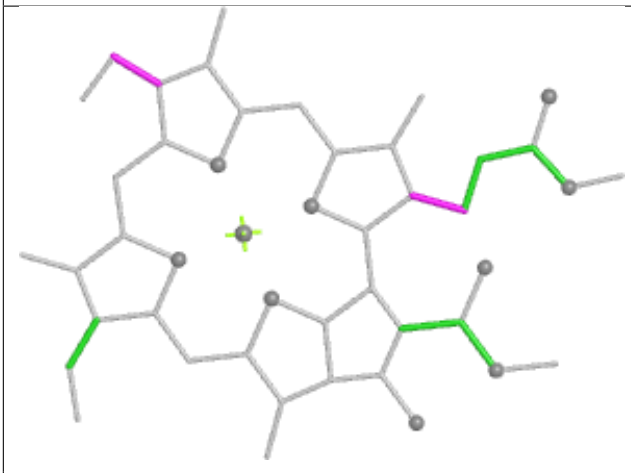


Bond angles



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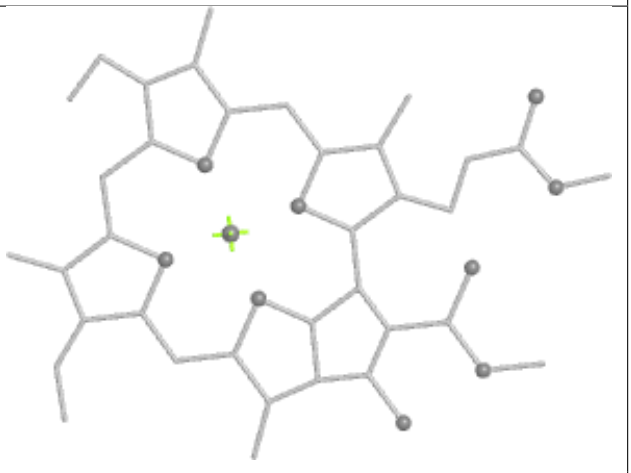
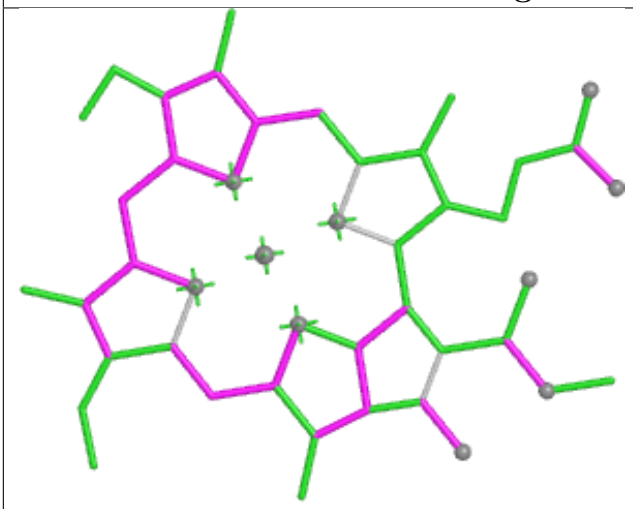


Rings

Ligand CLA bB 922



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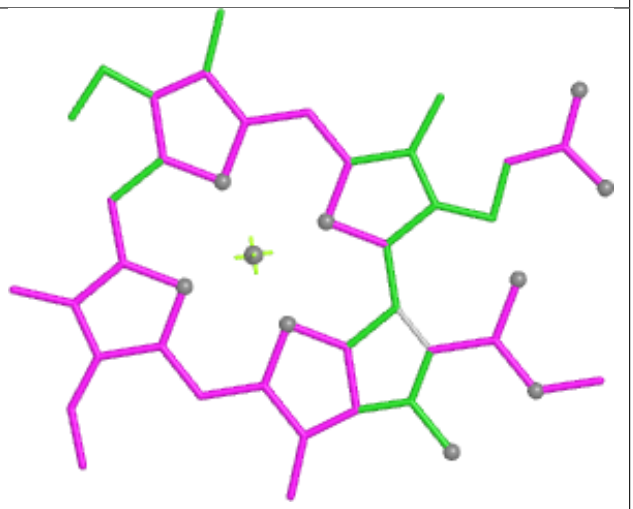
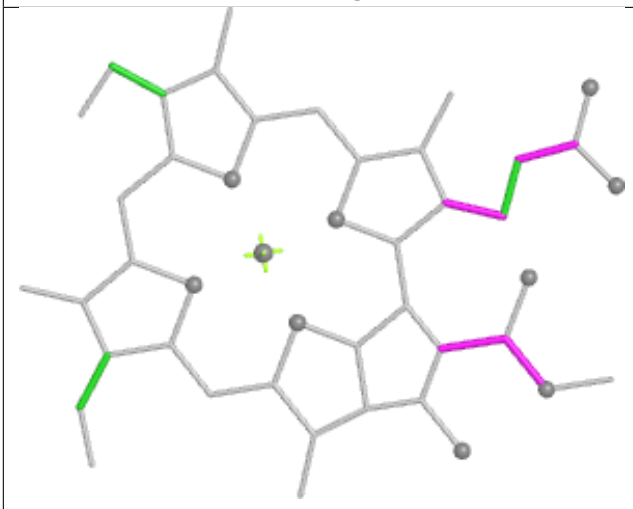


Bond angles

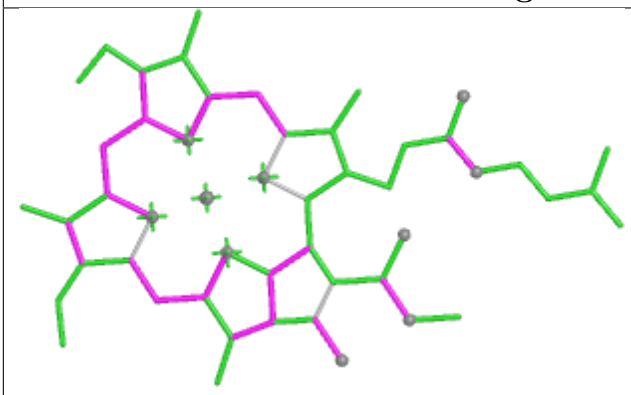


Torsions



Rings

Ligand CLA cA 821



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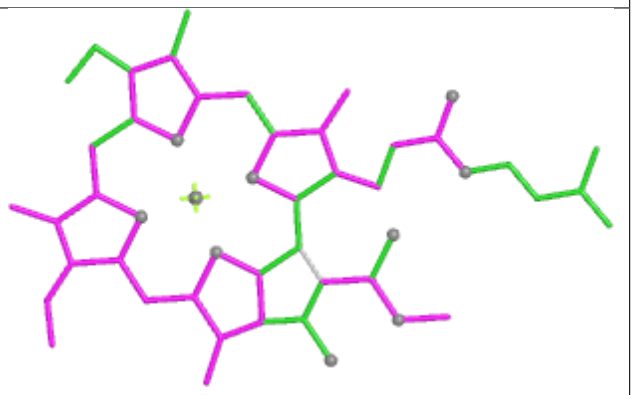
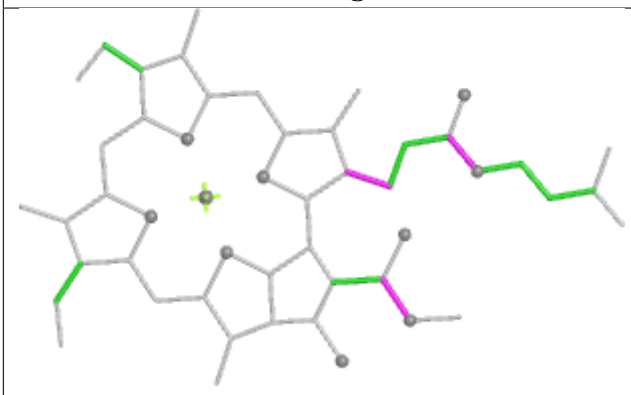


Bond angles



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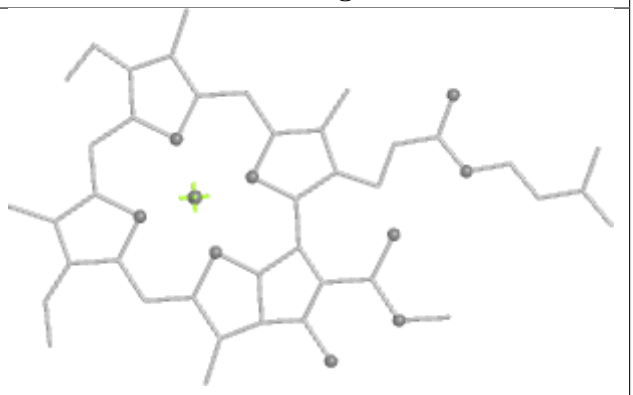
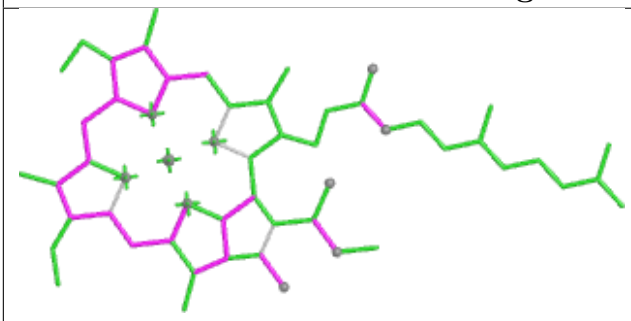


Rings

Ligand CLA cB 921



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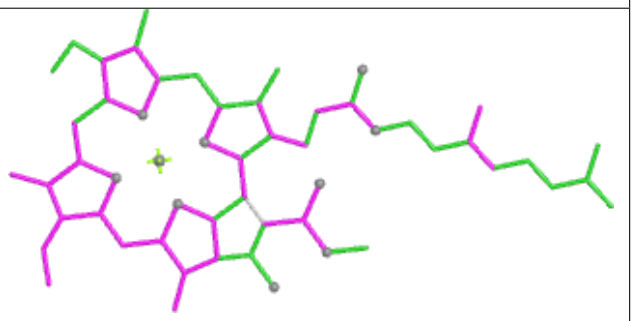
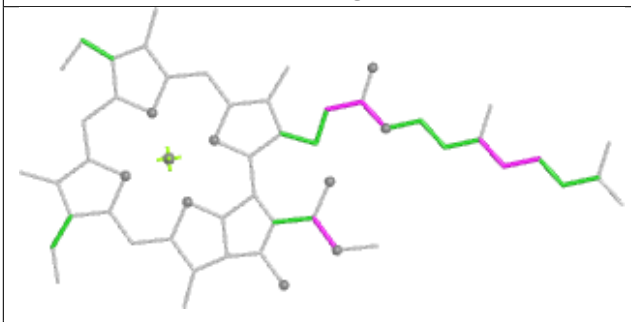


Bond angles



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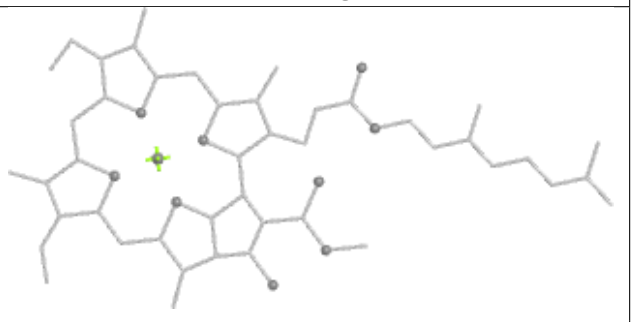
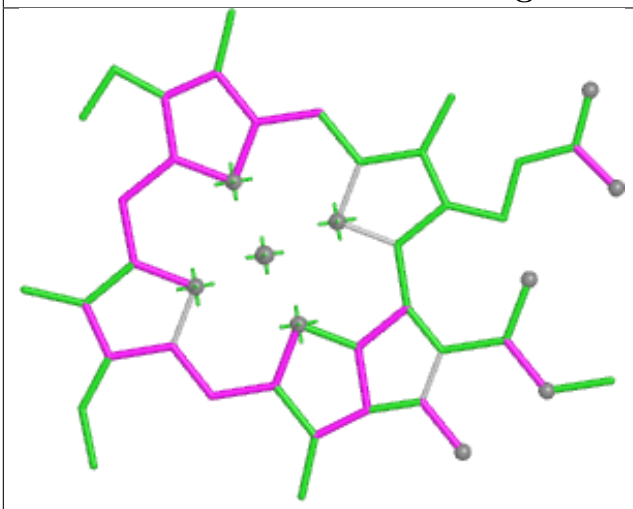


Rings

Ligand CLA aB 950



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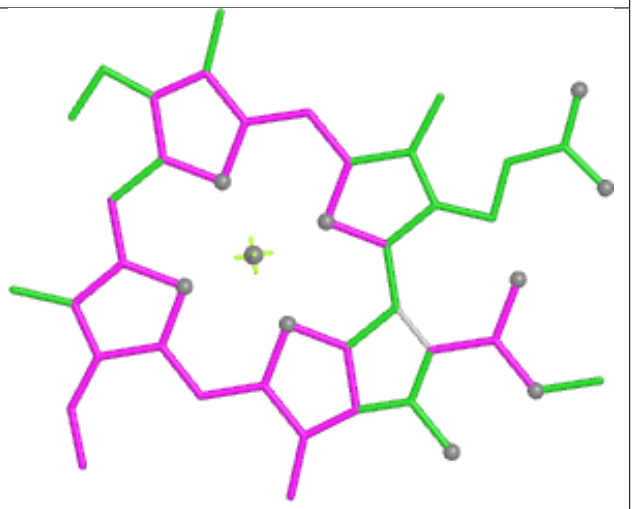
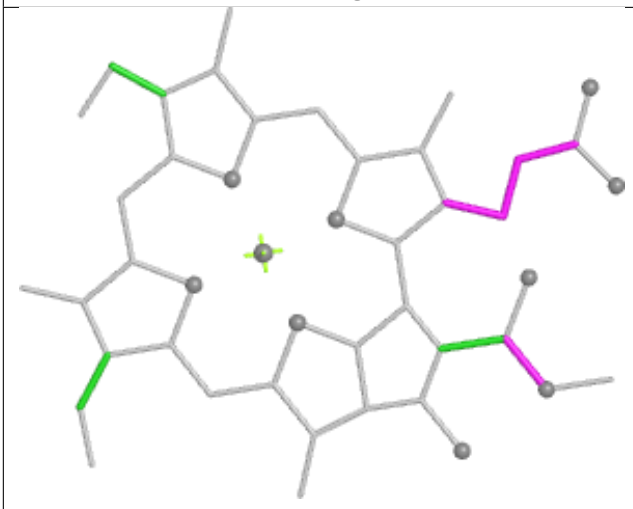


Bond angles

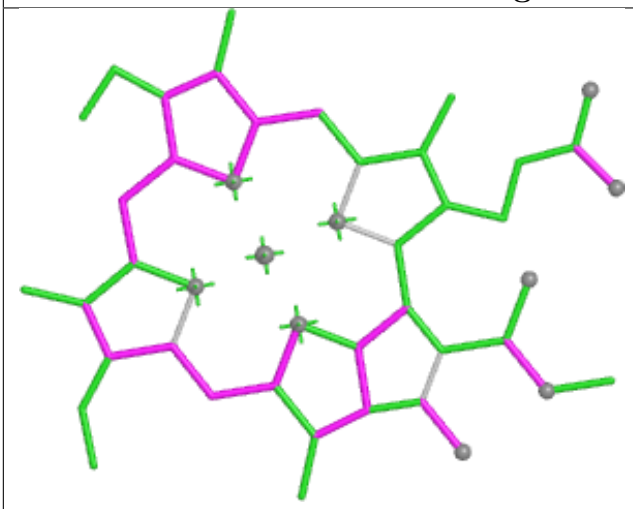


Torsions



Rings

Ligand CLA bA 815



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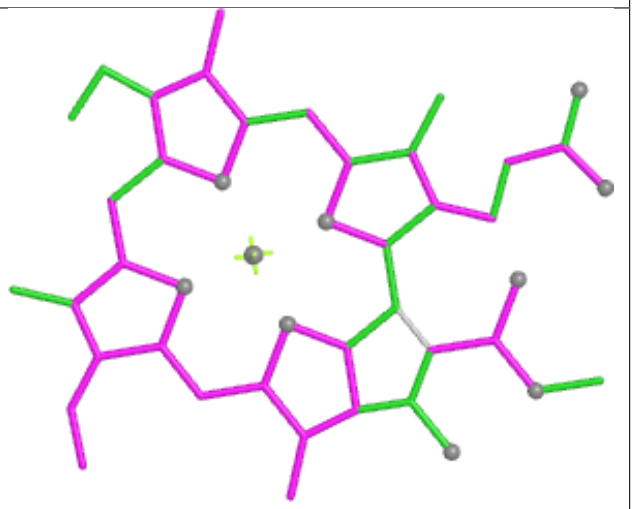
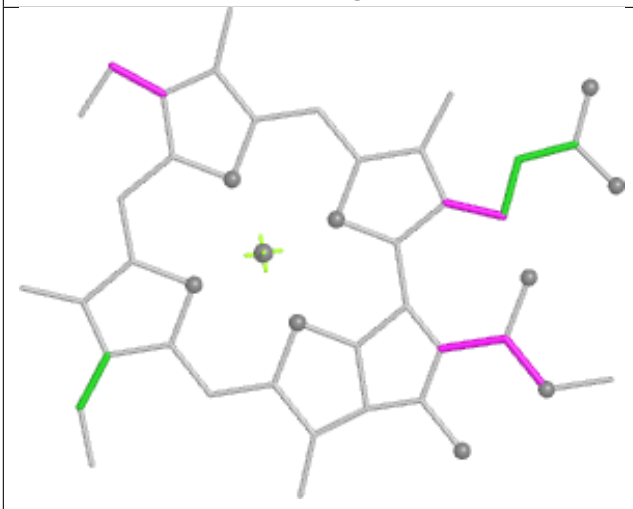


Bond angles

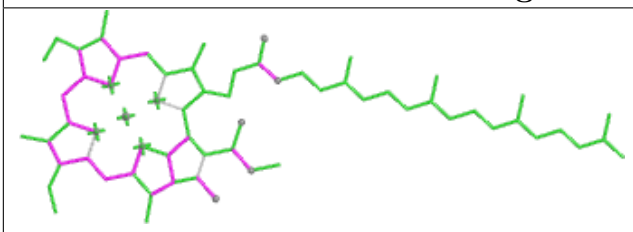


Torsions



Rings

Ligand CLA cA 840



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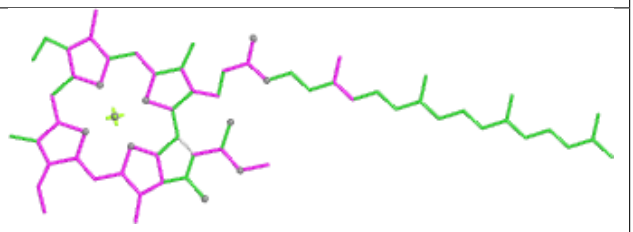
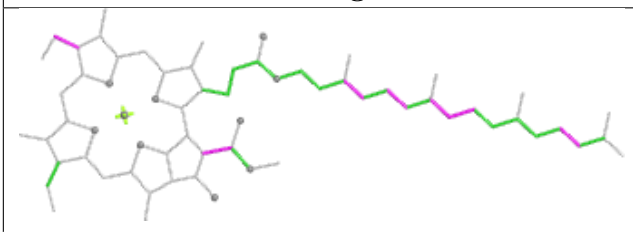


Bond angles



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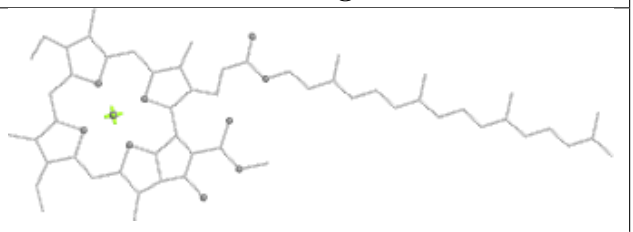
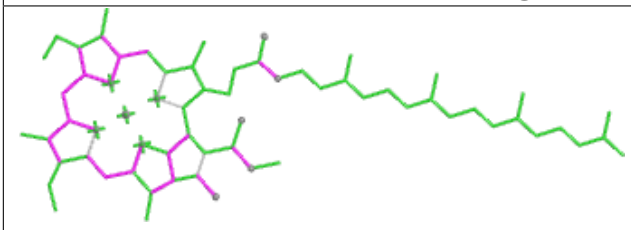


Rings

Ligand CLA cA 842



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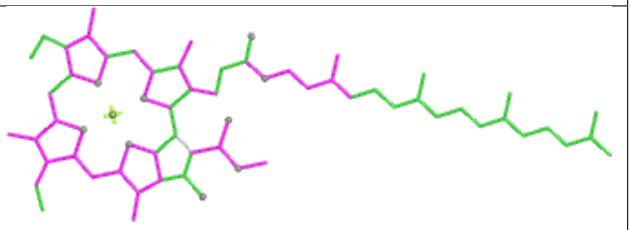
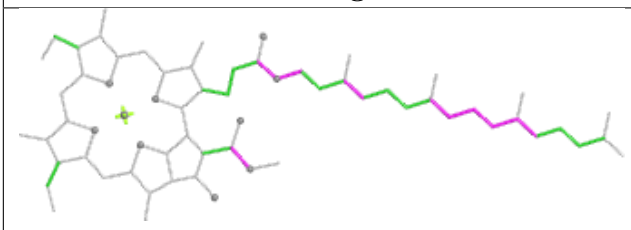


Bond angles



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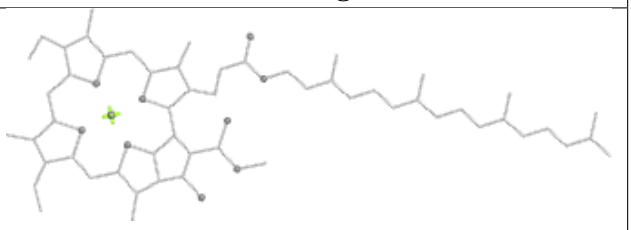
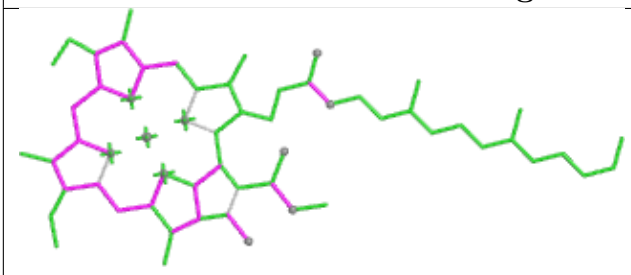


Rings

Ligand CLA cB 936



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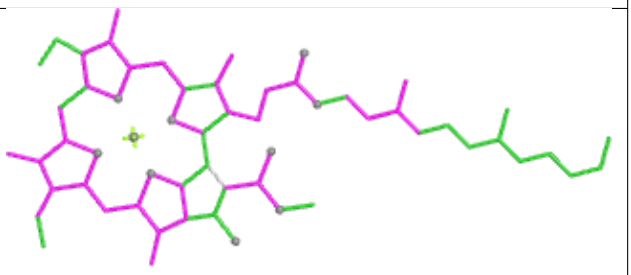
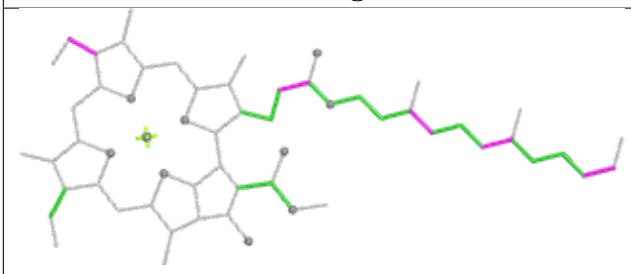


Bond angles



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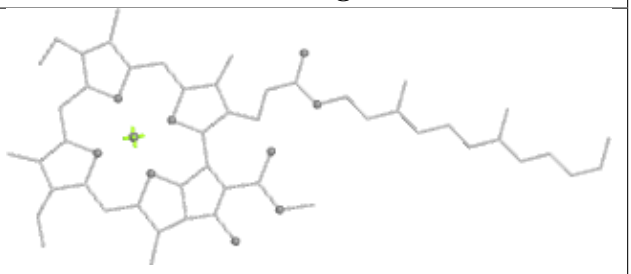
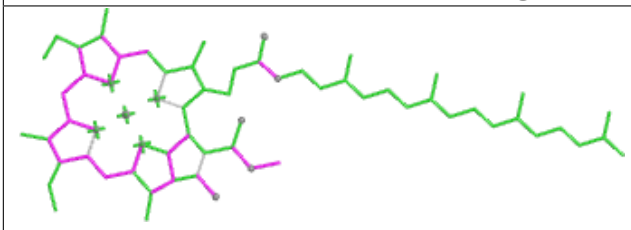


Rings

Ligand CLA bB 912



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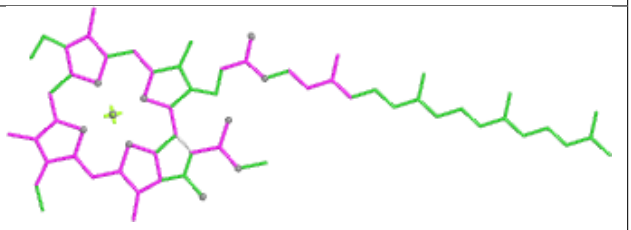
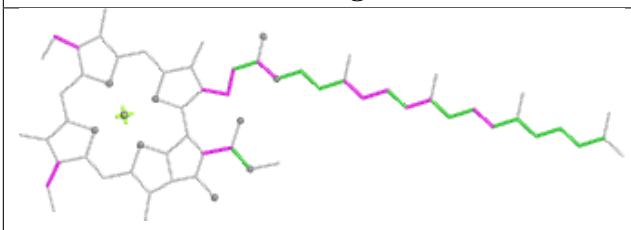
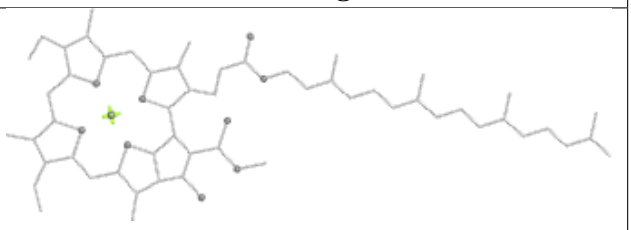


Bond angles

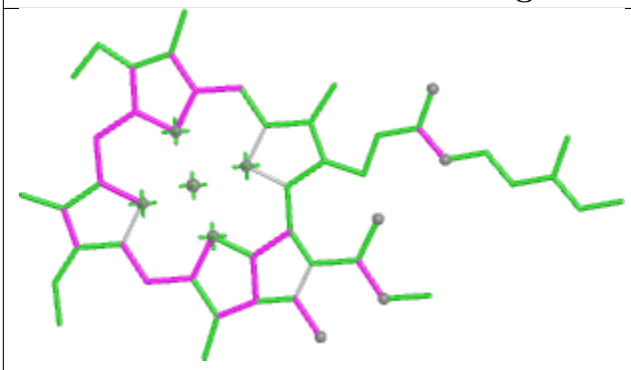


Torsions



Rings

Ligand CLA cA 833



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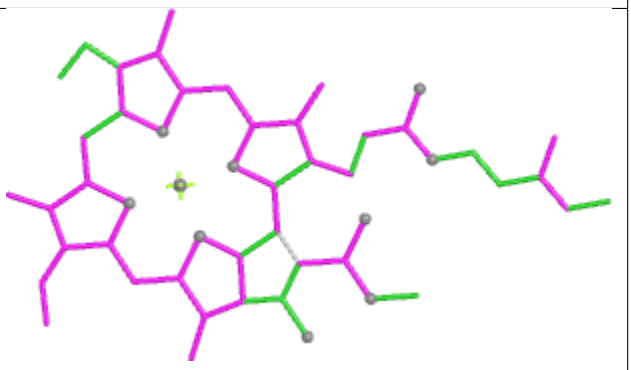
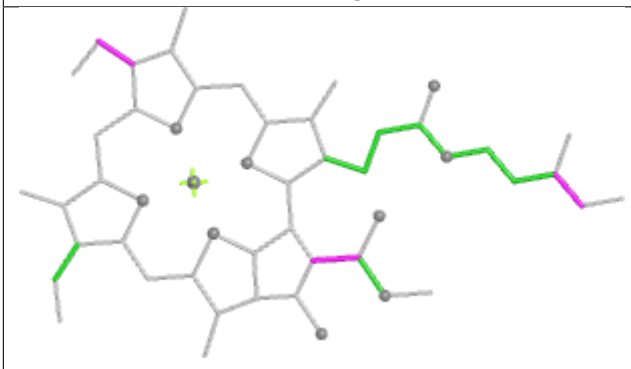


Bond angles



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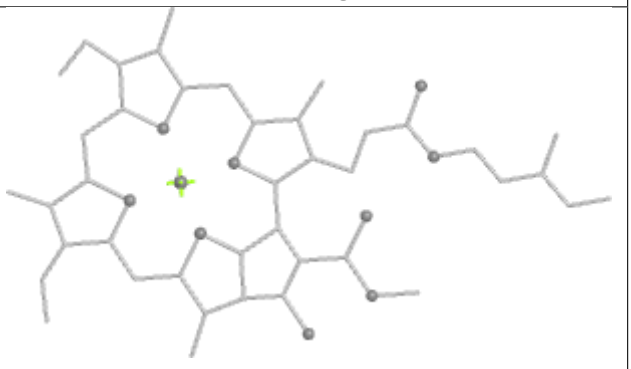
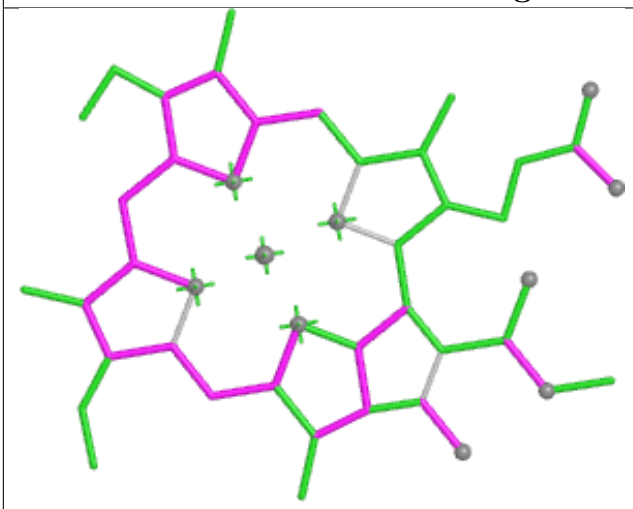


Rings

Ligand CLA bA 813



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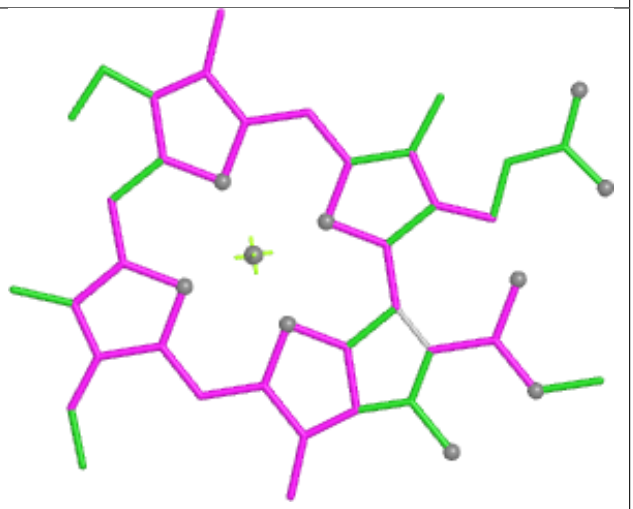
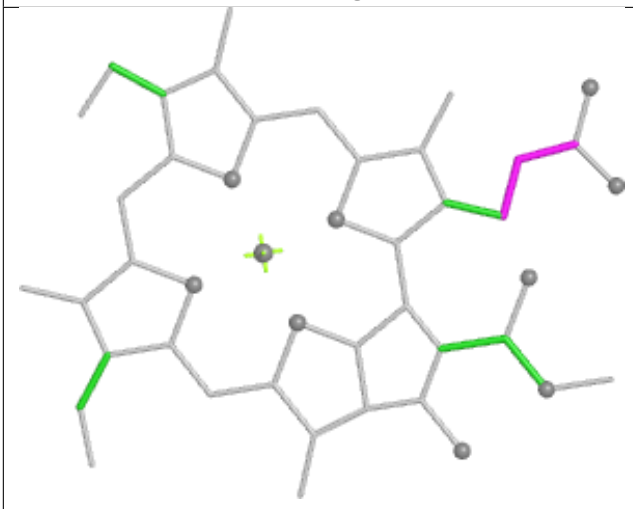


Bond angles

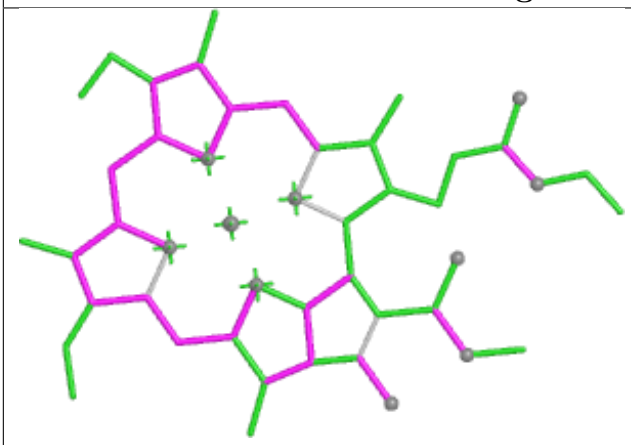


Torsions



Rings

Ligand CLA aB 937



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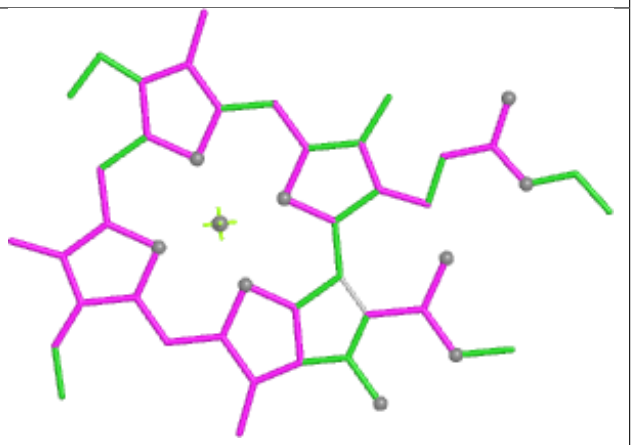
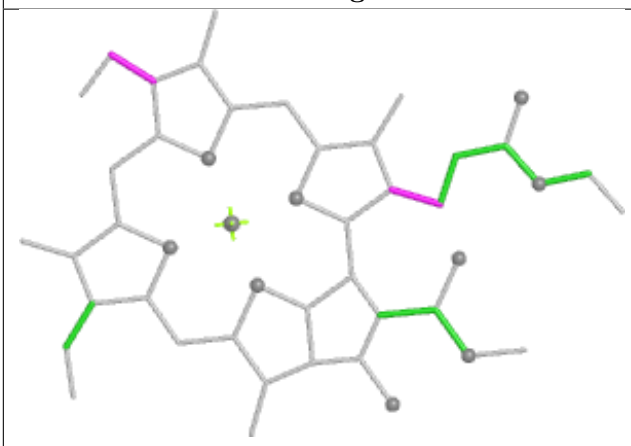
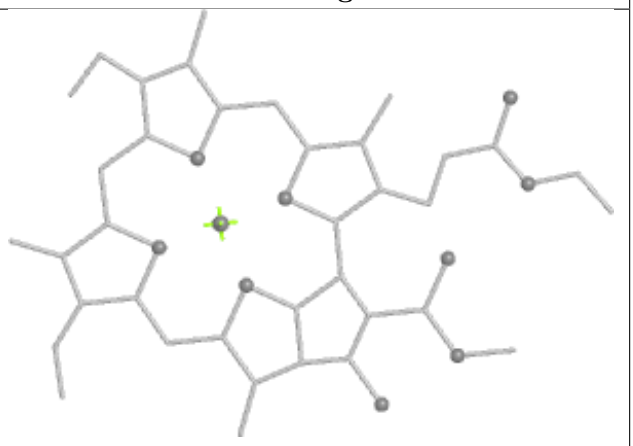


Bond angles

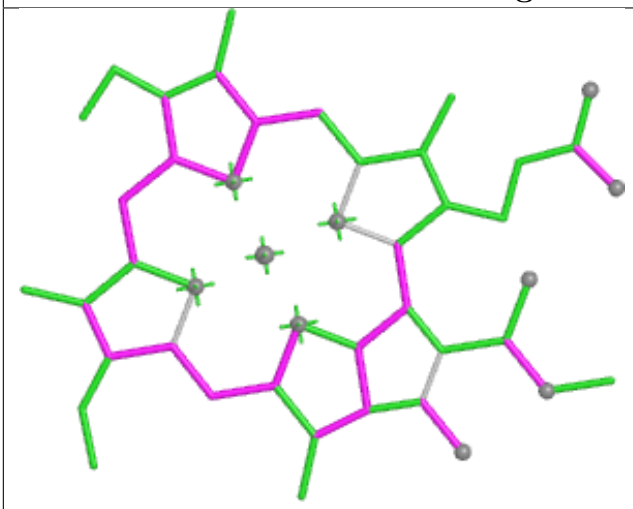


Torsions



Rings

Ligand CLA cA 836



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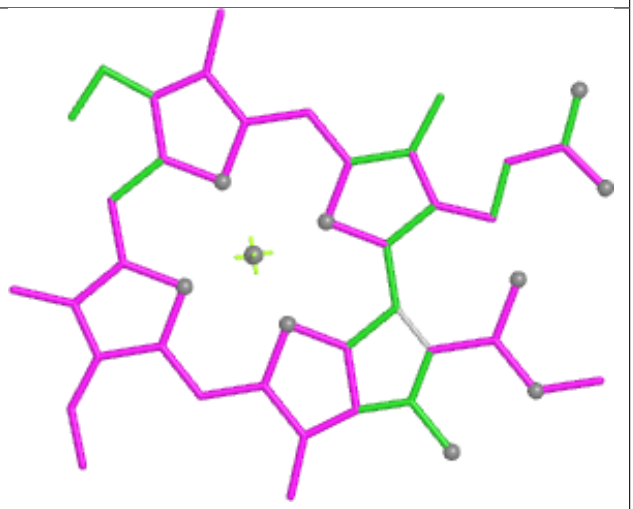
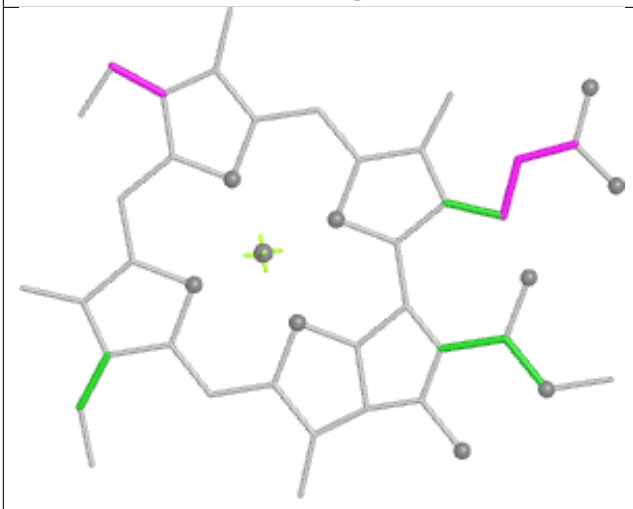


Bond angles

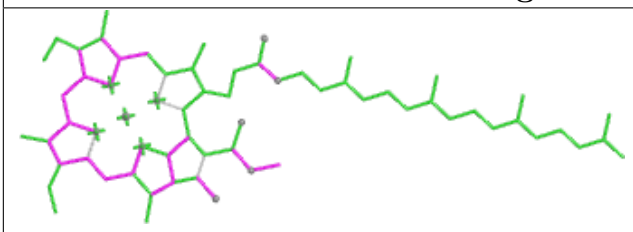


Torsions

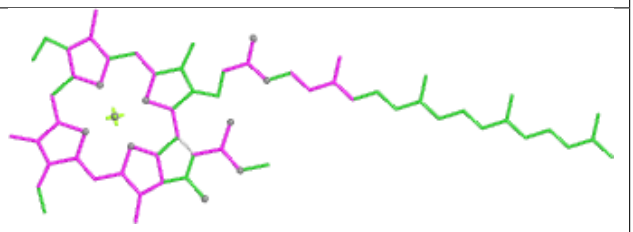


Rings

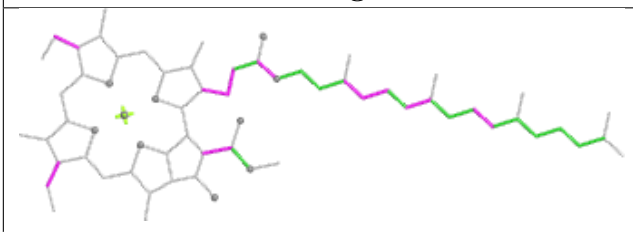
Ligand CLA cB 912



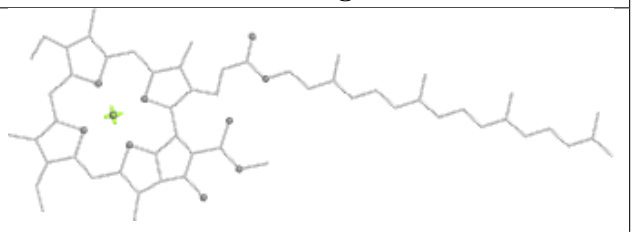
Bond lengths



Bond angles

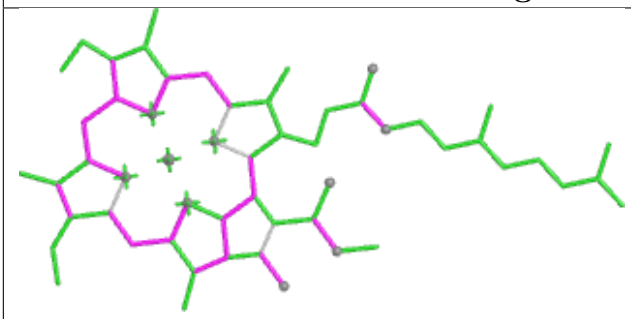


Torsions

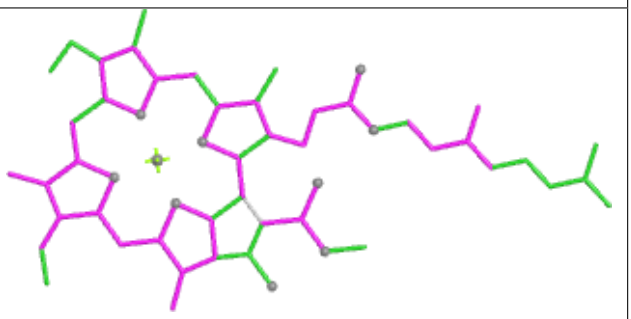


Rings

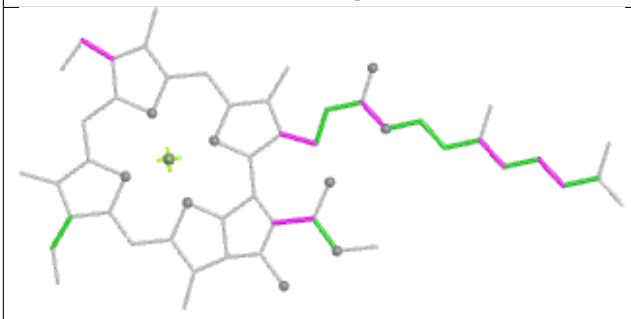
Ligand CLA bB 917



Bond lengths



Bond angles



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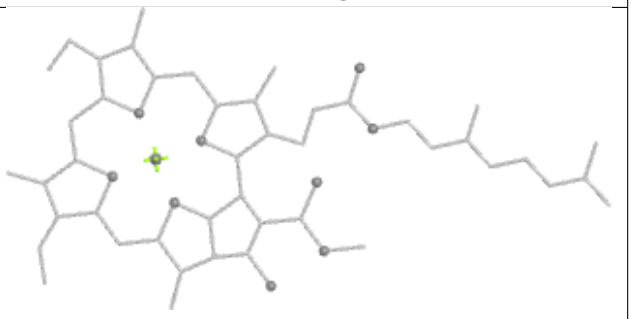
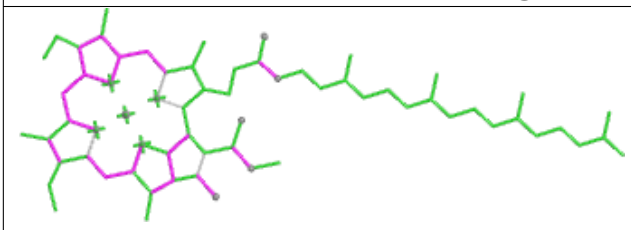


Rings

Ligand CLA cA 807



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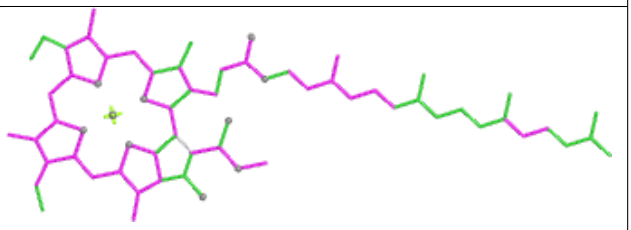
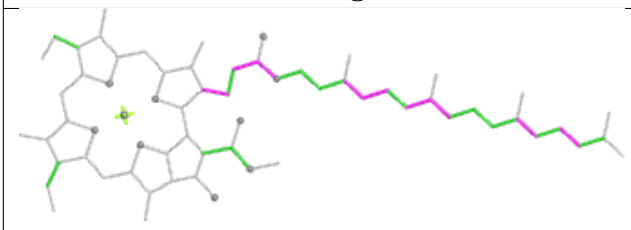


Bond angles



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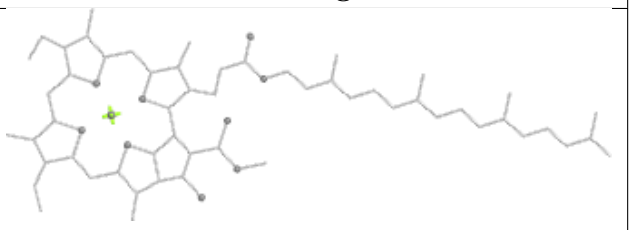
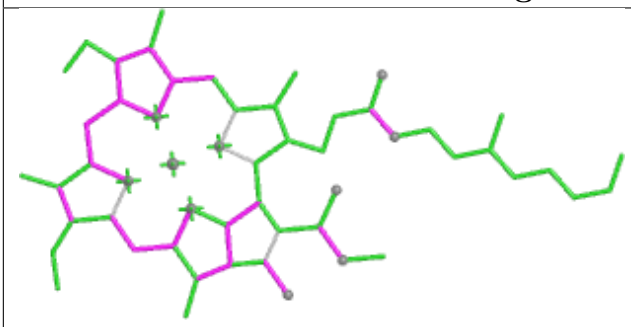


Rings

Ligand CLA aA 818



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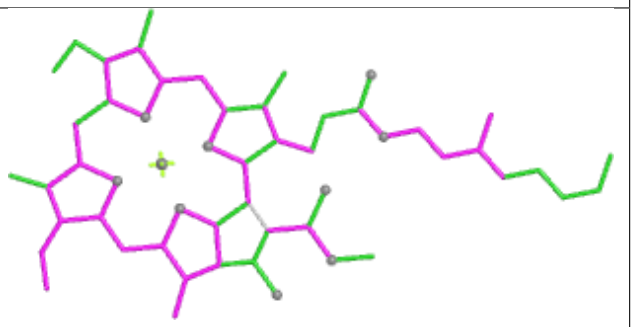
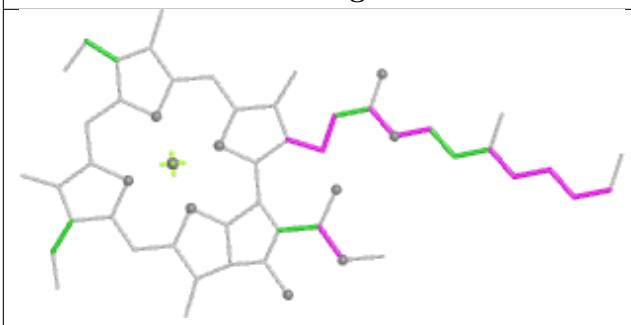
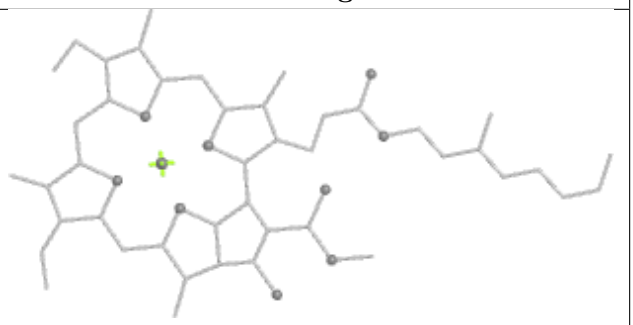


Bond angles

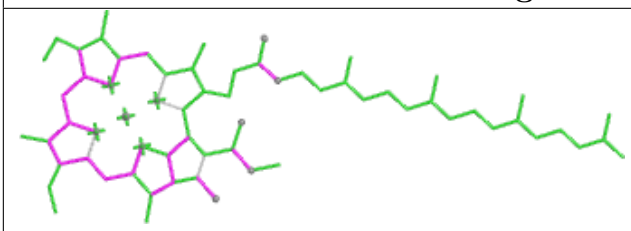


Torsions



Rings

Ligand CLA aB 927



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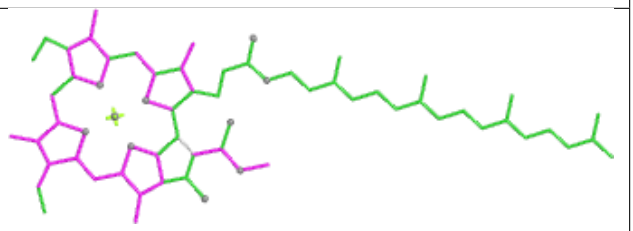
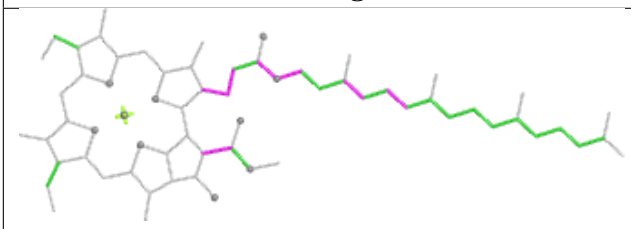


Bond angles



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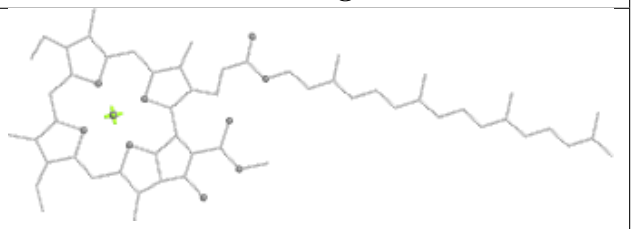
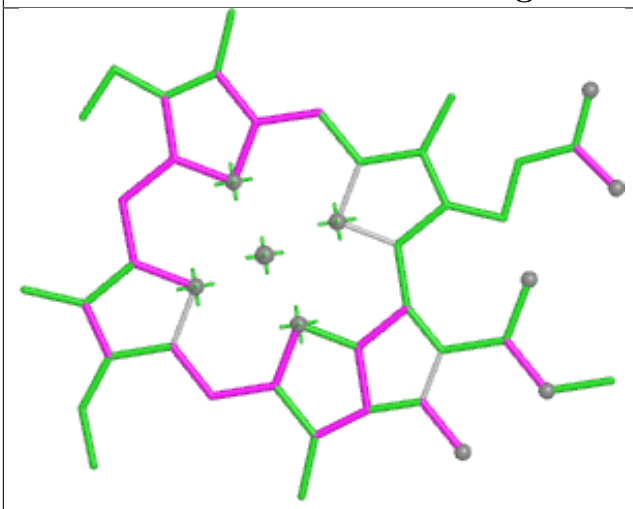


Rings

Ligand CLA aB 939



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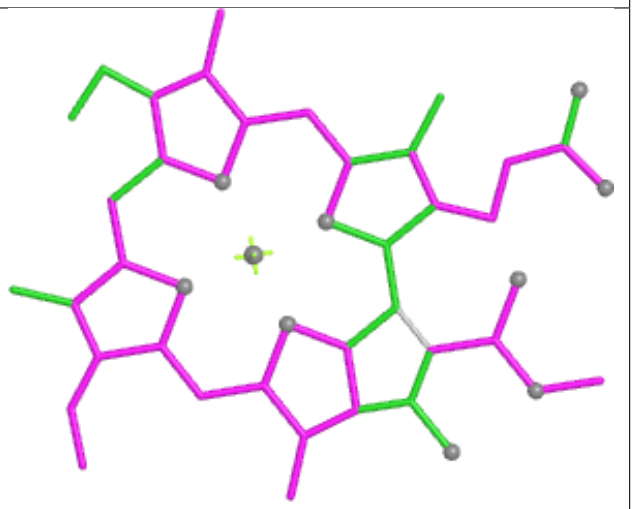
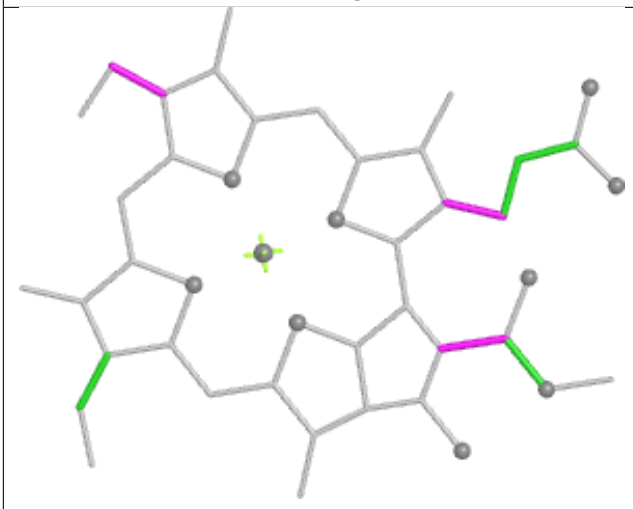


Bond angles

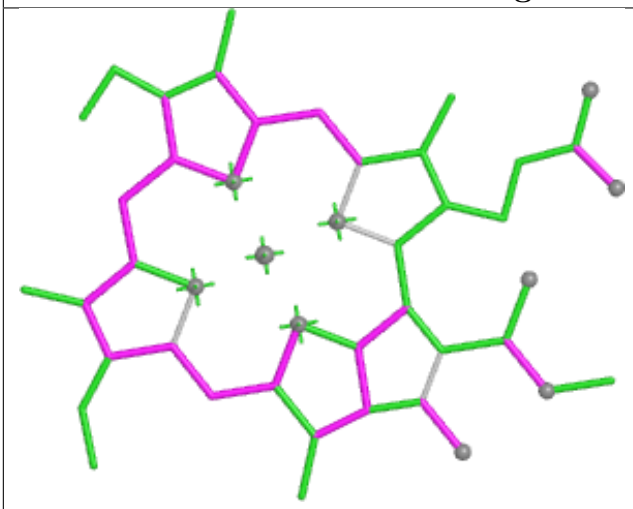


Torsions



Rings

Ligand CLA bB 929



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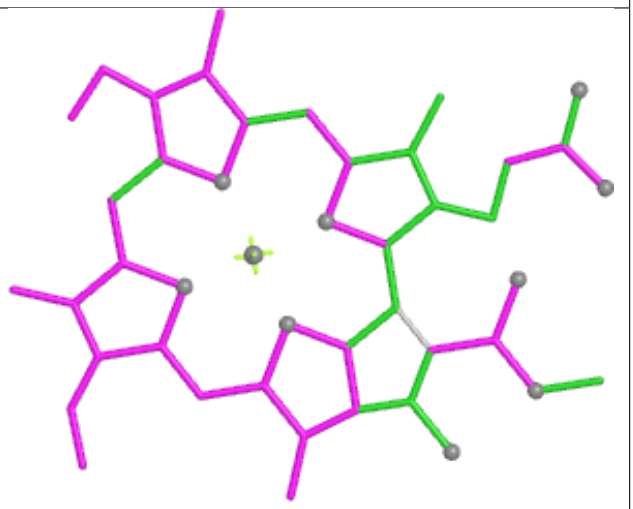
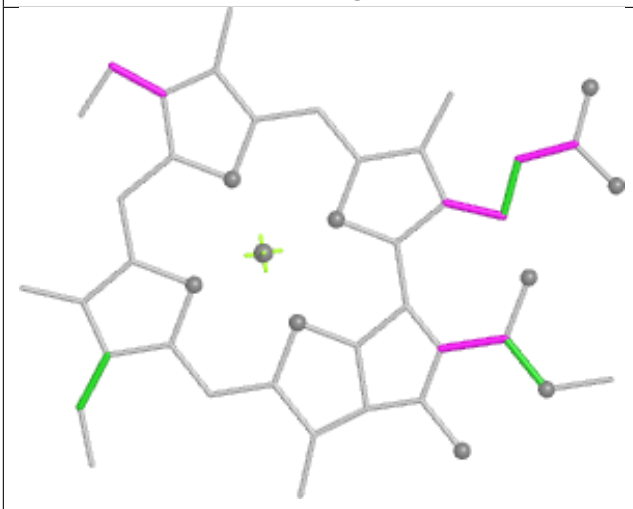


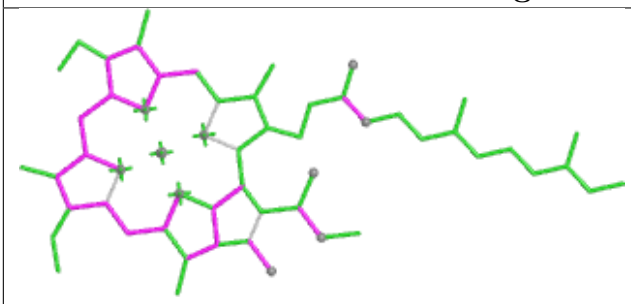
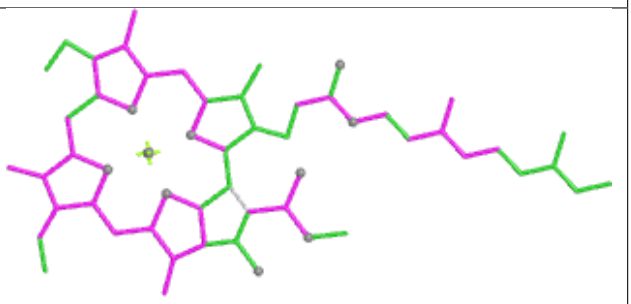
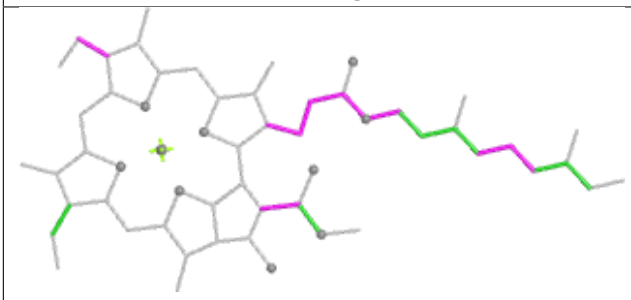
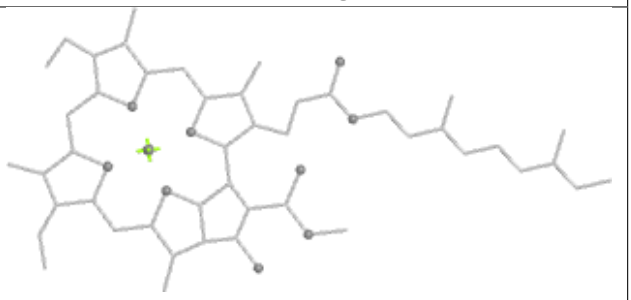
Bond angles



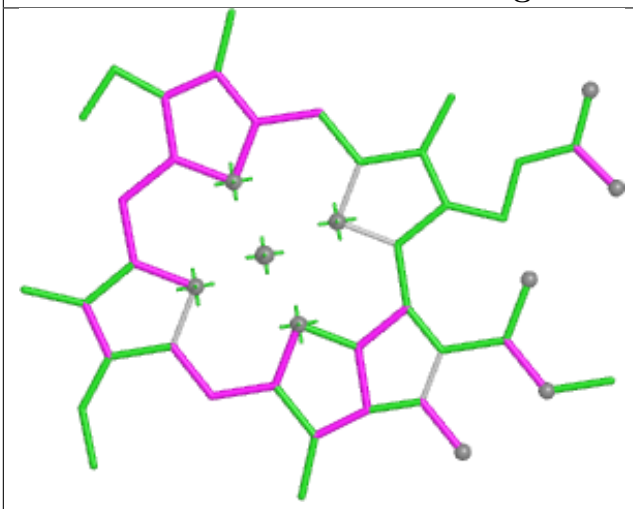
Torsions



Rings

Ligand CLA bA 820	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA bA 811



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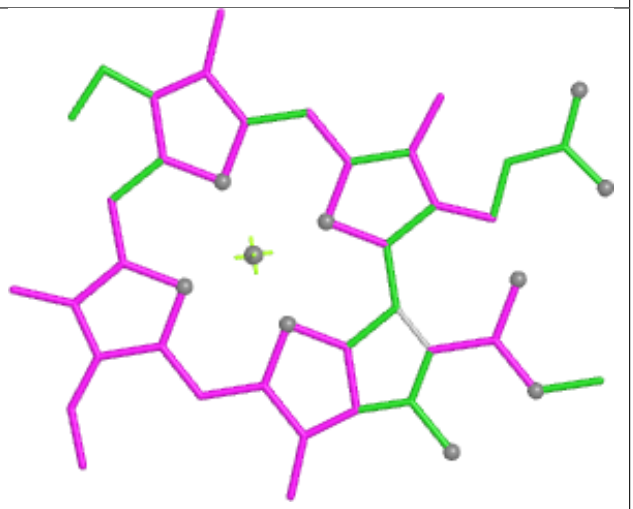
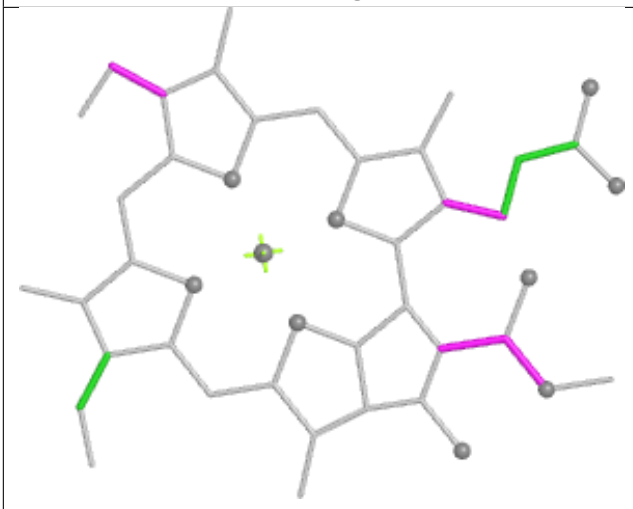


Bond angles

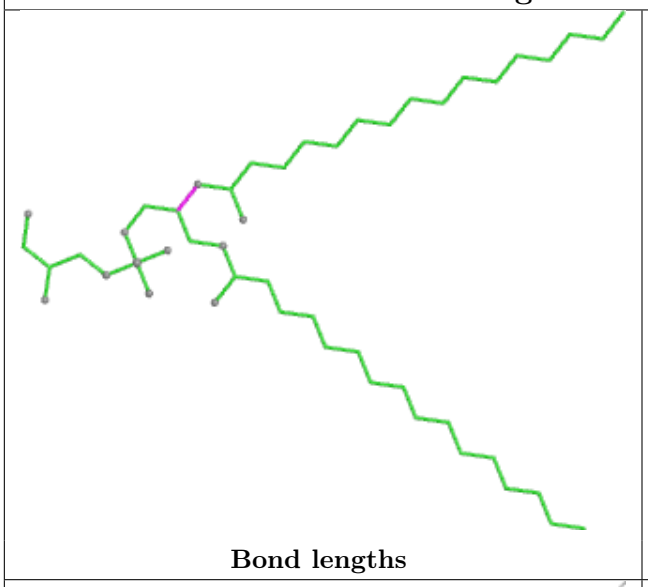


Torsions



Rings

Ligand LHG cA 851



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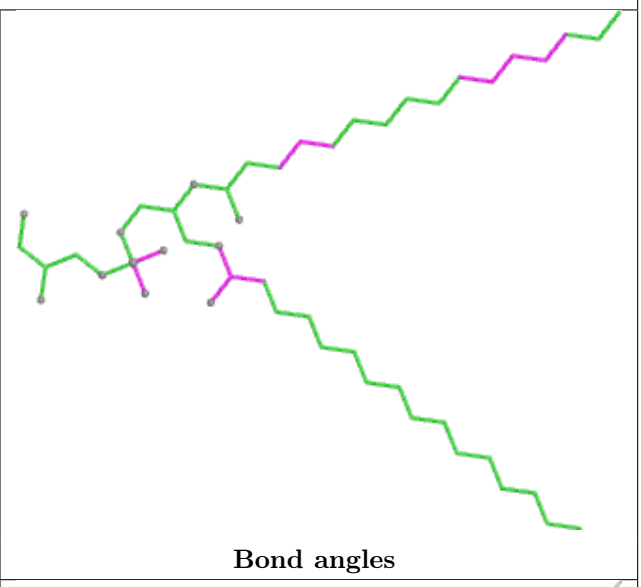
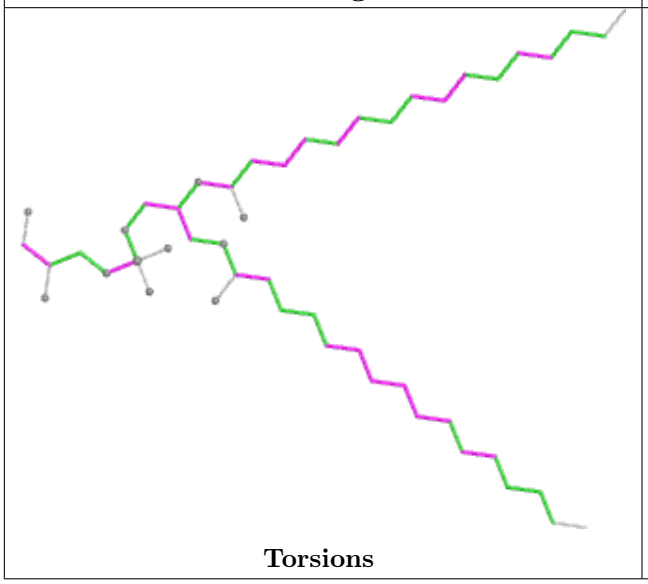
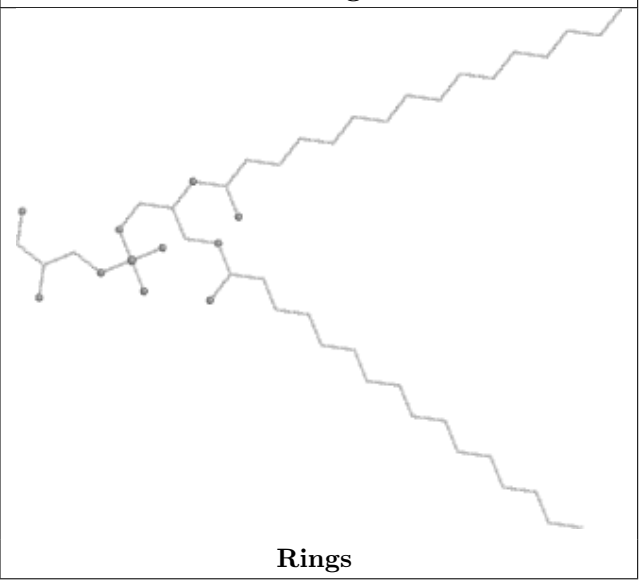


Bond angles

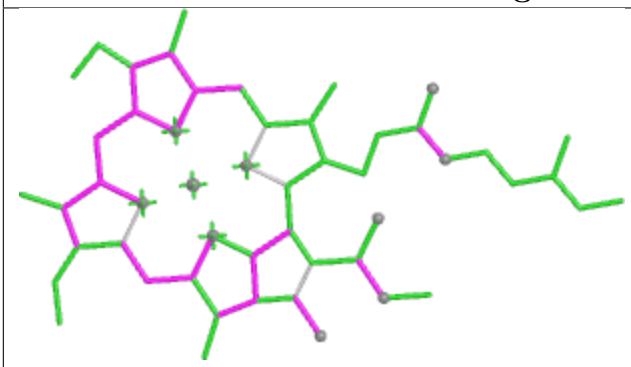


Torsions



Rings

Ligand CLA bA 823



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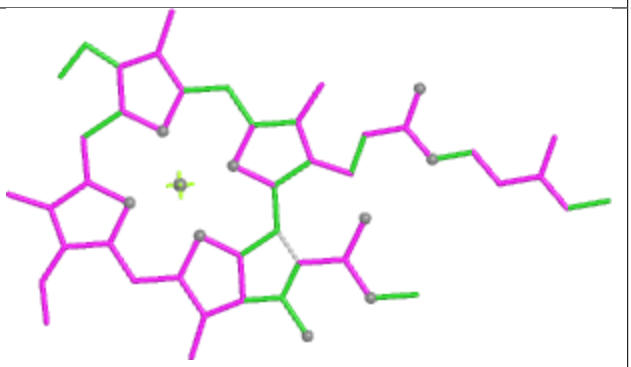
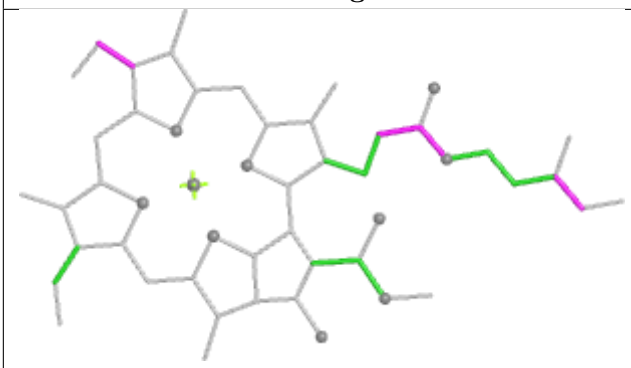
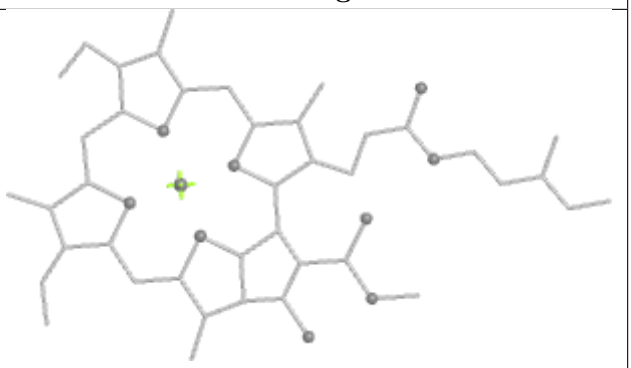


Bond angles

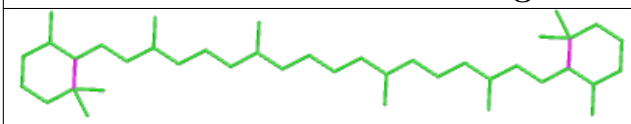


Torsions



Rings

Ligand BCR cA 850



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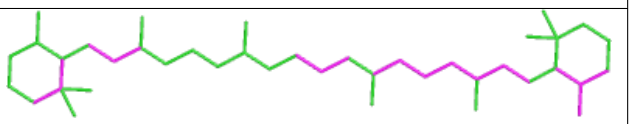
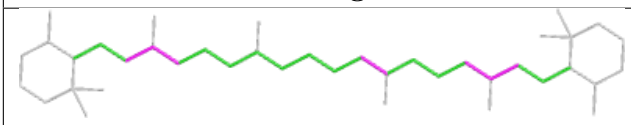
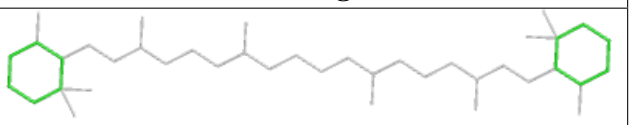


Bond angles

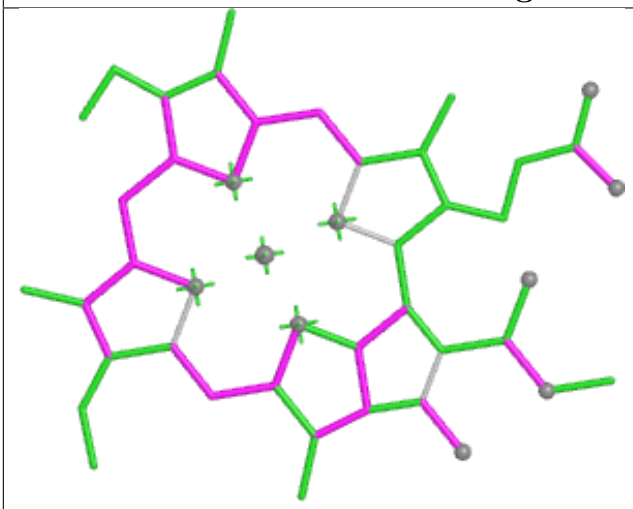


Torsions



Rings

Ligand CLA cA 809



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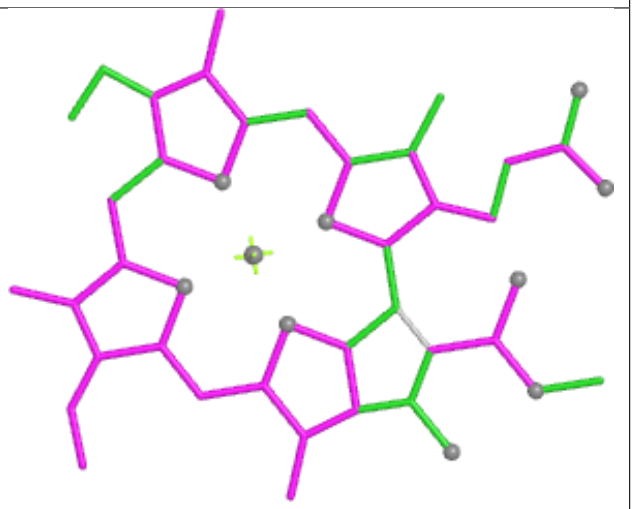
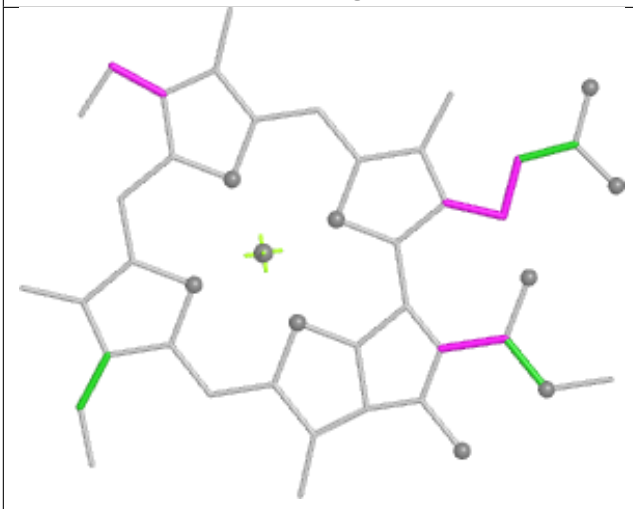


Bond angles

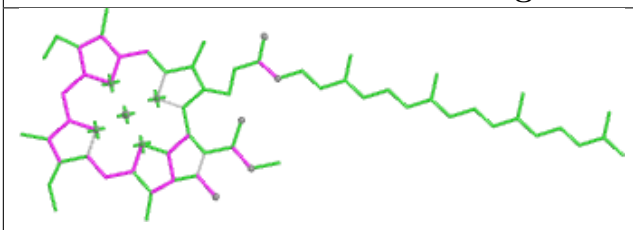


Torsions



Rings

Ligand CLA aA 828



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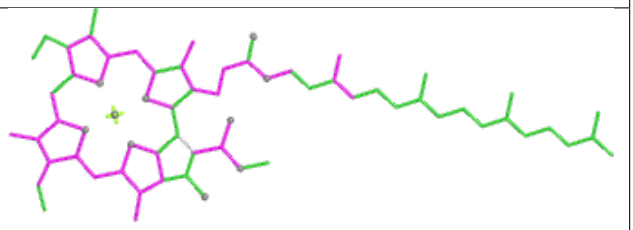
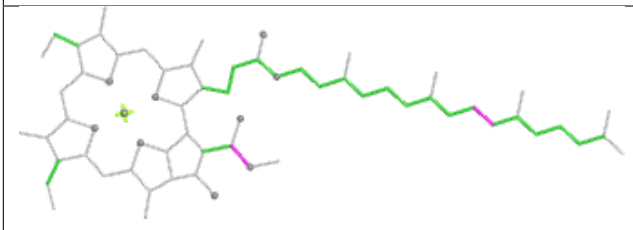
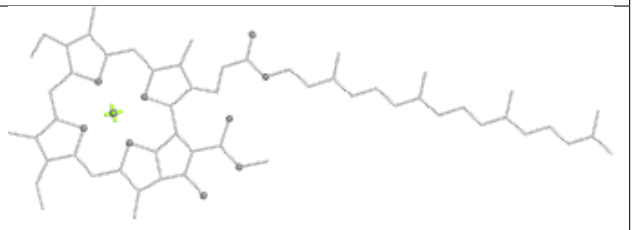


Bond angles

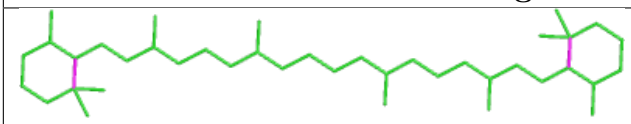


Torsions

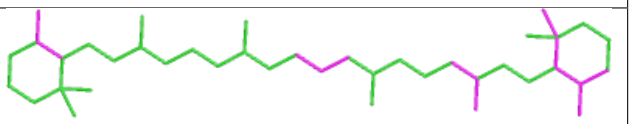


Rings

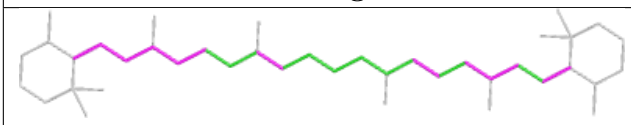
Ligand BCR cB 944



Bond lengths



Bond angles



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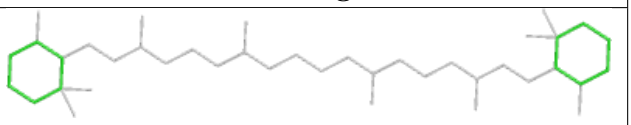
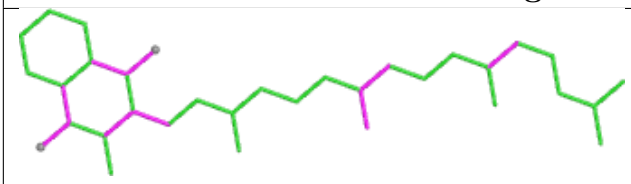
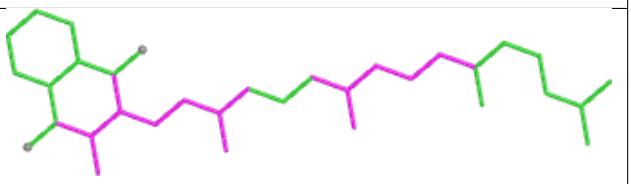


Rings

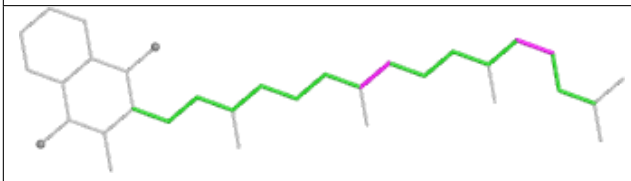
Ligand 1L3 cA 844



Bond lengths



Bond angles



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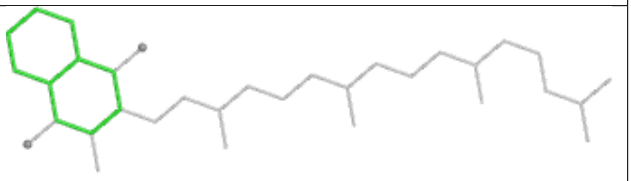
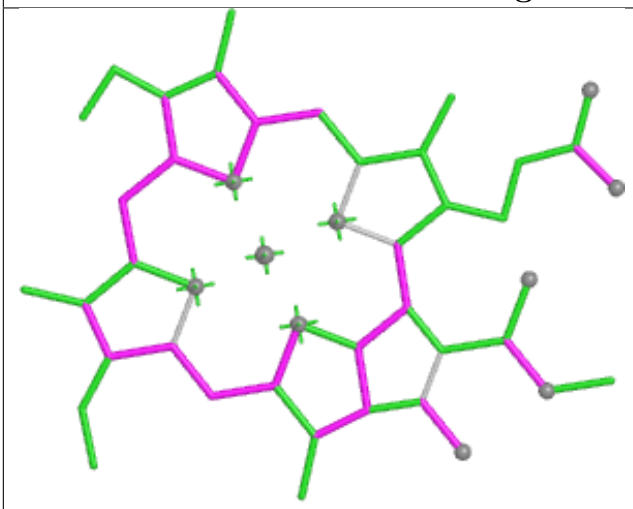
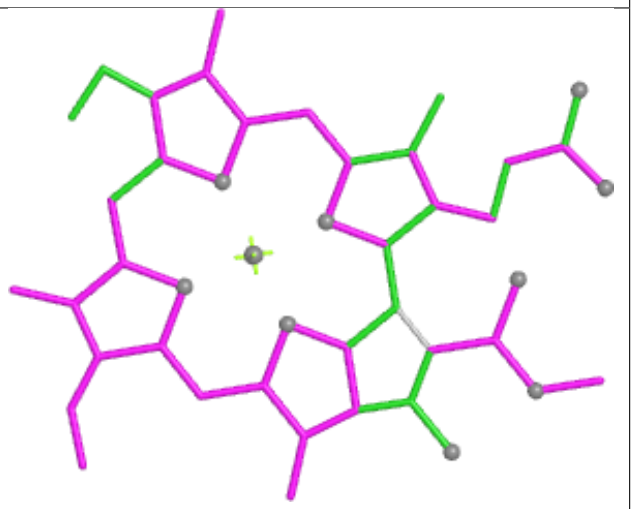


Rings

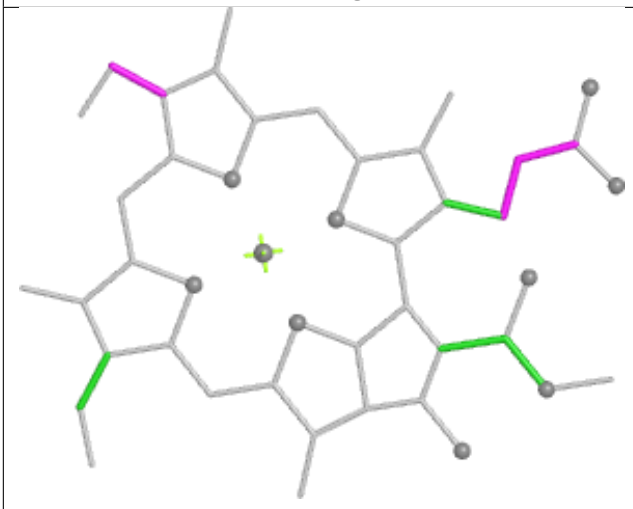
Ligand CLA aA 836



Bond lengths



Bond angles

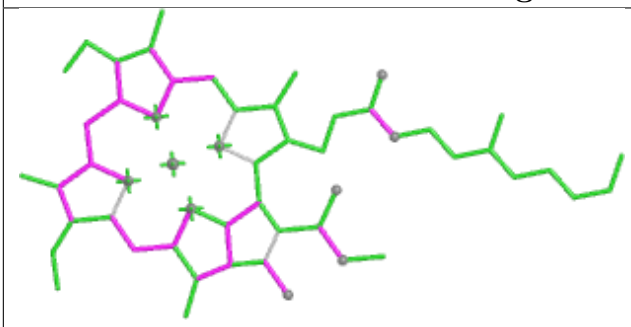


Torsions



Rings

Ligand CLA aB 923



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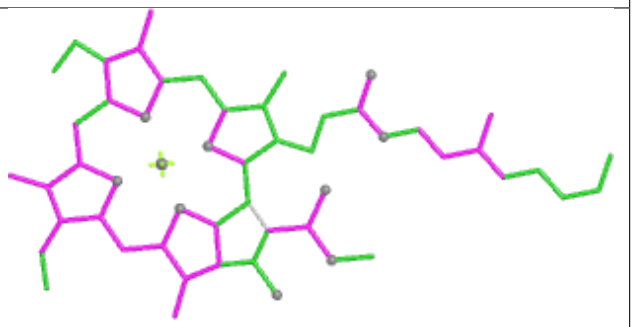
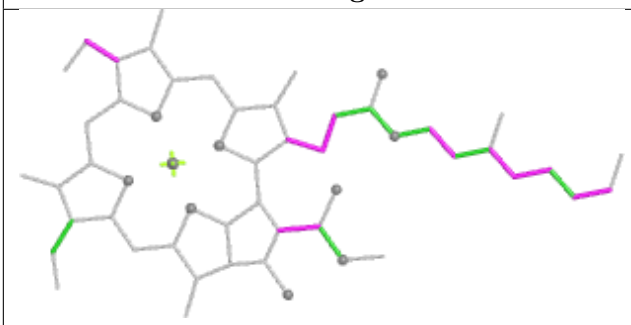
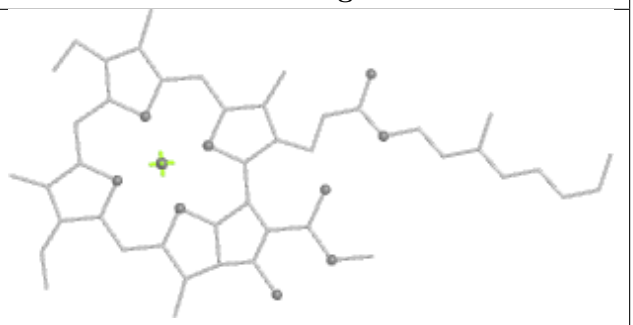


Bond angles

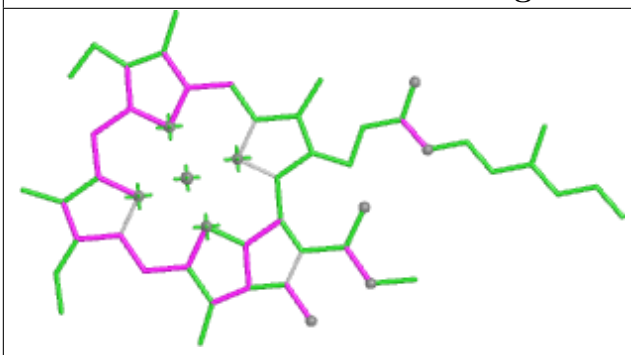


Torsions



Rings

Ligand CLA bB 907



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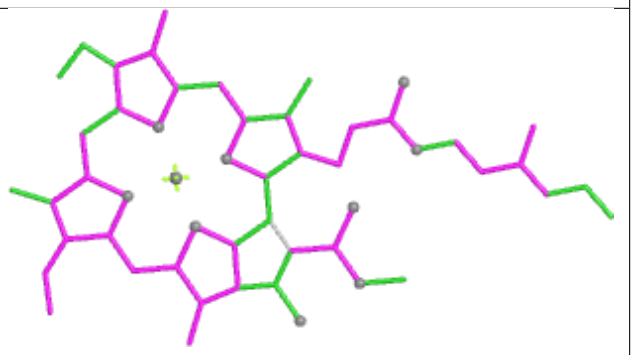
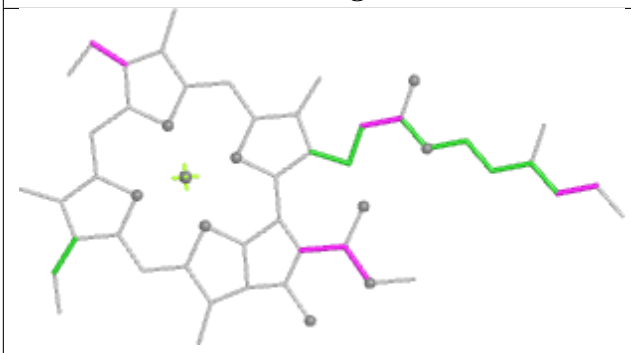


Bond angles



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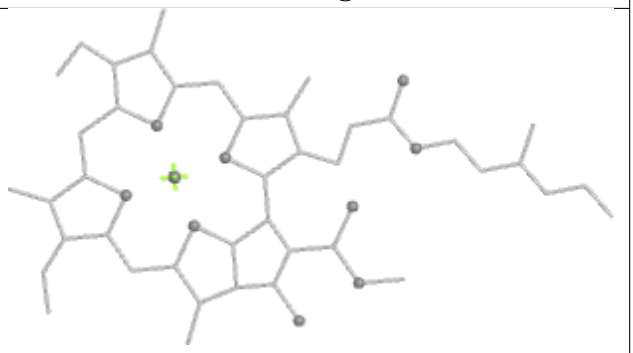
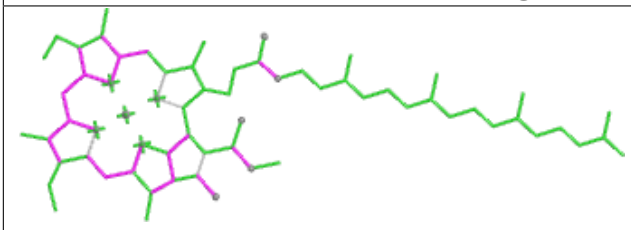


Rings

Ligand CLA aA 838



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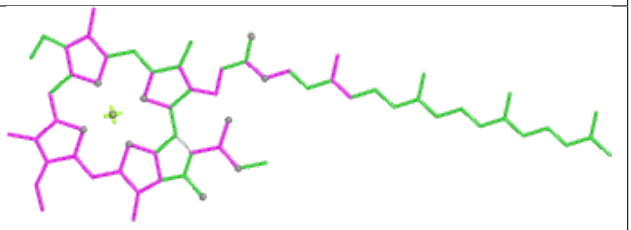
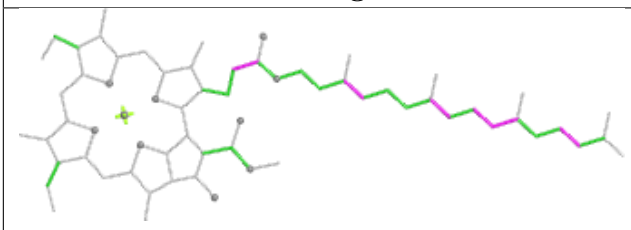


Bond angles



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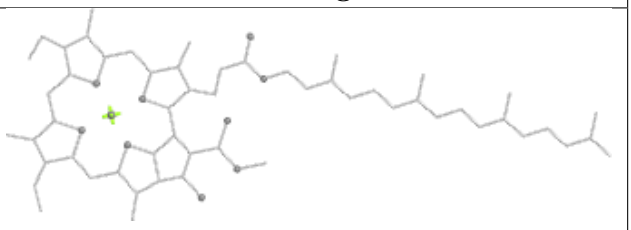
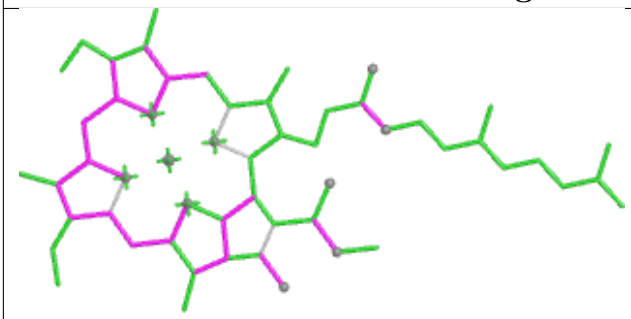


Rings

Ligand CLA aA 826



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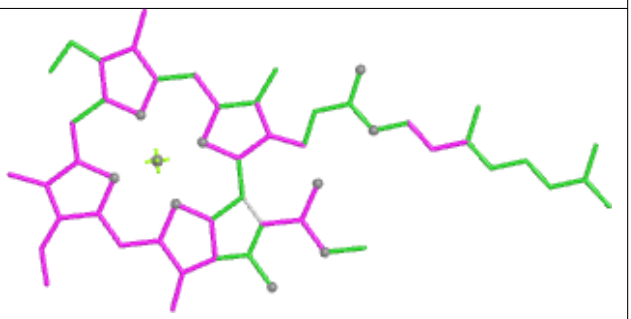
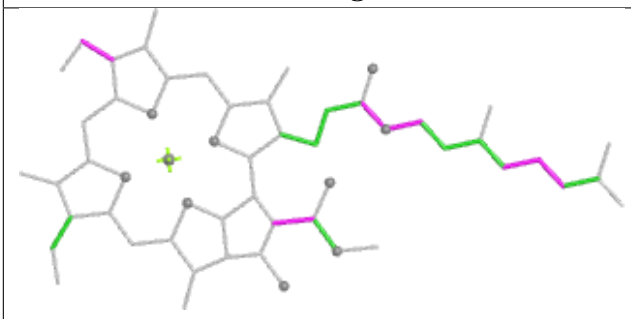


Bond angles



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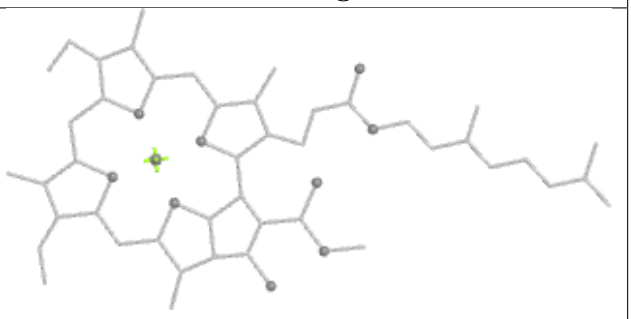
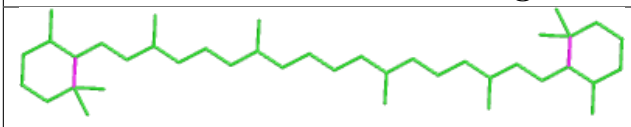


Rings

Ligand BCR cA 846



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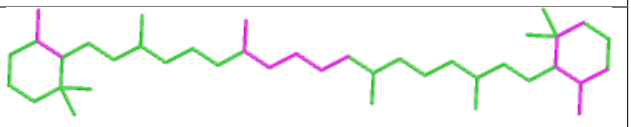

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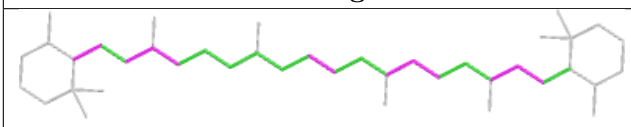

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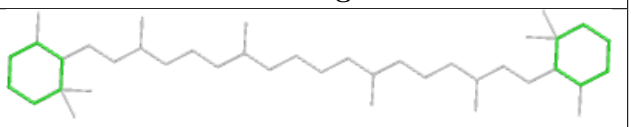
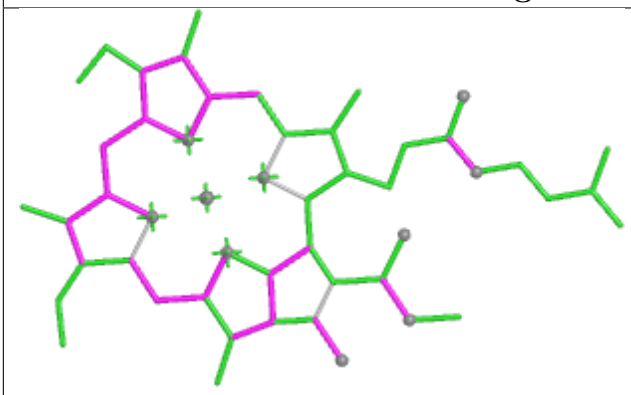


Rings

Ligand CLA bB 935



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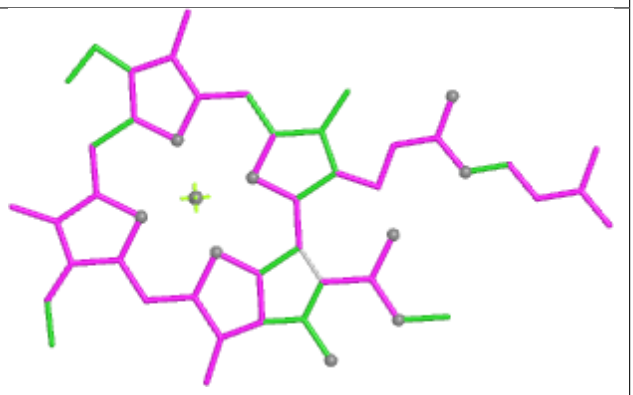
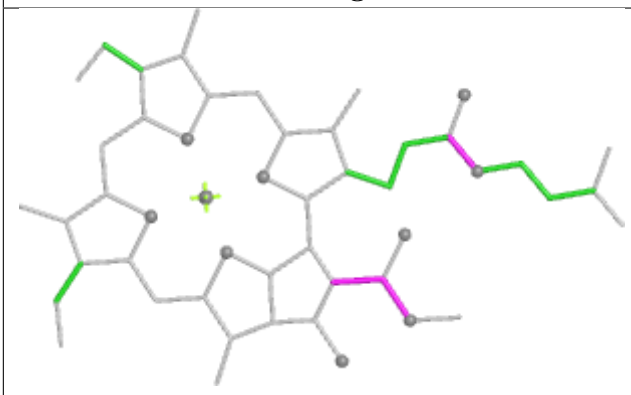


Bond angles



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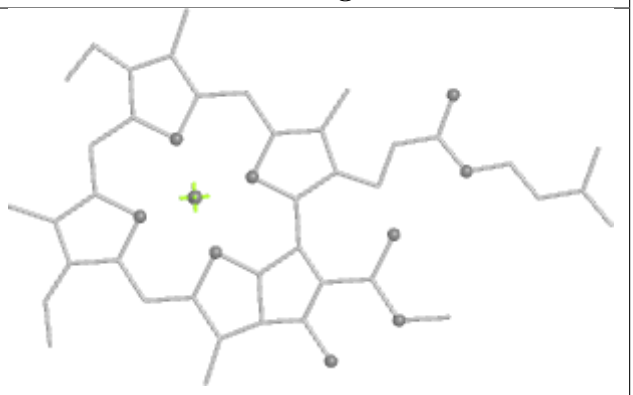
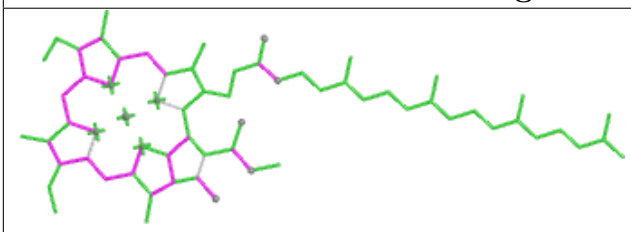


Rings

Ligand CLA aA 803



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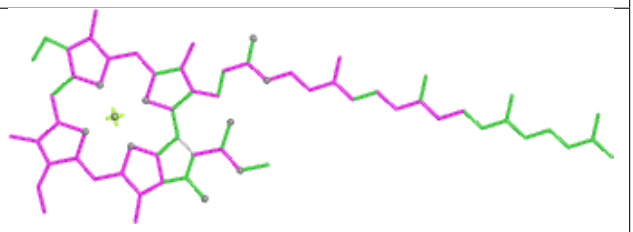
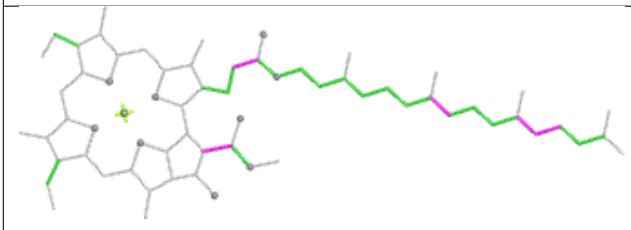


Bond angles



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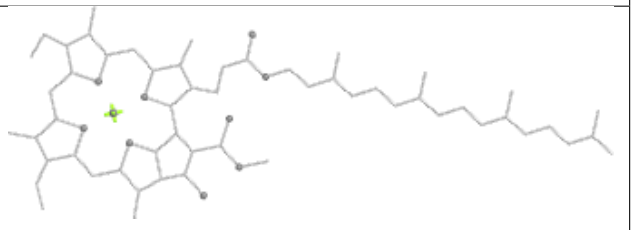
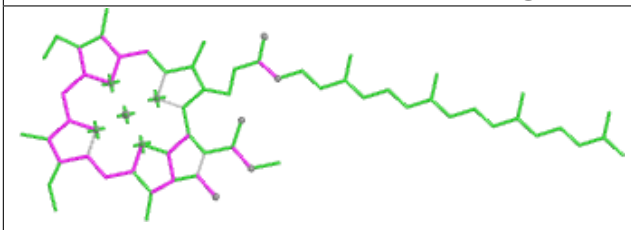


Rings

Ligand CL0 aA 801



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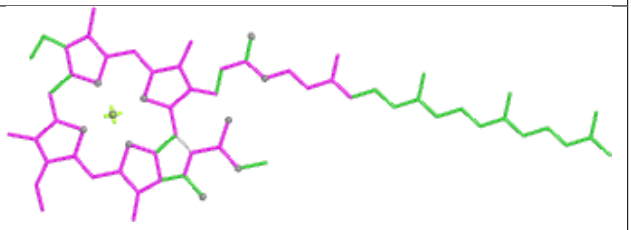
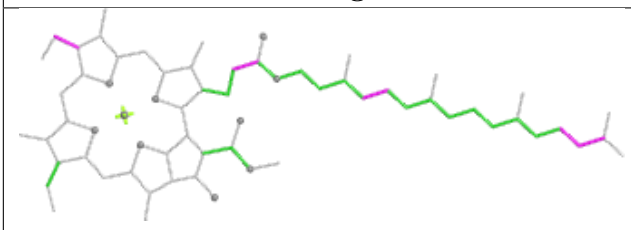


Bond angles



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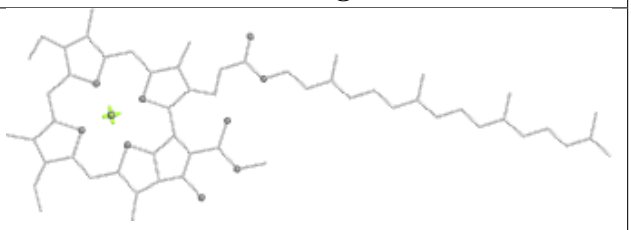
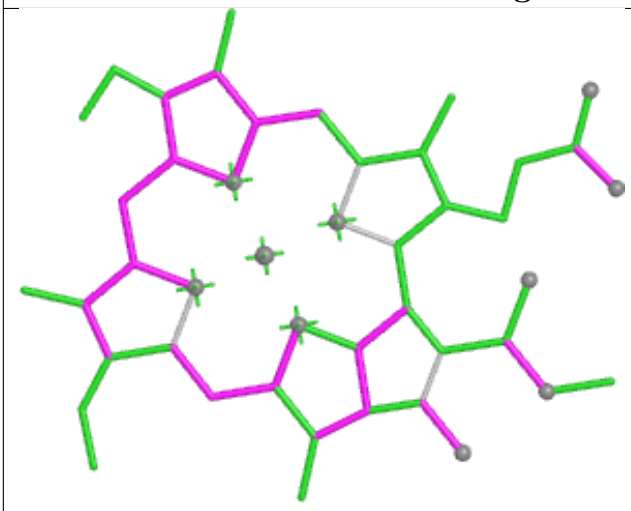


Rings

Ligand CLA bA 839



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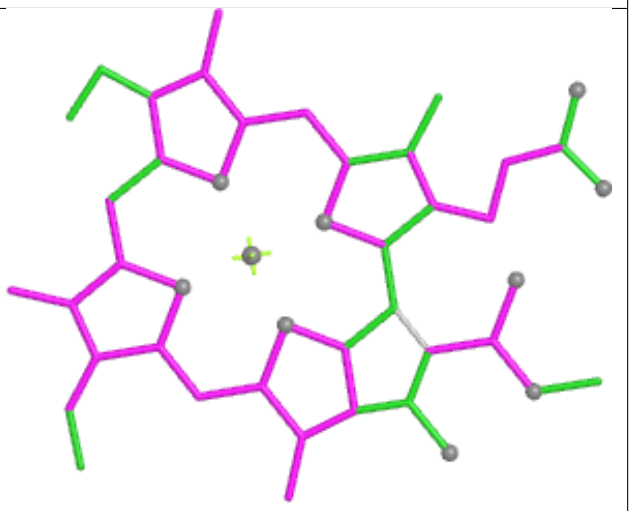
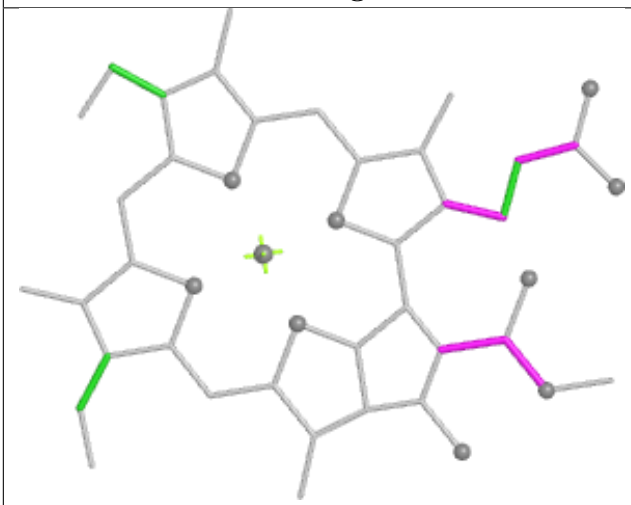


Bond angles



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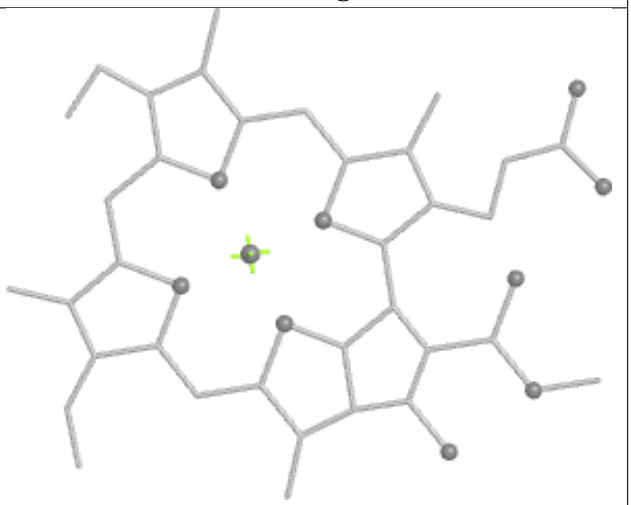
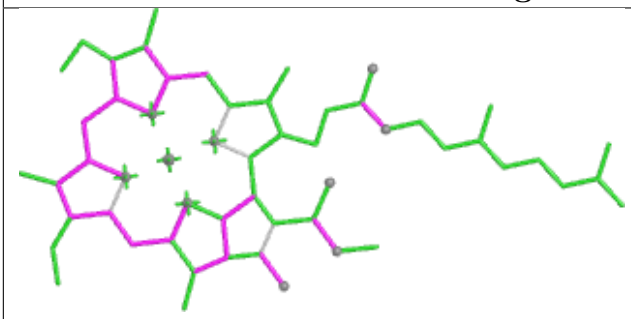


Rings

Ligand CLA bB 909



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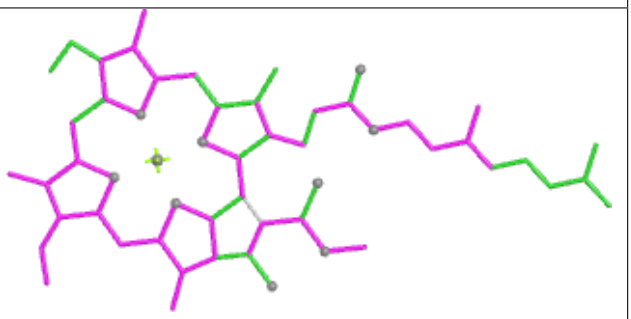
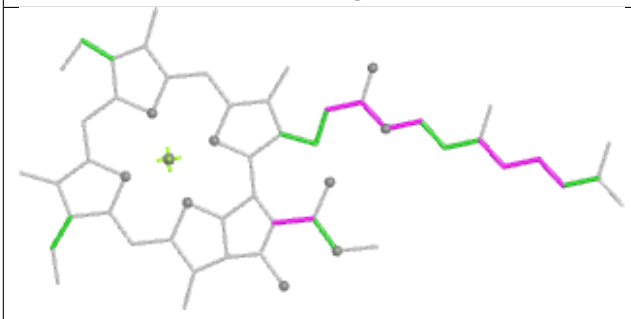
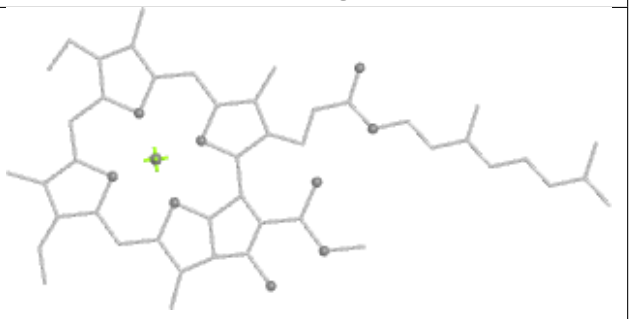


Bond angles

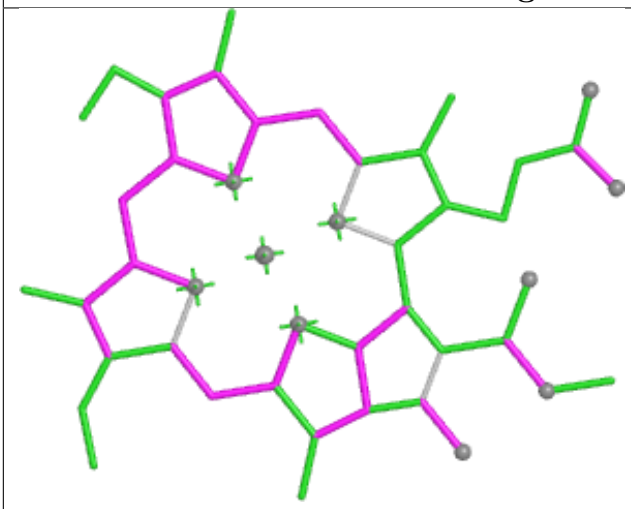


Torsions



Rings

Ligand CLA aL 203



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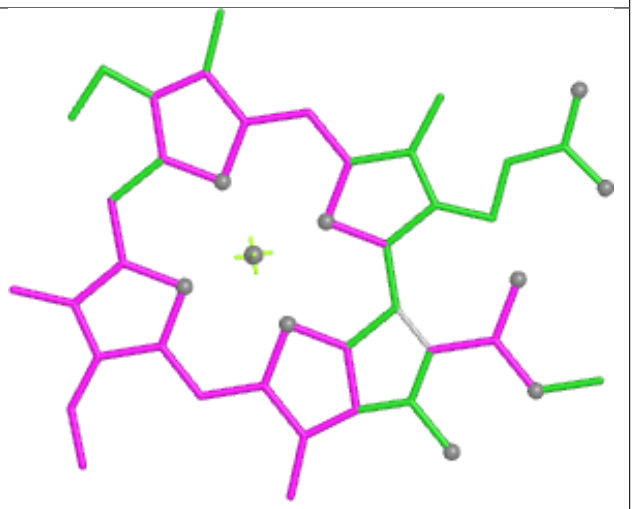
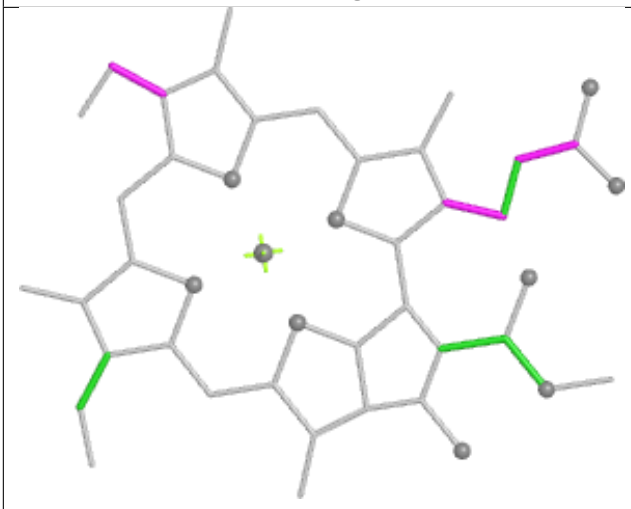


Bond angles

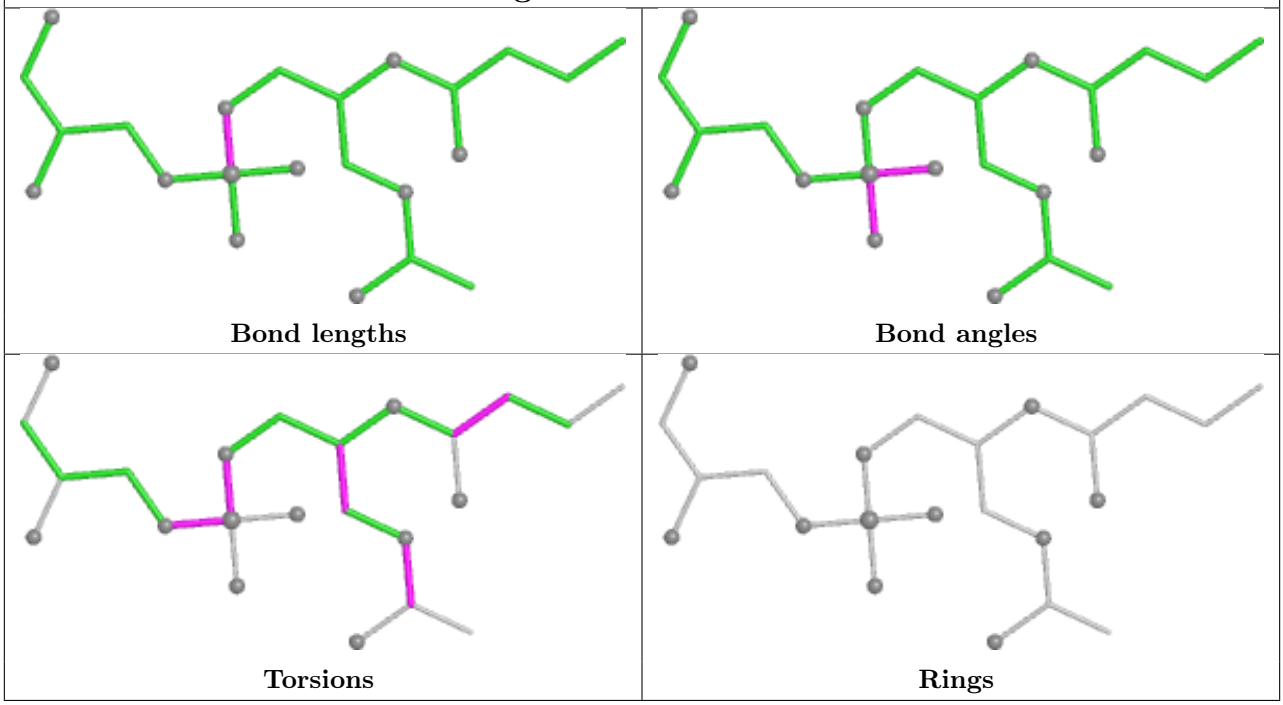


Torsions

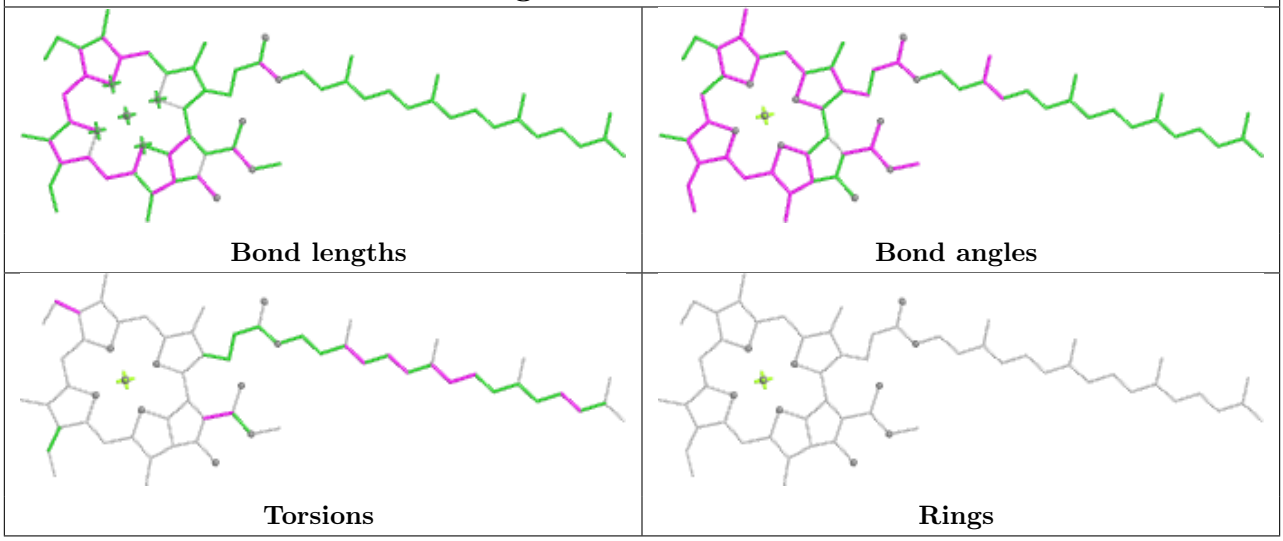


Rings

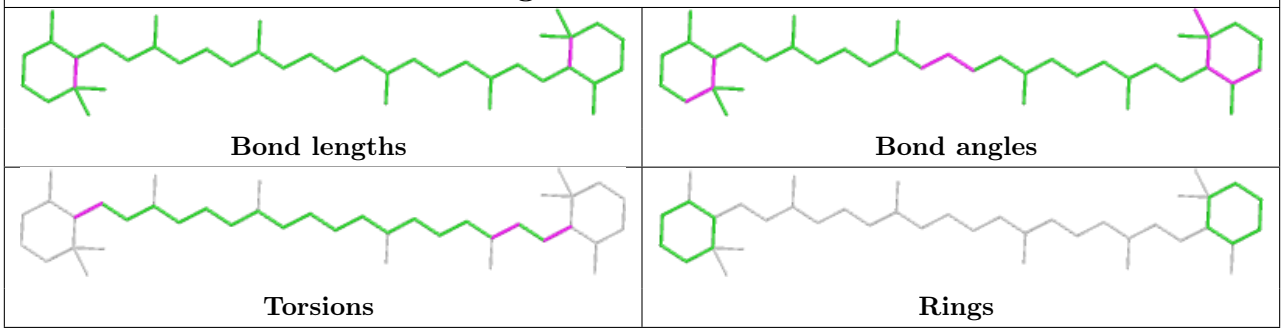
Ligand LHG bB 948



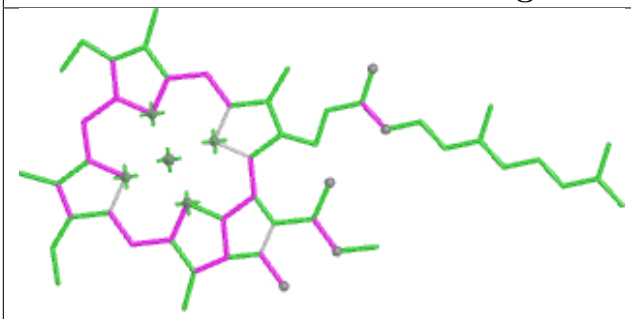
Ligand CLA bA 840



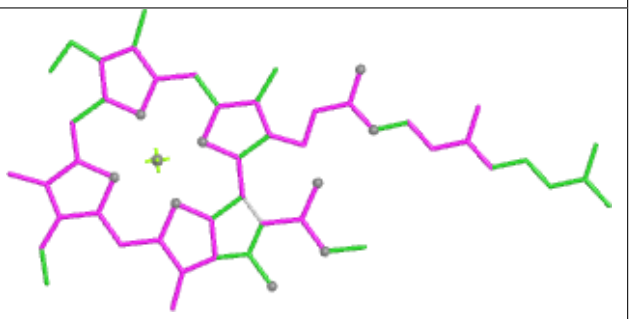
Ligand BCR aL 206



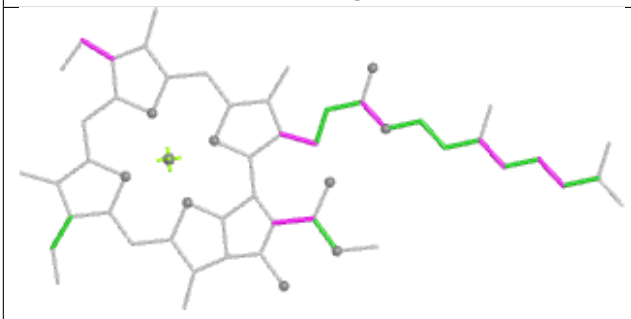
Ligand CLA cB 917



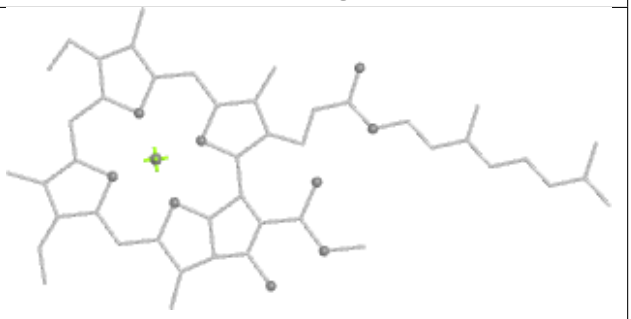
Bond lengths



Bond angles

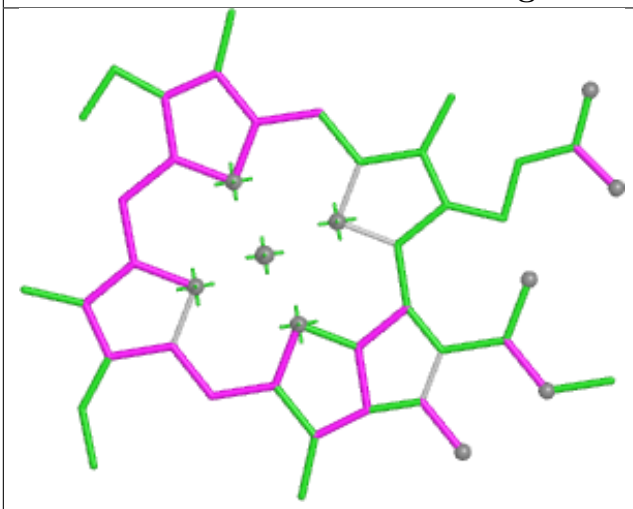


Torsions



Rings

Ligand CLA cF 202



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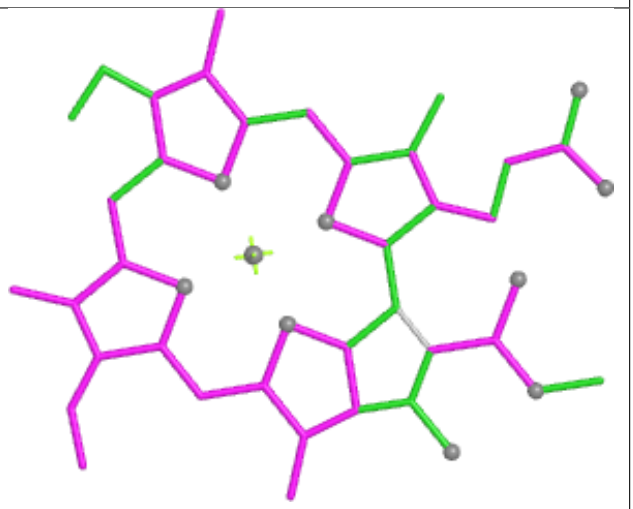
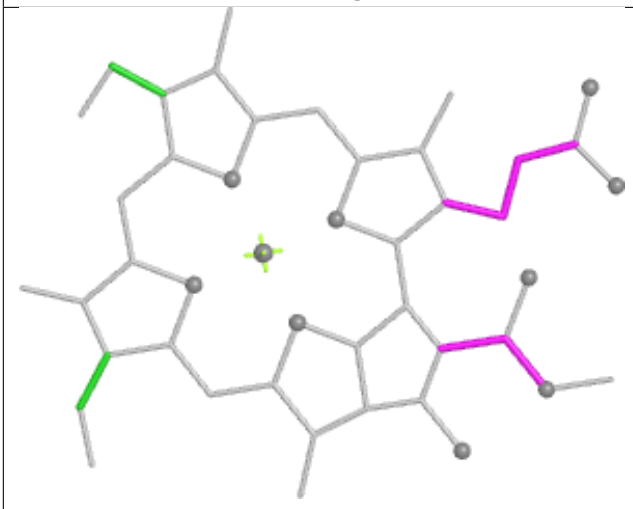


Bond angles

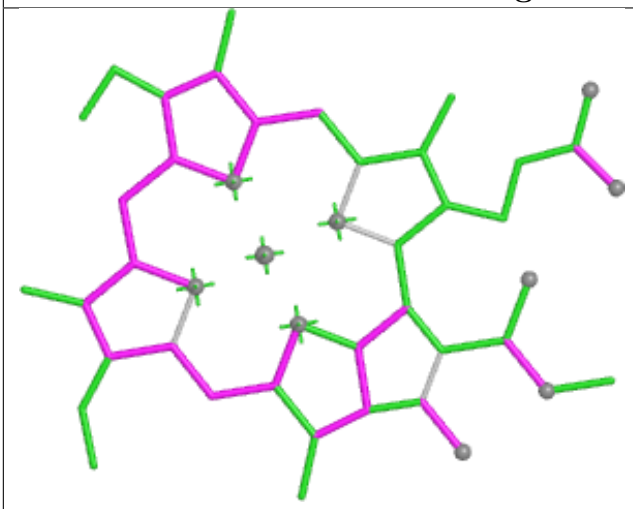


Torsions



Rings

Ligand CLA aA 816



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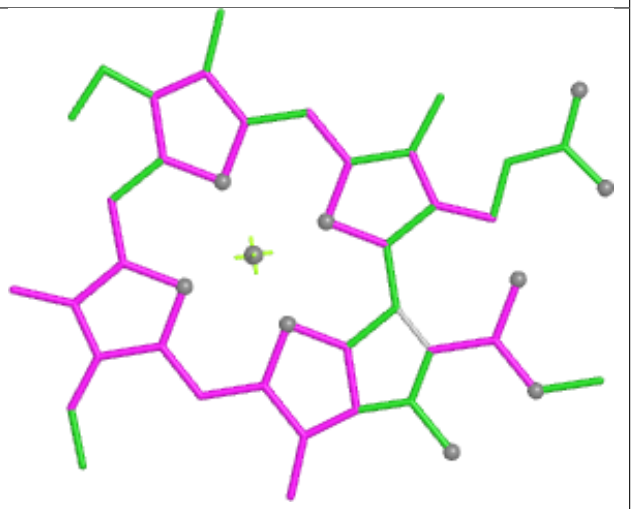
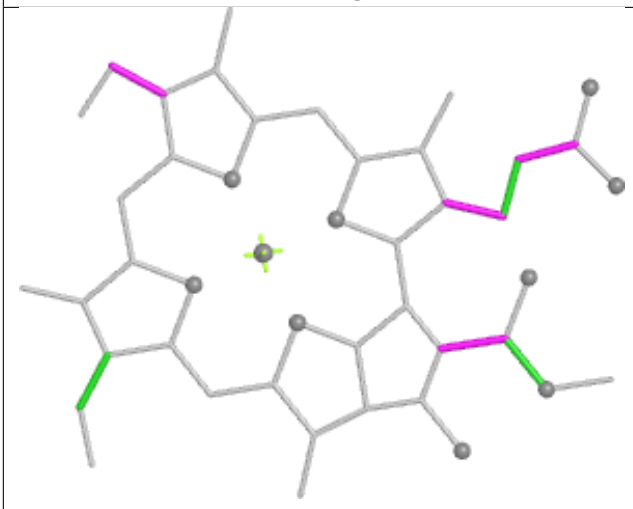


Bond angles

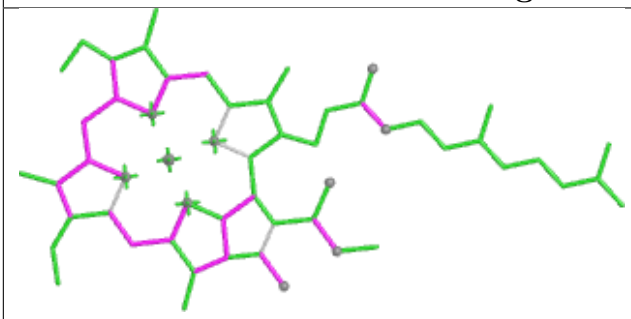


Torsions

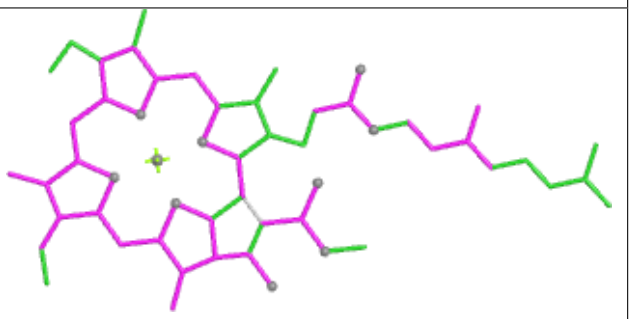


Rings

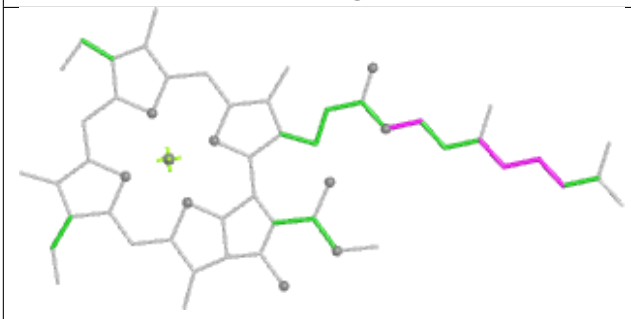
Ligand CLA aB 925



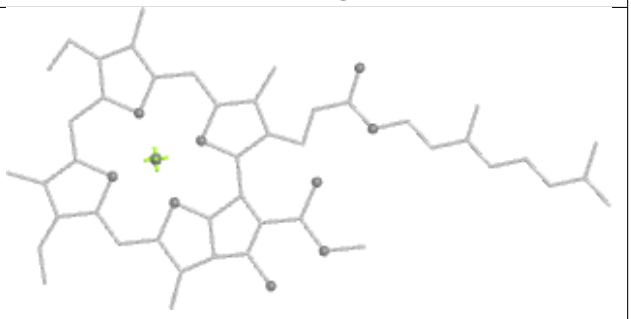
Bond lengths



Bond angles

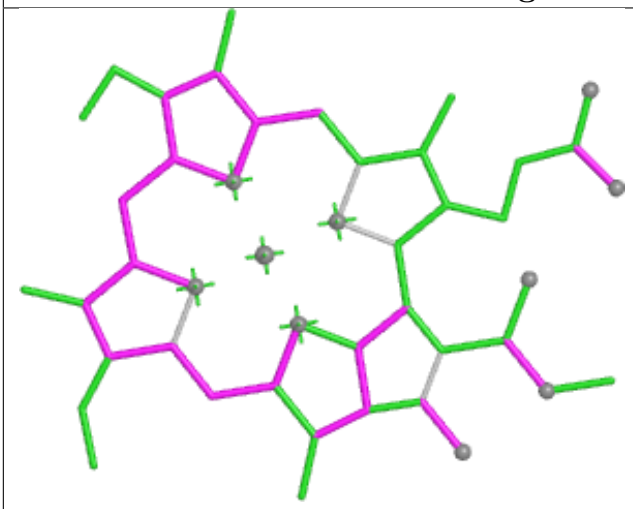


Torsions



Rings

Ligand CLA cL 204



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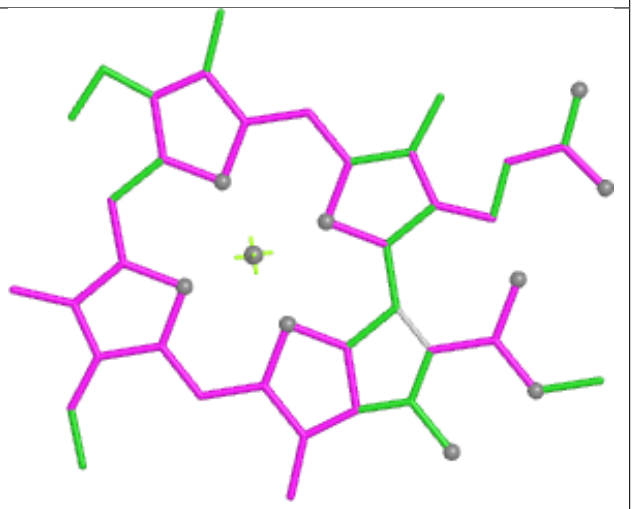
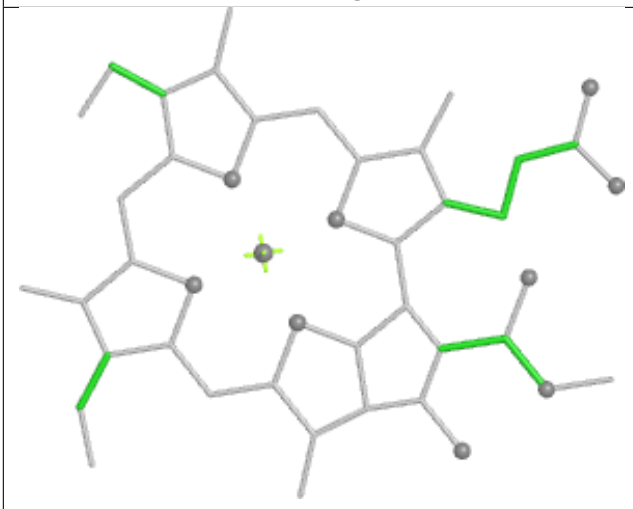


Bond angles

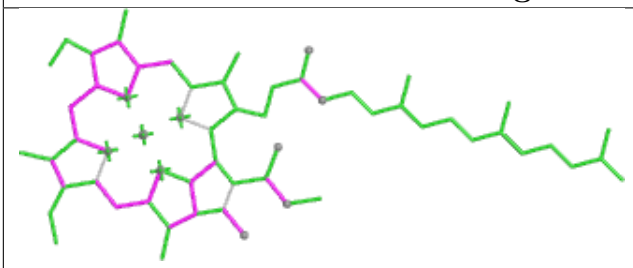


Torsions



Rings

Ligand CLA bA 829



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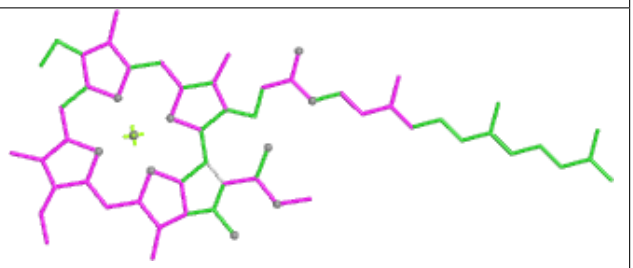
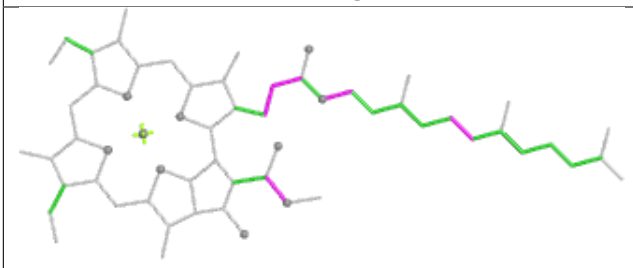


Bond angles



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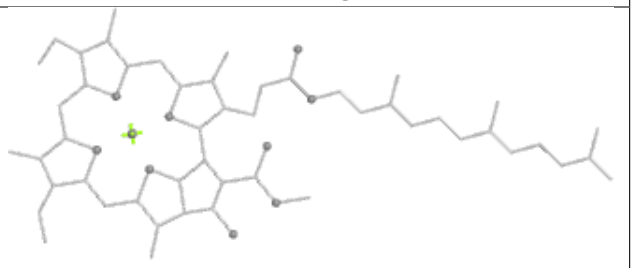
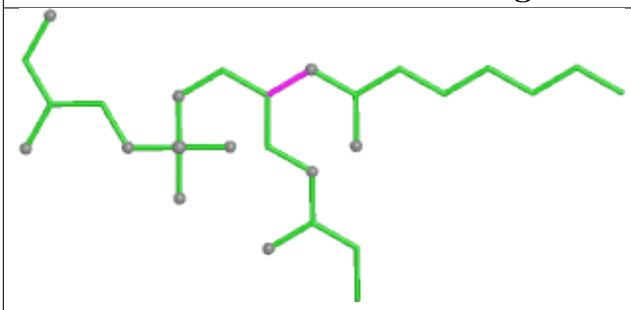


Rings

Ligand LHG cA 852



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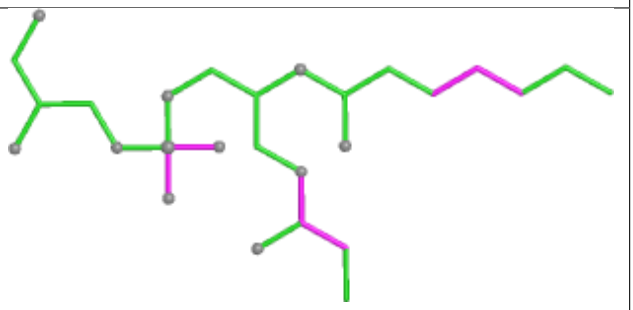
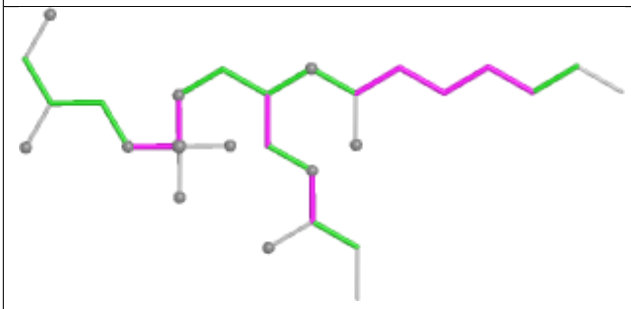


Bond angles



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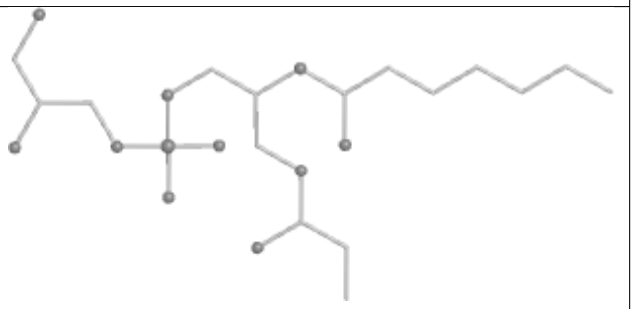
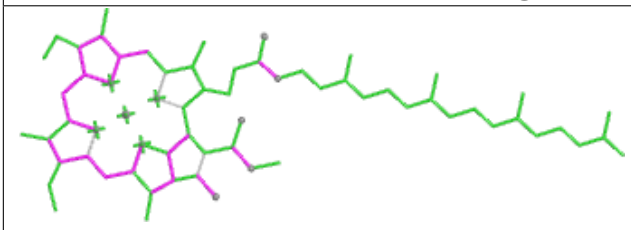
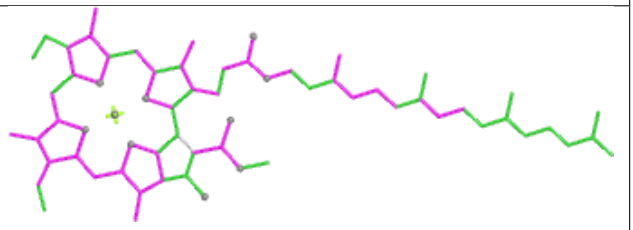


Rings

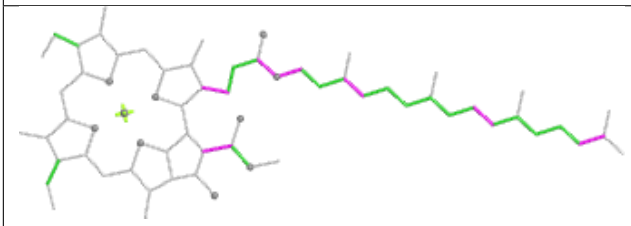
Ligand CLA cA 812



Bond lengths



Bond angles



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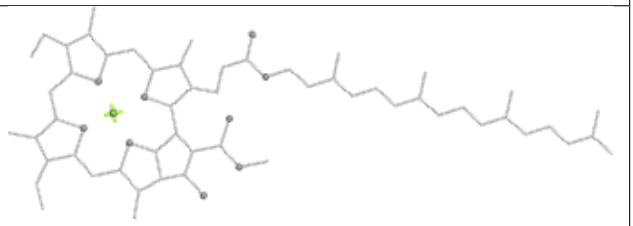
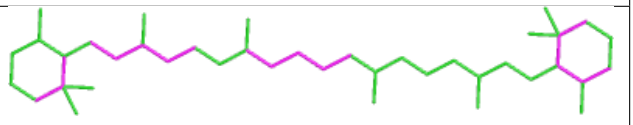


Rings

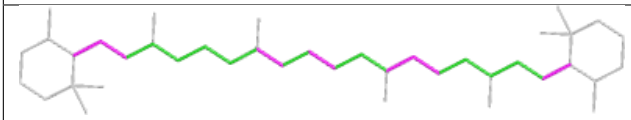
Ligand BCR cB 945



Bond lengths



Bond angles



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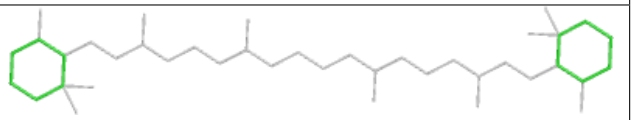
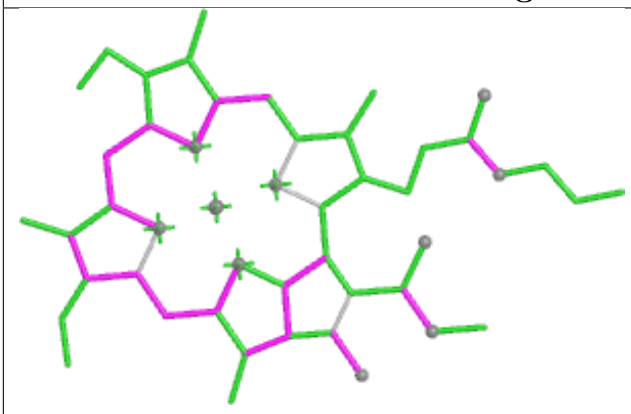
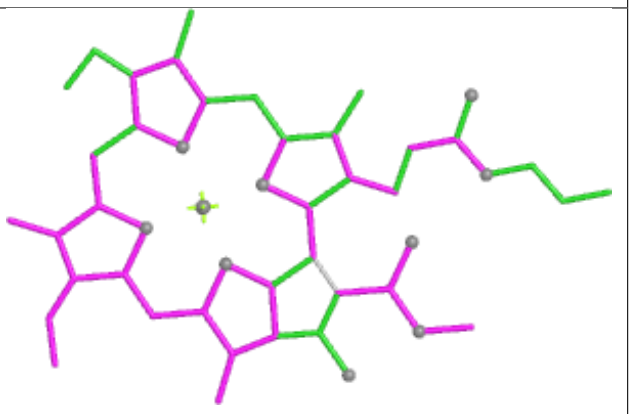
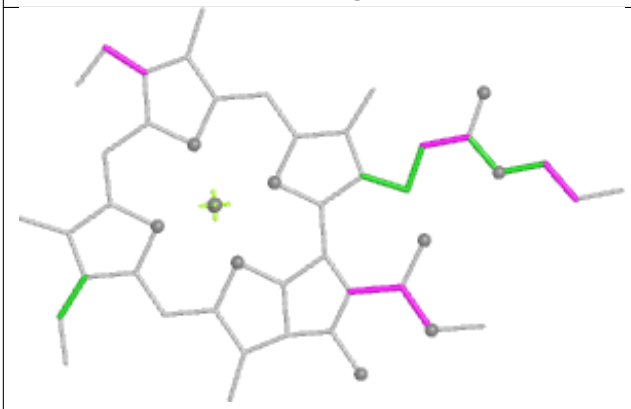
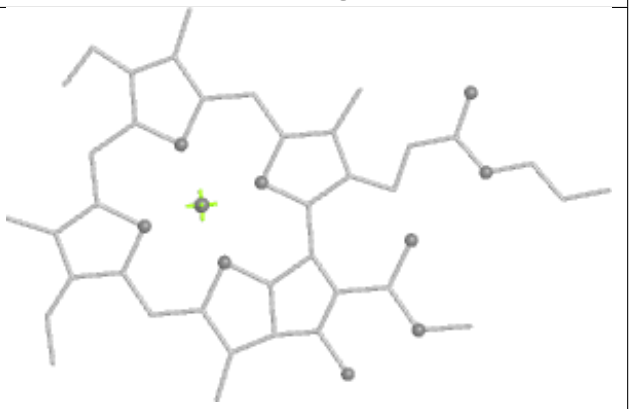
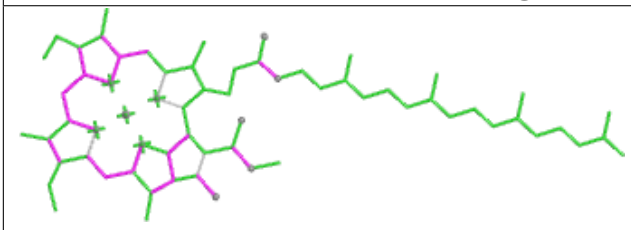
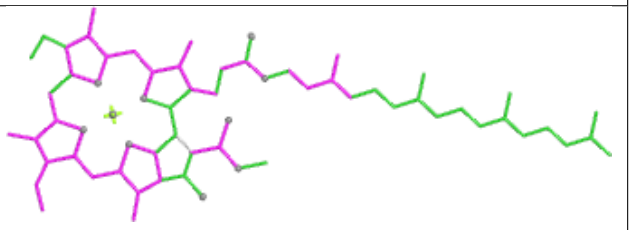
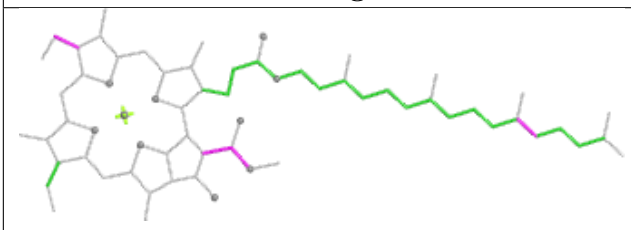
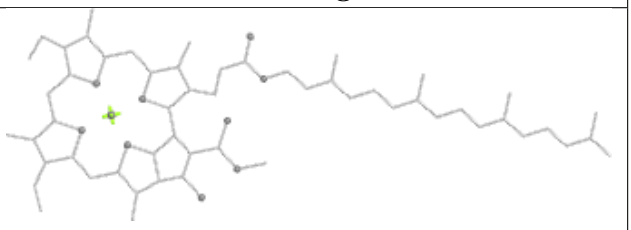
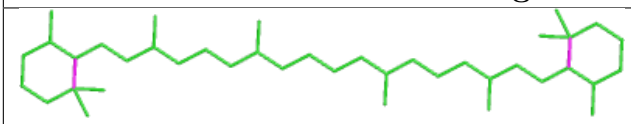


Rings

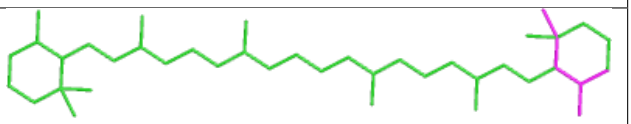
Ligand CLA aB 908	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 901	
	
Bond lengths	Bond angles
	
Torsions	Rings

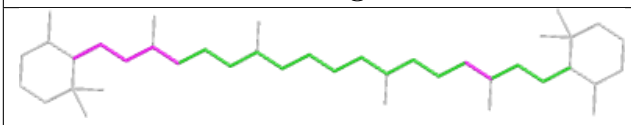
Ligand BCR bB 943



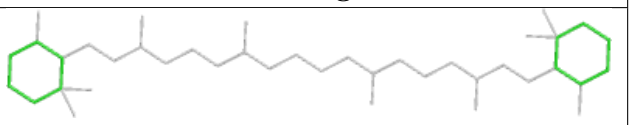
Bond lengths



Bond angles

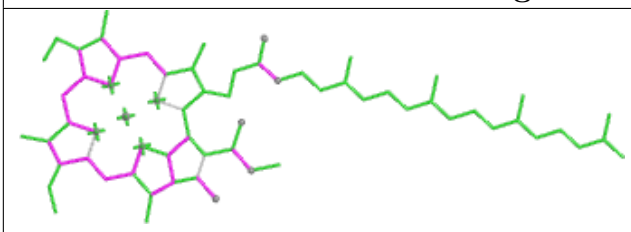


Torsions

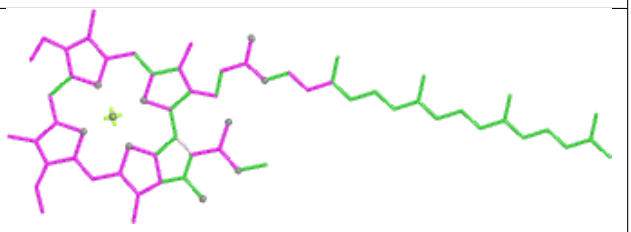


Rings

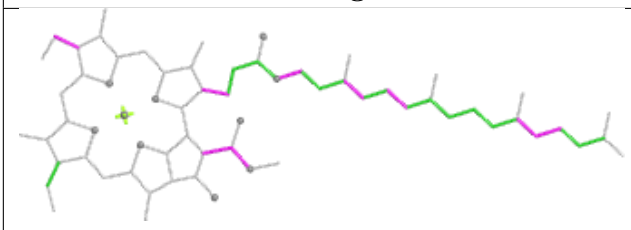
Ligand CLA bA 834



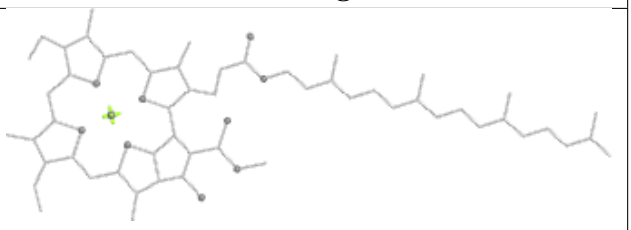
Bond lengths



Bond angles

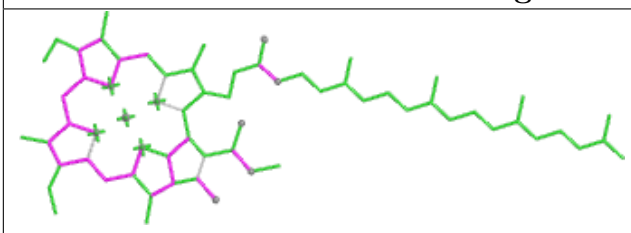


Torsions



Rings

Ligand CLA bB 927



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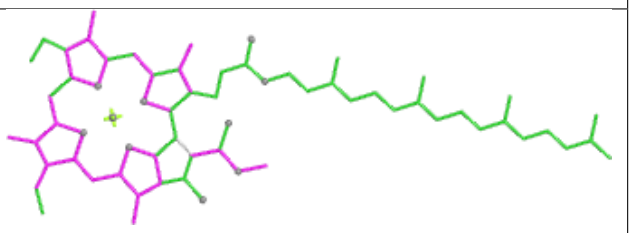
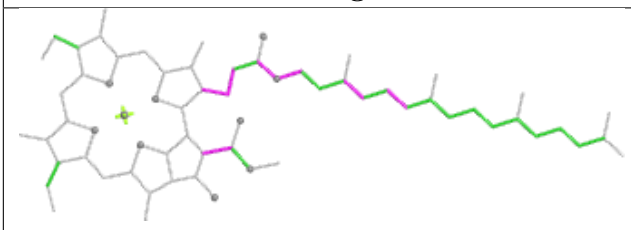


Bond angles



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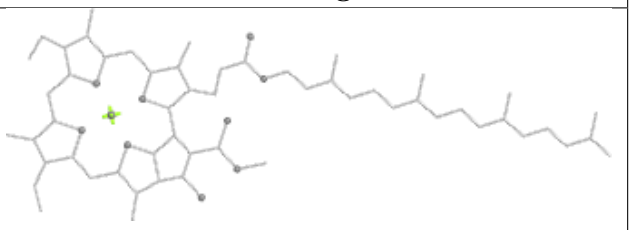
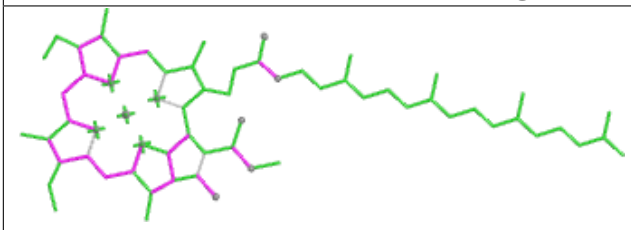


Rings

Ligand CLA bA 830



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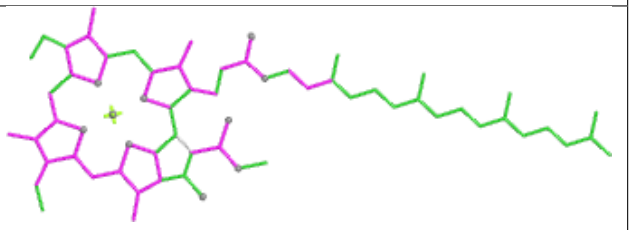
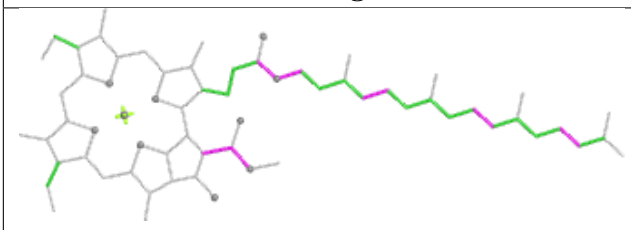
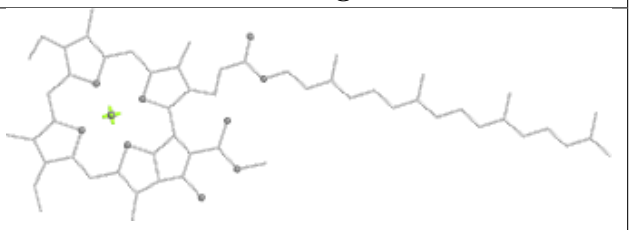


Bond angles

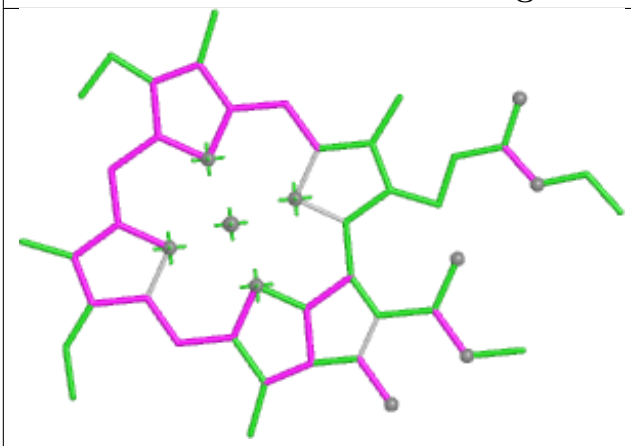


Torsions



Rings

Ligand CLA cB 937



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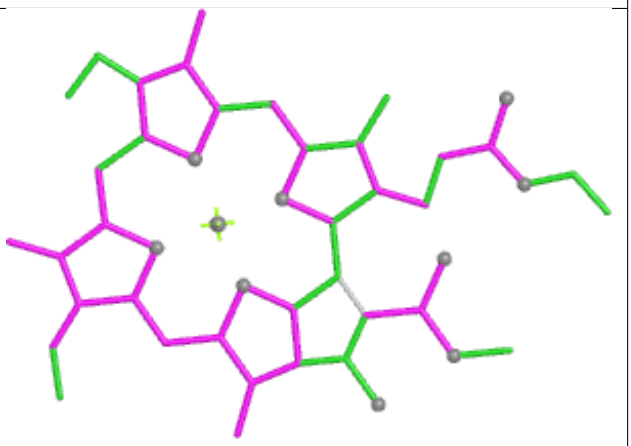
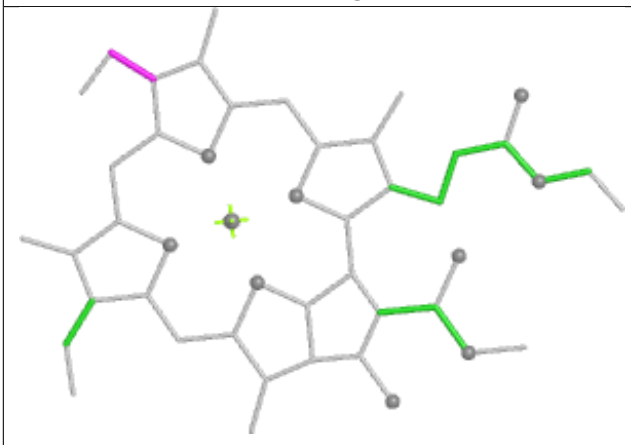


Bond angles



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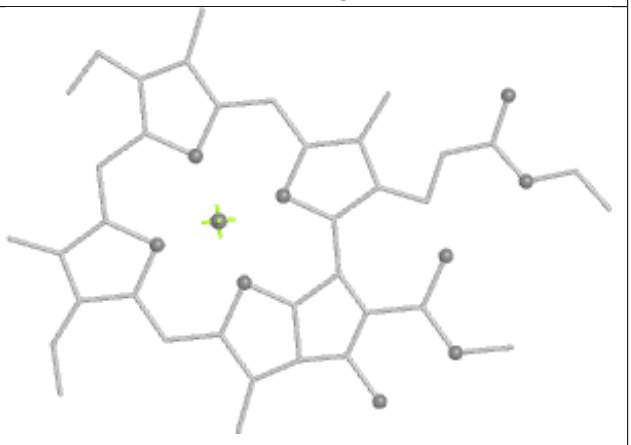
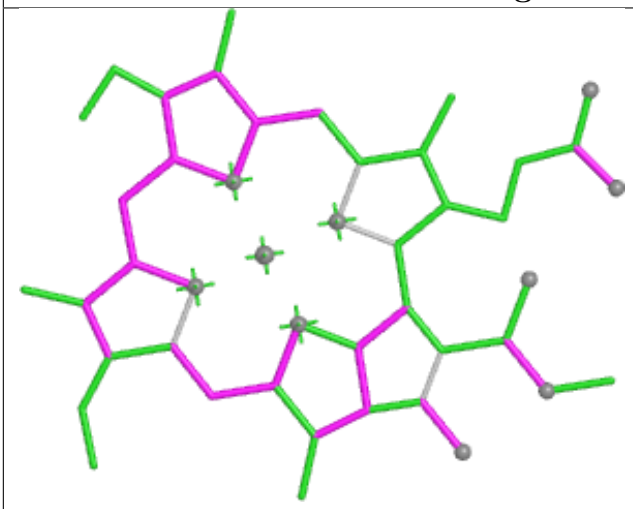
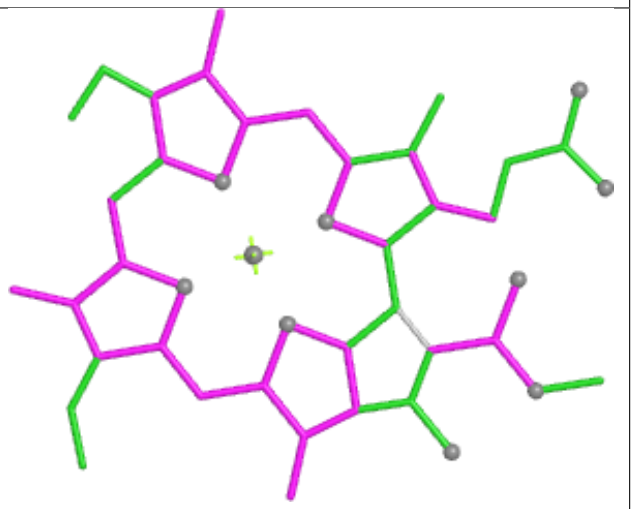


Rings

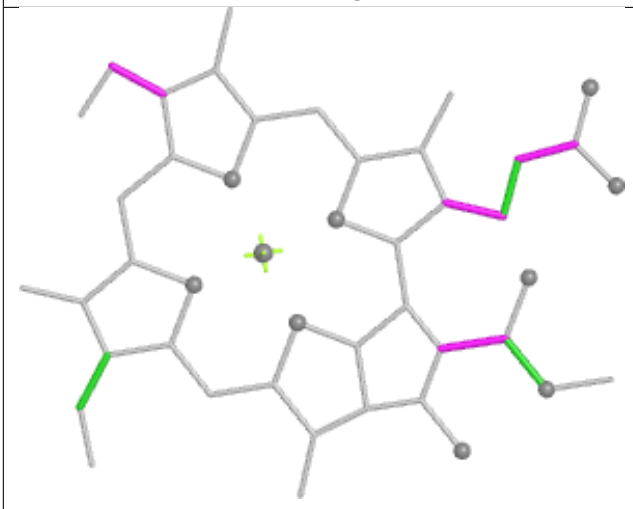
Ligand CLA bB 914



Bond lengths



Bond angles

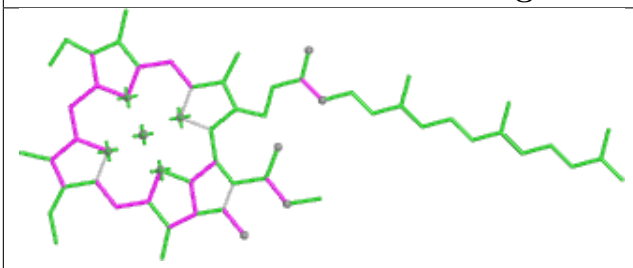


Torsions

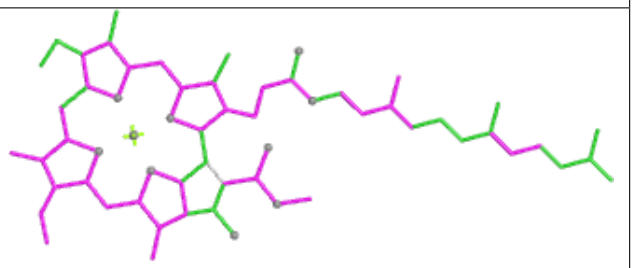


Rings

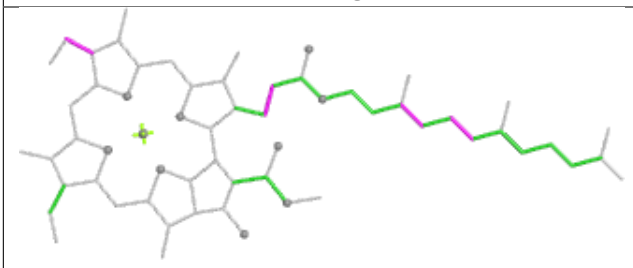
Ligand CLA cA 819



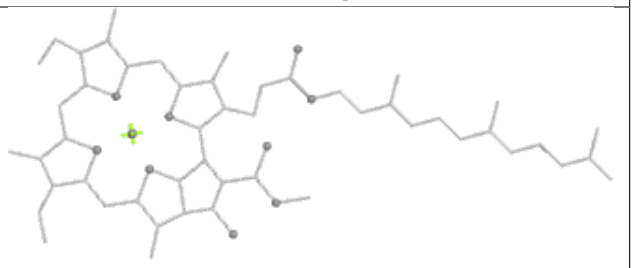
Bond lengths



Bond angles

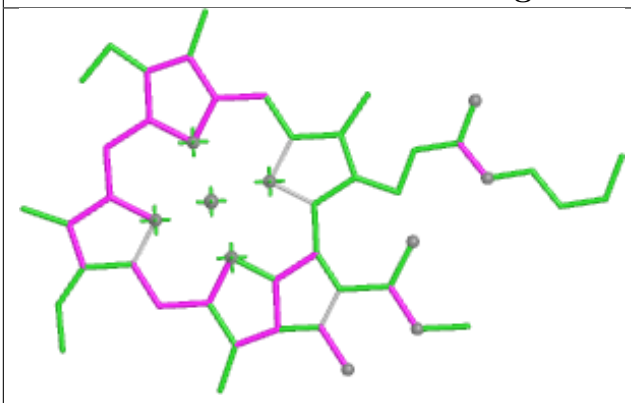


Torsions

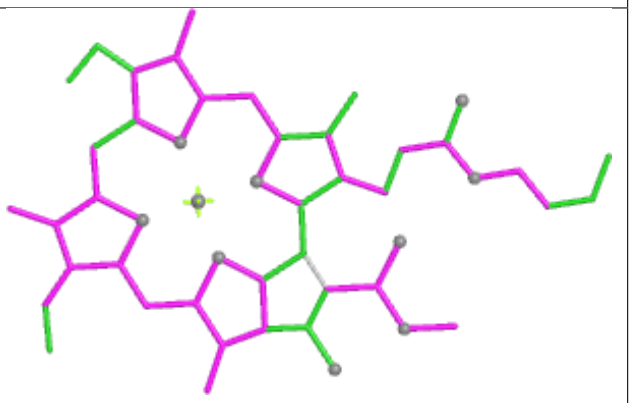


Rings

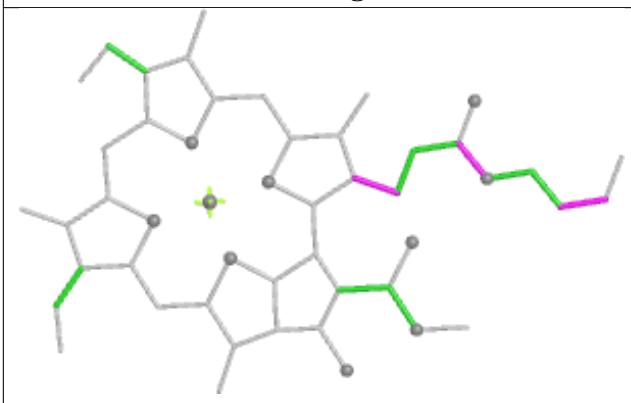
Ligand CLA bB 930



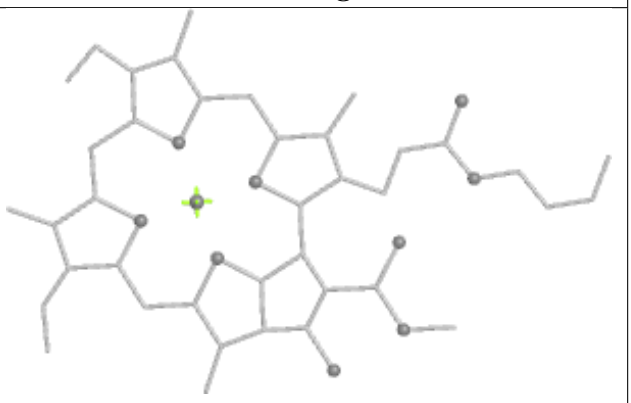
Bond lengths



Bond angles

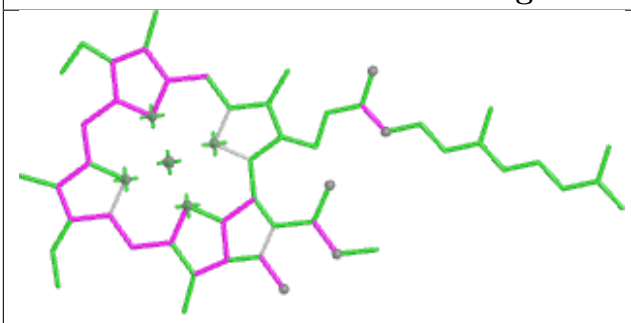


Torsions



Rings

Ligand CLA aB 921



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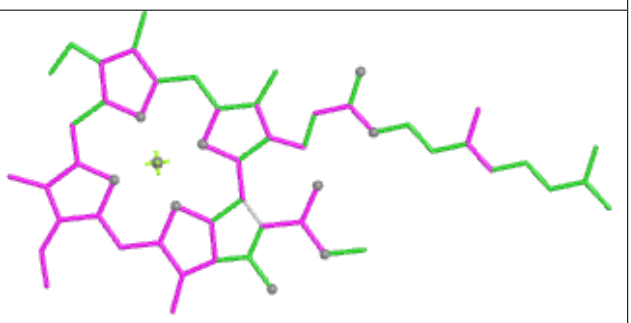
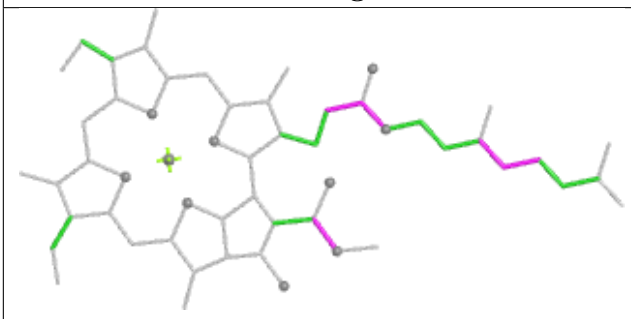


Bond angles



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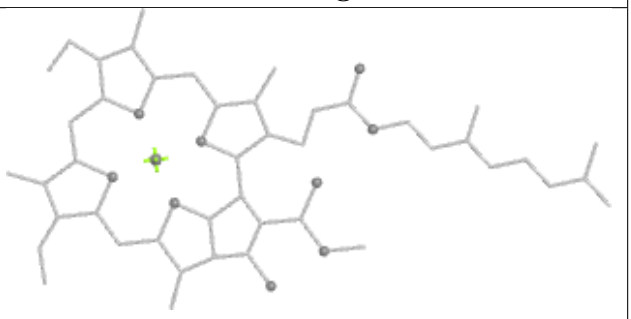
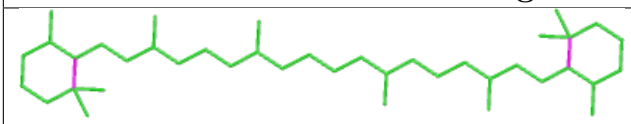


Rings

Ligand BCR cL 206



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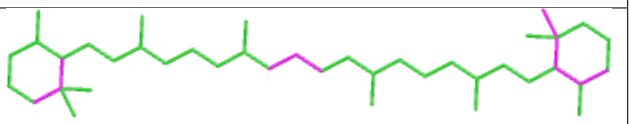
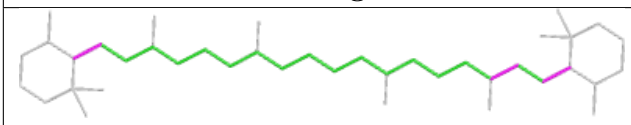


Bond angles



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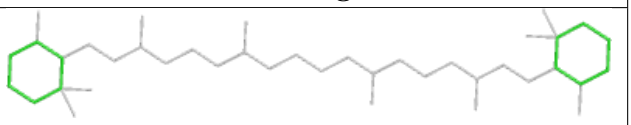
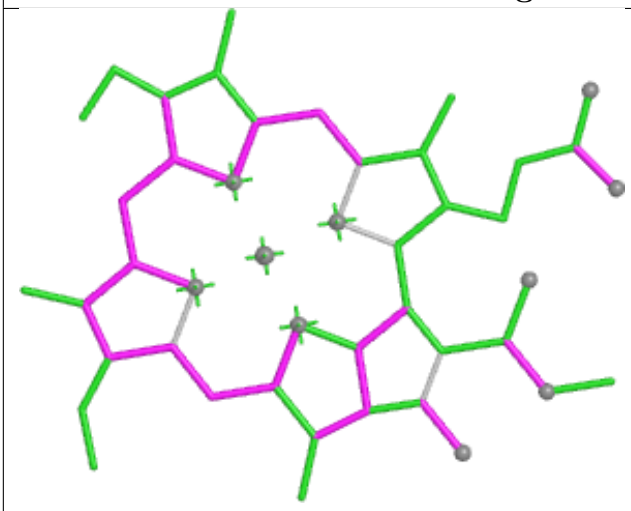


Rings

Ligand CLA cA 835



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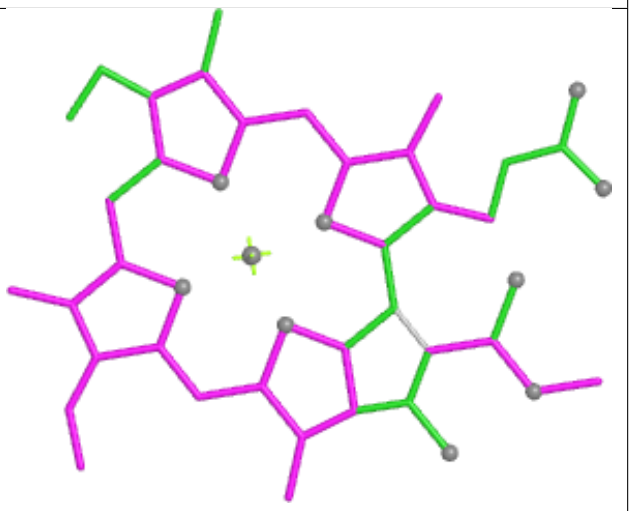
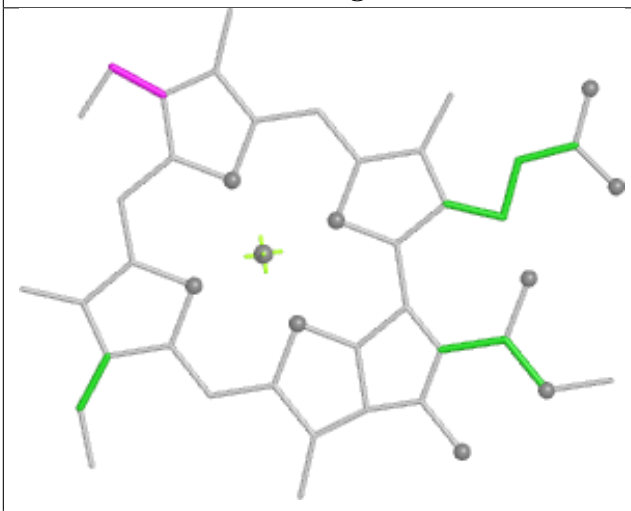


Bond angles



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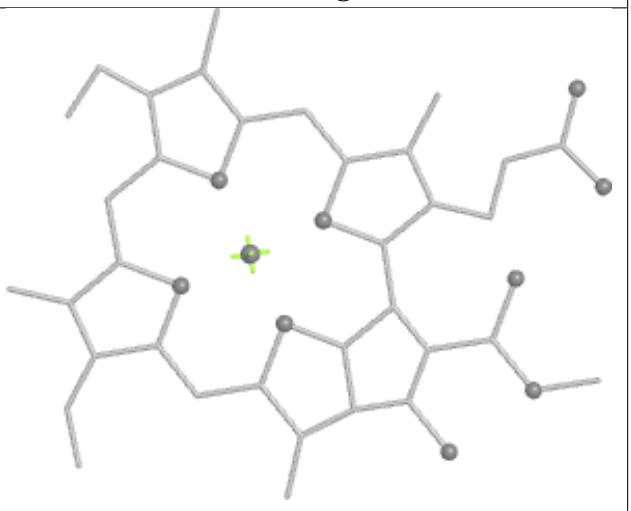
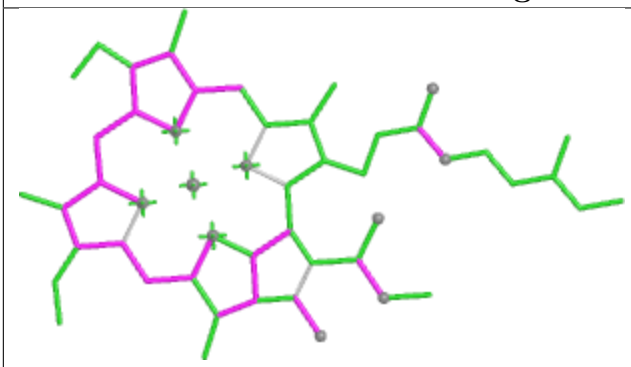
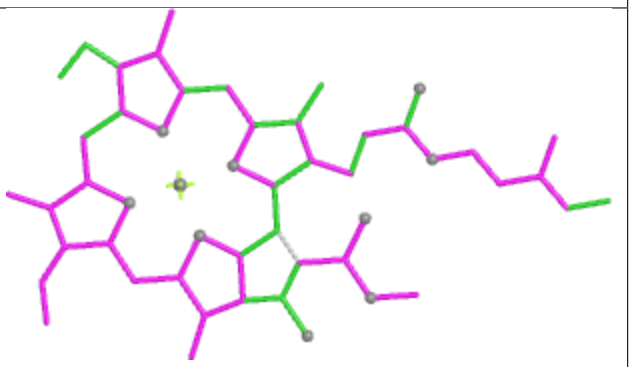
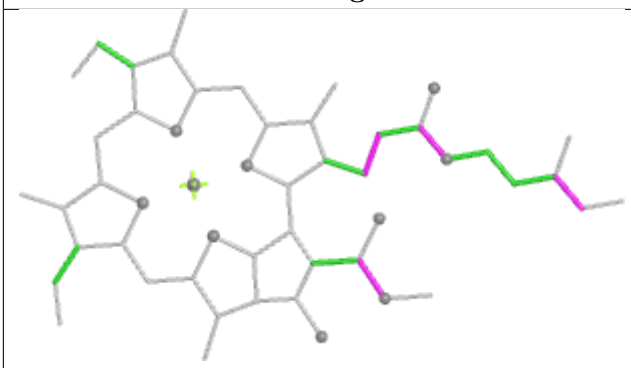
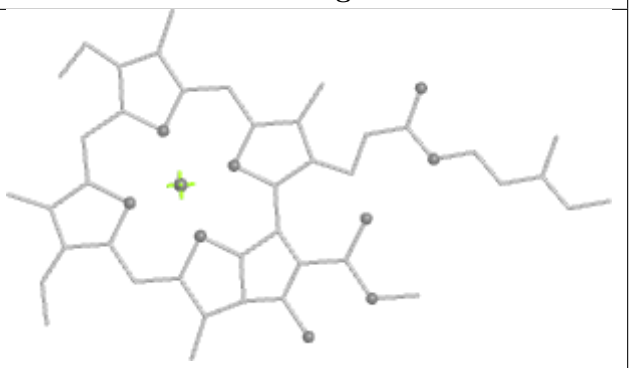
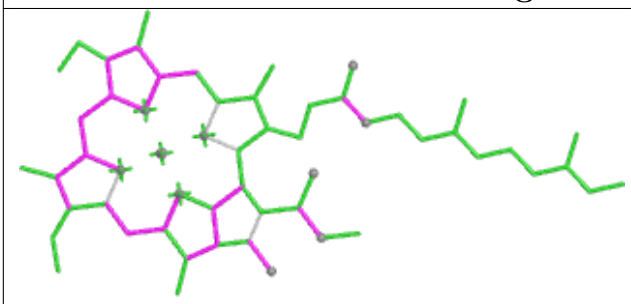
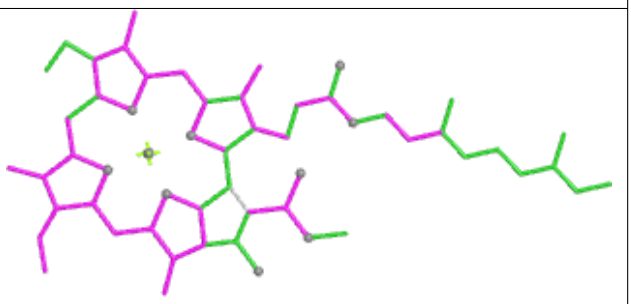
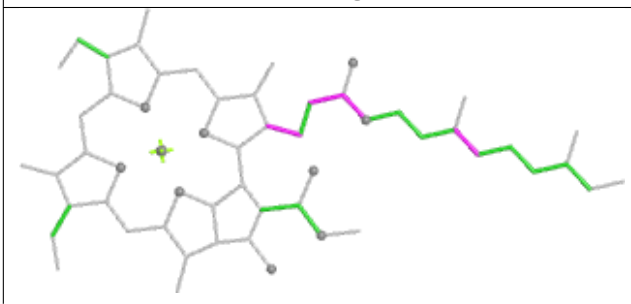
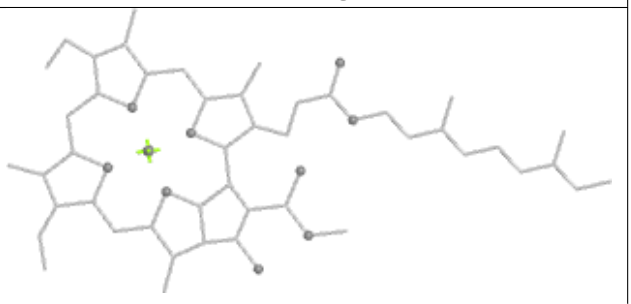
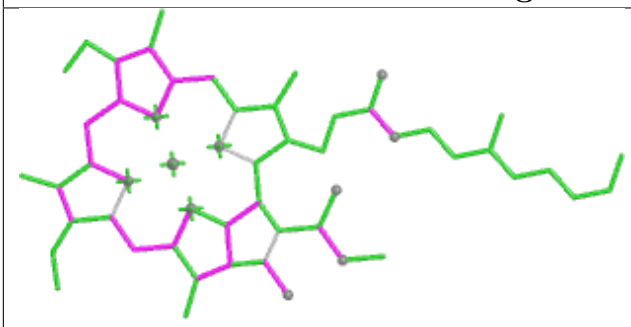


Rings

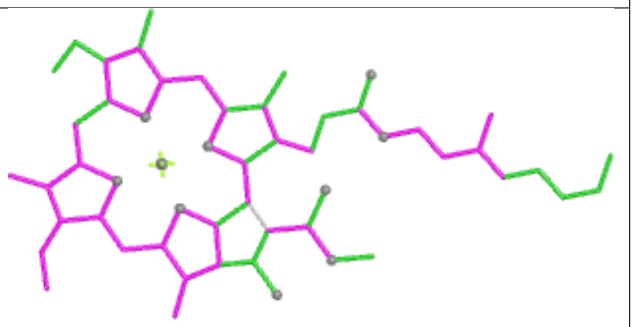
Ligand CLA bA 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aB 913	
 Bond lengths	 Bond angles
 Torsions	 Rings

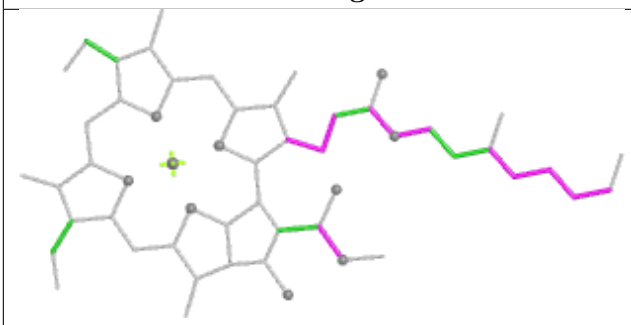
Ligand CLA cA 818



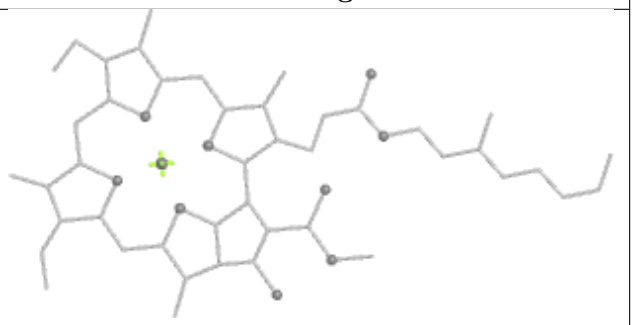
Bond lengths



Bond angles

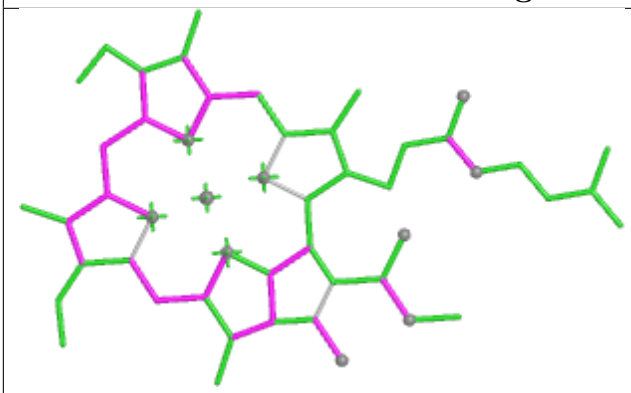


Torsions



Rings

Ligand CLA aA 831



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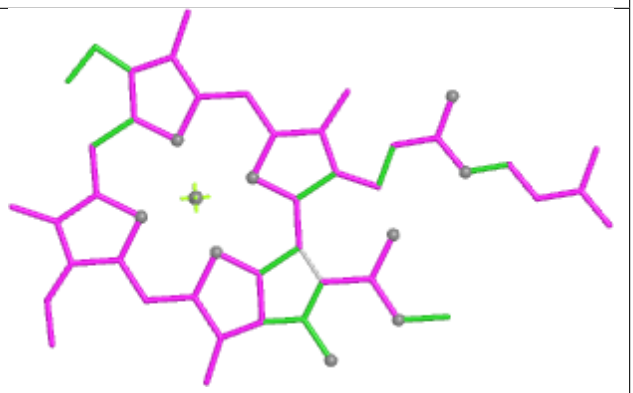
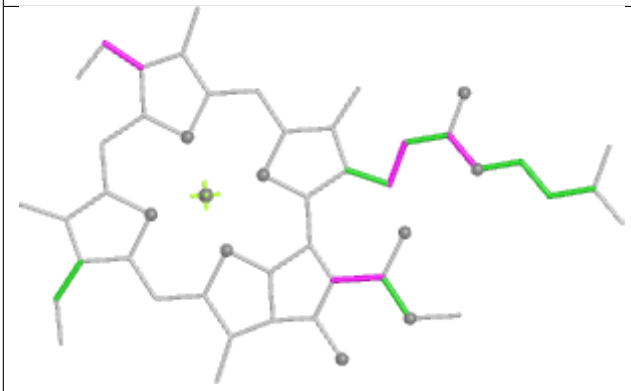


Bond angles



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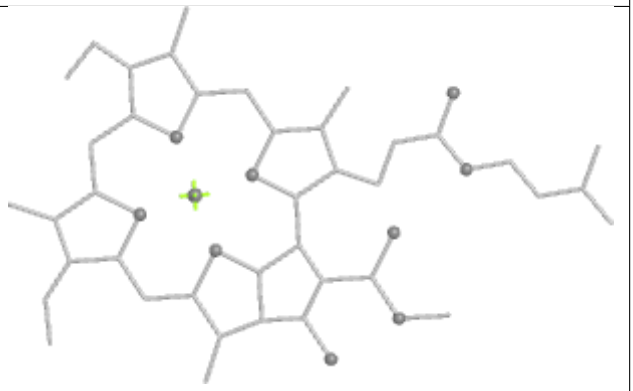
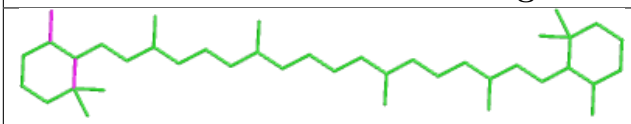


Rings

Ligand BCR aJ 101



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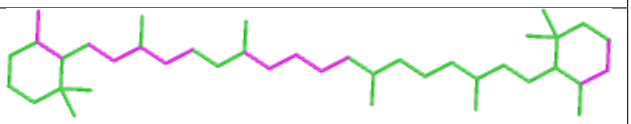
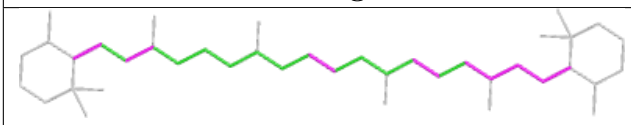


Bond angles



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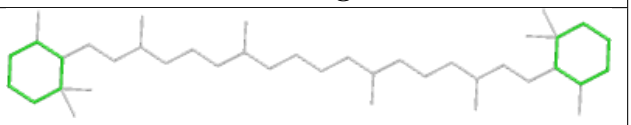
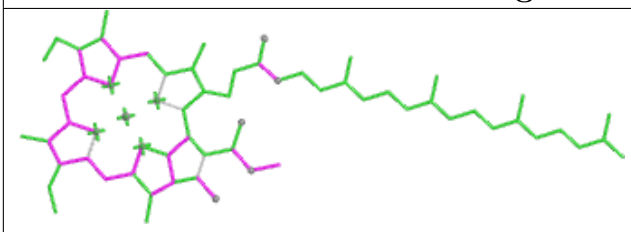
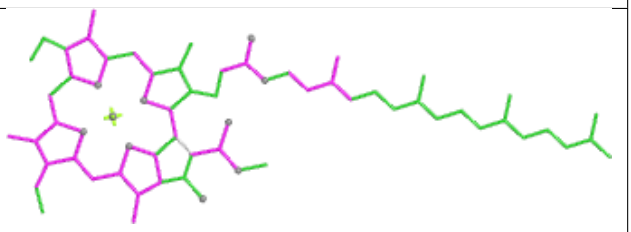


Rings

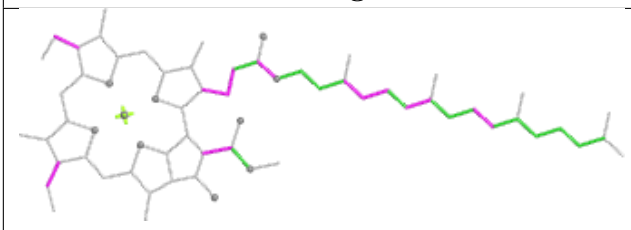
Ligand CLA aB 912



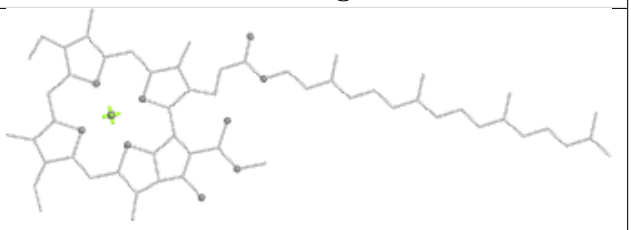
Bond lengths



Bond angles

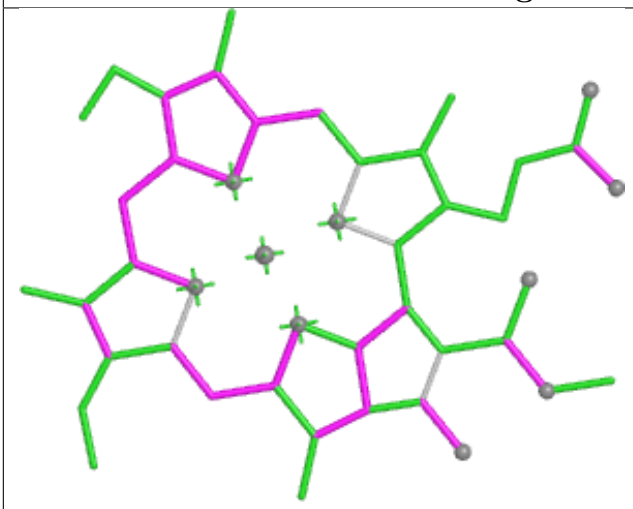


Torsions



Rings

Ligand CLA aB 922



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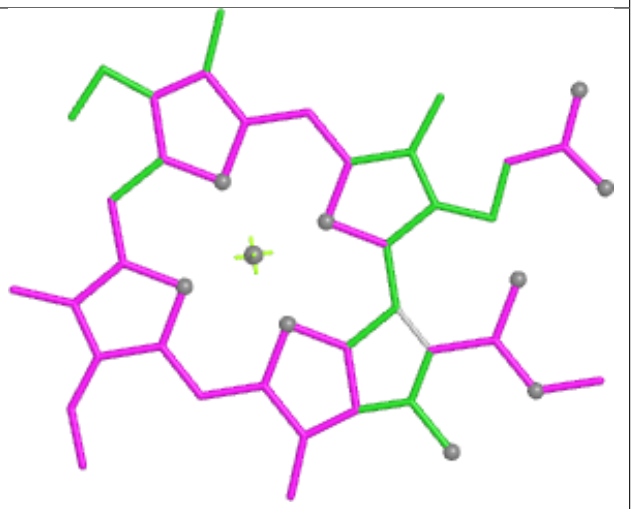
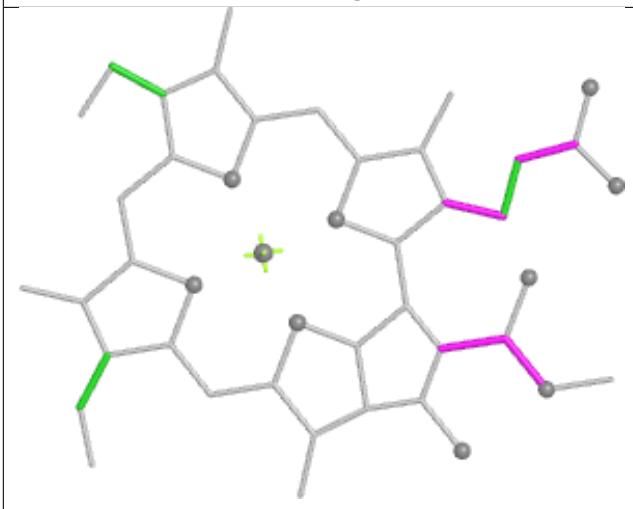


Bond angles

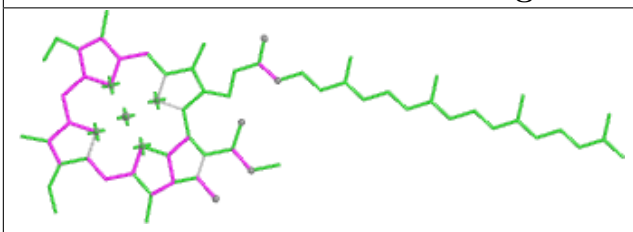


Torsions



Rings

Ligand CLA aB 926



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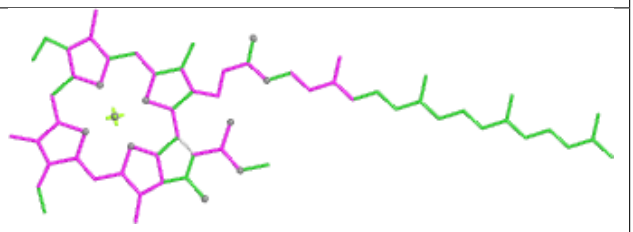
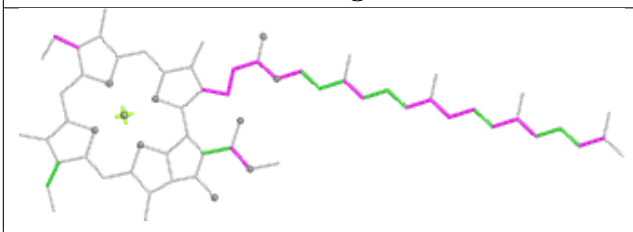


Bond angles



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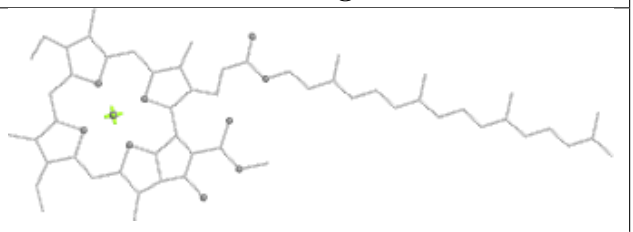
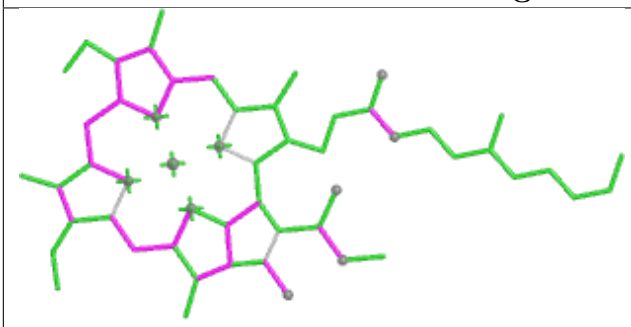


Rings

Ligand CLA bA 818



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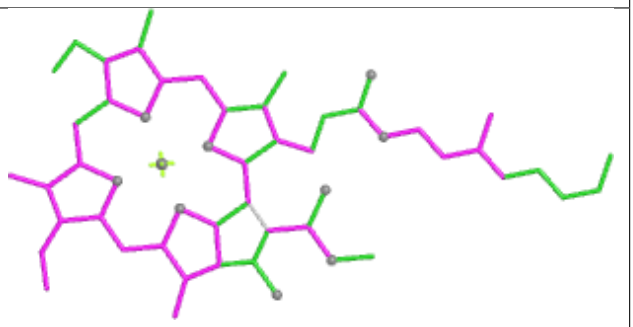
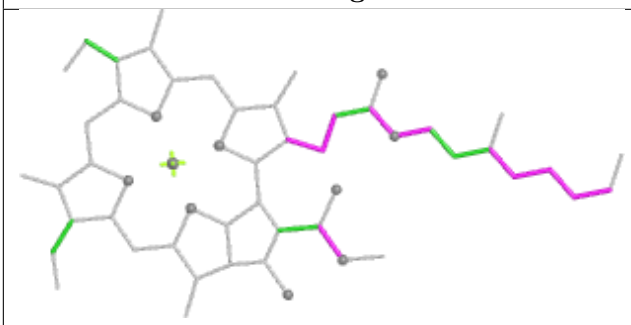


Bond angles



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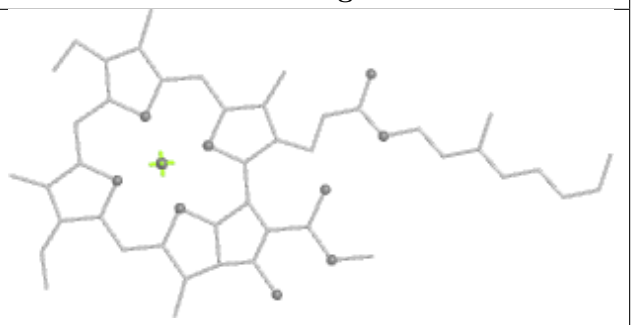
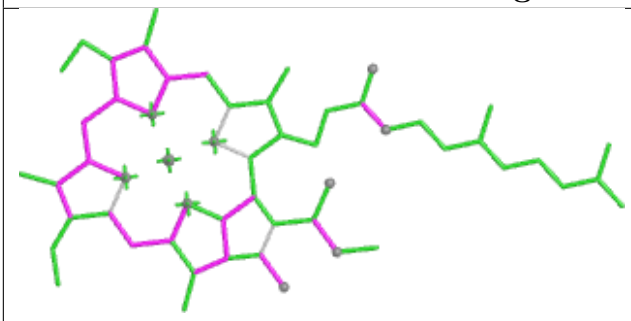
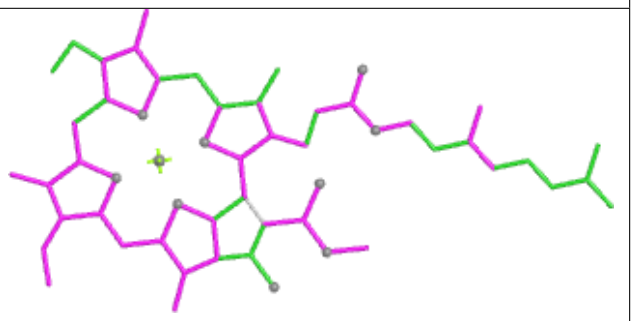


Rings

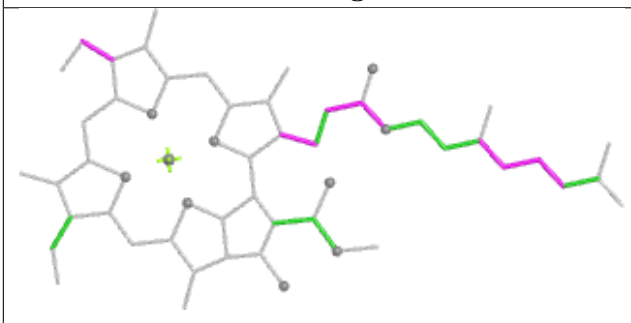
Ligand CLA bA 832



Bond lengths



Bond angles



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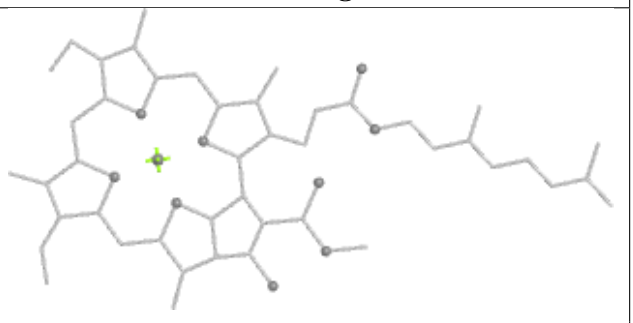
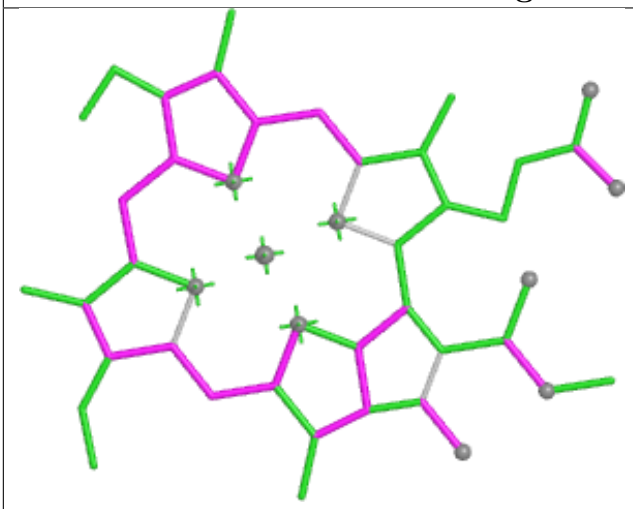


Rings

Ligand CLA cA 815



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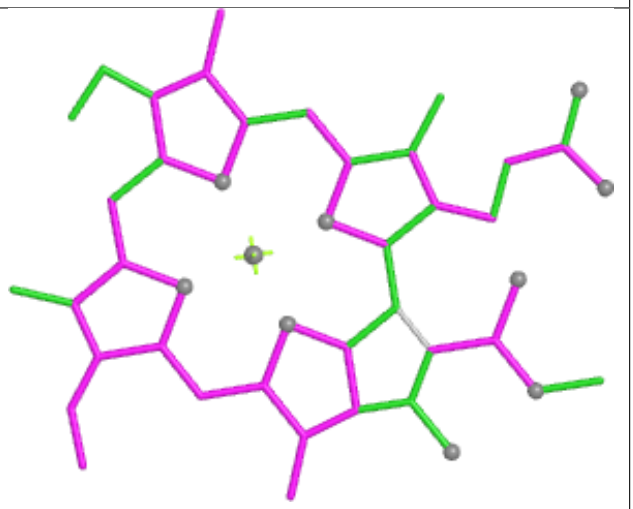
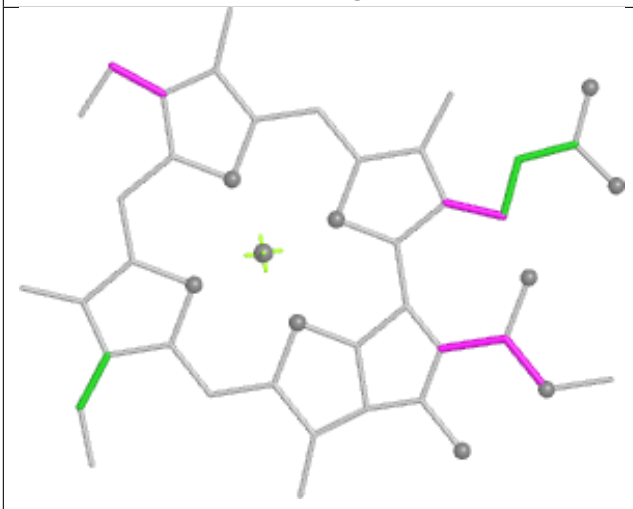


Bond angles

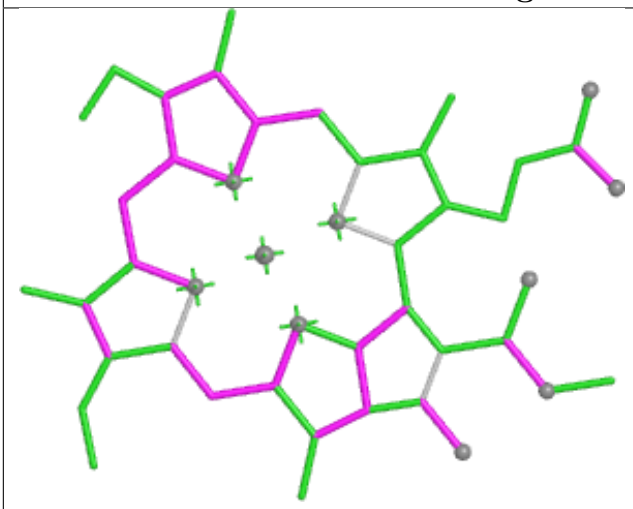


Torsions

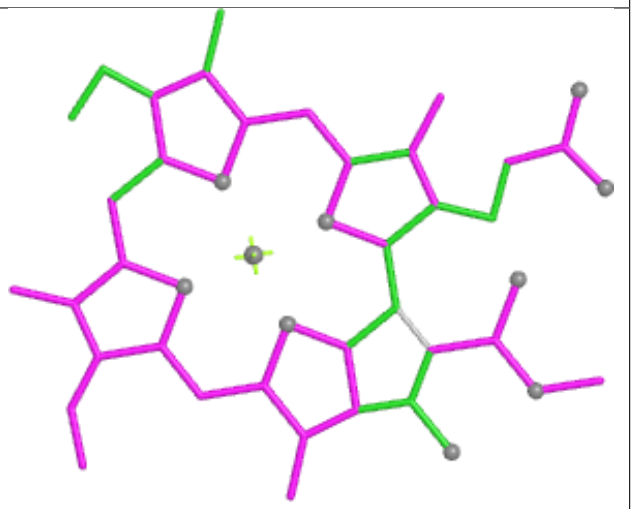


Rings

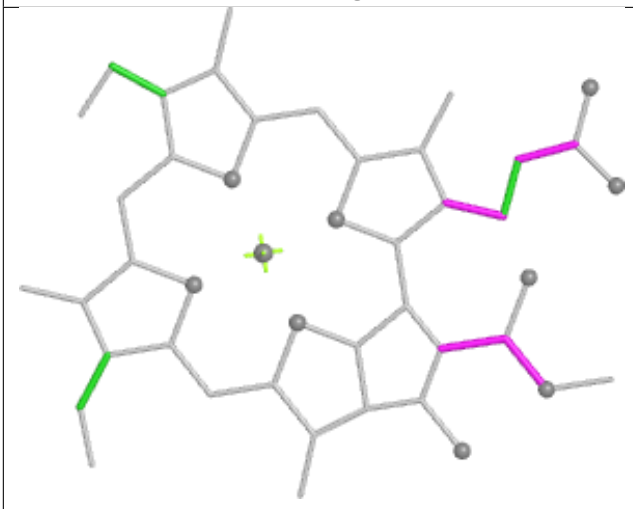
Ligand CLA cB 922



Bond lengths



Bond angles

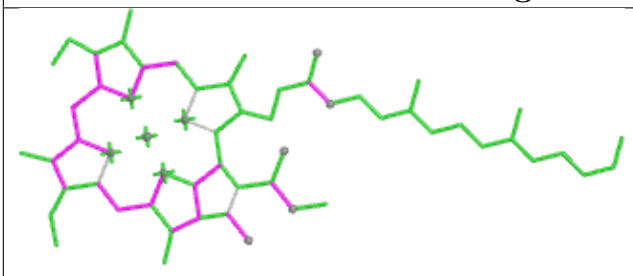


Torsions

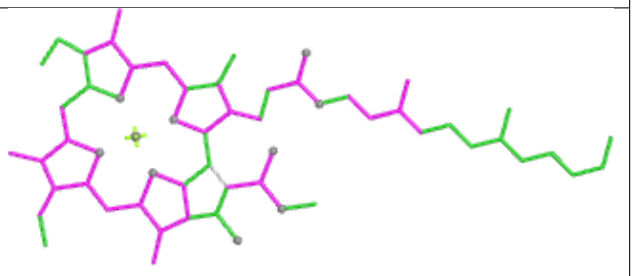


Rings

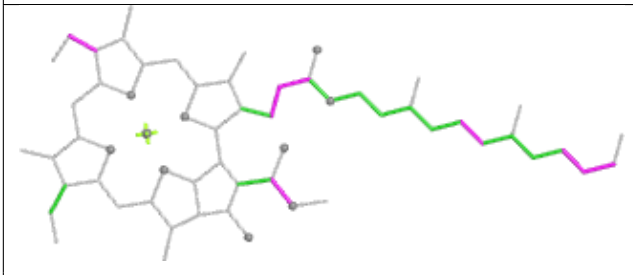
Ligand CLA bB 916



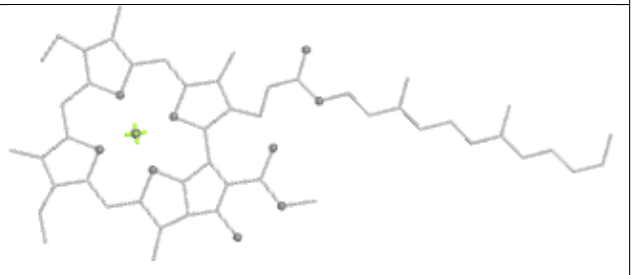
Bond lengths



Bond angles

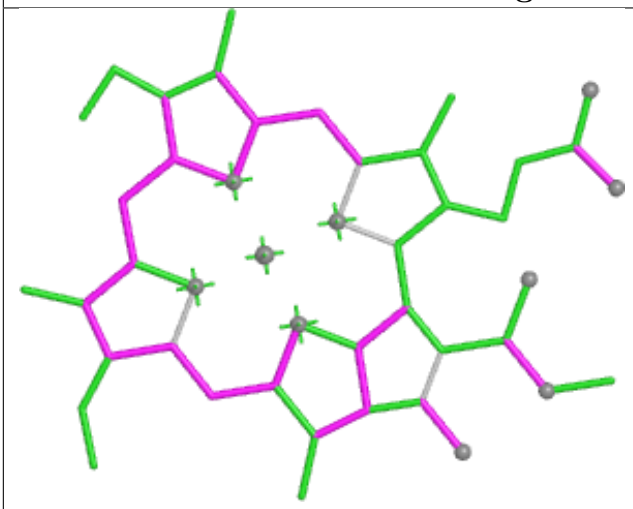


Torsions

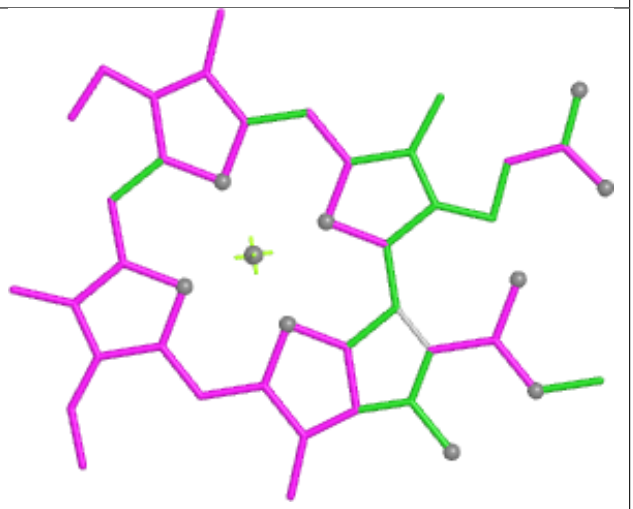


Rings

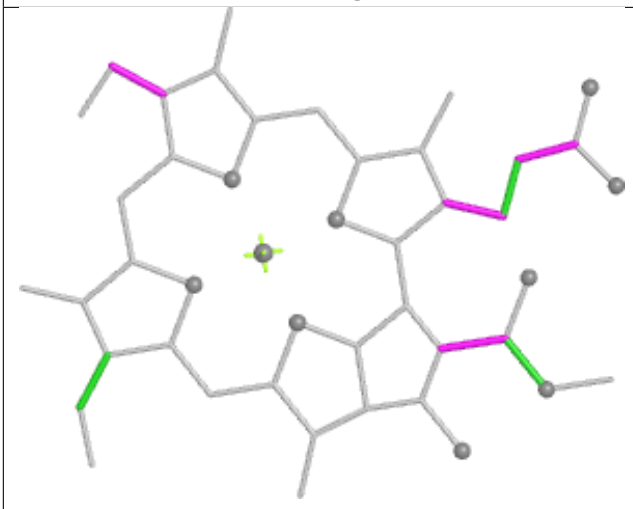
Ligand CLA aB 929



Bond lengths



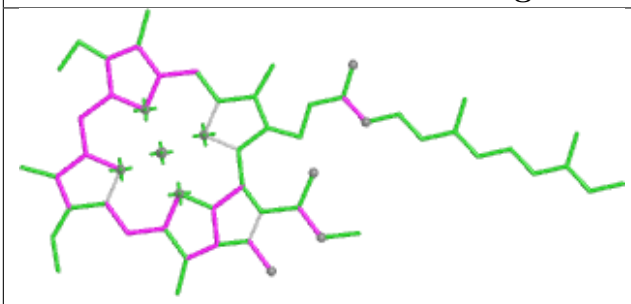
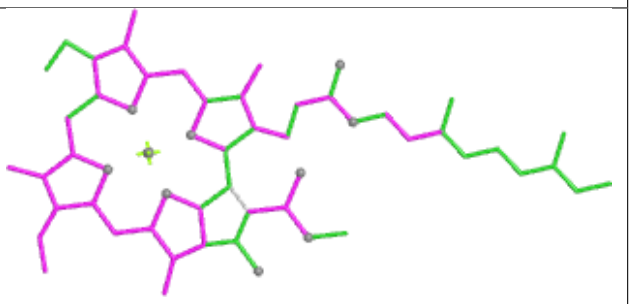
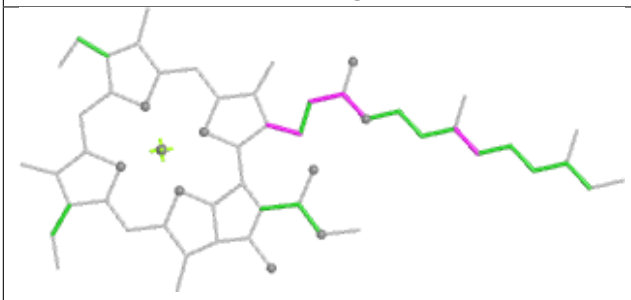
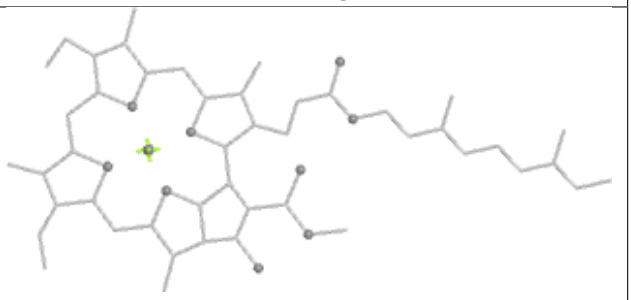
Bond angles

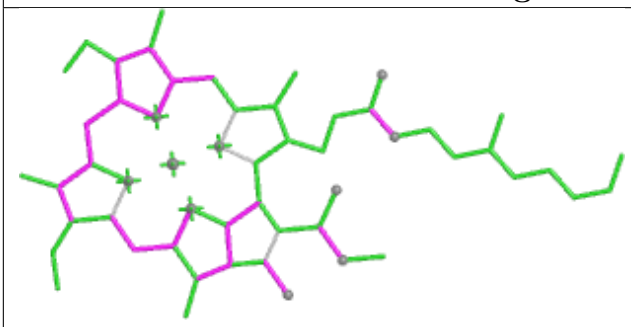
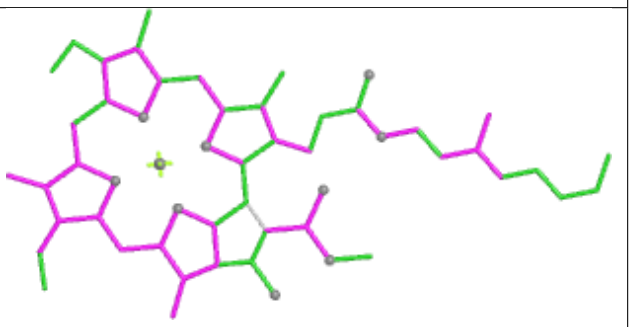
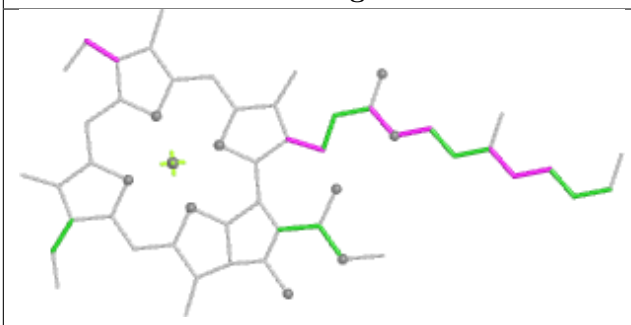
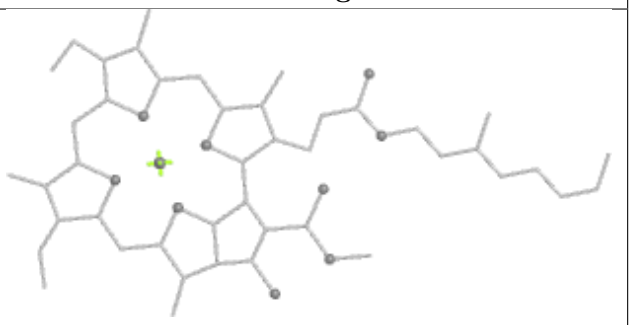


Torsions

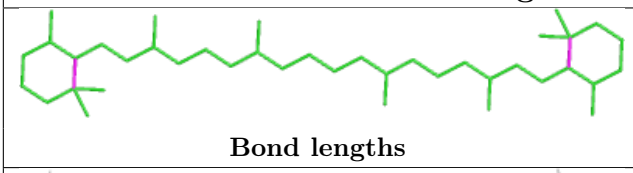


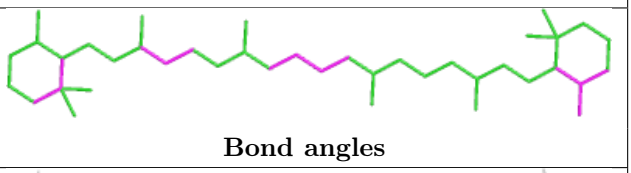
Rings

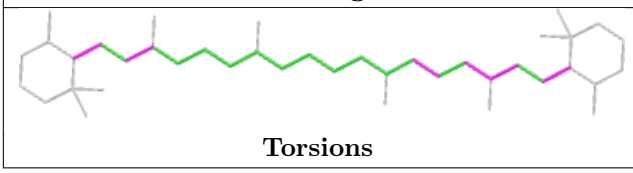
Ligand CLA bB 913	
	
Bond lengths	Bond angles
	
Torsions	Rings

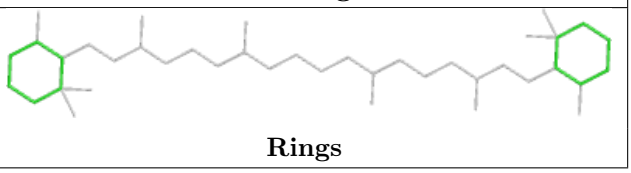
Ligand CLA bA 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cL 205

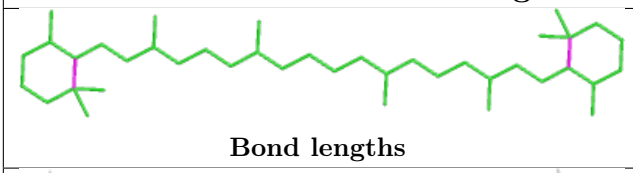

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR aA 851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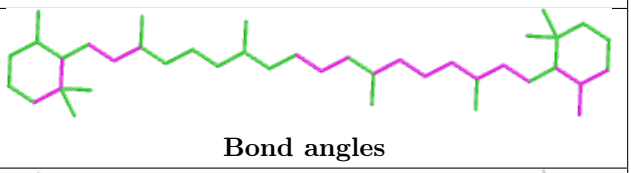
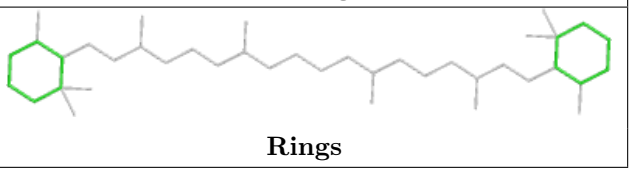
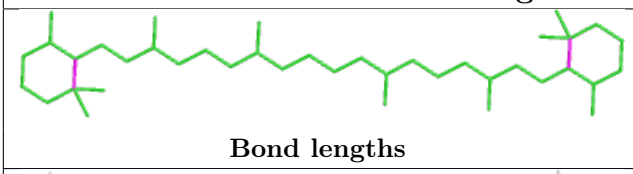

Bond angles


Torsions


Rings

Ligand BCR aL 205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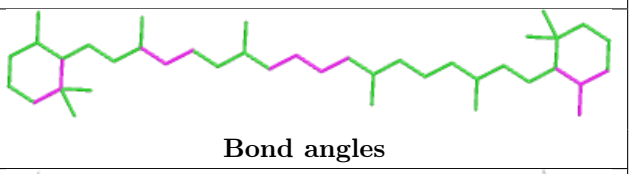
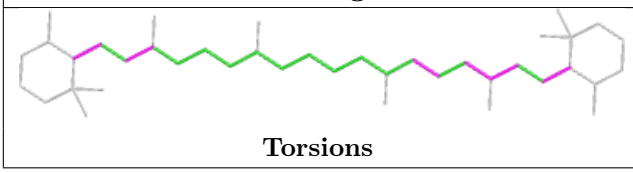

Bond angles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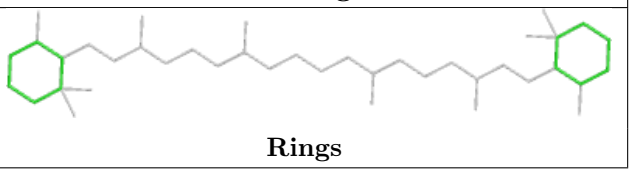
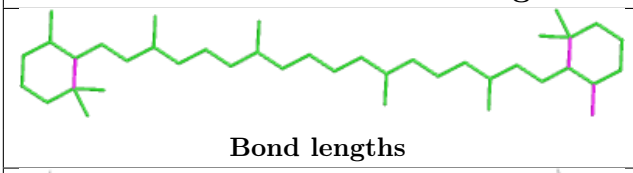

Rings

Ligand BCR bB 946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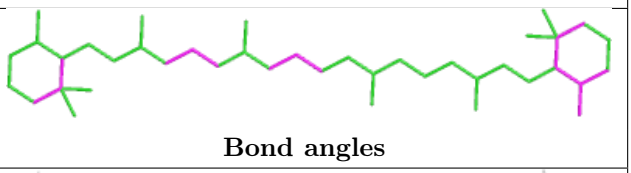
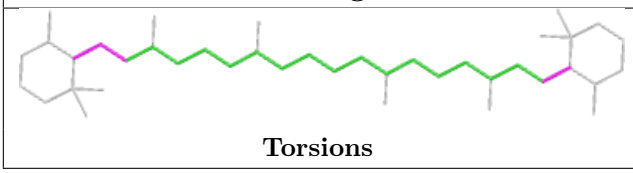

Bond angles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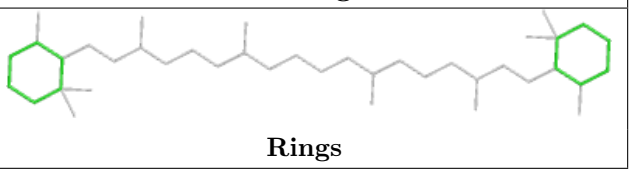
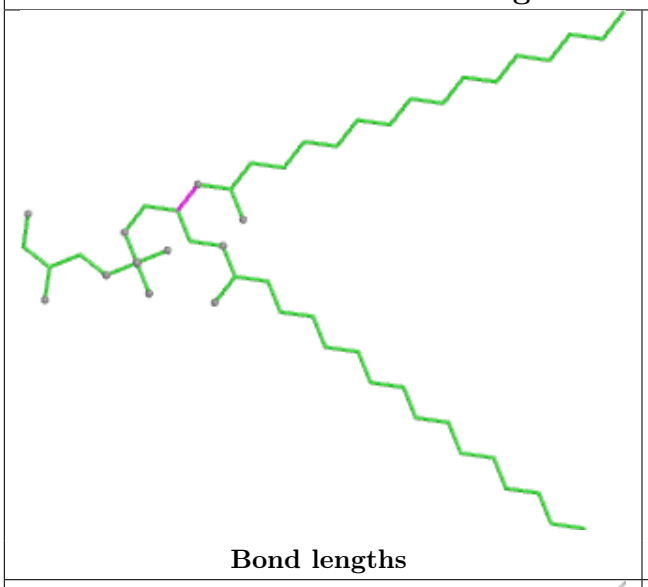
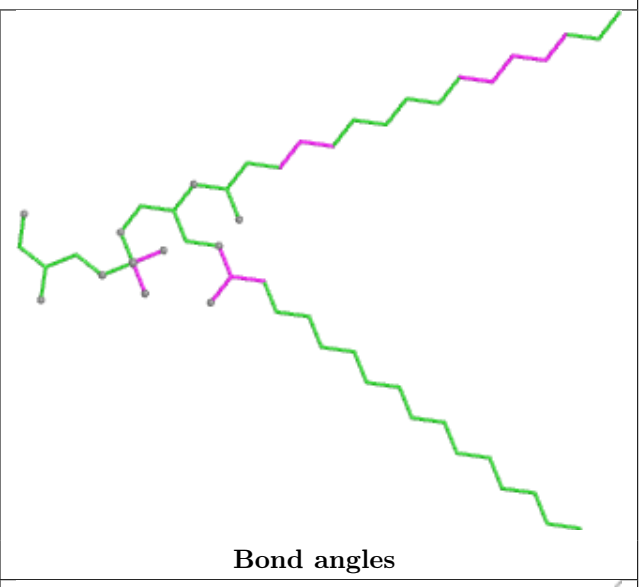

Rings

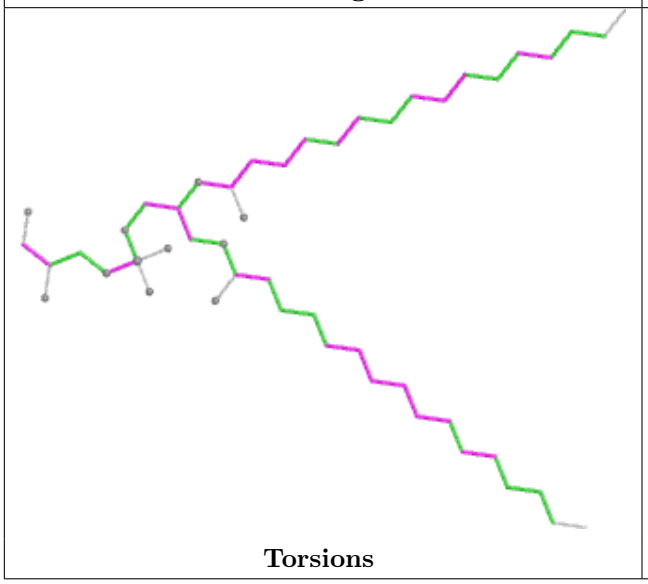
Ligand LHG bA 851



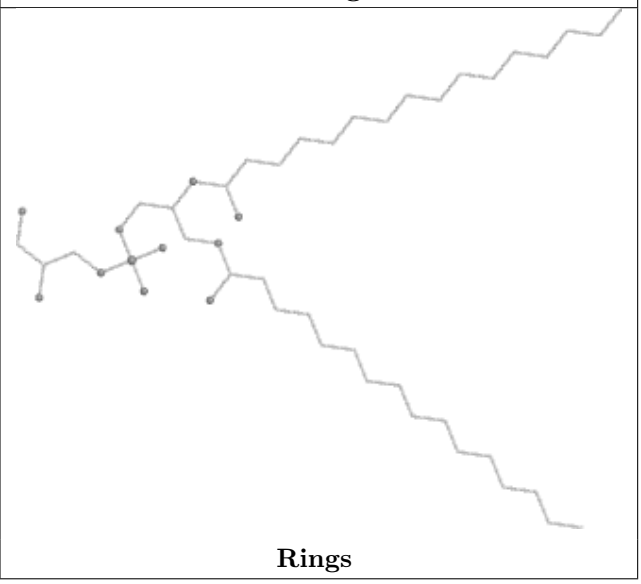
Bond lengths



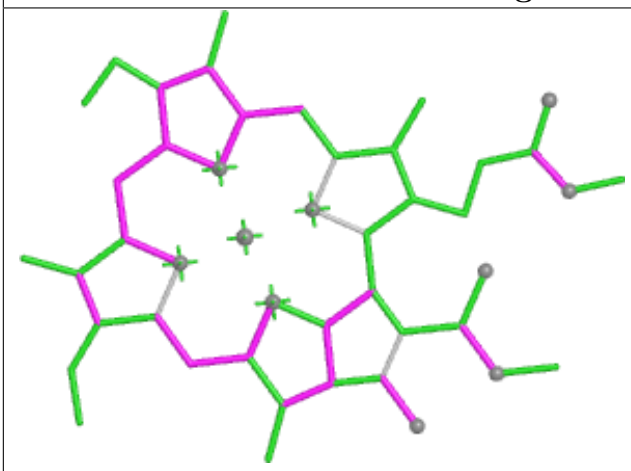
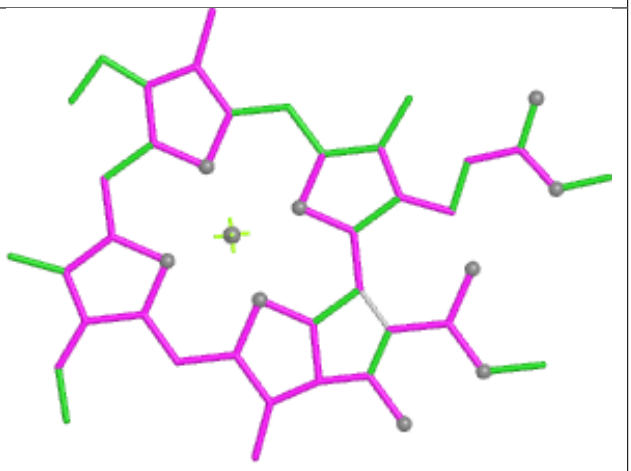
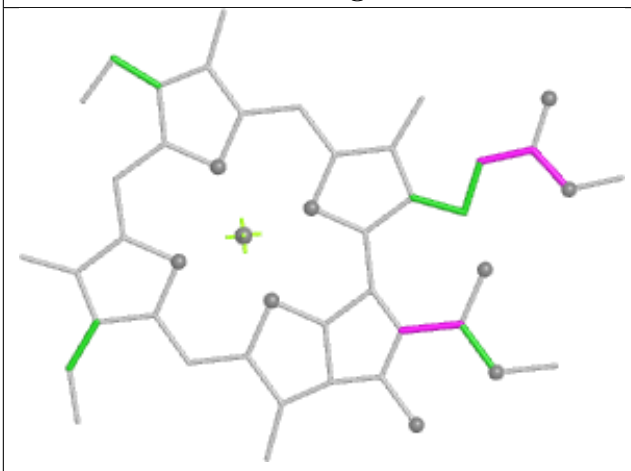
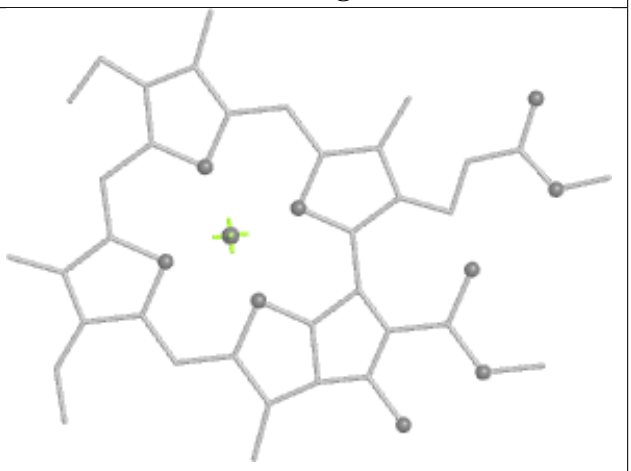
Bond angles



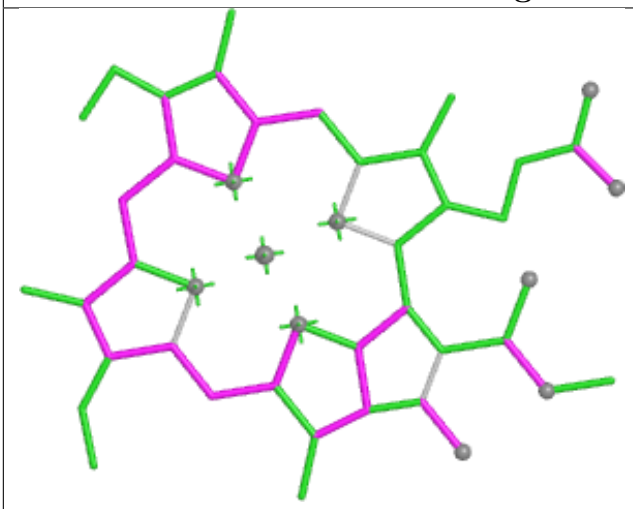
Torsions



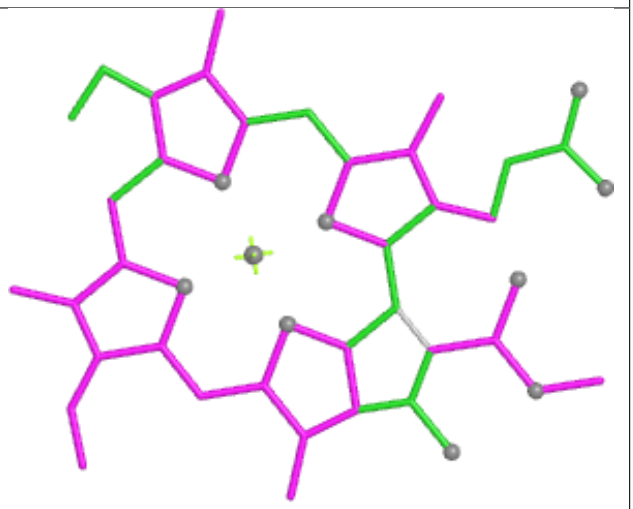
Rings

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

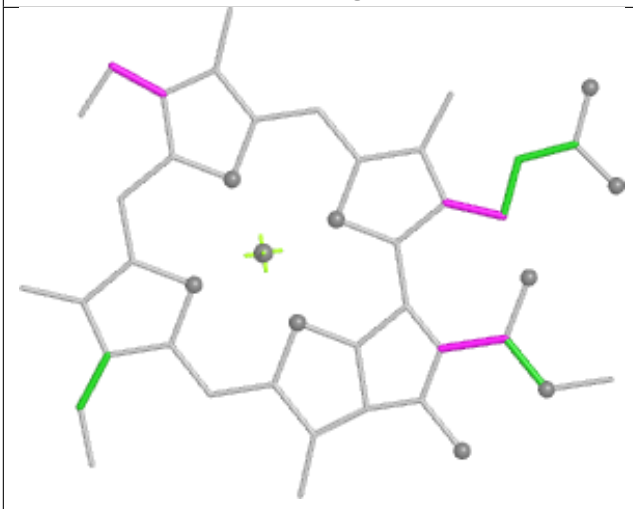
Ligand CLA bB 910



Bond lengths



Bond angles

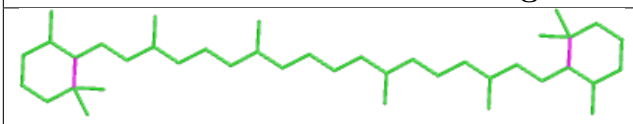


Torsions

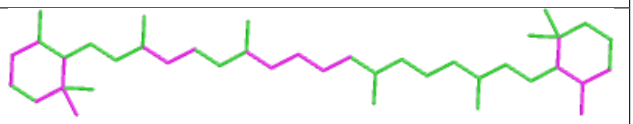


Rings

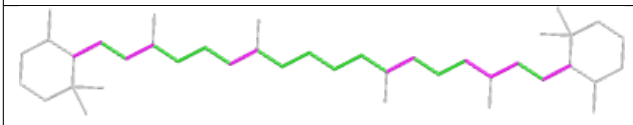
Ligand BCR cI 101



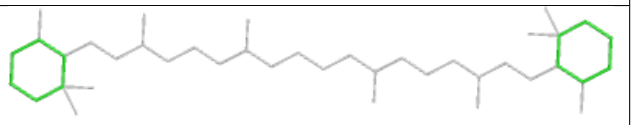
Bond lengths



Bond angles

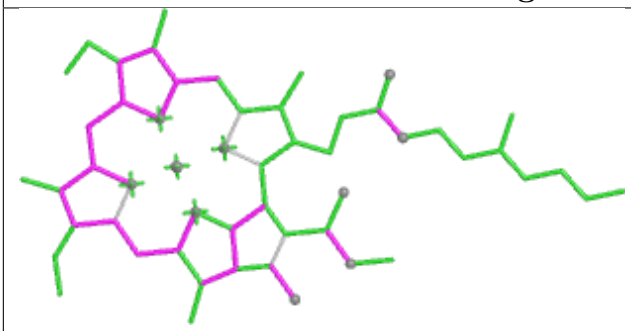


Torsions

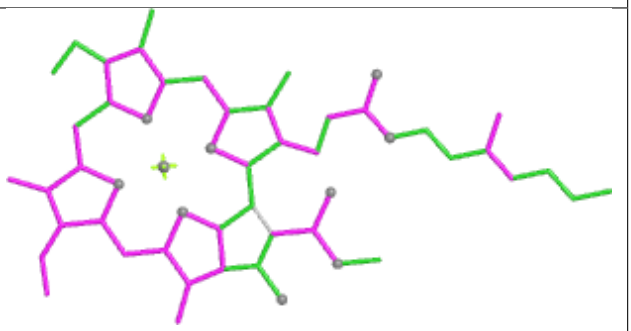


Rings

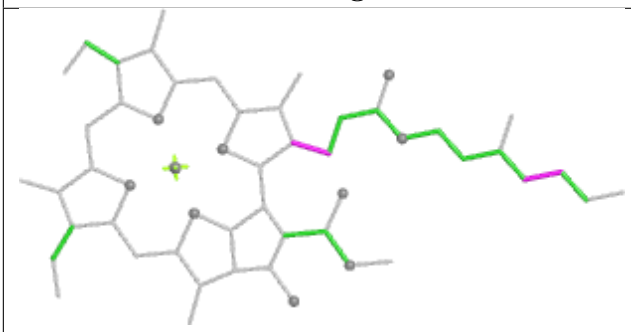
Ligand CLA aL 202



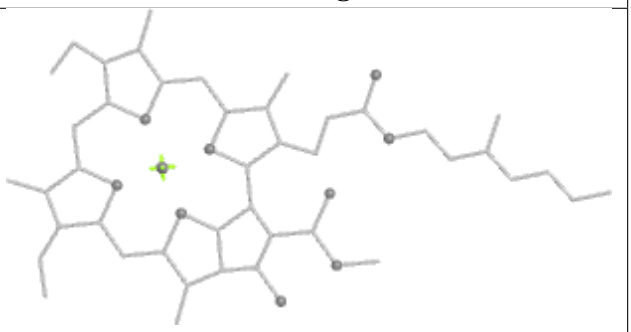
Bond lengths



Bond angles

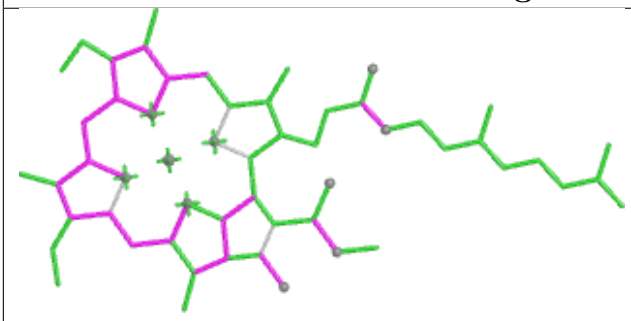


Torsions

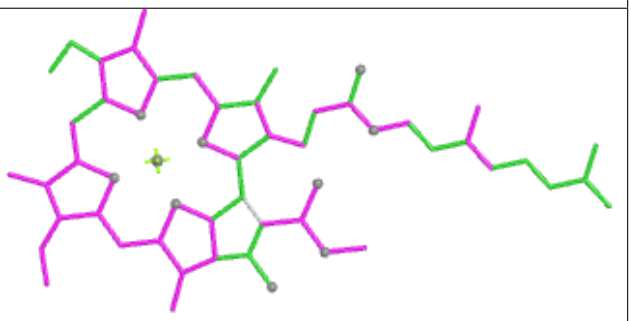


Rings

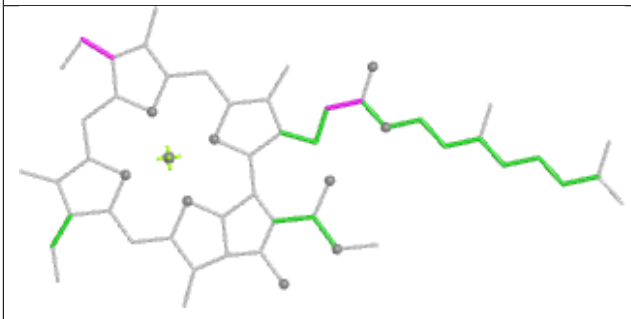
Ligand CLA bB 906



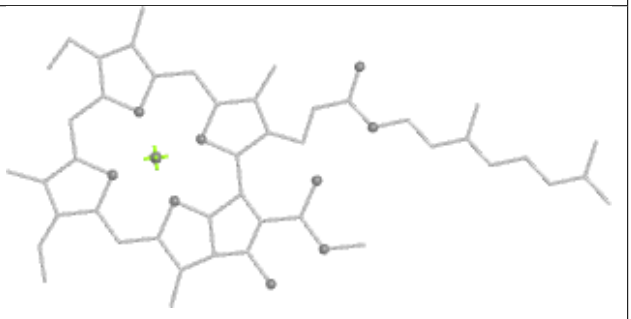
Bond lengths



Bond angles

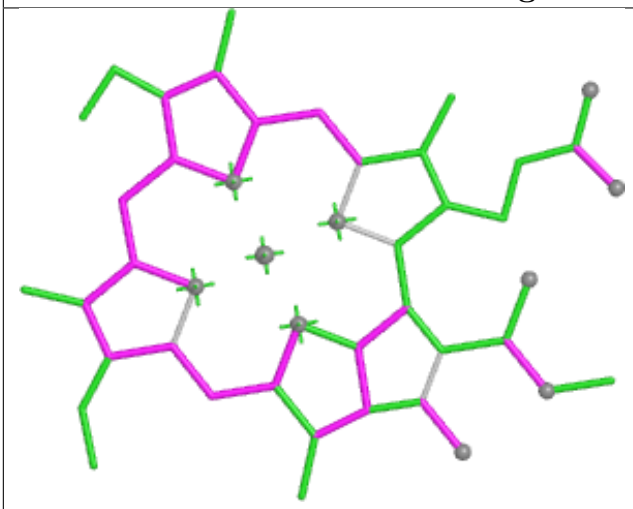


Torsions

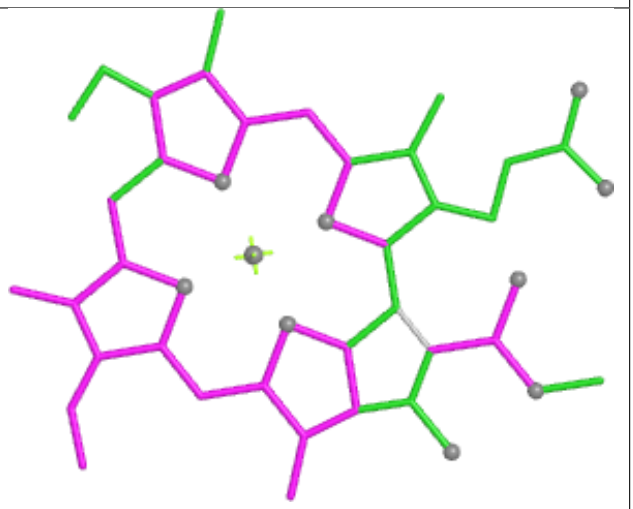


Rings

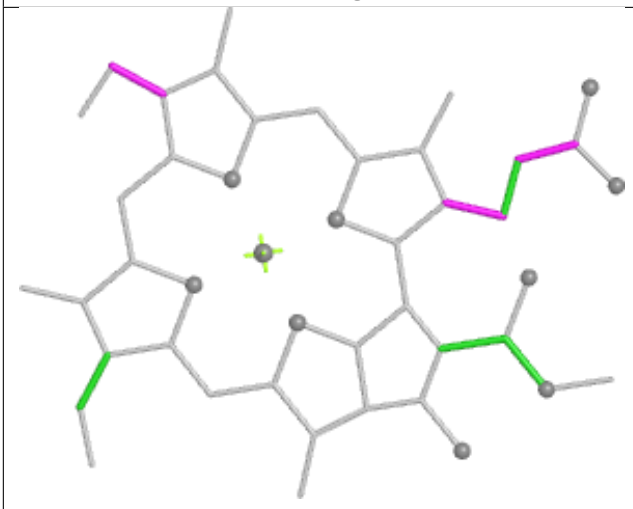
Ligand CLA cL 203



Bond lengths



Bond angles

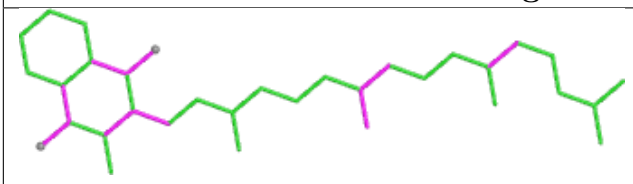


Torsions

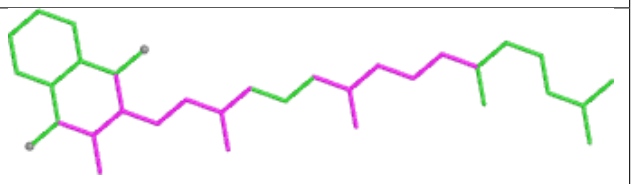


Rings

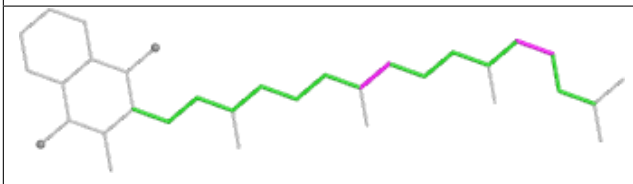
Ligand 1L3 bA 844



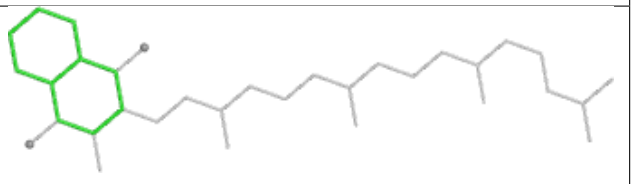
Bond lengths



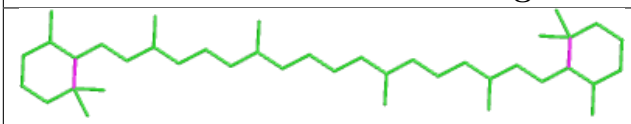
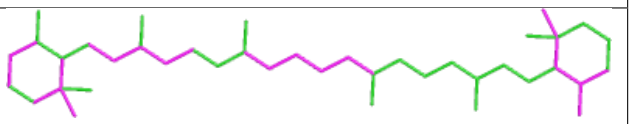
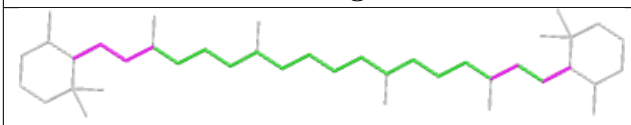
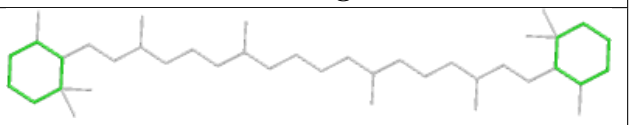
Bond angles

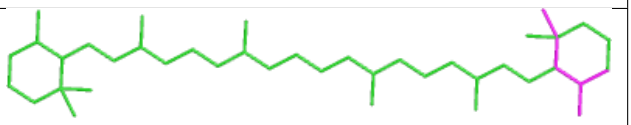
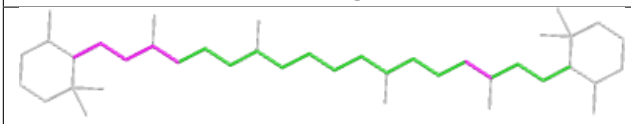
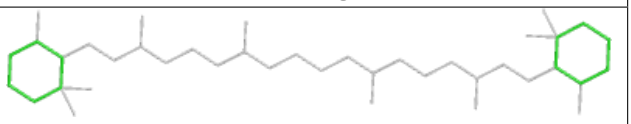


Torsions

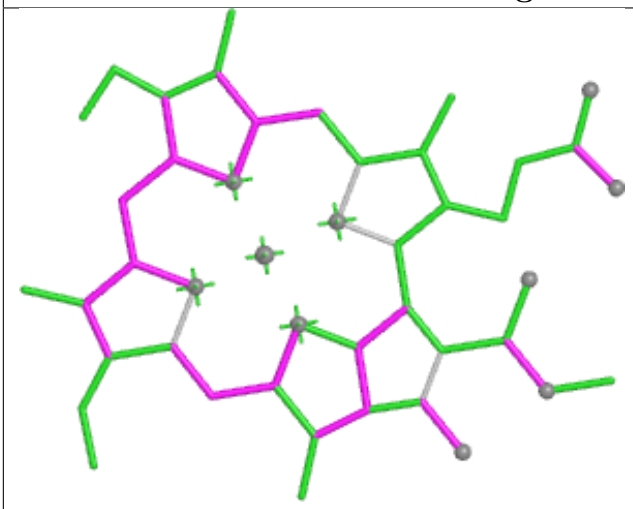


Rings

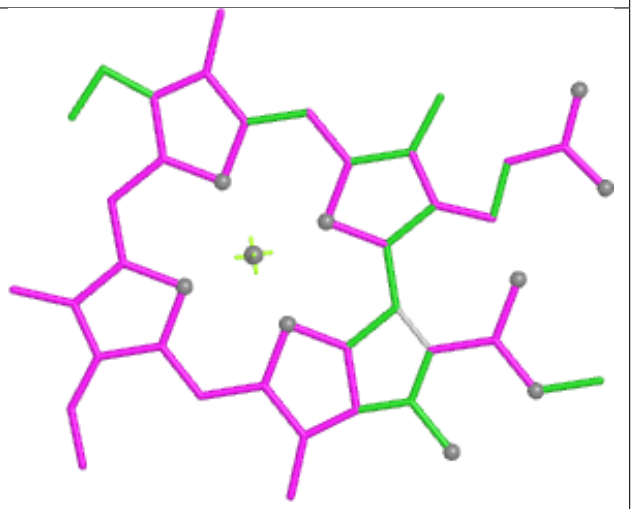
Ligand BCR cA 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR aB 943	
 Bond lengths	 Bond angles
 Torsions	 Rings

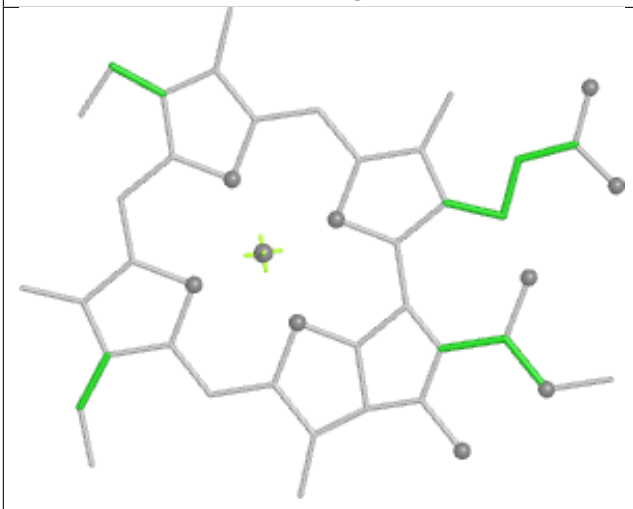
Ligand CLA aB 911



Bond lengths



Bond angles

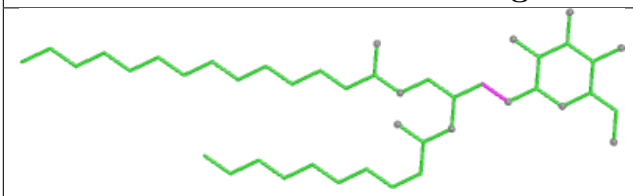


Torsions

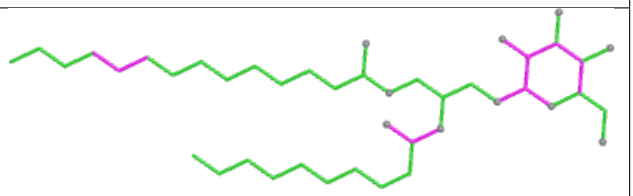


Rings

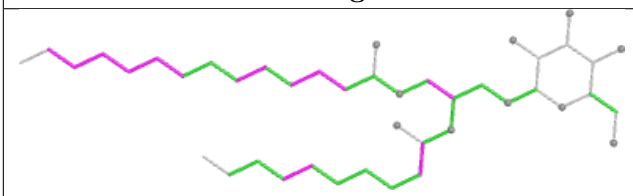
Ligand LMG aB 947



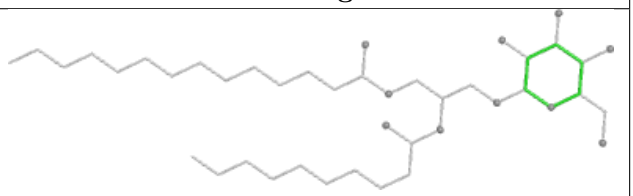
Bond lengths



Bond angles

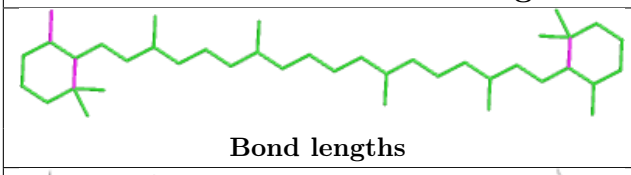


Torsions



Rings

Ligand BCR cB 941



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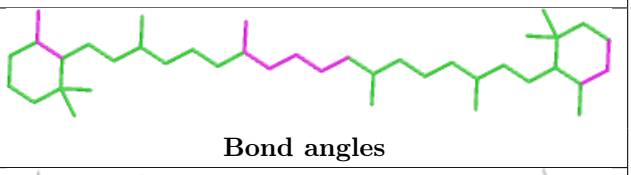
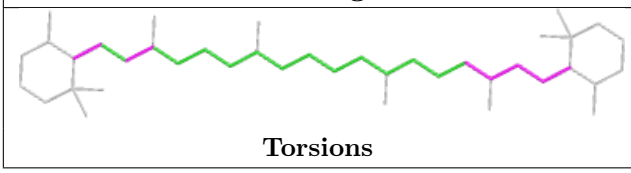


Bond angles



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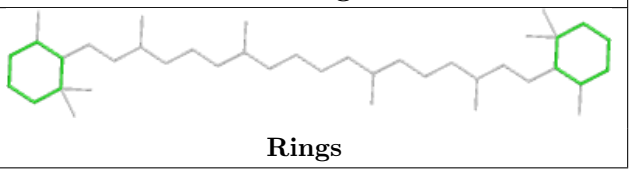
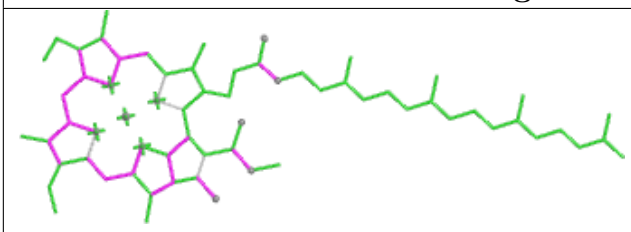
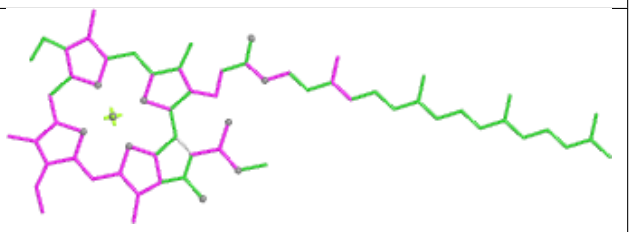


Rings

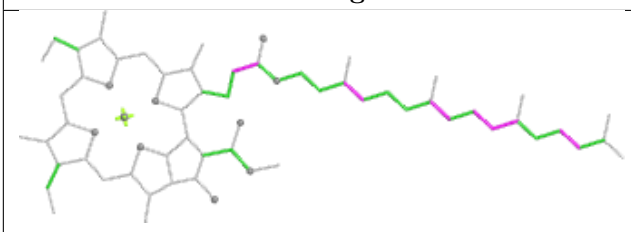
Ligand CLA bA 838



Bond lengths



Bond angles



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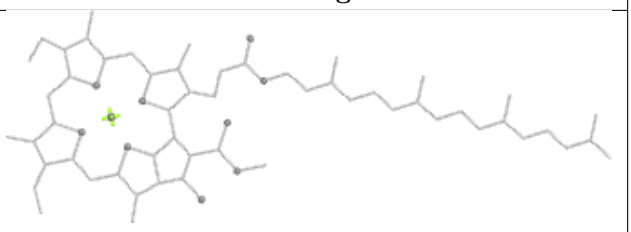
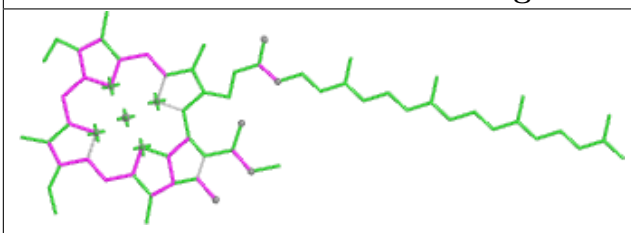
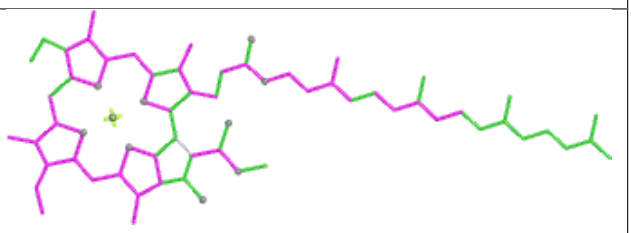


Rings

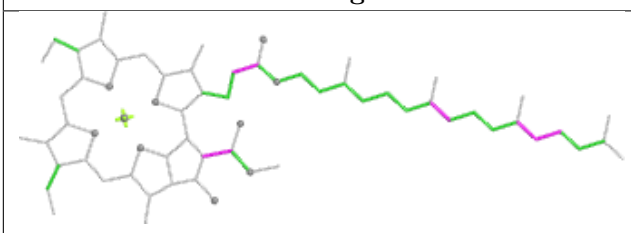
Ligand CLA bA 803



Bond lengths



Bond angles



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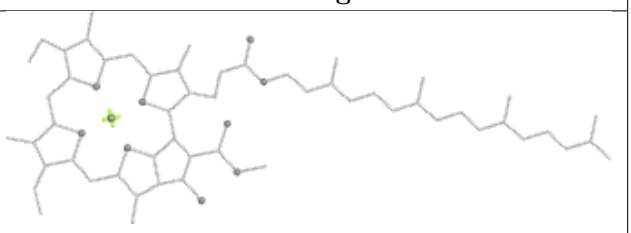
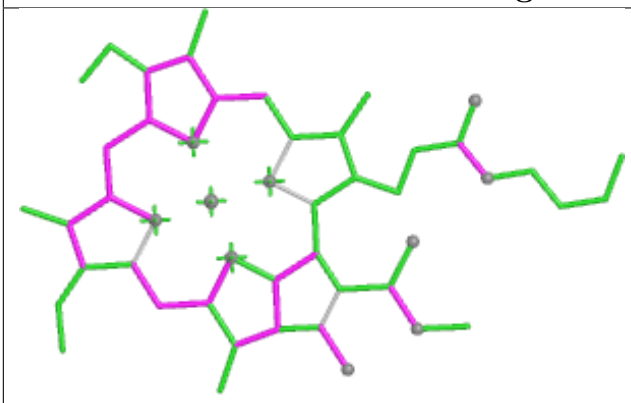


Rings

Ligand CLA aB 930



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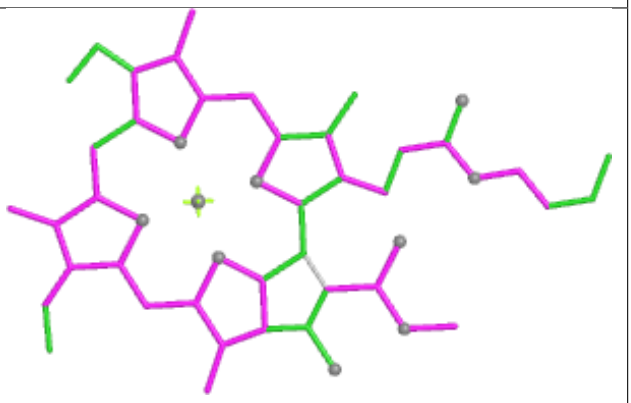
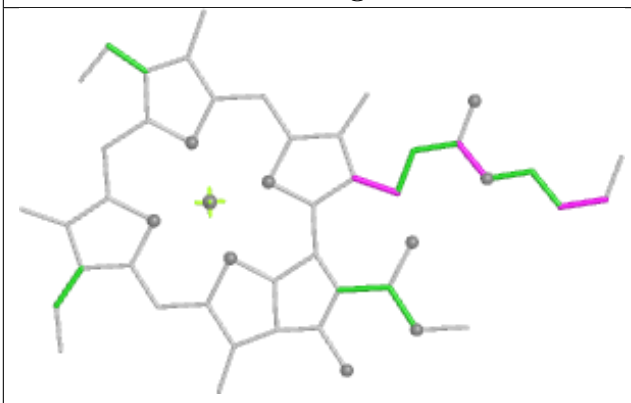


Bond angles



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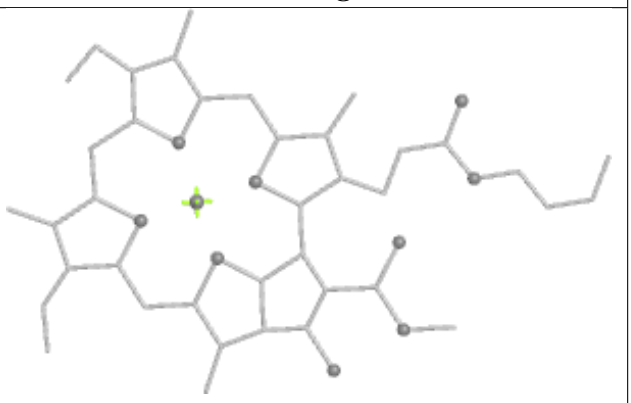
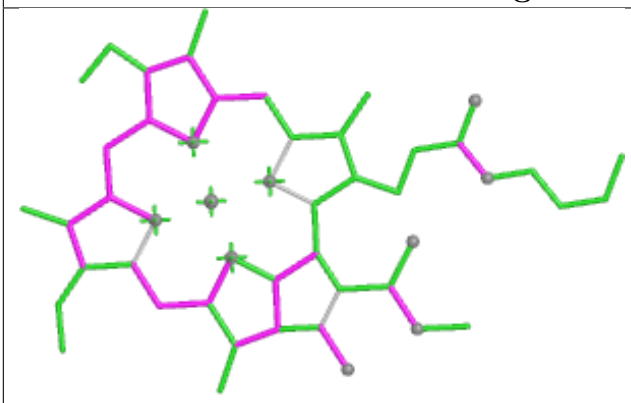


Rings

Ligand CLA bA 822



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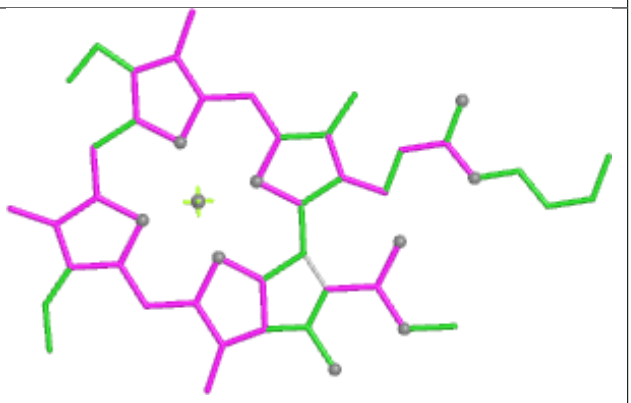
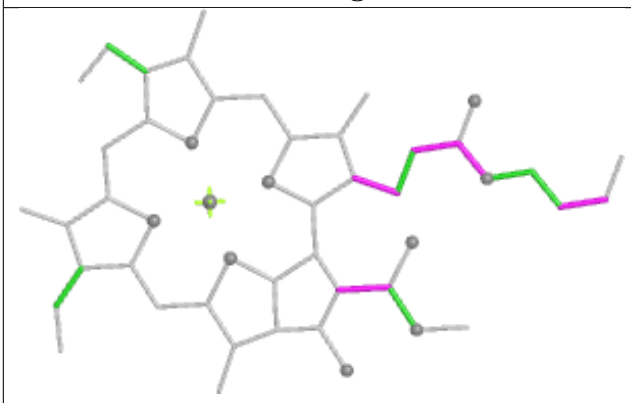


Bond angles



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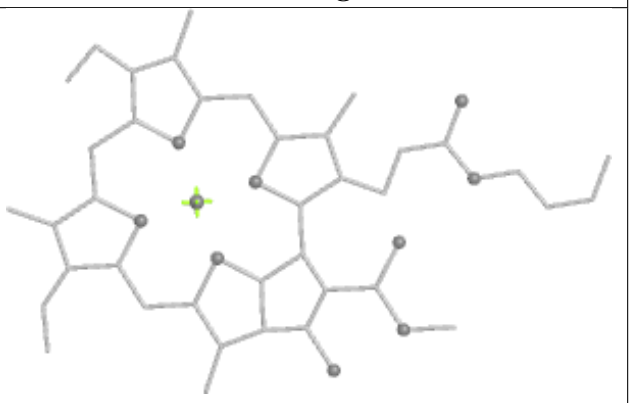
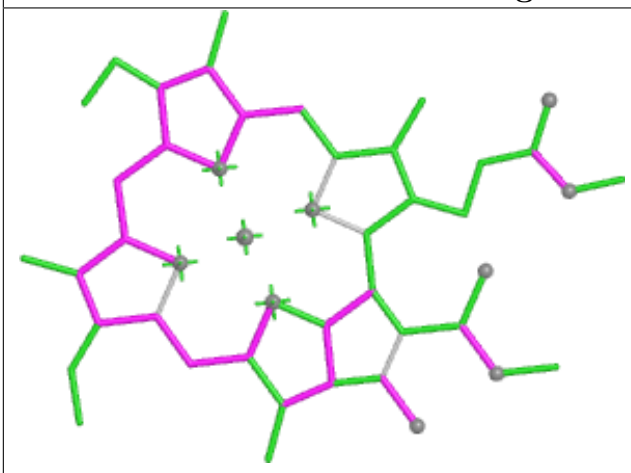


Rings

Ligand CLA aB 924



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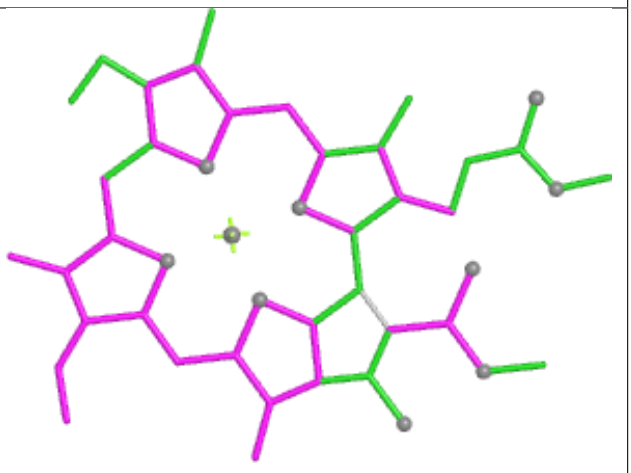
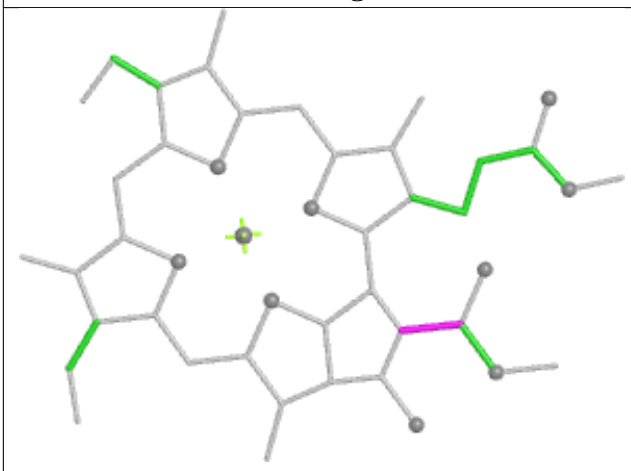


Bond angles



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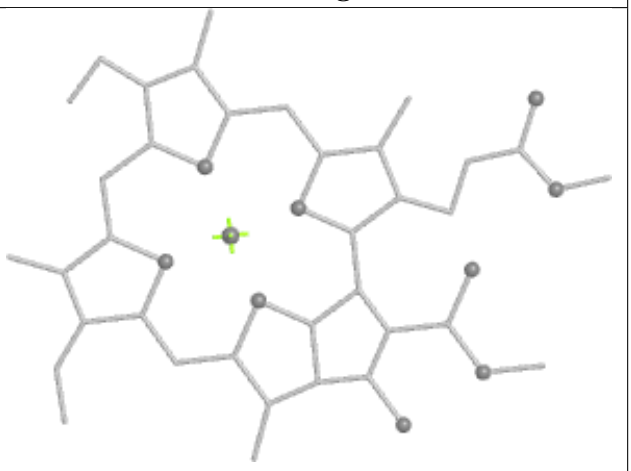
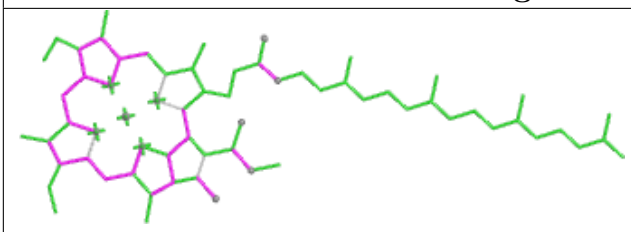


Rings

Ligand CLA bA 812



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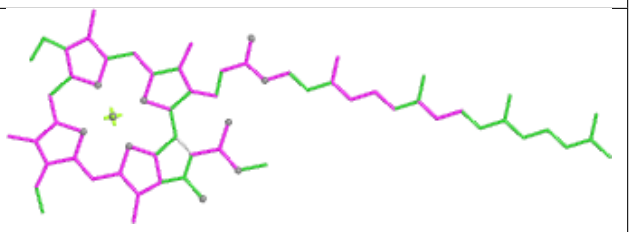
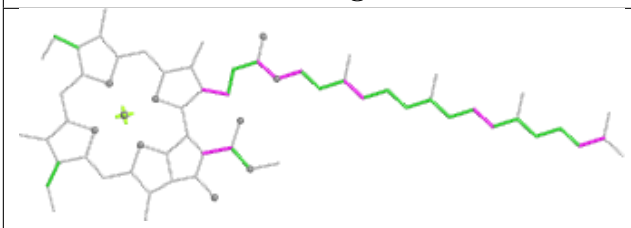


Bond angles



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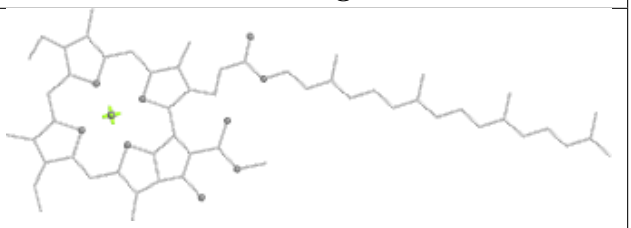
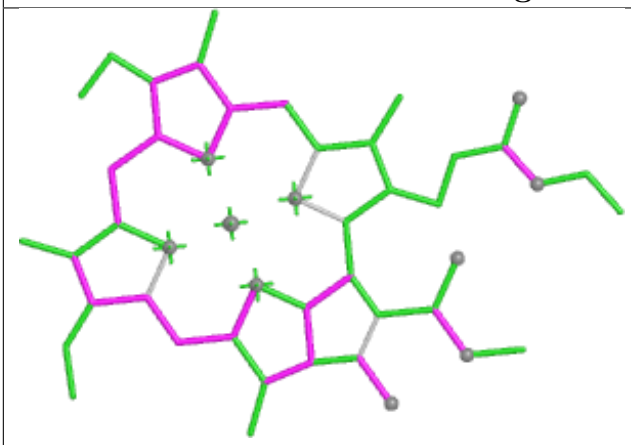


Rings

Ligand CLA bB 919



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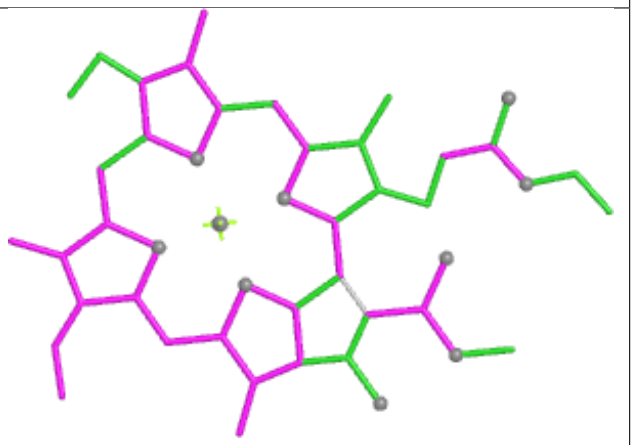
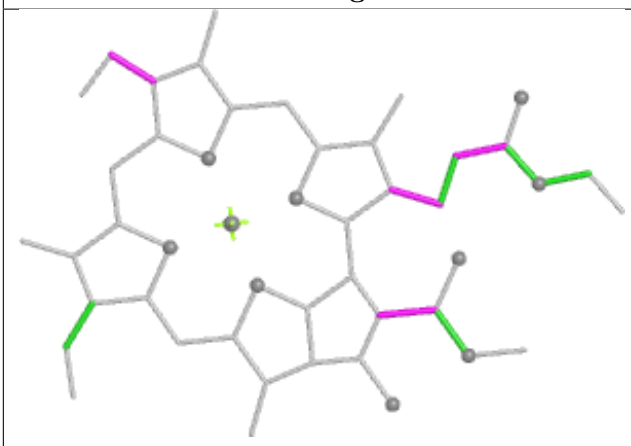


Bond angles



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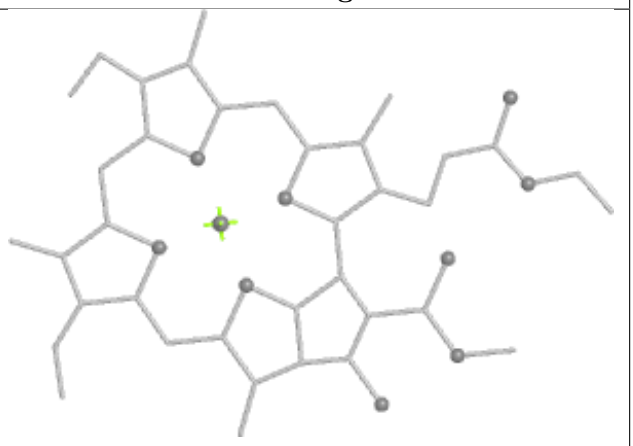
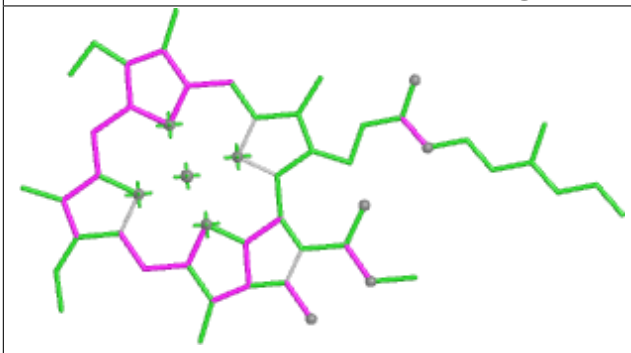
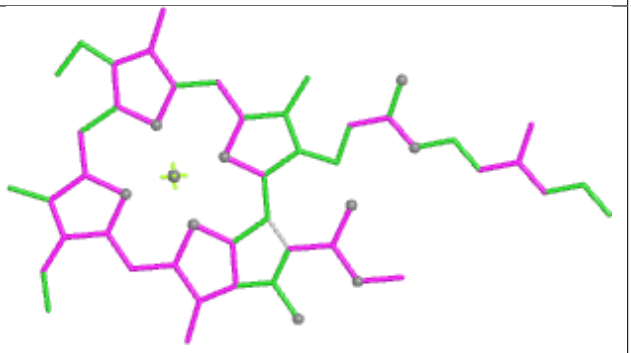
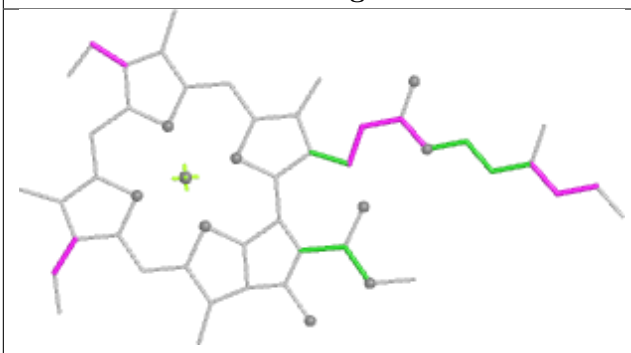
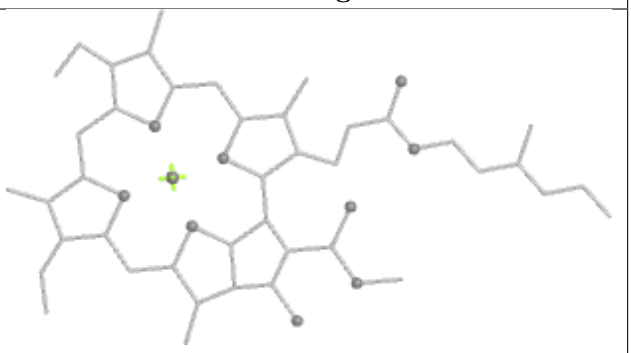
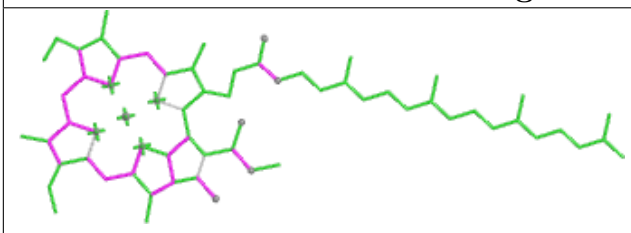
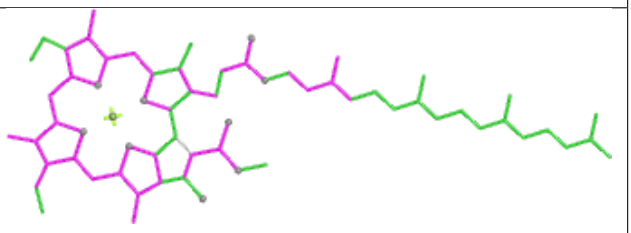
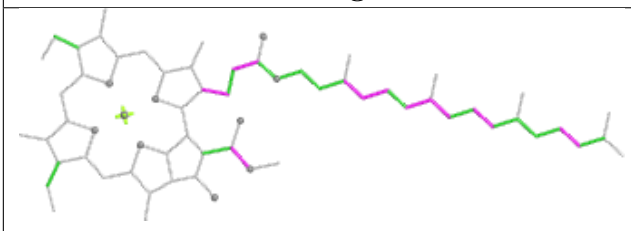
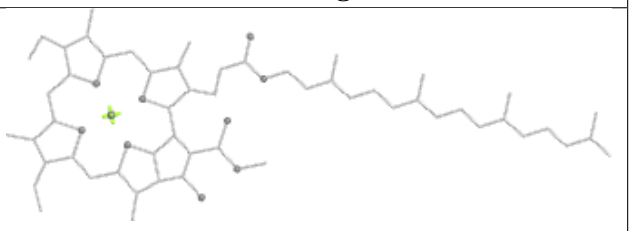
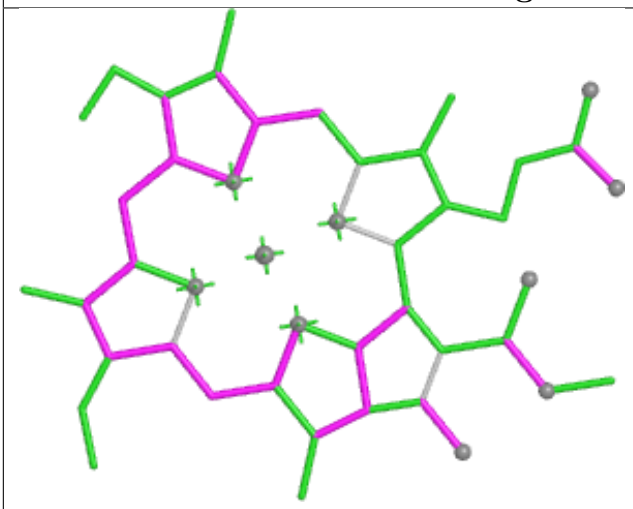


Rings

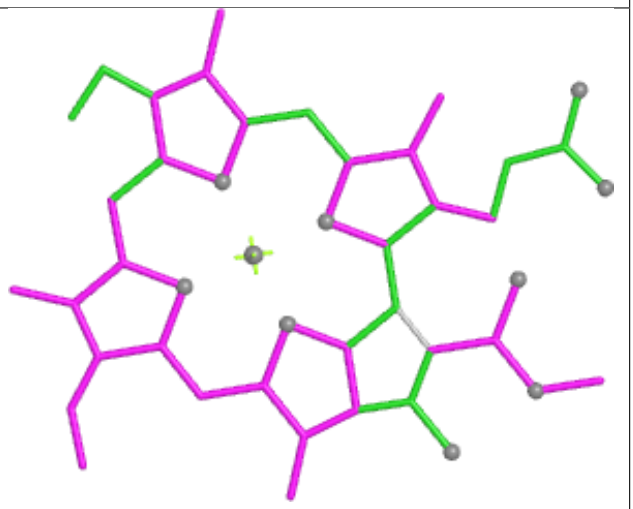
Ligand CLA aB 915	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 931	
	
Bond lengths	Bond angles
	
Torsions	Rings

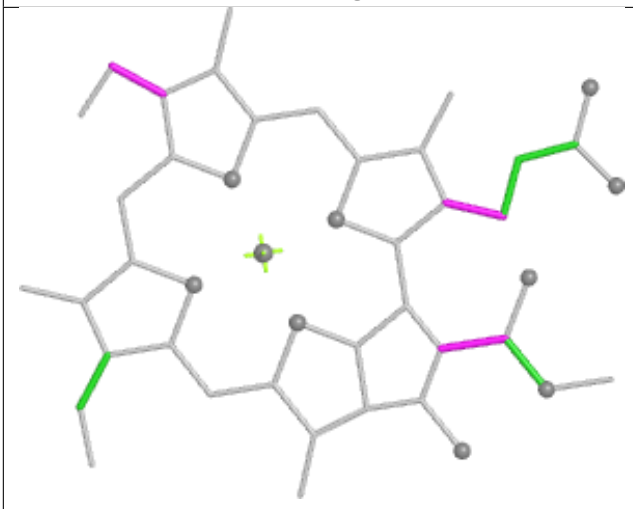
Ligand CLA aB 910



Bond lengths



Bond angles

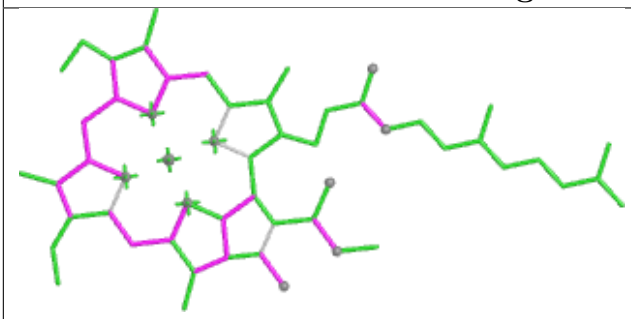


Torsions



Rings

Ligand CLA cB 925



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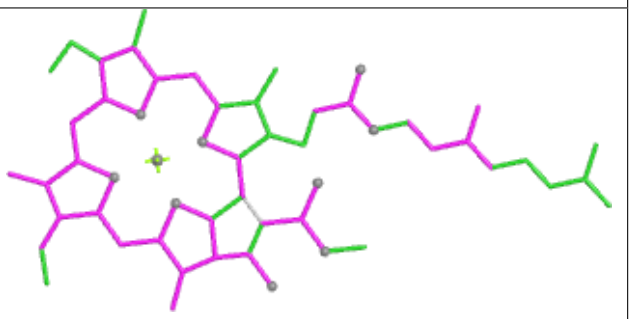
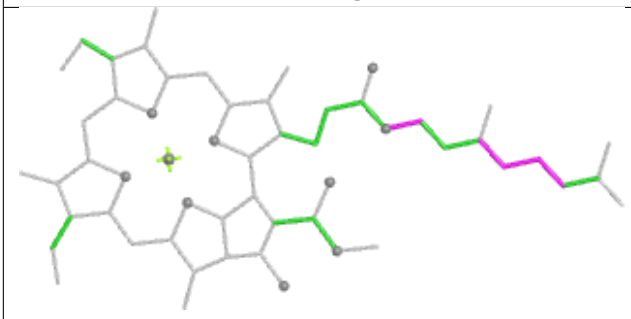
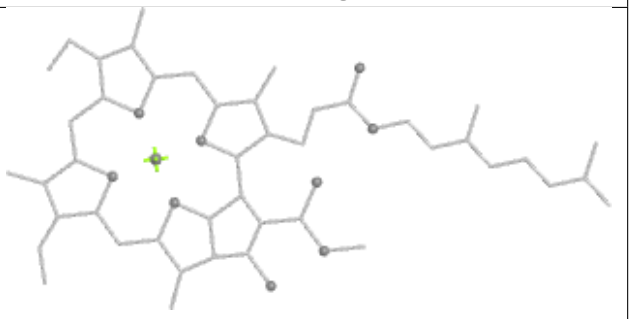


Bond angles

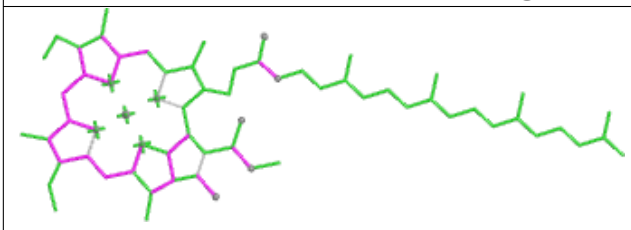


Torsions

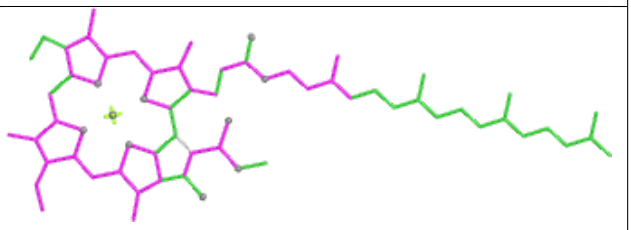


Rings

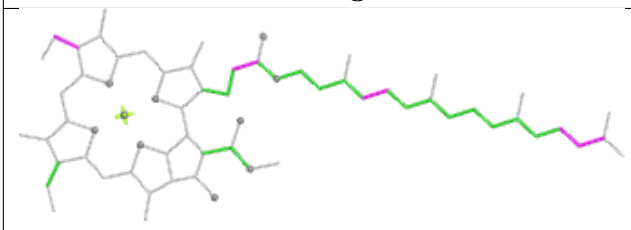
Ligand CL0 bA 801



Bond lengths



Bond angles



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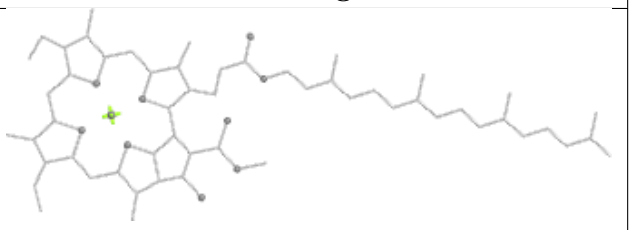
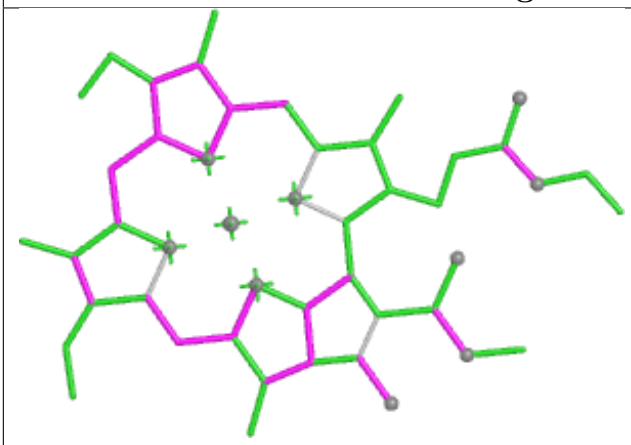


Rings

Ligand CLA cB 919



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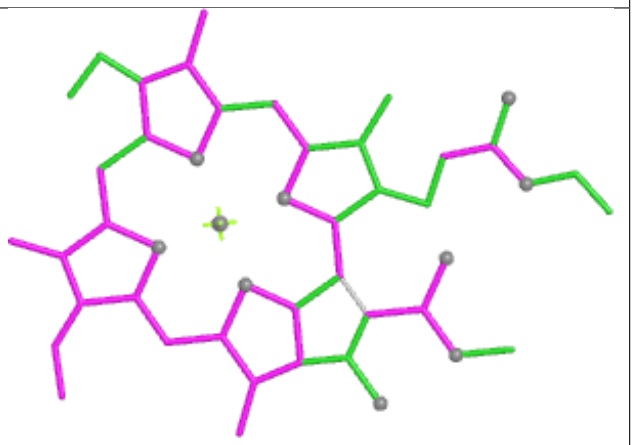
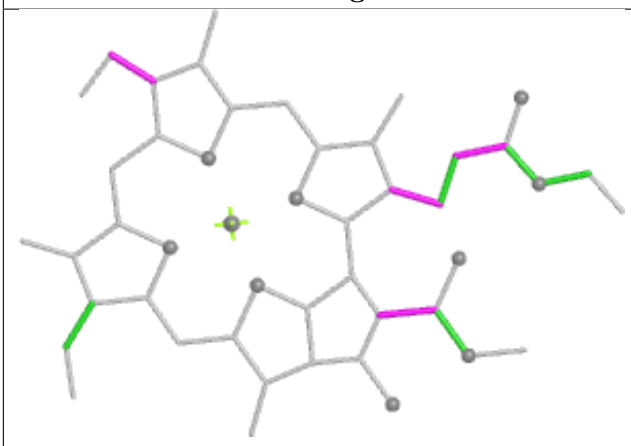
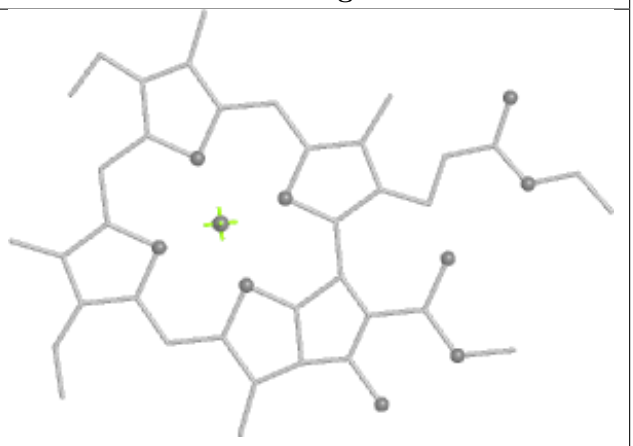


Bond angles

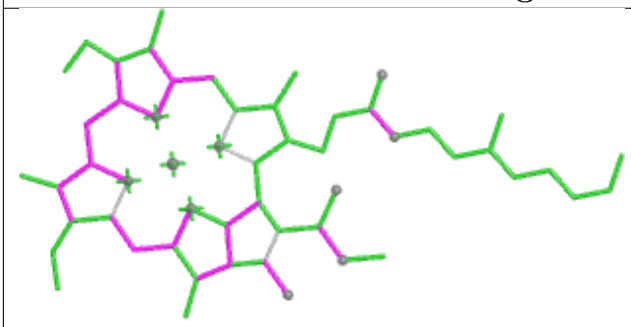


Torsions



Rings

Ligand CLA cB 923



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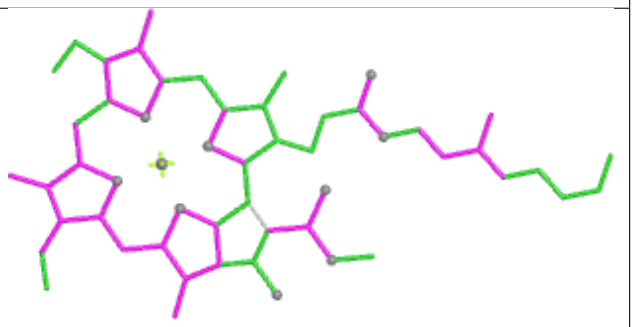
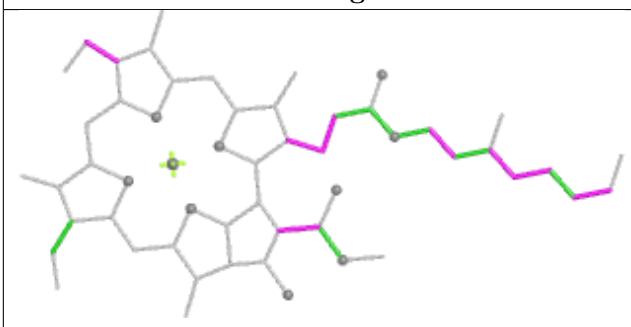
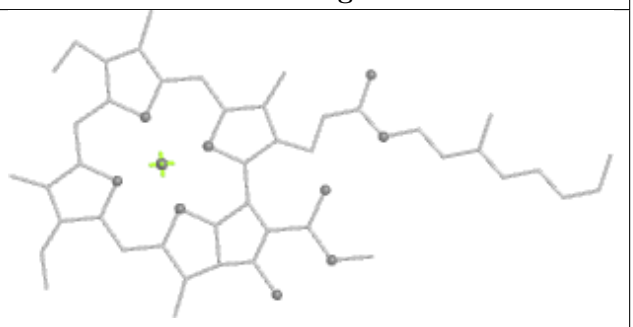


Bond angles

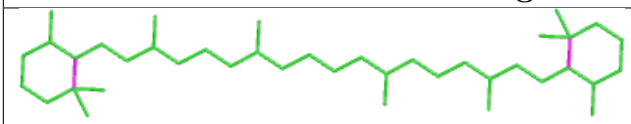


Torsions



Rings

Ligand BCR cF 201



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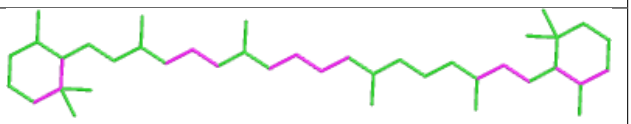
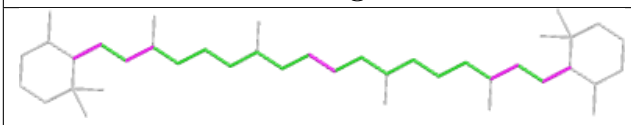


Bond angles



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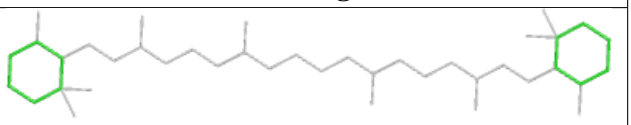
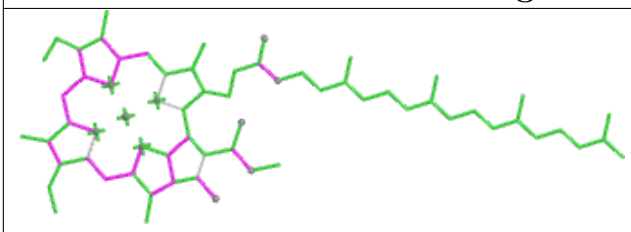


Rings

Ligand CLA cB 901



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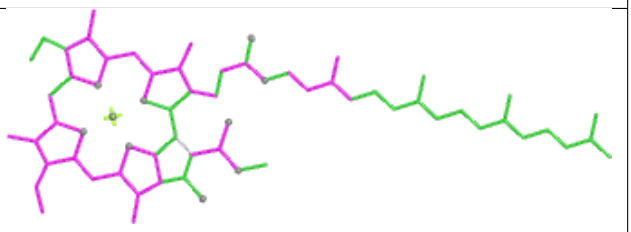
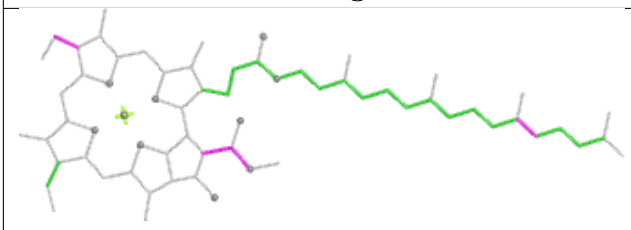


Bond angles



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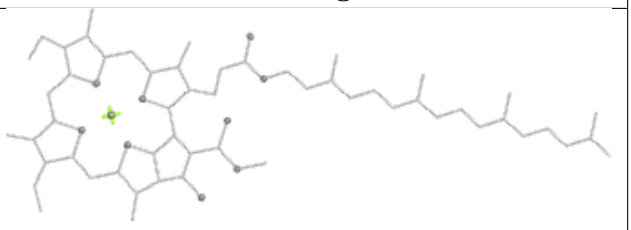
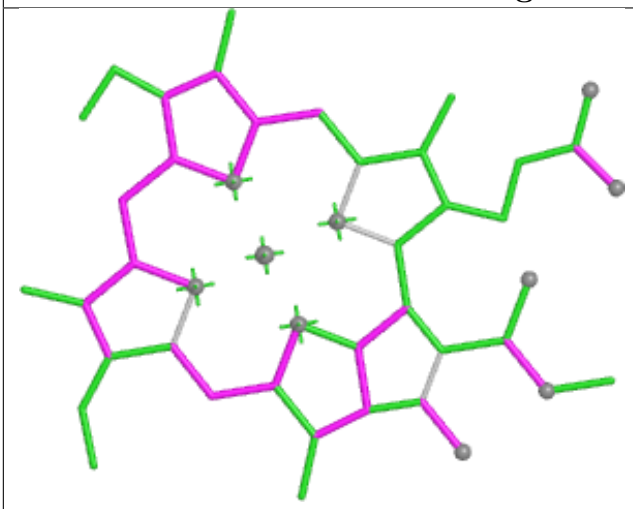


Rings

Ligand CLA cA 839



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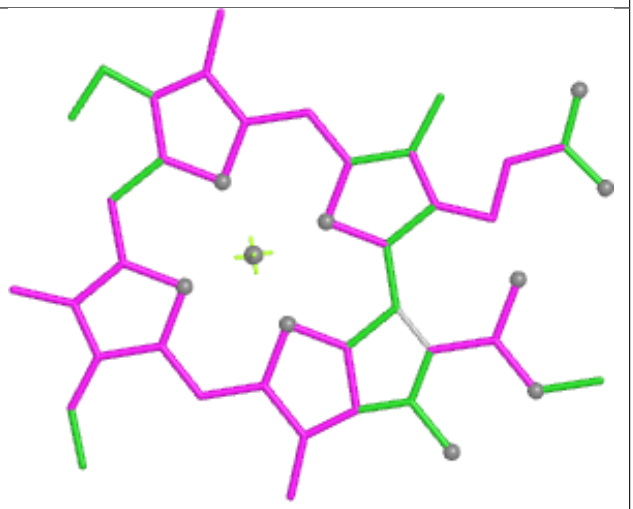
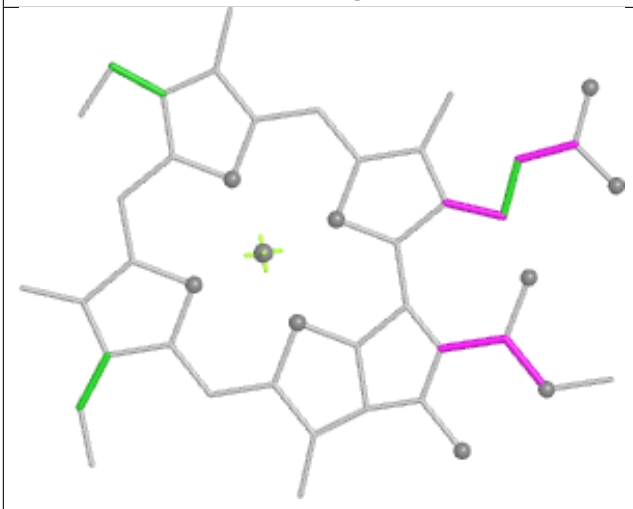


Bond angles

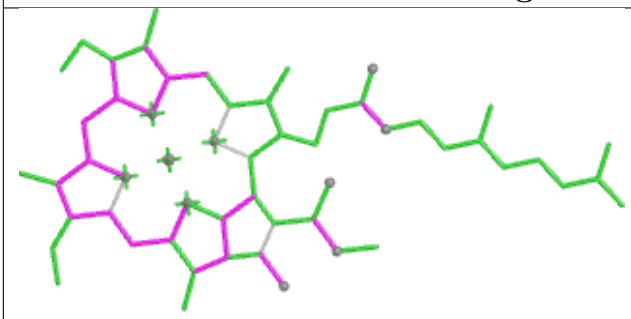


Torsions



Rings

Ligand CLA aB 909



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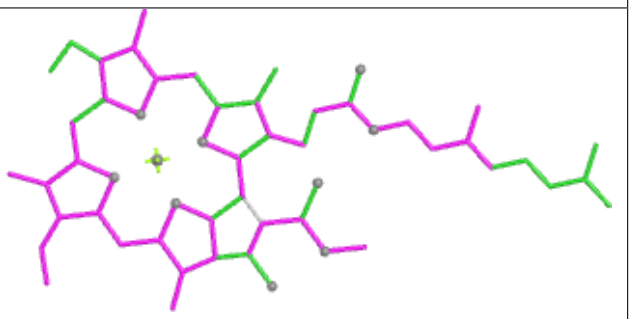
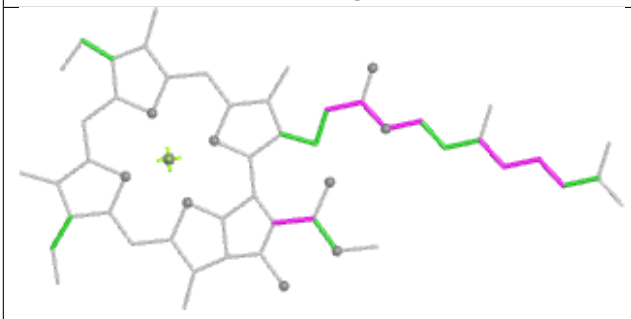


Bond angles



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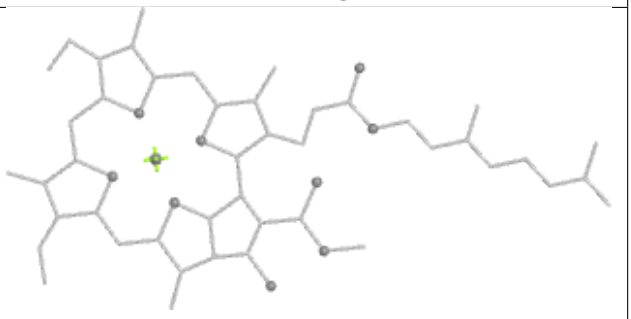
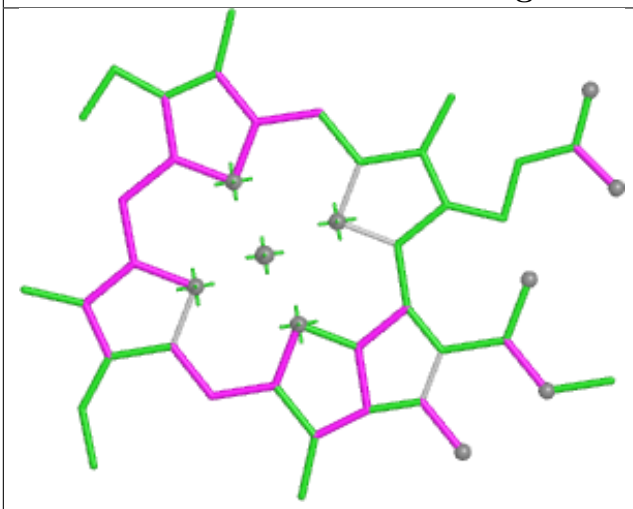


Rings

Ligand CLA aB 933



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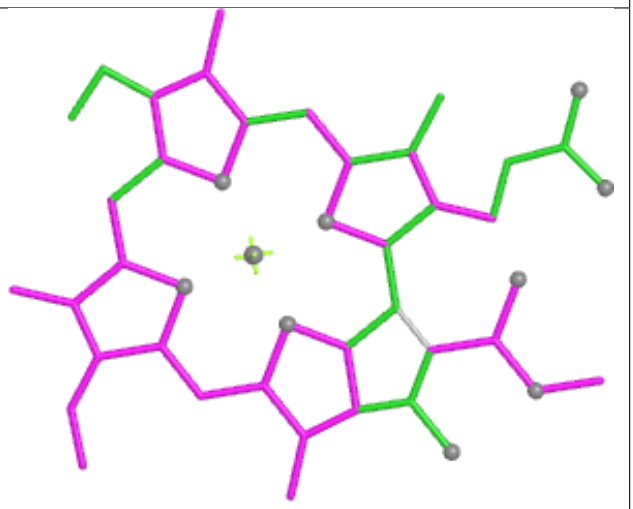
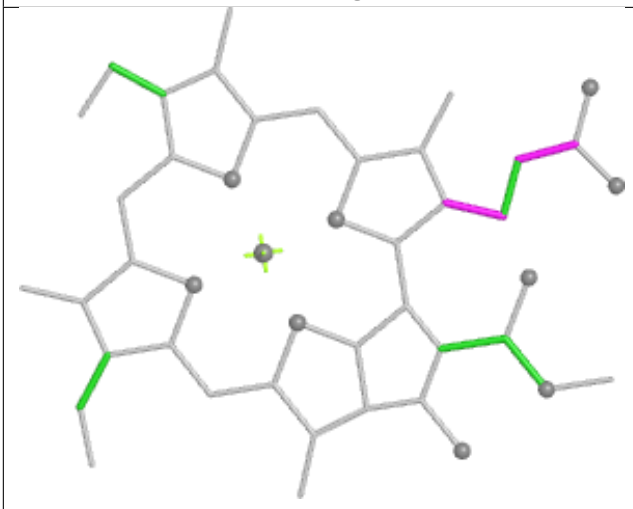


Bond angles

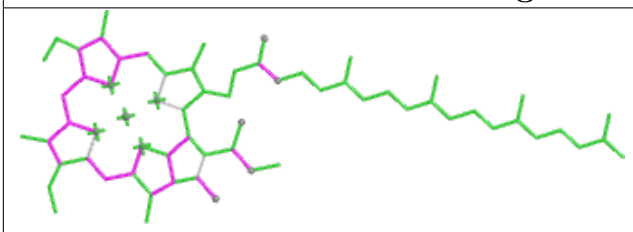


Torsions



Rings

Ligand CLA cB 905



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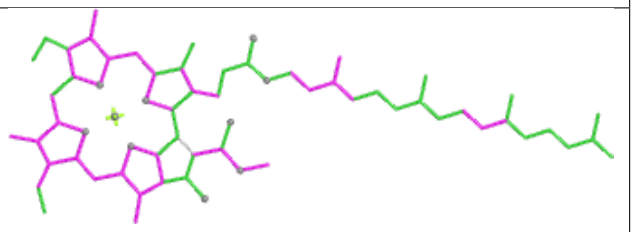
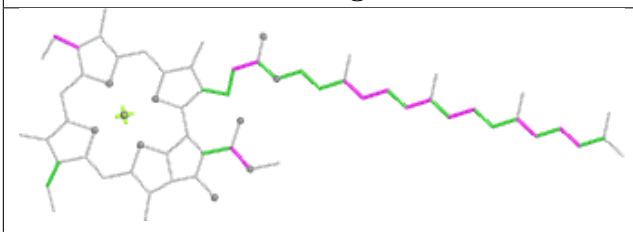


Bond angles



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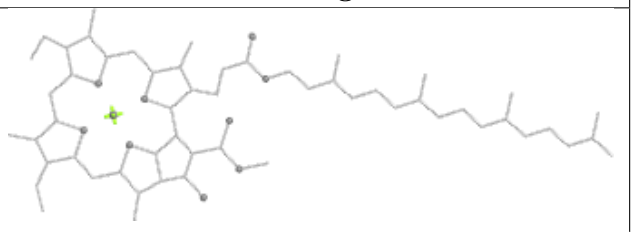
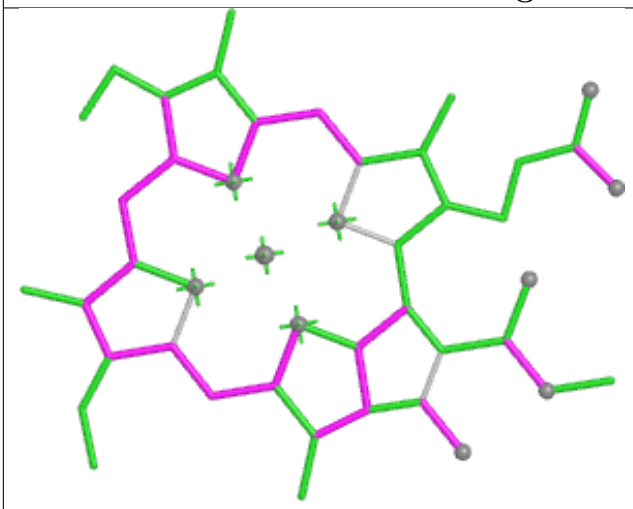


Rings

Ligand CLA cB 934



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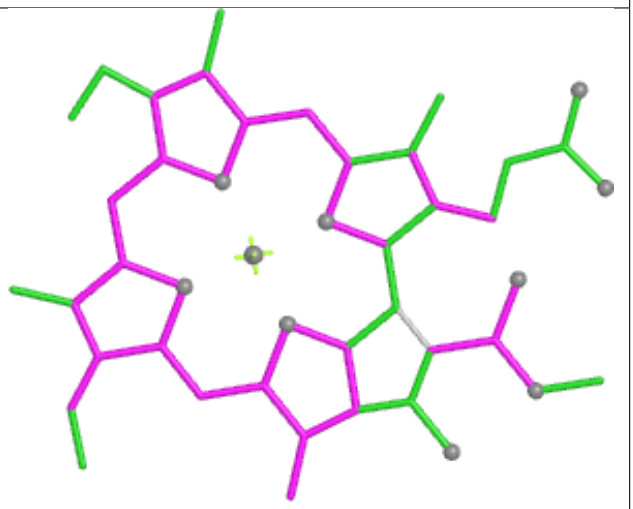
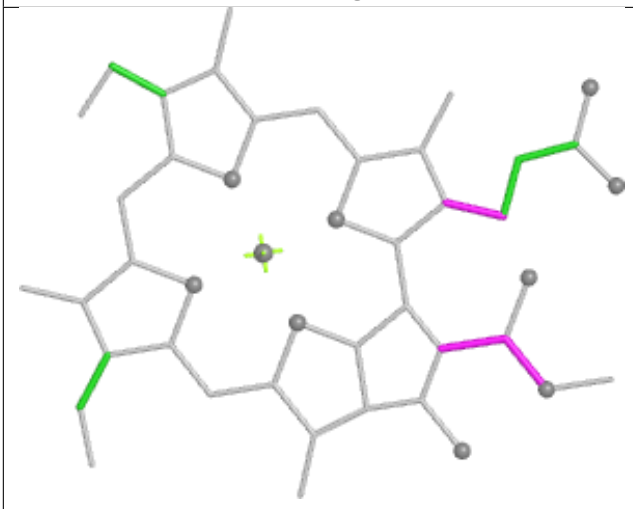


Bond angles

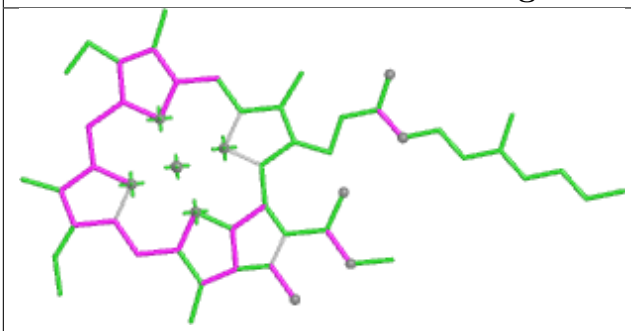


Torsions



Rings

Ligand CLA cL 202



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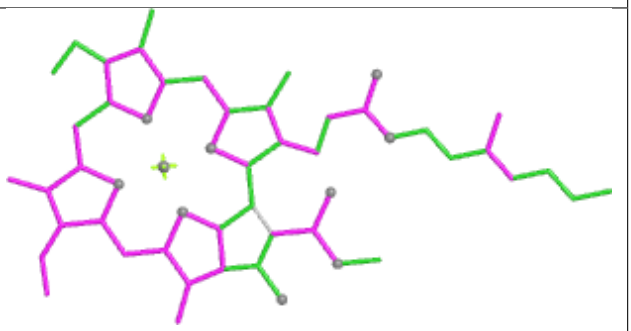
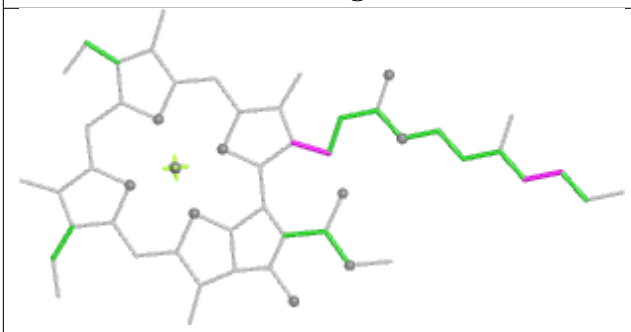
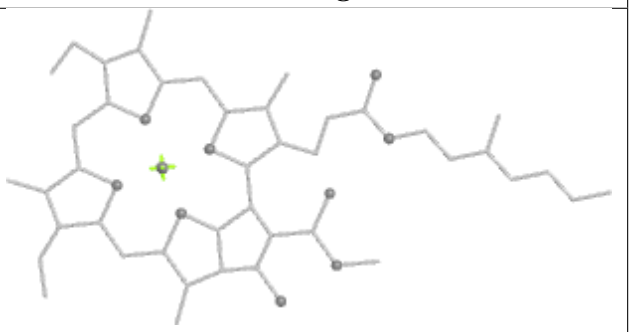


Bond angles



Torsions

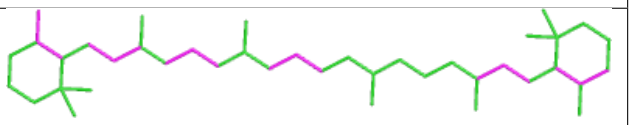


Rings

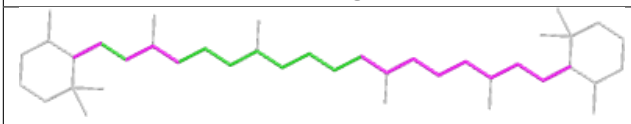
Ligand BCR aM 101



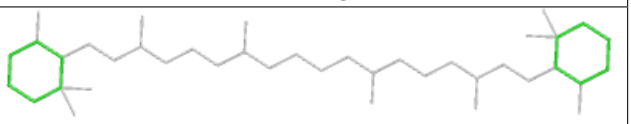
Bond lengths



Bond angles

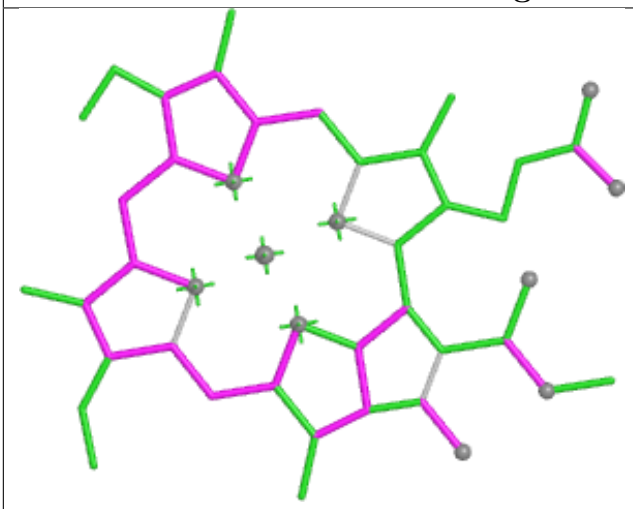


Torsions

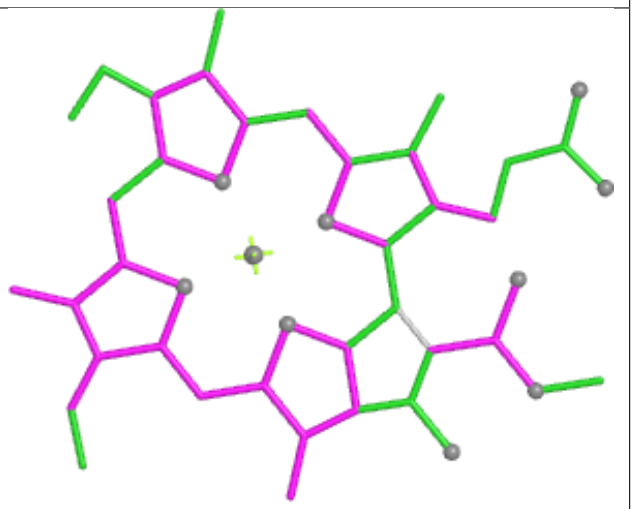


Rings

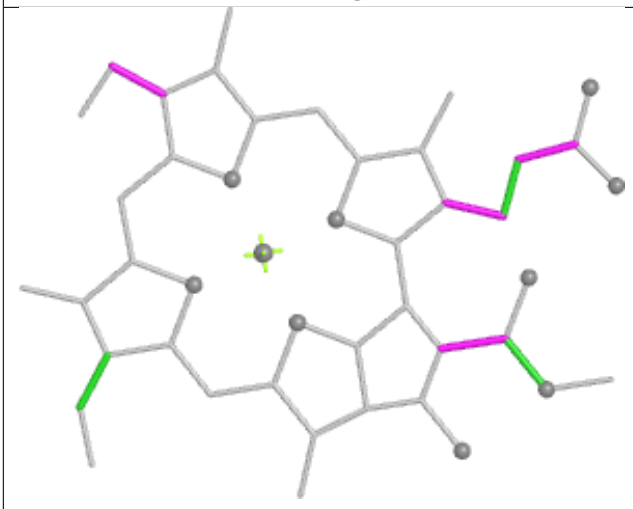
Ligand CLA bA 816



Bond lengths



Bond angles

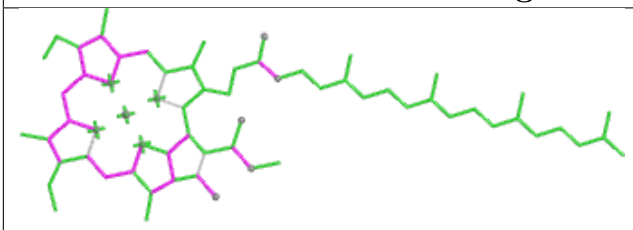


Torsions

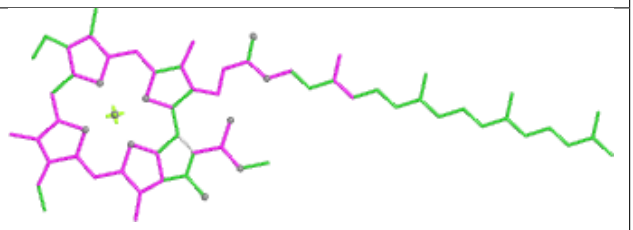


Rings

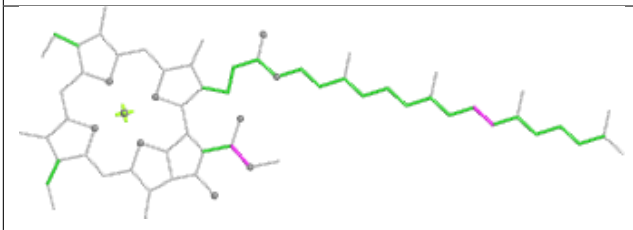
Ligand CLA cA 828



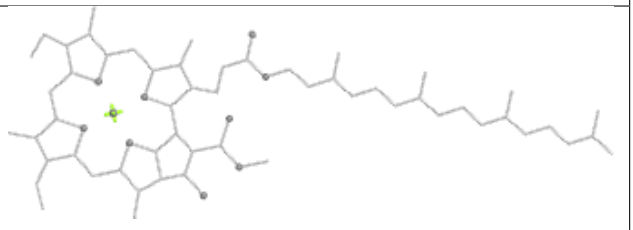
Bond lengths



Bond angles

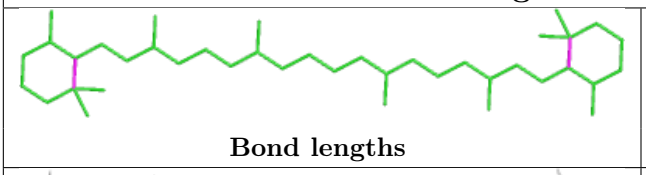


Torsions

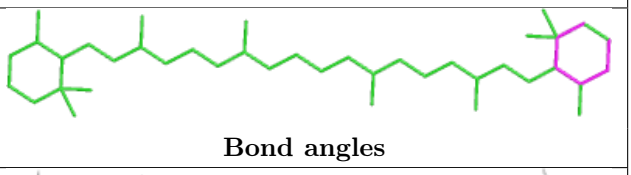


Rings

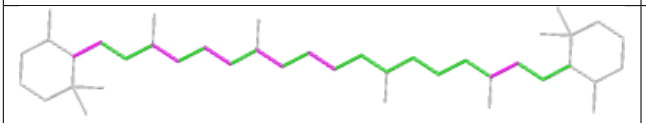
Ligand BCR bB 942



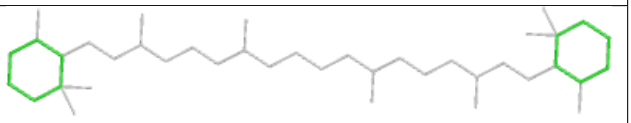
Bond lengths



Bond angles

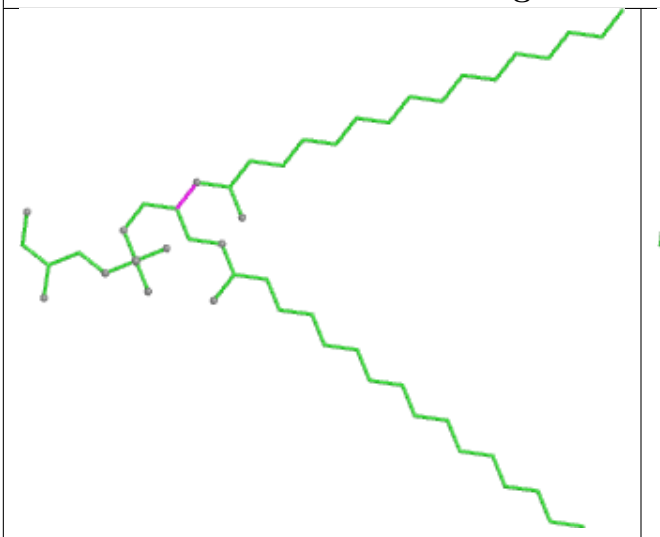


Torsions

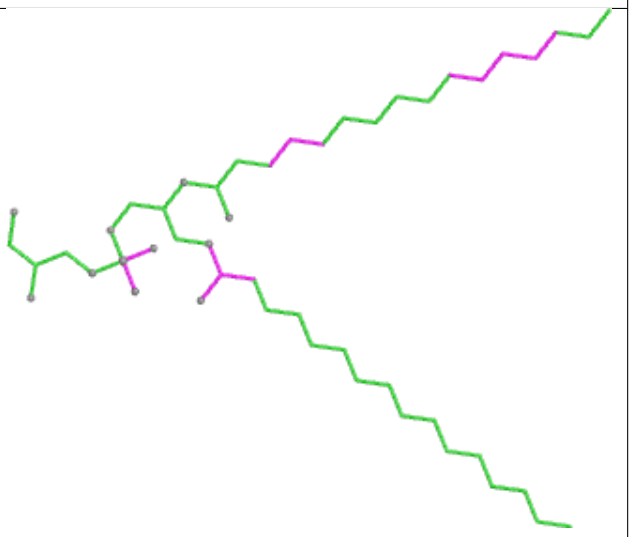


Rings

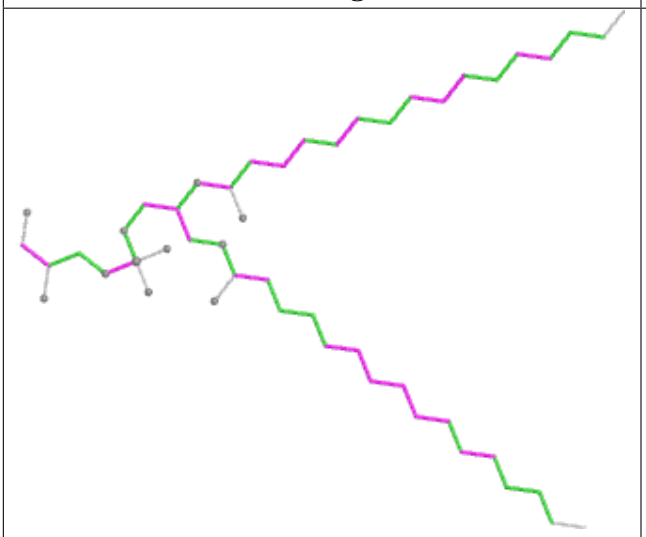
Ligand LHG aA 852



Bond lengths



Bond angles



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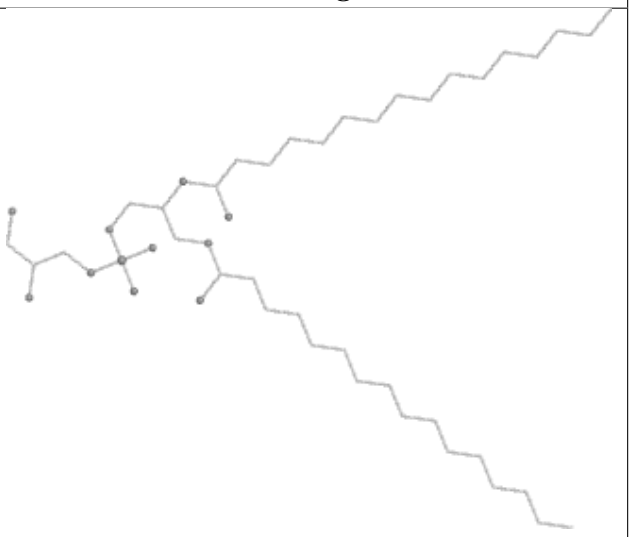
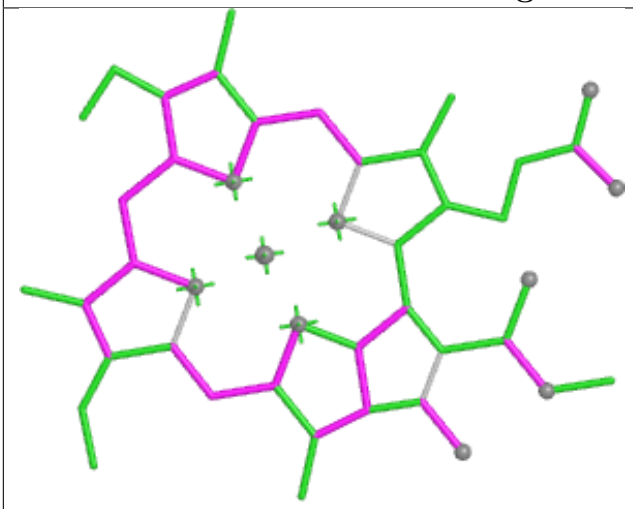


Rings

Ligand CLA bL 203



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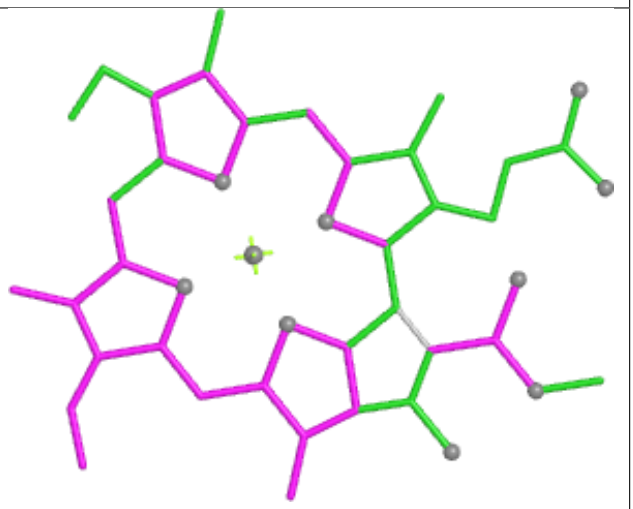
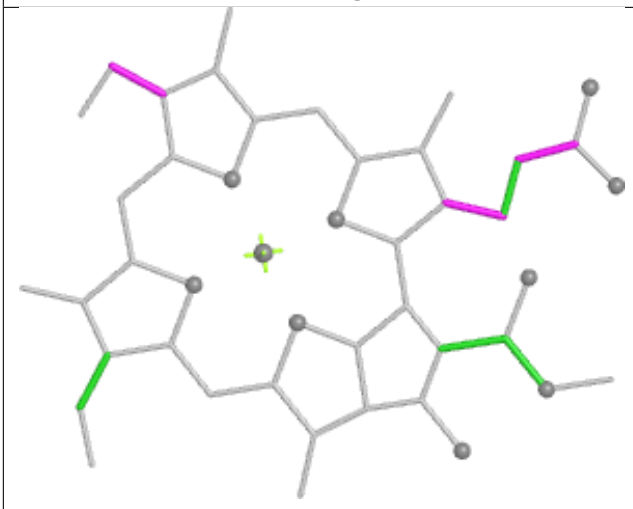


Bond angles

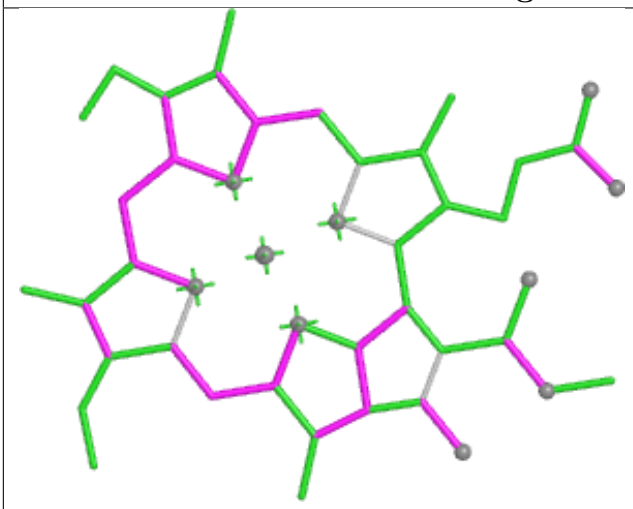


Torsions



Rings

Ligand CLA cB 939



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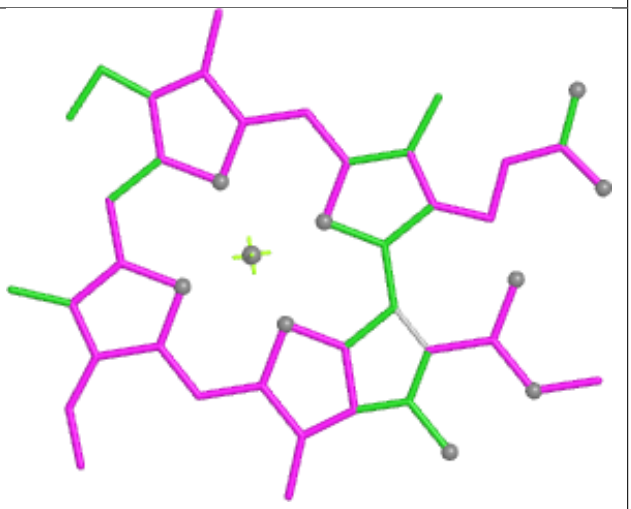
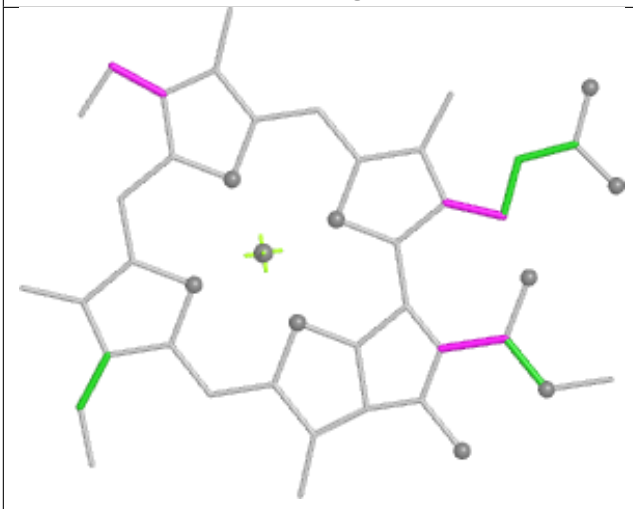


Bond angles

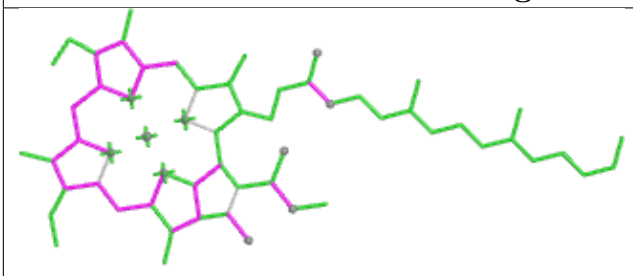


Torsions



Rings

Ligand CLA bB 936



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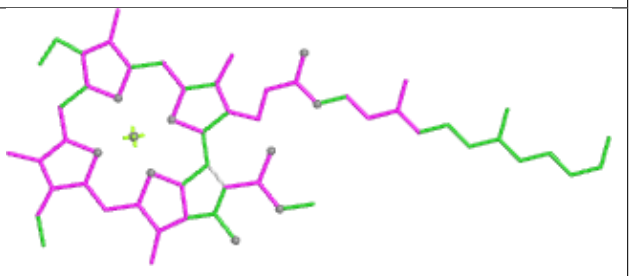
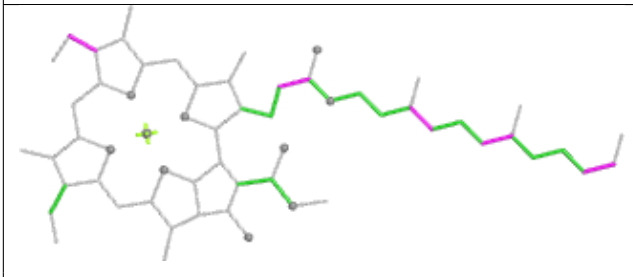
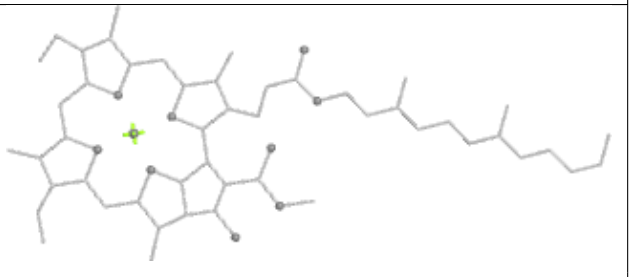


Bond angles

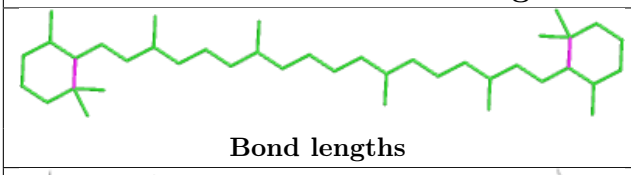


Torsions



Rings

Ligand BCR bA 846



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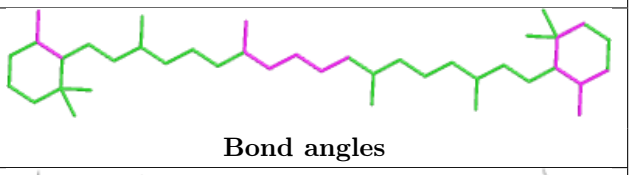
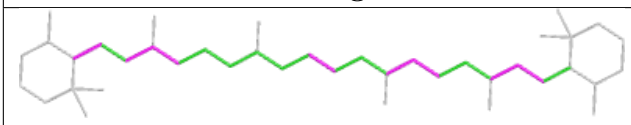
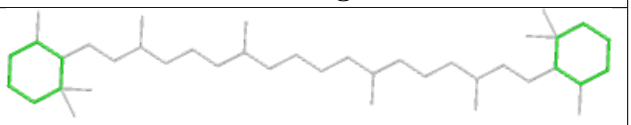


Bond angles

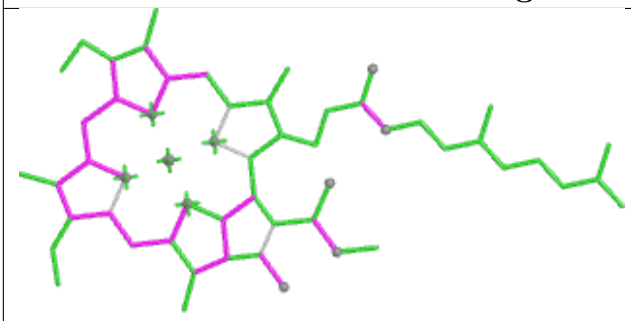


Torsions

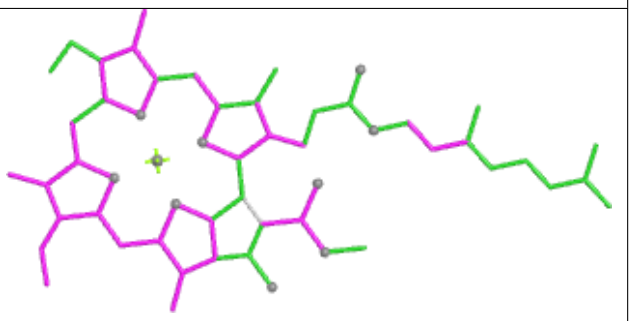


Rings

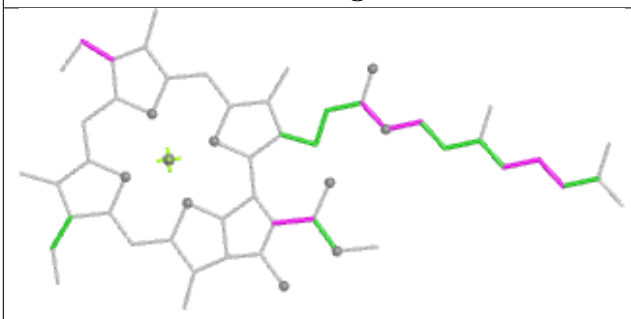
Ligand CLA cA 826



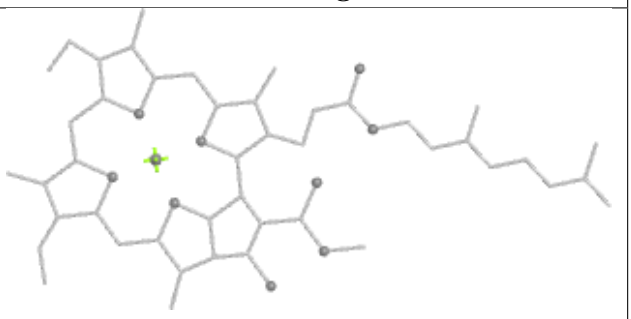
Bond lengths



Bond angles

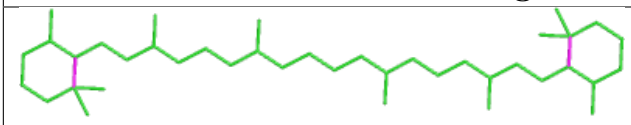


Torsions



Rings

Ligand BCR bF 204



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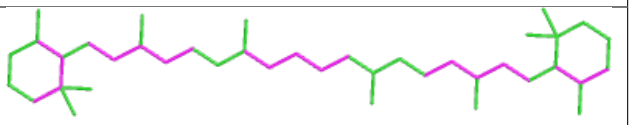
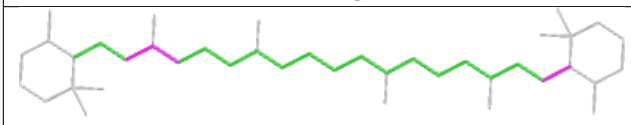


Bond angles



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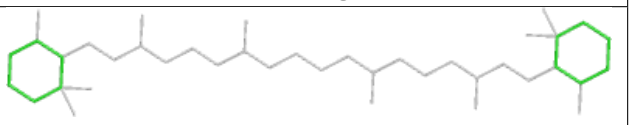
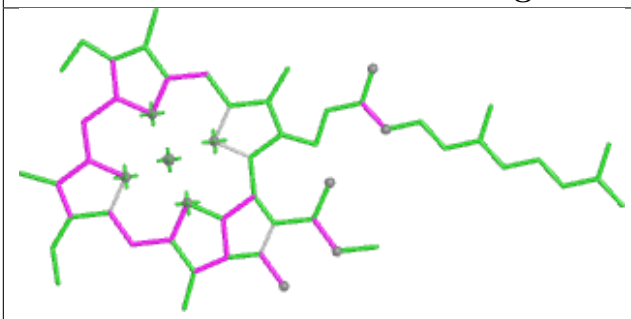


Rings

Ligand CLA bB 925



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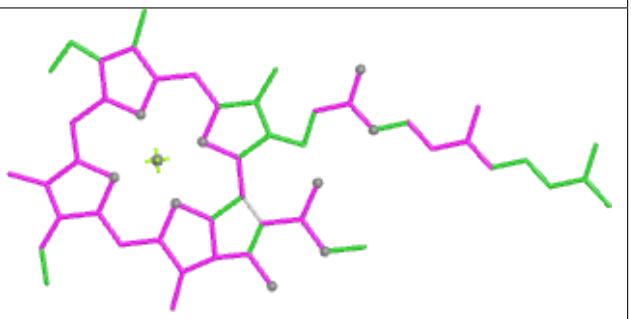
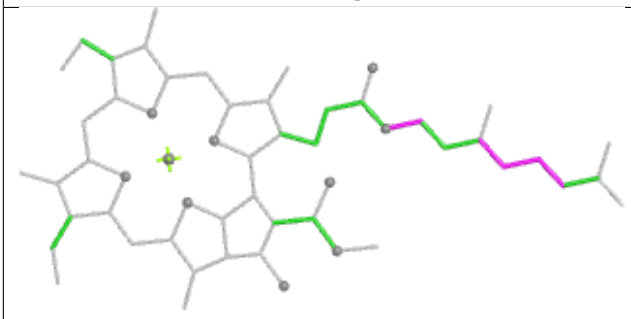


Bond angles



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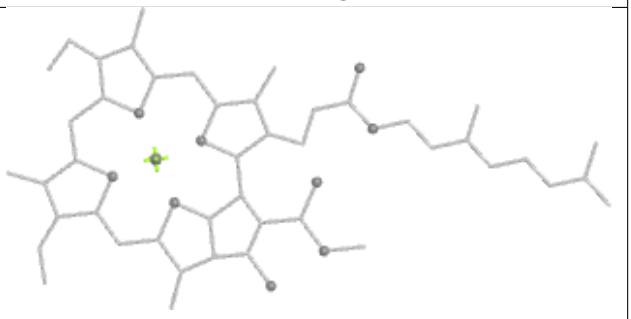
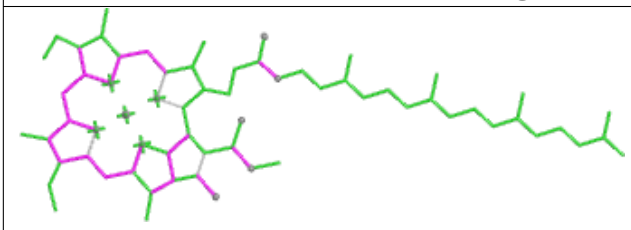
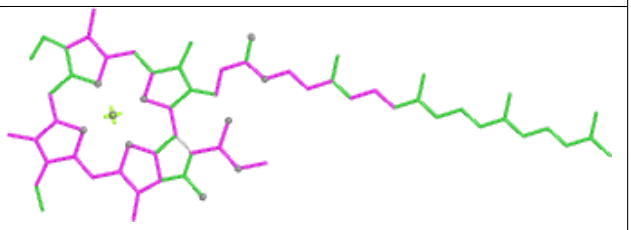


Rings

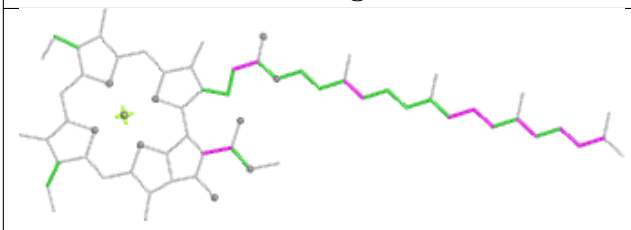
Ligand CLA bA 825



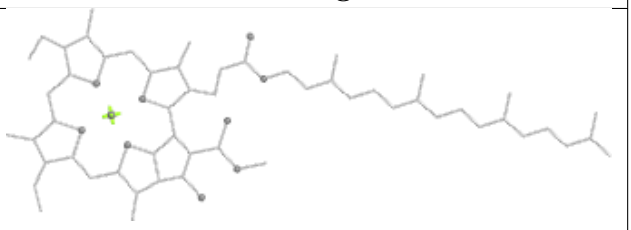
Bond lengths



Bond angles

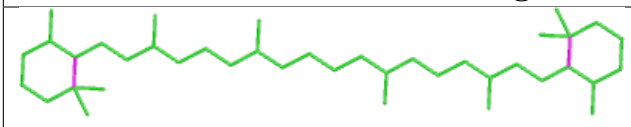


Torsions



Rings

Ligand BCR aA 848



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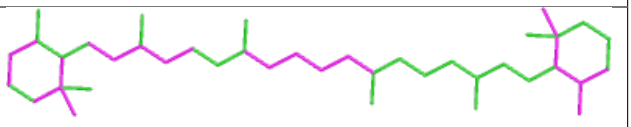
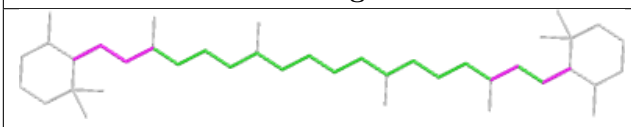


Bond angles



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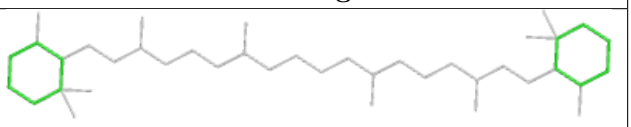
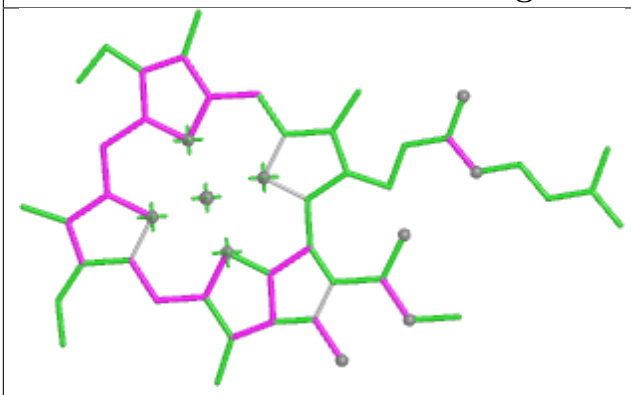
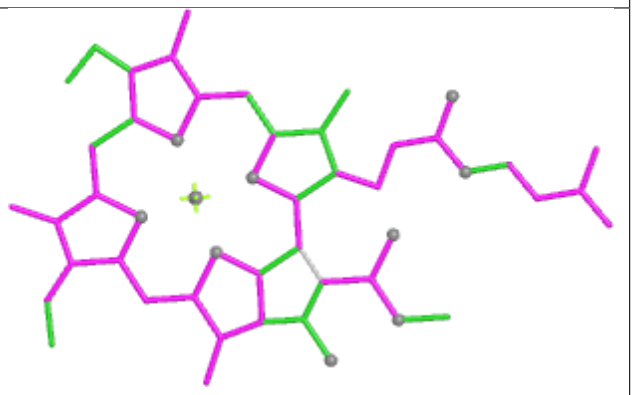


Rings

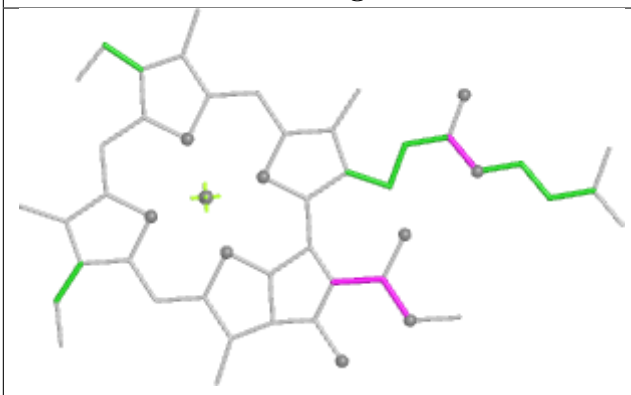
Ligand CLA aB 935



Bond lengths



Bond angles



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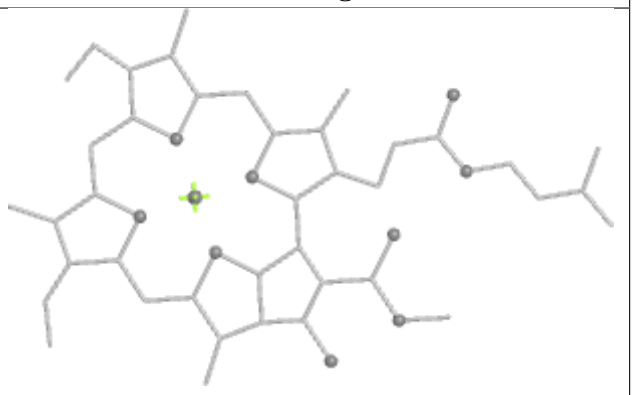
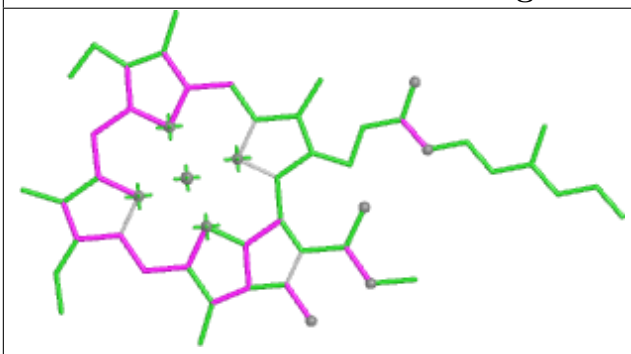
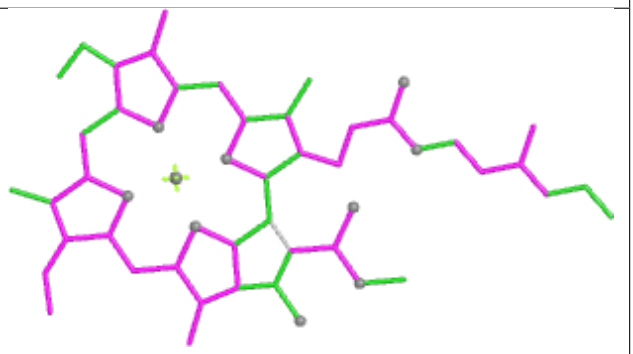


Rings

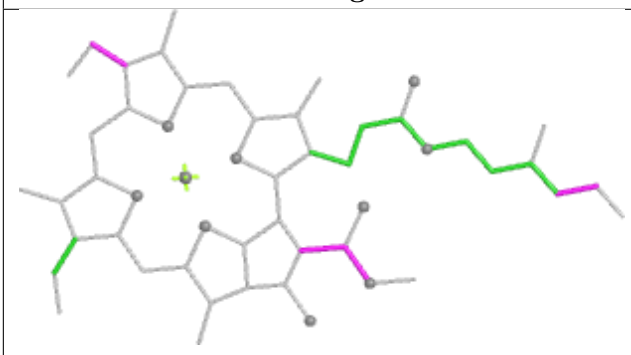
Ligand CLA cB 907



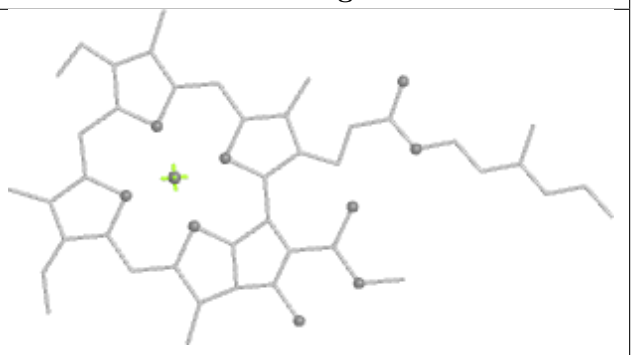
Bond lengths



Bond angles

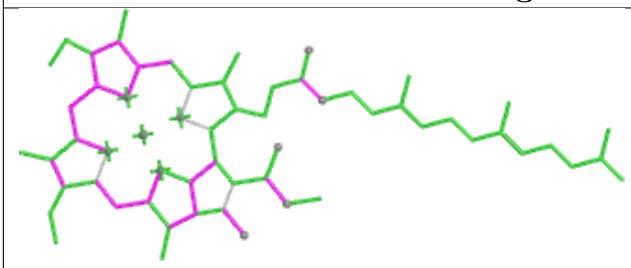


Torsions

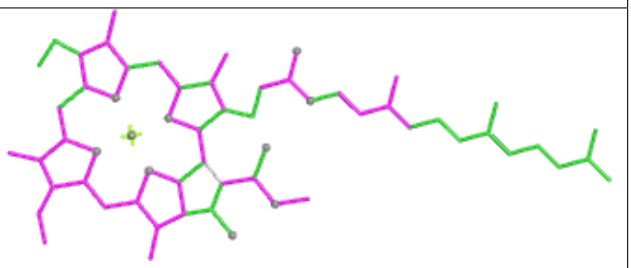


Rings

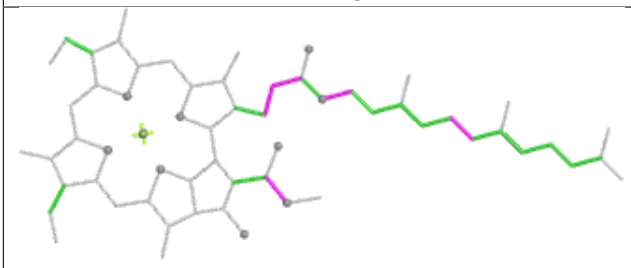
Ligand CLA cA 829



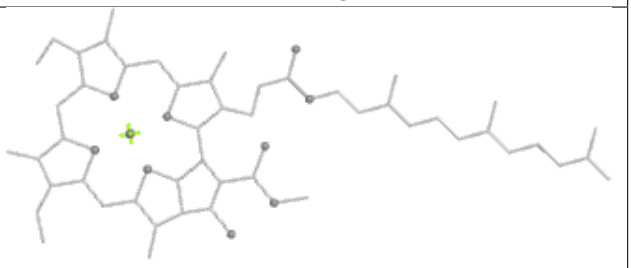
Bond lengths



Bond angles

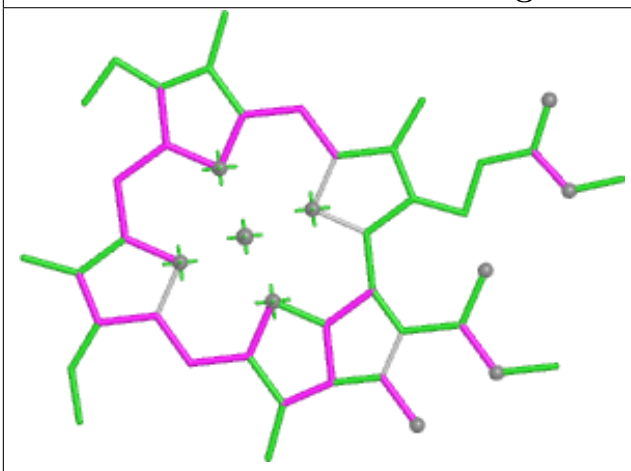


Torsions

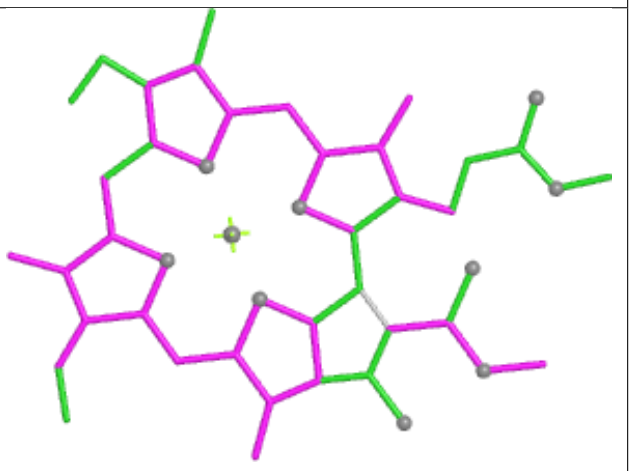


Rings

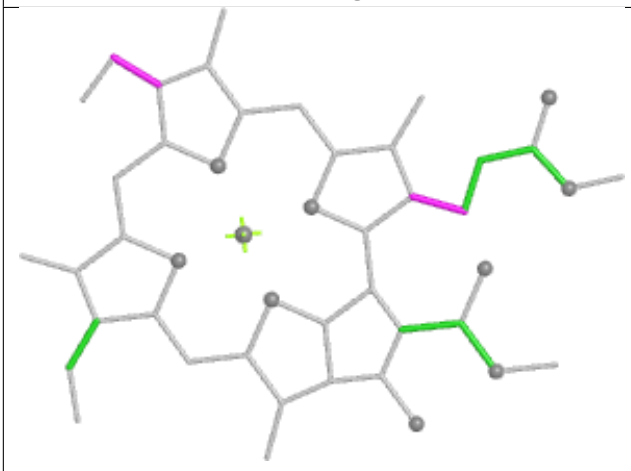
Ligand CLA aB 918



Bond lengths



Bond angles

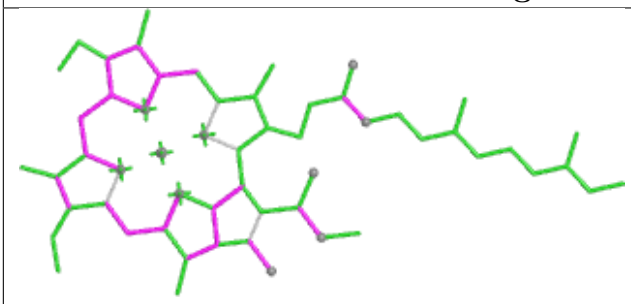


Torsions

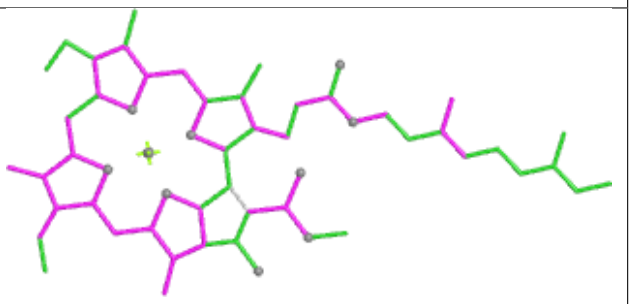


Rings

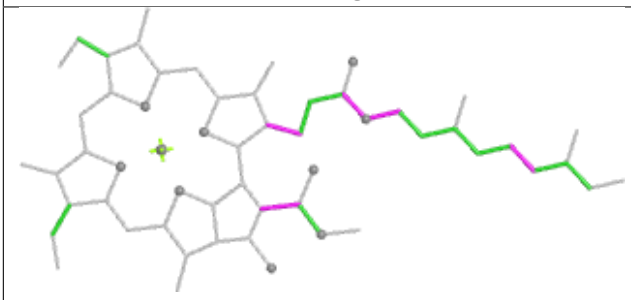
Ligand CLA bA 804



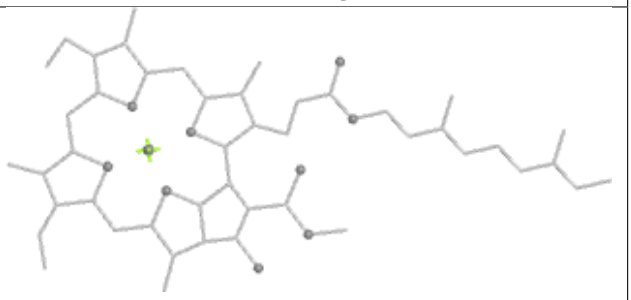
Bond lengths



Bond angles

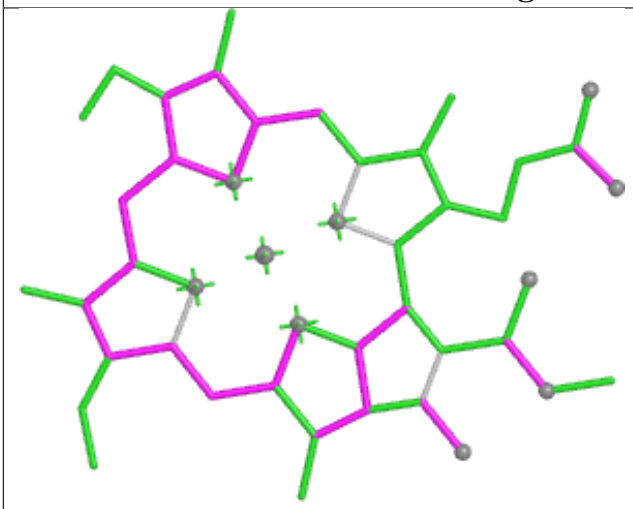


Torsions

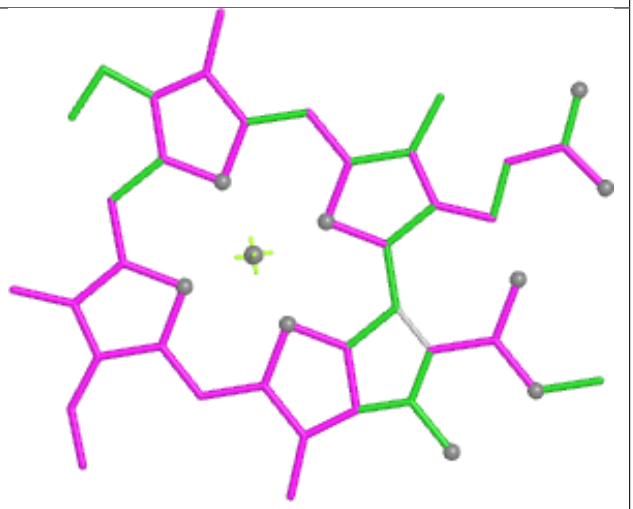


Rings

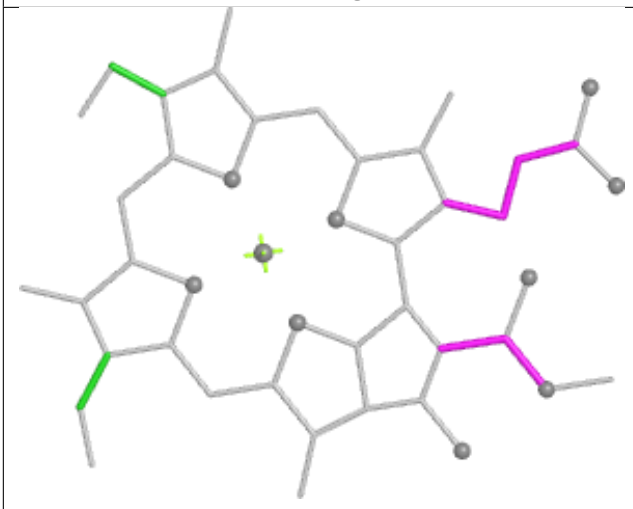
Ligand CLA aF 202



Bond lengths



Bond angles

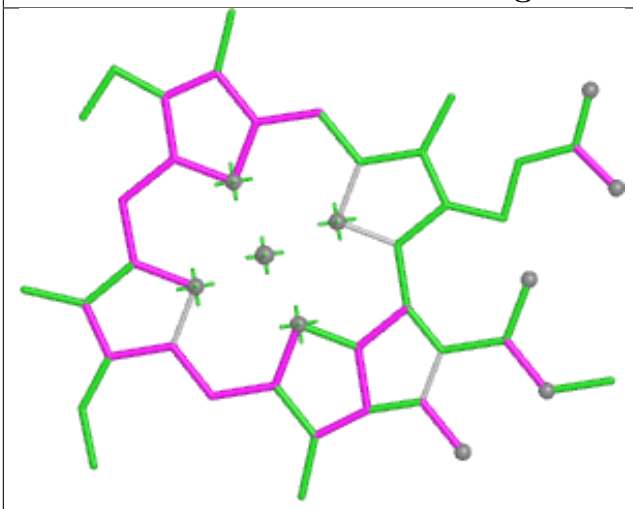


Torsions



Rings

Ligand CLA bB 950



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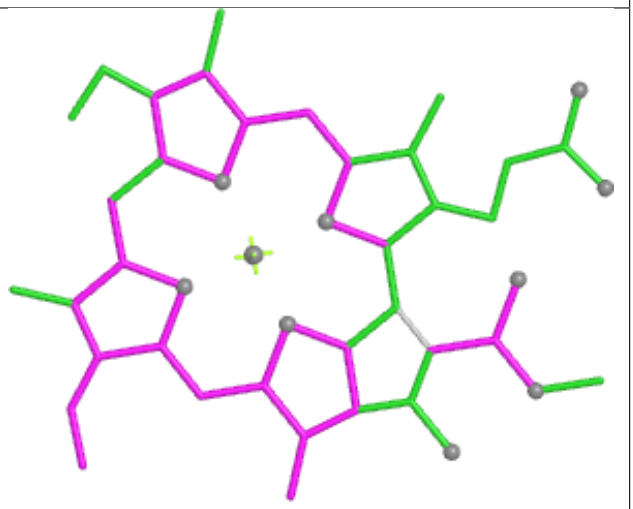
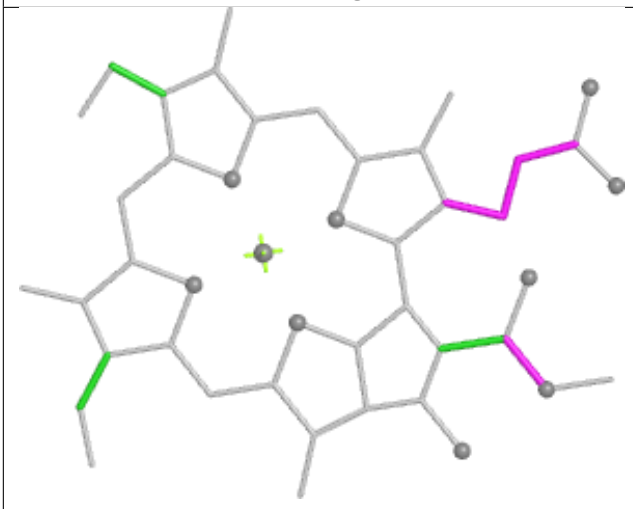


Bond angles

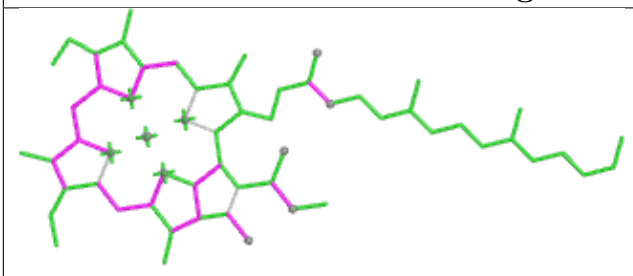


Torsions



Rings

Ligand CLA cB 916



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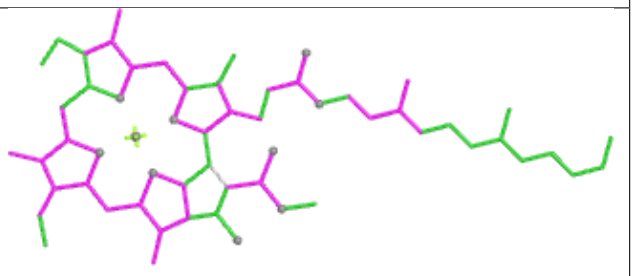
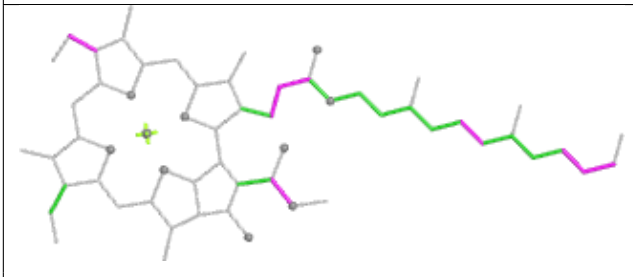
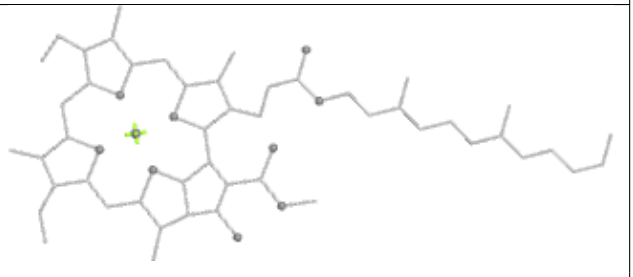


Bond angles

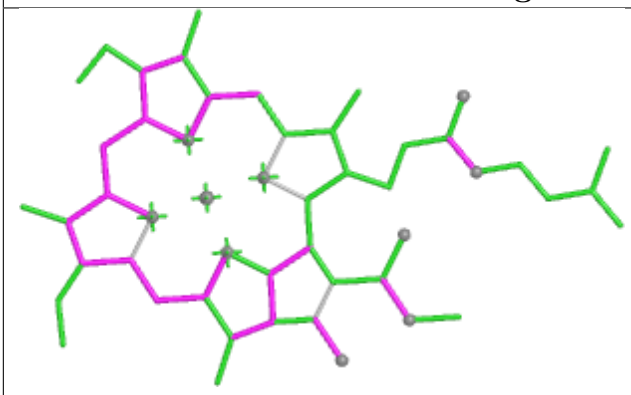


Torsions



Rings

Ligand CLA bB 928



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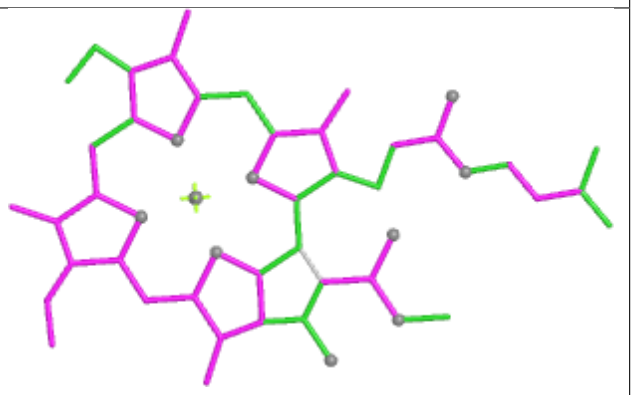
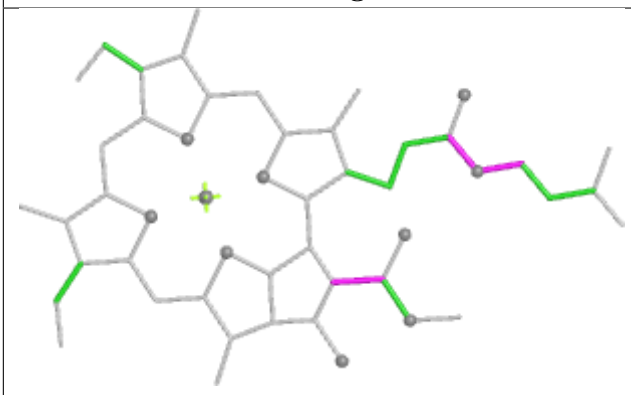


Bond angles



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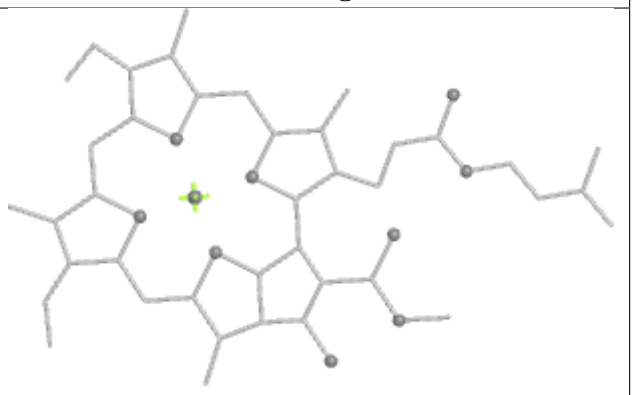
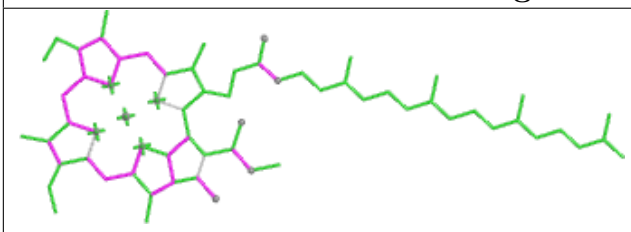


Rings

Ligand CLA bA 807



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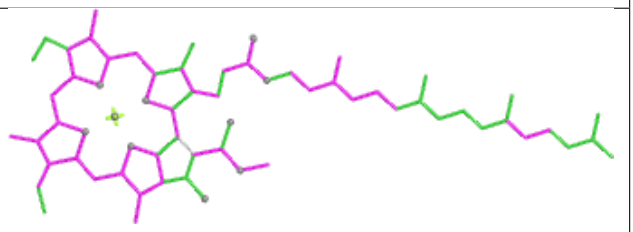
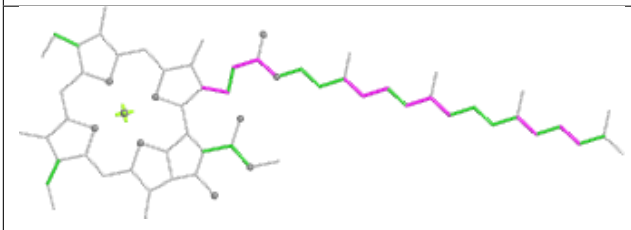


Bond angles



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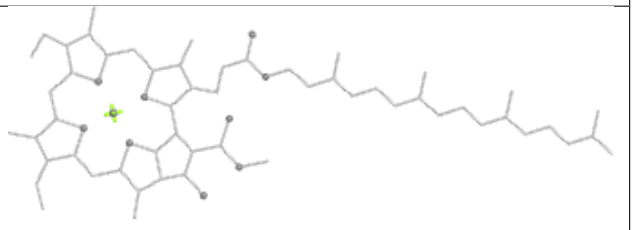
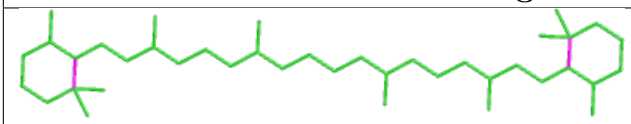


Rings

Ligand BCR cF 203



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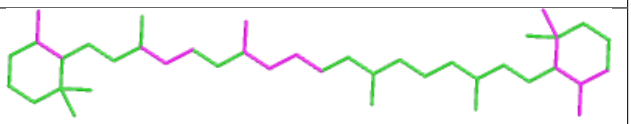
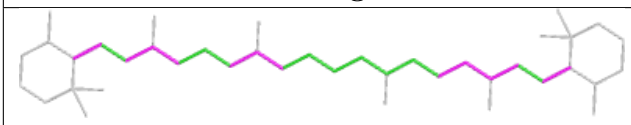
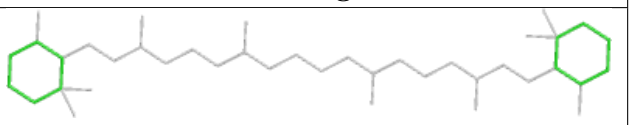


Bond angles

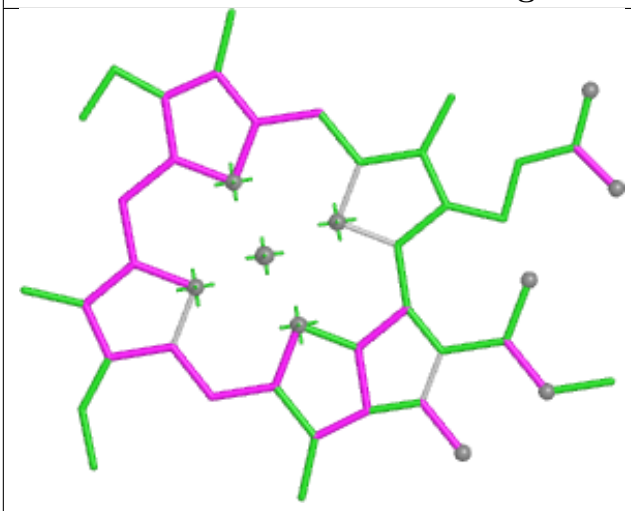


Torsions



Rings

Ligand CLA aL 204



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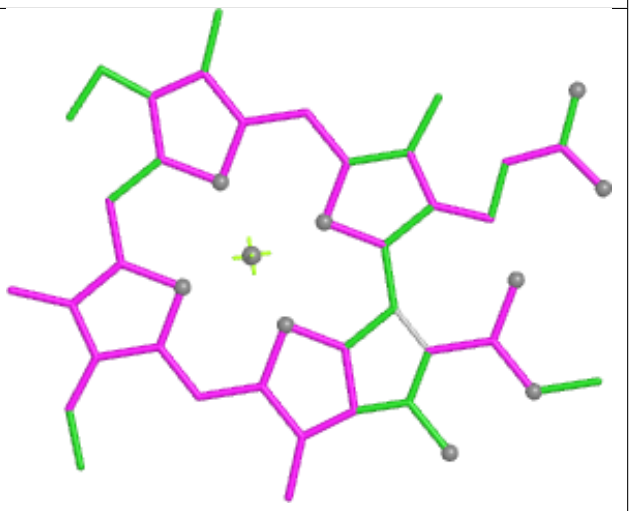
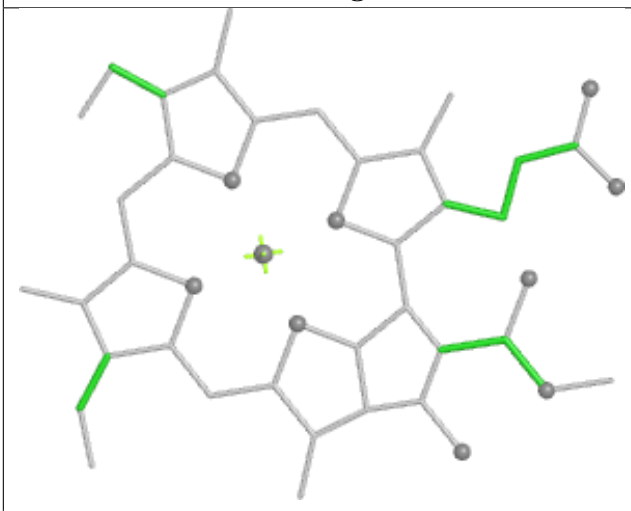


Bond angles



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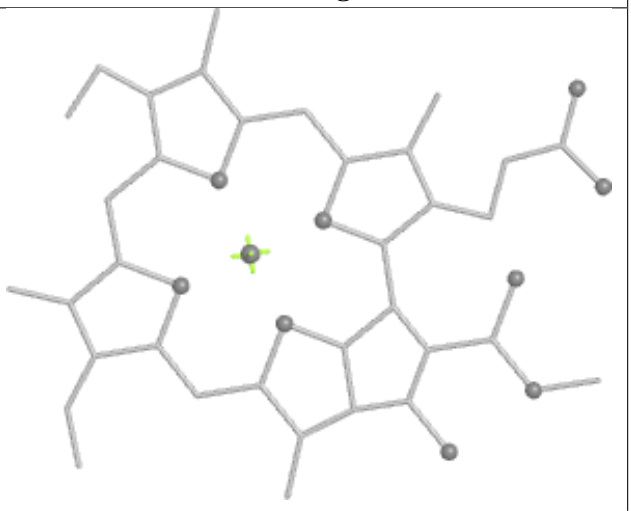
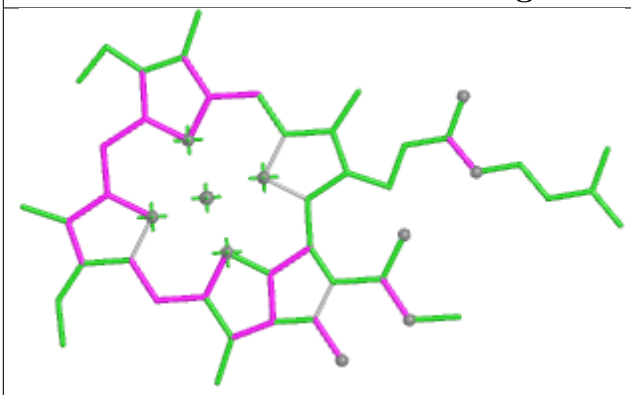


Rings

Ligand CLA cA 831



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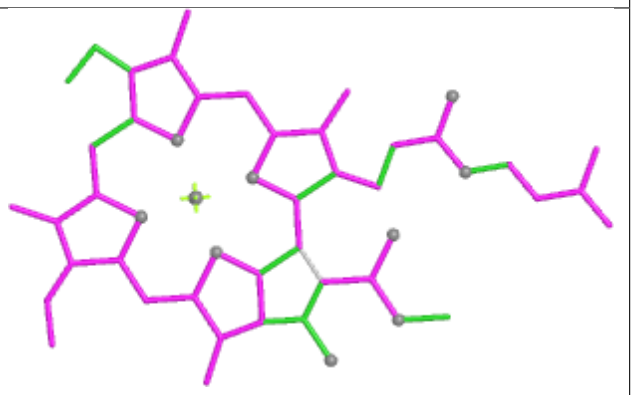
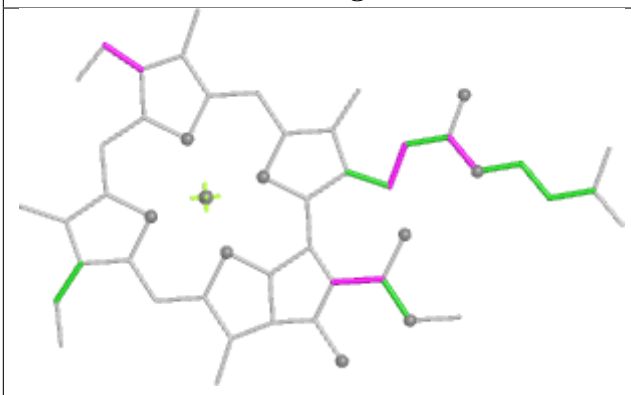


Bond angles



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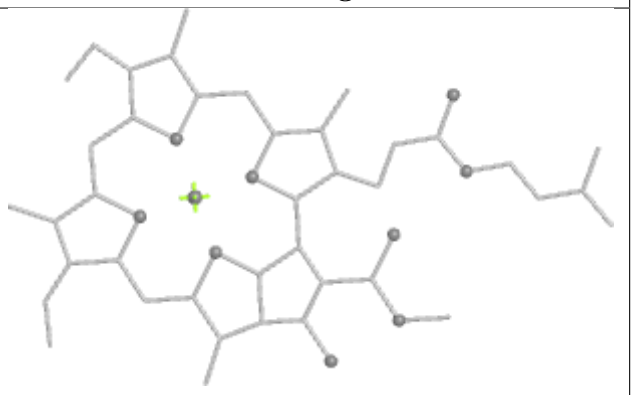
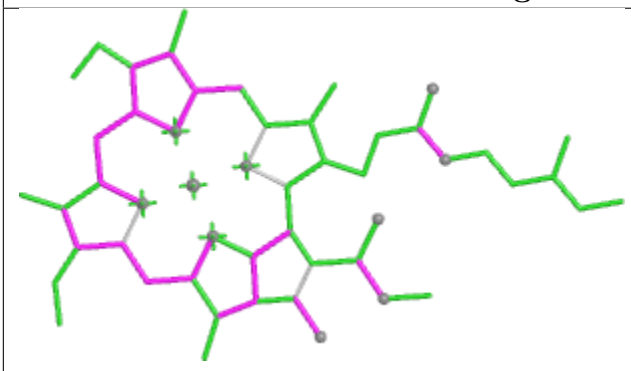


Rings

Ligand CLA bA 837



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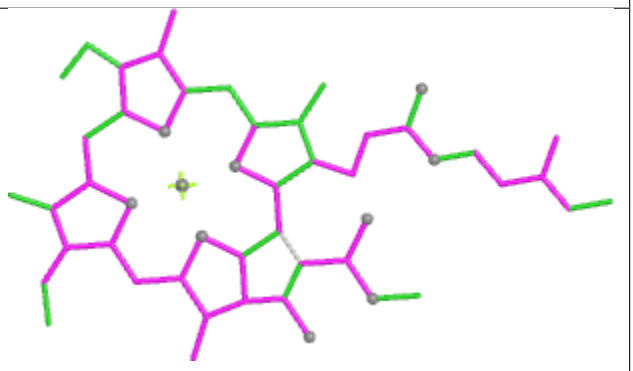
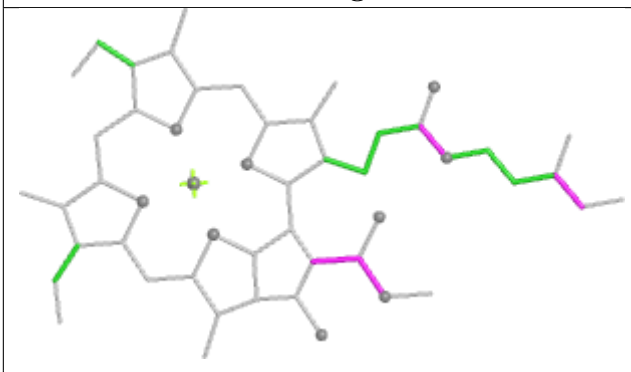
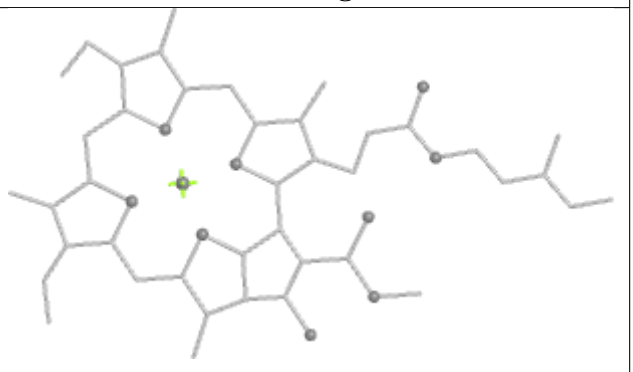


Bond angles

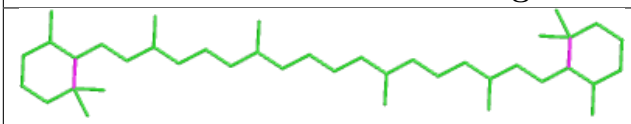


Torsions



Rings

Ligand BCR bA 847



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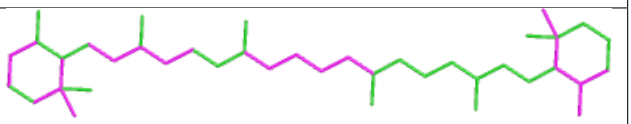
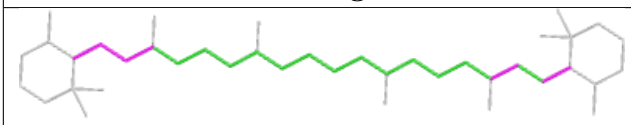


Bond angles



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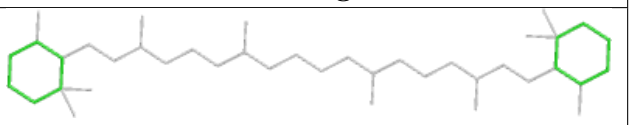
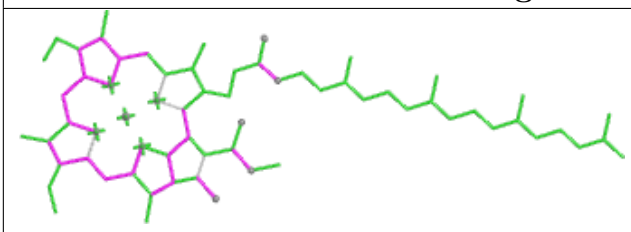


Rings

Ligand CLA aA 812



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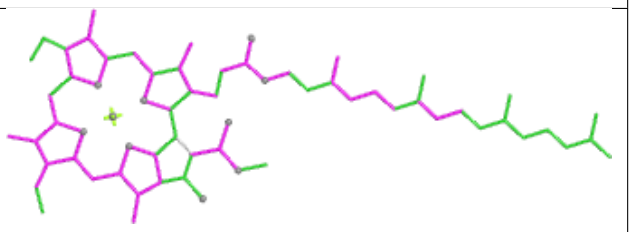
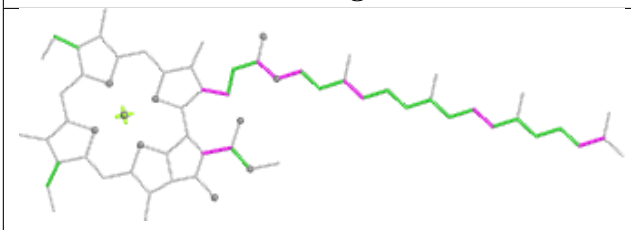
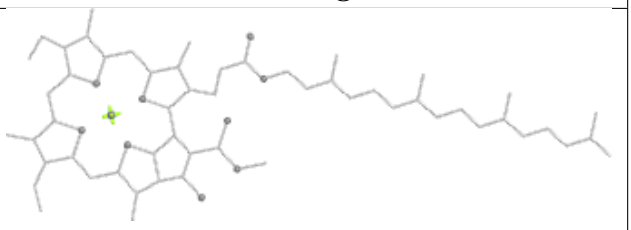


Bond angles

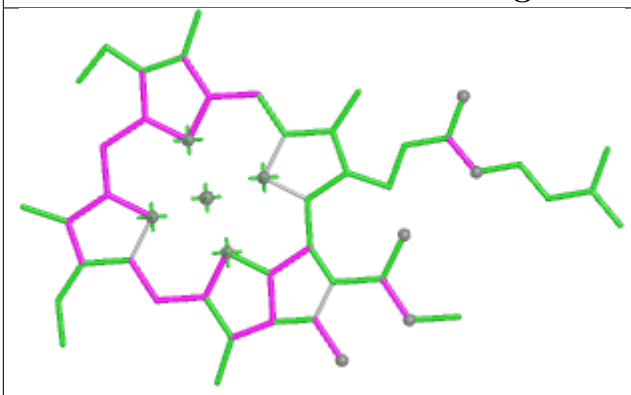


Torsions



Rings

Ligand CLA bA 831



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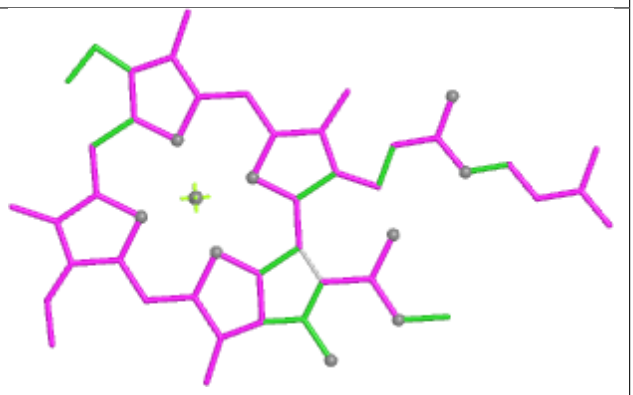
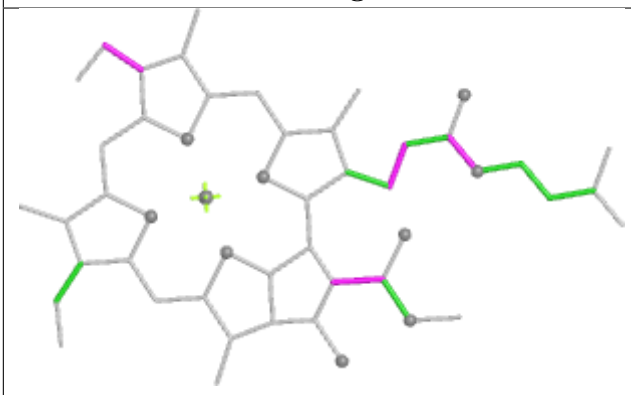
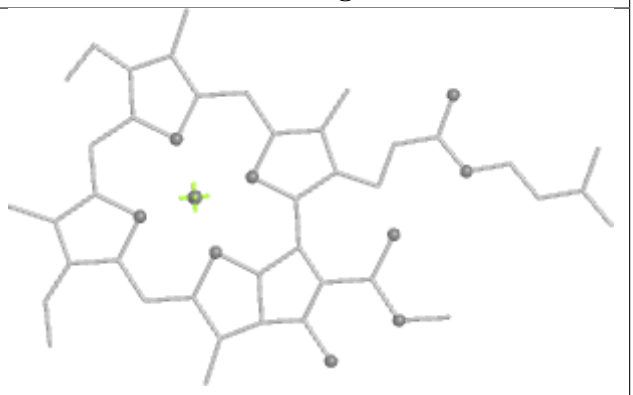


Bond angles

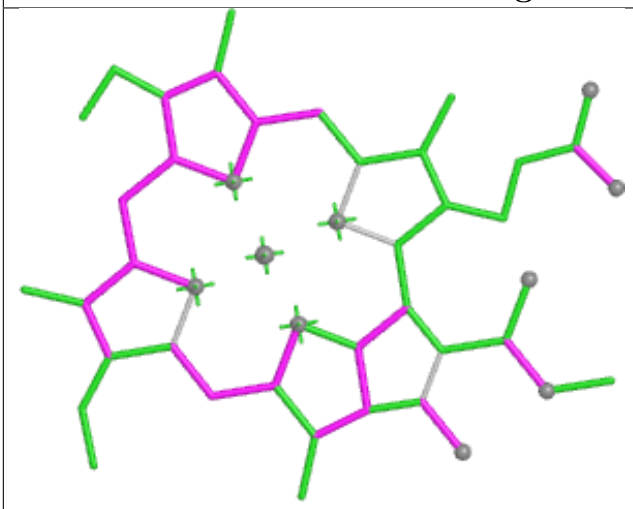


Torsions



Rings

Ligand CLA aA 810



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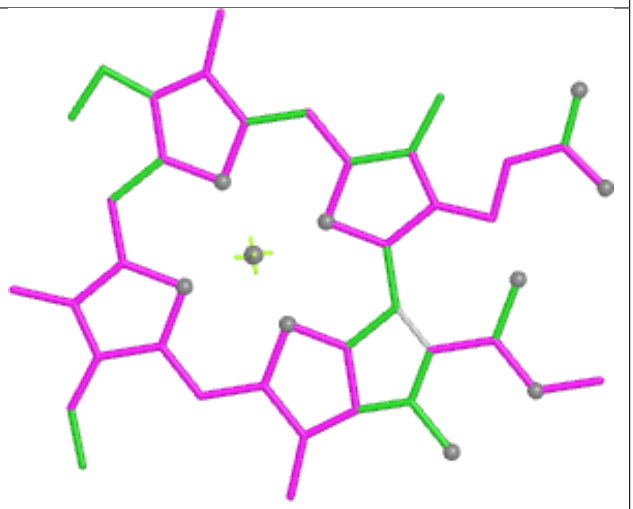
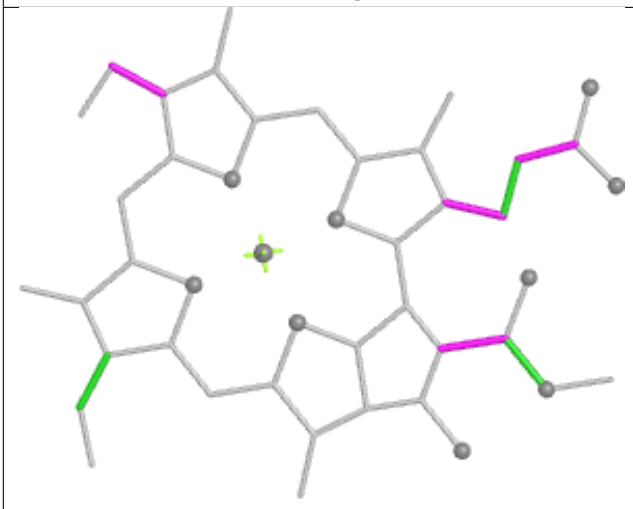


Bond angles

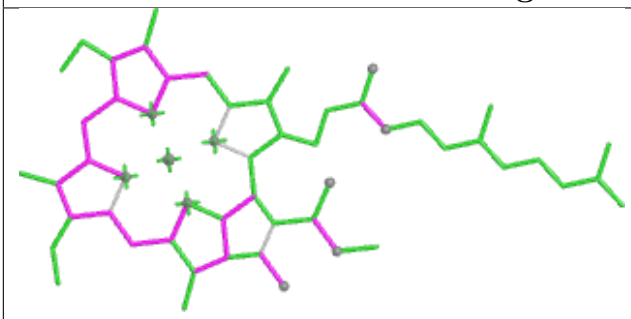


Torsions



Rings

Ligand CLA cB 906



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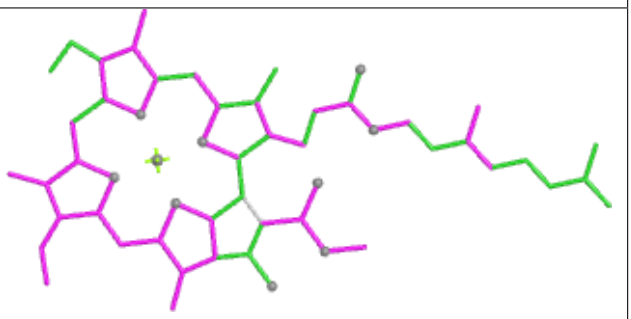
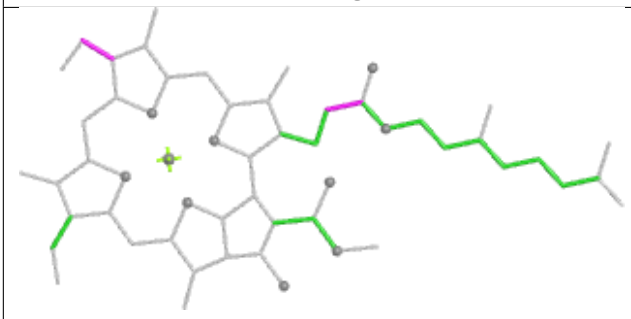


Bond angles



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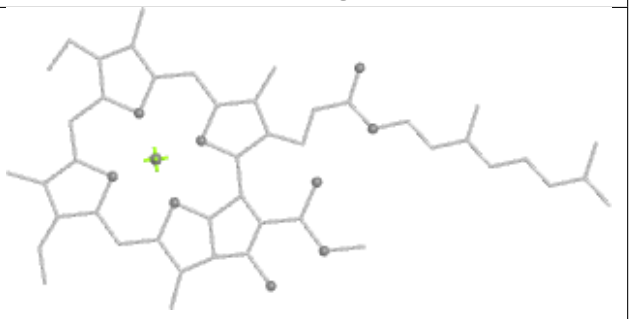
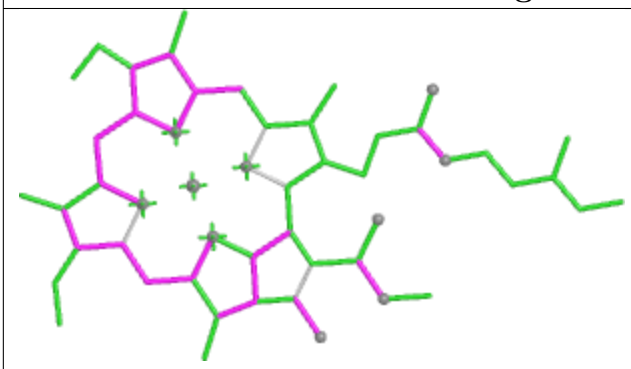


Rings

Ligand CLA aA 837



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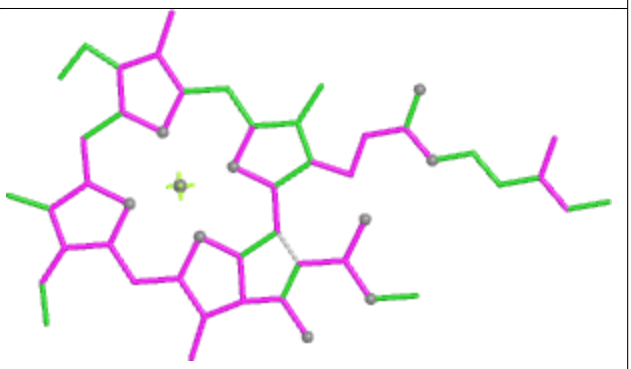
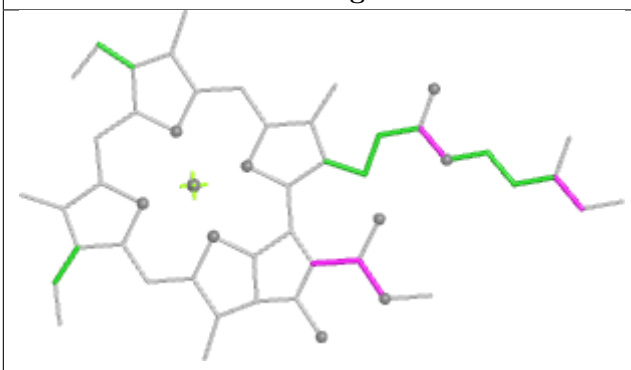
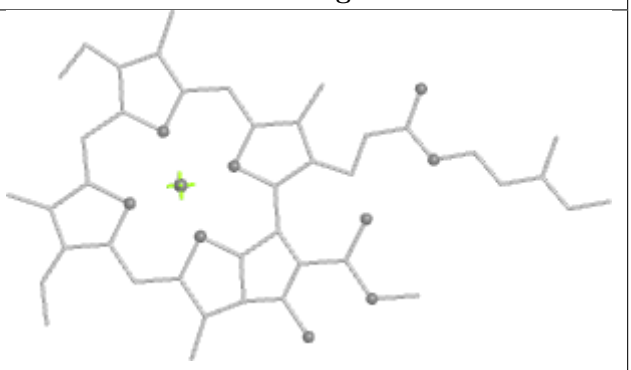


Bond angles

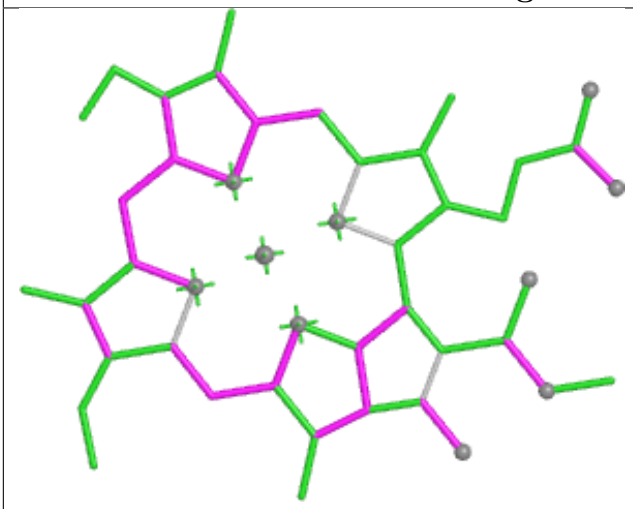


Torsions

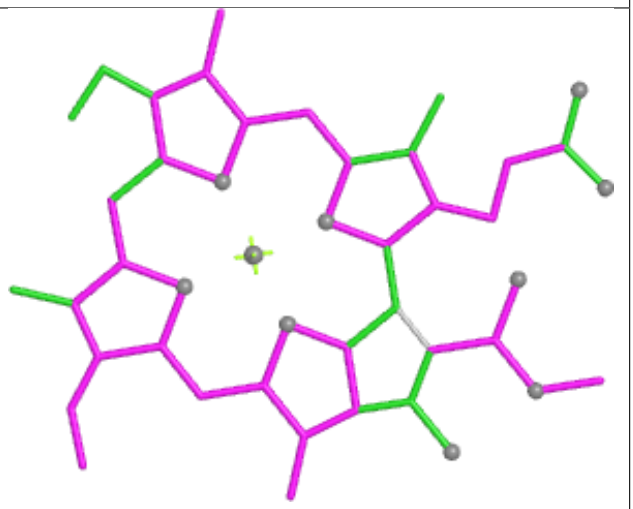


Rings

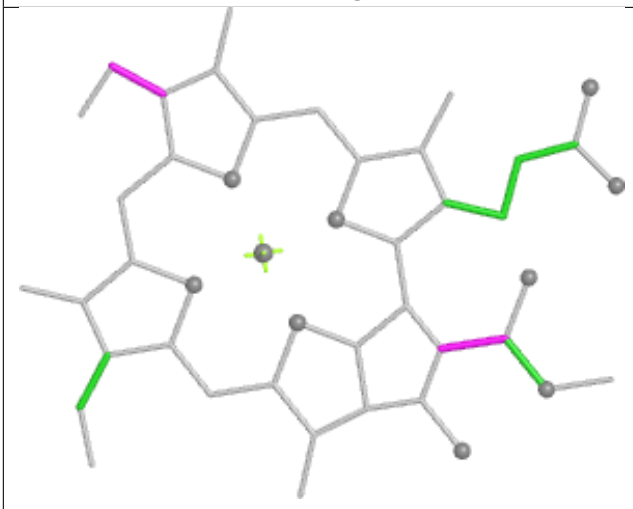
Ligand CLA cB 932



Bond lengths



Bond angles

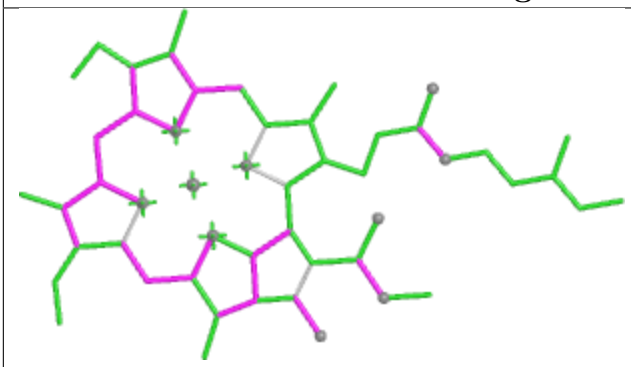


Torsions



Rings

Ligand CLA bB 938



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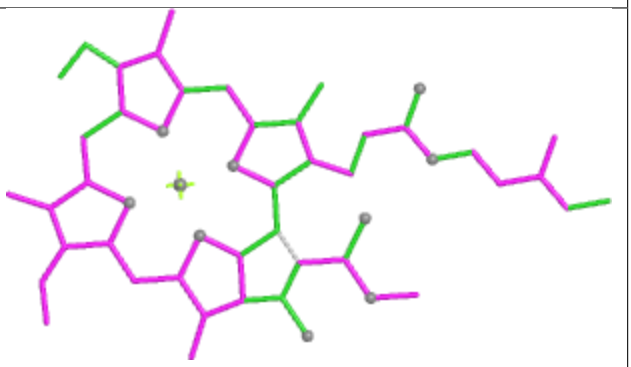

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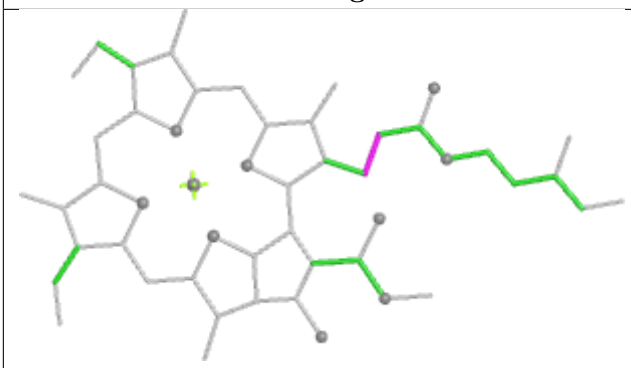

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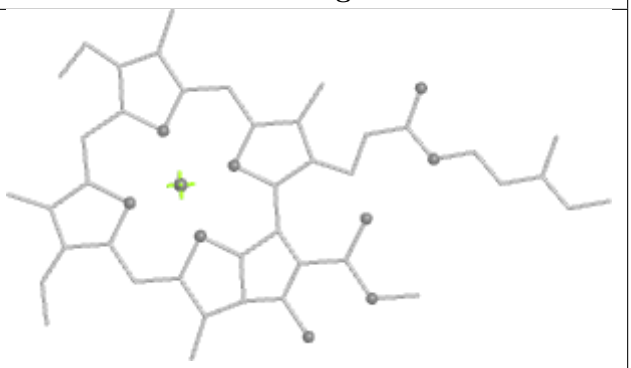
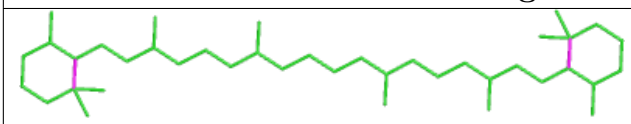


Rings

Ligand BCR bI 101



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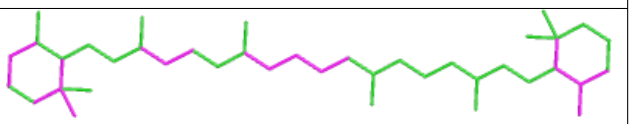
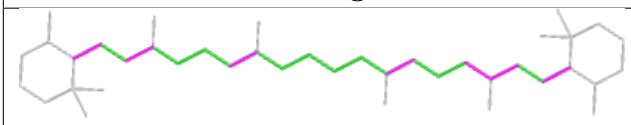


Bond angles



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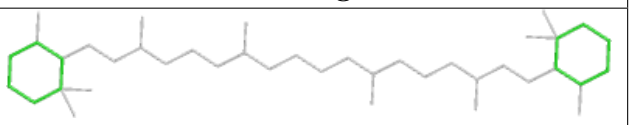
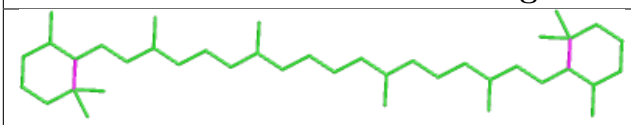


Rings

Ligand BCR aI 101



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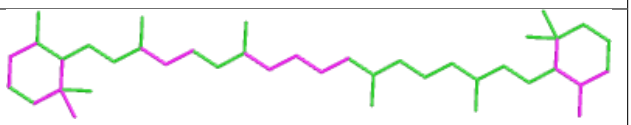
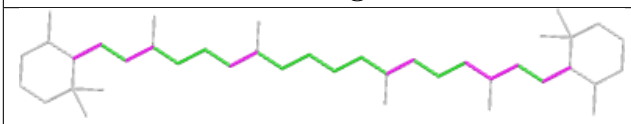


Bond angles



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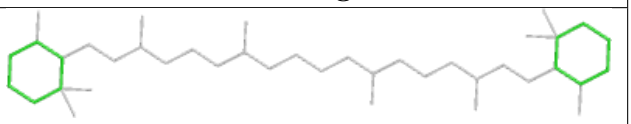
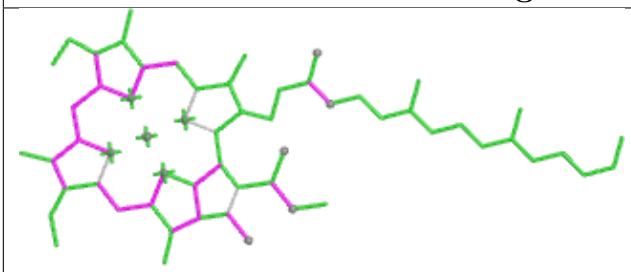


Rings

Ligand CLA aB 916



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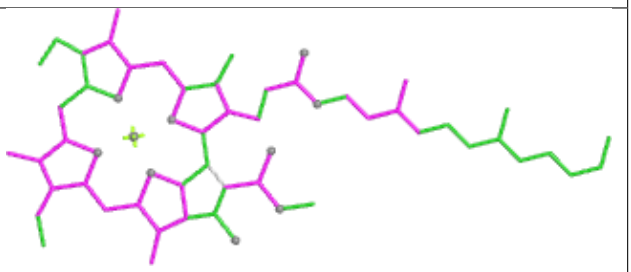
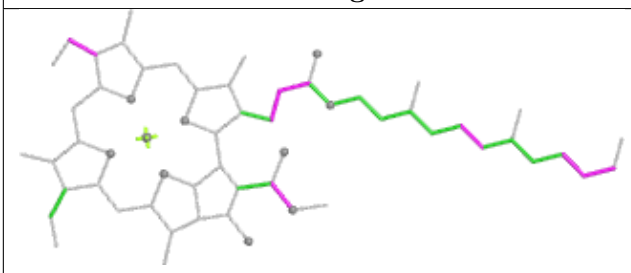


Bond angles



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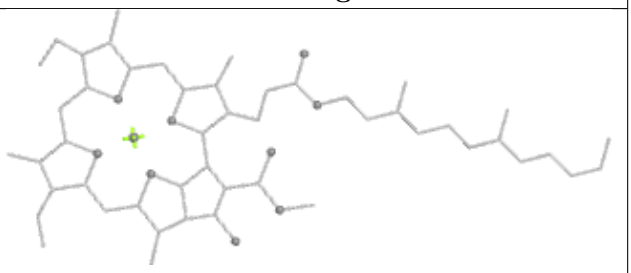
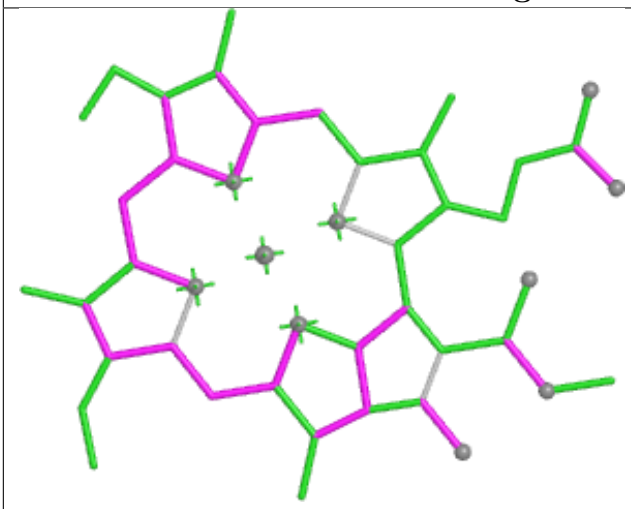


Rings

Ligand CLA bA 814



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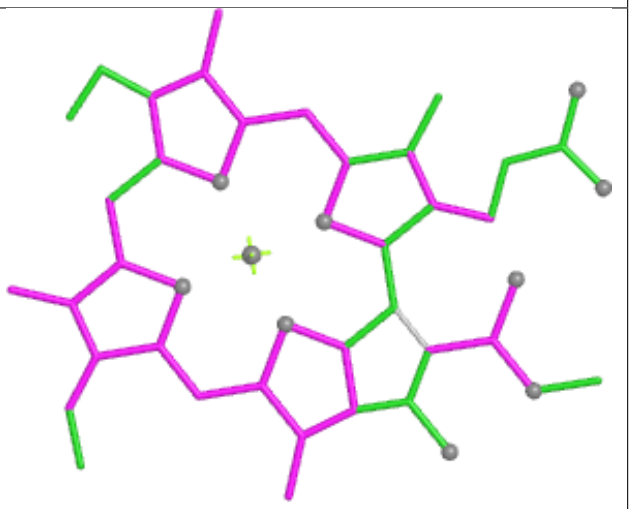
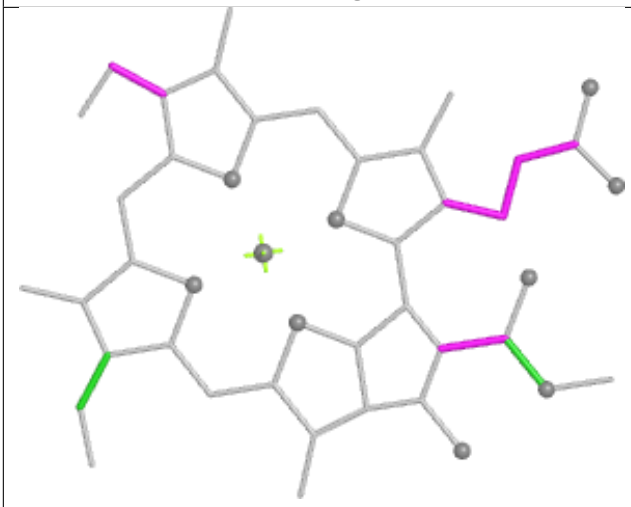


Bond angles

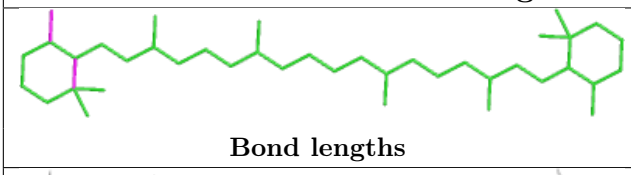


Torsions



Rings

Ligand BCR bJ 101



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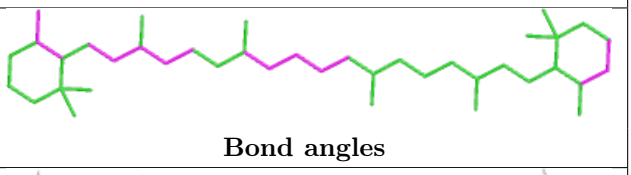
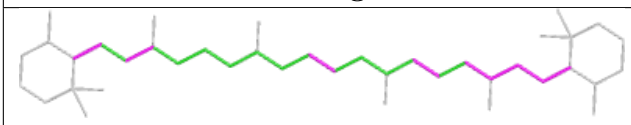


Bond angles



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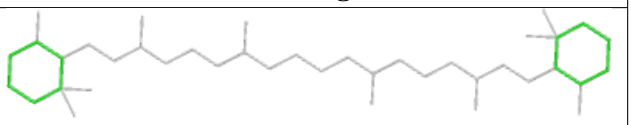
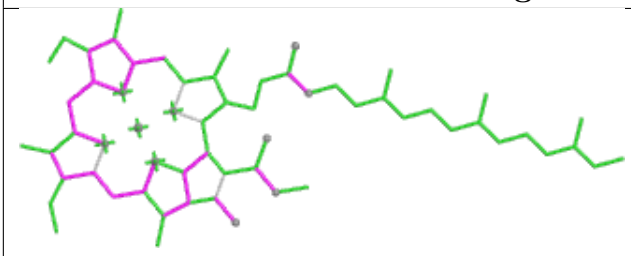


Rings

Ligand CLA bB 902



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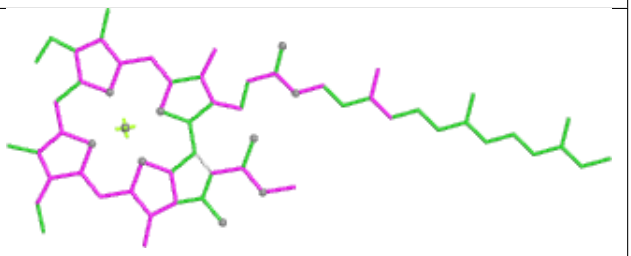
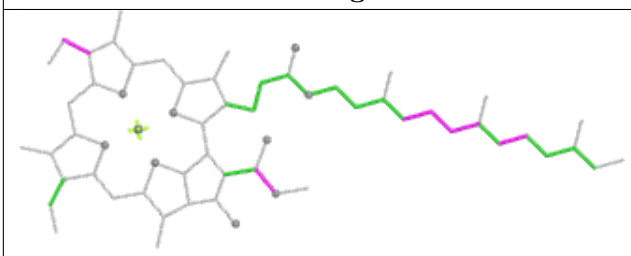


Bond angles



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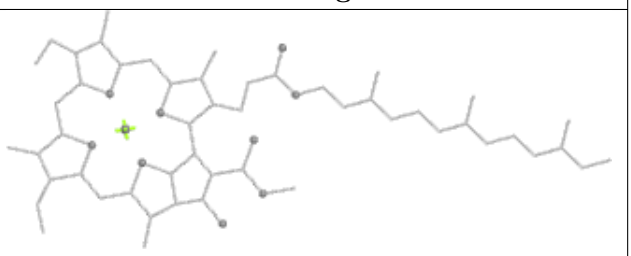
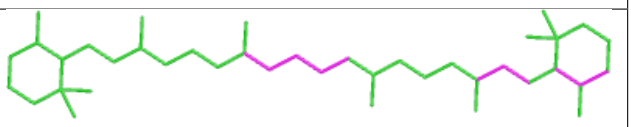


Rings

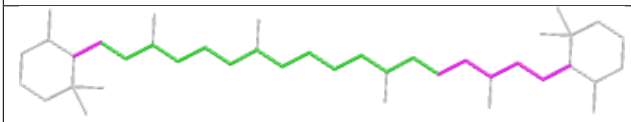
Ligand BCR aA 849



Bond lengths



Bond angles



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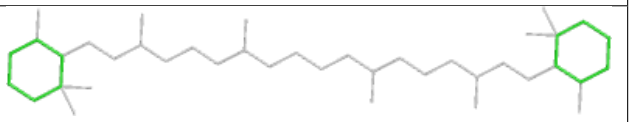
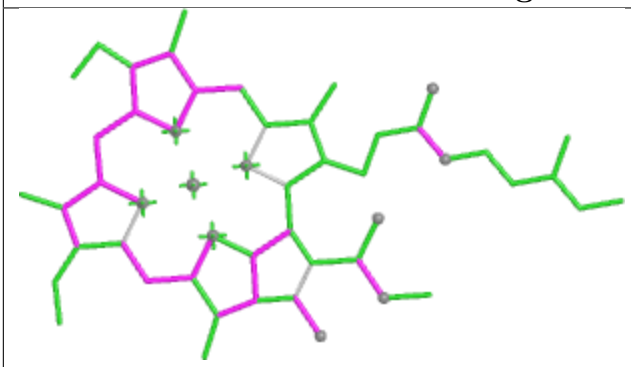
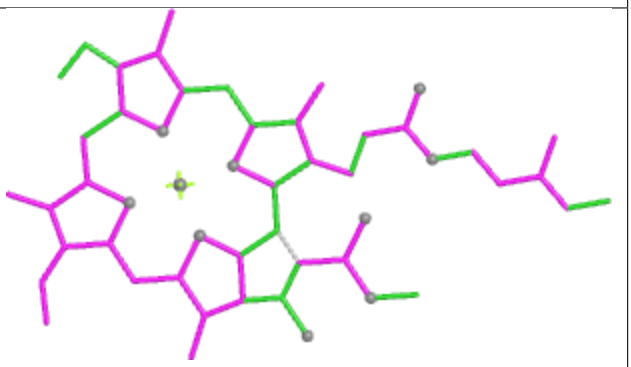
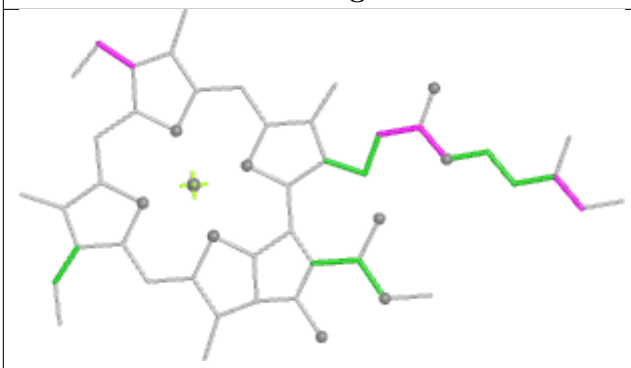
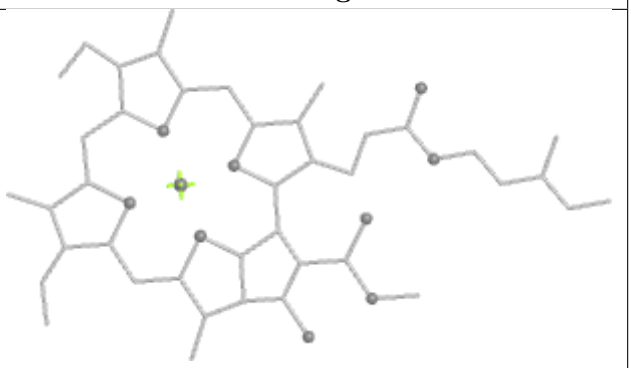


Rings

Ligand CLA cA 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

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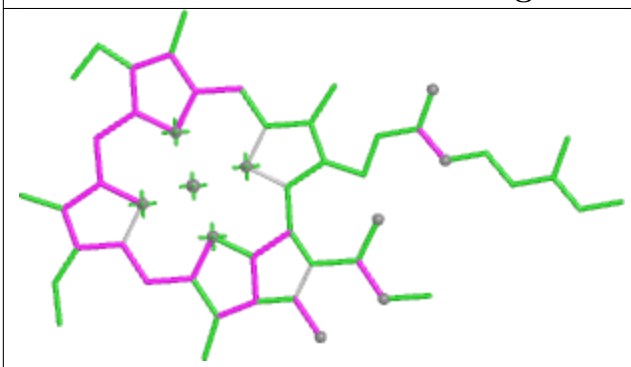
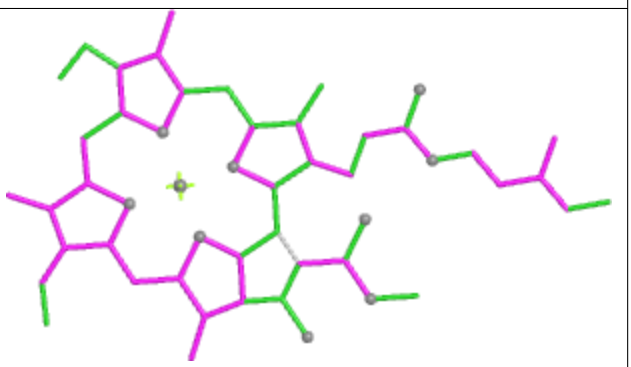
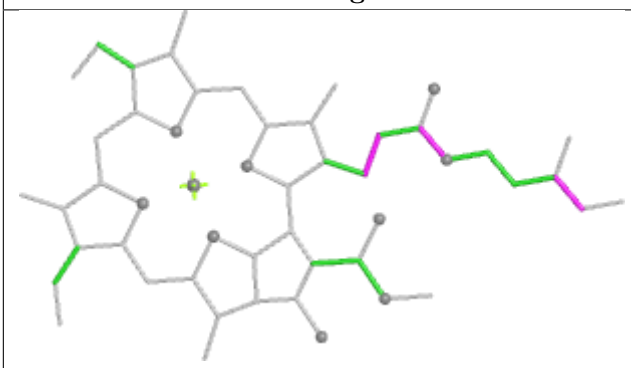
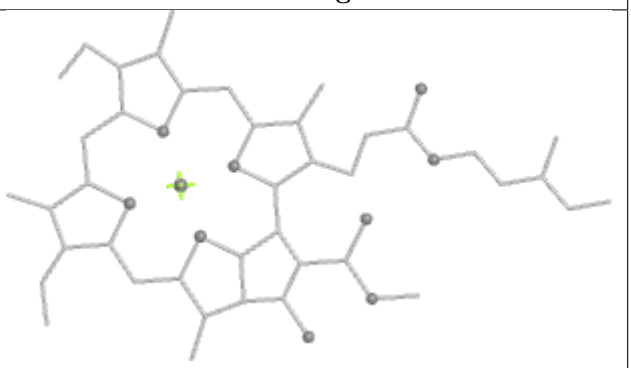
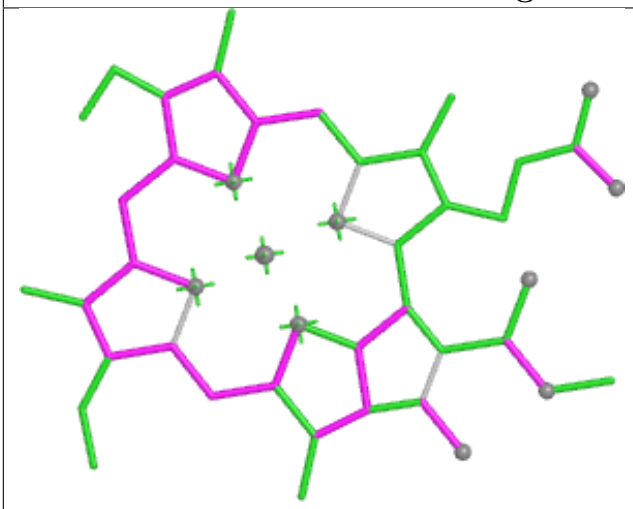
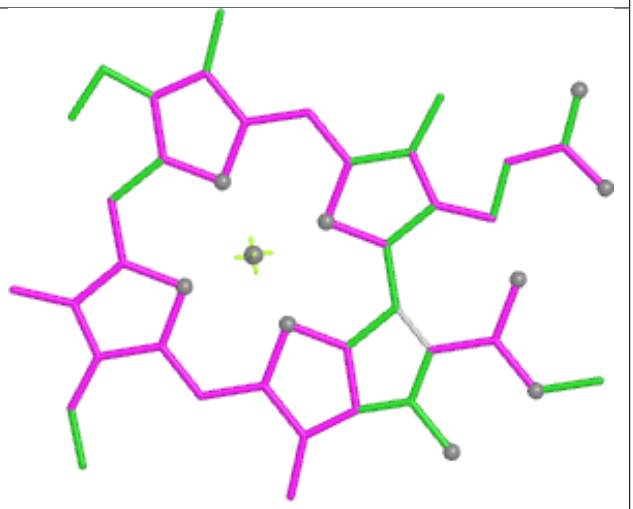
 Bond lengths	 Bond angles
 Torsions	 Rings

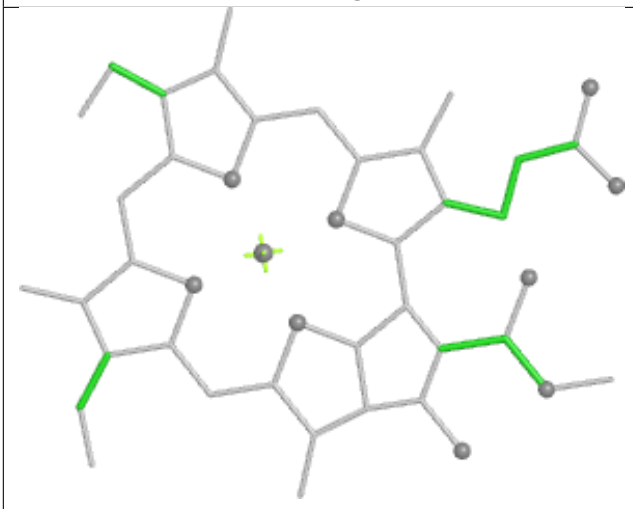
Ligand CLA bL 204



Bond lengths



Bond angles

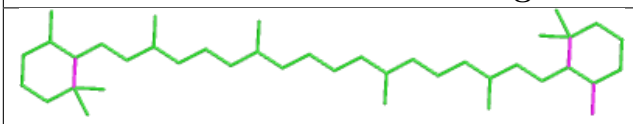


Torsions

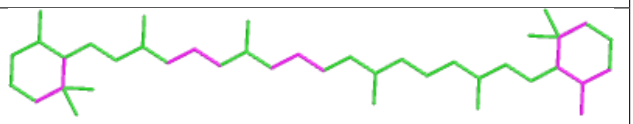


Rings

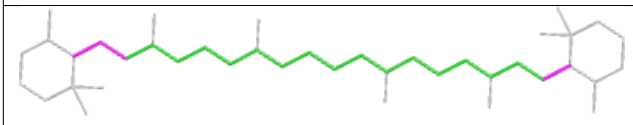
Ligand BCR aB 946



Bond lengths



Bond angles



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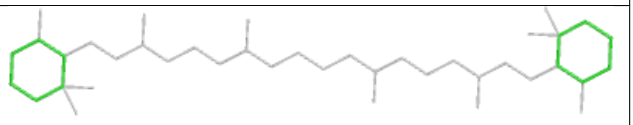
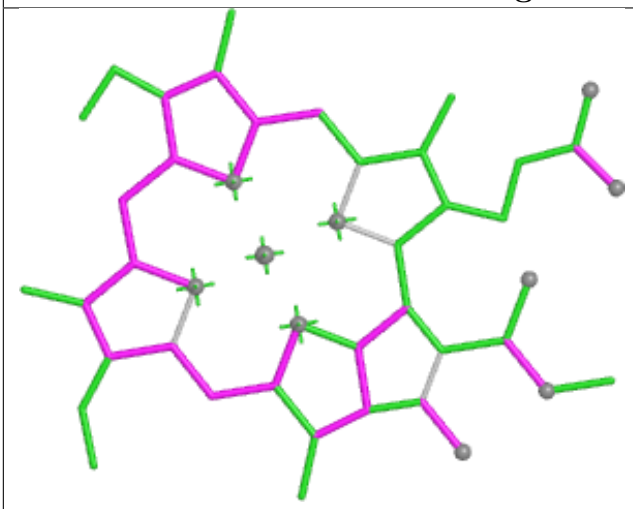


Rings

Ligand CLA aA 813



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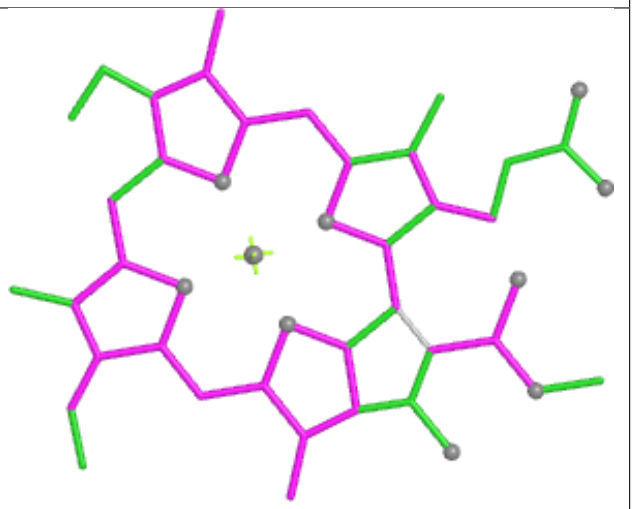
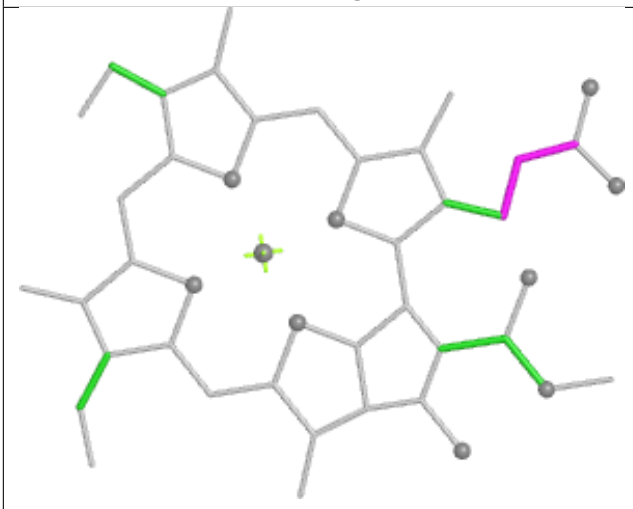


Bond angles

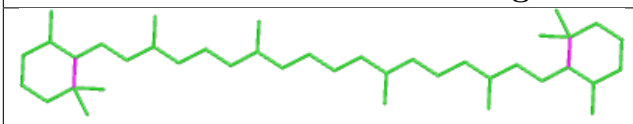


Torsions



Rings

Ligand BCR bA 850



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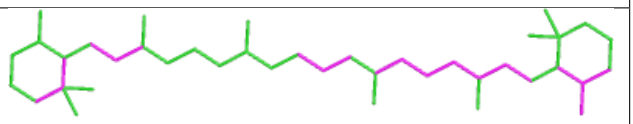
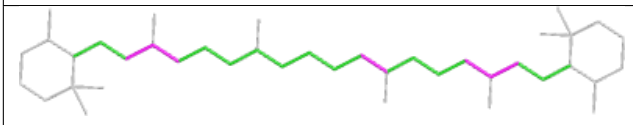
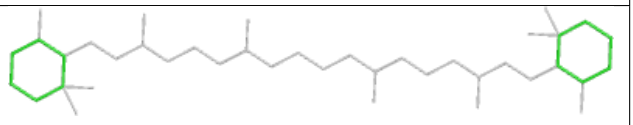


Bond angles

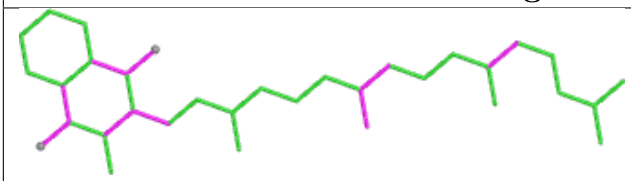


Torsions

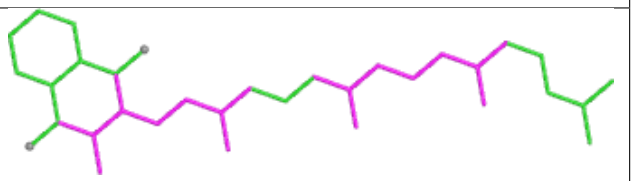


Rings

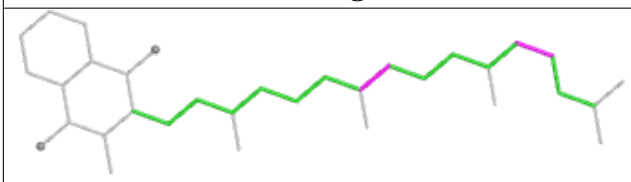
Ligand 1L3 aA 845



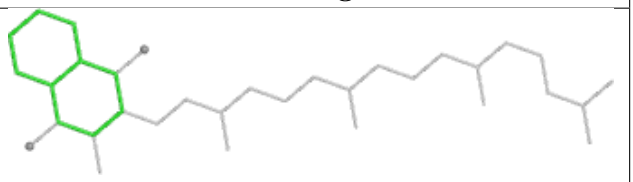
Bond lengths



Bond angles

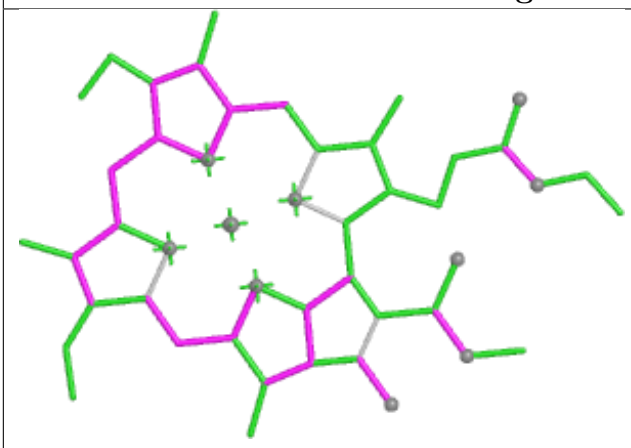


Torsions

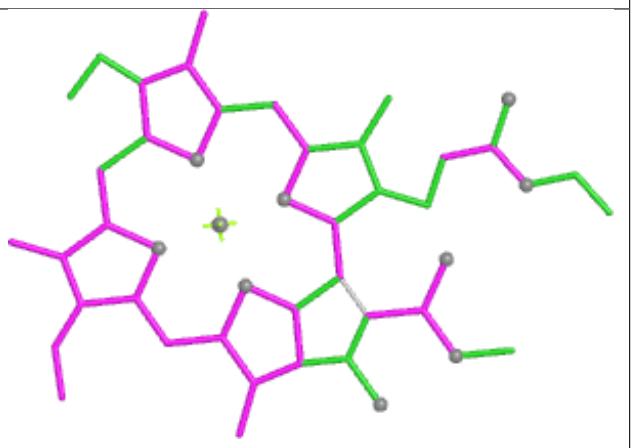


Rings

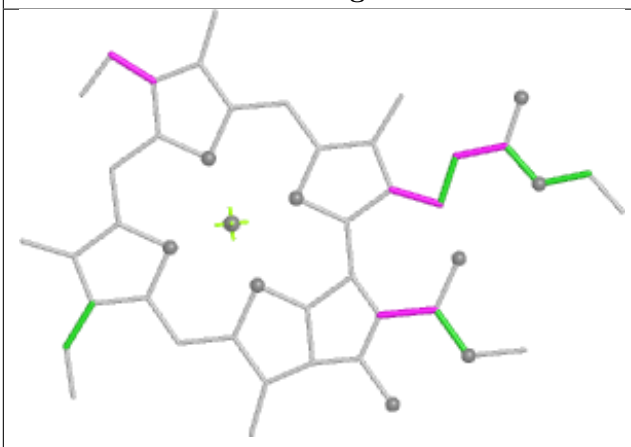
Ligand CLA aB 919



Bond lengths



Bond angles



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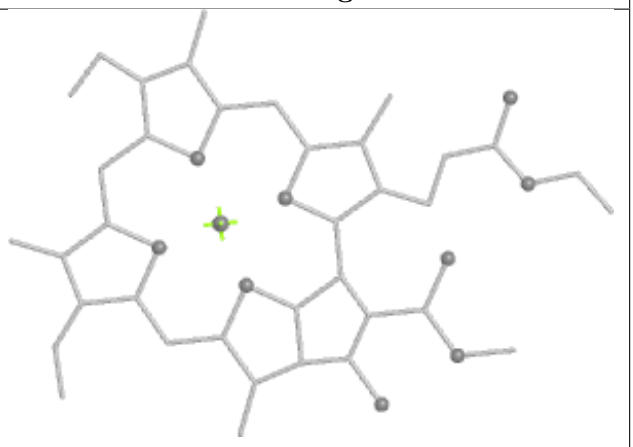
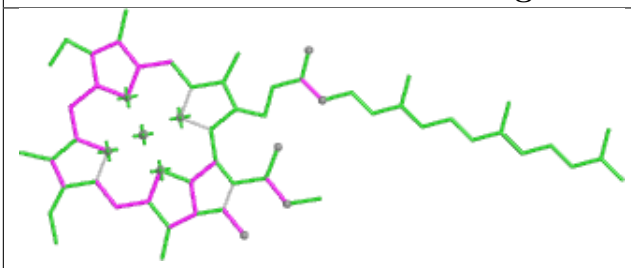
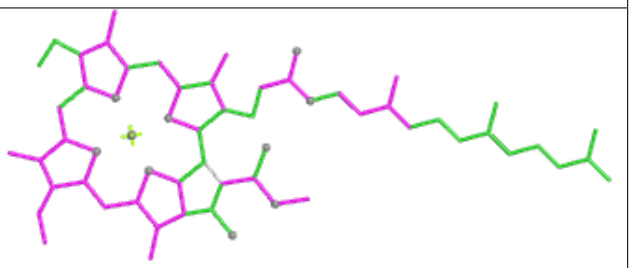


Rings

Ligand CLA aA 829	
	
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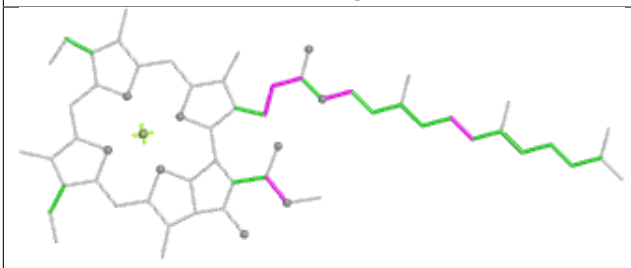
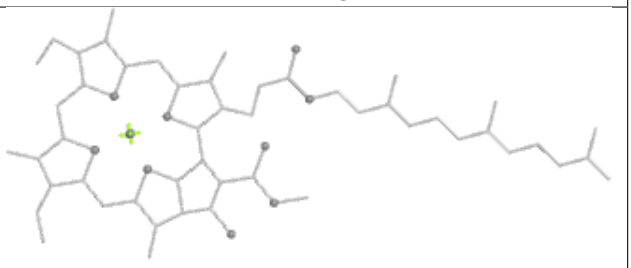
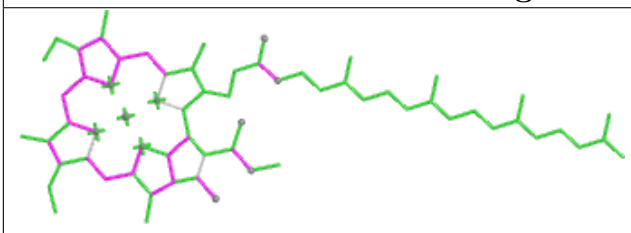
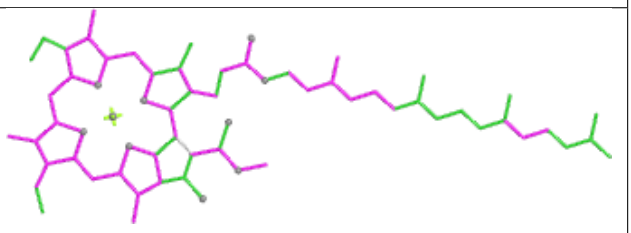
	
Torsions	**Rings**

Ligand CLA aA 807	
	
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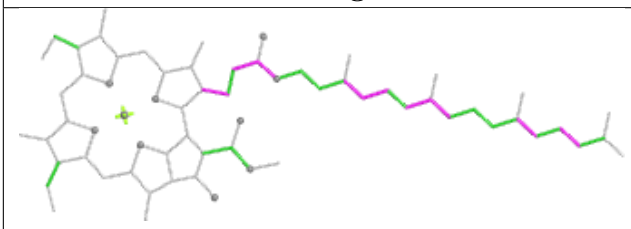
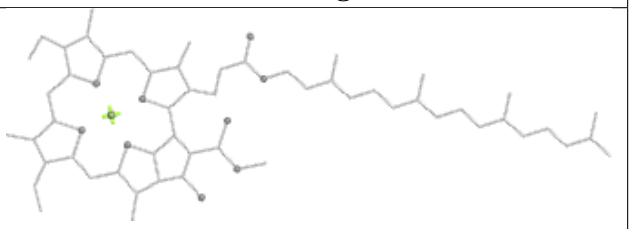
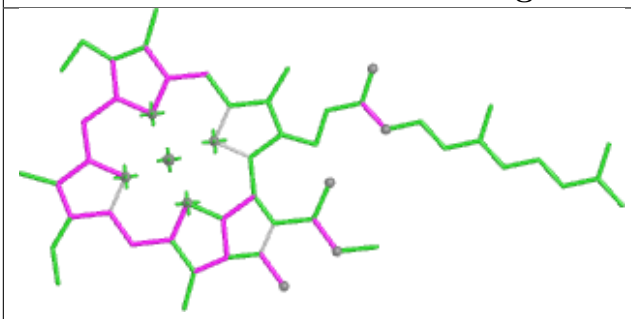
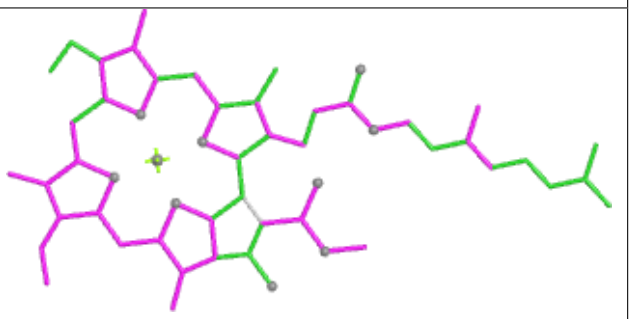
	
Torsions	**Rings**

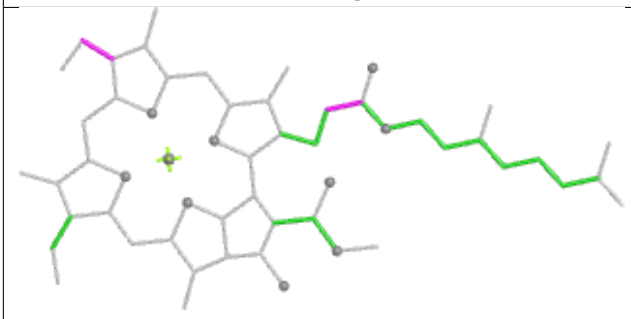
Ligand CLA aB 906



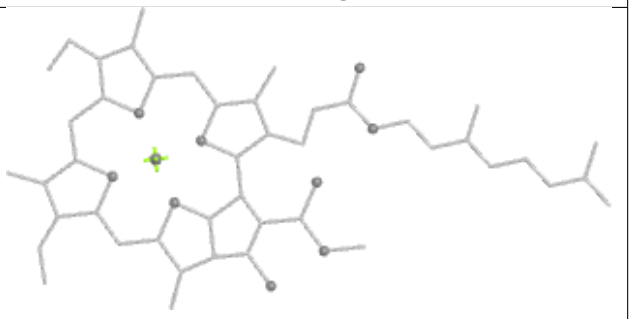
Bond lengths



Bond angles

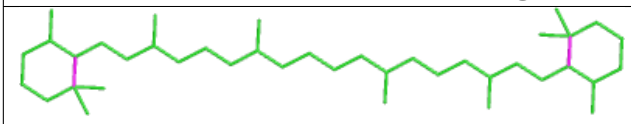


Torsions



Rings

Ligand BCR bF 201



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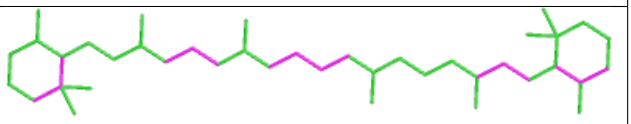
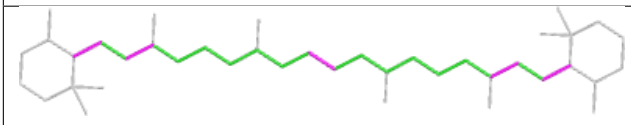


Bond angles



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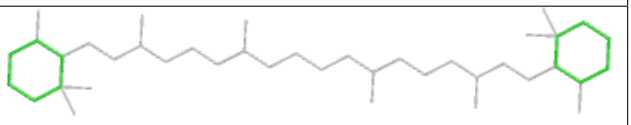
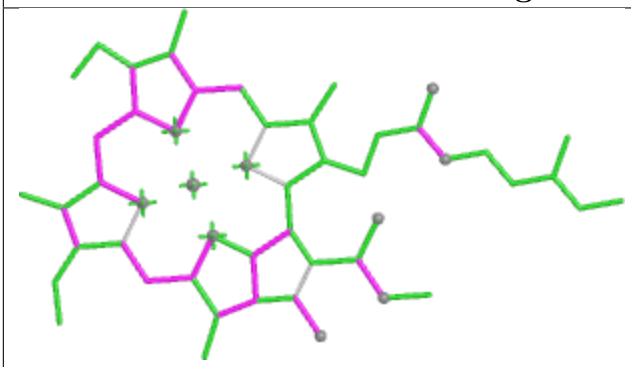


Rings

Ligand CLA aA 833



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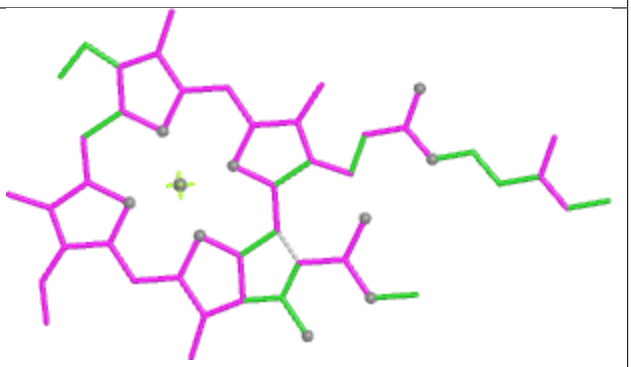
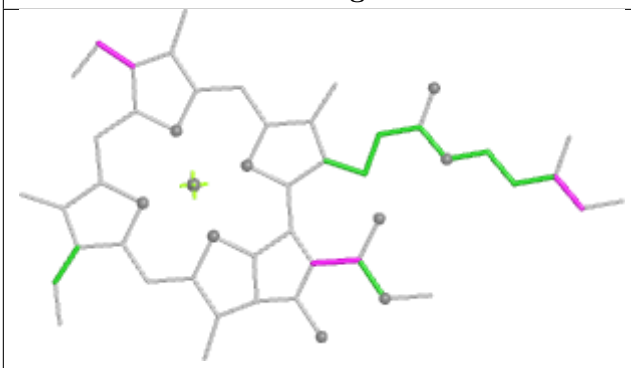


Bond angles



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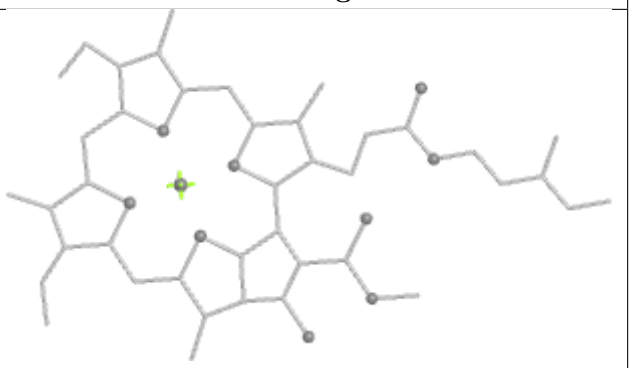
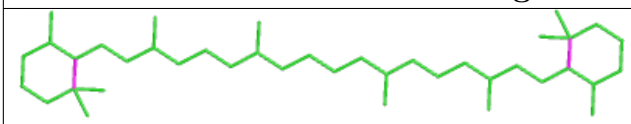


Rings

Ligand BCR aA 847



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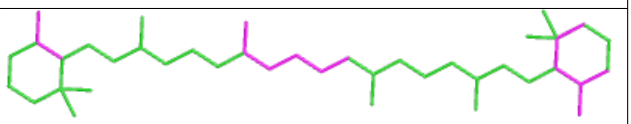
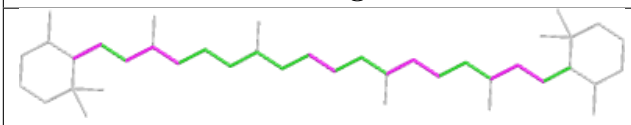


Bond angles



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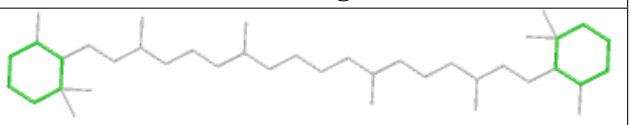
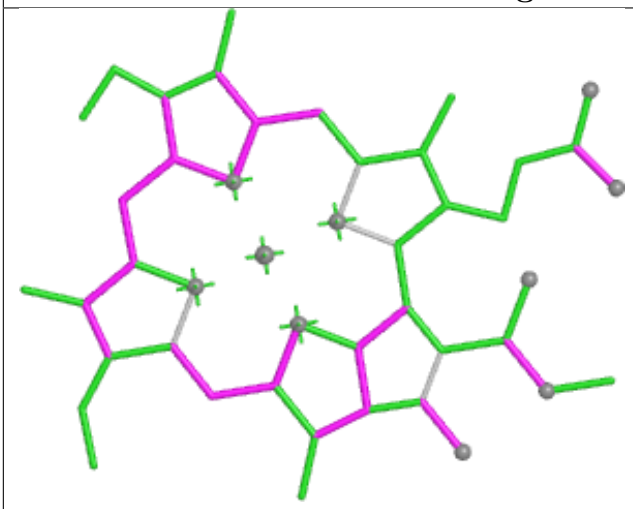


Rings

Ligand CLA cB 910



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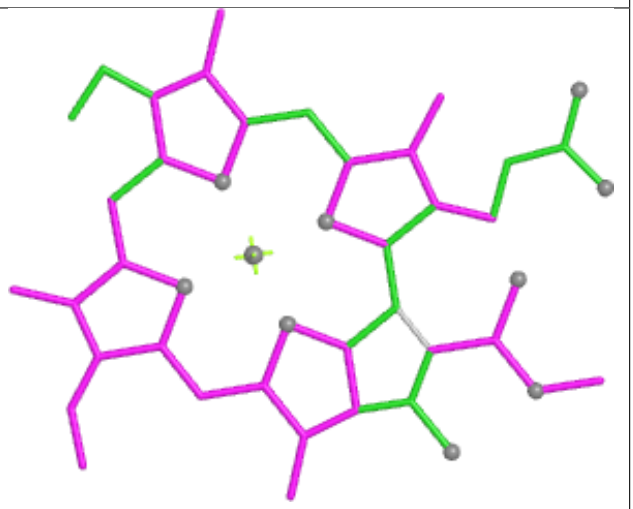
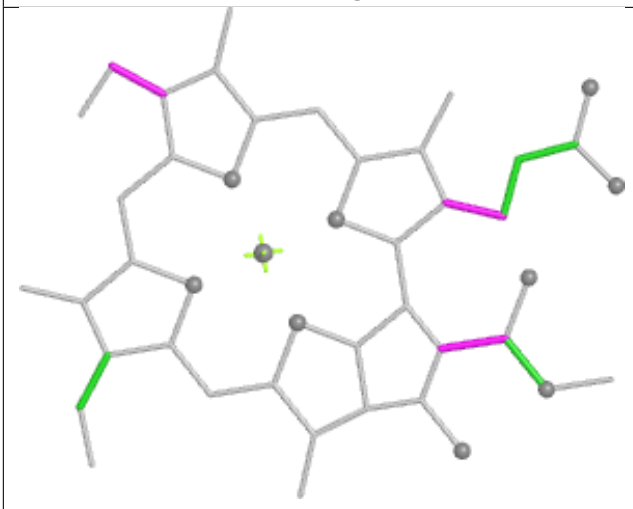


Bond angles

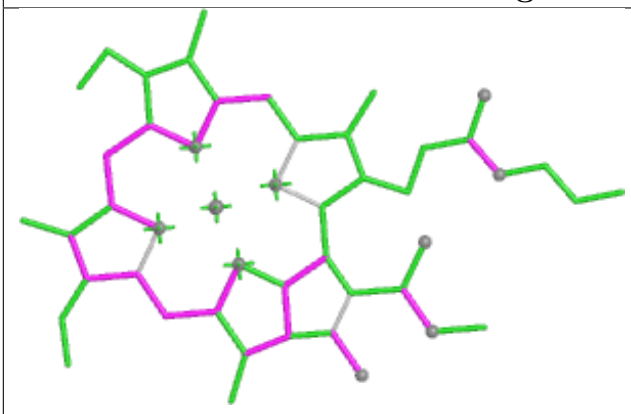


Torsions



Rings

Ligand CLA cB 908



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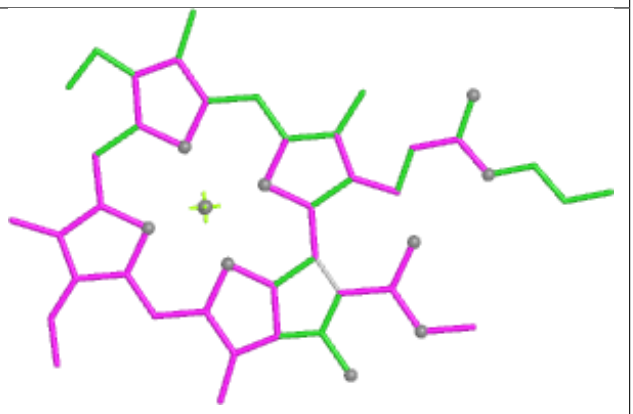
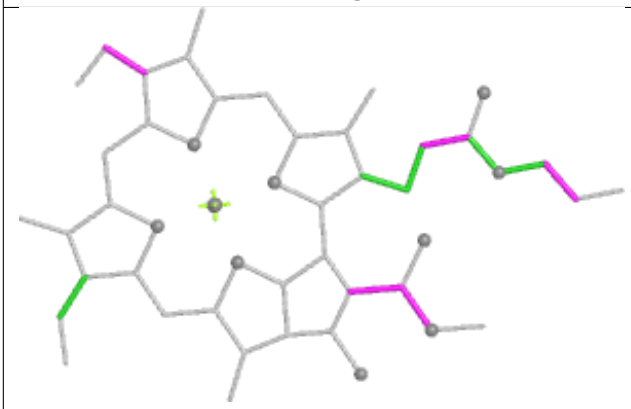


Bond angles



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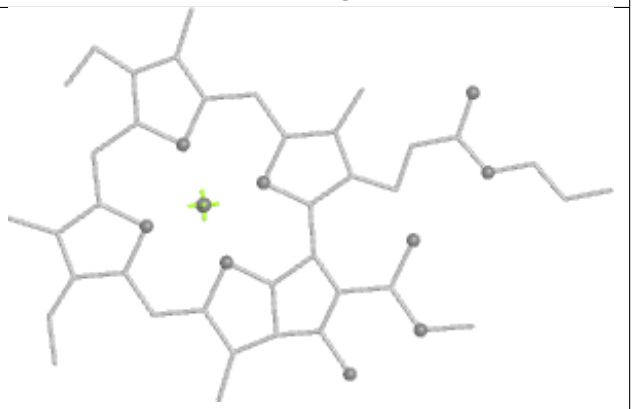
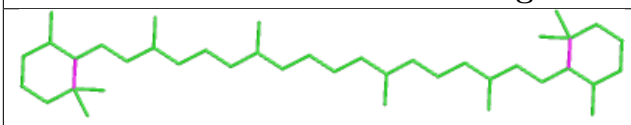


Rings

Ligand BCR cF 204



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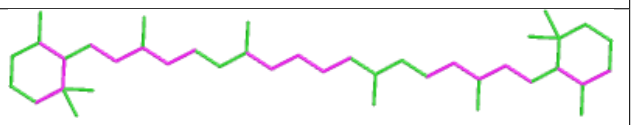
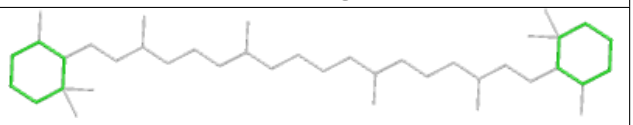


Bond angles

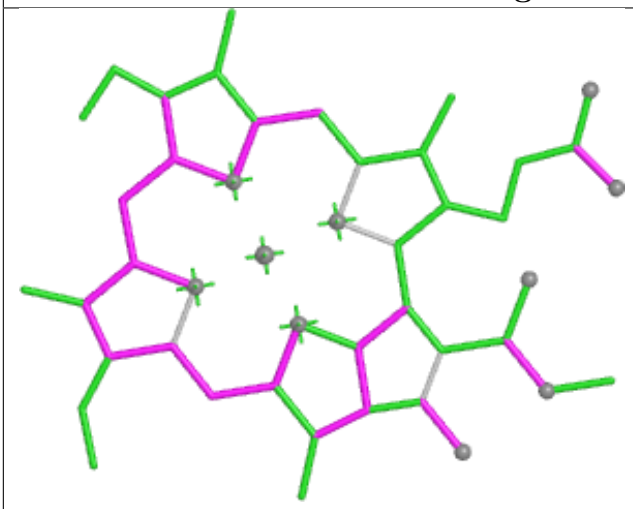


Torsions



Rings

Ligand CLA bB 933



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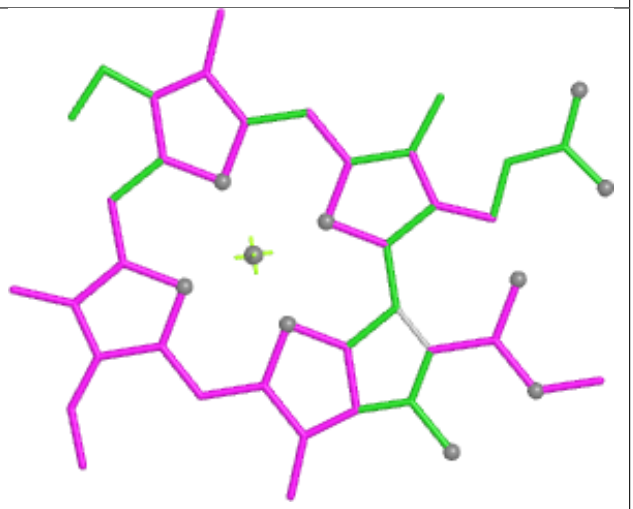
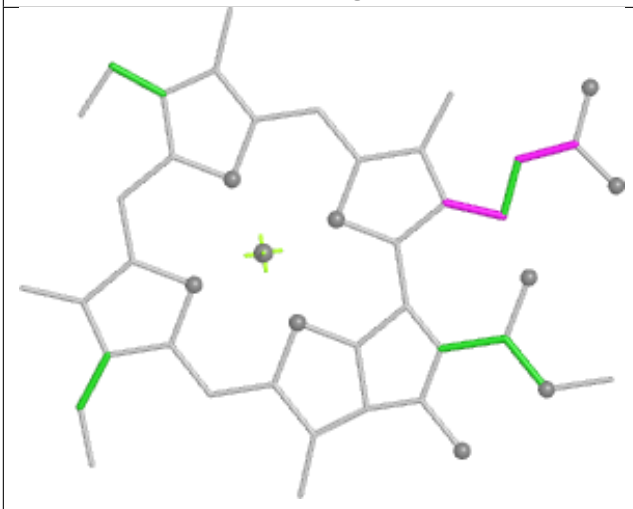


Bond angles

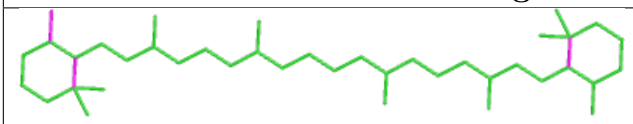


Torsions



Rings

Ligand BCR bB 941



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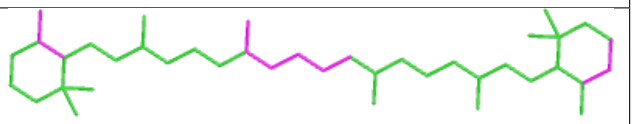
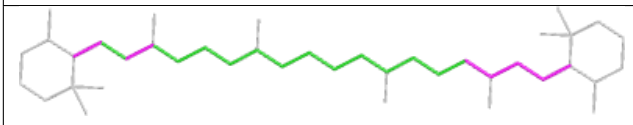
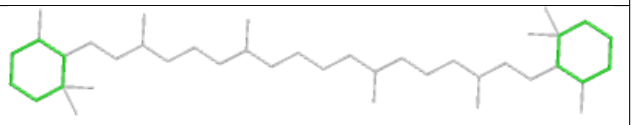


Bond angles

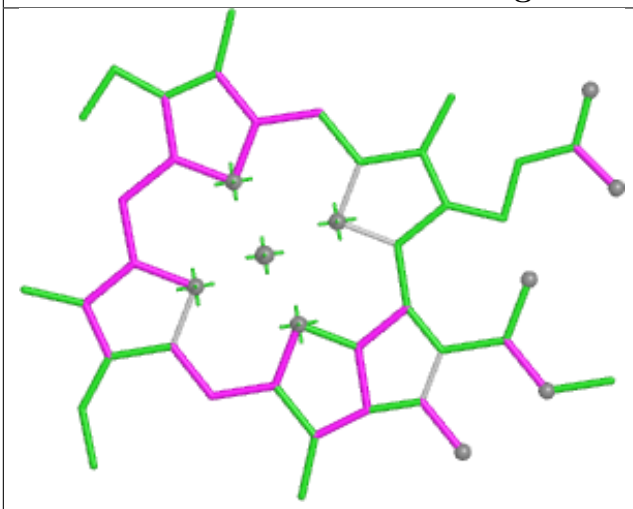


Torsions



Rings

Ligand CLA bB 911



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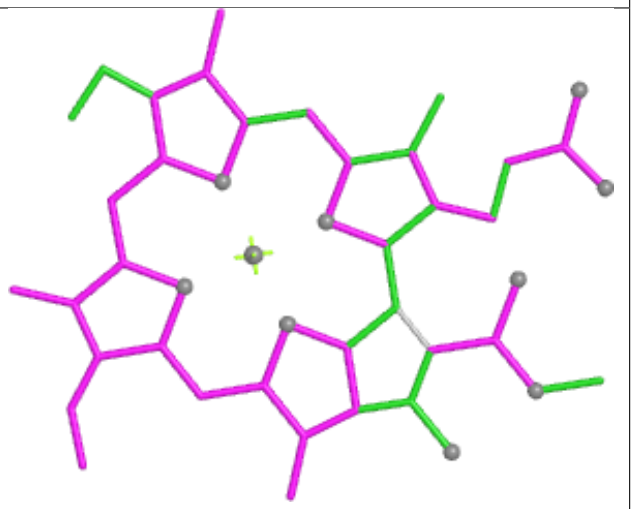
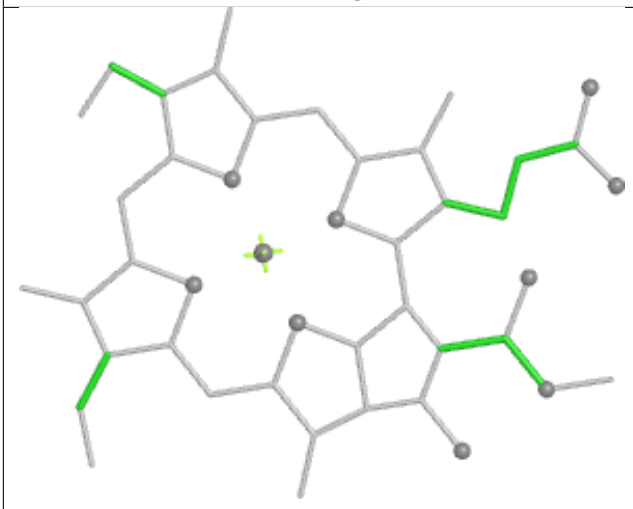


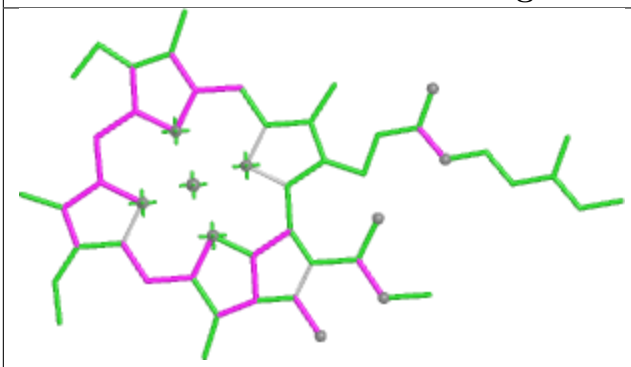
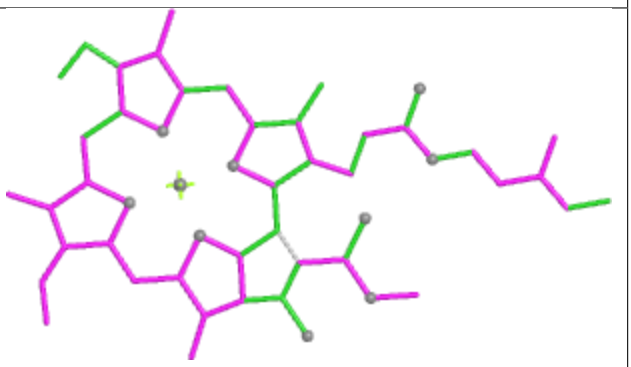
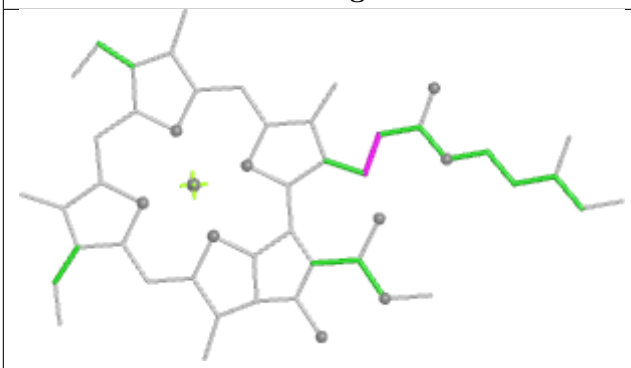
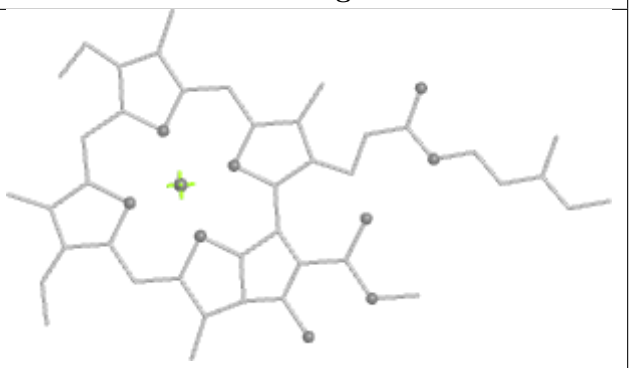
Bond angles



Torsions



Rings

Ligand CLA cB 938	
 Bond lengths	 Bond angles
 Torsions	 Rings

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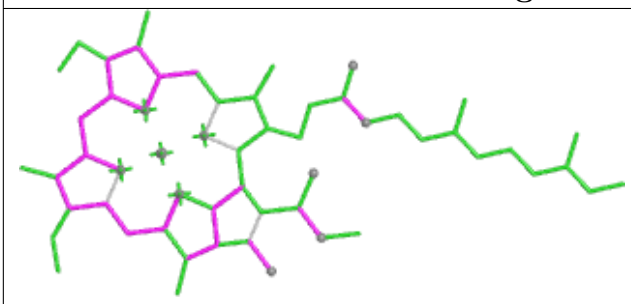
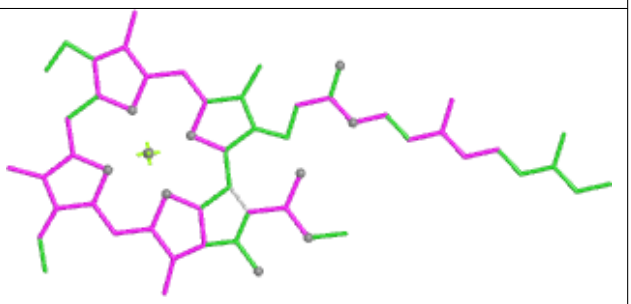
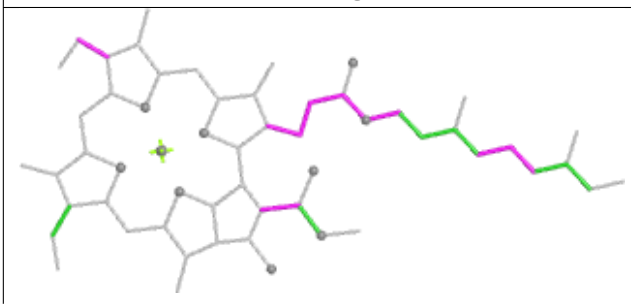
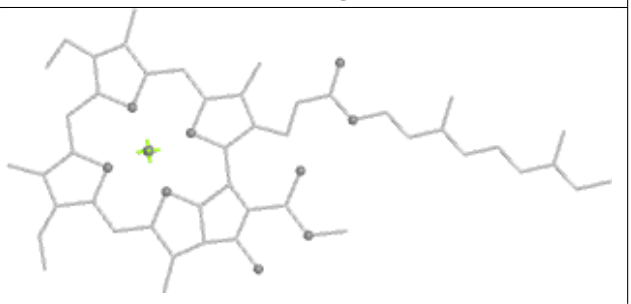
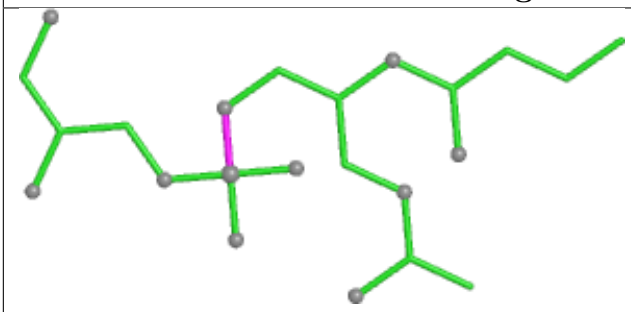
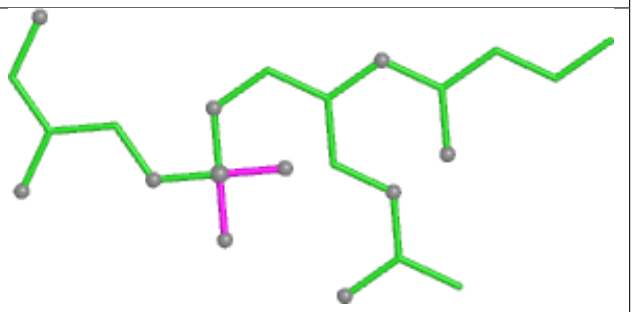
 Bond lengths	 Bond angles
 Torsions	 Rings

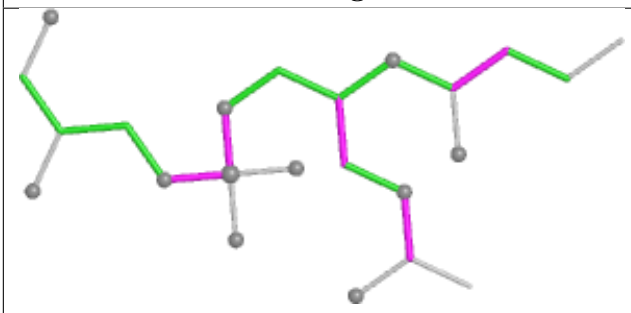
Ligand LHG cB 948



Bond lengths



Bond angles



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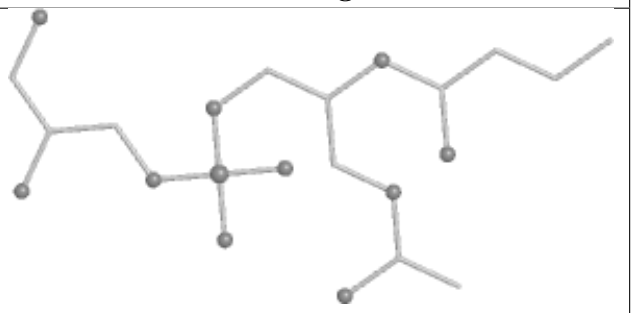
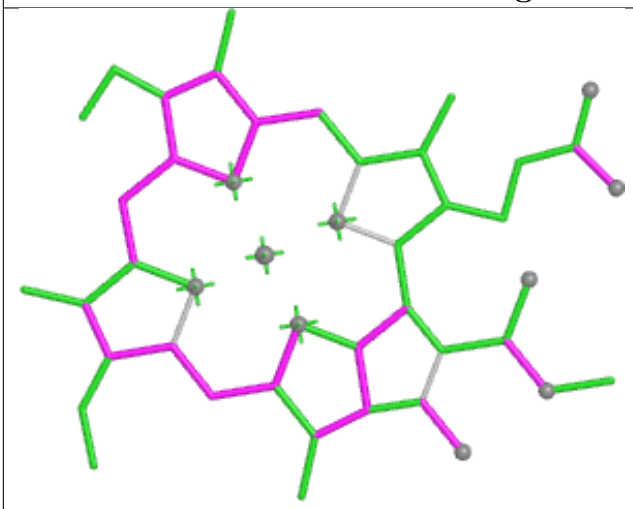


Rings

Ligand CLA aA 815



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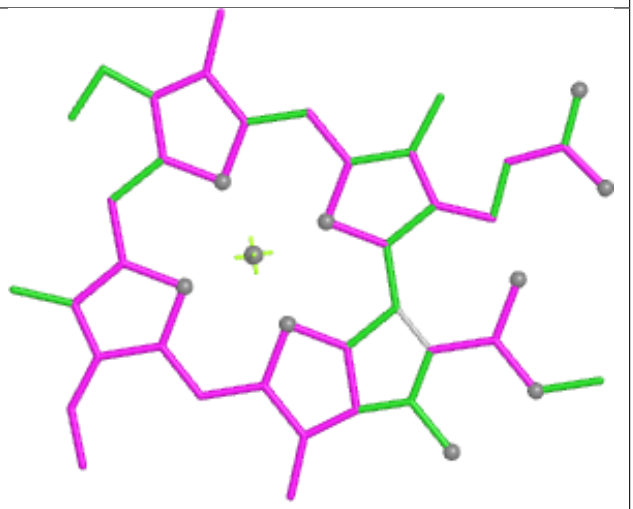

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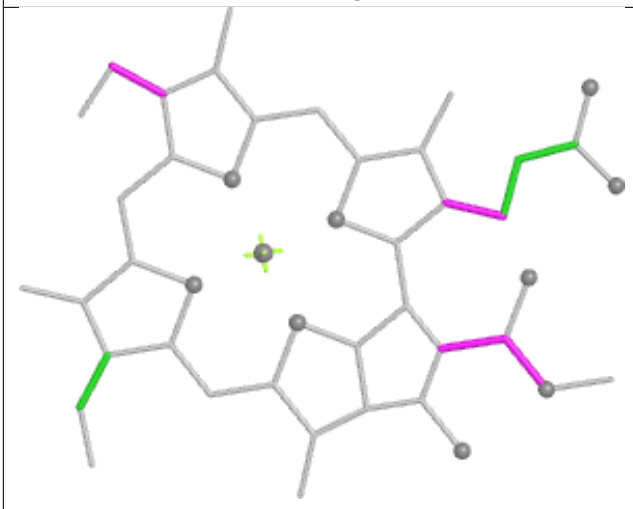
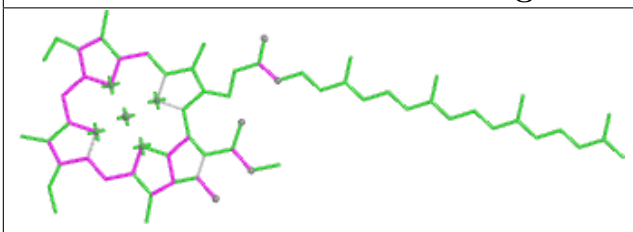


Torsions



Rings

Ligand CLA cA 830



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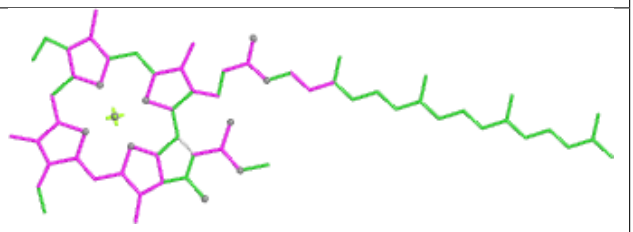

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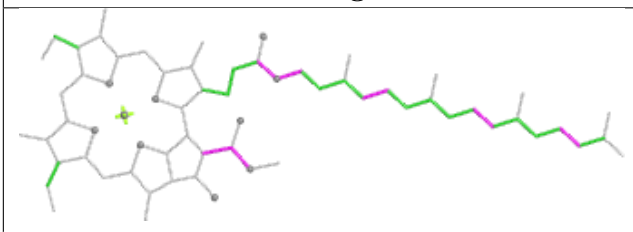

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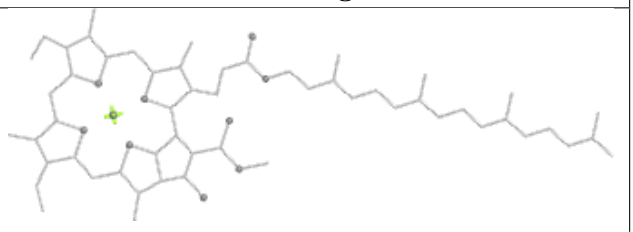
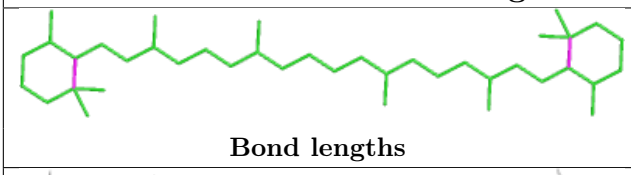


Rings

Ligand BCR bM 101



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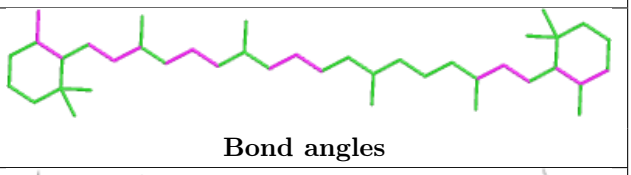

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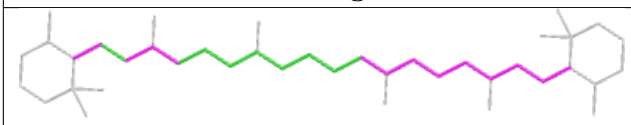

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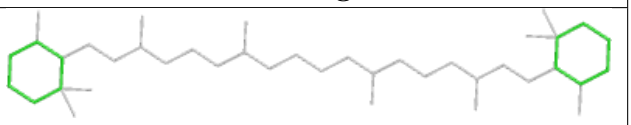
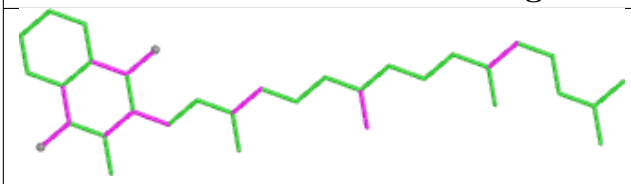


Rings

Ligand 1L3 cB 940



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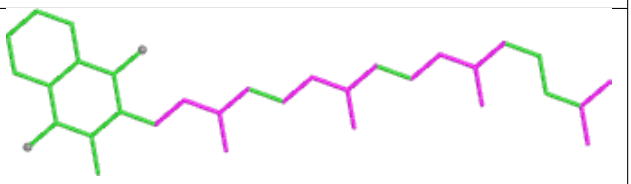
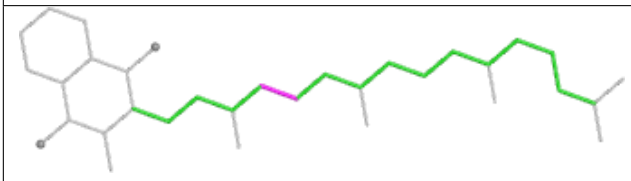


Bond angles



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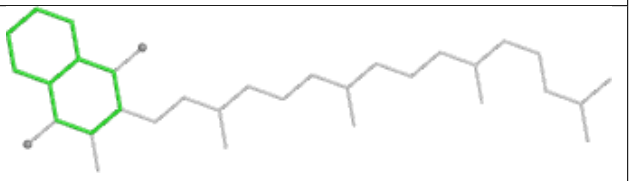
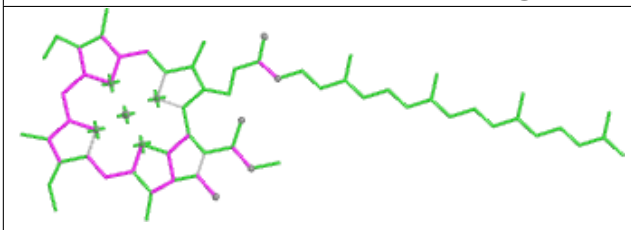


Rings

Ligand CLA cA 838



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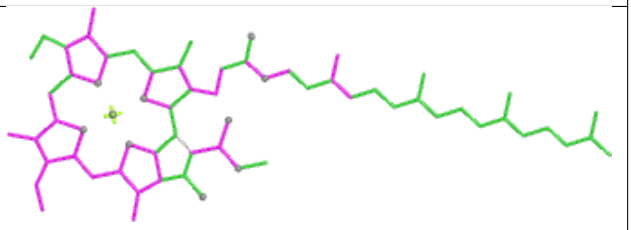
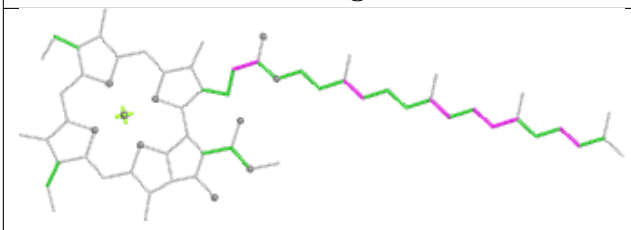


Bond angles



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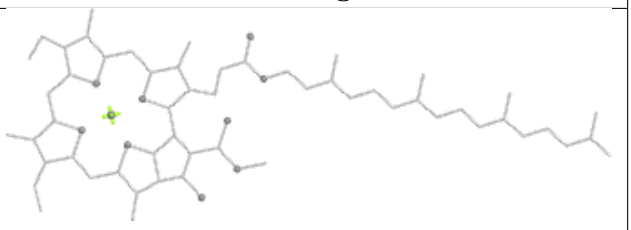
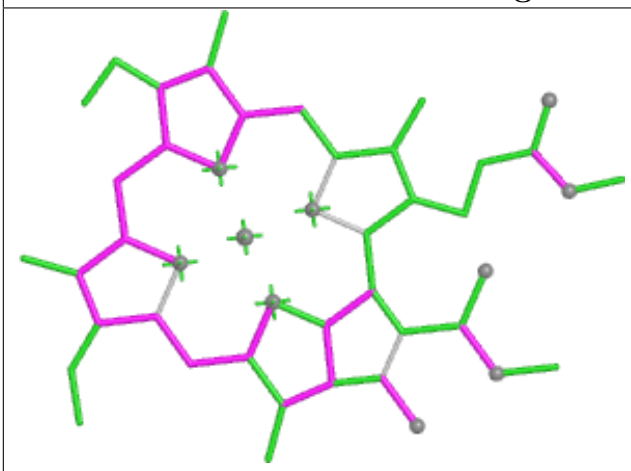


Rings

Ligand CLA bB 924



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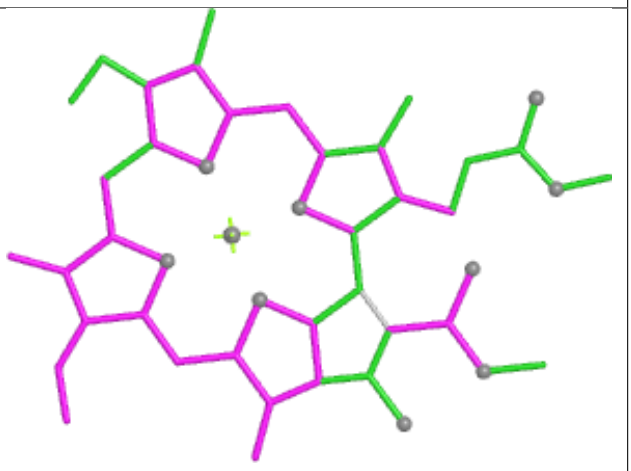
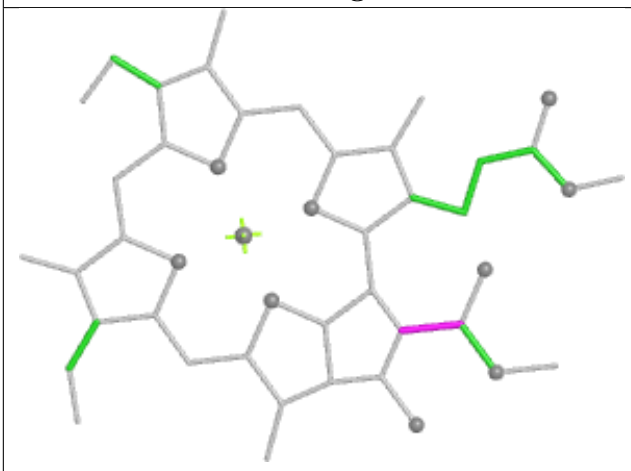


Bond angles



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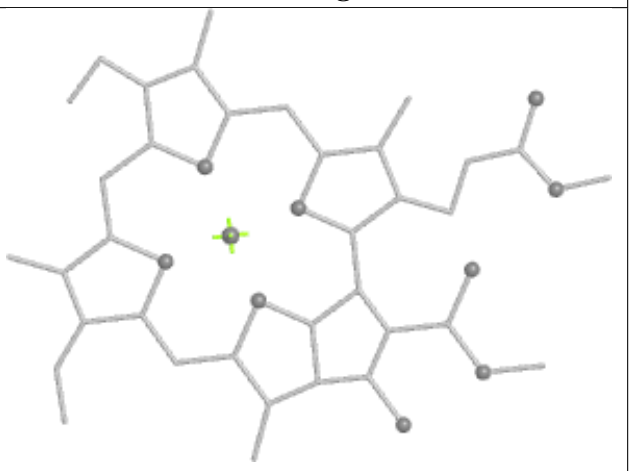
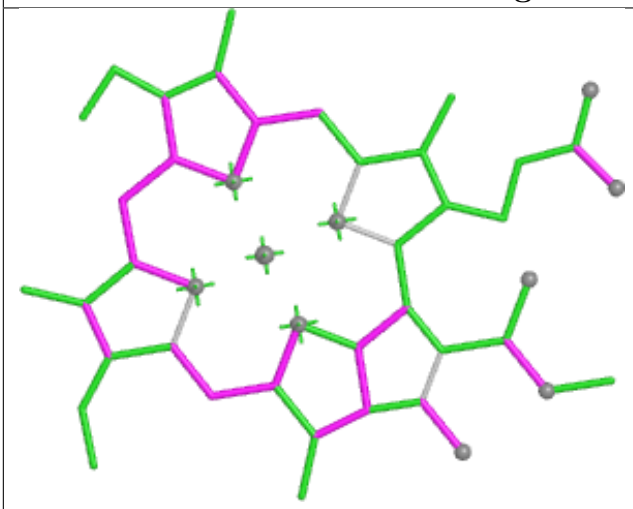


Rings

Ligand CLA bB 939



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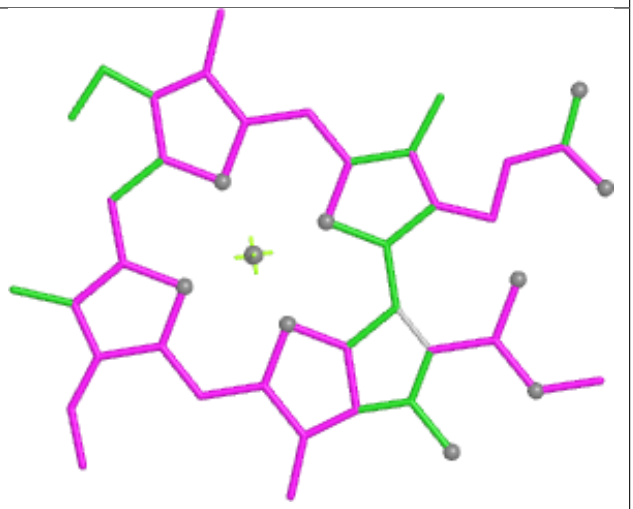
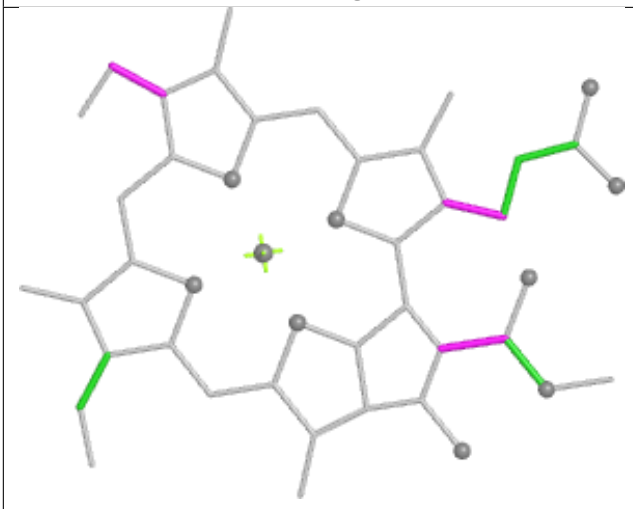


Bond angles

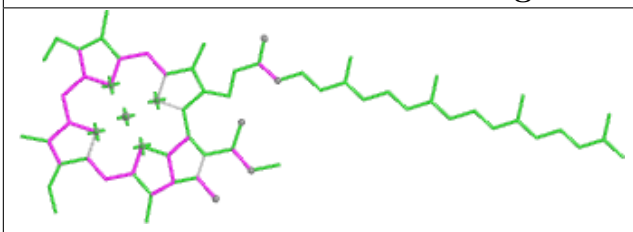


Torsions



Rings

Ligand CLA bB 931



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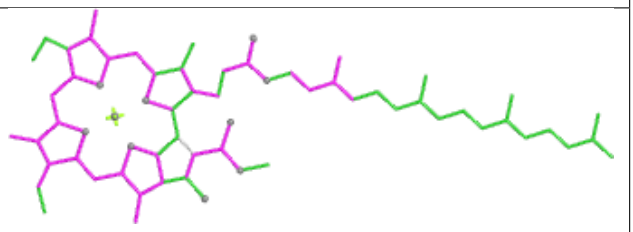
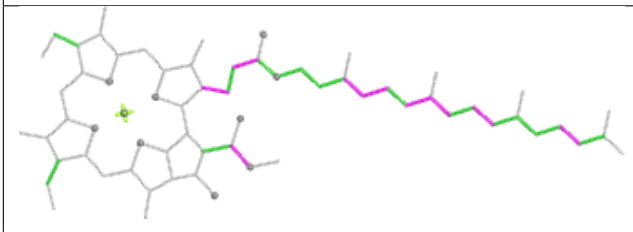


Bond angles



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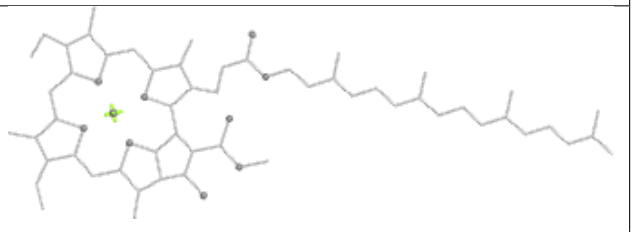
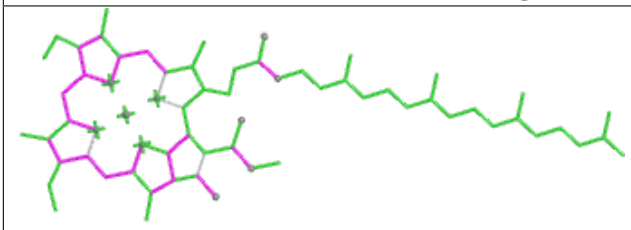


Rings

Ligand CLA cA 803



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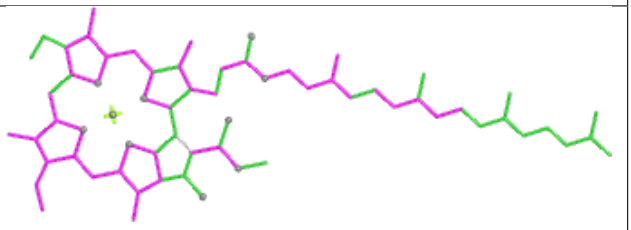
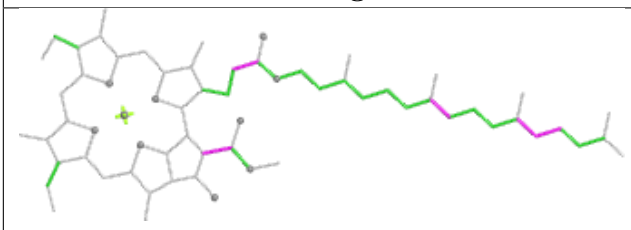


Bond angles



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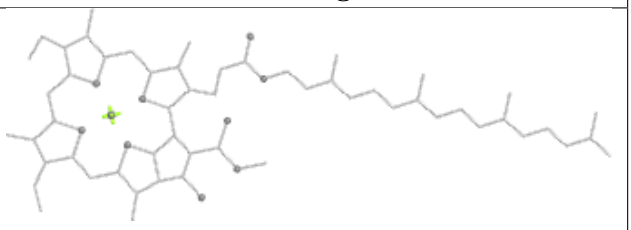
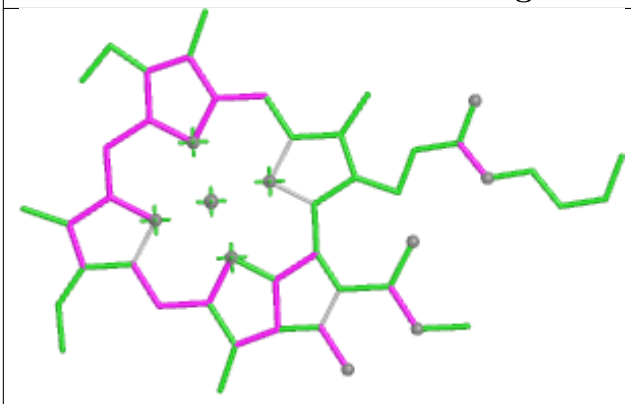


Rings

Ligand CLA aA 822



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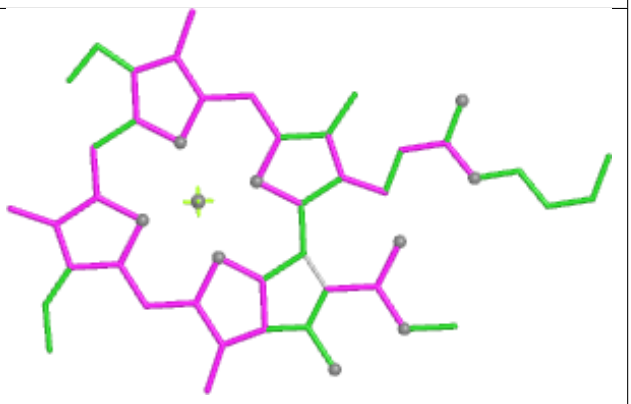
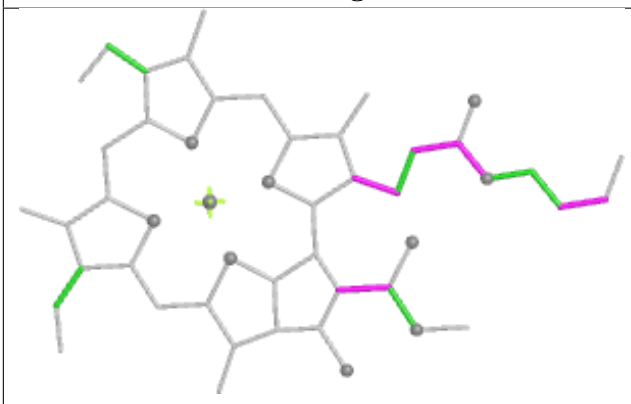


Bond angles



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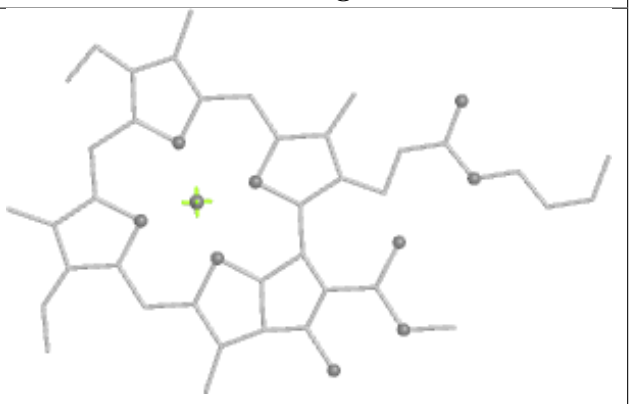
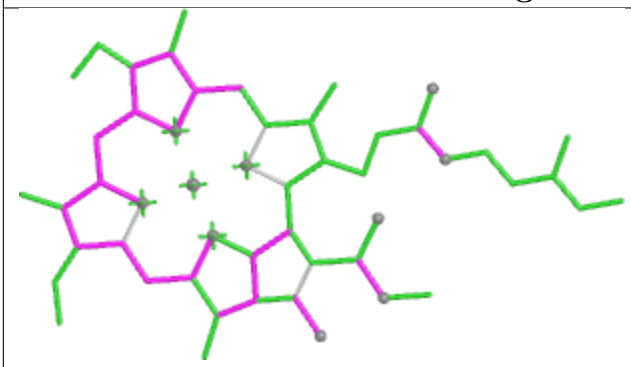


Rings

Ligand CLA cA 841



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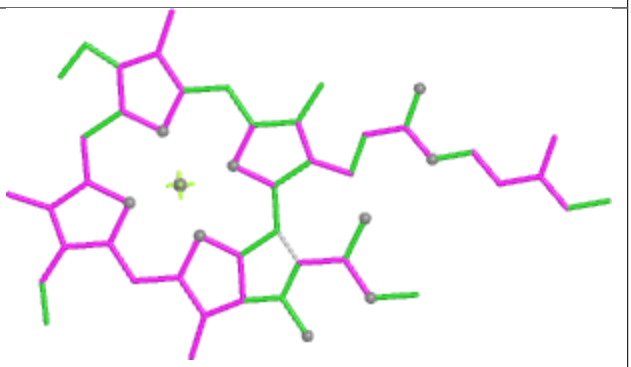

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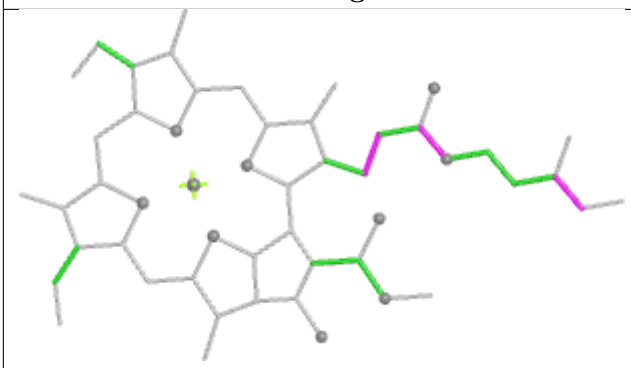

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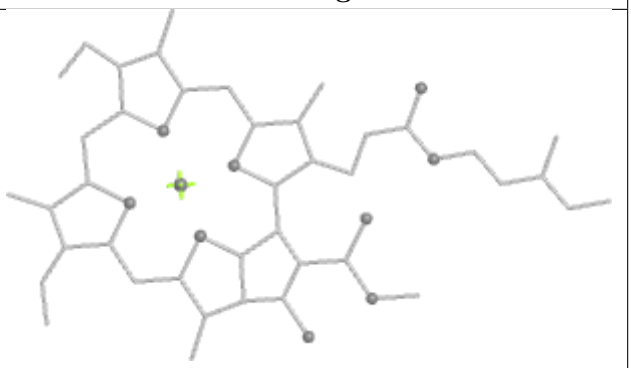
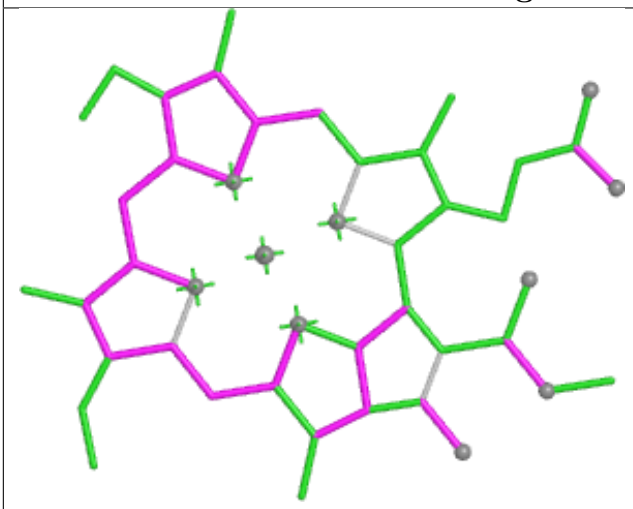


Rings

Ligand CLA cA 813



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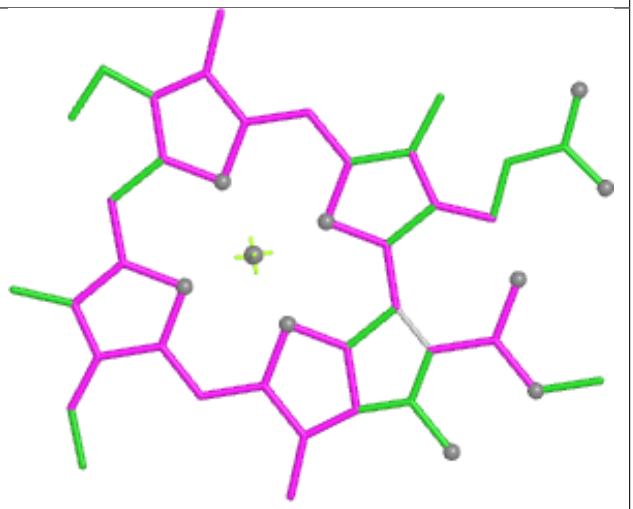
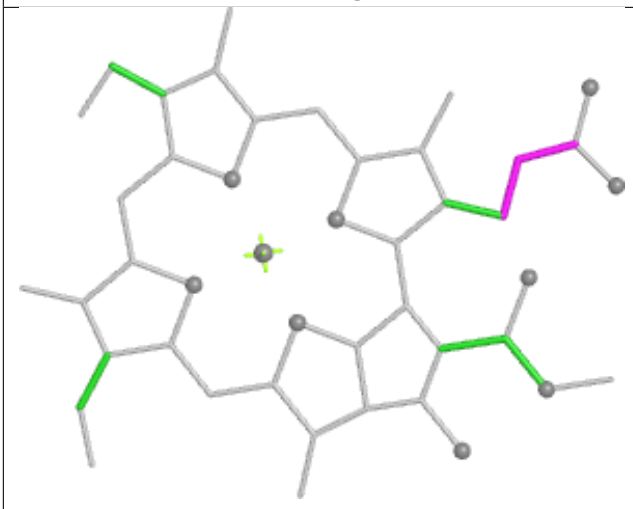


Bond angles

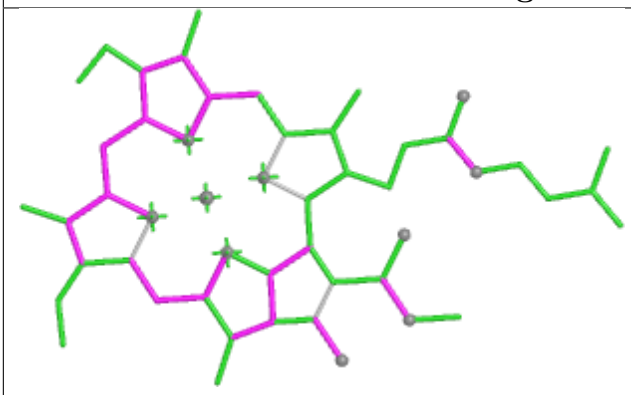


Torsions



Rings

Ligand CLA cB 935



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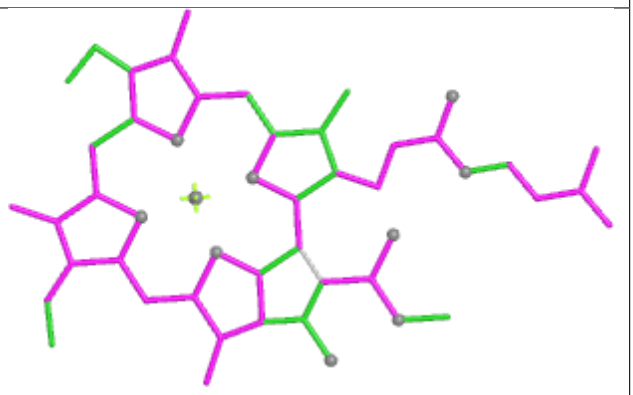
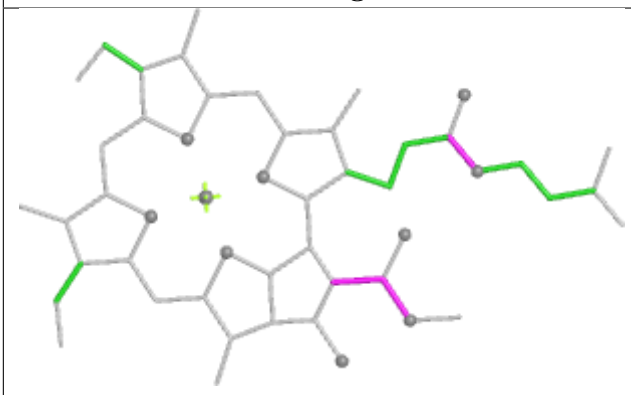
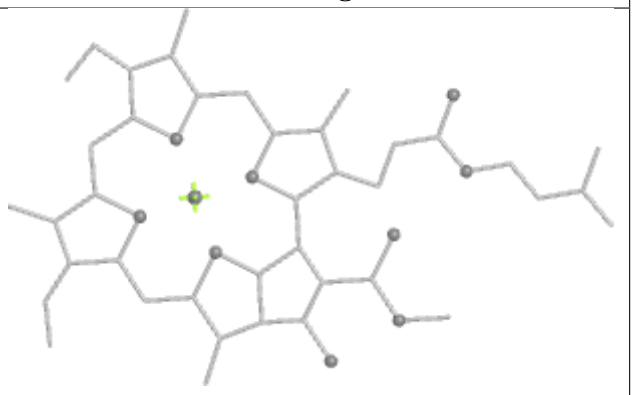


Bond angles

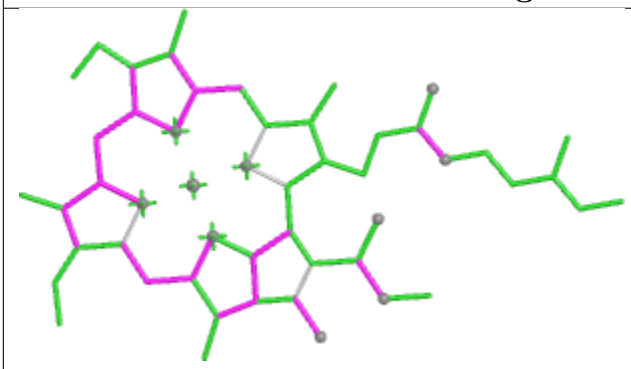


Torsions



Rings

Ligand CLA aB 938



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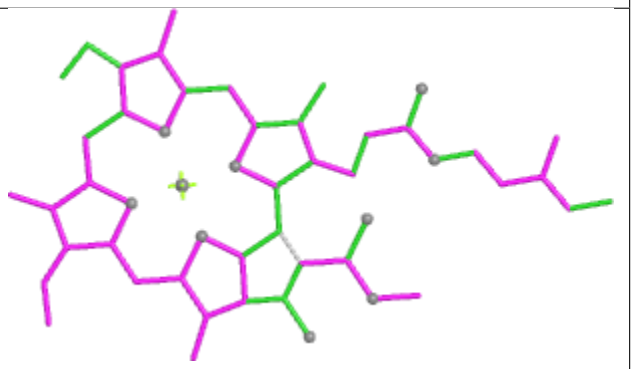
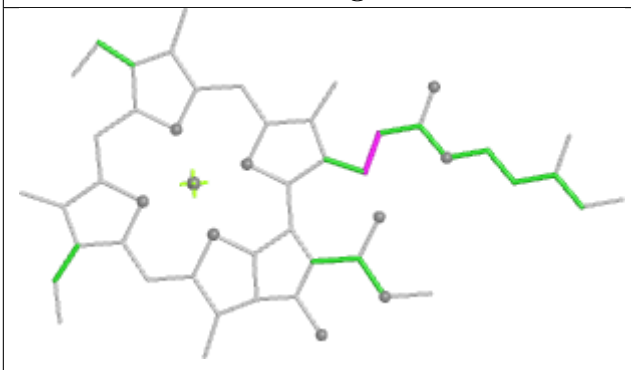


Bond angles



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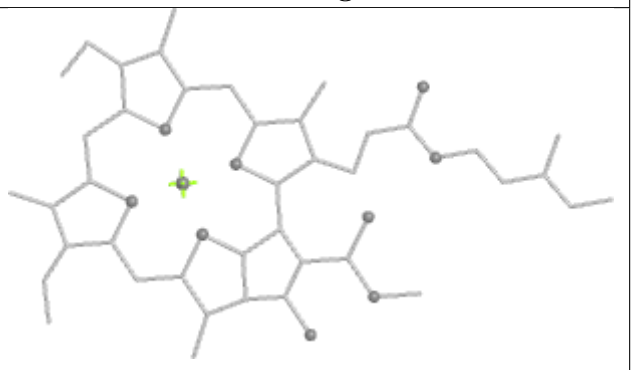
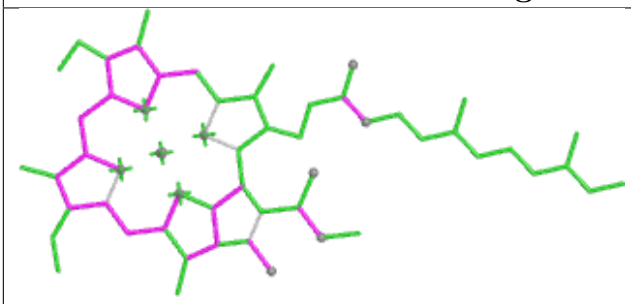
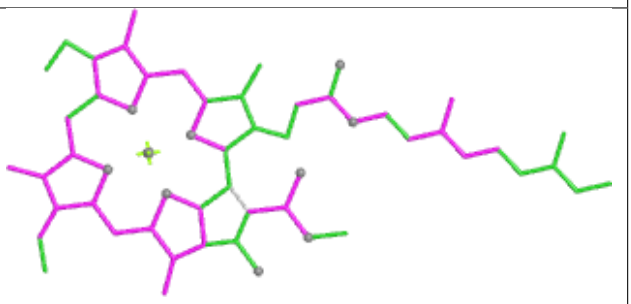


Rings

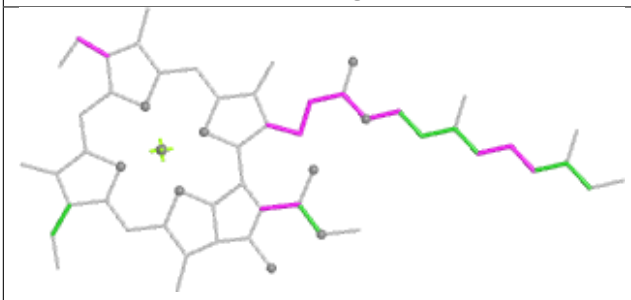
Ligand CLA aA 820



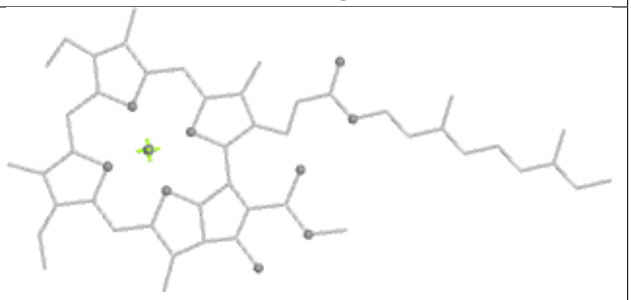
Bond lengths



Bond angles

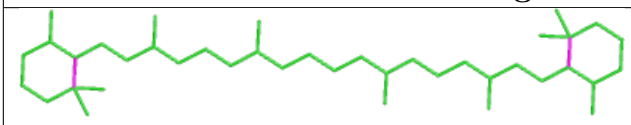


Torsions



Rings

Ligand BCR aB 942



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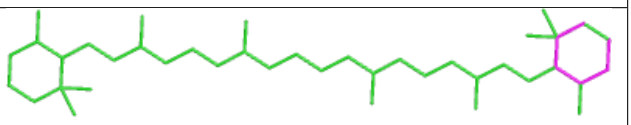

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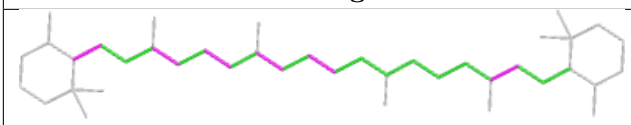

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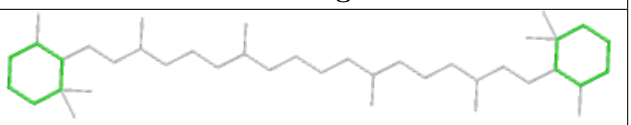
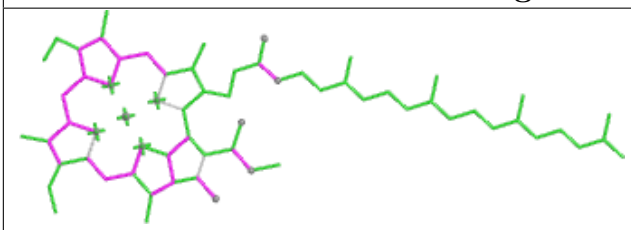


Rings

Ligand CLA bB 904



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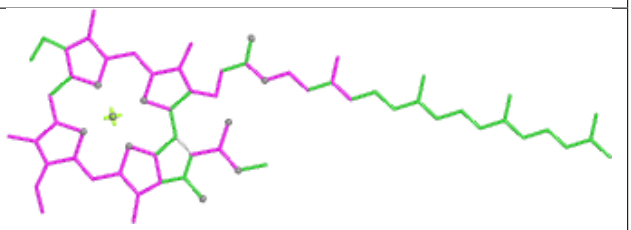

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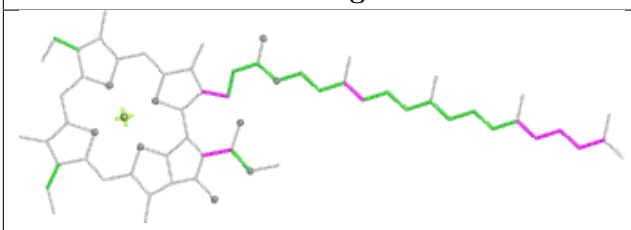

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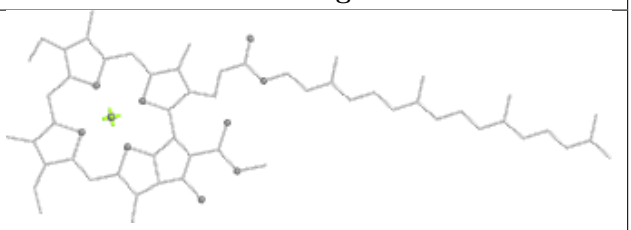
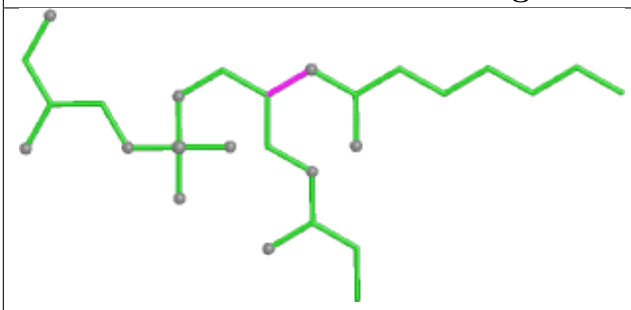
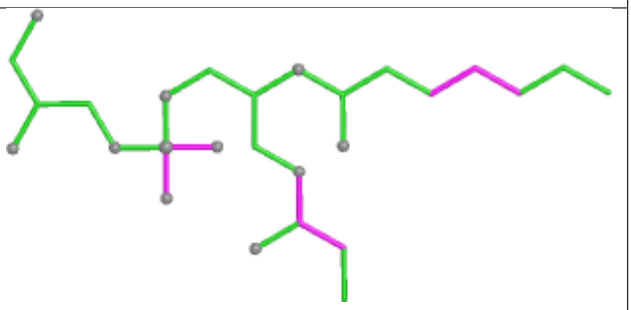
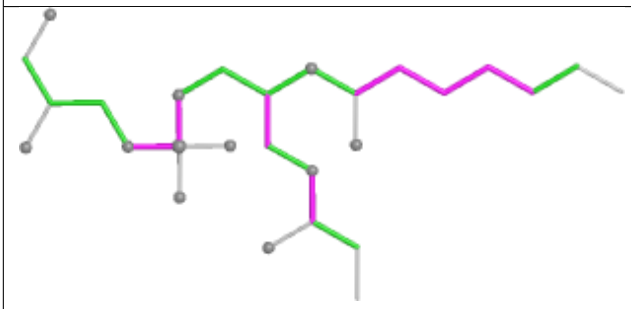
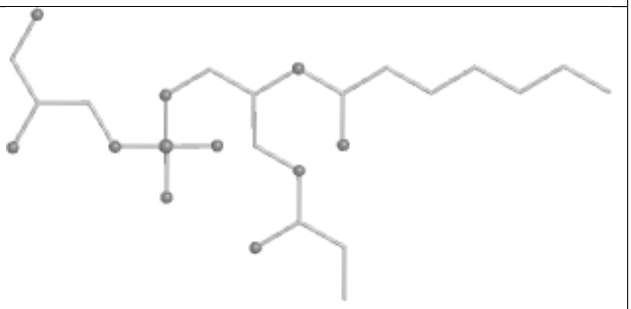


Rings

Ligand LHG bA 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

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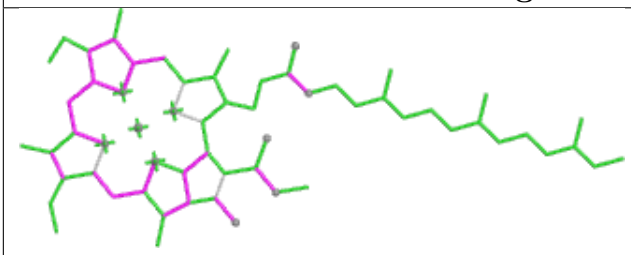
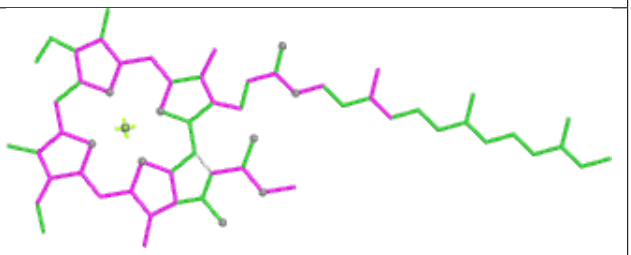
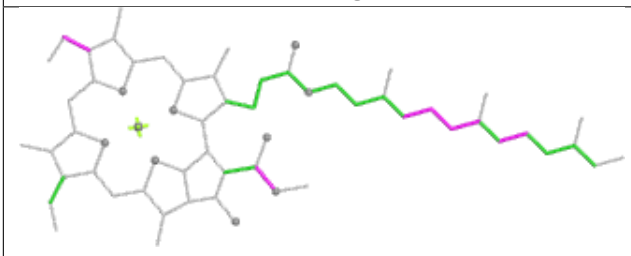
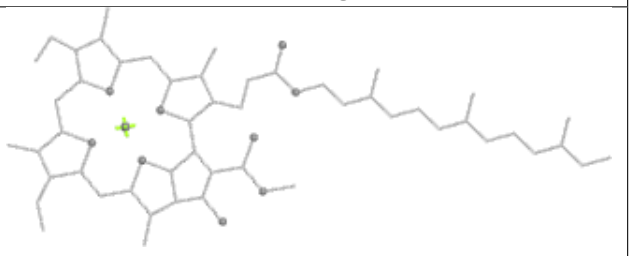
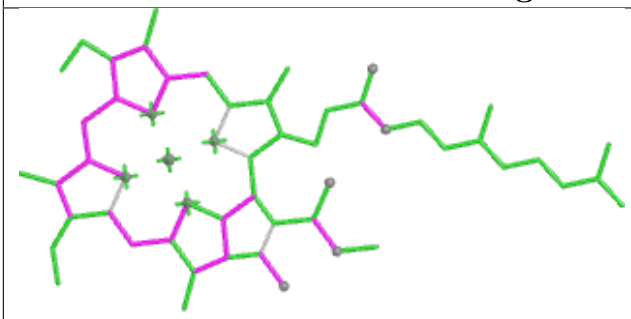
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cA 832



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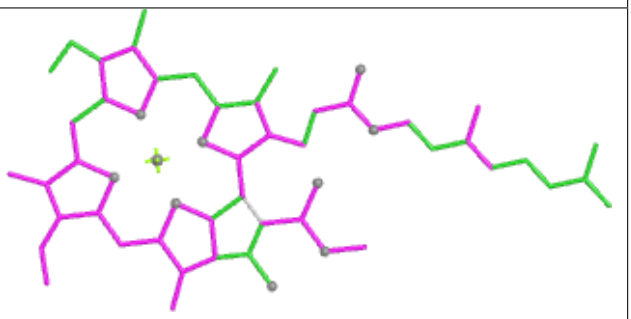

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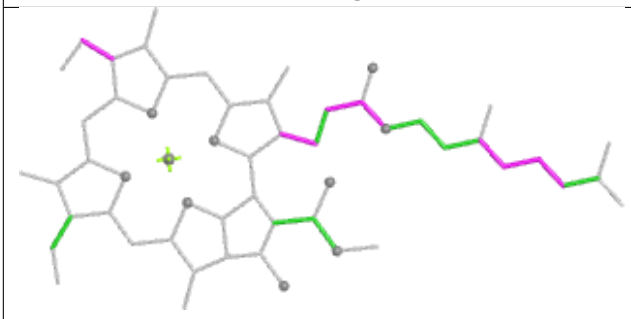

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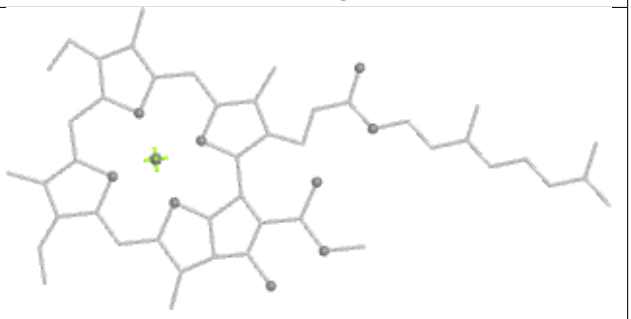
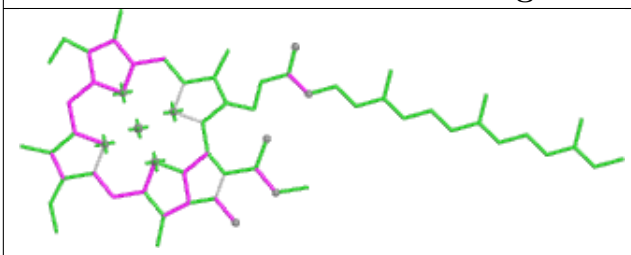


Rings

Ligand CLA cB 902



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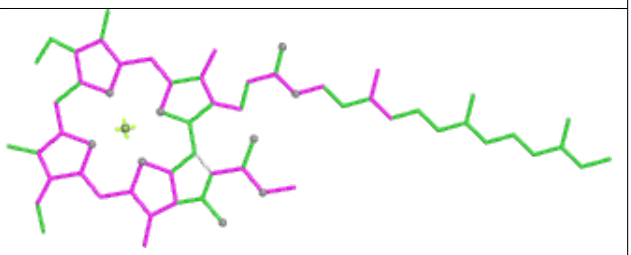

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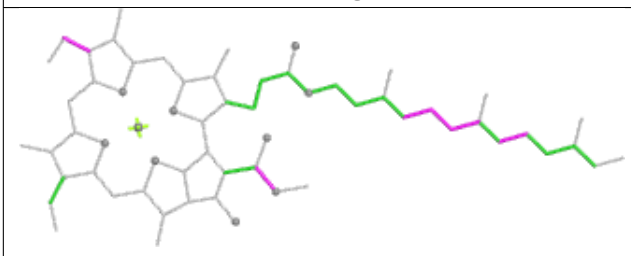

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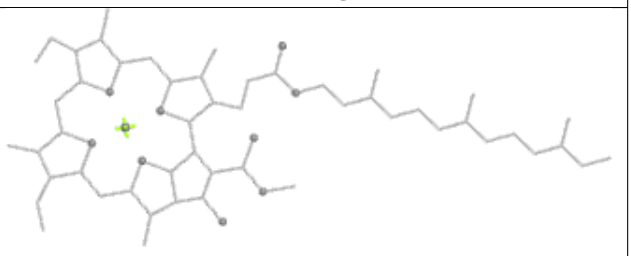
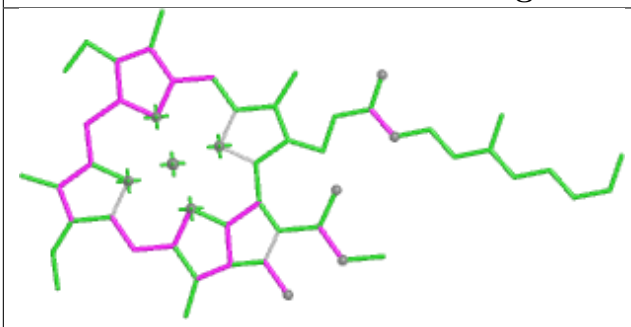


Rings

Ligand CLA cA 817



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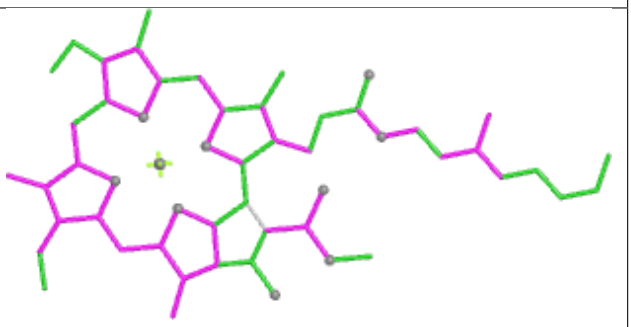

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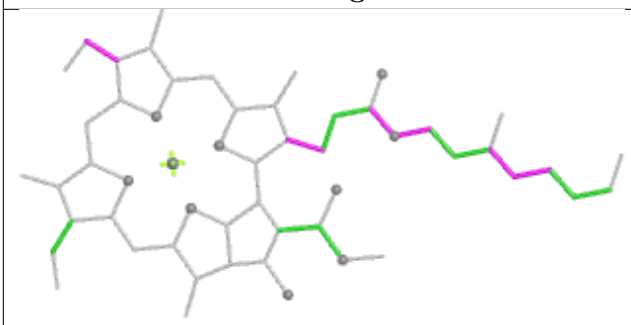

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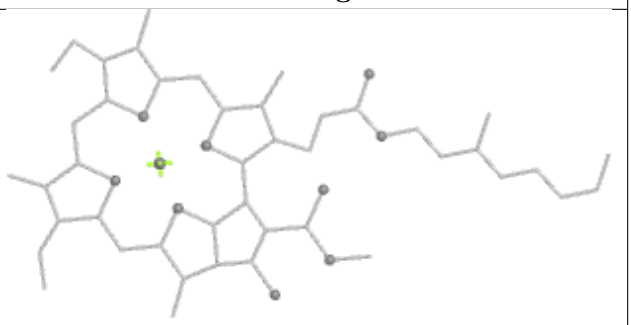
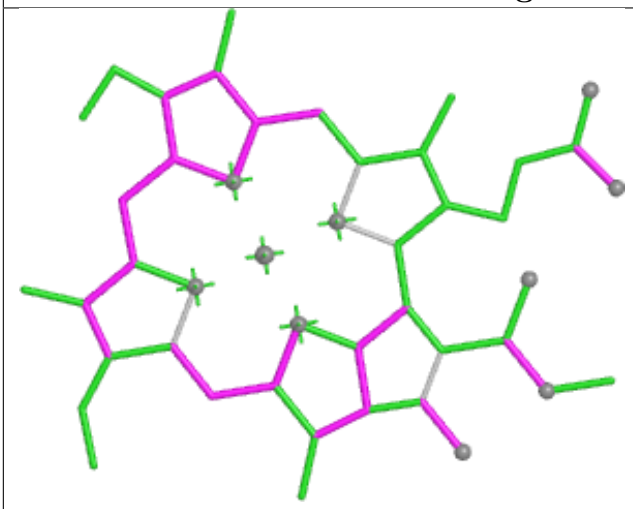


Rings

Ligand CLA aB 920



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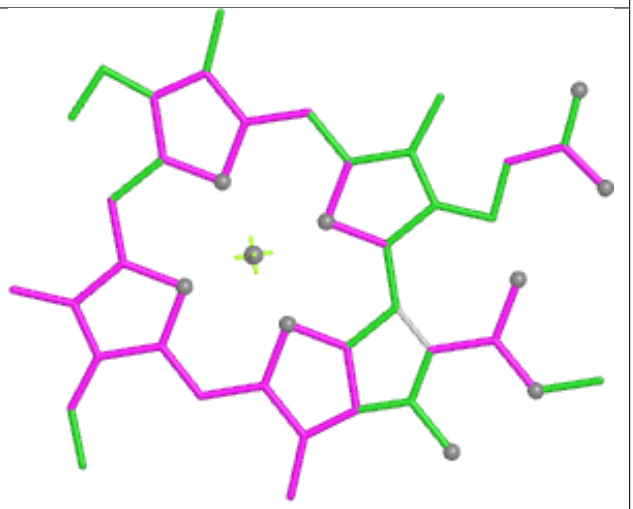
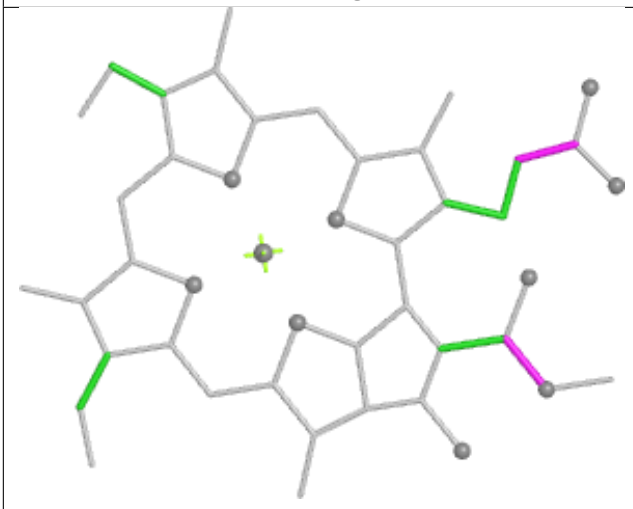


Bond angles

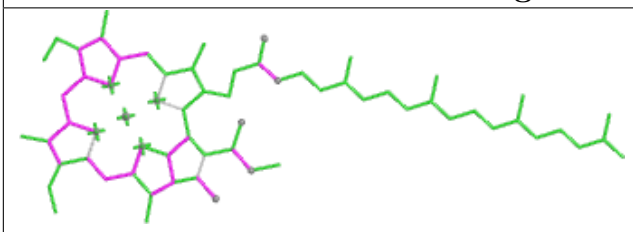


Torsions



Rings

Ligand CLA bB 926



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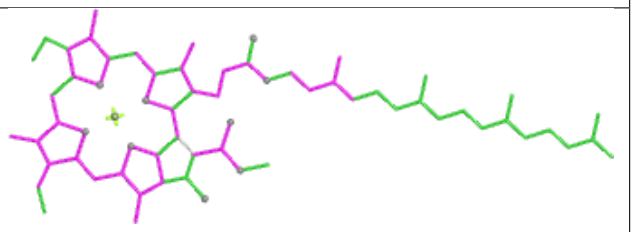
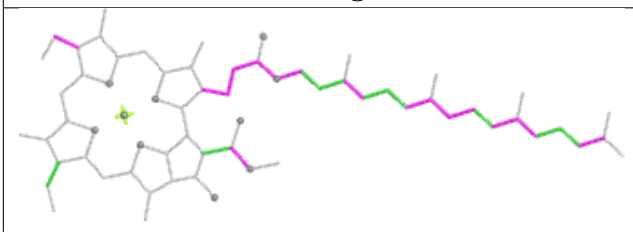


Bond angles



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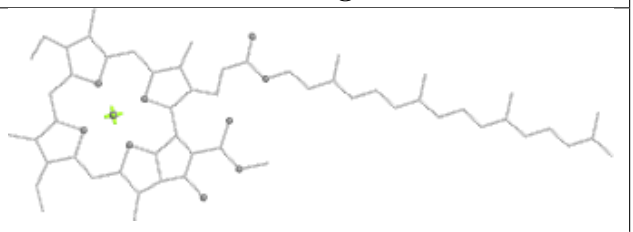
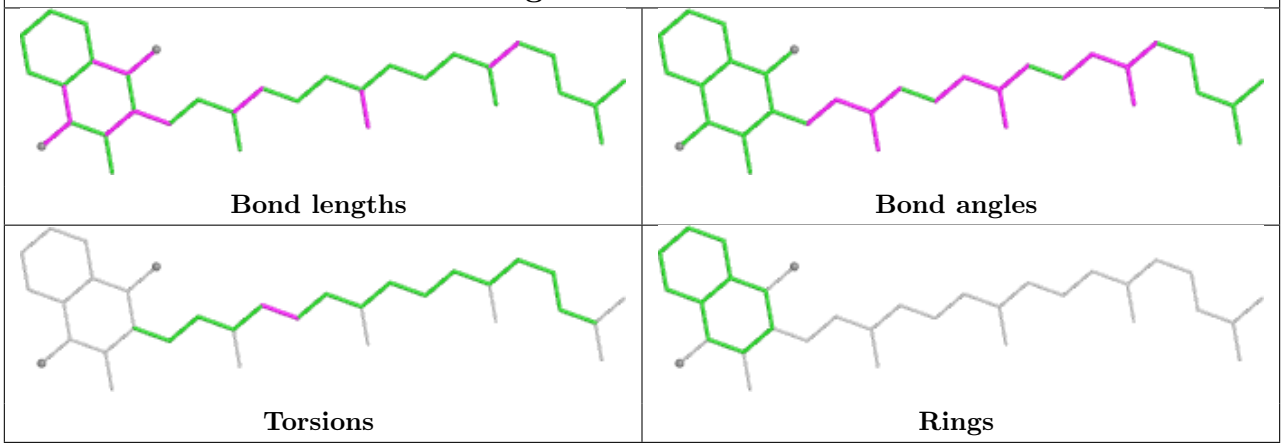
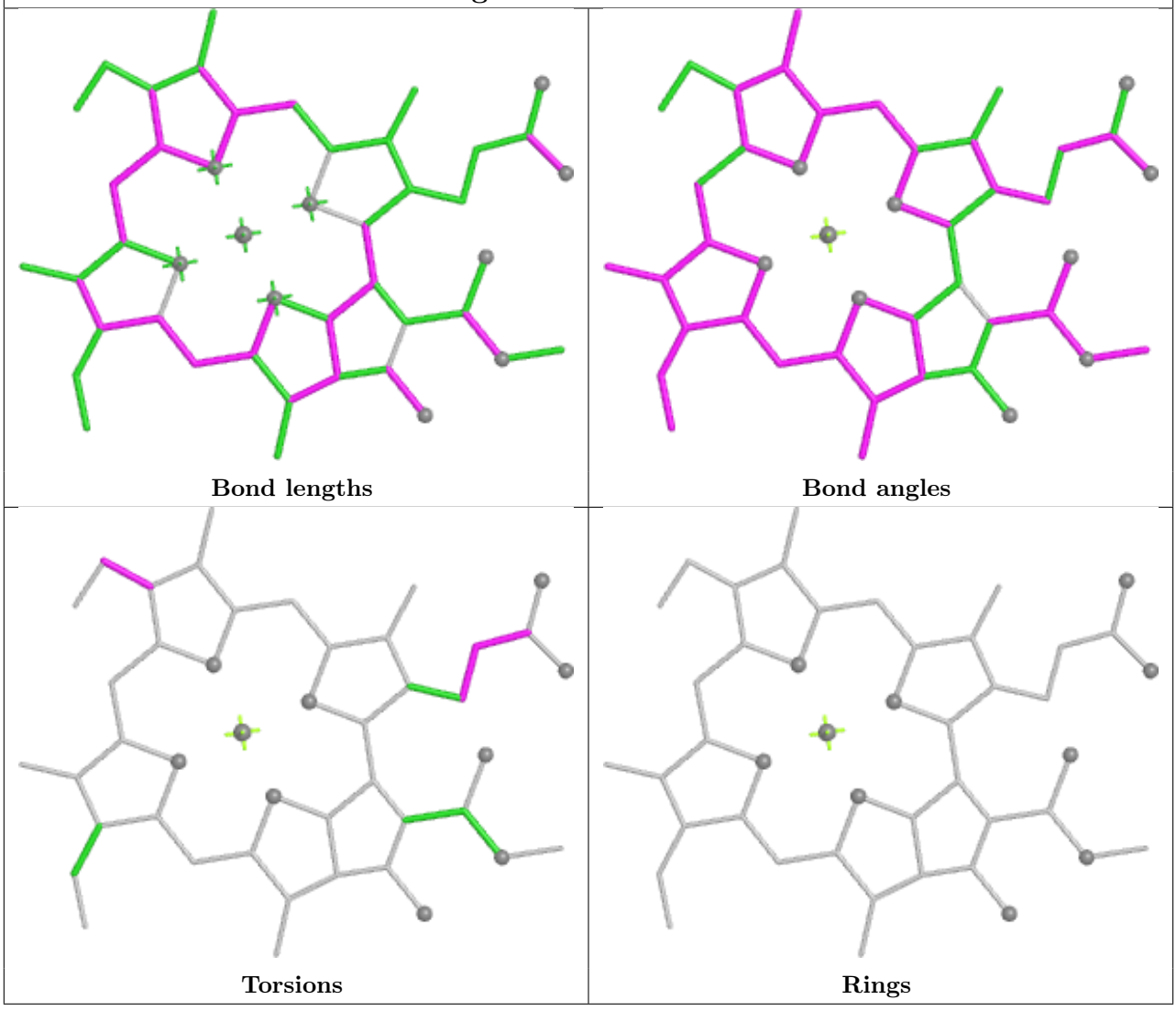


Rings

Ligand 1L3 aB 940



Ligand CLA bA 836



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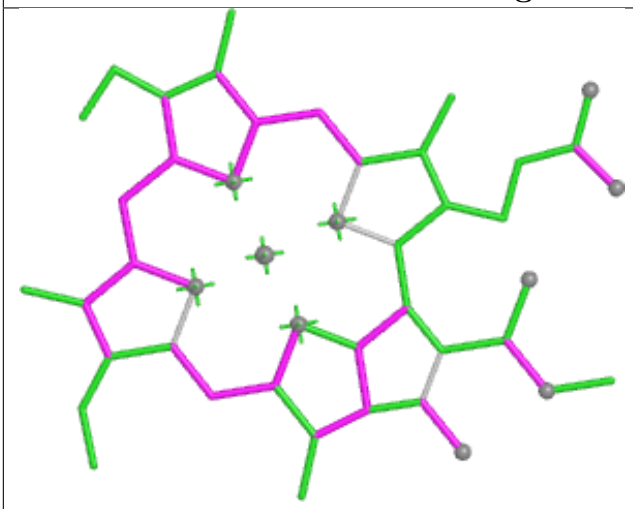

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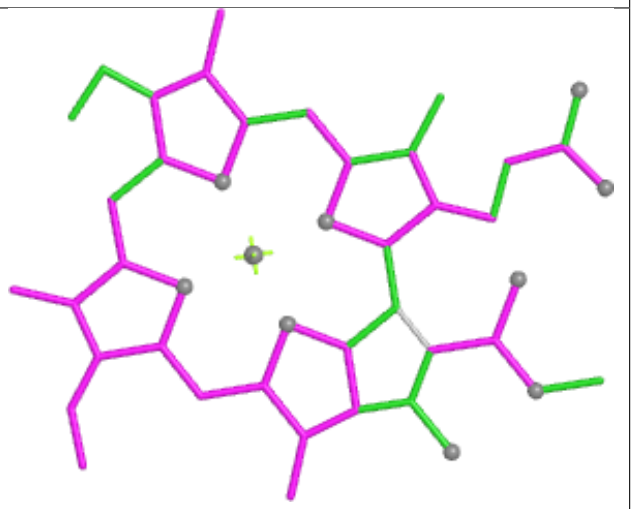
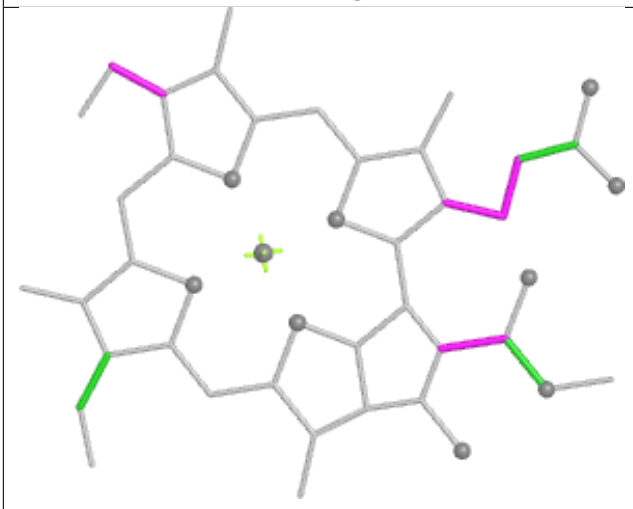


Bond angles

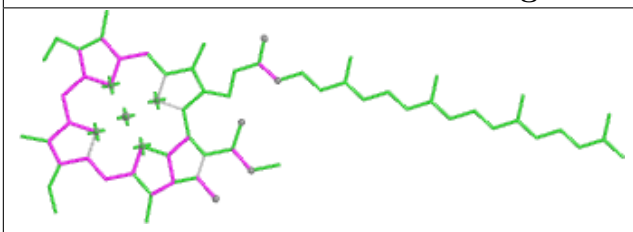


Torsions



Rings

Ligand CL0 cA 801



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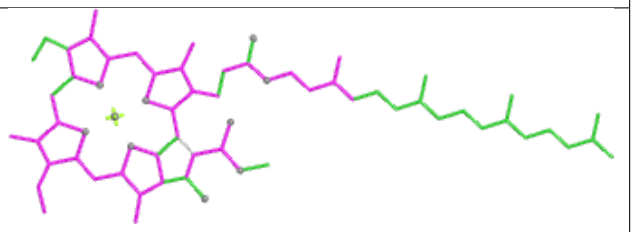

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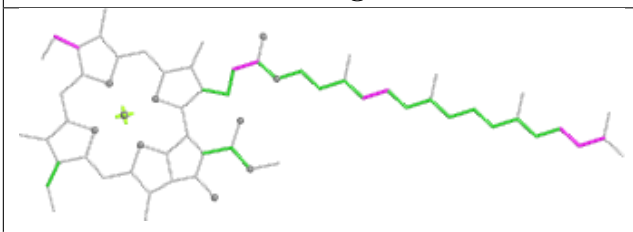

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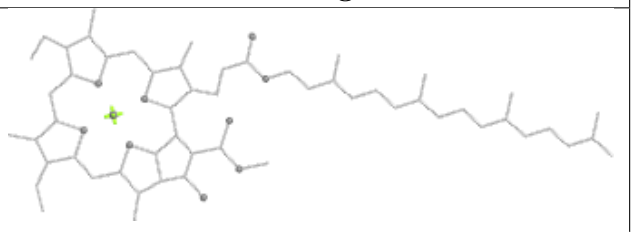
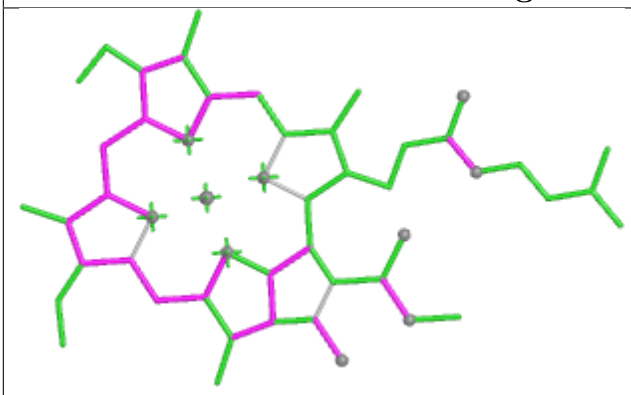


Rings

Ligand CLA aB 928



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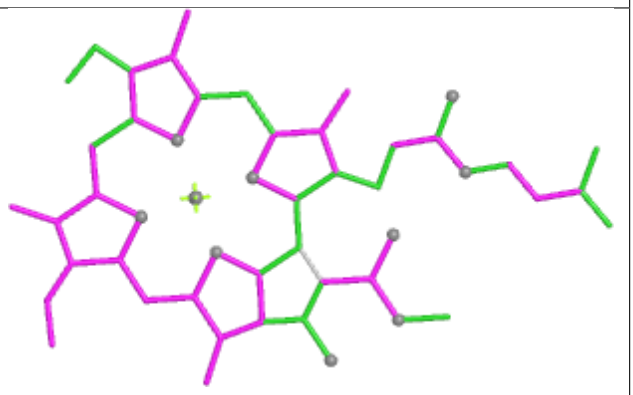
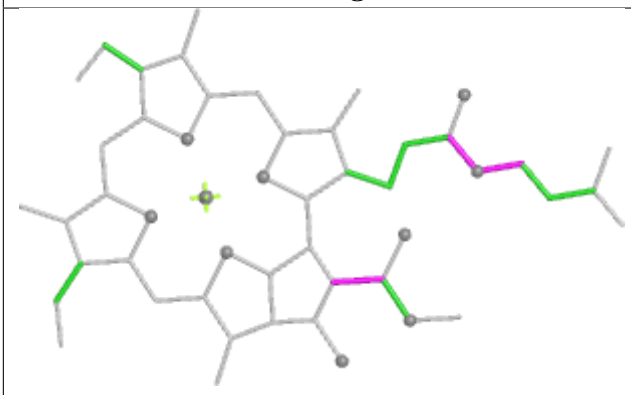


Bond angles



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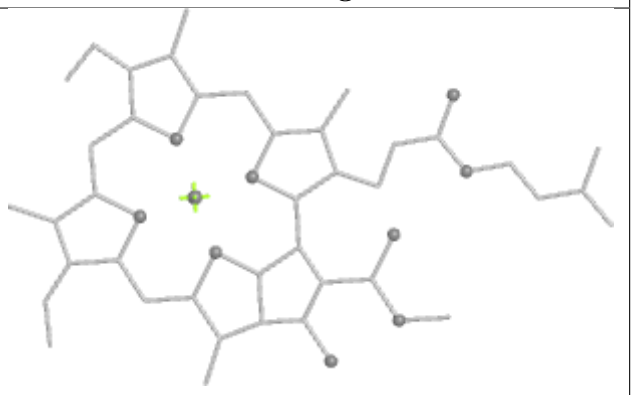
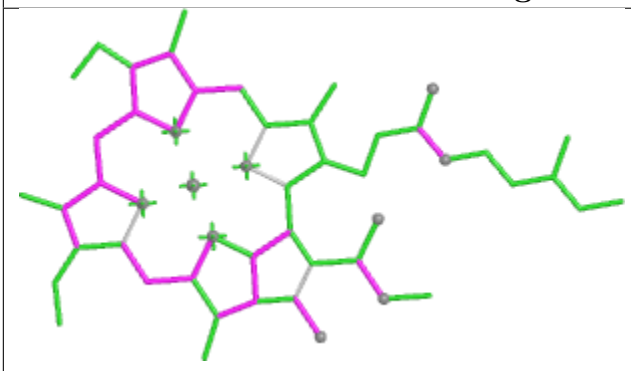
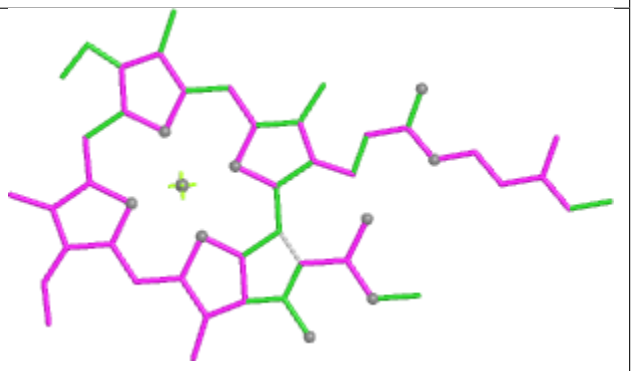


Rings

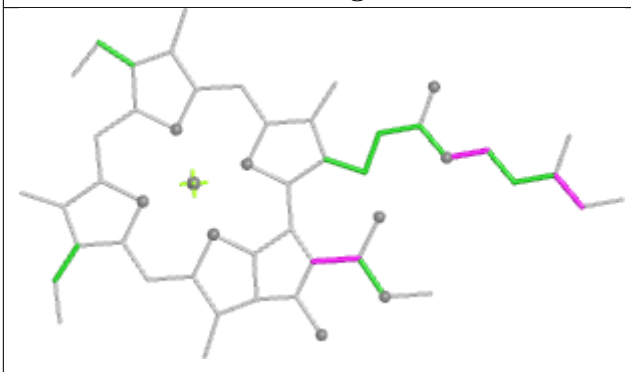
Ligand CLA bB 903



Bond lengths



Bond angles



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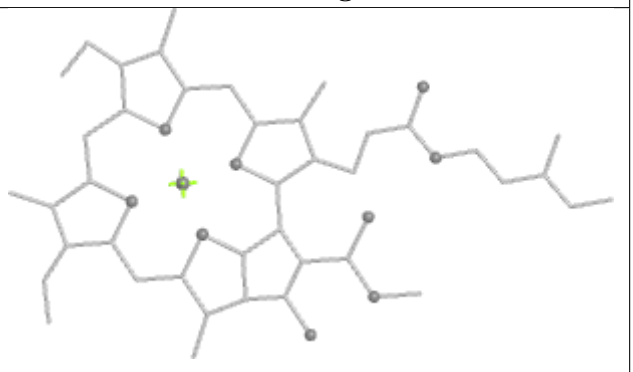
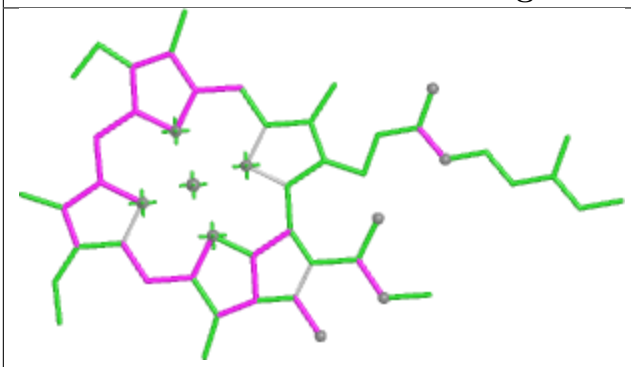


Rings

Ligand CLA cB 903



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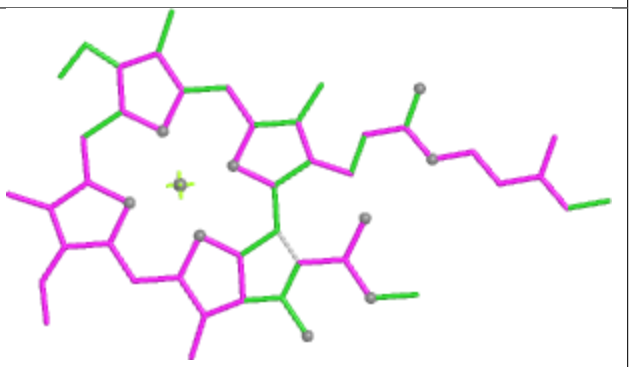
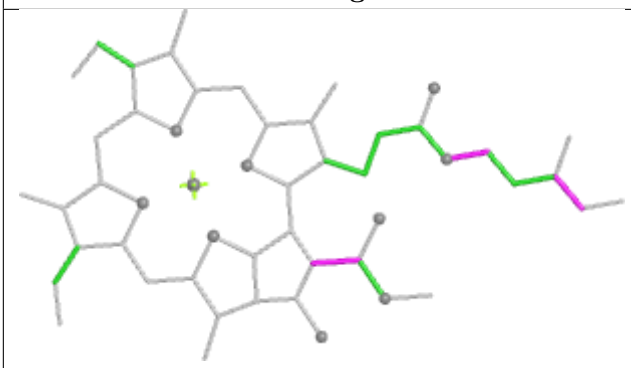
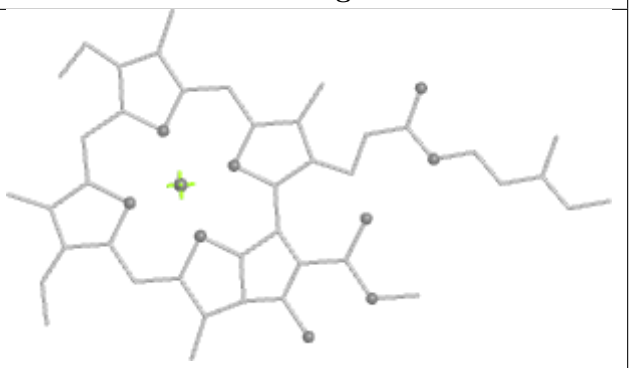


Bond angles

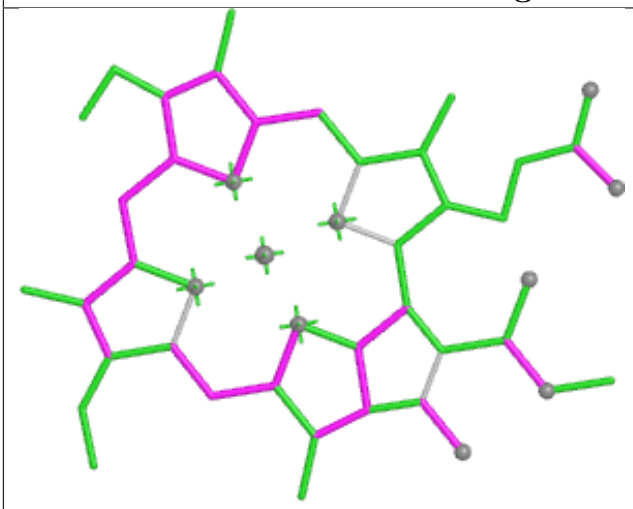


Torsions

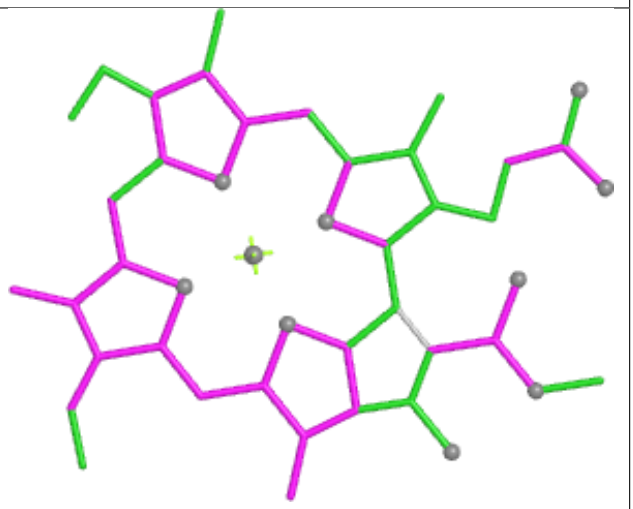


Rings

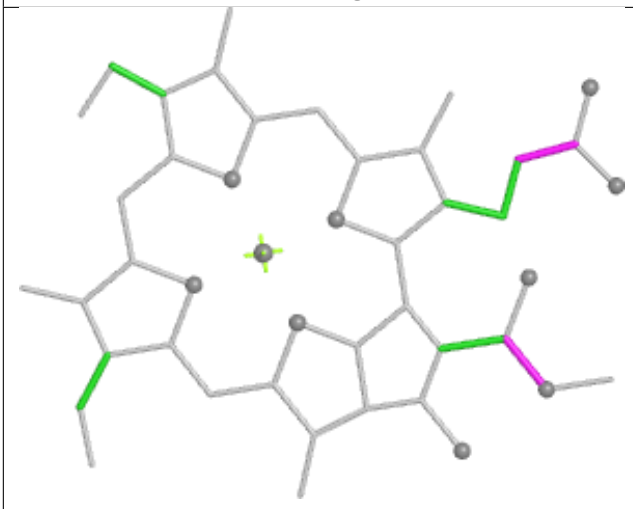
Ligand CLA bB 920



Bond lengths



Bond angles

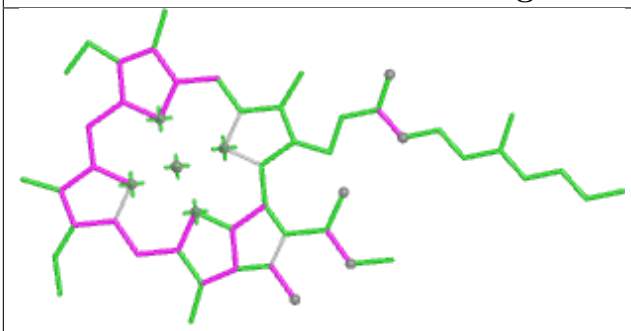


Torsions

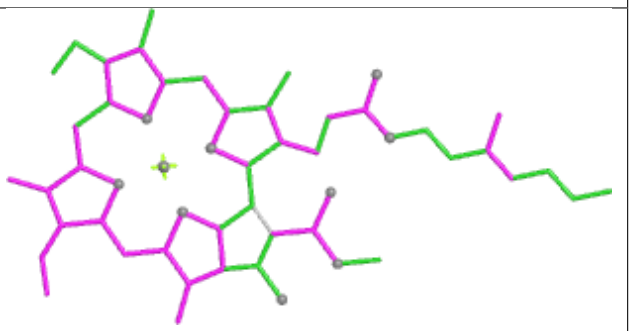


Rings

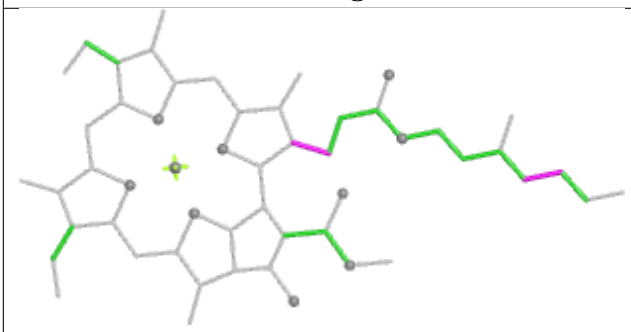
Ligand CLA bL 202



Bond lengths



Bond angles



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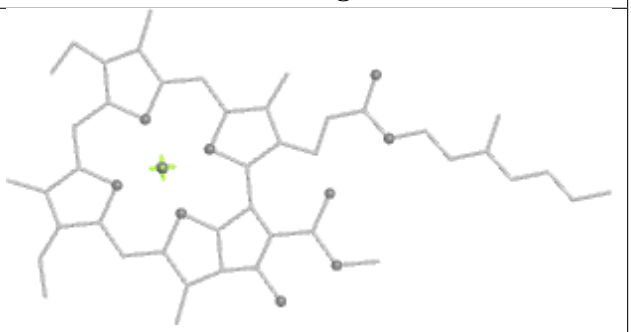
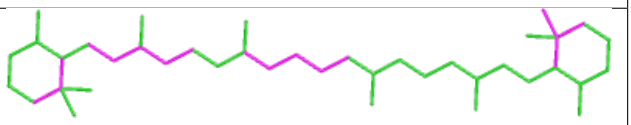


Rings

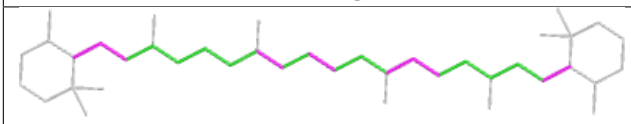
Ligand BCR aB 945



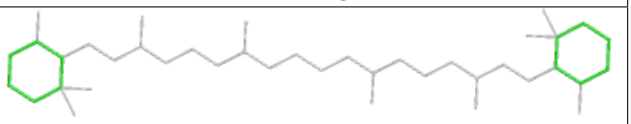
Bond lengths



Bond angles

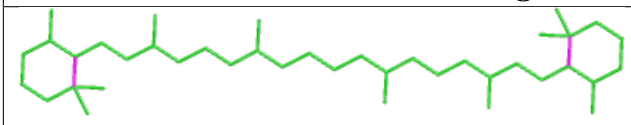


Torsions

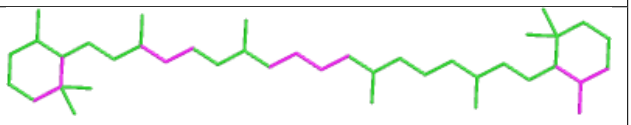


Rings

Ligand BCR bL 205



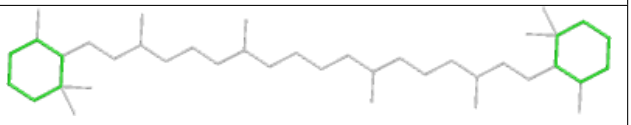
Bond lengths



Bond angles

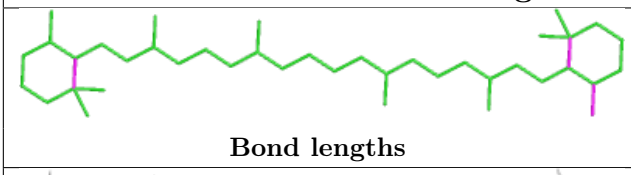


Torsions



Rings

Ligand BCR cB 946



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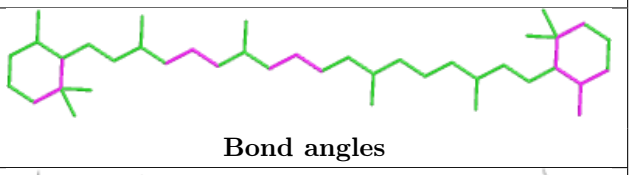
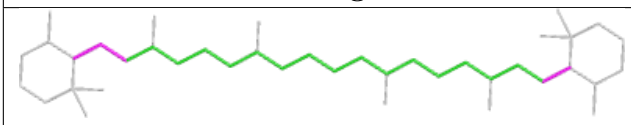
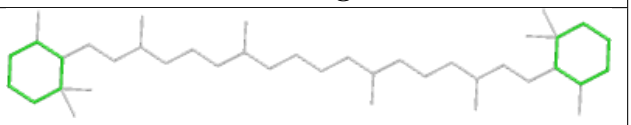


Bond angles

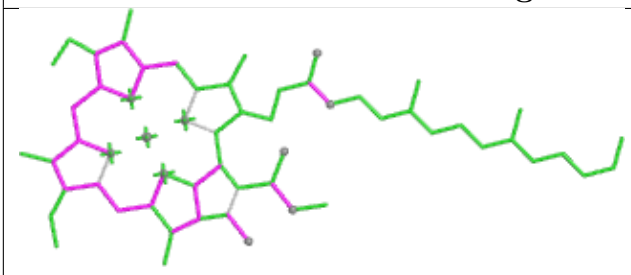


Torsions

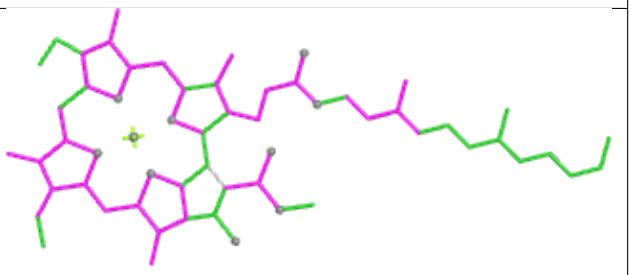


Rings

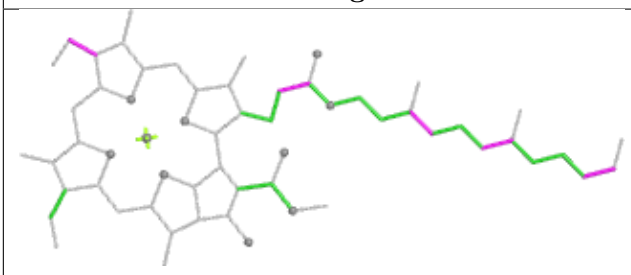
Ligand CLA aB 936



Bond lengths



Bond angles



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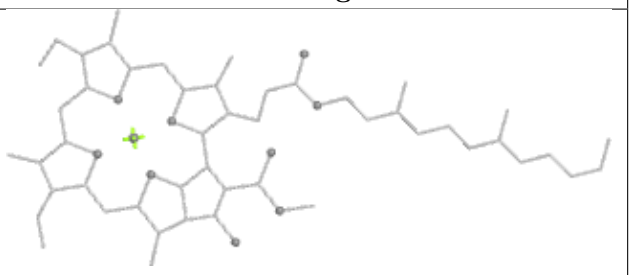
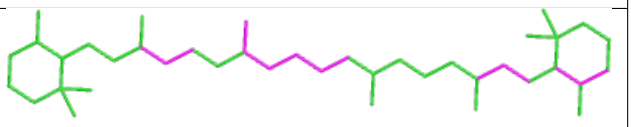


Rings

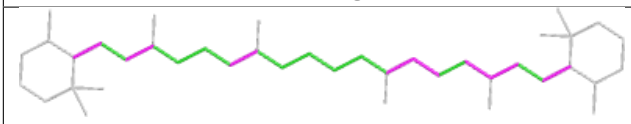
Ligand BCR cA 849



Bond lengths



Bond angles



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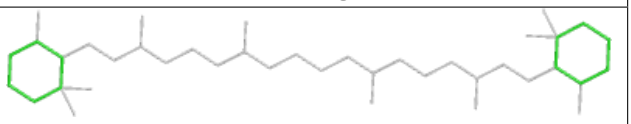
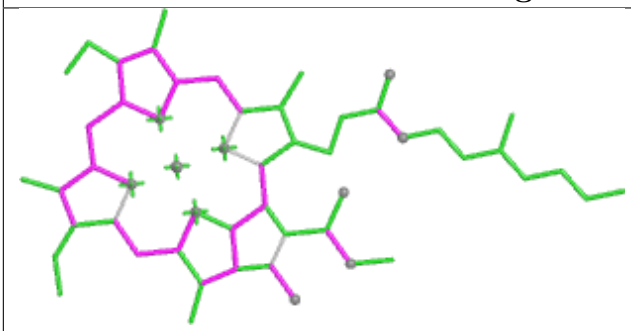


Rings

Ligand CLA aA 805



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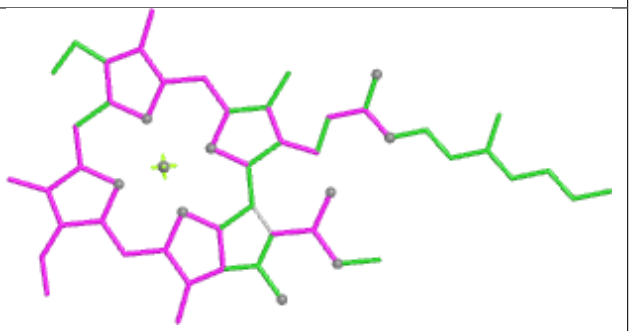
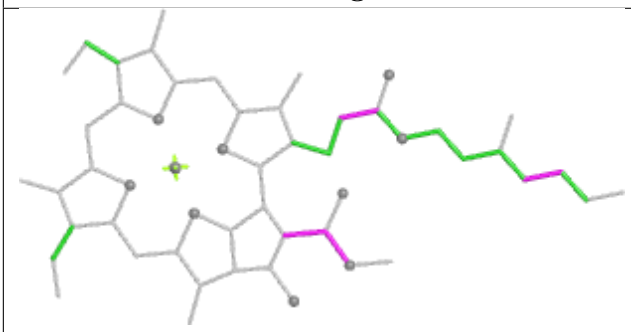


Bond angles



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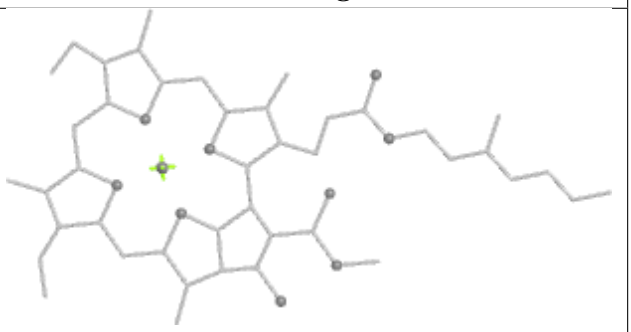
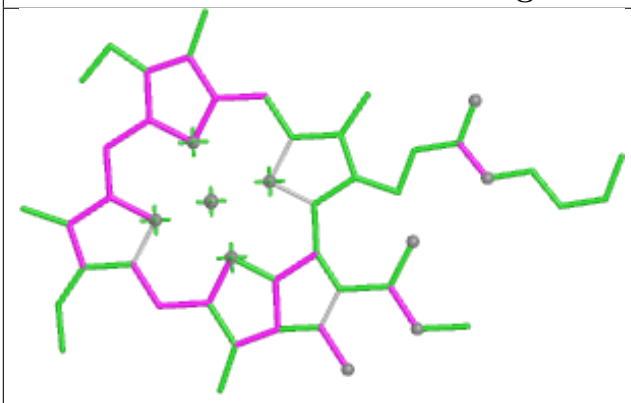
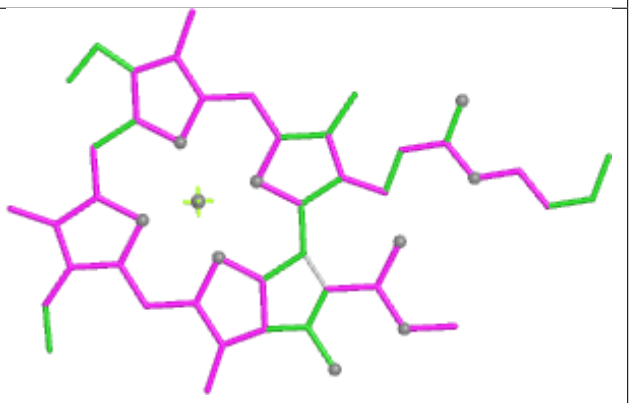


Rings

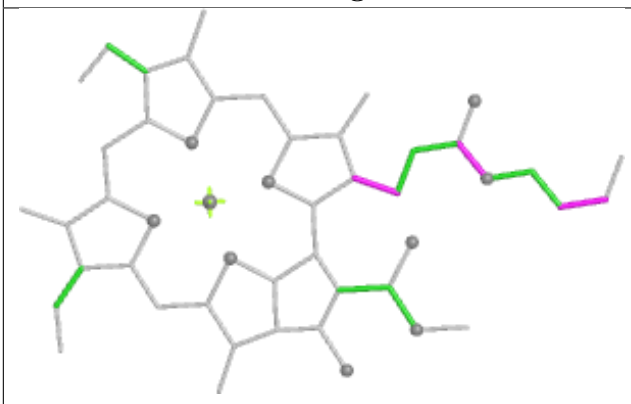
Ligand CLA cB 930



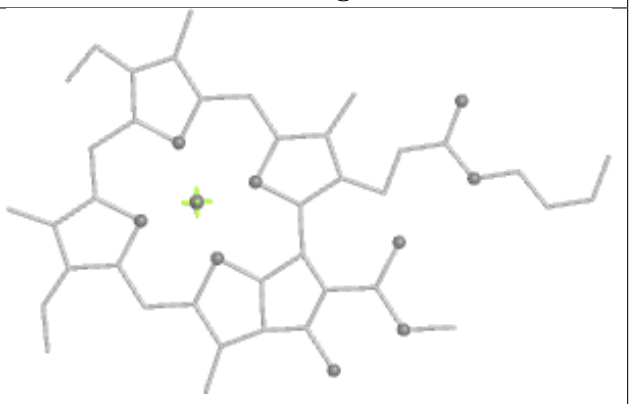
Bond lengths



Bond angles

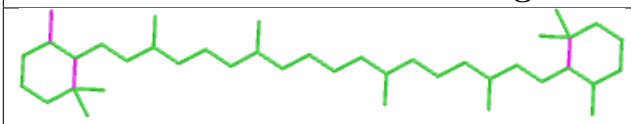


Torsions

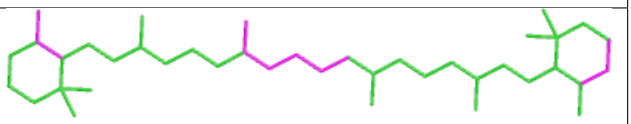


Rings

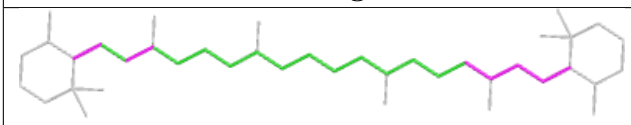
Ligand BCR aB 941



Bond lengths



Bond angles



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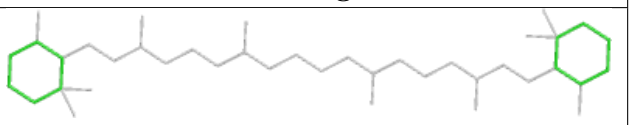
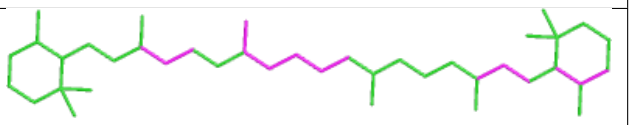


Rings

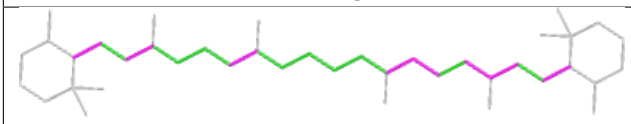
Ligand BCR bA 849



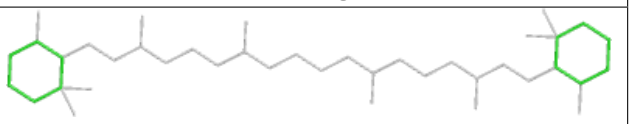
Bond lengths



Bond angles

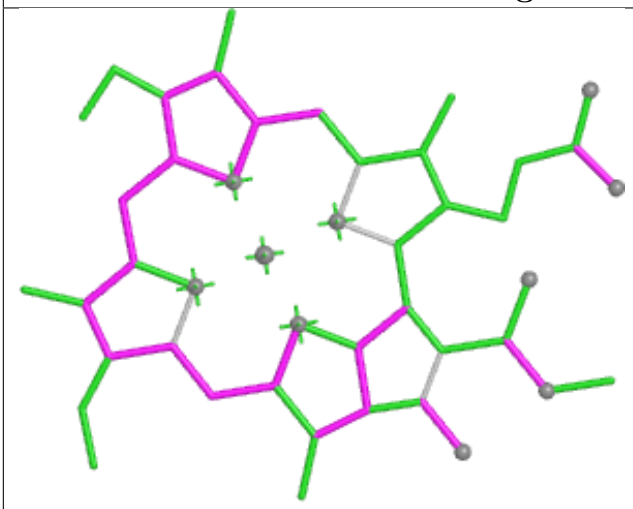


Torsions



Rings

Ligand CLA bF 202



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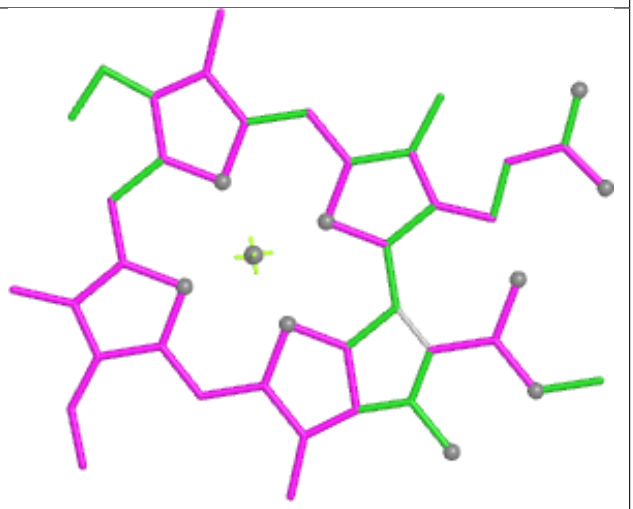
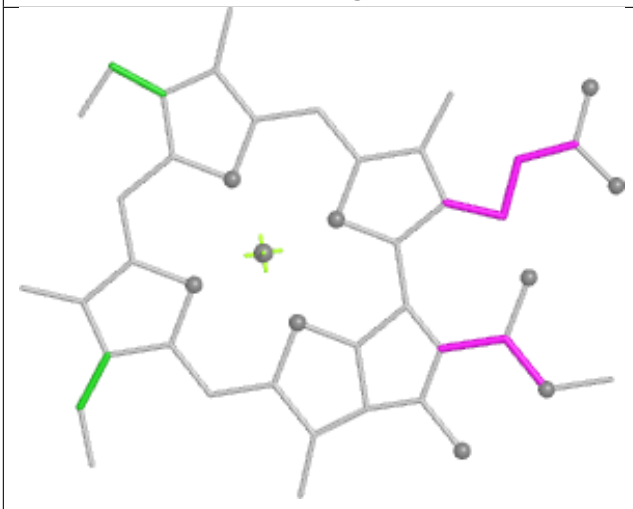


Bond angles

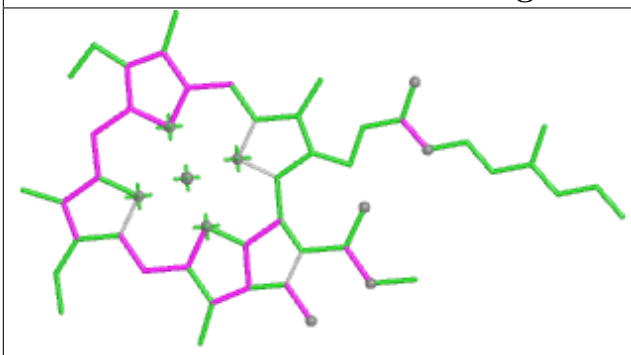


Torsions

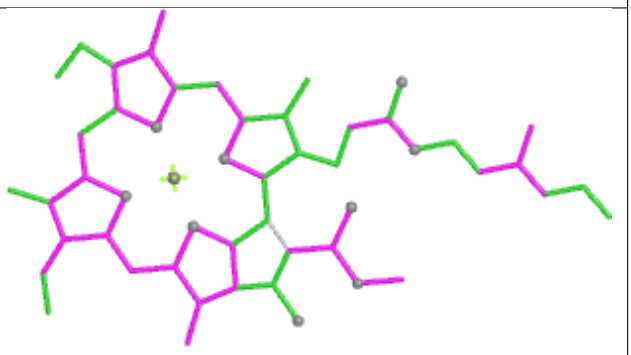


Rings

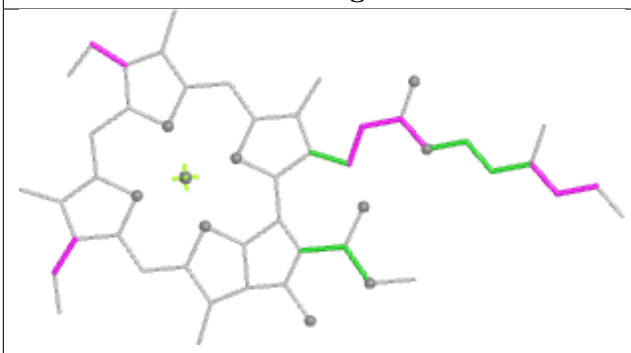
Ligand CLA cB 915



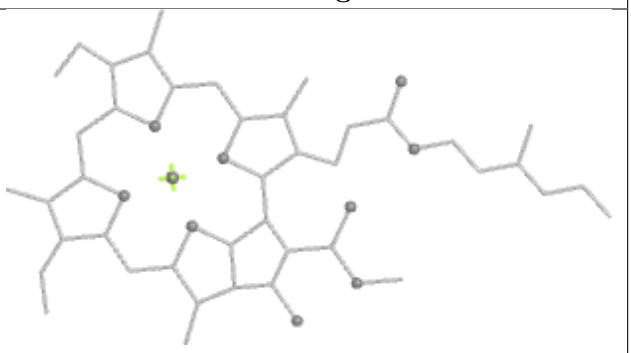
Bond lengths



Bond angles

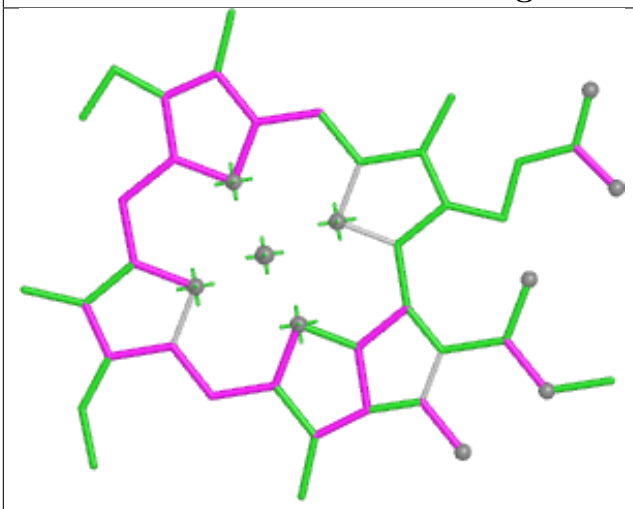


Torsions

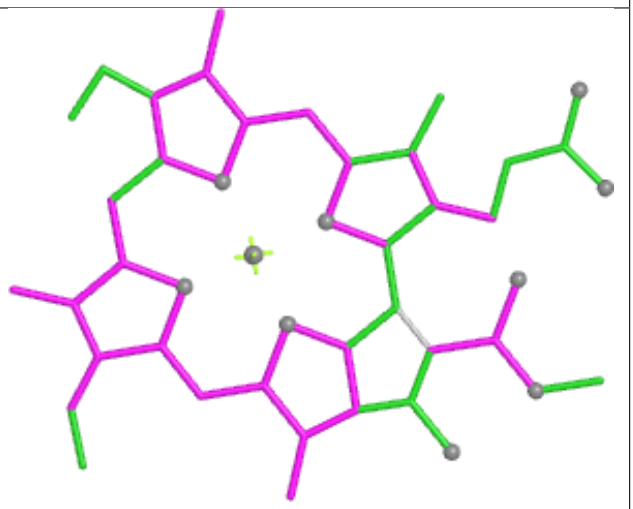


Rings

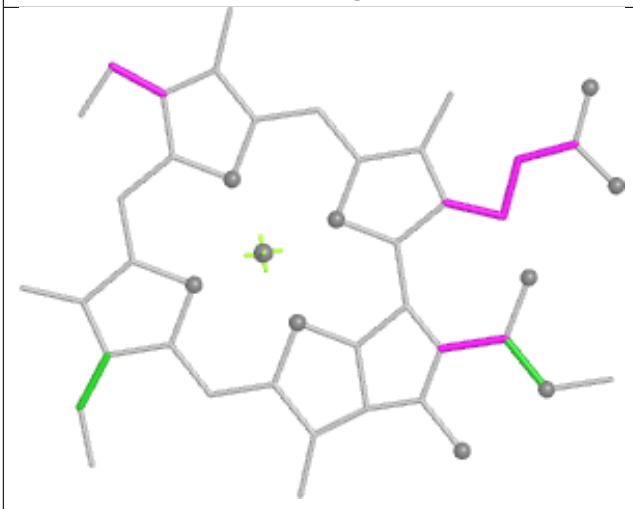
Ligand CLA cA 814



Bond lengths



Bond angles

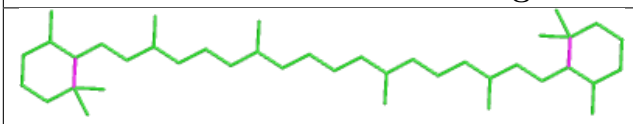


Torsions

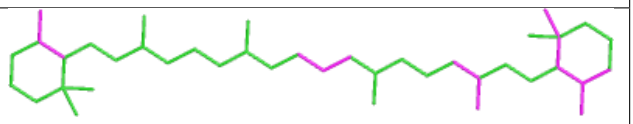


Rings

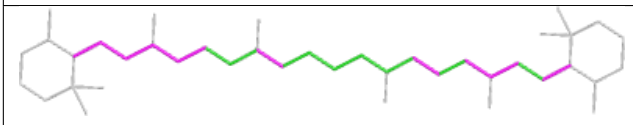
Ligand BCR bB 944



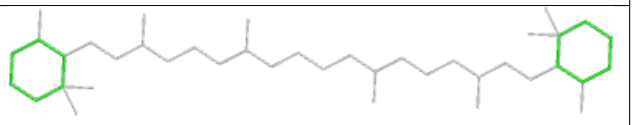
Bond lengths



Bond angles

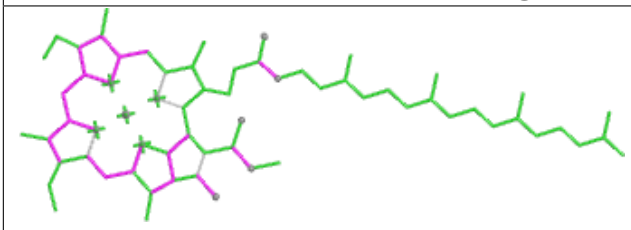


Torsions

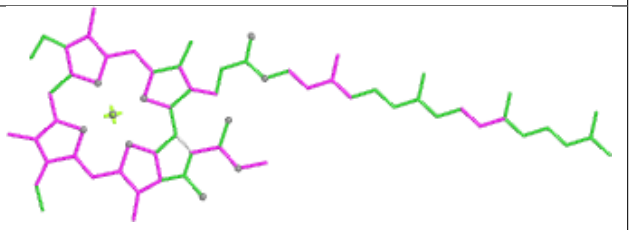


Rings

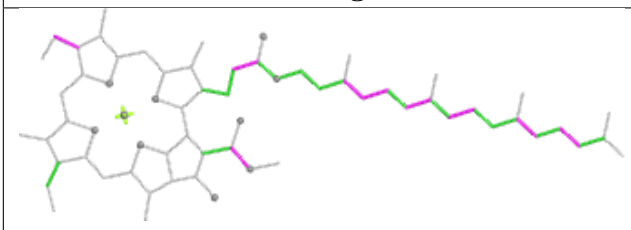
Ligand CLA aB 905



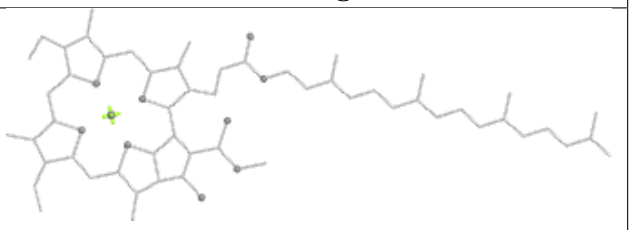
Bond lengths



Bond angles

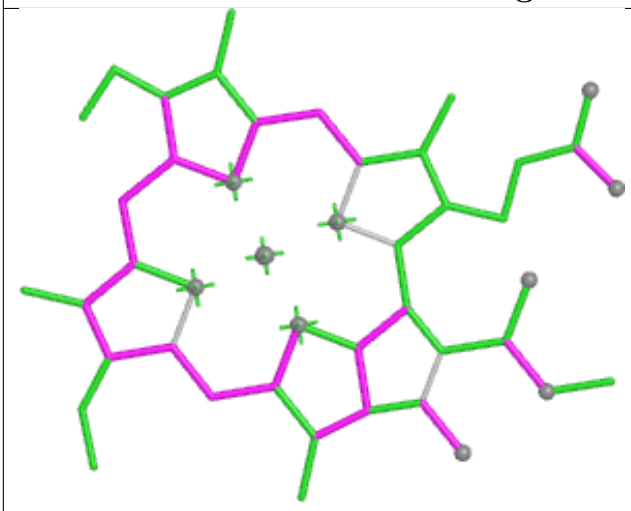


Torsions

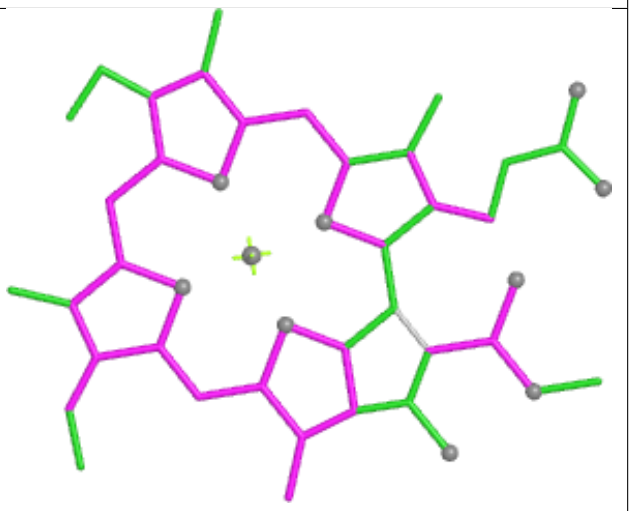


Rings

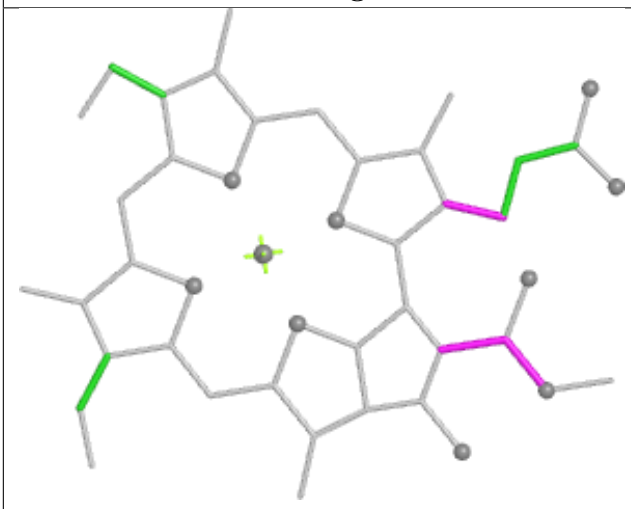
Ligand CLA aB 934



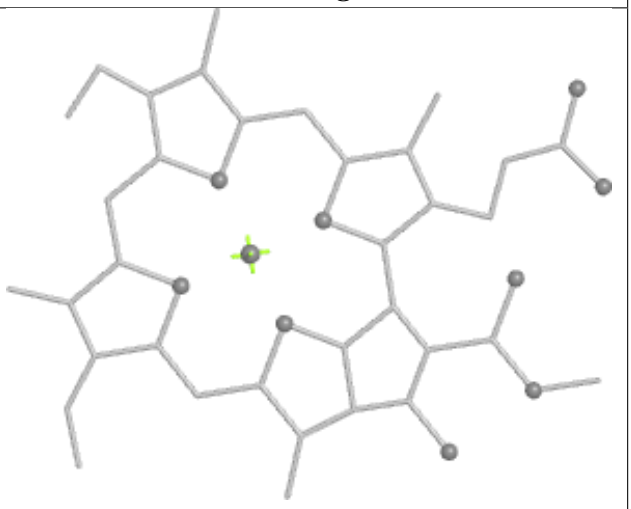
Bond lengths



Bond angles

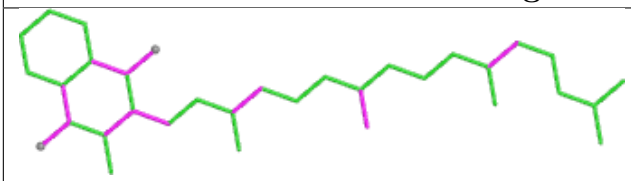


Torsions



Rings

Ligand 1L3 bB 940



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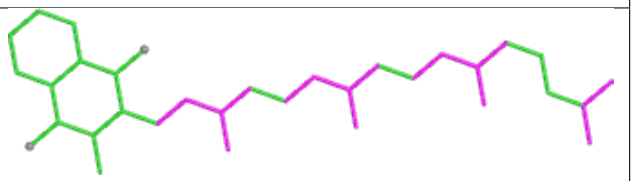

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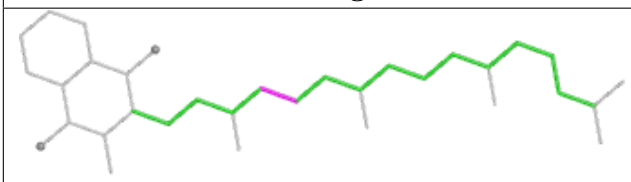

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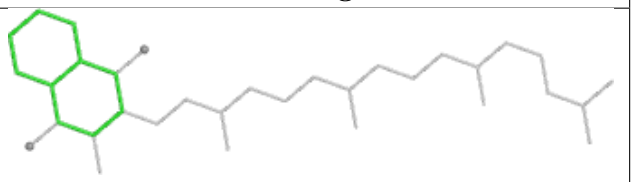
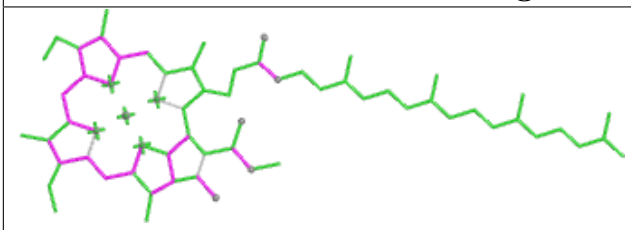


Rings

Ligand CLA cA 806



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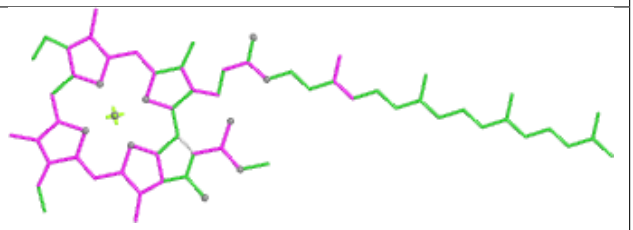
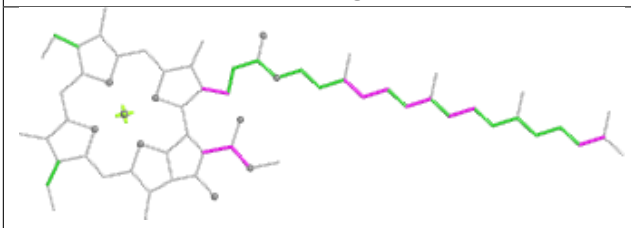


Bond angles



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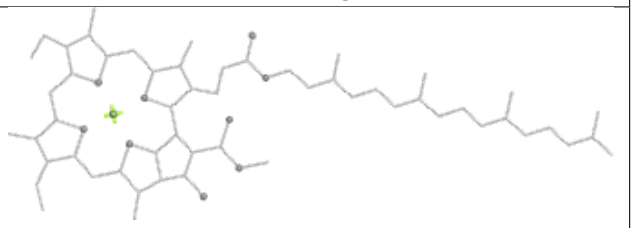
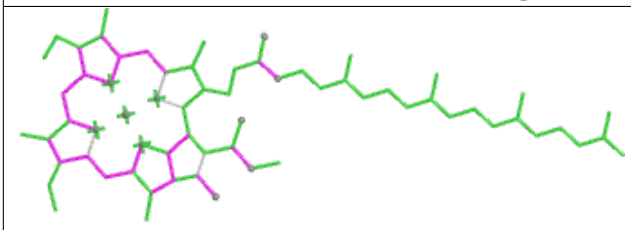


Rings

Ligand CLA aA 834



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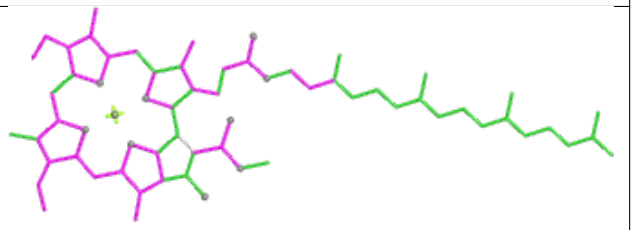
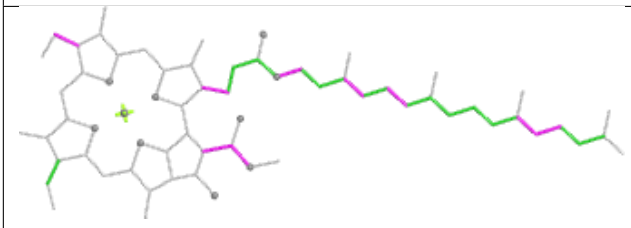


Bond angles



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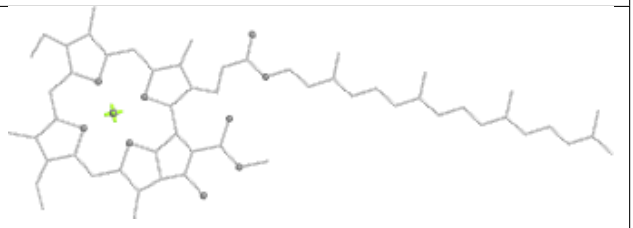
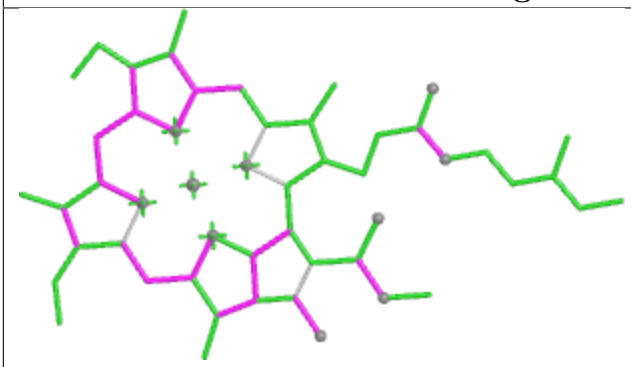


Rings

Ligand CLA bA 833



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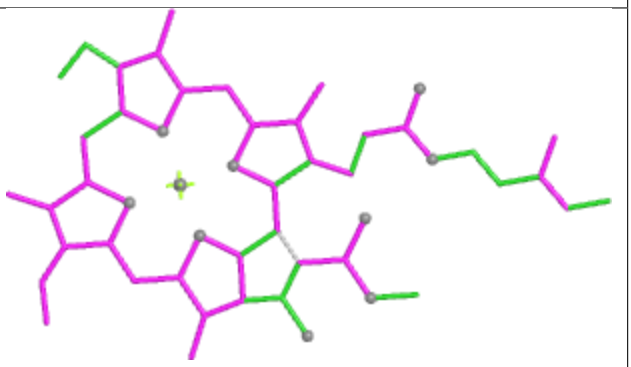

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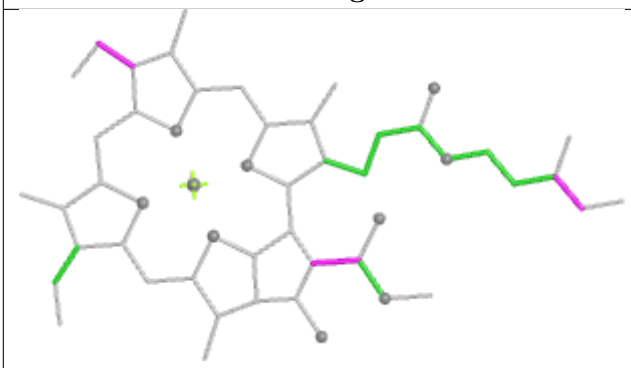

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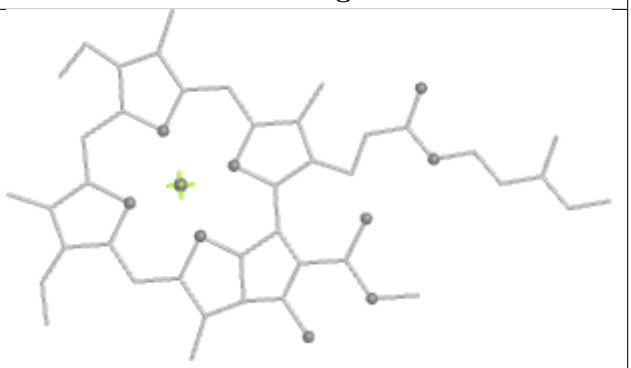
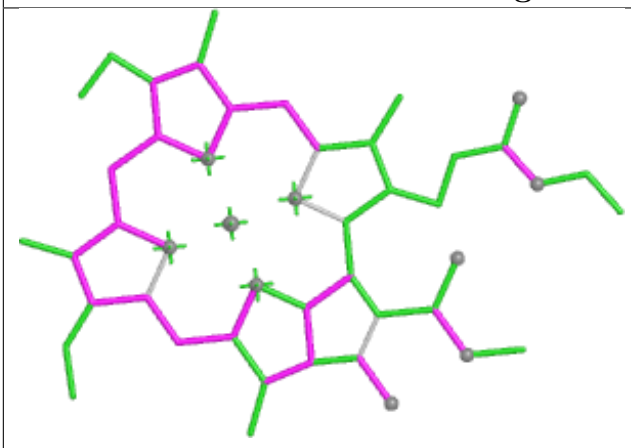


Rings

Ligand CLA bB 937



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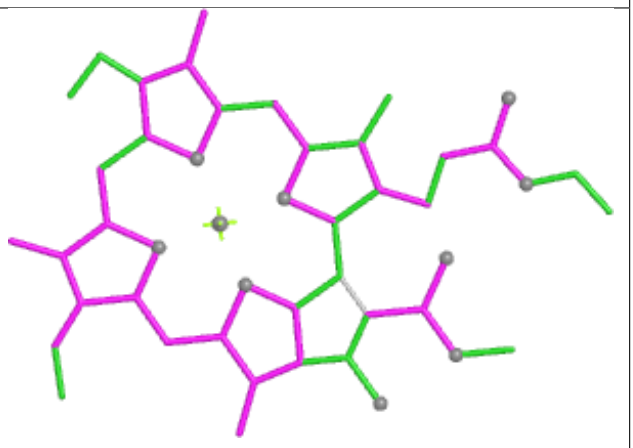

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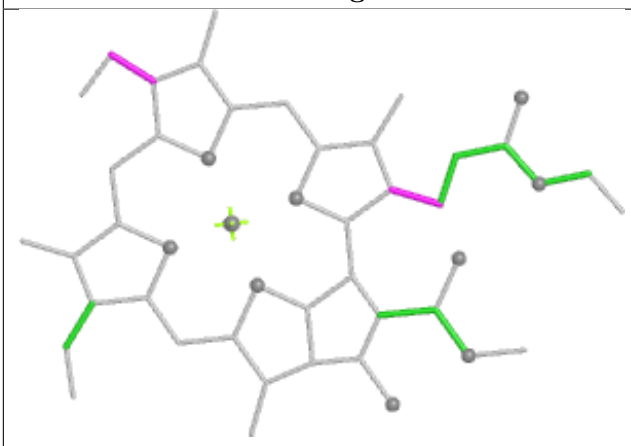

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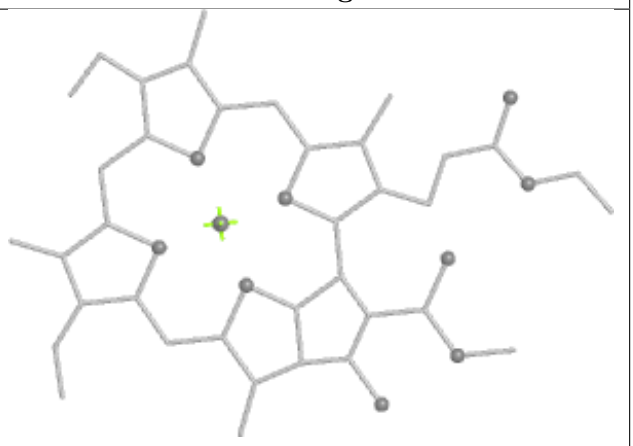
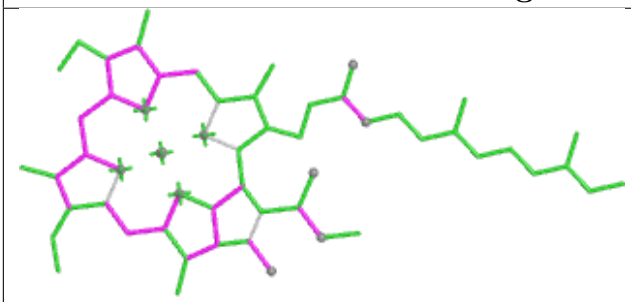


Rings

Ligand CLA cA 853



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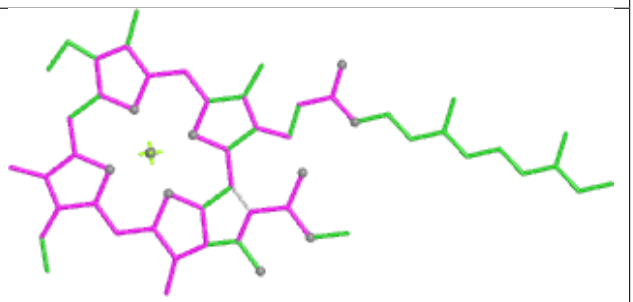
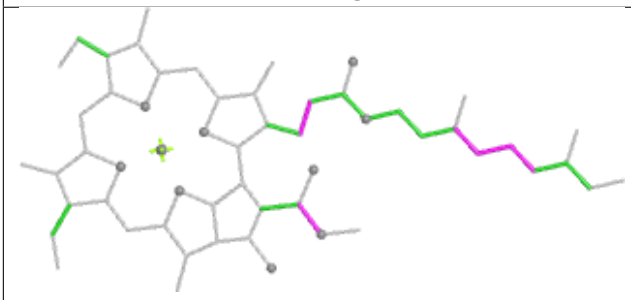


Bond angles



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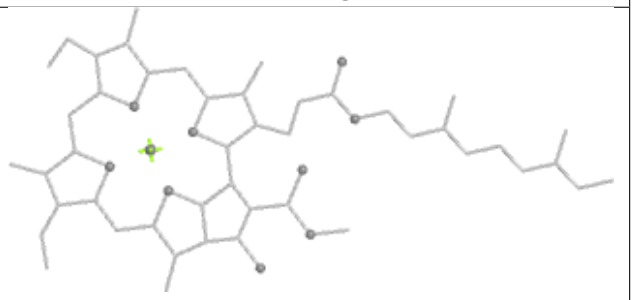
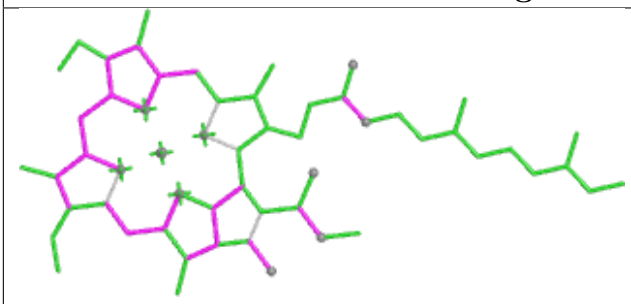
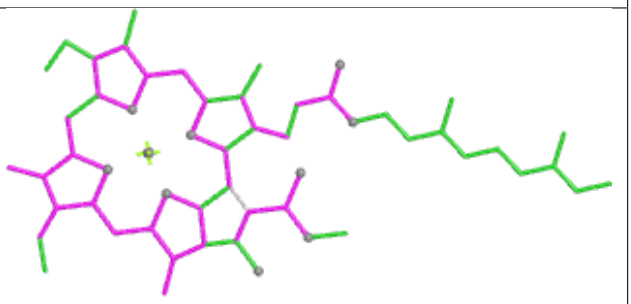
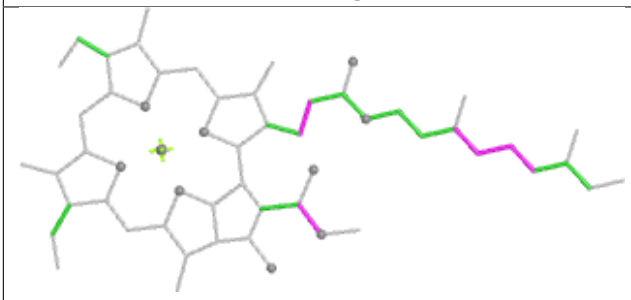
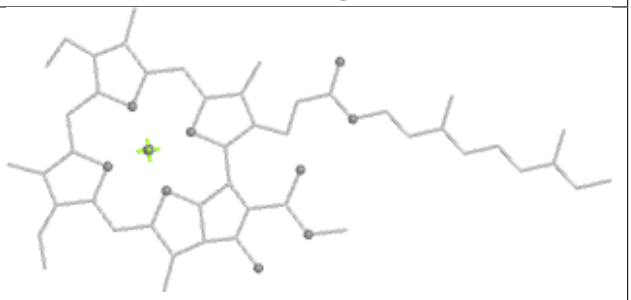
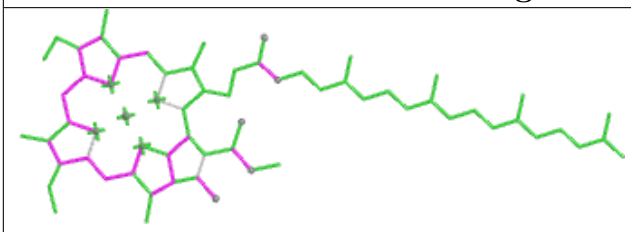
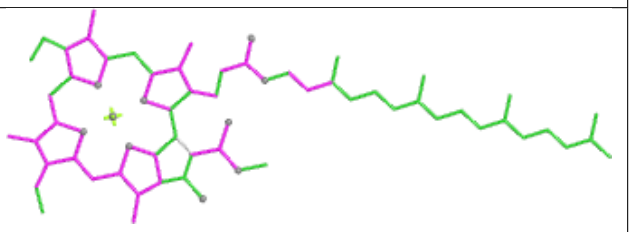
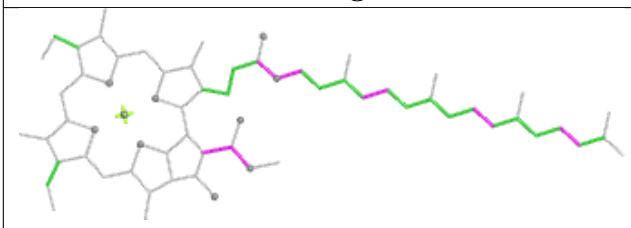
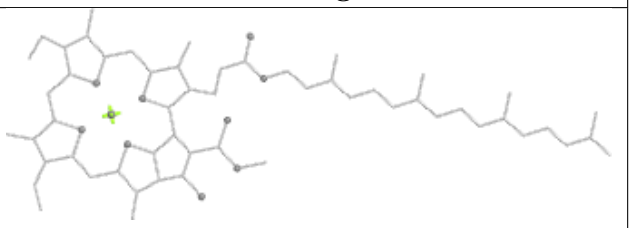
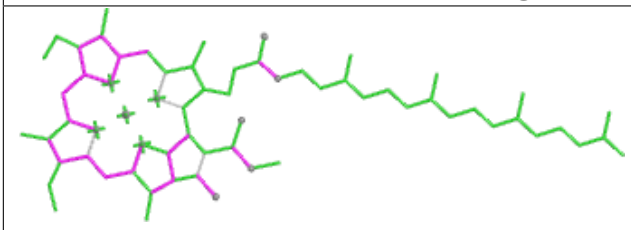


Rings

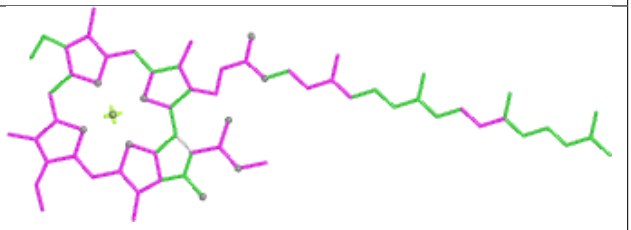
Ligand CLA aA 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aA 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

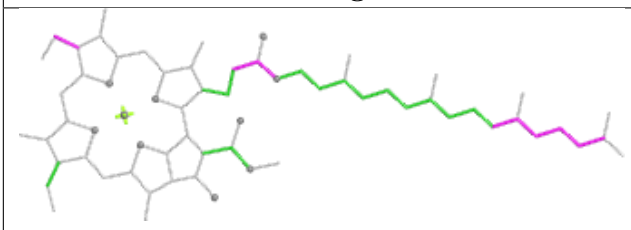
Ligand CLA aA 843



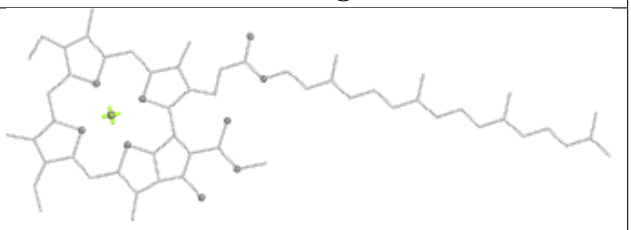
Bond lengths



Bond angles

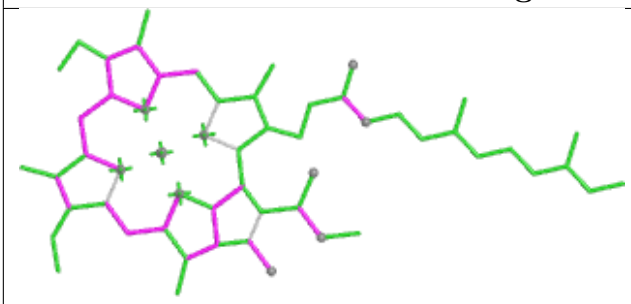


Torsions



Rings

Ligand CLA aA 804



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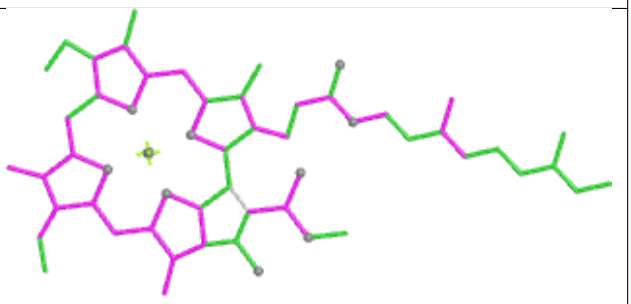

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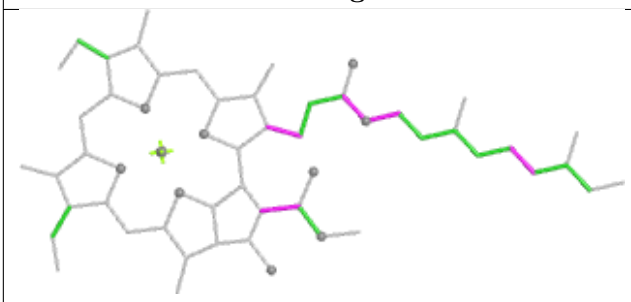

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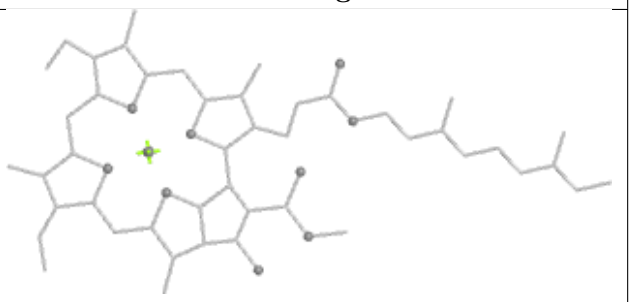
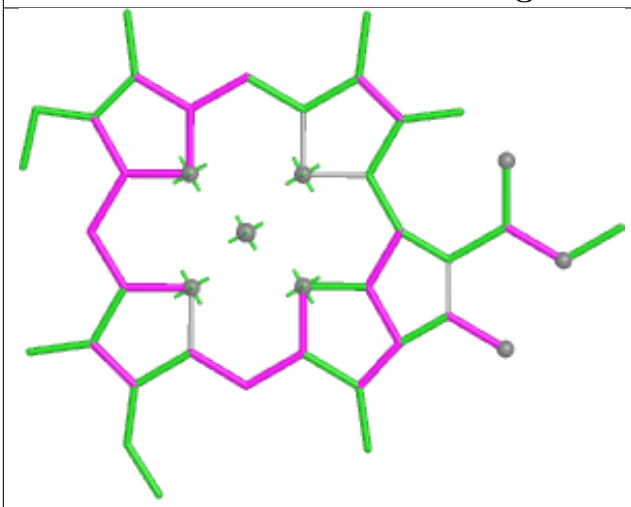


Rings

Ligand CLA aB 949



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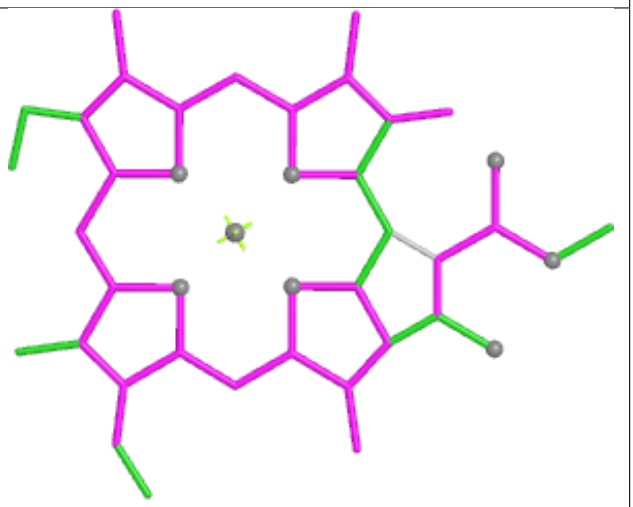
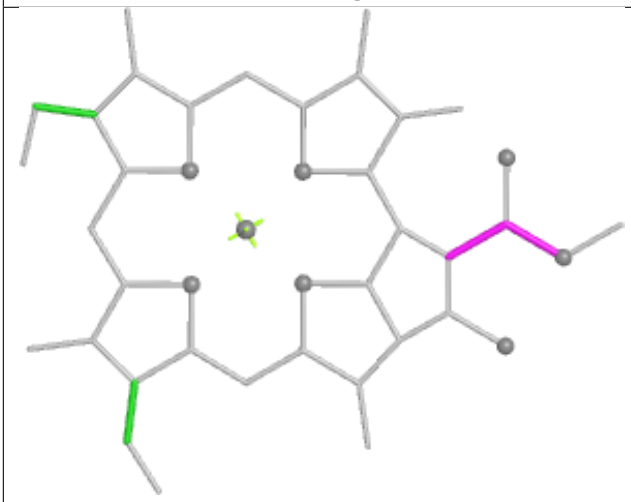


Bond angles



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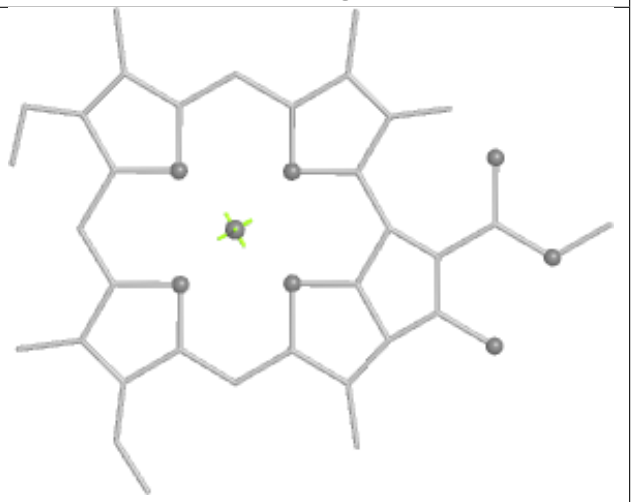
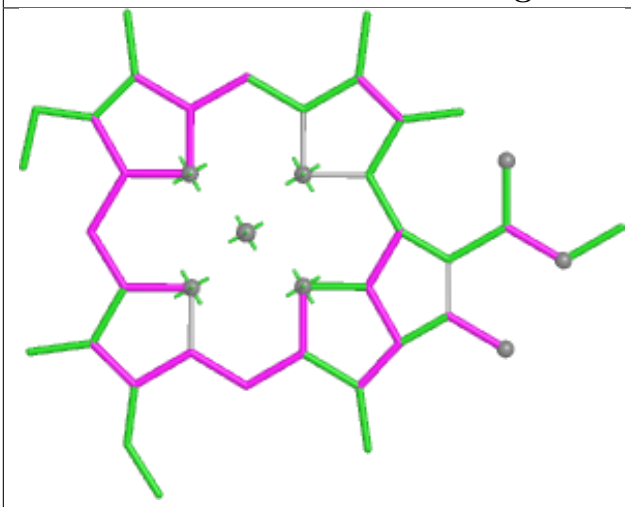


Rings

Ligand CLA bB 949



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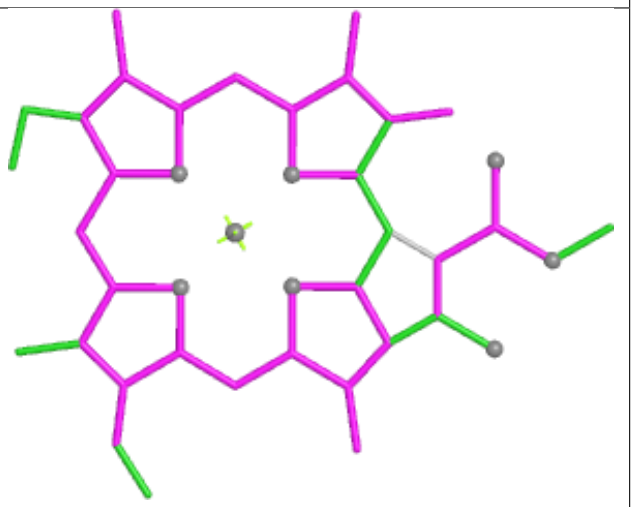
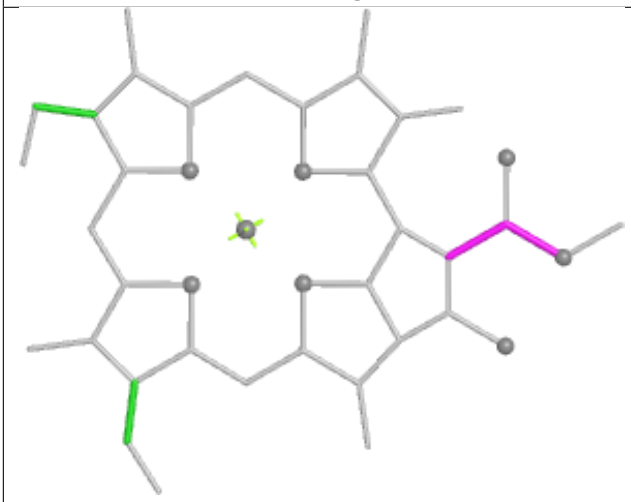
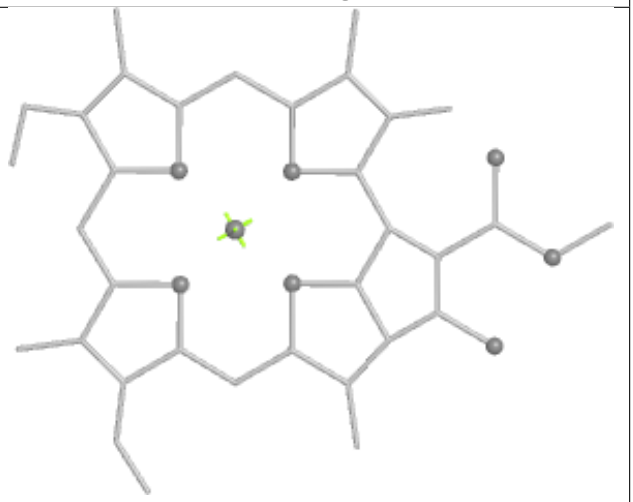


Bond angles

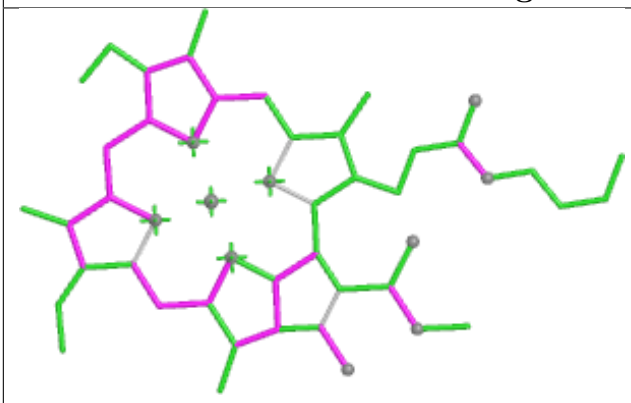


Torsions



Rings

Ligand CLA cA 822



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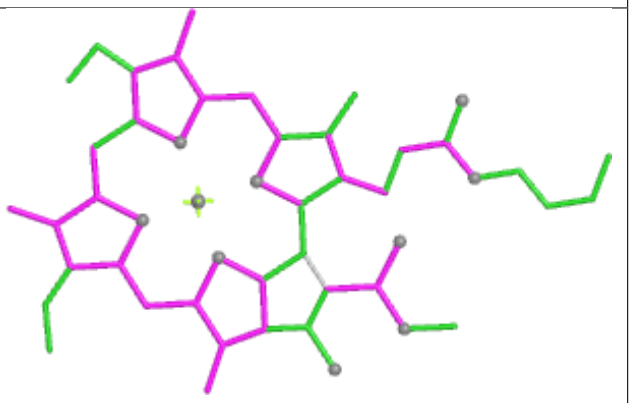
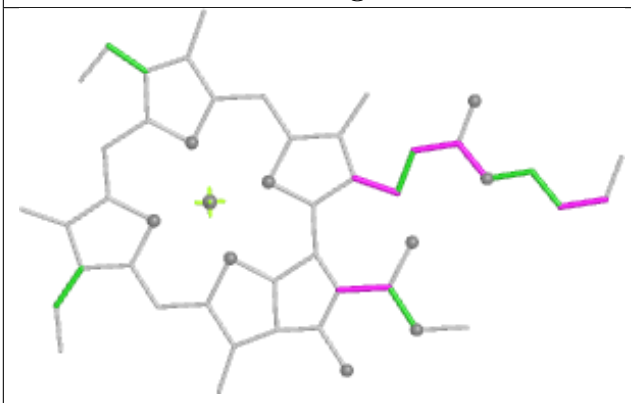


Bond angles



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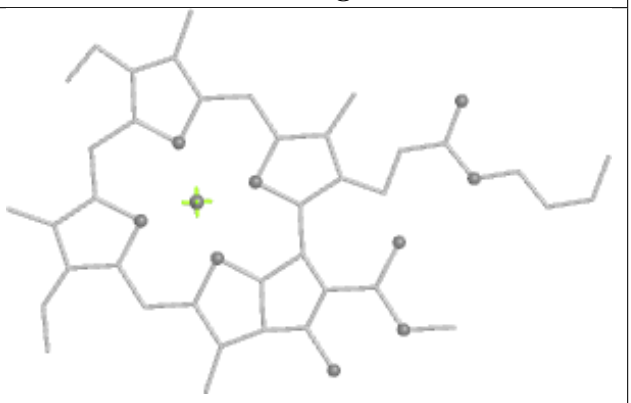
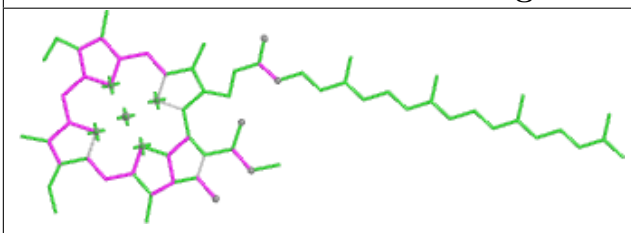
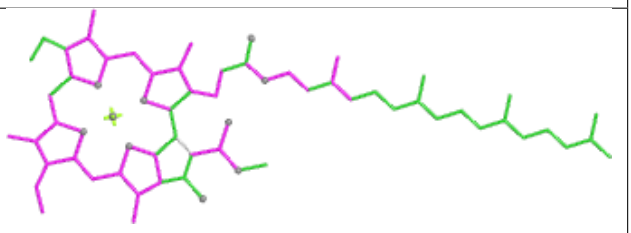


Rings

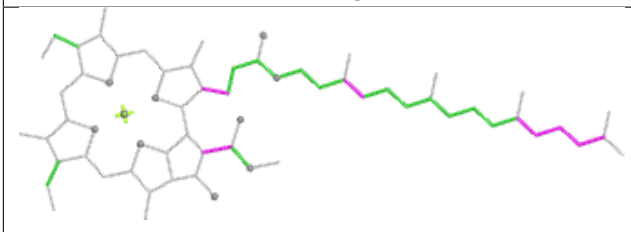
Ligand CLA aB 904



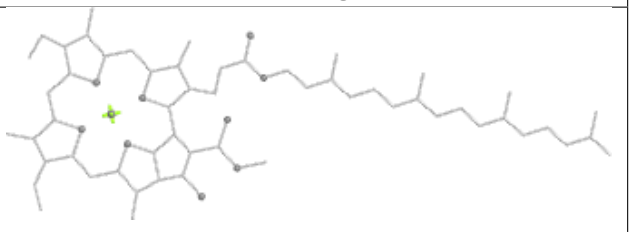
Bond lengths



Bond angles

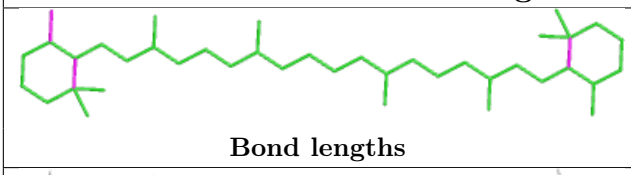


Torsions

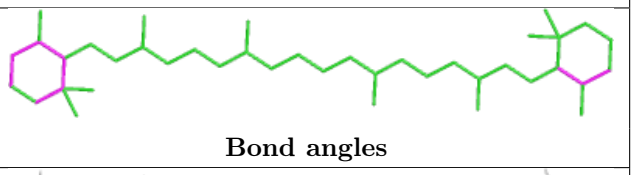


Rings

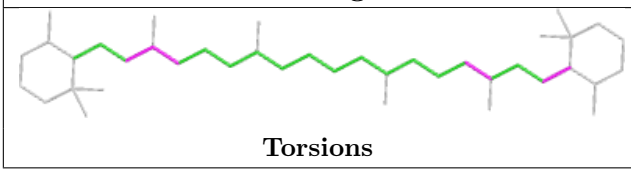
Ligand BCR bL 201



Bond lengths



Bond angles



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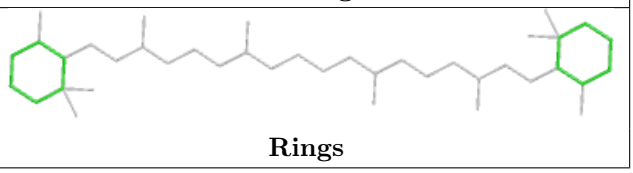
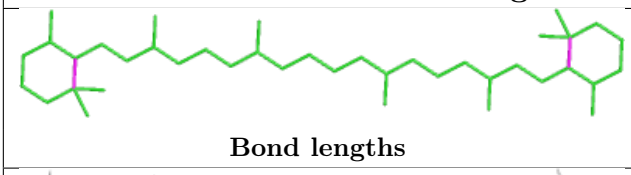


Rings

Ligand BCR cM 101



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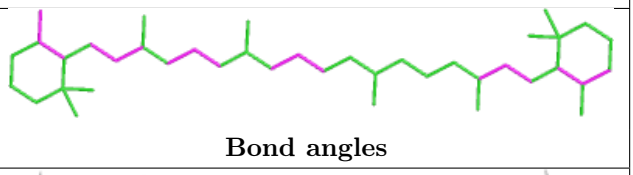

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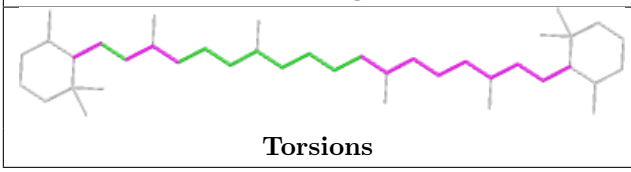

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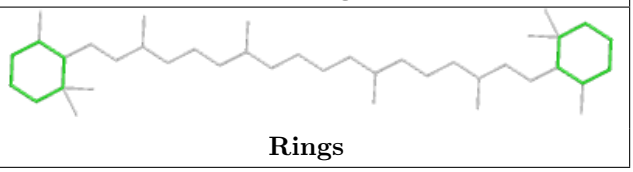
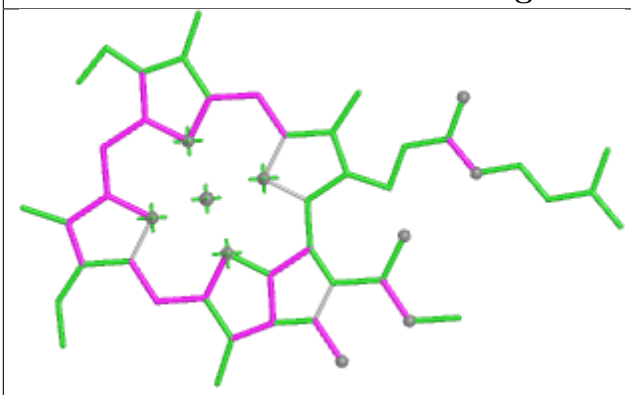


Rings

Ligand CLA aA 821



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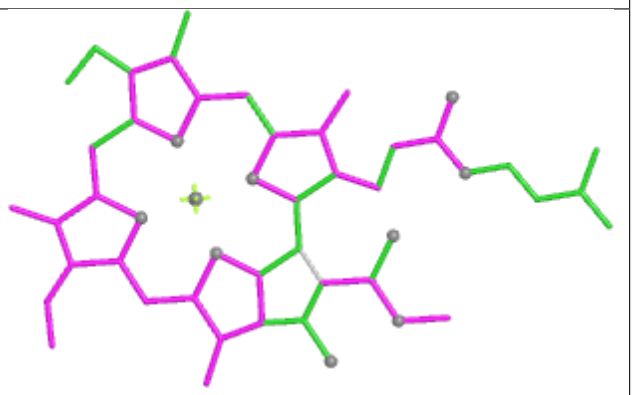

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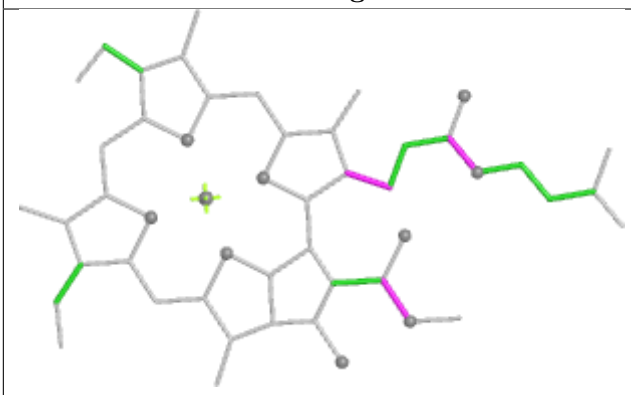

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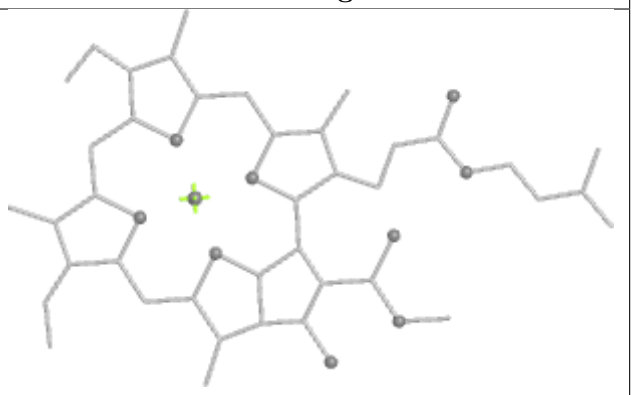
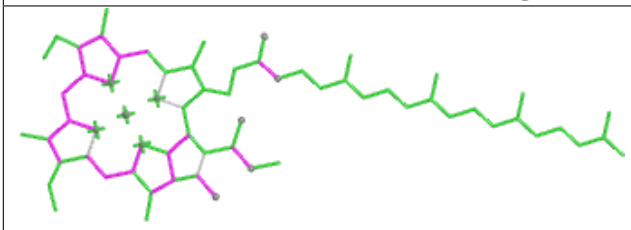


Rings

Ligand CLA cB 926



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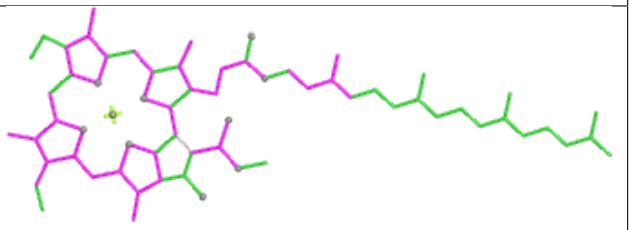

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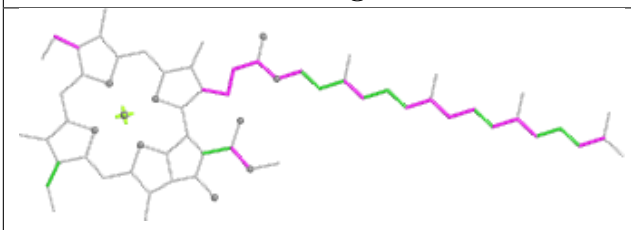

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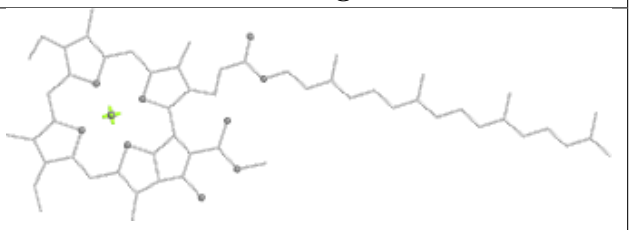
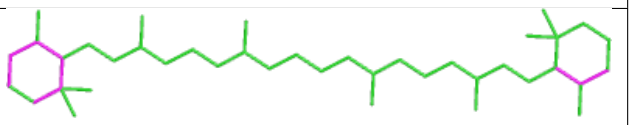


Rings

Ligand BCR aL 201



Bond lengths



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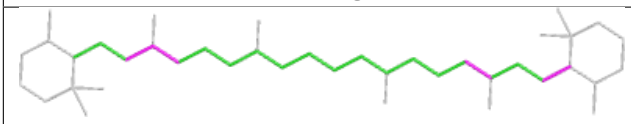

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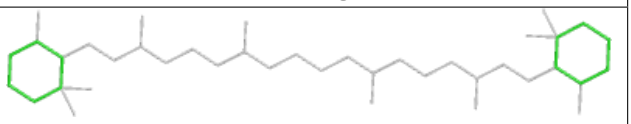
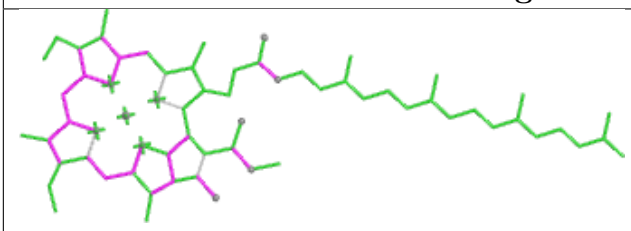


Rings

Ligand CLA aA 802



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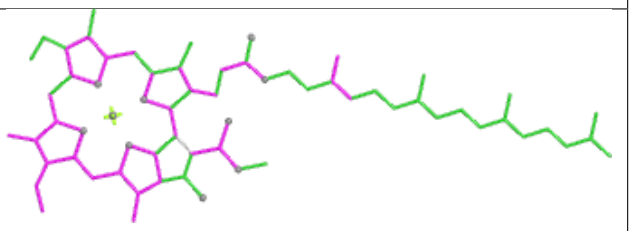

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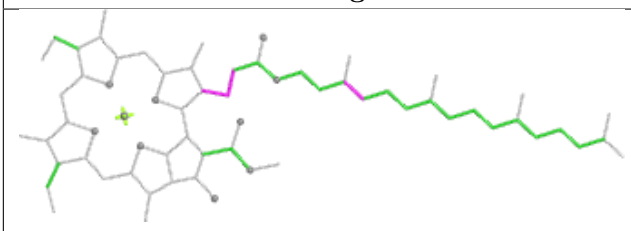

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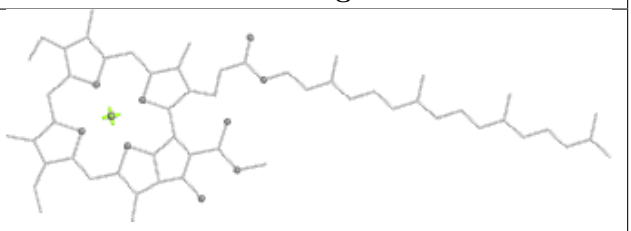
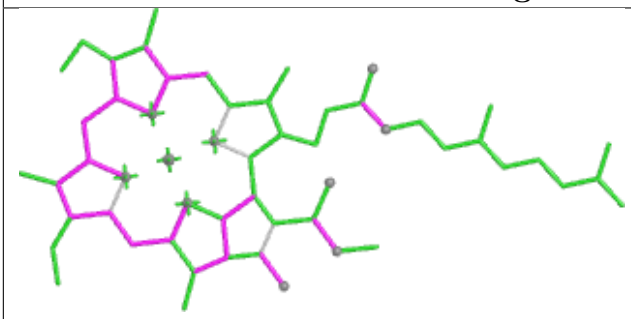


Rings

Ligand CLA bA 826



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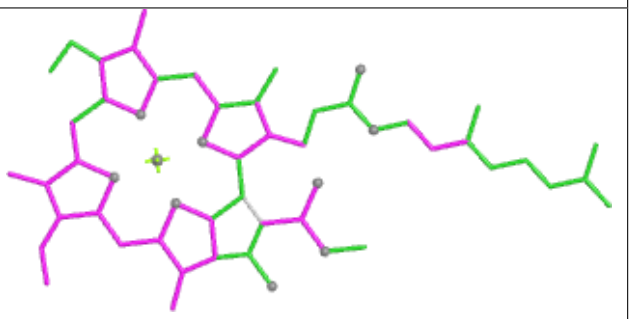
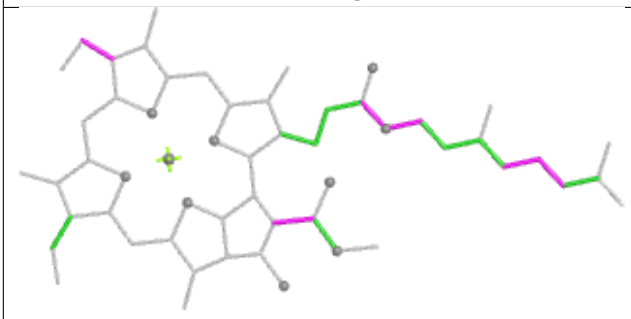


Bond angles



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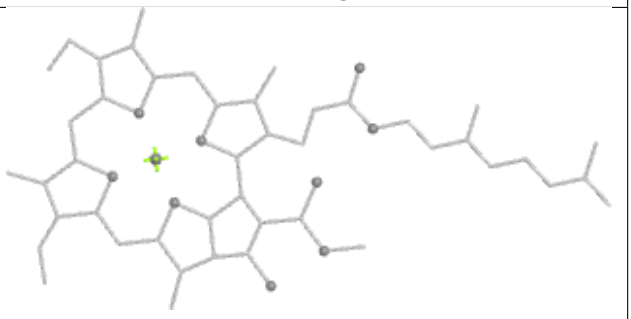
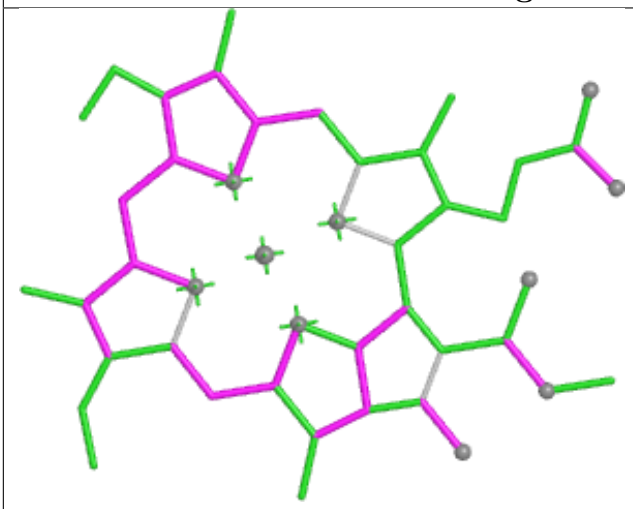


Rings

Ligand CLA aB 914



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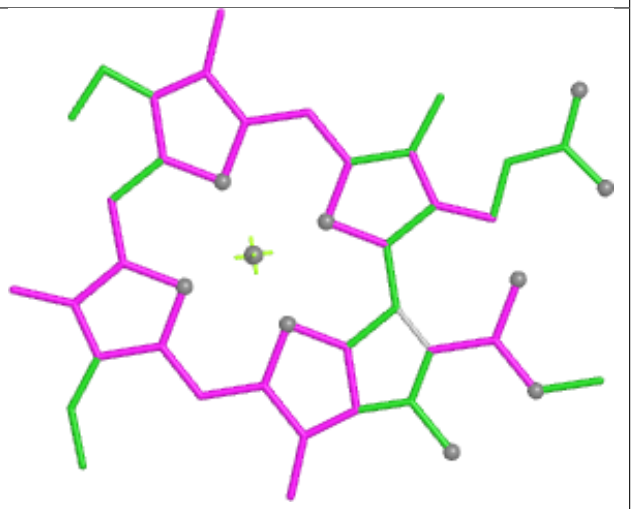
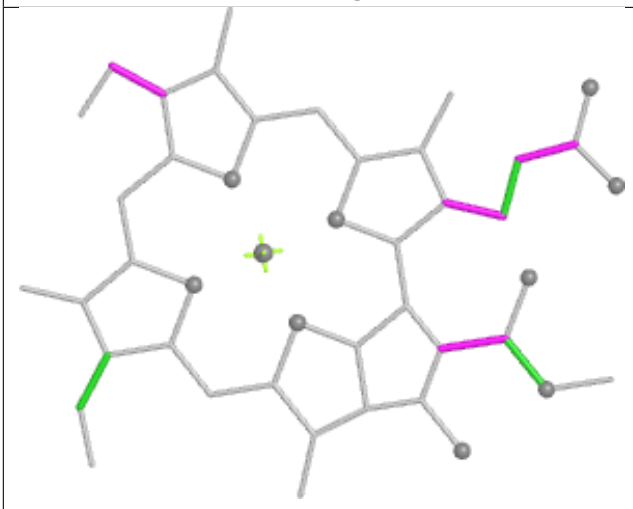


Bond angles

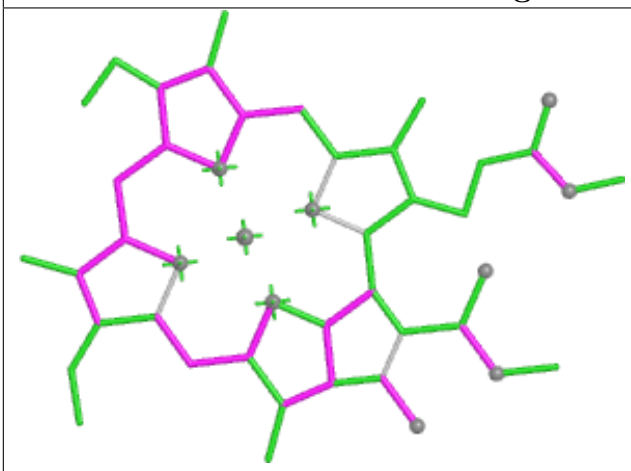


Torsions



Rings

Ligand CLA bA 827



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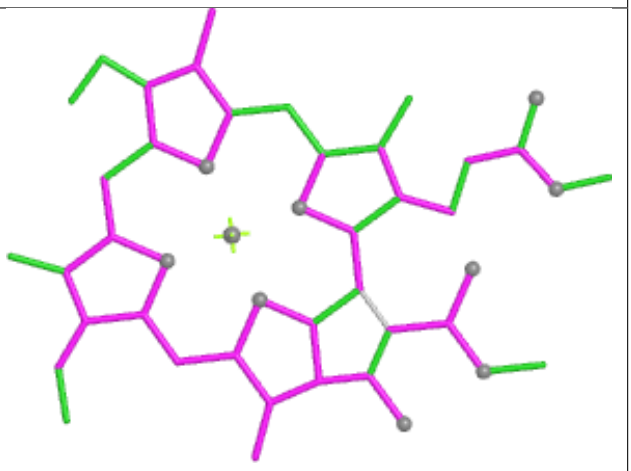
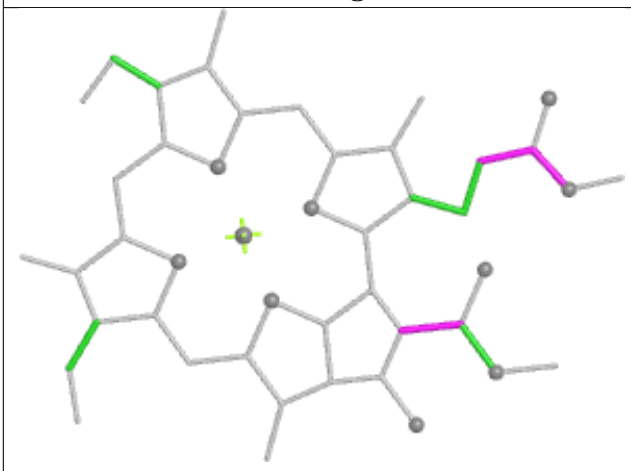


Bond angles



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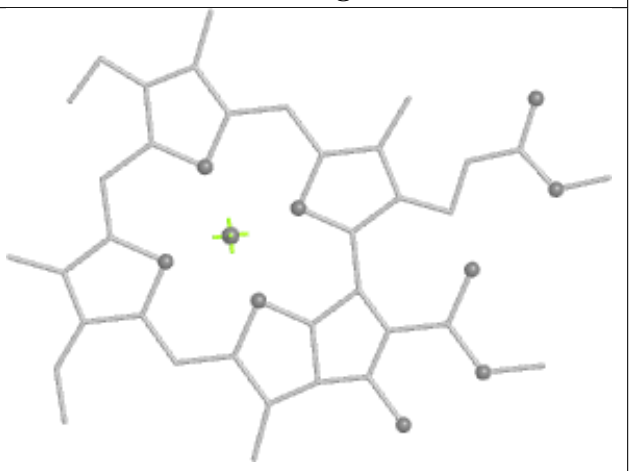
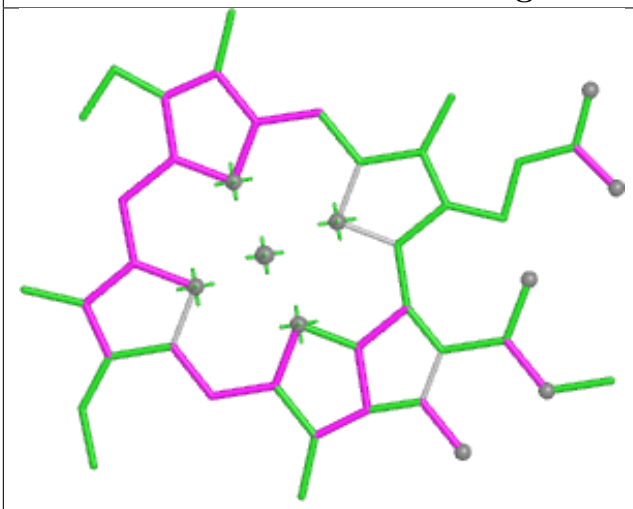


Rings

Ligand CLA cA 810



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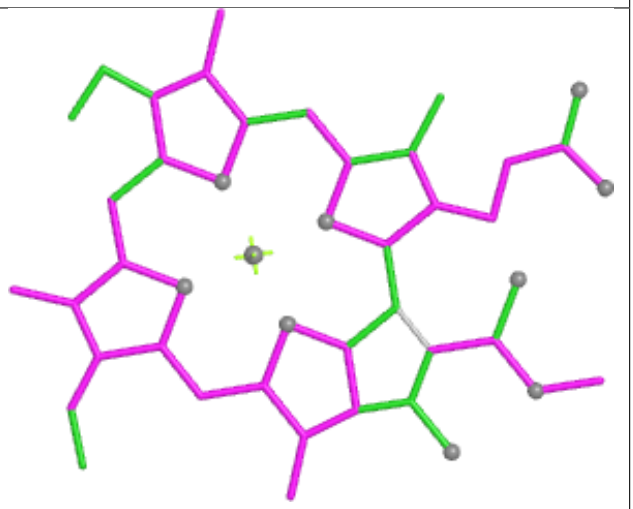

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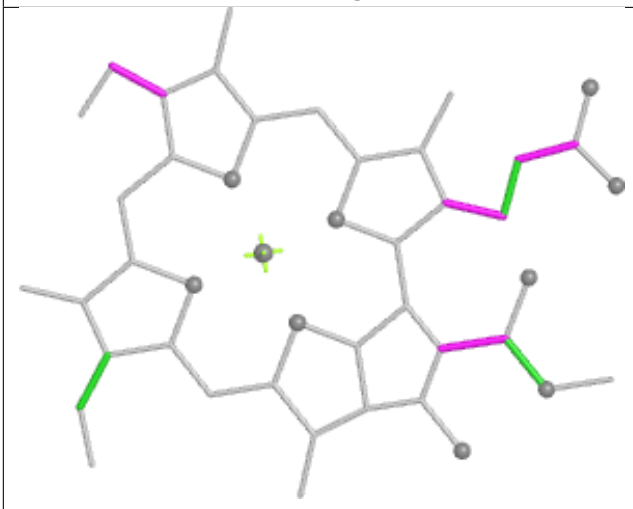
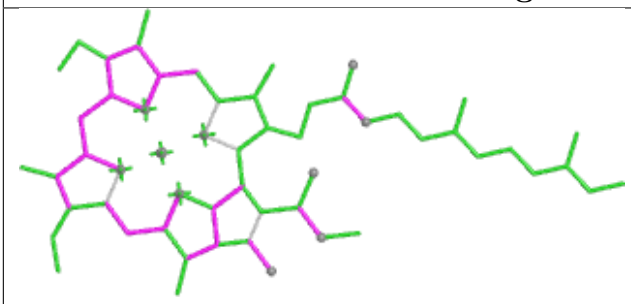
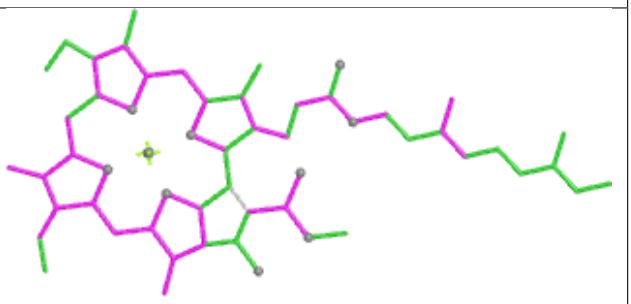
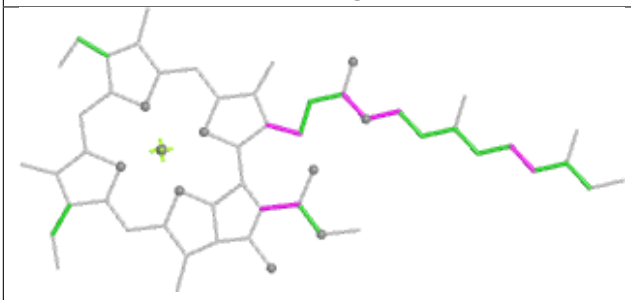
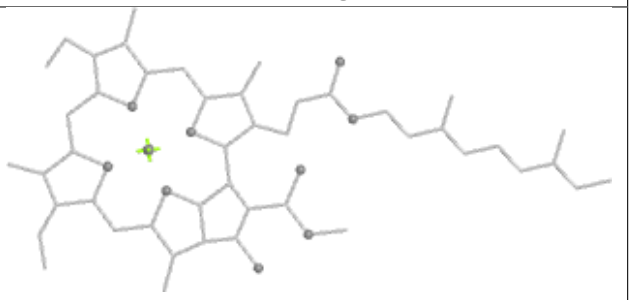


Torsions



Rings

Ligand CLA cA 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

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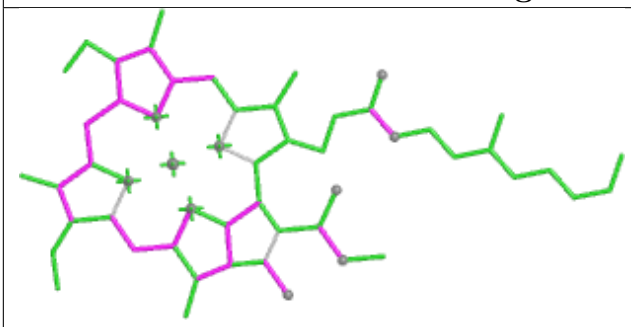
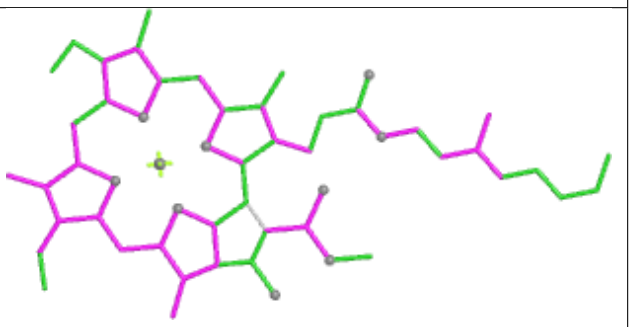
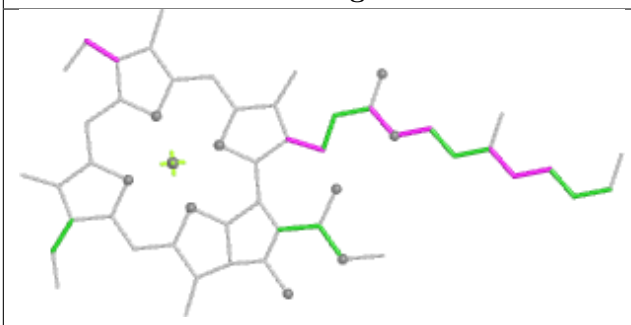
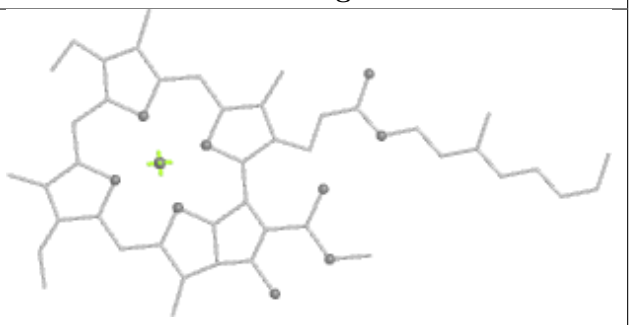
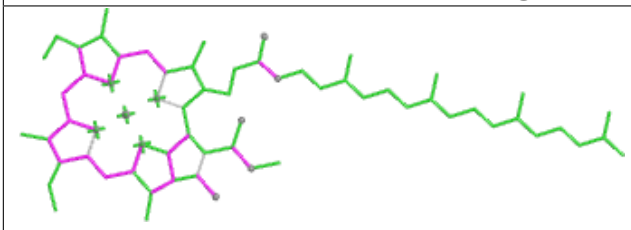
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aA 825



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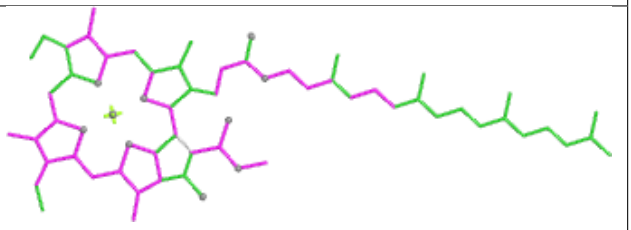
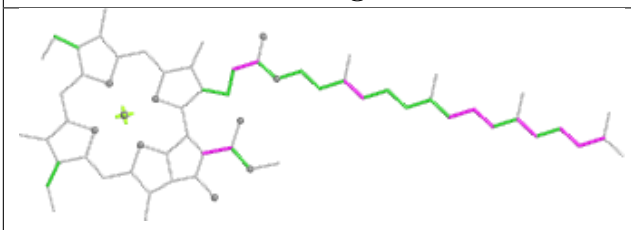


Bond angles



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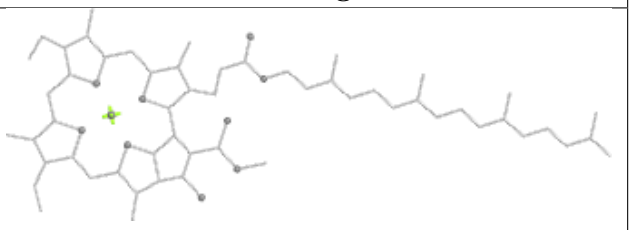
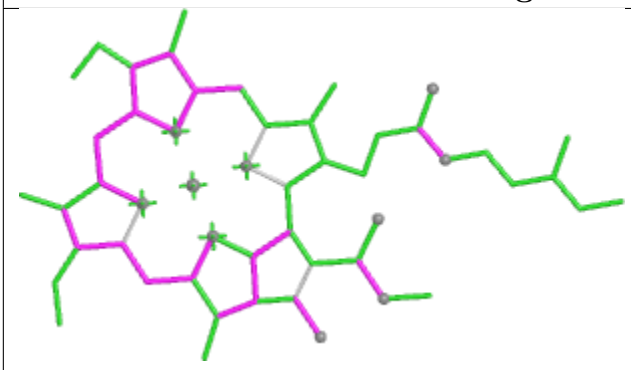


Rings

Ligand CLA cA 837



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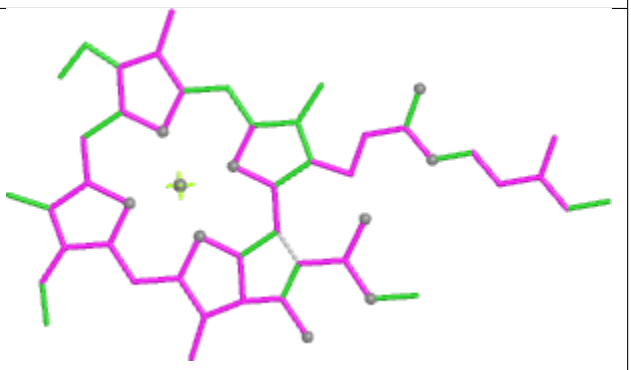
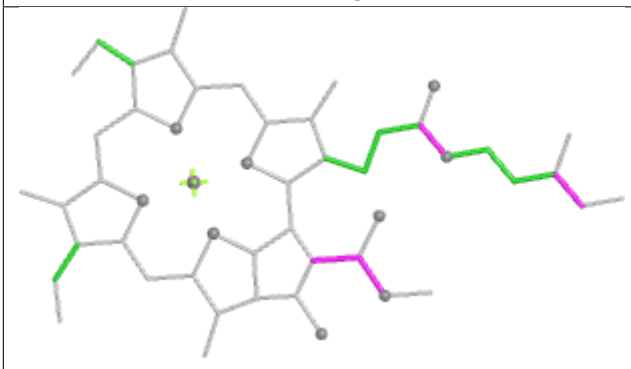


Bond angles



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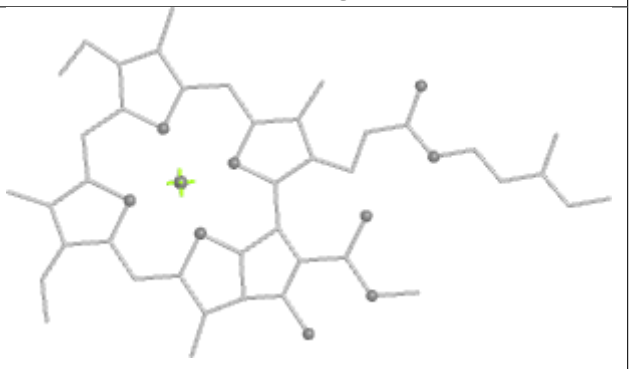
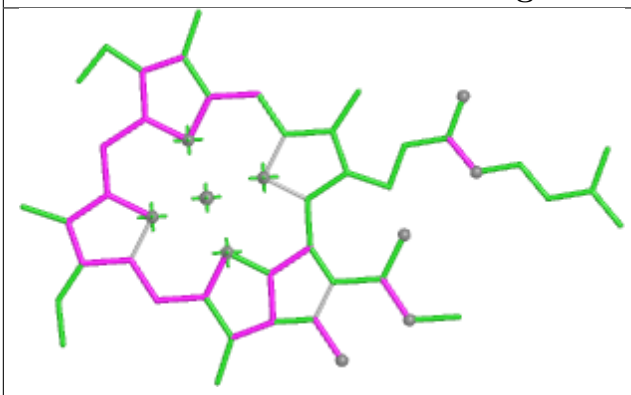


Rings

Ligand CLA cB 928



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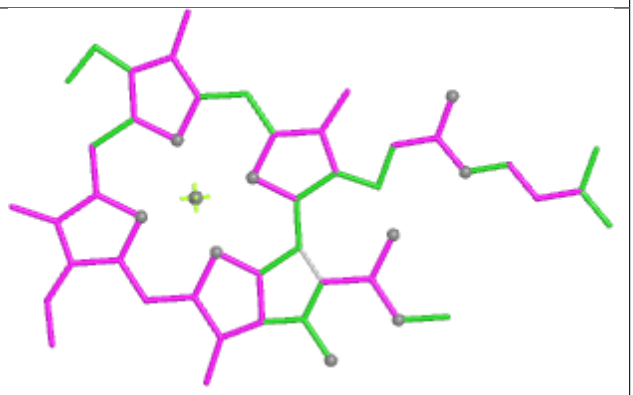
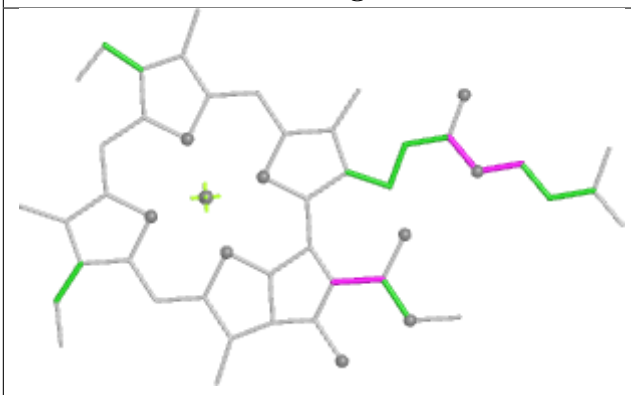


Bond angles



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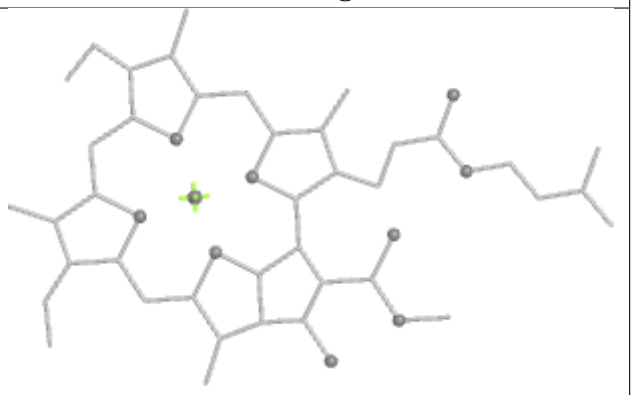
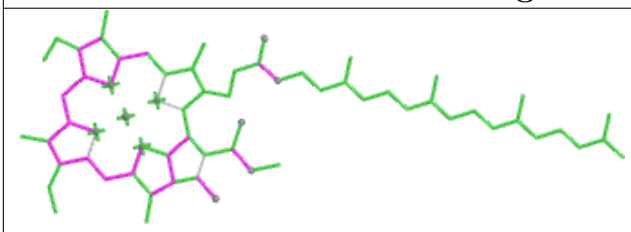
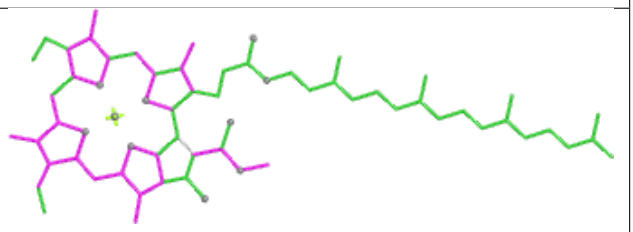


Rings

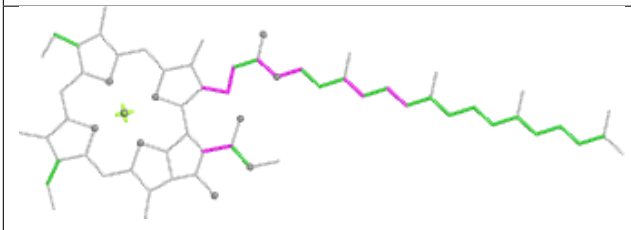
Ligand CLA cB 927



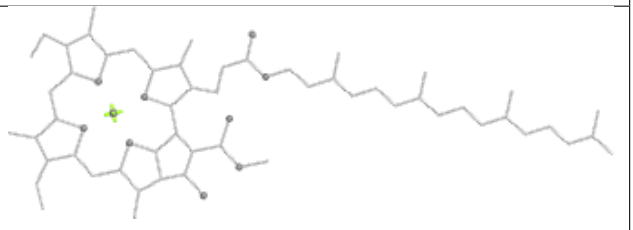
Bond lengths



Bond angles

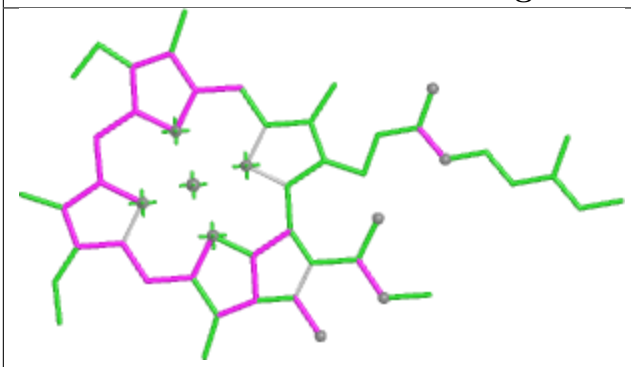


Torsions



Rings

Ligand CLA aA 808



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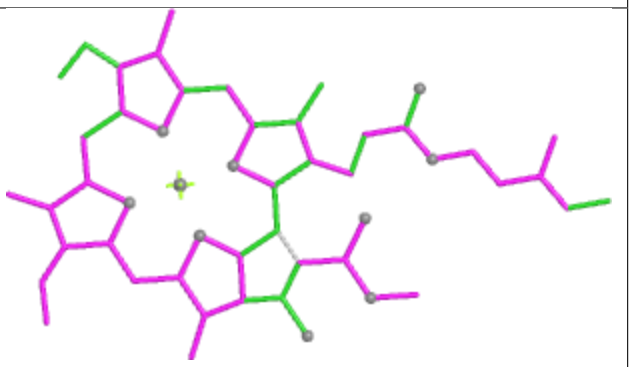
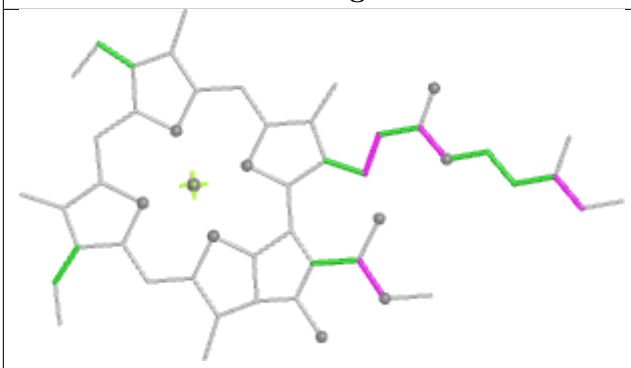


Bond angles



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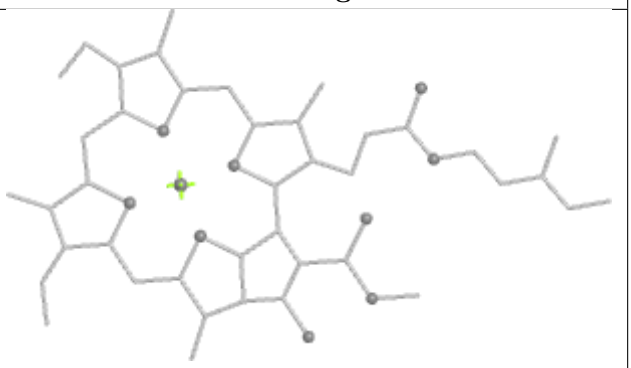
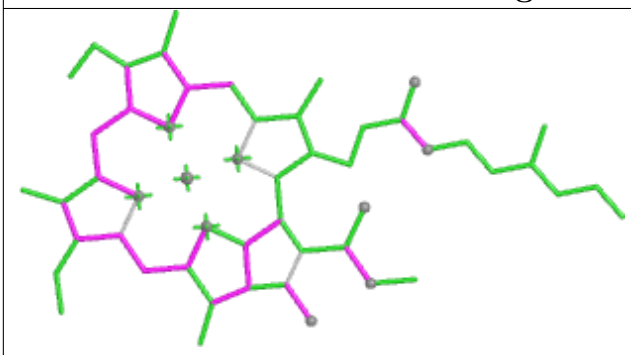


Rings

Ligand CLA aB 907



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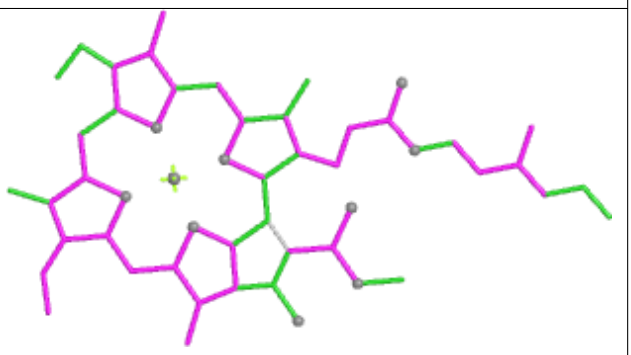
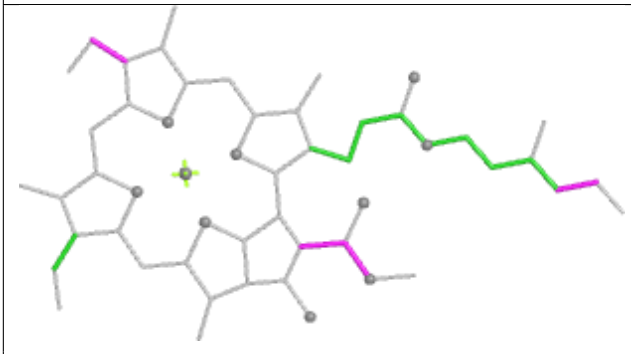


Bond angles



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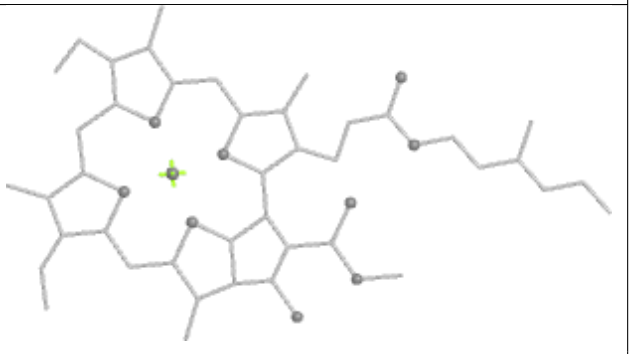
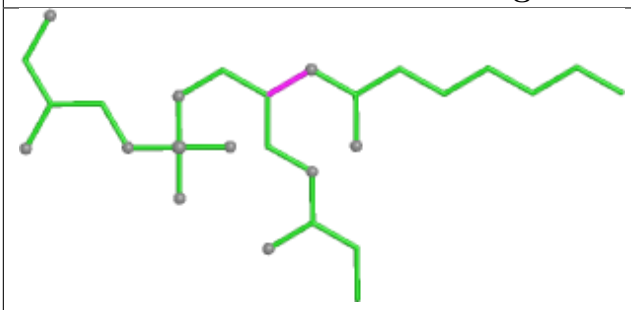


Rings

Ligand LHG aA 853



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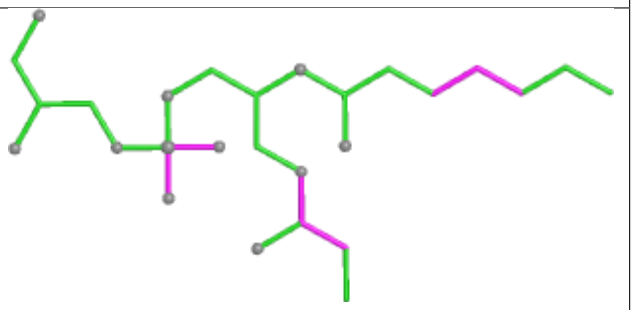
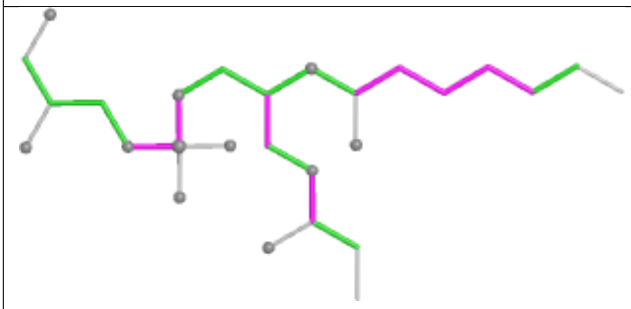


Bond angles



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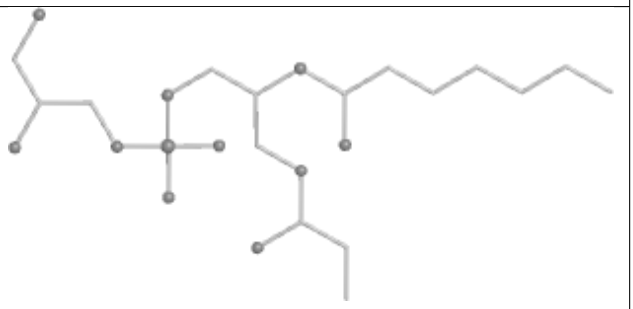
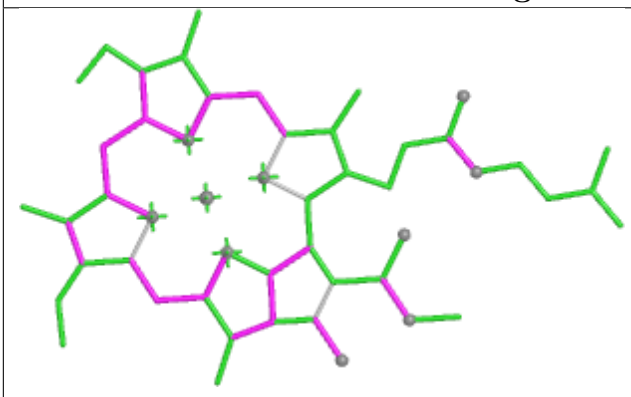


Rings

Ligand CLA bA 821



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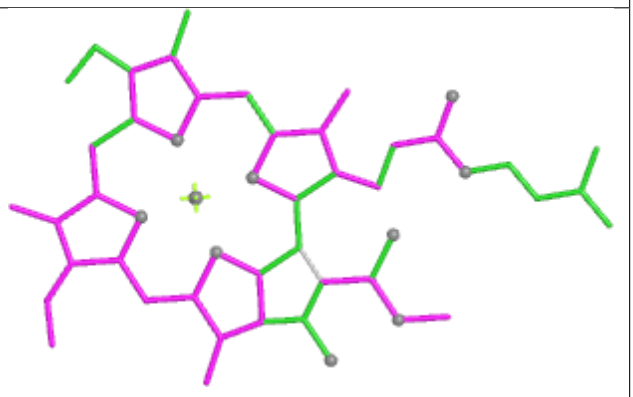
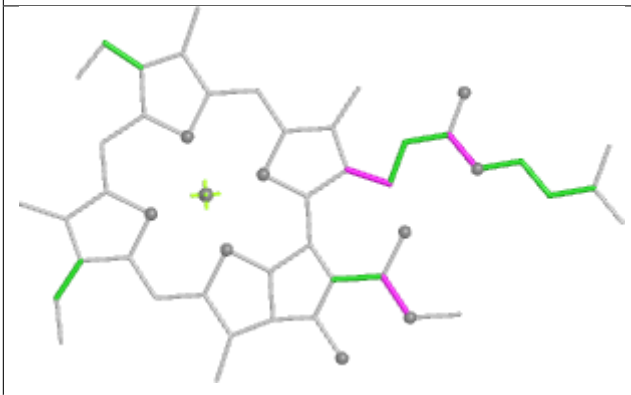


Bond angles



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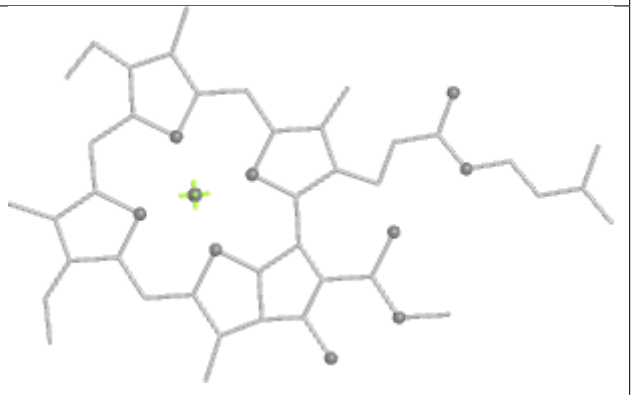
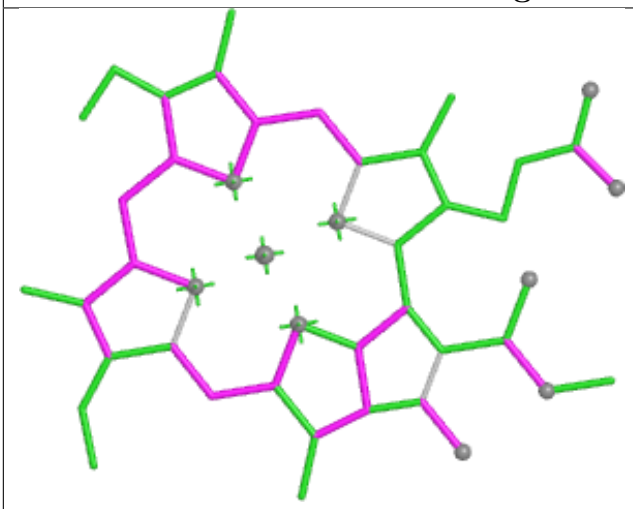


Rings

Ligand CLA bA 809



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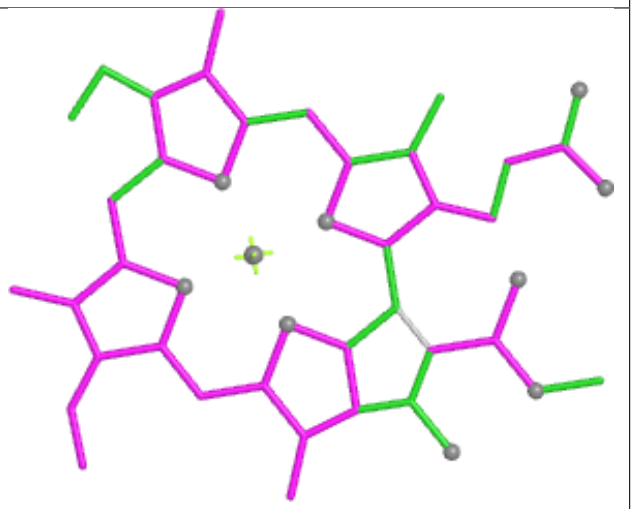
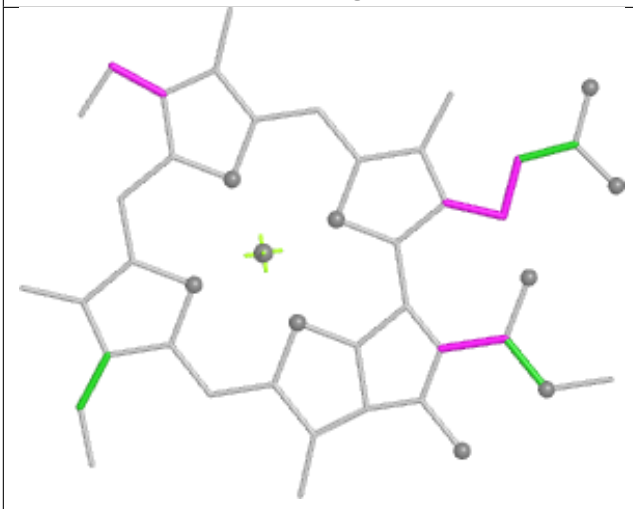


Bond angles

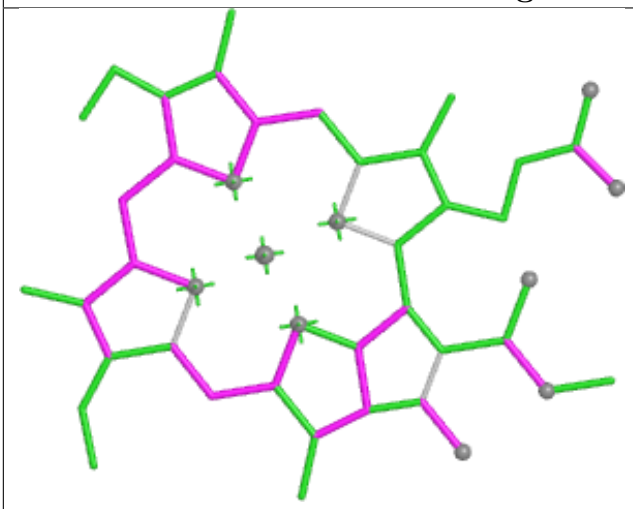


Torsions



Rings

Ligand CLA cB 911



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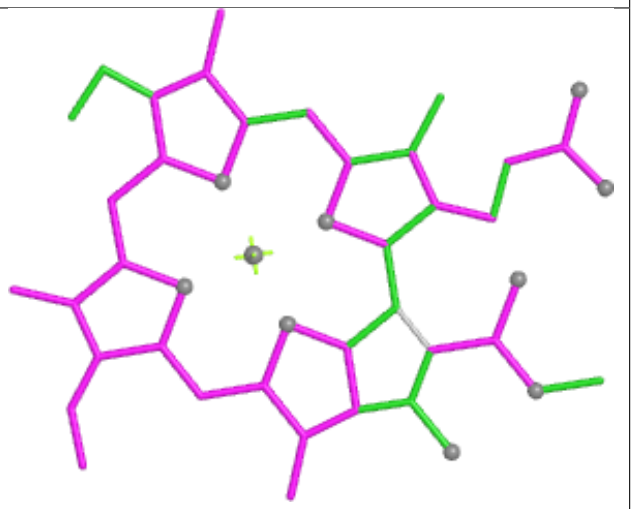
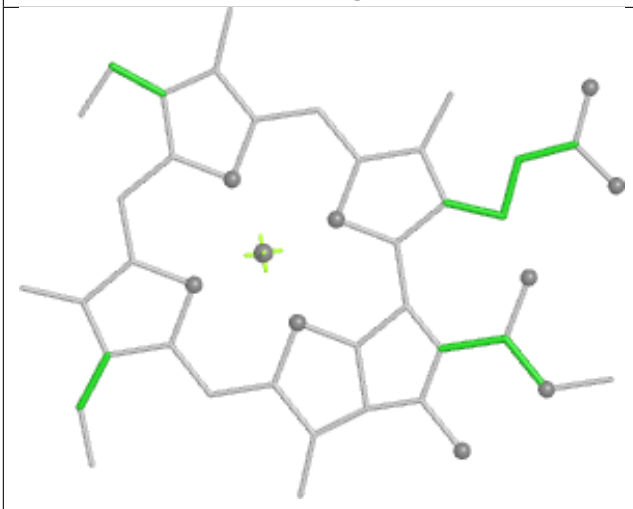


Bond angles

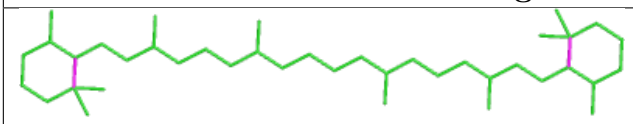


Torsions



Rings

Ligand BCR cB 943



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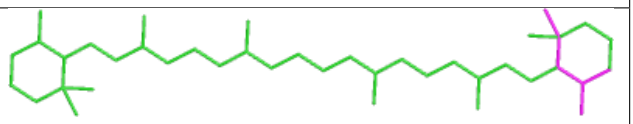
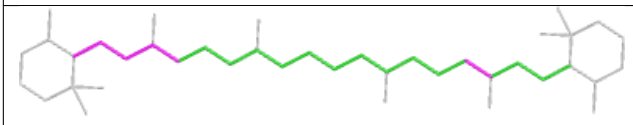


Bond angles



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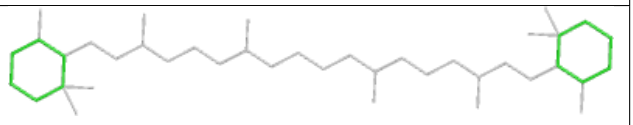
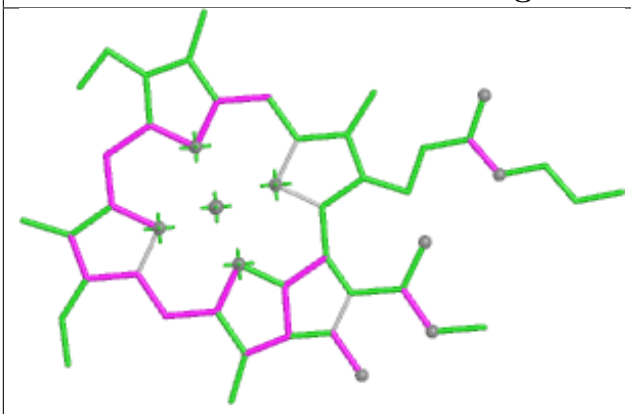
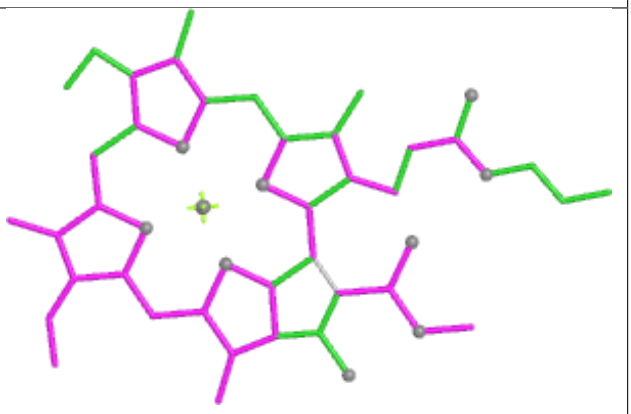
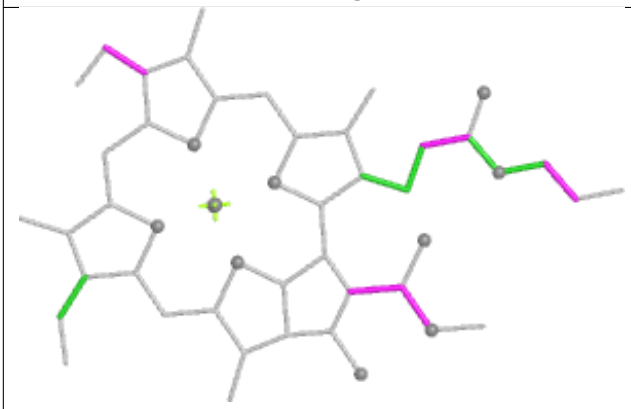
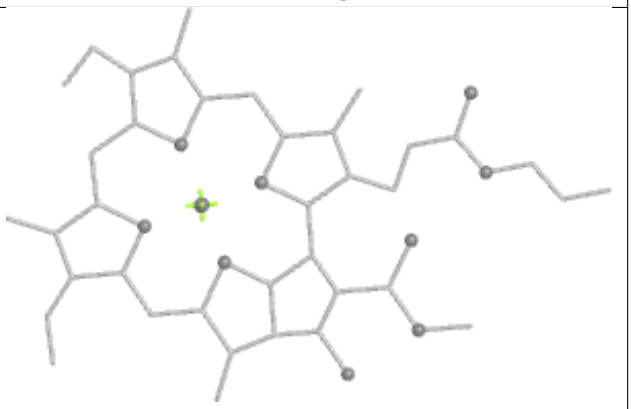
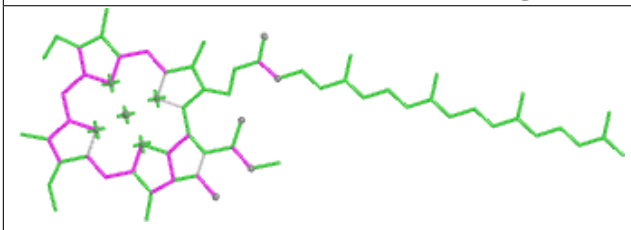
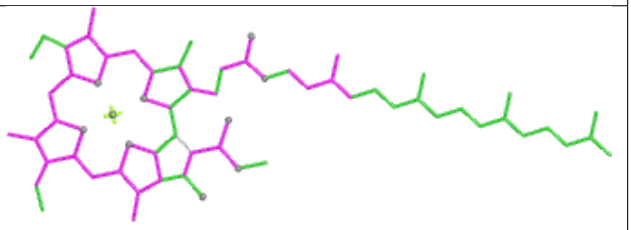
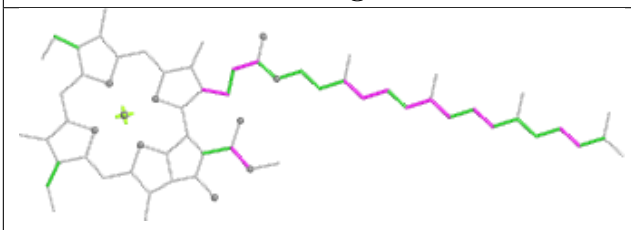
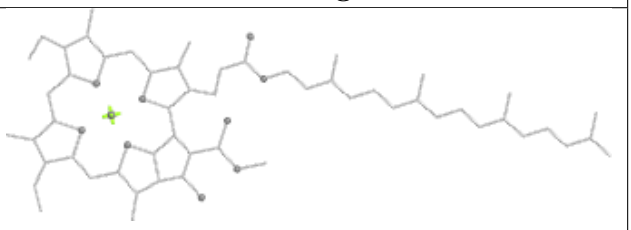
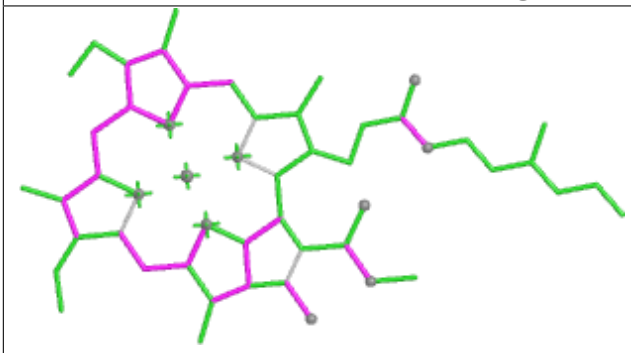


Rings

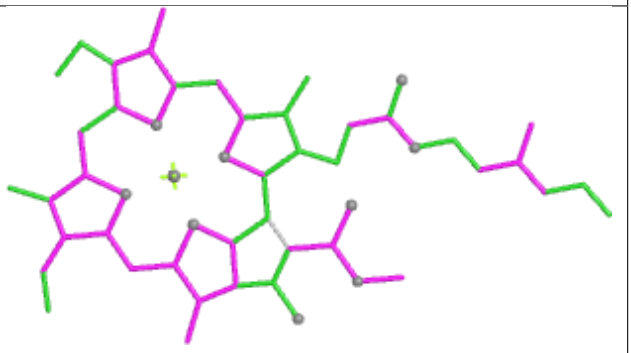
Ligand CLA bB 908	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 931	
	
Bond lengths	Bond angles
	
Torsions	Rings

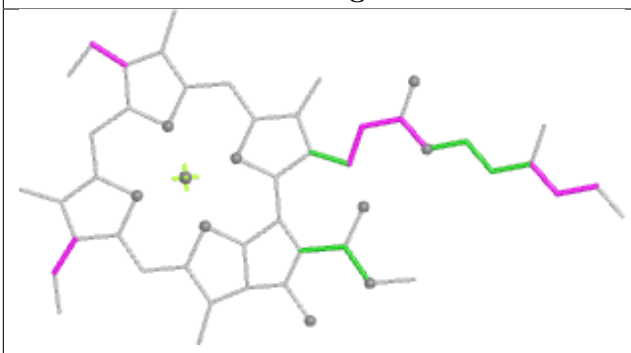
Ligand CLA bB 915



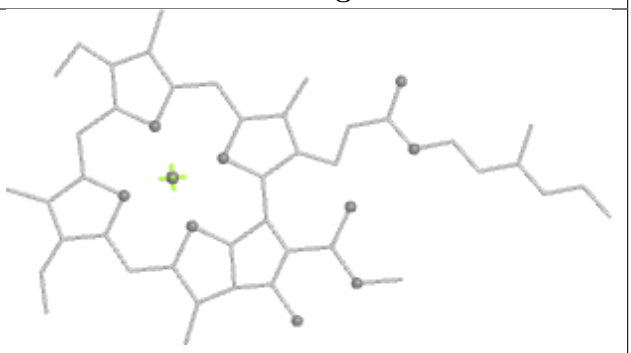
Bond lengths



Bond angles

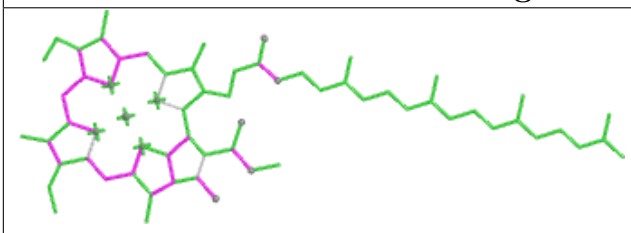


Torsions



Rings

Ligand CLA bB 901



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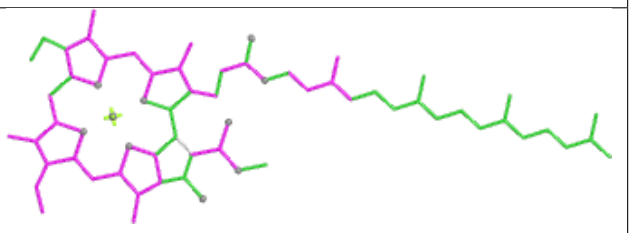
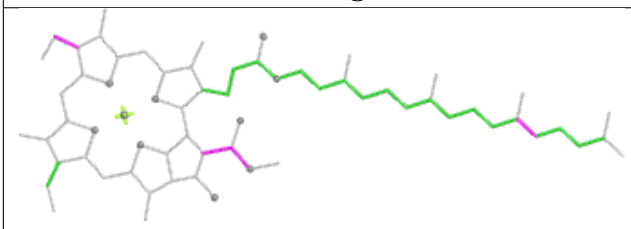


Bond angles



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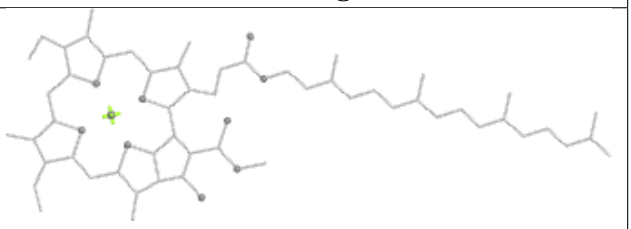
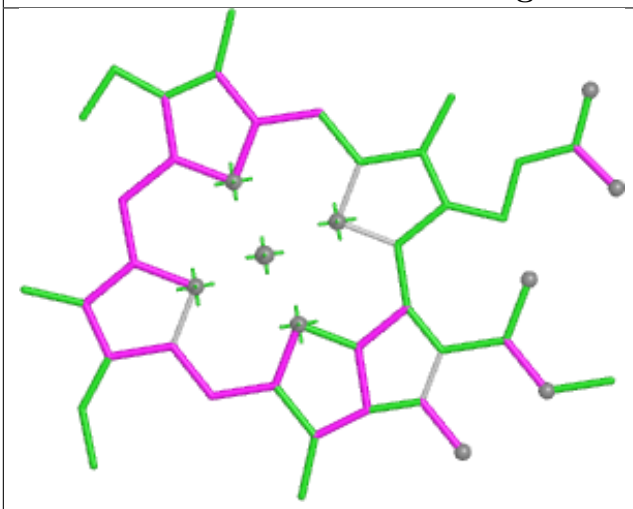


Rings

Ligand CLA cB 933



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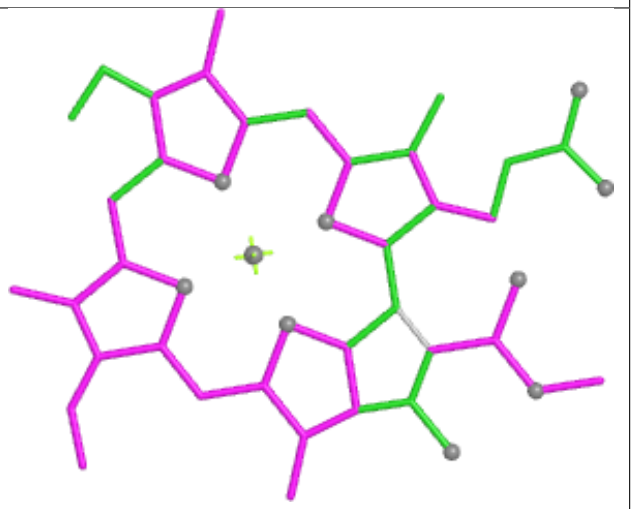
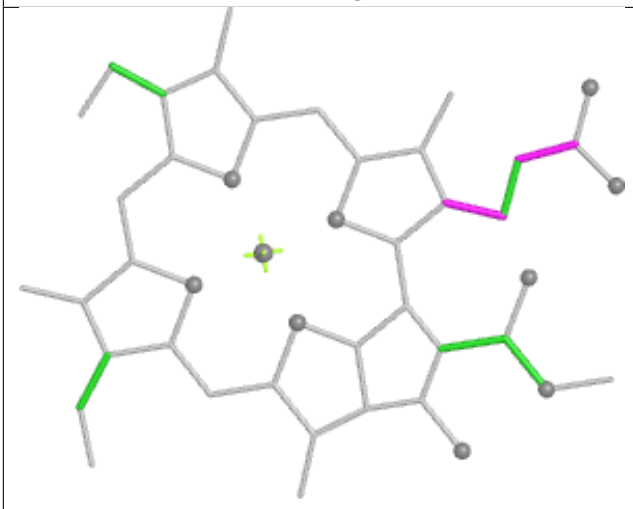


Bond angles

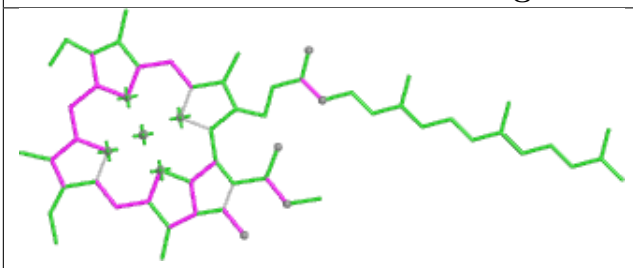


Torsions



Rings

Ligand CLA bA 819



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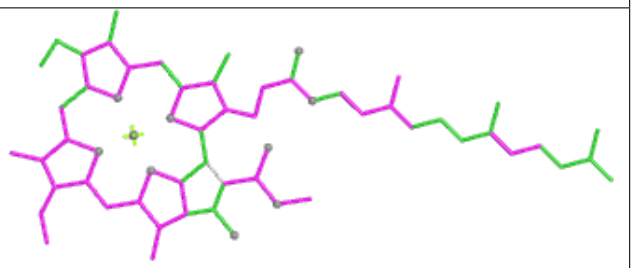
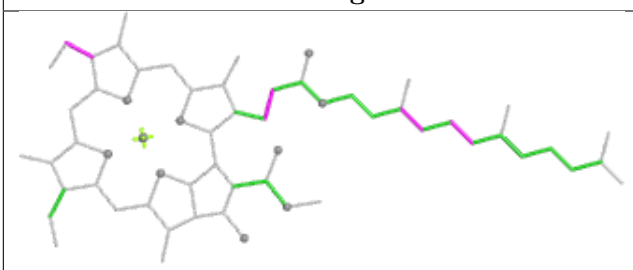
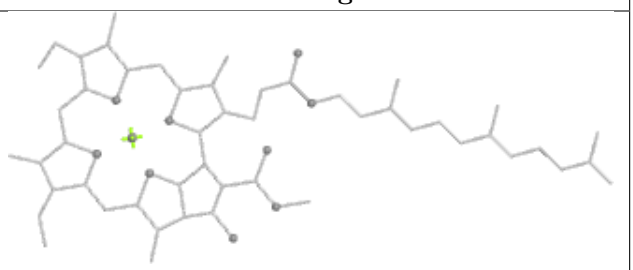


Bond angles

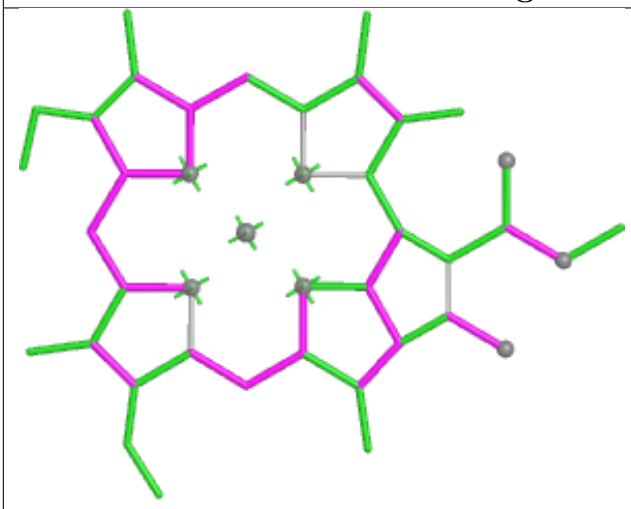


Torsions



Rings

Ligand CLA cB 949



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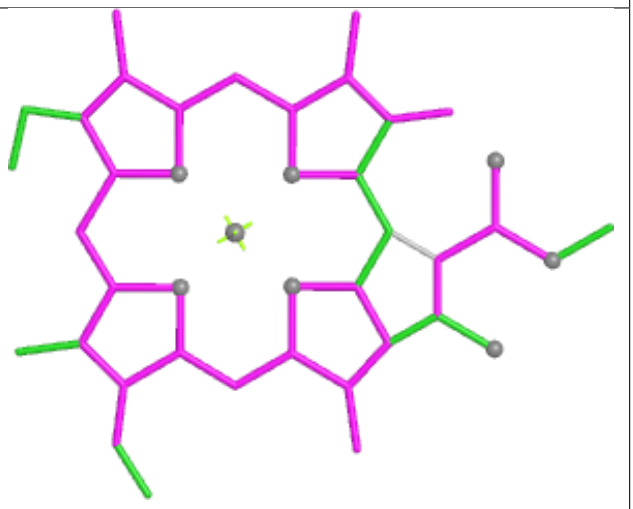
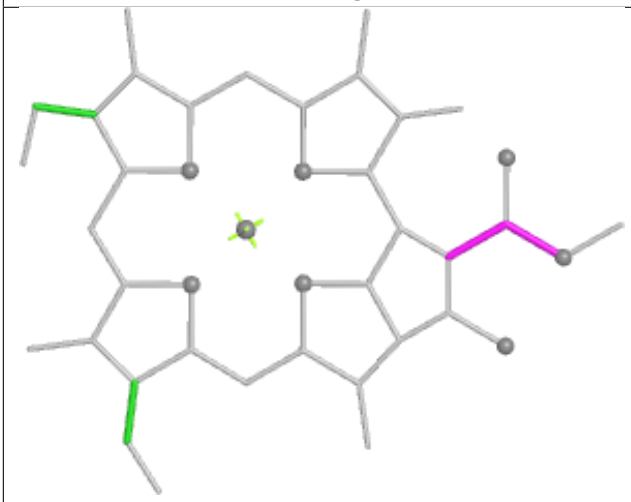


Bond angles



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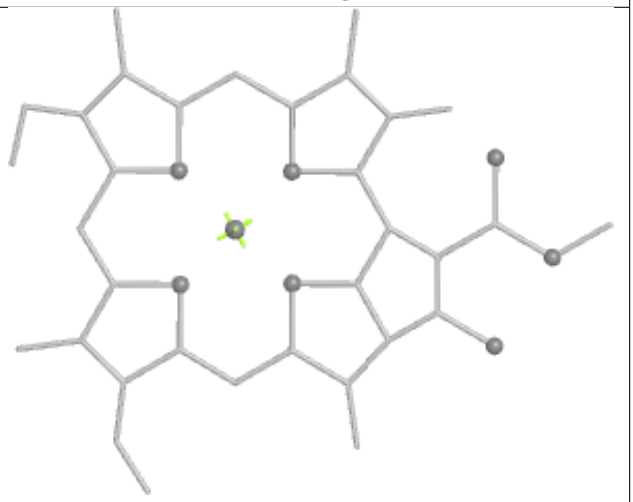
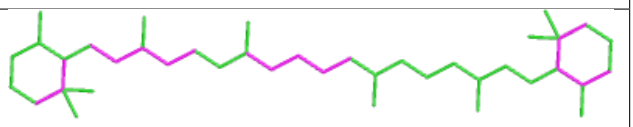


Rings

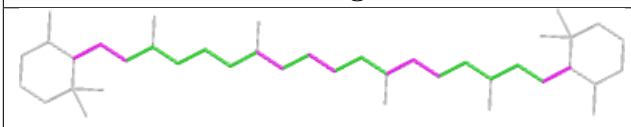
Ligand BCR bB 945



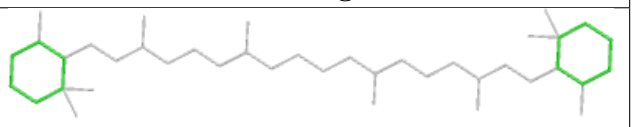
Bond lengths



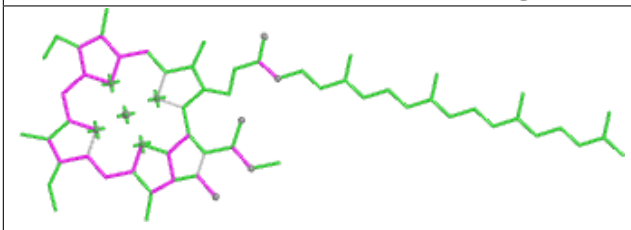
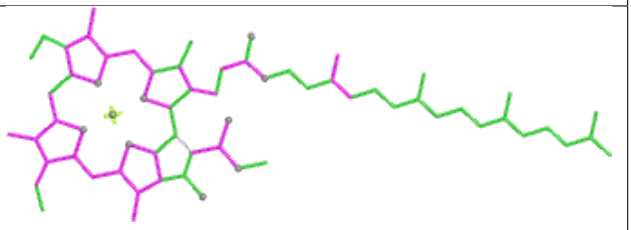
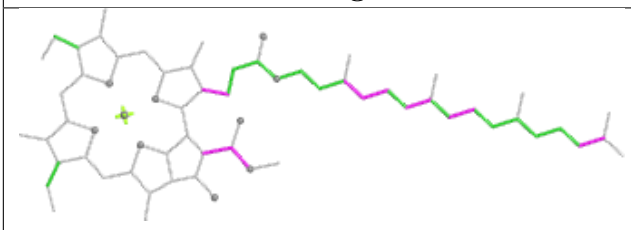
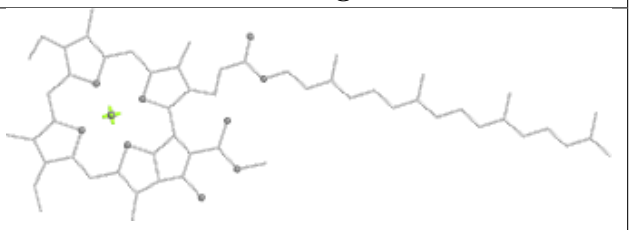
Bond angles

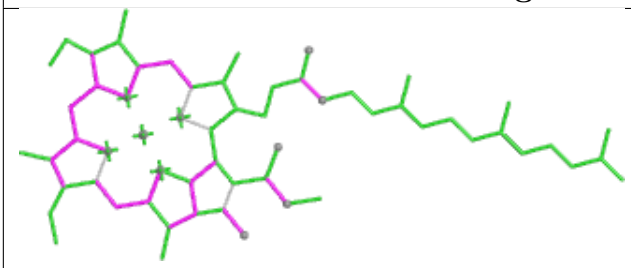
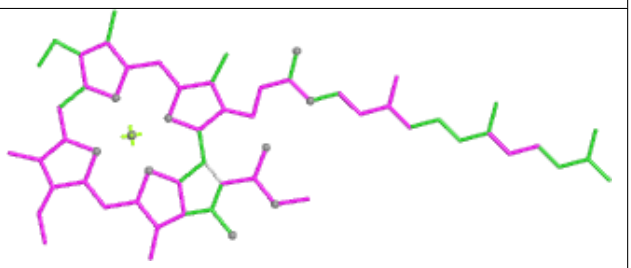
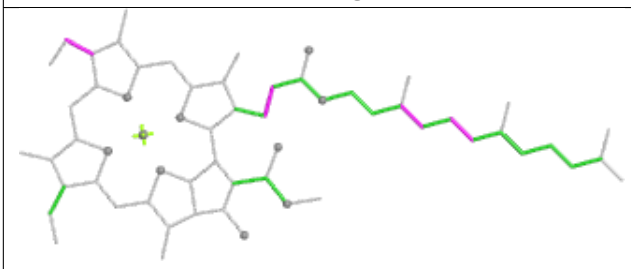
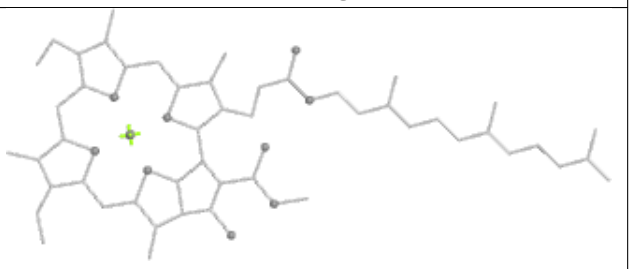


Torsions

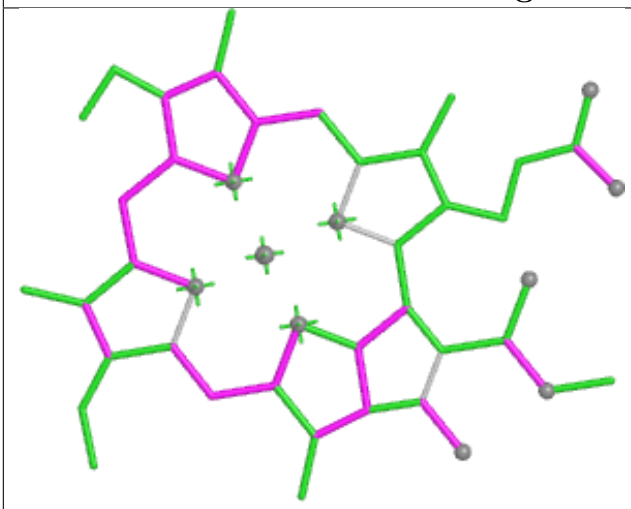


Rings

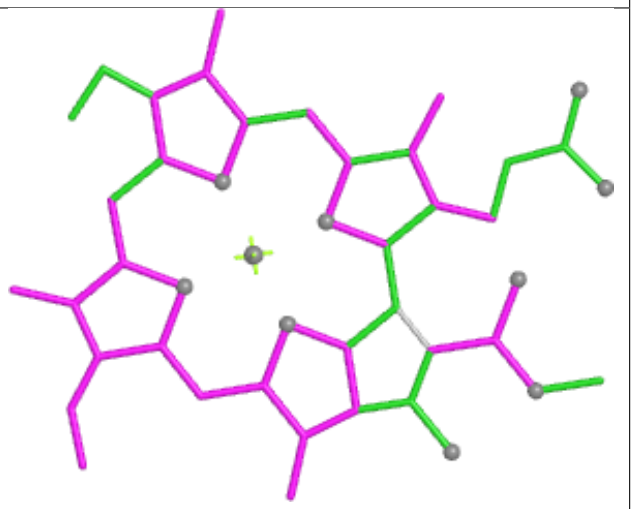
Ligand CLA aA 806	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA aA 819	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

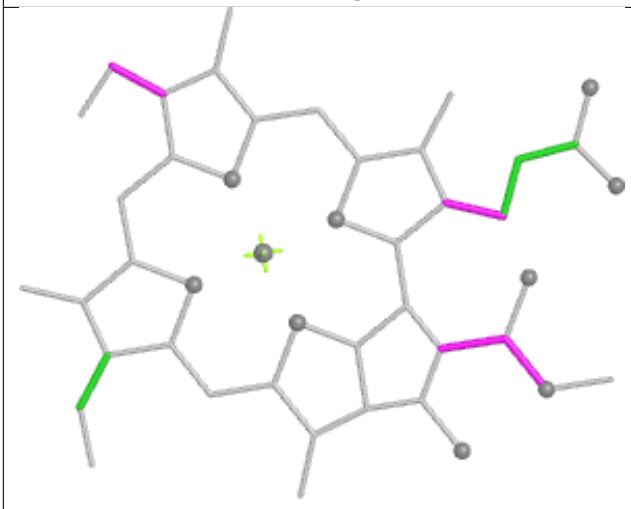
Ligand CLA cA 811



Bond lengths



Bond angles

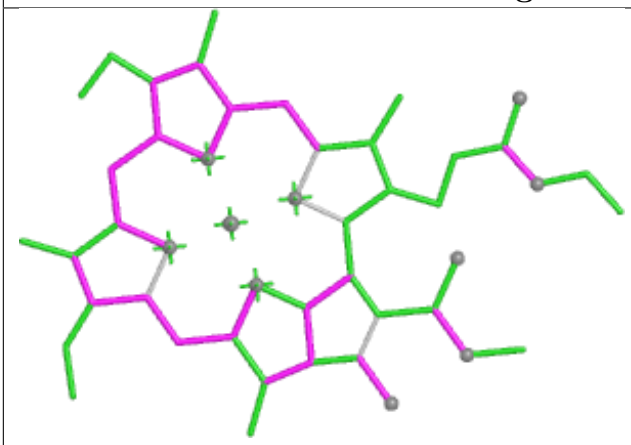


Torsions



Rings

Ligand CLA cA 824



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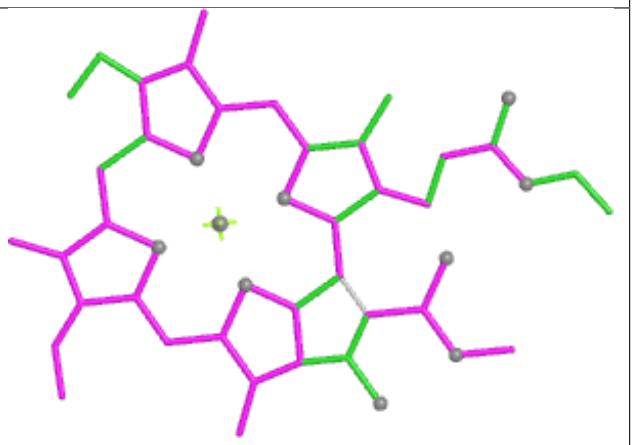
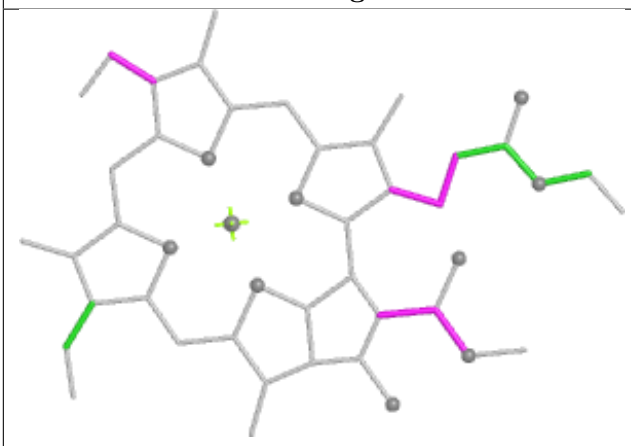
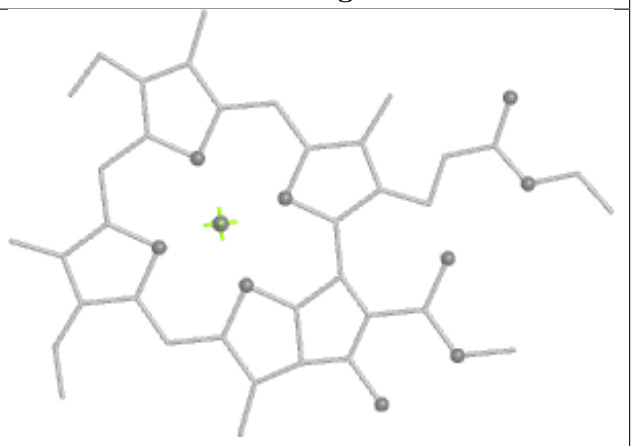


Bond angles

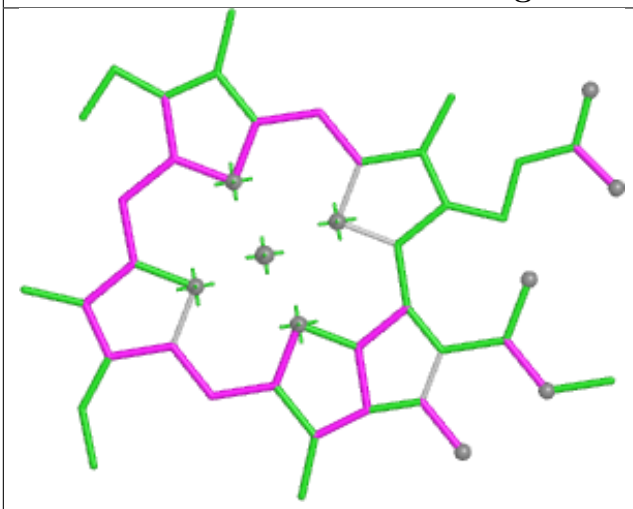


Torsions

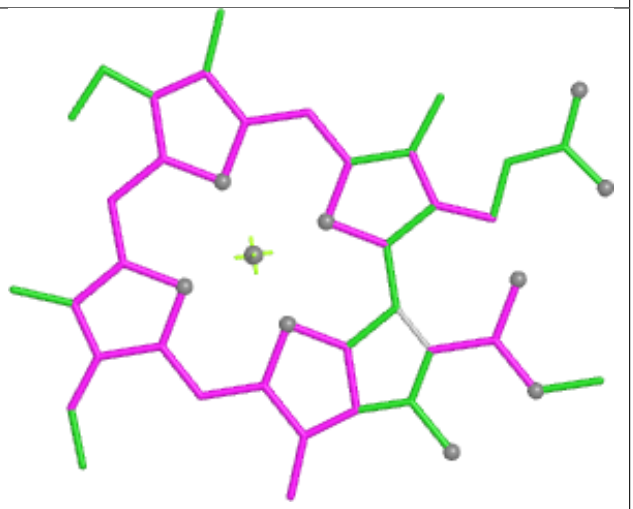


Rings

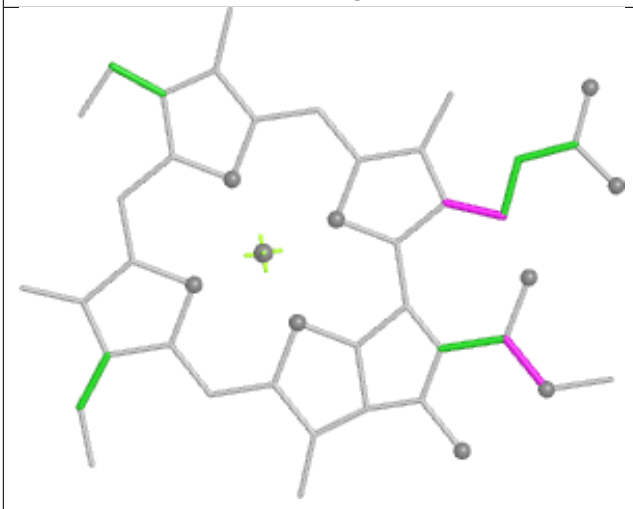
Ligand CLA bB 934



Bond lengths



Bond angles

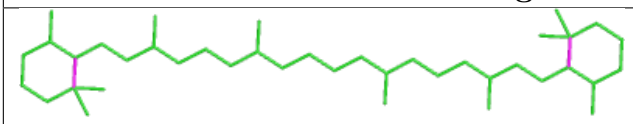


Torsions



Rings

Ligand BCR aF 203



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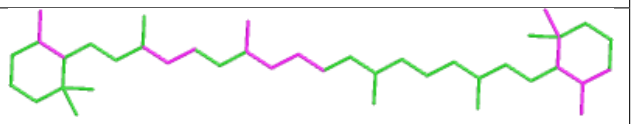
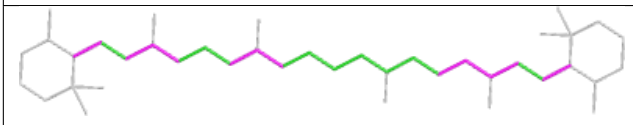


Bond angles



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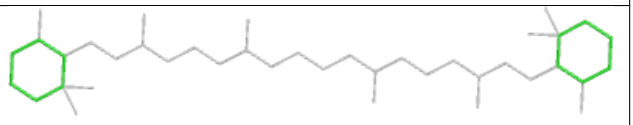
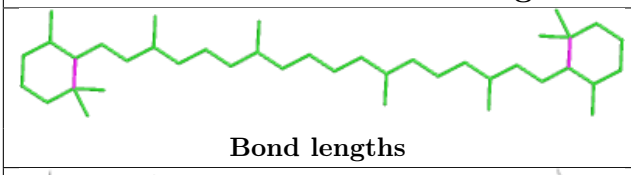


Rings

Ligand BCR cB 942



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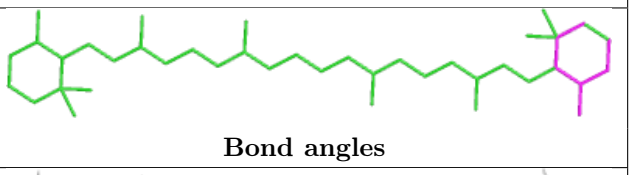
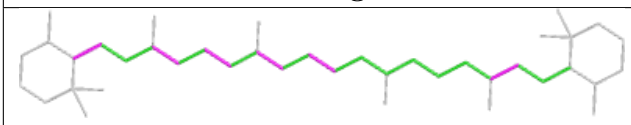


Bond angles



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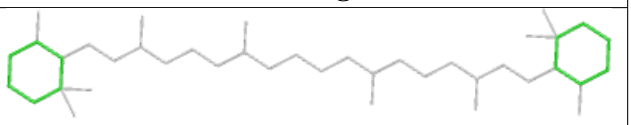
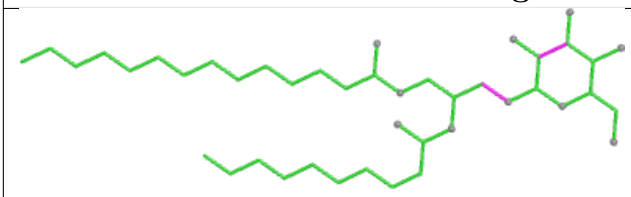


Rings

Ligand LMG cB 947



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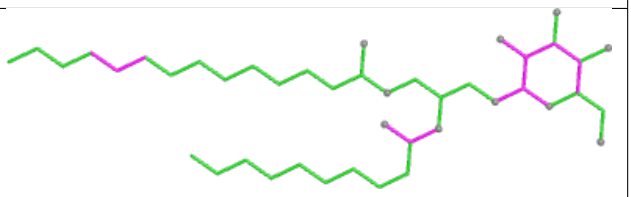
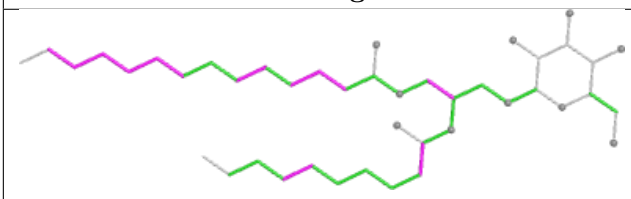


Bond angles



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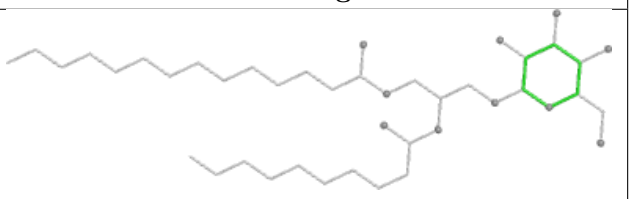
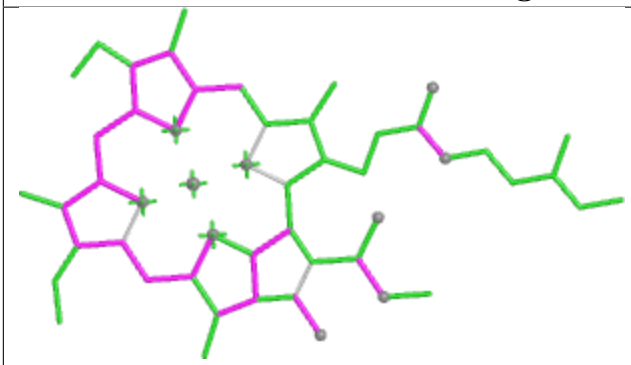


Rings

Ligand CLA cA 808



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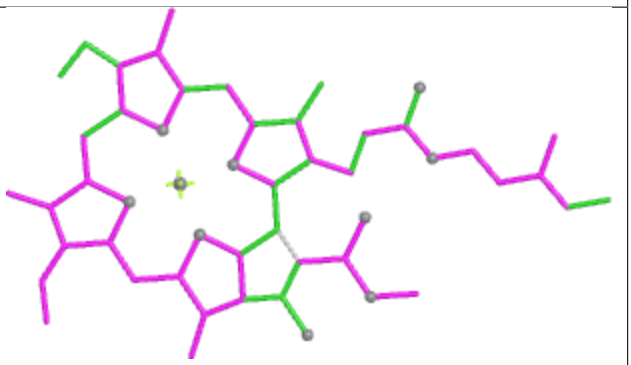
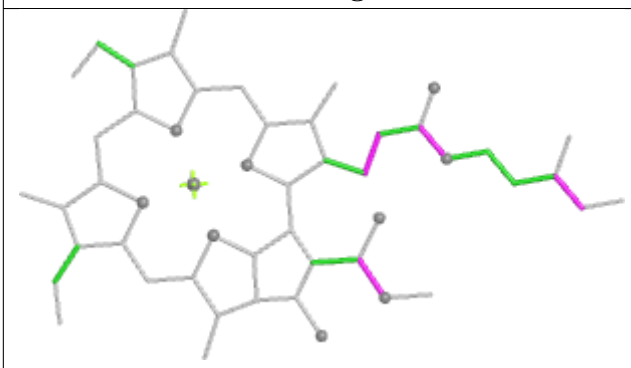
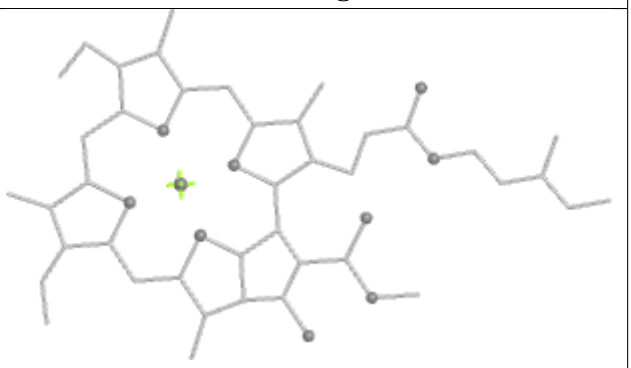


Bond angles

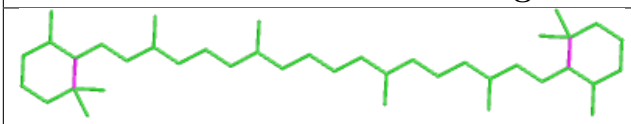


Torsions



Rings

Ligand BCR aB 944



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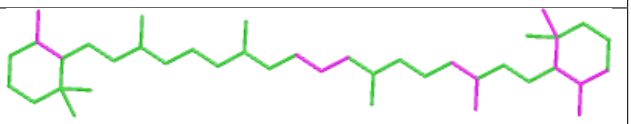
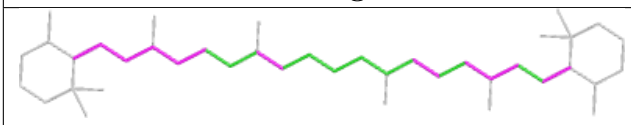
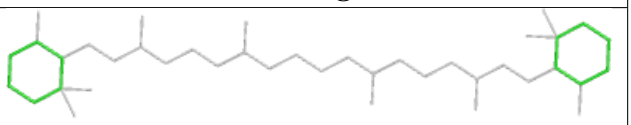


Bond angles

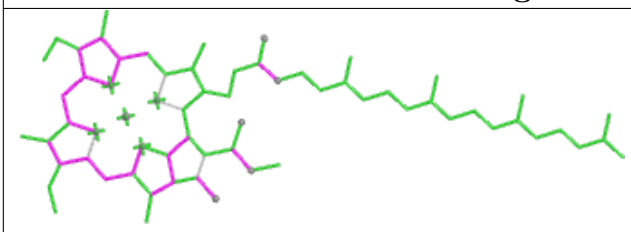


Torsions

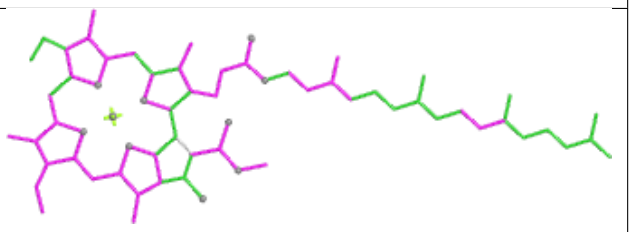


Rings

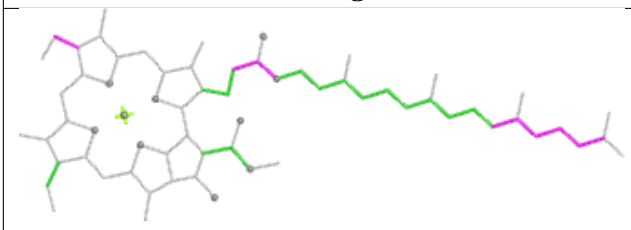
Ligand CLA bA 843



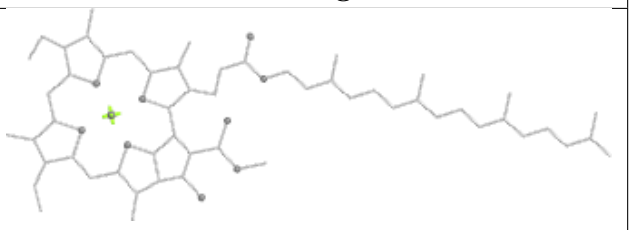
Bond lengths



Bond angles

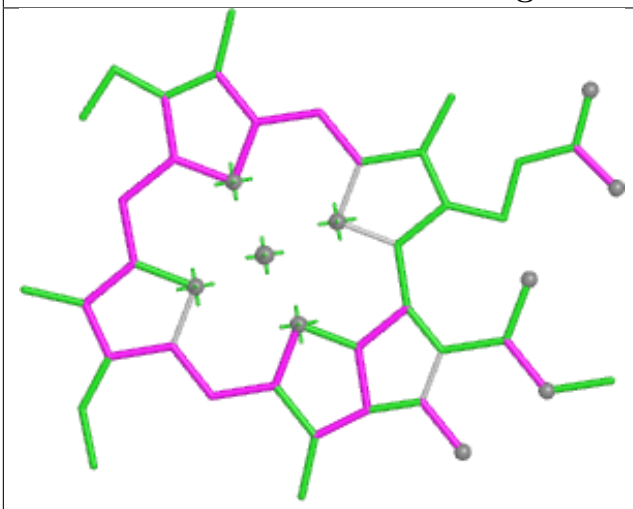


Torsions



Rings

Ligand CLA cB 929



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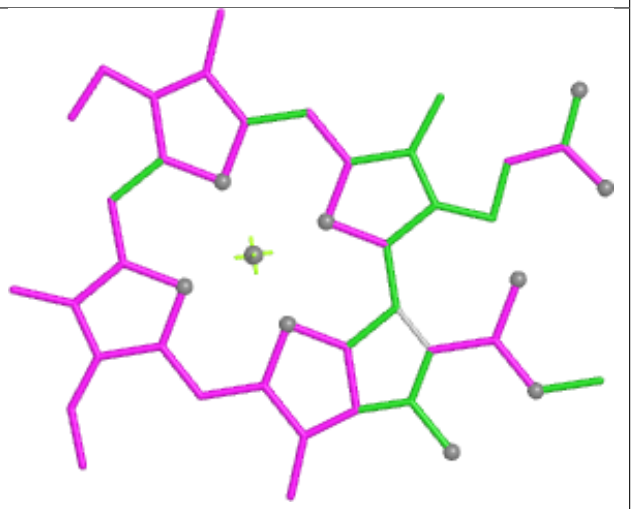
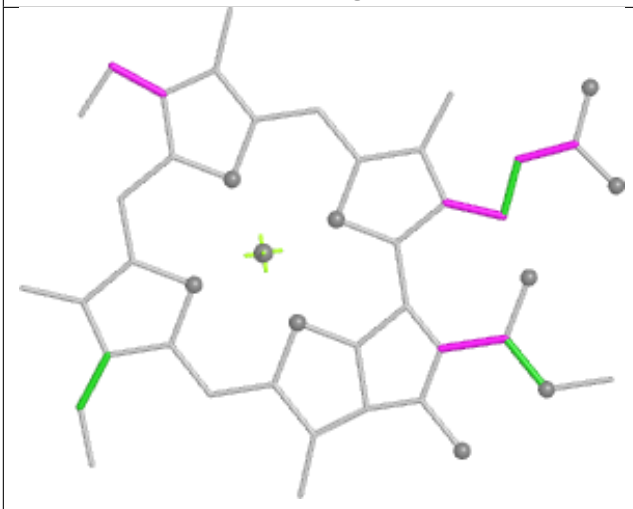


Bond angles

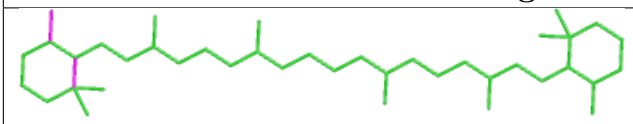


Torsions



Rings

Ligand BCR cJ 101



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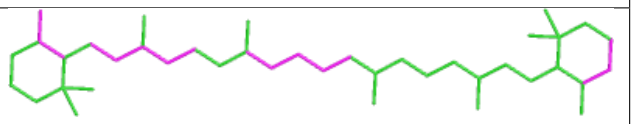
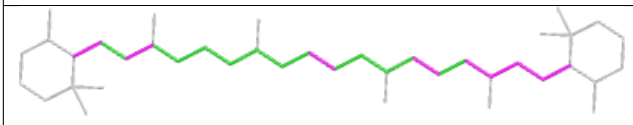
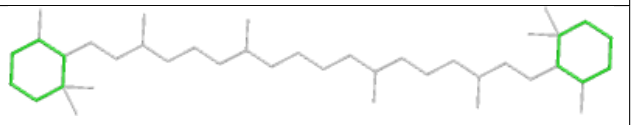


Bond angles

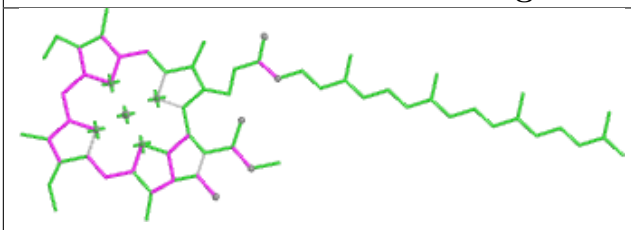


Torsions



Rings

Ligand CLA cA 802



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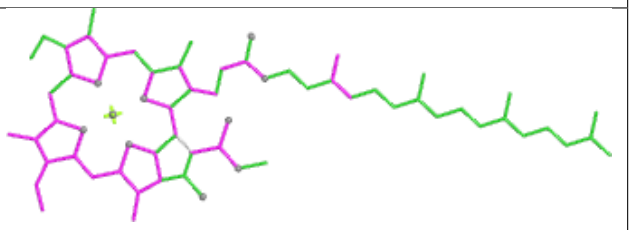
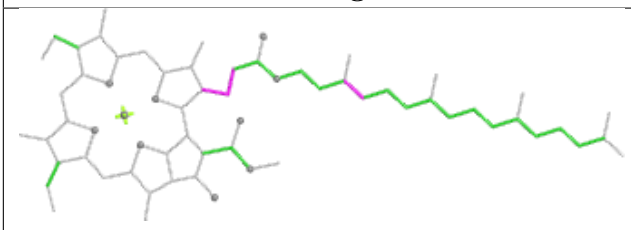


Bond angles



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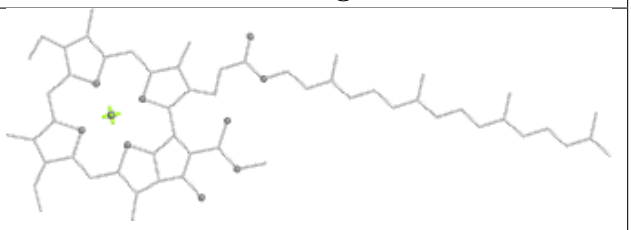
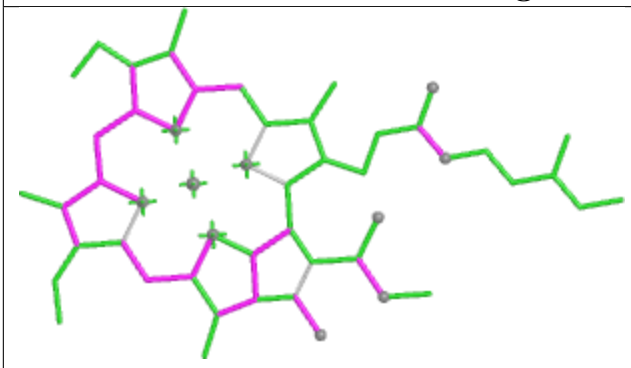
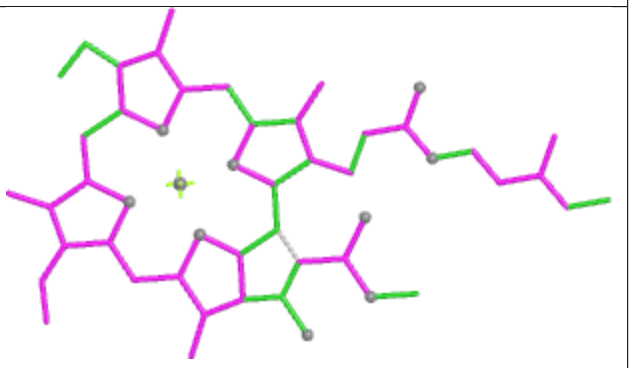


Rings

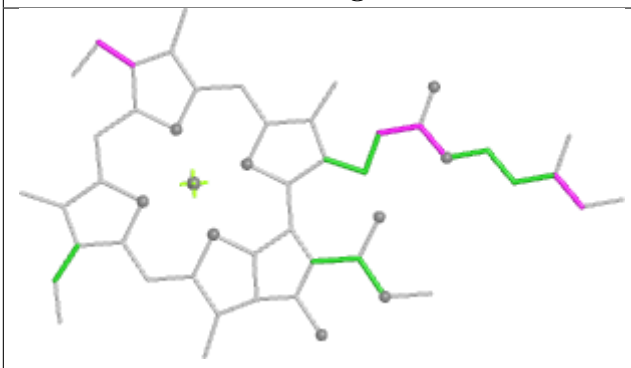
Ligand CLA aA 823



Bond lengths



Bond angles



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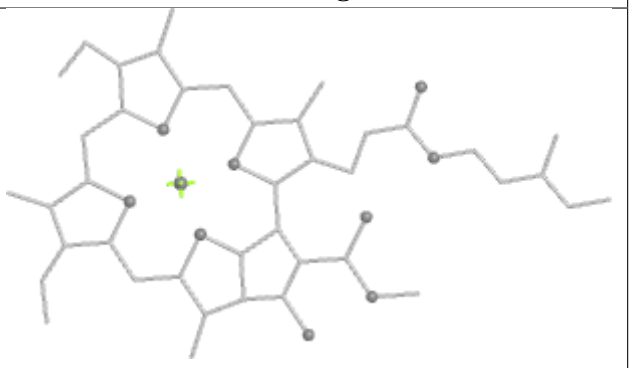
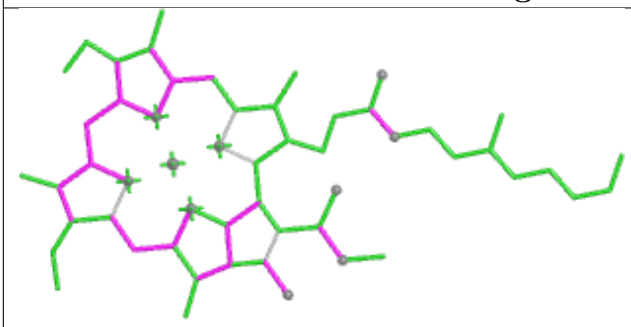
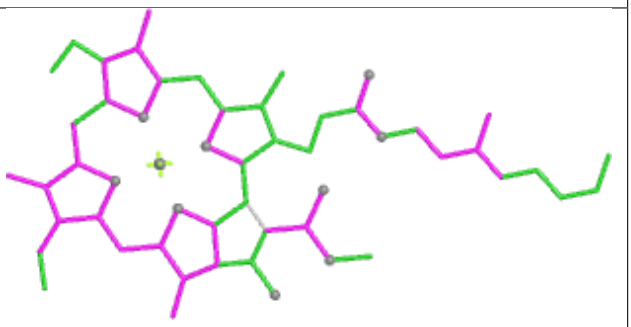


Rings

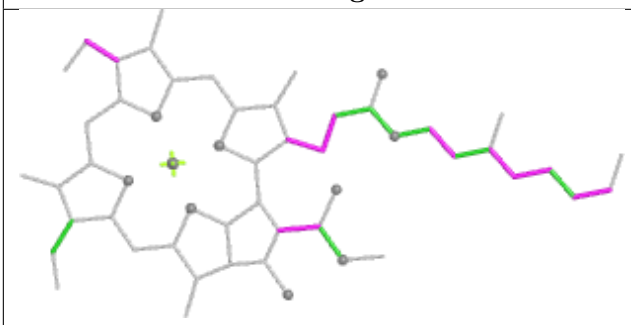
Ligand CLA bB 923



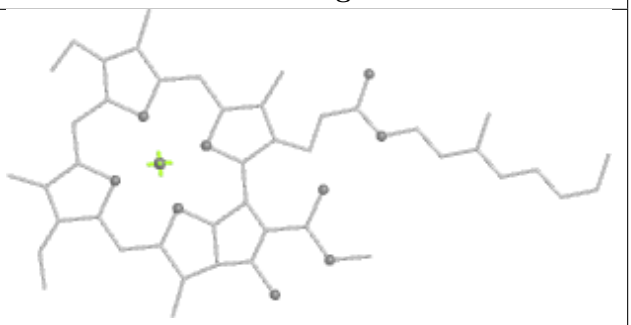
Bond lengths



Bond angles

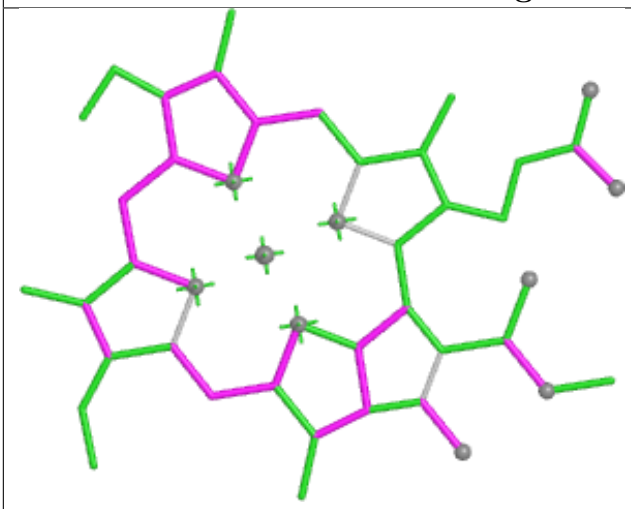


Torsions

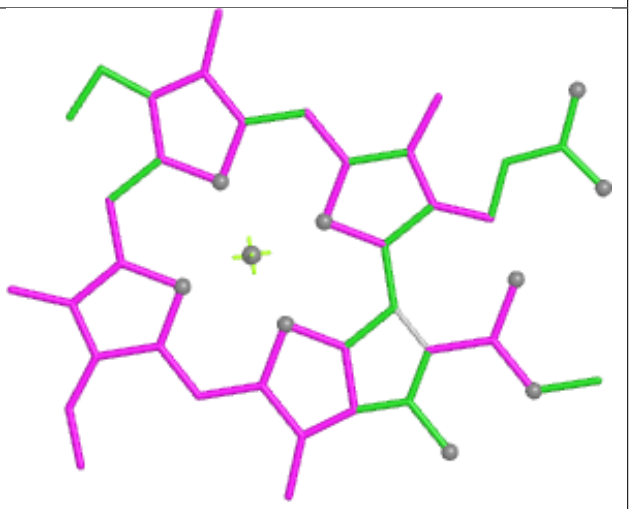


Rings

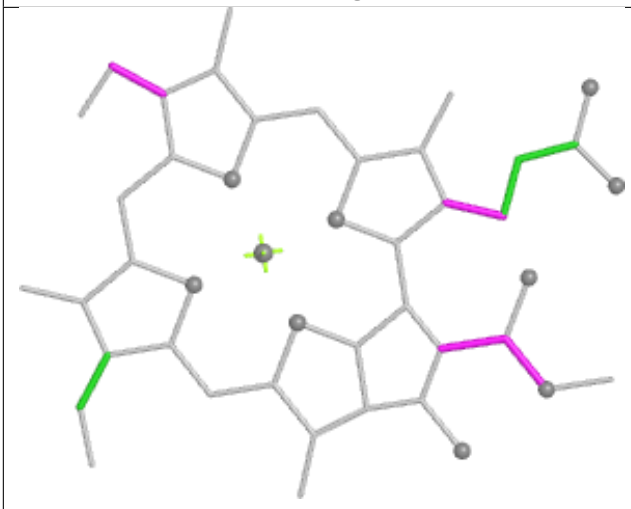
Ligand CLA aA 811



Bond lengths



Bond angles

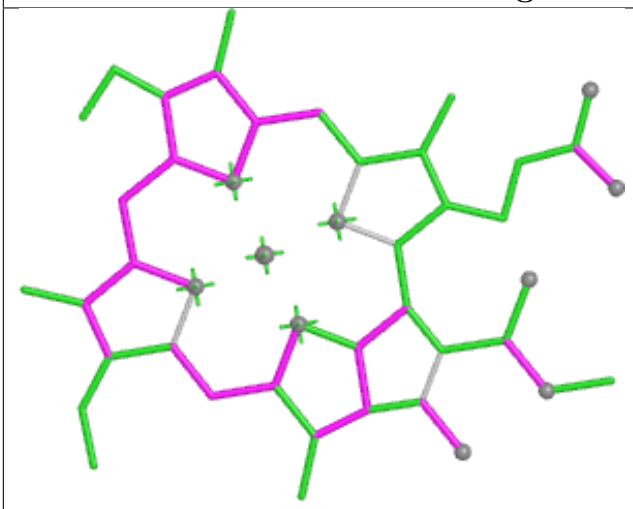


Torsions

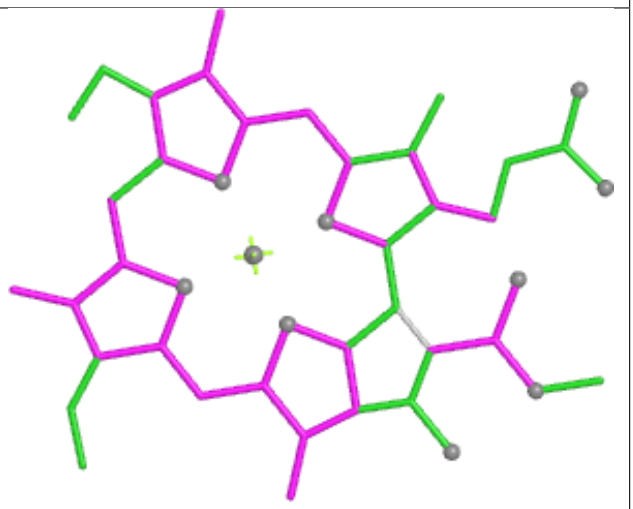


Rings

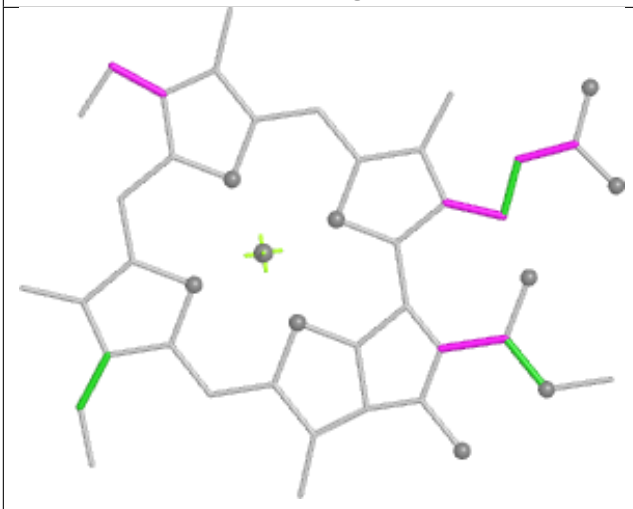
Ligand CLA cB 914



Bond lengths



Bond angles

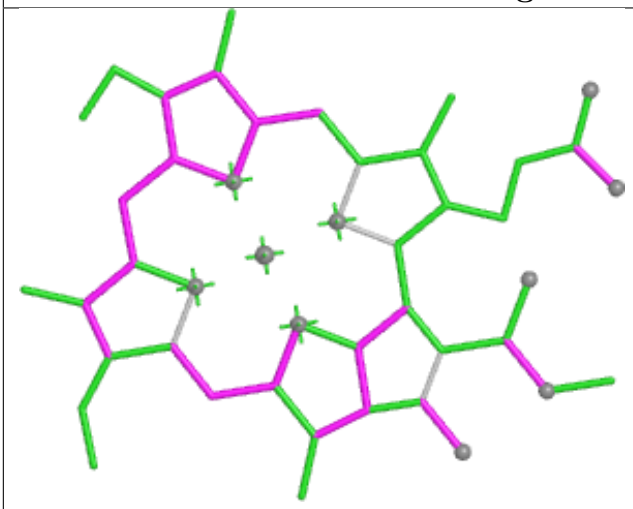


Torsions

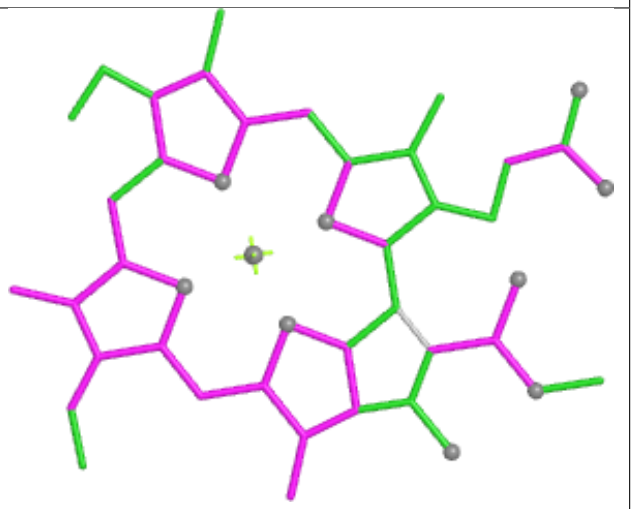


Rings

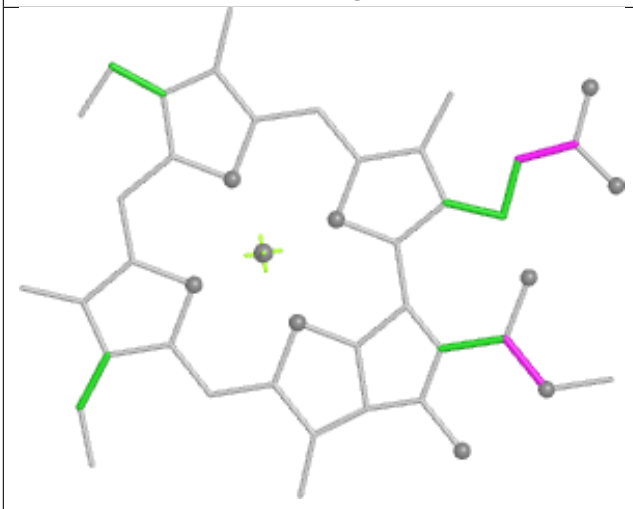
Ligand CLA cB 920



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.

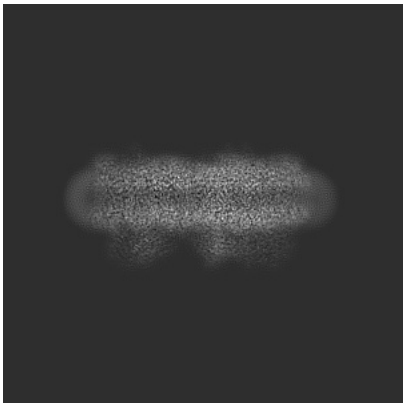
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31455. These allow visual inspection of the internal detail of the map and identification of artifacts.

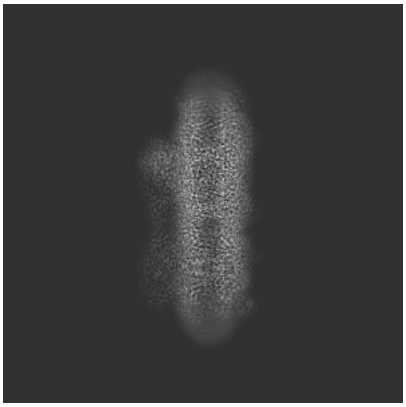
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

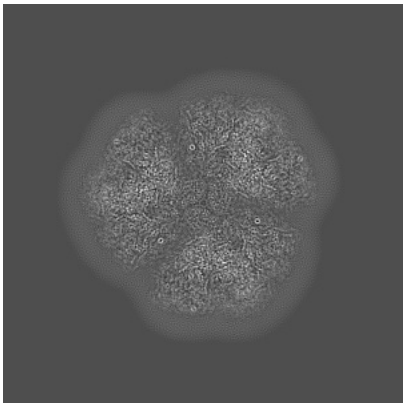
6.1.1 Primary map



X



Y



Z

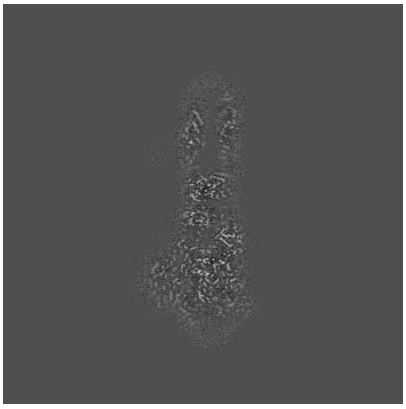
The images above show the map projected in three orthogonal directions.

6.2 Central slices

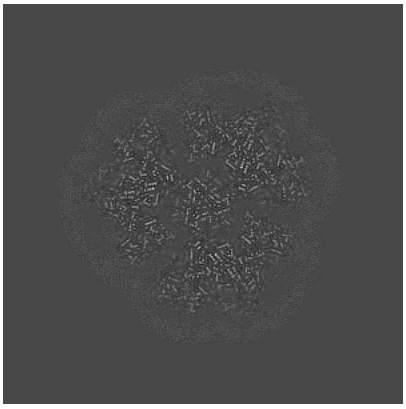
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

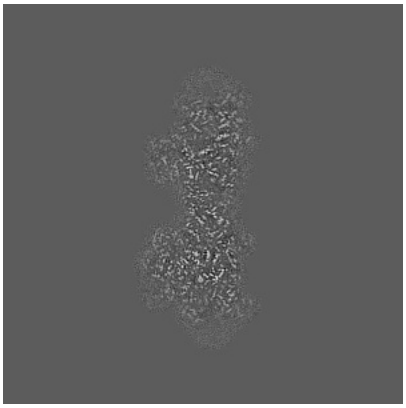
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

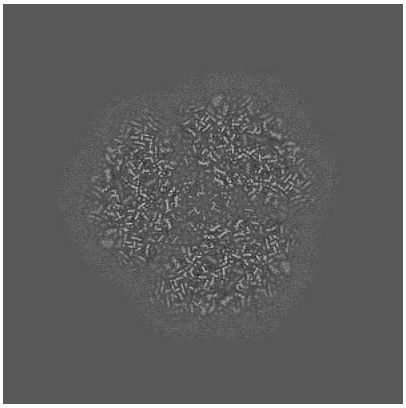
6.3.1 Primary map



X Index: 245



Y Index: 216

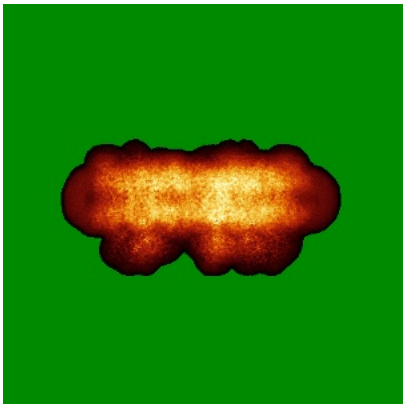


Z Index: 219

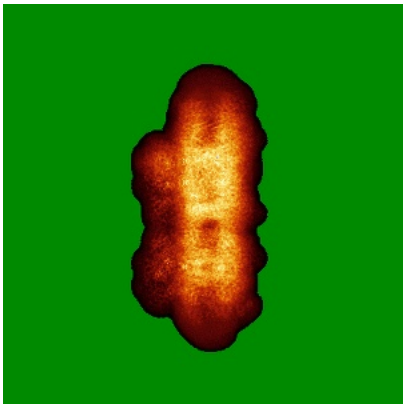
The images above show the largest variance slices of the map in three orthogonal directions.

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

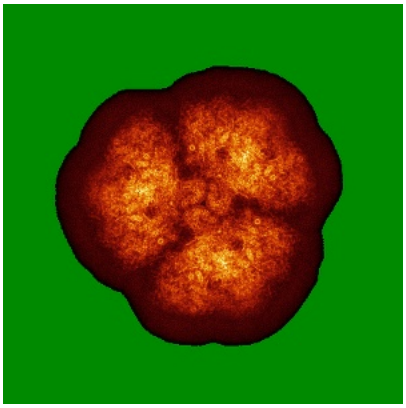
6.4.1 Primary map



X



Y

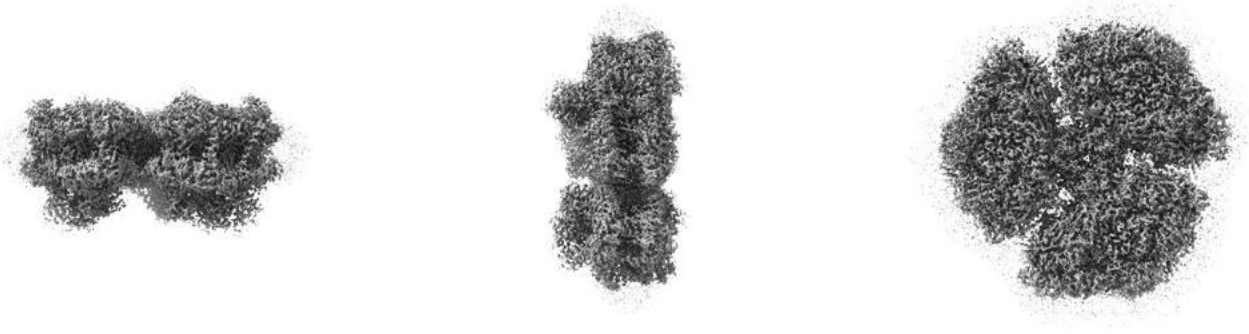


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

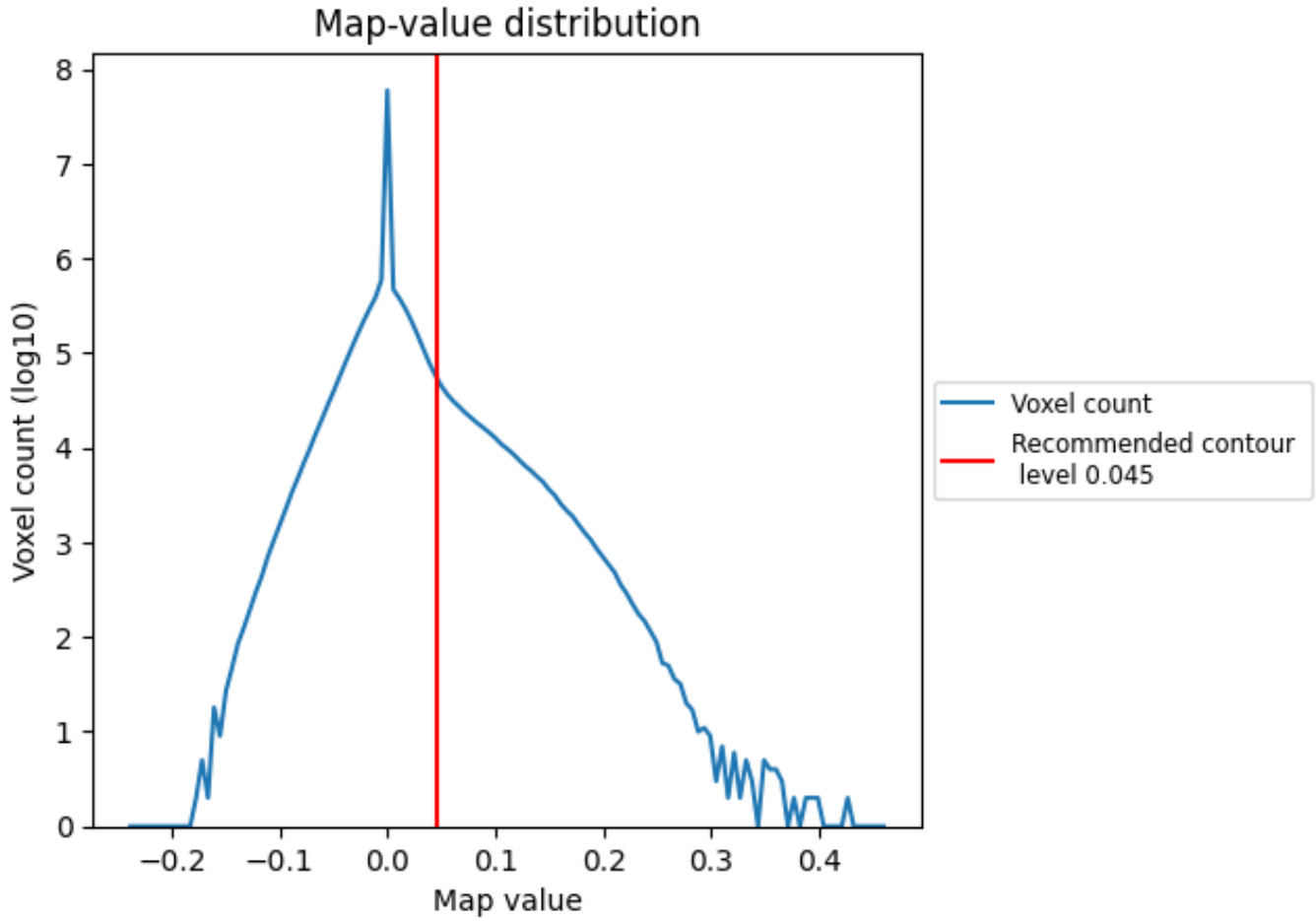
6.6 Mask visualisation (i)

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

7 Map analysis

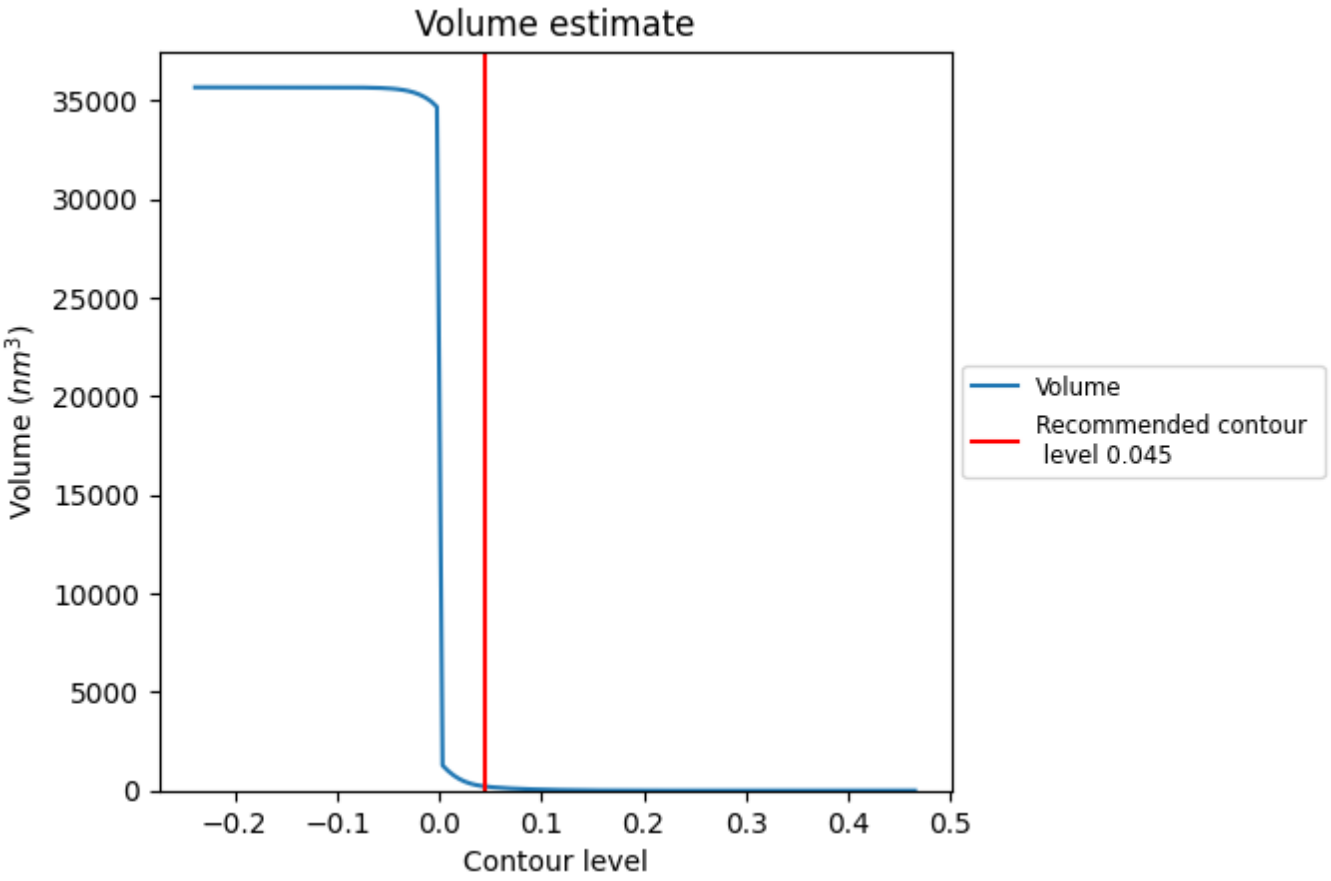
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

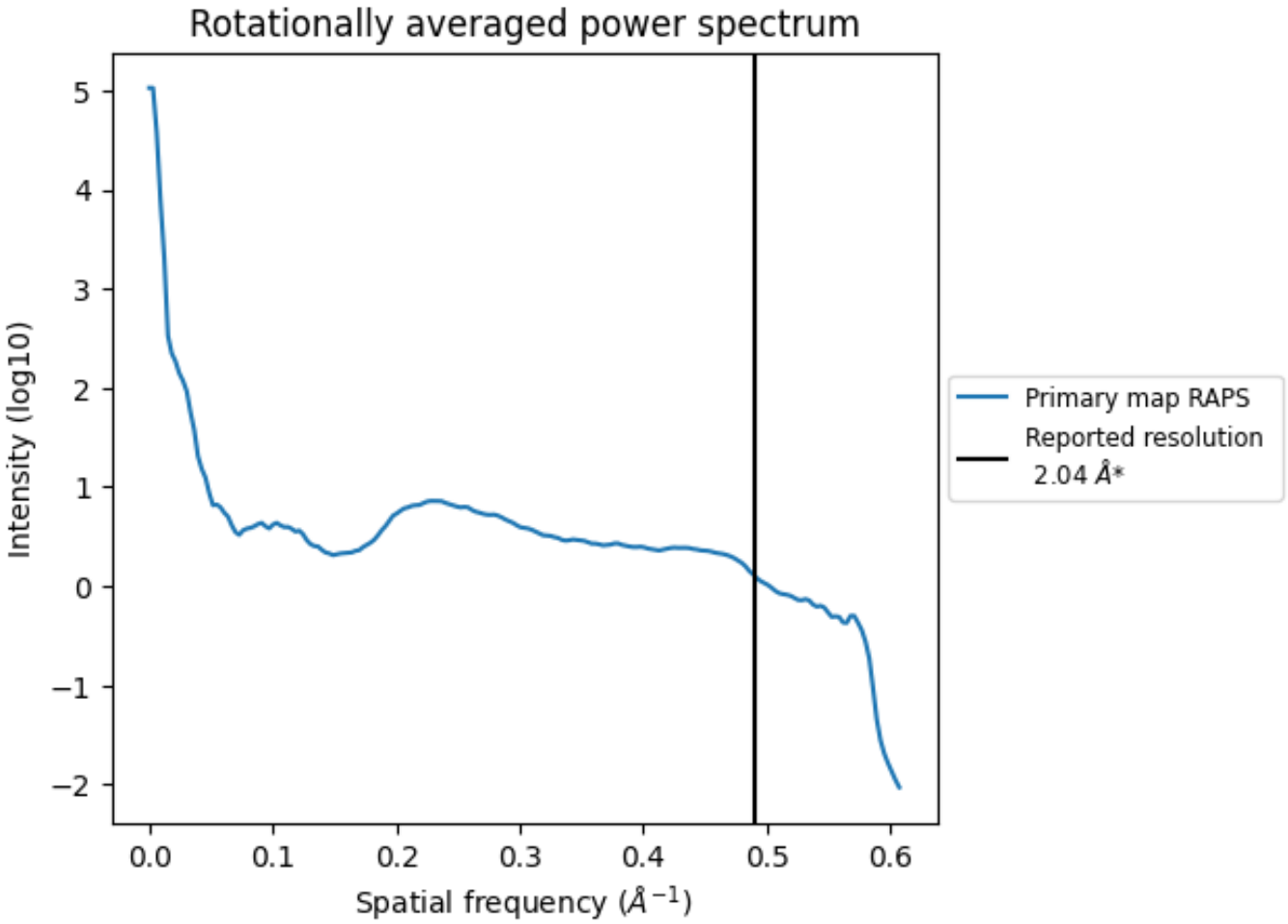
7.2 Volume estimate



The volume at the recommended contour level is 209 nm^3; this corresponds to an approximate mass of 189 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)

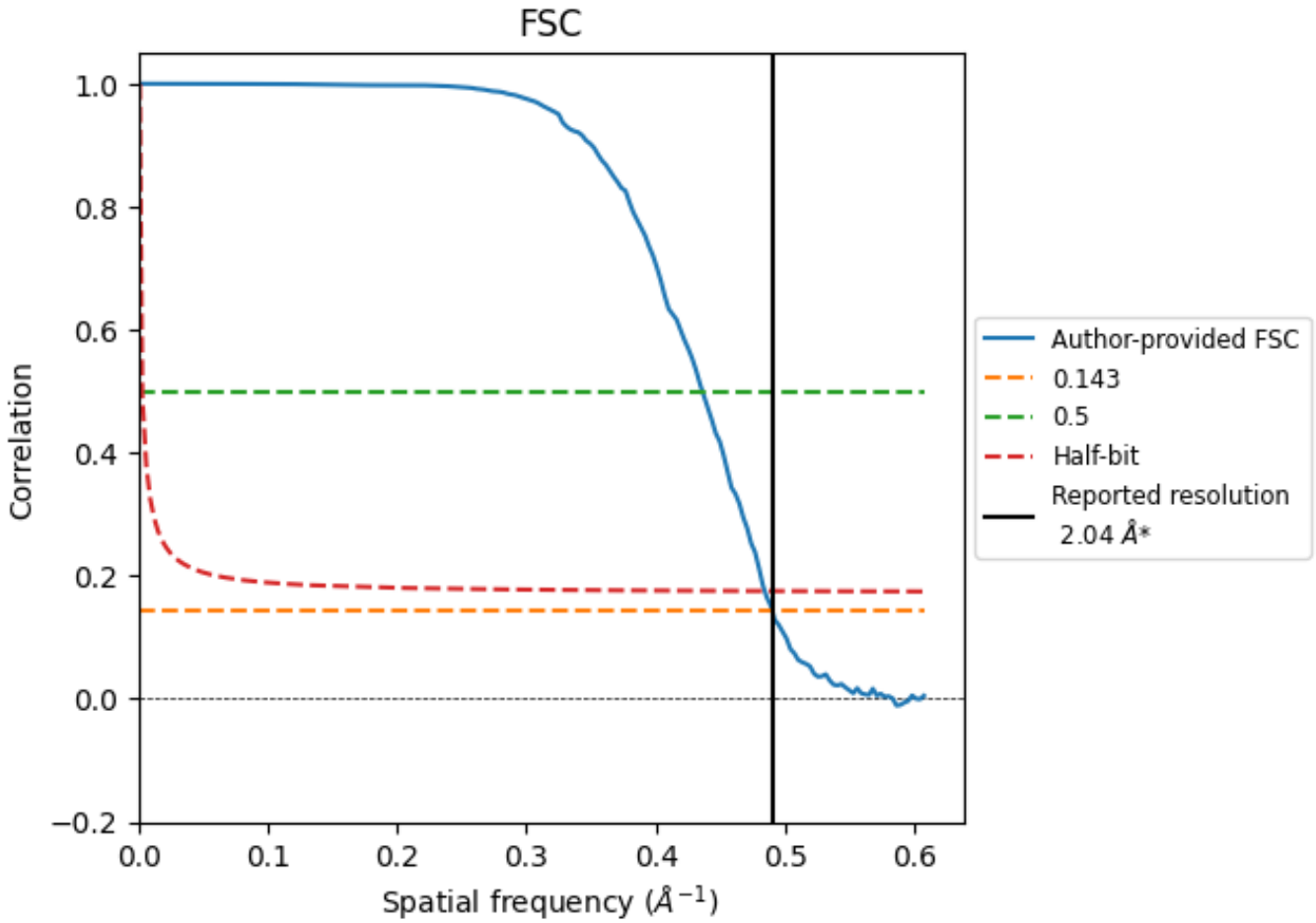


*Reported resolution corresponds to spatial frequency of 0.490 Å^{-1}

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 0.490 Å^{-1}

8.2 Resolution estimates (i)

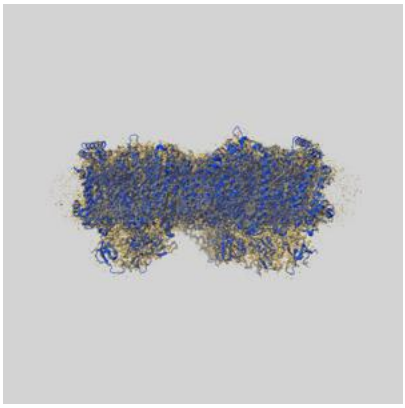
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.29	2.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

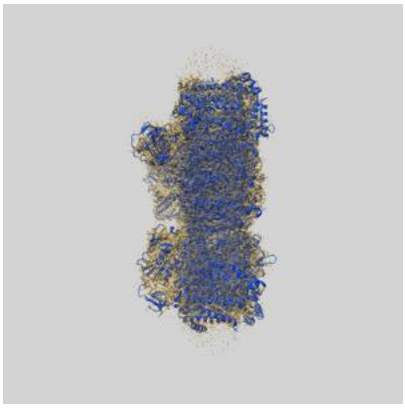
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31455 and PDB model 7F4V. Per-residue inclusion information can be found in section 3 on page 29.

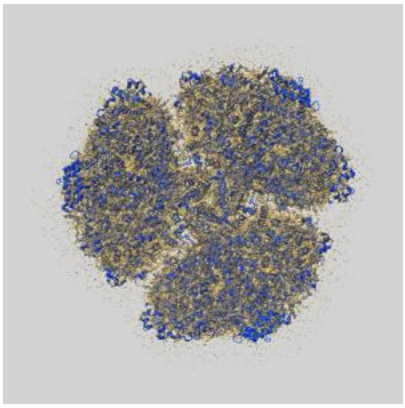
9.1 Map-model overlay



X



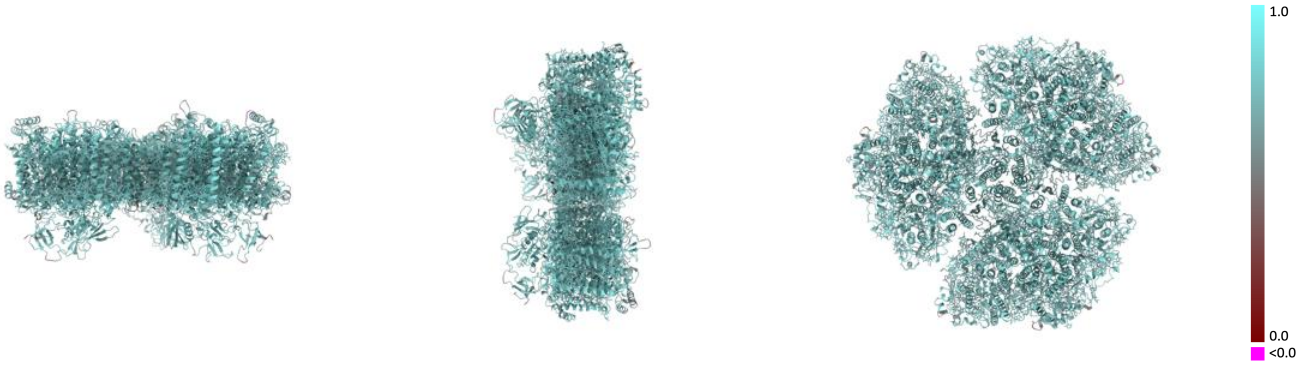
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

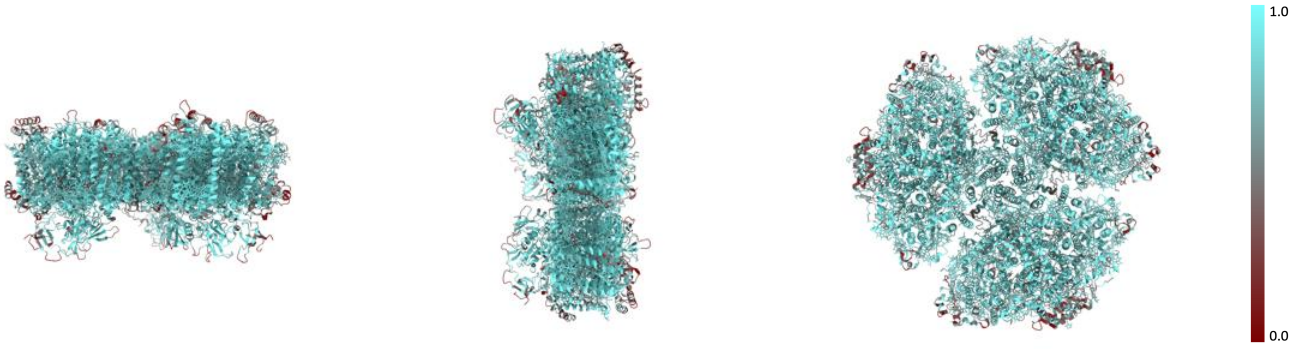
9.2 Q-score mapped to coordinate model



X Y Z

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

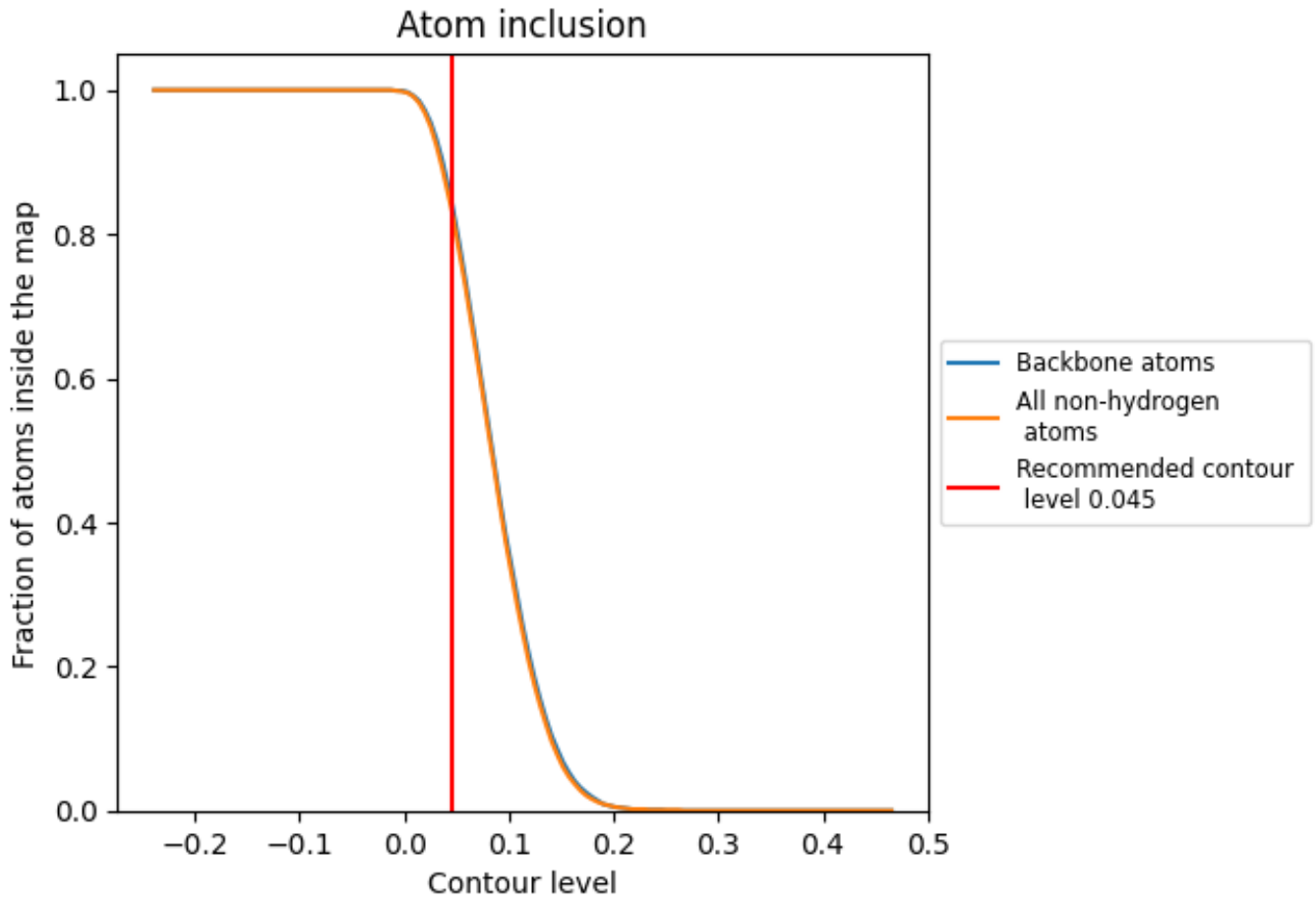
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.7520
aA	0.8580	0.7580
aB	0.8960	0.7710
aC	0.9170	0.7710
aD	0.6990	0.7180
aE	0.6140	0.6720
aF	0.5440	0.6770
aI	0.8340	0.7470
aJ	0.7450	0.7110
aL	0.8460	0.7570
aM	0.8480	0.7480
bA	0.8530	0.7560
bB	0.8940	0.7690
bC	0.9180	0.7680
bD	0.6930	0.7150
bE	0.5960	0.6670
bF	0.5280	0.6720
bI	0.8340	0.7450
bJ	0.7500	0.7120
bL	0.8400	0.7540
bM	0.8390	0.7460
cA	0.8500	0.7550
cB	0.8920	0.7690
cC	0.9320	0.7690
cD	0.6880	0.7150
cE	0.6020	0.6650
cF	0.5300	0.6720
cI	0.8300	0.7480
cJ	0.7450	0.7060
cL	0.8380	0.7500
cM	0.8480	0.7470

