wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 03:26 pm BST

PDB ID	:	6TRD / pdb_00006trd
EMDB ID	:	EMD-10559
Title	:	Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors	:	Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Mielke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on	:	2019-12-18
Resolution	:	3.16 Å(reported)
Based on initial model	:	1JB0

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:

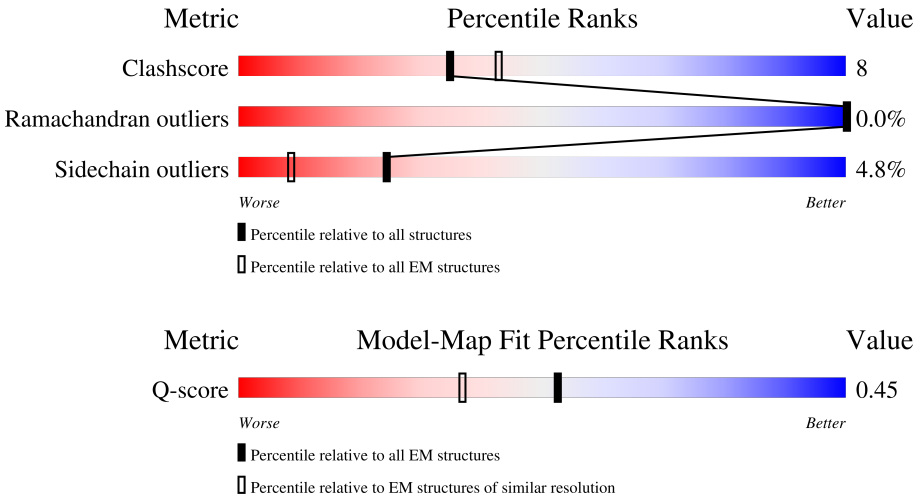
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 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	14474 (2.66 - 3.66)

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	1	755	27% 76% 22%
1	A	755	33% 76% 21%
1	a	755	36% 76% 21%

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Mol	Chain	Length	Quality of chain
2	2	741	24% 81% 18%
2	B	741	34% 82% 17%
2	b	741	22% 81% 18%
3	3	81	16% 81% 17%
3	C	81	11% 81% 17%
3	c	81	12% 85% 14%
4	4	139	24% 76% 22%
4	D	139	28% 76% 22%
4	d	139	35% 77% 21%
5	5	76	51% 70% 20% 8%
5	E	76	58% 74% 17% 8%
5	e	76	58% 72% 17% 8%
6	6	141	80% 56% 38% 6%
6	F	141	96% 57% 39%
6	f	141	91% 57% 37% 6%
7	7	38	16% 79% 21%
7	I	38	8% 79% 21%
7	i	38	11% 79% 21%
8	8	41	76% 73% 20% 5%
8	J	41	95% 73% 20% 5%
8	j	41	83% 68% 24% 5%
9	9	83	88% 59% 33% 5%
9	K	83	87% 64% 28% 5%
9	k	83	94% 64% 28% 5%
10	0	155	10% 76% 22%

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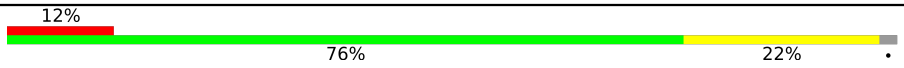
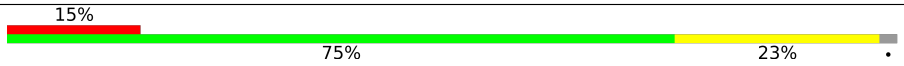
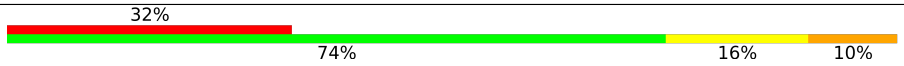
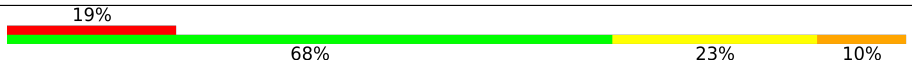
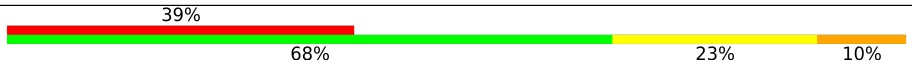
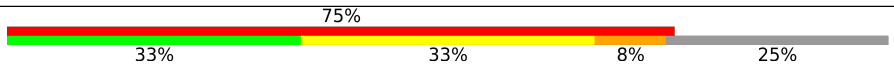
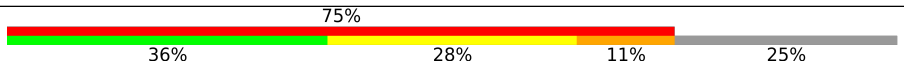
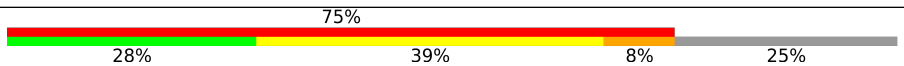
Mol	Chain	Length	Quality of chain
10	L	155	
10	l	155	
11	M	31	
11	m	31	
11	y	31	
12	X	36	
12	x	36	
12	z	36	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 74991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	a	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	1	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	b	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	2	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	4	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	70	Total	C	N	O	0	0
			546	347	94	105		
5	e	70	Total	C	N	O	0	0
			546	347	94	105		
5	5	70	Total	C	N	O	0	0
			546	347	94	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	6	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	i	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	7	38	Total	C	N	O	S	0	0
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		
8	j	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	k	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	9	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	l	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	0	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
l	143	LEU	SER	conflict	UNP Q8DGB4
0	143	LEU	SER	conflict	UNP Q8DGB4

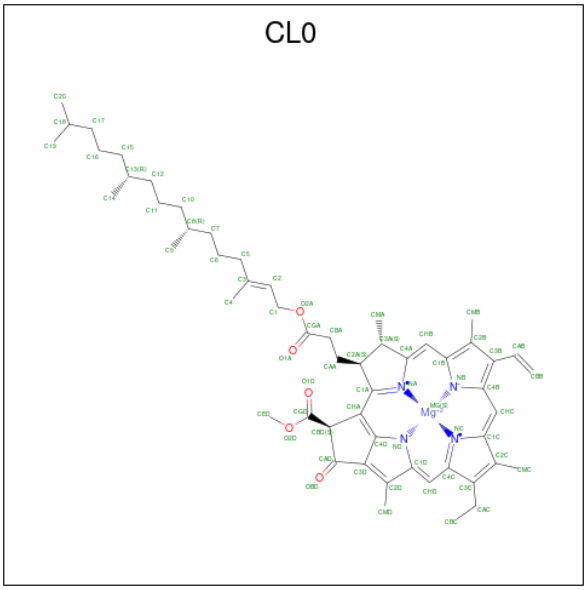
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	m	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	y	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

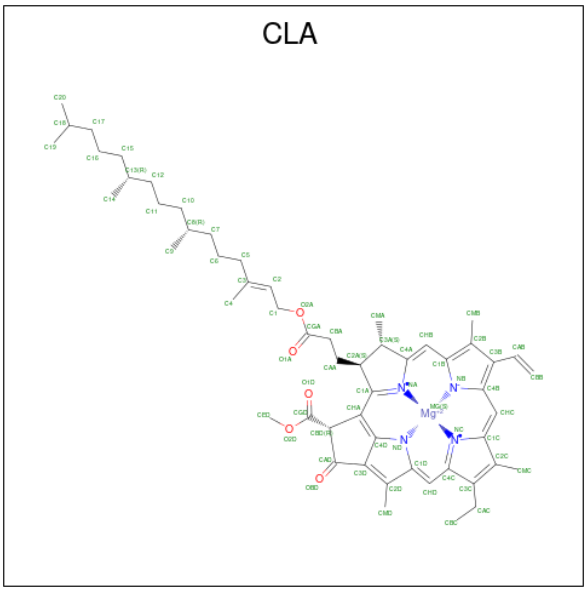
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total 228	C 163	N 33	O 32	0	0
12	x	27	Total 228	C 163	N 33	O 32	0	0
12	z	27	Total 228	C 163	N 33	O 32	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	M	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	9	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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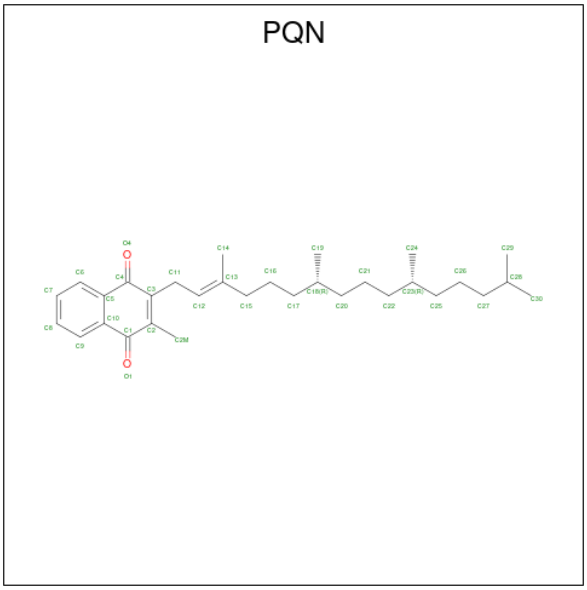
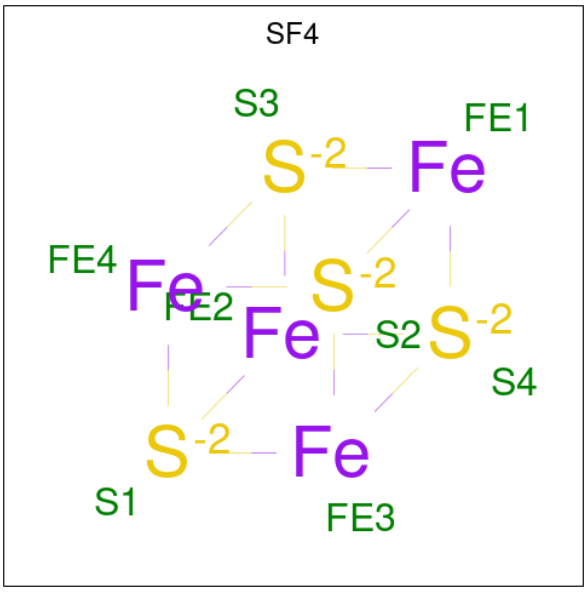
Mol	Chain	Residues	Atoms					AltConf
14	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



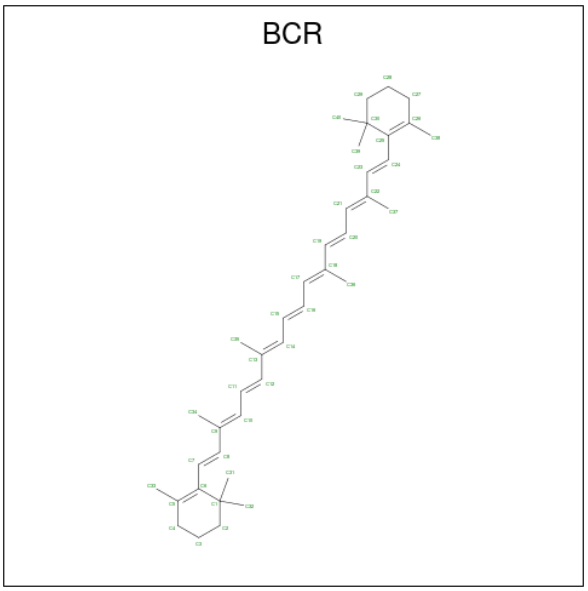
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	
15	1	1	Total	C	O	0
			33	31	2	
15	2	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	a	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	1	1	Total Fe S 8 4 4	0
16	3	1	Total Fe S 8 4 4	0
16	3	1	Total Fe S 8 4 4	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 25 25	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 25 25	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 25 25	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 25 25	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0

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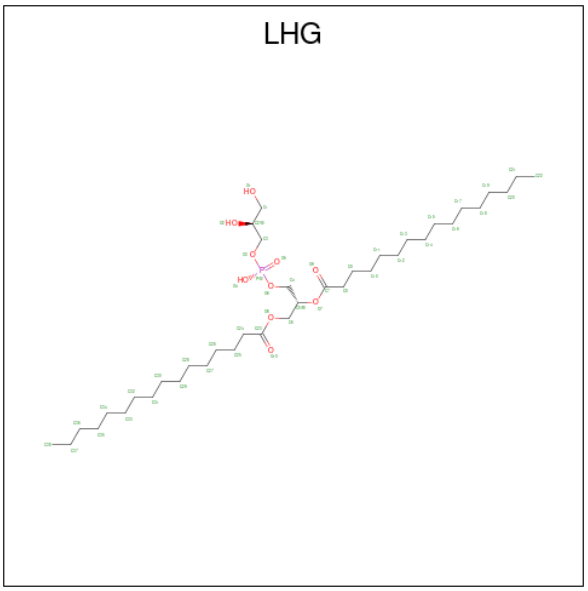
Mol	Chain	Residues	Atoms	AltConf
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	9	1	Total C 40 40	0
17	9	1	Total C 25 25	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	y	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	A	1	Total	C	O	P	0
			41	30	10	1	
18	B	1	Total	C	O	P	0
			49	38	10	1	
18	L	1	Total	C	O	P	0
			39	28	10	1	
18	M	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			41	30	10	1	
18	b	1	Total	C	O	P	0
			49	38	10	1	
18	l	1	Total	C	O	P	0
			39	28	10	1	
18	m	1	Total	C	O	P	0
			49	38	10	1	
18	1	1	Total	C	O	P	0
			49	38	10	1	
18	1	1	Total	C	O	P	0
			41	30	10	1	
18	0	1	Total	C	O	P	0
			39	28	10	1	
18	y	1	Total	C	O	P	0
			49	38	10	1	

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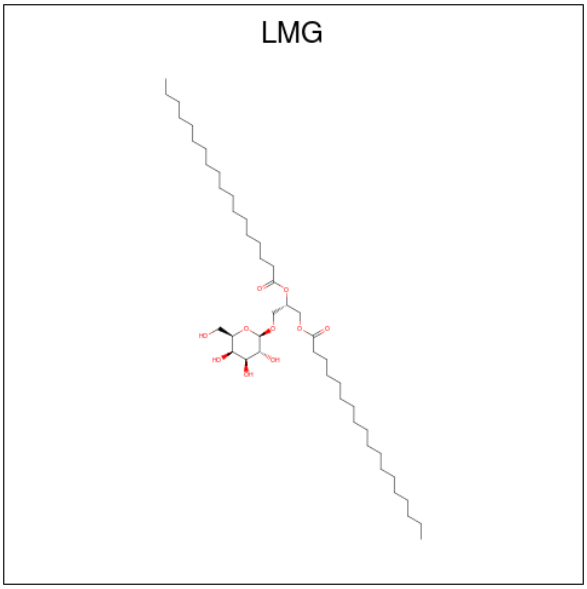
Mol	Chain	Residues	Atoms				AltConf
18	z	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Ca	0
			1	1	
19	L	1	Total	Ca	0
			1	1	
19	b	1	Total	Ca	0
			1	1	
19	l	1	Total	Ca	0
			1	1	
19	2	1	Total	Ca	0
			1	1	
19	0	1	Total	Ca	0
			1	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			55	45	10	
20	b	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms	AltConf
20	2	1	Total C O 55 45 10	0

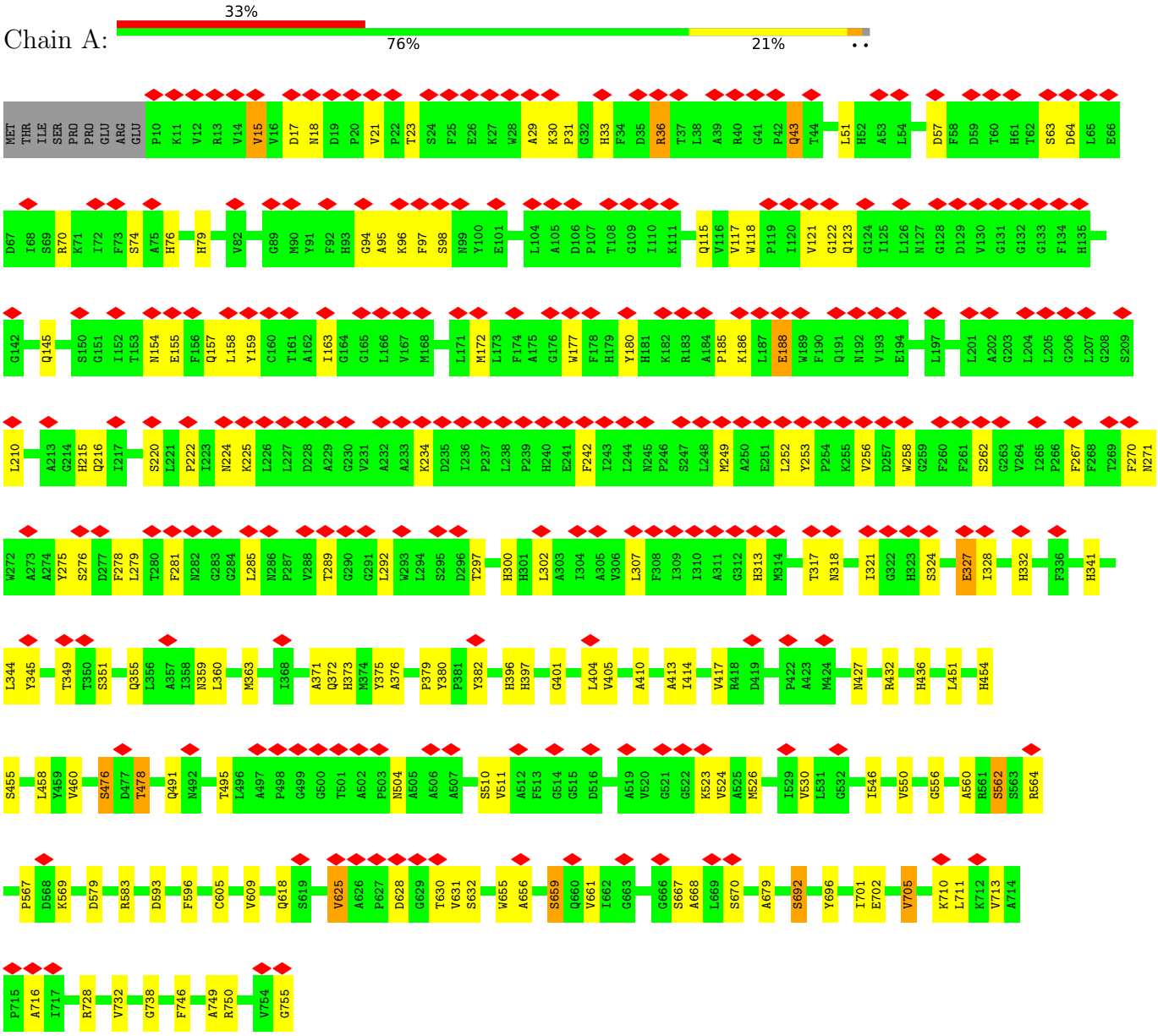
- Molecule 21 is water.

Mol	Chain	Residues	Atoms	AltConf
21	A	5	Total O 5 5	0
21	B	8	Total O 8 8	0
21	F	1	Total O 1 1	0
21	J	1	Total O 1 1	0
21	K	1	Total O 1 1	0
21	L	1	Total O 1 1	0
21	a	5	Total O 5 5	0
21	b	8	Total O 8 8	0
21	f	1	Total O 1 1	0
21	j	1	Total O 1 1	0
21	k	1	Total O 1 1	0
21	l	1	Total O 1 1	0
21	1	5	Total O 5 5	0
21	2	8	Total O 8 8	0
21	6	1	Total O 1 1	0
21	8	1	Total O 1 1	0
21	9	1	Total O 1 1	0
21	0	1	Total O 1 1	0

3 Residue-property plots (i)

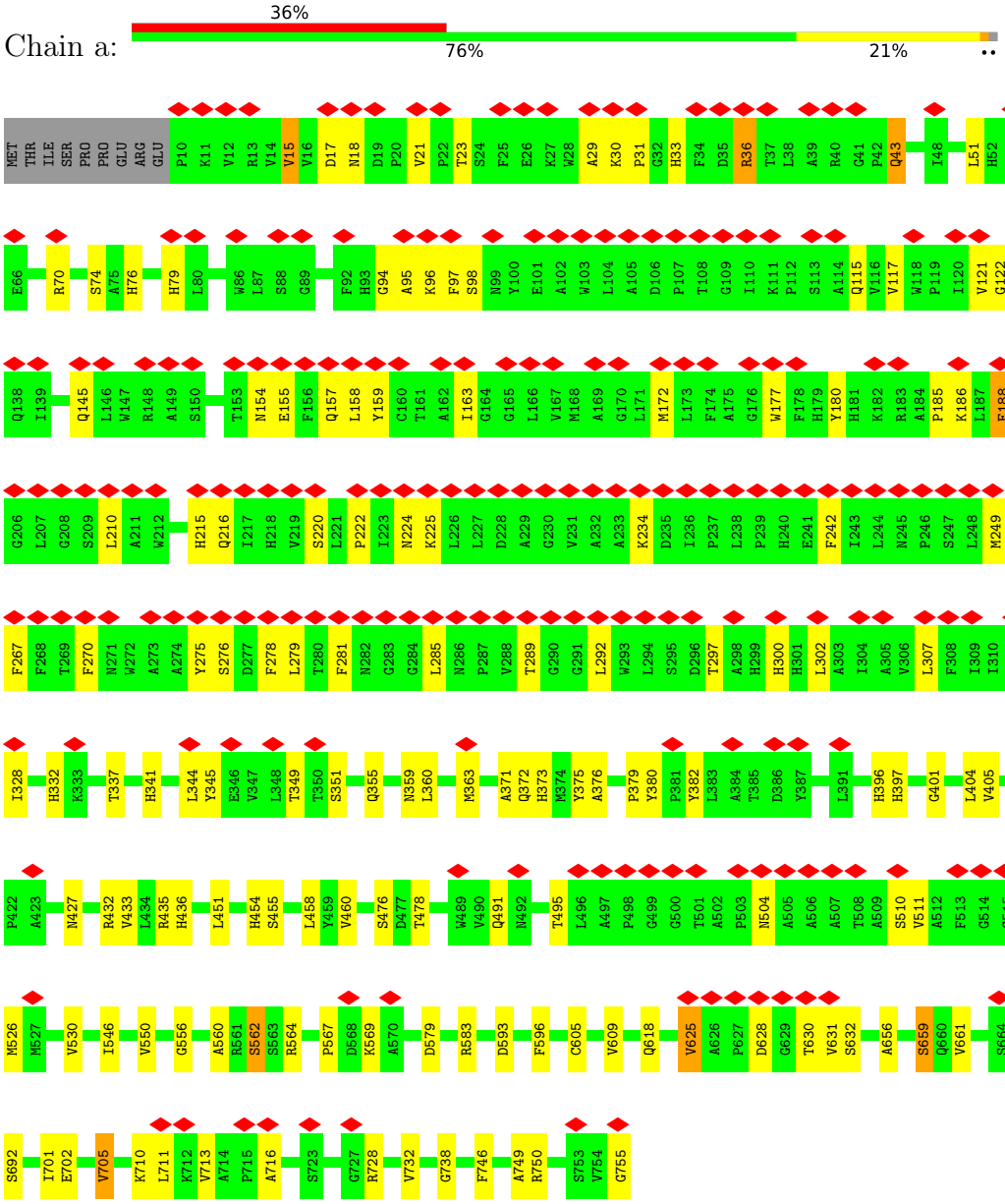
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



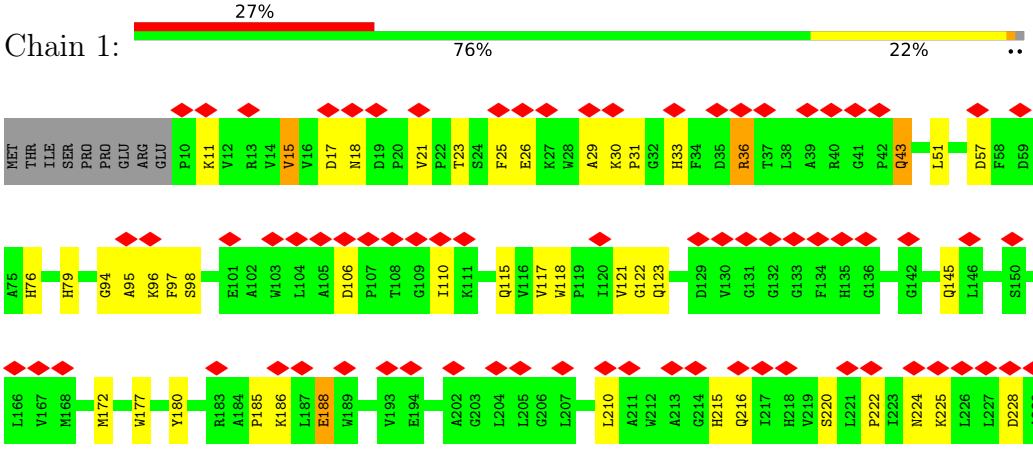
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

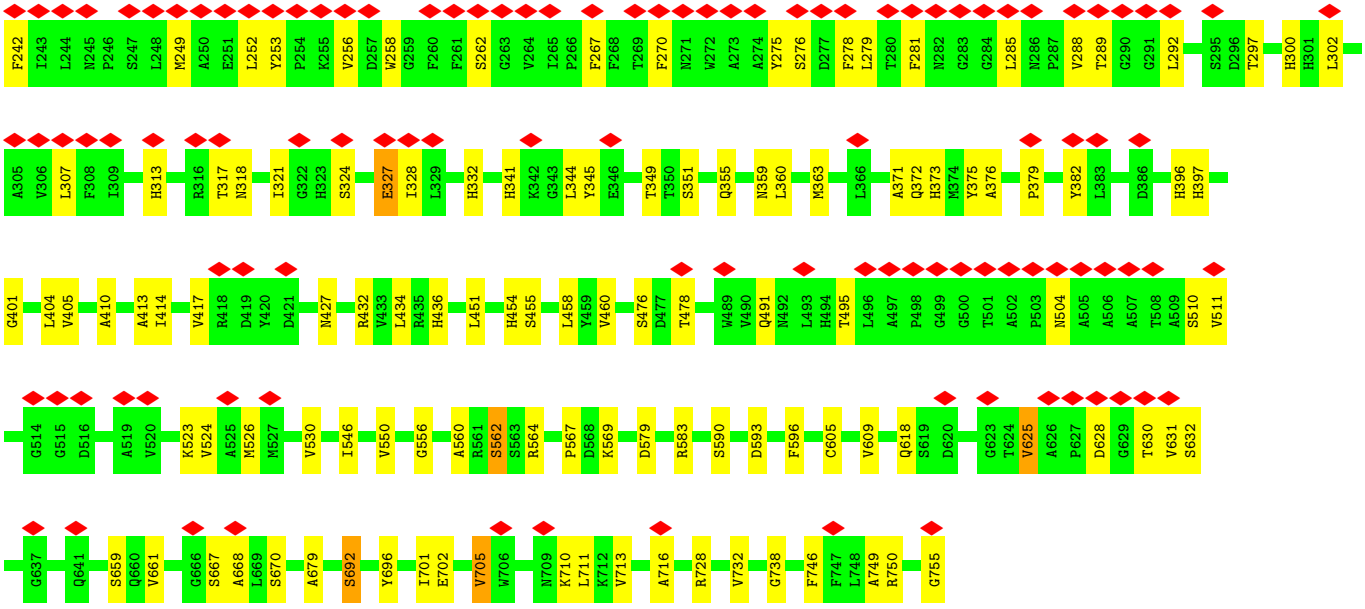
Chain a:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

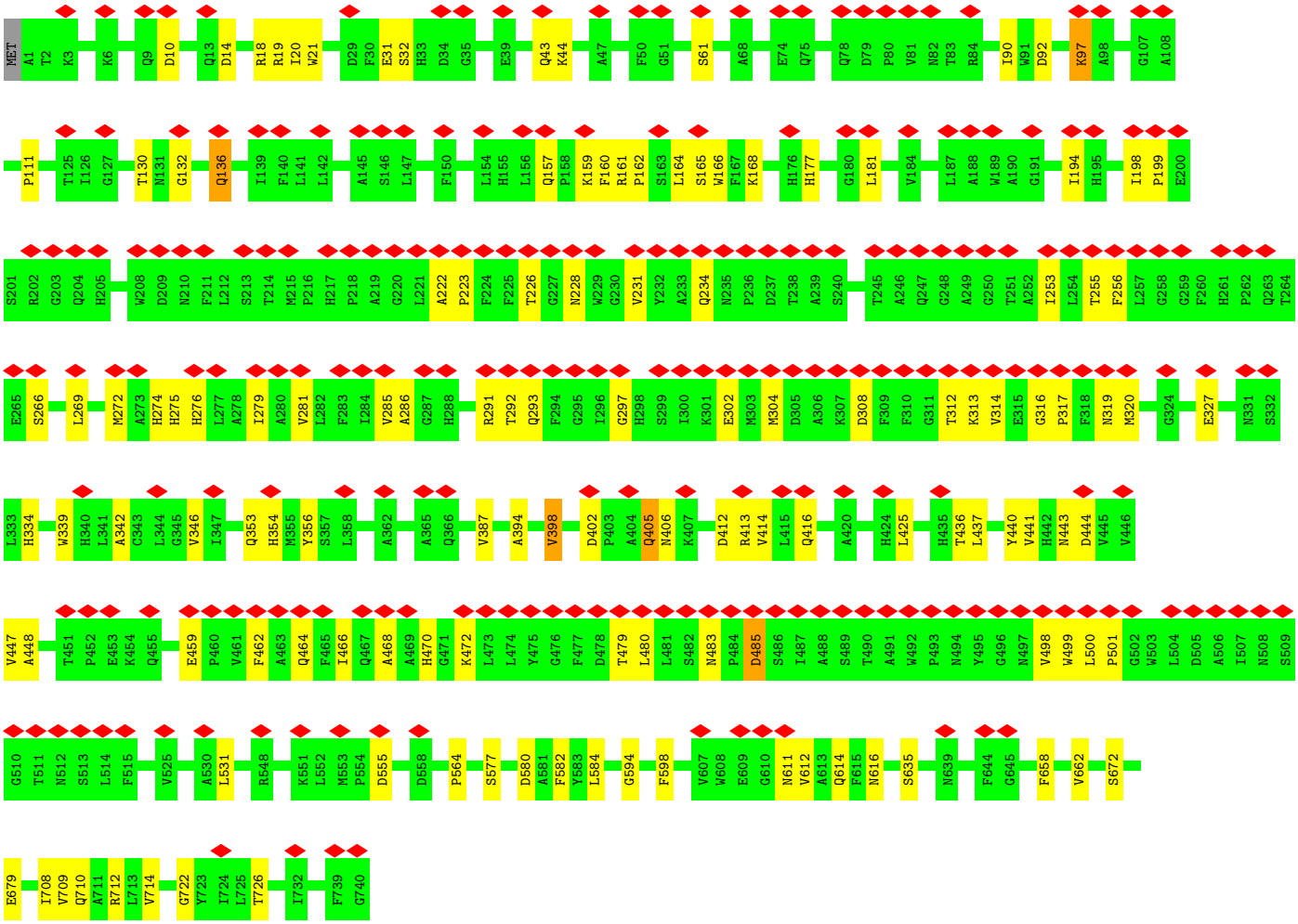
Chain 1:





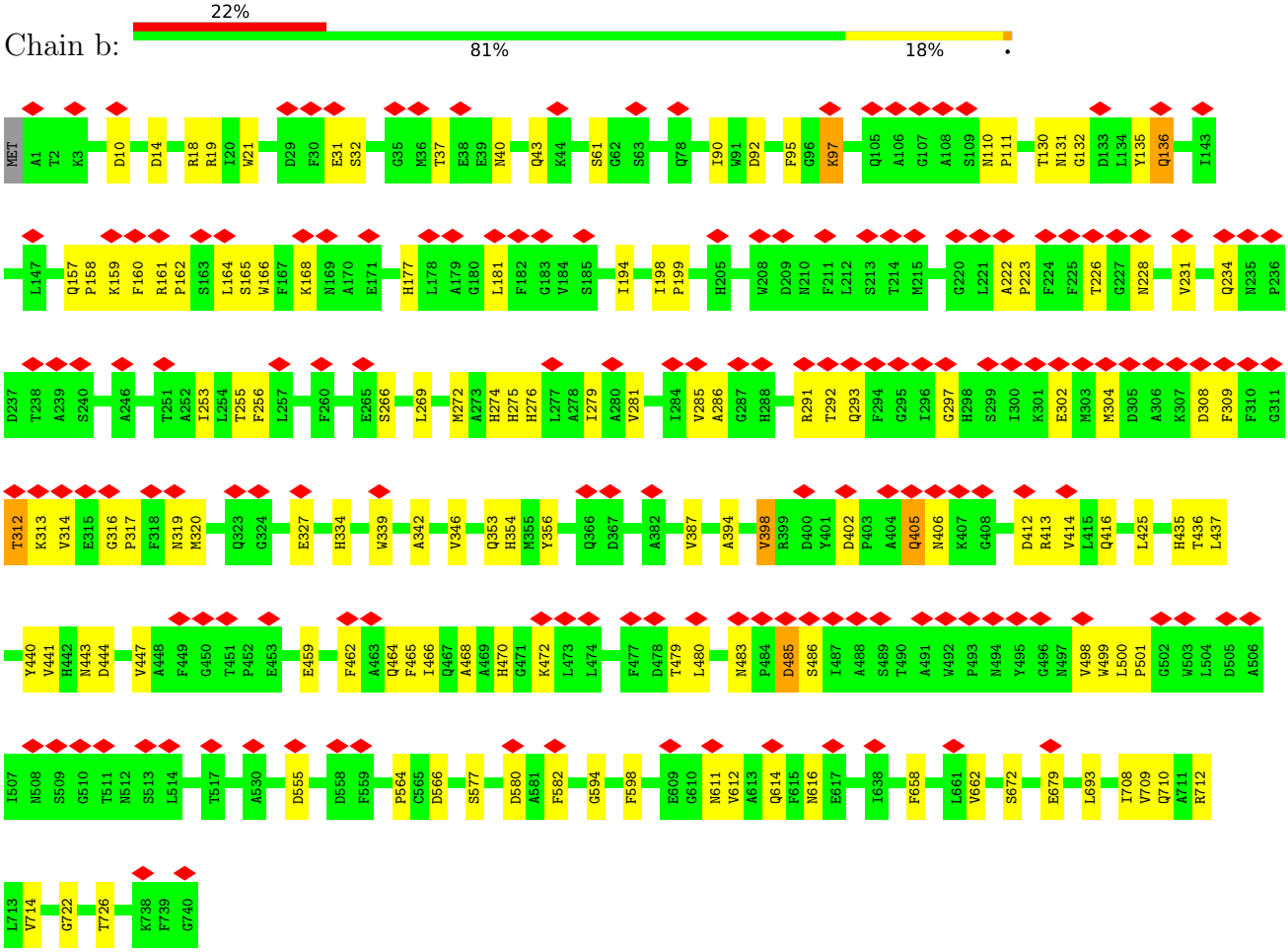
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 34% 82% 17%



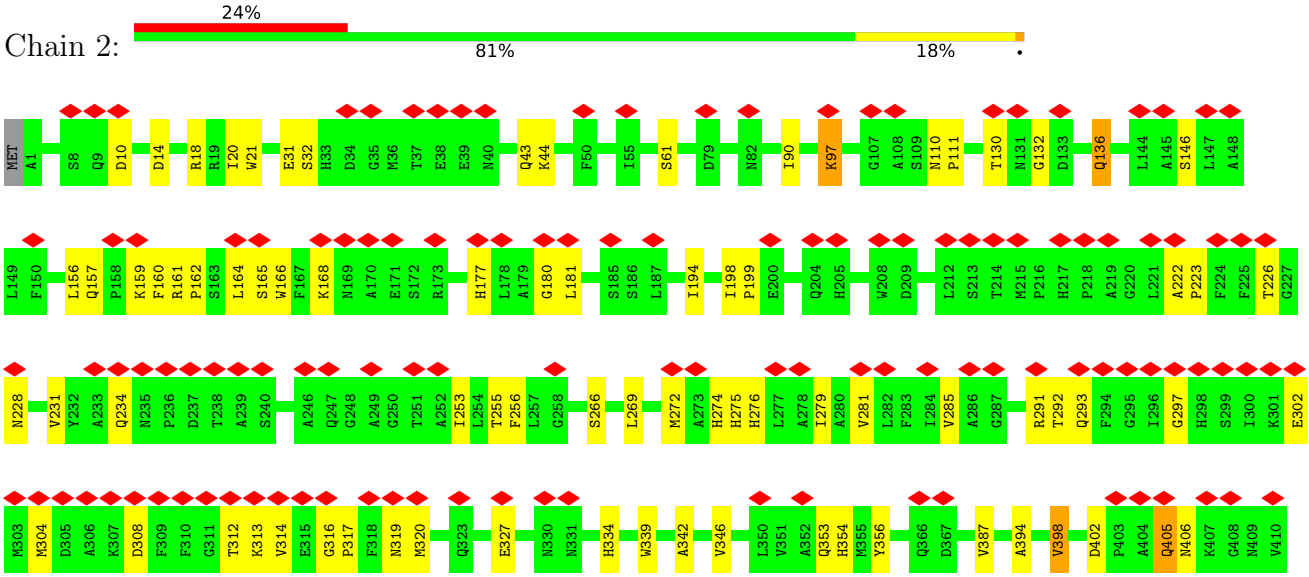
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

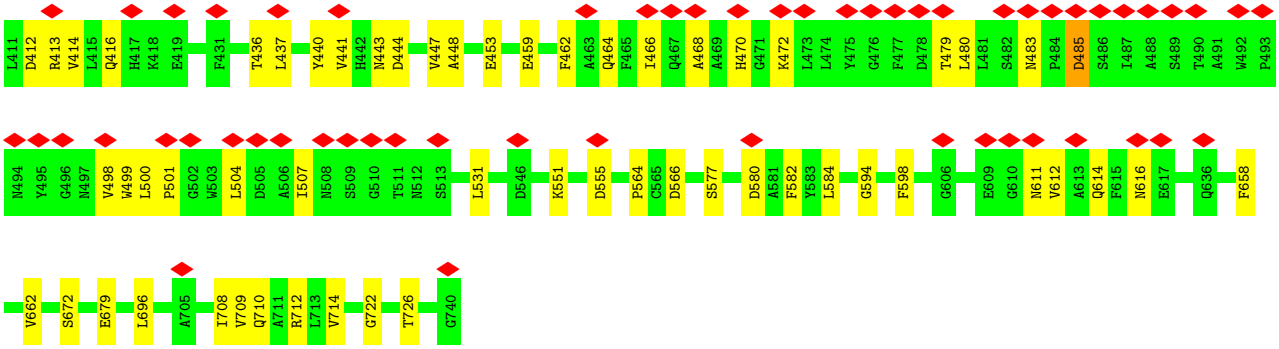
Chain b:



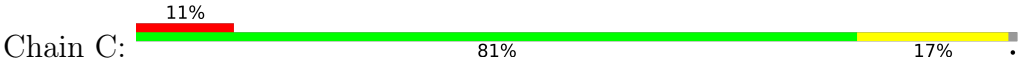
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

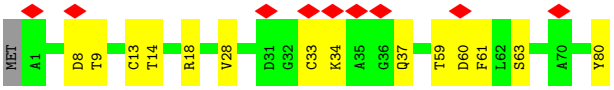
Chain 2:



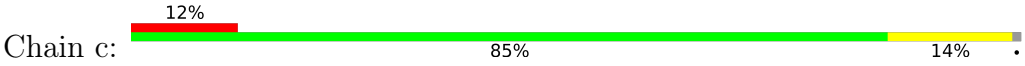


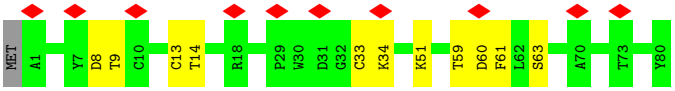
• Molecule 3: Photosystem I iron-sulfur center



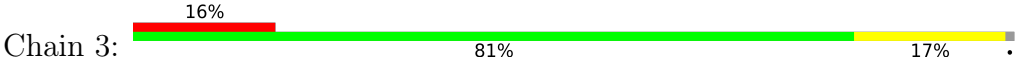


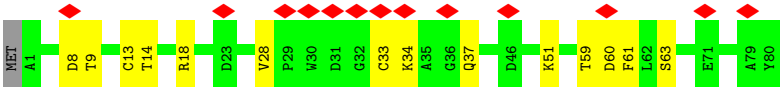
• Molecule 3: Photosystem I iron-sulfur center



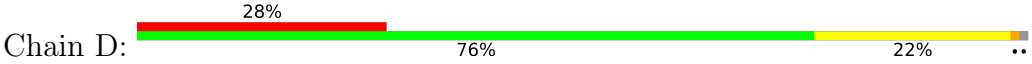


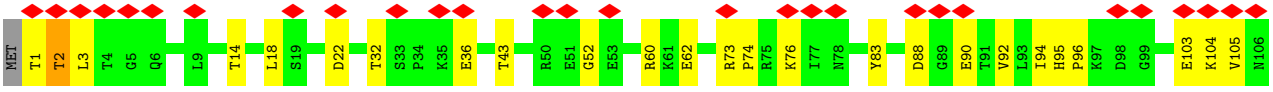
• Molecule 3: Photosystem I iron-sulfur center

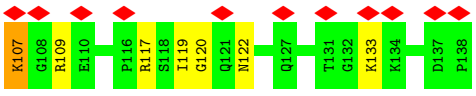




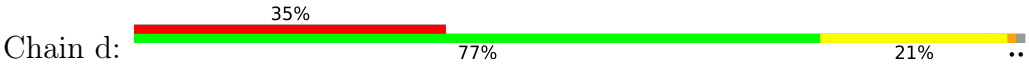
• Molecule 4: Photosystem I reaction center subunit II

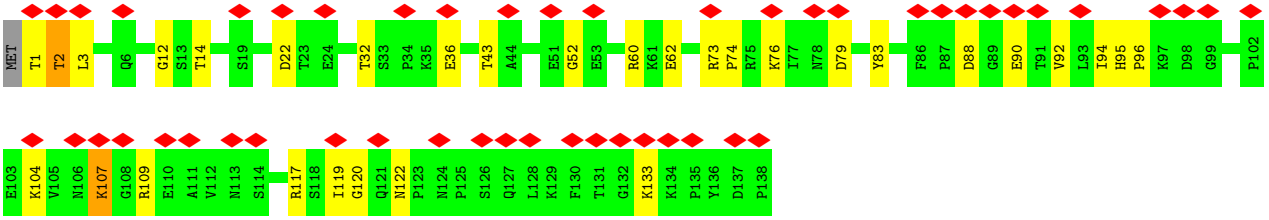






• Molecule 4: Photosystem I reaction center subunit II

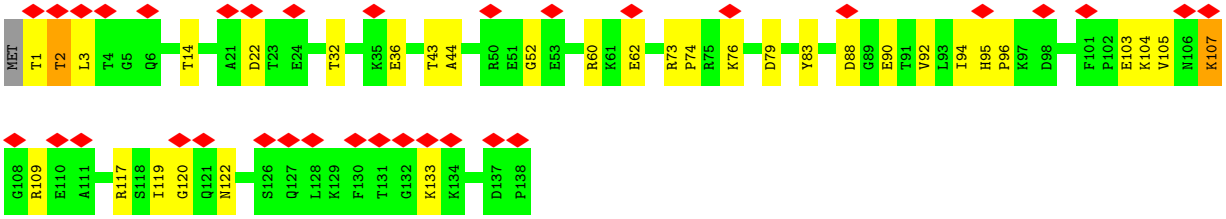




• Molecule 4: Photosystem I reaction center subunit II

Chain 4:

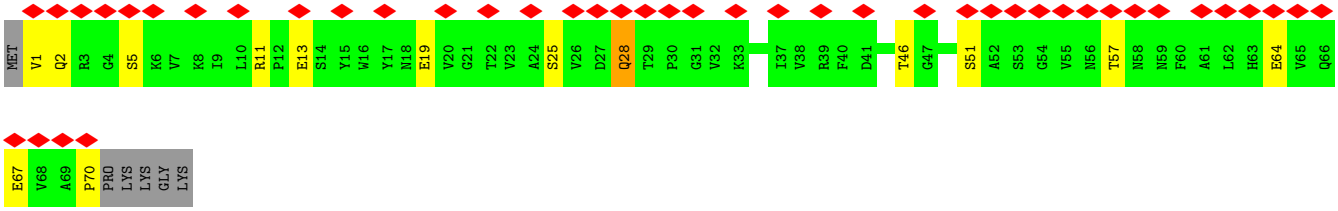




• Molecule 5: Photosystem I reaction center subunit IV

Chain E:

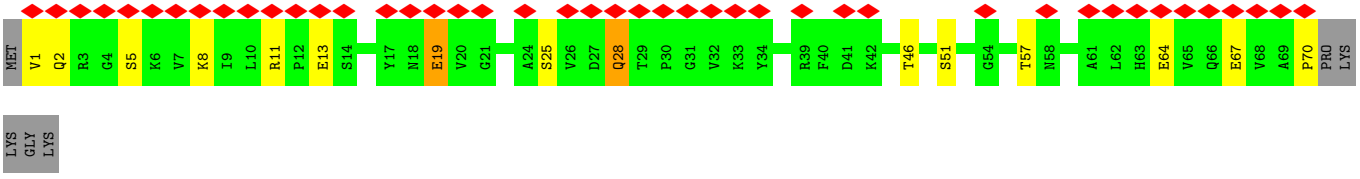




• Molecule 5: Photosystem I reaction center subunit IV

Chain e:

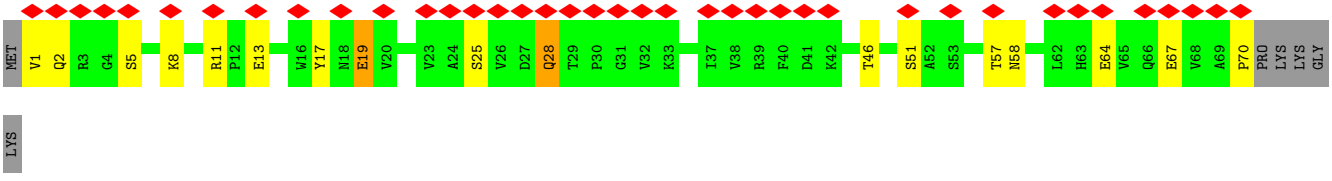




• Molecule 5: Photosystem I reaction center subunit IV

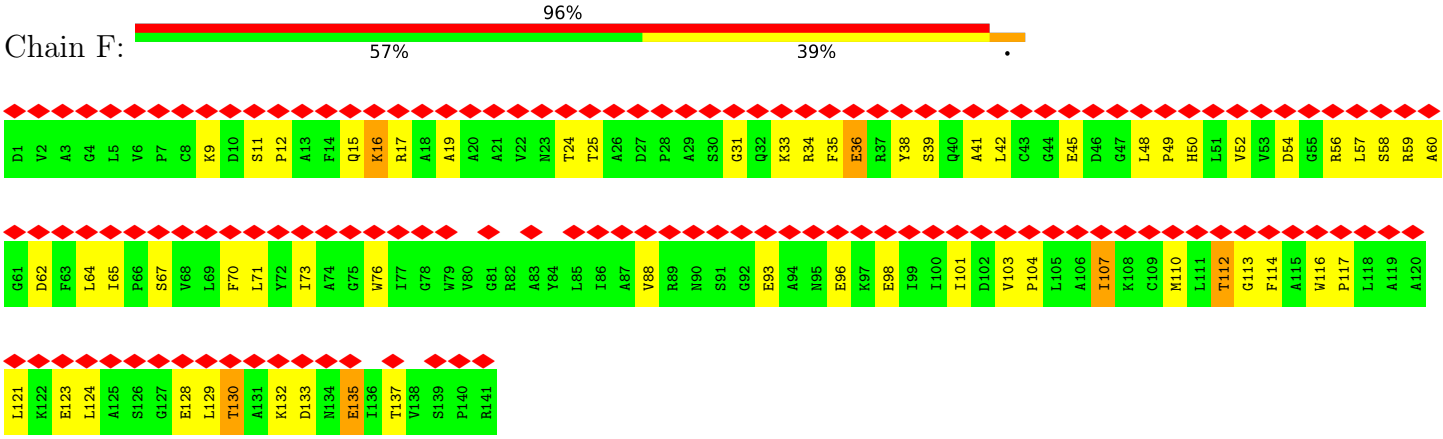
Chain 5:





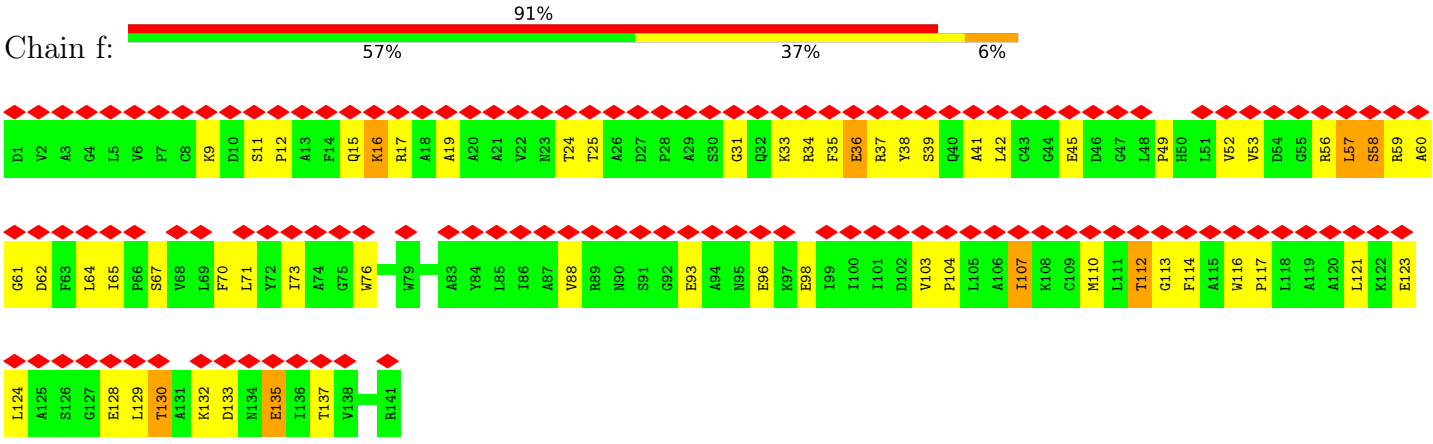
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



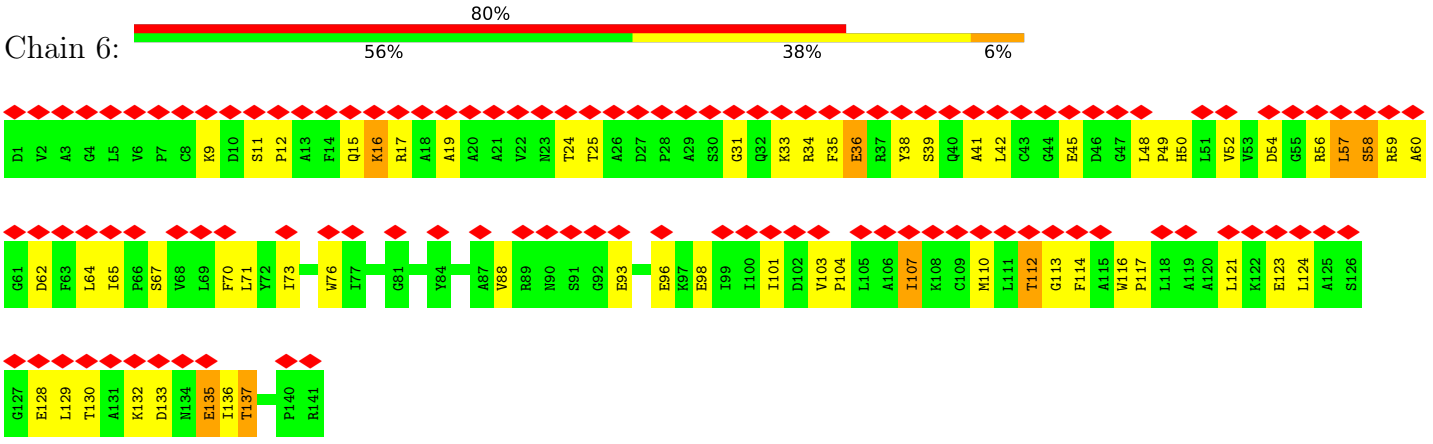
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



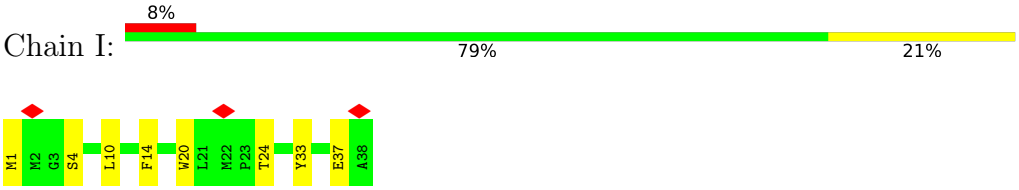
• Molecule 6: Photosystem I reaction center subunit III

Chain 6:



• Molecule 7: Photosystem I reaction center subunit VIII

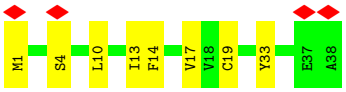
Chain I:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

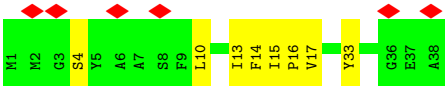




• Molecule 7: Photosystem I reaction center subunit VIII

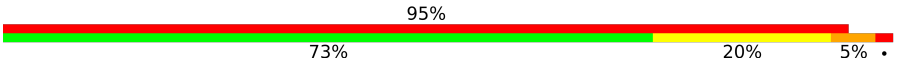
Chain 7:

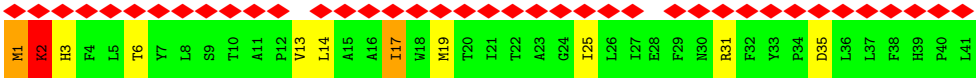




• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

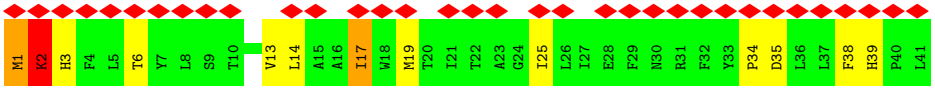




• Molecule 8: Photosystem I reaction center subunit IX

Chain j:





• Molecule 8: Photosystem I reaction center subunit IX

Chain 8:

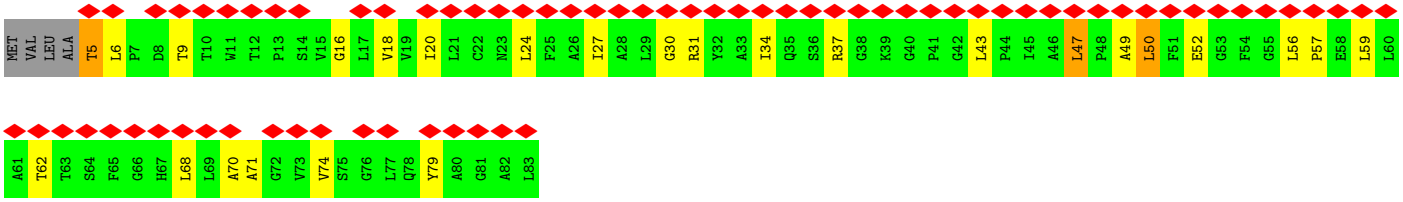




• Molecule 9: Photosystem I reaction center subunit PsaK

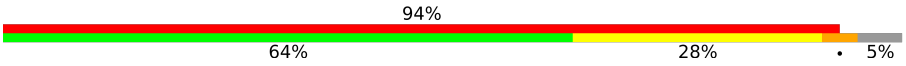
Chain K:

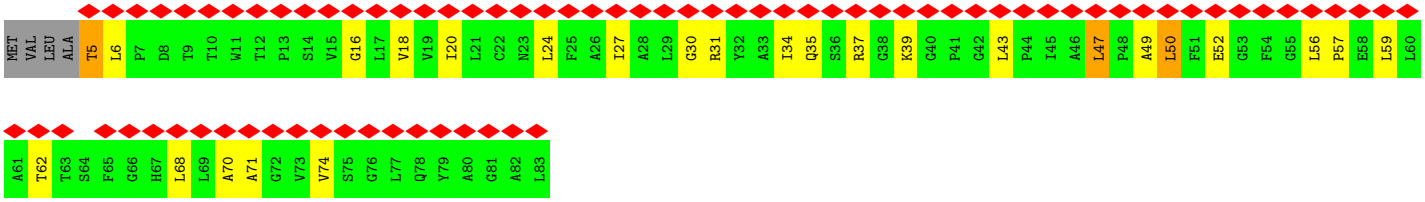




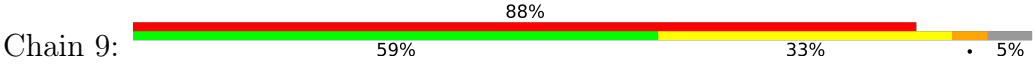
• Molecule 9: Photosystem I reaction center subunit PsaK

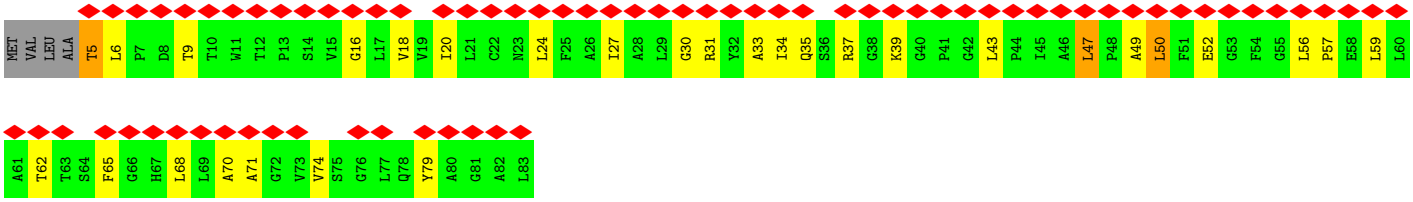
Chain k:



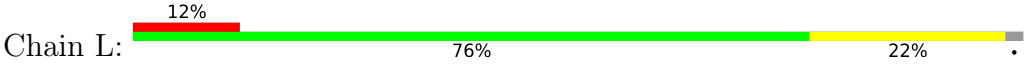


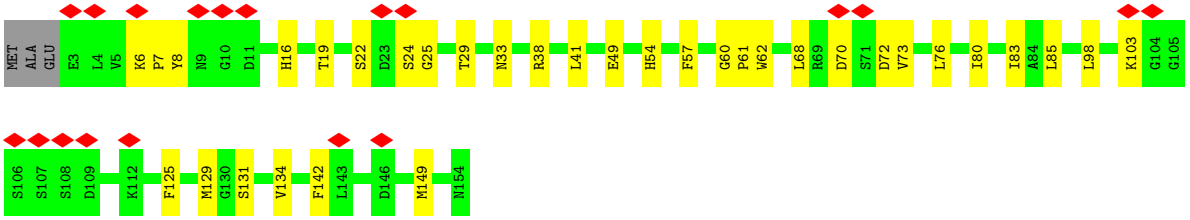
• Molecule 9: Photosystem I reaction center subunit PsaK





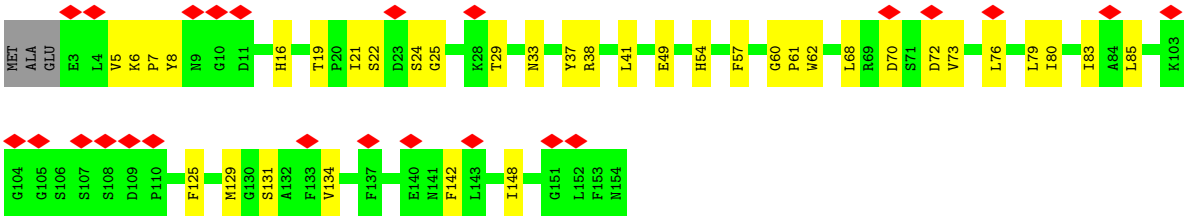
• Molecule 10: Photosystem I reaction center subunit XI





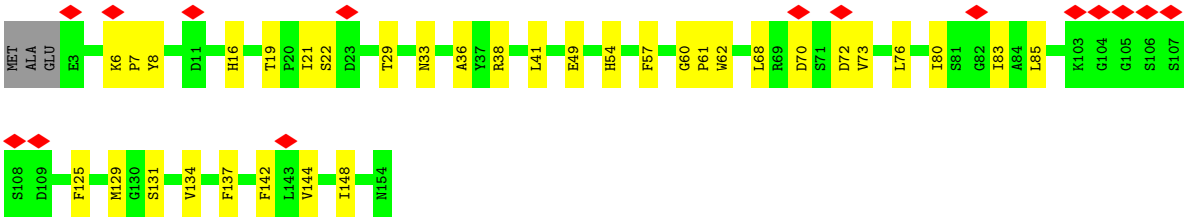
• Molecule 10: Photosystem I reaction center subunit XI





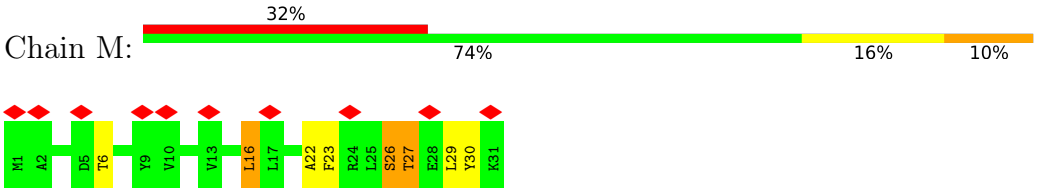
• Molecule 10: Photosystem I reaction center subunit XI





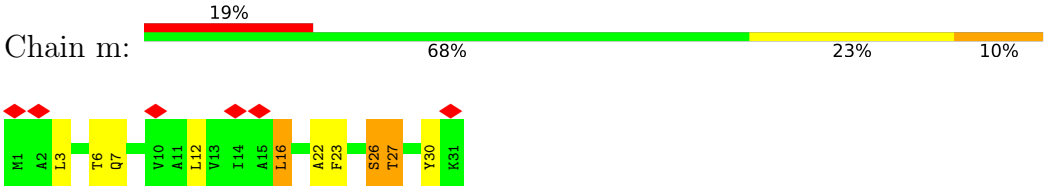
• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



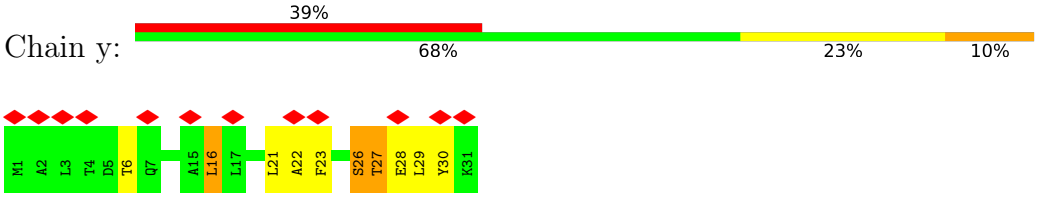
• Molecule 11: Photosystem I reaction center subunit XII

Chain m:



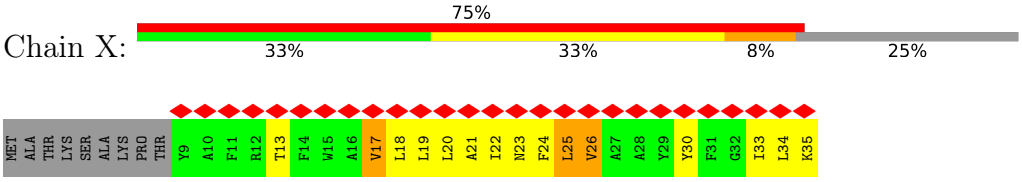
• Molecule 11: Photosystem I reaction center subunit XII

Chain y:



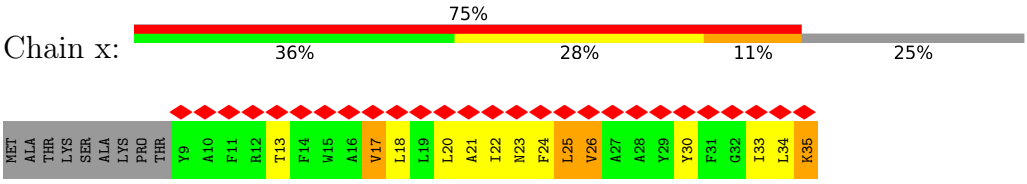
• Molecule 12: Photosystem I 4.8K protein

Chain X:



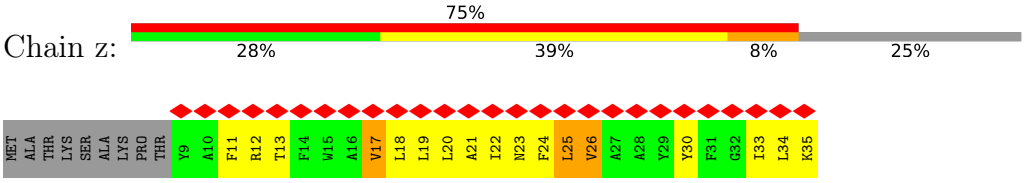
• Molecule 12: Photosystem I 4.8K protein

Chain x:



• Molecule 12: Photosystem I 4.8K protein

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.628, 0.628, 0.628	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.37	0/6027	0.48	2/8220 (0.0%)
1	A	0.37	0/6027	0.48	2/8220 (0.0%)
1	a	0.37	0/6027	0.48	2/8220 (0.0%)
2	2	0.37	0/6112	0.44	1/8350 (0.0%)
2	B	0.37	0/6112	0.44	1/8350 (0.0%)
2	b	0.37	0/6112	0.44	1/8350 (0.0%)
3	3	0.36	0/608	0.41	0/824
3	C	0.36	0/608	0.41	0/824
3	c	0.36	0/608	0.41	0/824
4	4	0.36	0/1101	0.60	2/1492 (0.1%)
4	D	0.36	0/1101	0.60	2/1492 (0.1%)
4	d	0.36	0/1101	0.60	2/1492 (0.1%)
5	5	0.29	0/559	0.56	1/762 (0.1%)
5	E	0.29	0/559	0.56	1/762 (0.1%)
5	e	0.29	0/559	0.56	1/762 (0.1%)
6	6	0.37	0/1087	0.89	5/1476 (0.3%)
6	F	0.37	0/1087	0.88	5/1476 (0.3%)
6	f	0.37	0/1087	0.88	5/1476 (0.3%)
7	7	0.41	0/304	0.50	0/415
7	I	0.41	0/304	0.50	0/415
7	i	0.41	0/304	0.50	0/415
8	8	0.30	0/342	0.55	0/467
8	J	0.31	0/342	0.55	0/467
8	j	0.30	0/342	0.55	0/467
9	9	0.28	0/585	0.68	1/800 (0.1%)
9	K	0.28	0/585	0.68	1/800 (0.1%)
9	k	0.28	0/585	0.68	1/800 (0.1%)
10	0	0.43	0/1153	0.43	0/1565
10	L	0.43	0/1153	0.43	0/1565
10	l	0.43	0/1153	0.43	0/1565
11	M	0.36	0/244	0.41	0/332
11	m	0.36	0/244	0.41	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	y	0.36	0/244	0.41	0/332
12	X	0.39	0/236	1.29	6/321 (1.9%)
12	x	0.38	0/236	1.29	6/321 (1.9%)
12	z	0.38	0/236	1.29	6/321 (1.9%)
All	All	0.37	0/55074	0.53	54/75072 (0.1%)

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
9	9	0	1
9	K	0	1
9	k	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	z	25	LEU	CA-CB-CG	11.29	155.81	116.30
12	X	25	LEU	CA-CB-CG	11.28	155.79	116.30
12	x	25	LEU	CA-CB-CG	11.28	155.77	116.30
6	f	121	LEU	CA-CB-CG	10.78	154.04	116.30
6	F	121	LEU	CA-CB-CG	10.78	154.03	116.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	47	LEU	Peptide
9	K	47	LEU	Peptide
9	k	47	LEU	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	1	5826	0	5692	121	0
1	A	5826	0	5692	120	0
1	a	5826	0	5692	114	0
2	2	5894	0	5653	100	0
2	B	5894	0	5653	92	0
2	b	5894	0	5653	102	0
3	3	598	0	580	15	0
3	C	598	0	580	13	0
3	c	598	0	580	8	0
4	4	1075	0	1077	27	0
4	D	1075	0	1077	24	0
4	d	1075	0	1077	21	0
5	5	546	0	535	11	0
5	E	546	0	535	6	0
5	e	546	0	535	5	0
6	6	1065	0	1077	53	0
6	F	1065	0	1077	48	0
6	f	1065	0	1077	50	0
7	7	303	0	305	7	0
7	I	303	0	305	8	0
7	i	303	0	305	10	0
8	8	340	0	346	13	0
8	J	340	0	346	10	0
8	j	340	0	346	12	0
9	9	571	0	593	17	0
9	K	571	0	593	16	0
9	k	571	0	593	13	0
10	0	1124	0	1127	25	0
10	L	1124	0	1127	24	0
10	l	1124	0	1127	30	0
11	M	241	0	264	5	0
11	m	241	0	264	10	0
11	y	241	0	264	8	0
12	X	228	0	234	12	0
12	x	228	0	234	16	0
12	z	228	0	234	28	0
13	1	65	0	72	0	0
13	A	65	0	72	0	0
13	a	65	0	72	2	0
14	0	195	0	216	4	0
14	1	2710	0	2873	50	0
14	2	2511	0	2634	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	6	108	0	94	2	0
14	8	127	0	91	2	0
14	9	104	0	88	1	0
14	A	2775	0	2945	47	0
14	B	2446	0	2562	32	0
14	F	153	0	127	4	0
14	J	82	0	58	1	0
14	K	104	0	88	1	0
14	L	195	0	216	4	0
14	M	36	0	24	1	0
14	X	45	0	33	3	0
14	a	2674	0	2849	41	0
14	b	2511	0	2634	39	0
14	f	108	0	94	3	0
14	j	127	0	91	2	0
14	k	104	0	88	0	0
14	l	195	0	216	4	0
14	x	45	0	33	4	0
14	z	45	0	33	3	0
15	1	33	0	46	1	0
15	2	33	0	46	0	0
15	A	33	0	46	1	0
15	B	33	0	46	0	0
15	a	33	0	46	1	0
15	b	33	0	46	0	0
16	1	8	0	0	0	0
16	3	16	0	0	0	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	a	8	0	0	0	0
16	c	16	0	0	0	0
17	0	160	0	224	4	0
17	1	225	0	313	5	0
17	2	240	0	336	1	0
17	6	80	0	112	2	0
17	7	40	0	56	0	0
17	8	120	0	168	2	0
17	9	65	0	89	1	0
17	A	265	0	369	7	0
17	B	280	0	392	1	0
17	F	80	0	112	1	0
17	I	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	40	0	56	0	0
17	K	65	0	89	0	0
17	L	120	0	168	1	0
17	M	40	0	56	4	0
17	a	225	0	313	5	0
17	b	280	0	392	2	0
17	f	80	0	112	1	0
17	i	40	0	56	0	0
17	j	80	0	112	0	0
17	k	65	0	89	0	0
17	l	80	0	112	1	0
17	m	40	0	56	2	0
17	y	40	0	56	2	0
18	0	39	0	51	1	0
18	1	90	0	129	1	0
18	A	90	0	129	1	0
18	B	49	0	74	3	0
18	L	39	0	51	1	0
18	M	49	0	74	1	0
18	a	90	0	129	1	0
18	b	49	0	74	3	0
18	l	39	0	51	1	0
18	m	49	0	74	1	0
18	y	49	0	74	2	0
18	z	49	0	74	13	0
19	0	1	0	0	0	0
19	2	1	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
19	b	1	0	0	0	0
19	l	1	0	0	0	0
20	2	55	0	86	0	0
20	B	55	0	86	0	0
20	b	55	0	86	0	0
21	0	1	0	0	0	0
21	1	5	0	0	1	0
21	2	8	0	0	0	0
21	6	1	0	0	0	0
21	8	1	0	0	0	0
21	9	1	0	0	0	0
21	A	5	0	0	1	0
21	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	F	1	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	1	0	0	0	0
21	a	5	0	0	1	0
21	b	8	0	0	0	0
21	f	1	0	0	0	0
21	j	1	0	0	0	0
21	k	1	0	0	0	0
21	l	1	0	0	0	0
All	All	74991	0	76164	1204	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 8.

The worst 5 of 1204 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)
2:2:483:ASN:ND2	2:2:485:ASP:OD2	1.92	1.03
2:B:483:ASN:ND2	2:B:485:ASP:OD2	1.92	1.01
2:b:483:ASN:ND2	2:b:485:ASP:OD2	1.92	1.00
1:1:157:GLN:NE2	14:1:1616:CLA:O1D	2.05	0.90
1:A:157:GLN:NE2	14:A:815:CLA:O1D	2.05	0.90

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	1	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
1	A	744/755 (98%)	684 (92%)	60 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
2	2	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
2	B	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
2	b	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
3	3	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	c	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	4	136/139 (98%)	121 (89%)	15 (11%)	0	100	100
4	D	136/139 (98%)	121 (89%)	15 (11%)	0	100	100
4	d	136/139 (98%)	120 (88%)	16 (12%)	0	100	100
5	5	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
5	E	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
5	e	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
6	6	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
6	F	139/141 (99%)	112 (81%)	27 (19%)	0	100	100
6	f	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
7	7	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	8	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	21
8	J	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	21
8	j	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	21
9	9	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
9	K	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
9	k	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
10	0	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	L	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	l	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	y	29/31 (94%)	27 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	X	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
12	x	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
12	z	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
All	All	6777/6951 (98%)	6181 (91%)	593 (9%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	2	LYS
8	j	2	LYS
8	8	2	LYS

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	1	594/603 (98%)	567 (96%)	27 (4%)	24	53
1	A	594/603 (98%)	567 (96%)	27 (4%)	24	53
1	a	594/603 (98%)	567 (96%)	27 (4%)	24	53
2	2	597/598 (100%)	582 (98%)	15 (2%)	42	65
2	B	597/598 (100%)	582 (98%)	15 (2%)	42	65
2	b	597/598 (100%)	582 (98%)	15 (2%)	42	65
3	3	67/68 (98%)	67 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	67 (100%)	0	100	100
4	4	115/116 (99%)	109 (95%)	6 (5%)	21	49
4	D	115/116 (99%)	109 (95%)	6 (5%)	21	49
4	d	115/116 (99%)	109 (95%)	6 (5%)	21	49
5	5	60/65 (92%)	53 (88%)	7 (12%)	5	20
5	E	60/65 (92%)	53 (88%)	7 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	60/65 (92%)	53 (88%)	7 (12%)	5	20
6	6	109/109 (100%)	96 (88%)	13 (12%)	5	20
6	F	109/109 (100%)	96 (88%)	13 (12%)	5	20
6	f	109/109 (100%)	96 (88%)	13 (12%)	5	20
7	7	31/31 (100%)	30 (97%)	1 (3%)	34	61
7	I	31/31 (100%)	30 (97%)	1 (3%)	34	61
7	i	31/31 (100%)	30 (97%)	1 (3%)	34	61
8	8	35/35 (100%)	33 (94%)	2 (6%)	18	47
8	J	35/35 (100%)	33 (94%)	2 (6%)	18	47
8	j	35/35 (100%)	33 (94%)	2 (6%)	18	47
9	9	58/61 (95%)	50 (86%)	8 (14%)	3	16
9	K	58/61 (95%)	50 (86%)	8 (14%)	3	16
9	k	58/61 (95%)	50 (86%)	8 (14%)	3	16
10	0	117/120 (98%)	115 (98%)	2 (2%)	53	70
10	L	117/120 (98%)	115 (98%)	2 (2%)	53	70
10	l	117/120 (98%)	115 (98%)	2 (2%)	53	70
11	M	26/26 (100%)	22 (85%)	4 (15%)	2	12
11	m	26/26 (100%)	22 (85%)	4 (15%)	2	12
11	y	26/26 (100%)	22 (85%)	4 (15%)	2	12
12	X	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	x	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	z	21/28 (75%)	19 (90%)	2 (10%)	8	29
All	All	5490/5580 (98%)	5229 (95%)	261 (5%)	24	52

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	36	GLU
6	6	112	THR
12	z	26	VAL
1	a	256	VAL
1	a	210	LEU

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

Mol	Chain	Res	Type
2	b	527	HIS
1	1	372	GLN
10	0	75	ASN
2	b	648	ASN
10	l	75	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
7	FME	i	1	7	8,9,10	1.00	0	7,9,11	0.82	0
7	FME	7	1	7	8,9,10	0.98	0	7,9,11	0.83	0
8	FME	j	1	8	8,9,10	1.01	0	7,9,11	1.37	2 (28%)
7	FME	I	1	7	8,9,10	0.98	0	7,9,11	0.83	0
8	FME	J	1	8	8,9,10	1.01	0	7,9,11	1.37	2 (28%)
8	FME	8	1	8	8,9,10	1.02	0	7,9,11	1.37	2 (28%)

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
7	FME	i	1	7	-	1/7/9/11	-
7	FME	7	1	7	-	1/7/9/11	-
8	FME	j	1	8	-	1/7/9/11	-
7	FME	I	1	7	-	1/7/9/11	-
8	FME	J	1	8	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	8	1	8	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	1	FME	C-CA-N	2.57	114.36	109.73
8	8	1	FME	C-CA-N	2.56	114.36	109.73
8	J	1	FME	C-CA-N	2.56	114.34	109.73
8	j	1	FME	O-C-CA	-2.06	119.38	124.78
8	J	1	FME	O-C-CA	-2.06	119.38	124.78

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	FME	CB-CA-N-CN
8	j	1	FME	CB-CA-N-CN
8	8	1	FME	CB-CA-N-CN
7	I	1	FME	N-CA-CB-CG
7	i	1	FME	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	i	1	FME	2	0
8	j	1	FME	1	0
7	I	1	FME	1	0
8	J	1	FME	1	0
8	8	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 402 ligands modelled in this entry, 6 are monoatomic - leaving 396 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	j	1303	-	42,45,73	1.59	9 (21%)	50,78,113	1.46	6 (12%)
14	CLA	b	832	2	53,57,73	1.41	9 (16%)	62,93,113	1.47	7 (11%)
14	CLA	b	818	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	7 (8%)
14	CLA	2	835	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	A	830	-	69,73,73	1.24	10 (14%)	83,113,113	1.40	7 (8%)
14	CLA	a	827	21	69,73,73	1.26	9 (13%)	83,113,113	1.40	11 (13%)
14	CLA	a	834	1	69,73,73	1.26	11 (15%)	83,113,113	1.45	12 (14%)
14	CLA	A	838	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	7 (8%)
16	SF4	a	846	1,2	0,12,12	-	-	-		
17	BCR	f	204	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	b	806	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	8 (9%)
14	CLA	B	838	2	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)
17	BCR	A	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
17	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	a	829	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
17	BCR	b	848	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	9 (16%)
14	CLA	2	809	2	69,73,73	1.23	9 (13%)	83,113,113	1.46	8 (9%)
14	CLA	1	1635	1	69,73,73	1.26	11 (15%)	83,113,113	1.44	12 (14%)
14	CLA	2	812	2	69,73,73	1.25	9 (13%)	83,113,113	1.39	9 (10%)
14	CLA	B	837	2	64,68,73	1.31	10 (15%)	77,107,113	1.39	6 (7%)
14	CLA	j	1301	21	49,53,73	1.50	10 (20%)	59,89,113	1.45	8 (13%)
14	CLA	1	1608	1	69,73,73	1.27	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	a	844	18	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	k	101	9	50,54,73	1.46	9 (18%)	60,90,113	1.44	5 (8%)
14	CLA	a	842	1	69,73,73	1.27	10 (14%)	83,113,113	1.41	8 (9%)
14	CLA	a	815	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
14	CLA	z	102	12	49,53,73	1.49	9 (18%)	59,89,113	1.47	5 (8%)
14	CLA	A	825	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	10 (12%)
14	CLA	b	822	2	49,53,73	1.48	10 (20%)	59,89,113	1.56	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	j	1302	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	6 (10%)
14	CLA	a	830	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	7 (8%)
17	BCR	8	1306	-	41,41,41	1.21	2 (4%)	56,56,56	1.34	9 (16%)
15	PQN	2	843	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	1	1623	21	69,73,73	1.26	10 (14%)	83,113,113	1.34	8 (9%)
17	BCR	B	847	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	9 (16%)
14	CLA	B	825	21	69,73,73	1.27	10 (14%)	83,113,113	1.43	9 (10%)
14	CLA	1	1634	1	69,73,73	1.27	11 (15%)	83,113,113	1.30	6 (7%)
14	CLA	a	813	1	49,53,73	1.50	10 (20%)	59,89,113	1.50	6 (10%)
17	BCR	6	202	-	41,41,41	1.25	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	A	816	1	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	1	1628	21	69,73,73	1.26	9 (13%)	83,113,113	1.40	11 (13%)
14	CLA	b	807	2	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)
13	CL0	a	801	1	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
14	CLA	b	811	2	69,73,73	1.25	11 (15%)	83,113,113	1.41	6 (7%)
14	CLA	B	817	2	69,73,73	1.27	9 (13%)	83,113,113	1.39	7 (8%)
14	CLA	F	204	-	54,58,73	1.41	6 (11%)	65,95,113	1.37	6 (9%)
14	CLA	B	820	2	69,73,73	1.25	10 (14%)	83,113,113	1.22	5 (6%)
14	CLA	a	806	1	69,73,73	1.27	11 (15%)	83,113,113	1.47	12 (14%)
14	CLA	1	1615	1	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
14	CLA	A	823	1	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
14	CLA	A	840	1	69,73,73	1.26	10 (14%)	83,113,113	1.36	6 (7%)
14	CLA	b	841	21	69,73,73	1.26	9 (13%)	83,113,113	1.34	9 (10%)
18	LHG	a	853	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	4 (7%)
14	CLA	a	831	1	69,73,73	1.28	11 (15%)	83,113,113	1.40	9 (10%)
17	BCR	A	848	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
17	BCR	1	1651	-	41,41,41	1.35	4 (9%)	56,56,56	1.28	7 (12%)
17	BCR	K	104	-	25,25,41	1.15	1 (4%)	33,33,56	1.15	4 (12%)
16	SF4	c	101	3	0,12,12	-	-	-		
14	CLA	1	1630	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
14	CLA	a	809	1	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
17	BCR	m	102	-	41,41,41	1.24	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	a	812	14,1	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
14	CLA	2	811	2	69,73,73	1.25	11 (15%)	83,113,113	1.41	7 (8%)
14	CLA	b	831	2	59,63,73	1.35	9 (15%)	71,101,113	1.42	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	SF4	c	102	3	0,12,12	-	-	-		
14	CLA	B	823	2	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
17	BCR	B	848	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	a	824	1	69,73,73	1.27	8 (11%)	83,113,113	1.30	7 (8%)
17	BCR	8	1304	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	7 (12%)
14	CLA	b	838	2	64,68,73	1.32	10 (15%)	77,107,113	1.39	6 (7%)
14	CLA	2	841	21	69,73,73	1.27	9 (13%)	83,113,113	1.34	9 (10%)
20	LMG	B	849	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	10 (15%)
14	CLA	A	807	1	69,73,73	1.27	11 (15%)	83,113,113	1.35	6 (7%)
14	CLA	a	835	1	69,73,73	1.24	9 (13%)	83,113,113	1.38	5 (6%)
14	CLA	L	205	21	69,73,73	1.26	10 (14%)	83,113,113	1.36	11 (13%)
14	CLA	b	839	2	69,73,73	1.27	9 (13%)	83,113,113	1.31	5 (6%)
14	CLA	1	1632	1	69,73,73	1.28	11 (15%)	83,113,113	1.41	9 (10%)
14	CLA	B	821	2	49,53,73	1.48	10 (20%)	59,89,113	1.56	10 (16%)
14	CLA	2	820	21	69,73,73	1.28	9 (13%)	83,113,113	1.26	8 (9%)
14	CLA	B	816	2	69,73,73	1.24	8 (11%)	83,113,113	1.37	7 (8%)
14	CLA	b	829	2	69,73,73	1.27	9 (13%)	83,113,113	1.20	4 (4%)
14	CLA	2	834	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	a	818	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	5 (6%)
14	CLA	l	204	10	69,73,73	1.29	10 (14%)	83,113,113	1.31	7 (8%)
14	CLA	b	814	2	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
18	LHG	b	851	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	F	203	21	49,53,73	1.50	10 (20%)	59,89,113	1.45	8 (13%)
14	CLA	b	809	2	69,73,73	1.23	9 (13%)	83,113,113	1.45	8 (9%)
17	BCR	I	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.25	3 (5%)
14	CLA	a	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.43	6 (9%)
14	CLA	2	819	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	10 (12%)
17	BCR	J	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	6 (10%)
14	CLA	b	812	2	69,73,73	1.25	9 (13%)	83,113,113	1.38	10 (12%)
13	CL0	1	1602	1	69,73,73	1.26	10 (14%)	83,113,113	1.38	6 (7%)
14	CLA	A	841	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
16	SF4	C	102	3	0,12,12	-	-	-		
14	CLA	2	814	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
15	PQN	B	842	-	34,34,34	0.45	0	42,45,45	0.38	0
17	BCR	1	1652	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	f	202	-	41,41,41	1.24	3 (7%)	56,56,56	1.26	6 (10%)
18	LHG	z	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	a	832	1	64,68,73	1.31	11 (17%)	77,107,113	1.33	6 (7%)
17	BCR	F	202	-	41,41,41	1.25	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	a	807	1	69,73,73	1.27	11 (15%)	83,113,113	1.34	5 (6%)
14	CLA	b	837	21	49,53,73	1.51	8 (16%)	59,89,113	1.44	5 (8%)
14	CLA	a	821	1	69,73,73	1.26	7 (10%)	83,113,113	1.35	7 (8%)
17	BCR	a	851	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	A	857	-	40,44,73	1.59	9 (22%)	47,76,113	1.44	3 (6%)
16	SF4	C	101	3	0,12,12	-	-	-		
15	PQN	A	845	-	34,34,34	0.39	0	42,45,45	0.35	0
14	CLA	B	841	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	6 (7%)
14	CLA	A	819	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
14	CLA	2	815	2	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
14	CLA	B	840	21	69,73,73	1.27	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	2	828	2	69,73,73	1.28	10 (14%)	83,113,113	1.32	8 (9%)
17	BCR	b	852	-	41,41,41	1.21	2 (4%)	56,56,56	1.33	9 (16%)
14	CLA	B	836	21	49,53,73	1.51	8 (16%)	59,89,113	1.43	4 (6%)
14	CLA	A	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
14	CLA	1	1620	1	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
14	CLA	2	840	2	51,55,73	1.46	10 (19%)	61,91,113	1.37	7 (11%)
14	CLA	x	1701	12	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
14	CLA	a	823	1	49,53,73	1.48	9 (18%)	59,89,113	1.52	8 (13%)
14	CLA	l	206	21	69,73,73	1.26	11 (15%)	83,113,113	1.36	11 (13%)
17	BCR	A	850	-	41,41,41	1.33	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	b	802	21	69,73,73	1.24	10 (14%)	83,113,113	1.42	8 (9%)
14	CLA	B	831	2	53,57,73	1.41	10 (18%)	62,93,113	1.48	8 (12%)
14	CLA	a	814	1	69,73,73	1.27	10 (14%)	83,113,113	1.27	7 (8%)
14	CLA	1	1643	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	8 (9%)
16	SF4	3	102	3	0,12,12	-	-	-		
14	CLA	B	819	21	69,73,73	1.28	9 (13%)	83,113,113	1.26	8 (9%)
14	CLA	A	833	1	69,73,73	1.26	11 (15%)	83,113,113	1.29	6 (7%)
14	CLA	b	820	21	69,73,73	1.27	9 (13%)	83,113,113	1.26	8 (9%)
14	CLA	a	816	1	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	1	1624	1	49,53,73	1.49	10 (20%)	59,89,113	1.51	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	839	2	51,55,73	1.47	10 (19%)	61,91,113	1.38	7 (11%)
14	CLA	A	837	1	49,53,73	1.49	9 (18%)	59,89,113	1.42	7 (11%)
14	CLA	a	841	1	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
14	CLA	K	103	21	62,66,73	1.33	9 (14%)	74,104,113	1.35	10 (13%)
15	PQN	b	843	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	1	1607	1	69,73,73	1.26	11 (15%)	83,113,113	1.47	12 (14%)
18	LHG	L	208	-	38,38,48	0.73	0	41,44,54	1.26	3 (7%)
14	CLA	1	1625	1	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
14	CLA	2	807	2	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)
18	LHG	a	854	14	40,40,48	0.77	1 (2%)	43,46,54	1.21	4 (9%)
14	CLA	B	814	2	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
14	CLA	1	1629	1	69,73,73	1.27	10 (14%)	83,113,113	1.30	8 (9%)
14	CLA	2	802	21	69,73,73	1.24	10 (14%)	83,113,113	1.42	7 (8%)
14	CLA	6	201	21	62,66,73	1.33	10 (16%)	74,104,113	1.37	8 (10%)
14	CLA	2	806	2	69,73,73	1.25	10 (14%)	83,113,113	1.40	8 (9%)
14	CLA	a	828	1	69,73,73	1.27	10 (14%)	83,113,113	1.30	8 (9%)
14	CLA	a	840	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	6 (7%)
17	BCR	a	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	6 (10%)
14	CLA	2	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.33	7 (8%)
14	CLA	a	819	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	9 (10%)
16	SF4	1	1647	1,2	0,12,12	-	-	-		
14	CLA	a	811	1	53,57,73	1.42	9 (16%)	62,93,113	1.40	6 (9%)
14	CLA	k	103	21	62,66,73	1.33	9 (14%)	74,104,113	1.36	10 (13%)
14	CLA	b	821	2	69,73,73	1.25	10 (14%)	83,113,113	1.22	6 (7%)
14	CLA	b	817	2	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
14	CLA	b	816	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
14	CLA	2	831	2	59,63,73	1.36	9 (15%)	71,101,113	1.43	8 (11%)
14	CLA	J	102	-	42,45,73	1.58	10 (23%)	50,78,113	1.46	6 (12%)
17	BCR	A	852	-	25,25,41	1.13	1 (4%)	33,33,56	1.28	4 (12%)
14	CLA	b	823	21	59,63,73	1.36	10 (16%)	71,101,113	1.34	6 (8%)
18	LHG	y	101	-	48,48,48	0.71	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	B	813	2	69,73,73	1.26	10 (14%)	83,113,113	1.34	9 (10%)
14	CLA	1	1627	21	69,73,73	1.25	10 (14%)	83,113,113	1.39	9 (10%)
14	CLA	A	802	-	69,73,73	1.27	12 (17%)	83,113,113	1.39	9 (10%)
14	CLA	K	101	9	50,54,73	1.46	9 (18%)	60,90,113	1.44	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	2	821	2	69,73,73	1.24	10 (14%)	83,113,113	1.21	5 (6%)
14	CLA	1	1613	14,1	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
14	CLA	A	827	21	69,73,73	1.26	10 (14%)	83,113,113	1.40	11 (13%)
14	CLA	A	834	1	69,73,73	1.26	11 (15%)	83,113,113	1.44	13 (15%)
17	BCR	A	851	-	41,41,41	1.27	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	B	804	2	69,73,73	1.26	10 (14%)	83,113,113	1.37	10 (12%)
14	CLA	A	836	1	69,73,73	1.25	9 (13%)	83,113,113	1.37	6 (7%)
14	CLA	B	802	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
14	CLA	A	828	1	69,73,73	1.27	10 (14%)	83,113,113	1.31	8 (9%)
14	CLA	1	1605	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
14	CLA	2	804	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	6 (7%)
17	BCR	F	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	2	833	2	69,73,73	1.26	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	B	806	2	69,73,73	1.28	9 (13%)	83,113,113	1.32	6 (7%)
14	CLA	1	1603	-	69,73,73	1.26	12 (17%)	83,113,113	1.39	9 (10%)
14	CLA	1	1604	21	69,73,73	1.29	10 (14%)	83,113,113	1.19	6 (7%)
14	CLA	L	204	10	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
14	CLA	A	831	1	69,73,73	1.28	11 (15%)	83,113,113	1.41	9 (10%)
14	CLA	A	829	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
14	CLA	1	1642	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	B	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.32	8 (9%)
14	CLA	b	810	2	69,73,73	1.26	11 (15%)	83,113,113	1.48	9 (10%)
14	CLA	2	832	2	53,57,73	1.41	10 (18%)	62,93,113	1.47	7 (11%)
14	CLA	b	836	21	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
14	CLA	L	203	10	69,73,73	1.28	10 (14%)	83,113,113	1.32	7 (8%)
14	CLA	A	826	21	69,73,73	1.25	10 (14%)	83,113,113	1.38	9 (10%)
17	BCR	A	856	-	41,41,41	1.23	3 (7%)	56,56,56	1.28	8 (14%)
14	CLA	1	1631	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	6 (7%)
14	CLA	1	1616	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
14	CLA	1	1619	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	5 (6%)
14	CLA	A	815	1	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
14	CLA	2	818	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	7 (8%)
14	CLA	a	843	21	69,73,73	1.28	10 (14%)	83,113,113	1.35	5 (6%)
18	LHG	M	101	-	48,48,48	0.70	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	A	805	14,1	63,67,73	1.29	10 (15%)	75,105,113	1.41	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	803	21	69,73,73	1.29	10 (14%)	83,113,113	1.19	6 (7%)
14	CLA	1	1610	1	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
14	CLA	a	804	1	69,73,73	1.23	9 (13%)	83,113,113	1.36	6 (7%)
17	BCR	B	846	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	7 (12%)
14	CLA	2	838	2	64,68,73	1.31	10 (15%)	77,107,113	1.39	6 (7%)
17	BCR	a	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.29	7 (12%)
14	CLA	0	206	10	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
18	LHG	B	850	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	2	836	21	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
14	CLA	B	805	2	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	b	830	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	7 (8%)
14	CLA	A	813	1	49,53,73	1.50	10 (20%)	59,89,113	1.50	7 (11%)
14	CLA	b	819	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	9 (10%)
14	CLA	8	1302	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
18	LHG	0	202	-	38,38,48	0.73	1 (2%)	41,44,54	1.26	3 (7%)
20	LMG	2	850	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
17	BCR	l	202	-	41,41,41	1.39	4 (9%)	56,56,56	1.32	7 (12%)
18	LHG	m	101	-	48,48,48	0.70	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	a	826	21	69,73,73	1.25	10 (14%)	83,113,113	1.38	9 (10%)
14	CLA	1	1606	14,1	63,67,73	1.29	10 (15%)	75,105,113	1.40	8 (10%)
14	CLA	2	813	2	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
14	CLA	B	826	2	69,73,73	1.28	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	B	832	2	69,73,73	1.26	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	A	842	1	69,73,73	1.26	11 (15%)	83,113,113	1.41	9 (10%)
15	PQN	a	845	-	34,34,34	0.40	0	42,45,45	0.35	0
14	CLA	a	838	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	7 (8%)
20	LMG	b	850	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	10 (15%)
14	CLA	a	833	1	69,73,73	1.26	11 (15%)	83,113,113	1.29	6 (7%)
17	BCR	j	1305	-	41,41,41	1.22	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	B	834	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	2	816	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
17	BCR	B	845	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	A	809	1	69,73,73	1.24	9 (13%)	83,113,113	1.39	8 (9%)
14	CLA	J	101	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	6 (10%)
17	BCR	0	201	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	810	2	69,73,73	1.25	10 (14%)	83,113,113	1.41	7 (8%)
14	CLA	A	812	14,1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
17	BCR	a	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	b	840	2	51,55,73	1.46	10 (19%)	61,91,113	1.37	6 (9%)
14	CLA	2	829	2	69,73,73	1.27	9 (13%)	83,113,113	1.21	5 (6%)
17	BCR	2	848	-	41,41,41	1.28	3 (7%)	56,56,56	1.31	8 (14%)
14	CLA	b	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	b	834	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	A	824	1	69,73,73	1.27	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	a	802	-	69,73,73	1.27	12 (17%)	83,113,113	1.39	9 (10%)
14	CLA	2	839	2	69,73,73	1.26	9 (13%)	83,113,113	1.31	6 (7%)
17	BCR	a	852	-	25,25,41	1.12	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	1	1644	21	69,73,73	1.28	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	2	825	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	6 (7%)
14	CLA	2	803	2	69,73,73	1.26	10 (14%)	83,113,113	1.36	7 (8%)
14	CLA	A	835	1	69,73,73	1.24	9 (13%)	83,113,113	1.37	4 (4%)
14	CLA	B	809	2	69,73,73	1.25	10 (14%)	83,113,113	1.48	9 (10%)
14	CLA	B	812	2	49,53,73	1.47	9 (18%)	59,89,113	1.46	4 (6%)
17	BCR	B	844	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	M	102	-	40,44,73	1.59	9 (22%)	47,76,113	1.43	3 (6%)
14	CLA	2	805	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	10 (12%)
17	BCR	B	851	-	41,41,41	1.21	2 (4%)	56,56,56	1.34	9 (16%)
14	CLA	B	815	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
17	BCR	2	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	A	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.43	6 (9%)
14	CLA	B	828	2	69,73,73	1.27	10 (14%)	83,113,113	1.20	5 (6%)
14	CLA	B	835	21	54,58,73	1.42	10 (18%)	65,95,113	1.44	7 (10%)
14	CLA	B	830	2	59,63,73	1.35	9 (15%)	71,101,113	1.42	8 (11%)
14	CLA	A	804	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
17	BCR	l	207	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	2	817	2	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
17	BCR	j	1304	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	7 (12%)
17	BCR	7	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.24	3 (5%)
14	CLA	1	1612	1	53,57,73	1.42	9 (16%)	62,93,113	1.40	6 (9%)
14	CLA	B	811	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	1	1640	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
17	BCR	9	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	7 (12%)
14	CLA	b	808	2	69,73,73	1.26	9 (13%)	83,113,113	1.34	7 (8%)
14	CLA	a	803	21	69,73,73	1.29	10 (14%)	83,113,113	1.18	5 (6%)
14	CLA	A	832	1	64,68,73	1.32	11 (17%)	77,107,113	1.32	6 (7%)
14	CLA	1	1601	-	40,44,73	1.59	8 (20%)	47,76,113	1.43	3 (6%)
14	CLA	b	825	2	69,73,73	1.26	10 (14%)	83,113,113	1.36	6 (7%)
17	BCR	L	201	-	41,41,41	1.39	4 (9%)	56,56,56	1.33	7 (12%)
14	CLA	b	824	2	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
14	CLA	A	806	1	69,73,73	1.27	11 (15%)	83,113,113	1.47	12 (14%)
17	BCR	M	103	-	41,41,41	1.23	3 (7%)	56,56,56	1.22	5 (8%)
17	BCR	b	846	-	41,41,41	1.25	3 (7%)	56,56,56	1.24	6 (10%)
17	BCR	k	104	-	25,25,41	1.14	1 (4%)	33,33,56	1.15	4 (12%)
14	CLA	a	825	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
14	CLA	2	830	2	69,73,73	1.24	11 (15%)	83,113,113	1.45	7 (8%)
14	CLA	2	824	2	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
14	CLA	b	803	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
14	CLA	0	207	21	69,73,73	1.26	11 (15%)	83,113,113	1.37	10 (12%)
14	CLA	1	1638	1	49,53,73	1.49	9 (18%)	59,89,113	1.42	7 (11%)
14	CLA	b	804	-	69,73,73	1.26	10 (14%)	83,113,113	1.39	6 (7%)
14	CLA	1	1639	1	69,73,73	1.25	11 (15%)	83,113,113	1.43	7 (8%)
17	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	2	810	2	69,73,73	1.26	11 (15%)	83,113,113	1.47	8 (9%)
14	CLA	a	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
17	BCR	1	1649	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	b	805	2	69,73,73	1.27	10 (14%)	83,113,113	1.37	11 (13%)
14	CLA	1	1618	21	69,73,73	1.24	10 (14%)	83,113,113	1.27	5 (6%)
17	BCR	0	208	-	41,41,41	1.22	3 (7%)	56,56,56	1.34	7 (12%)
18	LHG	A	854	14	40,40,48	0.77	1 (2%)	43,46,54	1.22	4 (9%)
17	BCR	b	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	b	842	2	69,73,73	1.26	9 (13%)	83,113,113	1.41	6 (7%)
14	CLA	2	808	2	69,73,73	1.27	9 (13%)	83,113,113	1.34	7 (8%)
14	CLA	l	205	10	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
14	CLA	A	820	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	10 (12%)
14	CLA	a	810	1	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	826	21	69,73,73	1.27	10 (14%)	83,113,113	1.44	9 (10%)
14	CLA	X	1701	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	f	203	-	54,58,73	1.42	6 (11%)	65,95,113	1.38	6 (9%)
14	CLA	f	201	21	62,66,73	1.33	10 (16%)	74,104,113	1.37	8 (10%)
14	CLA	A	811	1	53,57,73	1.42	9 (16%)	62,93,113	1.39	6 (9%)
17	BCR	1	1653	-	25,25,41	1.13	1 (4%)	33,33,56	1.28	4 (12%)
14	CLA	A	817	21	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)
14	CLA	6	203	-	54,58,73	1.42	5 (9%)	65,95,113	1.37	6 (9%)
14	CLA	9	101	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	5 (8%)
14	CLA	B	808	2	69,73,73	1.23	9 (13%)	83,113,113	1.46	8 (9%)
17	BCR	2	849	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	8	1303	-	42,45,73	1.58	9 (21%)	50,78,113	1.45	6 (12%)
14	CLA	1	1617	1	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
14	CLA	a	837	1	49,53,73	1.49	9 (18%)	59,89,113	1.43	7 (11%)
14	CLA	B	824	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	6 (7%)
17	BCR	1	1648	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	A	818	1	69,73,73	1.24	8 (11%)	83,113,113	1.33	5 (6%)
14	CLA	1	1636	1	69,73,73	1.24	9 (13%)	83,113,113	1.37	4 (4%)
14	CLA	9	103	21	62,66,73	1.33	9 (14%)	74,104,113	1.35	10 (13%)
14	CLA	B	803	-	69,73,73	1.26	9 (13%)	83,113,113	1.40	6 (7%)
14	CLA	B	818	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	9 (10%)
17	BCR	A	849	-	41,41,41	1.23	2 (4%)	56,56,56	1.20	6 (10%)
17	BCR	a	849	-	41,41,41	1.22	2 (4%)	56,56,56	1.20	6 (10%)
17	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
17	BCR	8	1305	-	41,41,41	1.22	2 (4%)	56,56,56	1.28	8 (14%)
17	BCR	K	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
17	BCR	b	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
17	BCR	0	203	-	41,41,41	1.39	4 (9%)	56,56,56	1.33	7 (12%)
15	PQN	1	1646	-	34,34,34	0.40	0	42,45,45	0.36	0
14	CLA	2	837	21	49,53,73	1.50	8 (16%)	59,89,113	1.42	5 (8%)
16	SF4	3	101	3	0,12,12	-	-	-		
14	CLA	b	833	2	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	b	828	2	69,73,73	1.28	10 (14%)	83,113,113	1.32	8 (9%)
14	CLA	b	835	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	B	807	2	69,73,73	1.27	9 (13%)	83,113,113	1.33	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	2	822	2	49,53,73	1.47	9 (18%)	59,89,113	1.56	10 (16%)
14	CLA	A	822	21	69,73,73	1.26	10 (14%)	83,113,113	1.34	8 (9%)
14	CLA	A	843	21	69,73,73	1.28	11 (15%)	83,113,113	1.35	5 (6%)
14	CLA	0	205	10	69,73,73	1.29	10 (14%)	83,113,113	1.31	7 (8%)
14	CLA	b	813	2	49,53,73	1.47	9 (18%)	59,89,113	1.45	4 (6%)
17	BCR	0	209	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	A	844	18	49,53,73	1.47	9 (18%)	59,89,113	1.50	7 (11%)
14	CLA	1	1622	1	69,73,73	1.26	7 (10%)	83,113,113	1.34	8 (9%)
14	CLA	1	1645	18	49,53,73	1.47	10 (20%)	59,89,113	1.50	7 (11%)
17	BCR	2	846	-	41,41,41	1.26	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	a	836	1	69,73,73	1.26	9 (13%)	83,113,113	1.37	6 (7%)
17	BCR	9	104	-	25,25,41	1.14	1 (4%)	33,33,56	1.15	4 (12%)
14	CLA	1	1637	1	69,73,73	1.26	9 (13%)	83,113,113	1.38	6 (7%)
14	CLA	1	1621	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	10 (12%)
14	CLA	B	822	21	59,63,73	1.37	10 (16%)	71,101,113	1.34	6 (8%)
14	CLA	2	823	21	59,63,73	1.36	10 (16%)	71,101,113	1.32	6 (8%)
14	CLA	1	1626	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
14	CLA	F	201	21	62,66,73	1.34	10 (16%)	74,104,113	1.36	8 (10%)
18	LHG	l	201	-	38,38,48	0.73	0	41,44,54	1.26	3 (7%)
14	CLA	b	815	2	69,73,73	1.24	10 (14%)	83,113,113	1.33	6 (7%)
14	CLA	1	1611	1	69,73,73	1.27	9 (13%)	83,113,113	1.31	6 (7%)
14	CLA	A	810	1	69,73,73	1.27	9 (13%)	83,113,113	1.33	6 (7%)
17	BCR	L	207	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	a	822	21	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
17	BCR	1	1650	-	41,41,41	1.22	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	A	814	1	69,73,73	1.27	9 (13%)	83,113,113	1.27	7 (8%)
18	LHG	A	853	-	48,48,48	0.75	2 (4%)	51,54,54	1.23	4 (7%)
14	CLA	8	1301	21	49,53,73	1.49	10 (20%)	59,89,113	1.45	8 (13%)
14	CLA	A	855	21	69,73,73	1.24	10 (14%)	83,113,113	1.42	8 (9%)
14	CLA	1	1609	1	55,59,73	1.40	10 (18%)	66,96,113	1.44	6 (9%)
14	CLA	2	826	21	69,73,73	1.27	10 (14%)	83,113,113	1.43	9 (10%)
18	LHG	1	1654	-	48,48,48	0.75	1 (2%)	51,54,54	1.23	4 (7%)
14	CLA	1	1614	1	49,53,73	1.49	10 (20%)	59,89,113	1.50	7 (11%)
17	BCR	L	206	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	1	1641	1	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	2	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	4 (7%)
14	CLA	2	842	2	69,73,73	1.26	9 (13%)	83,113,113	1.41	6 (7%)
14	CLA	B	833	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
18	LHG	1	1655	14	40,40,48	0.77	1 (2%)	43,46,54	1.21	4 (9%)
14	CLA	B	829	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	7 (8%)
16	SF4	A	846	1,2	0,12,12	-	-	-		
17	BCR	i	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.24	3 (5%)
17	BCR	6	204	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	1	1633	1	64,68,73	1.31	11 (17%)	77,107,113	1.33	6 (7%)
17	BCR	b	847	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	8 (14%)
17	BCR	b	849	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
17	BCR	y	102	-	41,41,41	1.24	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	a	817	21	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)
14	CLA	a	820	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	9 (10%)
14	CLA	A	821	1	69,73,73	1.25	7 (10%)	83,113,113	1.34	8 (9%)
13	CL0	A	801	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	6 (7%)
14	CLA	a	805	14,1	63,67,73	1.29	10 (15%)	75,105,113	1.40	9 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	j	1303	-	-	0/4/76/115	-
14	CLA	b	832	2	-	10/20/96/115	-
14	CLA	b	818	2	-	15/39/115/115	-
14	CLA	2	835	2	-	9/39/115/115	-
14	CLA	A	830	-	-	15/39/115/115	-
14	CLA	a	827	21	-	9/39/115/115	-
14	CLA	a	834	1	-	11/39/115/115	-
14	CLA	A	838	1	-	16/39/115/115	-
16	SF4	a	846	1,2	-	-	0/6/5/5
17	BCR	f	204	-	-	8/29/63/63	0/2/2/2
14	CLA	b	806	2	-	16/39/115/115	-
14	CLA	B	838	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	A	847	-	-	9/29/63/63	0/2/2/2
17	BCR	B	843	-	-	11/29/63/63	0/2/2/2
14	CLA	a	829	1	-	14/39/115/115	-
17	BCR	b	848	-	-	11/29/63/63	0/2/2/2
14	CLA	2	809	2	-	9/39/115/115	-
14	CLA	1	1635	1	-	11/39/115/115	-
14	CLA	2	812	2	-	10/39/115/115	-
14	CLA	B	837	2	-	5/33/109/115	-
14	CLA	j	1301	21	-	2/15/91/115	-
14	CLA	1	1608	1	-	15/39/115/115	-
14	CLA	a	844	18	-	5/15/91/115	-
14	CLA	k	101	9	-	12/17/93/115	-
14	CLA	a	842	1	-	12/39/115/115	-
14	CLA	a	815	1	-	14/39/115/115	-
14	CLA	z	102	12	-	7/15/91/115	-
14	CLA	A	825	1	-	14/39/115/115	-
14	CLA	b	822	2	-	5/15/91/115	-
14	CLA	j	1302	-	-	5/15/91/115	-
14	CLA	a	830	-	-	15/39/115/115	-
17	BCR	8	1306	-	-	15/29/63/63	0/2/2/2
15	PQN	2	843	-	-	1/23/43/43	0/2/2/2
14	CLA	1	1623	21	-	12/39/115/115	-
17	BCR	B	847	-	-	11/29/63/63	0/2/2/2
14	CLA	B	825	21	-	11/39/115/115	-
14	CLA	1	1634	1	-	12/39/115/115	-
14	CLA	a	813	1	-	4/15/91/115	-
17	BCR	6	202	-	-	12/29/63/63	0/2/2/2
14	CLA	A	816	1	-	19/39/115/115	-
14	CLA	1	1628	21	-	9/39/115/115	-
14	CLA	b	807	2	-	9/39/115/115	-
13	CL0	a	801	1	-	12/39/115/115	-
14	CLA	b	811	2	-	15/39/115/115	-
14	CLA	B	817	2	-	15/39/115/115	-
14	CLA	F	204	-	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	820	2	-	21/39/115/115	-
14	CLA	a	806	1	-	21/39/115/115	-
14	CLA	1	1615	1	-	17/39/115/115	-
14	CLA	A	823	1	-	8/15/91/115	-
14	CLA	A	840	1	-	18/39/115/115	-
14	CLA	b	841	21	-	9/39/115/115	-
18	LHG	a	853	-	-	21/53/53/53	-
14	CLA	a	831	1	-	7/39/115/115	-
17	BCR	A	848	-	-	15/29/63/63	0/2/2/2
17	BCR	1	1651	-	-	8/29/63/63	0/2/2/2
17	BCR	K	104	-	-	4/18/35/63	0/1/1/2
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	1	1630	1	-	14/39/115/115	-
14	CLA	a	809	1	-	11/39/115/115	-
17	BCR	m	102	-	-	9/29/63/63	0/2/2/2
14	CLA	a	812	14,1	-	13/39/115/115	-
14	CLA	2	811	2	-	15/39/115/115	-
14	CLA	b	831	2	-	13/27/103/115	-
16	SF4	c	102	3	-	-	0/6/5/5
14	CLA	B	823	2	-	5/15/91/115	-
17	BCR	B	848	-	-	5/29/63/63	0/2/2/2
14	CLA	a	824	1	-	12/39/115/115	-
17	BCR	8	1304	-	-	11/29/63/63	0/2/2/2
14	CLA	b	838	2	-	6/33/109/115	-
14	CLA	2	841	21	-	9/39/115/115	-
20	LMG	B	849	-	-	27/50/70/70	0/1/1/1
14	CLA	A	807	1	-	15/39/115/115	-
14	CLA	a	835	1	-	10/39/115/115	-
14	CLA	L	205	21	-	11/39/115/115	-
14	CLA	b	839	2	-	9/39/115/115	-
14	CLA	1	1632	1	-	7/39/115/115	-
14	CLA	B	821	2	-	5/15/91/115	-
14	CLA	2	820	21	-	17/39/115/115	-
14	CLA	B	816	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	829	2	-	11/39/115/115	-
14	CLA	2	834	2	-	11/39/115/115	-
14	CLA	a	818	1	-	10/39/115/115	-
14	CLA	l	204	10	-	17/39/115/115	-
14	CLA	b	814	2	-	16/39/115/115	-
18	LHG	b	851	-	-	18/53/53/53	-
14	CLA	F	203	21	-	2/15/91/115	-
14	CLA	b	809	2	-	9/39/115/115	-
17	BCR	I	101	-	-	7/29/63/63	0/2/2/2
14	CLA	a	808	1	-	6/23/99/115	-
14	CLA	2	819	2	-	17/39/115/115	-
17	BCR	J	103	-	-	11/29/63/63	0/2/2/2
14	CLA	b	812	2	-	10/39/115/115	-
13	CL0	1	1602	1	-	12/39/115/115	-
14	CLA	A	841	1	-	14/39/115/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	2	814	2	-	16/39/115/115	-
15	PQN	B	842	-	-	1/23/43/43	0/2/2/2
17	BCR	1	1652	-	-	18/29/63/63	0/2/2/2
17	BCR	f	202	-	-	12/29/63/63	0/2/2/2
18	LHG	z	101	-	-	18/53/53/53	-
14	CLA	a	832	1	-	6/33/109/115	-
17	BCR	F	202	-	-	12/29/63/63	0/2/2/2
14	CLA	a	807	1	-	15/39/115/115	-
14	CLA	b	837	21	-	3/15/91/115	-
14	CLA	a	821	1	-	16/39/115/115	-
17	BCR	a	851	-	-	18/29/63/63	0/2/2/2
14	CLA	A	857	-	-	0/4/72/115	-
16	SF4	C	101	3	-	-	0/6/5/5
15	PQN	A	845	-	-	1/23/43/43	0/2/2/2
14	CLA	B	841	2	-	10/39/115/115	-
14	CLA	A	819	1	-	19/39/115/115	-
14	CLA	2	815	2	-	13/39/115/115	-
14	CLA	B	840	21	-	9/39/115/115	-
14	CLA	2	828	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	852	-	-	15/29/63/63	0/2/2/2
14	CLA	B	836	21	-	3/15/91/115	-
14	CLA	A	839	1	-	20/39/115/115	-
14	CLA	1	1620	1	-	19/39/115/115	-
14	CLA	2	840	2	-	2/18/94/115	-
14	CLA	x	1701	12	-	7/15/91/115	-
14	CLA	a	823	1	-	8/15/91/115	-
14	CLA	l	206	21	-	11/39/115/115	-
17	BCR	A	850	-	-	8/29/63/63	0/2/2/2
14	CLA	b	802	21	-	18/39/115/115	-
14	CLA	B	831	2	-	10/20/96/115	-
14	CLA	a	814	1	-	17/39/115/115	-
14	CLA	1	1643	1	-	12/39/115/115	-
16	SF4	3	102	3	-	-	0/6/5/5
14	CLA	B	819	21	-	17/39/115/115	-
14	CLA	A	833	1	-	12/39/115/115	-
14	CLA	b	820	21	-	17/39/115/115	-
14	CLA	a	816	1	-	19/39/115/115	-
14	CLA	1	1624	1	-	8/15/91/115	-
14	CLA	B	839	2	-	2/18/94/115	-
14	CLA	A	837	1	-	5/15/91/115	-
14	CLA	a	841	1	-	14/39/115/115	-
14	CLA	K	103	21	-	9/31/107/115	-
15	PQN	b	843	-	-	1/23/43/43	0/2/2/2
14	CLA	1	1607	1	-	21/39/115/115	-
18	LHG	L	208	-	-	27/43/43/53	-
14	CLA	1	1625	1	-	12/39/115/115	-
14	CLA	2	807	2	-	9/39/115/115	-
18	LHG	a	854	14	-	13/45/45/53	-
14	CLA	B	814	2	-	13/39/115/115	-
14	CLA	1	1629	1	-	7/39/115/115	-
14	CLA	2	802	21	-	18/39/115/115	-
14	CLA	6	201	21	-	6/31/107/115	-
14	CLA	2	806	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	828	1	-	7/39/115/115	-
14	CLA	a	840	1	-	18/39/115/115	-
17	BCR	a	848	-	-	15/29/63/63	0/2/2/2
14	CLA	2	827	2	-	6/39/115/115	-
14	CLA	a	819	1	-	19/39/115/115	-
16	SF4	1	1647	1,2	-	-	0/6/5/5
14	CLA	a	811	1	-	8/20/96/115	-
14	CLA	k	103	21	-	9/31/107/115	-
14	CLA	b	821	2	-	21/39/115/115	-
14	CLA	b	817	2	-	12/39/115/115	-
14	CLA	b	816	2	-	13/39/115/115	-
14	CLA	2	831	2	-	13/27/103/115	-
14	CLA	J	102	-	-	0/4/76/115	-
17	BCR	A	852	-	-	11/18/35/63	0/1/1/2
14	CLA	b	823	21	-	5/27/103/115	-
18	LHG	y	101	-	-	27/53/53/53	-
14	CLA	B	813	2	-	16/39/115/115	-
14	CLA	1	1627	21	-	13/39/115/115	-
14	CLA	A	802	-	-	15/39/115/115	-
14	CLA	K	101	9	-	12/17/93/115	-
14	CLA	2	821	2	-	21/39/115/115	-
14	CLA	1	1613	14,1	-	13/39/115/115	-
14	CLA	A	827	21	-	9/39/115/115	-
14	CLA	A	834	1	-	11/39/115/115	-
17	BCR	A	851	-	-	18/29/63/63	0/2/2/2
14	CLA	B	804	2	-	17/39/115/115	-
14	CLA	A	836	1	-	8/39/115/115	-
14	CLA	B	802	2	-	18/39/115/115	-
14	CLA	A	828	1	-	7/39/115/115	-
14	CLA	1	1605	1	-	16/39/115/115	-
14	CLA	2	804	-	-	12/39/115/115	-
17	BCR	F	205	-	-	8/29/63/63	0/2/2/2
14	CLA	2	833	2	-	16/39/115/115	-
14	CLA	B	806	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	1603	-	-	15/39/115/115	-
14	CLA	1	1604	21	-	6/39/115/115	-
14	CLA	L	204	10	-	11/39/115/115	-
14	CLA	A	831	1	-	7/39/115/115	-
14	CLA	A	829	1	-	14/39/115/115	-
14	CLA	1	1642	1	-	14/39/115/115	-
14	CLA	B	827	2	-	15/39/115/115	-
14	CLA	b	810	2	-	11/39/115/115	-
14	CLA	2	832	2	-	10/20/96/115	-
14	CLA	b	836	21	-	11/21/97/115	-
14	CLA	L	203	10	-	17/39/115/115	-
14	CLA	A	826	21	-	13/39/115/115	-
17	BCR	A	856	-	-	13/29/63/63	0/2/2/2
14	CLA	1	1631	-	-	15/39/115/115	-
14	CLA	1	1616	1	-	14/39/115/115	-
14	CLA	1	1619	1	-	10/39/115/115	-
14	CLA	A	815	1	-	14/39/115/115	-
14	CLA	2	818	2	-	15/39/115/115	-
14	CLA	a	843	21	-	16/39/115/115	-
18	LHG	M	101	-	-	27/53/53/53	-
14	CLA	A	805	14,1	-	10/32/108/115	-
14	CLA	A	803	21	-	6/39/115/115	-
14	CLA	1	1610	1	-	11/39/115/115	-
14	CLA	a	804	1	-	16/39/115/115	-
17	BCR	B	846	-	-	12/29/63/63	0/2/2/2
14	CLA	2	838	2	-	6/33/109/115	-
17	BCR	a	850	-	-	8/29/63/63	0/2/2/2
14	CLA	0	206	10	-	11/39/115/115	-
18	LHG	B	850	-	-	18/53/53/53	-
14	CLA	2	836	21	-	11/21/97/115	-
14	CLA	B	805	2	-	16/39/115/115	-
14	CLA	b	830	2	-	7/39/115/115	-
14	CLA	A	813	1	-	4/15/91/115	-
14	CLA	b	819	2	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	8	1302	-	-	5/15/91/115	-
18	LHG	0	202	-	-	27/43/43/53	-
20	LMG	2	850	-	-	27/50/70/70	0/1/1/1
17	BCR	l	202	-	-	8/29/63/63	0/2/2/2
18	LHG	m	101	-	-	27/53/53/53	-
14	CLA	a	826	21	-	13/39/115/115	-
14	CLA	1	1606	14,1	-	10/32/108/115	-
14	CLA	2	813	2	-	2/15/91/115	-
14	CLA	B	826	2	-	6/39/115/115	-
14	CLA	B	832	2	-	16/39/115/115	-
14	CLA	A	842	1	-	12/39/115/115	-
15	PQN	a	845	-	-	1/23/43/43	0/2/2/2
14	CLA	a	838	1	-	16/39/115/115	-
20	LMG	b	850	-	-	27/50/70/70	0/1/1/1
14	CLA	a	833	1	-	12/39/115/115	-
17	BCR	j	1305	-	-	13/29/63/63	0/2/2/2
14	CLA	B	834	2	-	9/39/115/115	-
14	CLA	2	816	2	-	13/39/115/115	-
17	BCR	B	845	-	-	11/29/63/63	0/2/2/2
14	CLA	A	809	1	-	11/39/115/115	-
14	CLA	J	101	-	-	5/15/91/115	-
17	BCR	0	201	-	-	5/29/63/63	0/2/2/2
14	CLA	B	810	2	-	15/39/115/115	-
14	CLA	A	812	14,1	-	13/39/115/115	-
17	BCR	a	847	-	-	9/29/63/63	0/2/2/2
14	CLA	b	840	2	-	2/18/94/115	-
14	CLA	2	829	2	-	11/39/115/115	-
17	BCR	2	848	-	-	11/29/63/63	0/2/2/2
14	CLA	b	827	2	-	6/39/115/115	-
14	CLA	b	834	2	-	11/39/115/115	-
14	CLA	A	824	1	-	12/39/115/115	-
14	CLA	a	802	-	-	15/39/115/115	-
14	CLA	2	839	2	-	9/39/115/115	-
17	BCR	a	852	-	-	11/18/35/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	1644	21	-	16/39/115/115	-
14	CLA	2	825	2	-	14/39/115/115	-
14	CLA	2	803	2	-	18/39/115/115	-
14	CLA	A	835	1	-	10/39/115/115	-
14	CLA	B	809	2	-	11/39/115/115	-
14	CLA	B	812	2	-	2/15/91/115	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	M	102	-	-	0/4/72/115	-
14	CLA	2	805	2	-	17/39/115/115	-
17	BCR	B	851	-	-	15/29/63/63	0/2/2/2
14	CLA	B	815	2	-	13/39/115/115	-
17	BCR	2	845	-	-	8/29/63/63	0/2/2/2
14	CLA	A	808	1	-	6/23/99/115	-
14	CLA	B	828	2	-	11/39/115/115	-
14	CLA	B	835	21	-	11/21/97/115	-
14	CLA	B	830	2	-	13/27/103/115	-
14	CLA	A	804	1	-	16/39/115/115	-
17	BCR	l	207	-	-	10/29/63/63	0/2/2/2
14	CLA	2	817	2	-	12/39/115/115	-
17	BCR	j	1304	-	-	11/29/63/63	0/2/2/2
17	BCR	7	101	-	-	7/29/63/63	0/2/2/2
14	CLA	1	1612	1	-	8/20/96/115	-
14	CLA	B	811	2	-	10/39/115/115	-
14	CLA	1	1640	1	-	20/39/115/115	-
17	BCR	9	102	-	-	6/29/63/63	0/2/2/2
14	CLA	b	808	2	-	8/39/115/115	-
14	CLA	a	803	21	-	6/39/115/115	-
14	CLA	A	832	1	-	6/33/109/115	-
14	CLA	1	1601	-	-	0/4/72/115	-
14	CLA	b	825	2	-	14/39/115/115	-
17	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	b	824	2	-	5/15/91/115	-
14	CLA	A	806	1	-	21/39/115/115	-
17	BCR	M	103	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	846	-	-	11/29/63/63	0/2/2/2
17	BCR	k	104	-	-	4/18/35/63	0/1/1/2
14	CLA	a	825	1	-	14/39/115/115	-
14	CLA	2	830	2	-	7/39/115/115	-
14	CLA	2	824	2	-	5/15/91/115	-
14	CLA	b	803	2	-	18/39/115/115	-
14	CLA	0	207	21	-	11/39/115/115	-
14	CLA	1	1638	1	-	5/15/91/115	-
14	CLA	b	804	-	-	12/39/115/115	-
14	CLA	1	1639	1	-	16/39/115/115	-
17	BCR	2	847	-	-	12/29/63/63	0/2/2/2
14	CLA	2	810	2	-	11/39/115/115	-
14	CLA	a	839	1	-	20/39/115/115	-
17	BCR	1	1649	-	-	15/29/63/63	0/2/2/2
14	CLA	b	805	2	-	17/39/115/115	-
14	CLA	1	1618	21	-	14/39/115/115	-
17	BCR	0	208	-	-	10/29/63/63	0/2/2/2
18	LHG	A	854	14	-	13/45/45/53	-
17	BCR	b	845	-	-	8/29/63/63	0/2/2/2
14	CLA	b	842	2	-	10/39/115/115	-
14	CLA	2	808	2	-	8/39/115/115	-
14	CLA	l	205	10	-	11/39/115/115	-
14	CLA	A	820	1	-	10/39/115/115	-
14	CLA	a	810	1	-	12/39/115/115	-
14	CLA	b	826	21	-	11/39/115/115	-
14	CLA	X	1701	12	-	7/15/91/115	-
14	CLA	f	203	-	-	6/21/97/115	-
14	CLA	f	201	21	-	6/31/107/115	-
14	CLA	A	811	1	-	8/20/96/115	-
17	BCR	1	1653	-	-	11/18/35/63	0/1/1/2
14	CLA	A	817	21	-	14/39/115/115	-
14	CLA	6	203	-	-	6/21/97/115	-
14	CLA	9	101	-	-	12/17/93/115	-
14	CLA	B	808	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	2	849	-	-	5/29/63/63	0/2/2/2
14	CLA	8	1303	-	-	0/4/76/115	-
14	CLA	1	1617	1	-	19/39/115/115	-
14	CLA	a	837	1	-	5/15/91/115	-
14	CLA	B	824	2	-	14/39/115/115	-
17	BCR	1	1648	-	-	9/29/63/63	0/2/2/2
14	CLA	A	818	1	-	10/39/115/115	-
14	CLA	1	1636	1	-	10/39/115/115	-
14	CLA	9	103	21	-	9/31/107/115	-
14	CLA	B	803	-	-	12/39/115/115	-
14	CLA	B	818	2	-	17/39/115/115	-
17	BCR	A	849	-	-	5/29/63/63	0/2/2/2
17	BCR	a	849	-	-	5/29/63/63	0/2/2/2
17	BCR	k	102	-	-	6/29/63/63	0/2/2/2
17	BCR	8	1305	-	-	13/29/63/63	0/2/2/2
17	BCR	K	102	-	-	6/29/63/63	0/2/2/2
17	BCR	b	844	-	-	11/29/63/63	0/2/2/2
17	BCR	0	203	-	-	8/29/63/63	0/2/2/2
15	PQN	1	1646	-	-	1/23/43/43	0/2/2/2
14	CLA	2	837	21	-	3/15/91/115	-
16	SF4	3	101	3	-	-	0/6/5/5
14	CLA	b	833	2	-	16/39/115/115	-
14	CLA	b	828	2	-	15/39/115/115	-
14	CLA	b	835	2	-	9/39/115/115	-
14	CLA	B	807	2	-	8/39/115/115	-
14	CLA	2	822	2	-	5/15/91/115	-
14	CLA	A	822	21	-	12/39/115/115	-
14	CLA	A	843	21	-	16/39/115/115	-
14	CLA	0	205	10	-	17/39/115/115	-
14	CLA	b	813	2	-	2/15/91/115	-
17	BCR	0	209	-	-	5/29/63/63	0/2/2/2
14	CLA	A	844	18	-	5/15/91/115	-
14	CLA	1	1622	1	-	16/39/115/115	-
14	CLA	1	1645	18	-	5/15/91/115	-
17	BCR	2	846	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	836	1	-	8/39/115/115	-
17	BCR	9	104	-	-	4/18/35/63	0/1/1/2
14	CLA	1	1637	1	-	8/39/115/115	-
14	CLA	1	1621	1	-	10/39/115/115	-
14	CLA	B	822	21	-	5/27/103/115	-
14	CLA	2	823	21	-	5/27/103/115	-
14	CLA	1	1626	1	-	14/39/115/115	-
14	CLA	F	201	21	-	6/31/107/115	-
18	LHG	l	201	-	-	27/43/43/53	-
14	CLA	b	815	2	-	13/39/115/115	-
14	CLA	1	1611	1	-	12/39/115/115	-
14	CLA	A	810	1	-	12/39/115/115	-
17	BCR	L	207	-	-	5/29/63/63	0/2/2/2
14	CLA	a	822	21	-	12/39/115/115	-
17	BCR	1	1650	-	-	5/29/63/63	0/2/2/2
14	CLA	A	814	1	-	17/39/115/115	-
18	LHG	A	853	-	-	21/53/53/53	-
14	CLA	8	1301	21	-	2/15/91/115	-
14	CLA	A	855	21	-	18/39/115/115	-
14	CLA	1	1609	1	-	6/23/99/115	-
14	CLA	2	826	21	-	11/39/115/115	-
18	LHG	1	1654	-	-	21/53/53/53	-
14	CLA	1	1614	1	-	4/15/91/115	-
17	BCR	L	206	-	-	10/29/63/63	0/2/2/2
14	CLA	1	1641	1	-	18/39/115/115	-
17	BCR	2	844	-	-	11/29/63/63	0/2/2/2
14	CLA	2	842	2	-	10/39/115/115	-
14	CLA	B	833	2	-	11/39/115/115	-
18	LHG	1	1655	14	-	13/45/45/53	-
14	CLA	B	829	2	-	7/39/115/115	-
17	BCR	i	101	-	-	7/29/63/63	0/2/2/2
16	SF4	A	846	1,2	-	-	0/6/5/5
17	BCR	6	204	-	-	8/29/63/63	0/2/2/2
14	CLA	1	1633	1	-	6/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	847	-	-	12/29/63/63	0/2/2/2
17	BCR	b	849	-	-	5/29/63/63	0/2/2/2
17	BCR	y	102	-	-	9/29/63/63	0/2/2/2
14	CLA	a	817	21	-	14/39/115/115	-
14	CLA	a	820	1	-	10/39/115/115	-
14	CLA	A	821	1	-	16/39/115/115	-
13	CL0	A	801	1	-	12/39/115/115	-
14	CLA	a	805	14,1	-	10/32/108/115	-

The worst 5 of 2998 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	845	BCR	C30-C25	-4.08	1.48	1.53
17	1	1651	BCR	C30-C25	-4.06	1.48	1.53
17	a	850	BCR	C30-C25	-4.02	1.48	1.53
17	b	846	BCR	C30-C25	-4.01	1.48	1.53
17	2	844	BCR	C1-C6	-4.01	1.48	1.53

The worst 5 of 2628 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	808	CLA	C4A-NA-C1A	8.39	110.48	106.71
14	2	809	CLA	C4A-NA-C1A	8.34	110.46	106.71
14	b	809	CLA	C4A-NA-C1A	8.29	110.43	106.71
14	B	803	CLA	C4A-NA-C1A	8.28	110.43	106.71
14	a	835	CLA	C4A-NA-C1A	8.24	110.41	106.71

There are no chirality outliers.

5 of 4325 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	C6-C7-C8-C9
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

221 monomers are involved in 322 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	818	CLA	4	0
14	2	835	CLA	2	0
14	A	830	CLA	2	0
14	a	827	CLA	2	0
14	b	806	CLA	1	0
14	a	829	CLA	2	0
14	2	809	CLA	1	0
14	1	1635	CLA	2	0
14	2	812	CLA	2	0
14	B	837	CLA	1	0
14	j	1301	CLA	1	0
14	1	1608	CLA	1	0
14	a	815	CLA	2	0
14	z	102	CLA	3	0
14	A	825	CLA	1	0
14	j	1302	CLA	1	0
14	a	830	CLA	1	0
14	1	1634	CLA	2	0
14	a	813	CLA	1	0
14	A	816	CLA	1	0
14	1	1628	CLA	2	0
13	a	801	CL0	2	0
14	b	811	CLA	4	0
14	B	817	CLA	3	0
14	a	806	CLA	1	0
14	1	1615	CLA	2	0
14	A	840	CLA	1	0
18	a	853	LHG	1	0
14	a	831	CLA	1	0
14	1	1630	CLA	2	0
17	m	102	BCR	2	0
14	a	812	CLA	1	0
14	2	811	CLA	2	0
14	a	824	CLA	2	0
14	b	838	CLA	2	0
14	A	807	CLA	1	0
14	a	835	CLA	1	0
14	L	205	CLA	2	0
14	b	839	CLA	1	0
14	1	1632	CLA	1	0
14	B	816	CLA	1	0
14	a	818	CLA	2	0
14	l	204	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	814	CLA	1	0
18	b	851	LHG	3	0
14	F	203	CLA	2	0
14	b	809	CLA	1	0
17	I	101	BCR	3	0
14	b	812	CLA	3	0
14	A	841	CLA	3	0
17	1	1652	BCR	3	0
17	f	202	BCR	1	0
18	z	101	LHG	13	0
14	a	832	CLA	1	0
17	F	202	BCR	1	0
14	a	807	CLA	1	0
14	a	821	CLA	2	0
17	a	851	BCR	4	0
14	A	857	CLA	1	0
15	A	845	PQN	1	0
14	B	841	CLA	1	0
14	A	819	CLA	3	0
14	2	815	CLA	2	0
14	B	840	CLA	1	0
14	2	828	CLA	1	0
17	b	852	BCR	1	0
14	A	839	CLA	1	0
14	1	1620	CLA	5	0
14	x	1701	CLA	4	0
14	a	823	CLA	1	0
14	l	206	CLA	2	0
14	b	802	CLA	4	0
14	B	831	CLA	3	0
14	a	814	CLA	2	0
14	B	819	CLA	1	0
14	A	833	CLA	1	0
14	b	820	CLA	1	0
14	a	816	CLA	1	0
14	1	1624	CLA	3	0
14	B	839	CLA	1	0
14	a	841	CLA	3	0
14	1	1607	CLA	1	0
18	L	208	LHG	1	0
14	1	1625	CLA	2	0
14	B	814	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	1629	CLA	1	0
14	2	802	CLA	2	0
14	6	201	CLA	2	0
14	a	828	CLA	1	0
14	a	840	CLA	1	0
14	a	819	CLA	3	0
14	b	817	CLA	1	0
14	b	823	CLA	1	0
18	y	101	LHG	2	0
14	A	802	CLA	2	0
14	K	101	CLA	1	0
14	1	1613	CLA	1	0
14	A	827	CLA	2	0
14	A	834	CLA	1	0
17	A	851	BCR	4	0
14	B	804	CLA	1	0
14	B	802	CLA	1	0
14	A	828	CLA	1	0
14	1	1605	CLA	1	0
14	2	804	CLA	2	0
14	2	833	CLA	1	0
14	1	1603	CLA	2	0
14	1	1604	CLA	1	0
14	L	204	CLA	1	0
14	A	831	CLA	1	0
14	A	829	CLA	2	0
14	1	1642	CLA	3	0
14	B	827	CLA	1	0
14	2	832	CLA	2	0
14	b	836	CLA	3	0
14	L	203	CLA	1	0
17	A	856	BCR	2	0
14	1	1616	CLA	2	0
14	1	1619	CLA	3	0
14	A	815	CLA	2	0
14	2	818	CLA	3	0
14	a	843	CLA	2	0
18	M	101	LHG	1	0
14	a	804	CLA	1	0
17	B	846	BCR	1	0
14	0	206	CLA	1	0
18	B	850	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	836	CLA	1	0
14	B	805	CLA	1	0
14	A	813	CLA	1	0
14	8	1302	CLA	1	0
18	0	202	LHG	1	0
18	m	101	LHG	1	0
14	B	832	CLA	2	0
15	a	845	PQN	1	0
14	a	833	CLA	2	0
14	B	834	CLA	2	0
14	A	809	CLA	1	0
14	J	101	CLA	1	0
17	0	201	BCR	1	0
14	B	810	CLA	2	0
14	A	812	CLA	1	0
14	b	840	CLA	1	0
14	b	834	CLA	2	0
14	A	824	CLA	2	0
14	2	839	CLA	2	0
14	1	1644	CLA	1	0
14	2	825	CLA	1	0
14	2	803	CLA	1	0
14	A	835	CLA	1	0
14	M	102	CLA	1	0
14	2	805	CLA	1	0
14	B	835	CLA	1	0
14	A	804	CLA	2	0
17	l	207	BCR	1	0
14	2	817	CLA	2	0
14	B	811	CLA	3	0
14	1	1640	CLA	1	0
17	9	102	BCR	1	0
14	b	808	CLA	1	0
14	1	1601	CLA	1	0
14	b	825	CLA	2	0
14	A	806	CLA	1	0
17	M	103	BCR	4	0
14	a	825	CLA	1	0
14	b	803	CLA	1	0
14	0	207	CLA	2	0
14	b	804	CLA	1	0
17	2	847	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	839	CLA	1	0
14	b	805	CLA	1	0
17	0	208	BCR	1	0
14	2	808	CLA	2	0
14	l	205	CLA	1	0
14	A	820	CLA	1	0
14	a	810	CLA	1	0
14	X	1701	CLA	3	0
14	f	201	CLA	3	0
17	1	1653	BCR	1	0
14	B	808	CLA	1	0
14	1	1617	CLA	1	0
14	B	824	CLA	2	0
14	A	818	CLA	3	0
14	1	1636	CLA	1	0
14	9	103	CLA	1	0
14	B	803	CLA	1	0
17	A	849	BCR	1	0
17	a	849	BCR	1	0
17	8	1305	BCR	2	0
17	0	203	BCR	2	0
15	1	1646	PQN	1	0
14	b	833	CLA	2	0
14	b	828	CLA	1	0
14	b	835	CLA	2	0
14	A	843	CLA	1	0
14	0	205	CLA	1	0
14	1	1622	CLA	2	0
14	1	1621	CLA	1	0
14	B	822	CLA	1	0
14	2	823	CLA	1	0
14	1	1626	CLA	1	0
14	F	201	CLA	2	0
18	l	201	LHG	1	0
14	b	815	CLA	1	0
14	1	1611	CLA	2	0
14	A	810	CLA	1	0
17	1	1650	BCR	1	0
14	A	814	CLA	2	0
18	A	853	LHG	1	0
14	8	1301	CLA	1	0
14	A	855	CLA	2	0

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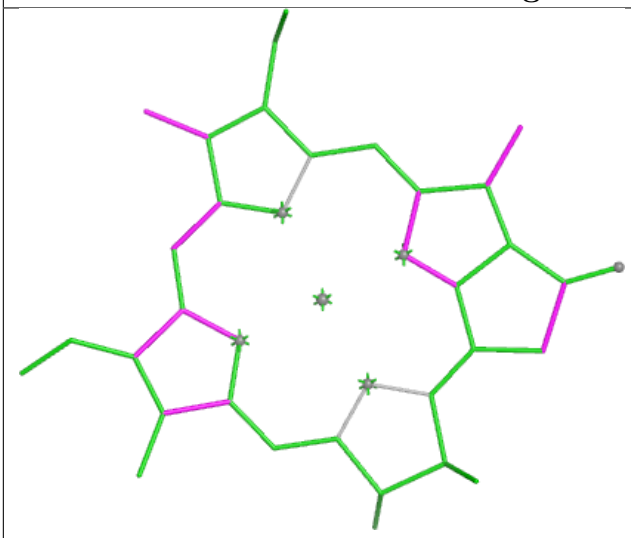
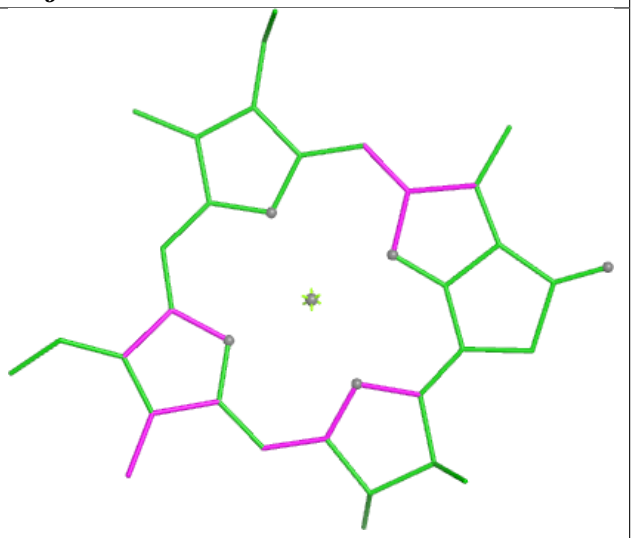
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	1654	LHG	1	0
14	1	1614	CLA	1	0
17	L	206	BCR	1	0
14	1	1641	CLA	1	0
14	B	833	CLA	2	0
17	6	204	BCR	2	0
17	b	847	BCR	1	0
17	y	102	BCR	2	0
14	a	820	CLA	1	0
14	A	821	CLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

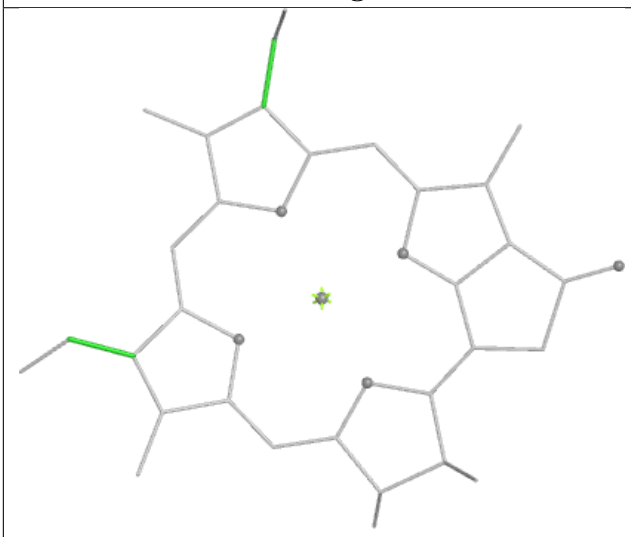
Ligand CLA j 1303



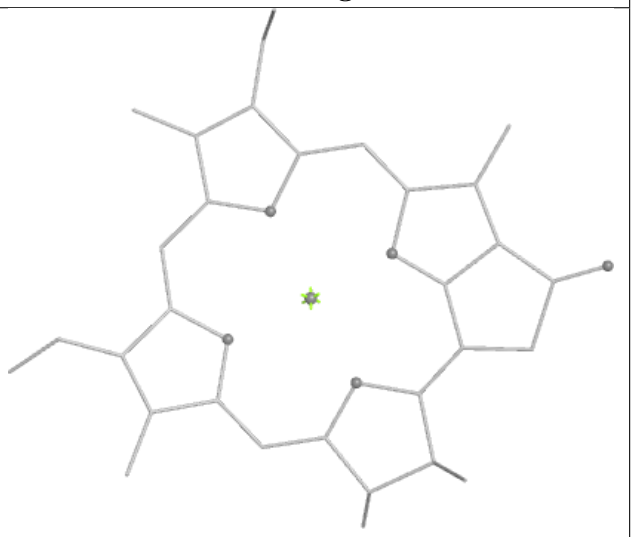
Bond lengths



Bond angles

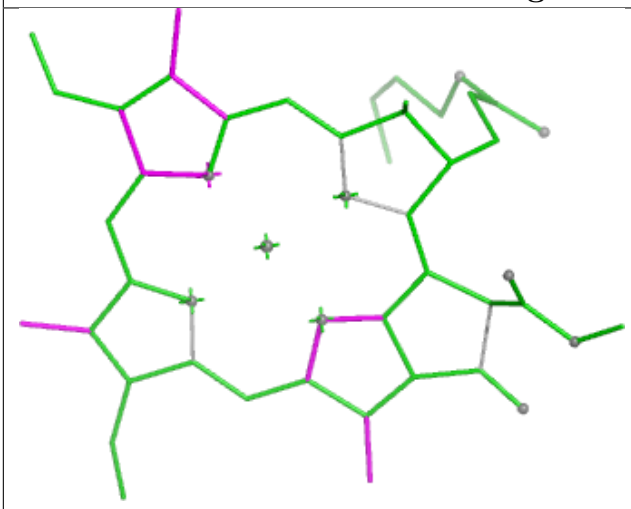


Torsions



Rings

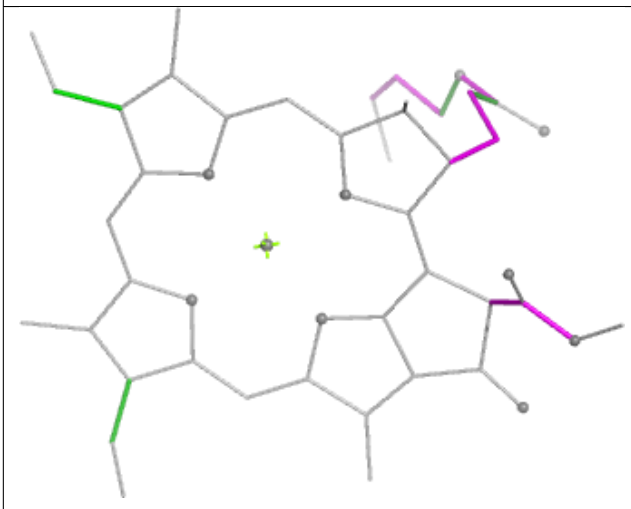
Ligand CLA b 832



Bond lengths



Bond angles

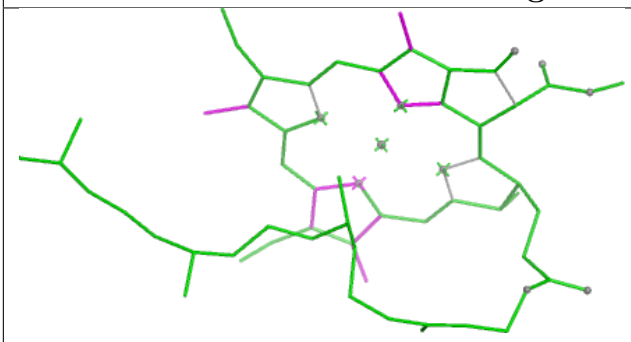


Torsions



Rings

Ligand CLA b 818



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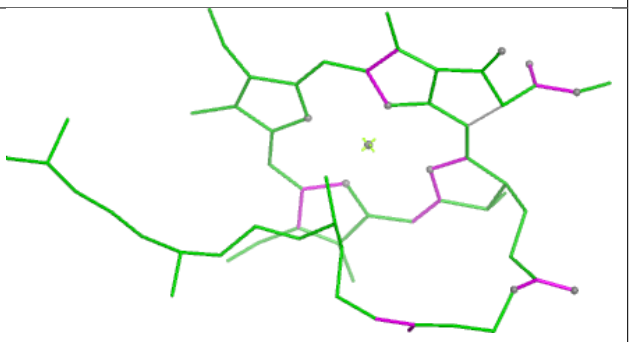
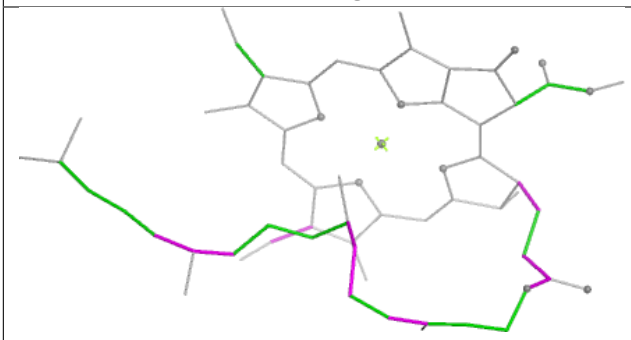
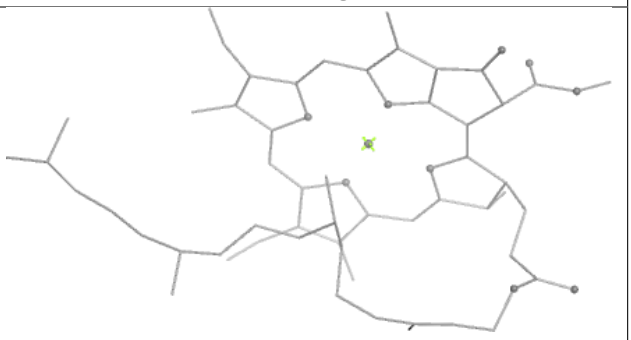


Bond angles

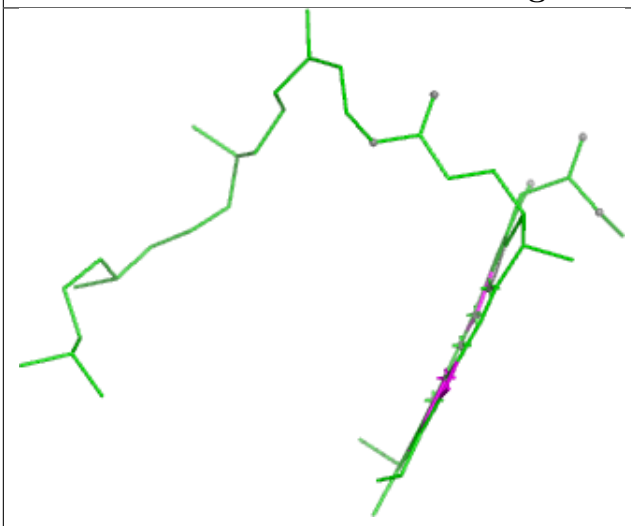


Torsions

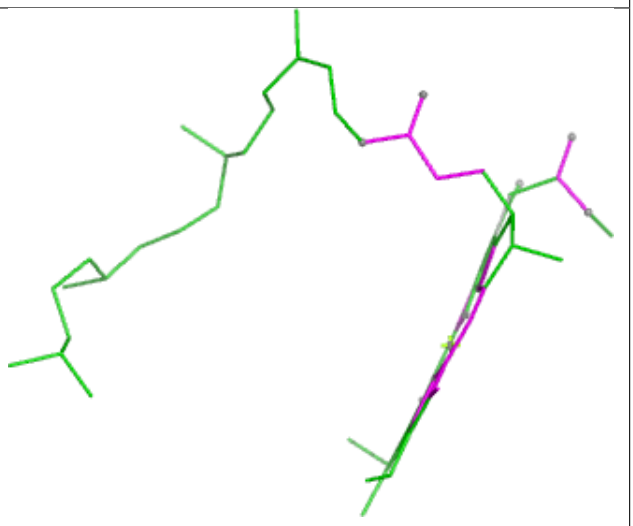


Rings

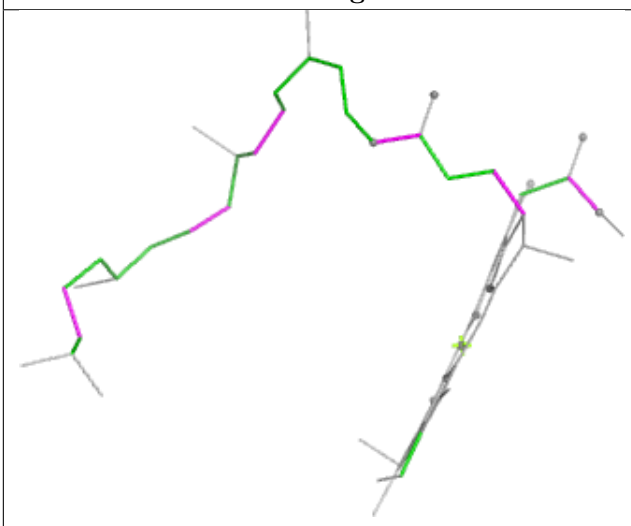
Ligand CLA 2 835



Bond lengths



Bond angles



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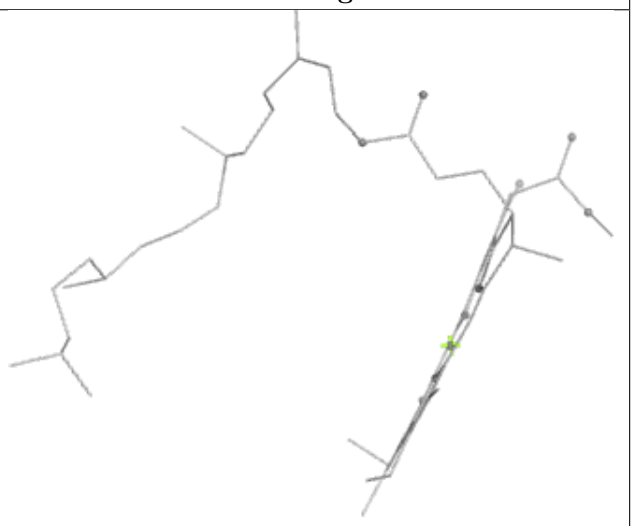
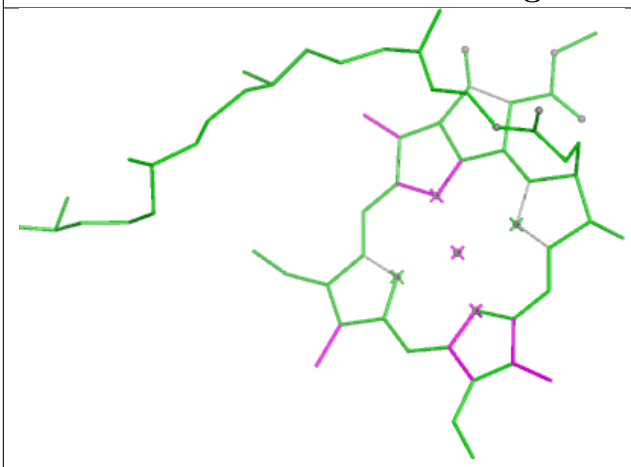


Rings

Ligand CLA A 830



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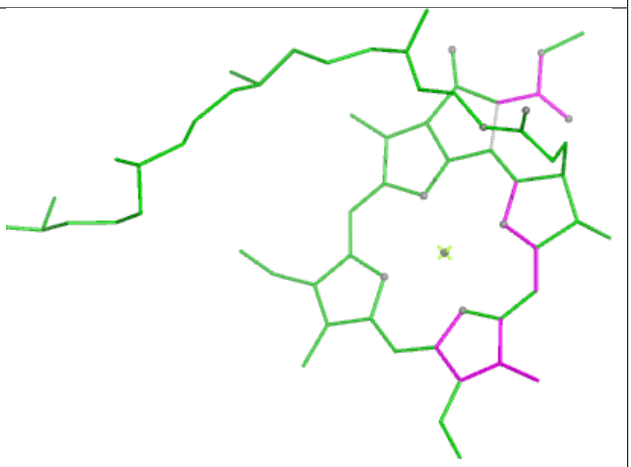
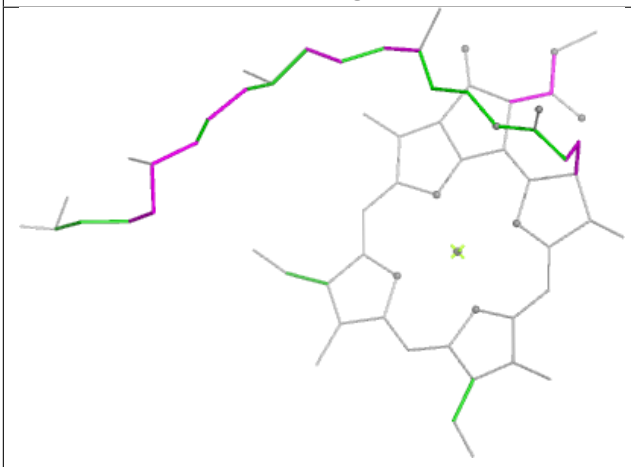


Bond angles

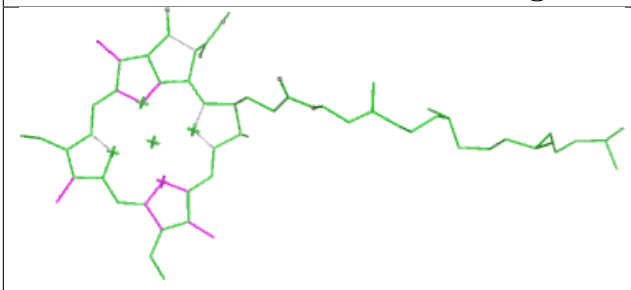


Torsions



Rings

Ligand CLA a 827



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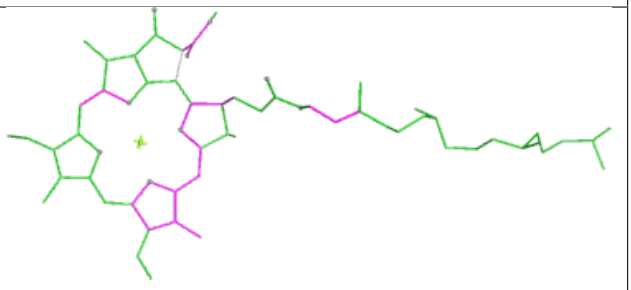

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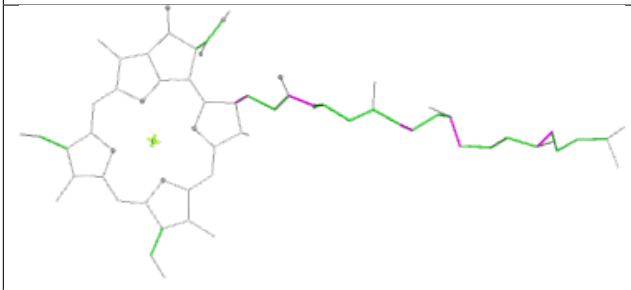

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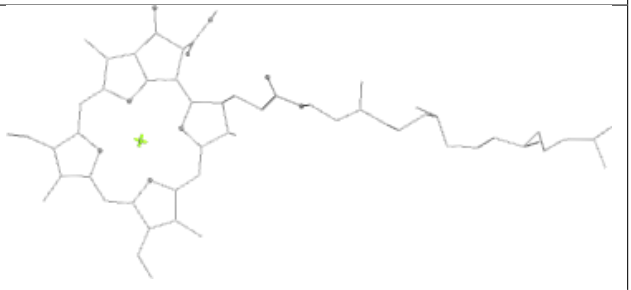

Rings

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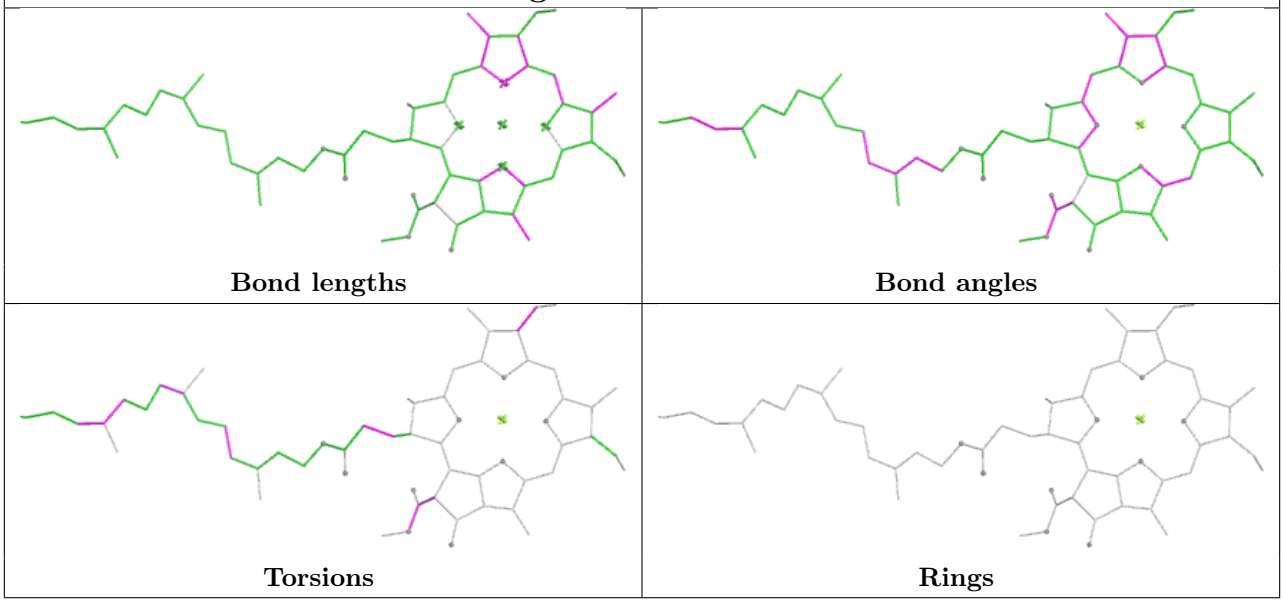
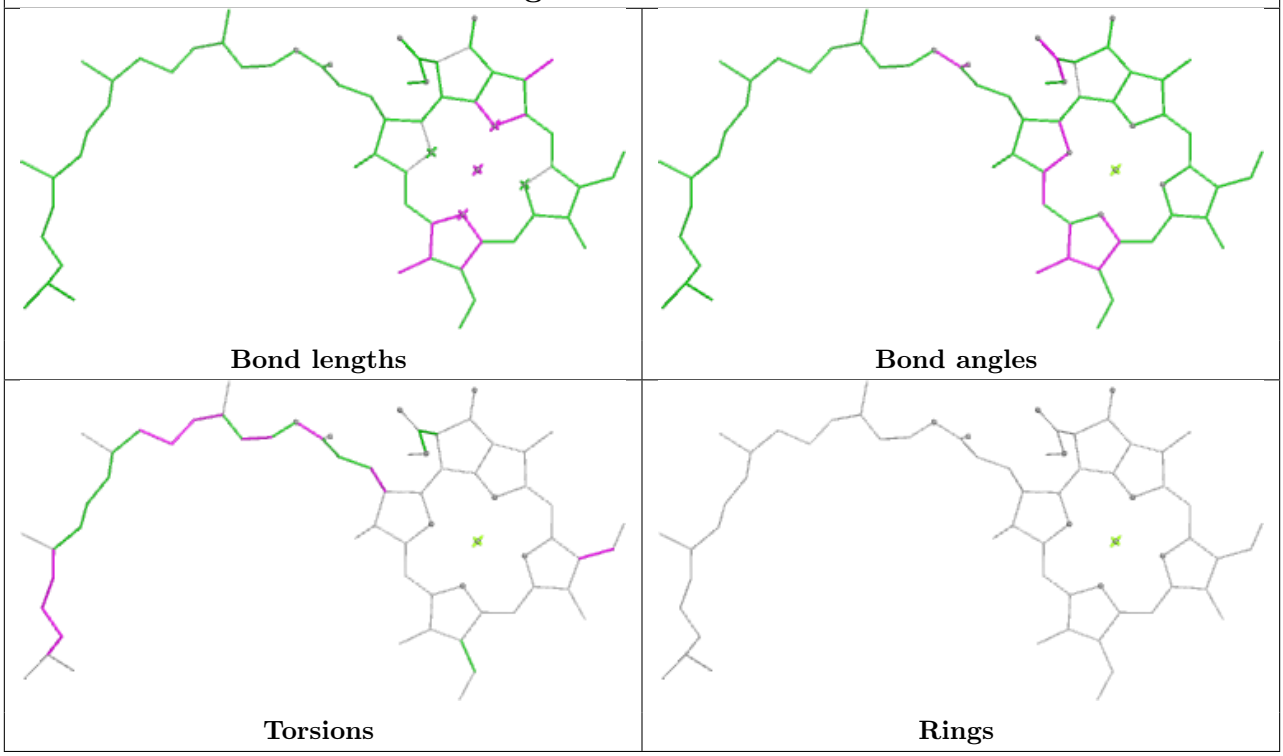
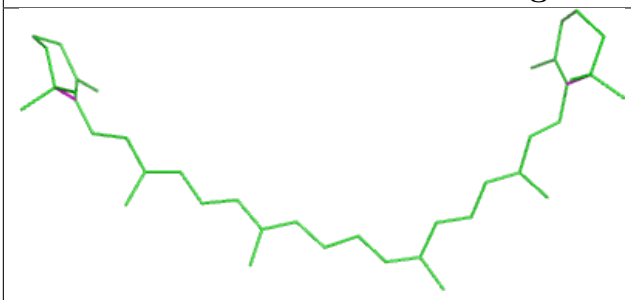


Ligand CLA A 838



Ligand BCR f 204



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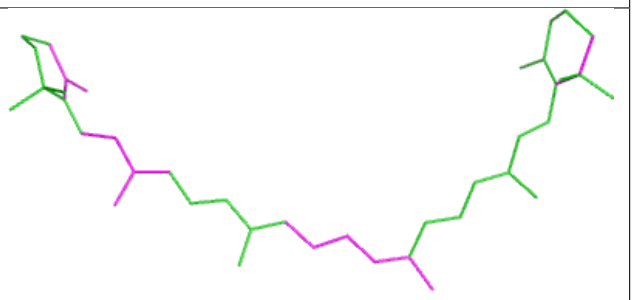

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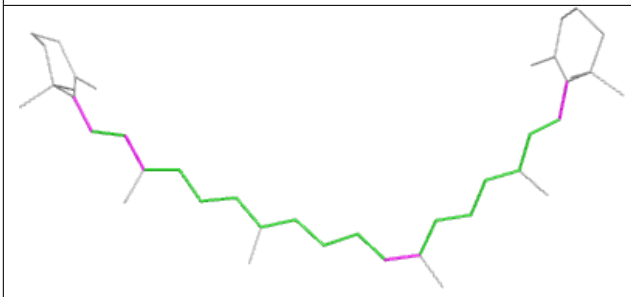
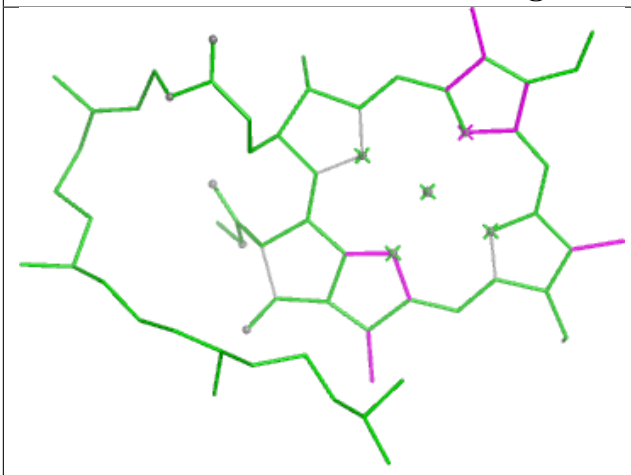


Torsions



Rings

Ligand CLA b 806



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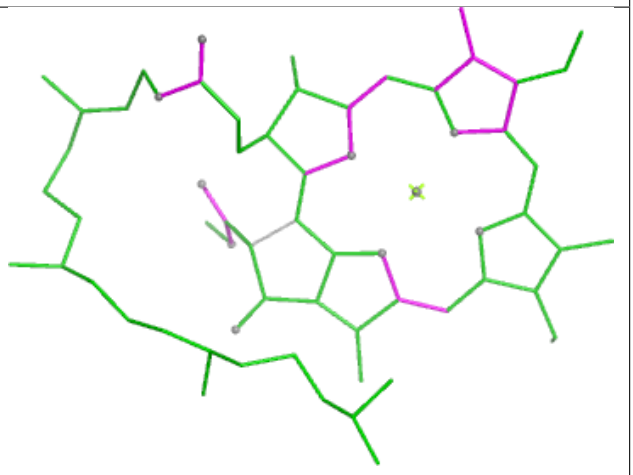

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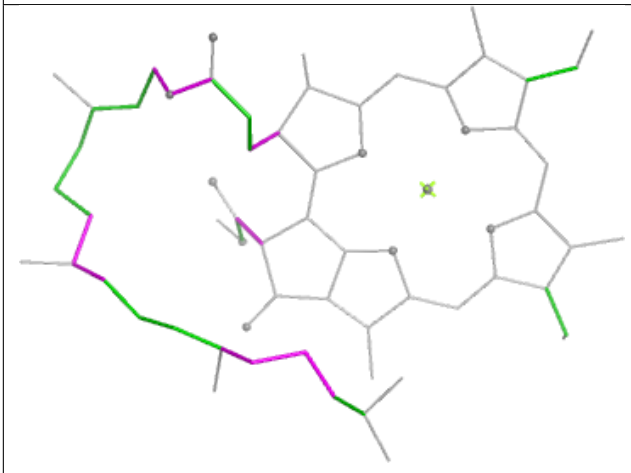

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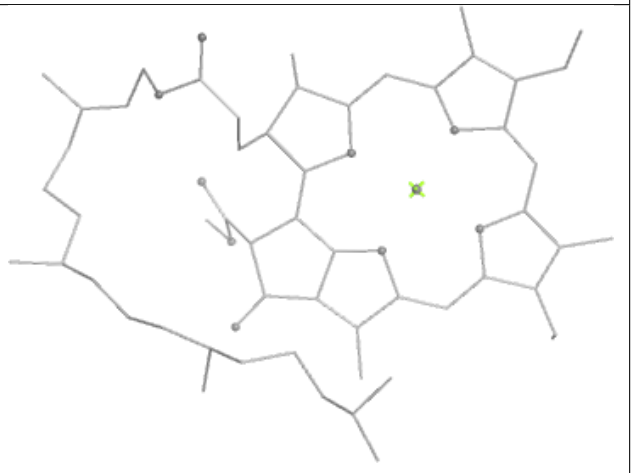

Rings

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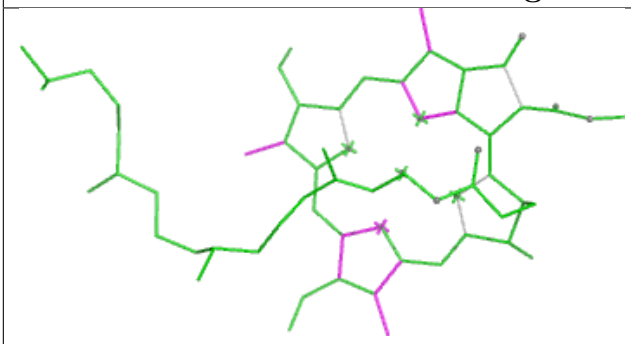

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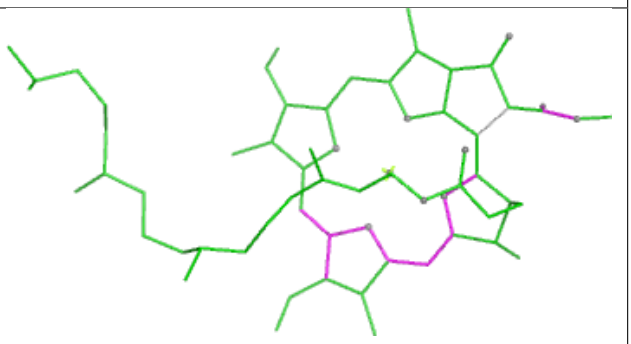

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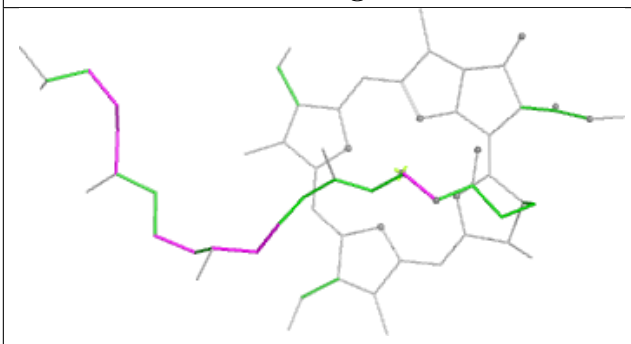

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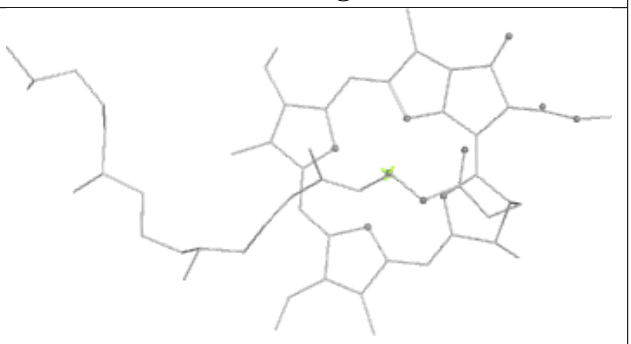
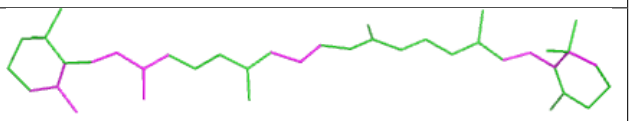


Rings

Ligand BCR A 847



Bond lengths



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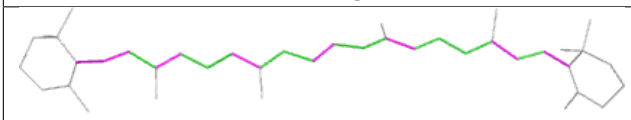

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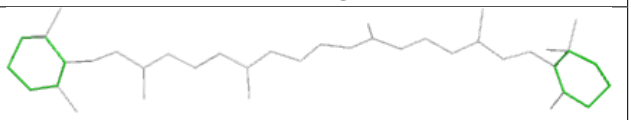
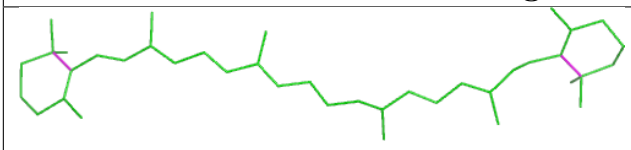


Rings

Ligand BCR B 843



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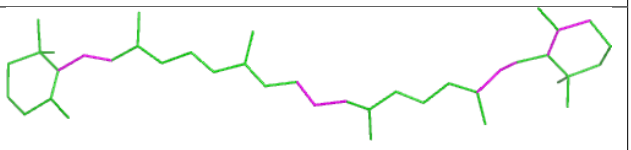

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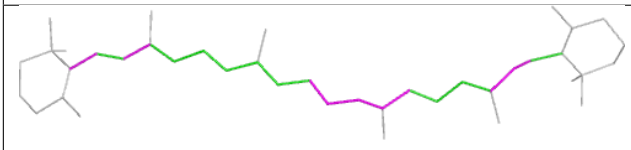

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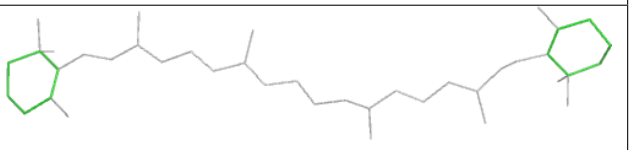
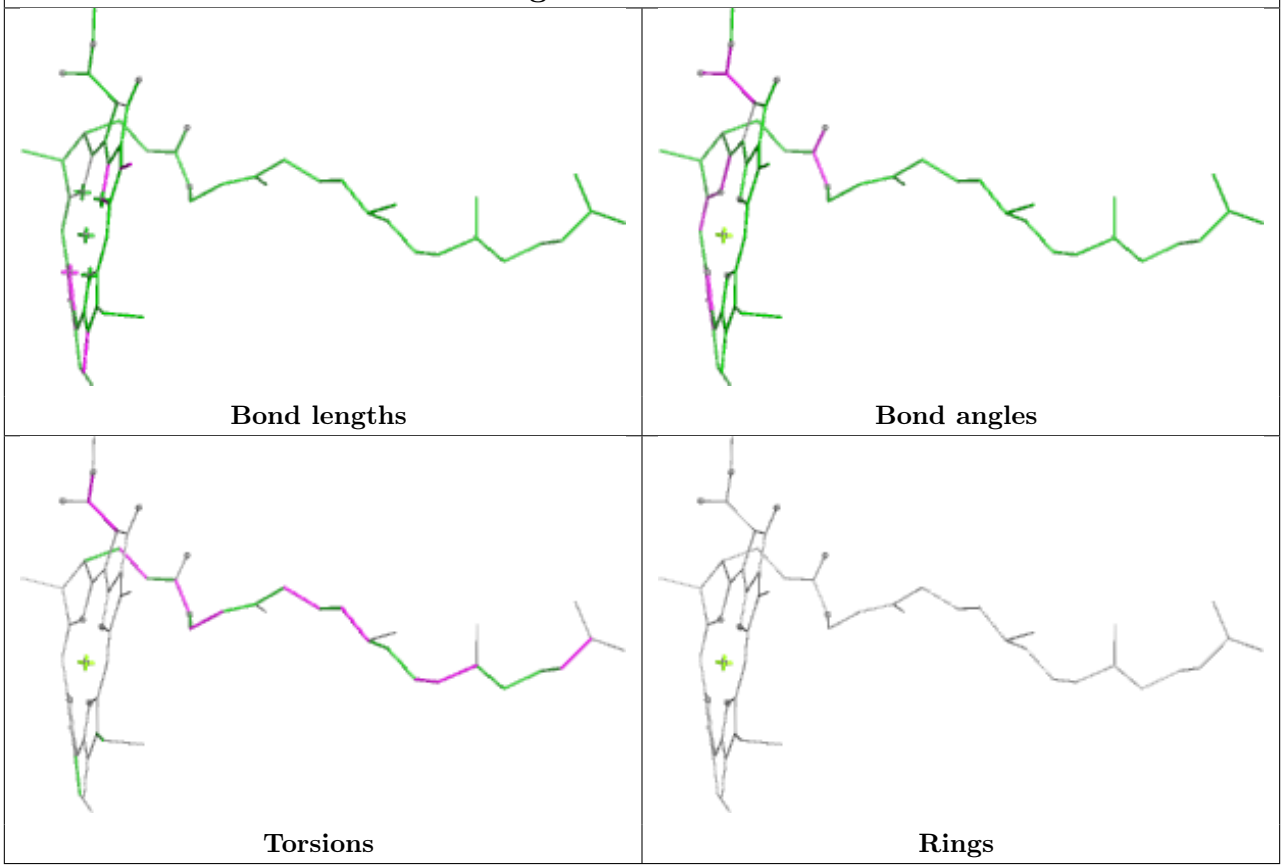


Rings

Ligand CLA a 829



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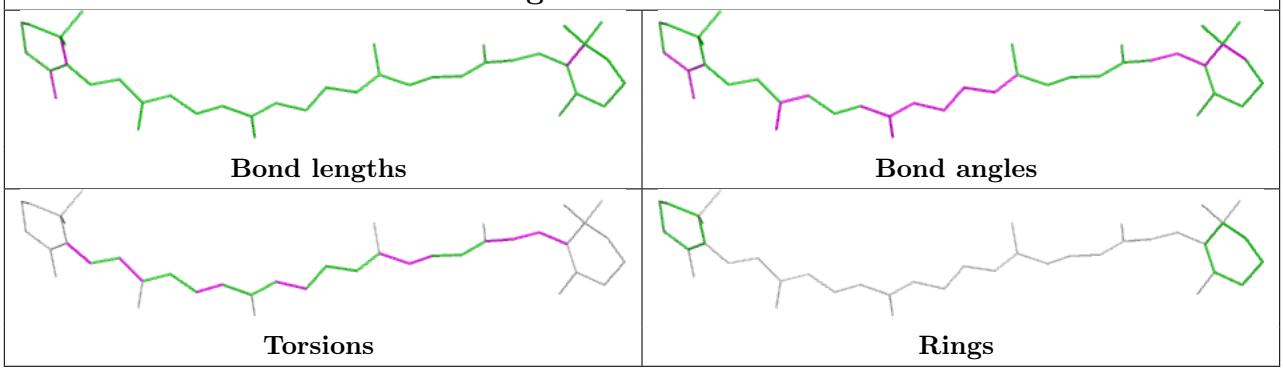
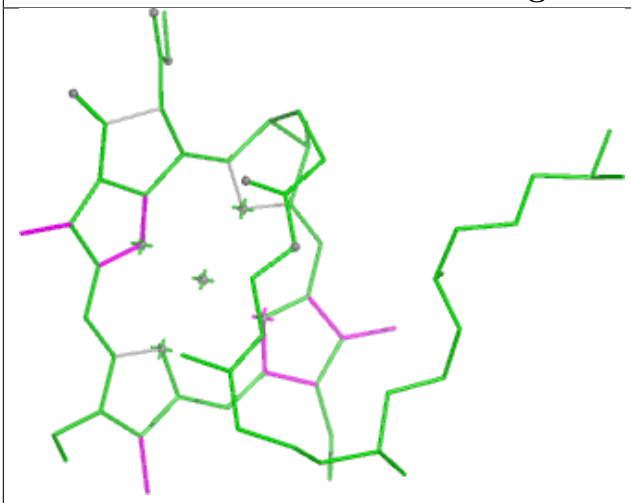


Ligand CLA 2 809



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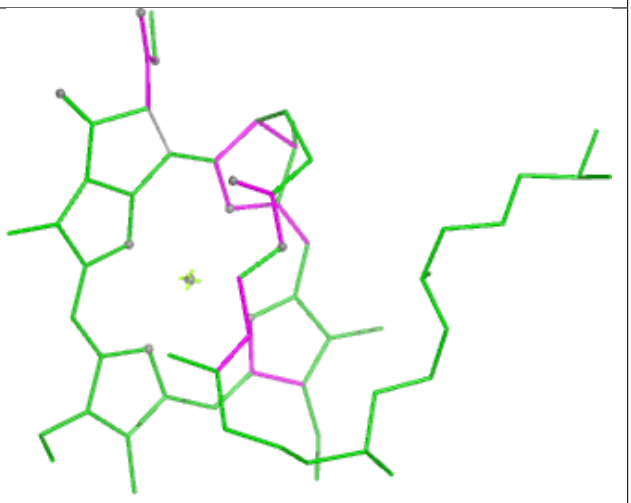

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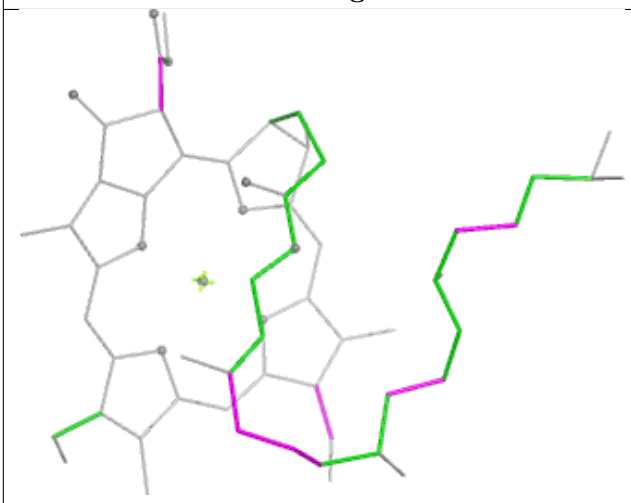

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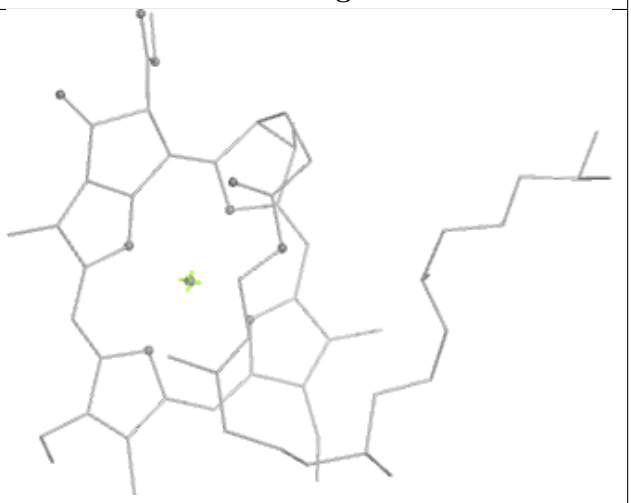
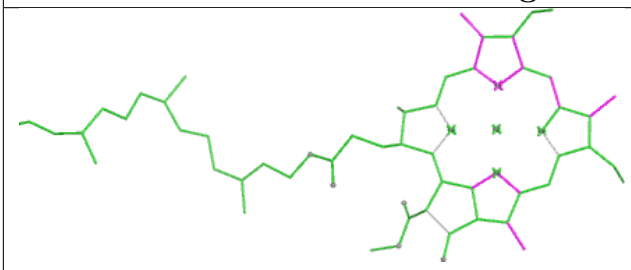


Rings

Ligand CLA 1 1635



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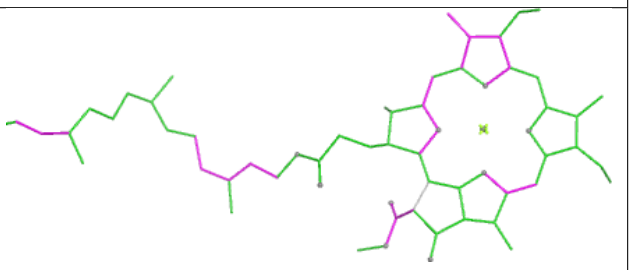
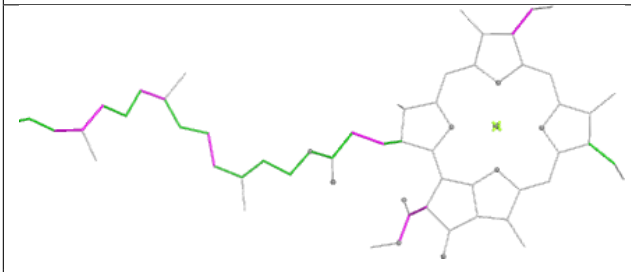


Bond angles



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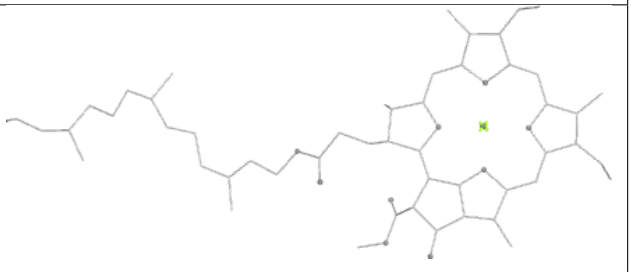


Rings

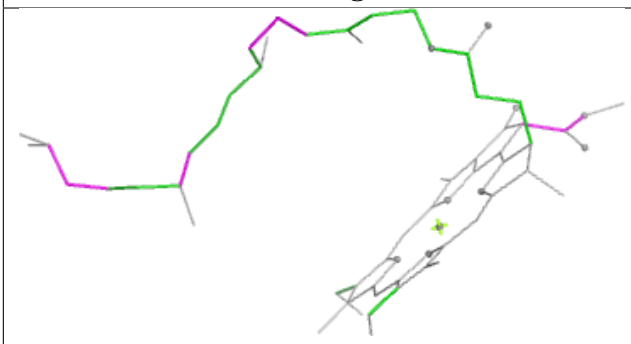
Ligand CLA 2 812



Bond lengths



Bond angles

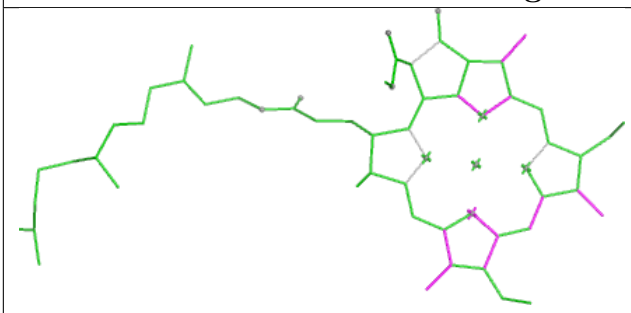


Torsions

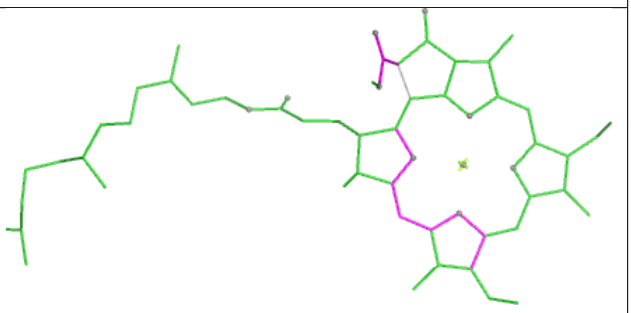


Rings

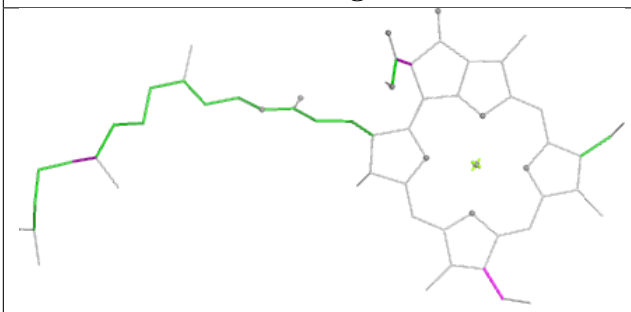
Ligand CLA B 837



Bond lengths



Bond angles



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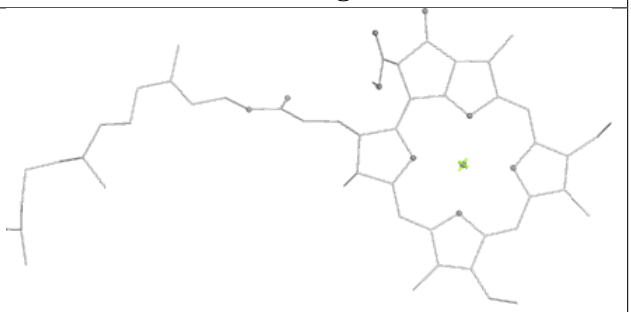
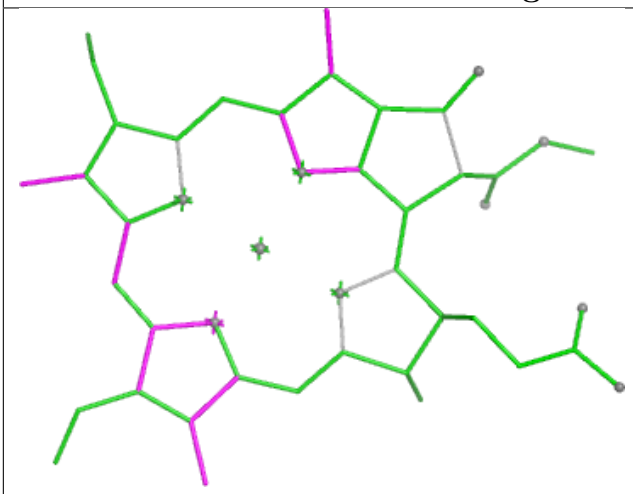
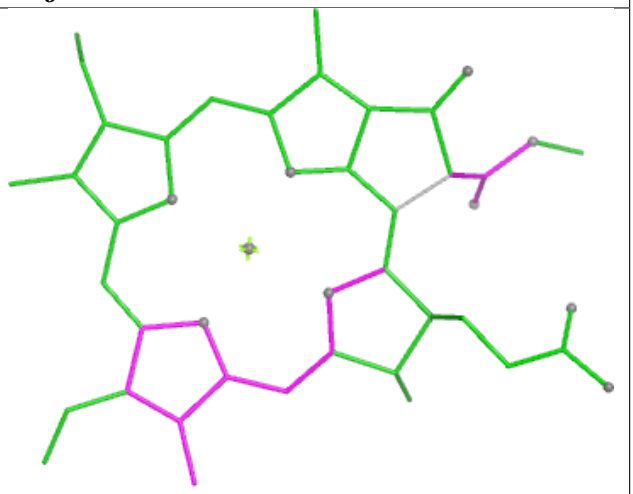


Rings

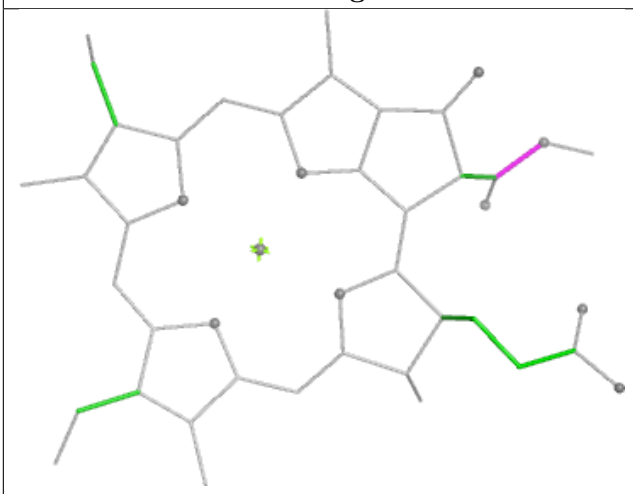
Ligand CLA j 1301



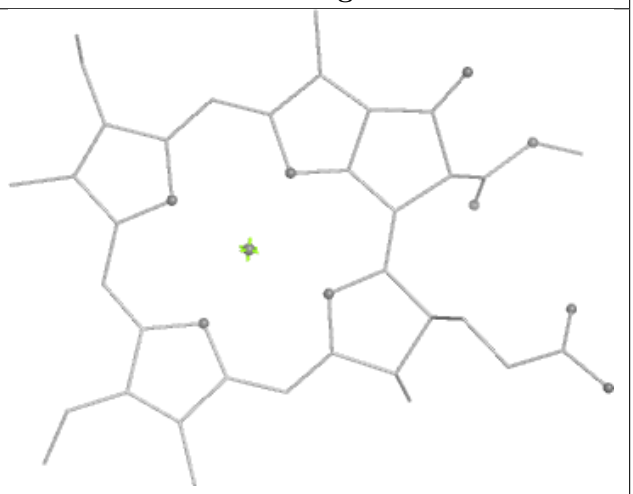
Bond lengths



Bond angles

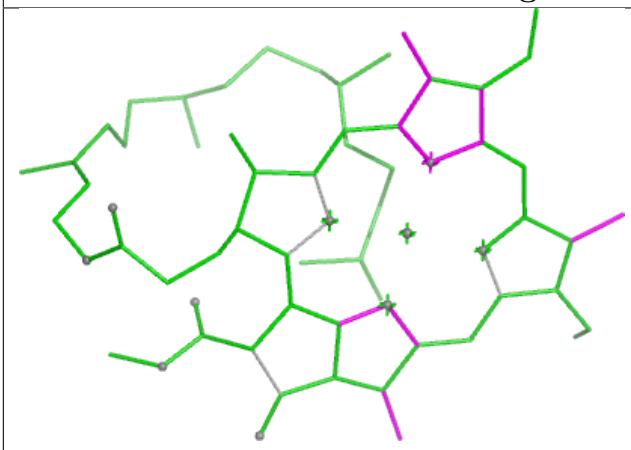


Torsions



Rings

Ligand CLA 1 1608



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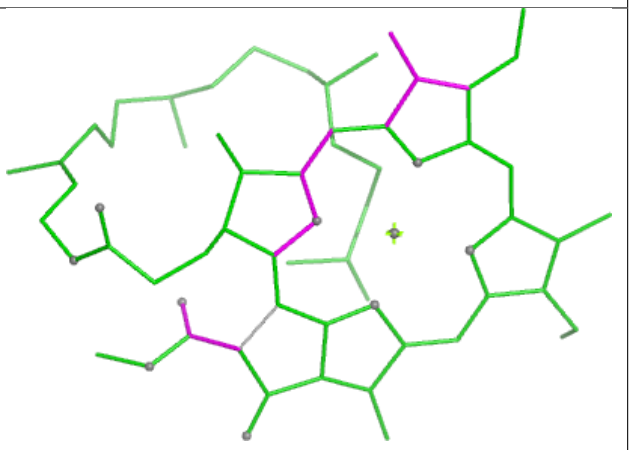

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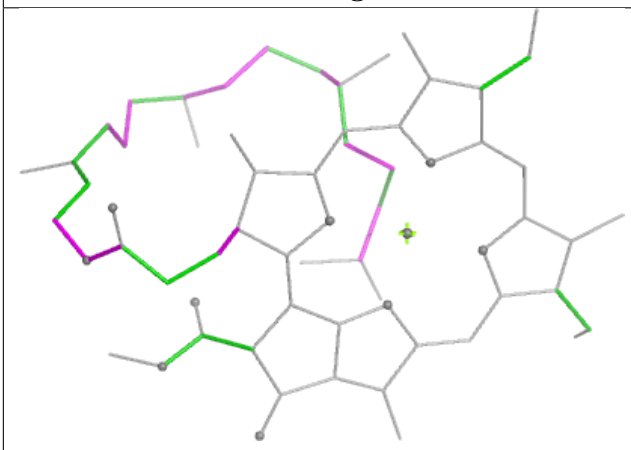

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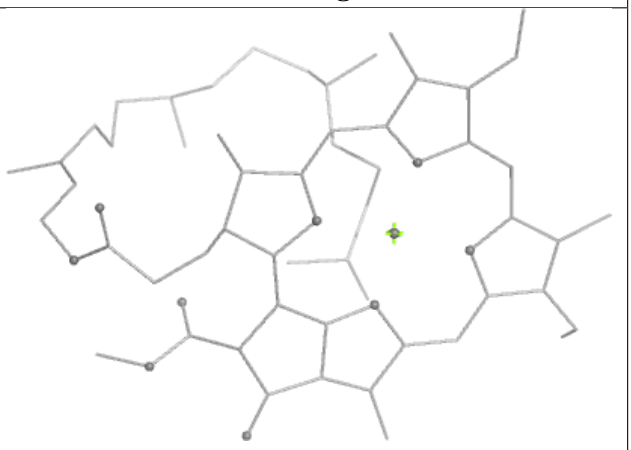
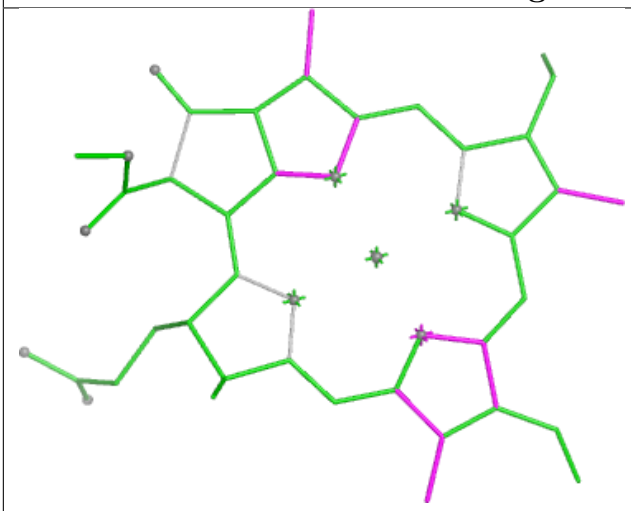


Rings

Ligand CLA a 844



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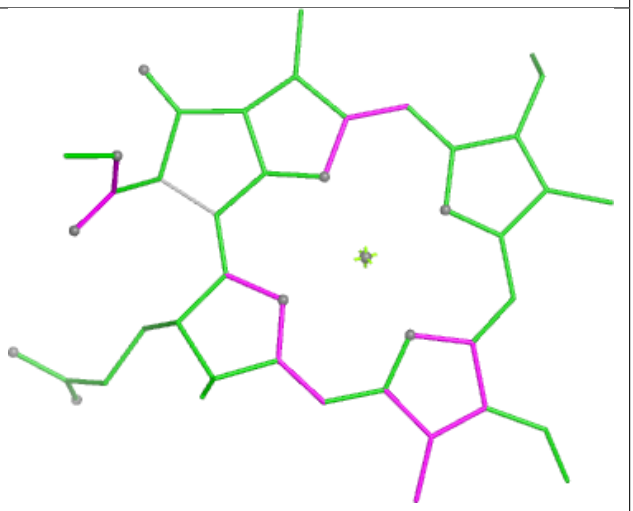

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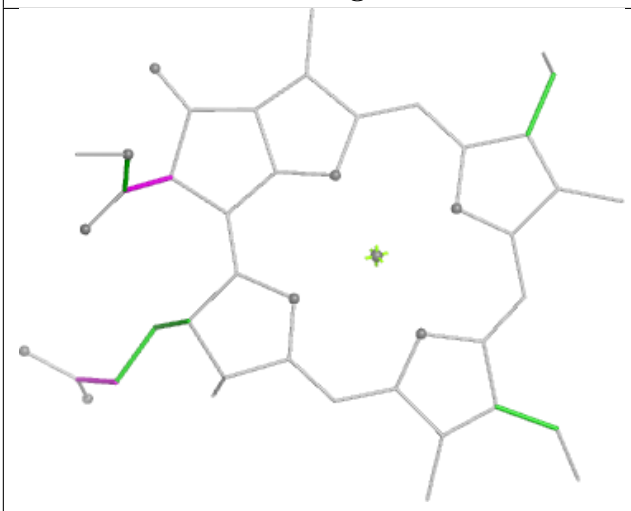

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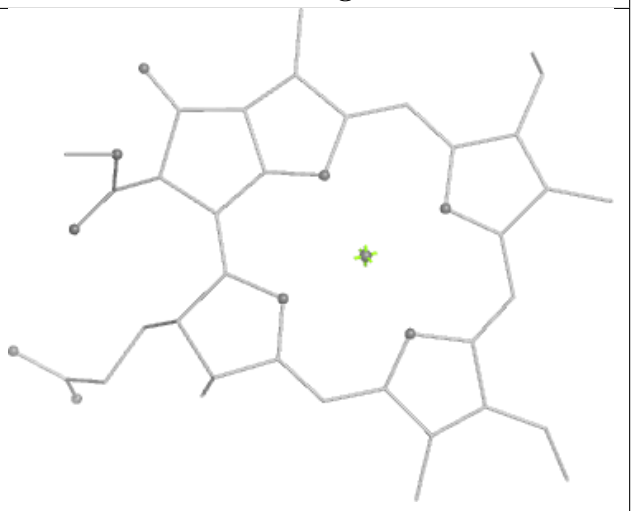
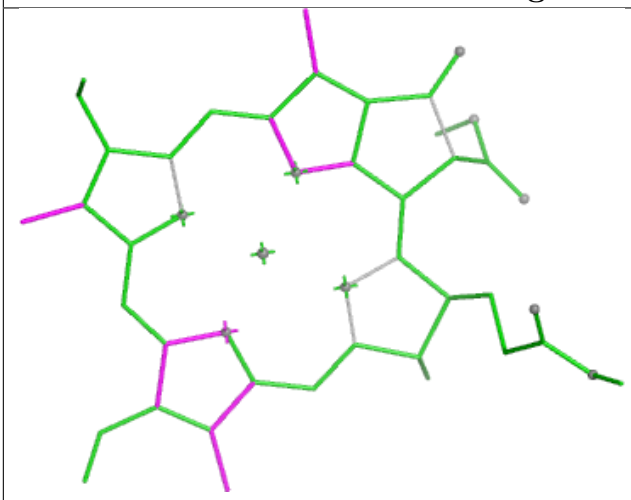


Rings

Ligand CLA k 101



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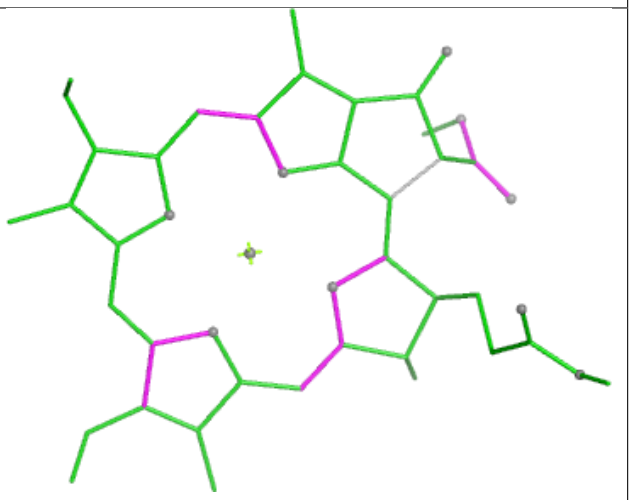

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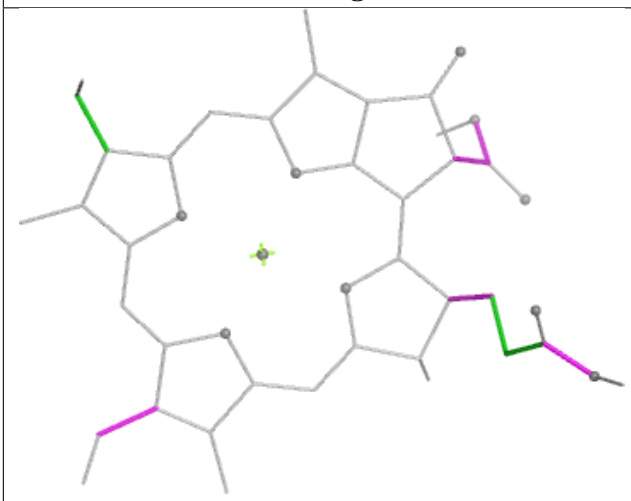

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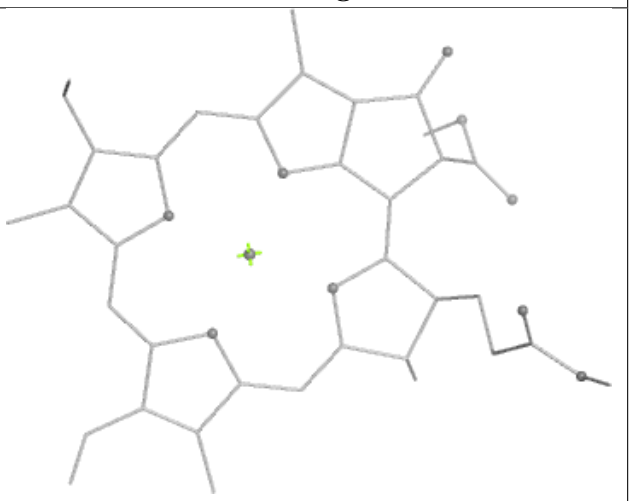
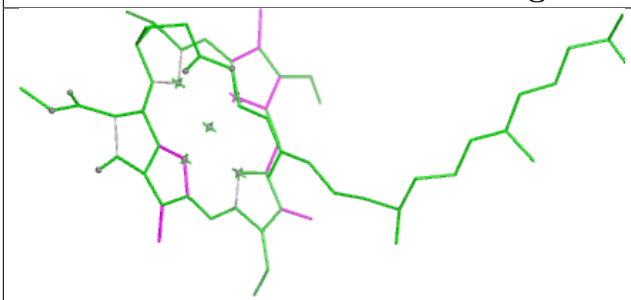


Rings

Ligand CLA a 842



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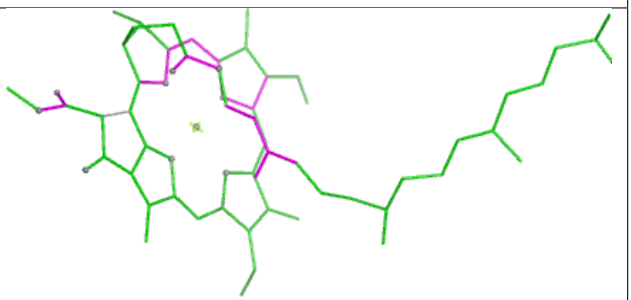

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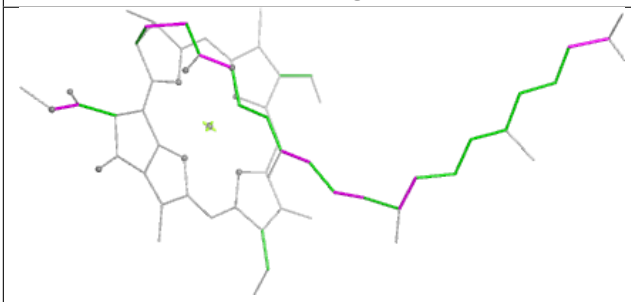

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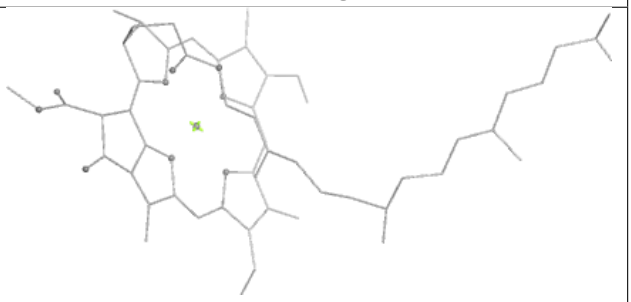
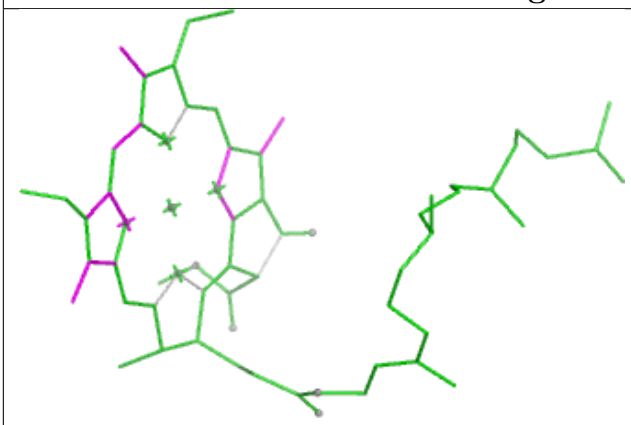


Rings

Ligand CLA a 815



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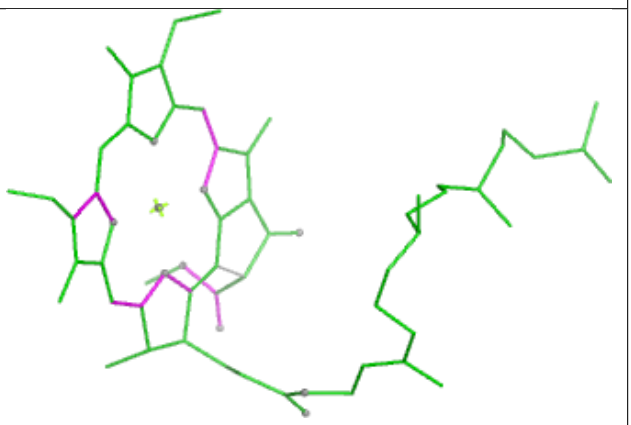

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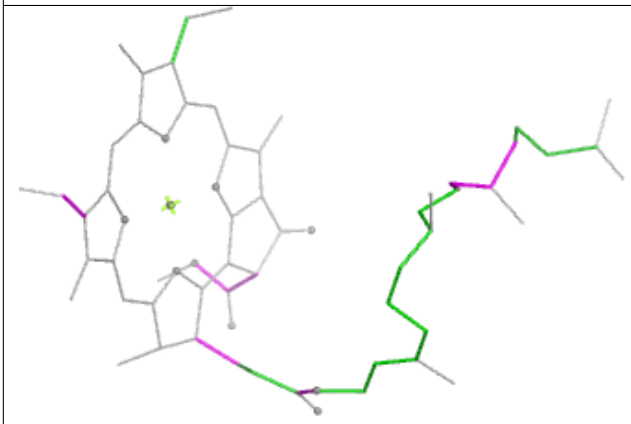

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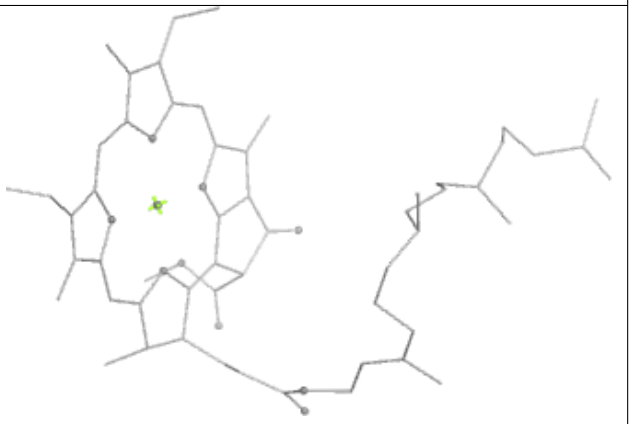
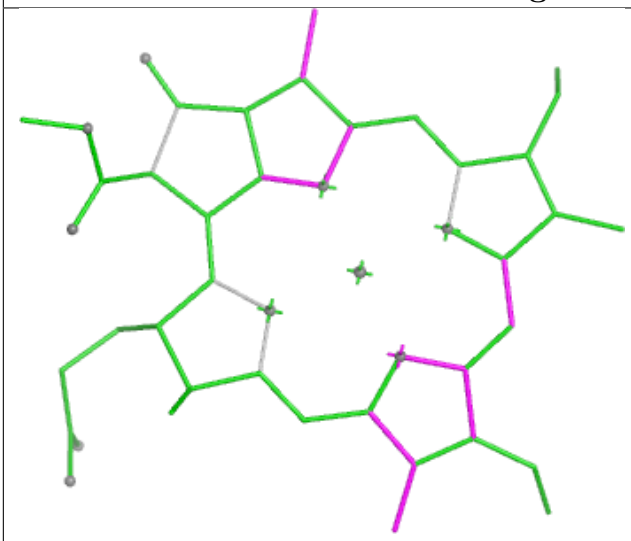


Rings

Ligand CLA z 102



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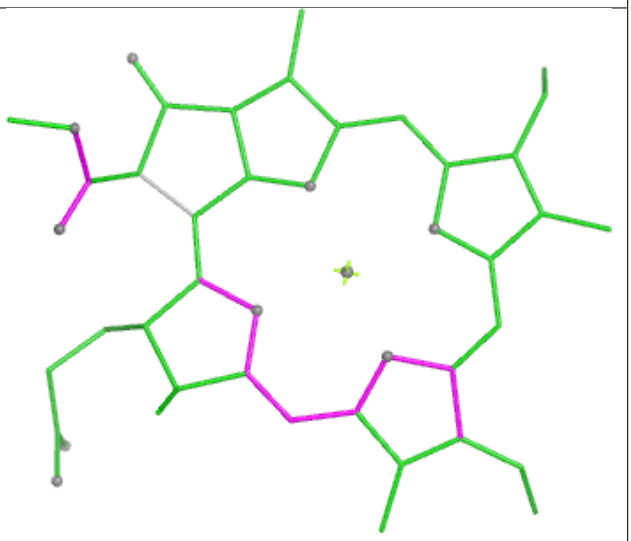

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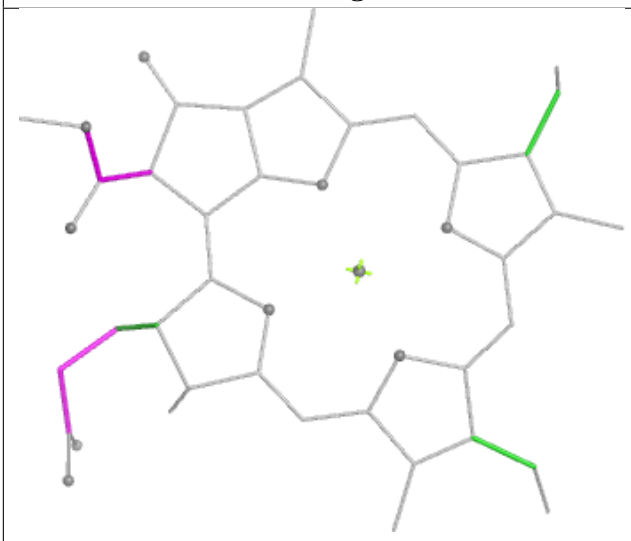

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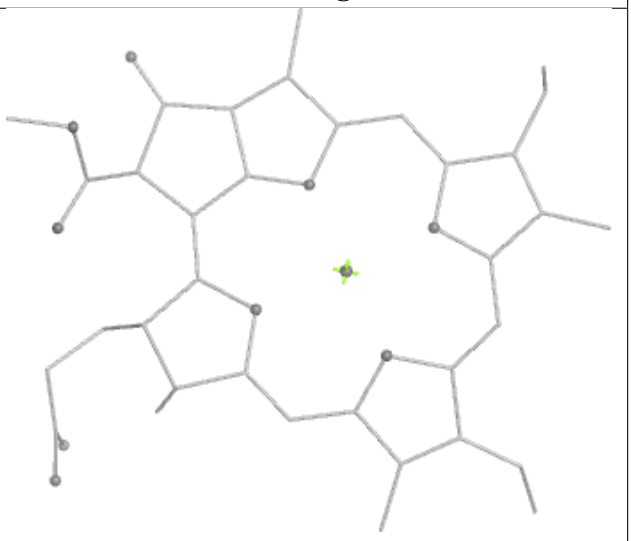
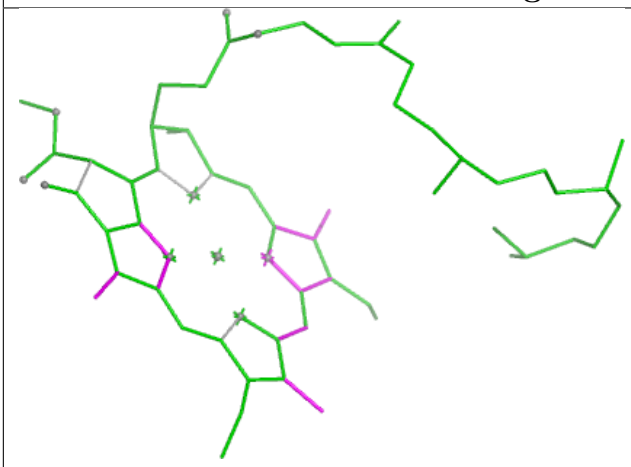


Rings

Ligand CLA A 825



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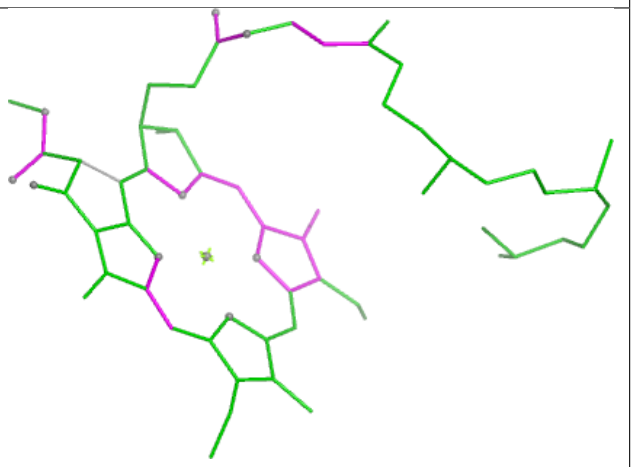

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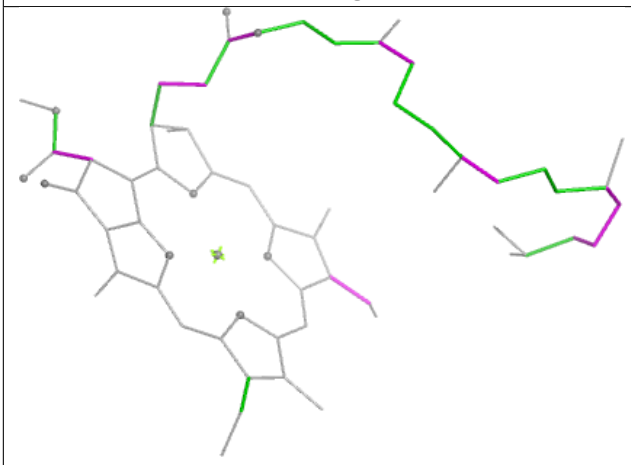
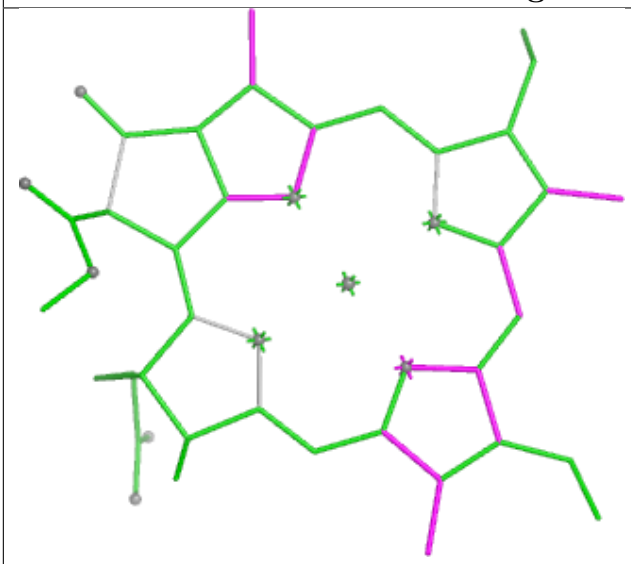


Torsions



Rings

Ligand CLA b 822



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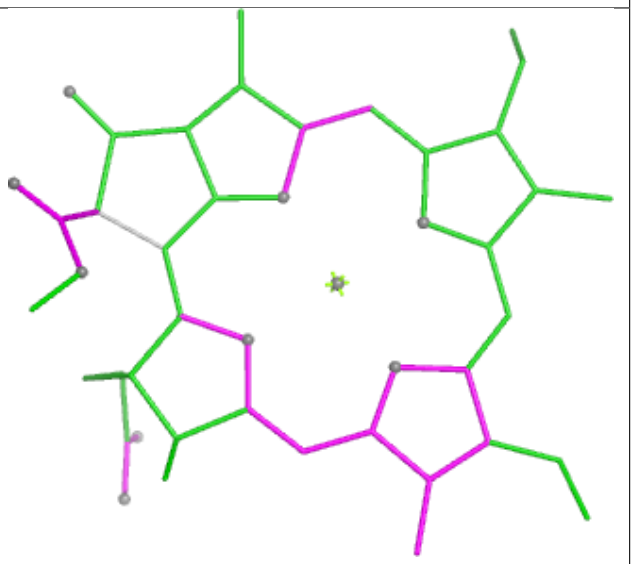

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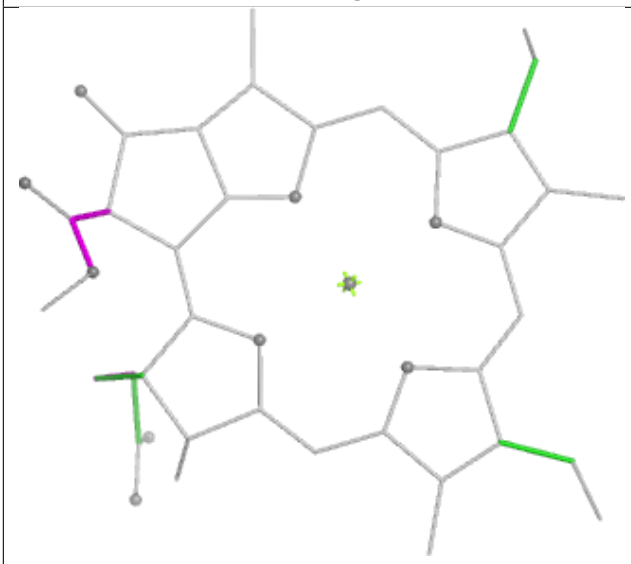

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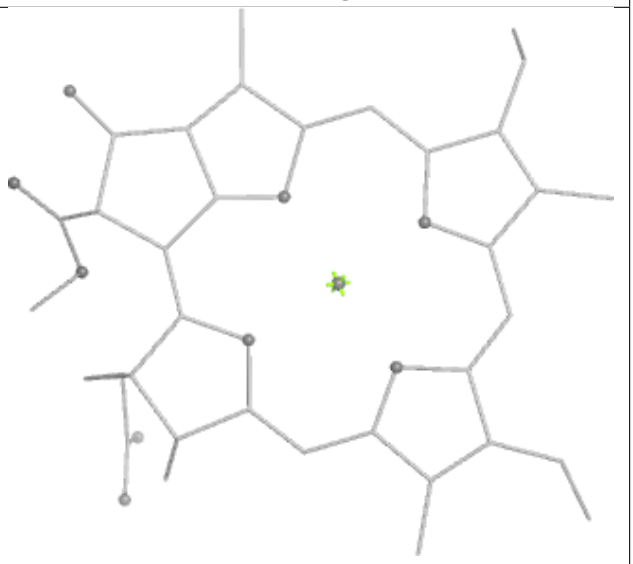
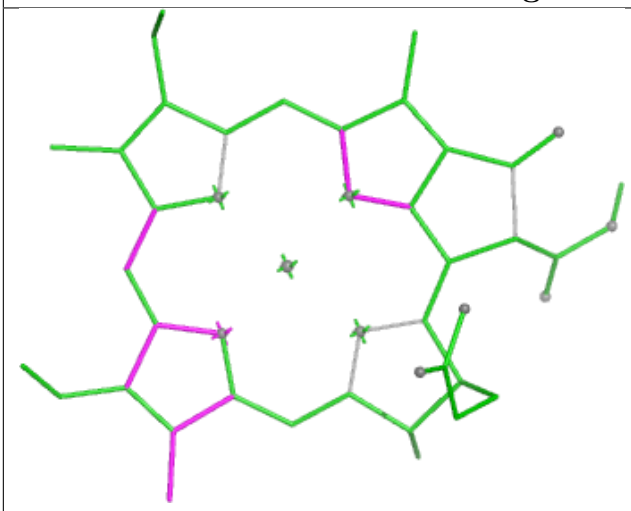


Rings

Ligand CLA j 1302



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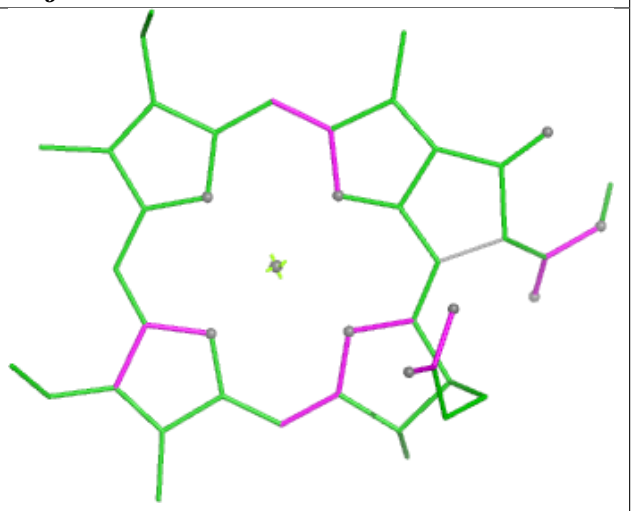
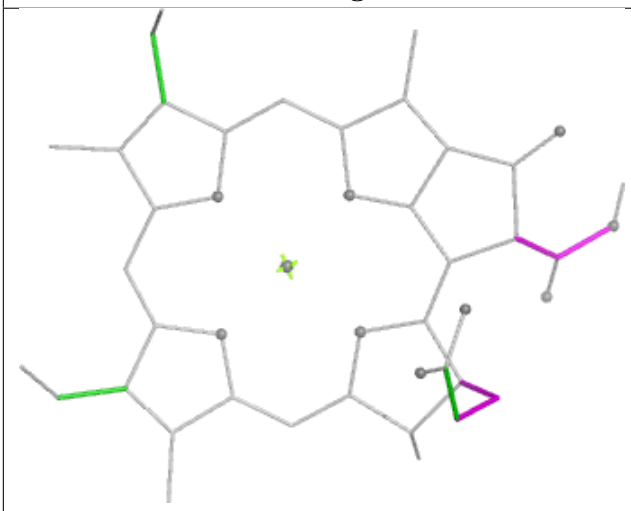


Bond angles



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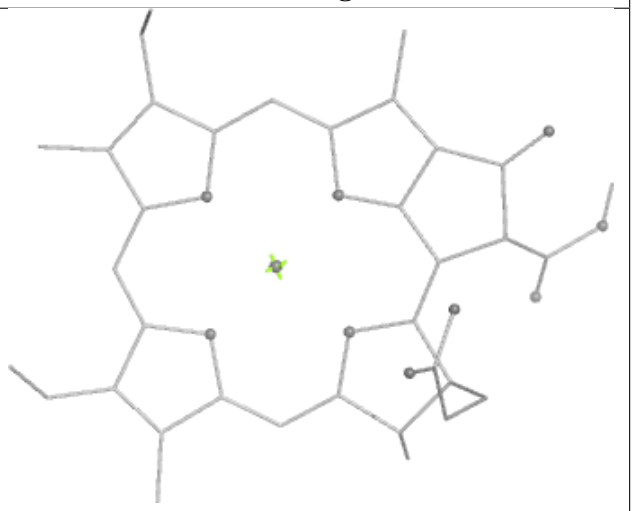
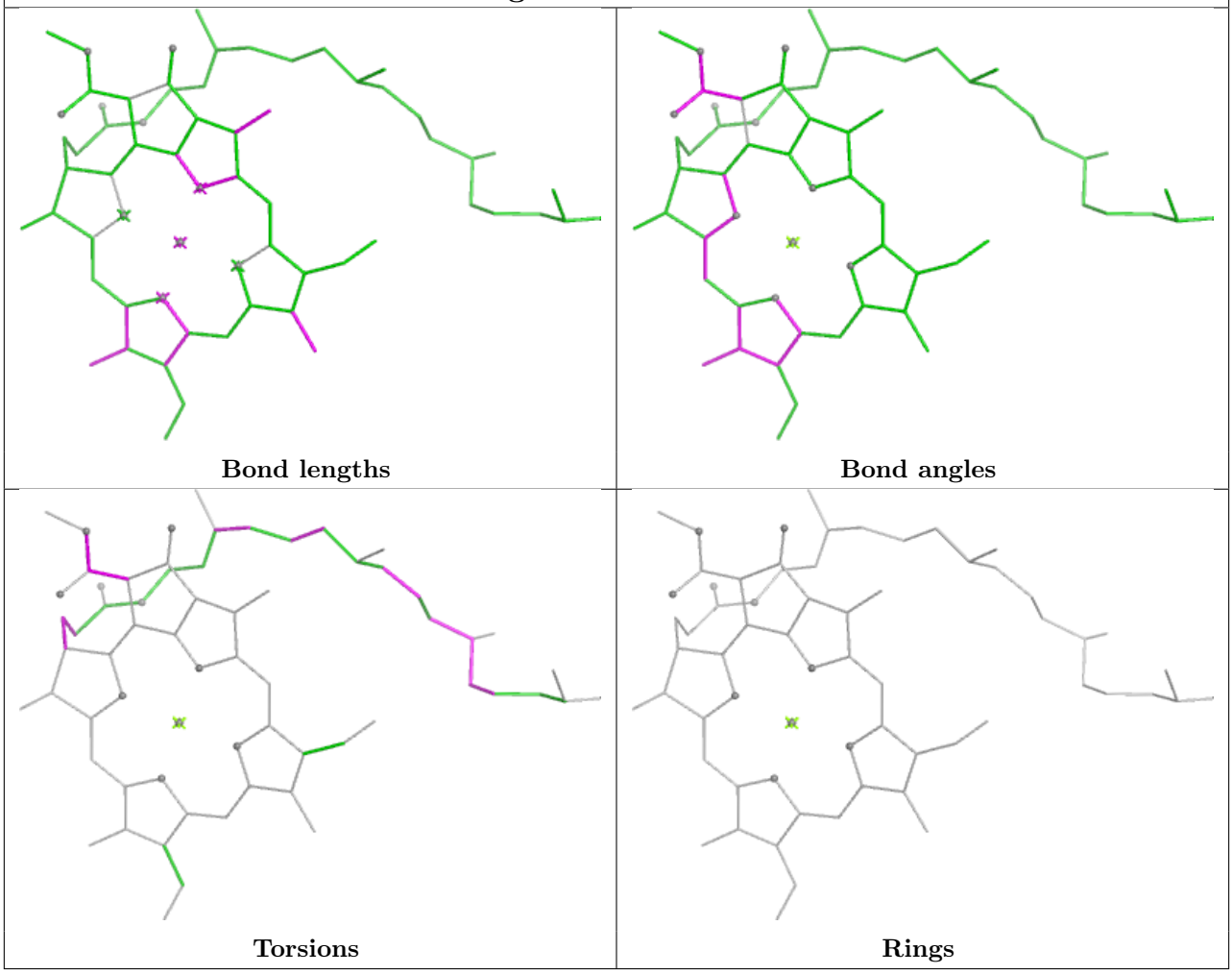
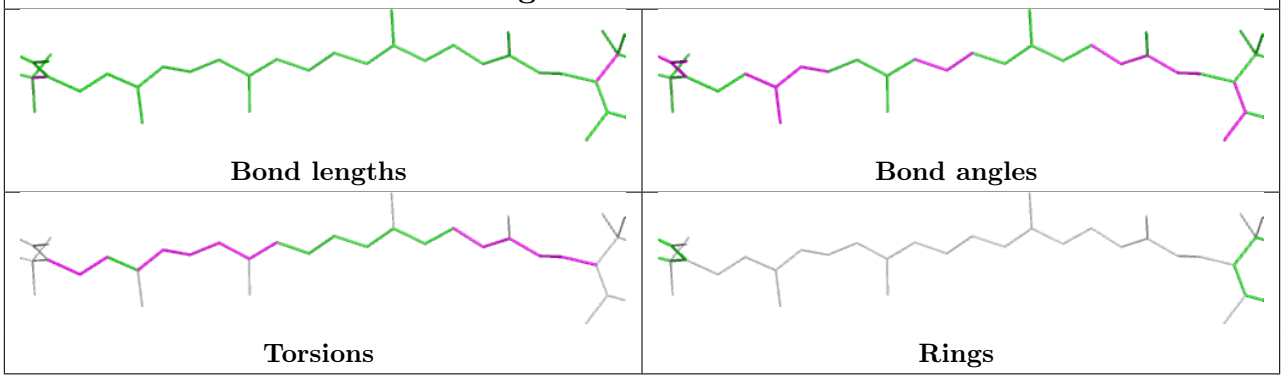


Rings

Ligand CLA a 830



Ligand BCR 8 1306



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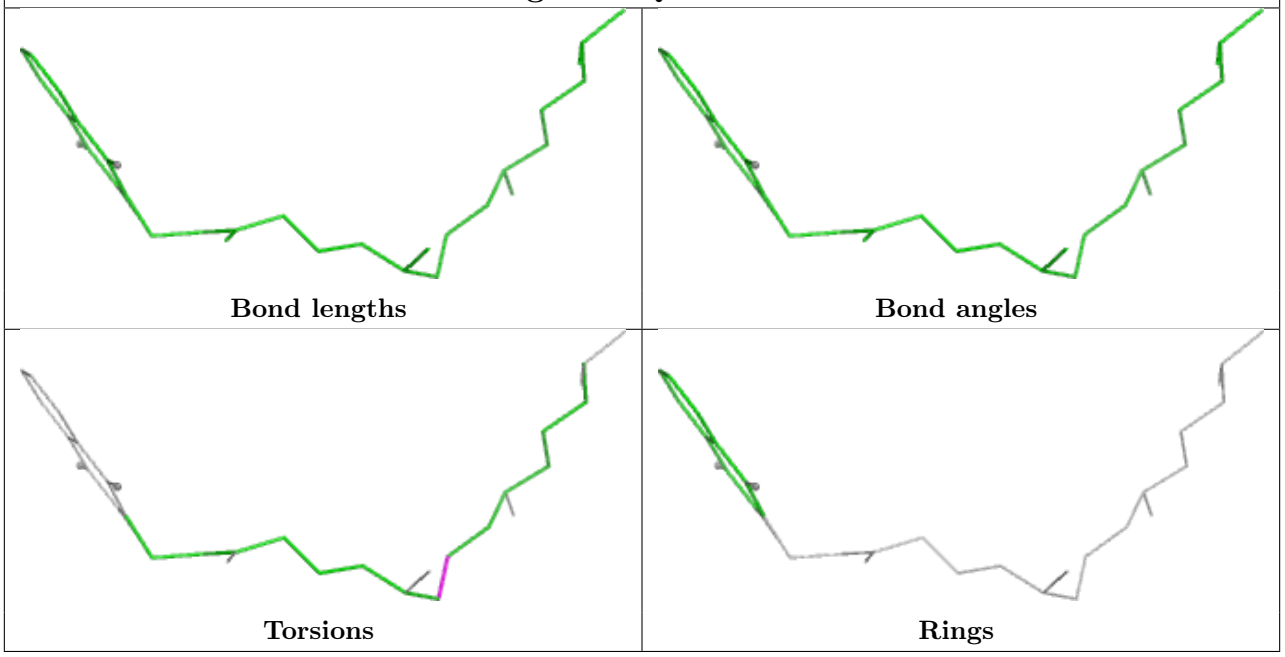

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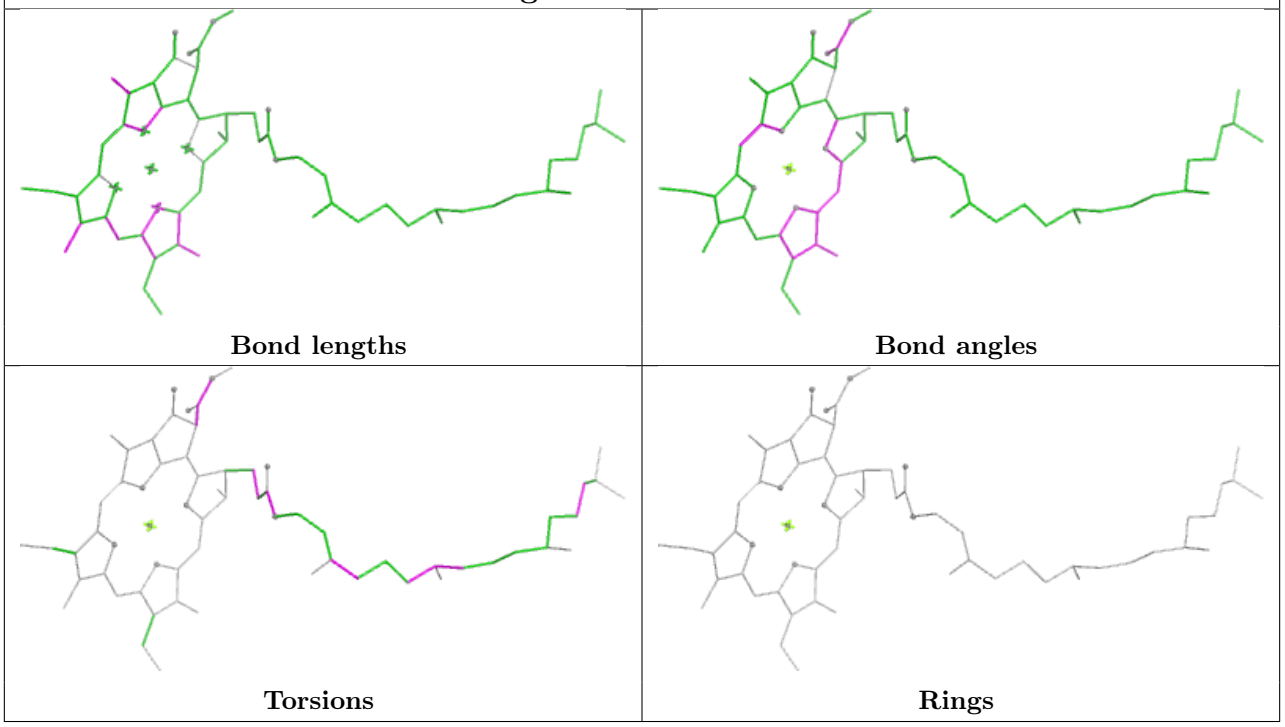

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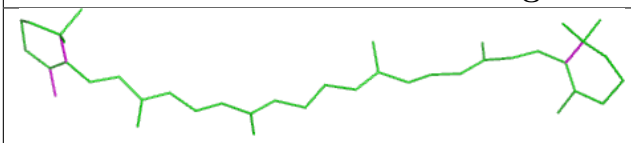
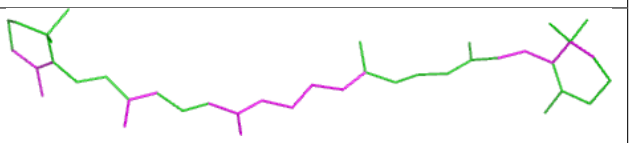
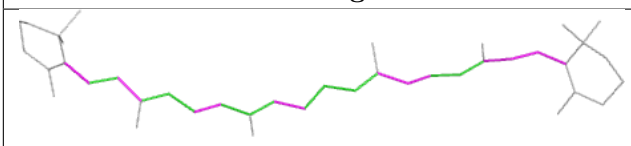


Bond lengths



Bond angles



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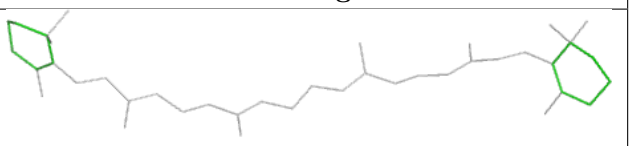
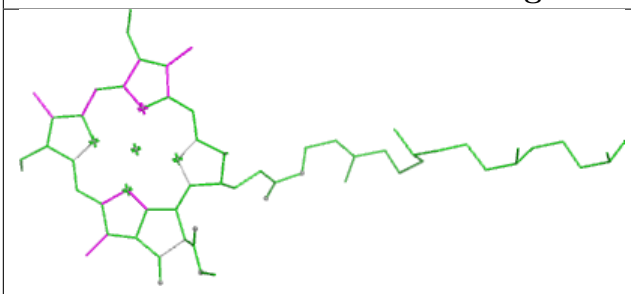


Rings

Ligand CLA B 825



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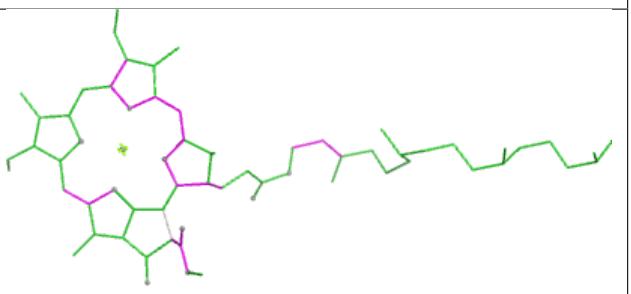

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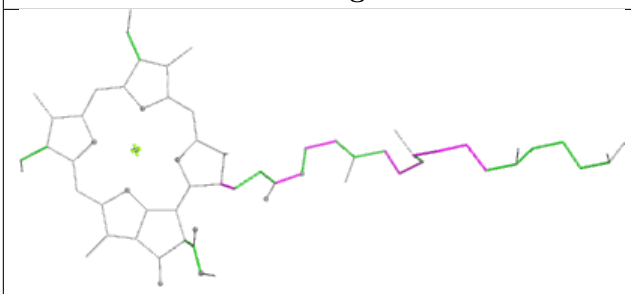

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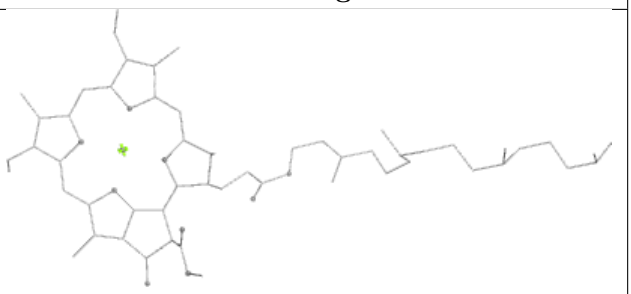

Rings

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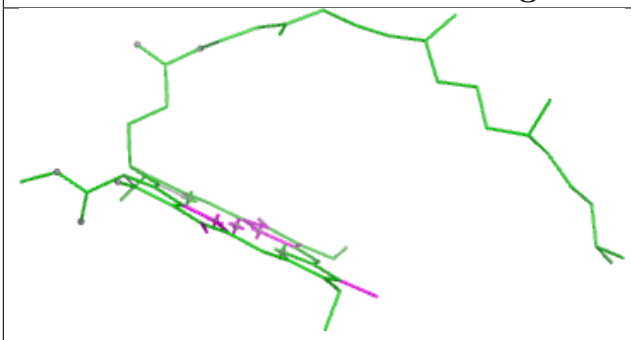

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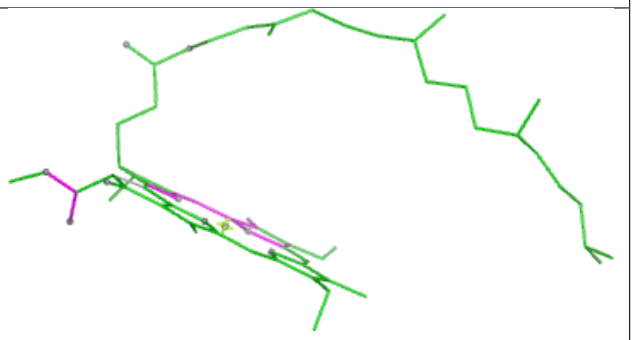
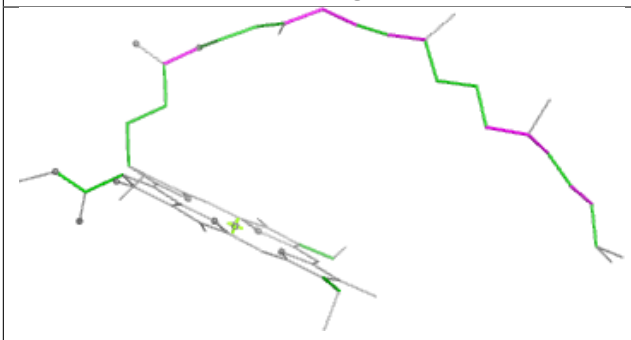


Bond angles

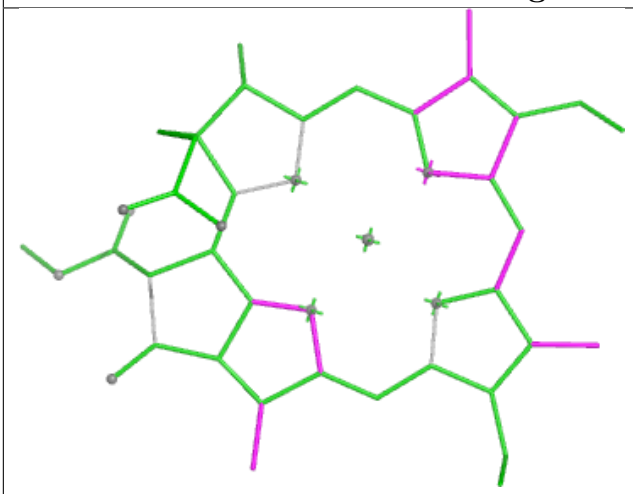


Torsions



Rings

Ligand CLA a 813



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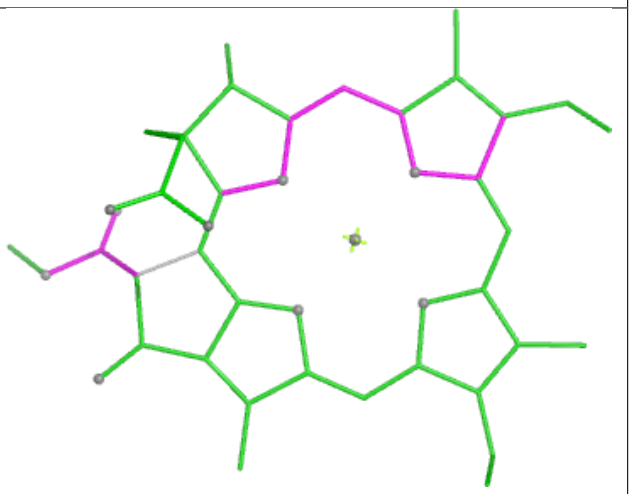
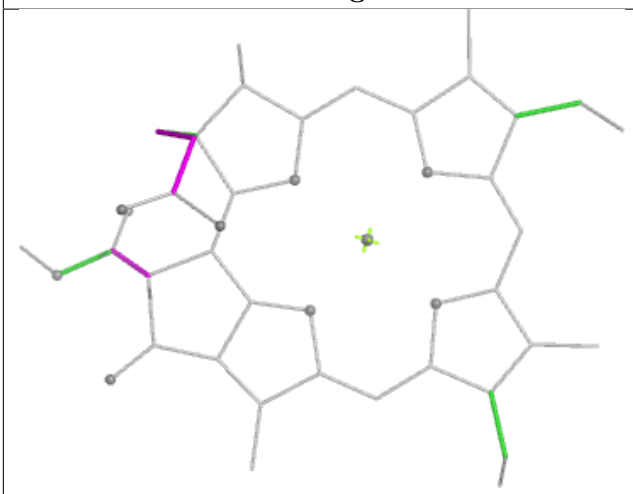


Bond angles



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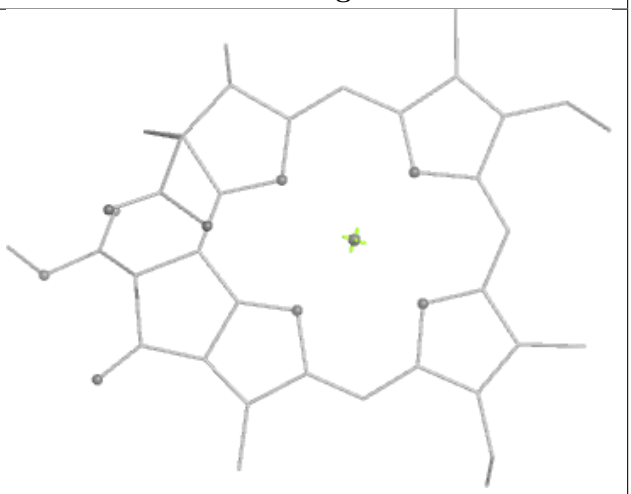
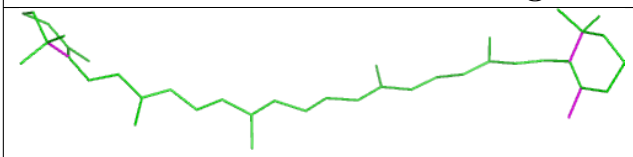
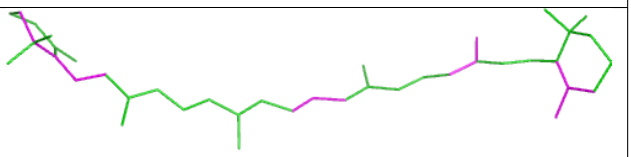


Rings

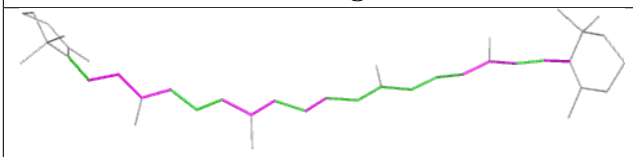
Ligand BCR 6 202



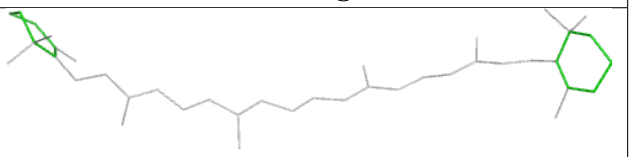
Bond lengths



Bond angles

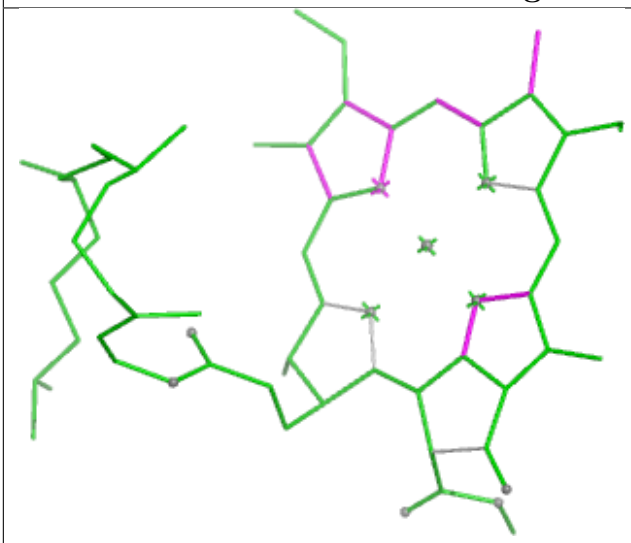


Torsions



Rings

Ligand CLA A 816



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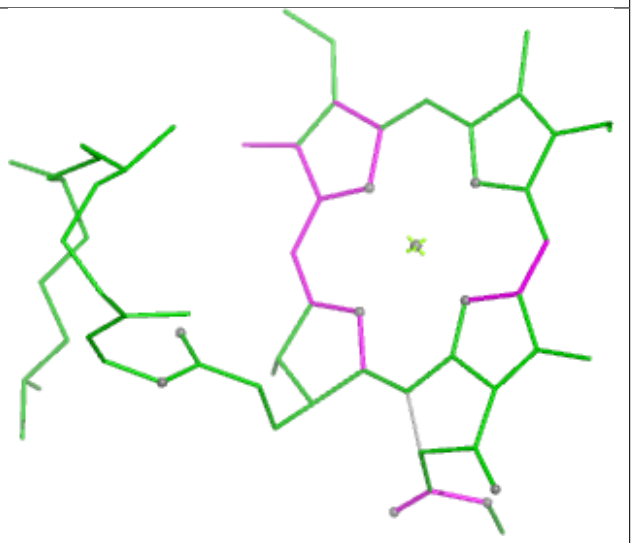
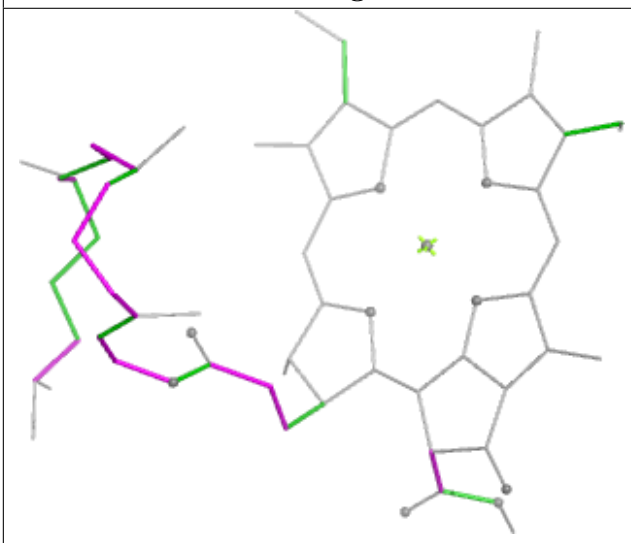


Bond angles

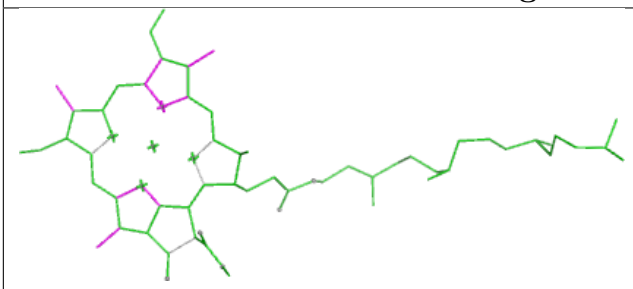


Torsions



Rings

Ligand CLA 1 1628



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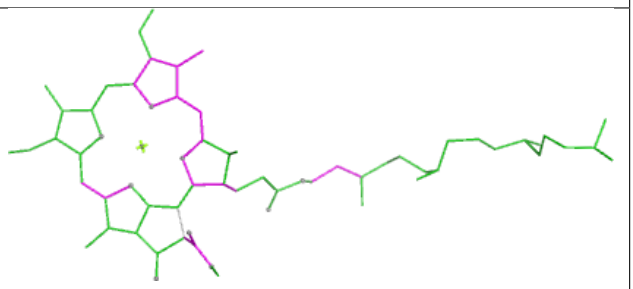
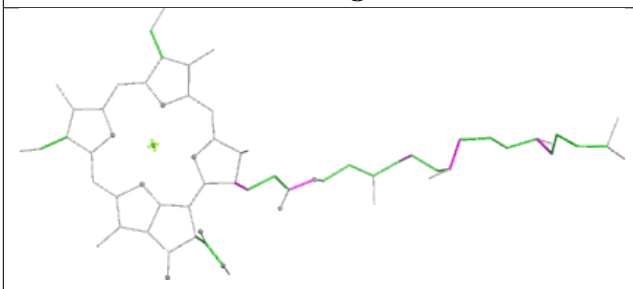


Bond angles



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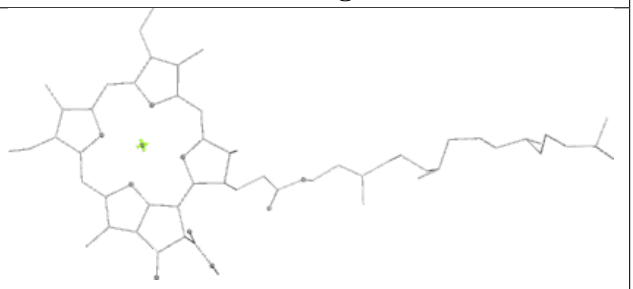
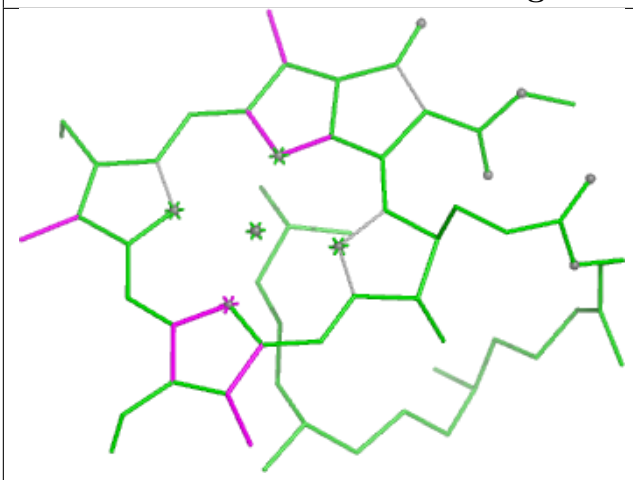


Rings

Ligand CLA b 807



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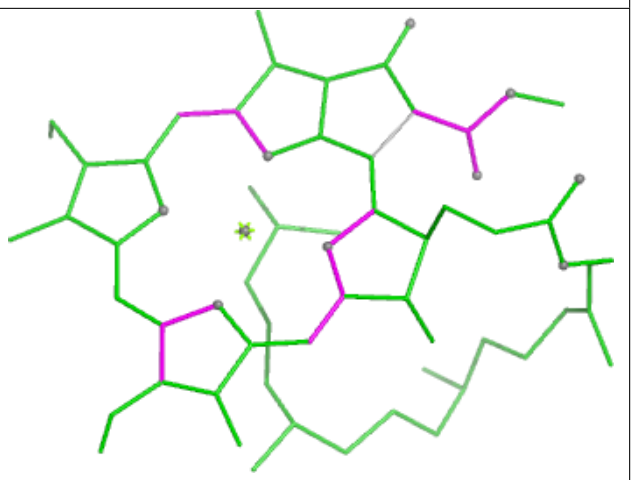
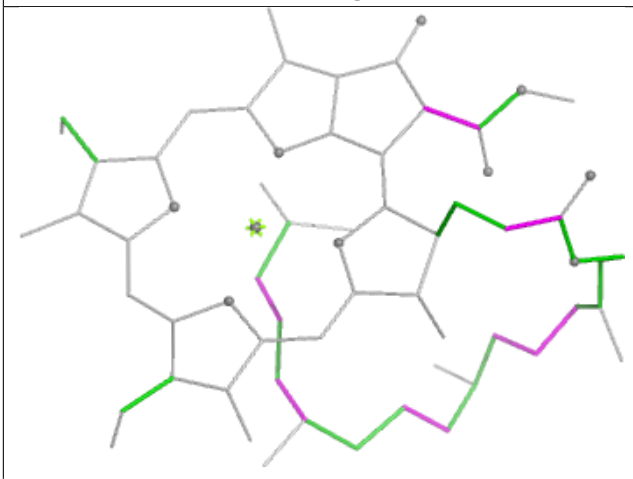


Bond angles



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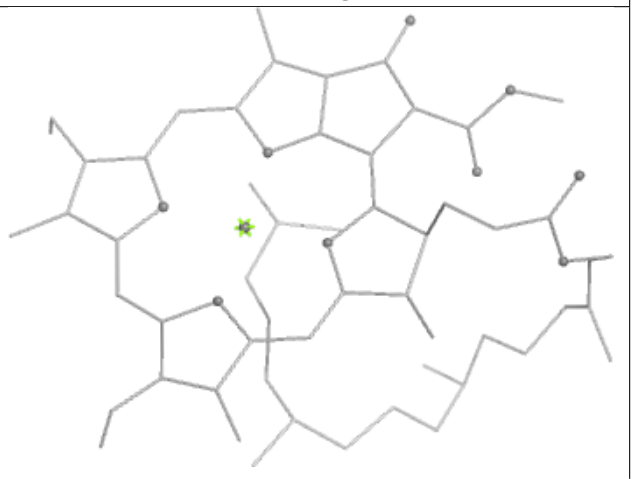
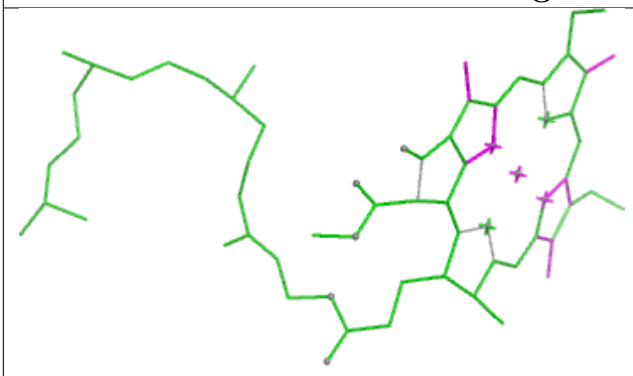


Rings

Ligand CL0 a 801



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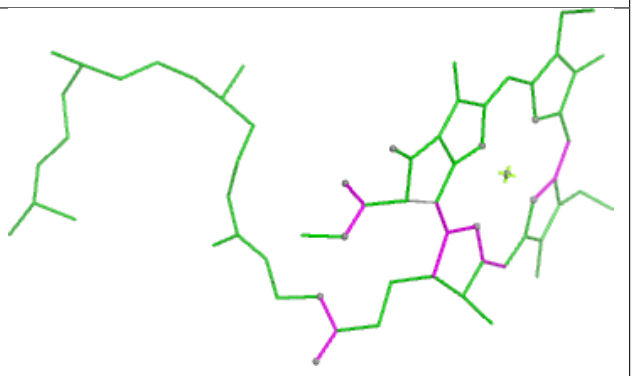
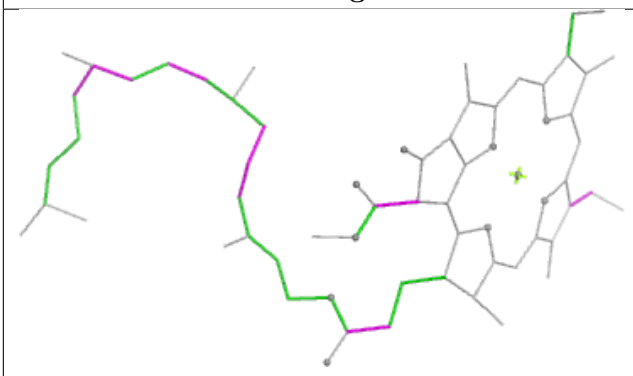


Bond angles



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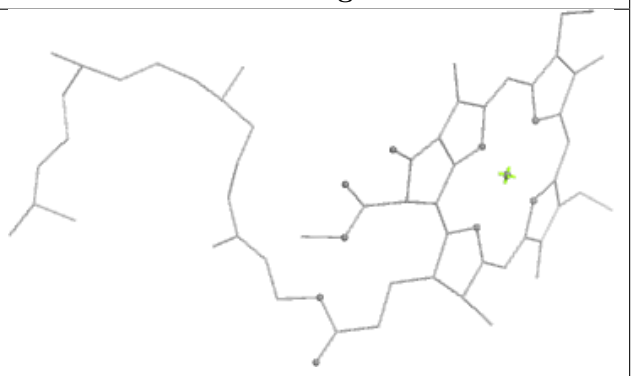
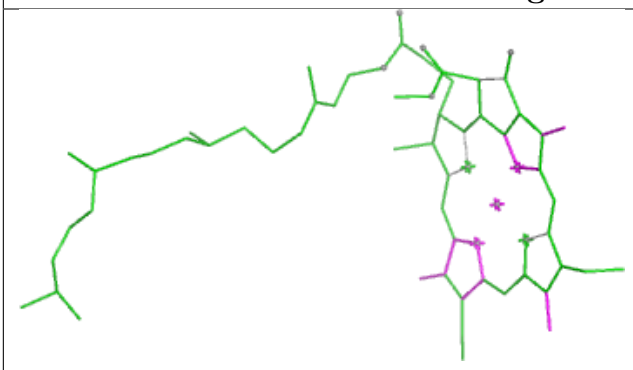


Rings

Ligand CLA b 811



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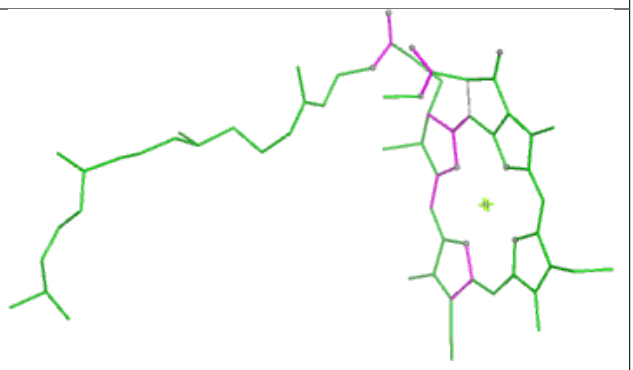
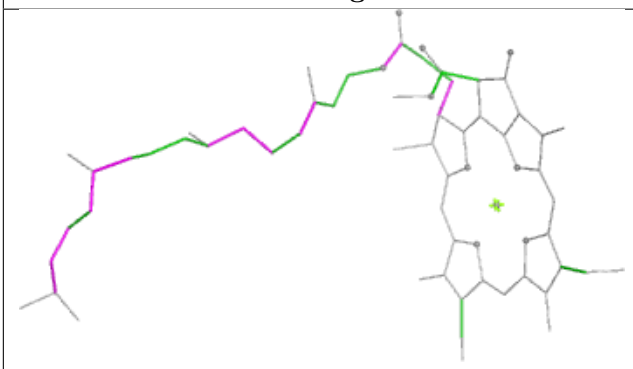


Bond angles



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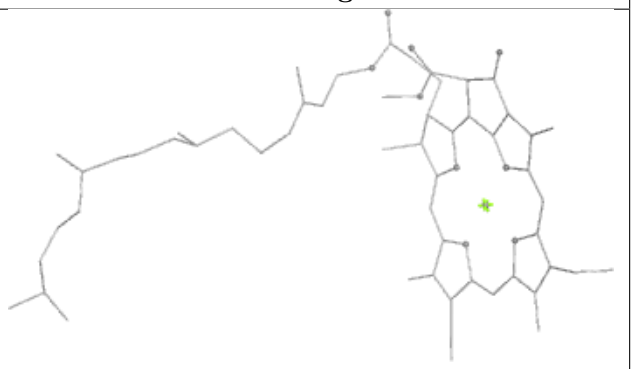
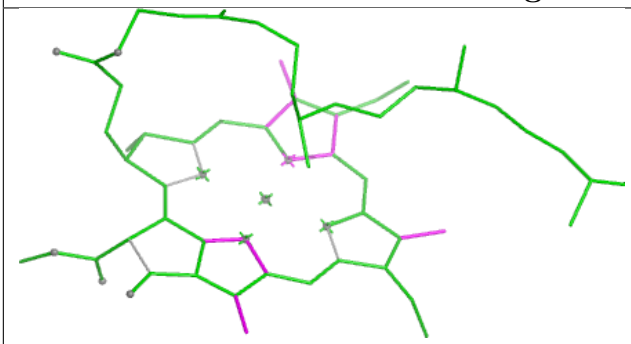


Rings

Ligand CLA B 817



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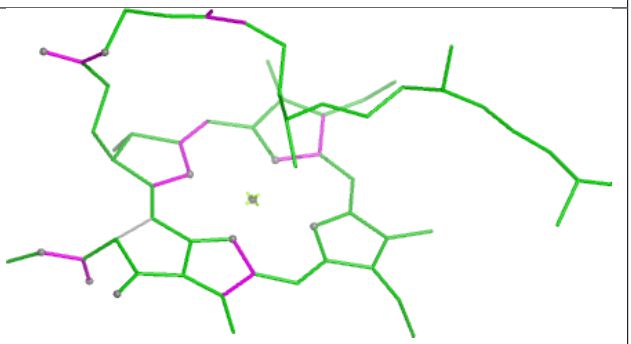
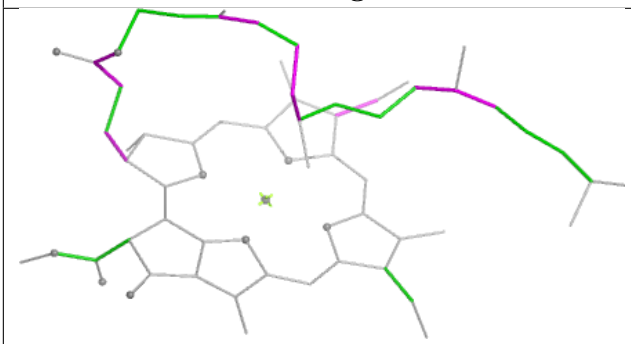


Bond angles

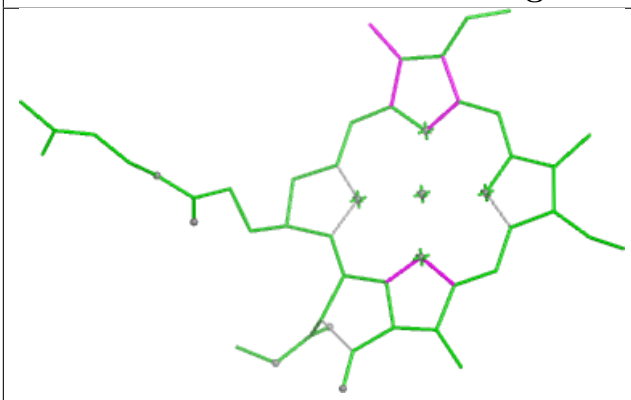


Torsions

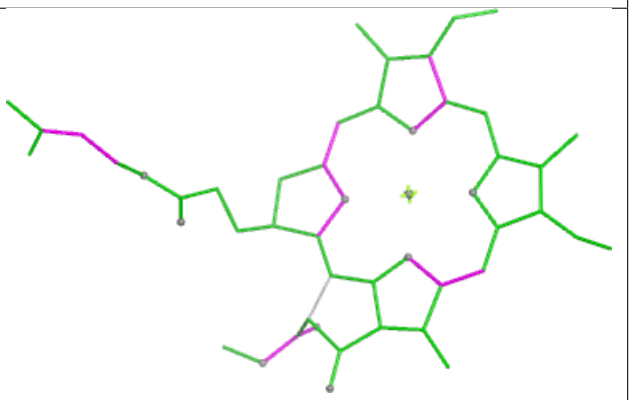


Rings

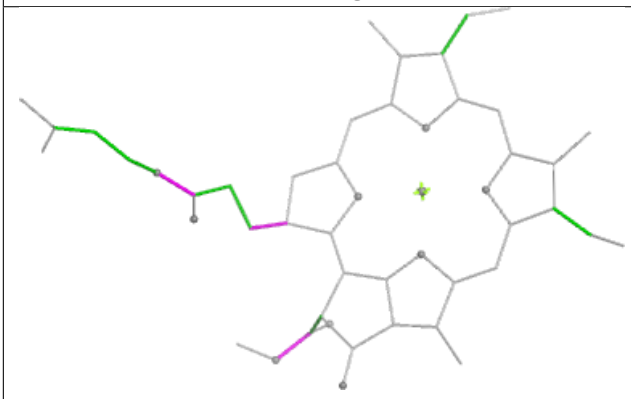
Ligand CLA F 204



Bond lengths



Bond angles



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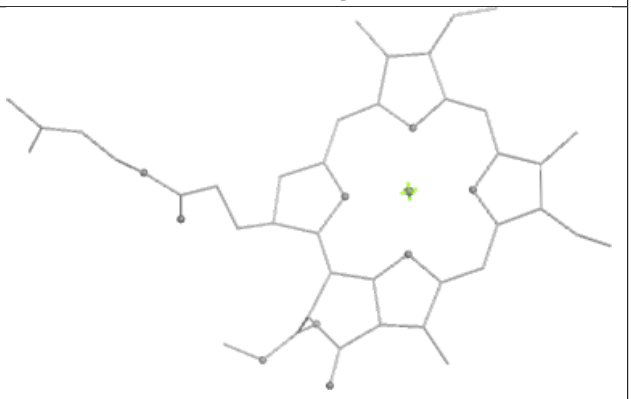
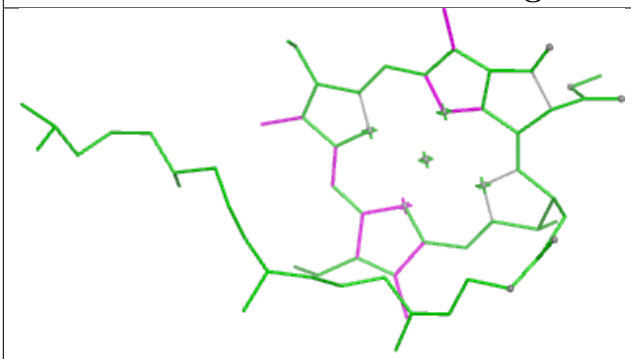


Rings

Ligand CLA B 820



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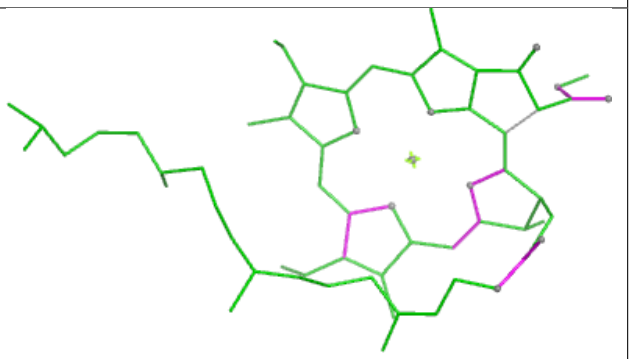
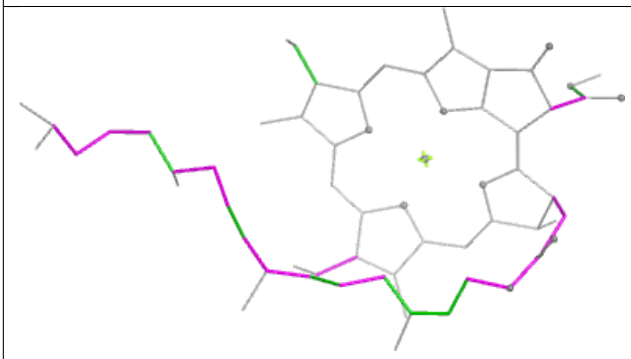


Bond angles



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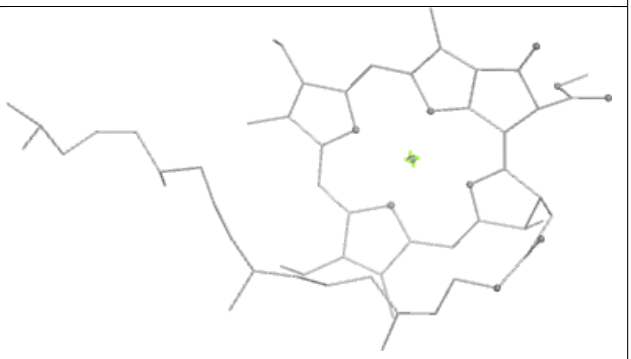
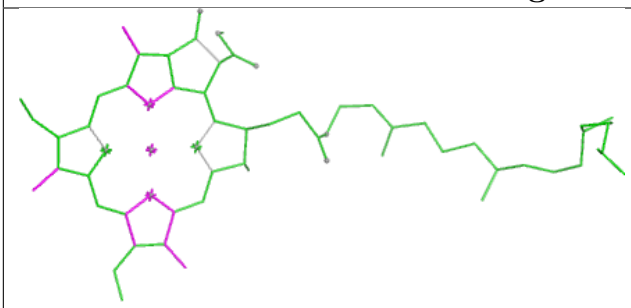


Rings

Ligand CLA a 806



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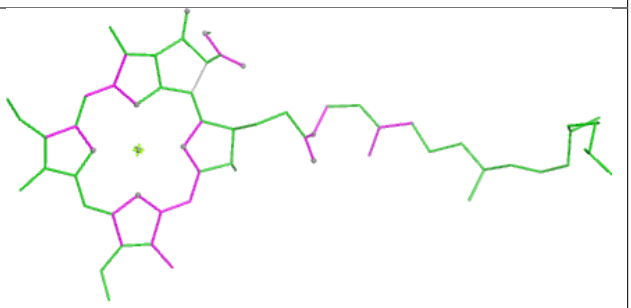
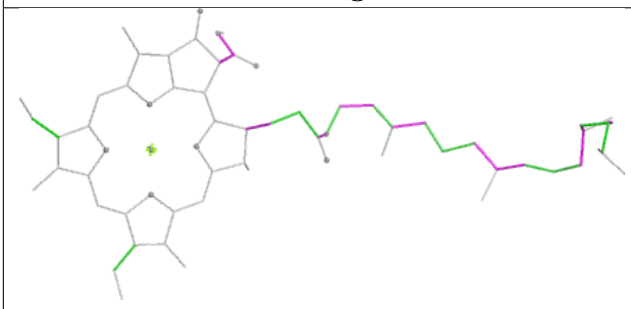


Bond angles



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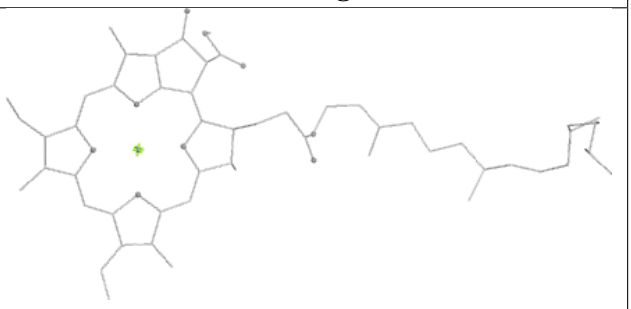
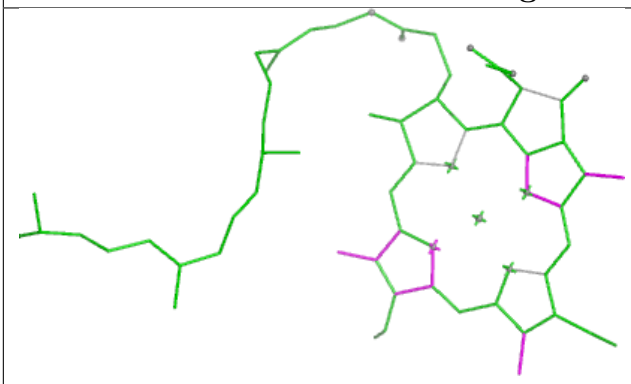


Rings

Ligand CLA 1 1615



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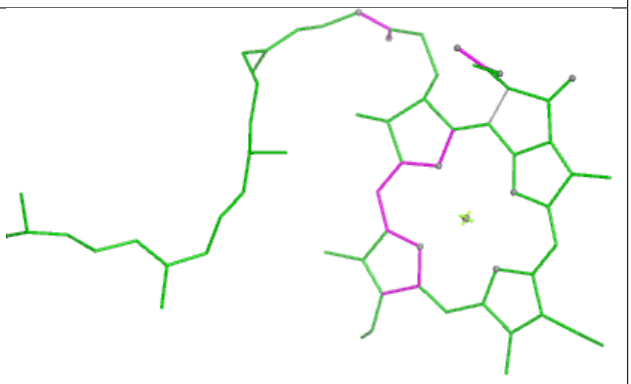
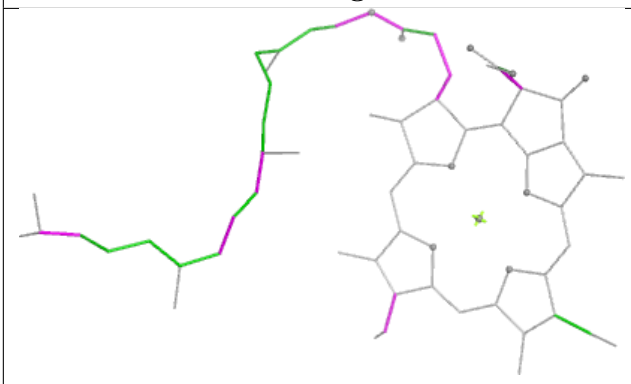


Bond angles

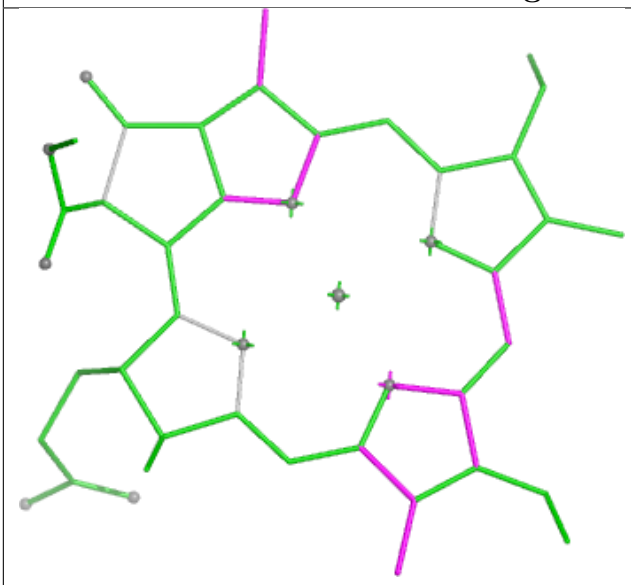


Torsions



Rings

Ligand CLA A 823



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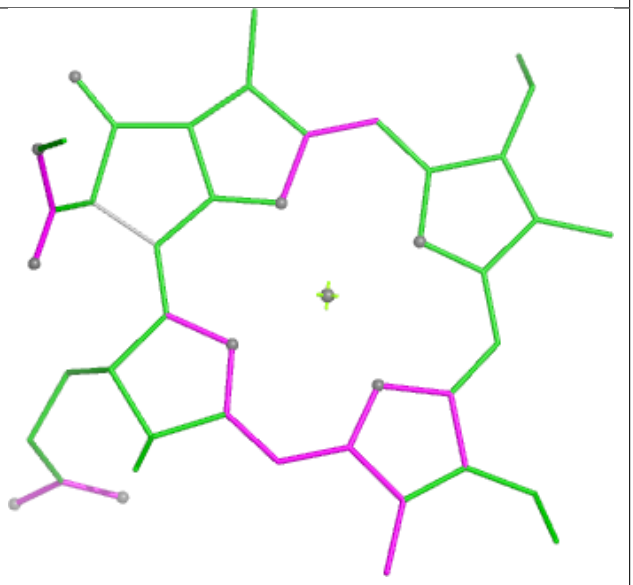
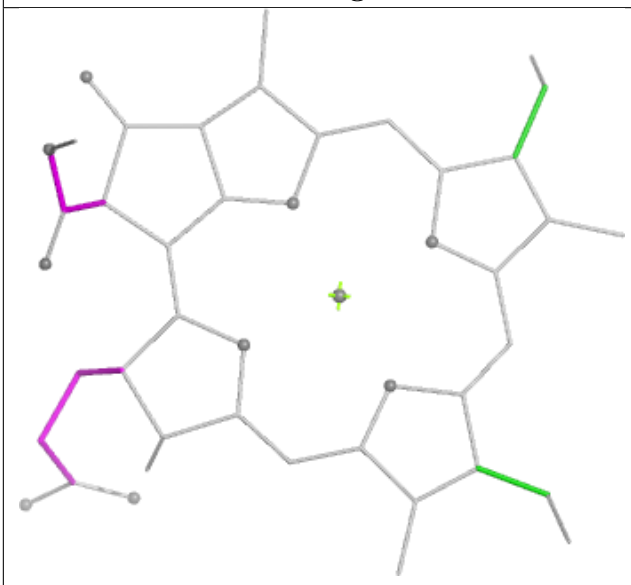


Bond angles



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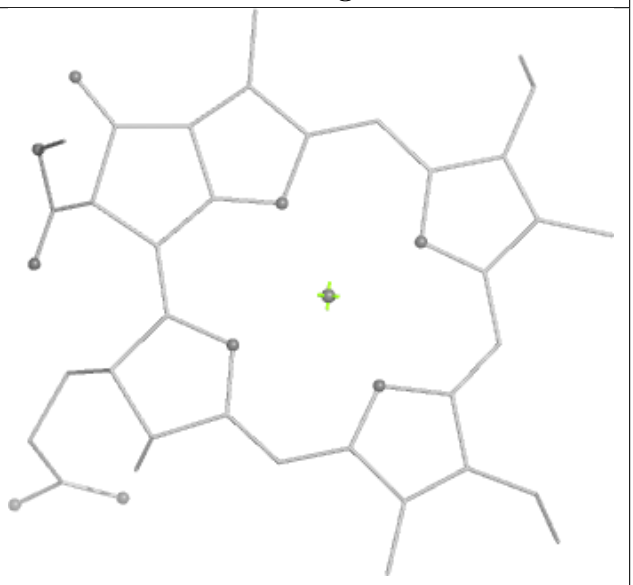
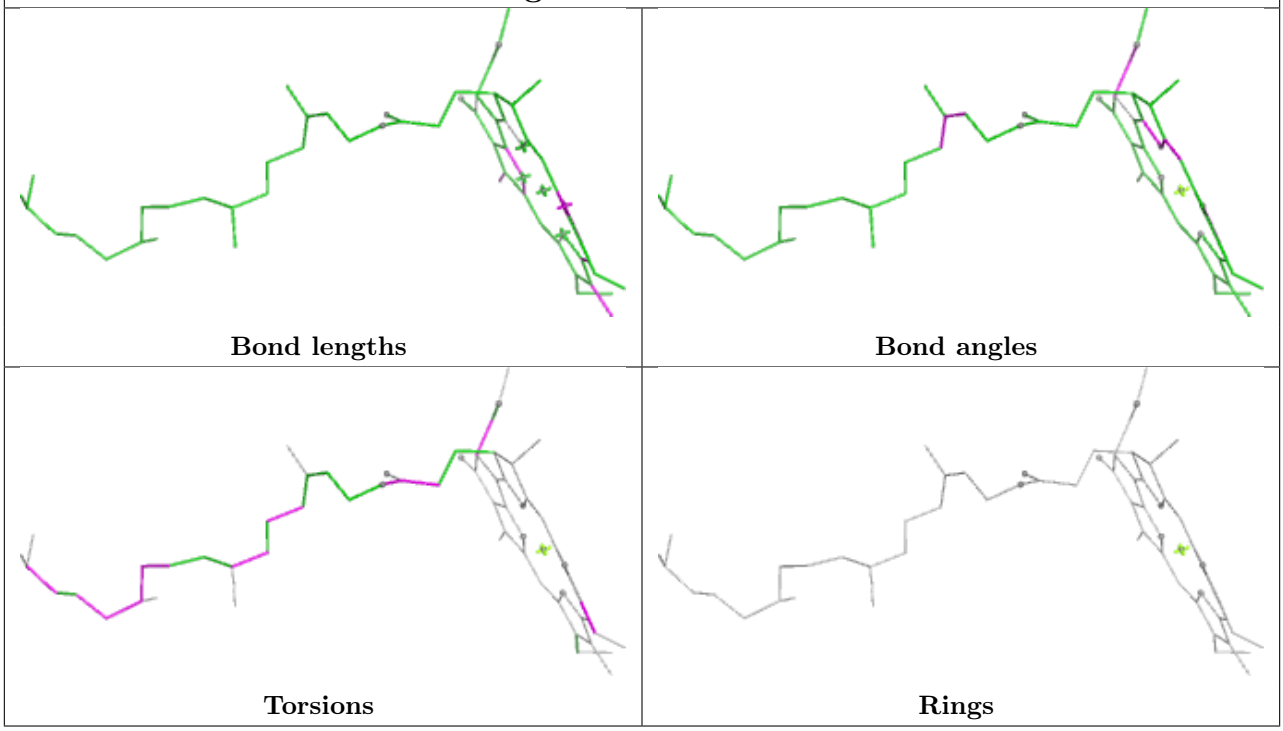
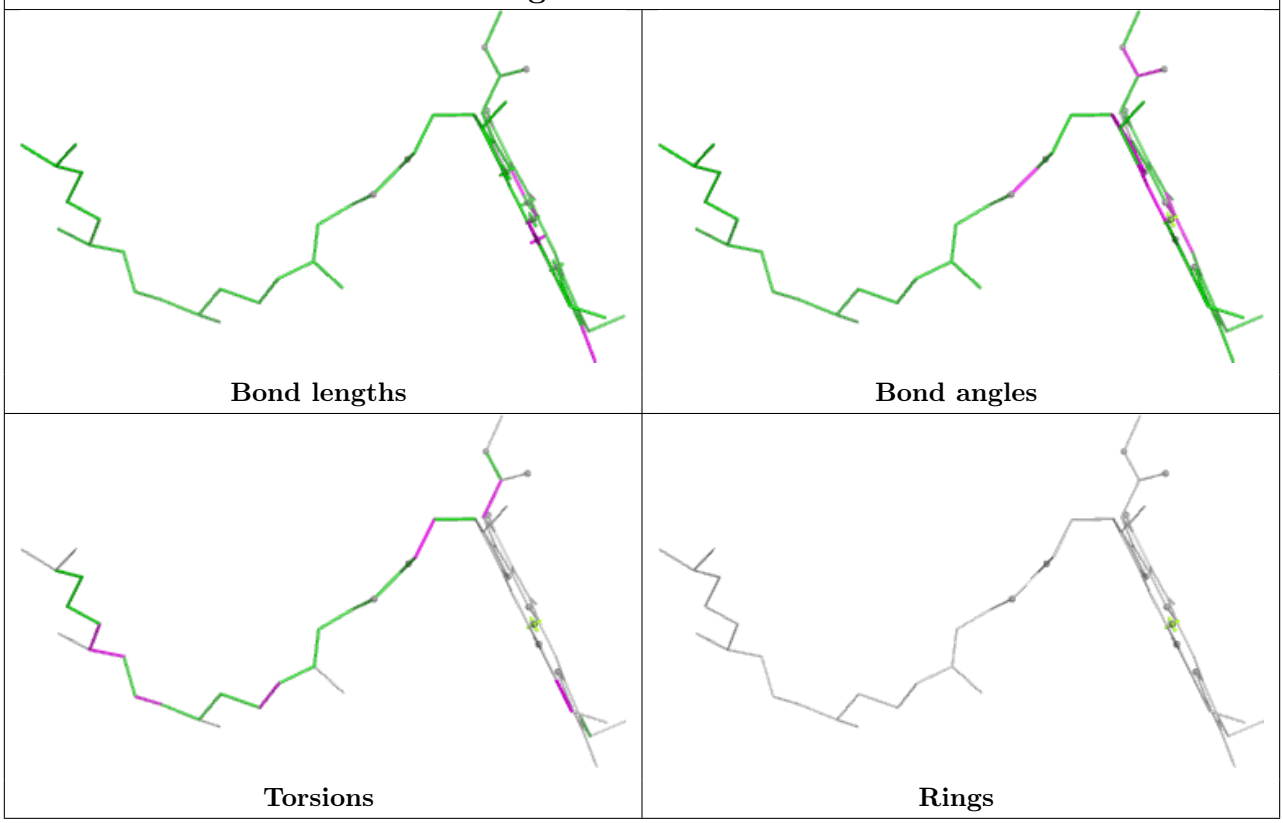


Rings

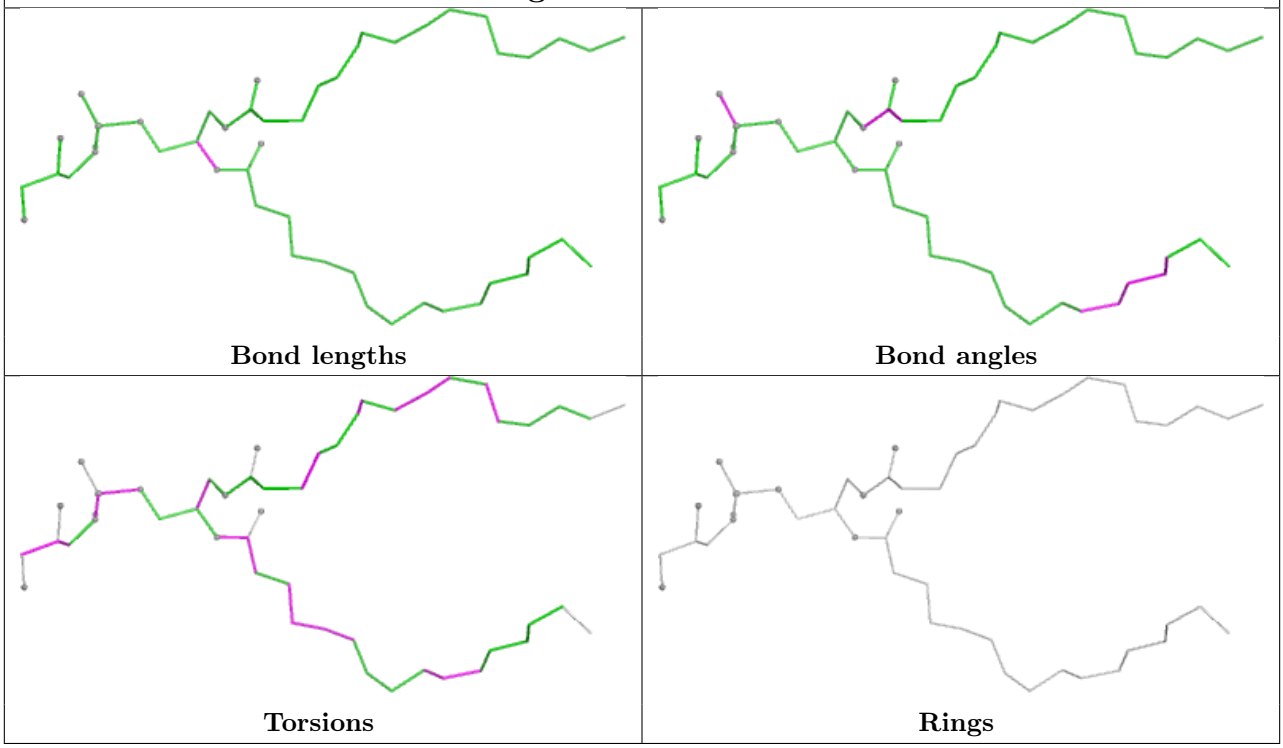
Ligand CLA A 840



Ligand CLA b 841



Ligand LHG a 853



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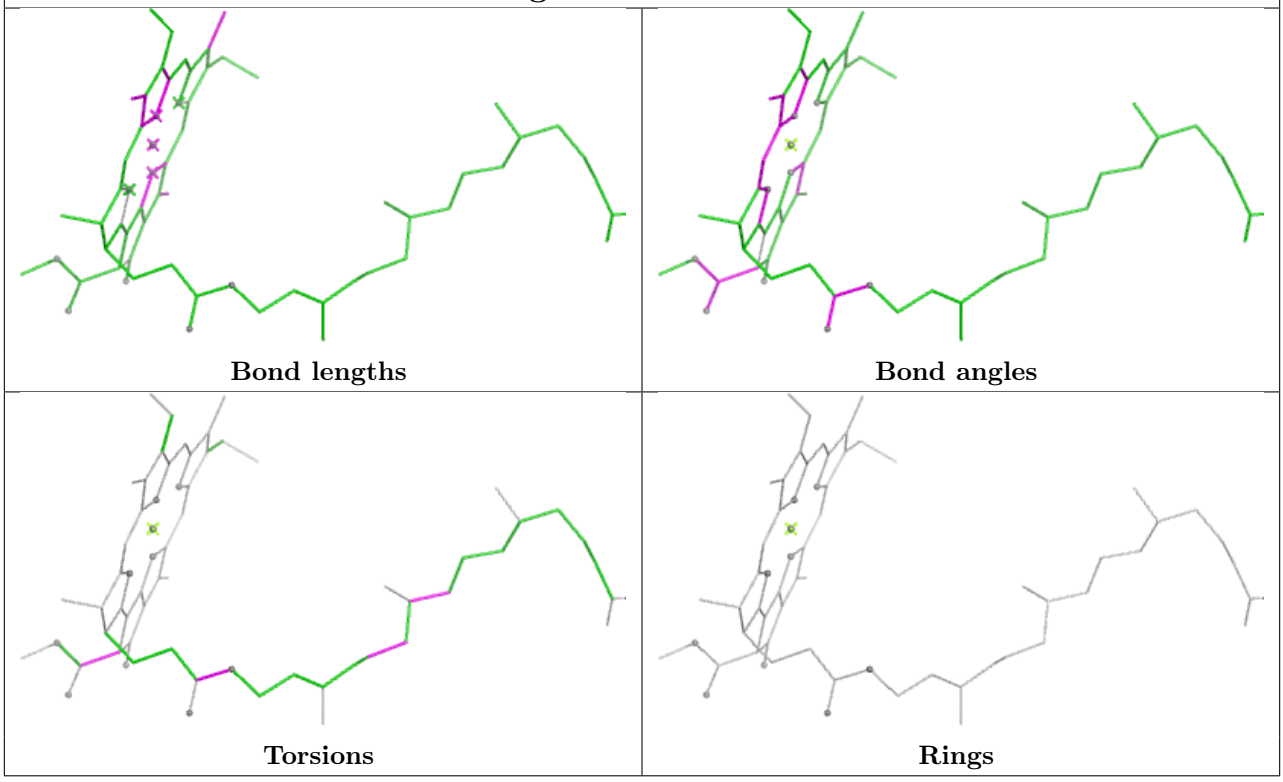
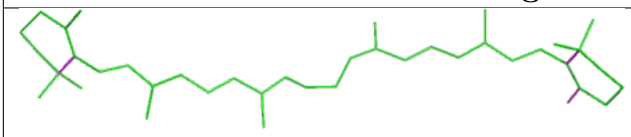
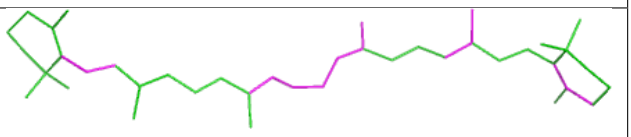
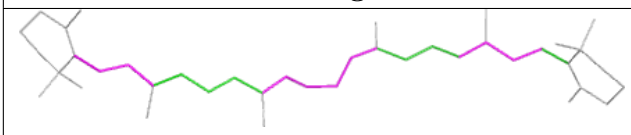
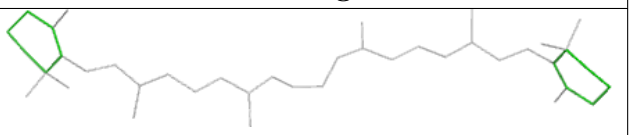
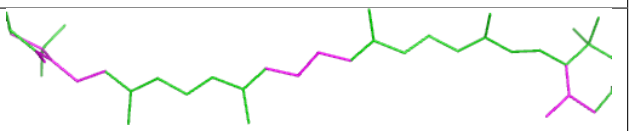
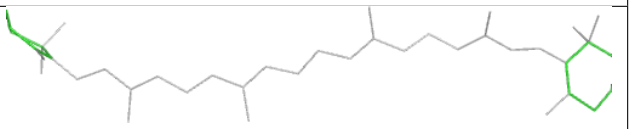


Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 1 1651	
 Bond lengths	 Bond angles
 Torsions	 Rings

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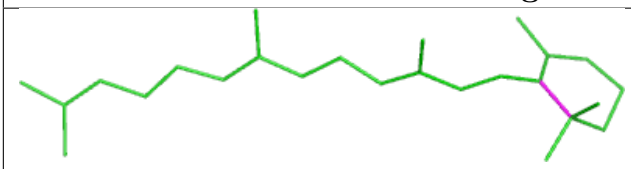
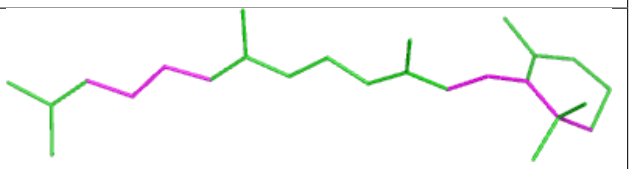
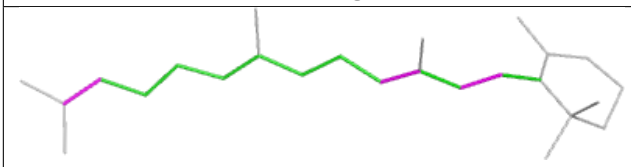
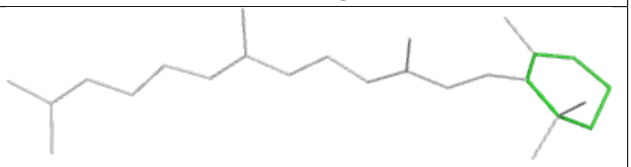
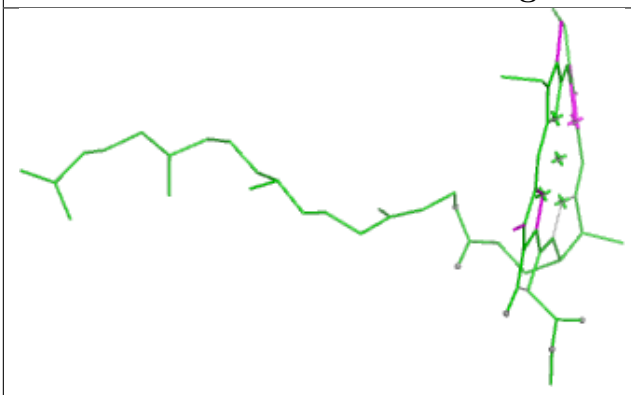
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1630



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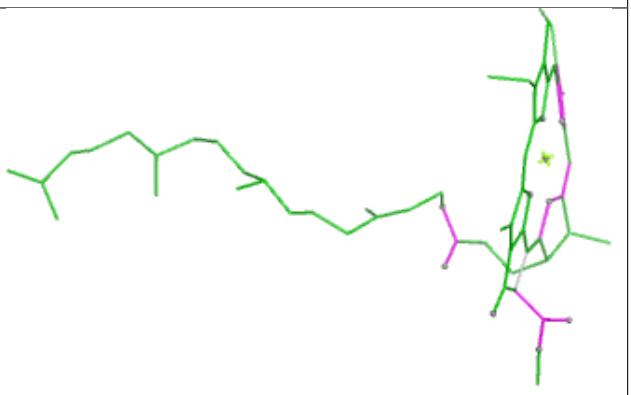
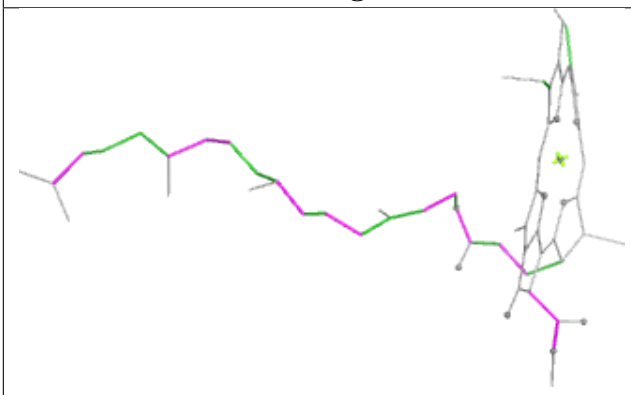


Bond angles



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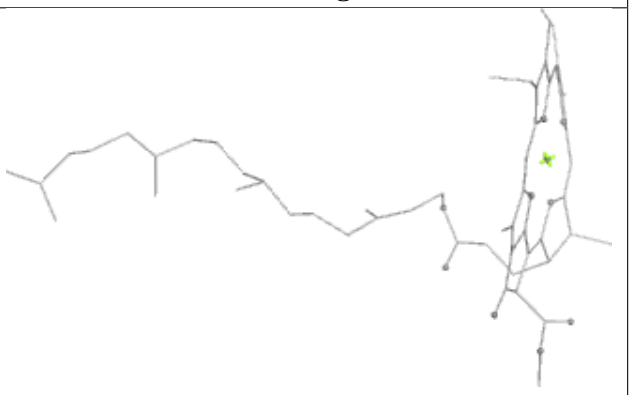
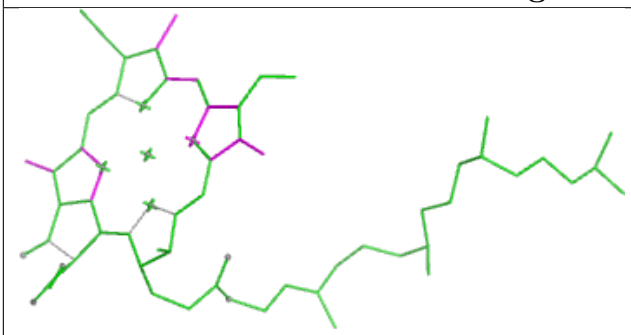


Rings

Ligand CLA a 809



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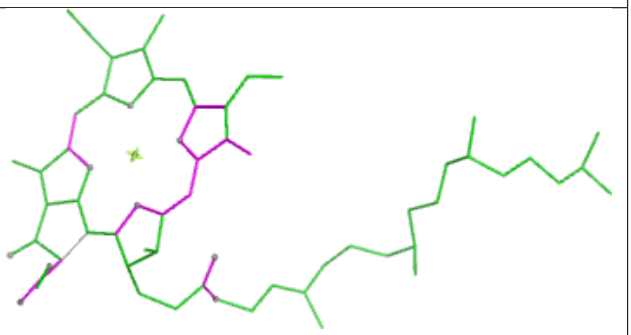
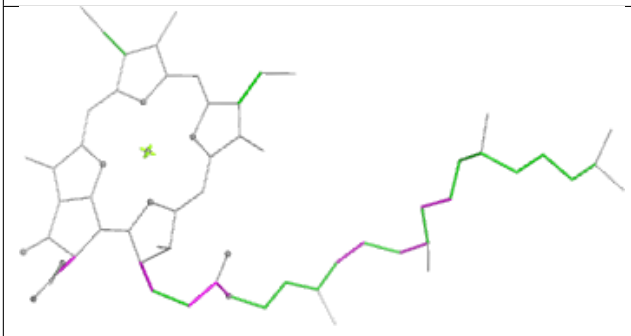


Bond angles



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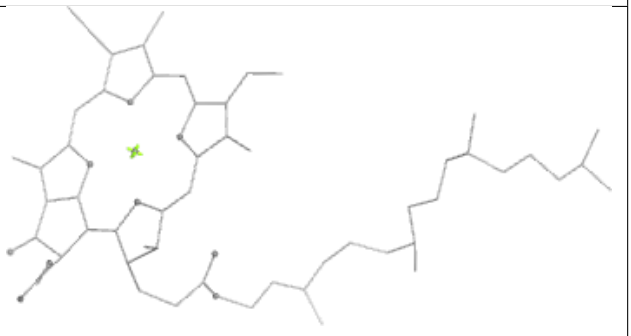
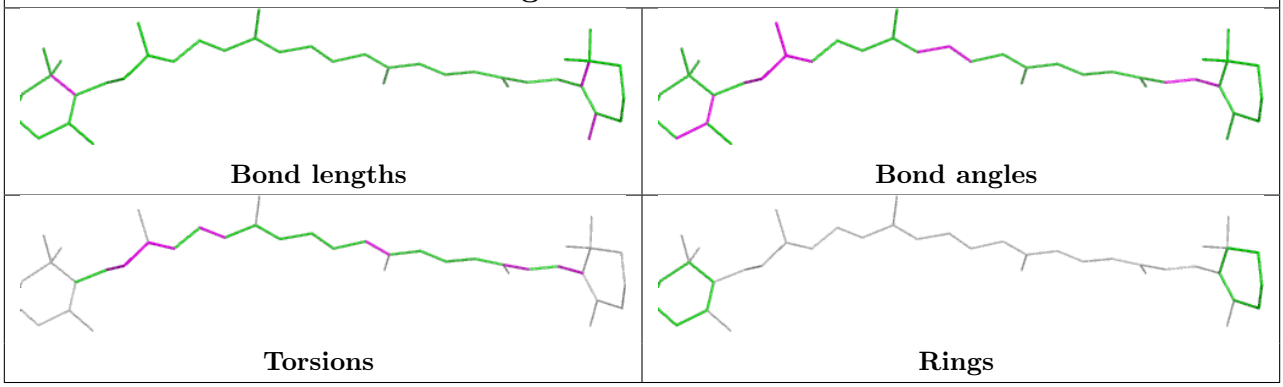


Rings

Ligand BCR m 102



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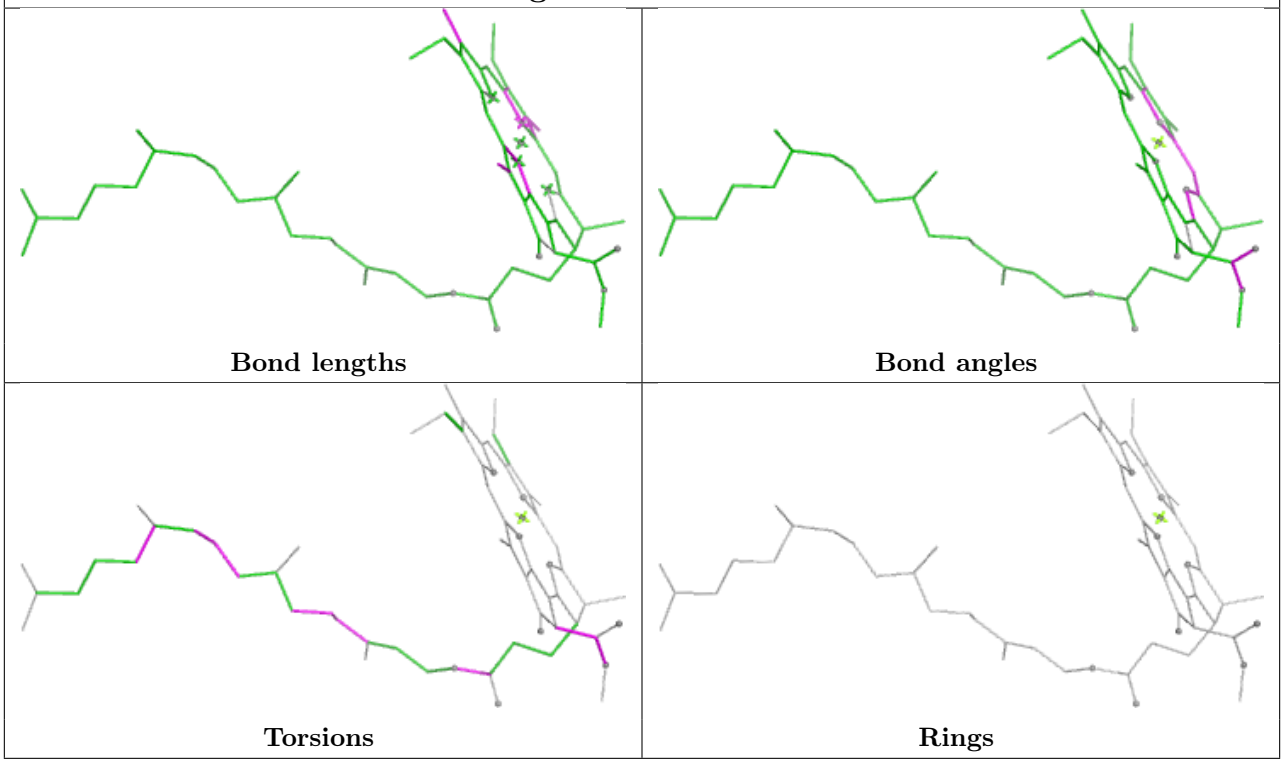
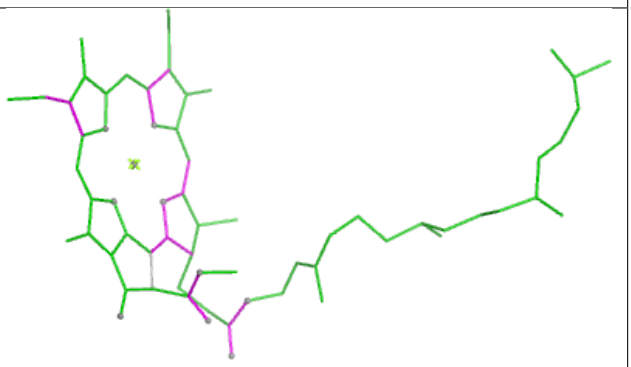


Ligand CLA 2 811



Bond lengths



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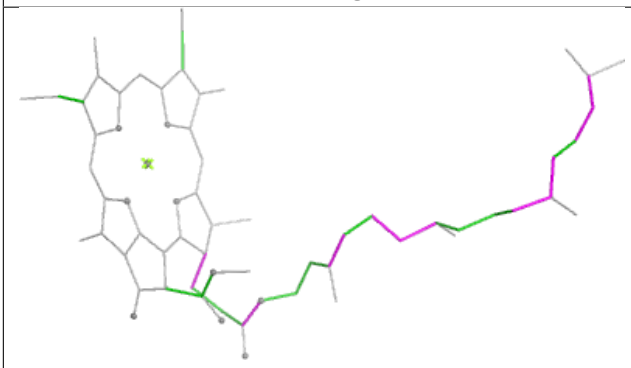

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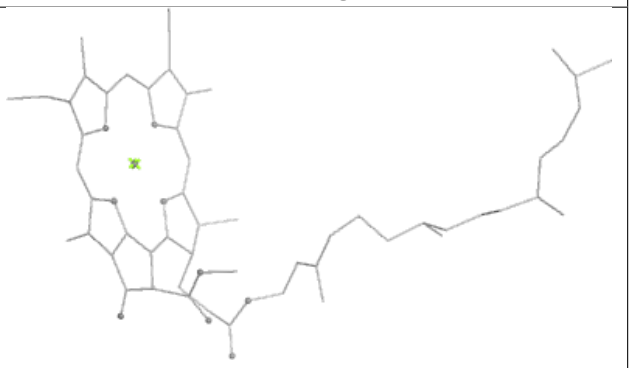
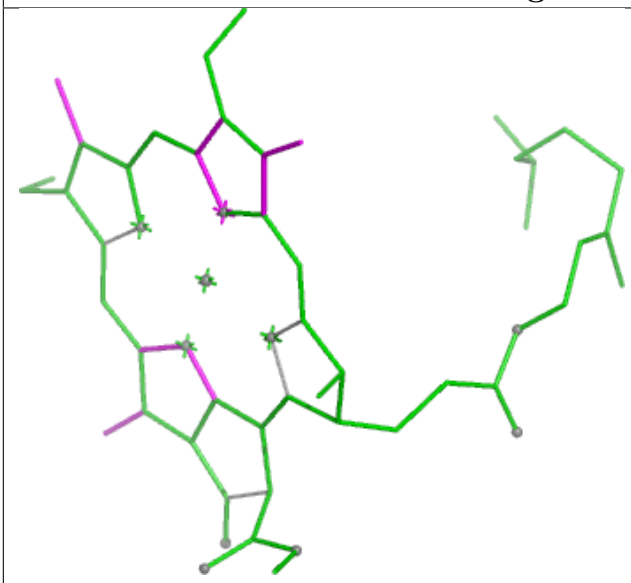


Rings

Ligand CLA b 831



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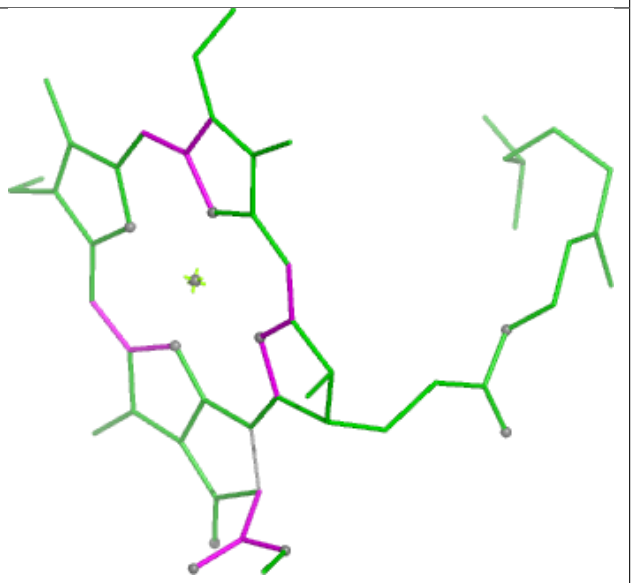
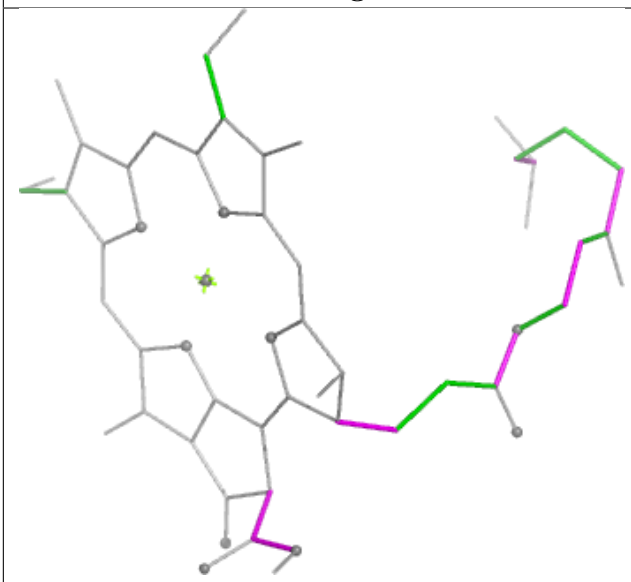


Bond angles



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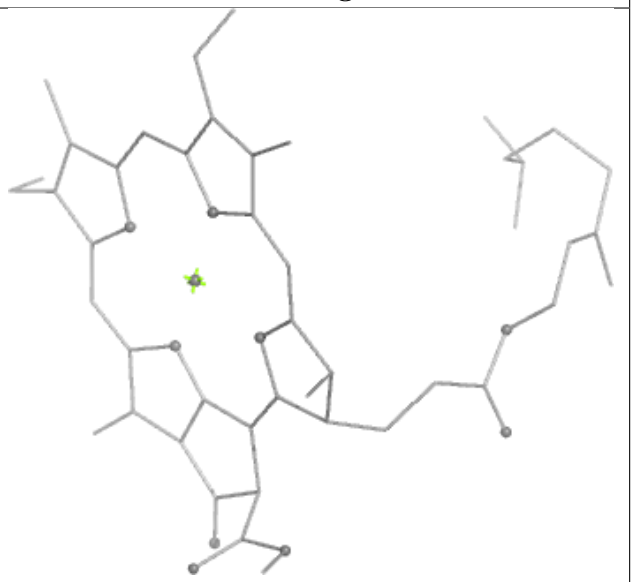
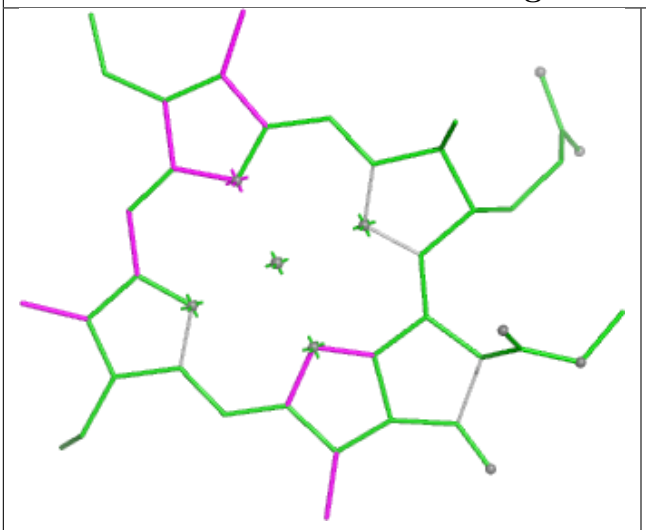


Rings

Ligand CLA B 823



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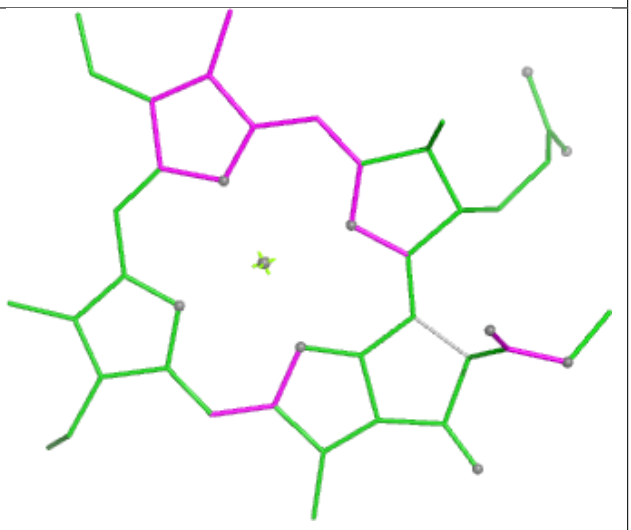

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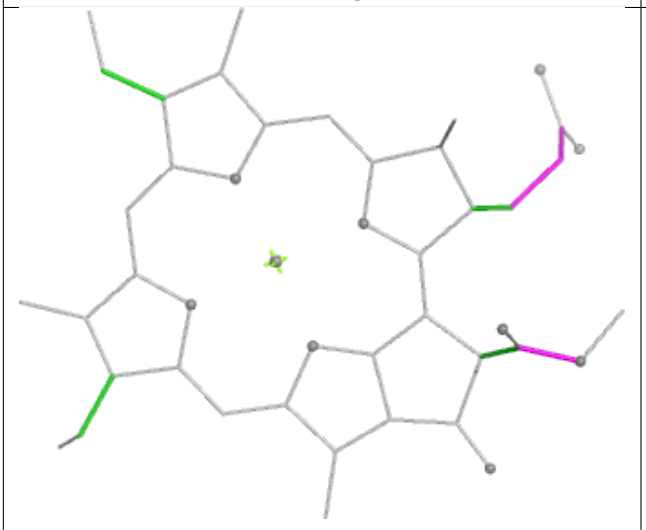

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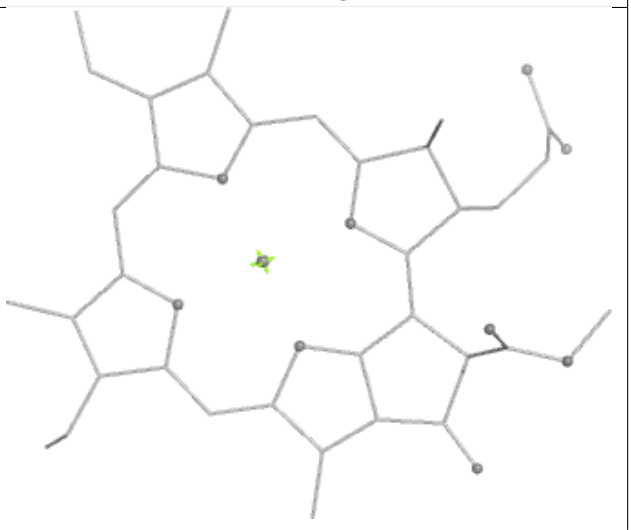
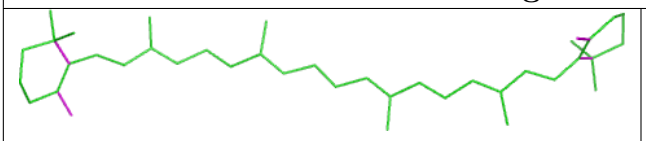


Rings

Ligand BCR B 848



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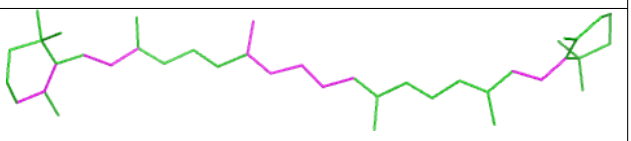
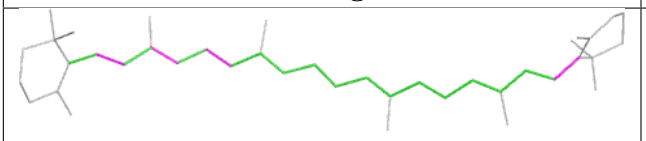


Bond angles



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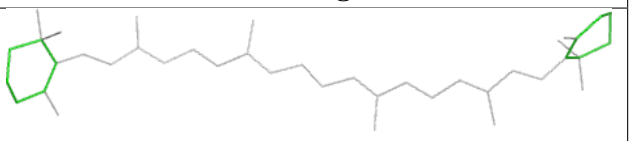
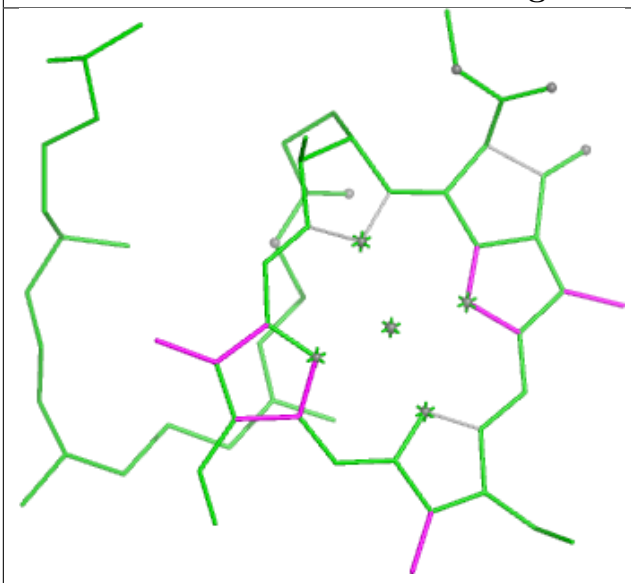


Rings

Ligand CLA a 824



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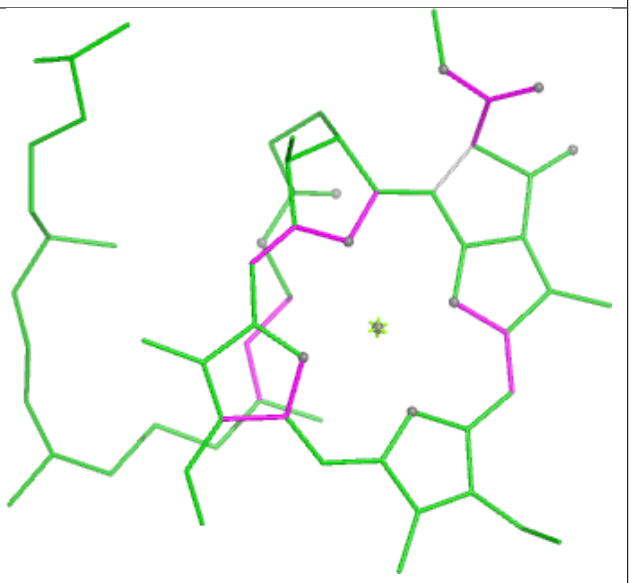
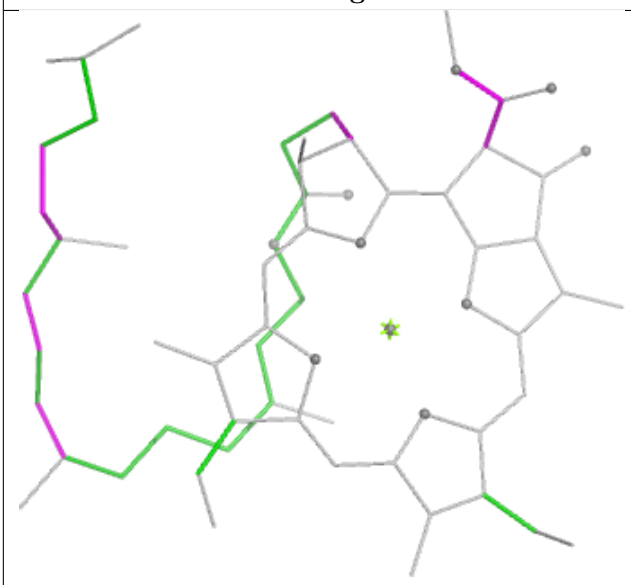


Bond angles



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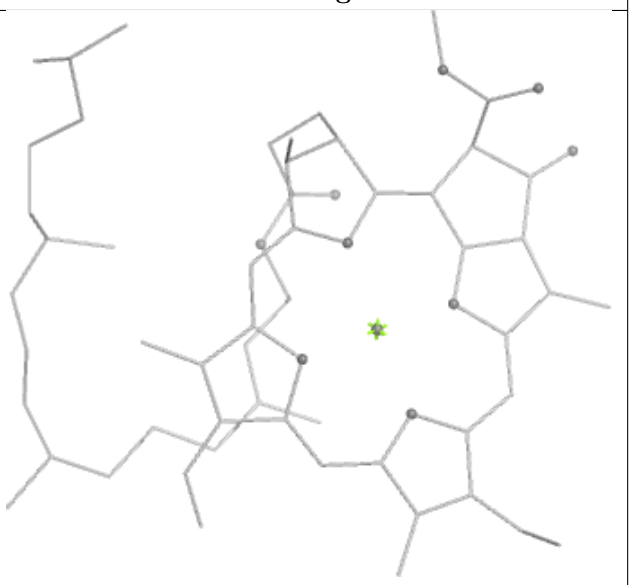
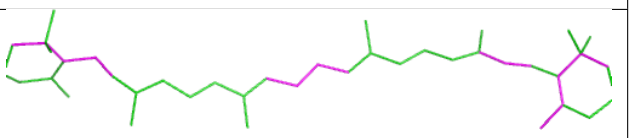


Rings

Ligand BCR 8 1304



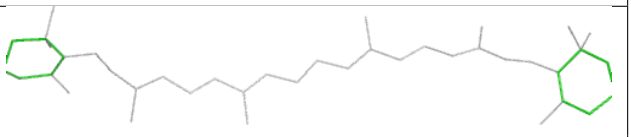
Bond lengths



Bond angles

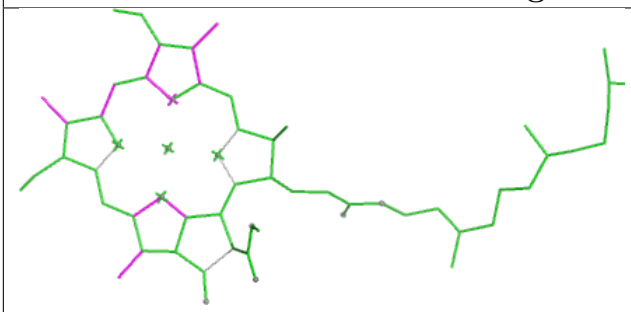


Torsions



Rings

Ligand CLA b 838



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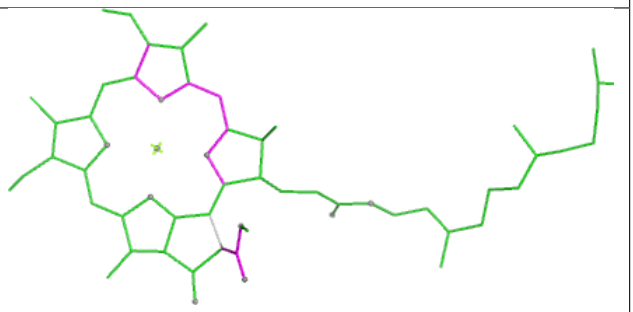

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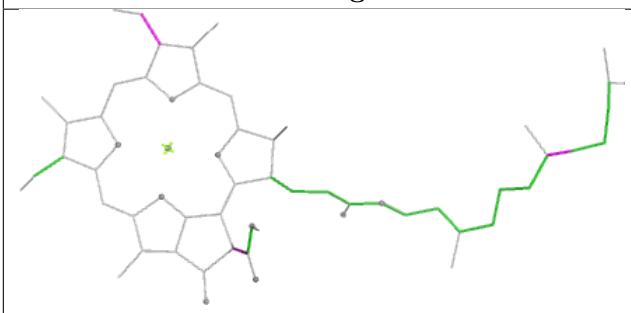

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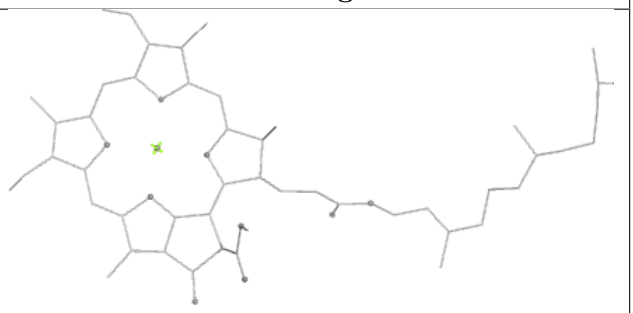
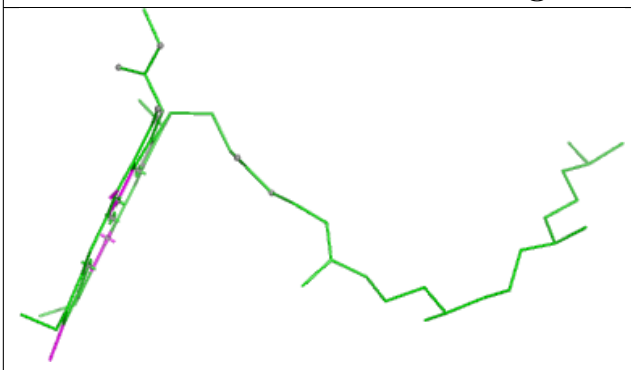


Rings

Ligand CLA 2 841



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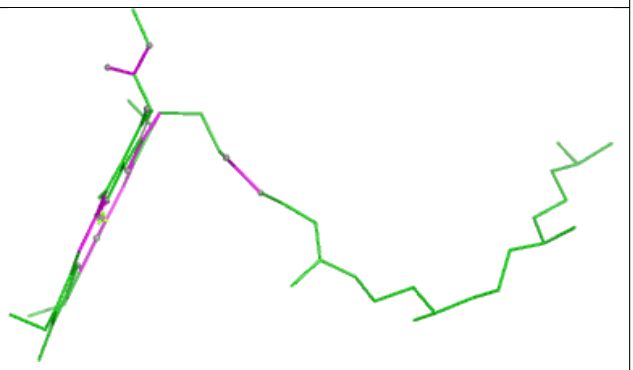

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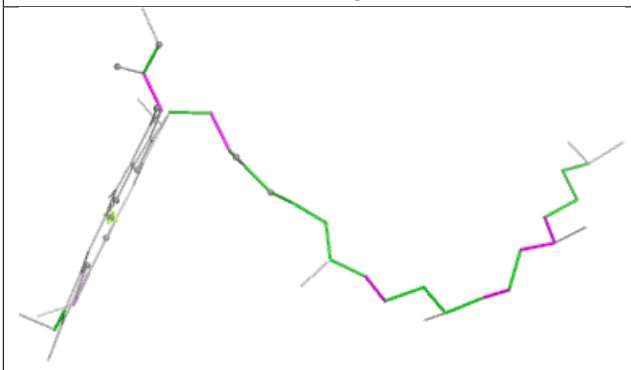
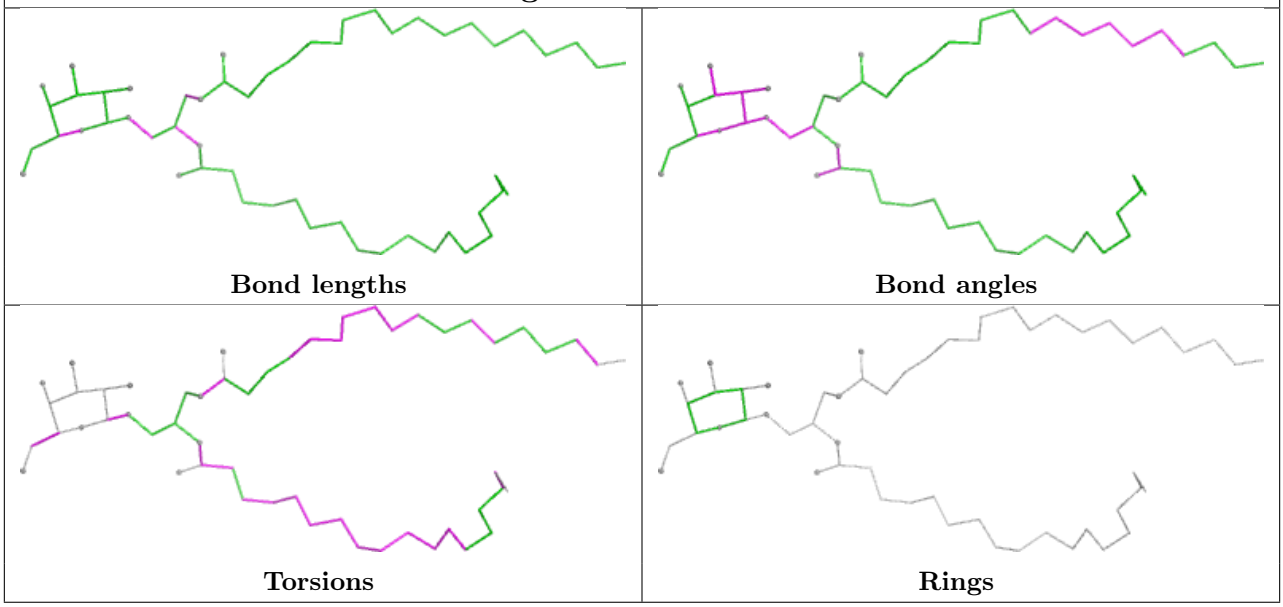


Torsions



Rings

Ligand LMG B 849



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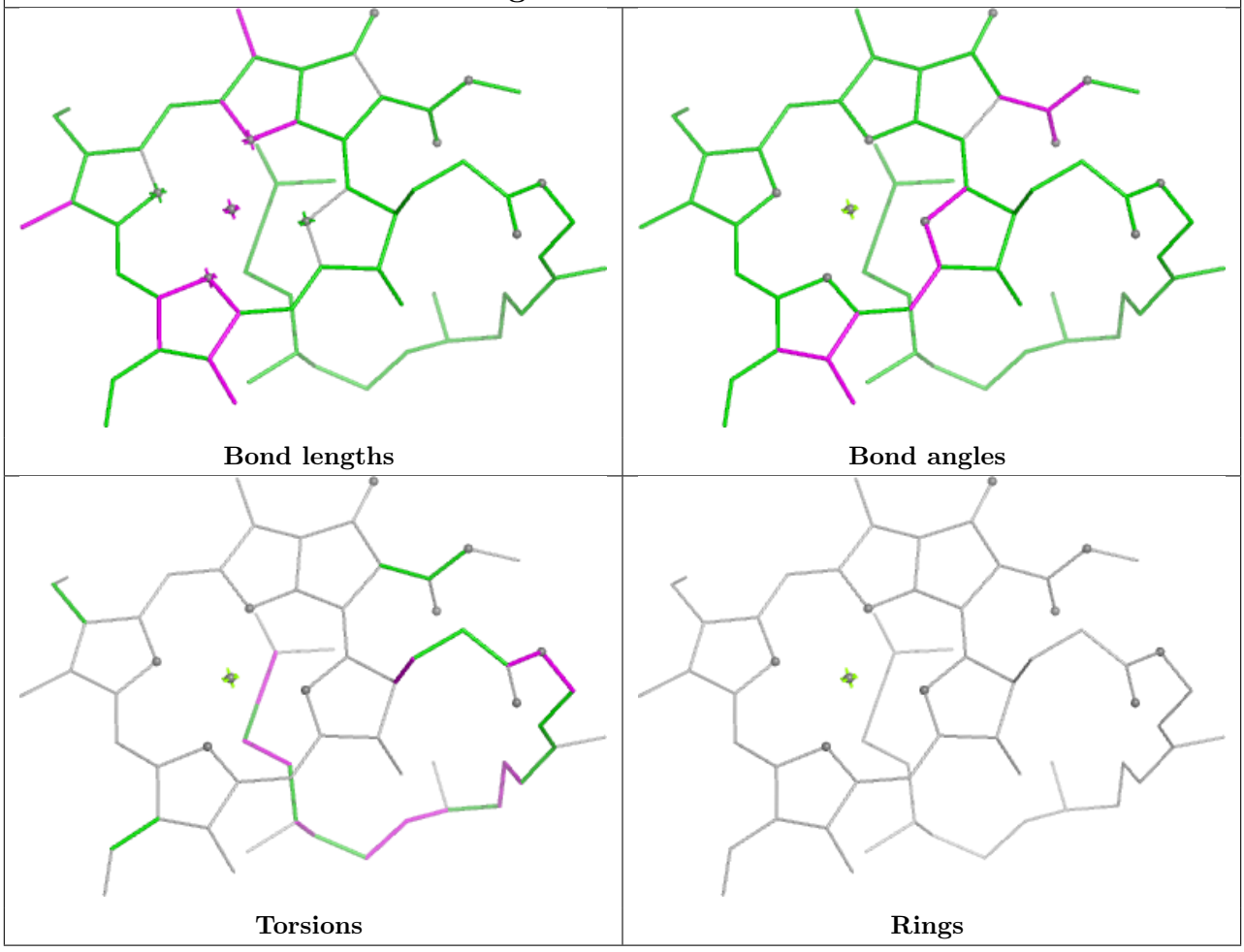
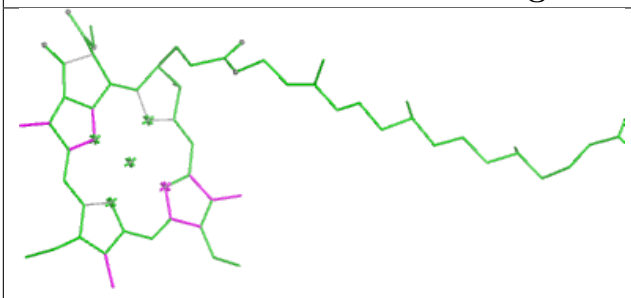


Ligand CLA a 835



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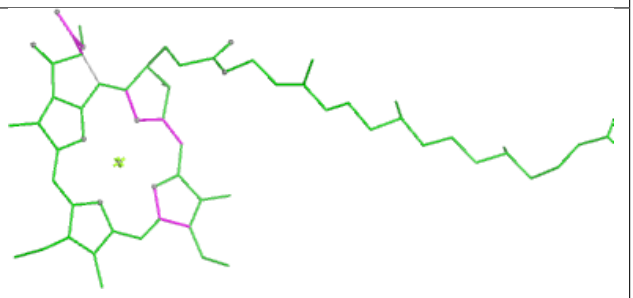
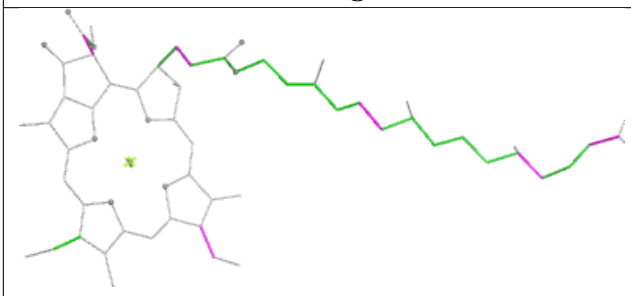


Bond angles



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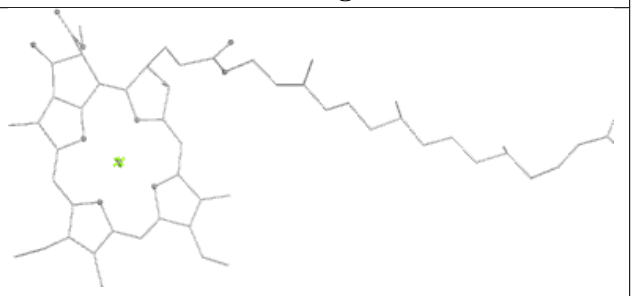
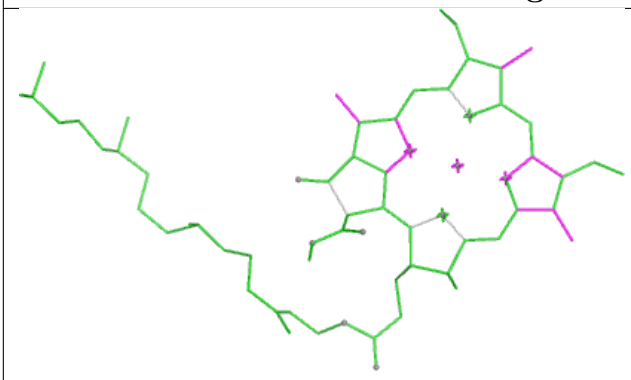


Rings

Ligand CLA L 205



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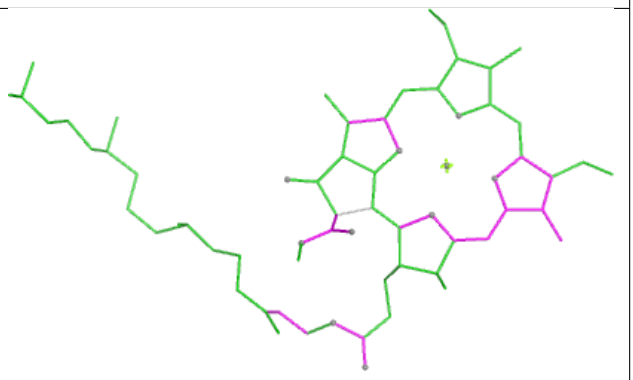
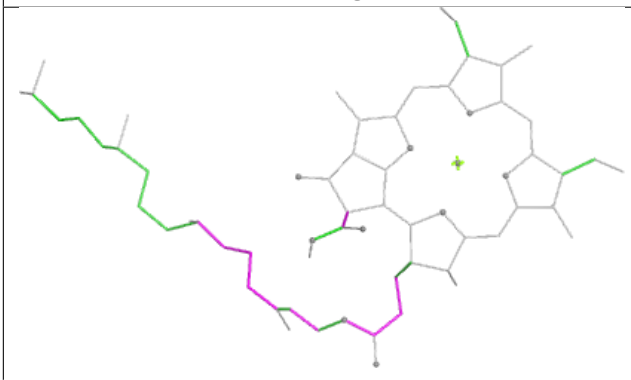


Bond angles

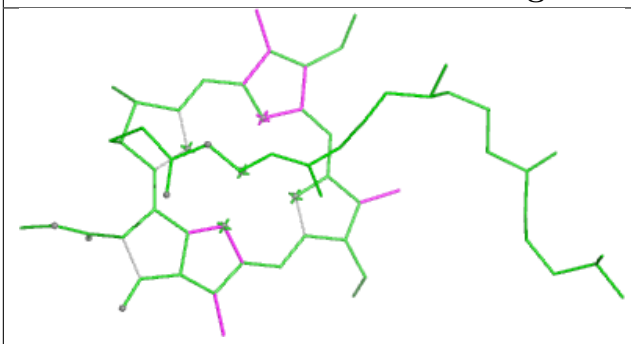


Torsions



Rings

Ligand CLA b 839



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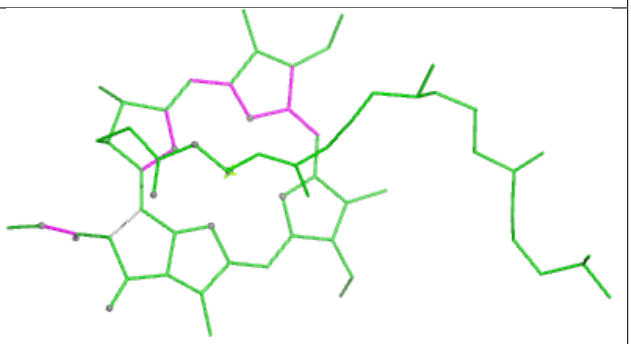
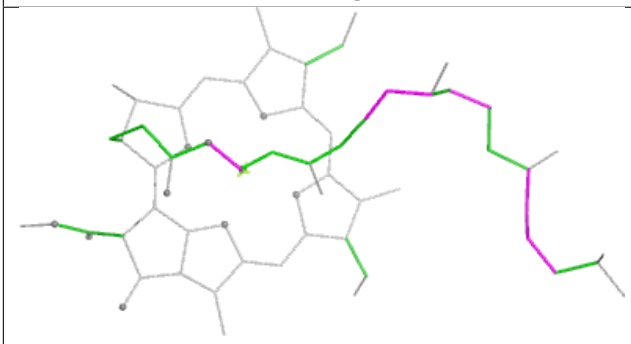


Bond angles

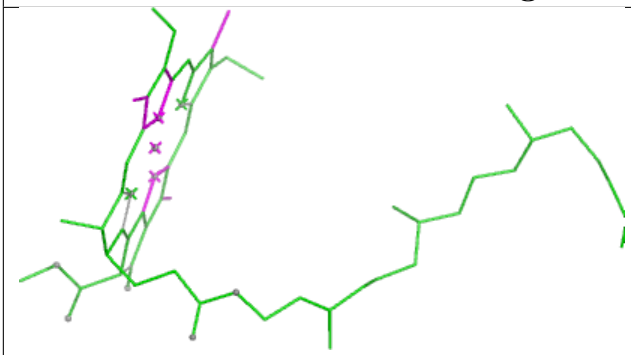


Torsions



Rings

Ligand CLA 1 1632



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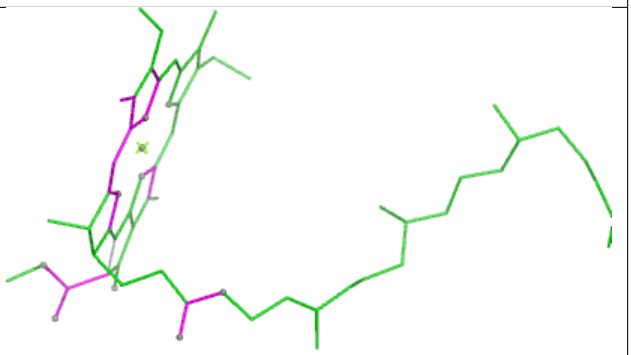

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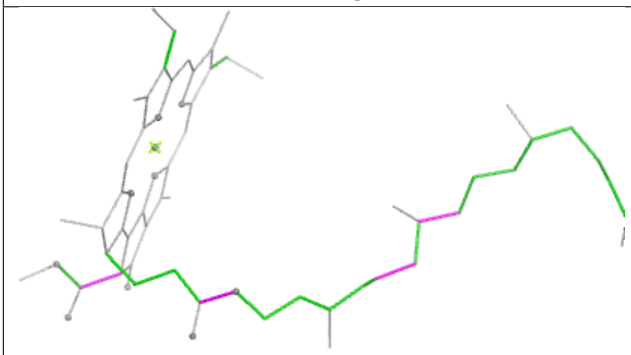
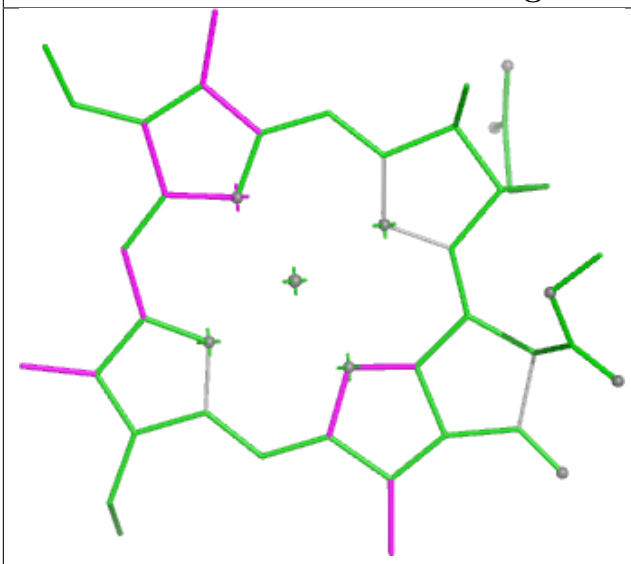


Torsions



Rings

Ligand CLA B 821



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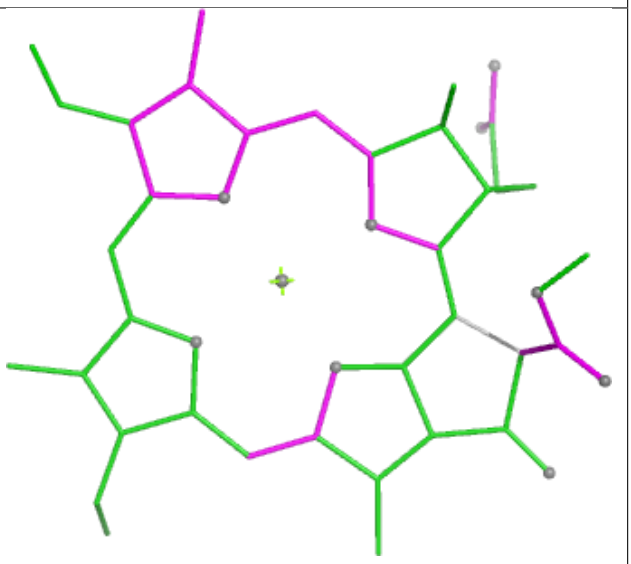
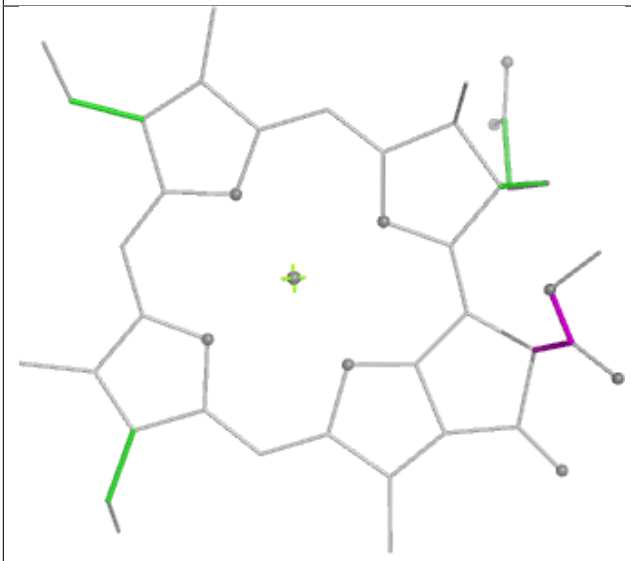


Bond angles



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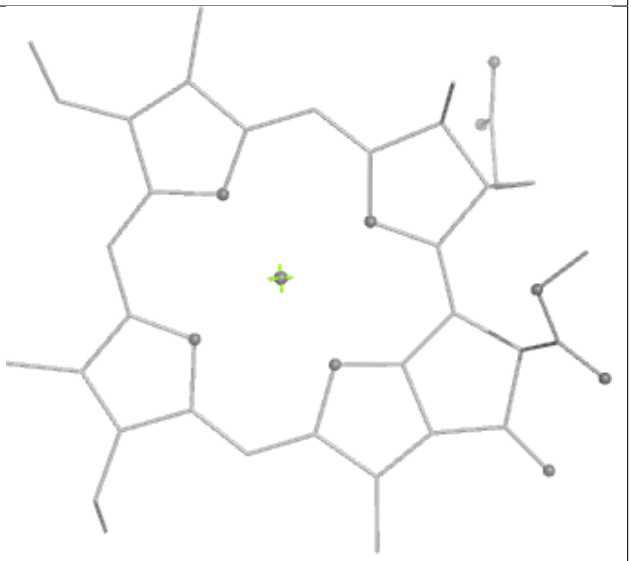
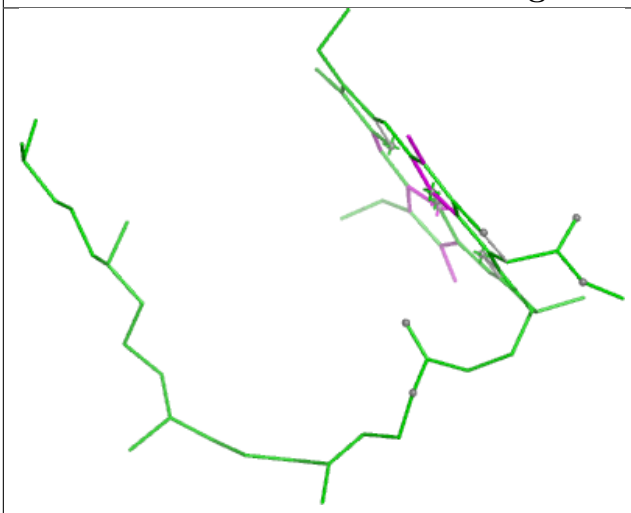
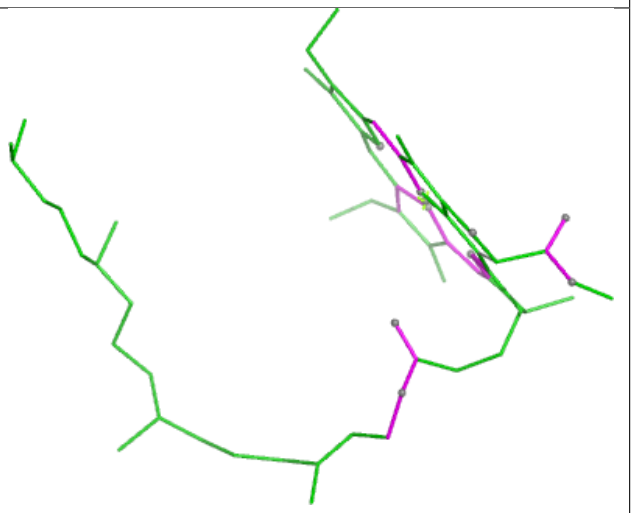


Rings

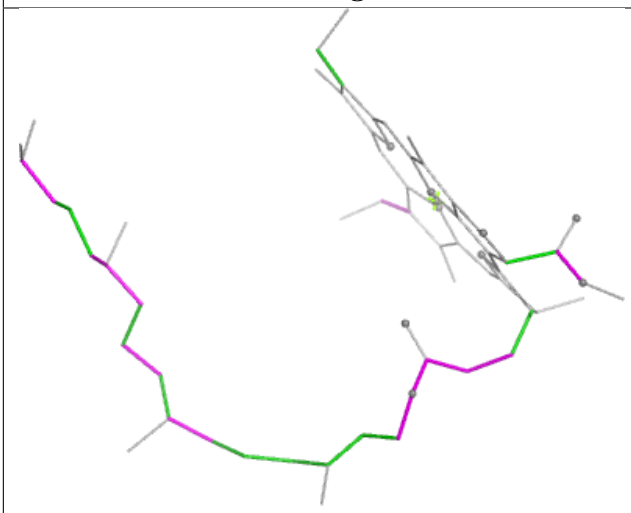
Ligand CLA 2 820



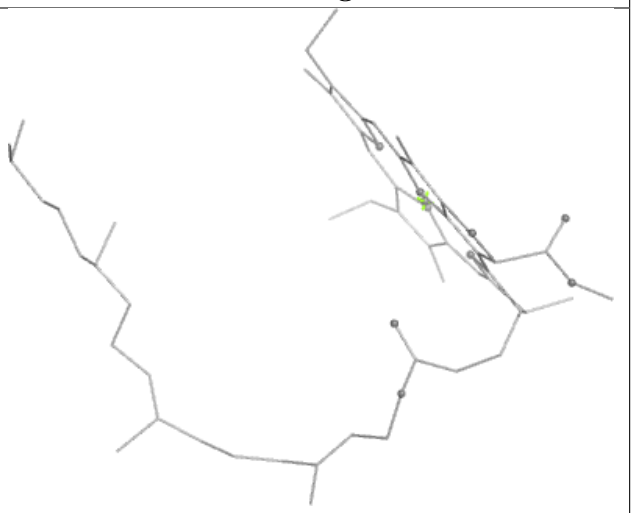
Bond lengths



Bond angles

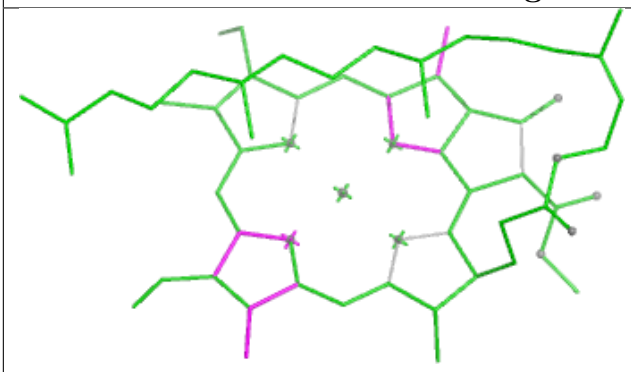


Torsions



Rings

Ligand CLA B 816



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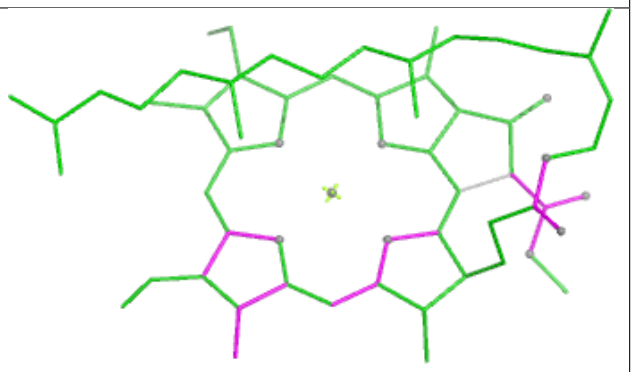

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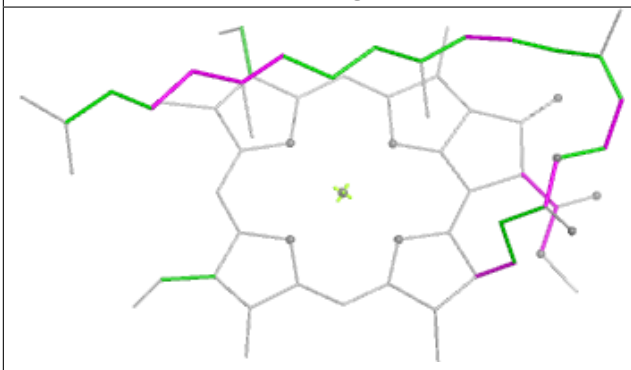

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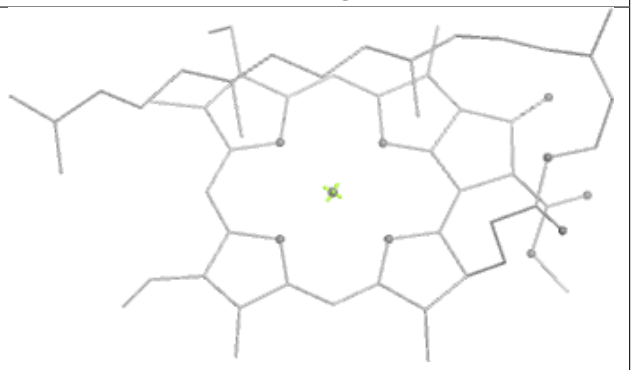
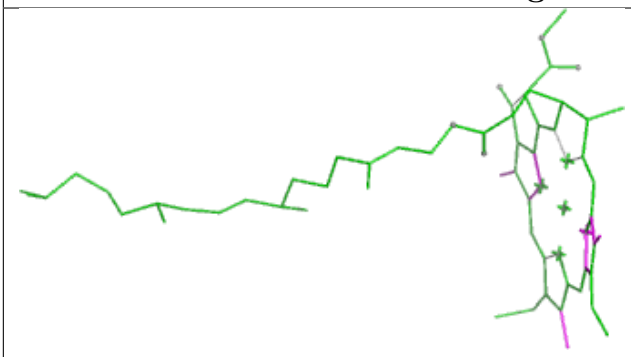


Rings

Ligand CLA b 829



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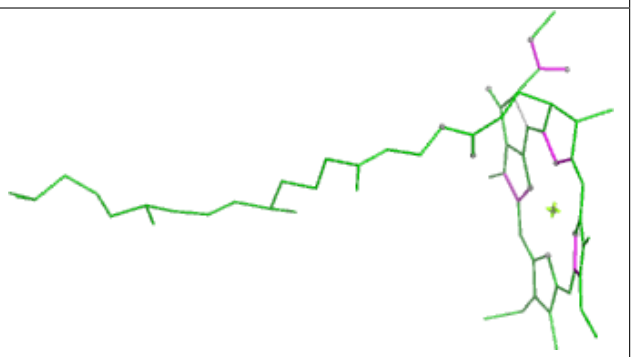
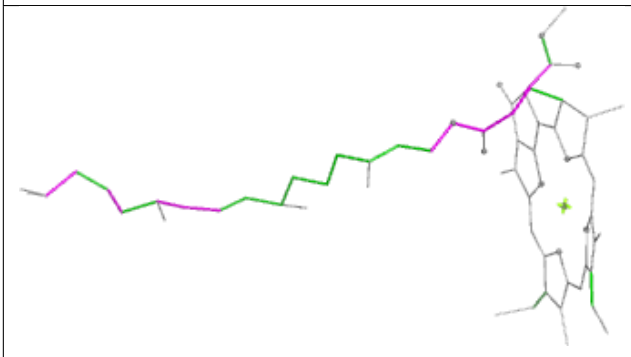


Bond angles



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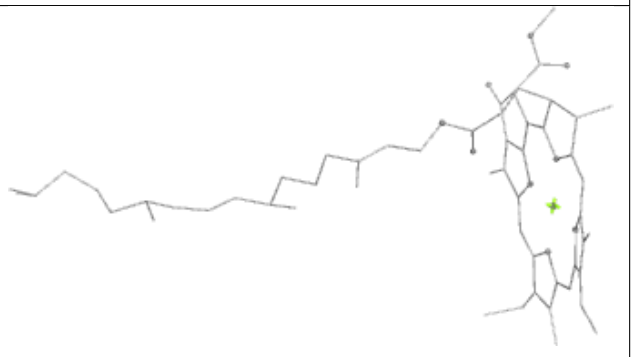
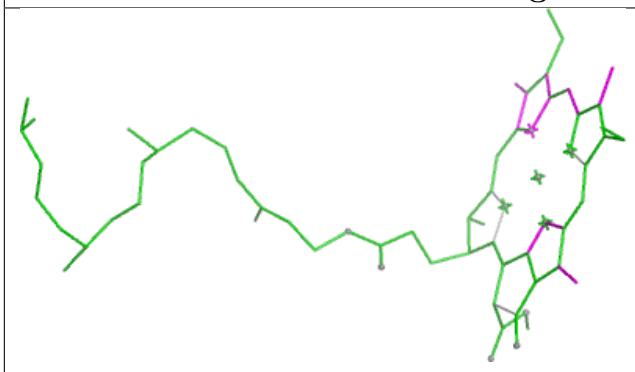


Rings

Ligand CLA 2 834



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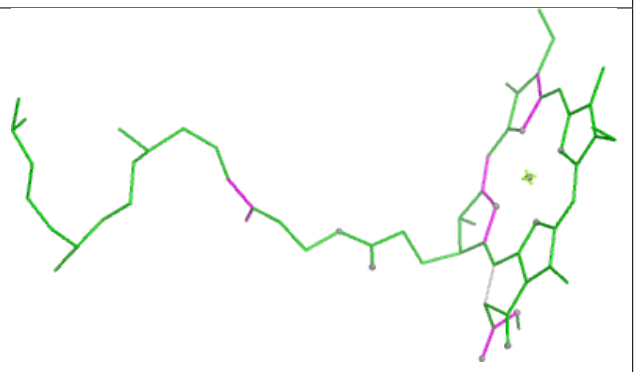
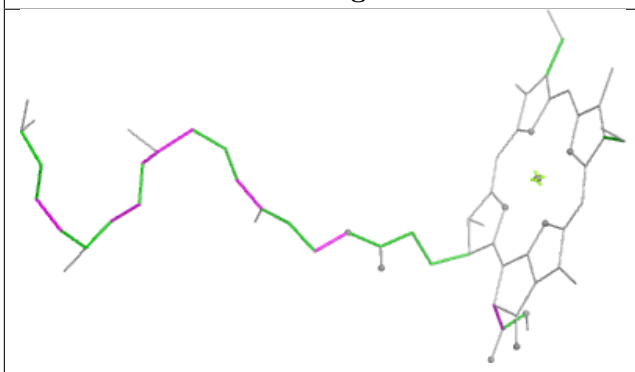


Bond angles



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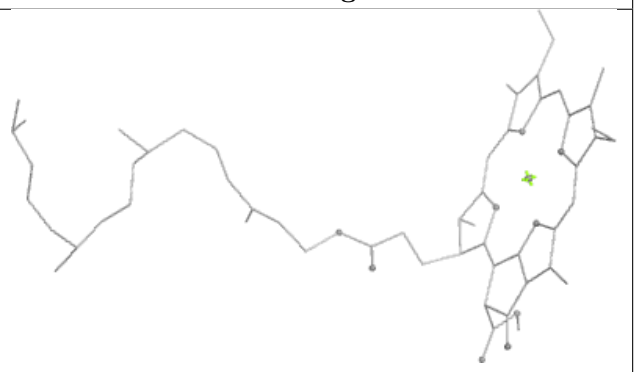
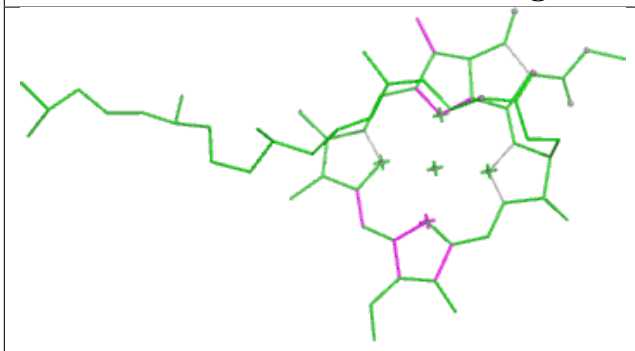


Rings

Ligand CLA a 818



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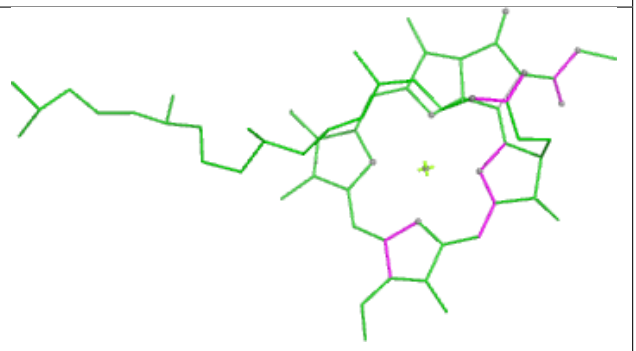

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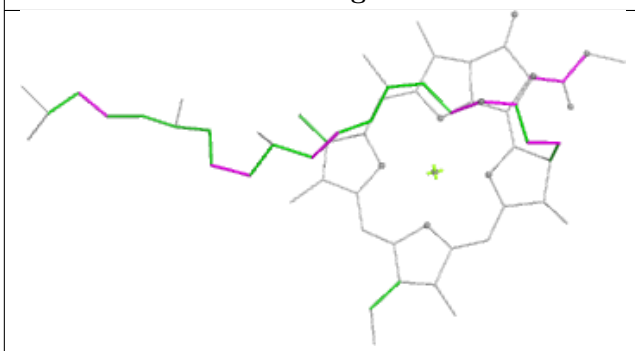

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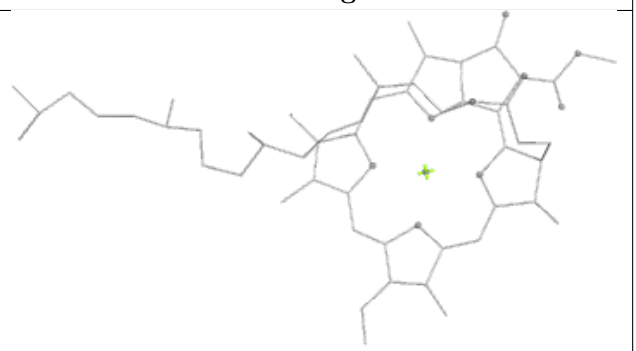
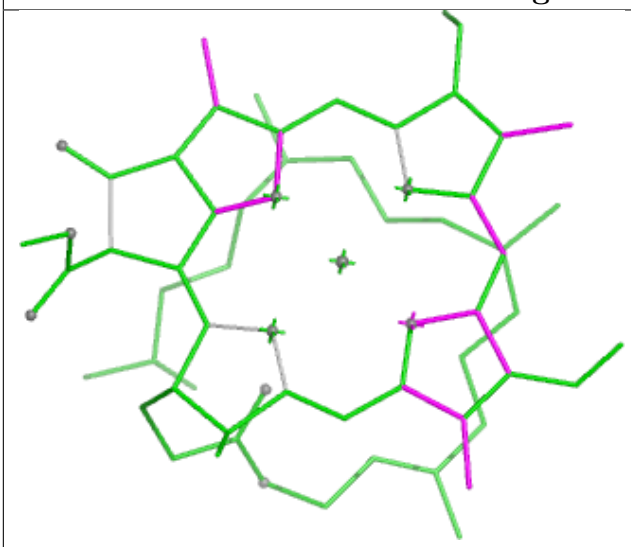


Rings

Ligand CLA l 204



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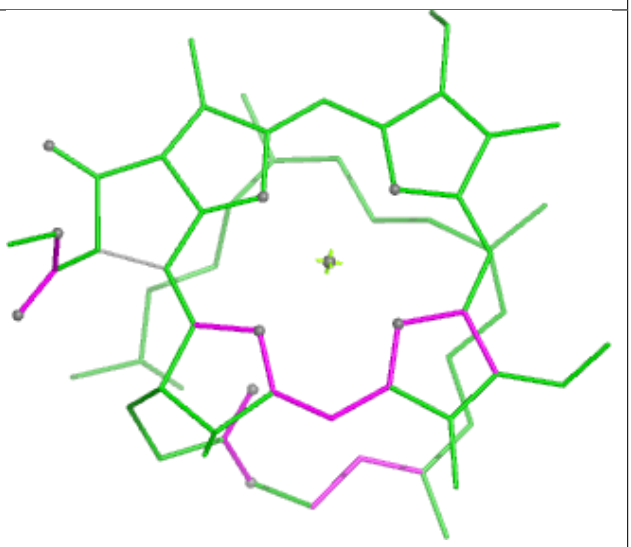

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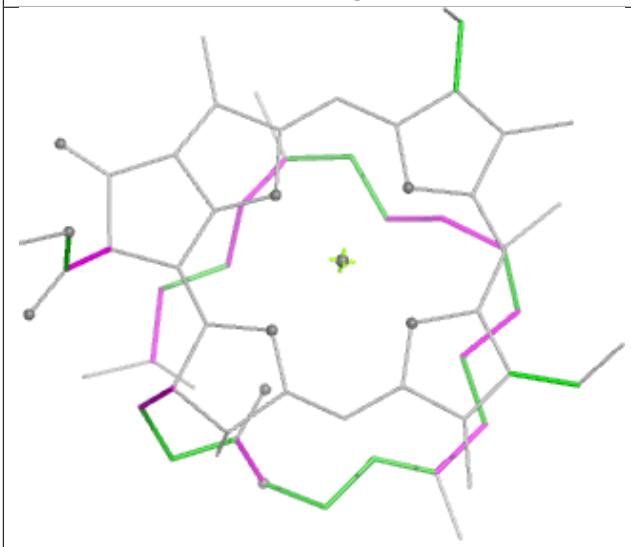

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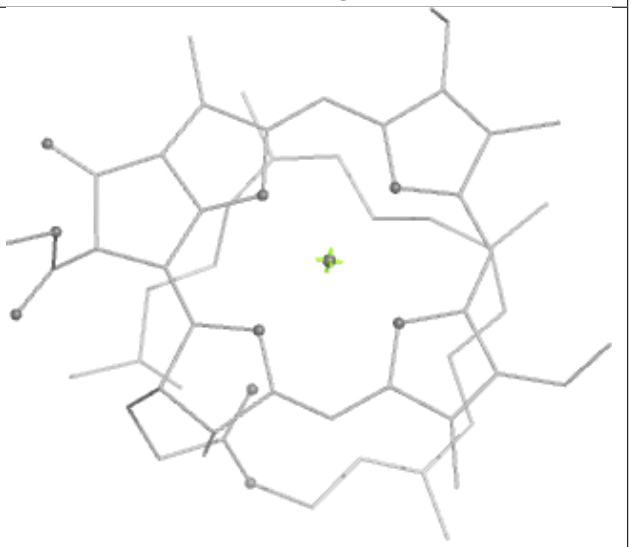
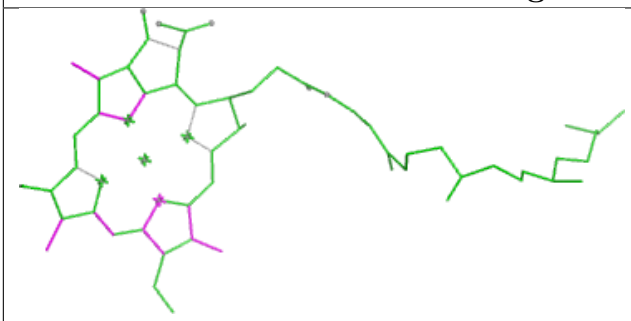


Rings

Ligand CLA b 814



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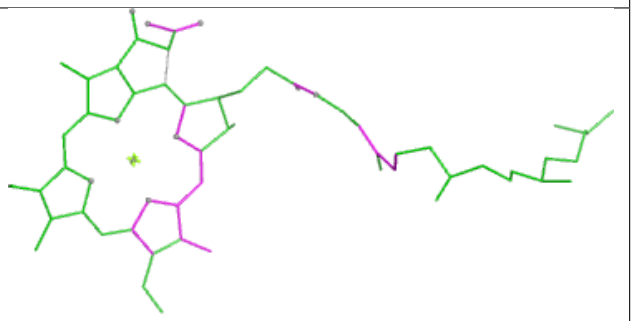
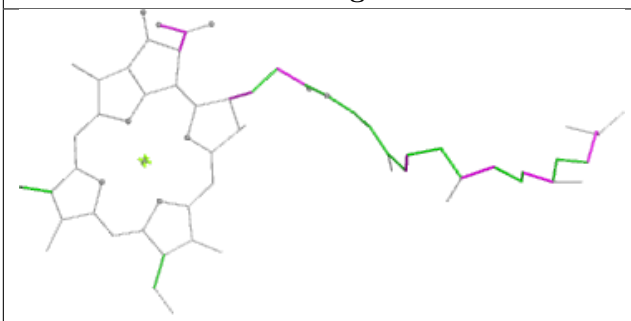


Bond angles



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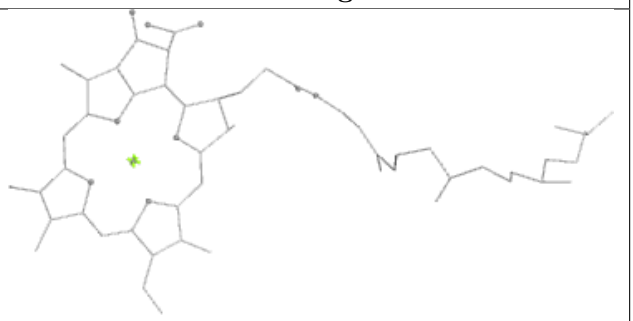
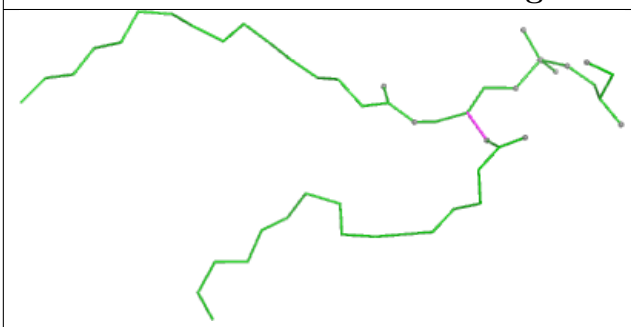


Rings

Ligand LHG b 851



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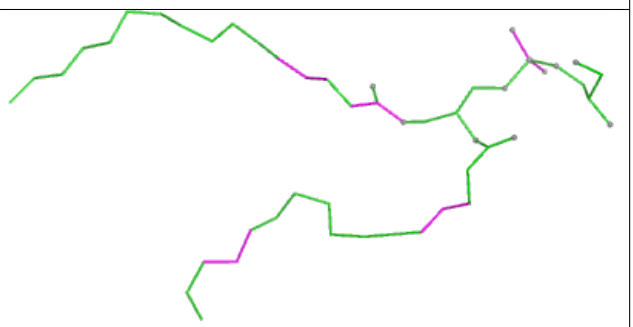

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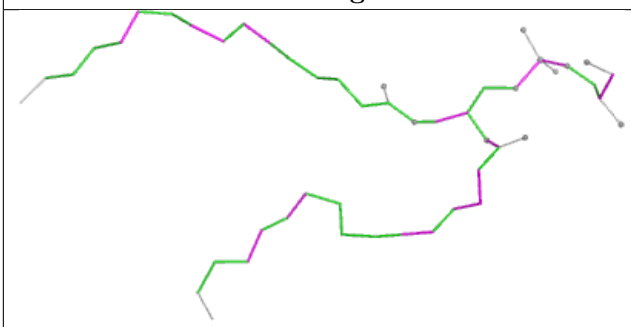

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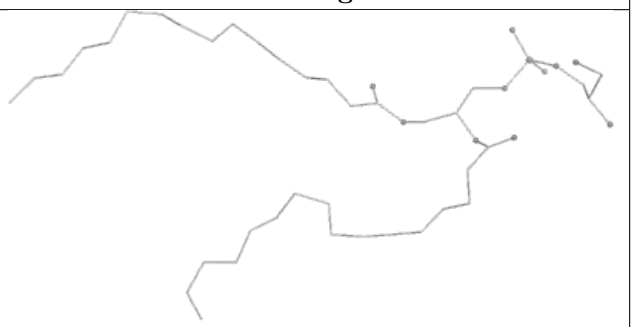
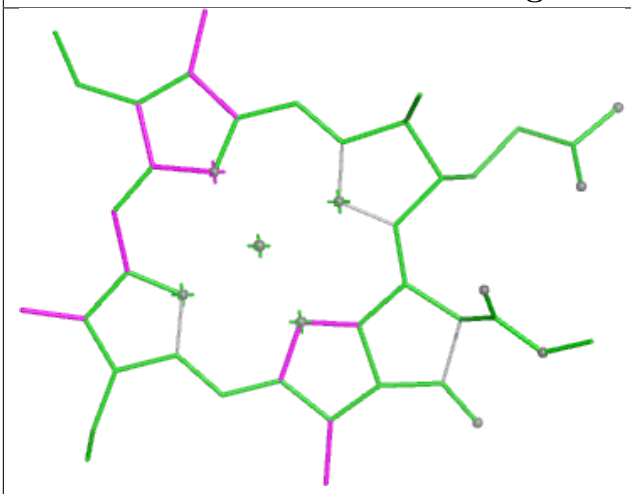


Rings

Ligand CLA F 203



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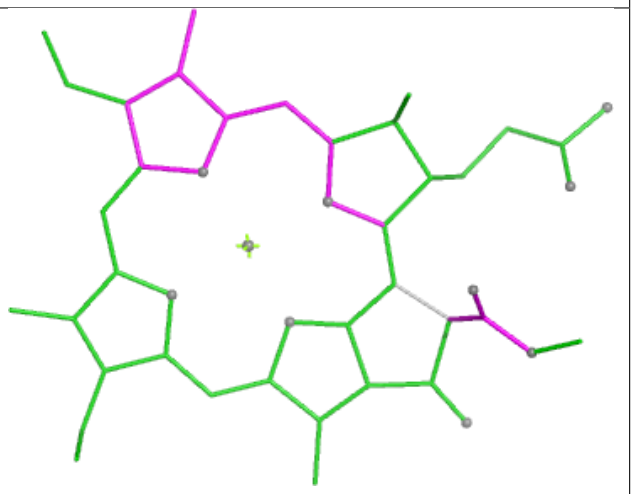
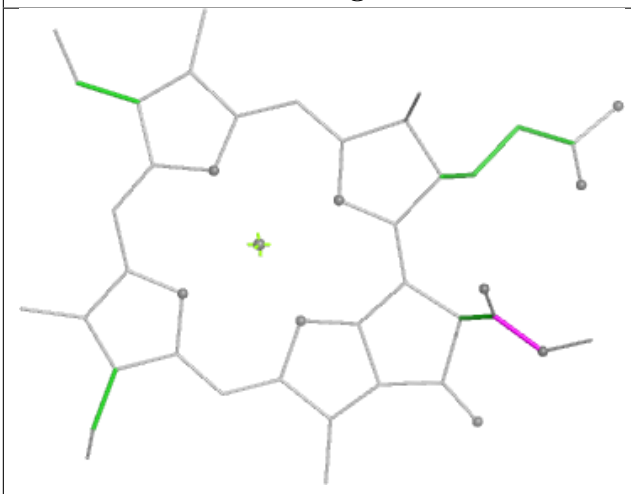


Bond angles



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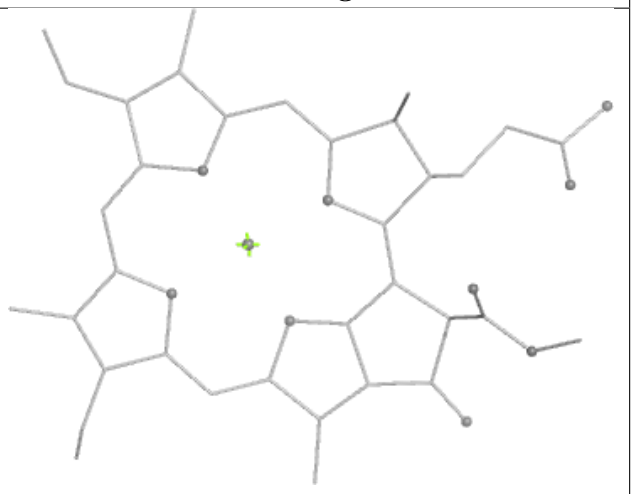
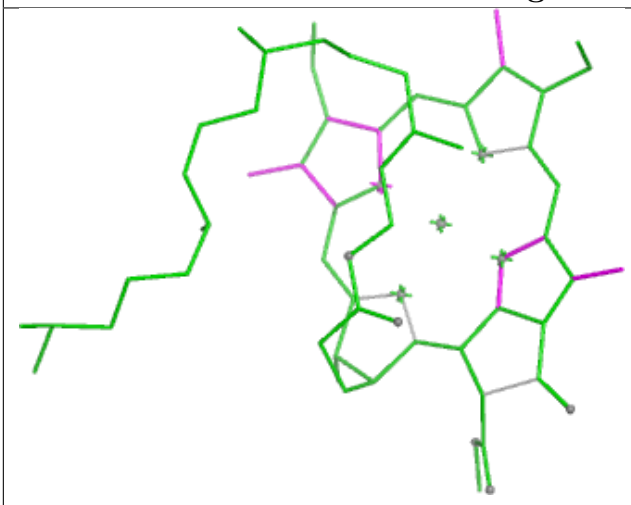


Rings

Ligand CLA b 809



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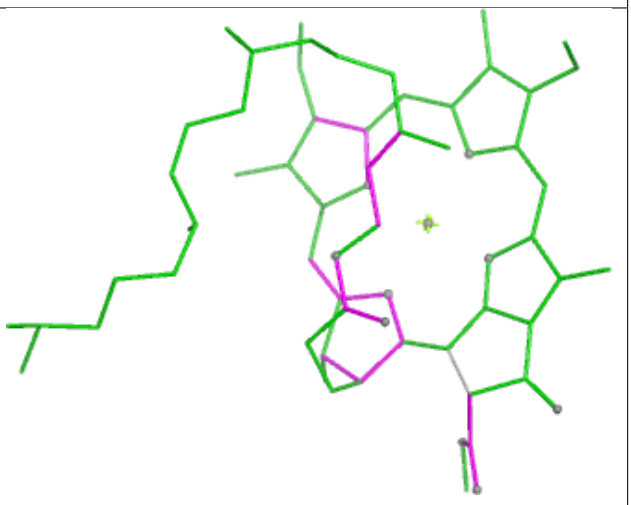
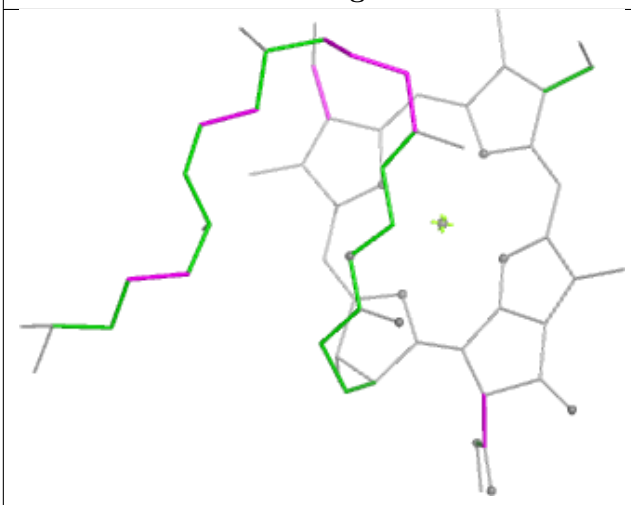


Bond angles



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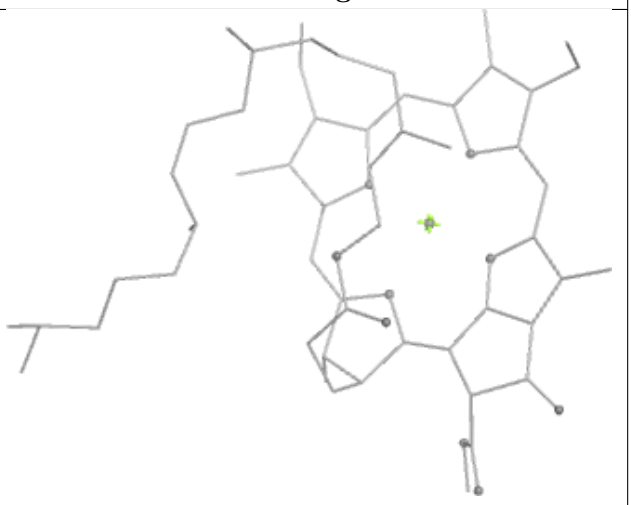
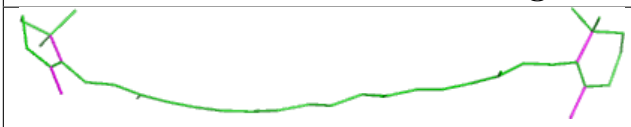


Rings

Ligand BCR I 101



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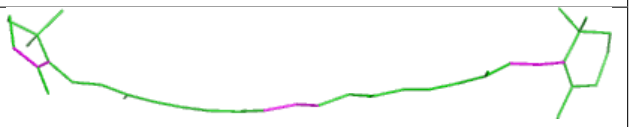

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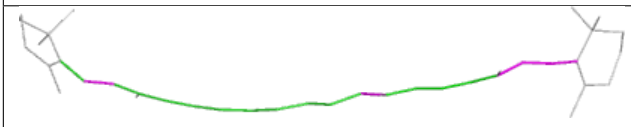

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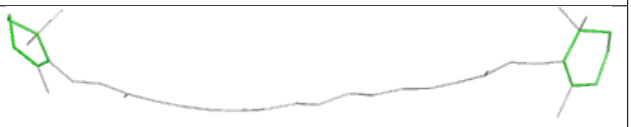
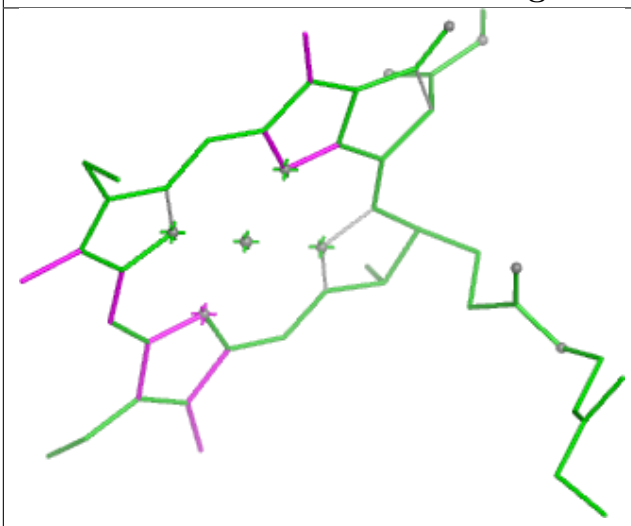


Rings

Ligand CLA a 808



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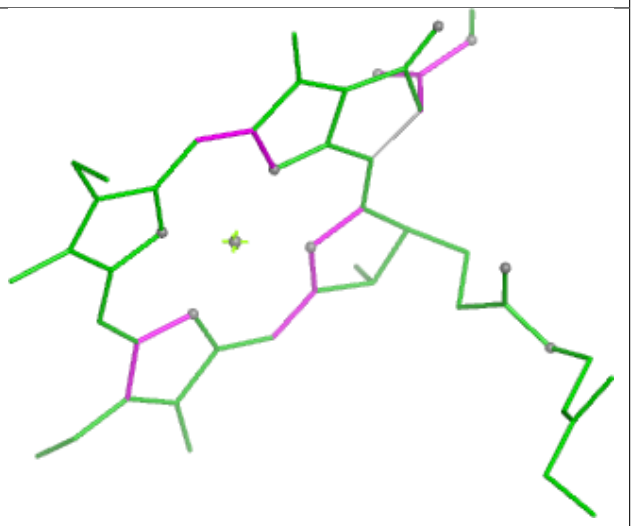
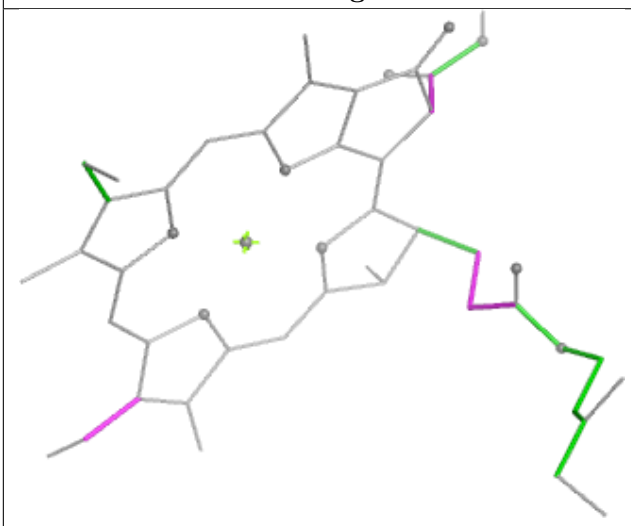


Bond angles



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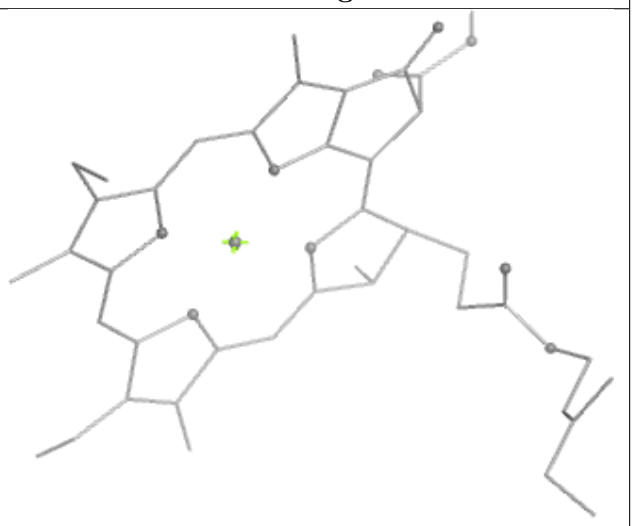
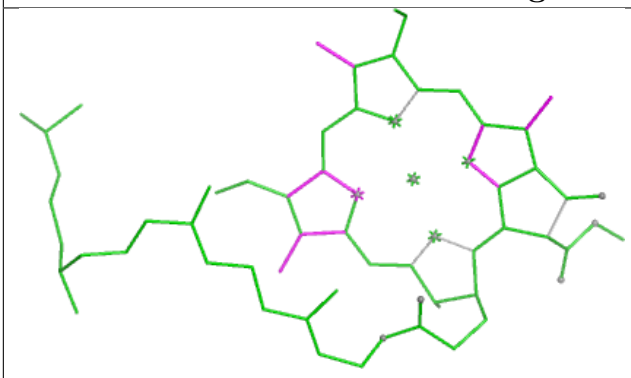


Rings

Ligand CLA 2 819



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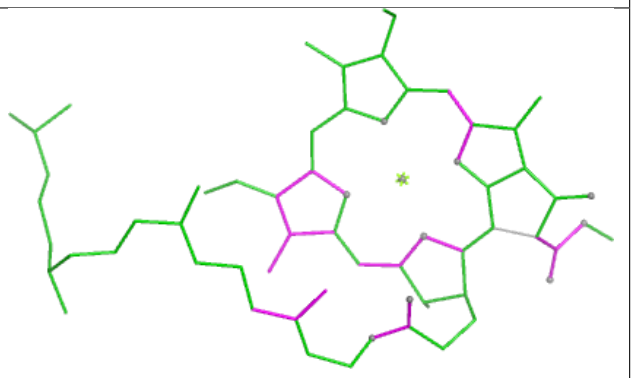
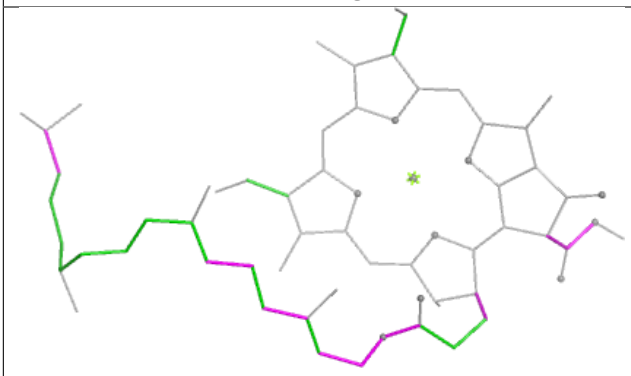


Bond angles



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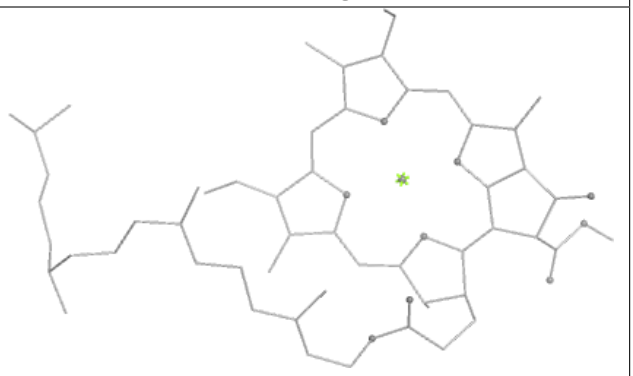
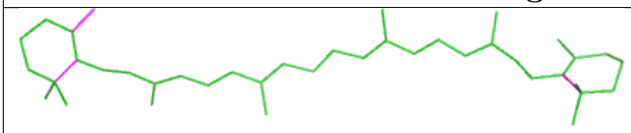


Rings

Ligand BCR J 103



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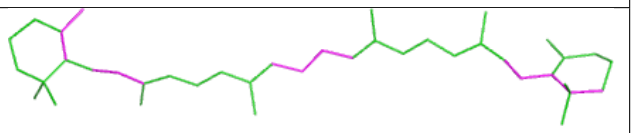
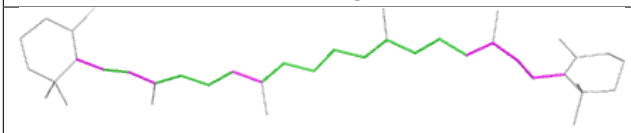


Bond angles



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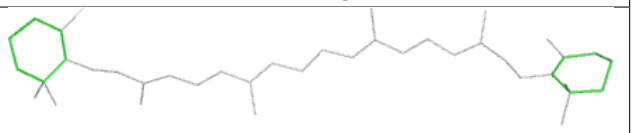
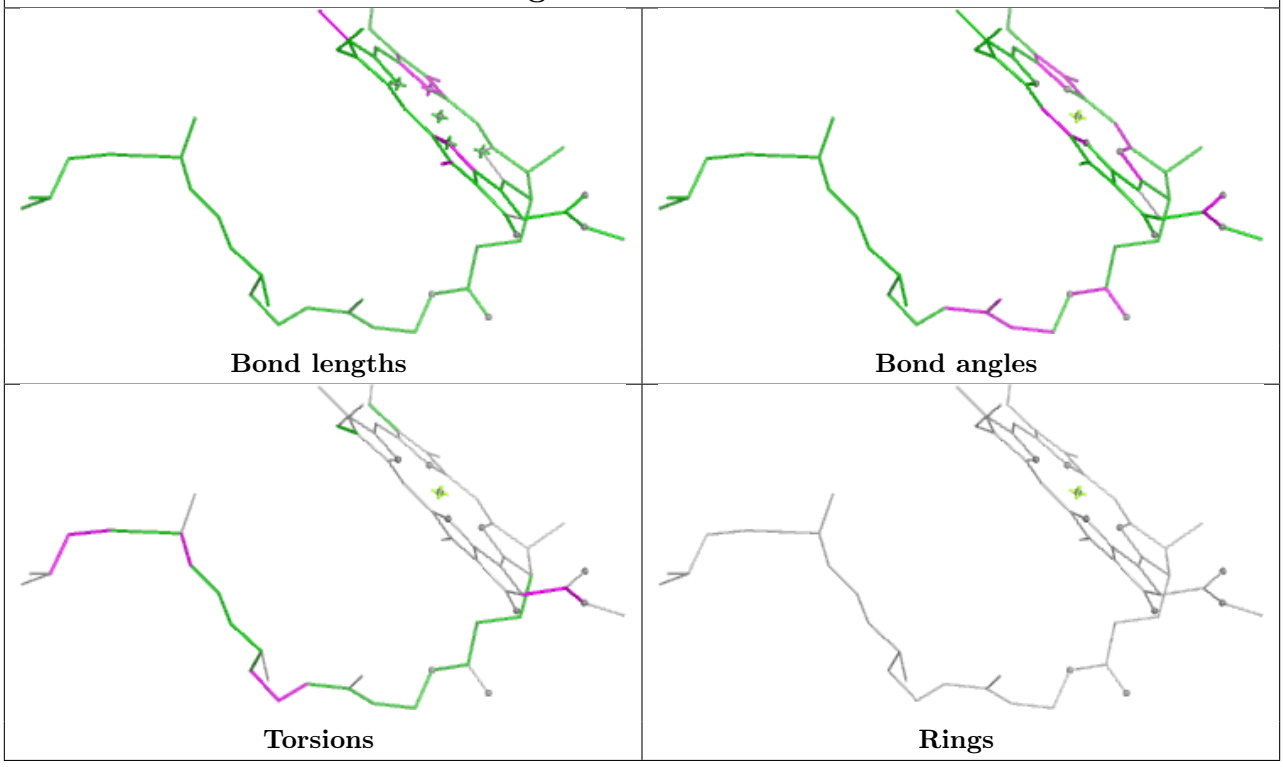
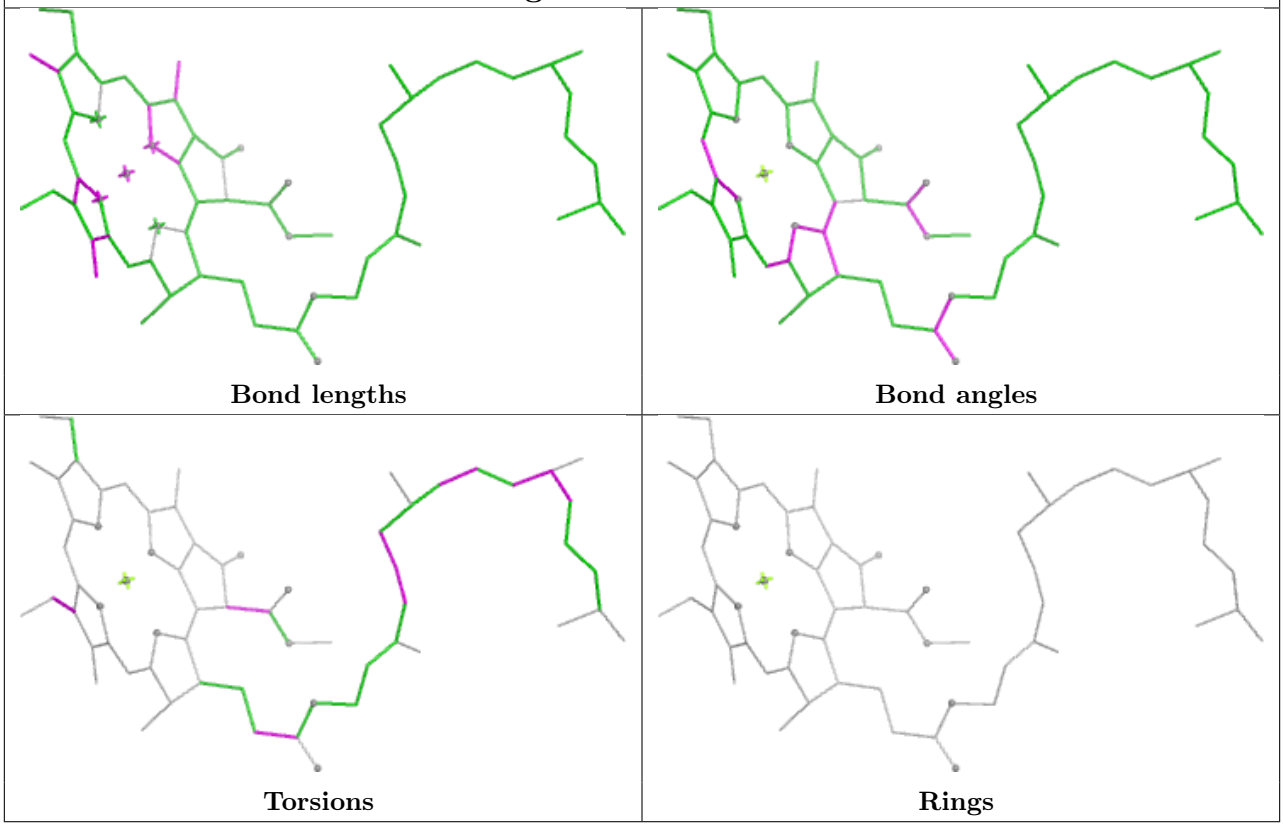


Rings

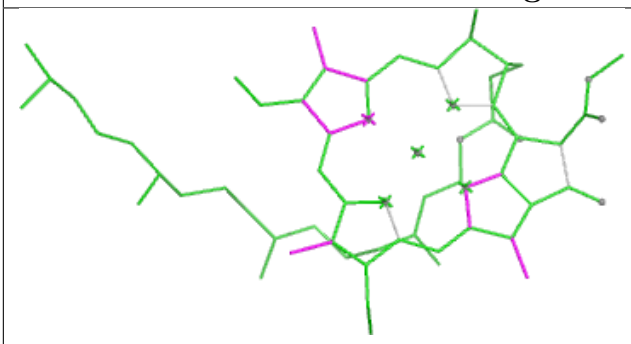
Ligand CLA b 812



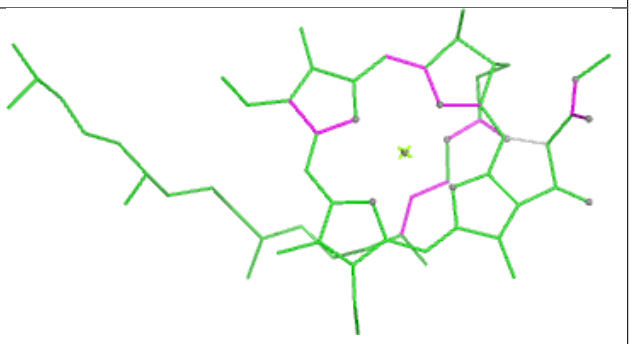
Ligand CL0 1 1602



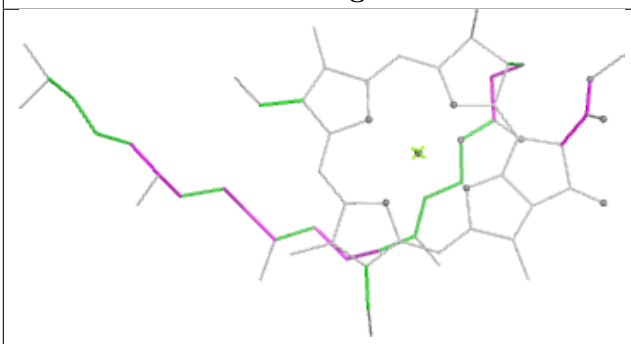
Ligand CLA A 841



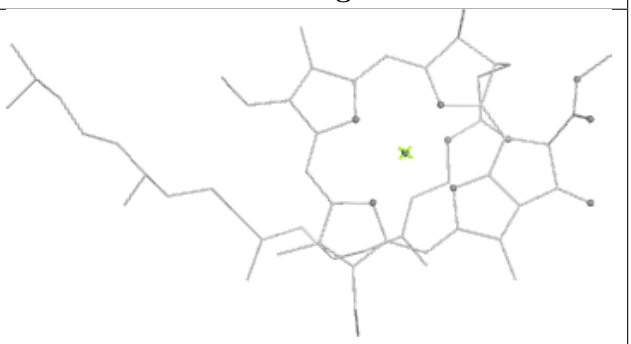
Bond lengths



Bond angles

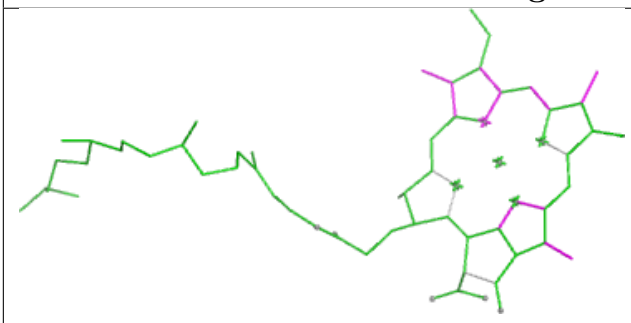


Torsions



Rings

Ligand CLA 2 814



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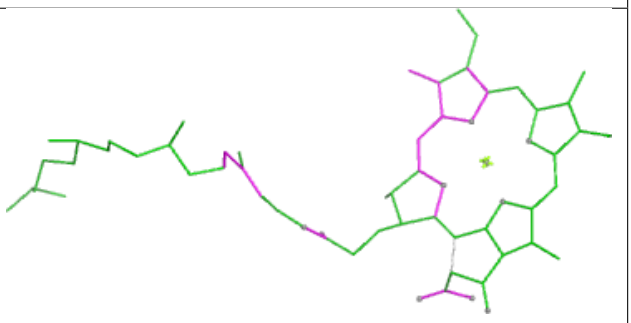
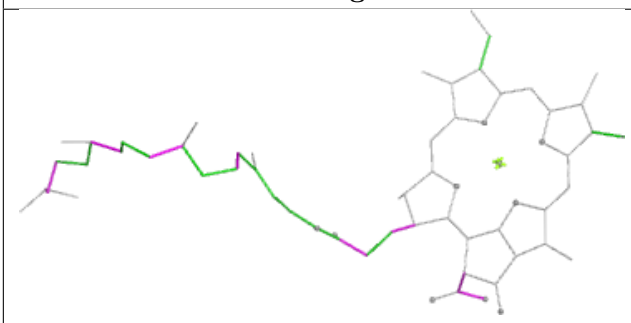


Bond angles



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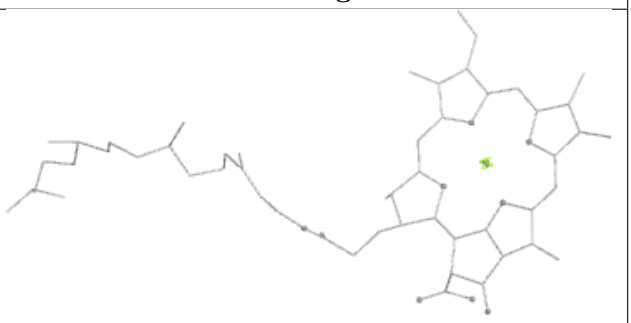
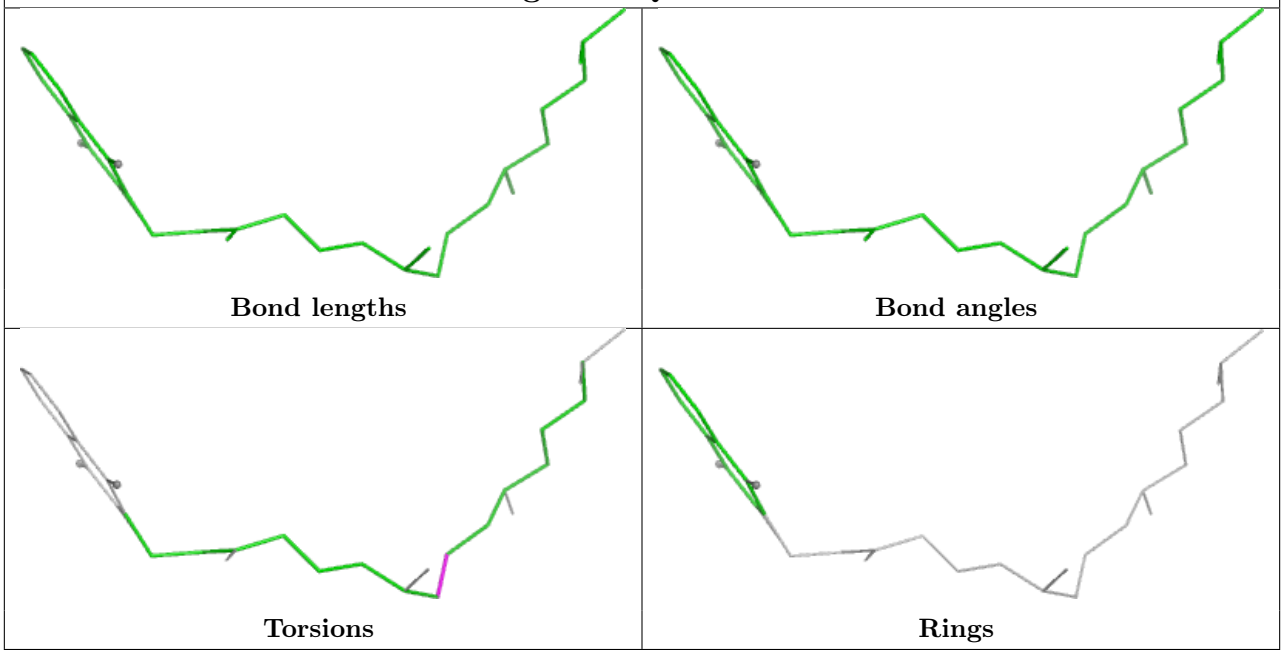
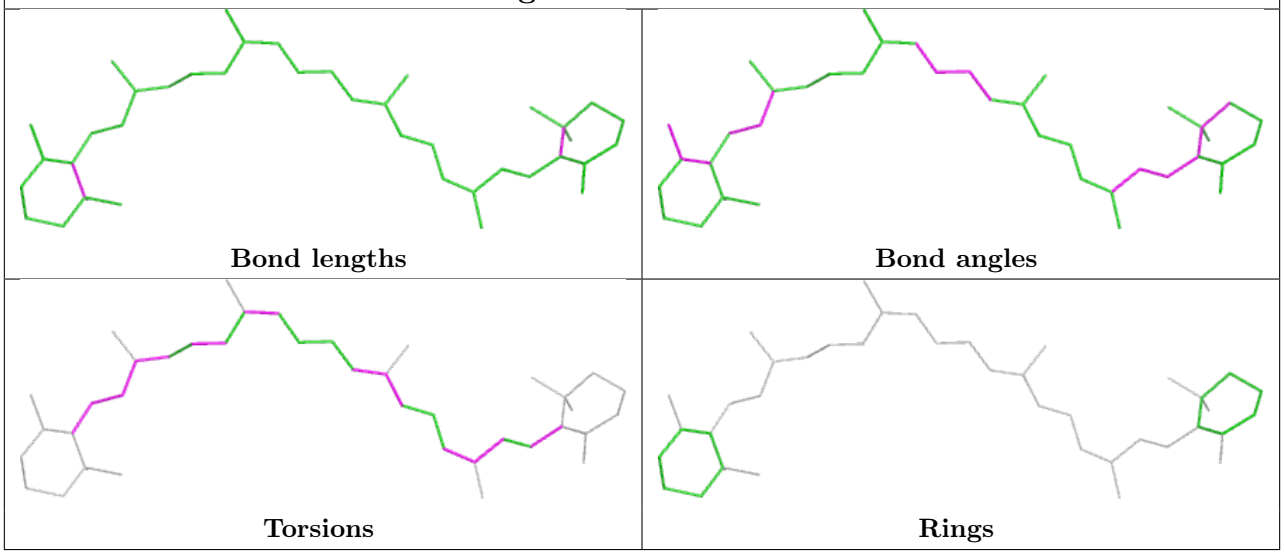


Rings

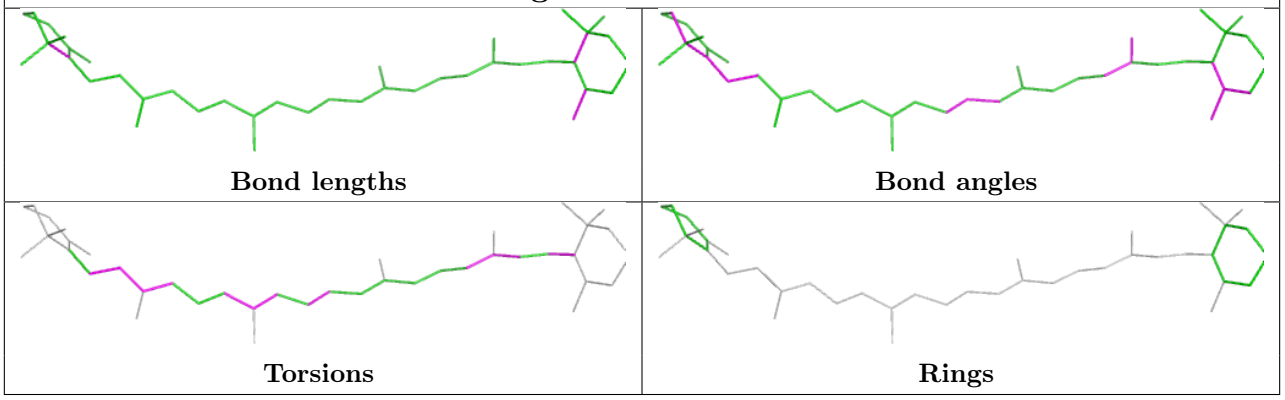
Ligand PQN B 842



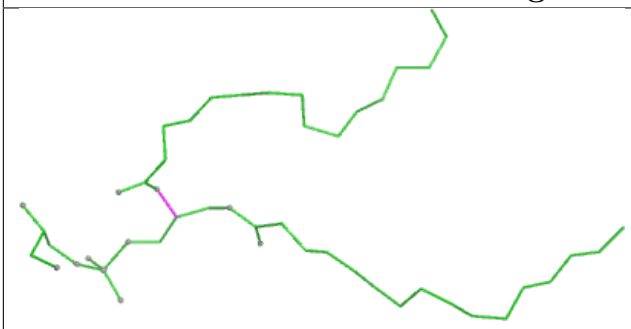
Ligand BCR 1 1652



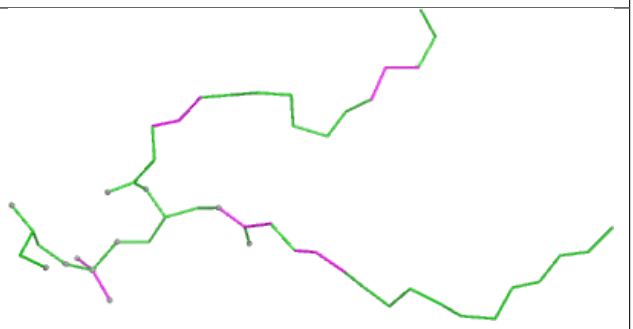
Ligand BCR f 202



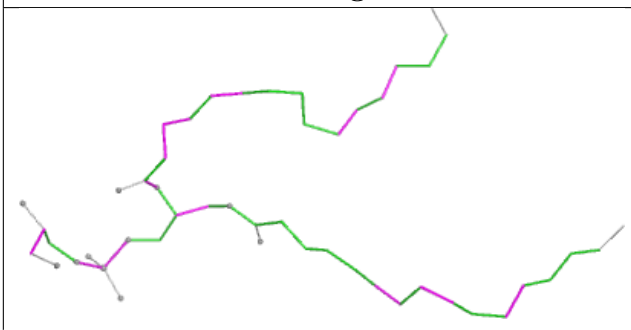
Ligand LHG z 101



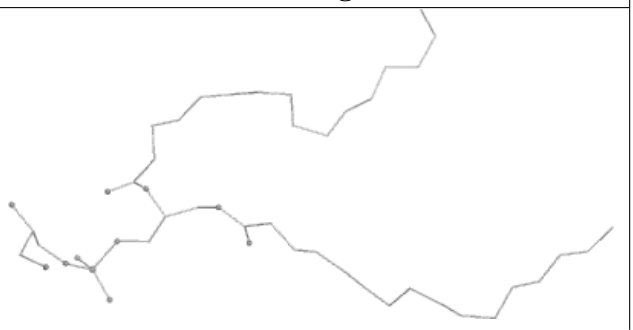
Bond lengths



Bond angles

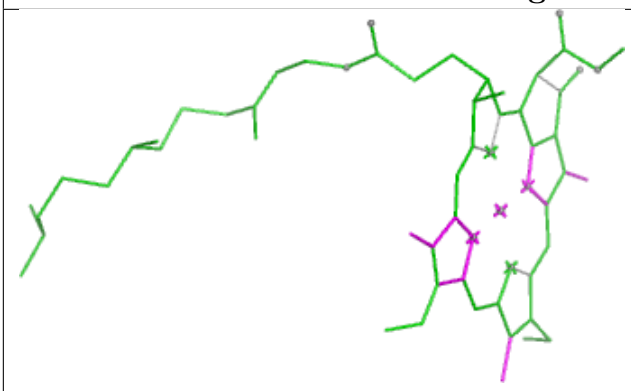


Torsions



Rings

Ligand CLA a 832



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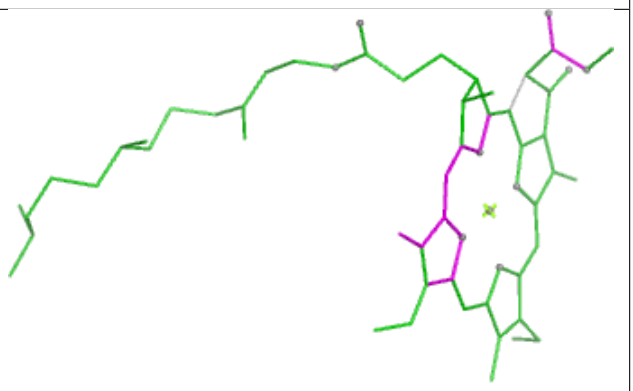
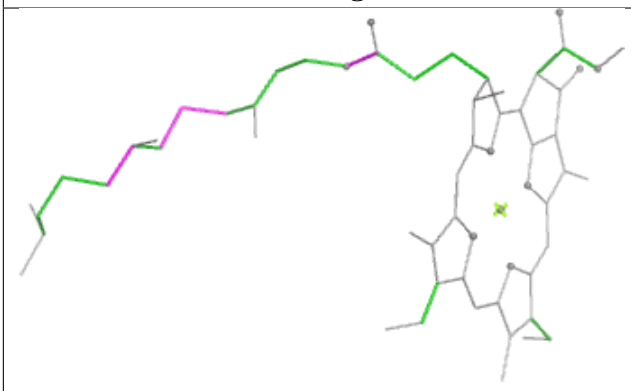


Bond angles

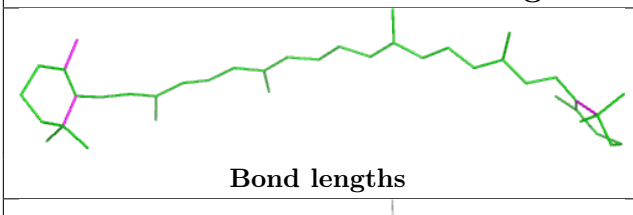


Torsions



Rings

Ligand BCR F 202



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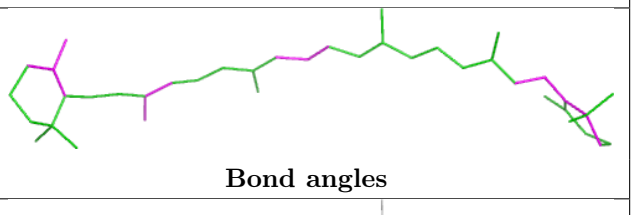
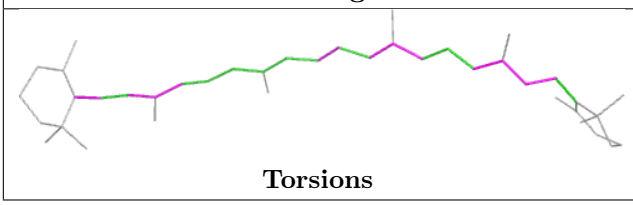


Bond angles



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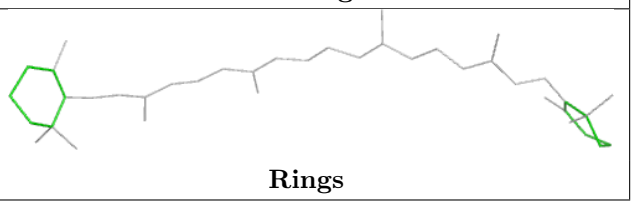
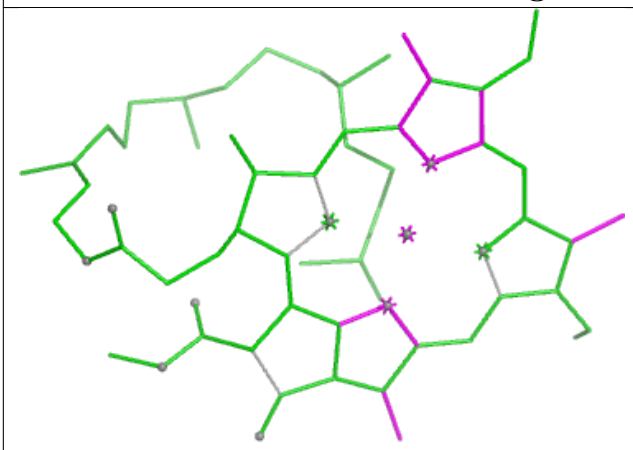


Rings

Ligand CLA a 807



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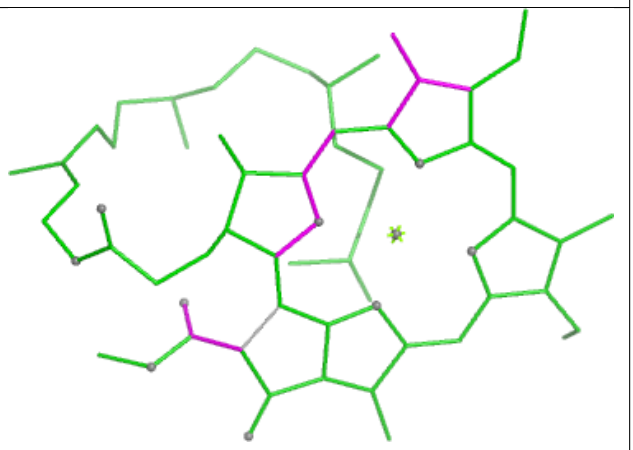
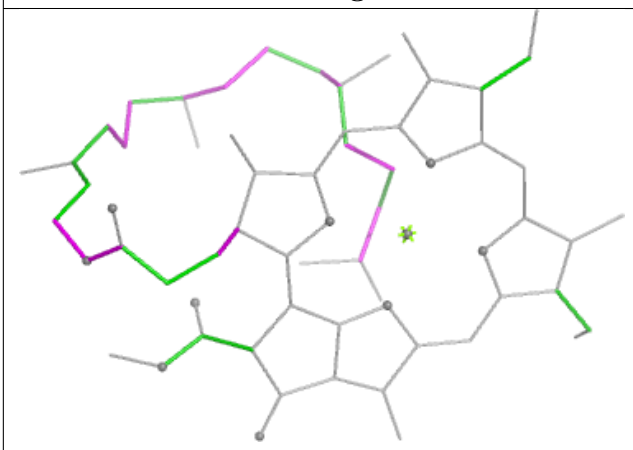
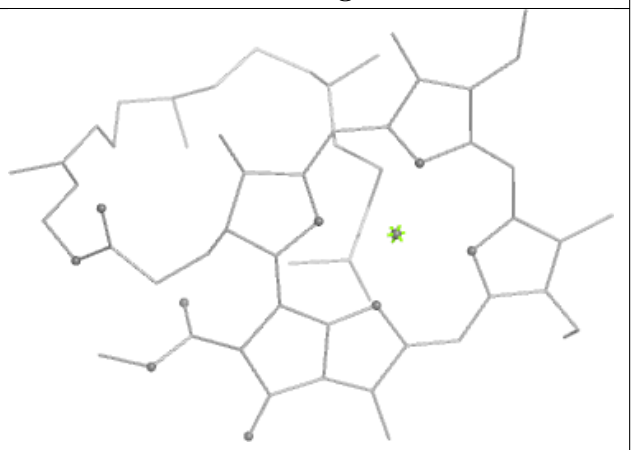


Bond angles

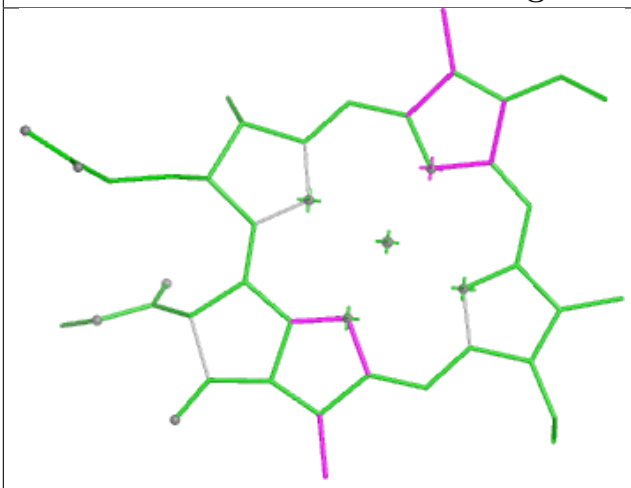


Torsions



Rings

Ligand CLA b 837



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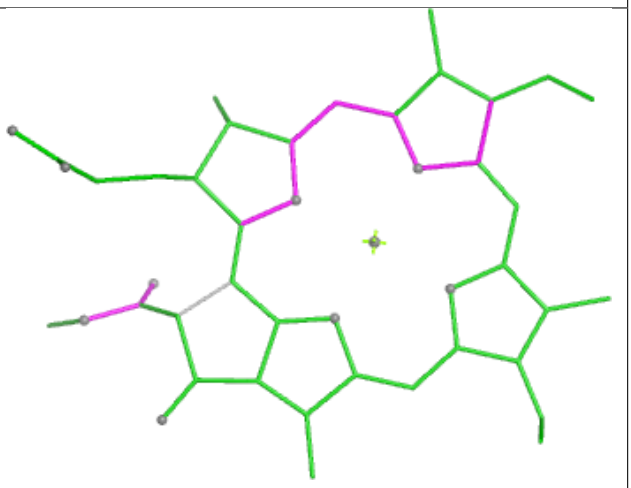
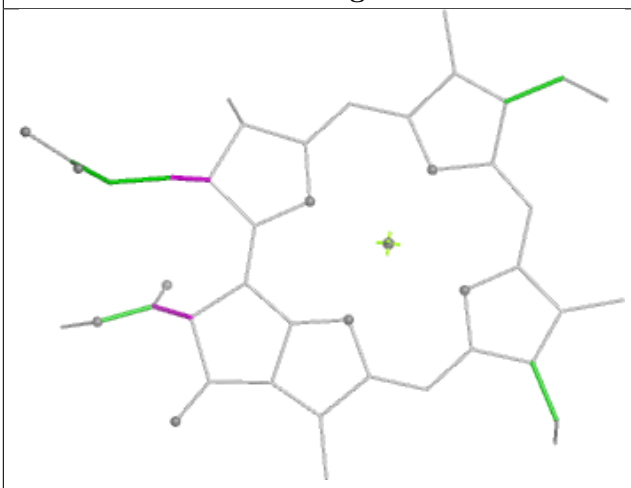


Bond angles



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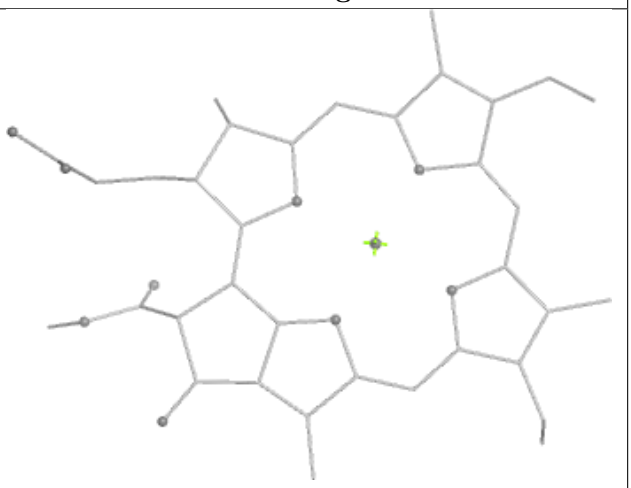
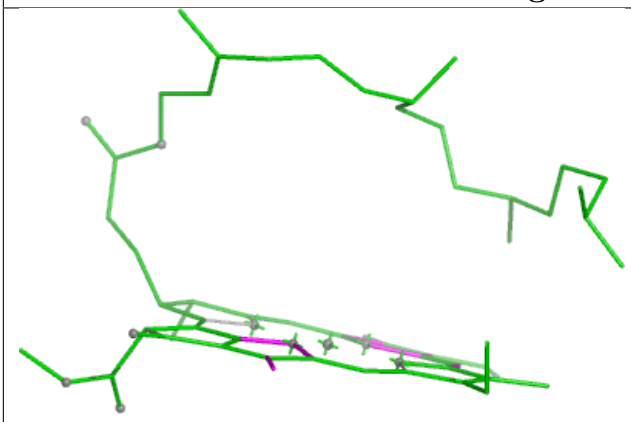


Rings

Ligand CLA a 821



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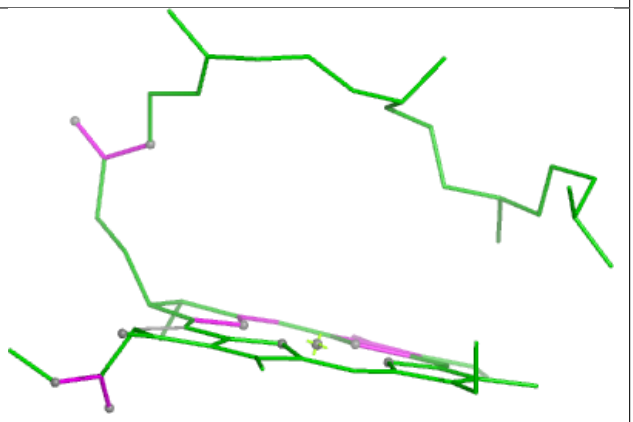
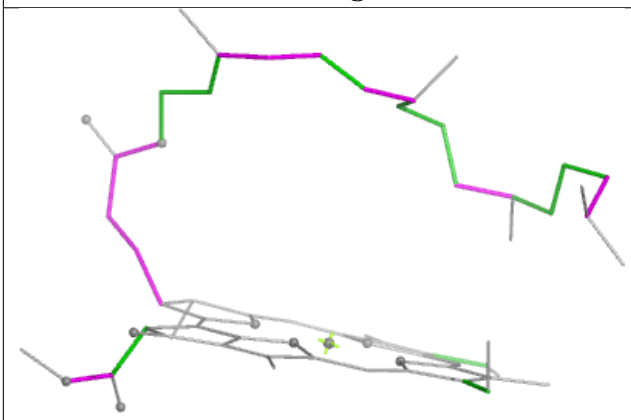


Bond angles

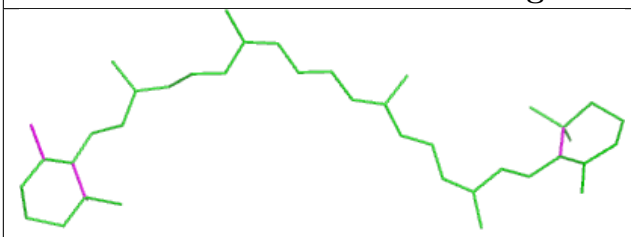


Torsions



Rings

Ligand BCR a 851



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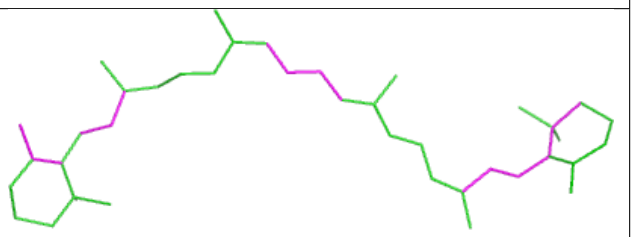
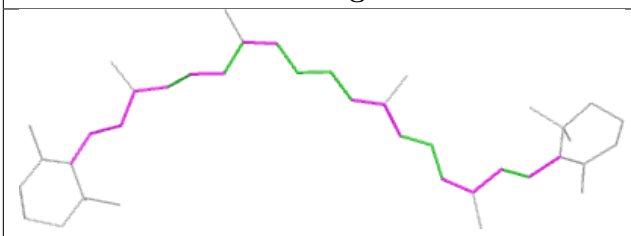
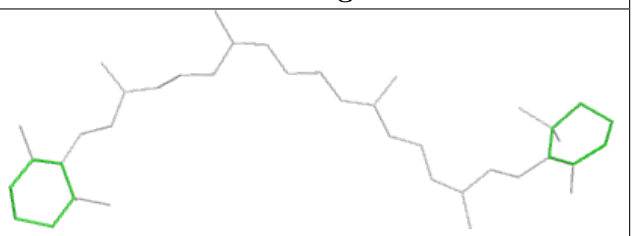


Bond angles

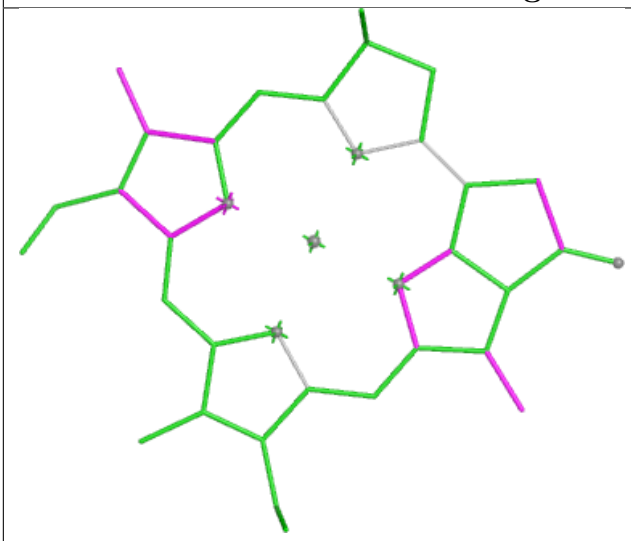


Torsions



Rings

Ligand CLA A 857



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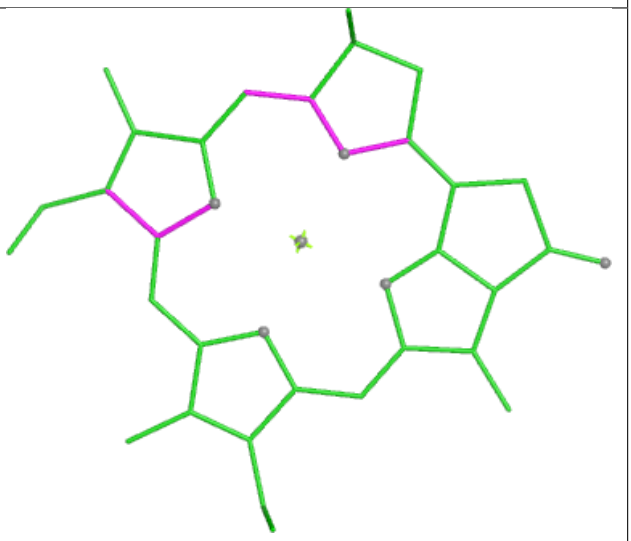
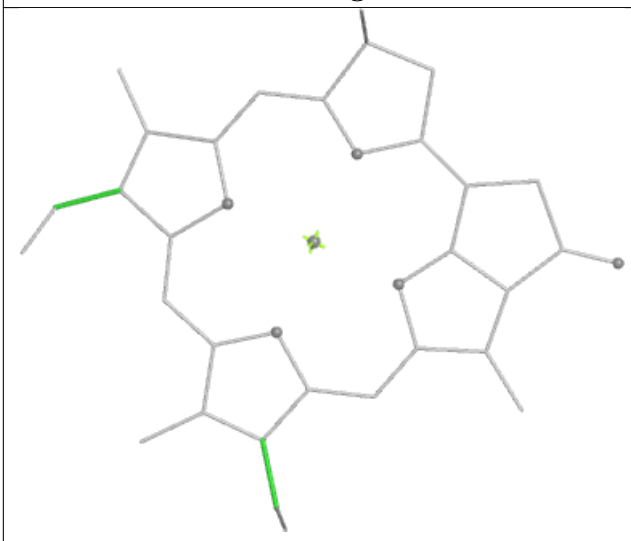


Bond angles



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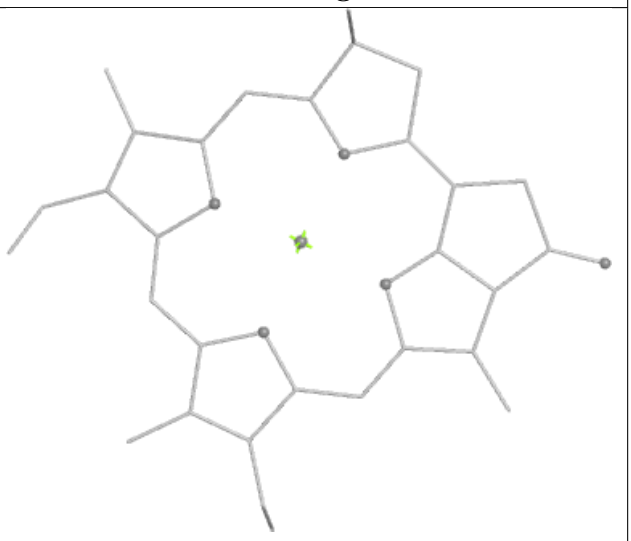
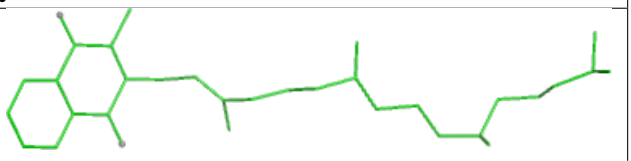


Rings

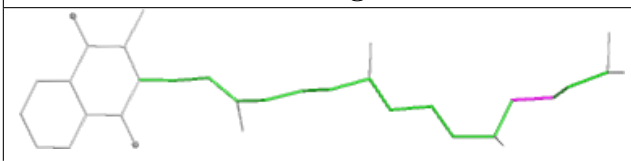
Ligand PQN A 845



Bond lengths



Bond angles



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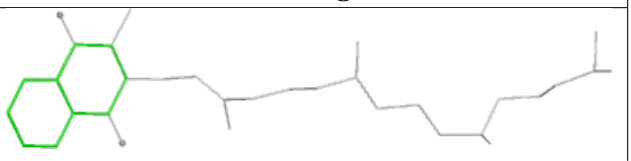
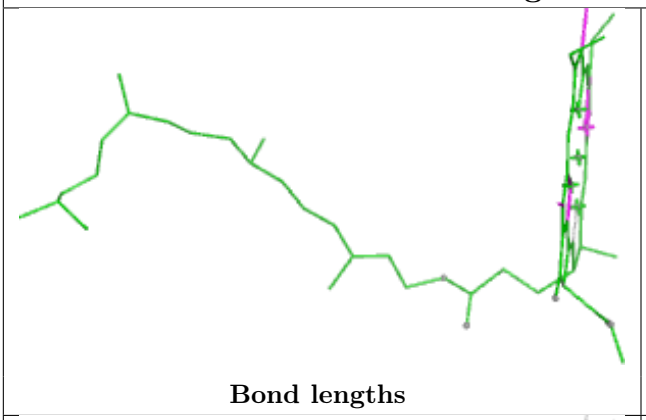


Rings

Ligand CLA B 841



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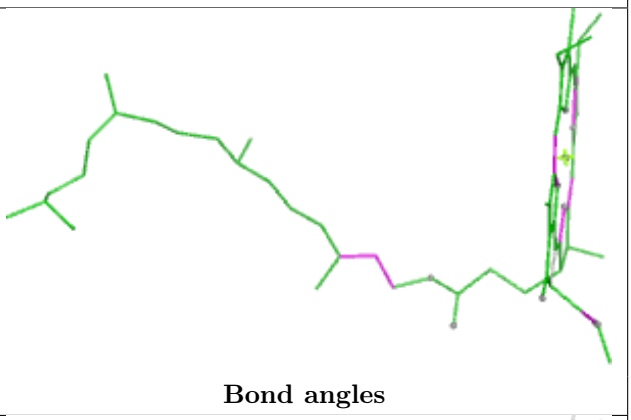
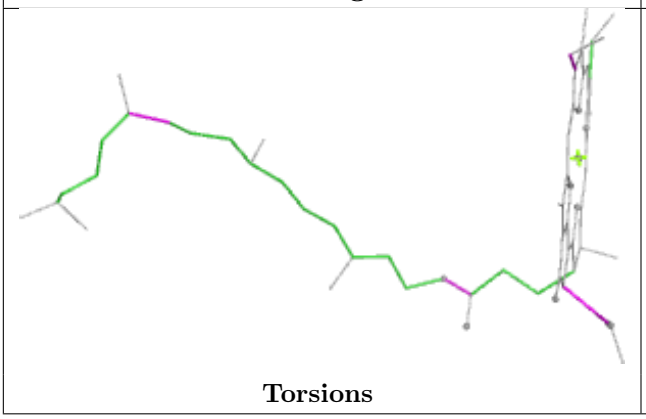


Bond angles



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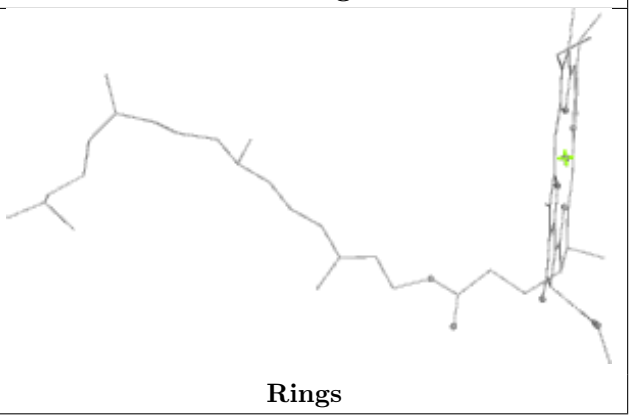
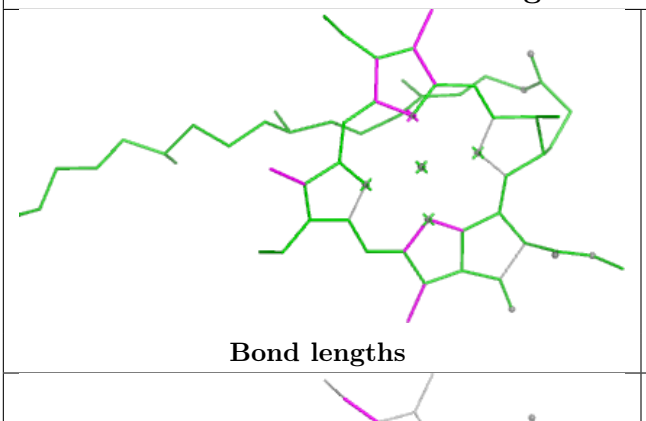


Rings

Ligand CLA A 819



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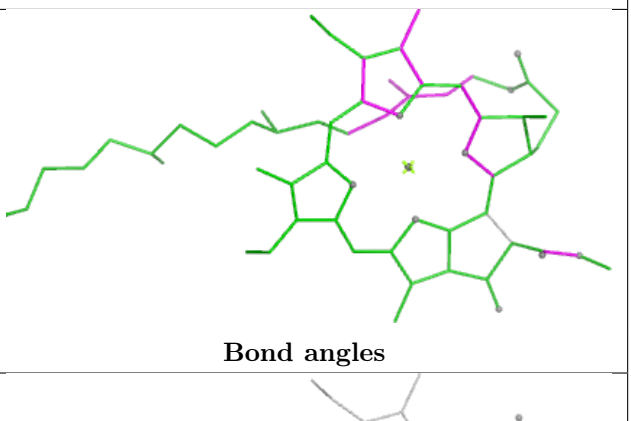
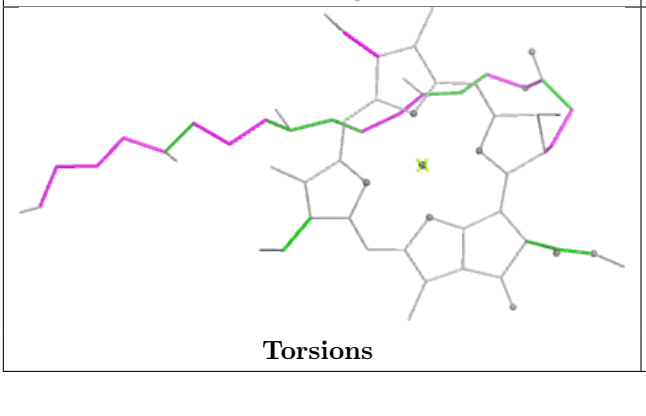


Bond angles



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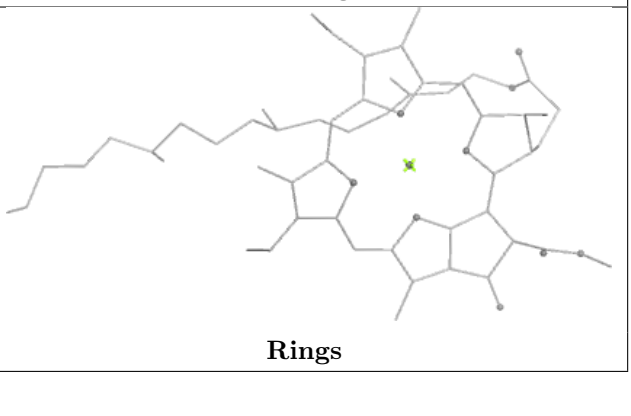
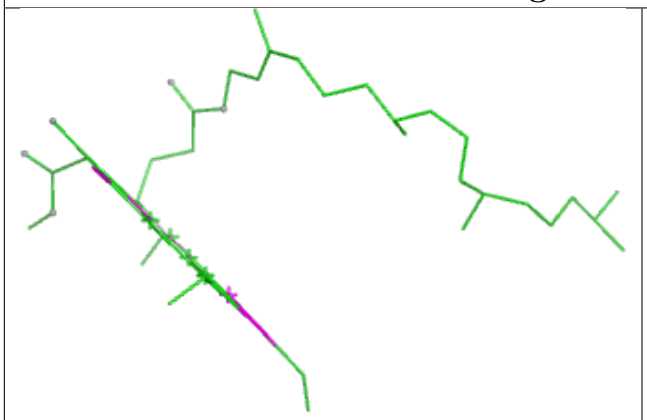


Rings

Ligand CLA 2 815



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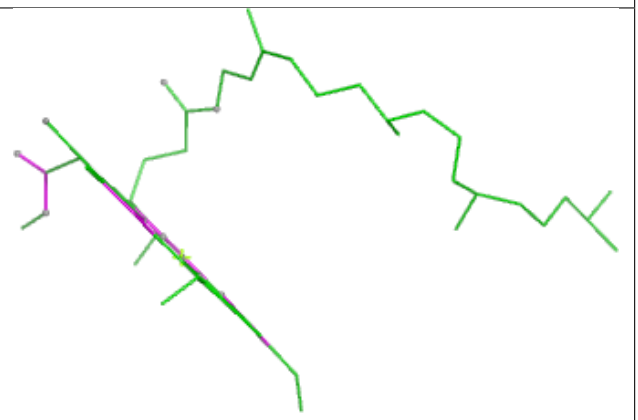
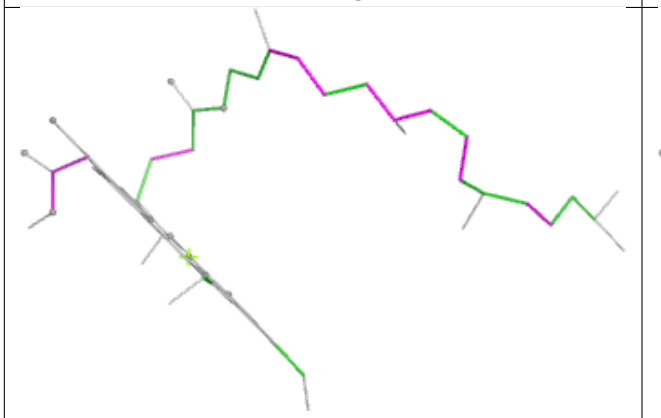


Bond angles

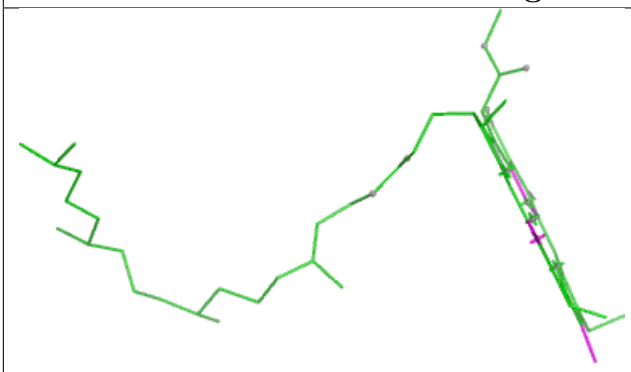


Torsions

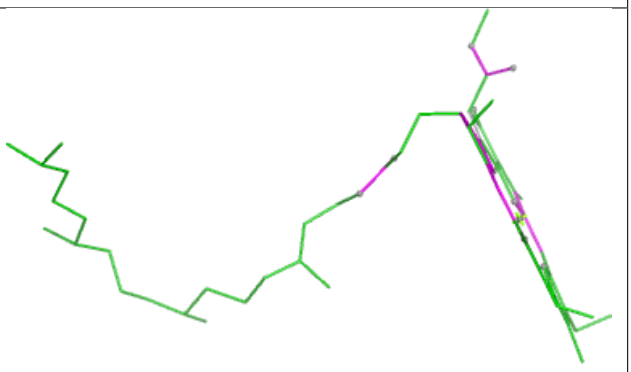


Rings

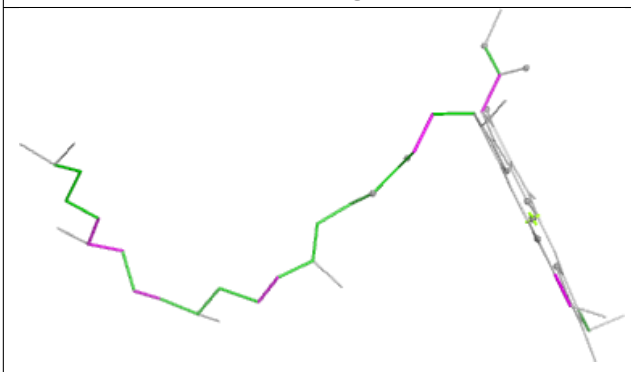
Ligand CLA B 840



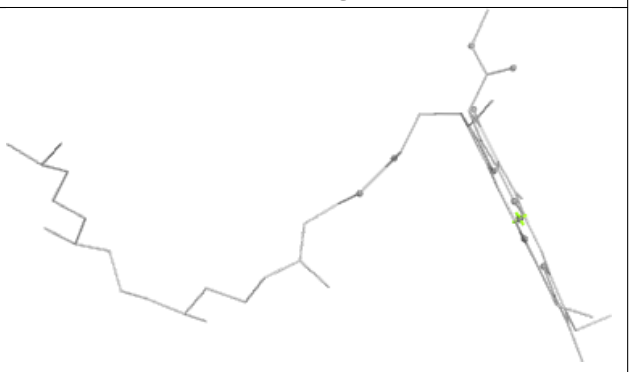
Bond lengths



Bond angles

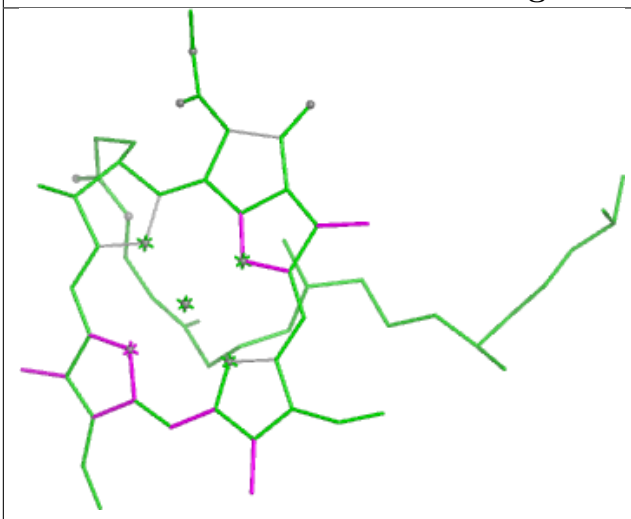


Torsions

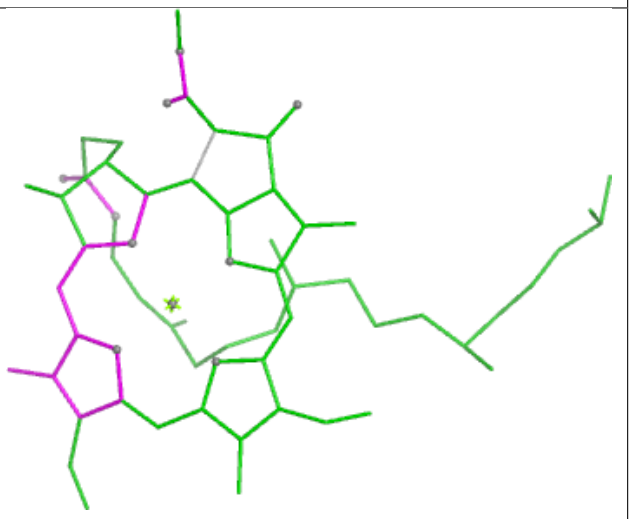


Rings

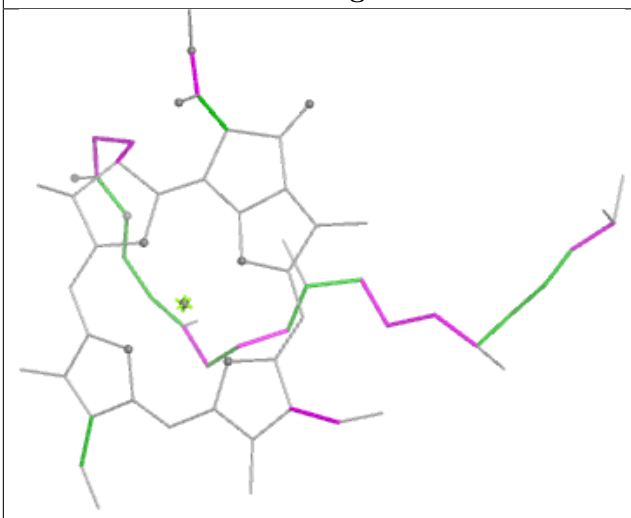
Ligand CLA 2 828



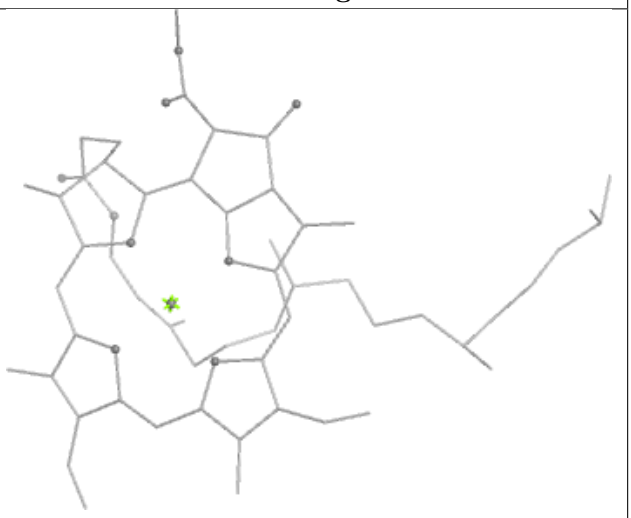
Bond lengths



Bond angles

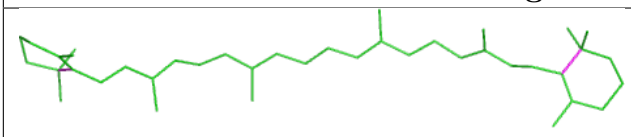


Torsions



Rings

Ligand BCR b 852



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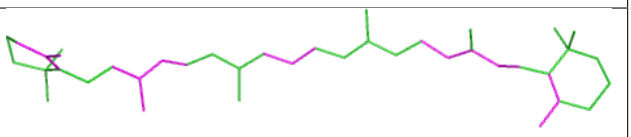

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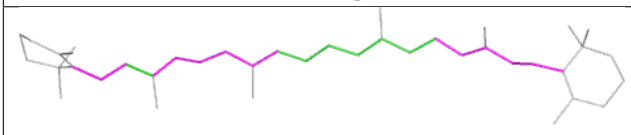

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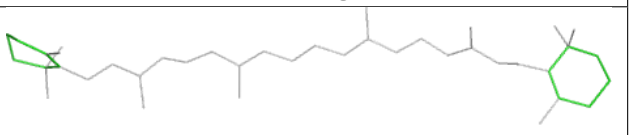
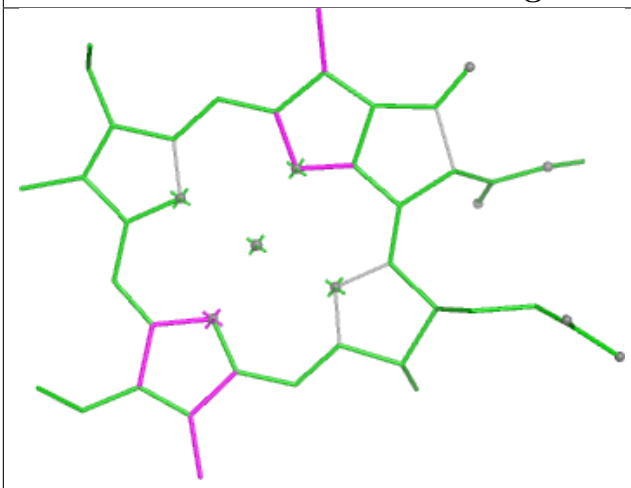


Rings

Ligand CLA B 836



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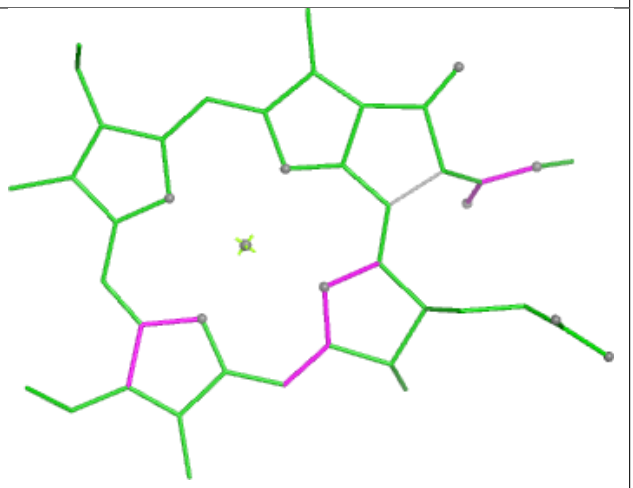
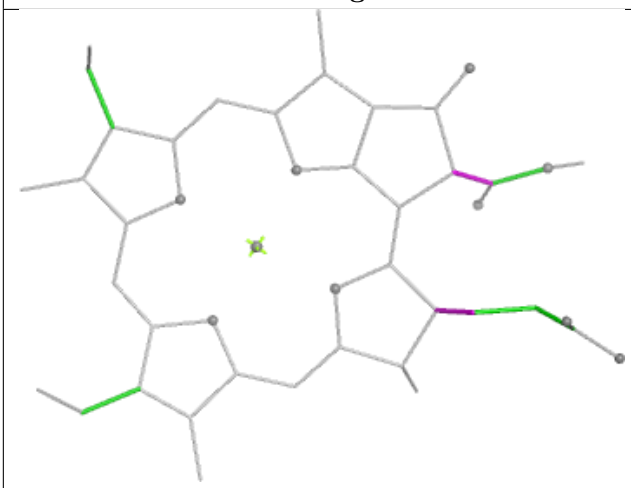


Bond angles



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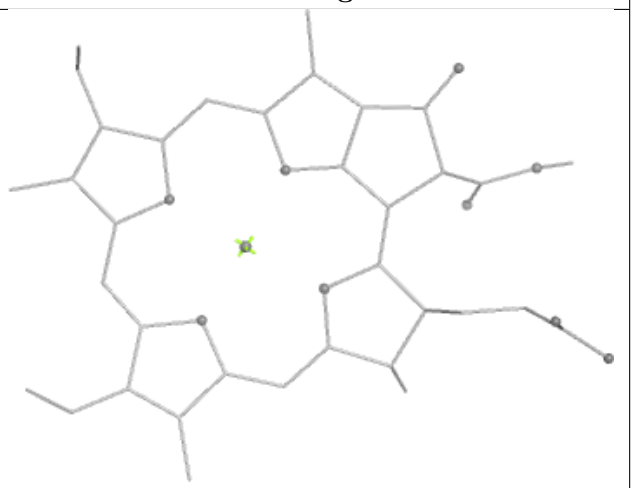
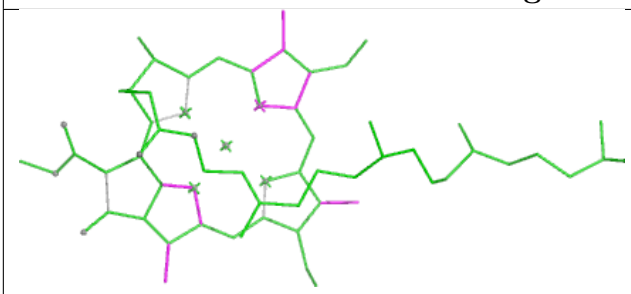


Rings

Ligand CLA A 839



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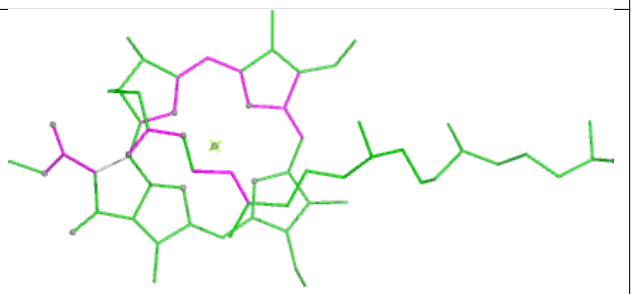
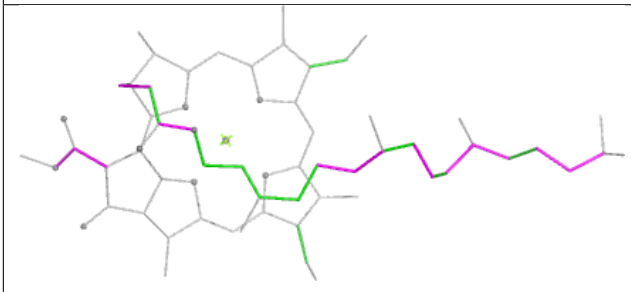


Bond angles



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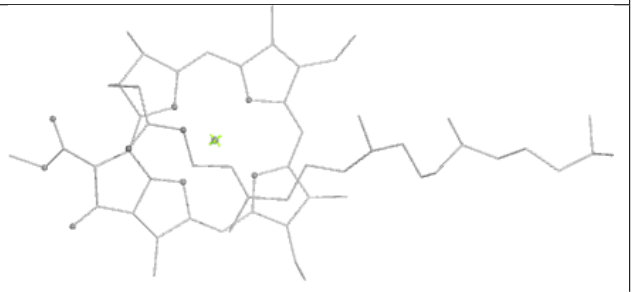
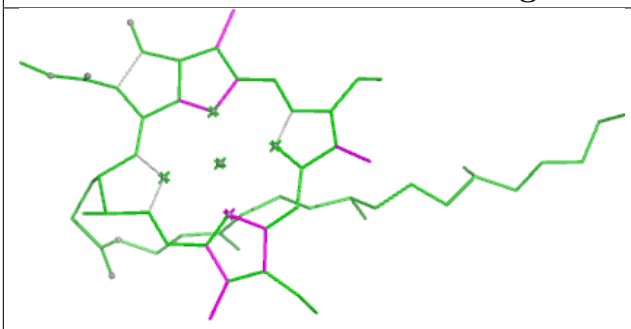
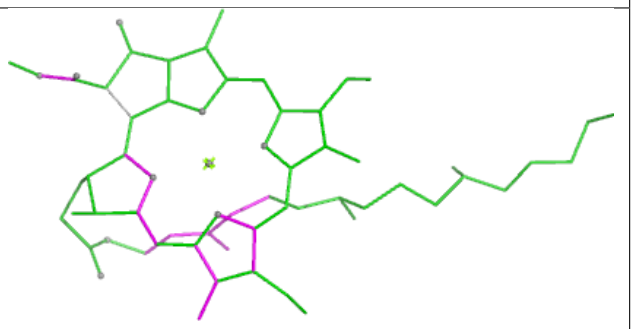
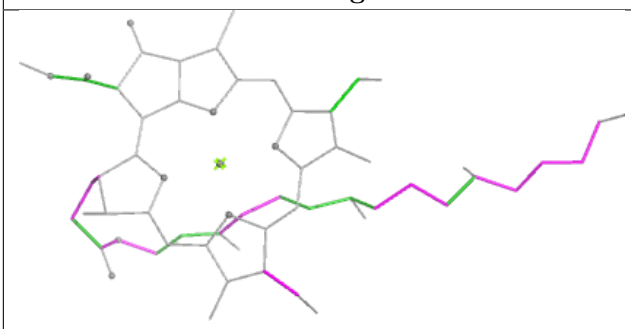
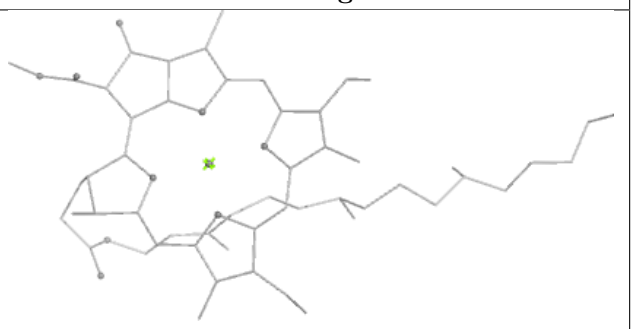
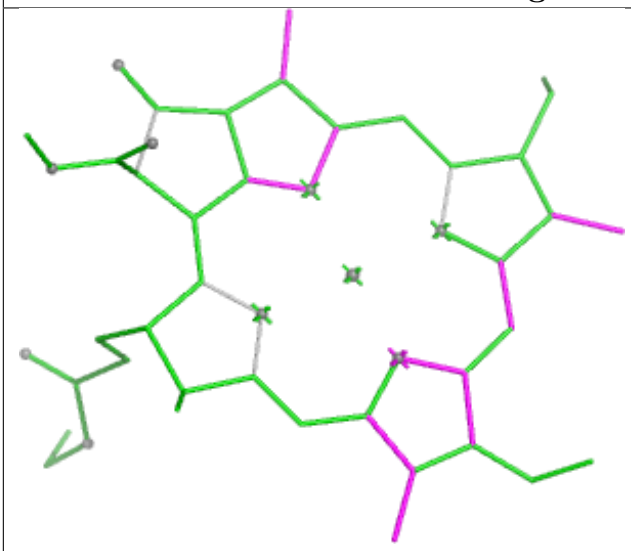


Rings

Ligand CLA 1 1620	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 2 840



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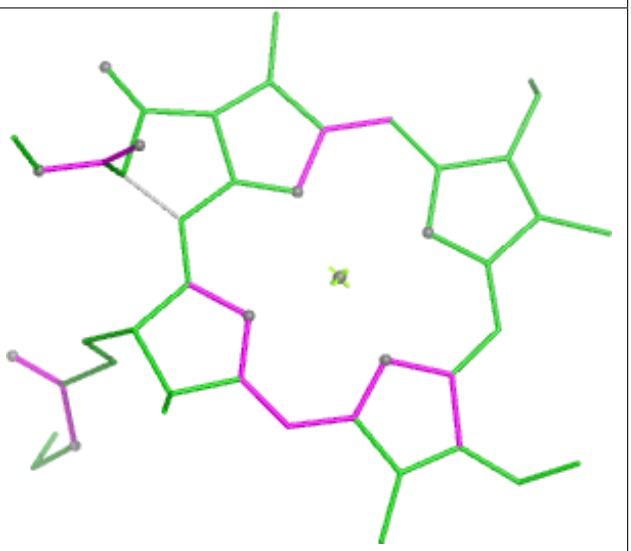
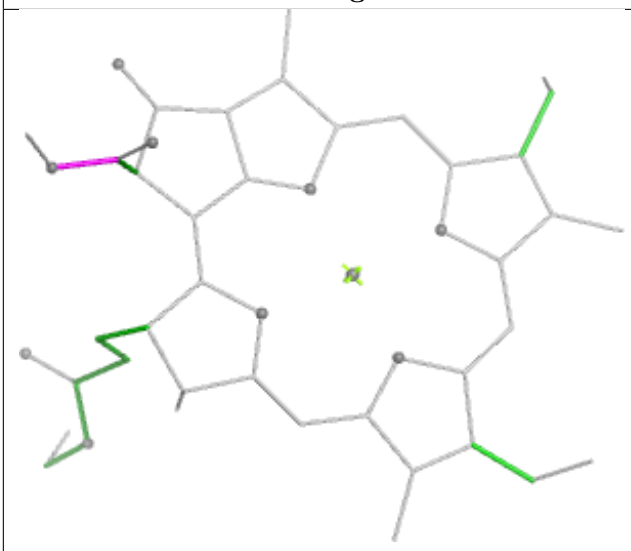


Bond angles



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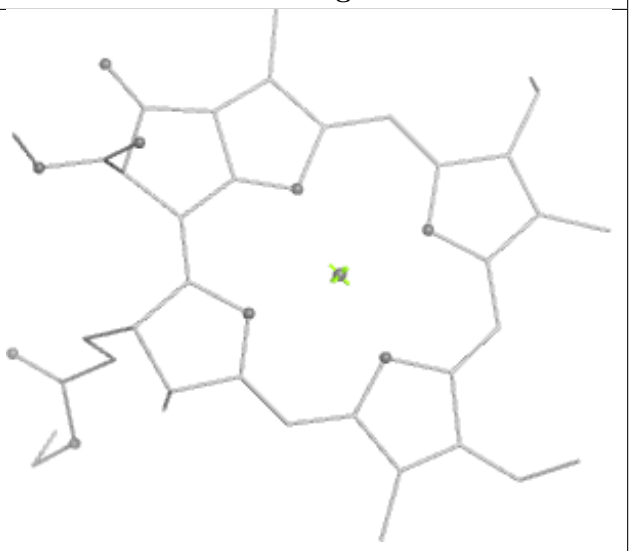
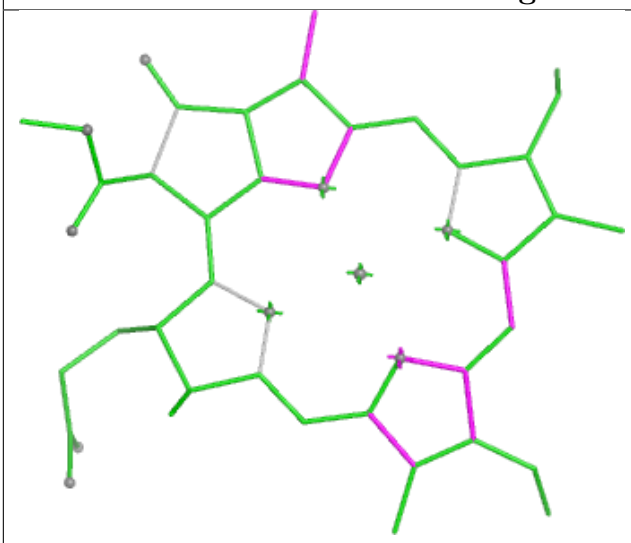


Rings

Ligand CLA x 1701



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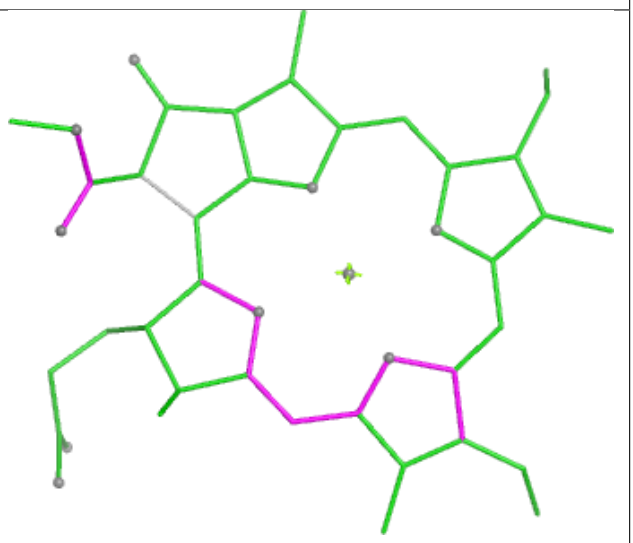

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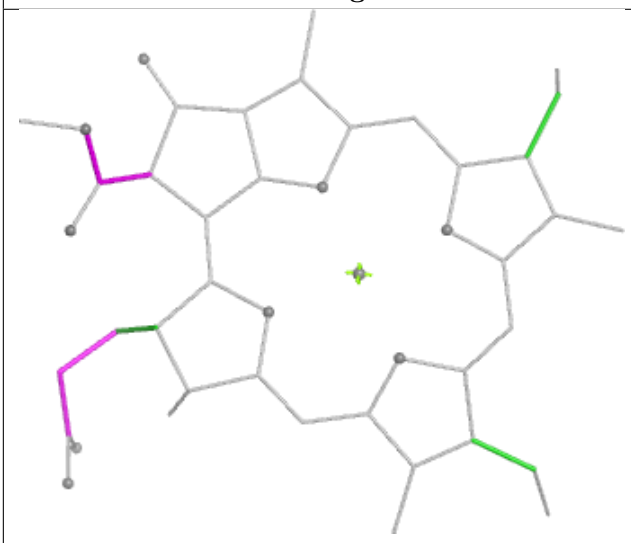

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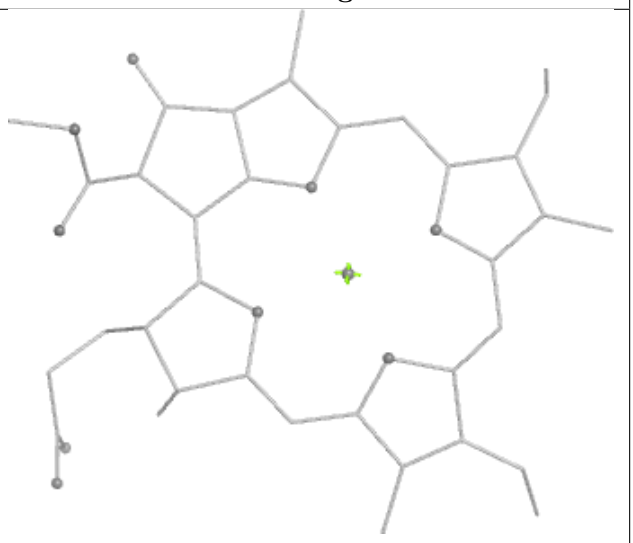
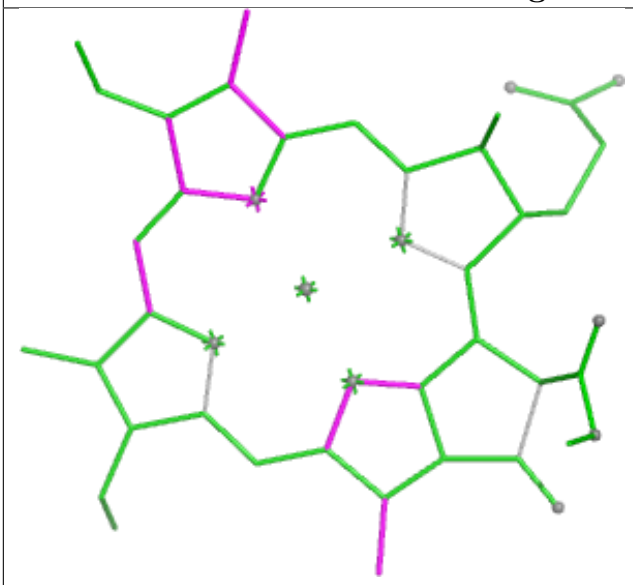


Rings

Ligand CLA a 823



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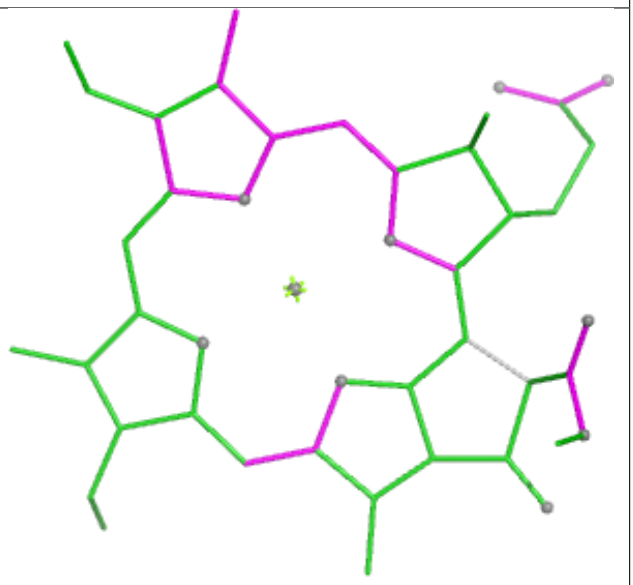

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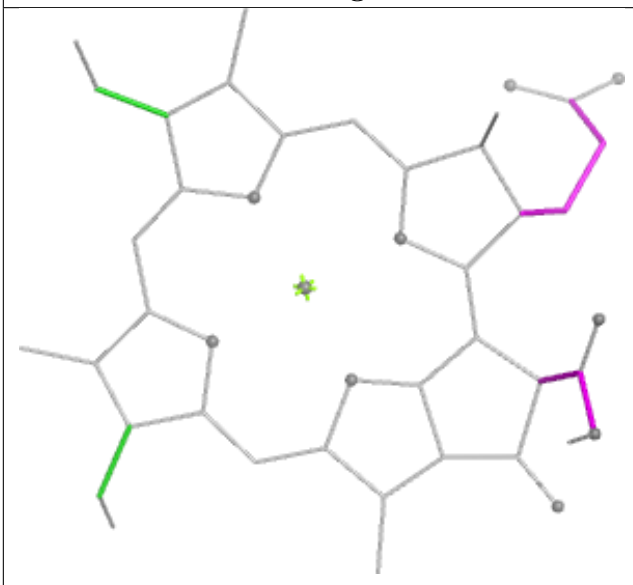

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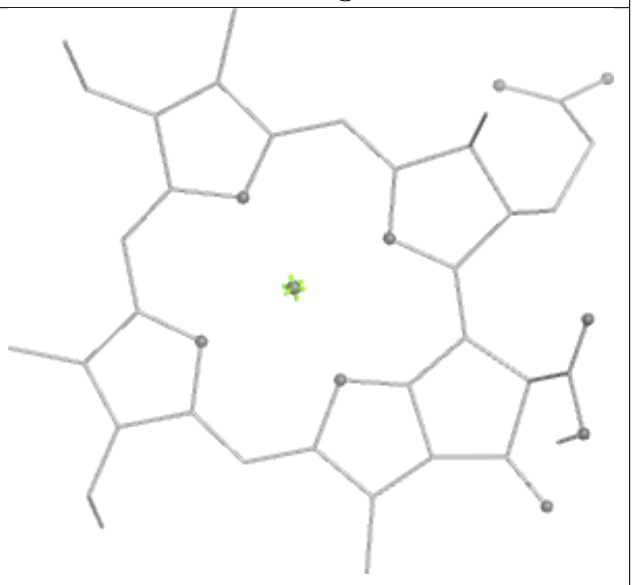
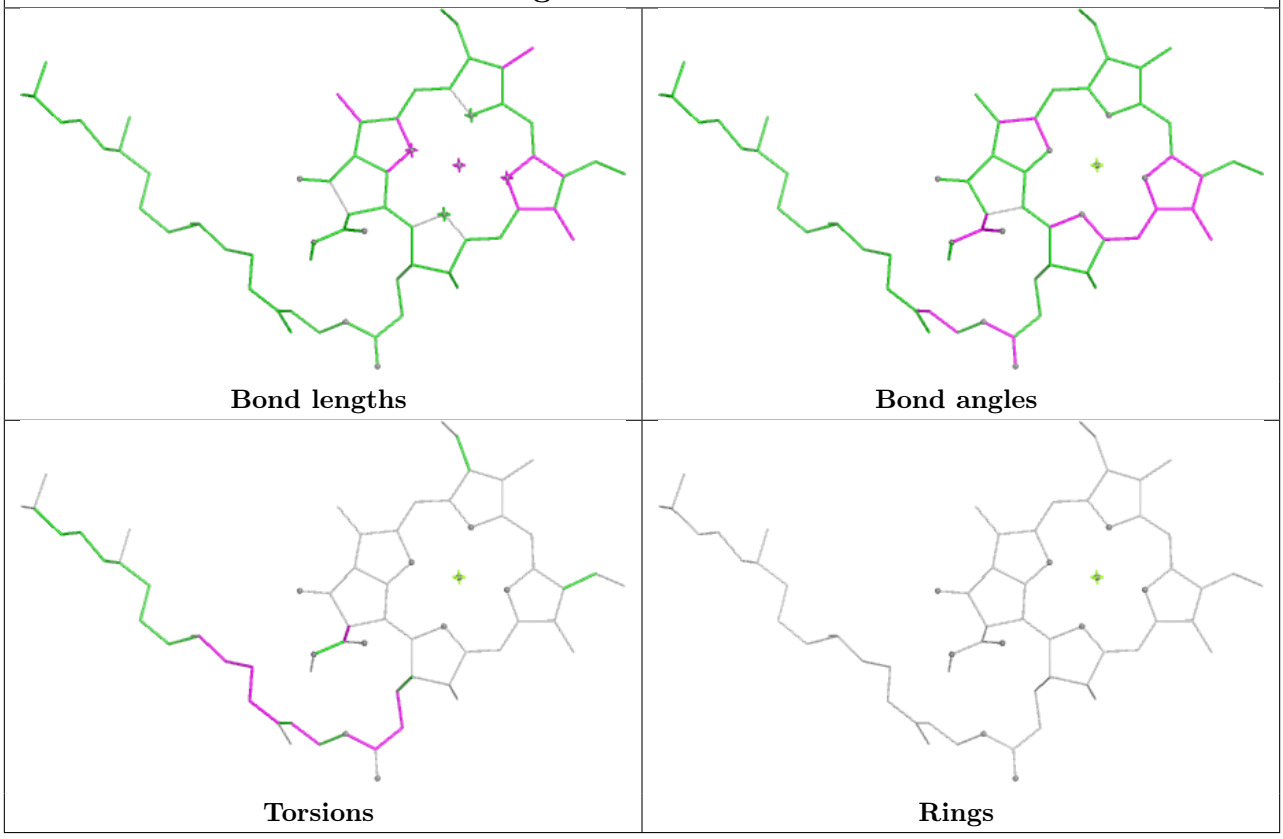
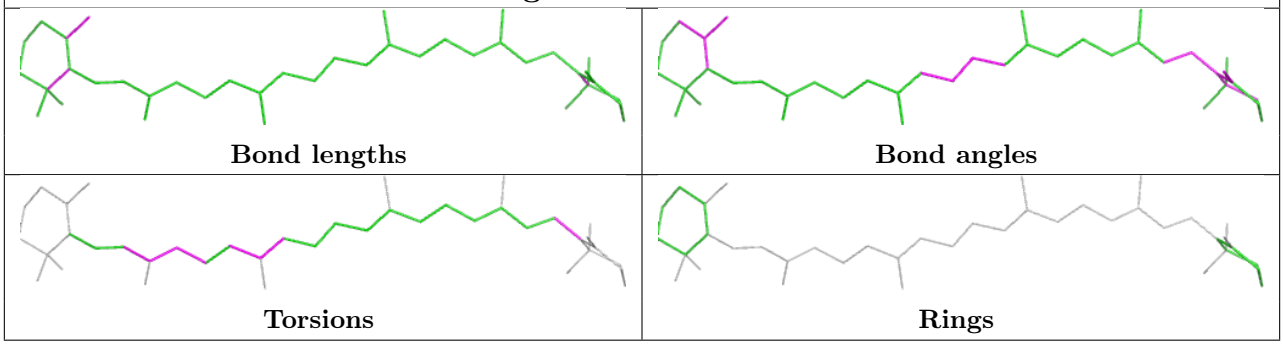


Rings

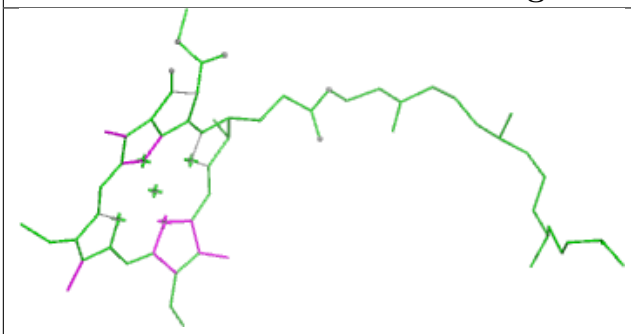
Ligand CLA l 206



Ligand BCR A 850



Ligand CLA b 802



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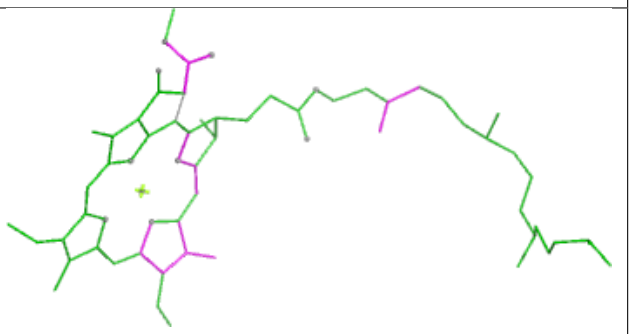
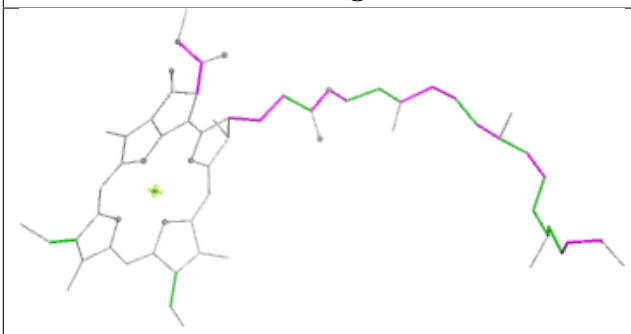


Bond angles



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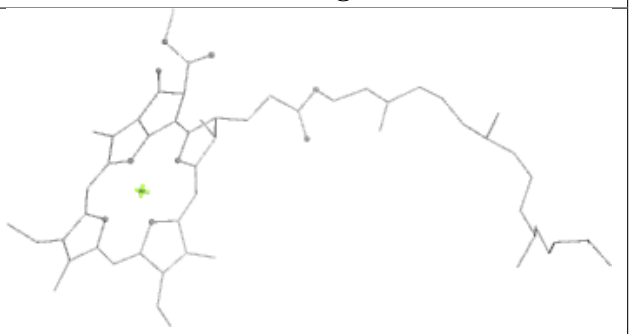
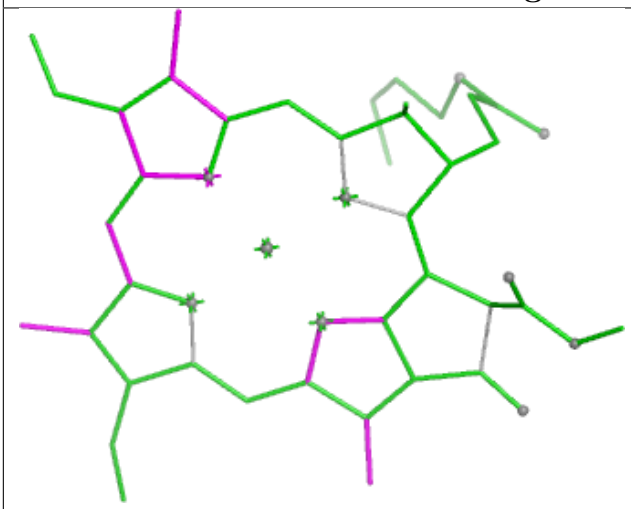


Rings

Ligand CLA B 831



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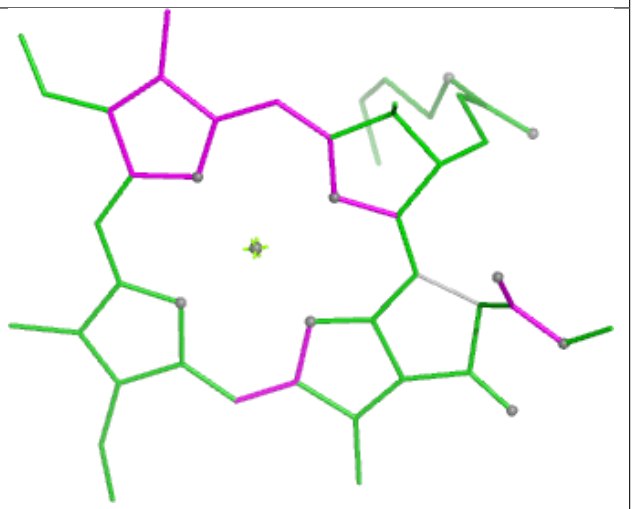

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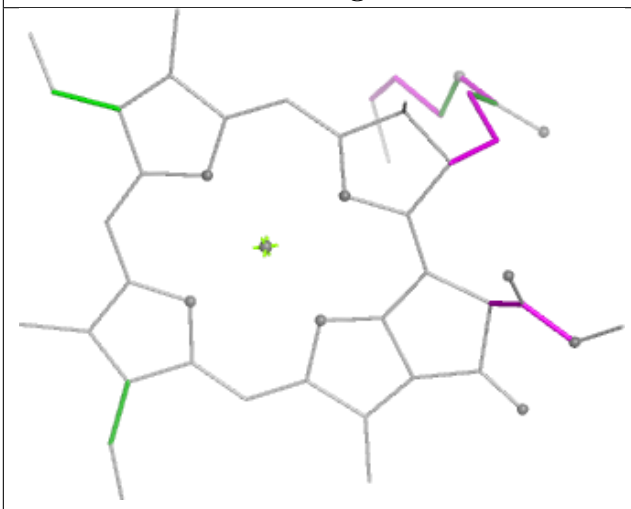

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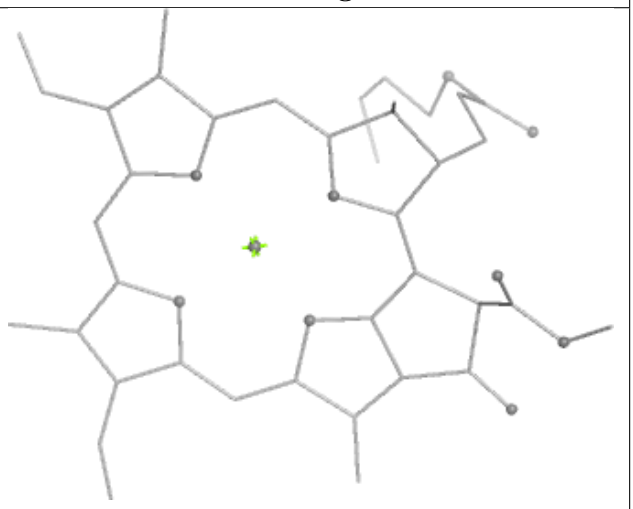
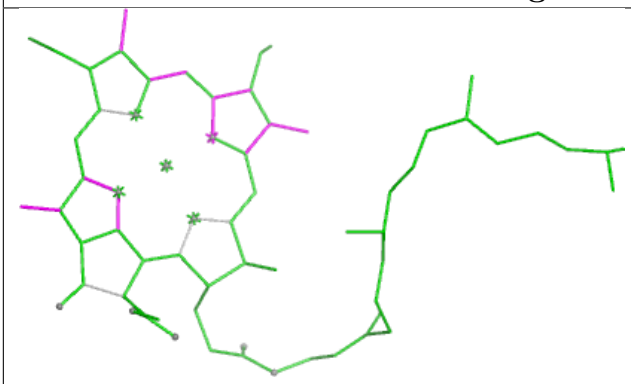


Rings

Ligand CLA a 814



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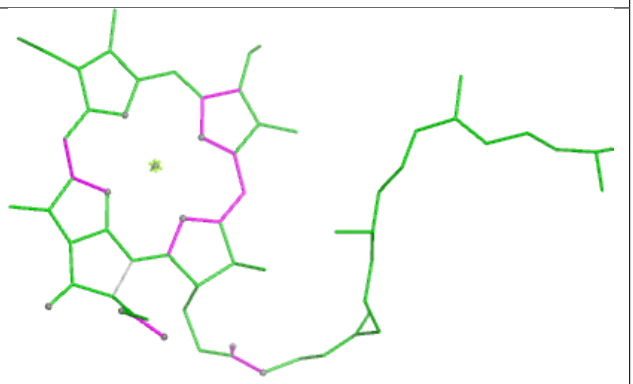
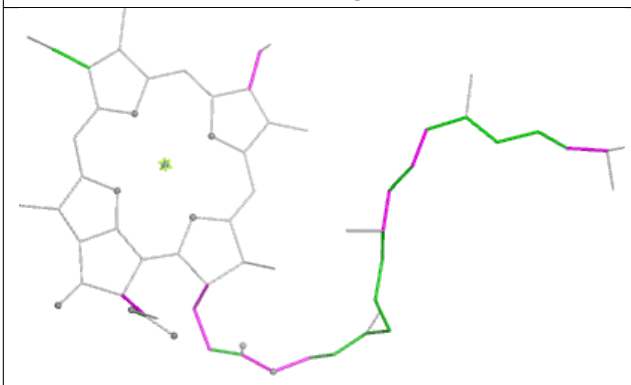


Bond angles



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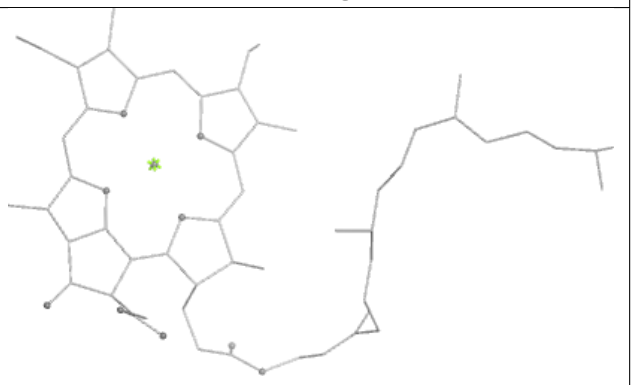
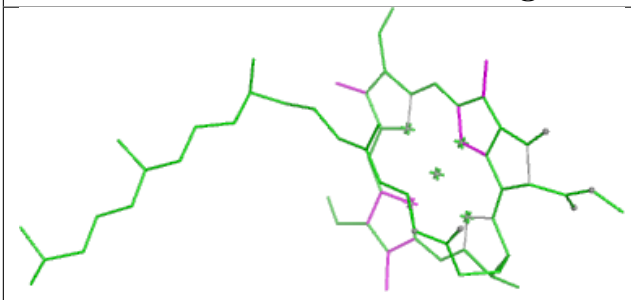


Rings

Ligand CLA 1 1643



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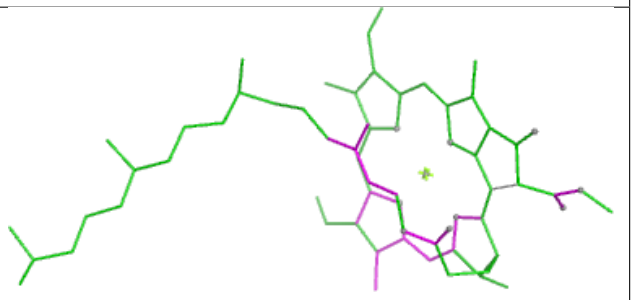
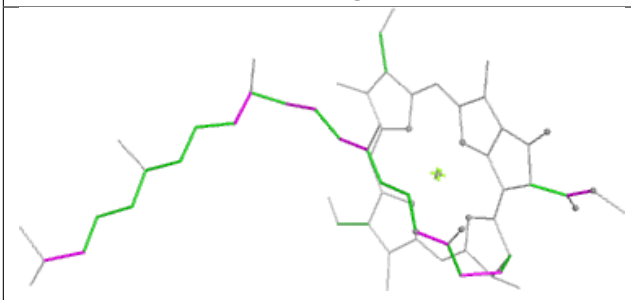


Bond angles



Torsions

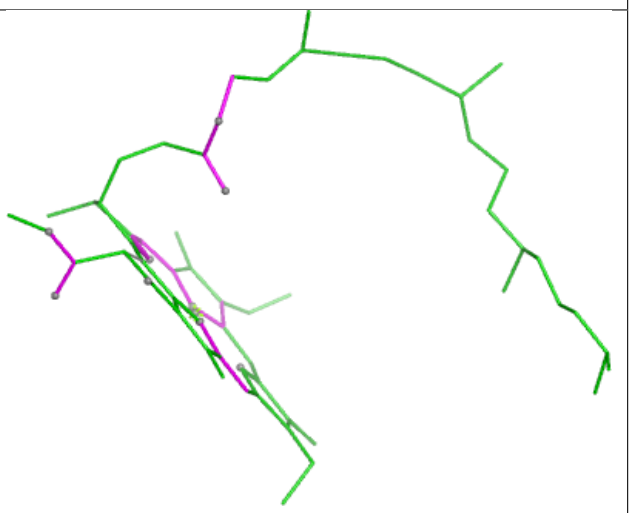


Rings

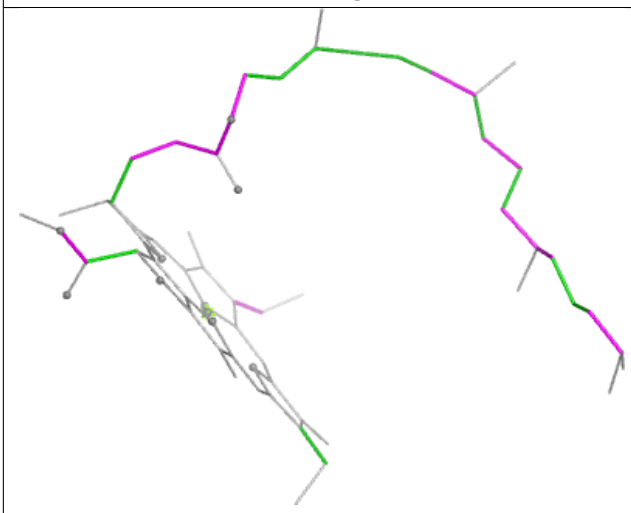
Ligand CLA B 819



Bond lengths



Bond angles

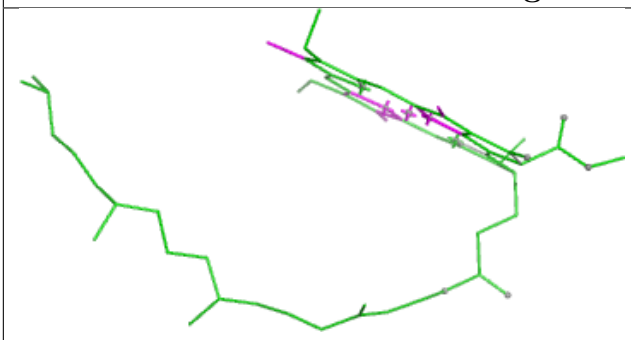


Torsions

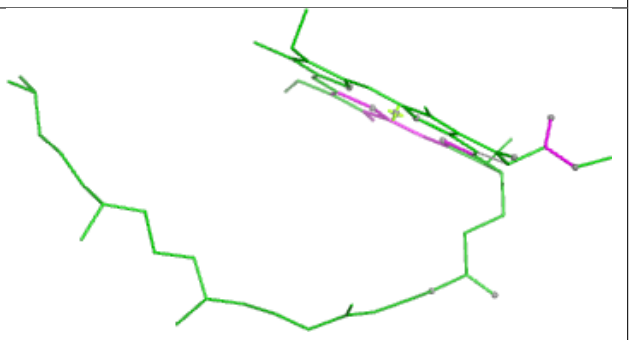


Rings

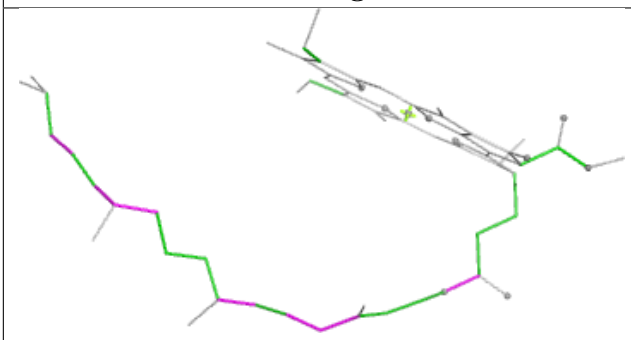
Ligand CLA A 833



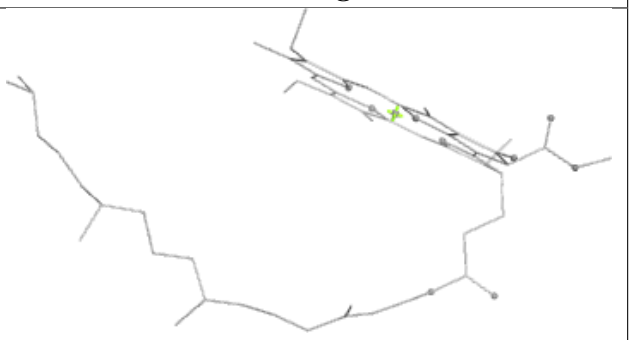
Bond lengths



Bond angles

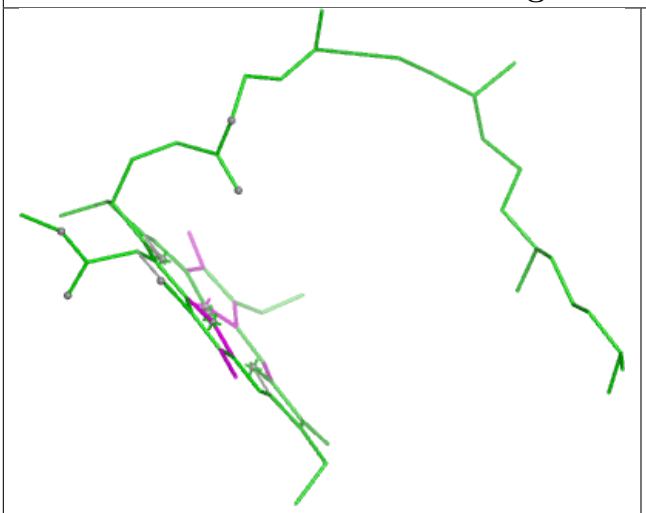


Torsions



Rings

Ligand CLA b 820



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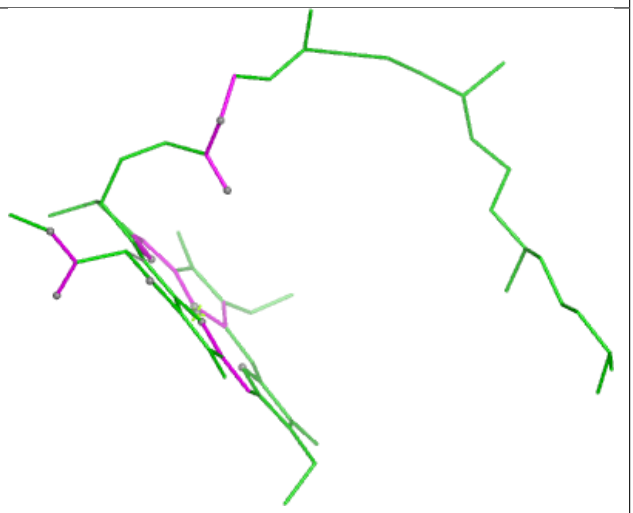
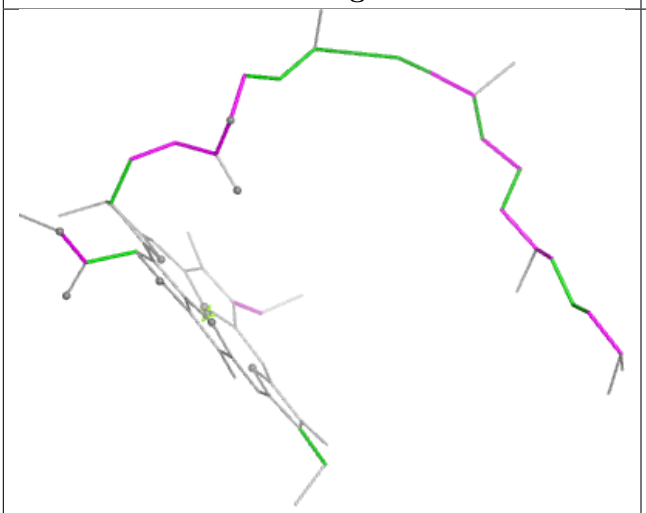


Bond angles

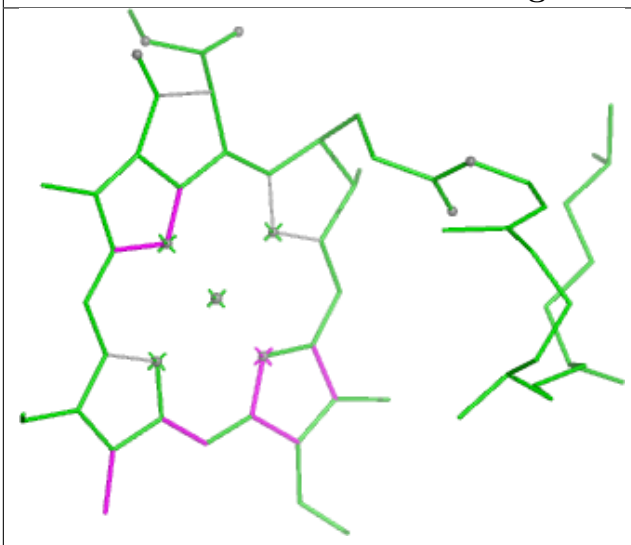


Torsions

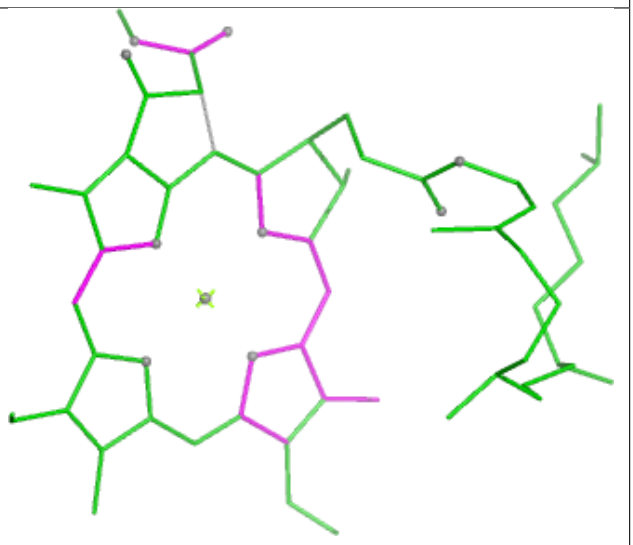


Rings

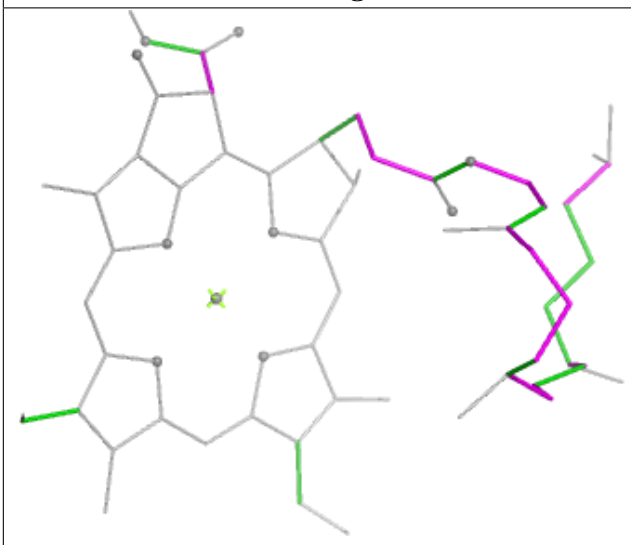
Ligand CLA a 816



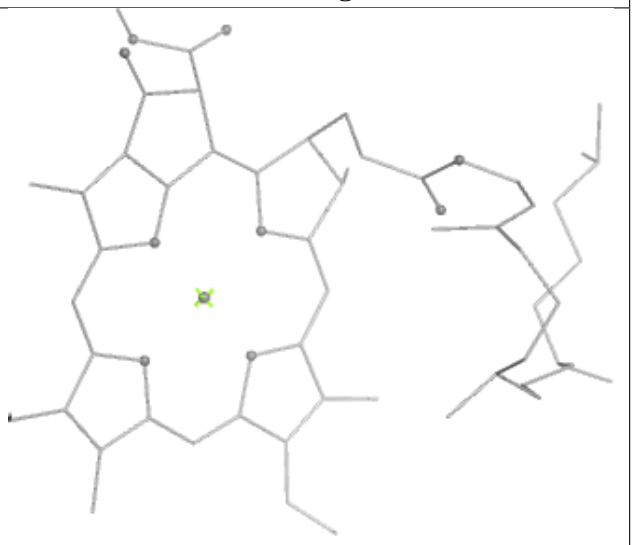
Bond lengths



Bond angles

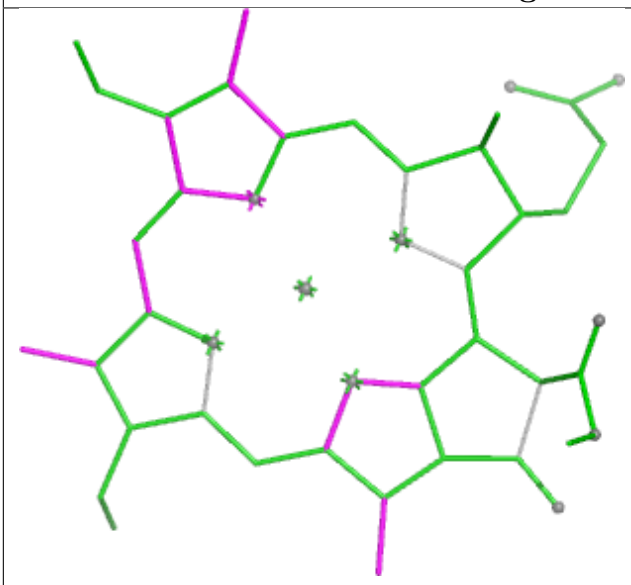


Torsions



Rings

Ligand CLA 1 1624



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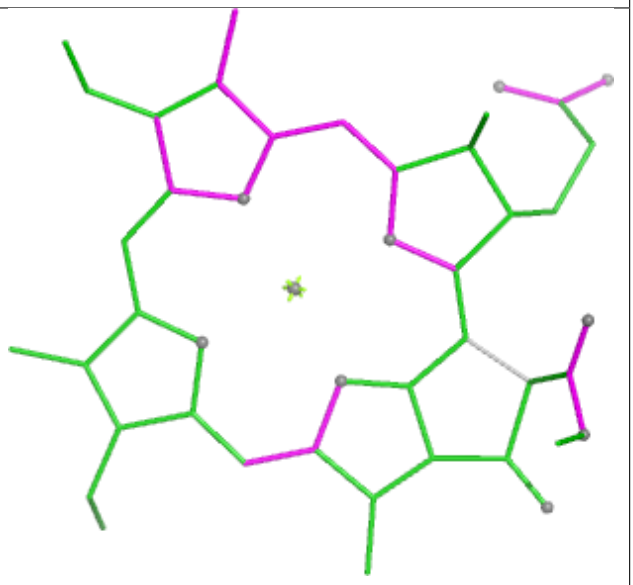

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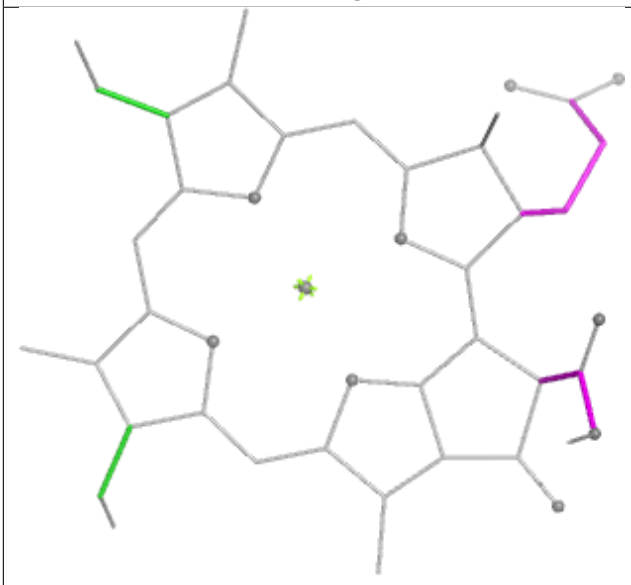

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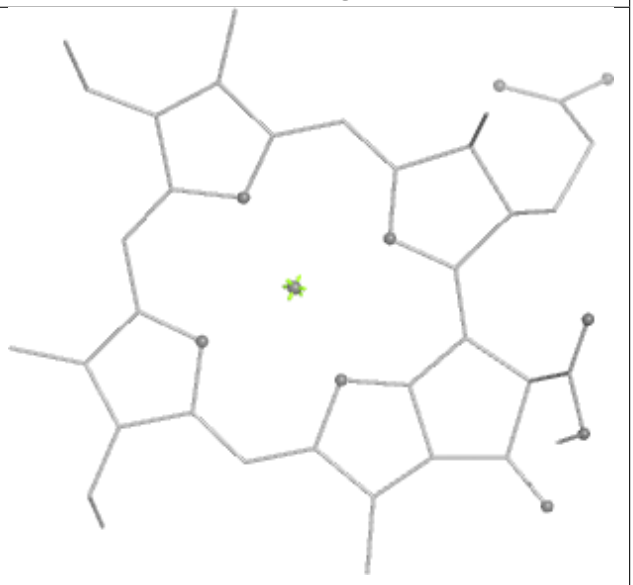
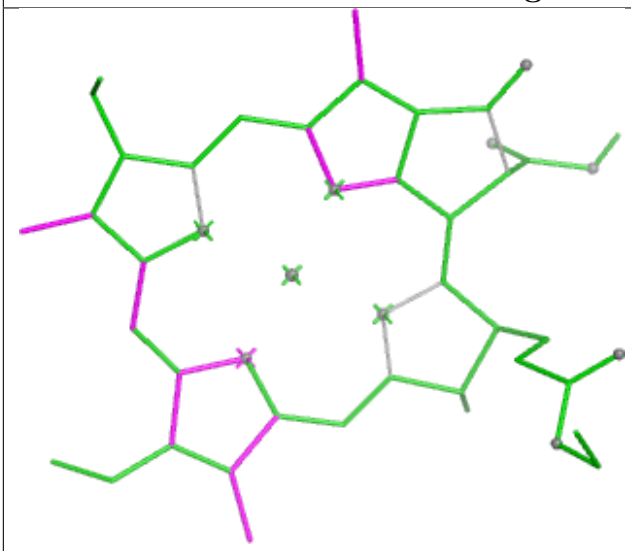


Rings

Ligand CLA B 839



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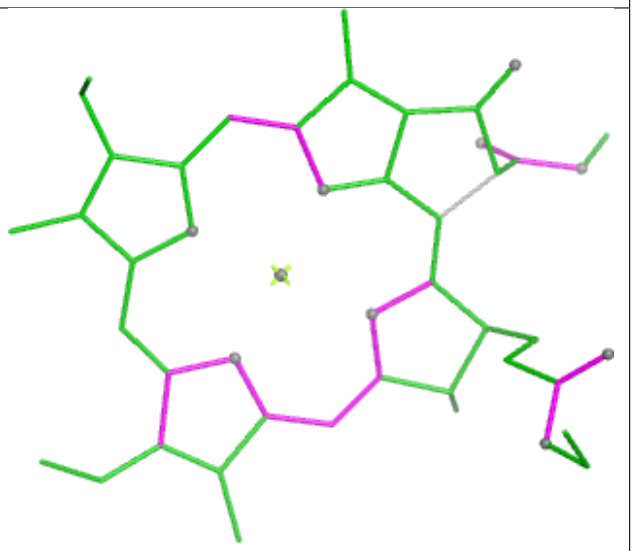
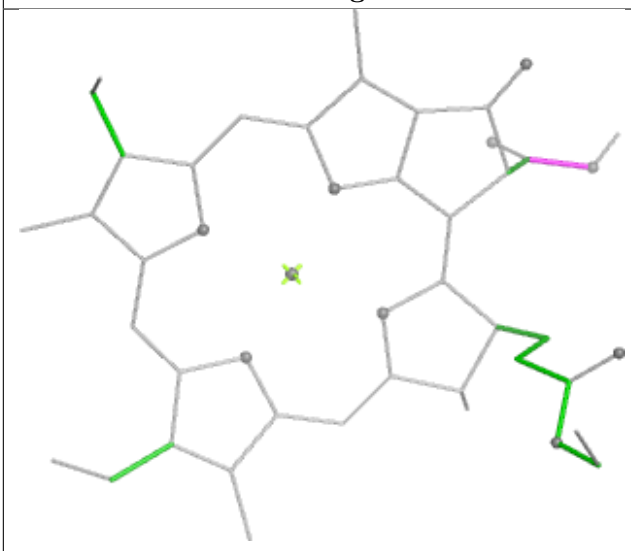


Bond angles



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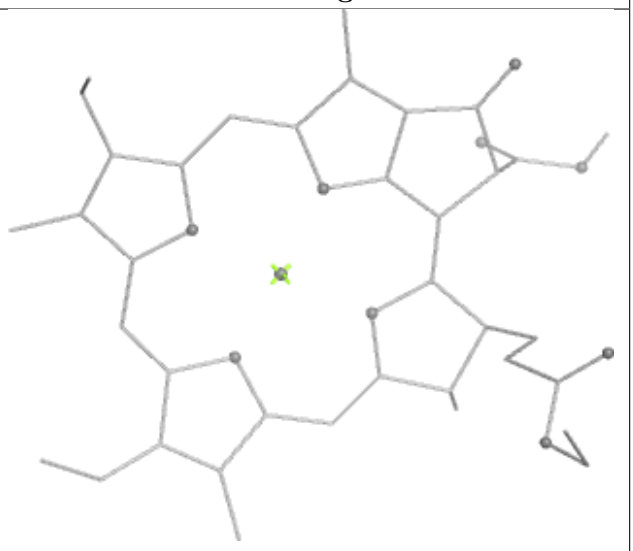
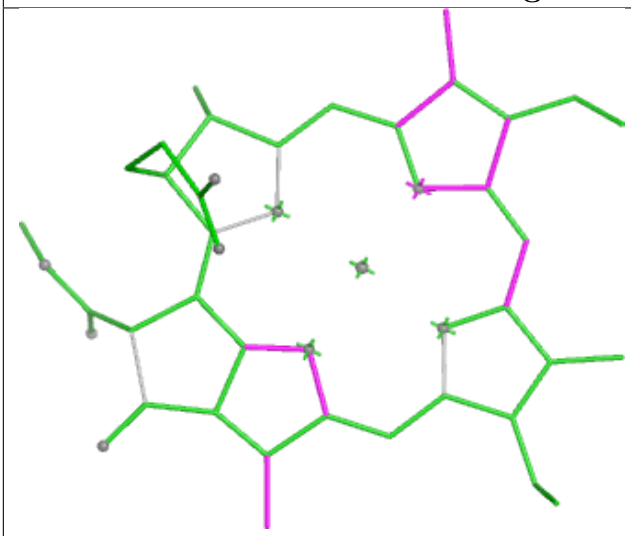


Rings

Ligand CLA A 837



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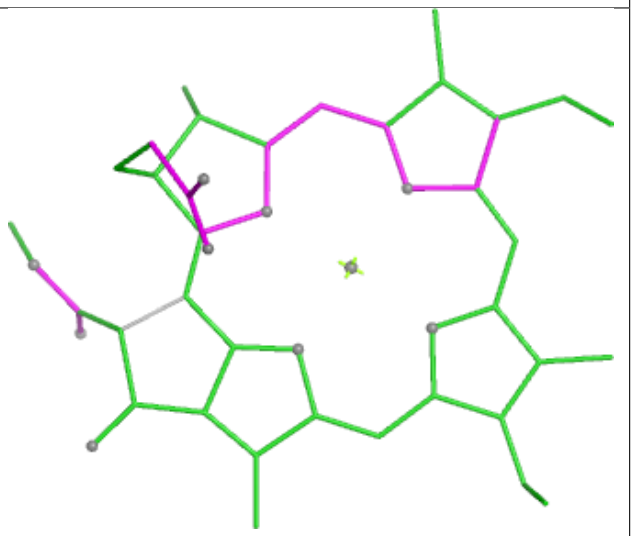
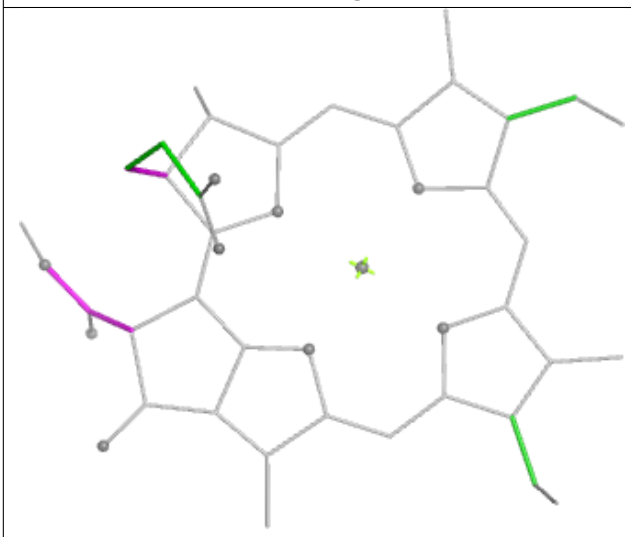


Bond angles



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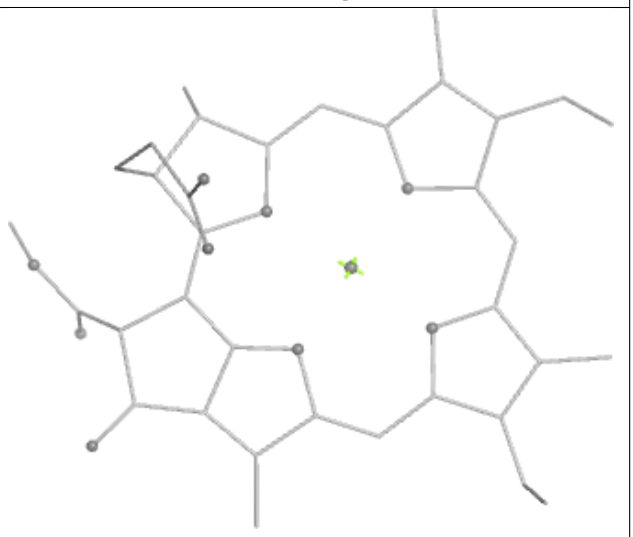
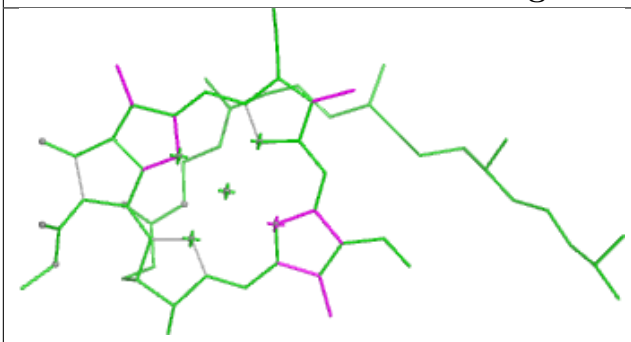


Rings

Ligand CLA a 841



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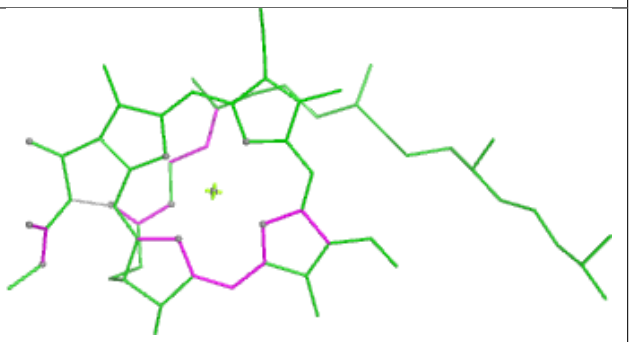
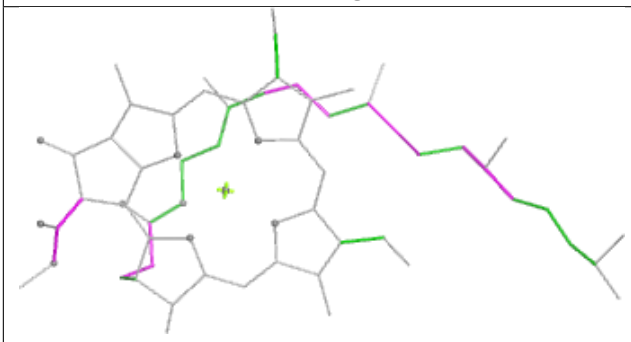


Bond angles



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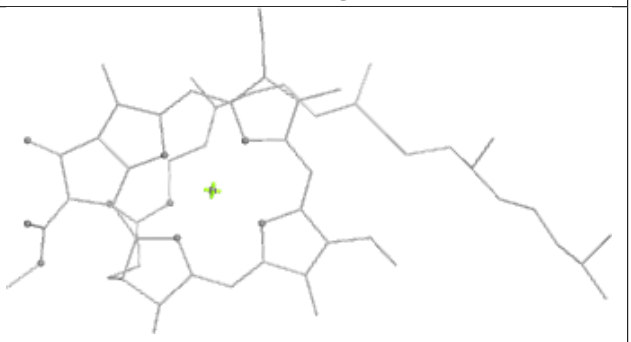
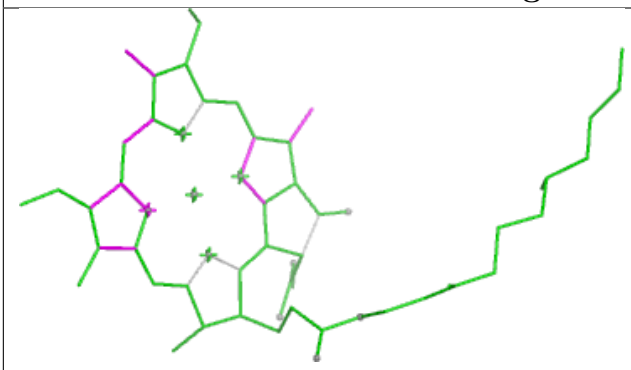


Rings

Ligand CLA K 103



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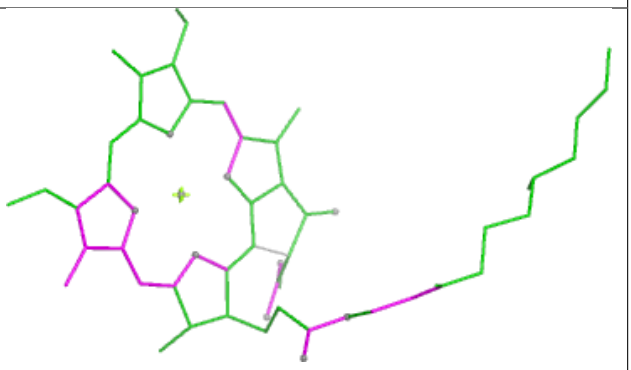
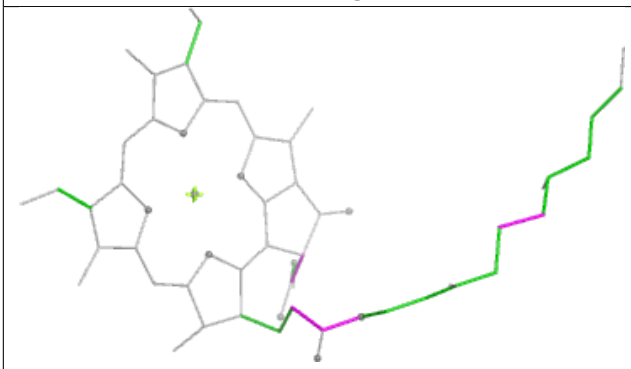


Bond angles

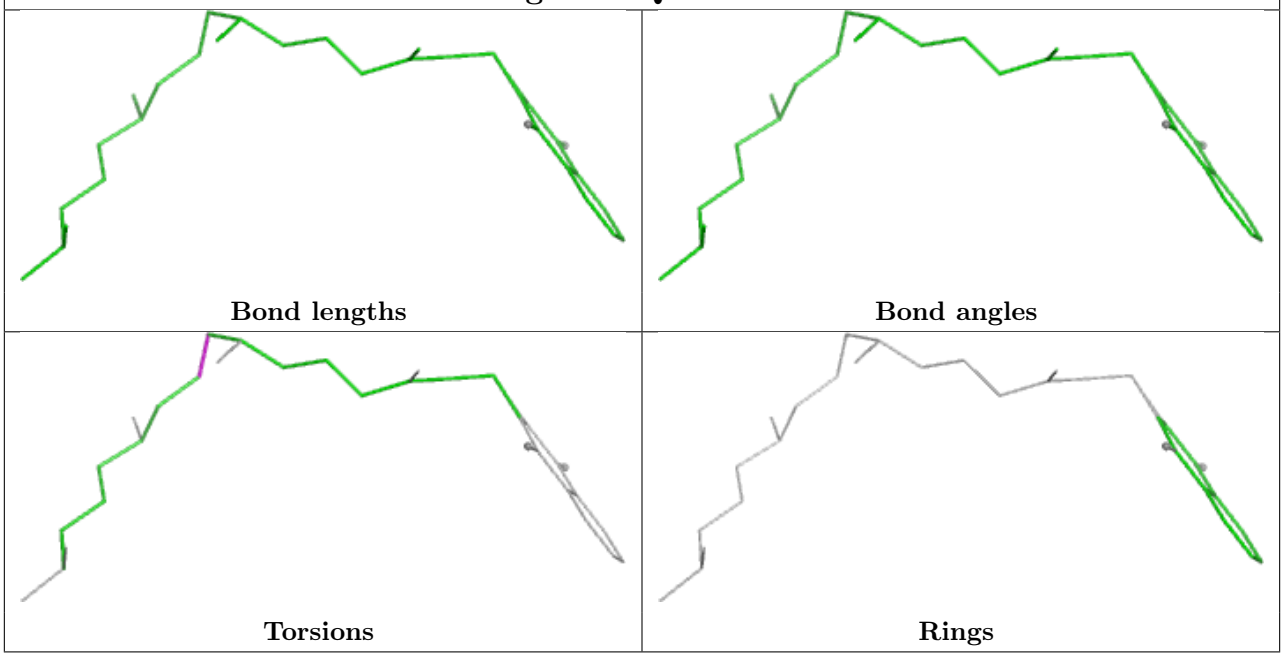


Torsions

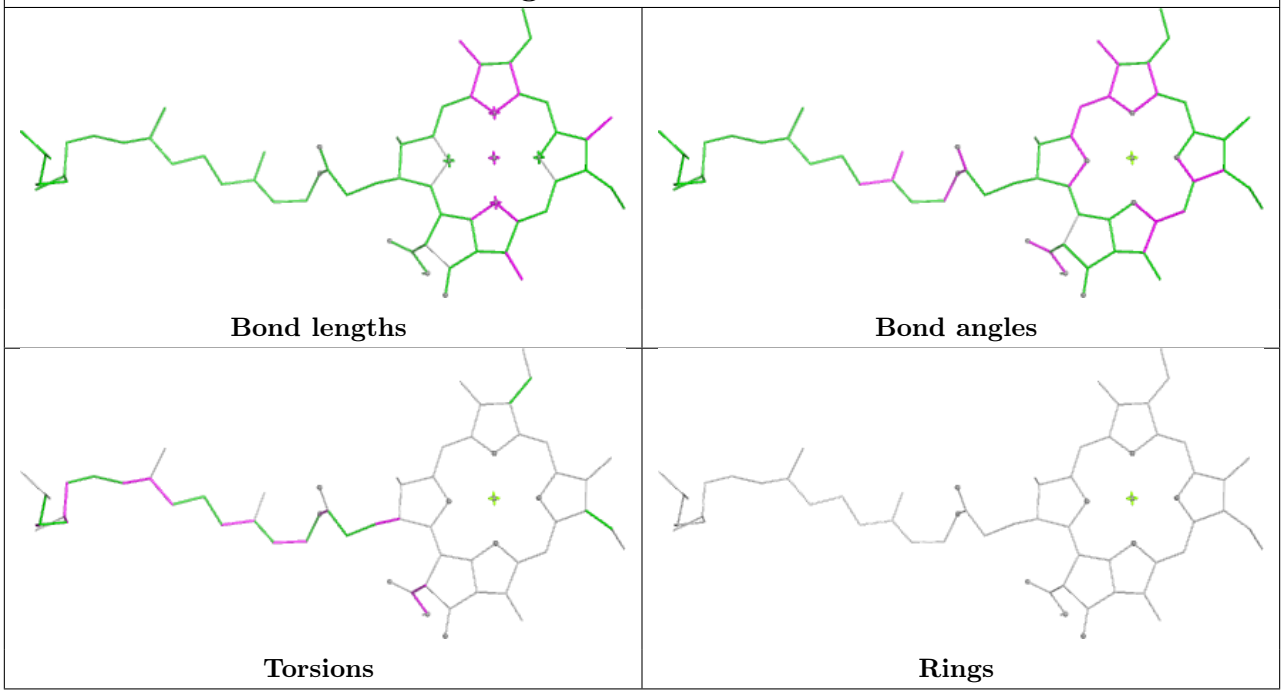


Rings

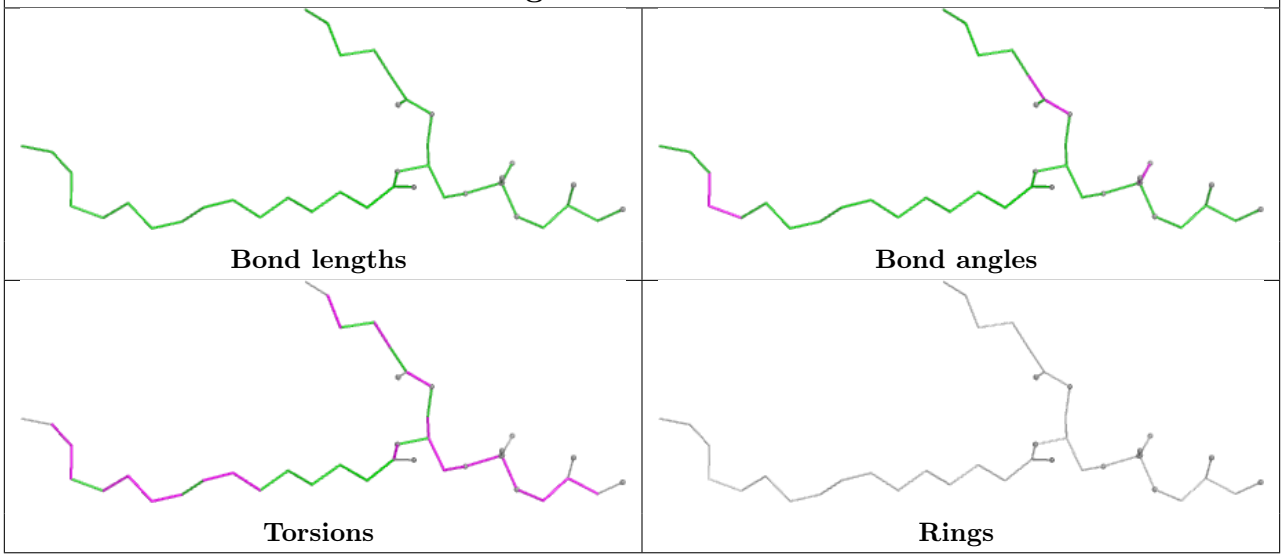
Ligand PQN b 843



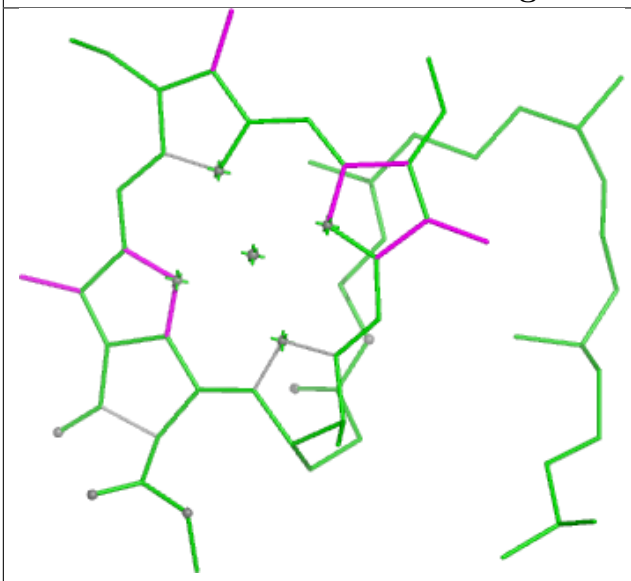
Ligand CLA 1 1607



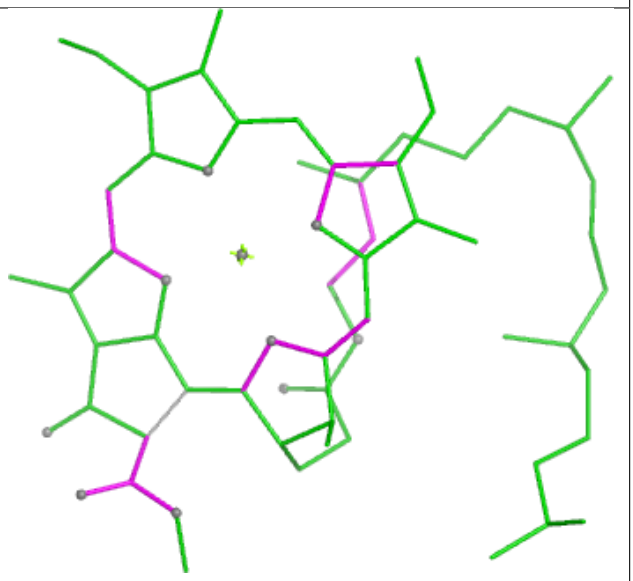
Ligand LHG L 208



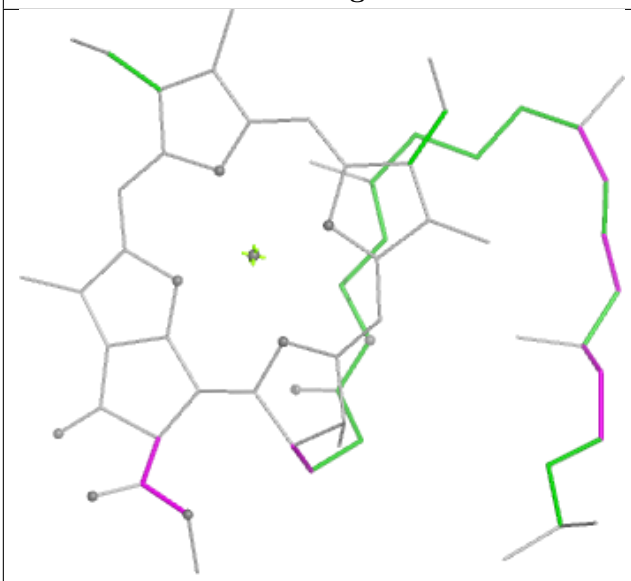
Ligand CLA 1 1625



Bond lengths



Bond angles

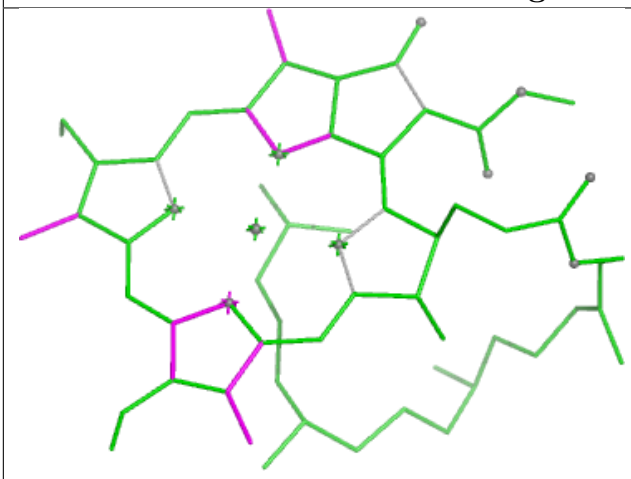


Torsions



Rings

Ligand CLA 2 807



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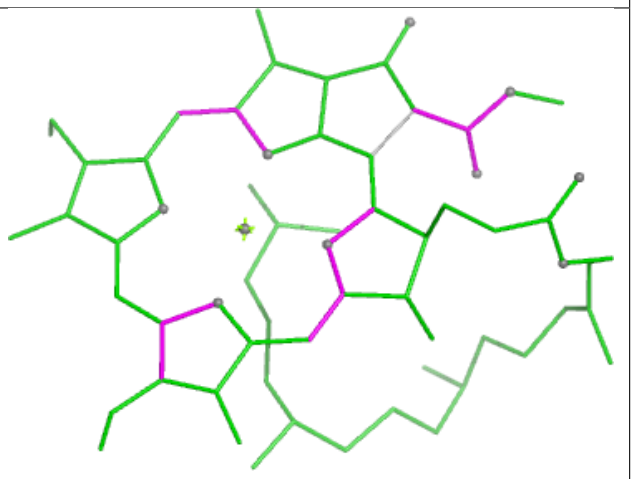
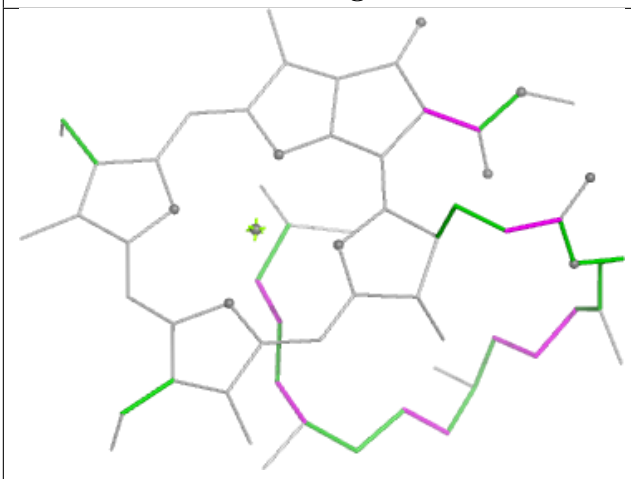


Bond angles



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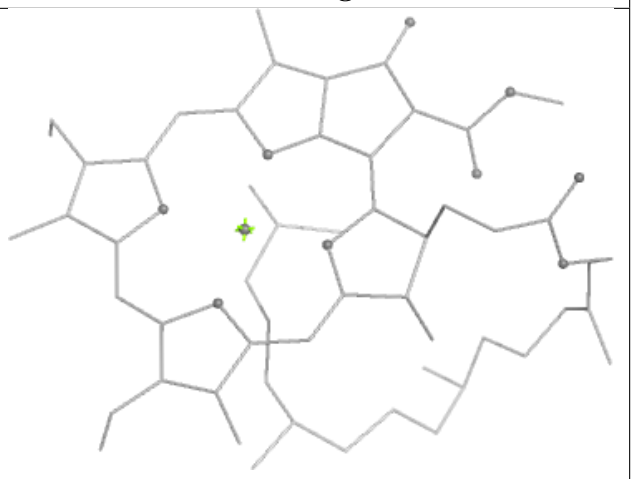
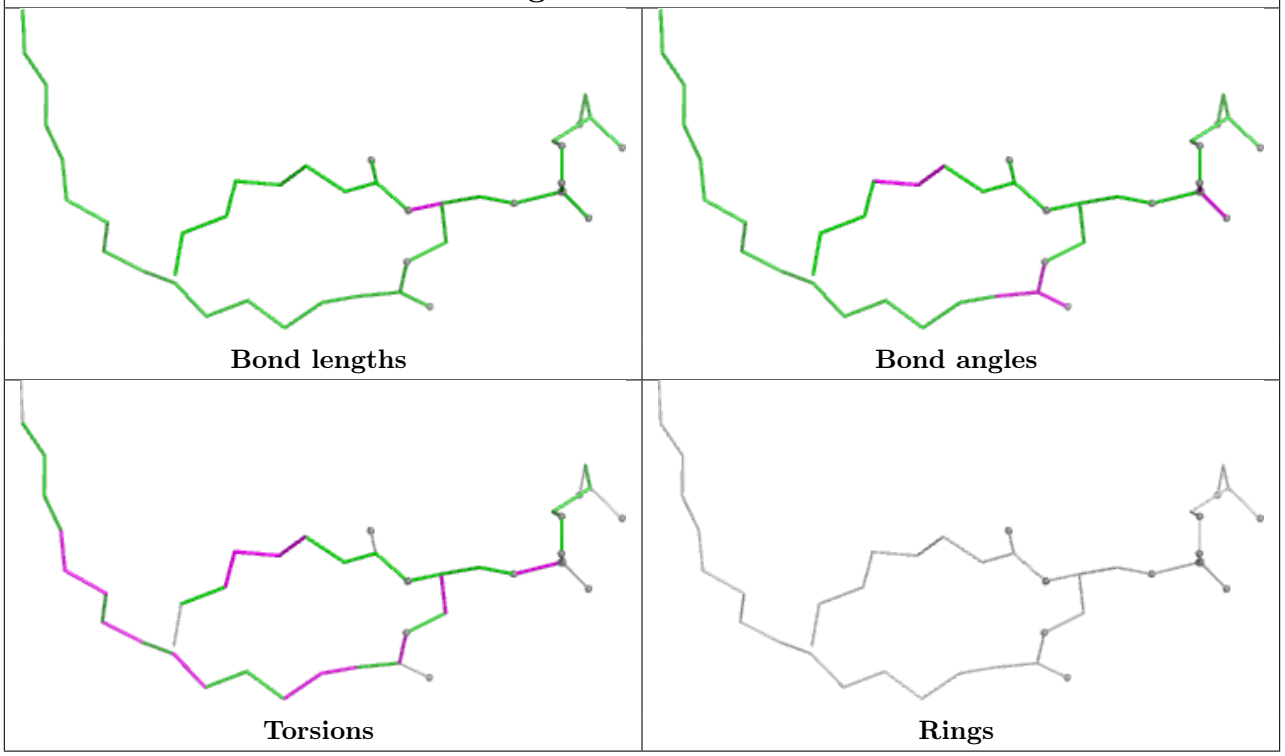
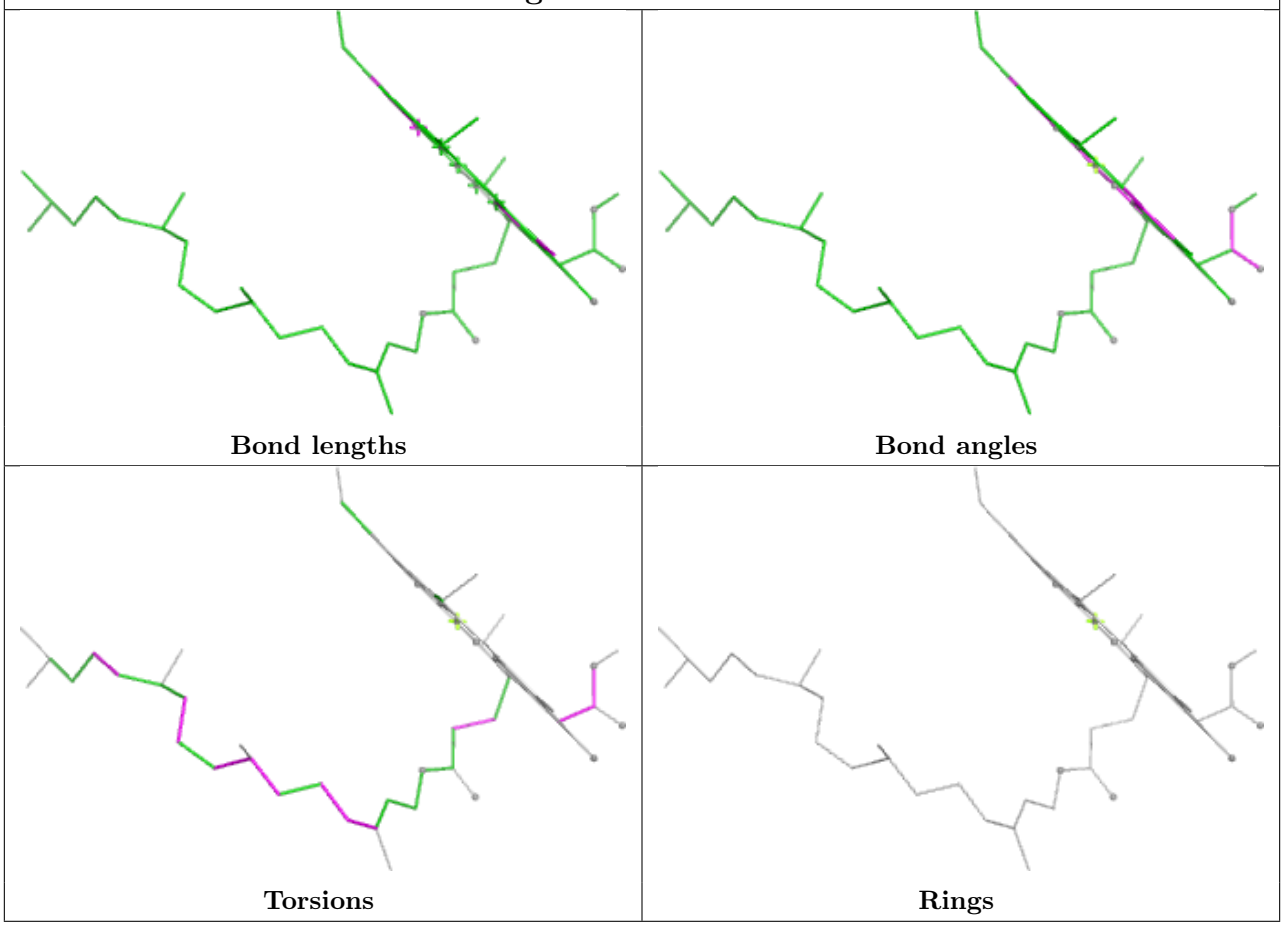


Rings

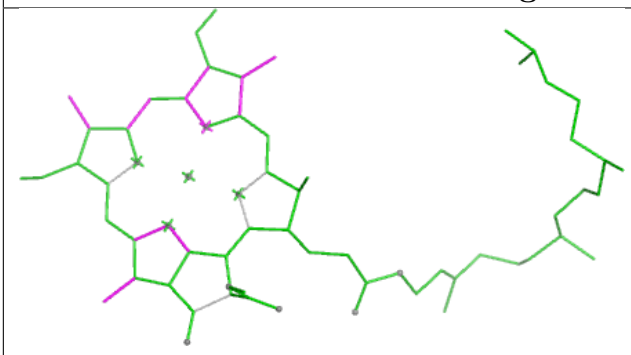
Ligand LHG a 854



Ligand CLA B 814



Ligand CLA 1 1629



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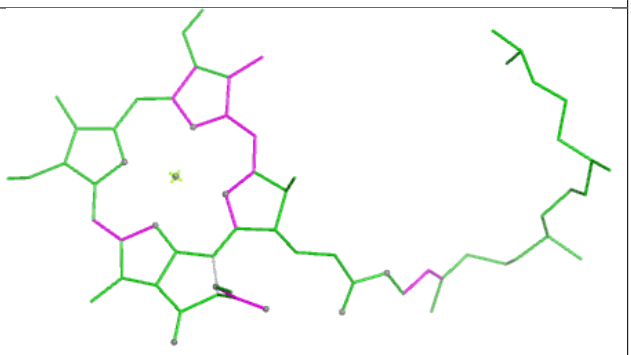
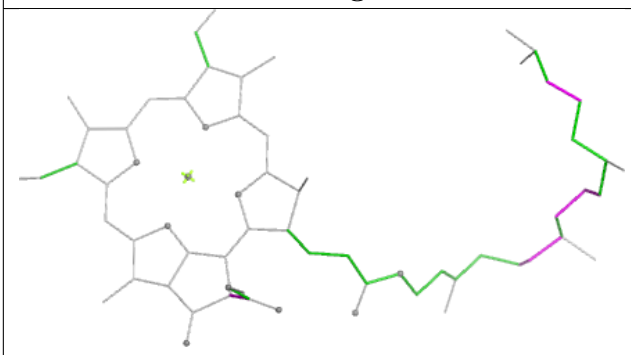
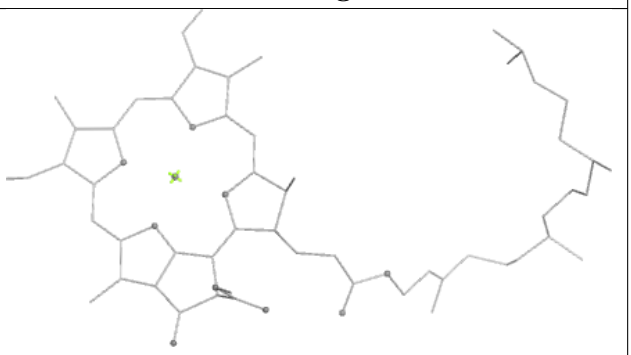


Bond angles

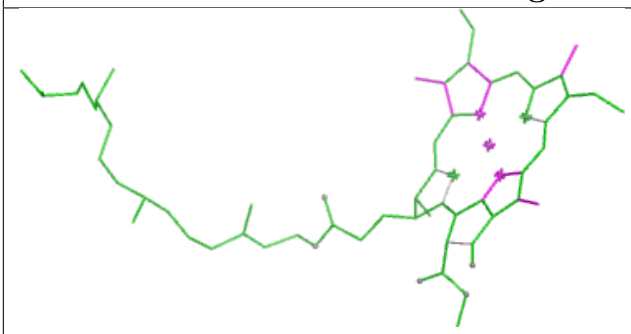


Torsions



Rings

Ligand CLA 2 802



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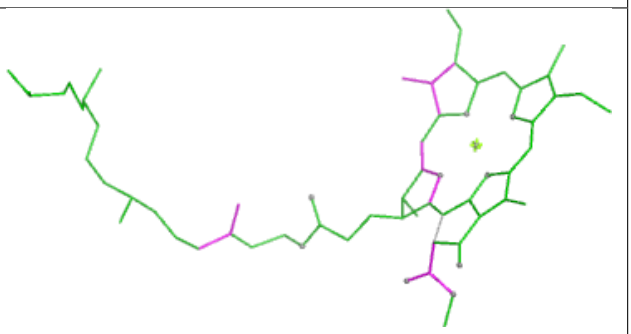
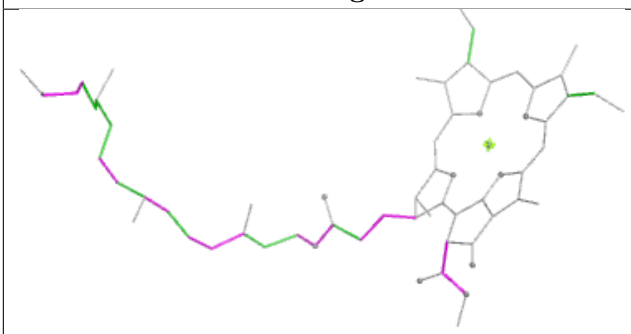


Bond angles



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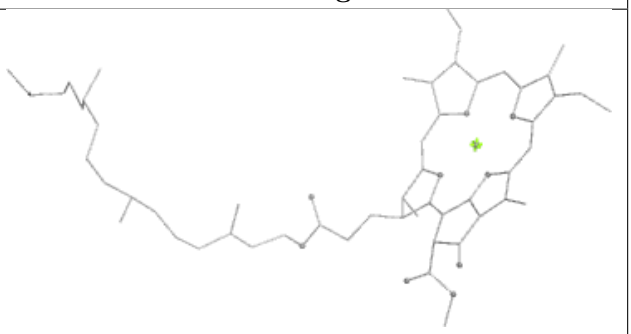
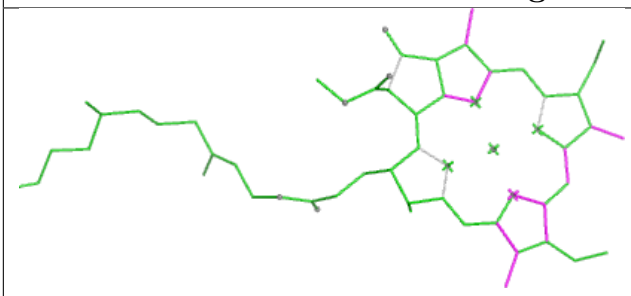


Rings

Ligand CLA 6 201



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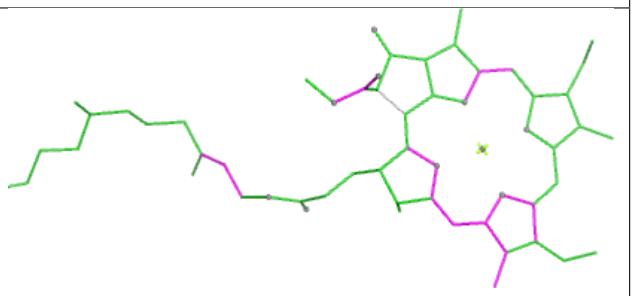
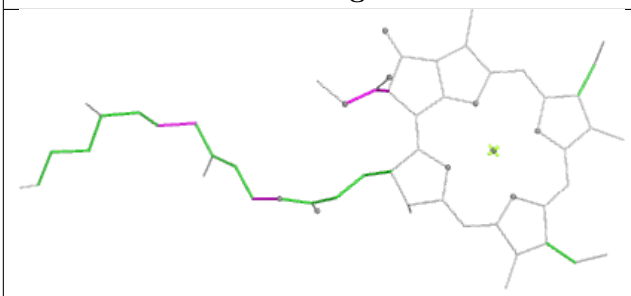


Bond angles



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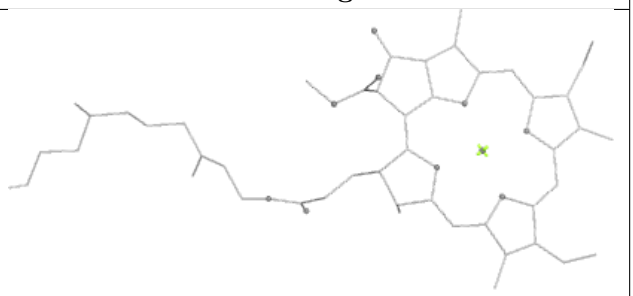
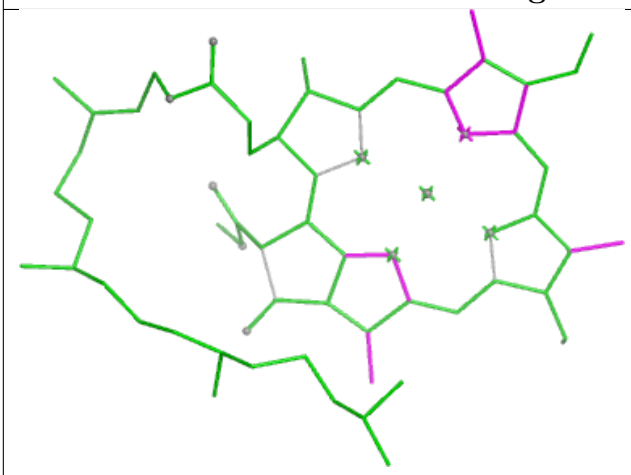


Rings

Ligand CLA 2 806



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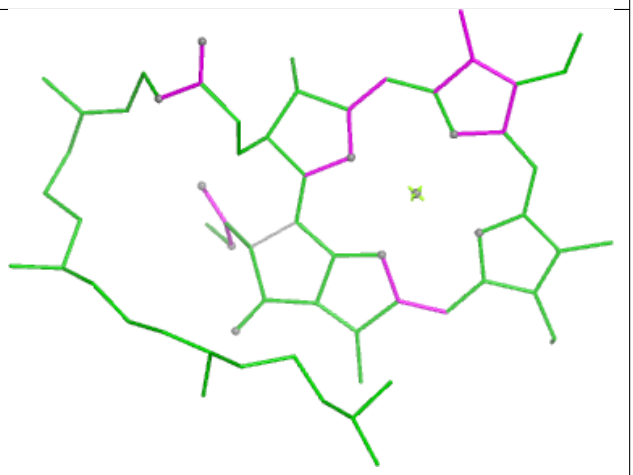
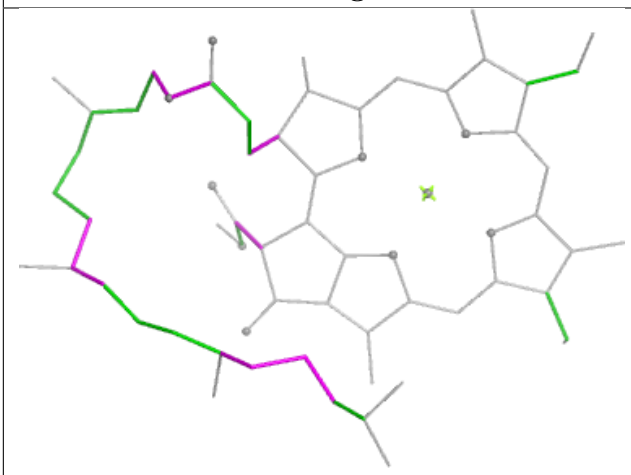


Bond angles



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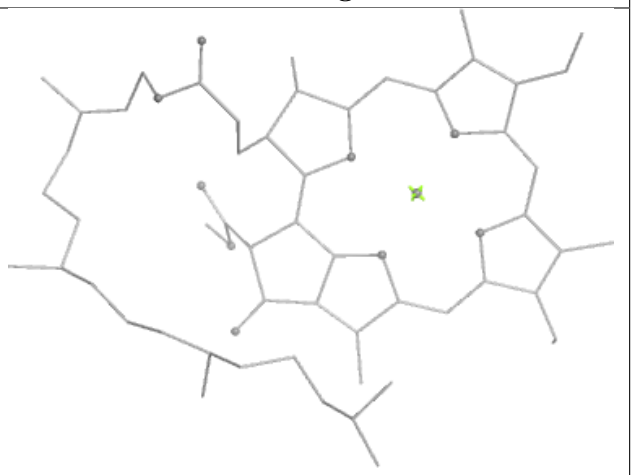
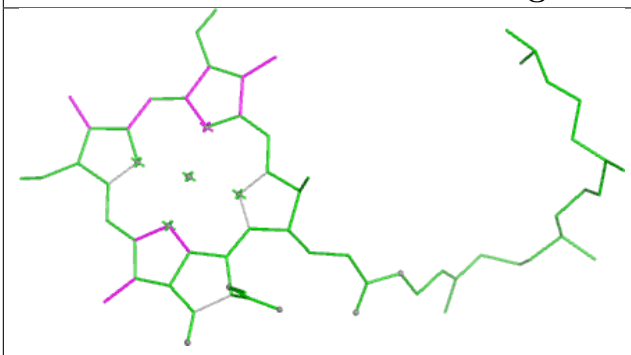
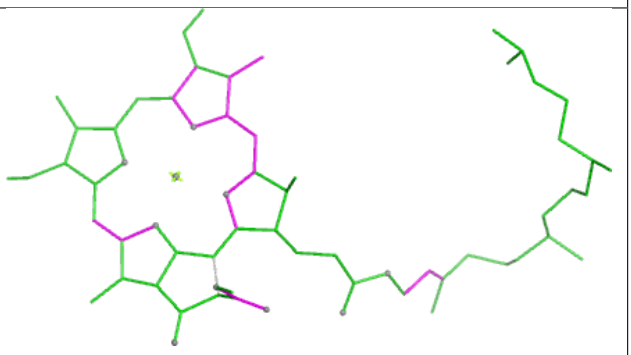


Rings

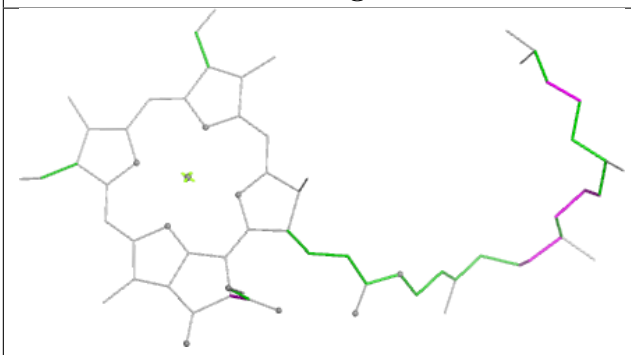
Ligand CLA a 828



Bond lengths



Bond angles



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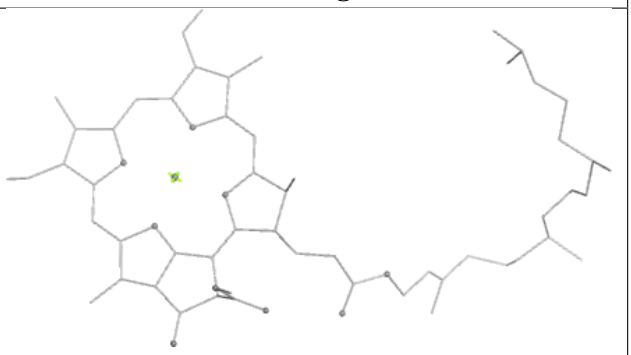
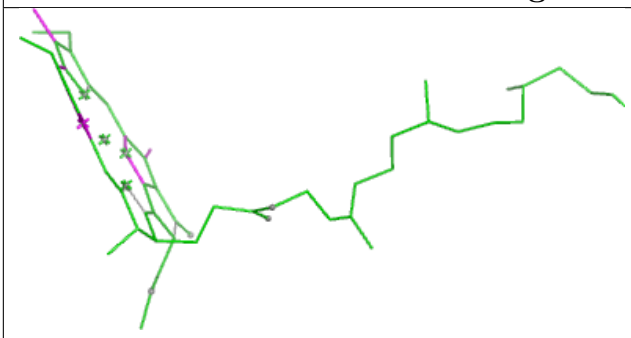
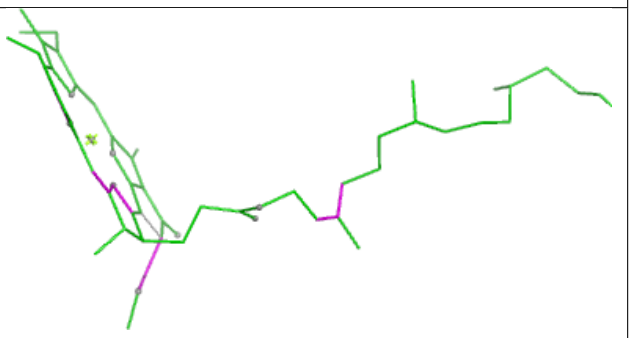


Rings

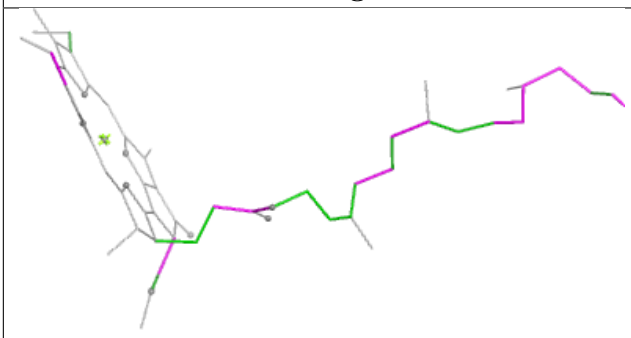
Ligand CLA a 840



Bond lengths



Bond angles



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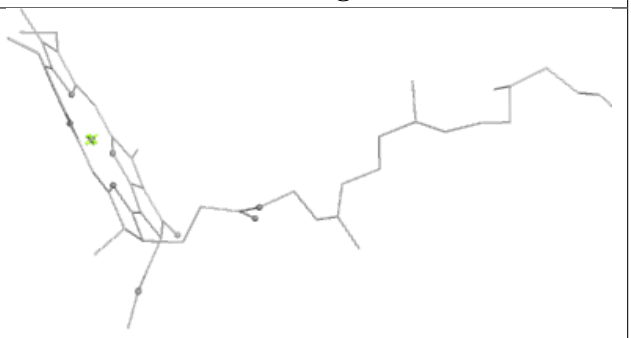
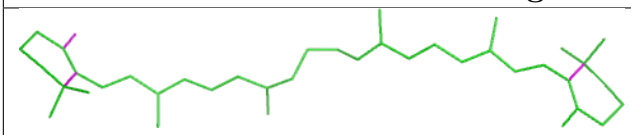
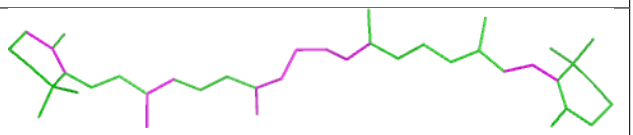


Rings

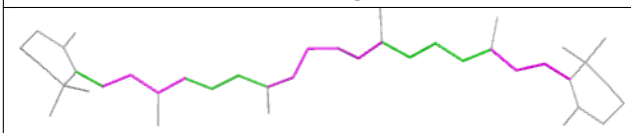
Ligand BCR a 848



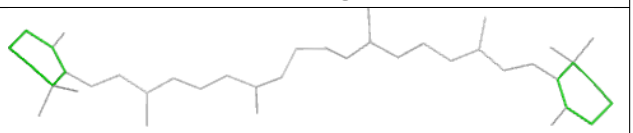
Bond lengths



Bond angles

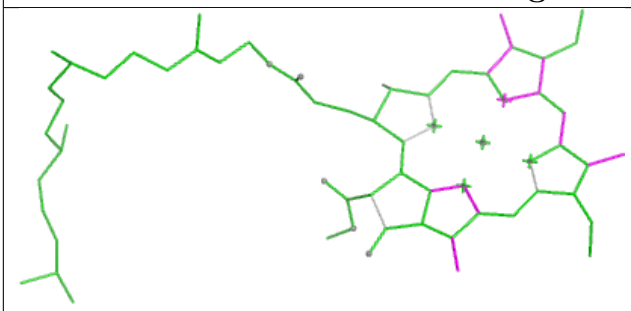


Torsions



Rings

Ligand CLA 2 827



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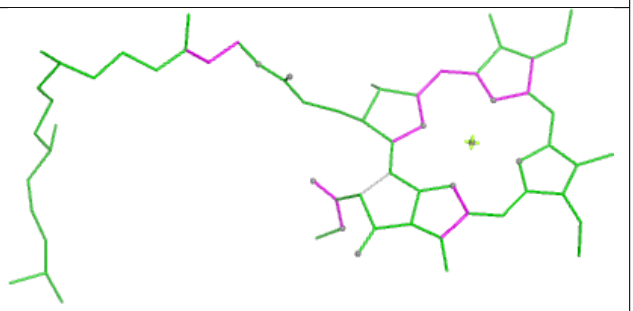

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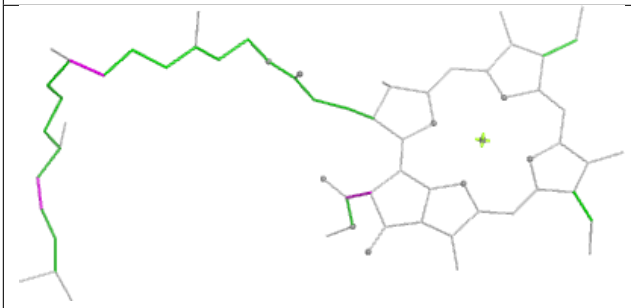

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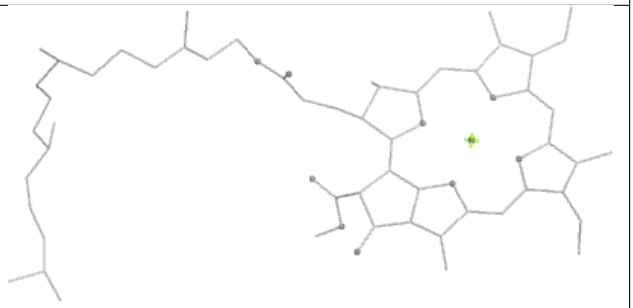
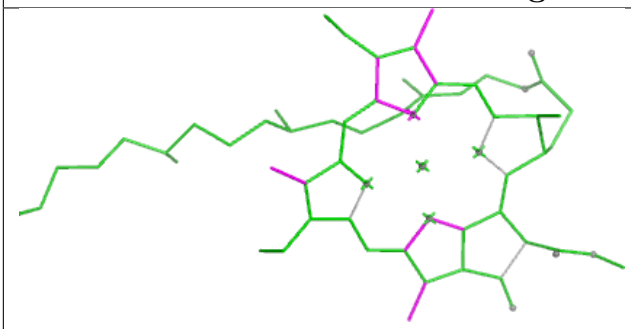


Rings

Ligand CLA a 819



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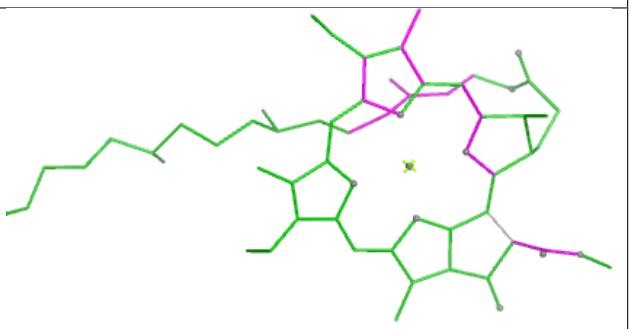

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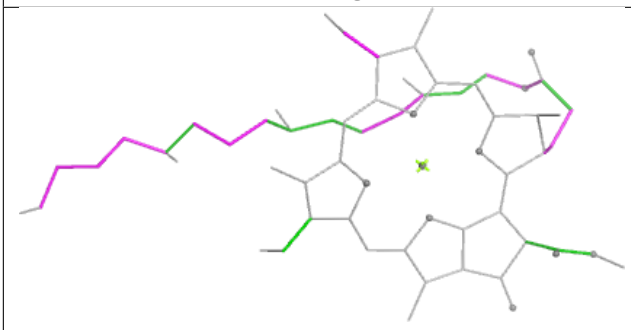
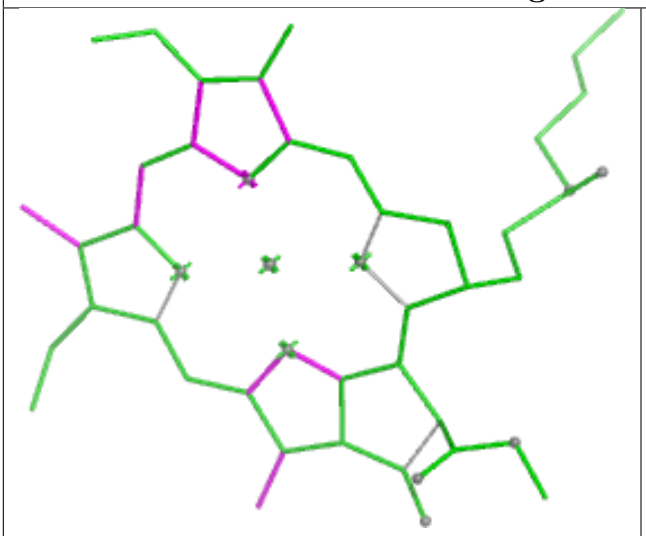


Torsions



Rings

Ligand CLA a 811



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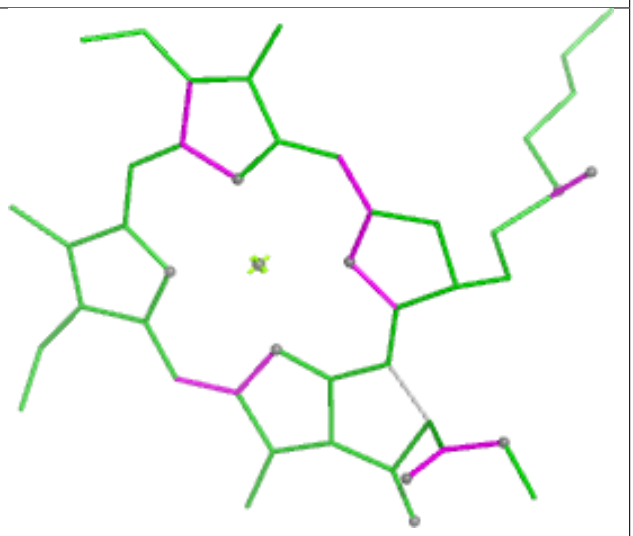

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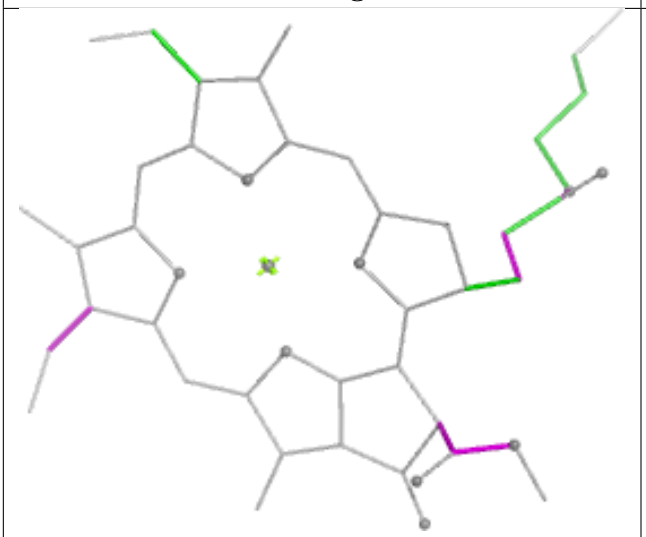
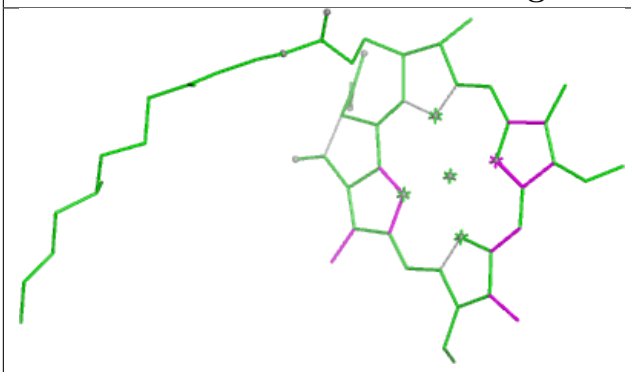


Torsions



Rings

Ligand CLA k 103



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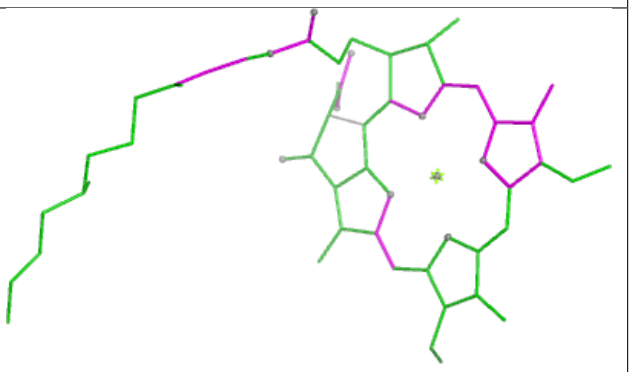

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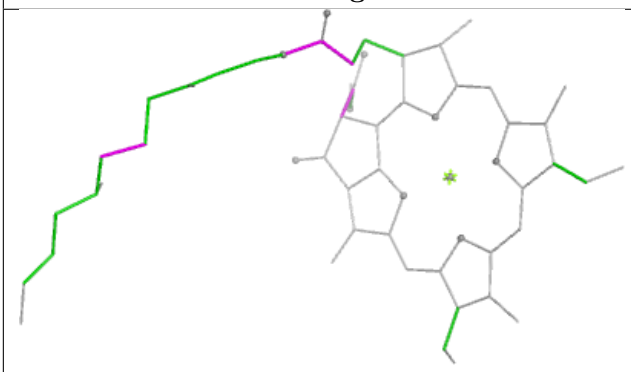

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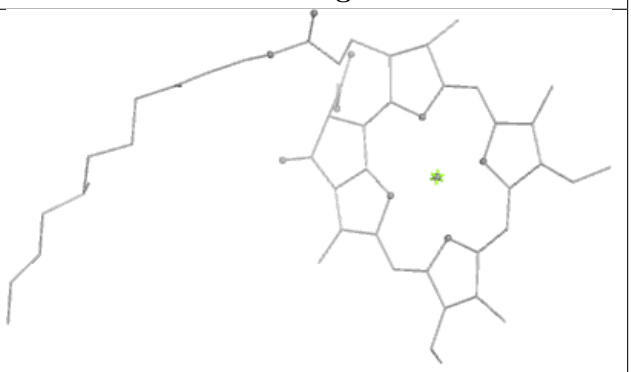
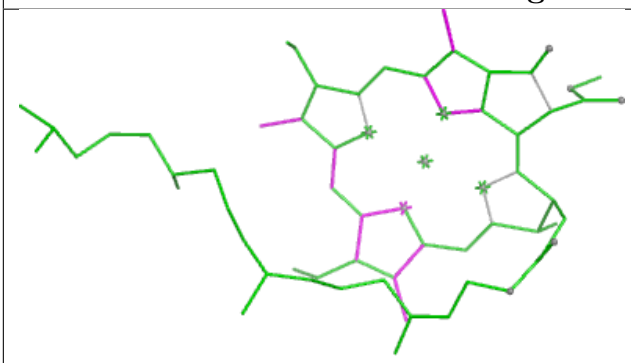


Rings

Ligand CLA b 821



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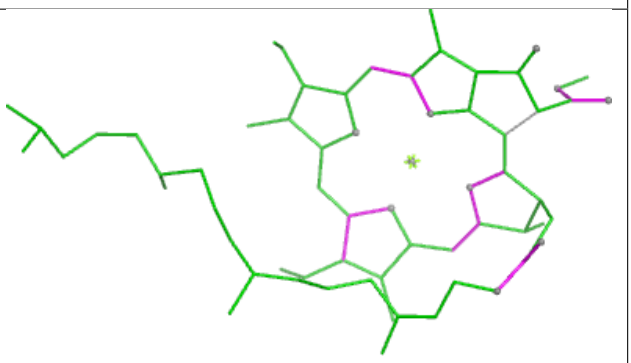

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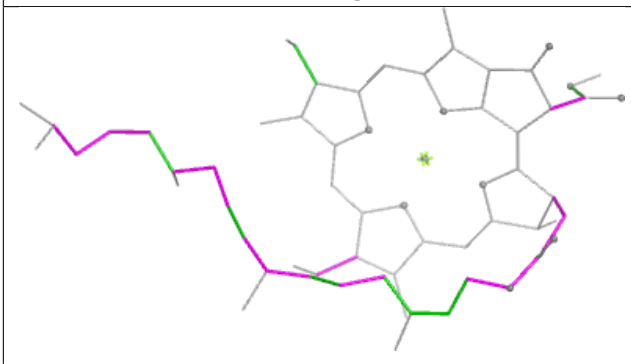

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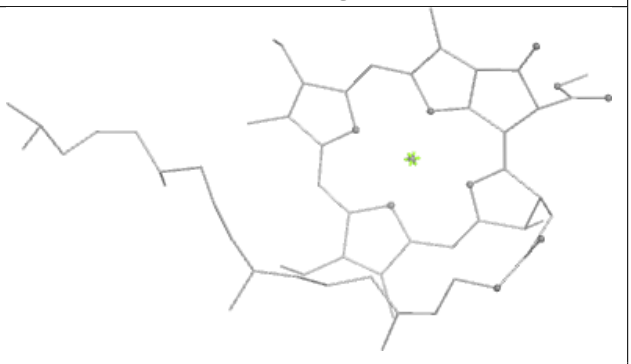

Rings

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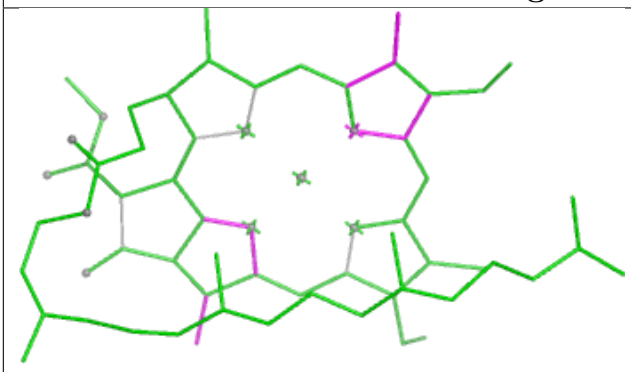

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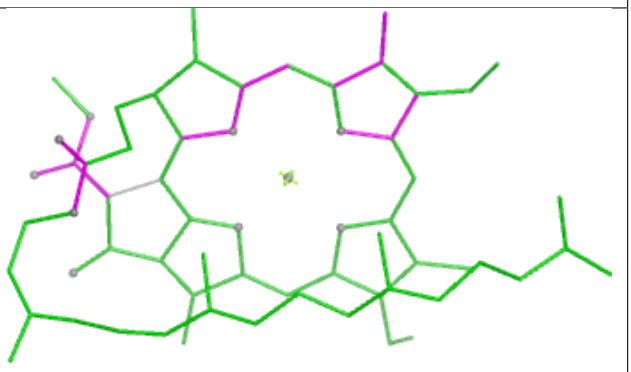
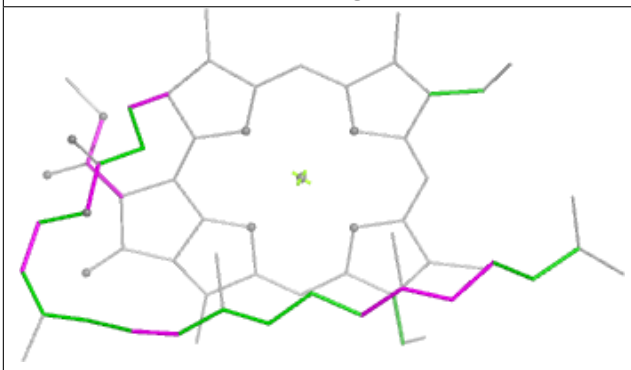


Bond angles



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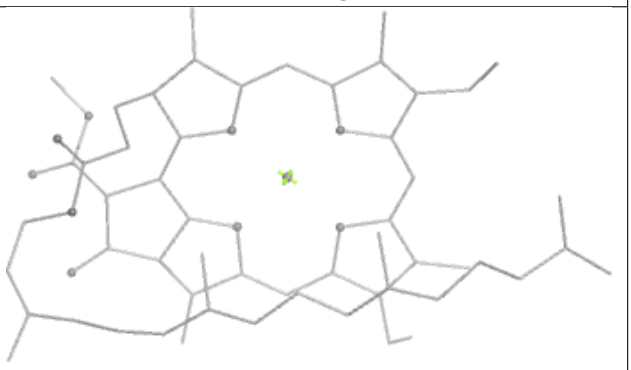
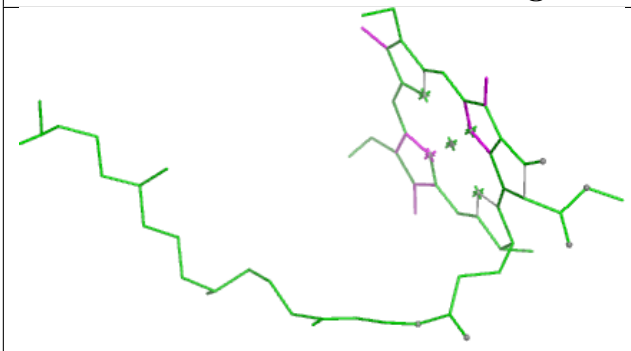


Rings

Ligand CLA b 816



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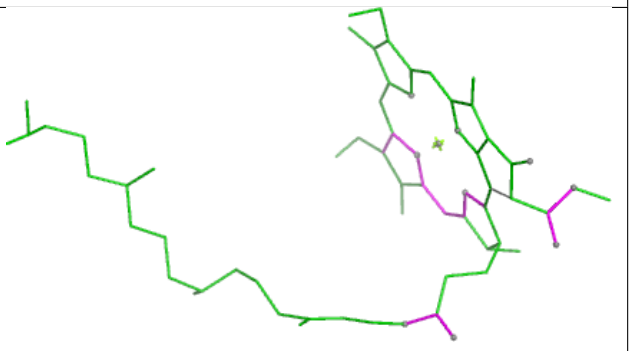


Bond angles

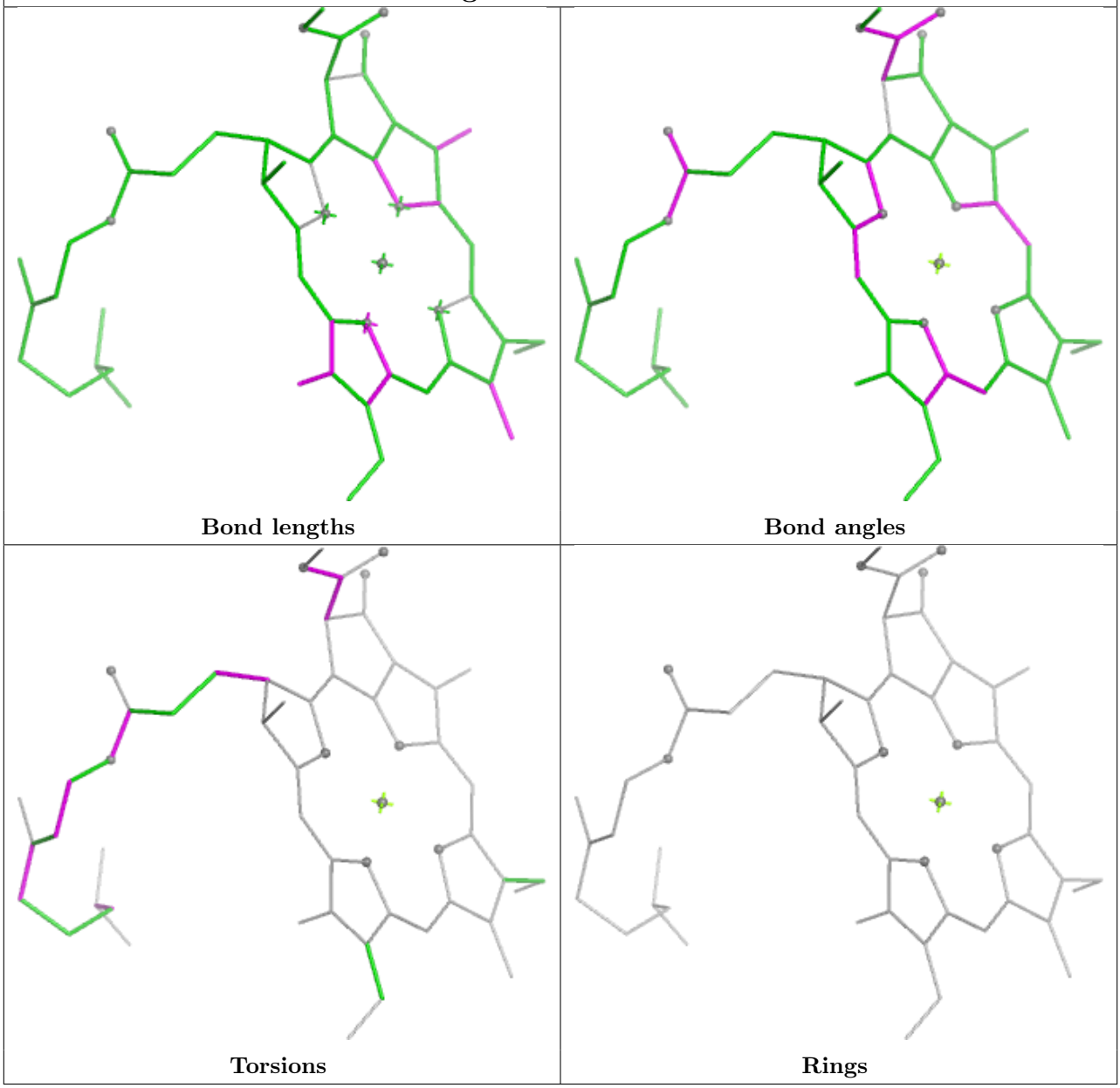


Torsions



Rings

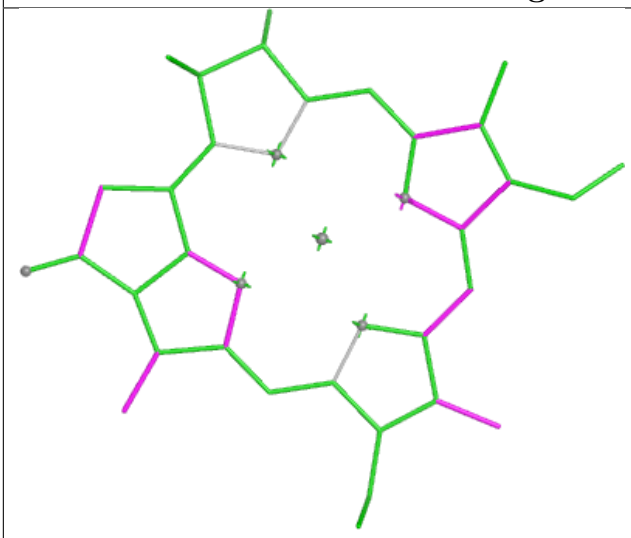
Ligand CLA 2 831



Bond lengths | **Bond angles**

Torsions | **Rings**

Ligand CLA J 102



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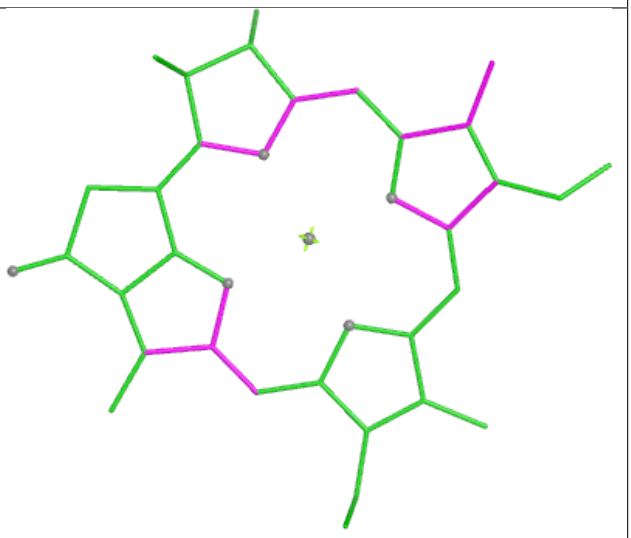
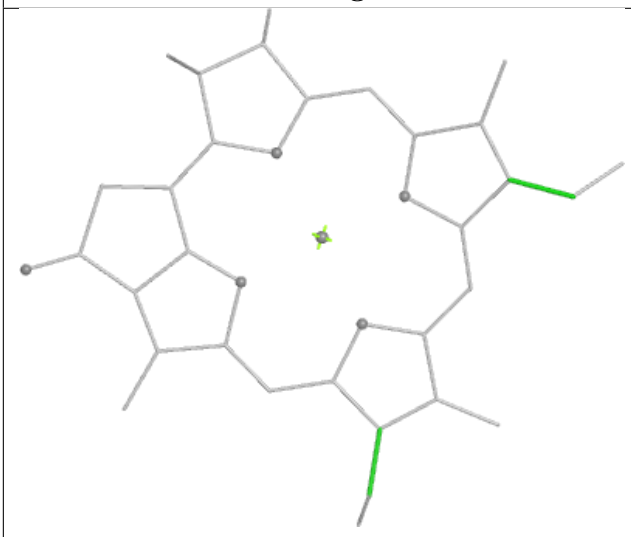


Bond angles



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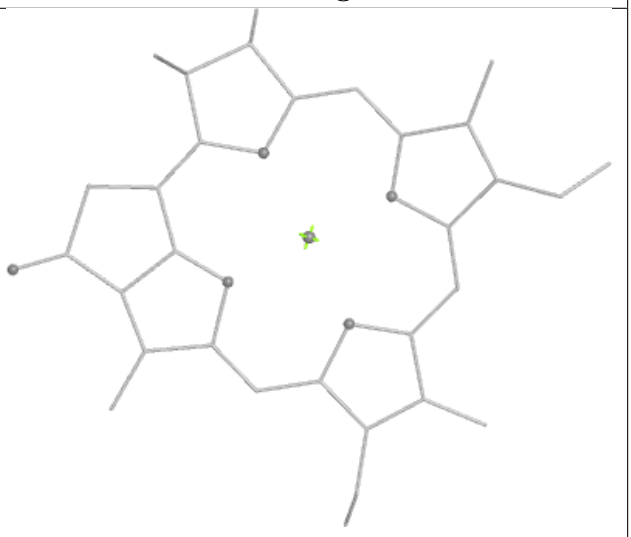
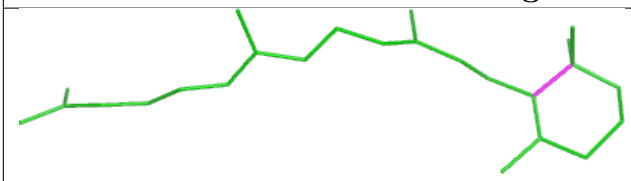


Rings

Ligand BCR A 852



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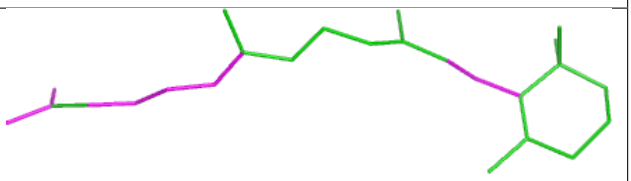
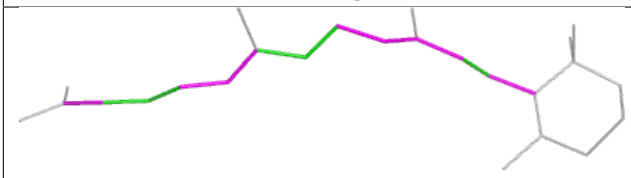


Bond angles

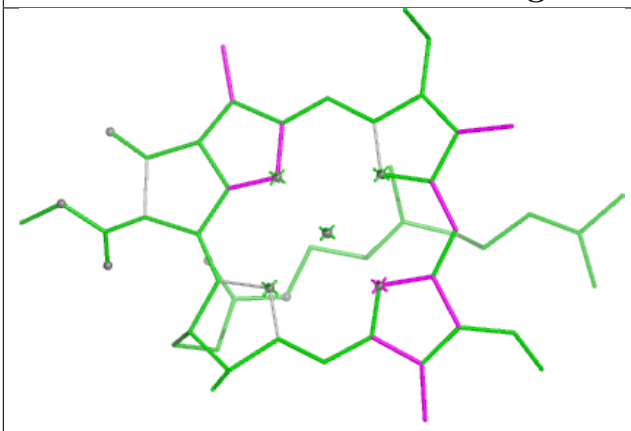


Torsions



Rings

Ligand CLA b 823



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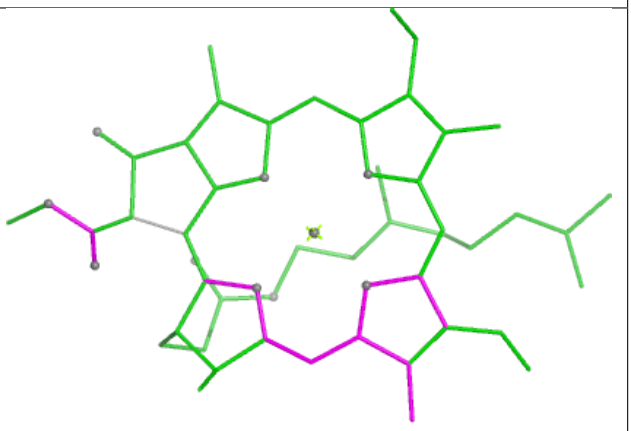
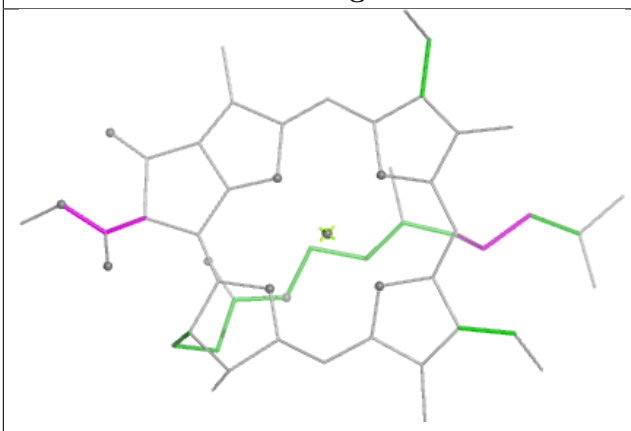


Bond angles



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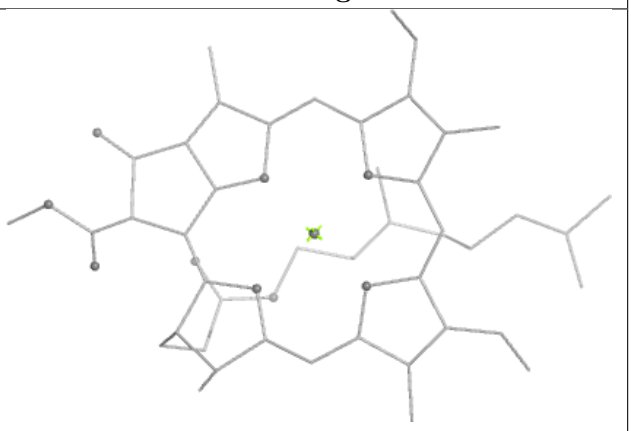
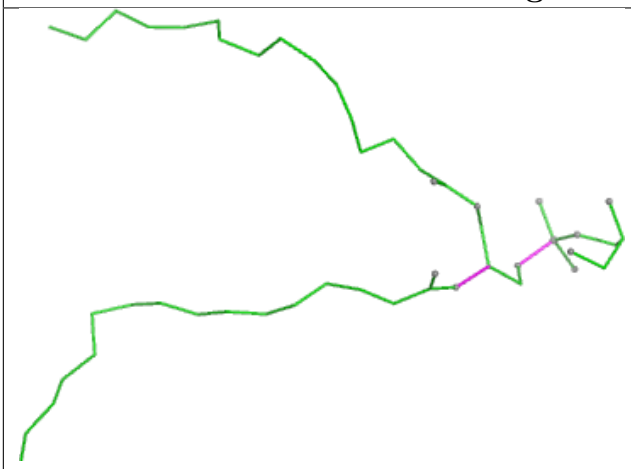


Rings

Ligand LHG y 101



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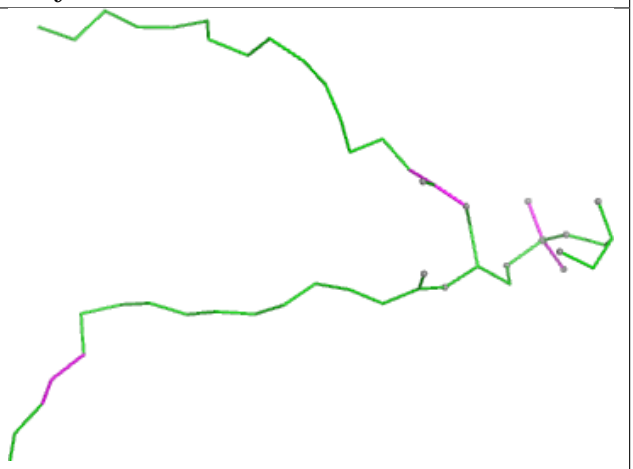

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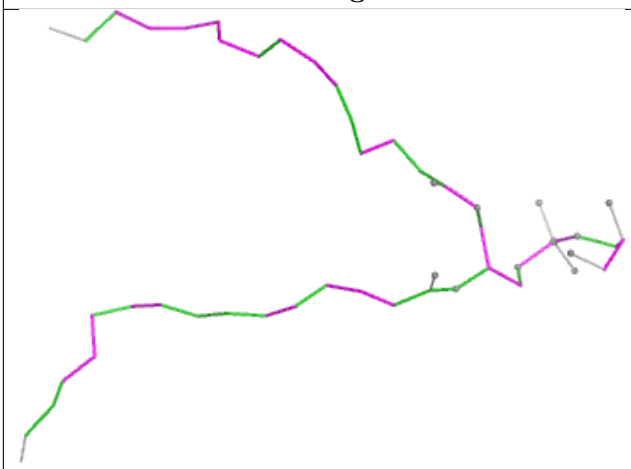
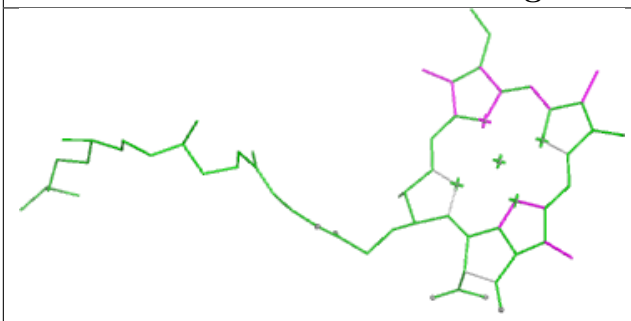


Torsions



Rings

Ligand CLA B 813



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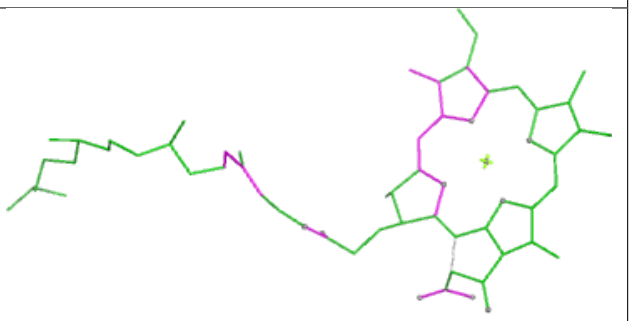

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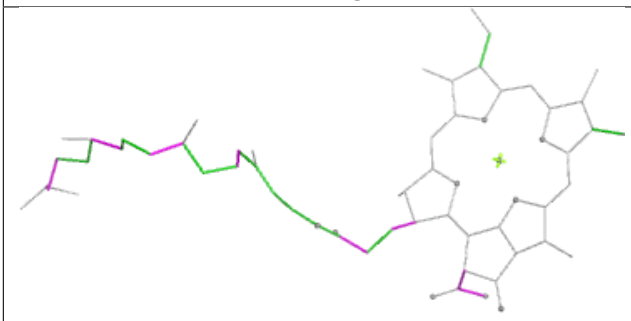
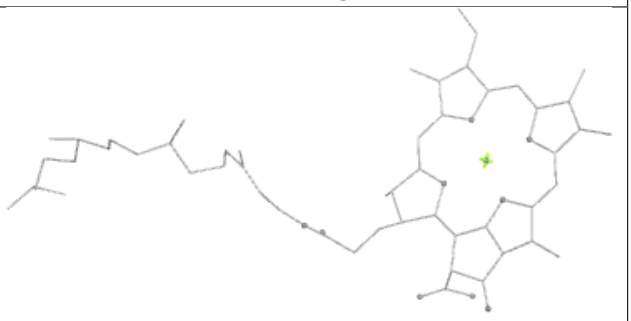
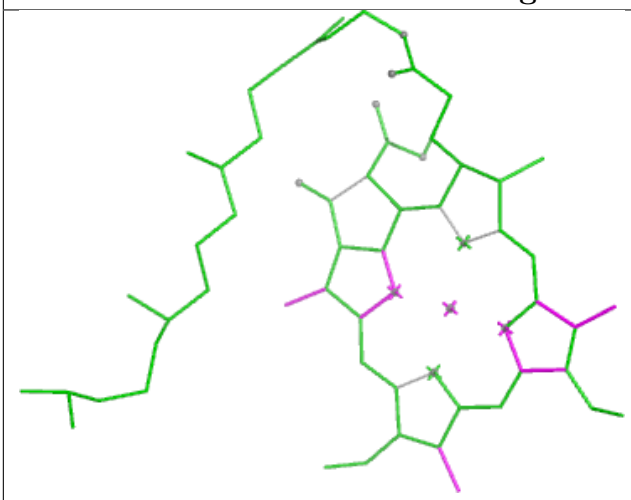


Torsions



Rings

Ligand CLA 1 1627



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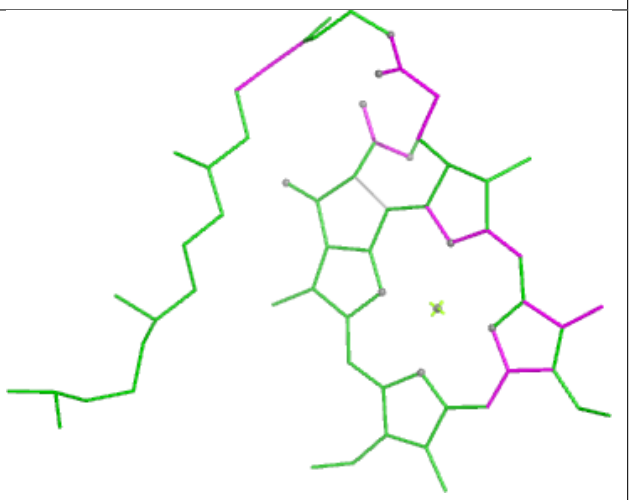

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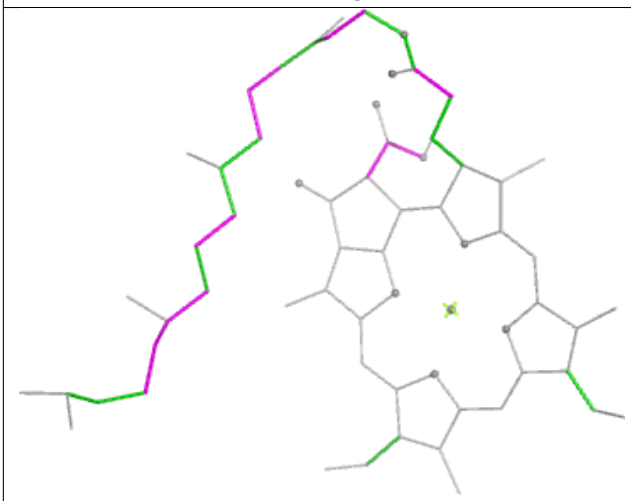

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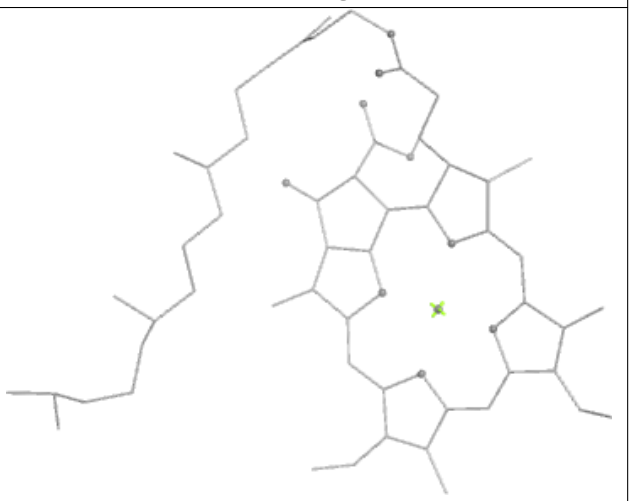
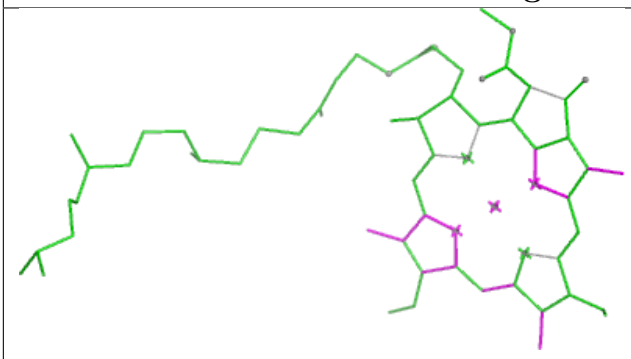


Rings

Ligand CLA A 802



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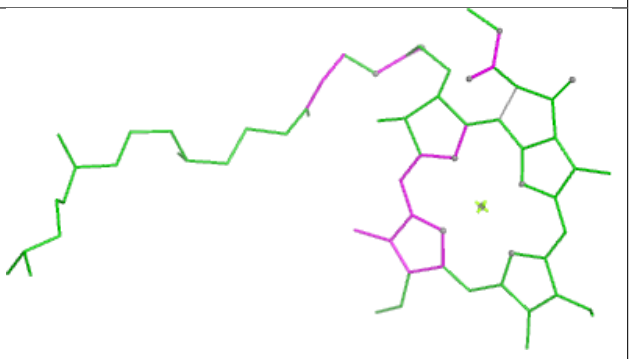
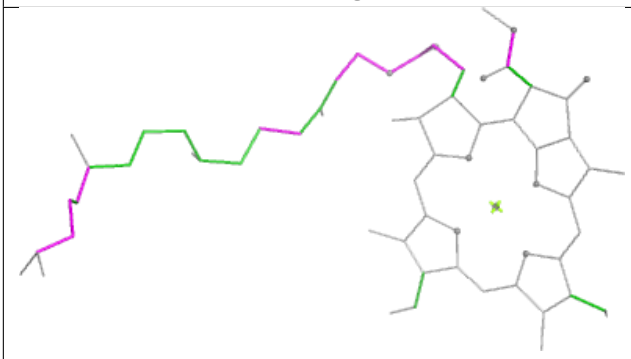


Bond angles

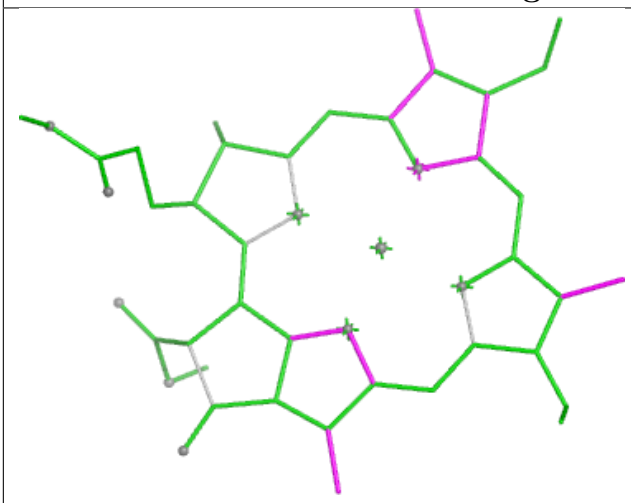


Torsions



Rings

Ligand CLA K 101



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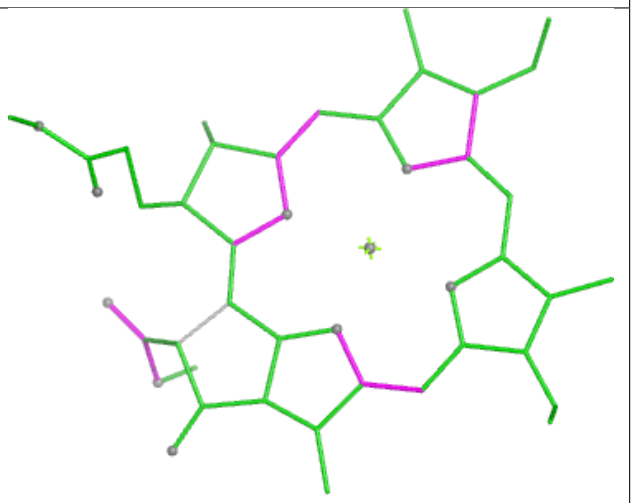
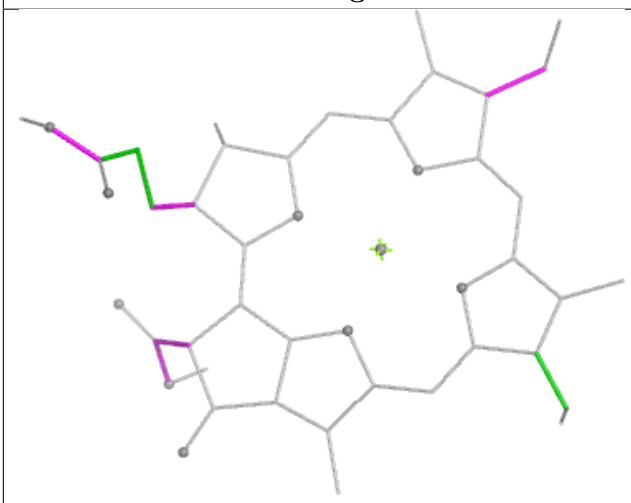


Bond angles



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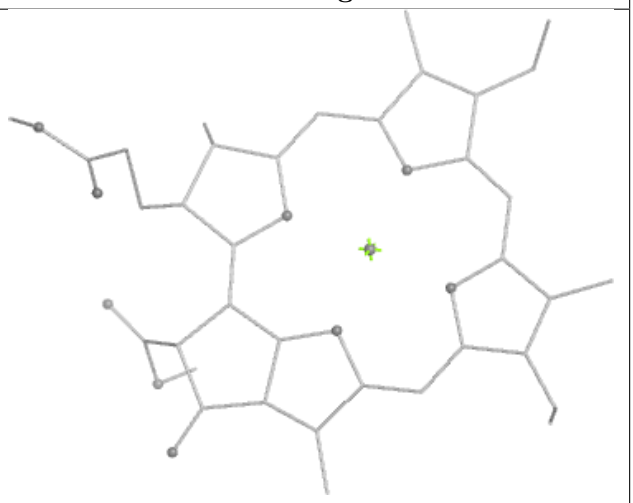
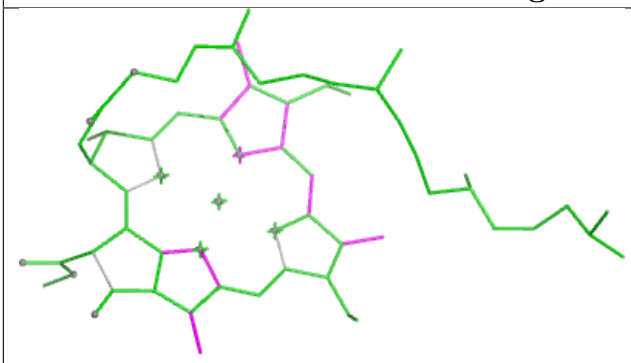
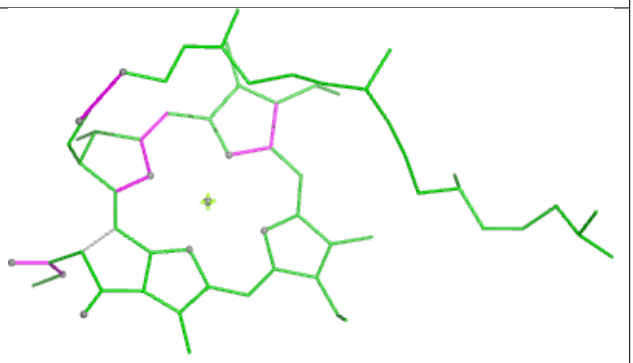


Rings

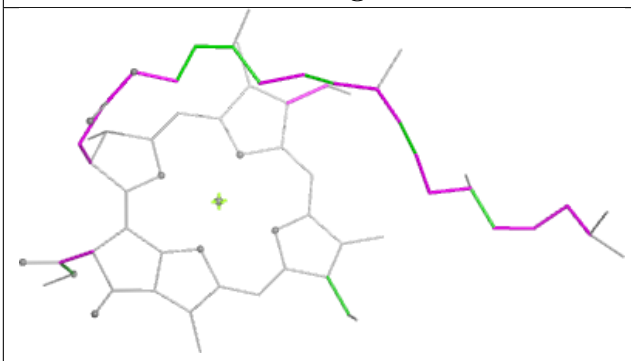
Ligand CLA 2 821



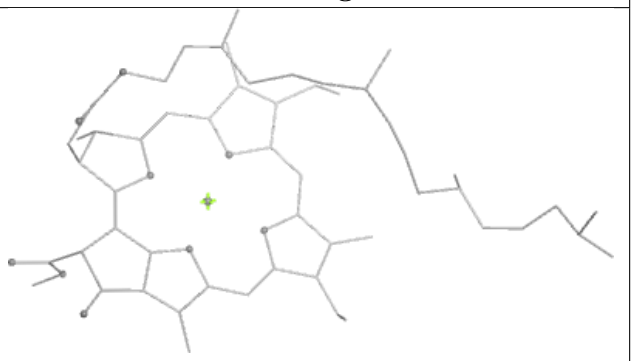
Bond lengths



Bond angles

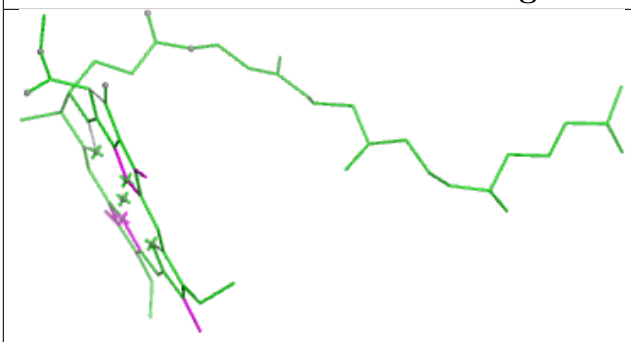


Torsions



Rings

Ligand CLA 1 1613



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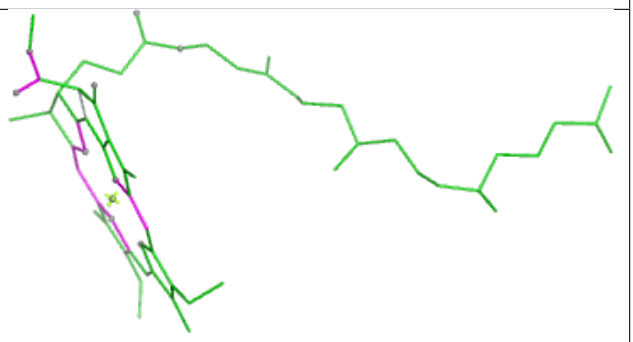
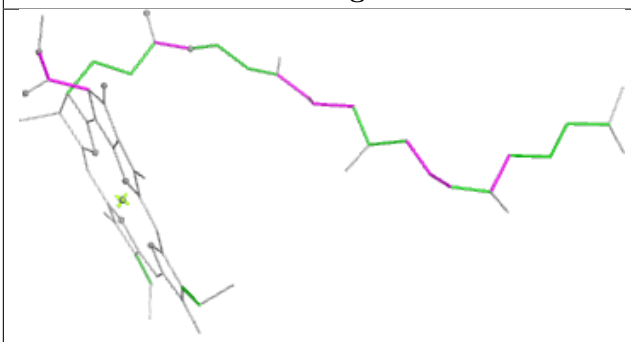


Bond angles



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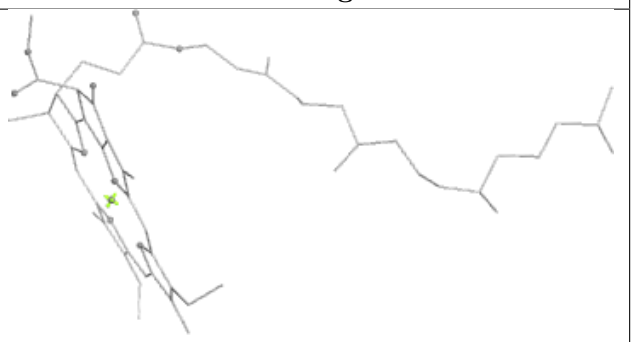
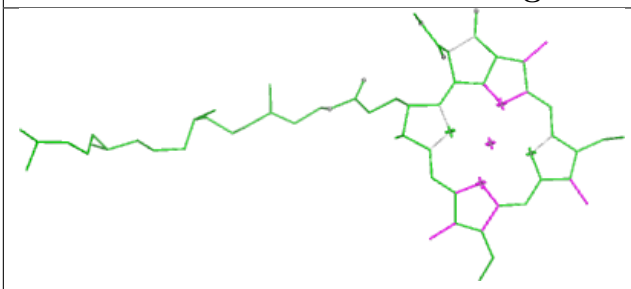


Rings

Ligand CLA A 827



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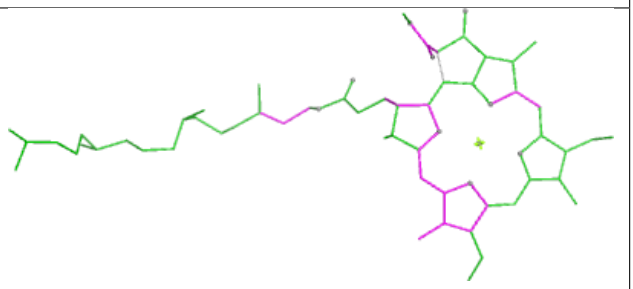
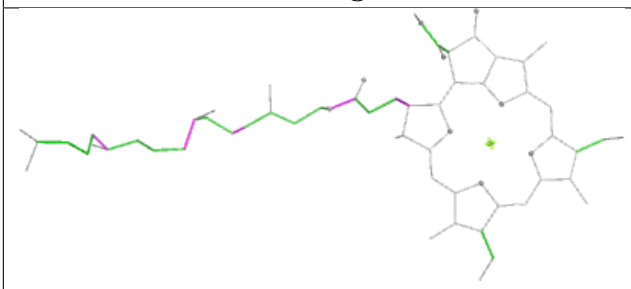


Bond angles



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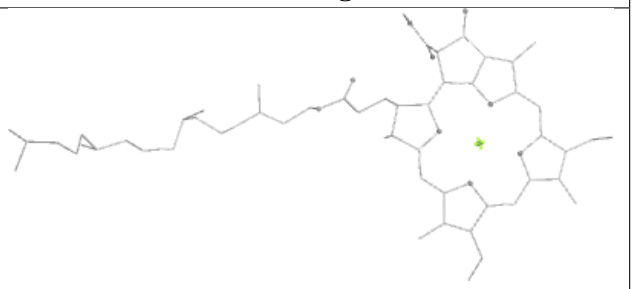
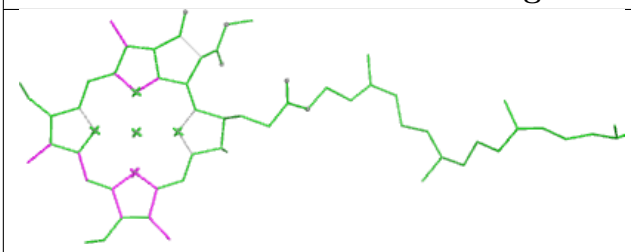


Rings

Ligand CLA A 834



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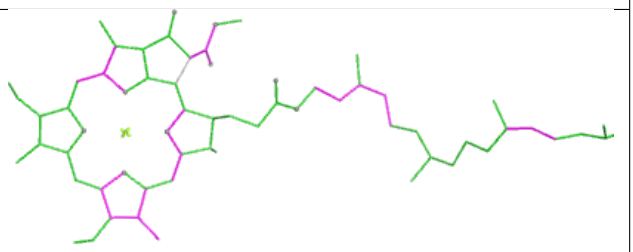
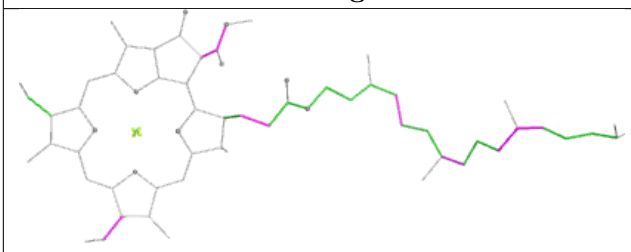


Bond angles



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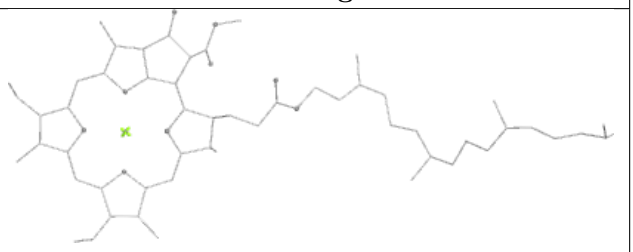
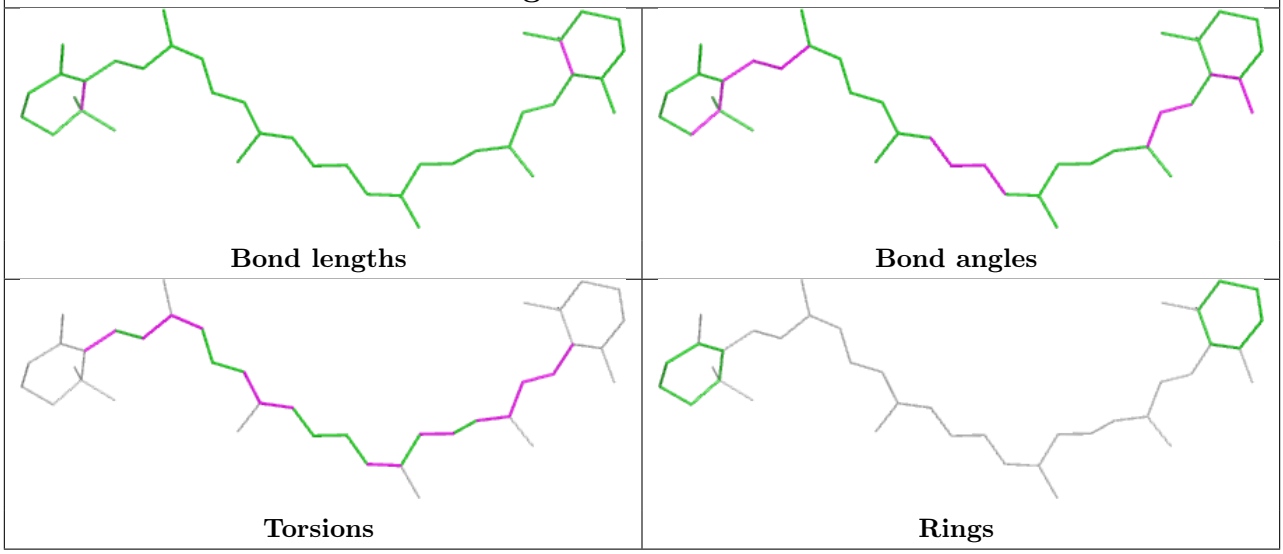
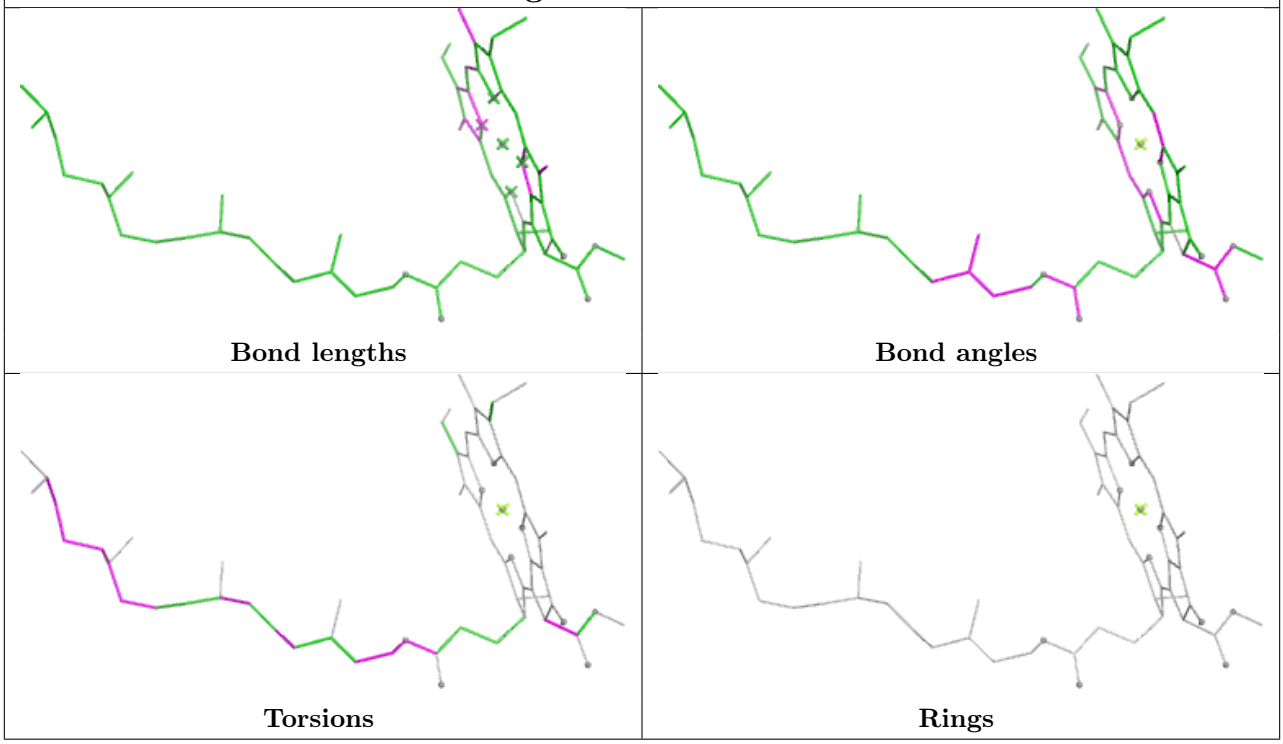


Rings

Ligand BCR A 851



Ligand CLA B 804



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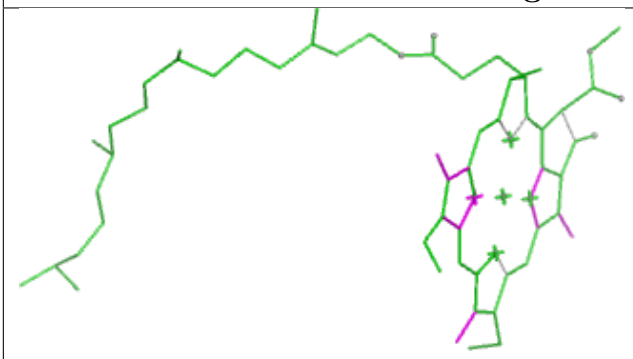

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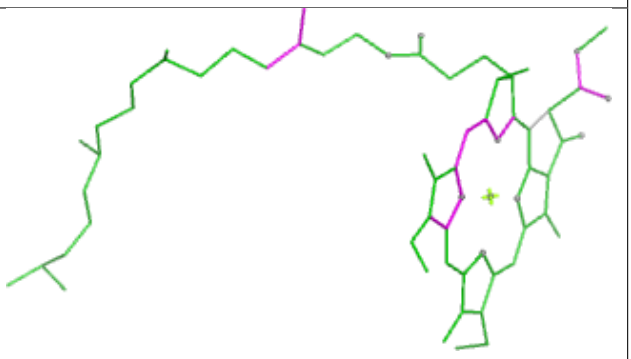
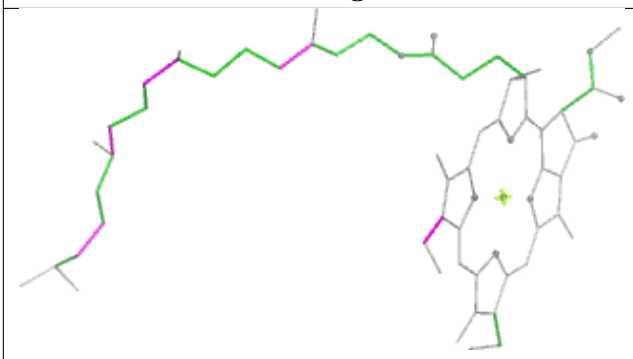


Bond angles



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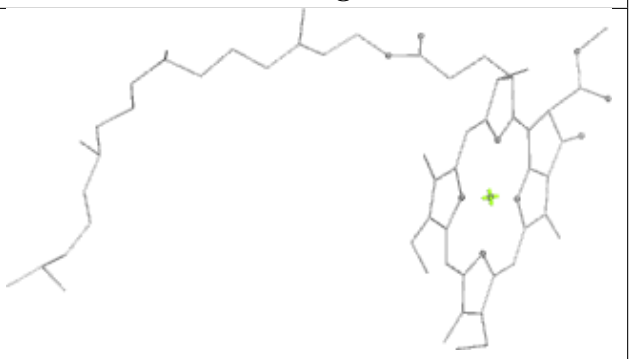
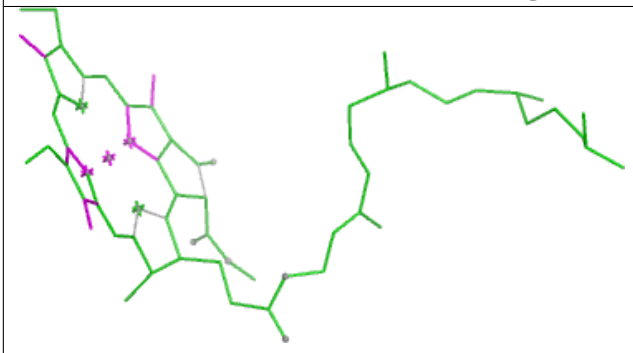


Rings

Ligand CLA B 802



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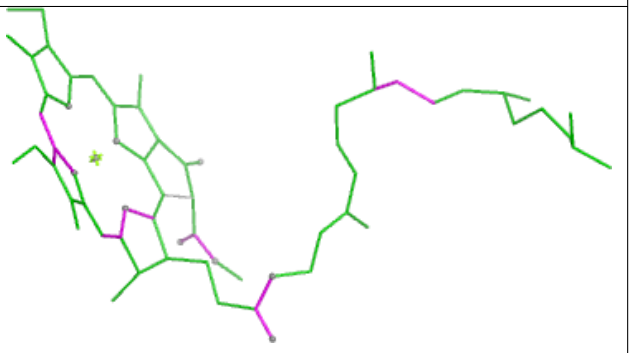
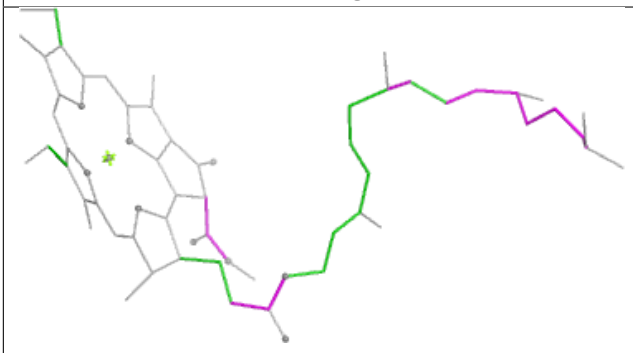


Bond angles



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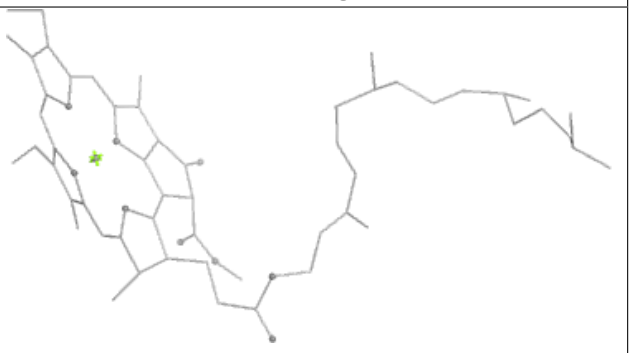
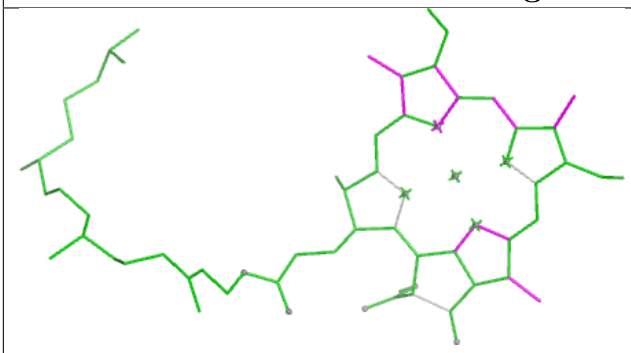


Rings

Ligand CLA A 828



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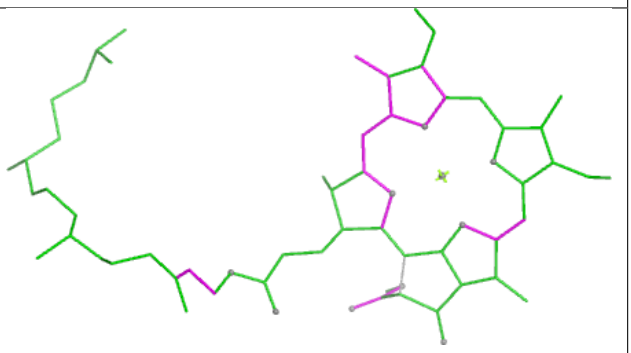
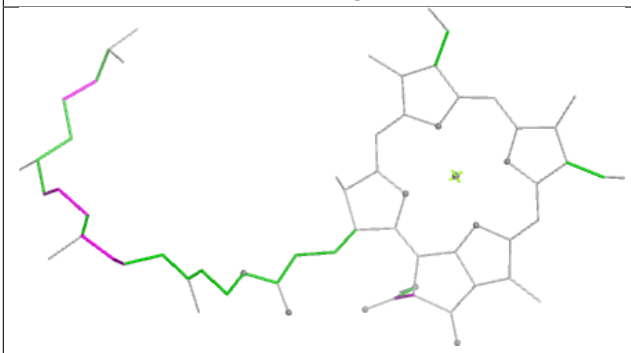


Bond angles



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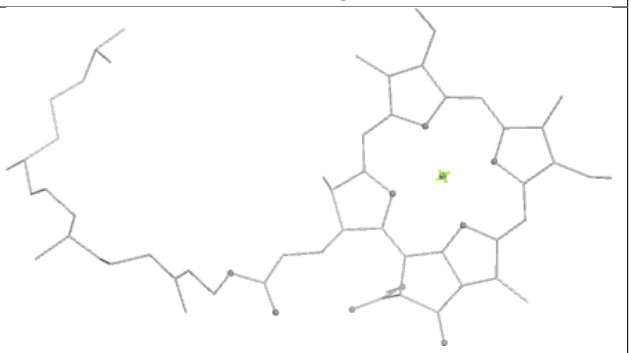
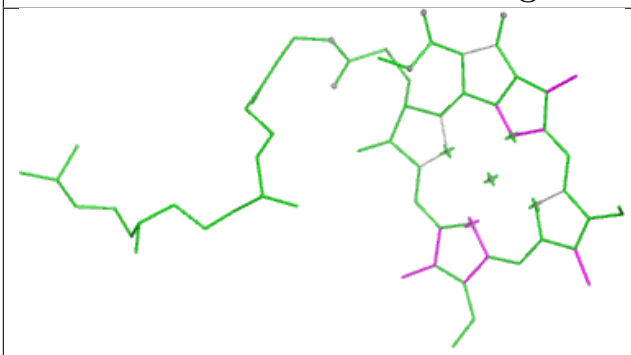


Rings

Ligand CLA 1 1605



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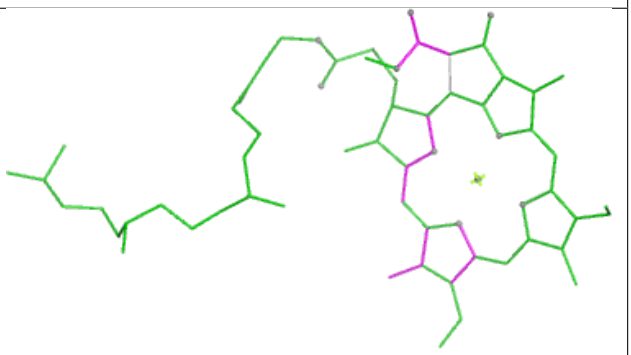
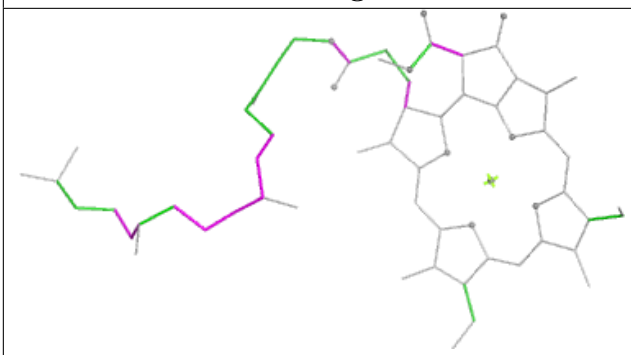


Bond angles



Torsions

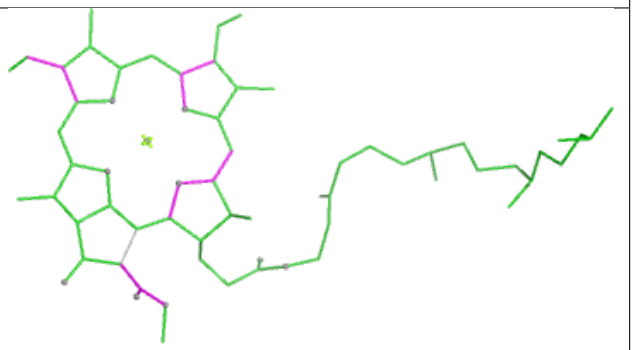


Rings

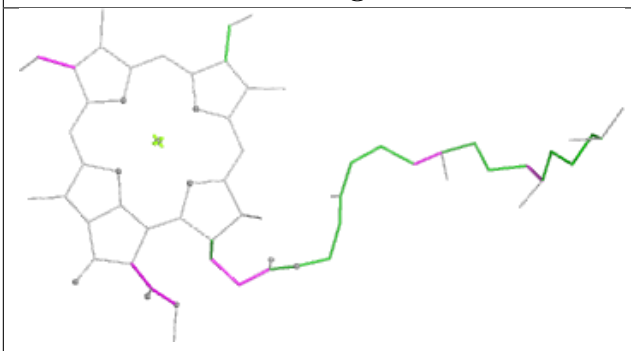
Ligand CLA 2 804



Bond lengths



Bond angles



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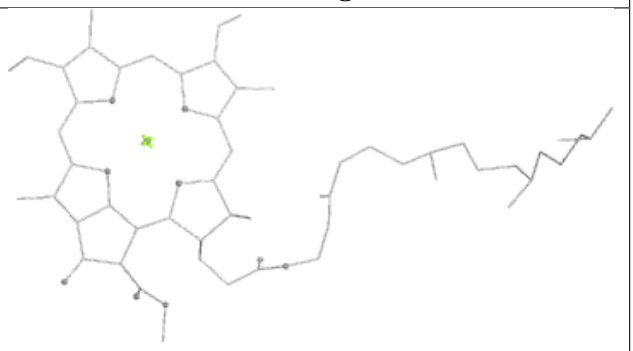
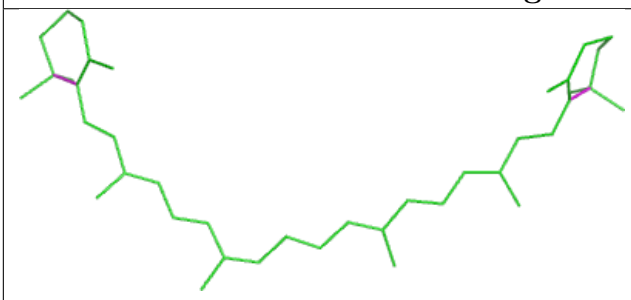


Rings

Ligand BCR F 205



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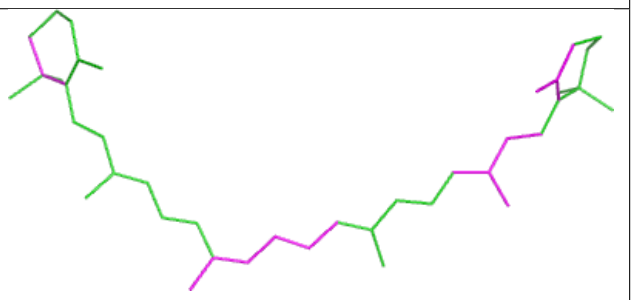


Bond angles

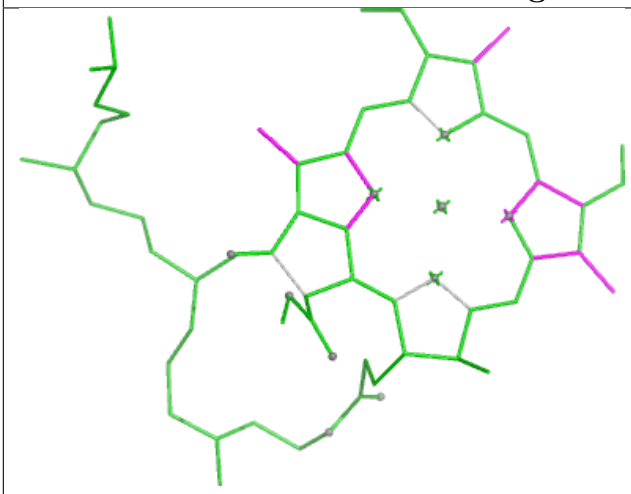


Torsions



Rings

Ligand CLA 2 833



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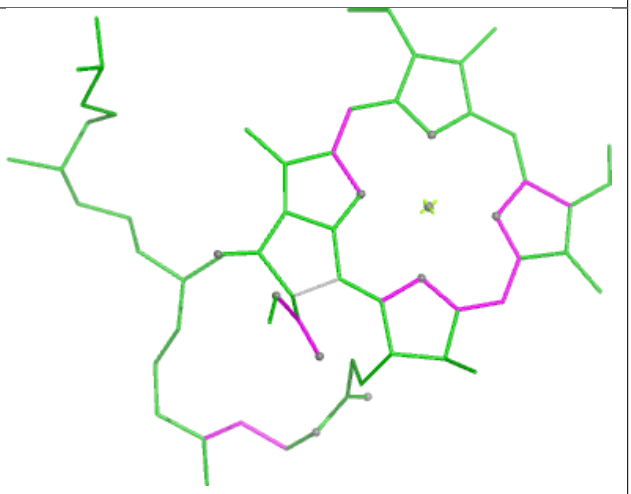
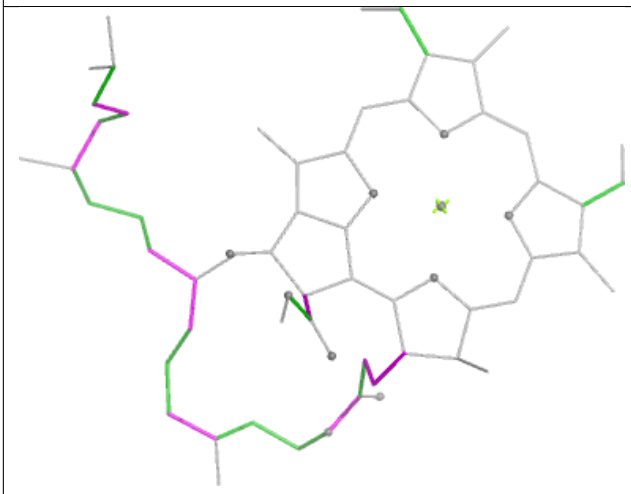
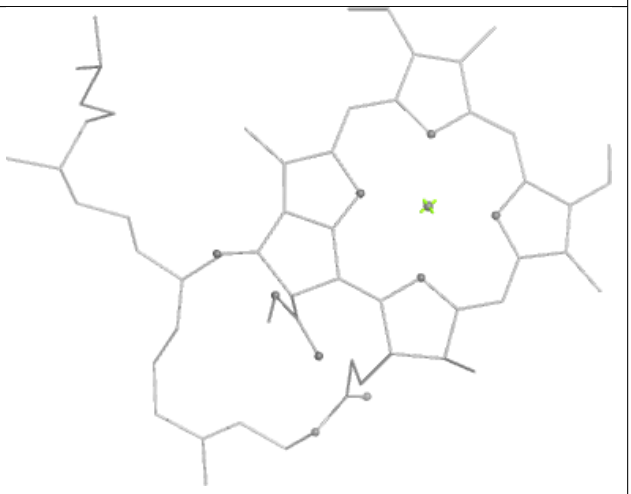


Bond angles

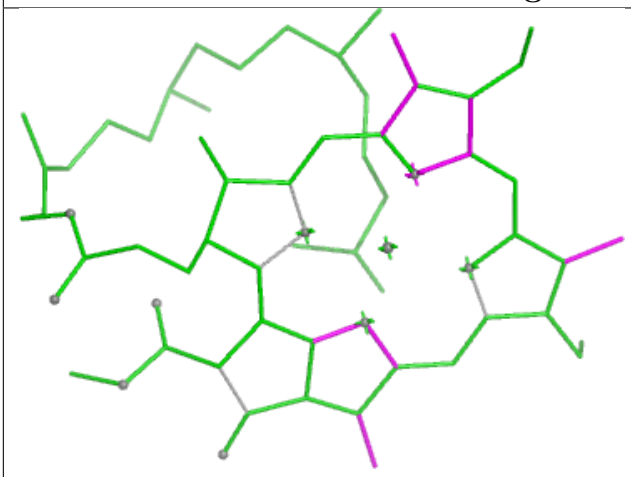


Torsions



Rings

Ligand CLA B 806



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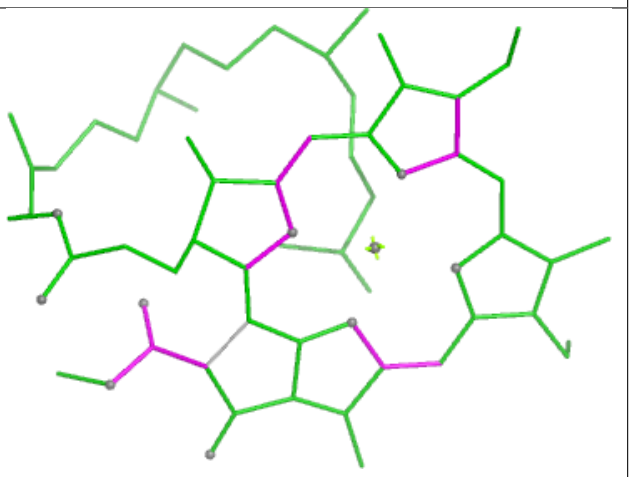
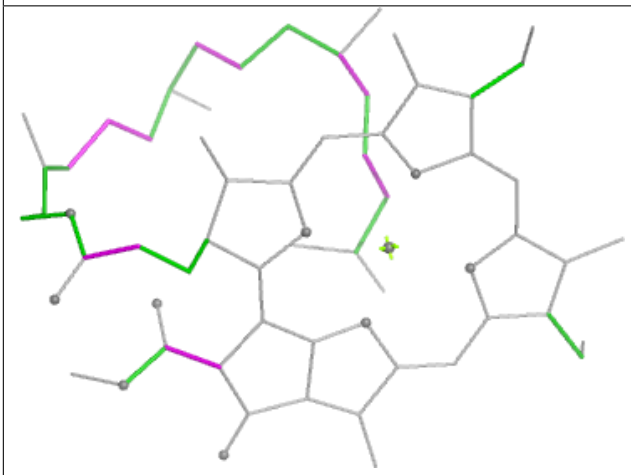


Bond angles



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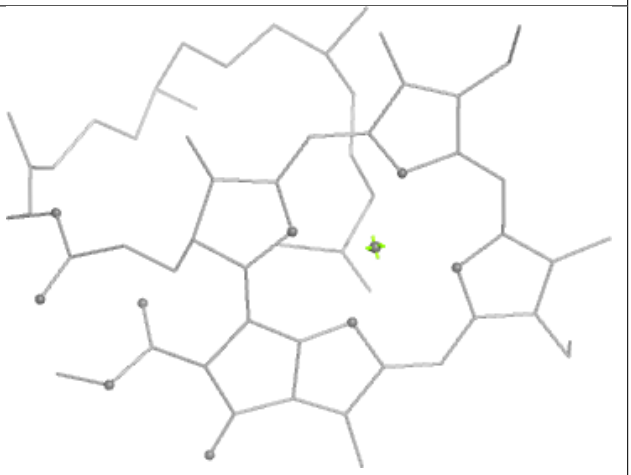
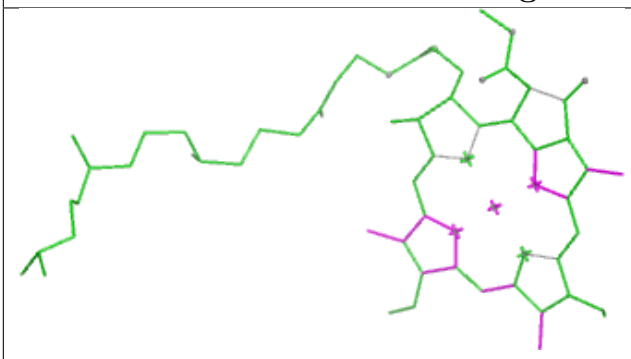
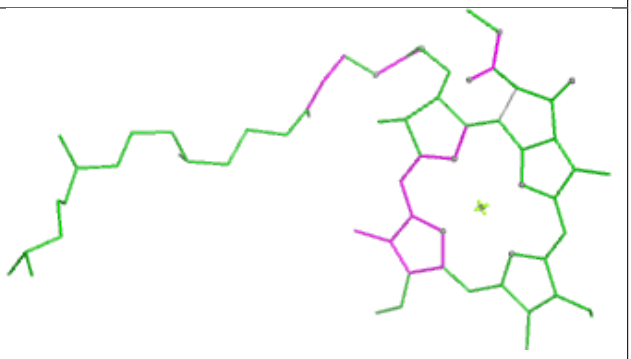


Rings

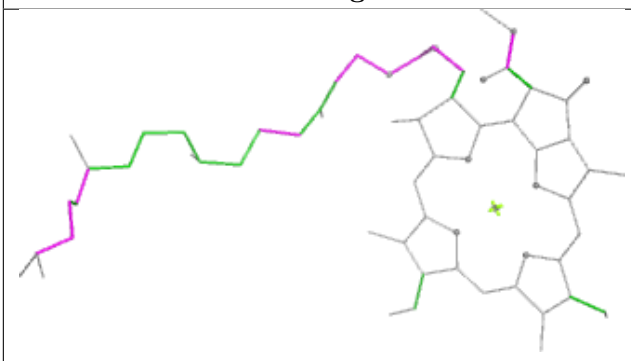
Ligand CLA 1 1603



Bond lengths



Bond angles



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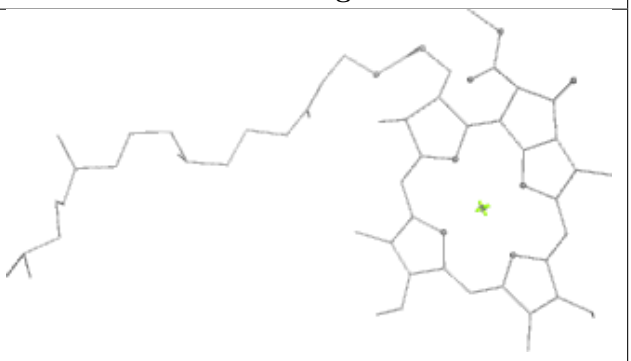
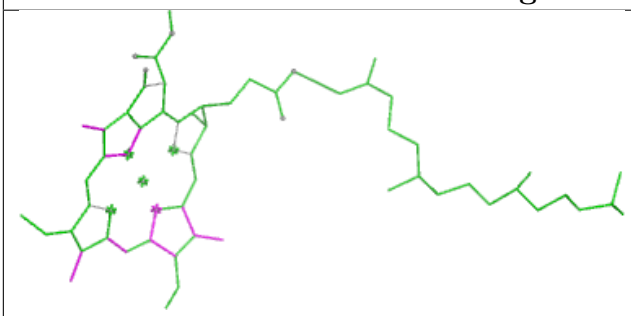


Rings

Ligand CLA 1 1604



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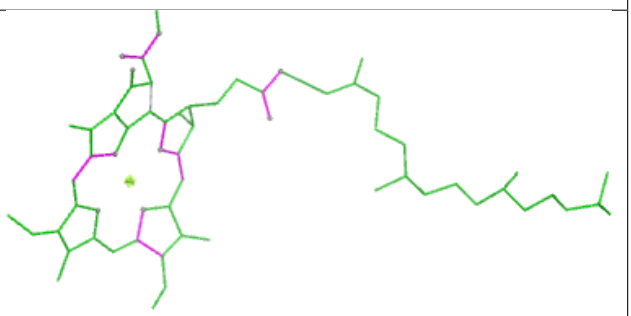
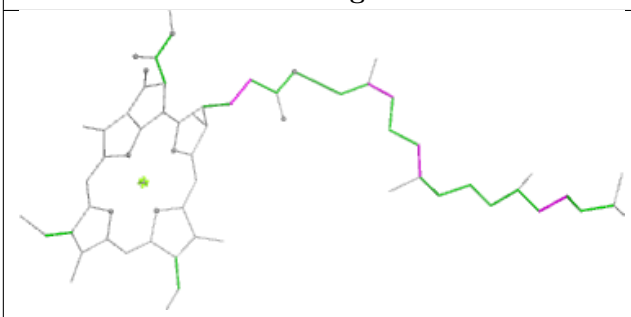


Bond angles



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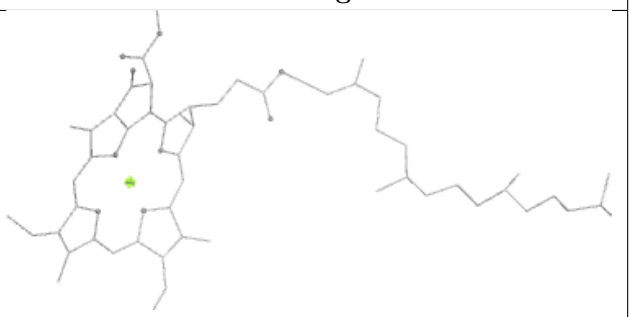
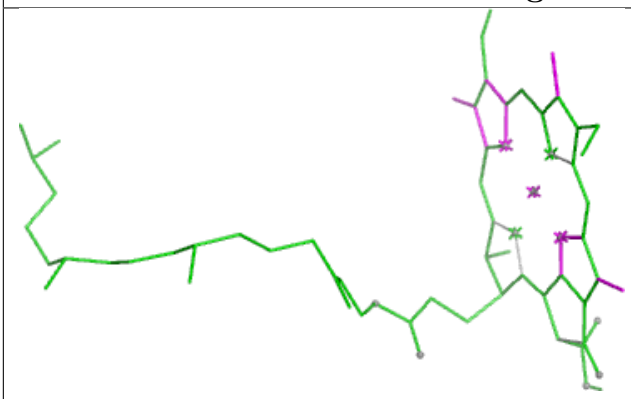


Rings

Ligand CLA L 204



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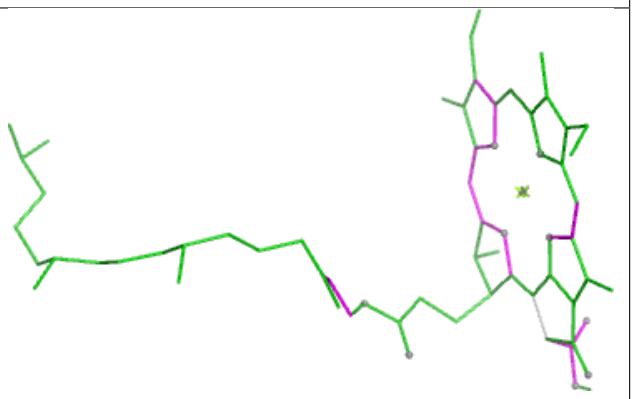
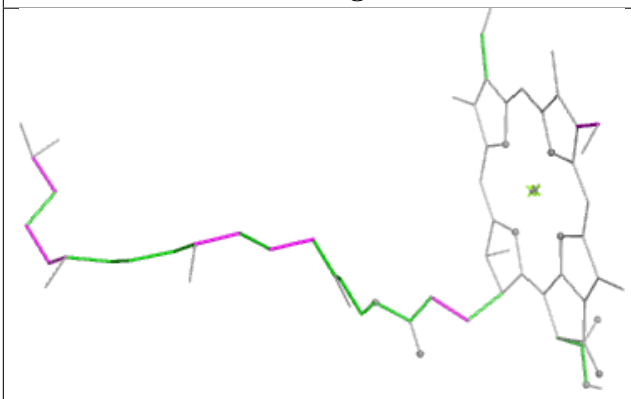


Bond angles

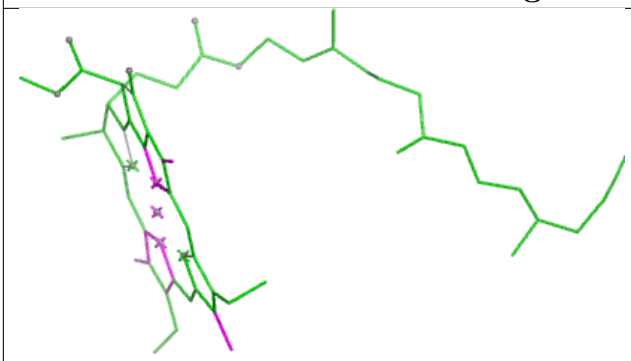


Torsions



Rings

Ligand CLA A 831



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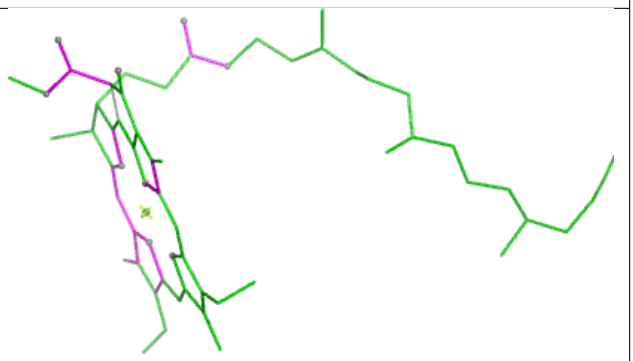
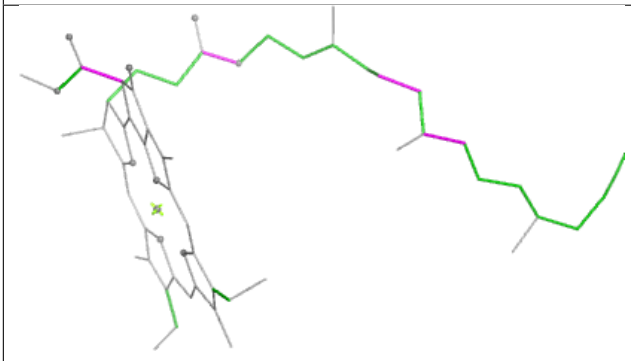
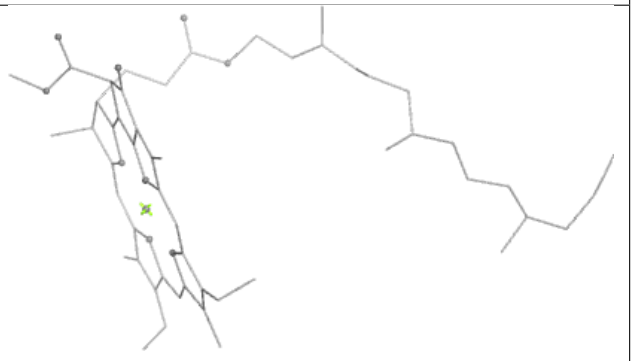


Bond angles

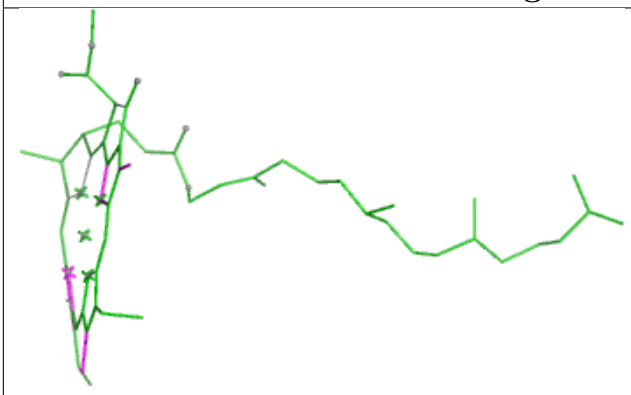


Torsions

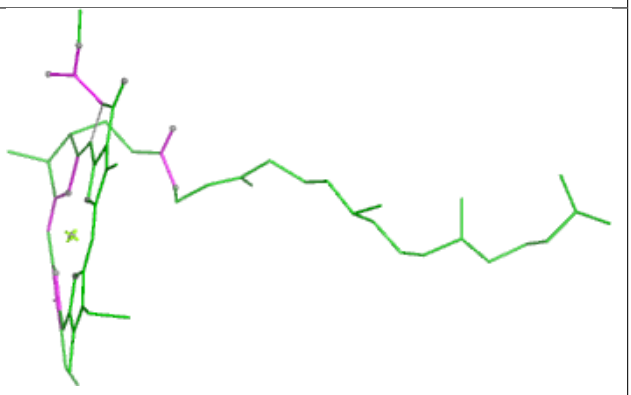


Rings

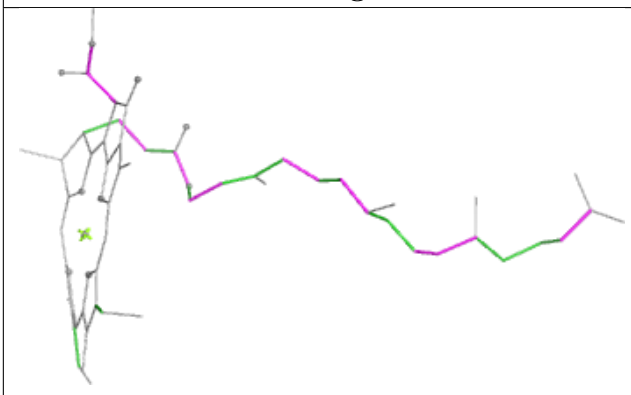
Ligand CLA A 829



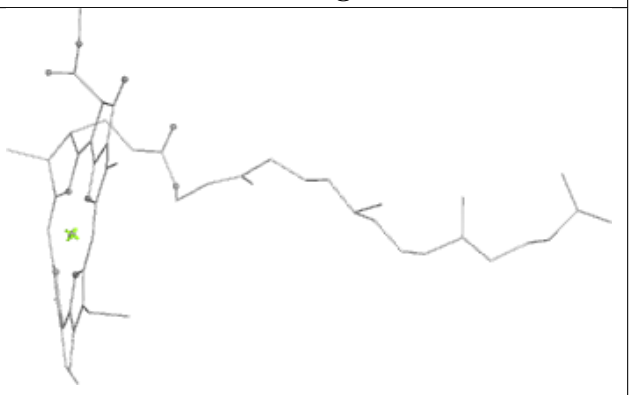
Bond lengths



Bond angles

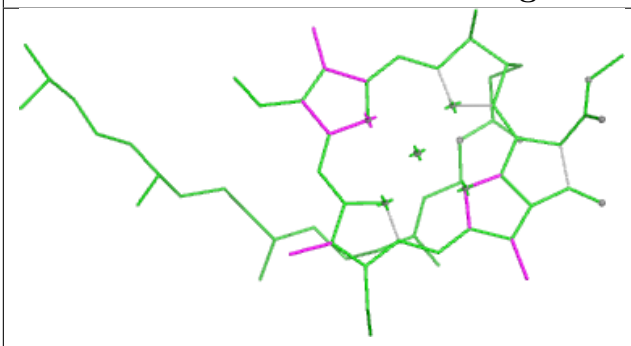


Torsions



Rings

Ligand CLA 1 1642



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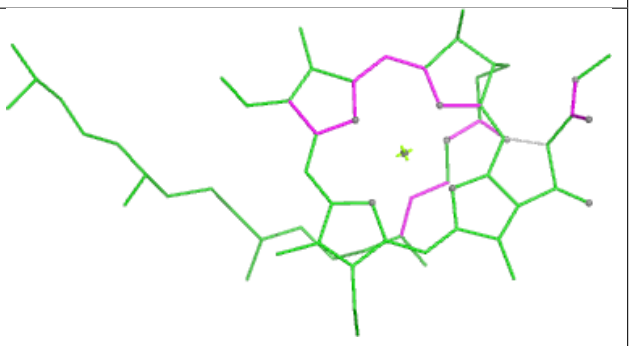
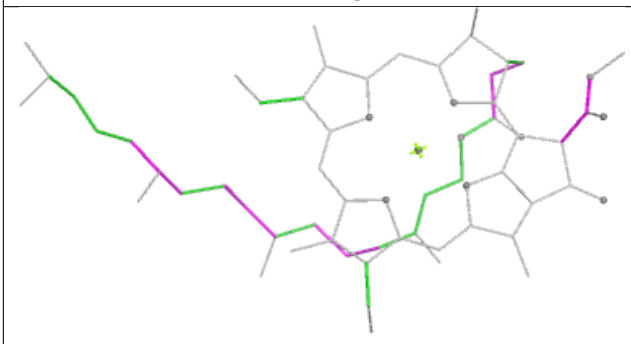


Bond angles



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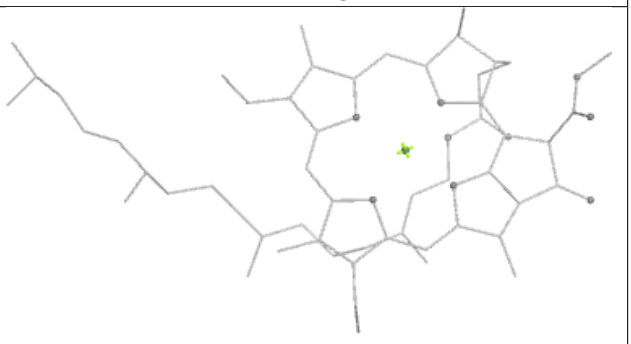
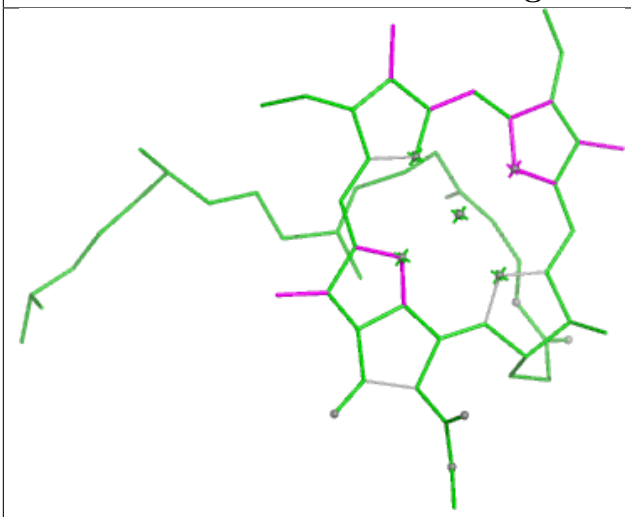


Rings

Ligand CLA B 827



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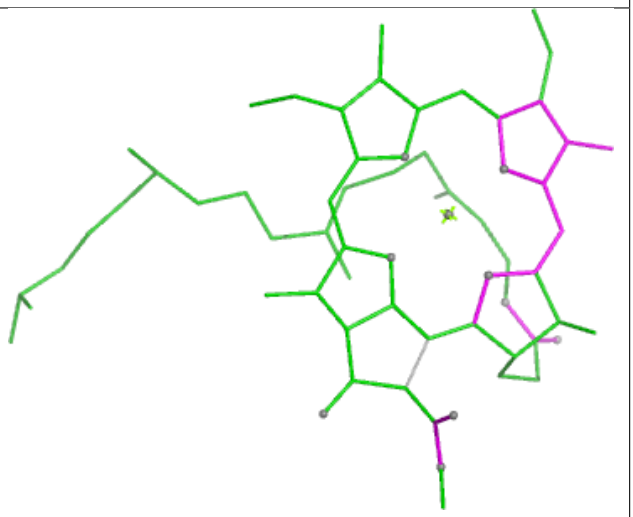
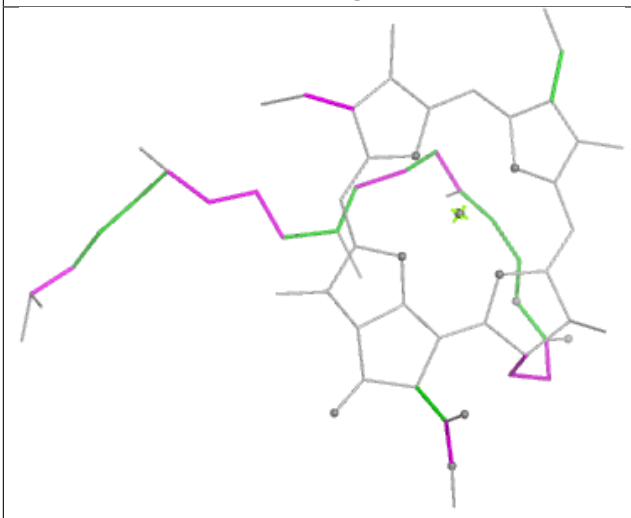


Bond angles



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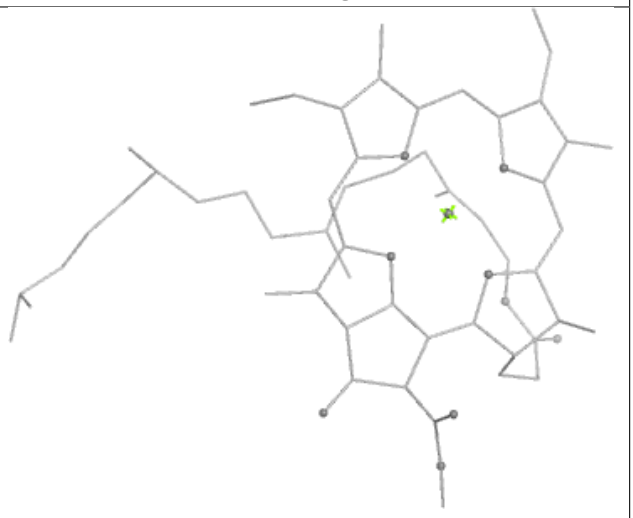
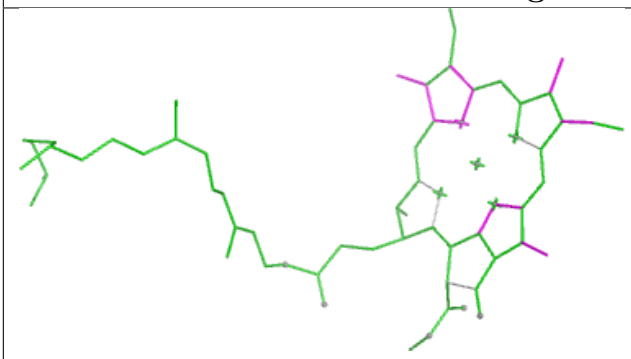


Rings

Ligand CLA b 810



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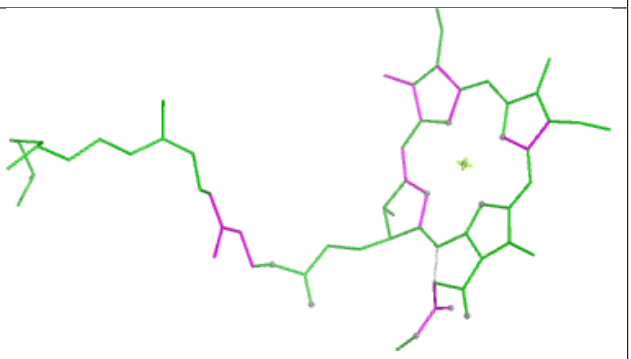
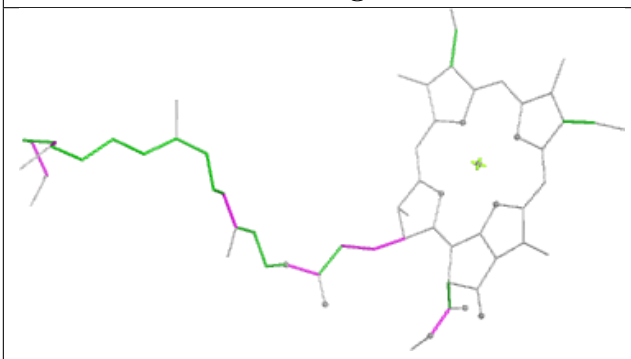


Bond angles



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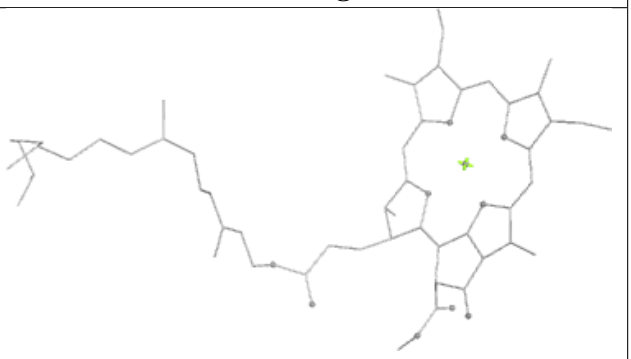
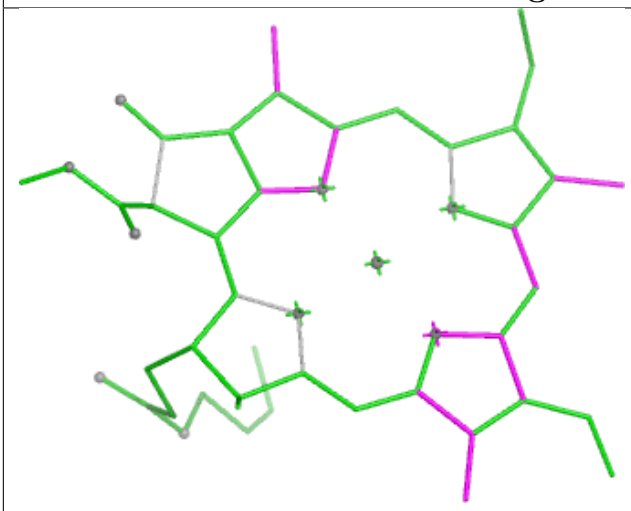


Rings

Ligand CLA 2 832



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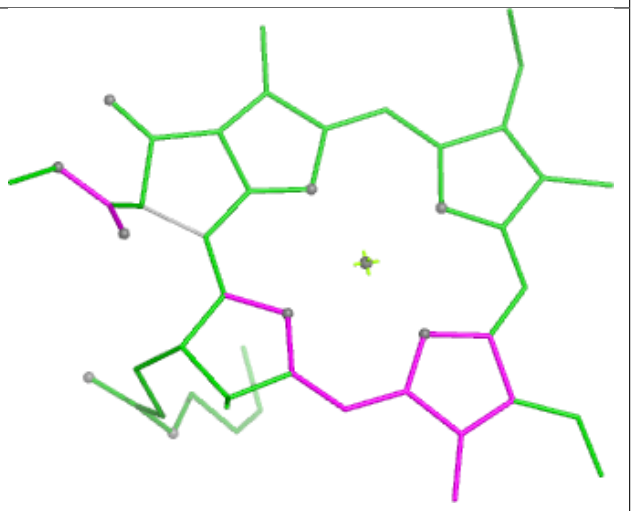
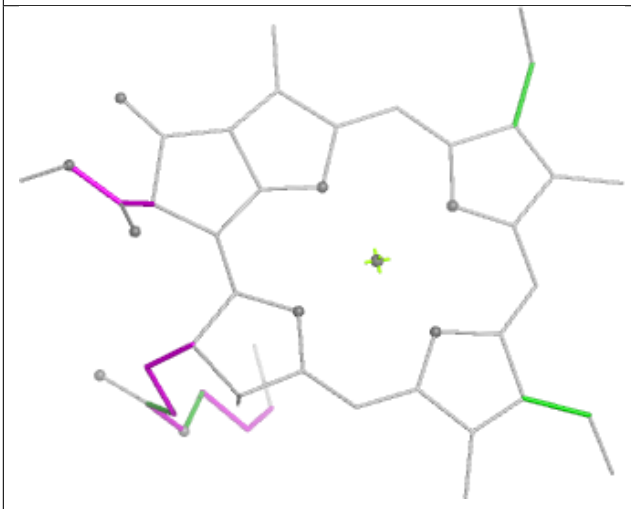


Bond angles



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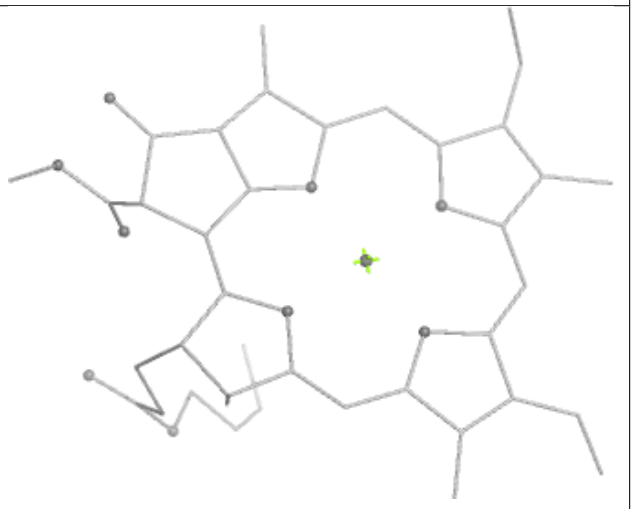
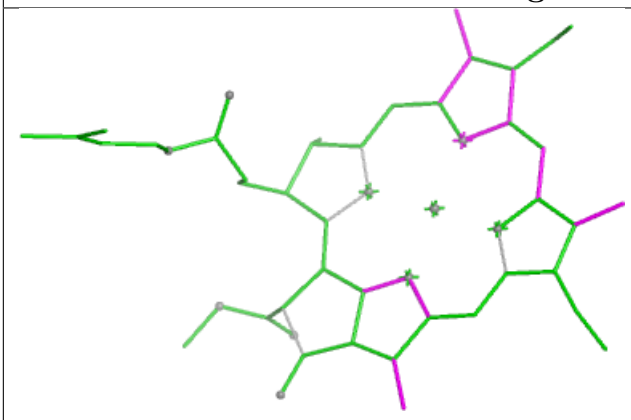


Rings

Ligand CLA b 836



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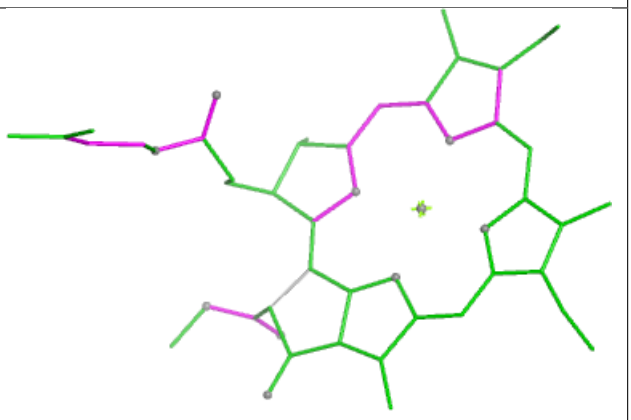
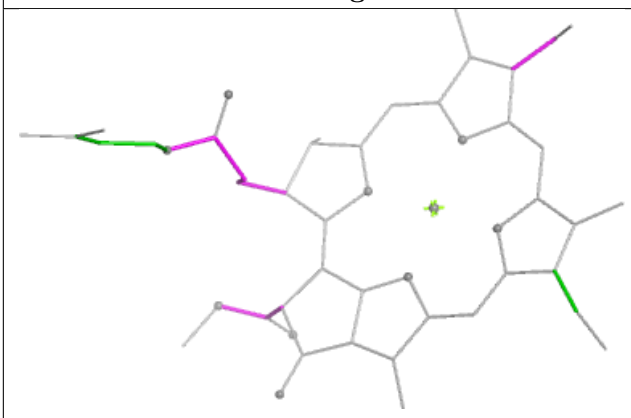


Bond angles



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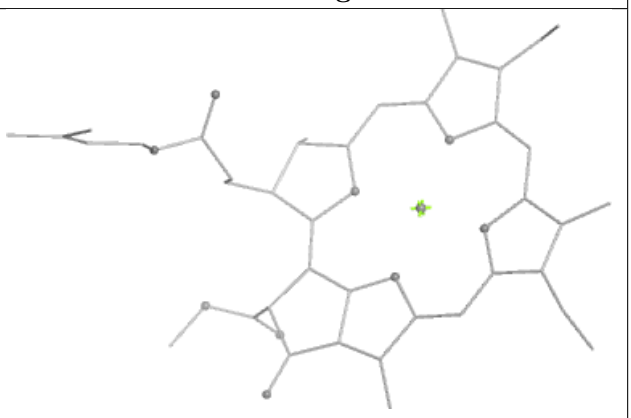
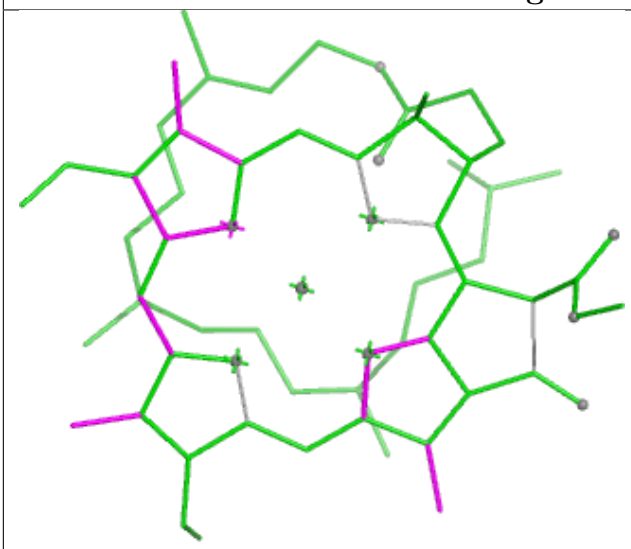


Rings

Ligand CLA L 203



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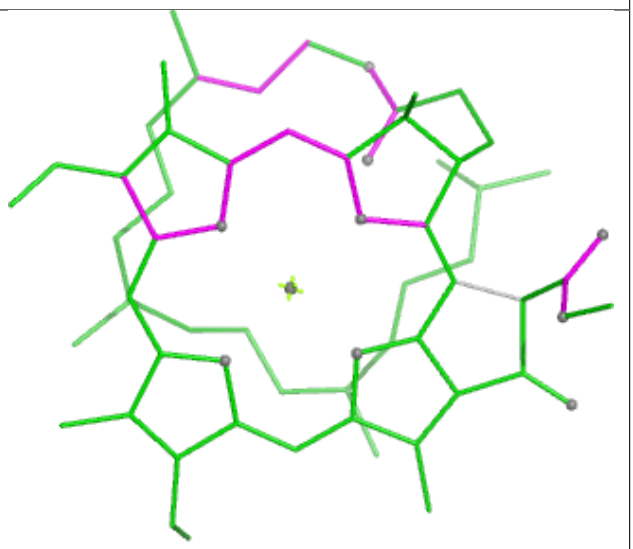
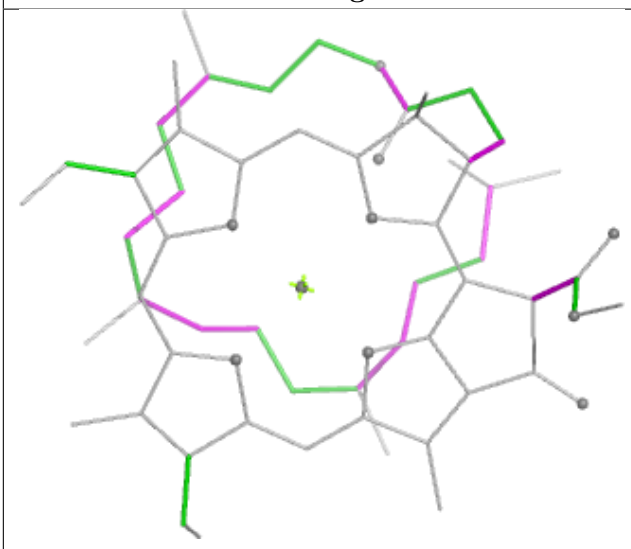


Bond angles



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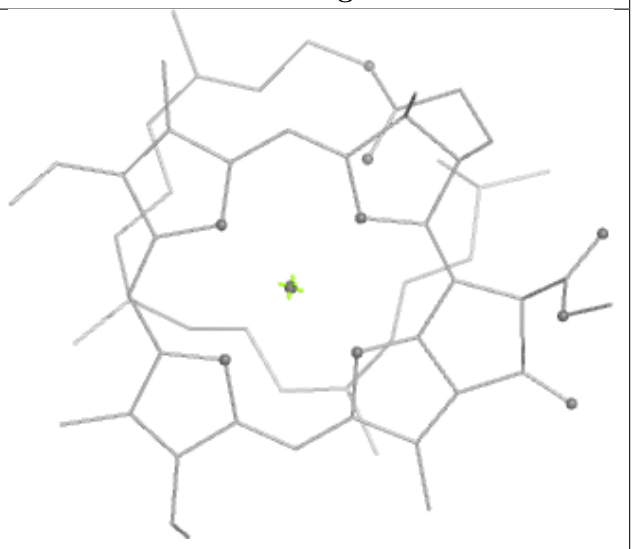
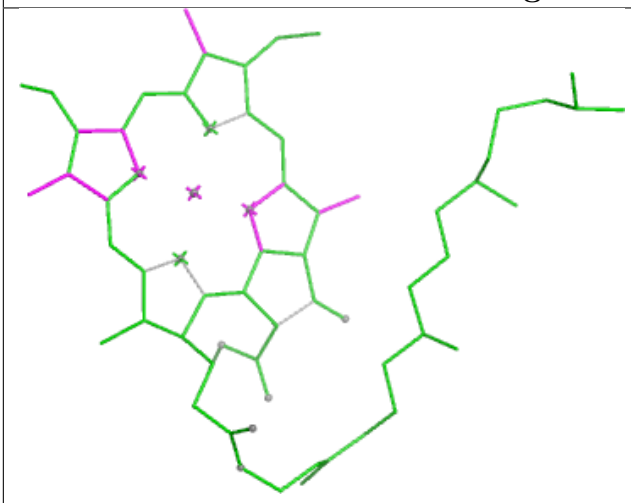


Rings

Ligand CLA A 826



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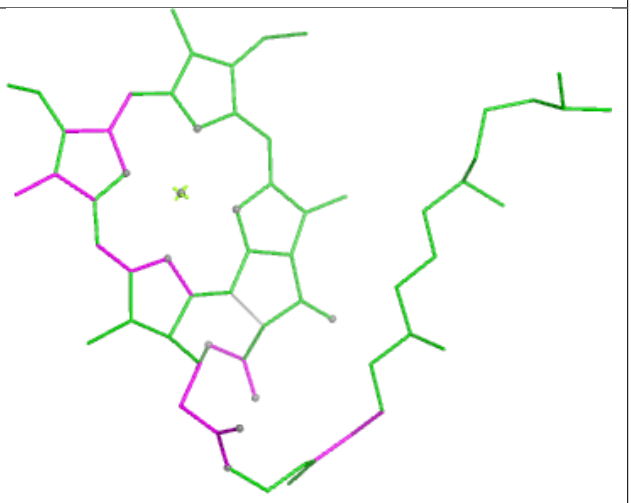
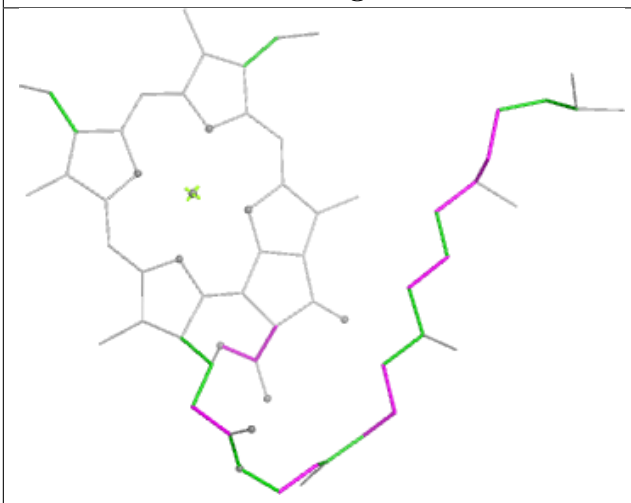


Bond angles



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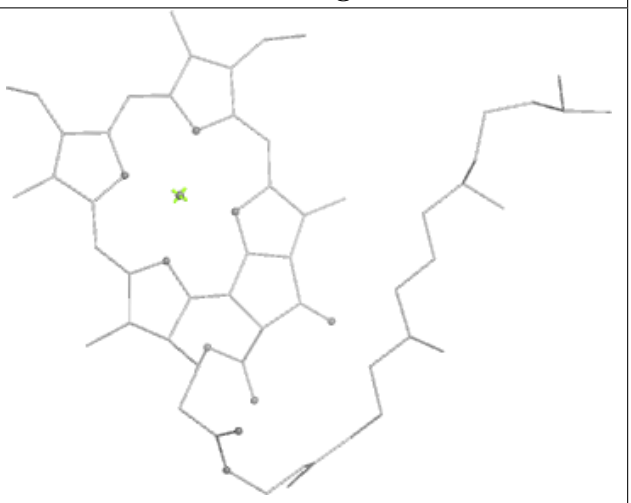
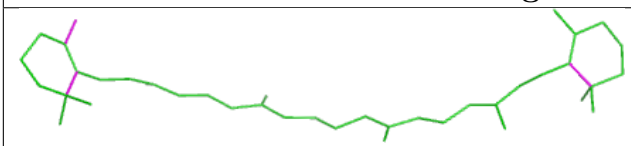


Rings

Ligand BCR A 856



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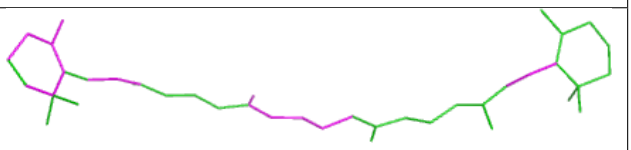
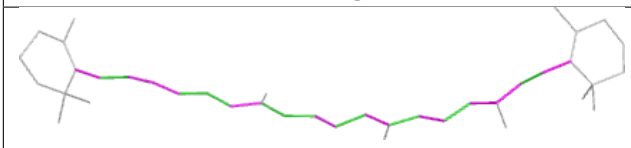


Bond angles



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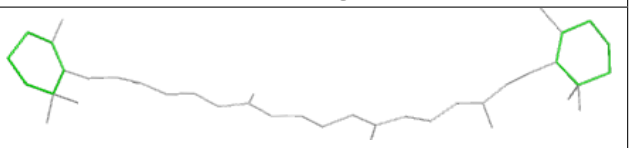
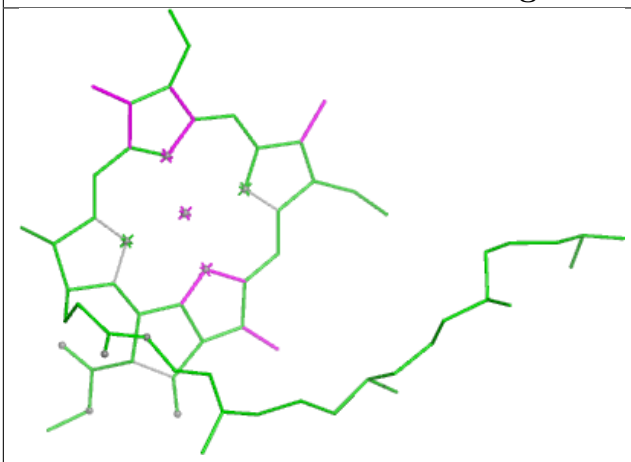


Rings

Ligand CLA 1 1631



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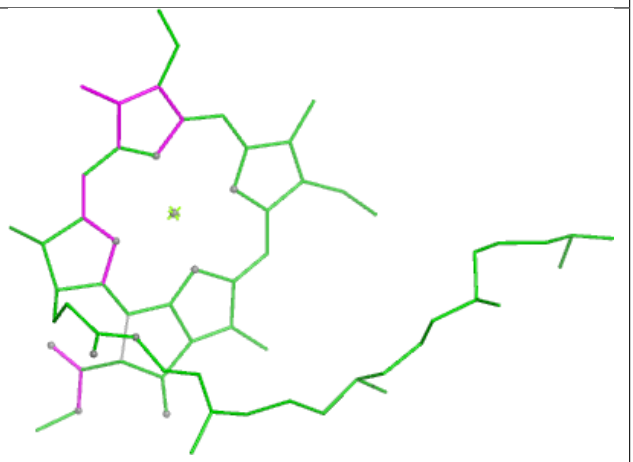
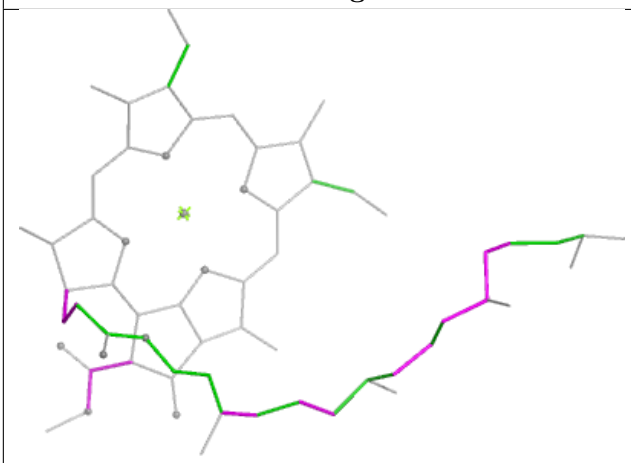
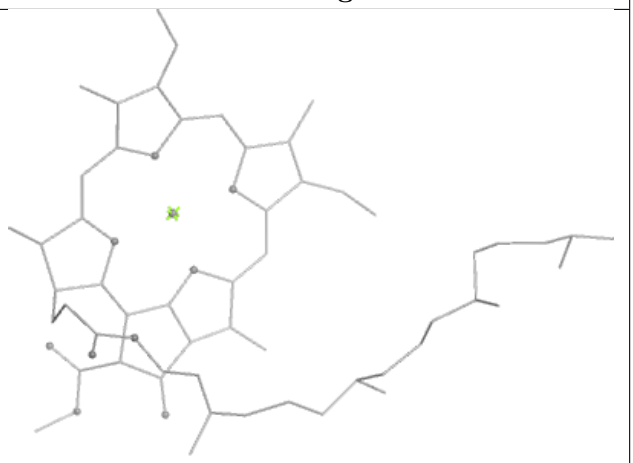


Bond angles

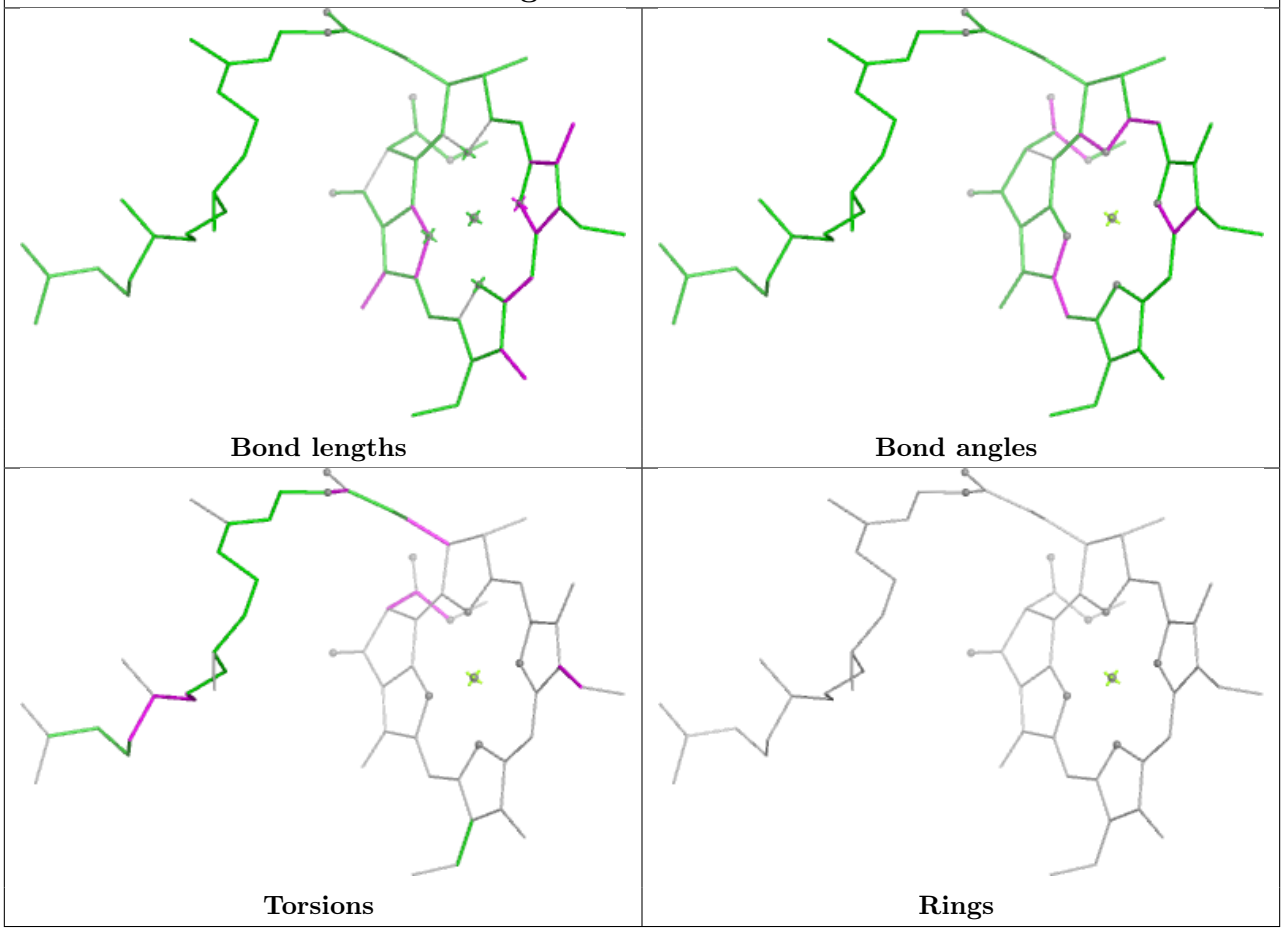


Torsions



Rings

Ligand CLA 1 1616



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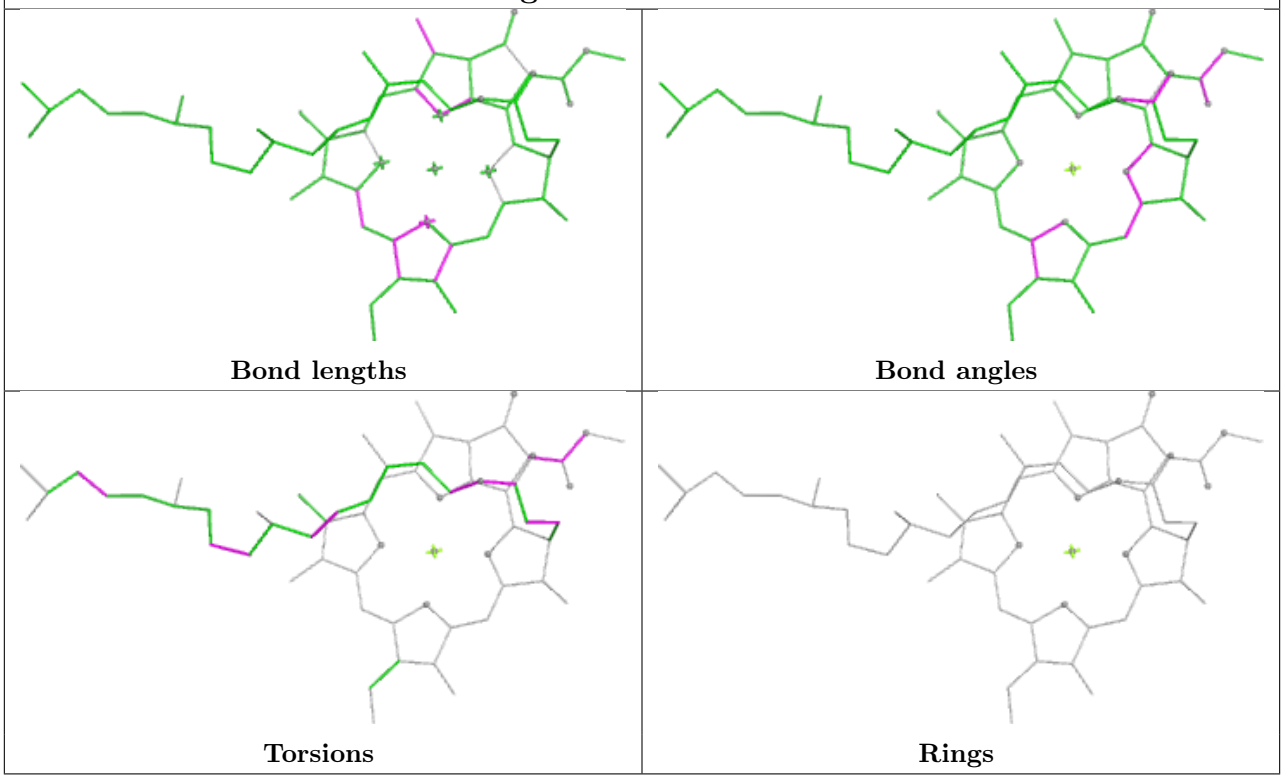
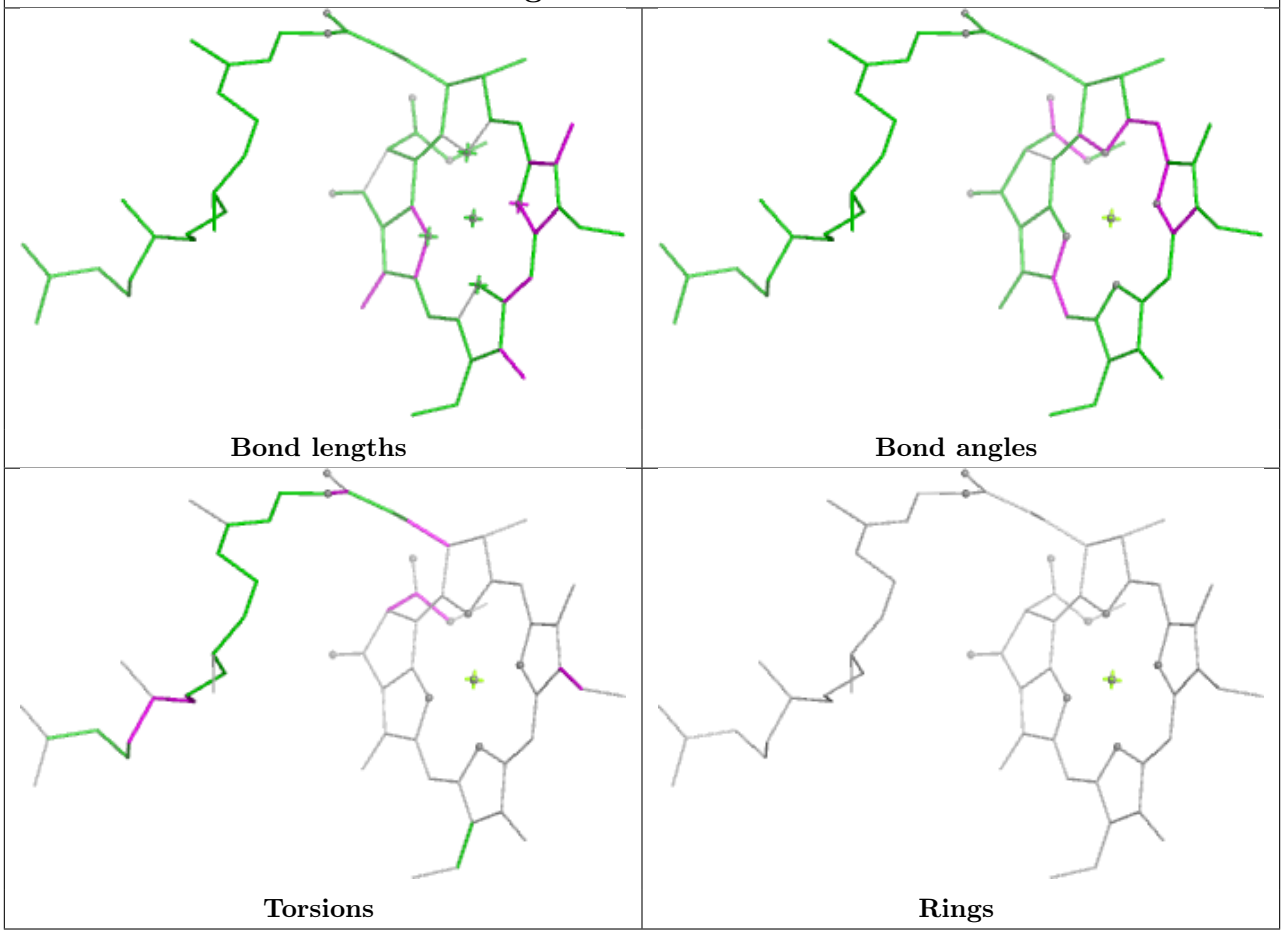


Ligand CLA A 815



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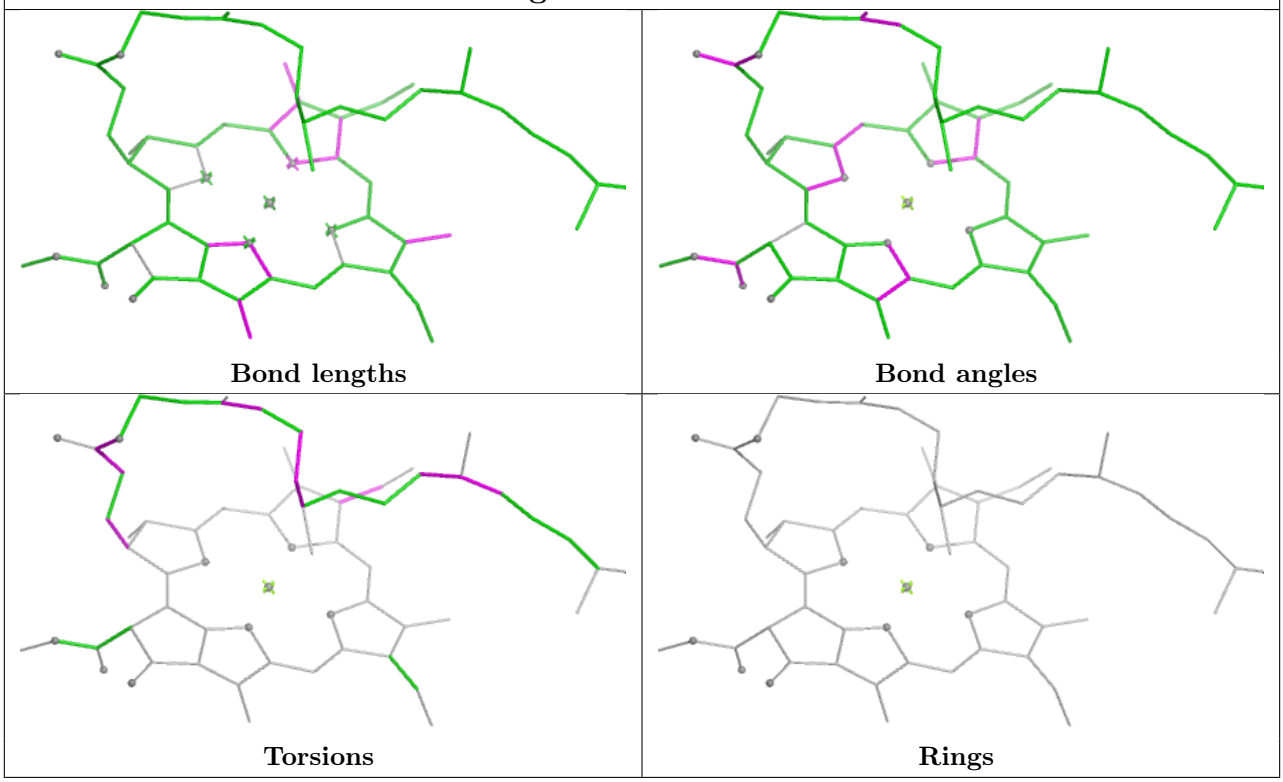
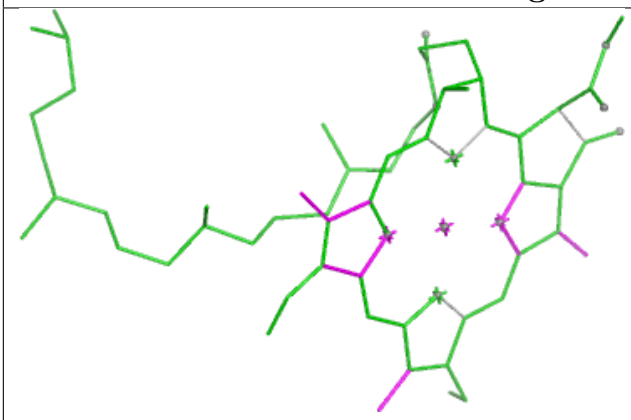
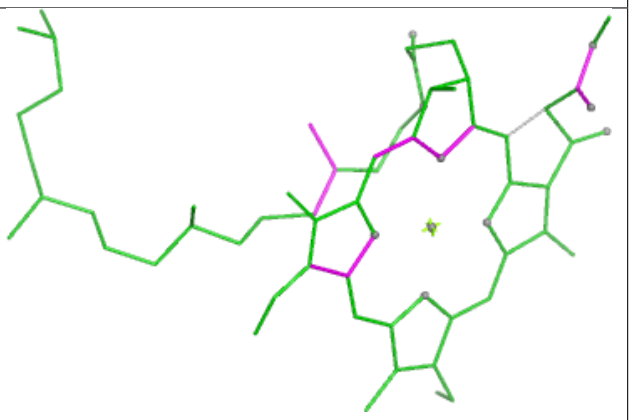


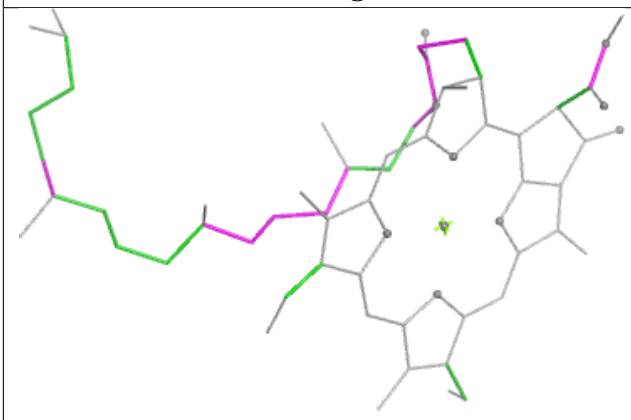
Ligand CLA a 843



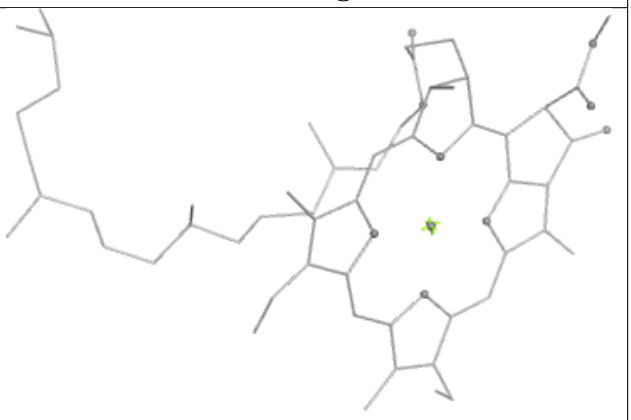
Bond lengths



Bond angles

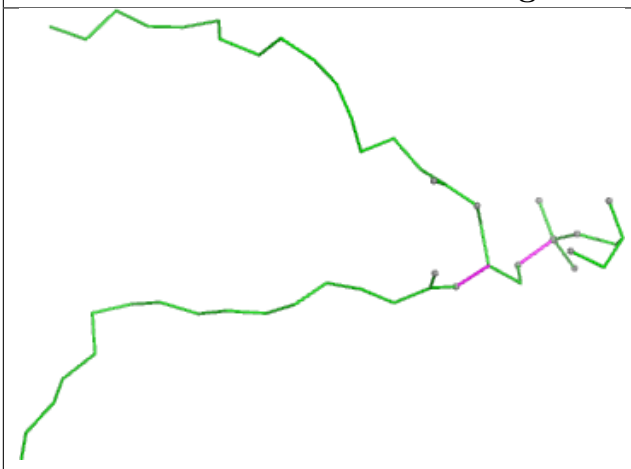


Torsions



Rings

Ligand LHG M 101



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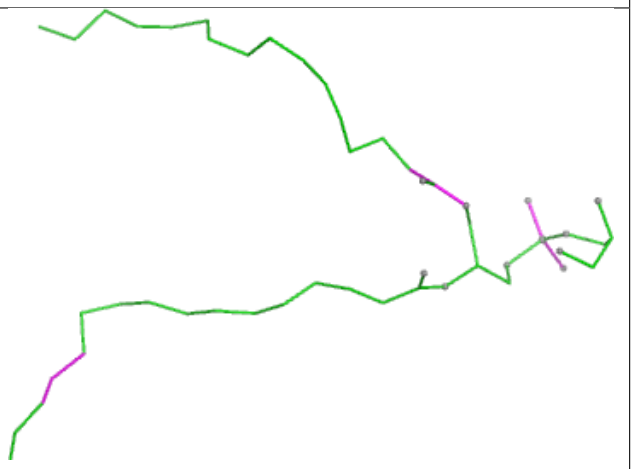
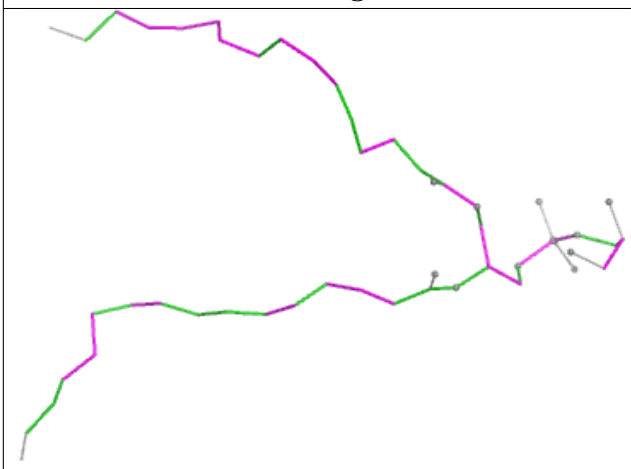


Bond angles

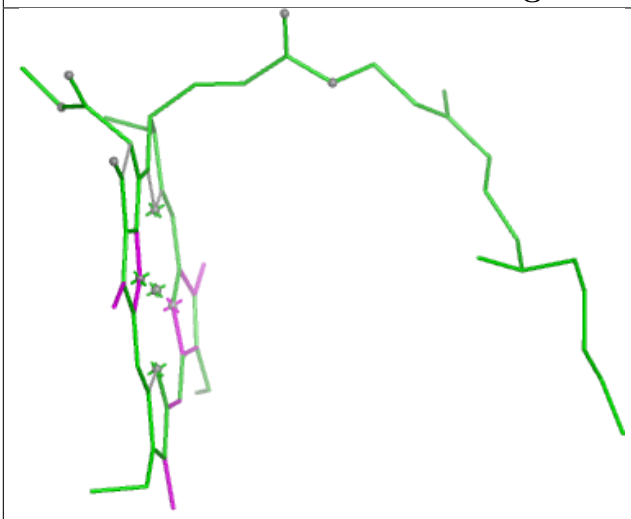


Torsions

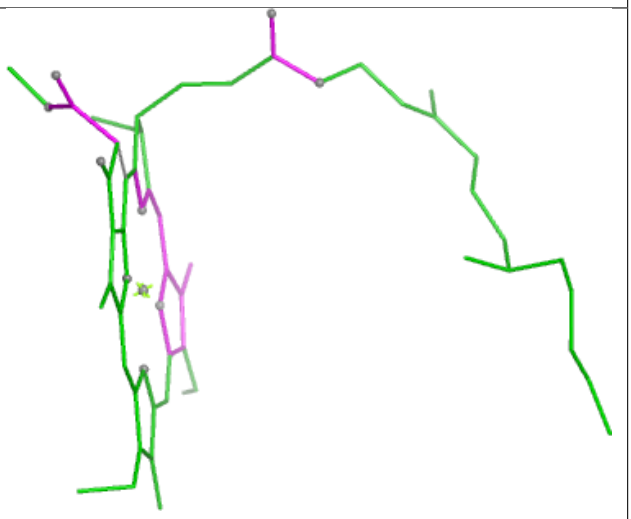


Rings

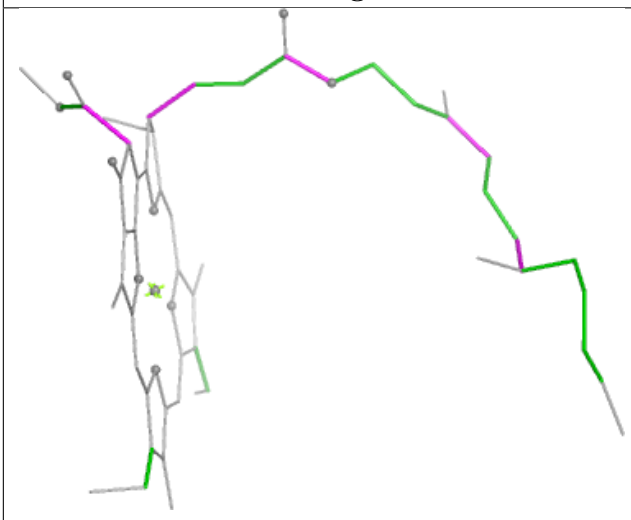
Ligand CLA A 805



Bond lengths



Bond angles

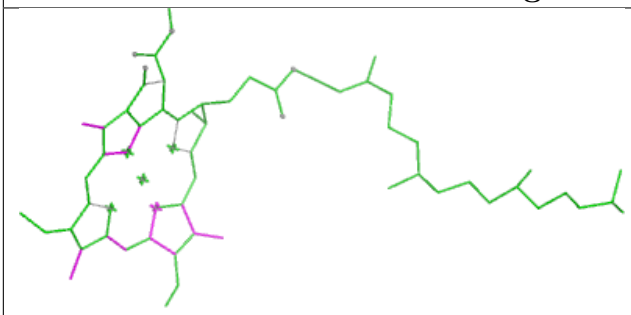


Torsions

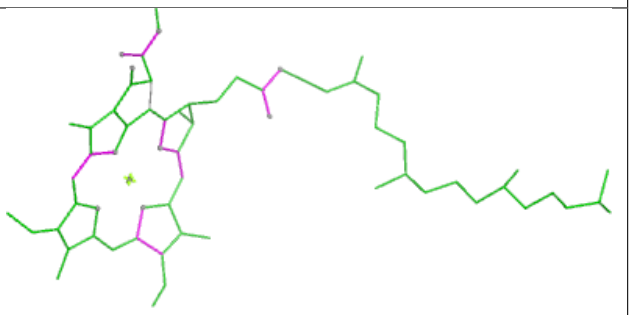


Rings

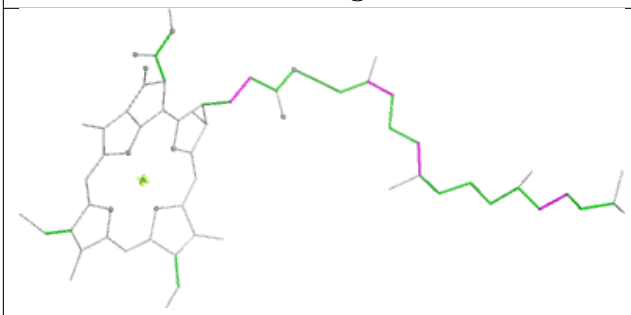
Ligand CLA A 803



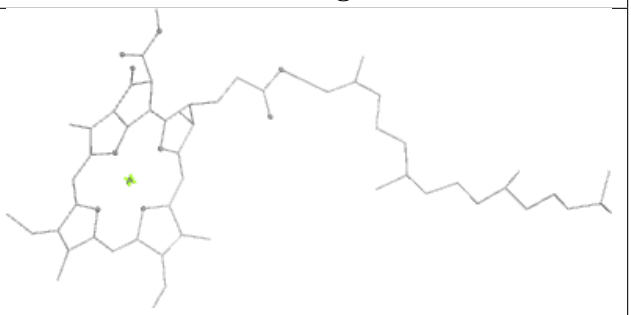
Bond lengths



Bond angles

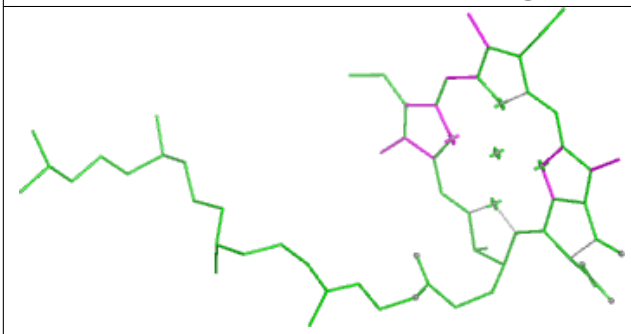


Torsions

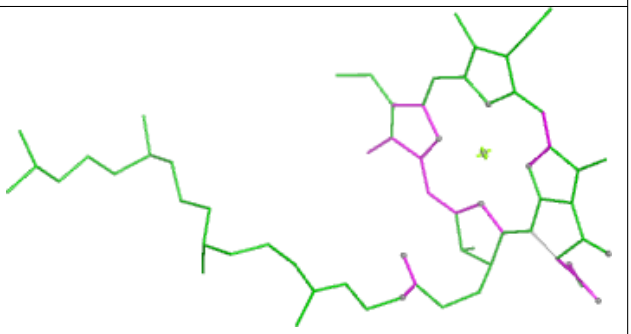


Rings

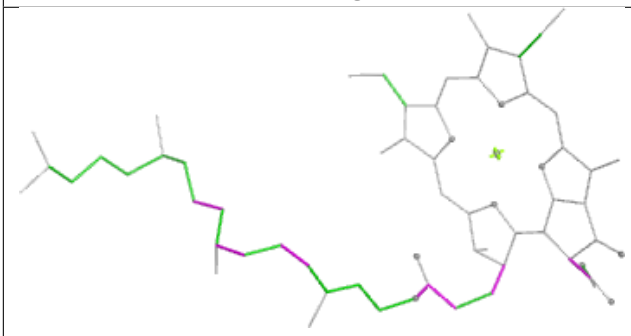
Ligand CLA 1 1610



Bond lengths



Bond angles

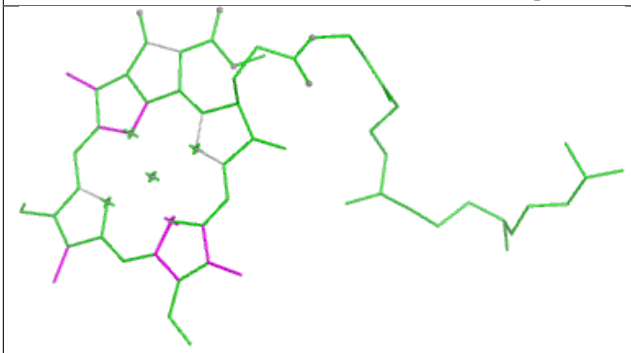


Torsions



Rings

Ligand CLA a 804



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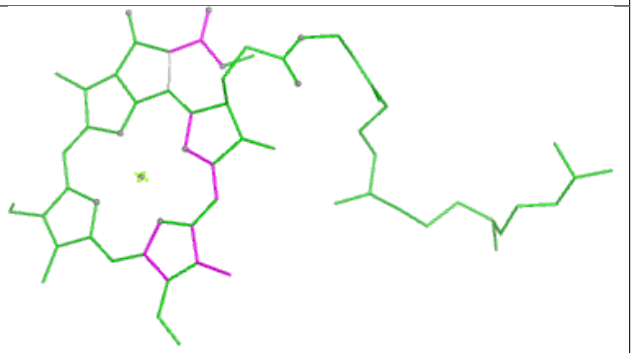
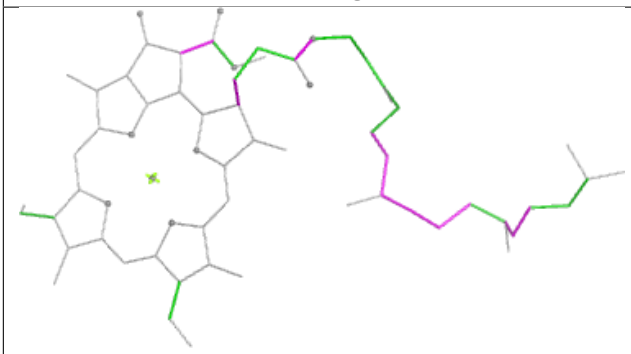


Bond angles

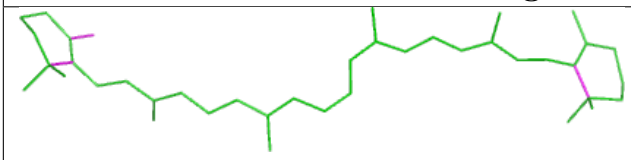


Torsions



Rings

Ligand BCR B 846



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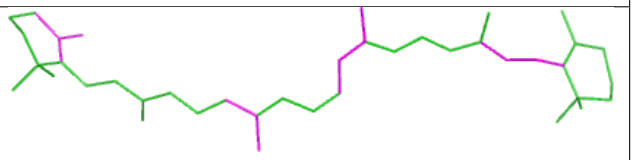
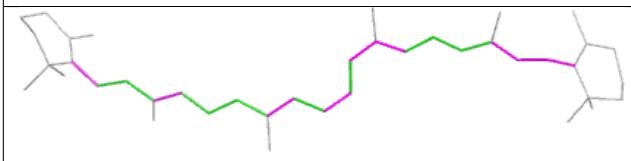
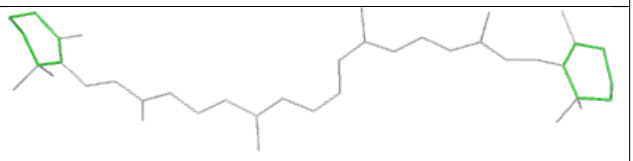


Bond angles

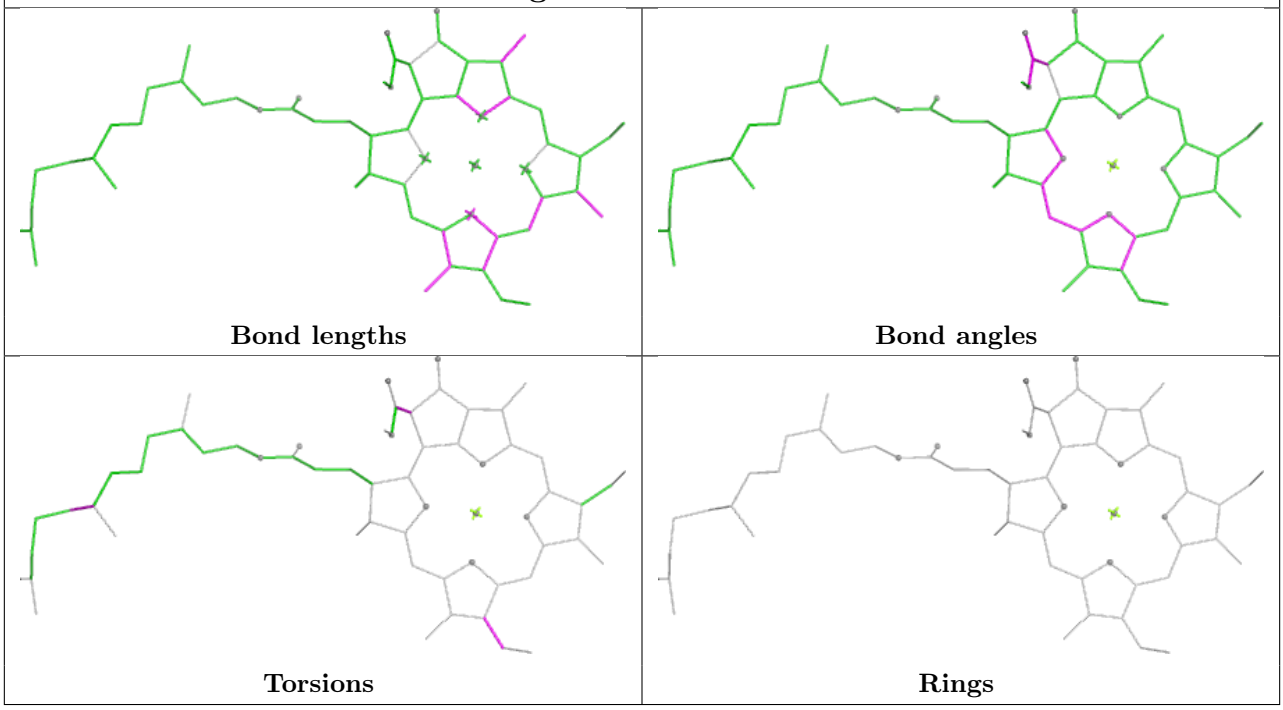


Torsions

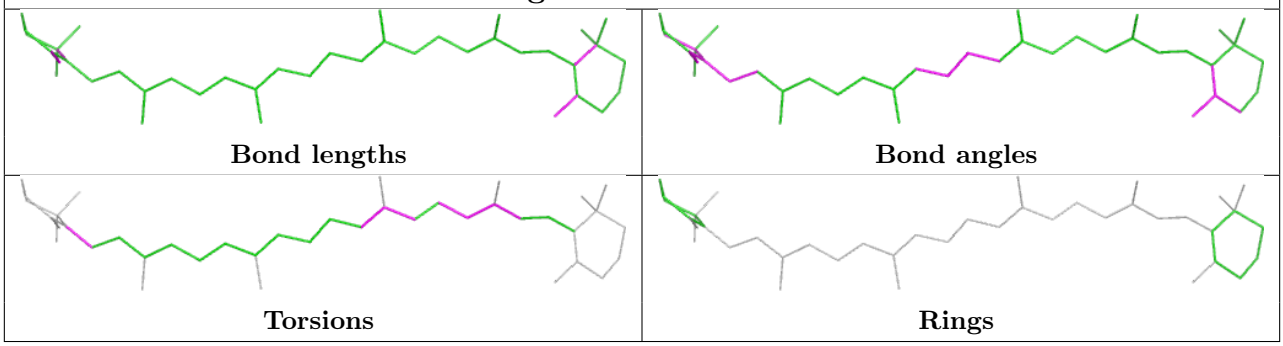


Rings

Ligand CLA 2 838



Ligand BCR a 850



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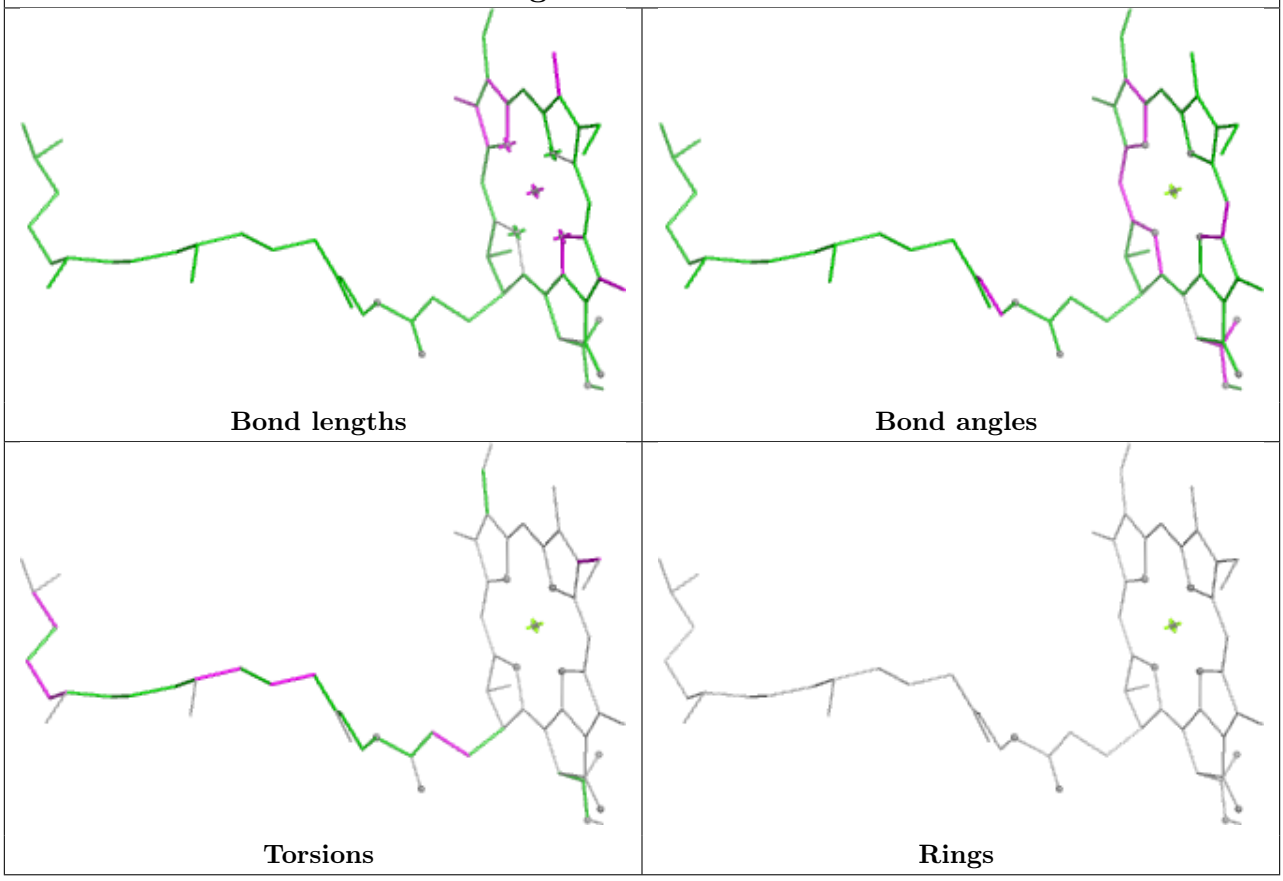

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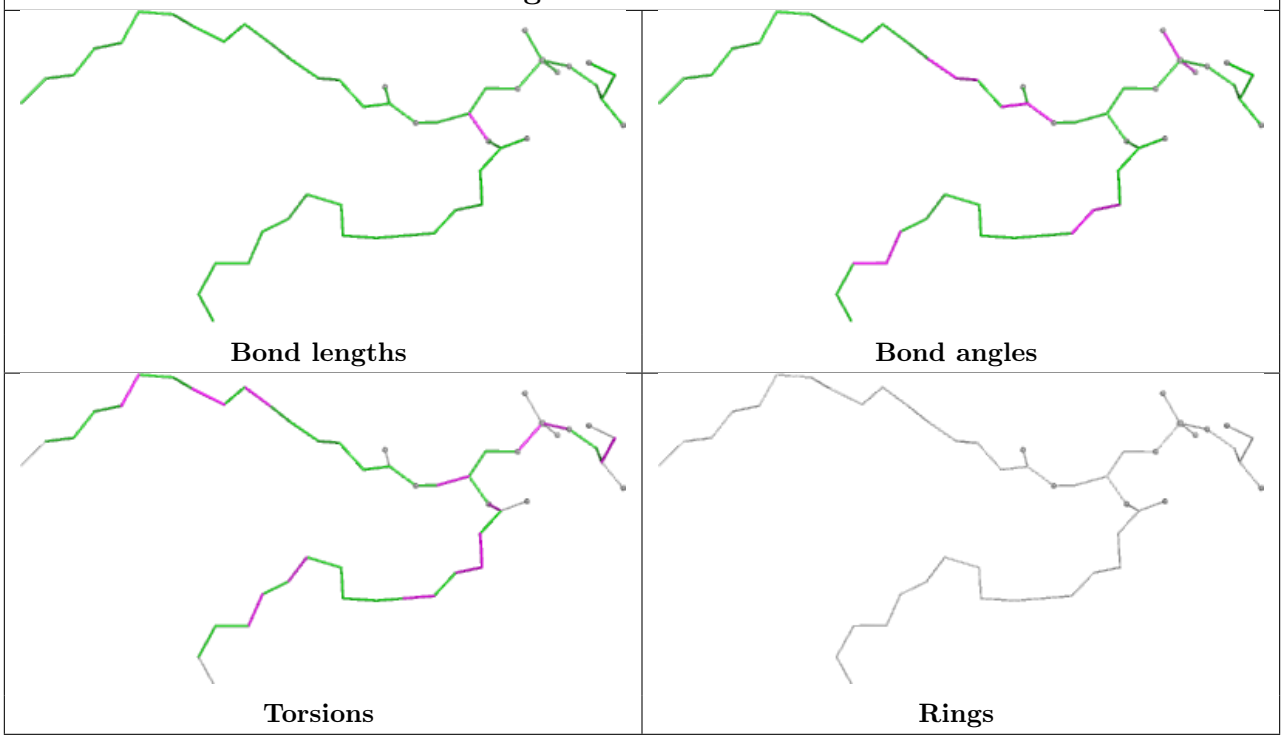

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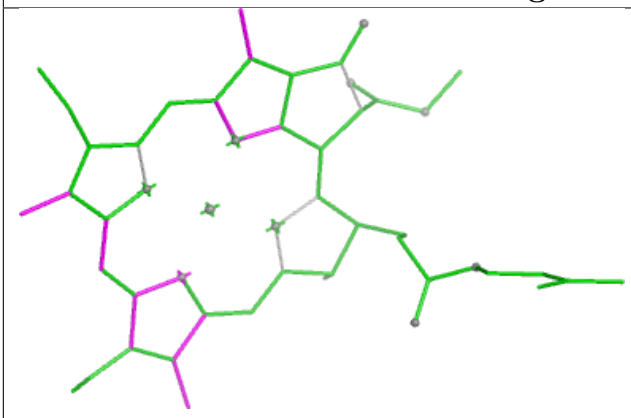
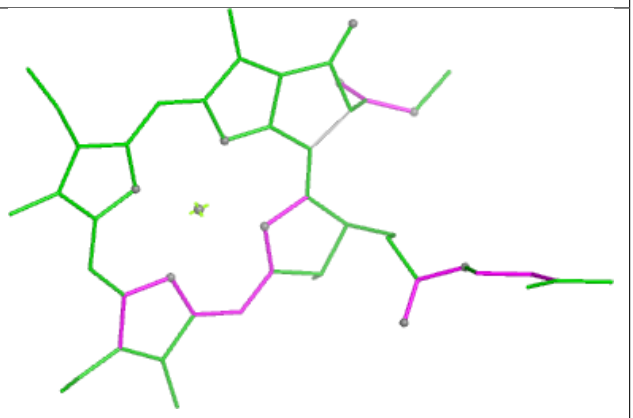
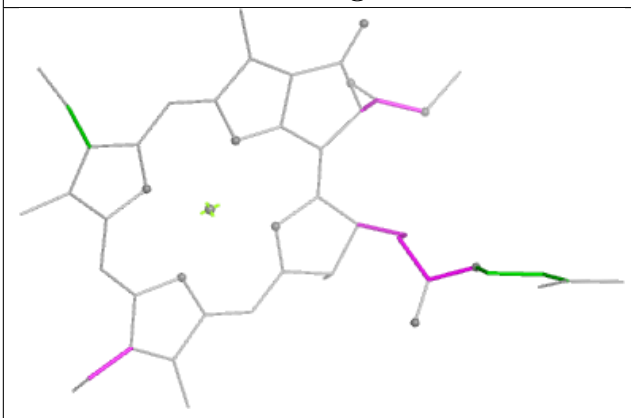


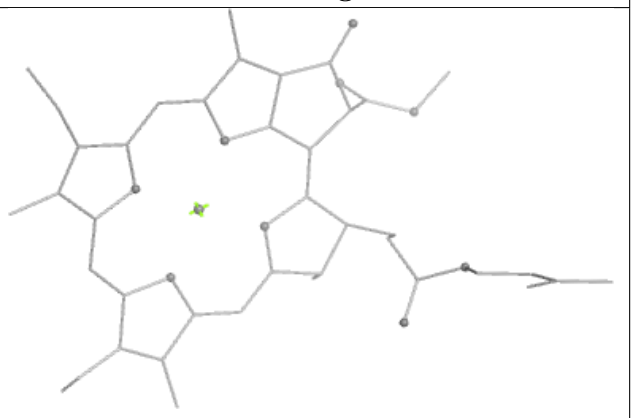
Bond lengths



Bond angles

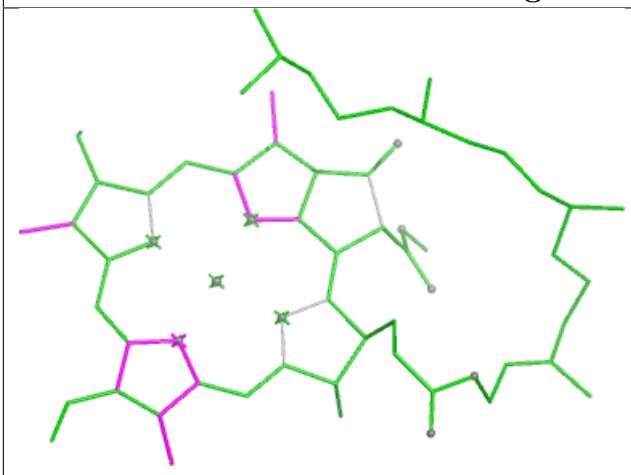


Torsions



Rings

Ligand CLA B 805



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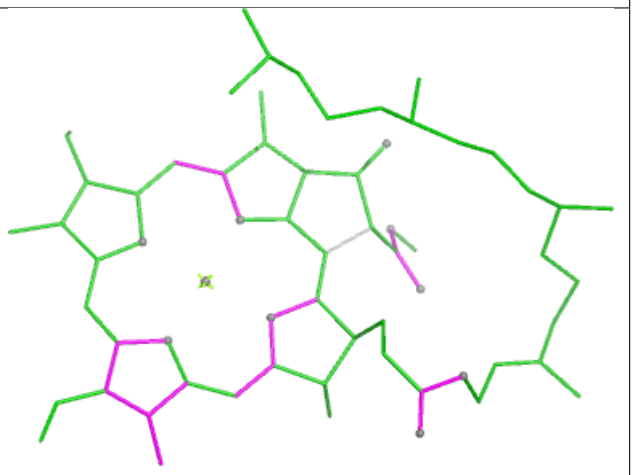
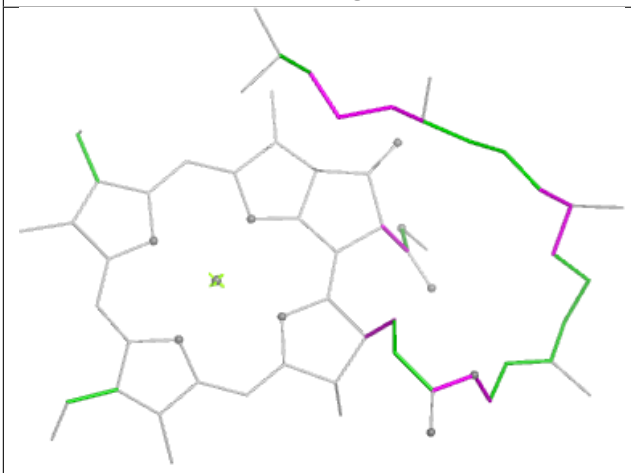
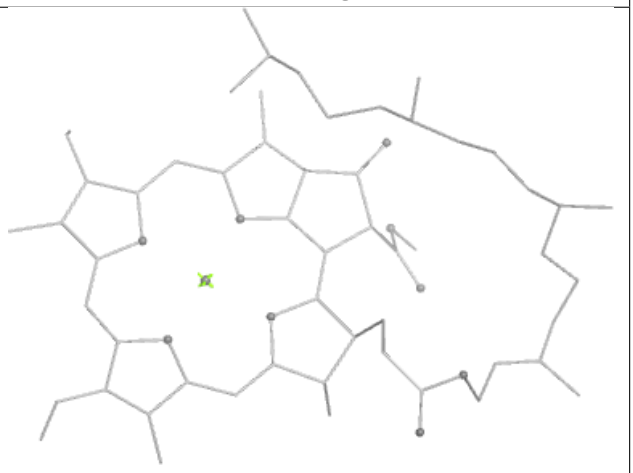


Bond angles

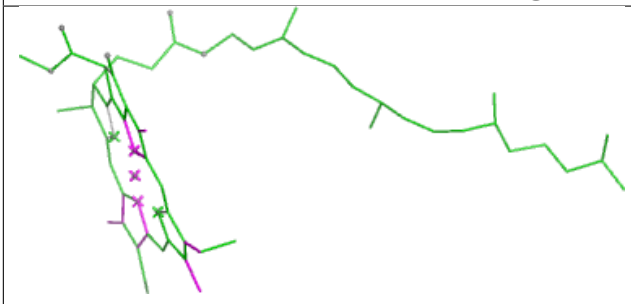


Torsions



Rings

Ligand CLA b 830



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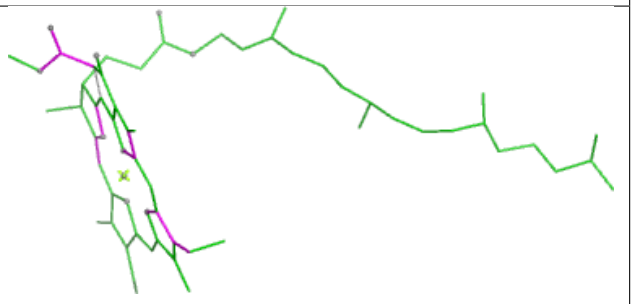
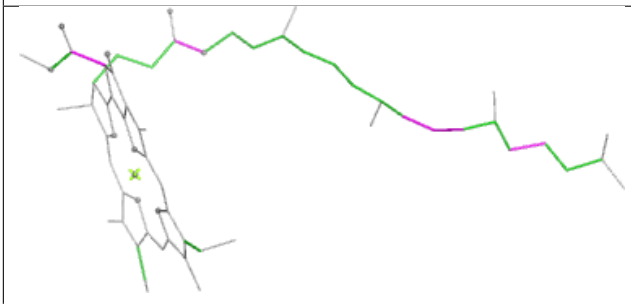


Bond angles

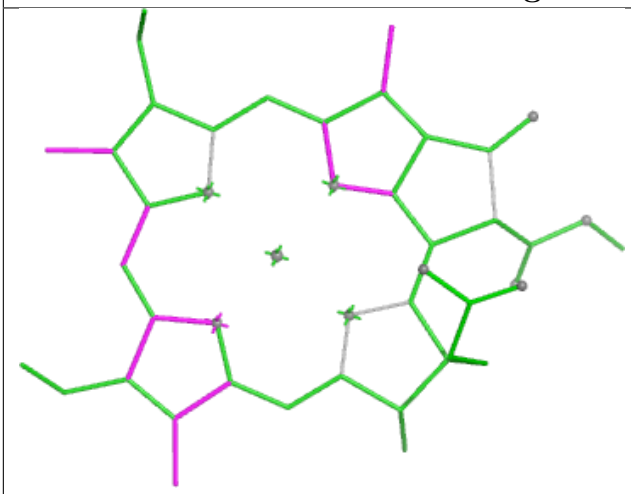


Torsions



Rings

Ligand CLA A 813



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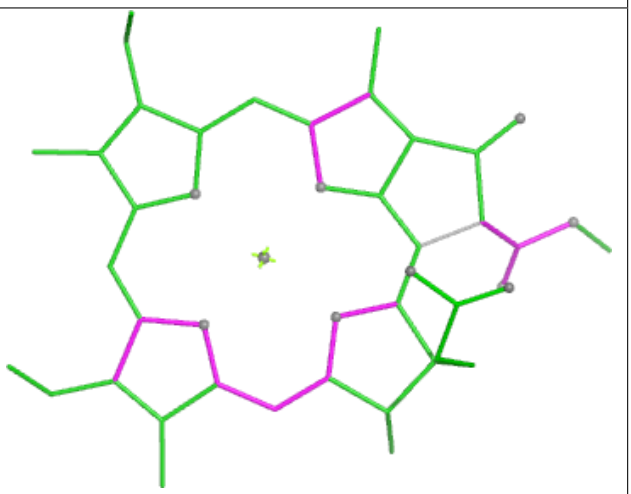
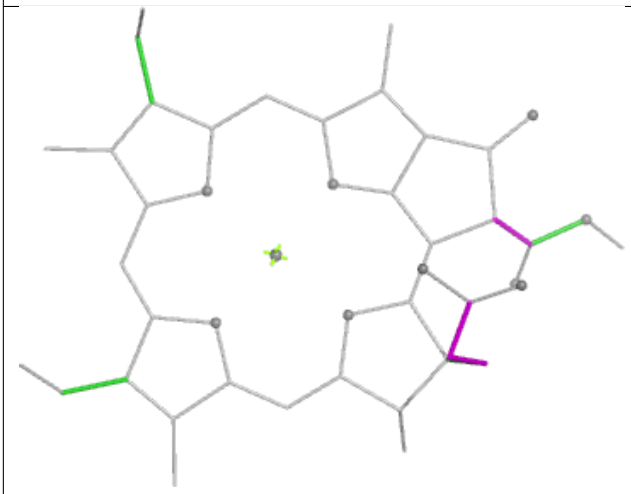


Bond angles



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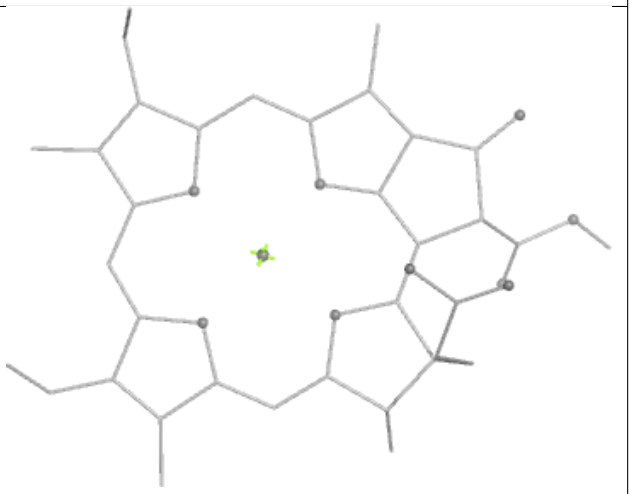
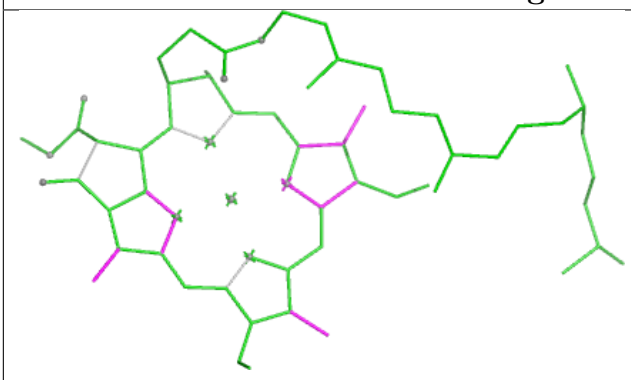


Rings

Ligand CLA b 819



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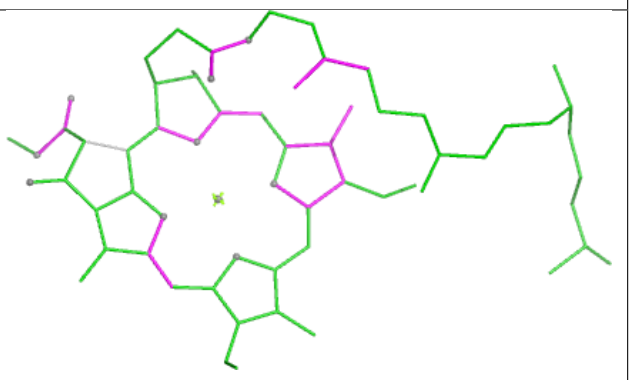
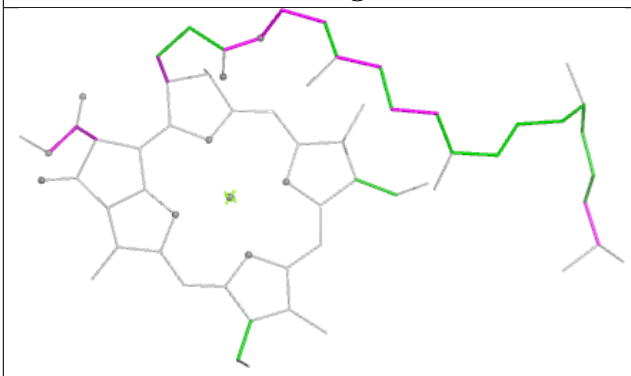
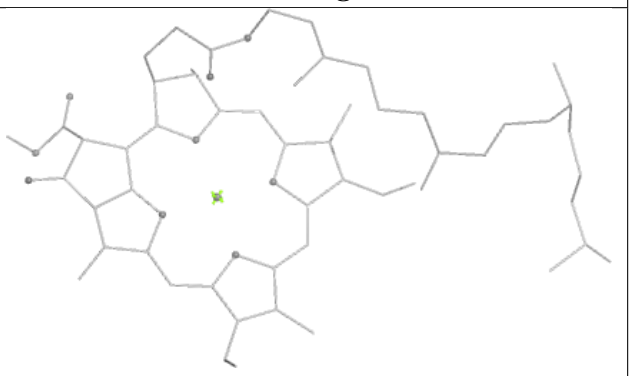


Bond angles

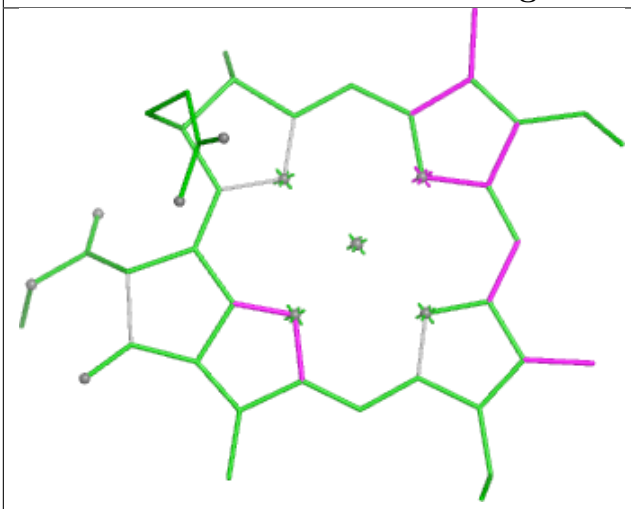


Torsions



Rings

Ligand CLA 8 1302



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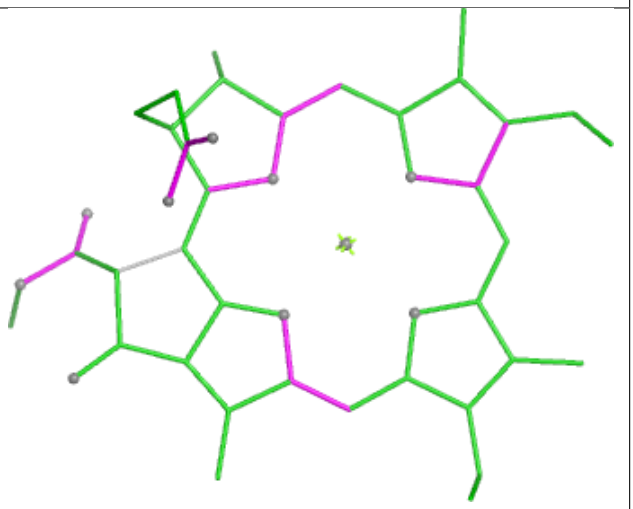
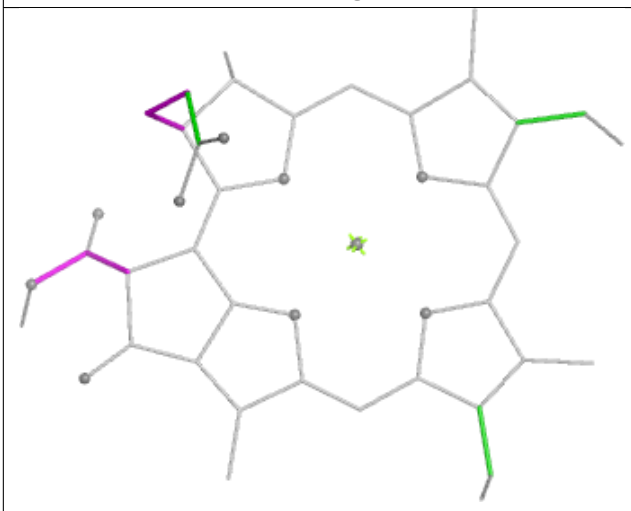


Bond angles



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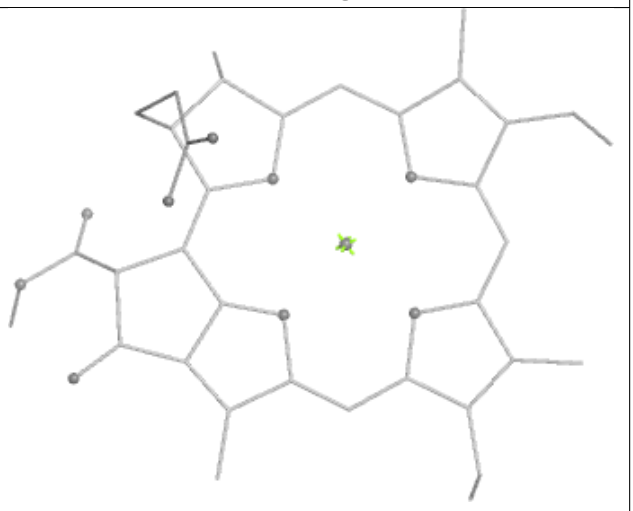
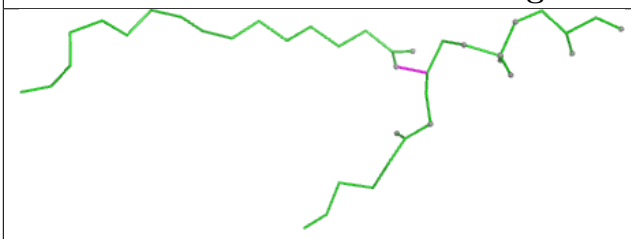


Rings

Ligand LHG 0 202



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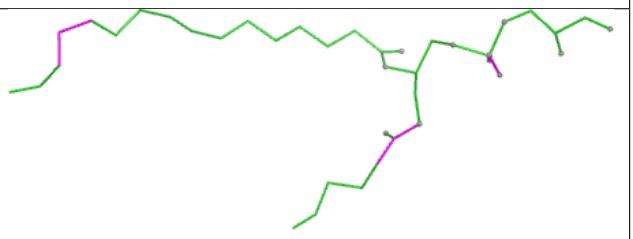
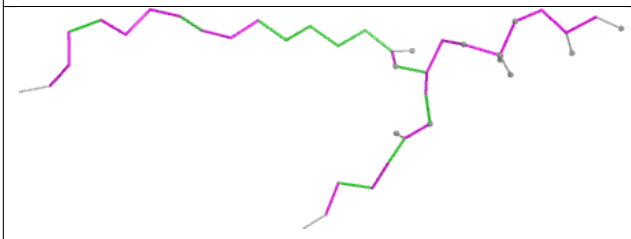


Bond angles

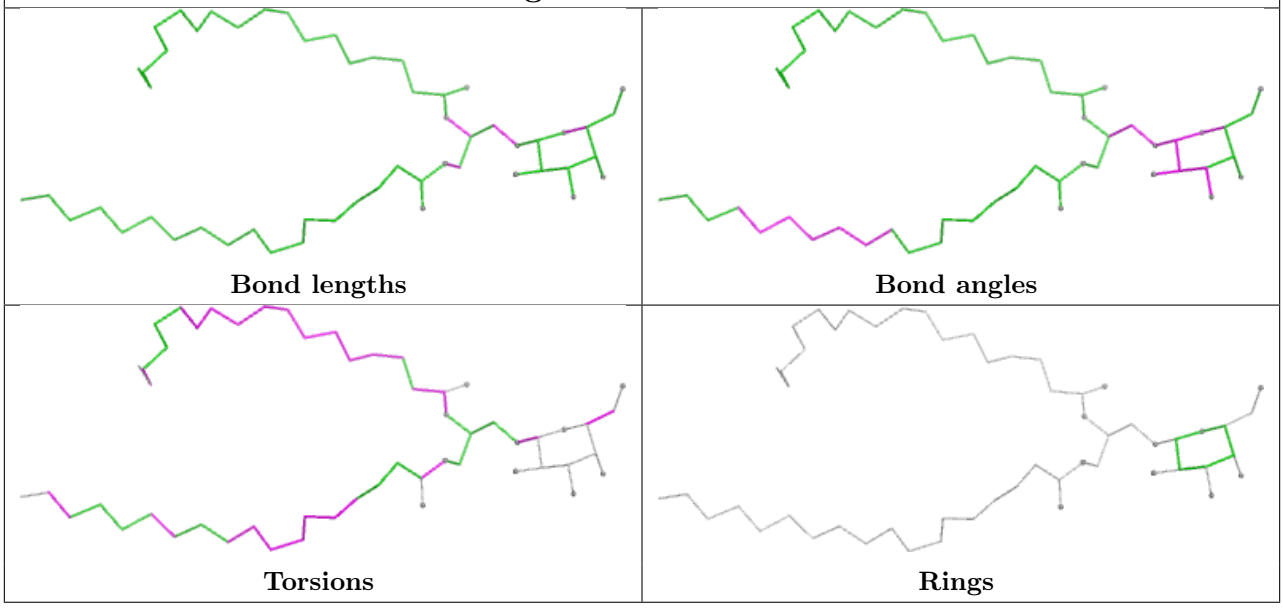


Torsions



Rings

Ligand LMG 2 850



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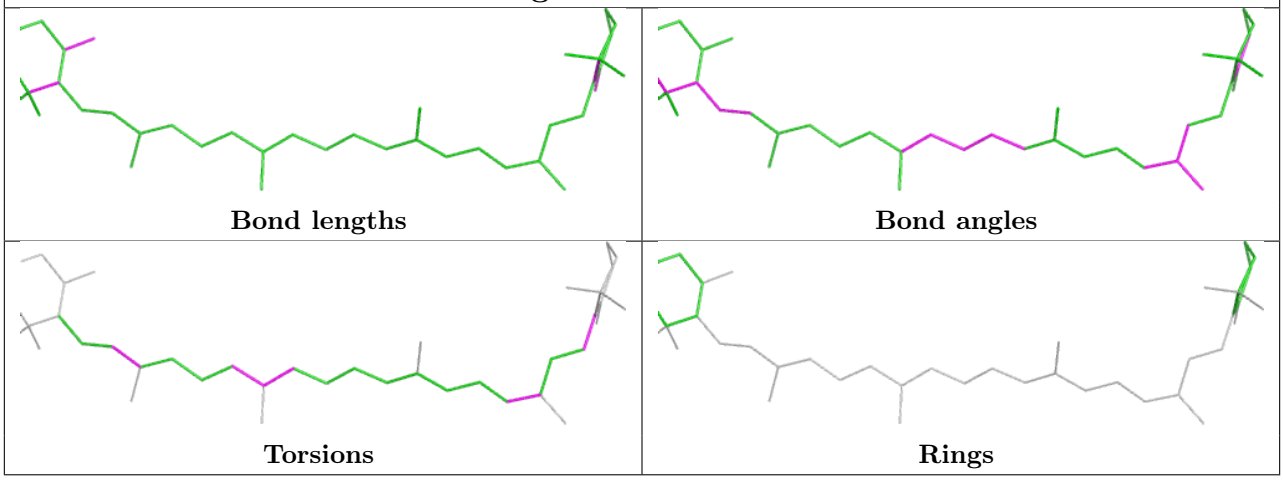
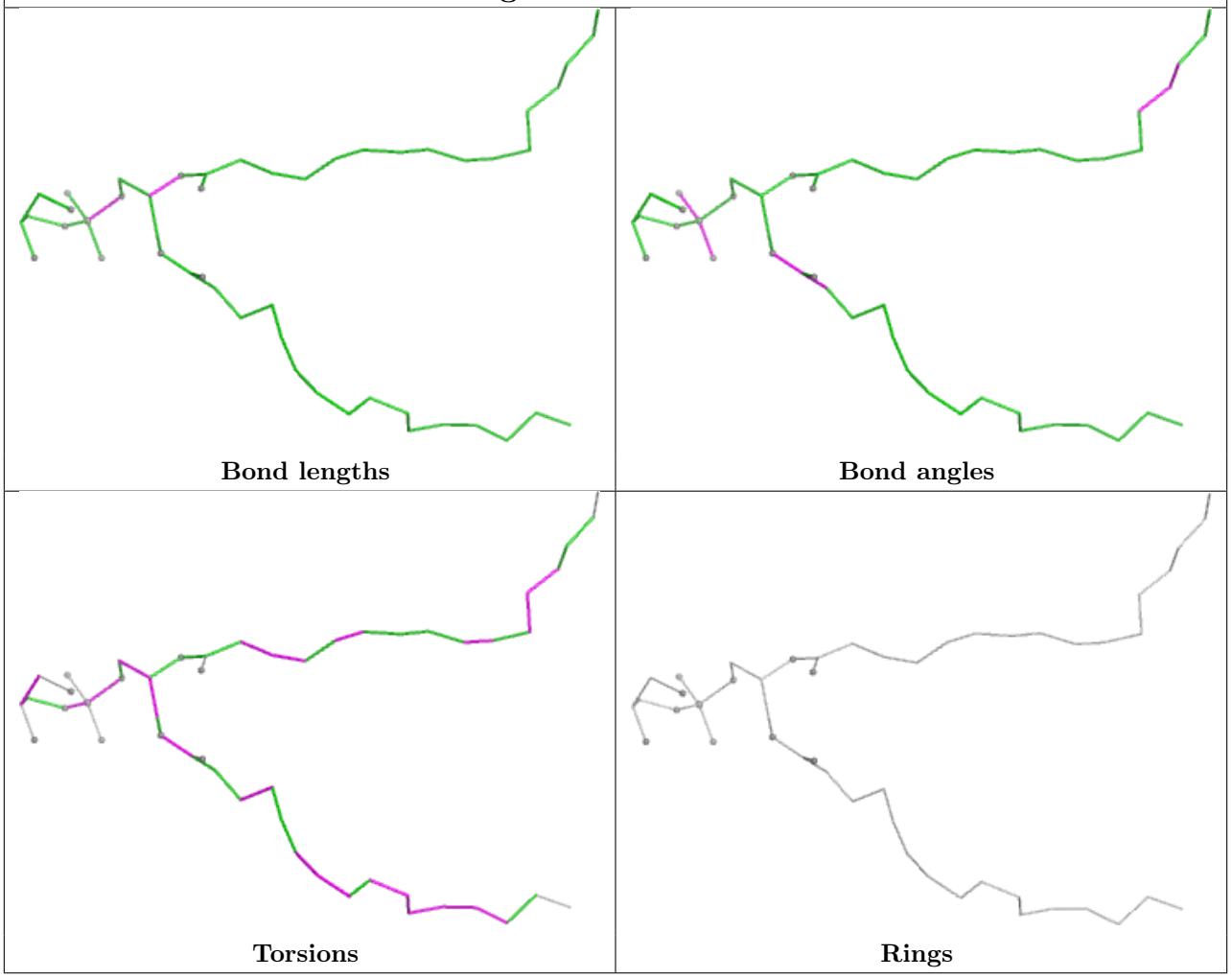
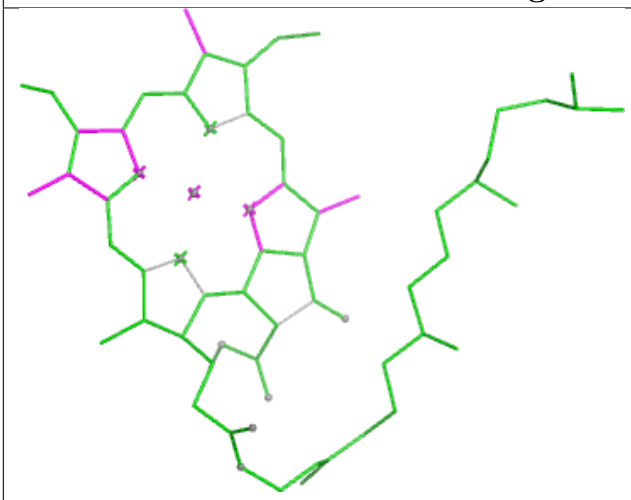


Ligand LHG m 101



Ligand CLA a 826



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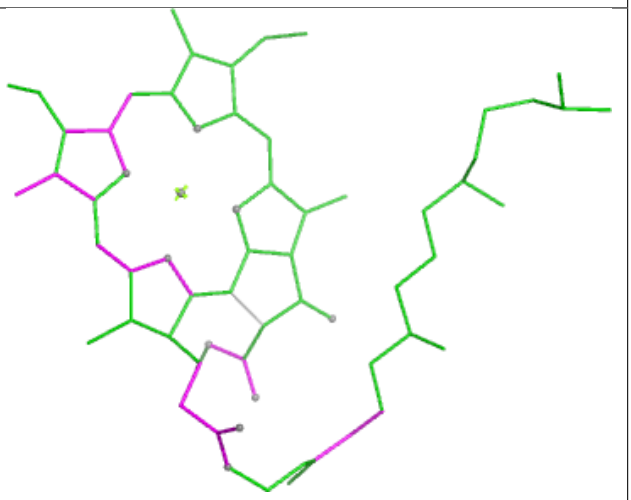
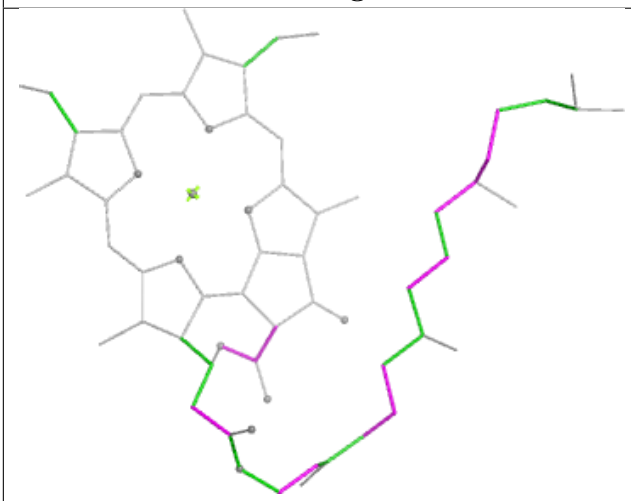


Bond angles



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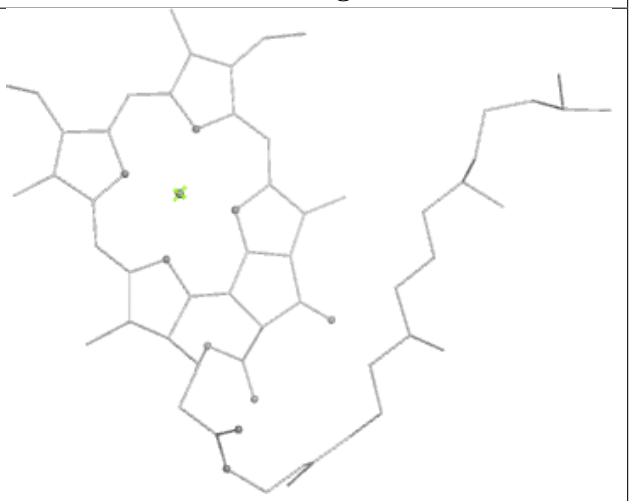
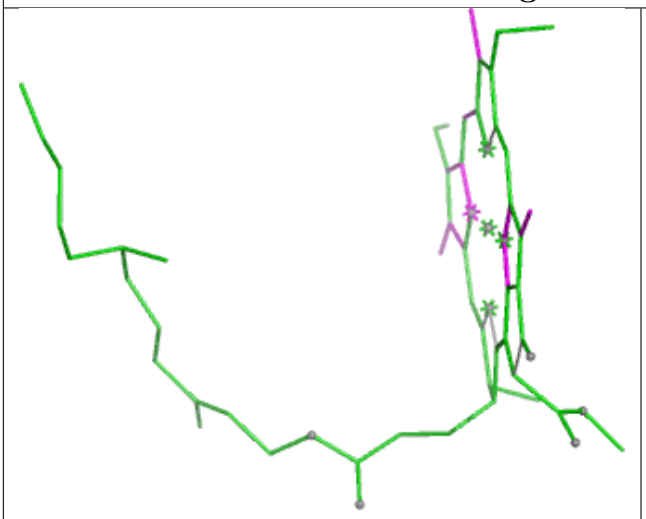


Rings

Ligand CLA 1 1606



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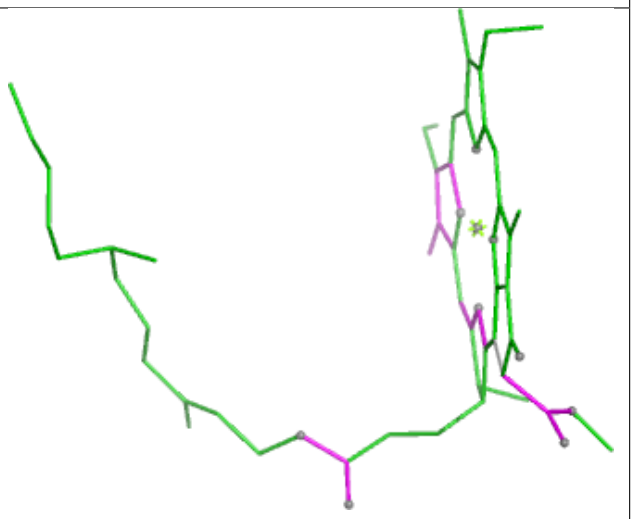

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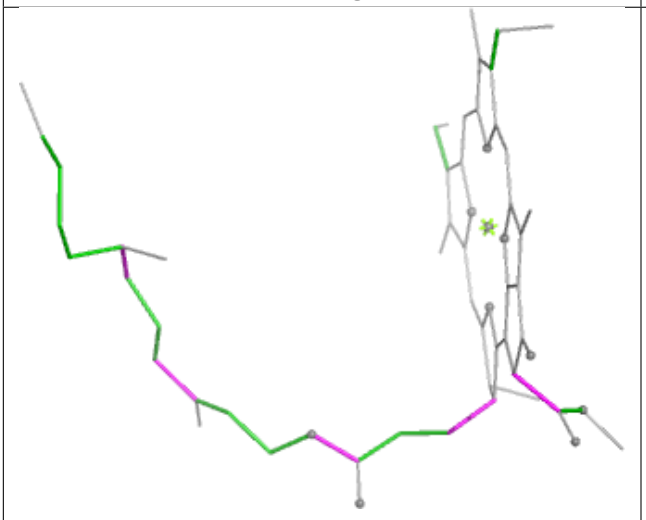
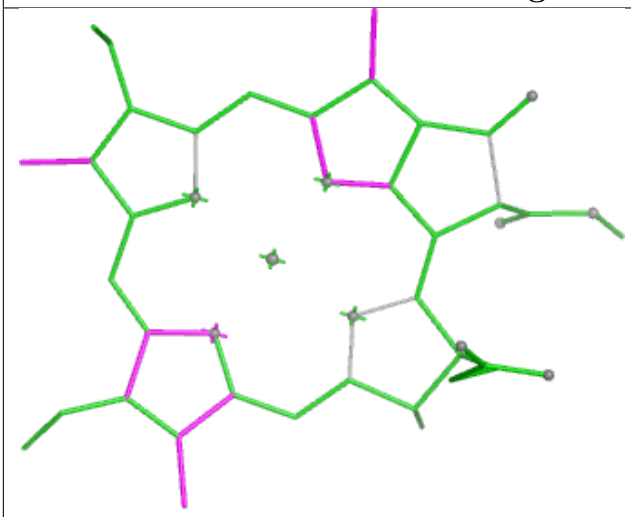


Torsions



Rings

Ligand CLA 2 813



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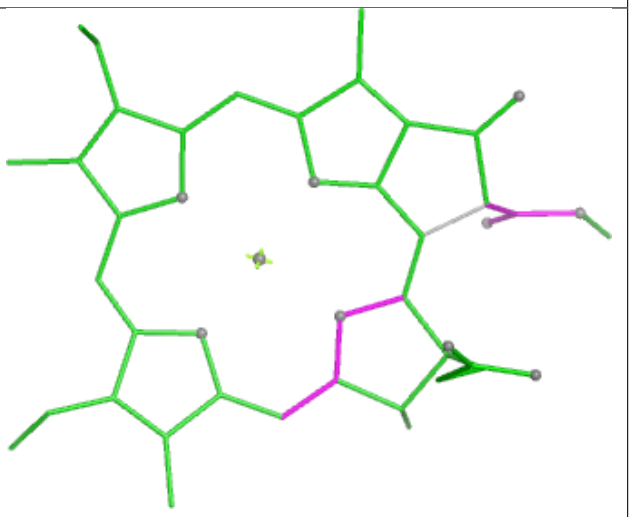
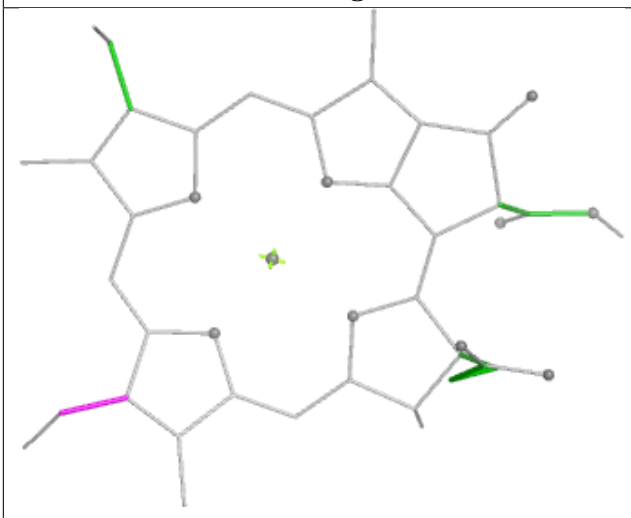


Bond angles



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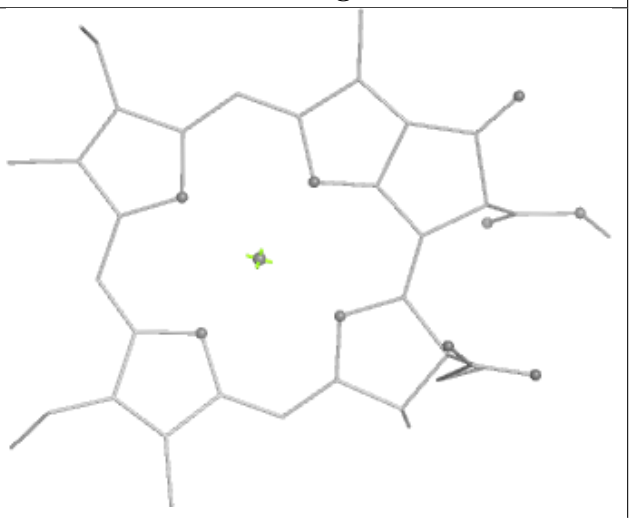
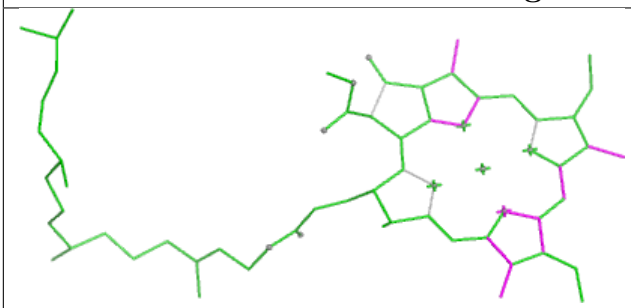


Rings

Ligand CLA B 826



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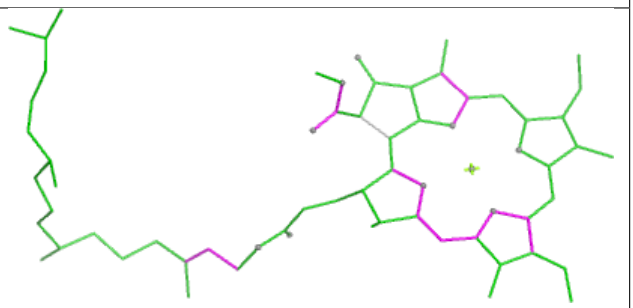
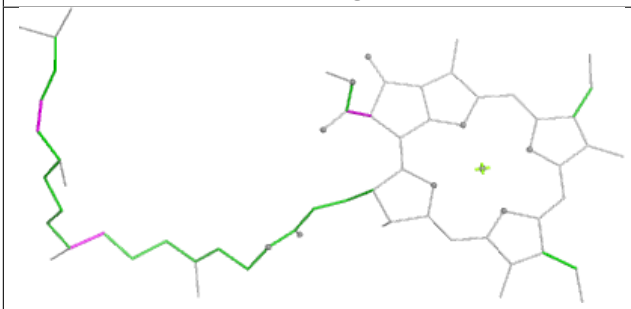
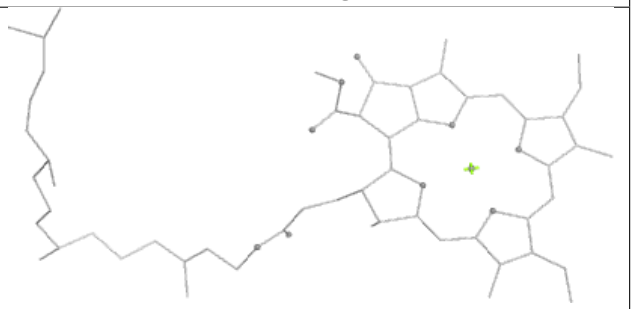


Bond angles

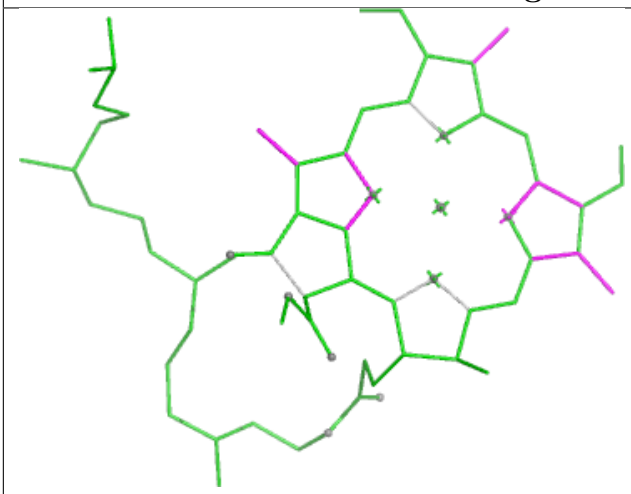


Torsions

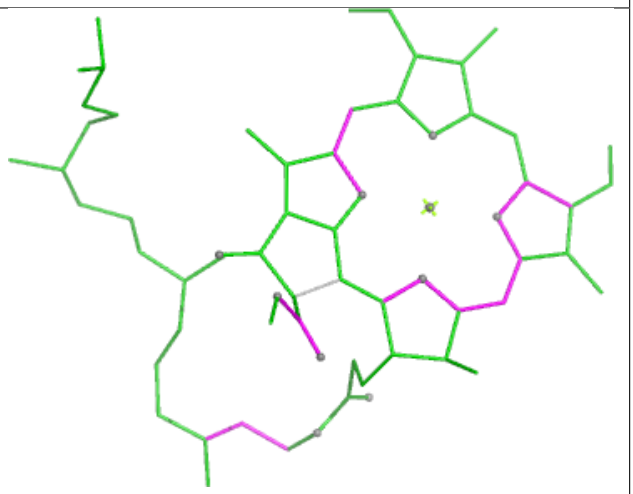


Rings

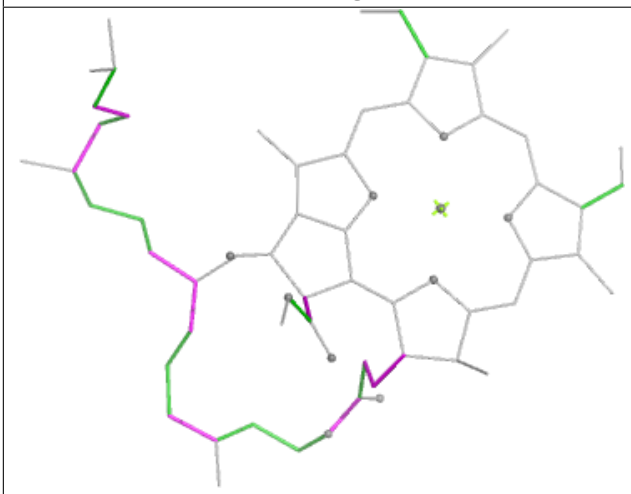
Ligand CLA B 832



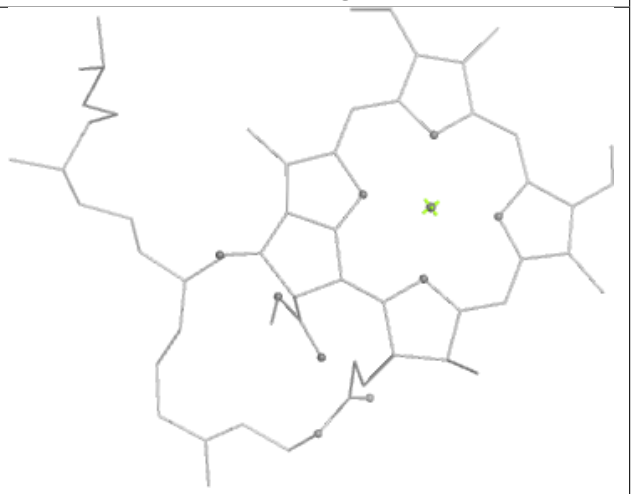
Bond lengths



Bond angles

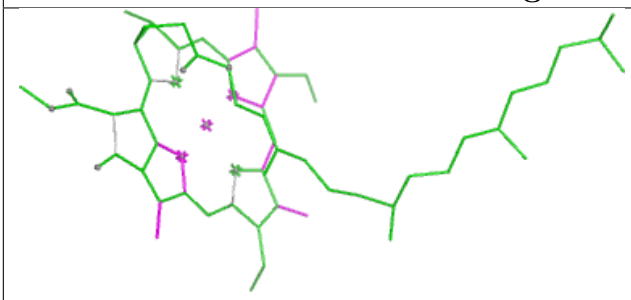


Torsions



Rings

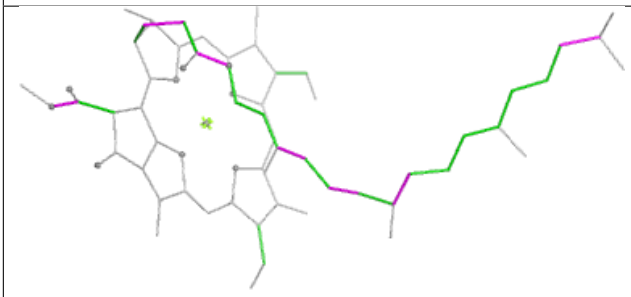
Ligand CLA A 842



Bond lengths



Bond angles



Torsions

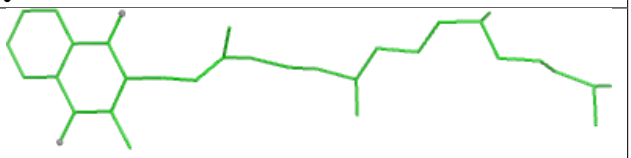


Rings

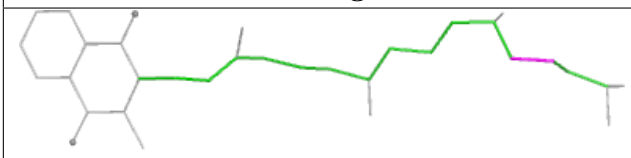
Ligand PQN a 845



Bond lengths



Bond angles

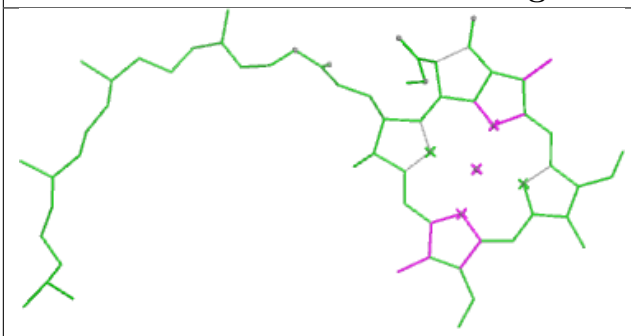


Torsions



Rings

Ligand CLA a 838



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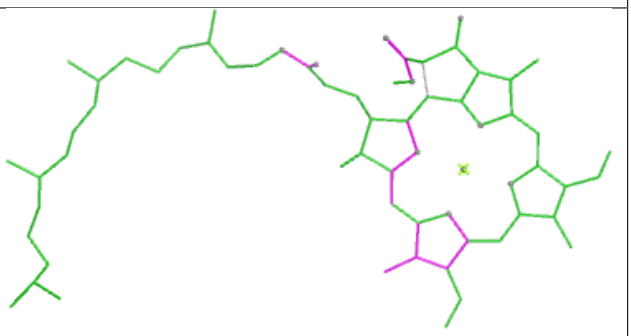
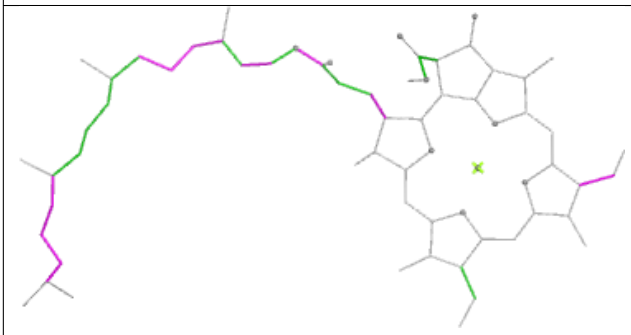


Bond angles

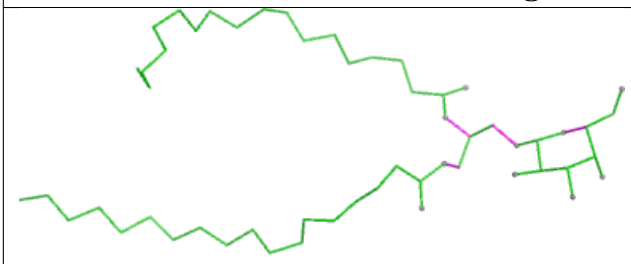


Torsions



Rings

Ligand LMG b 850



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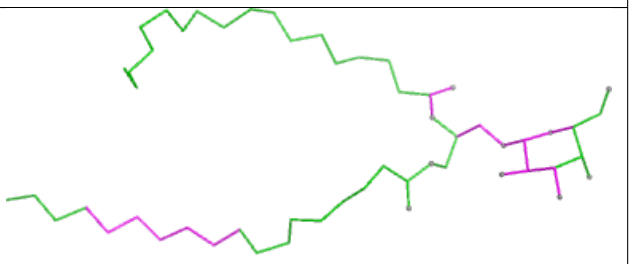
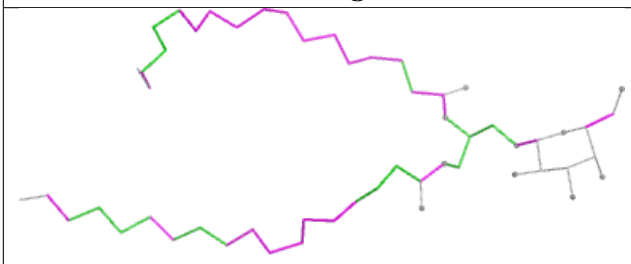


Bond angles

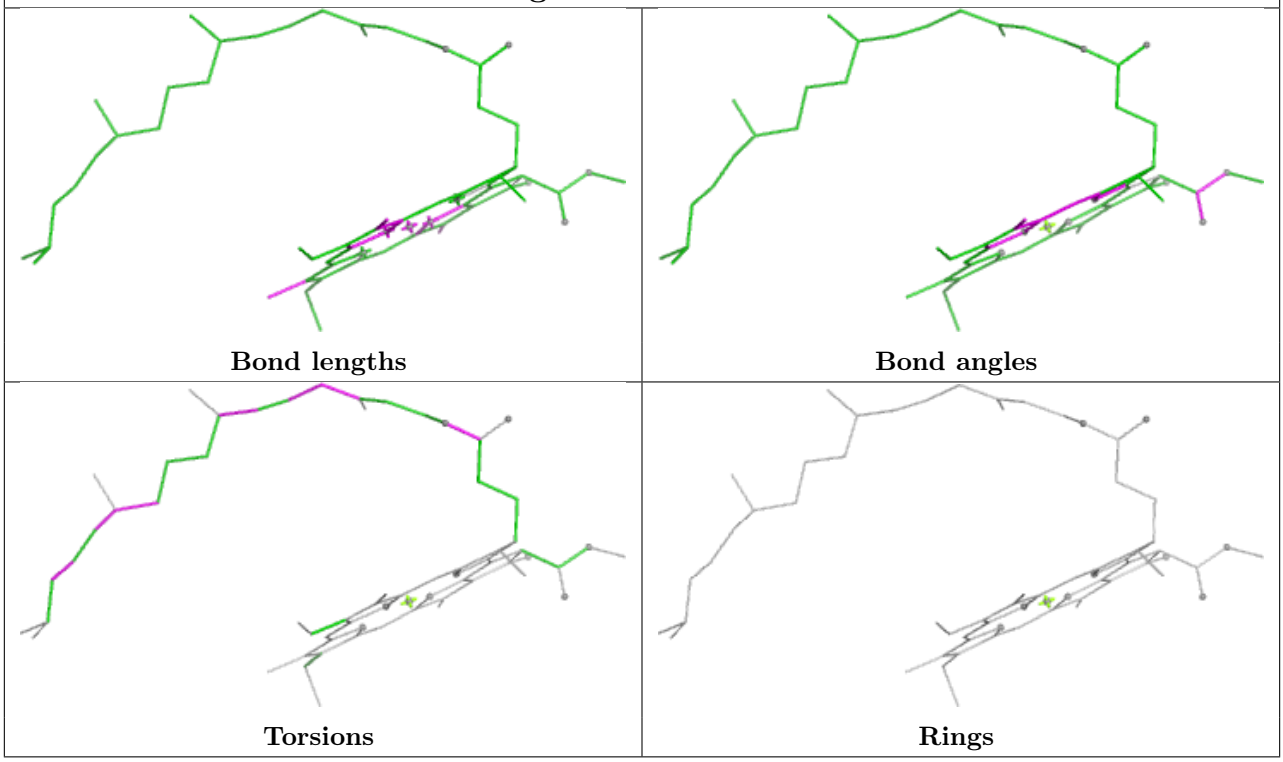


Torsions

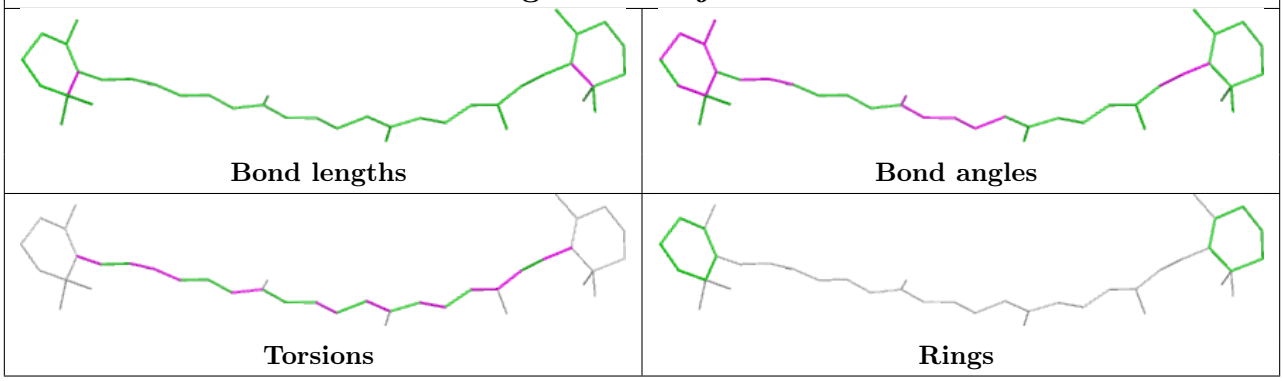


Rings

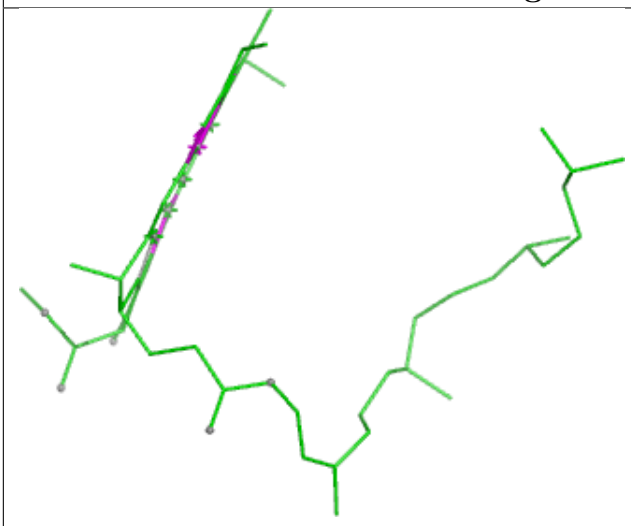
Ligand CLA a 833



Ligand BCR j 1305



Ligand CLA B 834



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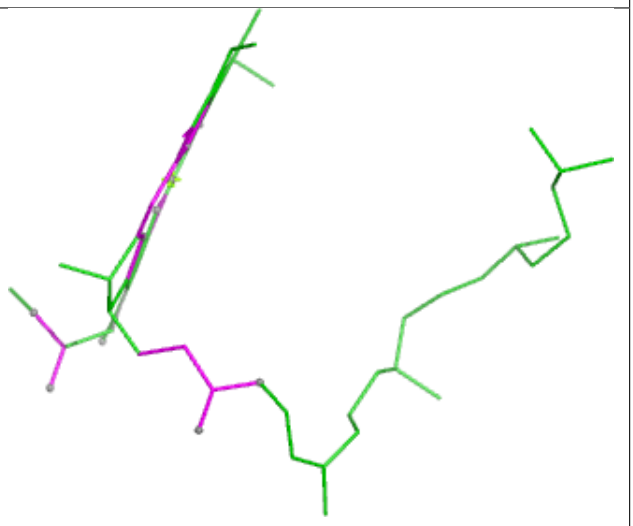
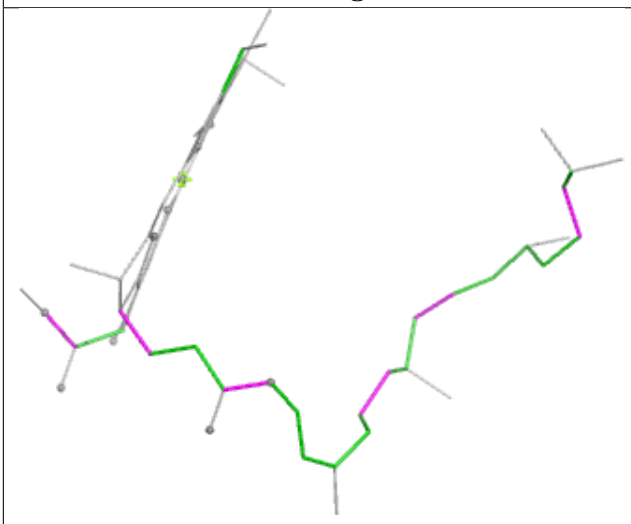
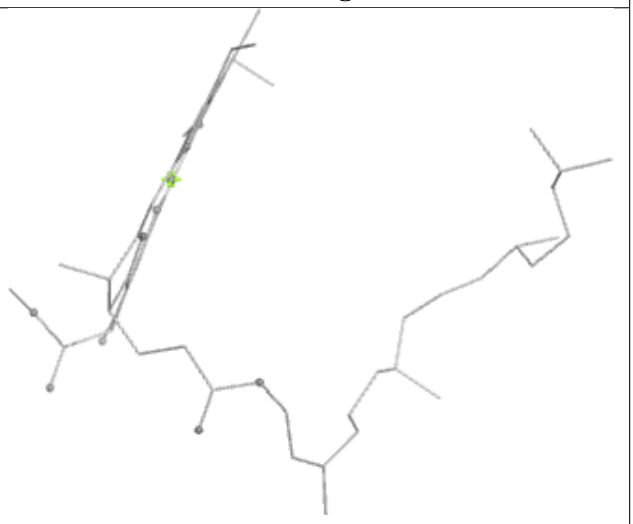


Bond angles

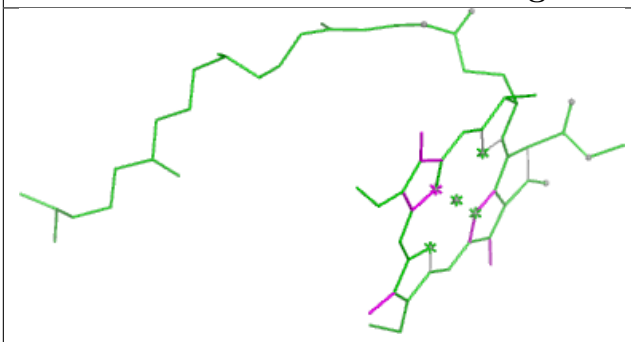


Torsions



Rings

Ligand CLA 2 816



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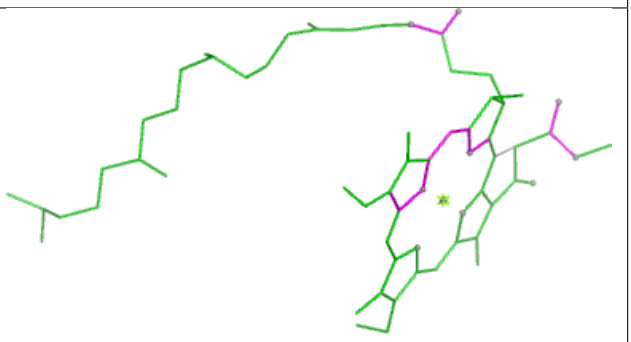
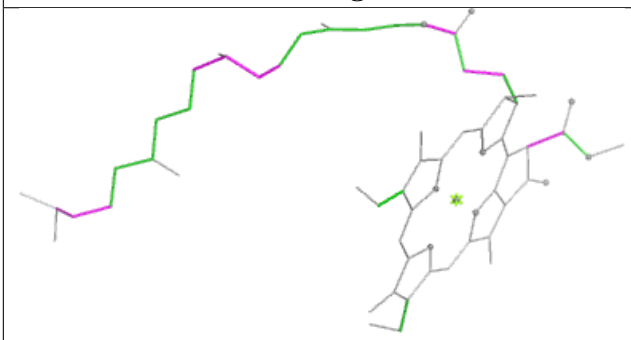


Bond angles

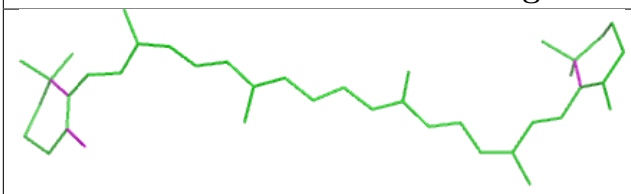


Torsions



Rings

Ligand BCR B 845



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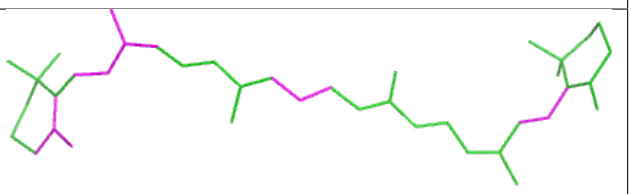
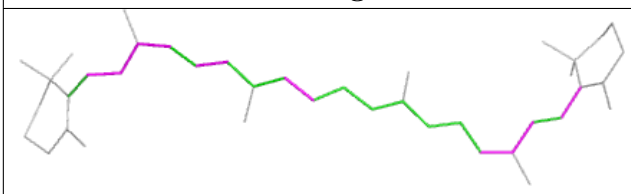


Bond angles



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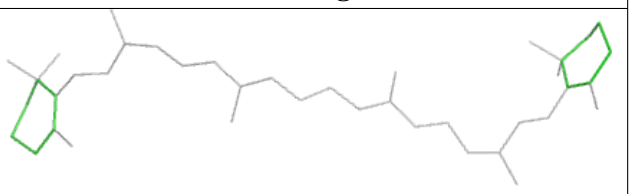
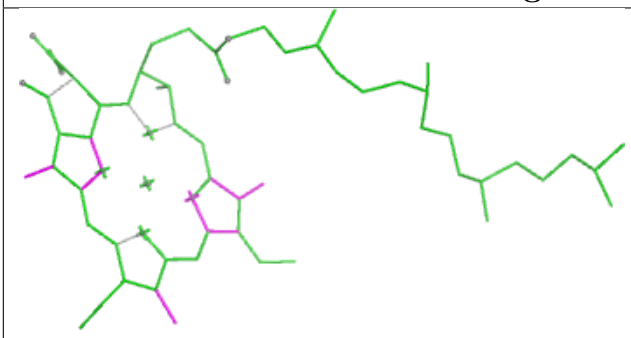


Rings

Ligand CLA A 809



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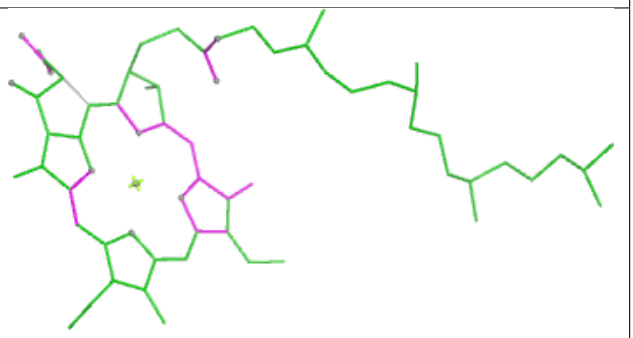
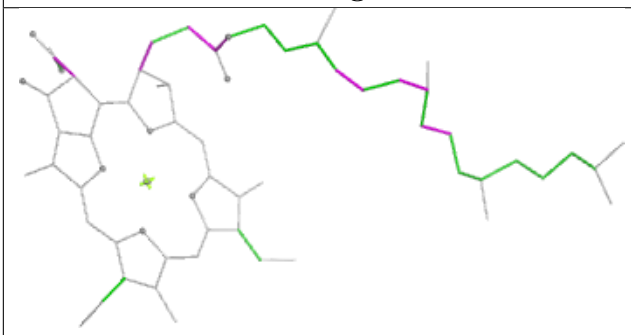


Bond angles

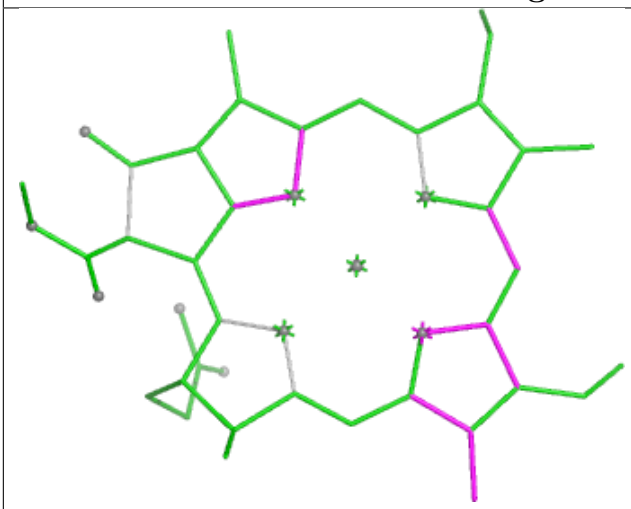


Torsions



Rings

Ligand CLA J 101



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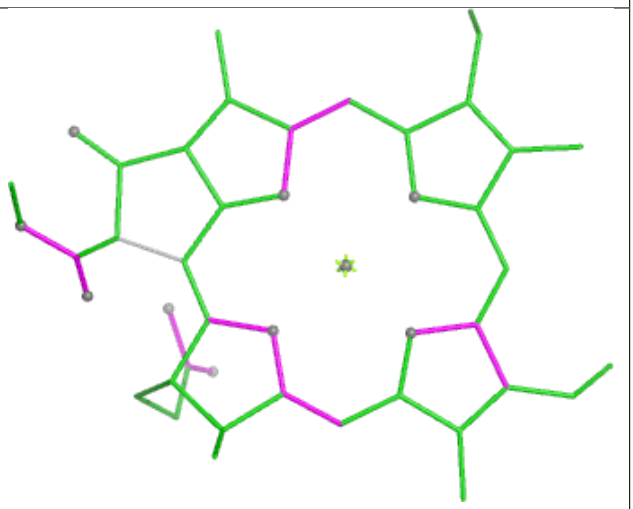
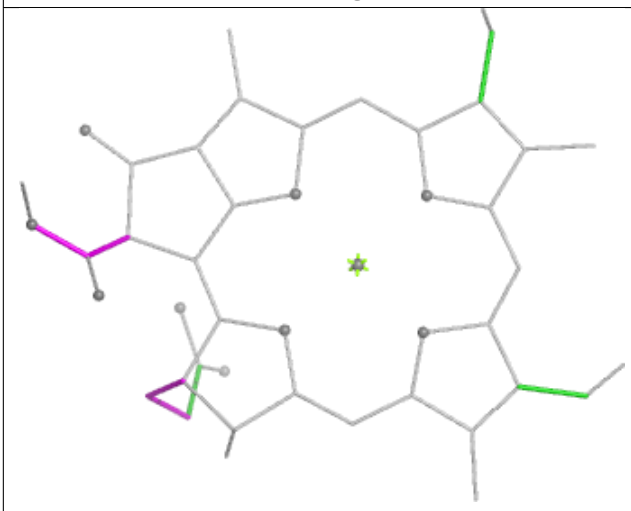


Bond angles



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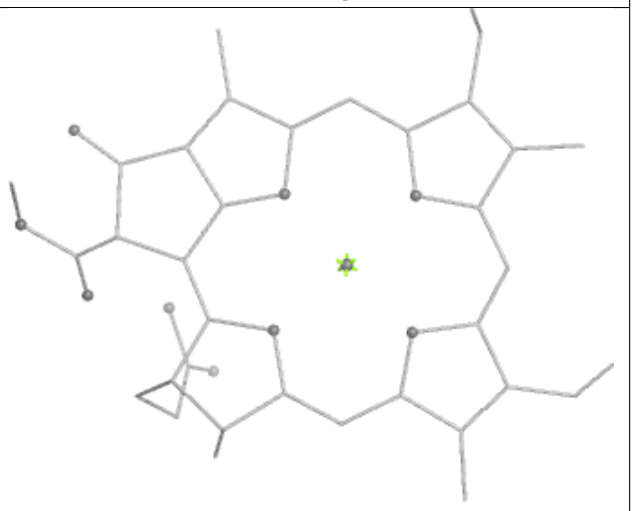
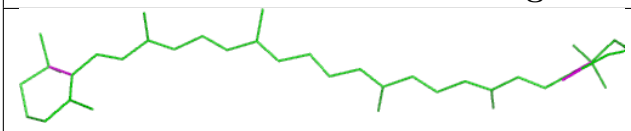


Rings

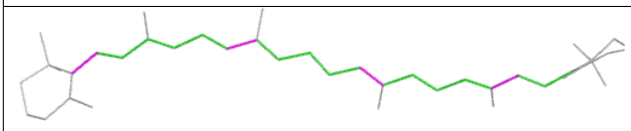
Ligand BCR 0 201



Bond lengths



Bond angles



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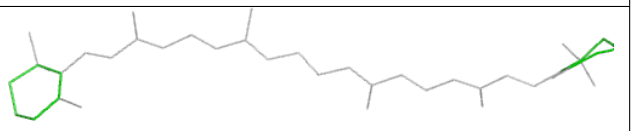
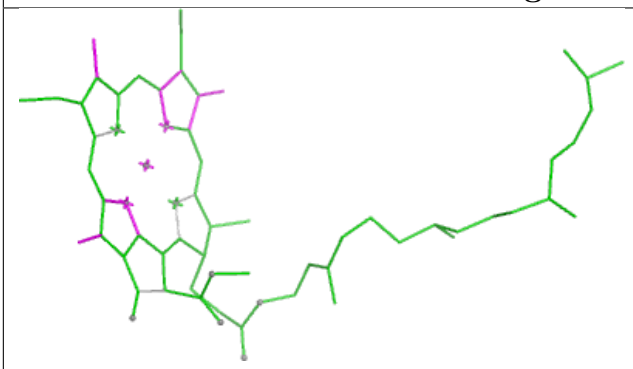
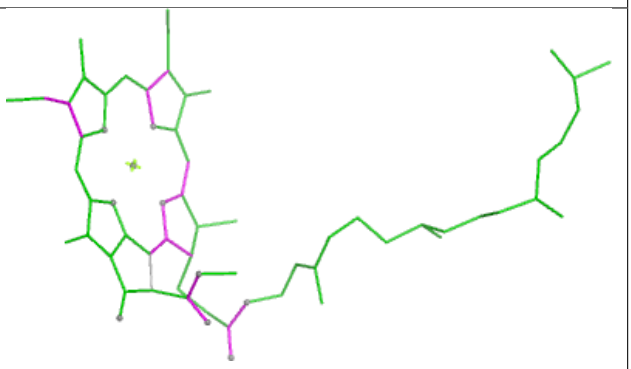


Rings

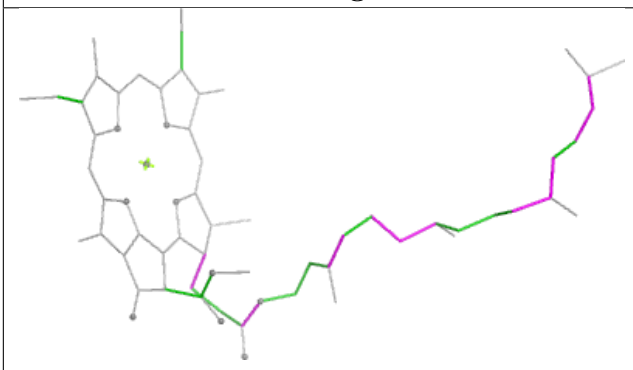
Ligand CLA B 810



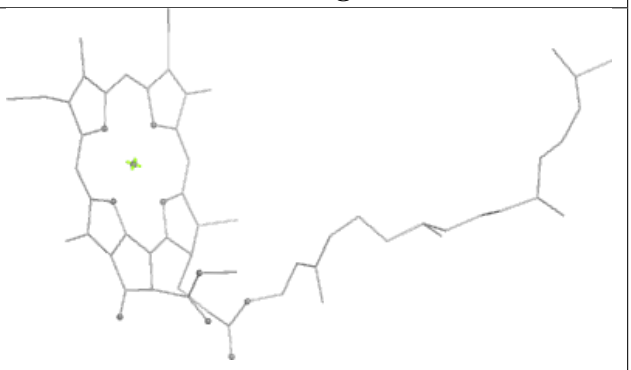
Bond lengths



Bond angles

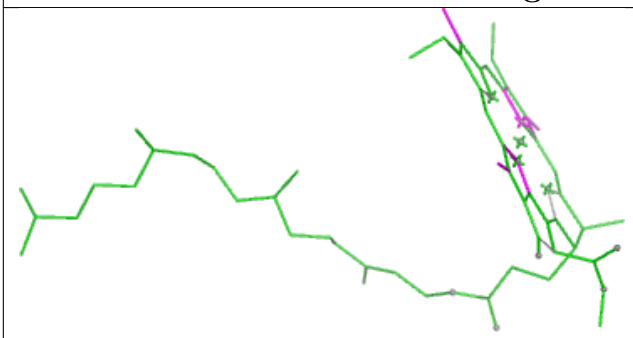


Torsions



Rings

Ligand CLA A 812



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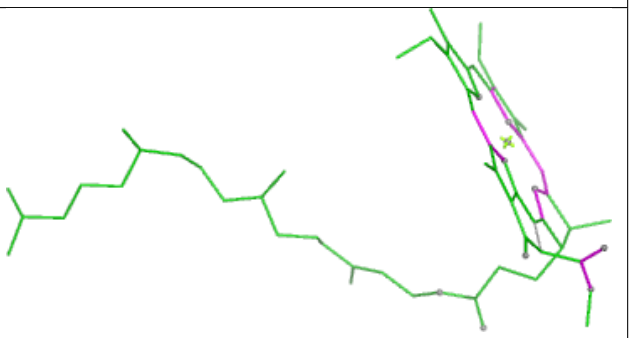
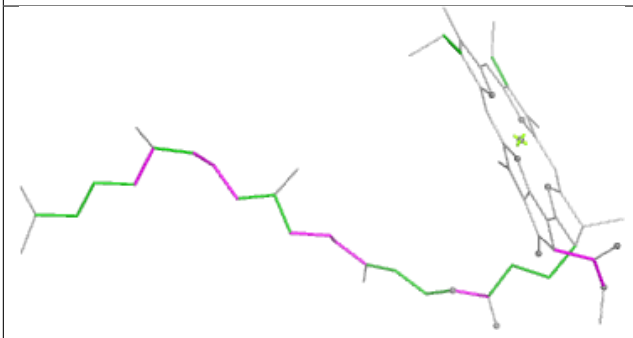


Bond angles

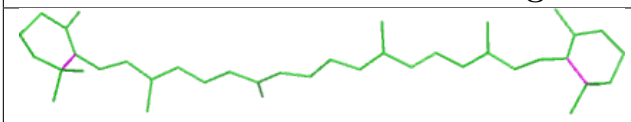


Torsions



Rings

Ligand BCR a 847



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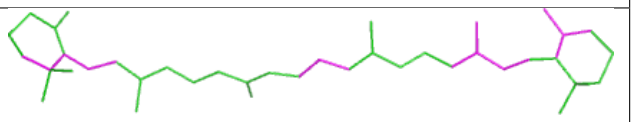
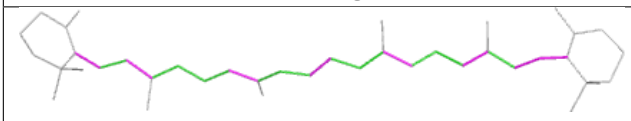
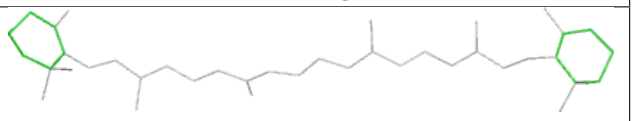


Bond angles

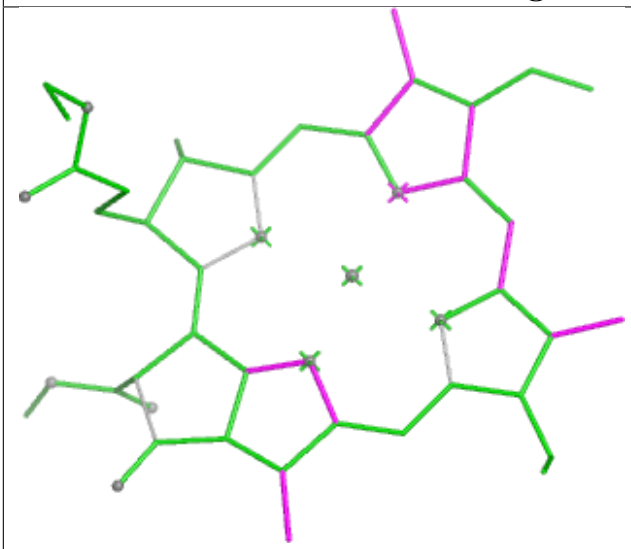


Torsions



Rings

Ligand CLA b 840



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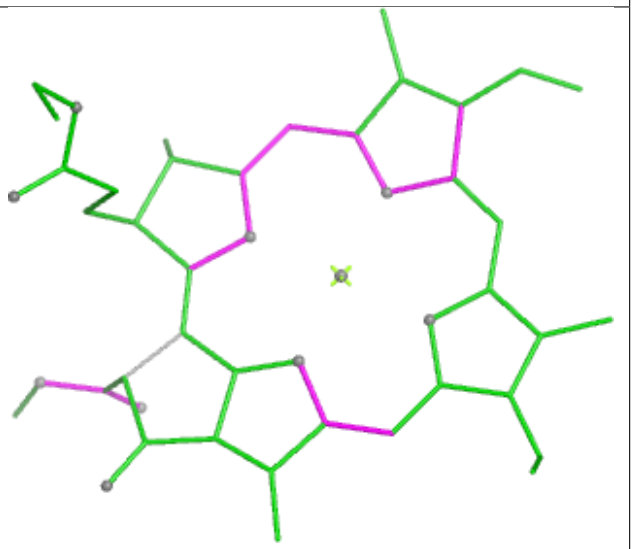
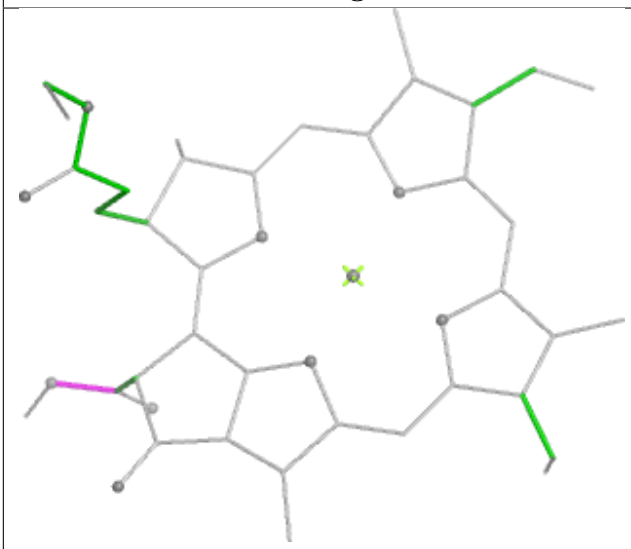
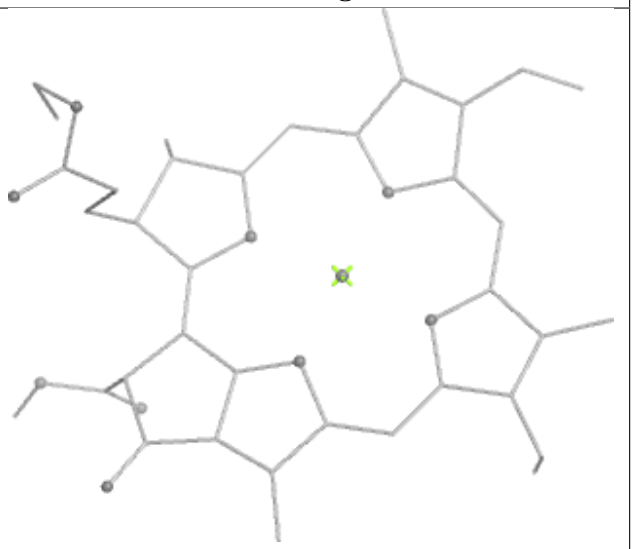


Bond angles

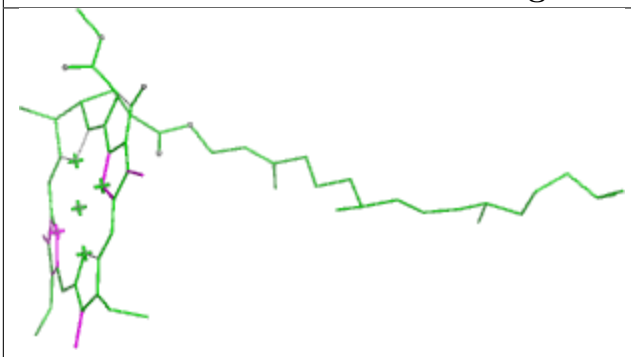


Torsions



Rings

Ligand CLA 2 829



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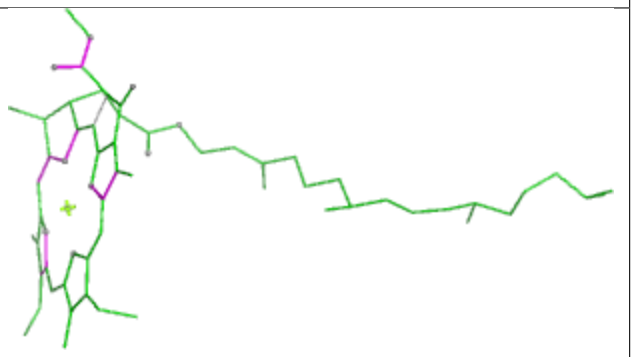
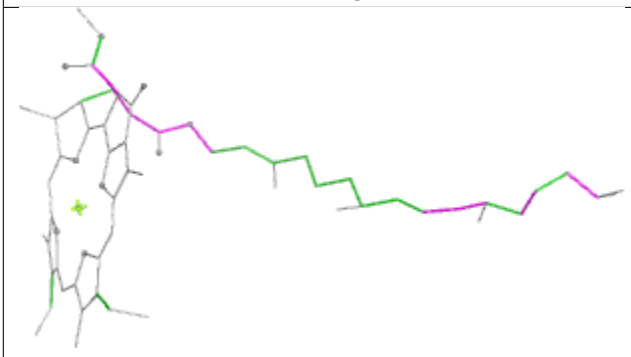


Bond angles

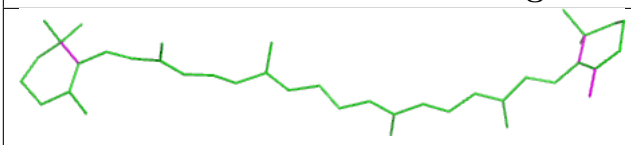


Torsions



Rings

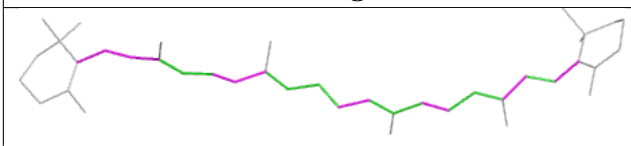
Ligand BCR 2 848



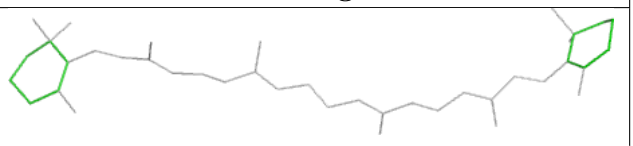
Bond lengths



Bond angles

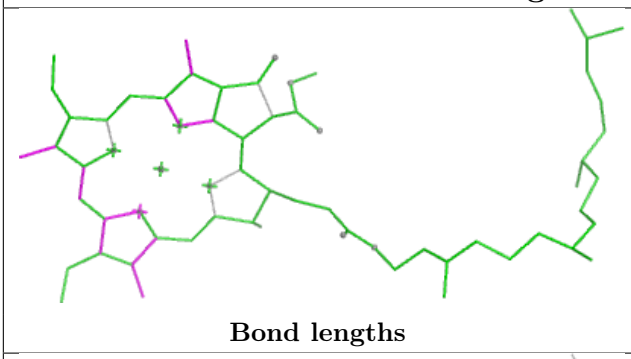


Torsions

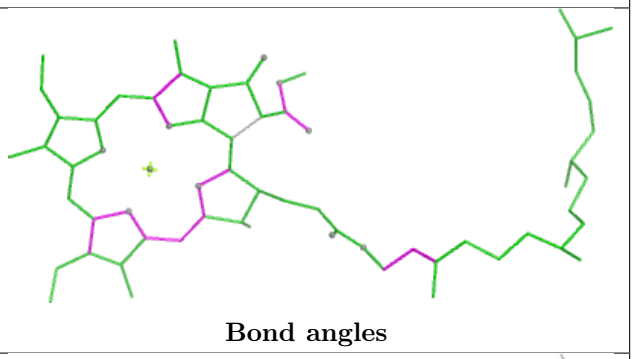


Rings

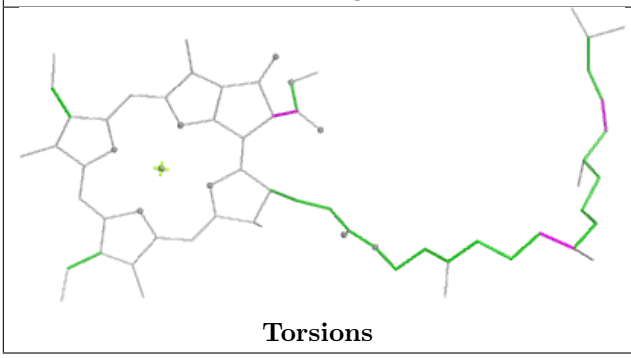
Ligand CLA b 827



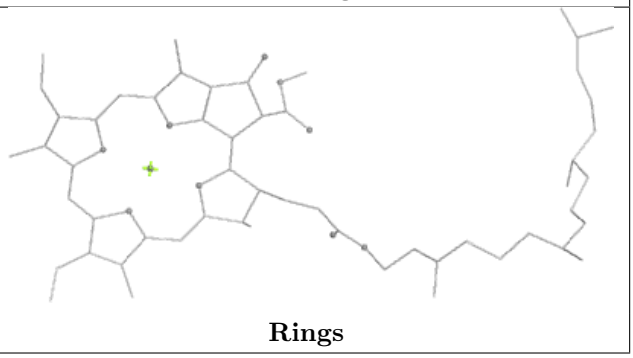
Bond lengths



Bond angles

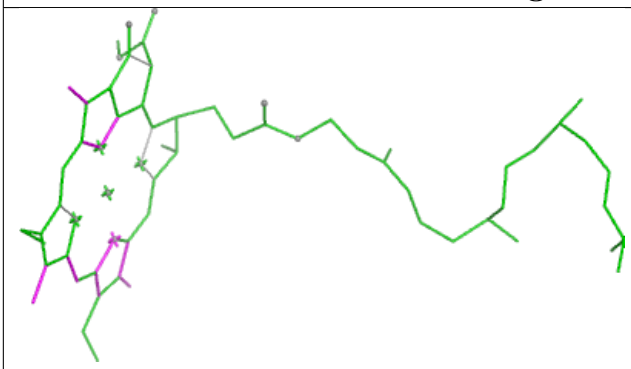


Torsions



Rings

Ligand CLA b 834



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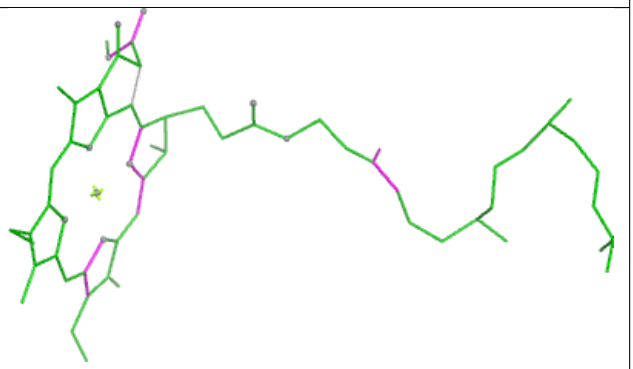
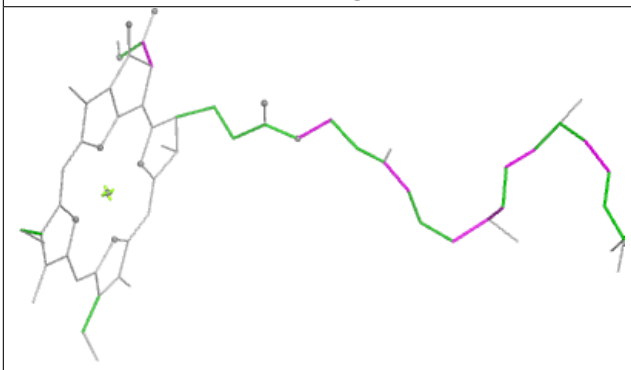


Bond angles



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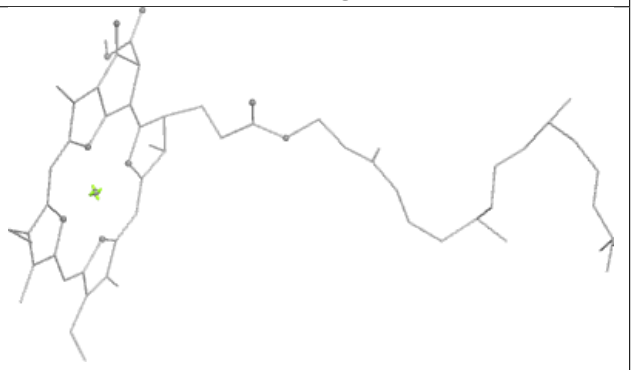
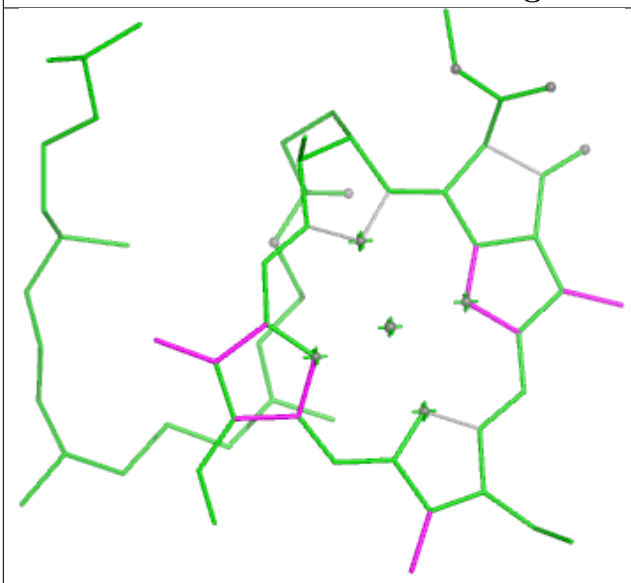


Rings

Ligand CLA A 824



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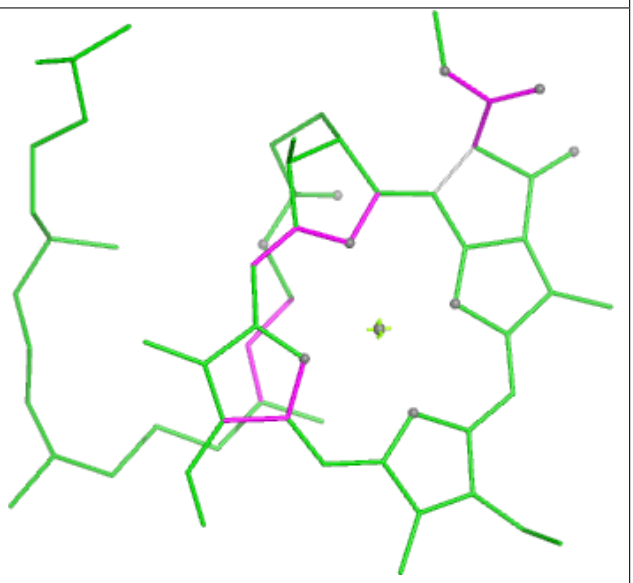
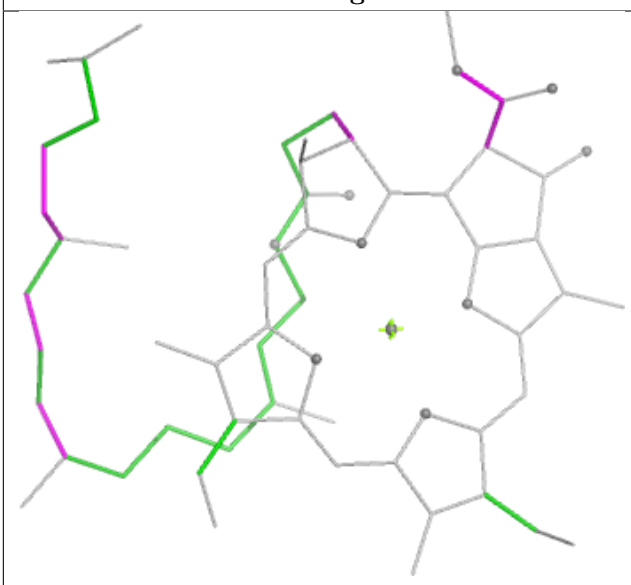


Bond angles



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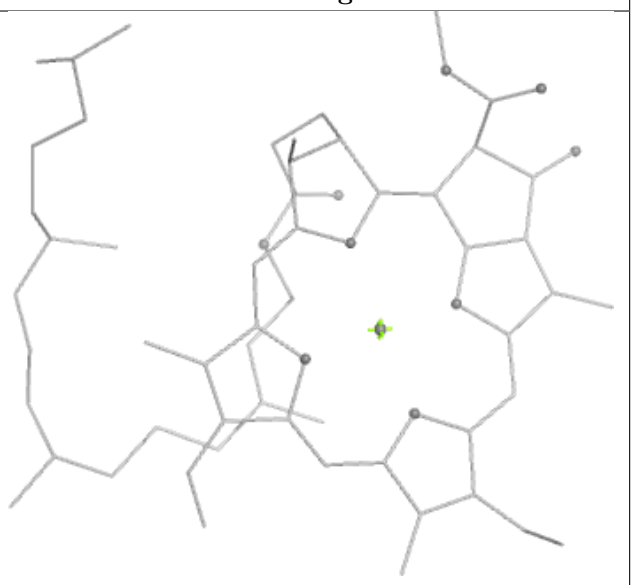
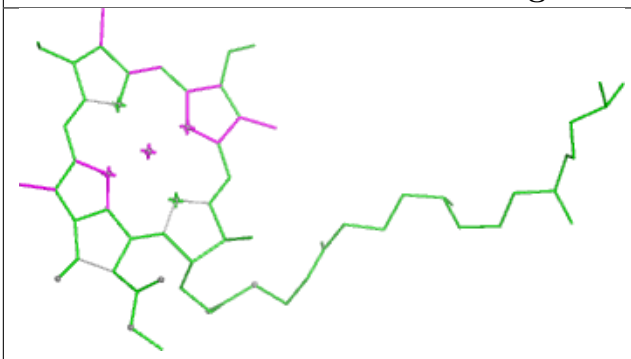


Rings

Ligand CLA a 802



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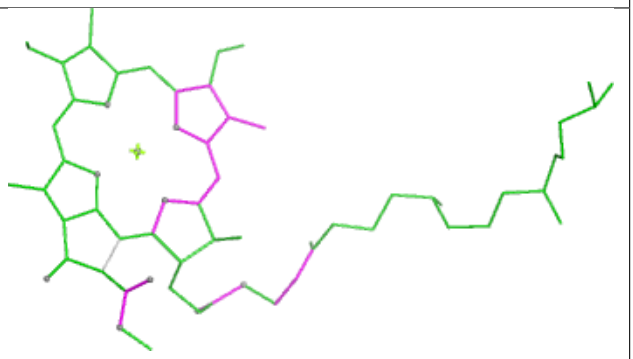
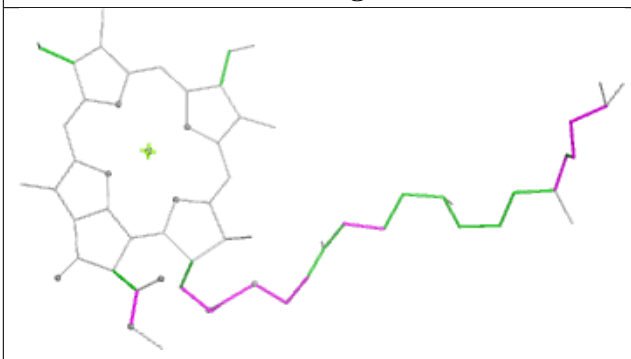


Bond angles



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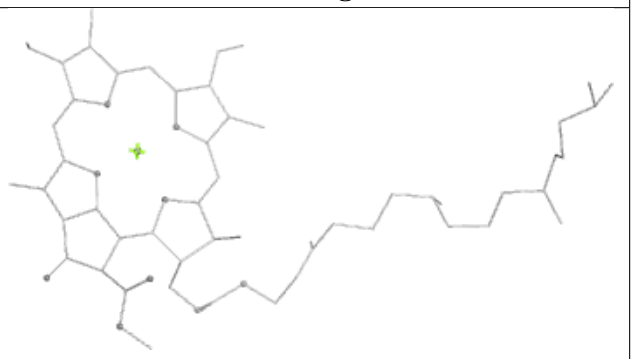
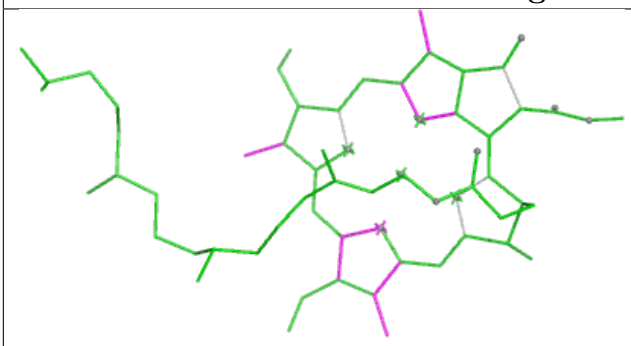


Rings

Ligand CLA 2 839



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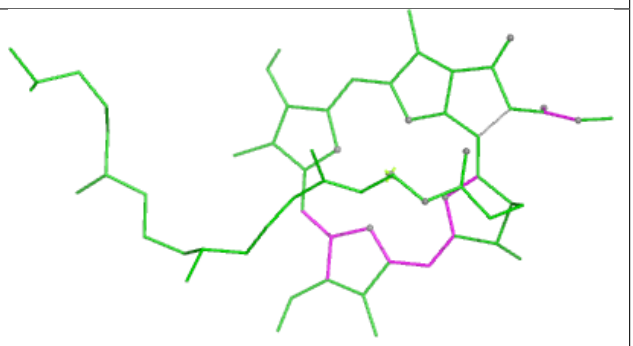
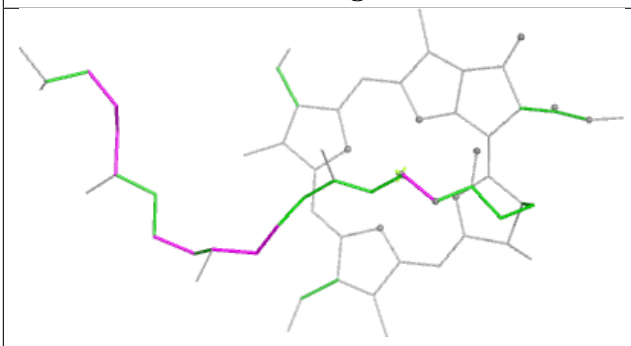


Bond angles



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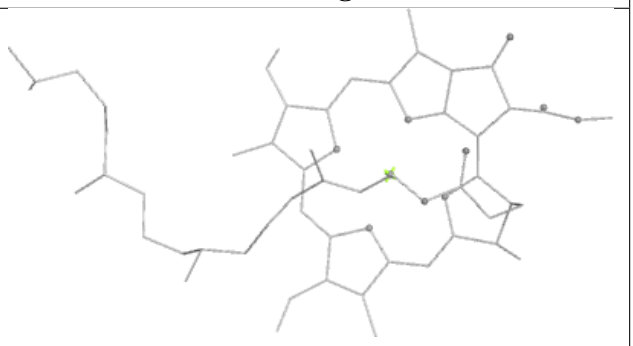
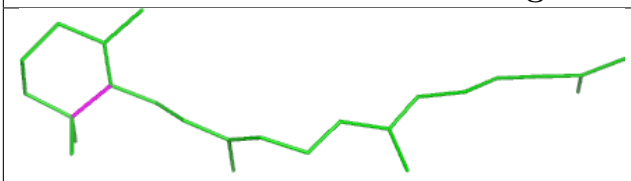


Rings

Ligand BCR a 852



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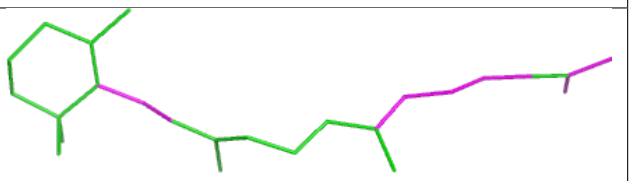
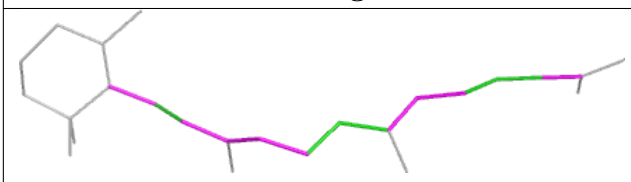


Bond angles



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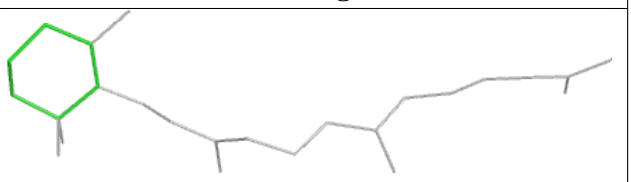
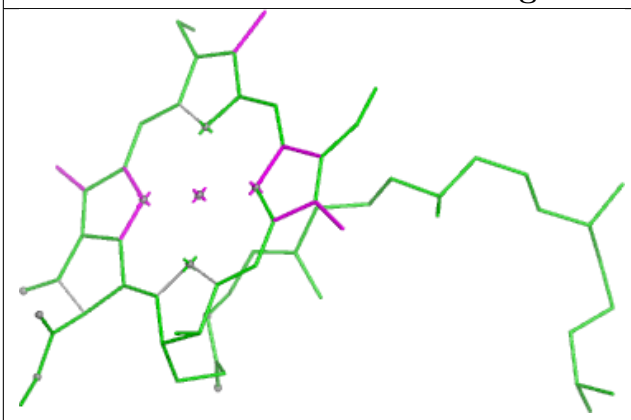


Rings

Ligand CLA 1 1644



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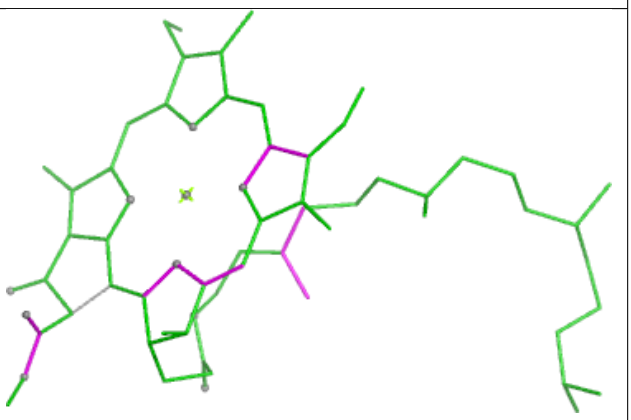
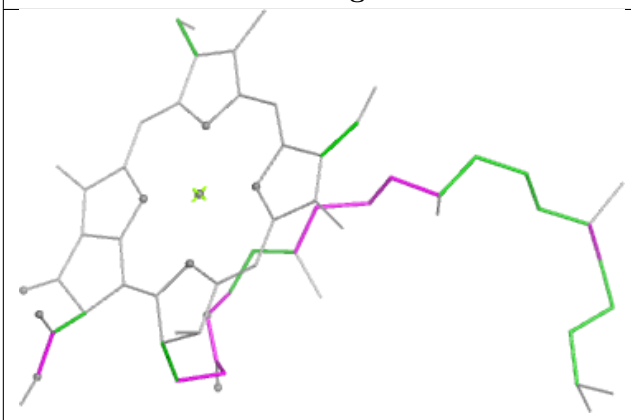


Bond angles



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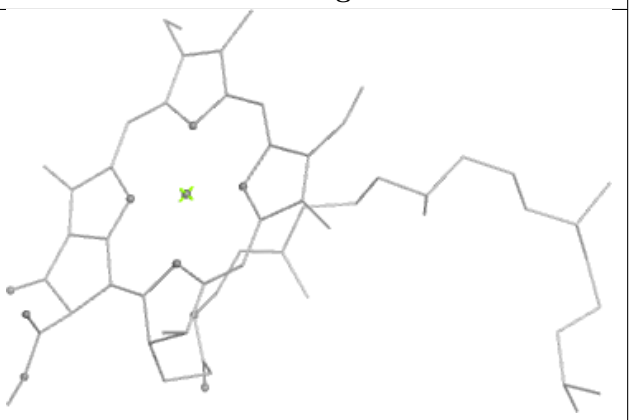
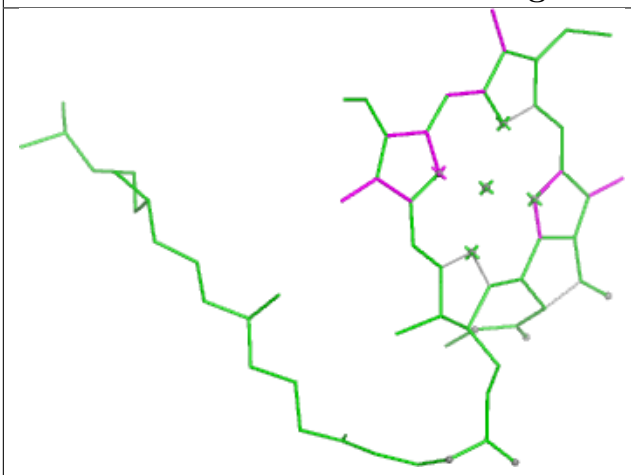


Rings

Ligand CLA 2 825



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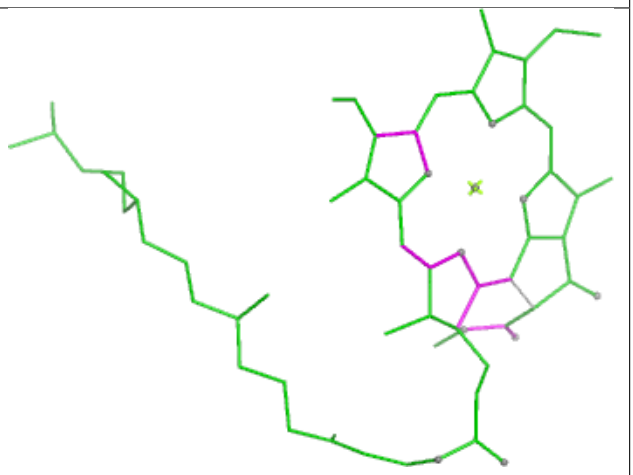
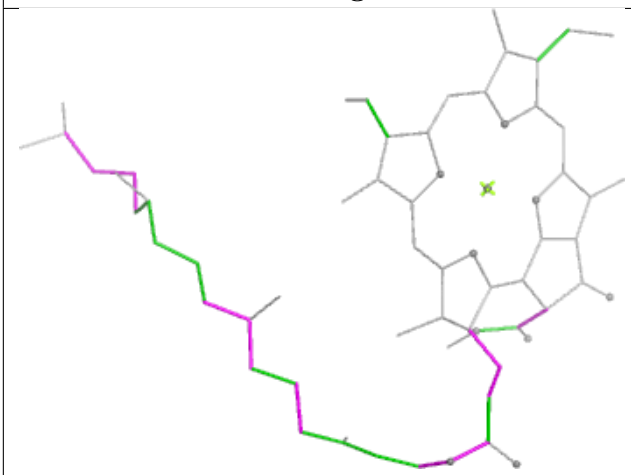


Bond angles



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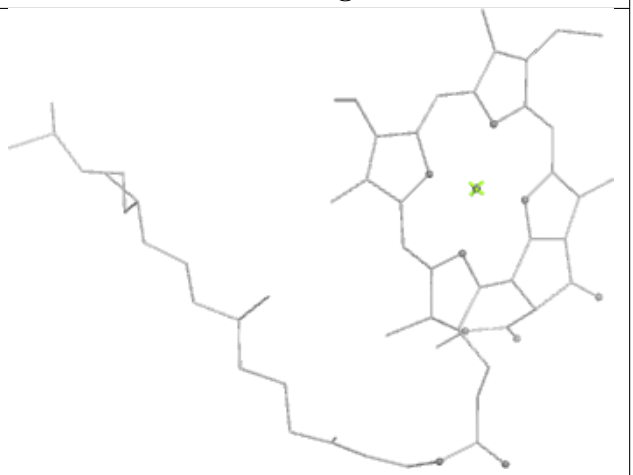
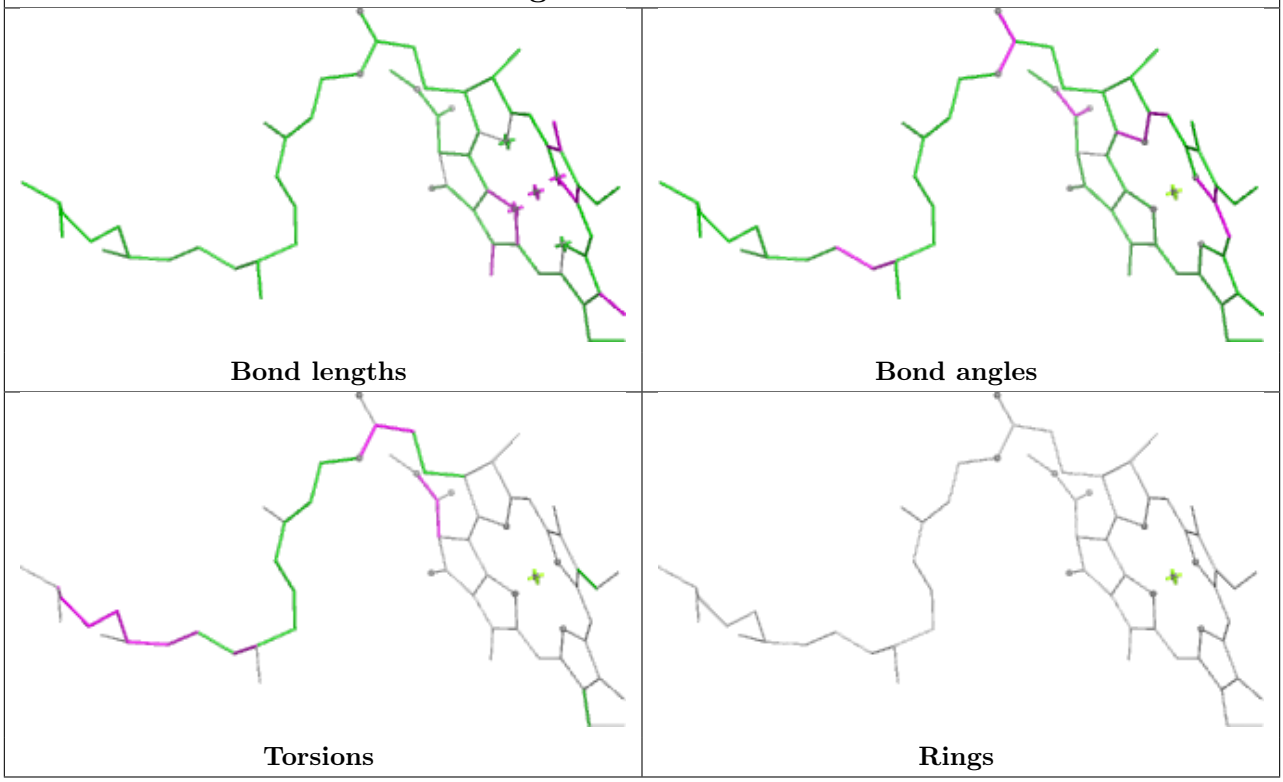
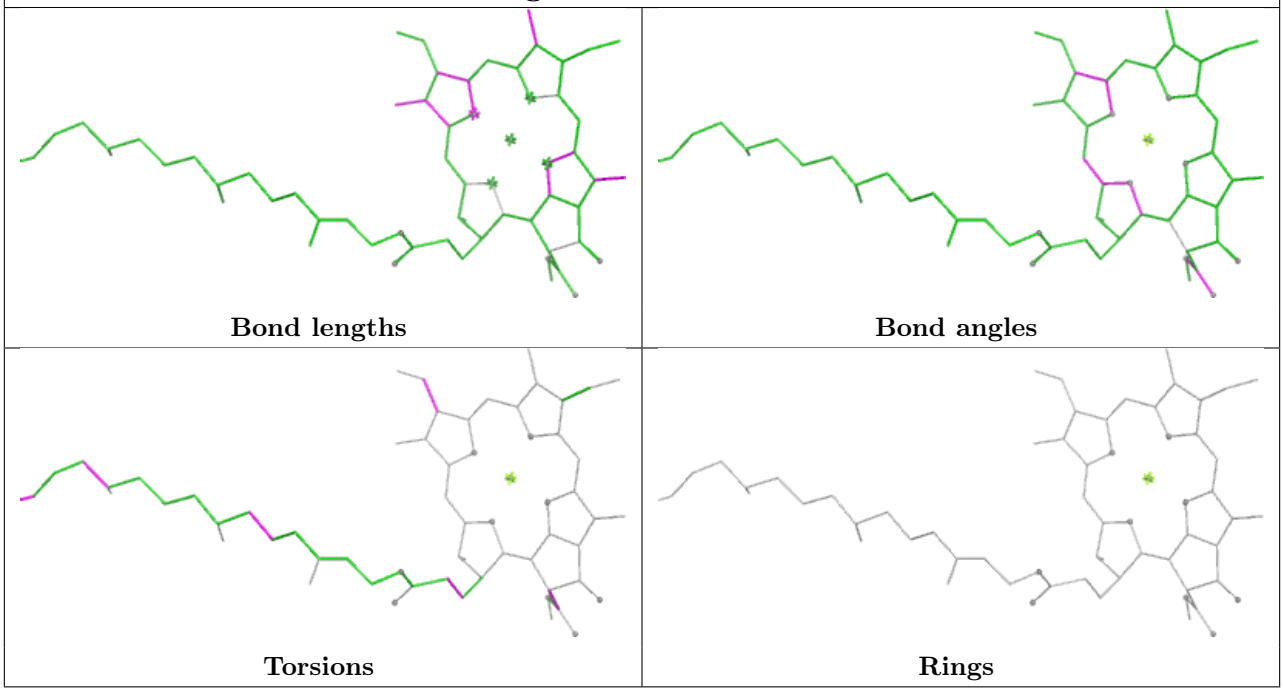


Rings

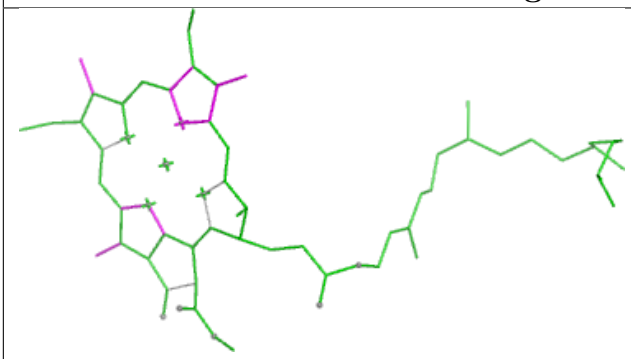
Ligand CLA 2 803



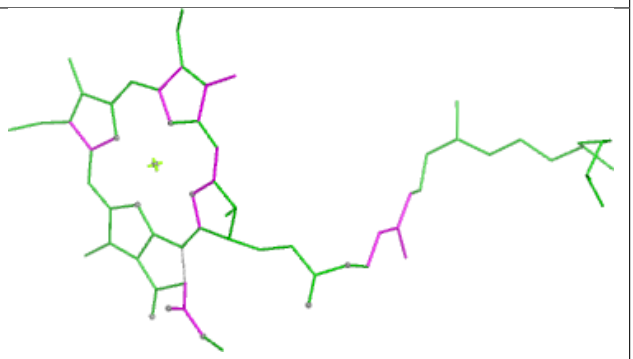
Ligand CLA A 835



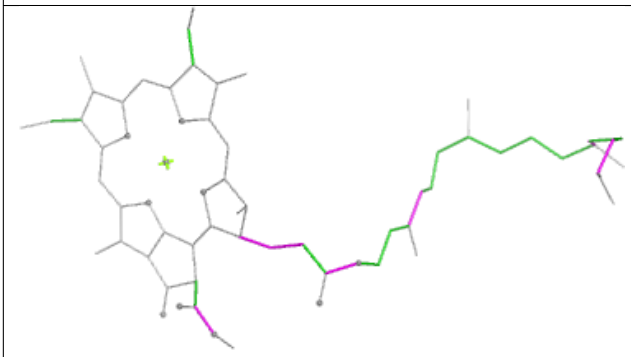
Ligand CLA B 809



Bond lengths



Bond angles



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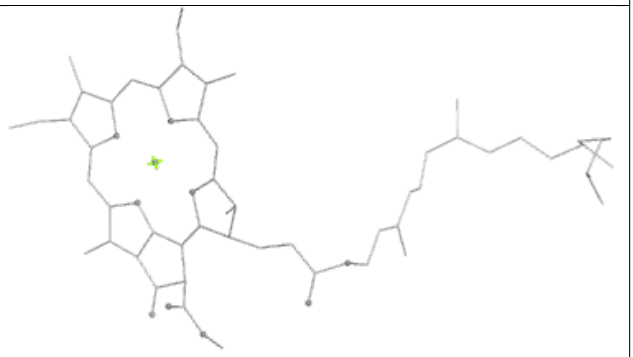
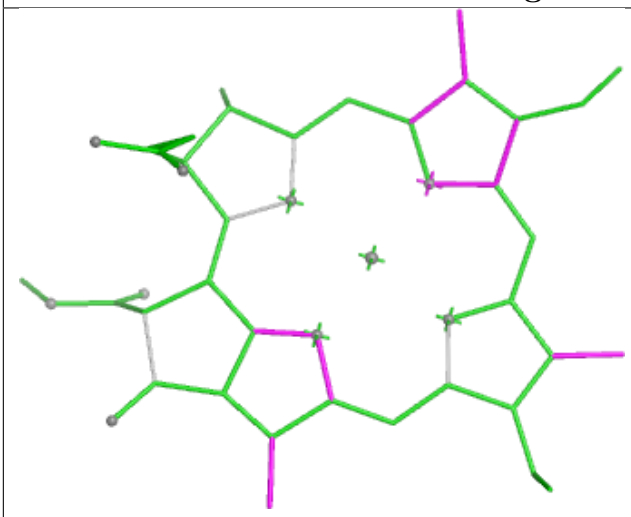


Rings

Ligand CLA B 812



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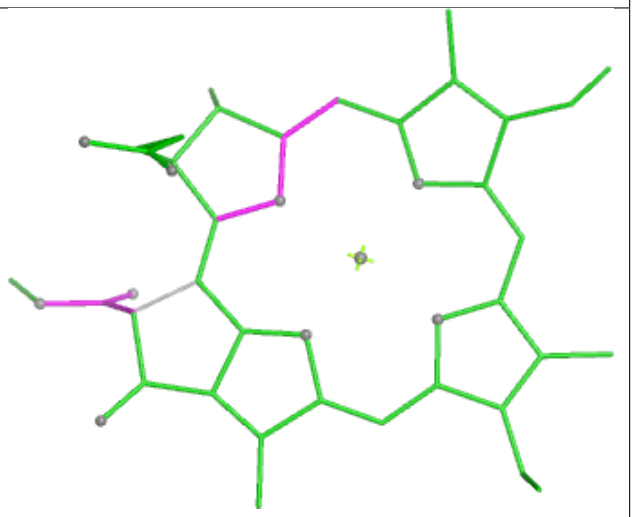
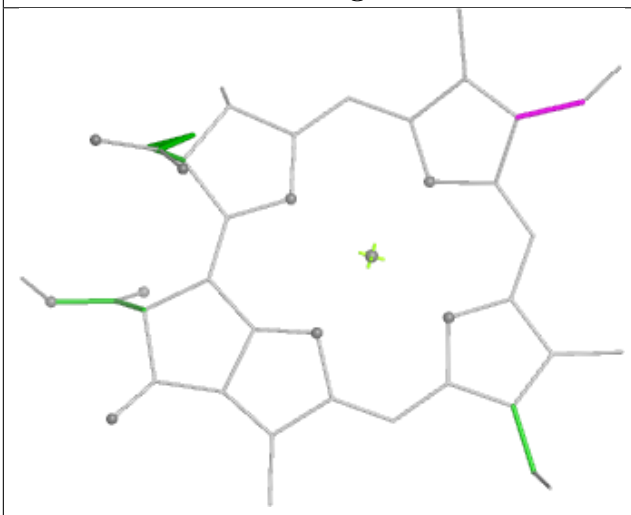


Bond angles



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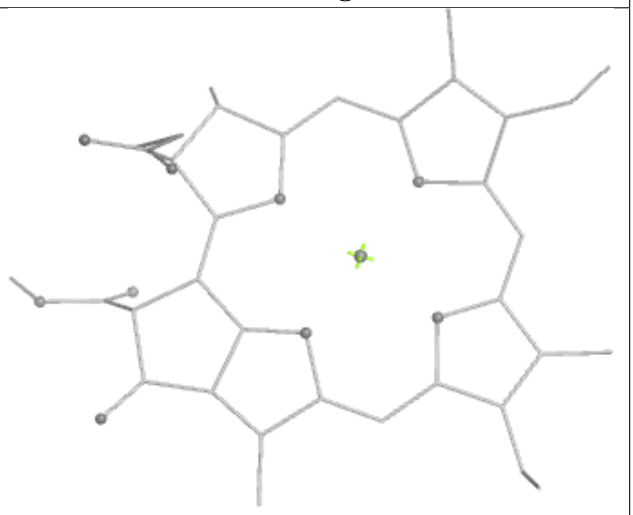


Rings

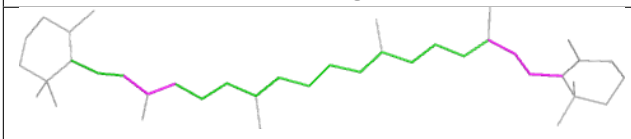
Ligand BCR B 844



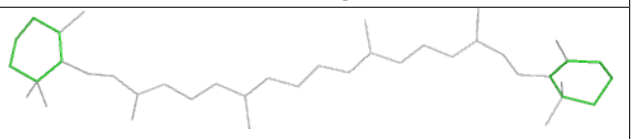
Bond lengths



Bond angles



Torsions

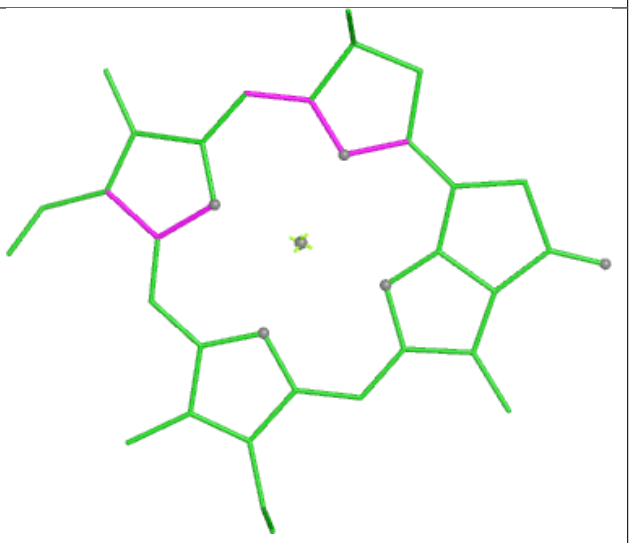


Rings

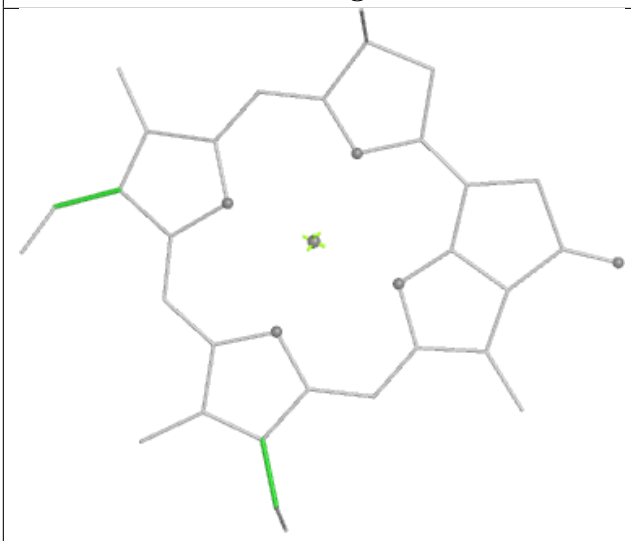
Ligand CLA M 102



Bond lengths



Bond angles



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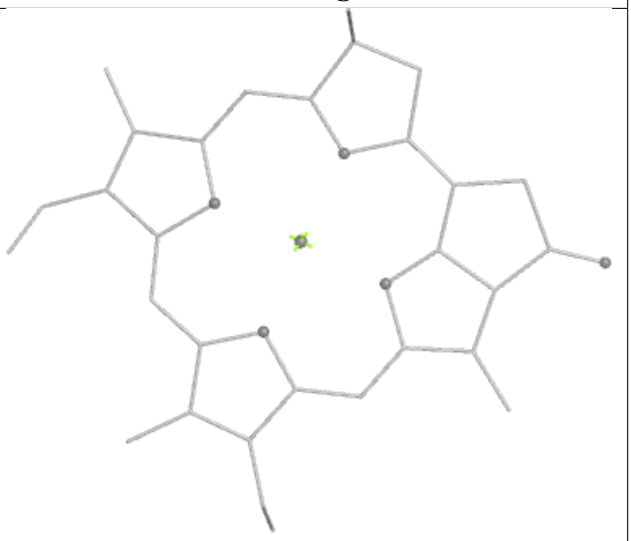
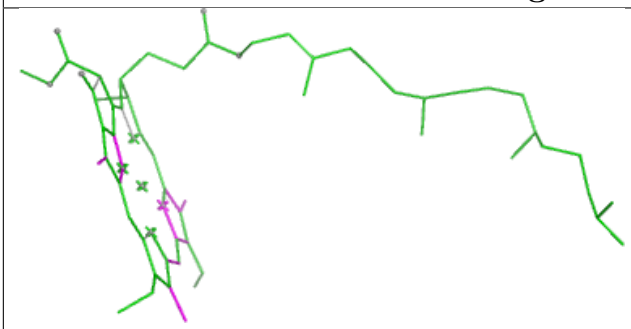
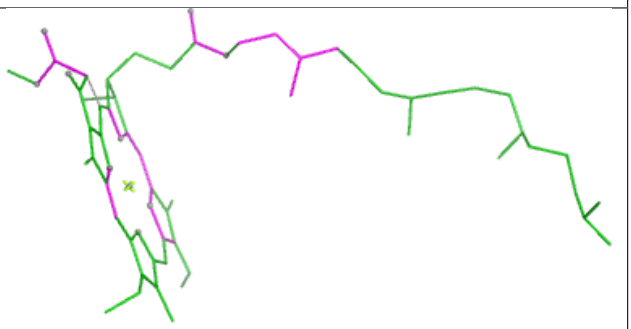


Rings

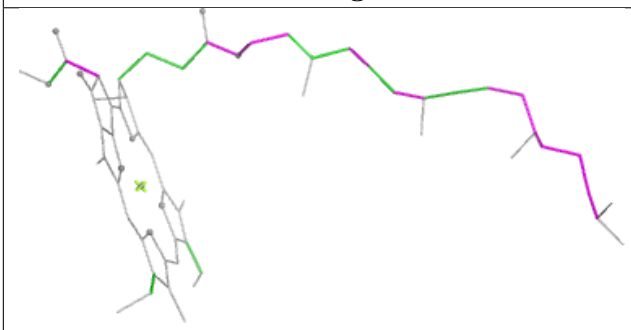
Ligand CLA 2 805



Bond lengths



Bond angles

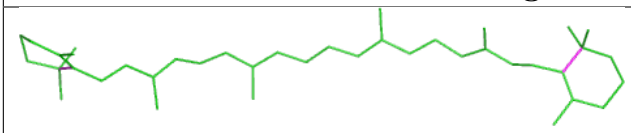


Torsions

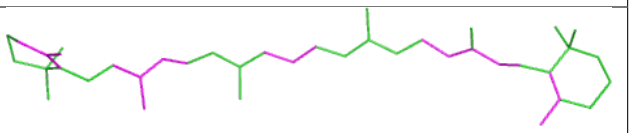


Rings

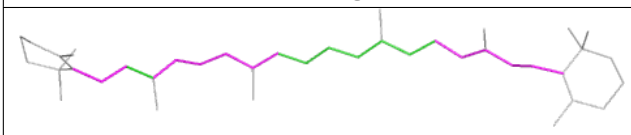
Ligand BCR B 851



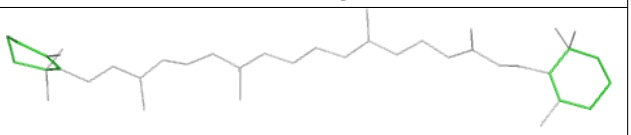
Bond lengths



Bond angles

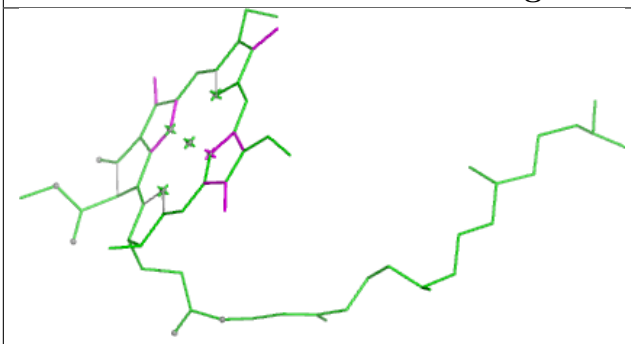


Torsions

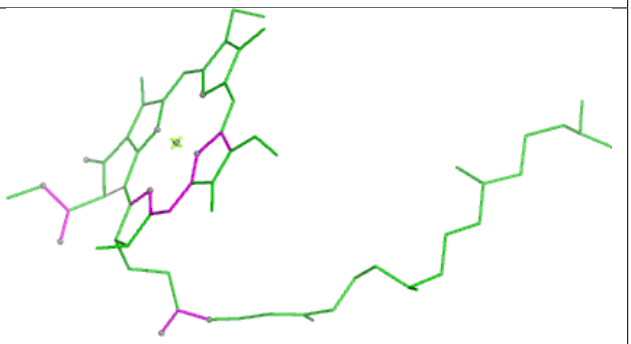


Rings

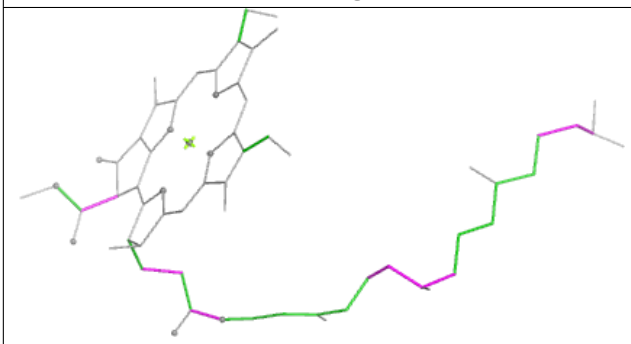
Ligand CLA B 815



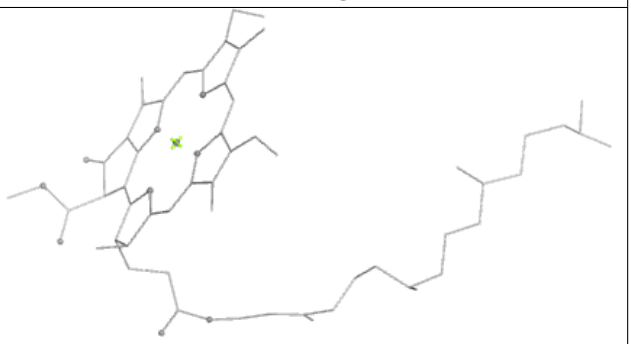
Bond lengths



Bond angles



Torsions

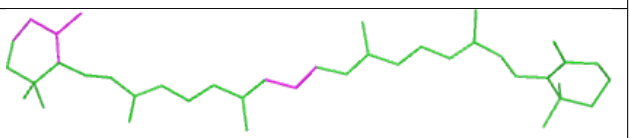


Rings

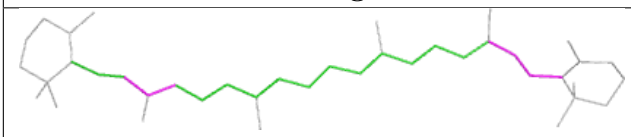
Ligand BCR 2 845



Bond lengths



Bond angles



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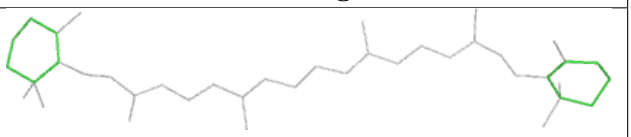
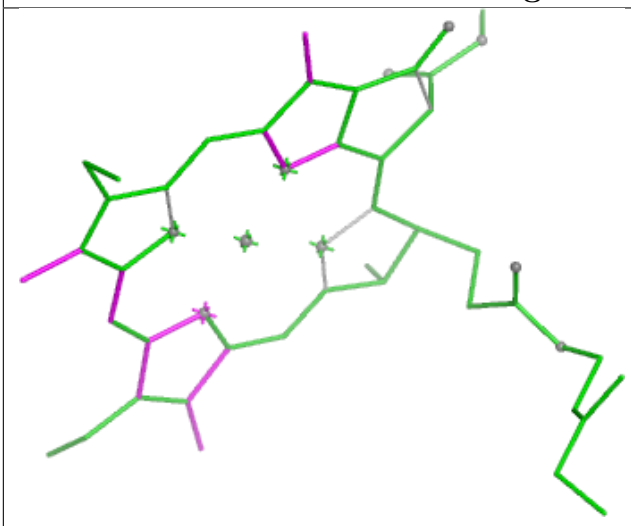


Rings

Ligand CLA A 808



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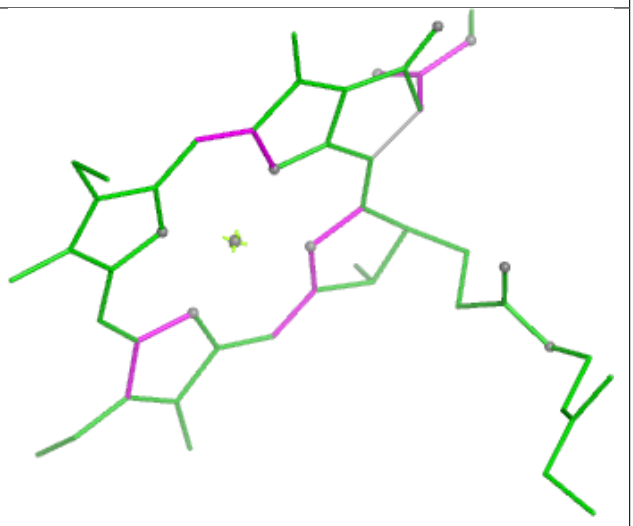
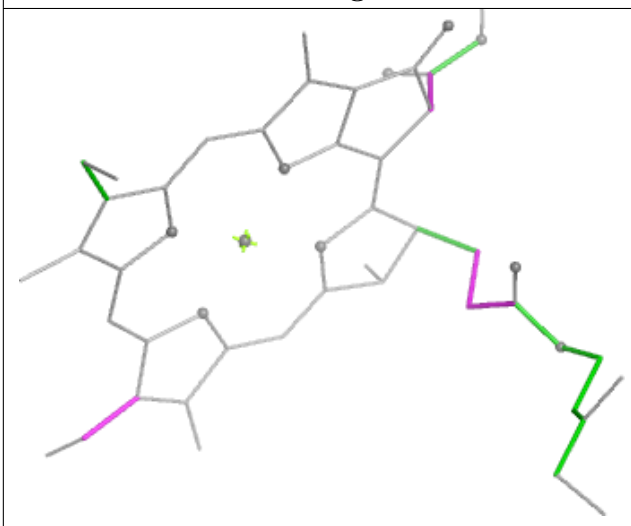


Bond angles



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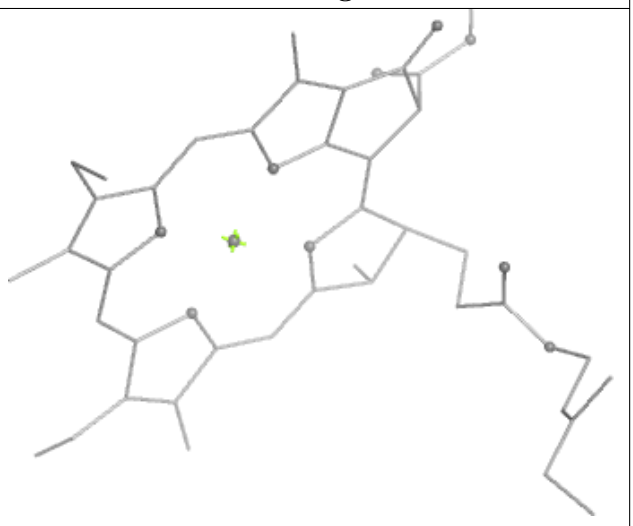
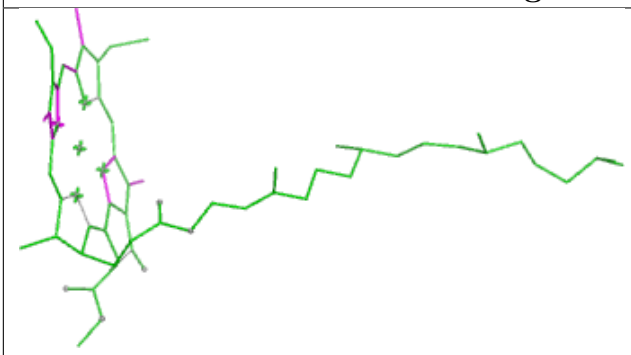


Rings

Ligand CLA B 828



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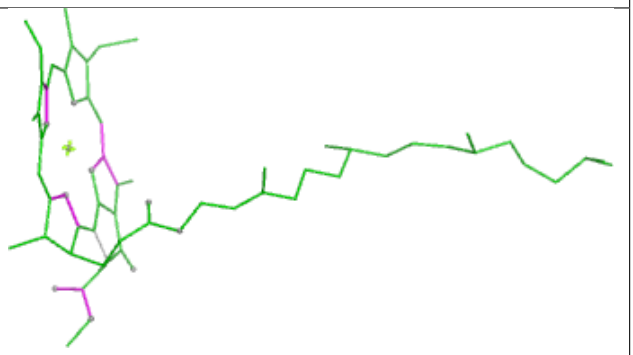

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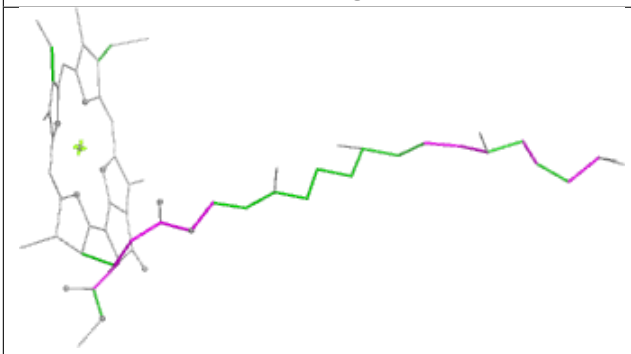

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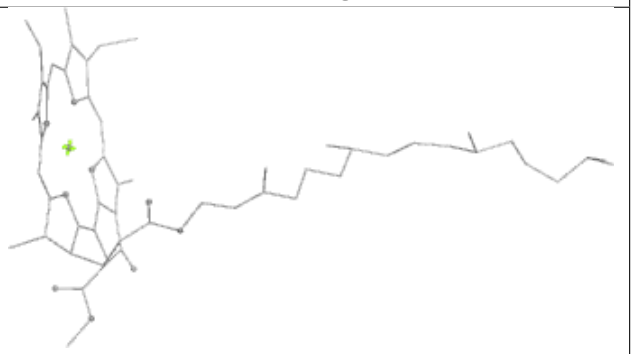
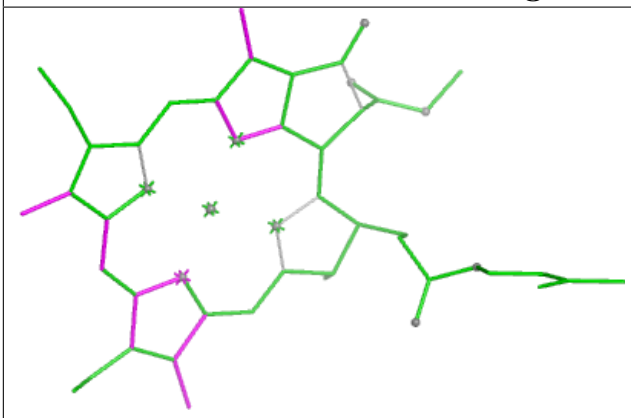


Rings

Ligand CLA B 835



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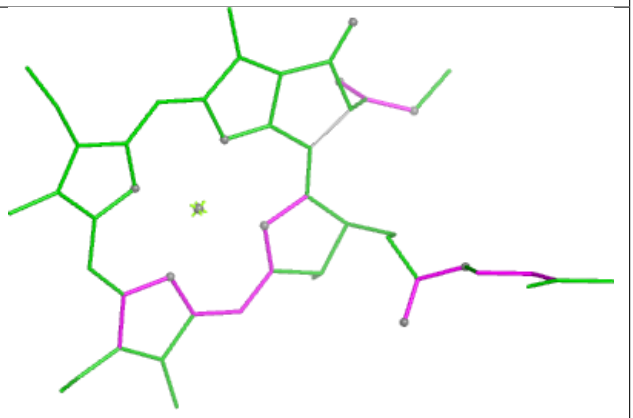

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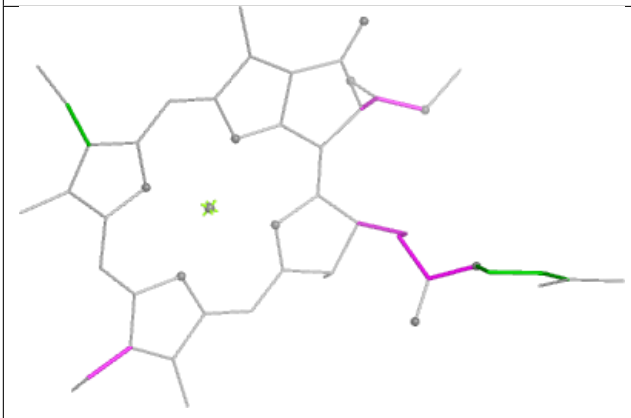
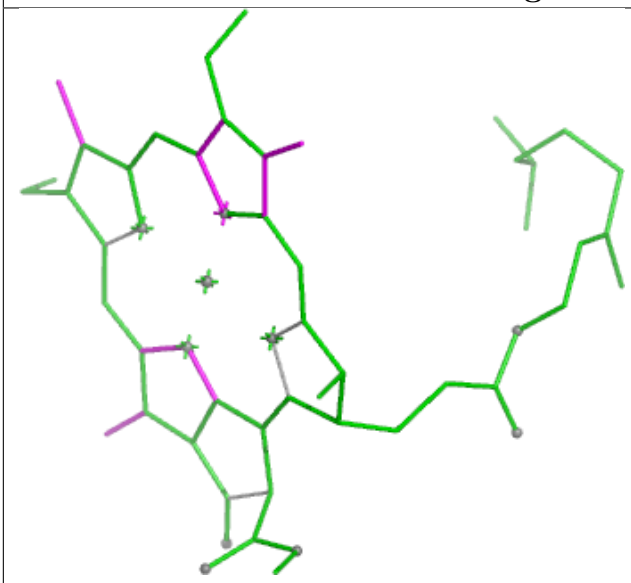


Torsions



Rings

Ligand CLA B 830



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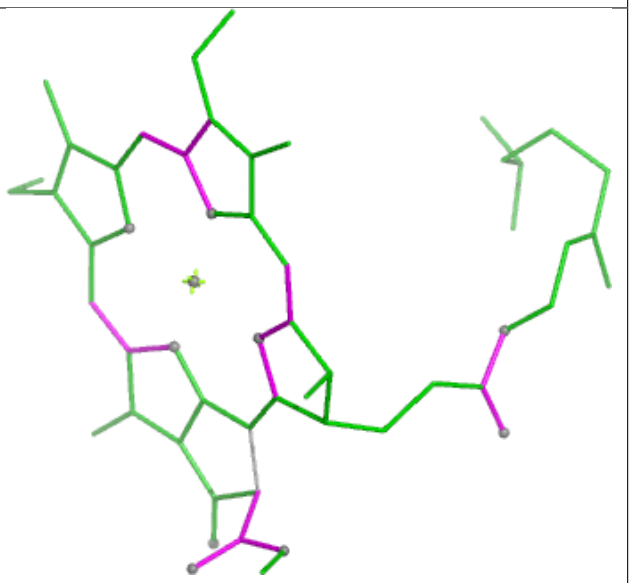
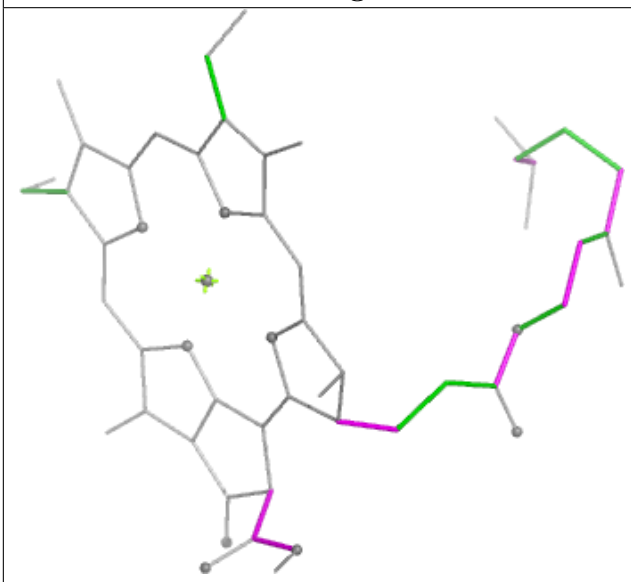


Bond angles



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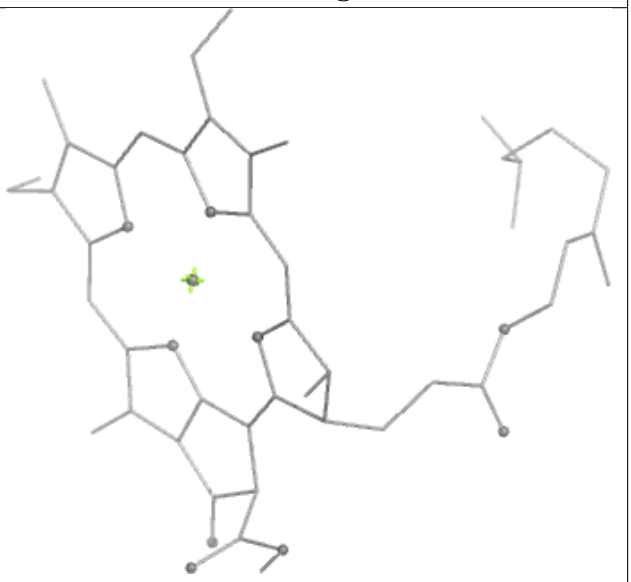
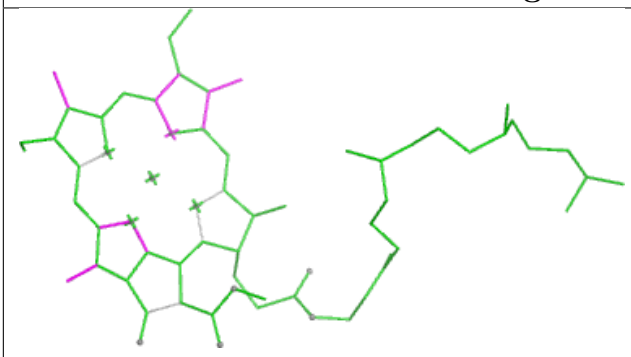


Rings

Ligand CLA A 804



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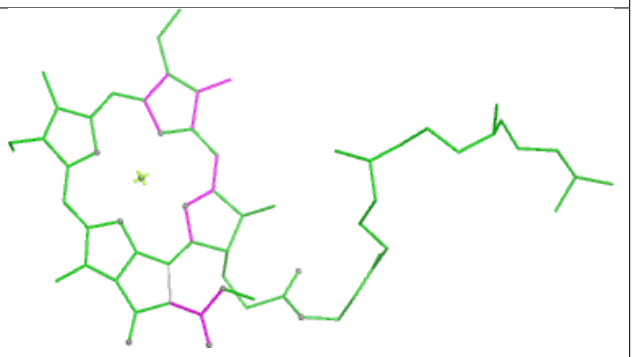
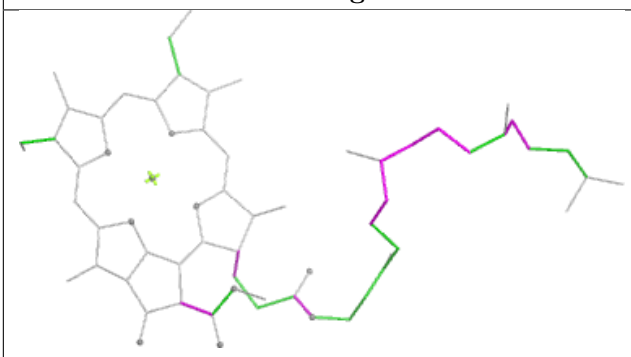


Bond angles



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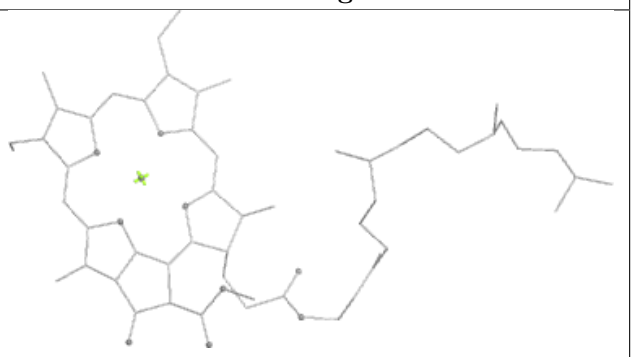
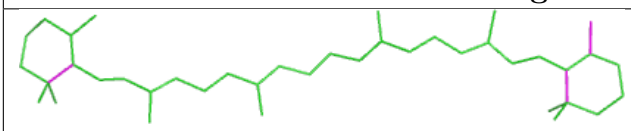


Rings

Ligand BCR l 207



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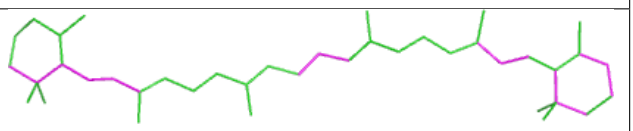
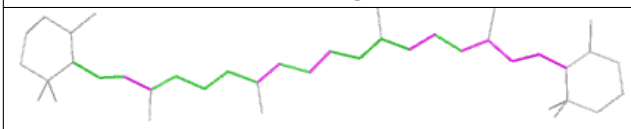


Bond angles



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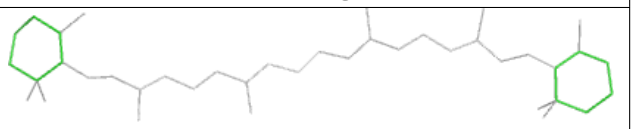
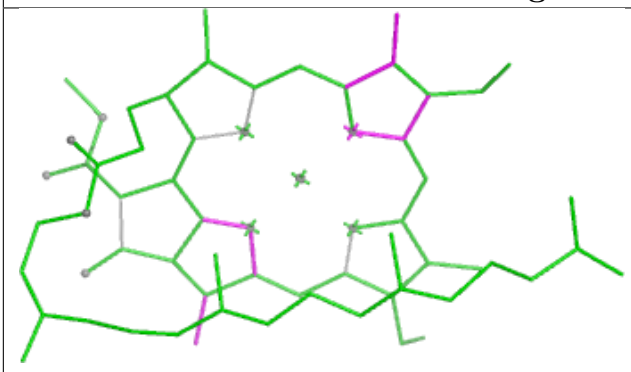


Rings

Ligand CLA 2 817



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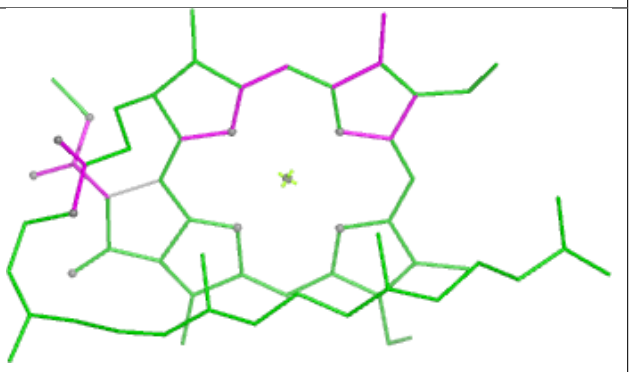
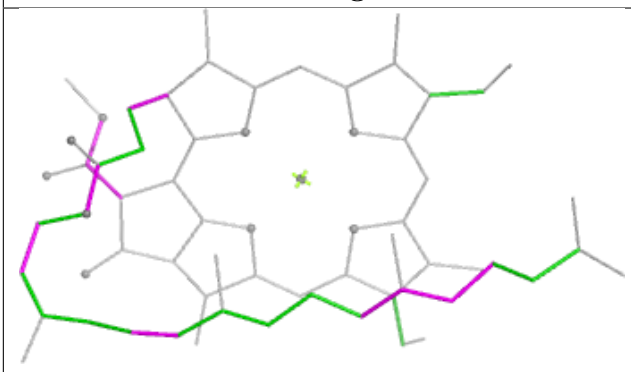


Bond angles



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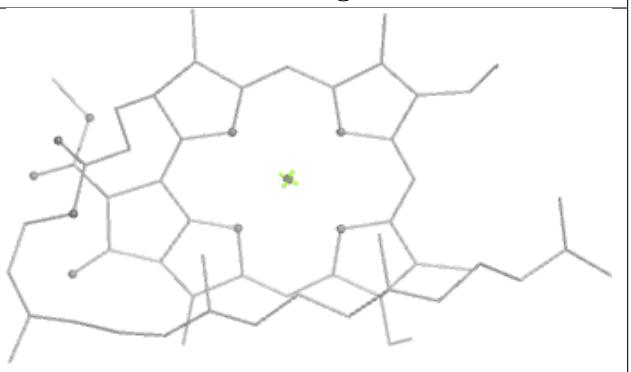
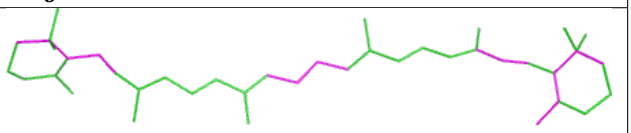


Rings

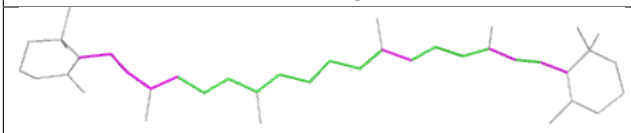
Ligand BCR j 1304



Bond lengths



Bond angles



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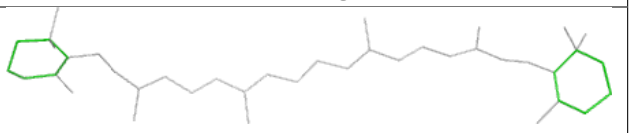
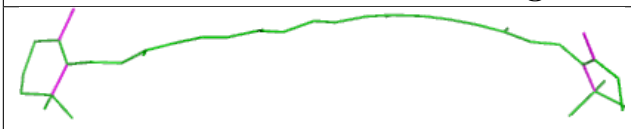


Rings

Ligand BCR 7 101



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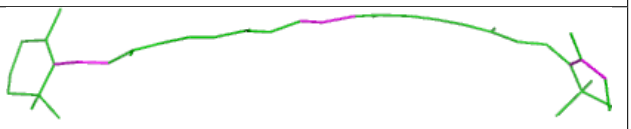
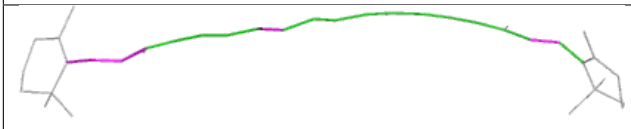


Bond angles



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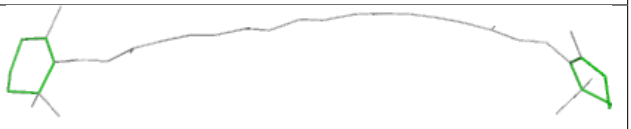
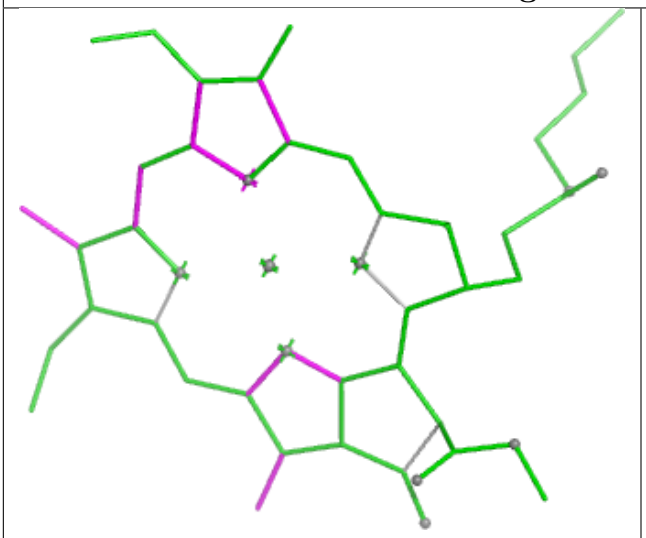


Rings

Ligand CLA 1 1612



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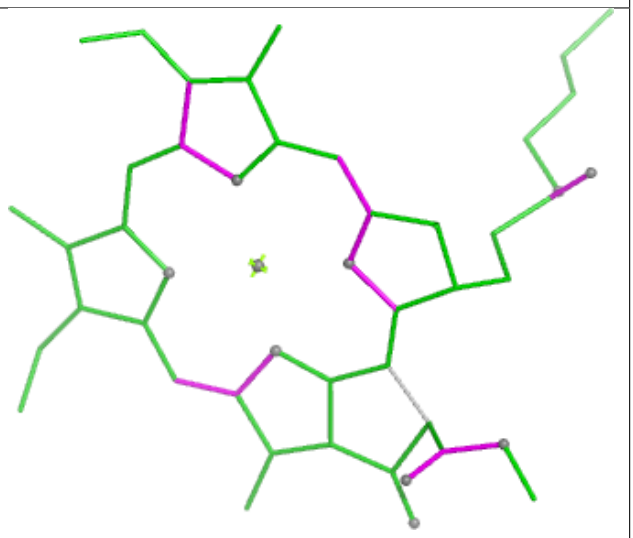
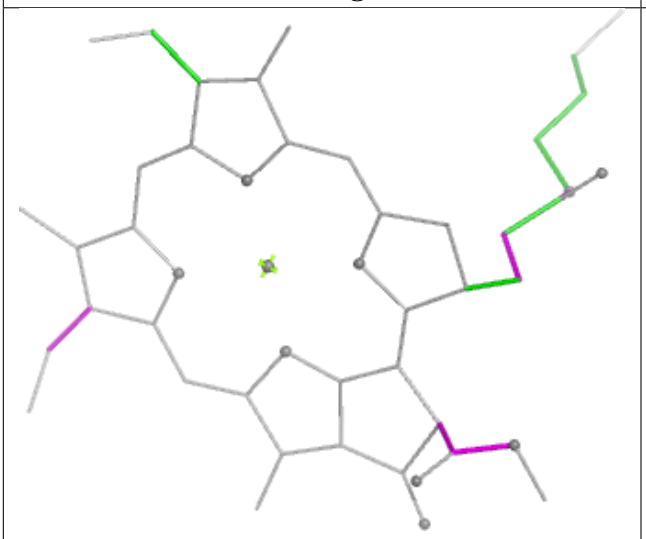


Bond angles



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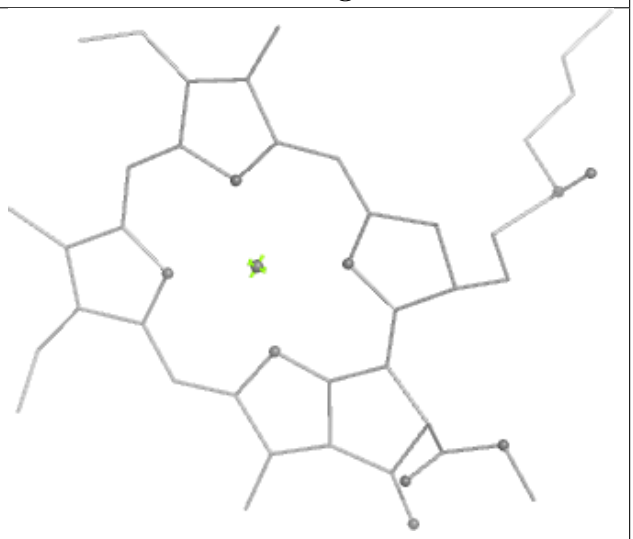
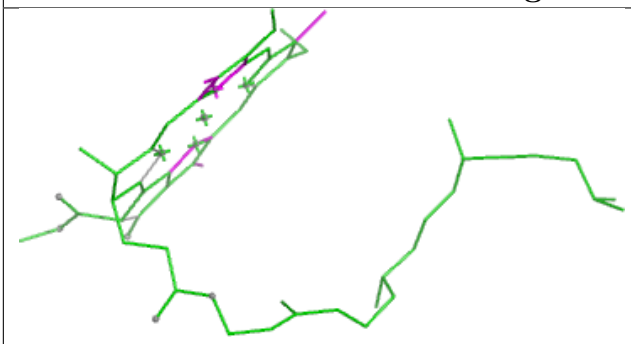


Rings

Ligand CLA B 811



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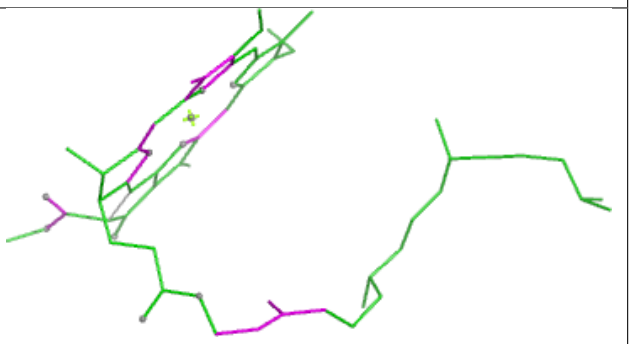
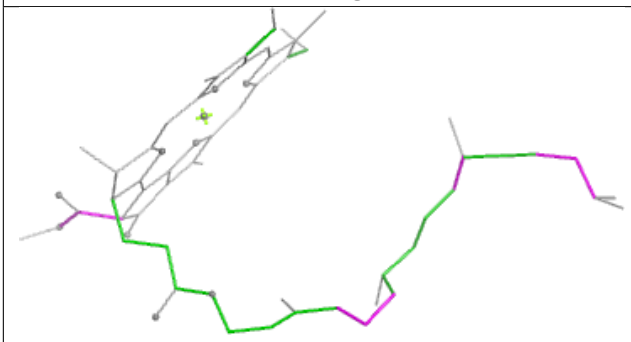


Bond angles



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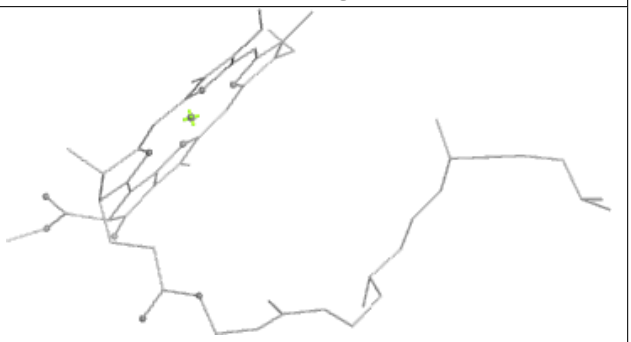
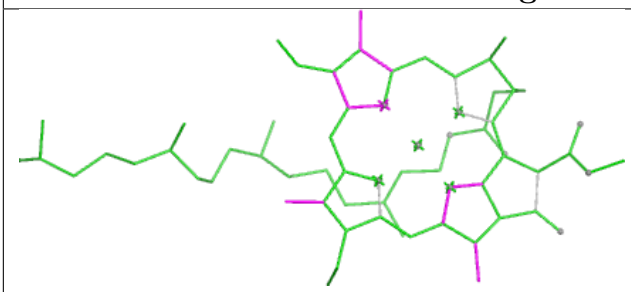


Rings

Ligand CLA 1 1640



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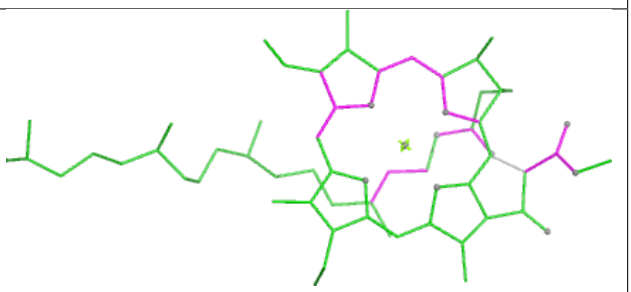
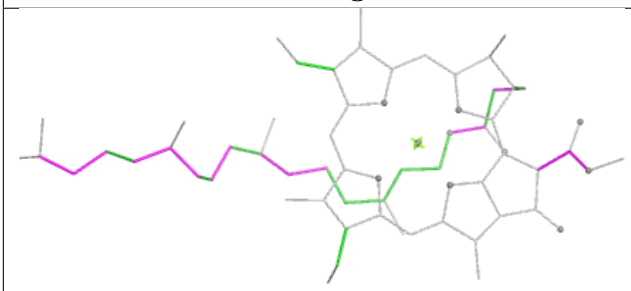


Bond angles

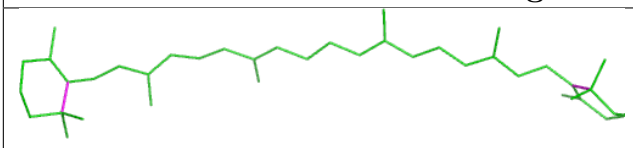


Torsions



Rings

Ligand BCR 9 102



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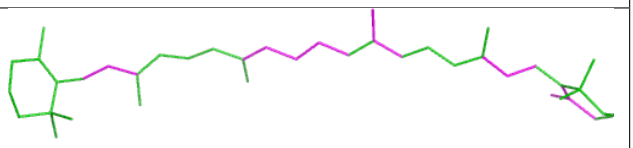
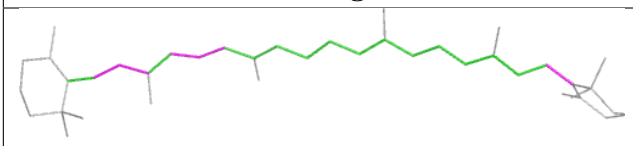


Bond angles



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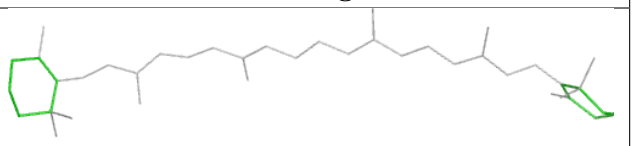
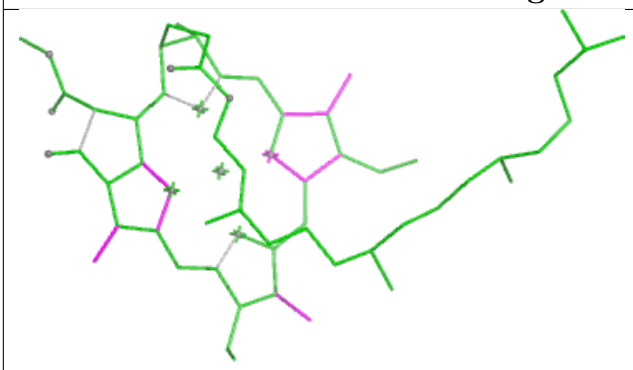


Rings

Ligand CLA b 808



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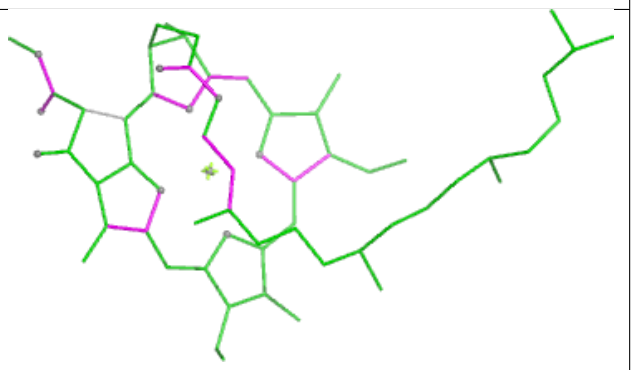
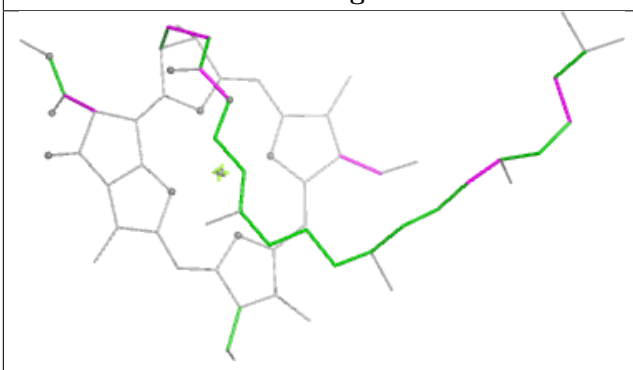


Bond angles



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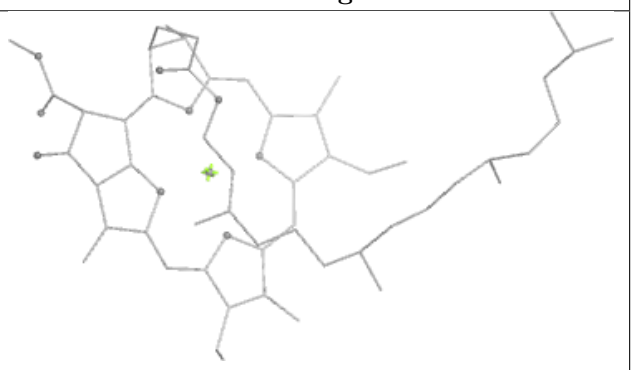
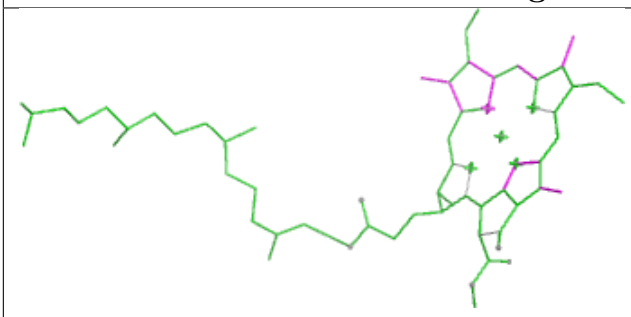
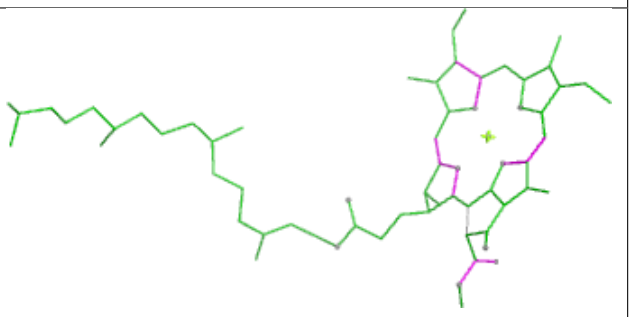


Rings

Ligand CLA a 803



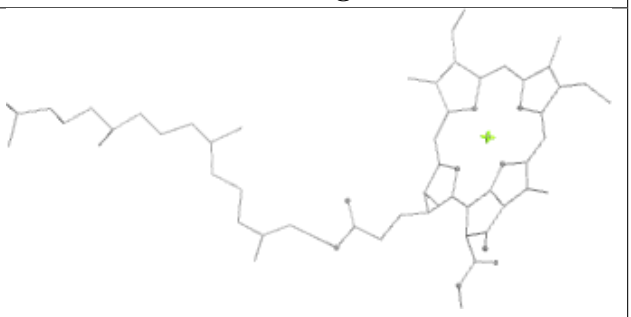
Bond lengths



Bond angles

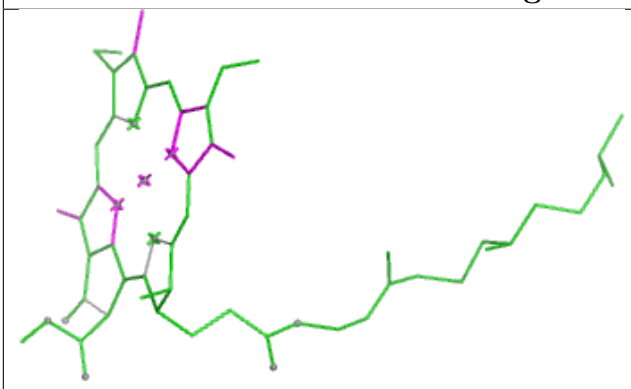


Torsions



Rings

Ligand CLA A 832



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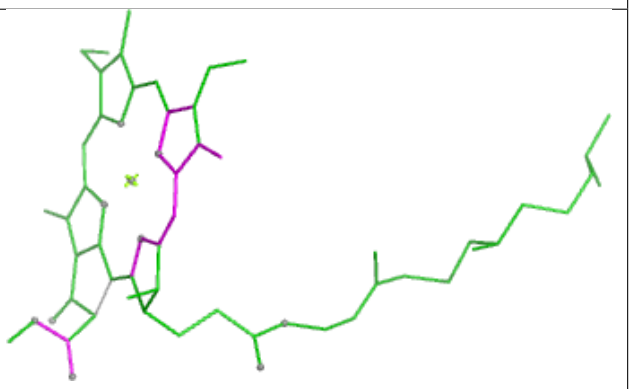

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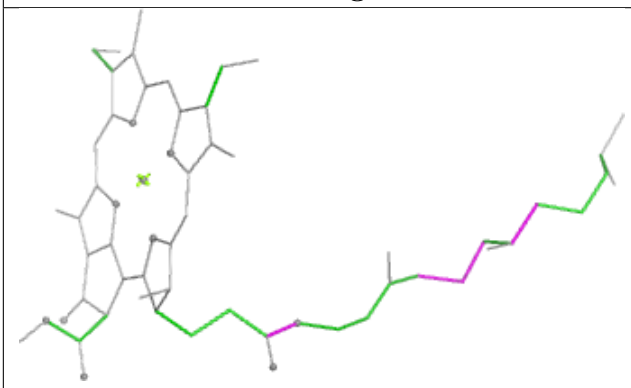

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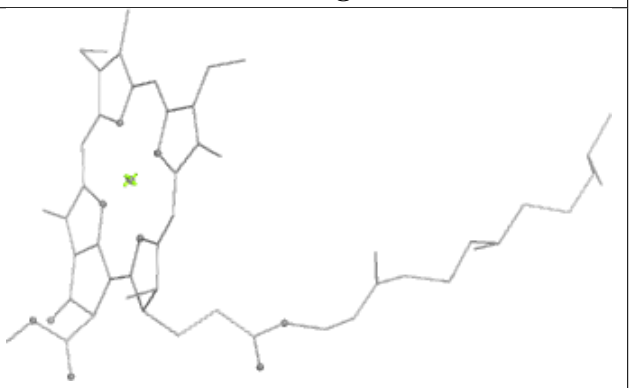
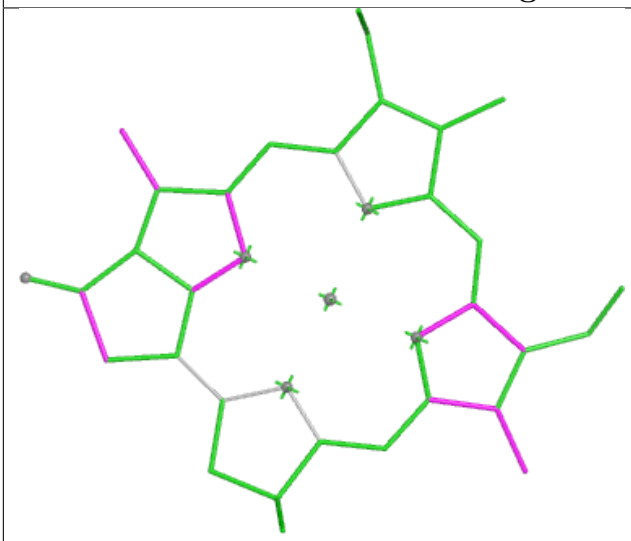


Rings

Ligand CLA 1 1601



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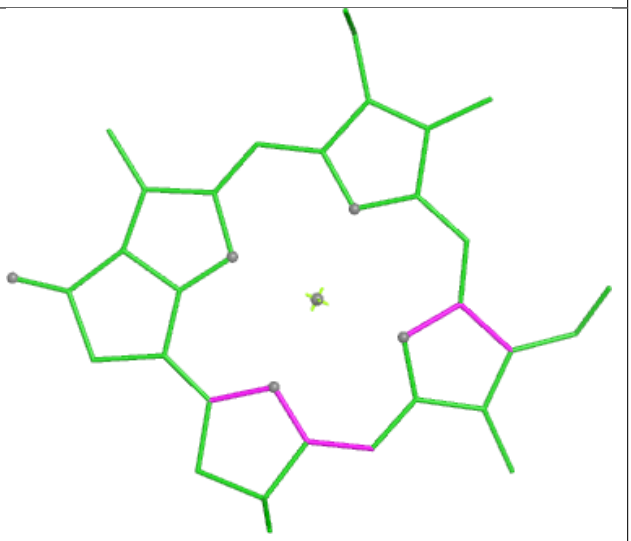

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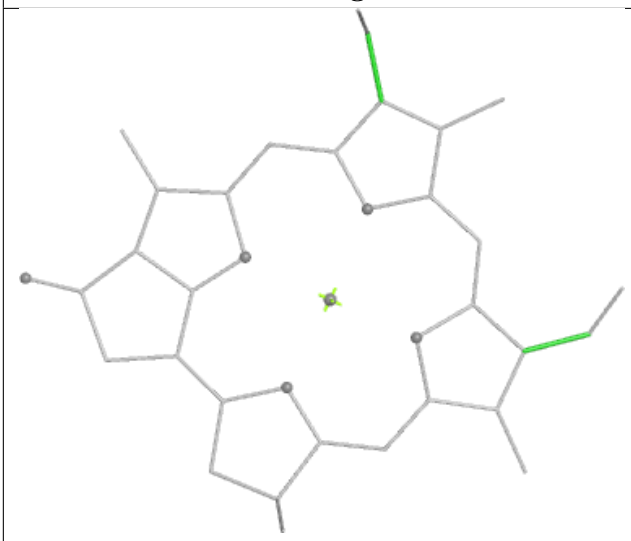

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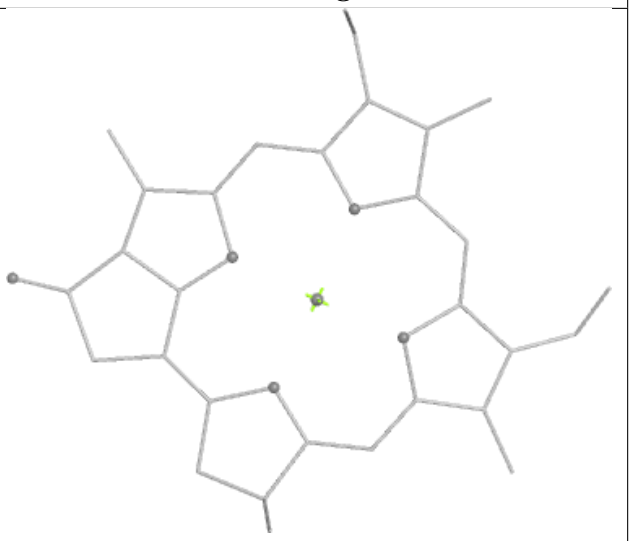
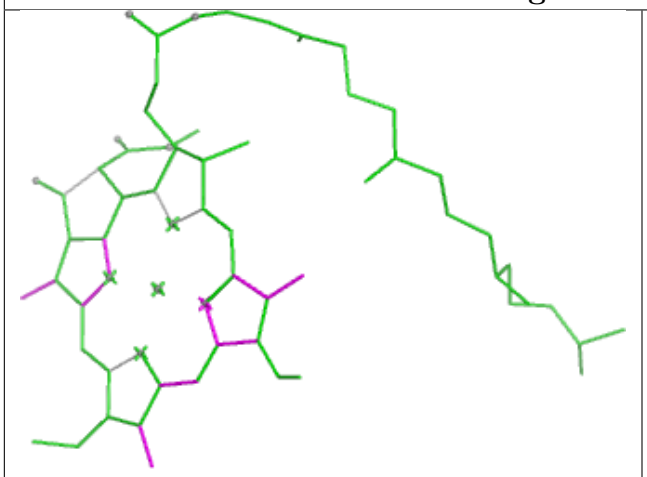


Rings

Ligand CLA b 825



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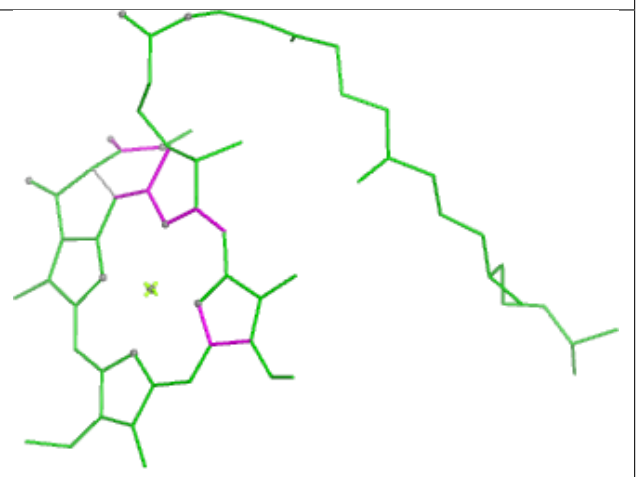
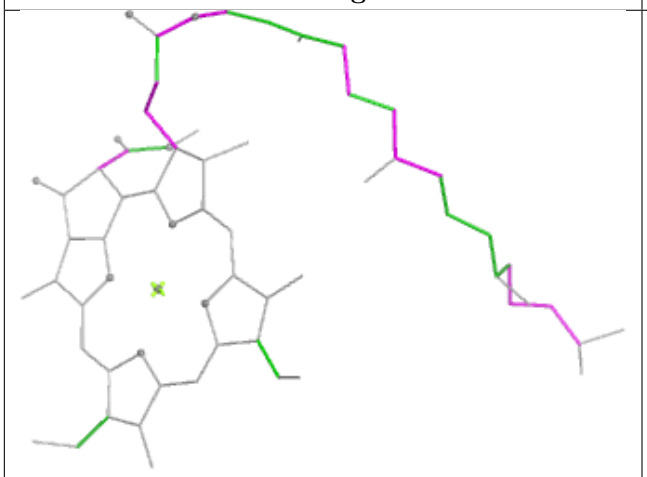


Bond angles



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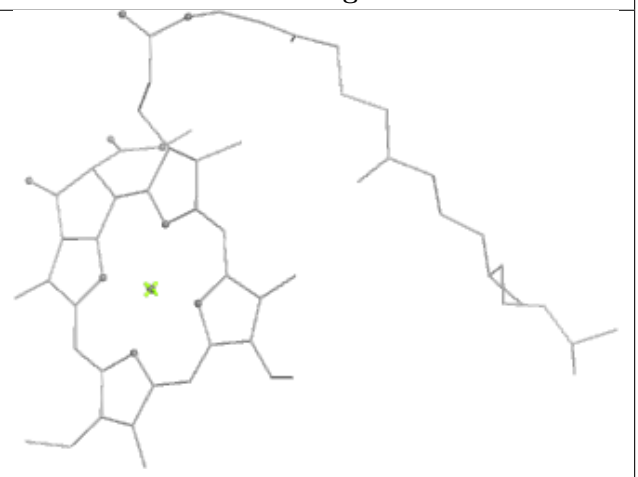
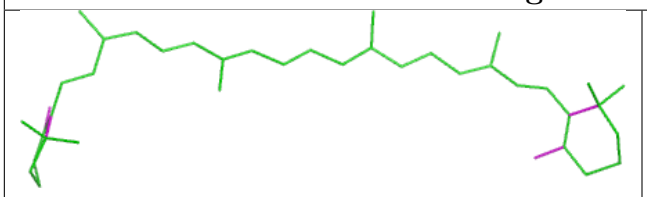


Rings

Ligand BCR L 201



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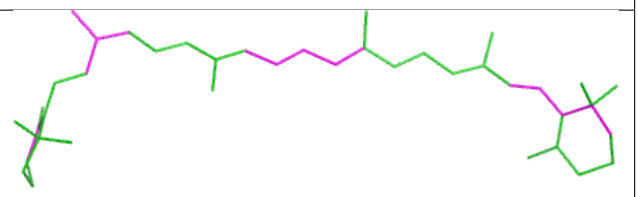
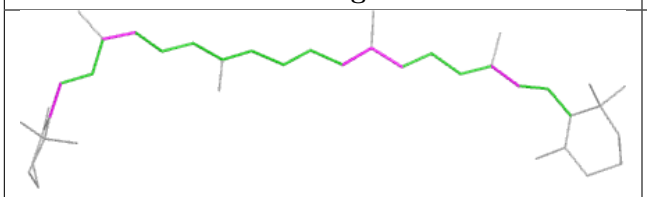


Bond angles



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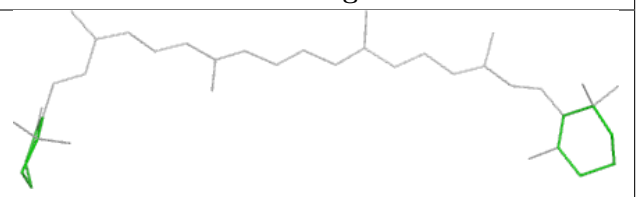
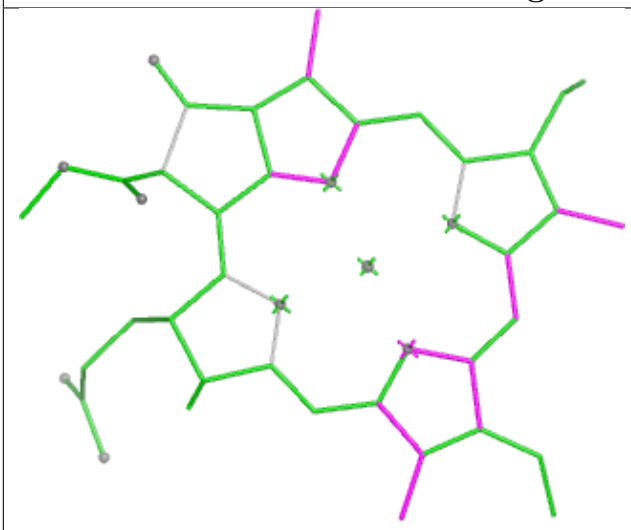


Rings

Ligand CLA b 824



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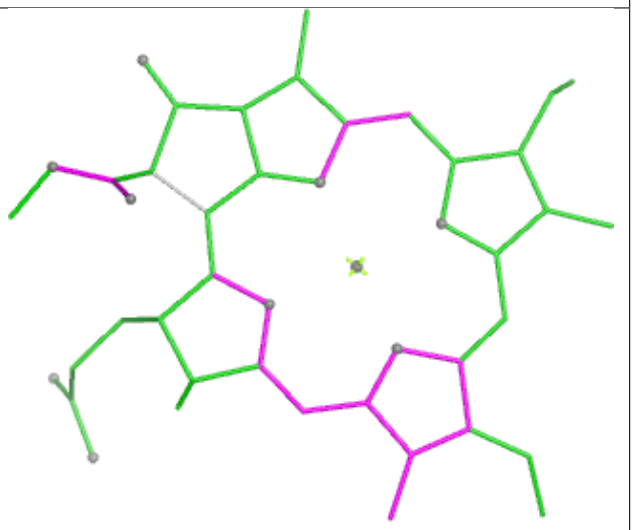
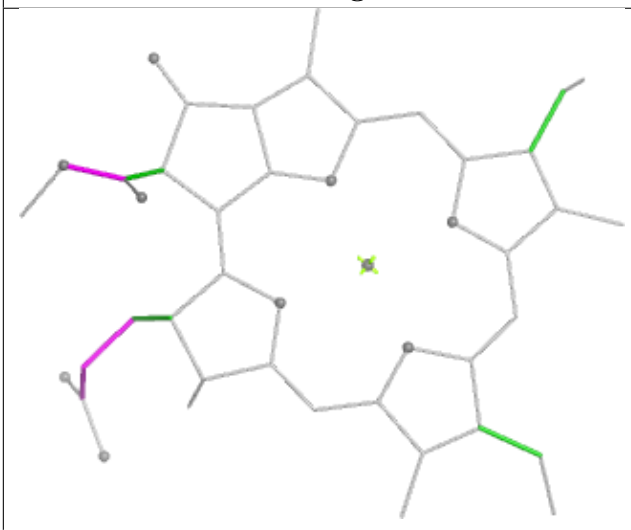


Bond angles



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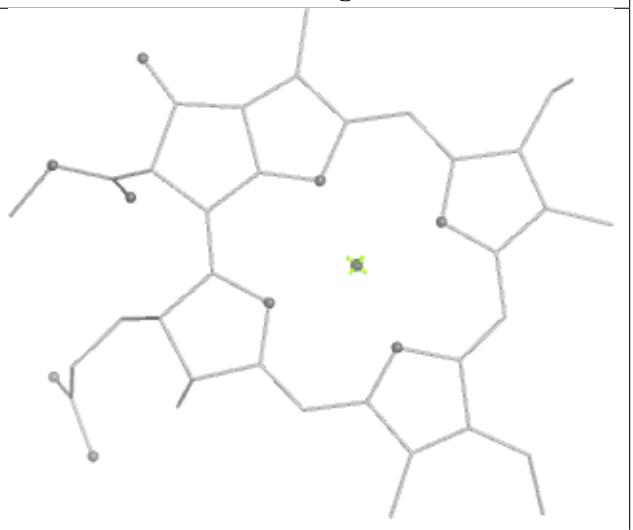
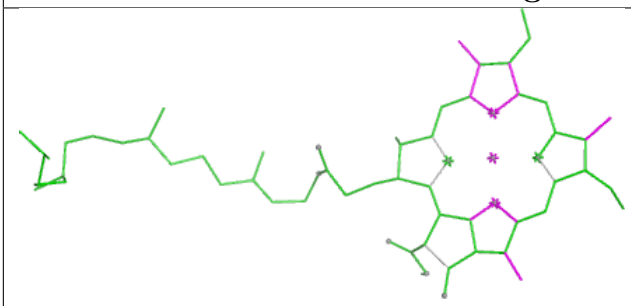


Rings

Ligand CLA A 806



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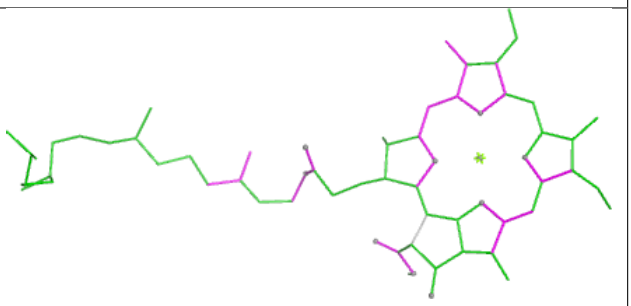
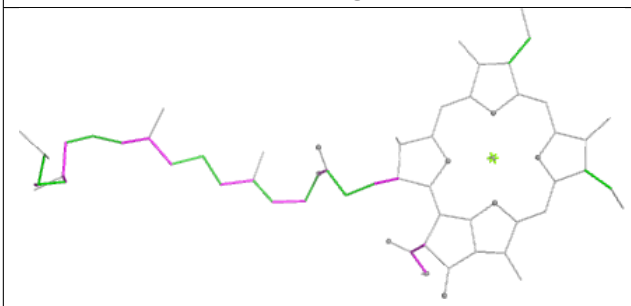


Bond angles



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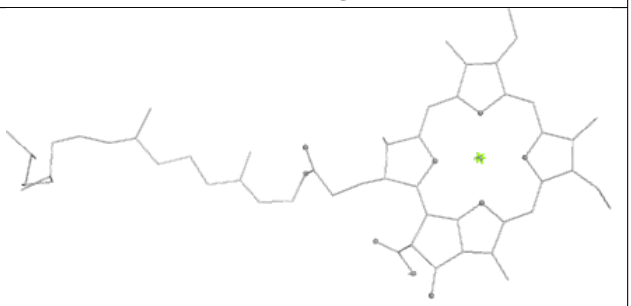
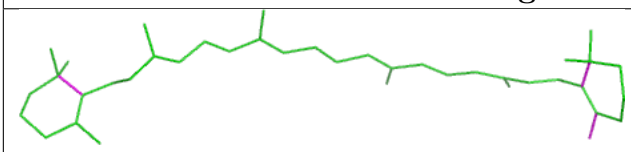


Rings

Ligand BCR M 103



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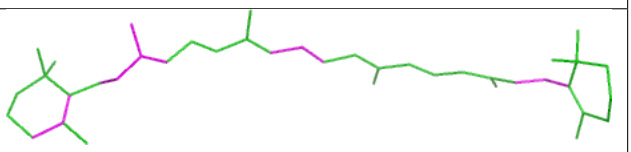
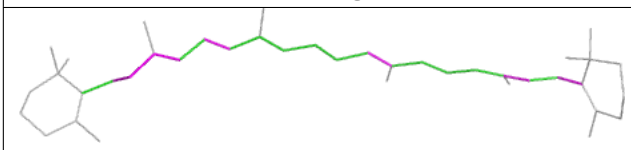


Bond angles



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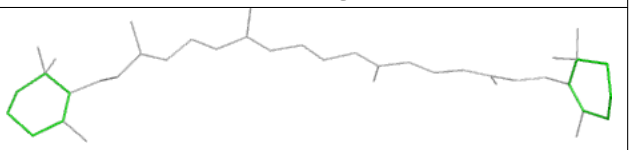
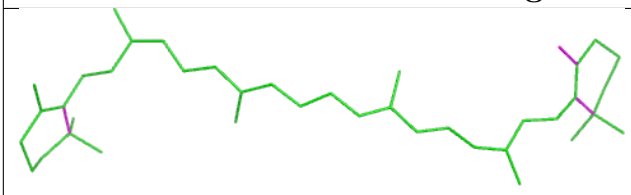


Rings

Ligand BCR b 846



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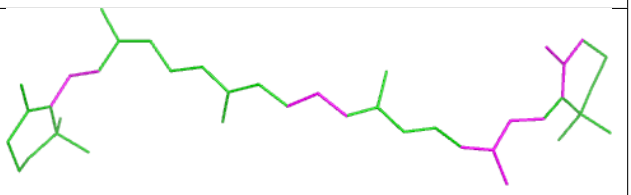
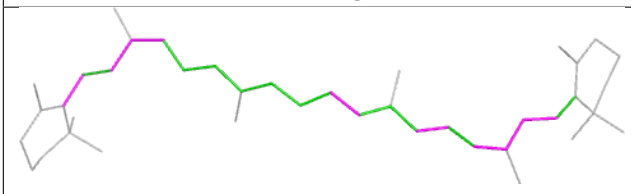


Bond angles



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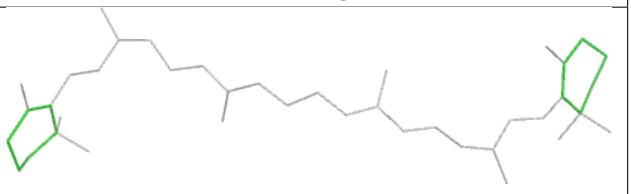
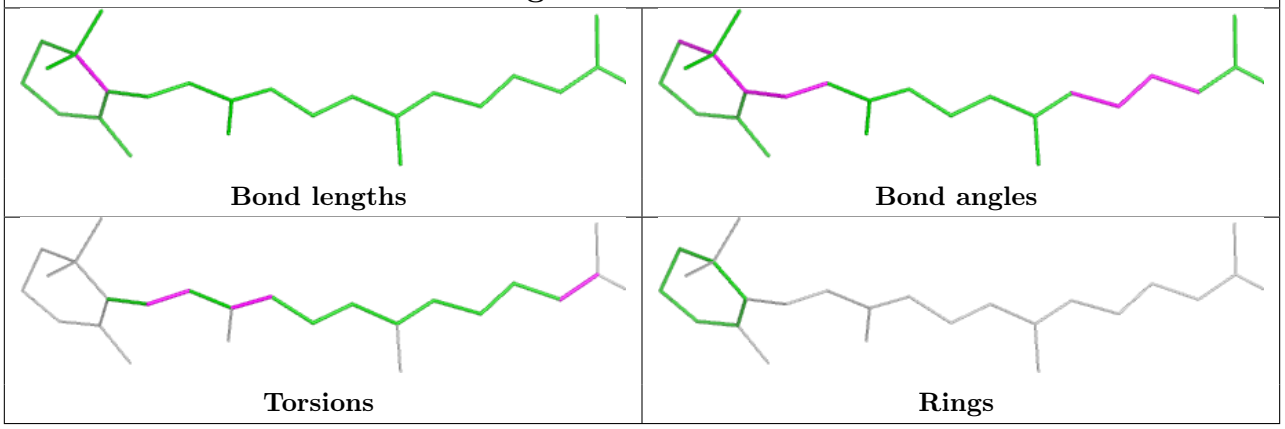
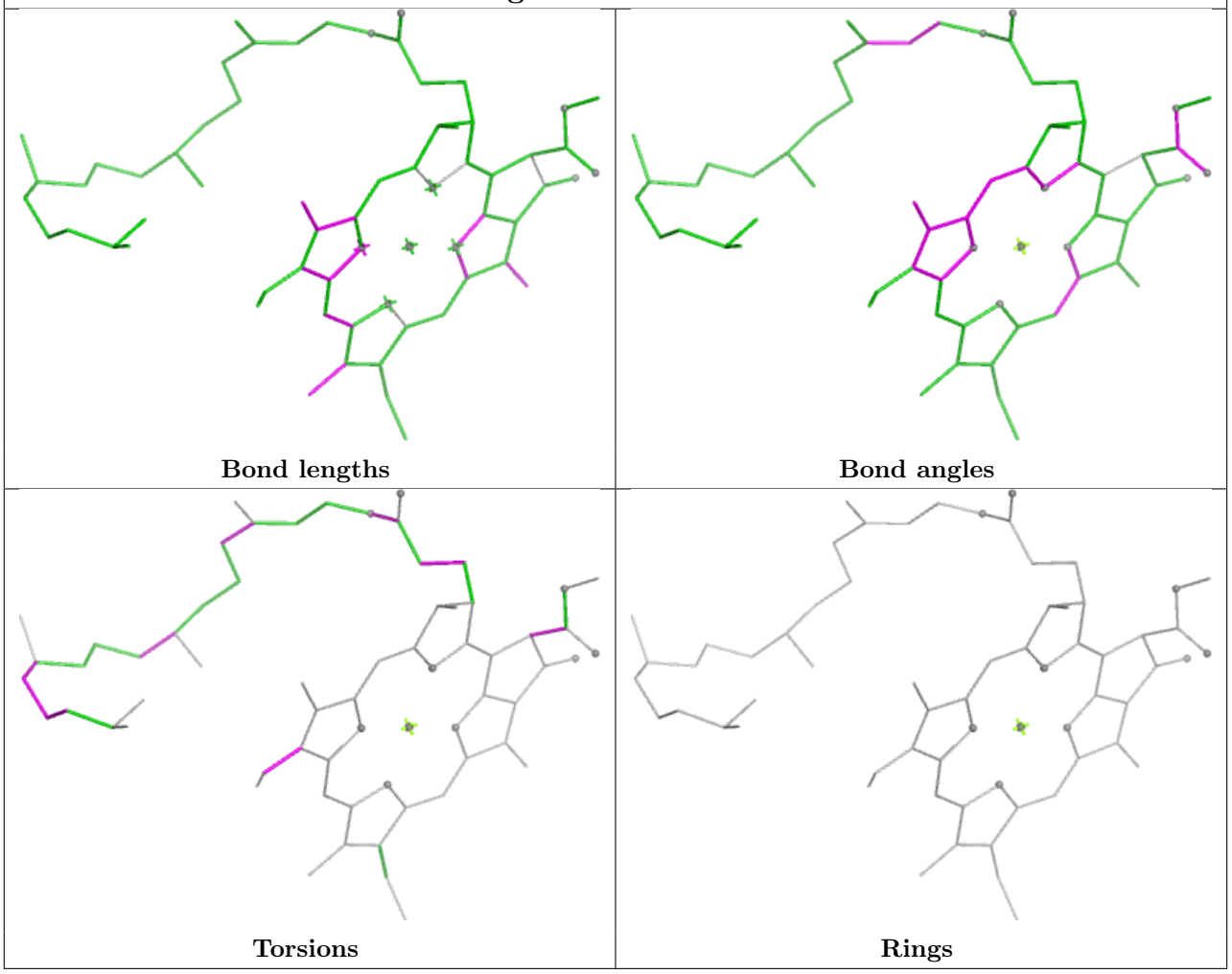


Rings

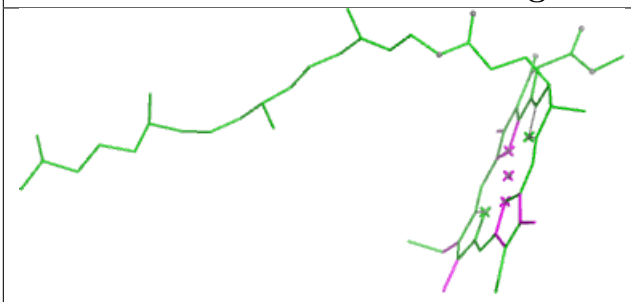
Ligand BCR k 104



Ligand CLA a 825



Ligand CLA 2 830



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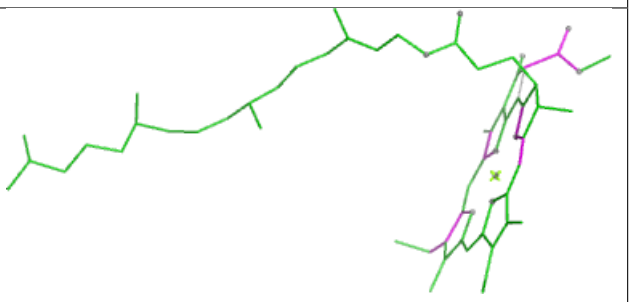
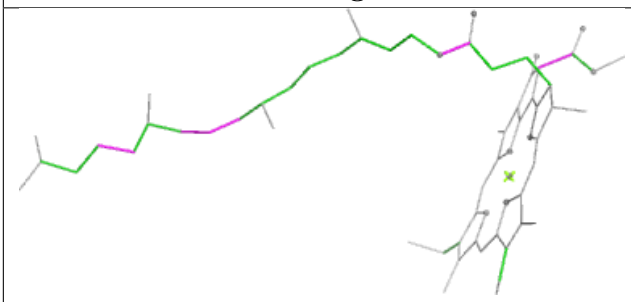


Bond angles

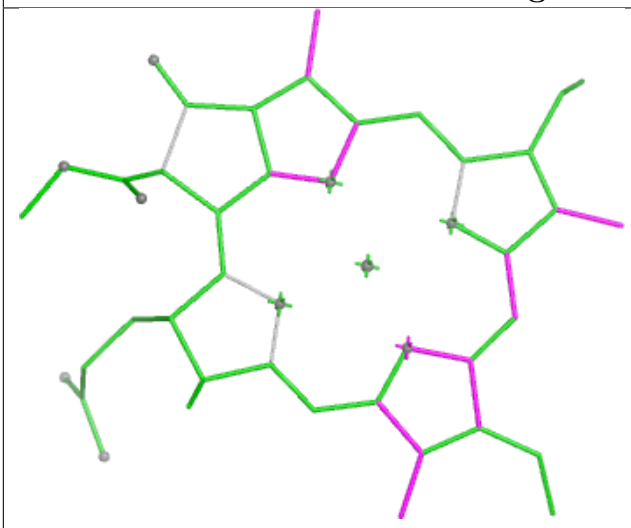


Torsions



Rings

Ligand CLA 2 824



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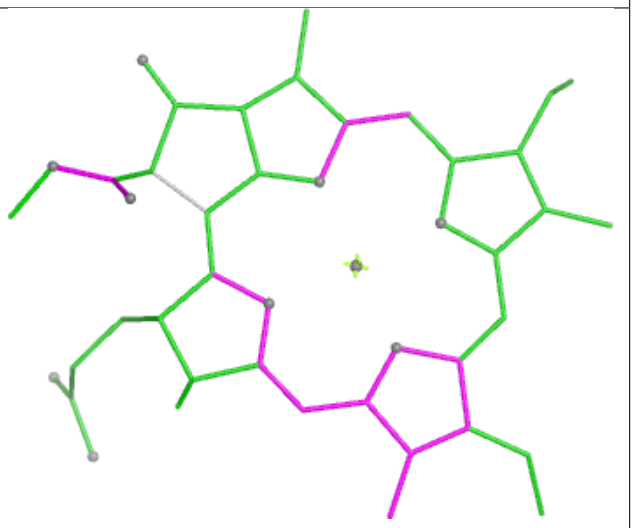
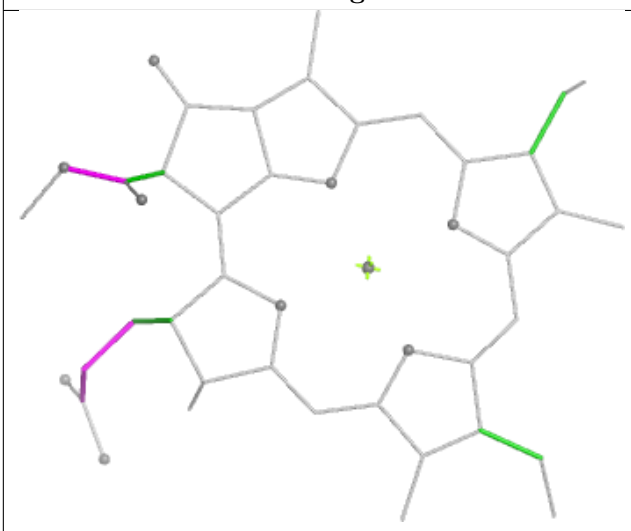


Bond angles



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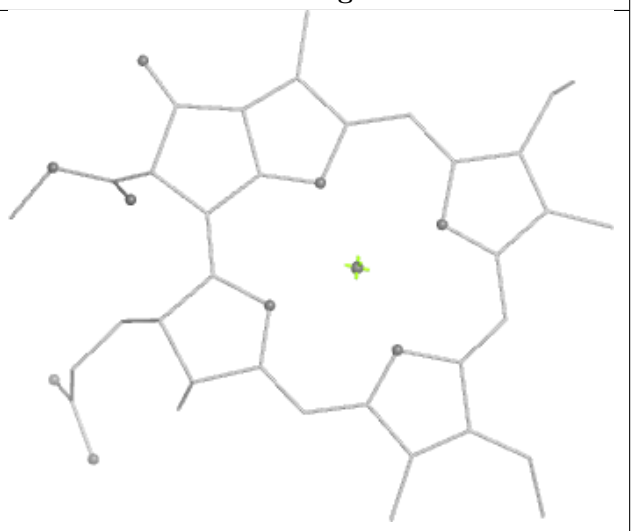
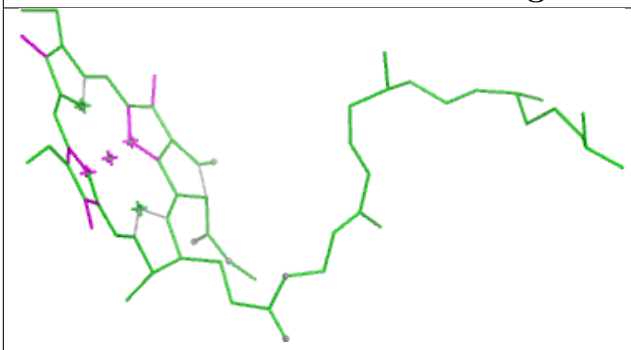


Rings

Ligand CLA b 803



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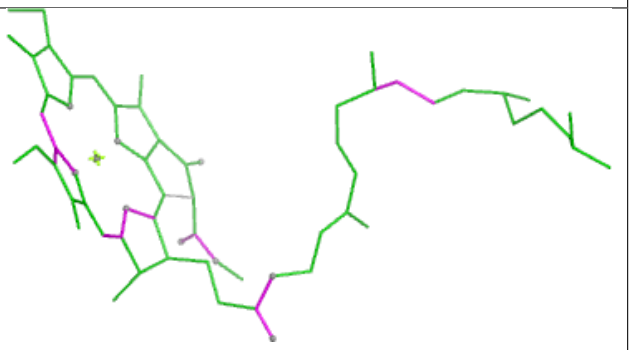
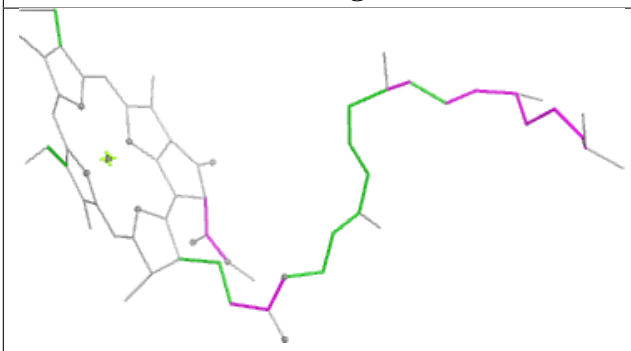


Bond angles



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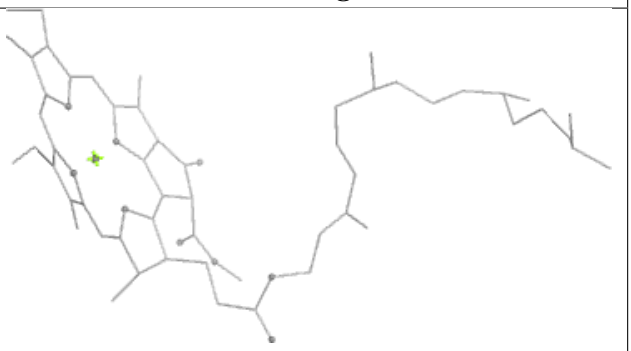
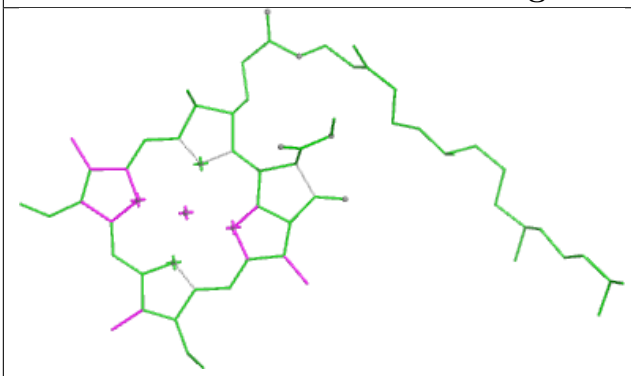


Rings

Ligand CLA 0 207



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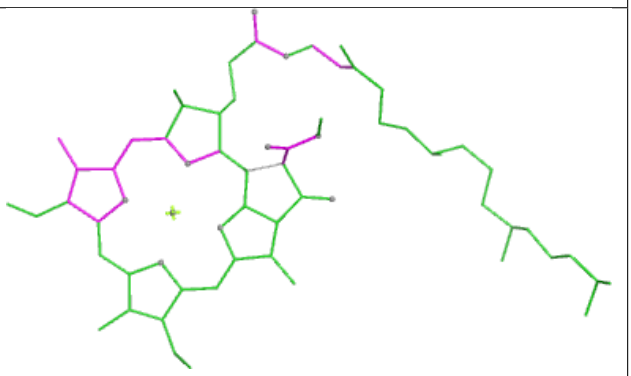
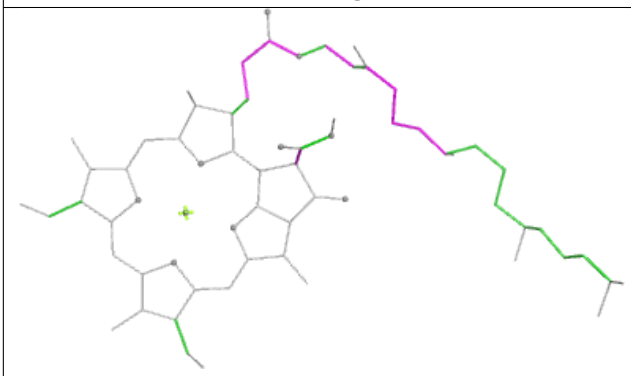
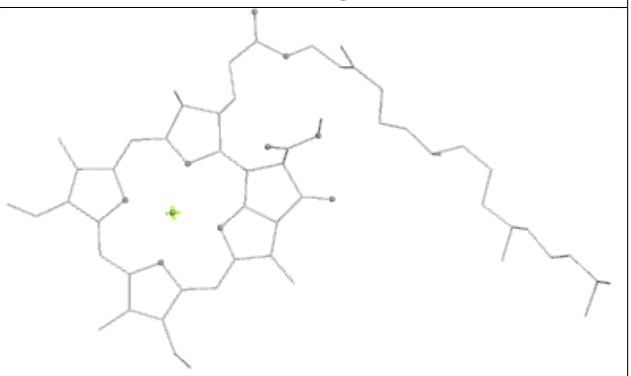


Bond angles

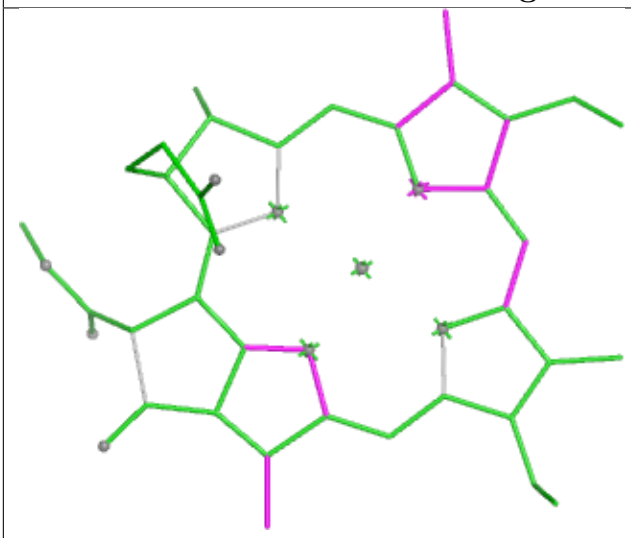


Torsions



Rings

Ligand CLA 1 1638



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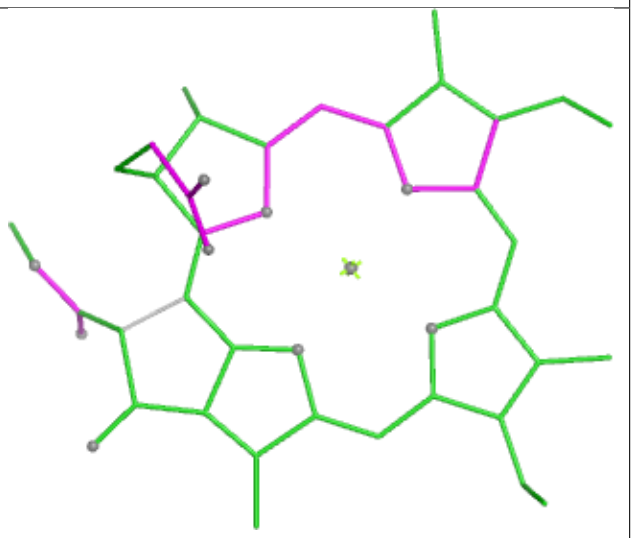
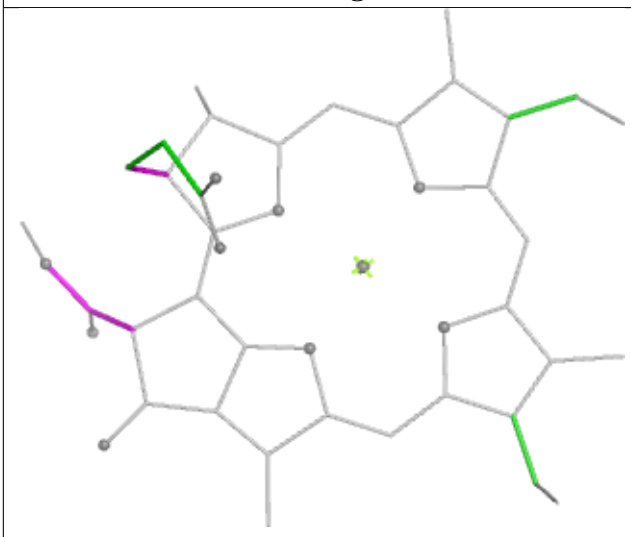


Bond angles



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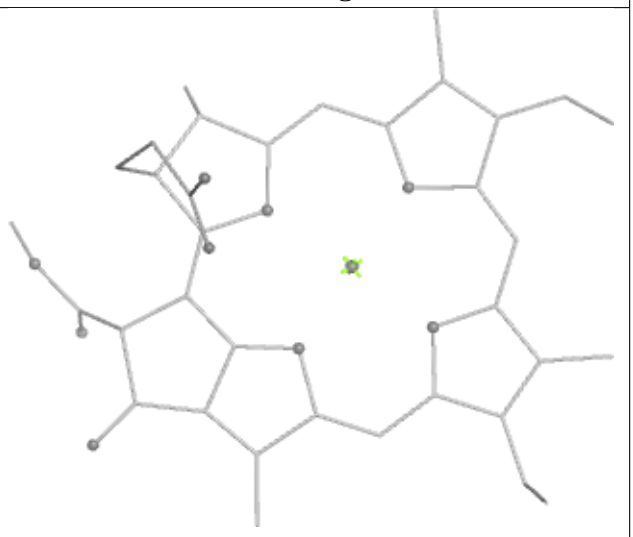
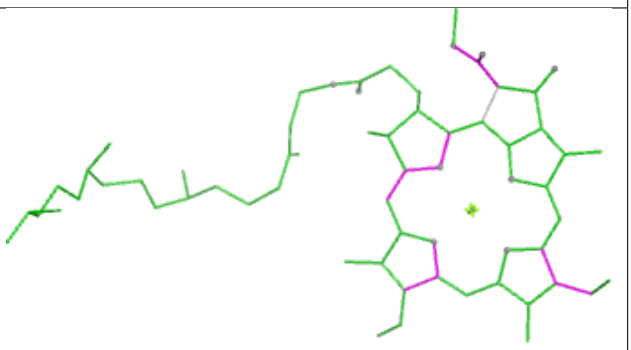


Rings

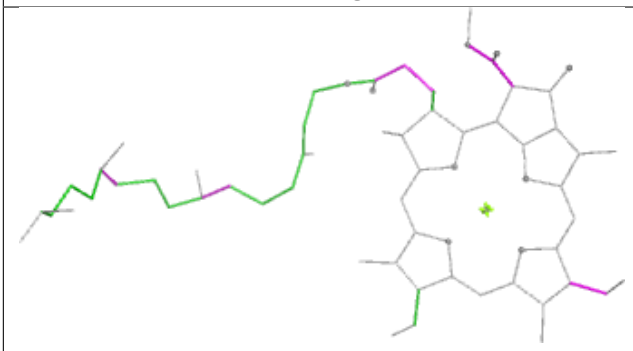
Ligand CLA b 804



Bond lengths



Bond angles

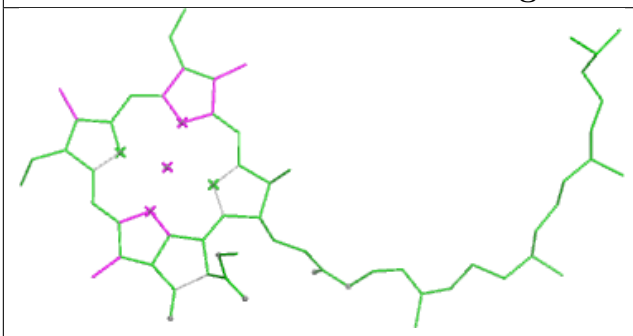


Torsions

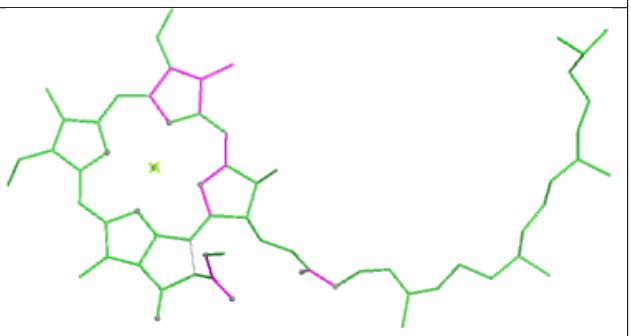


Rings

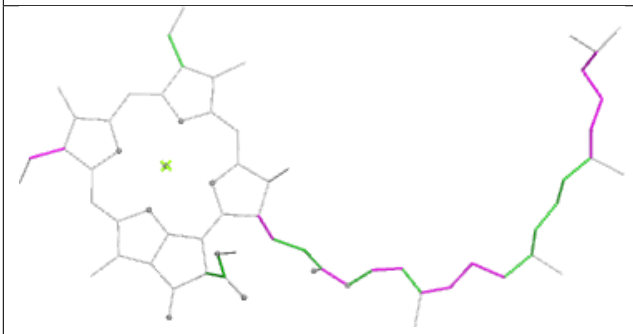
Ligand CLA 1 1639



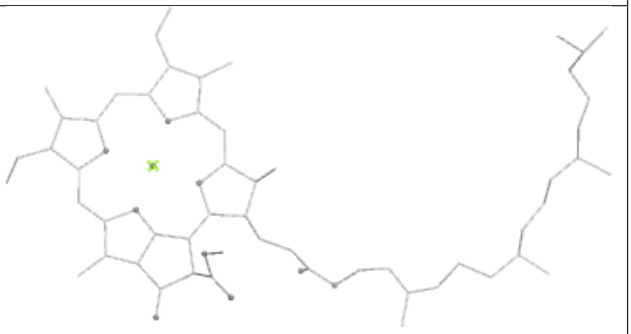
Bond lengths



Bond angles

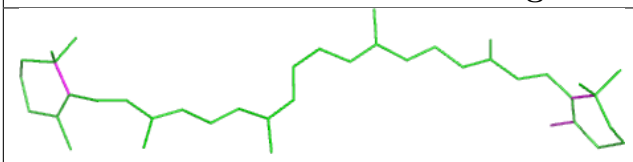


Torsions



Rings

Ligand BCR 2 847



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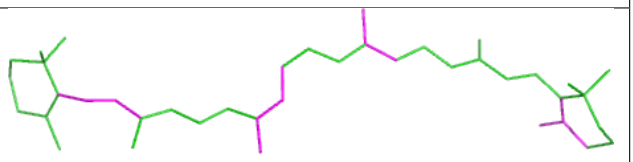
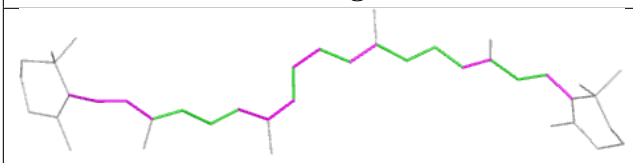


Bond angles



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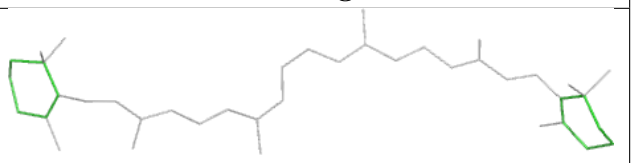
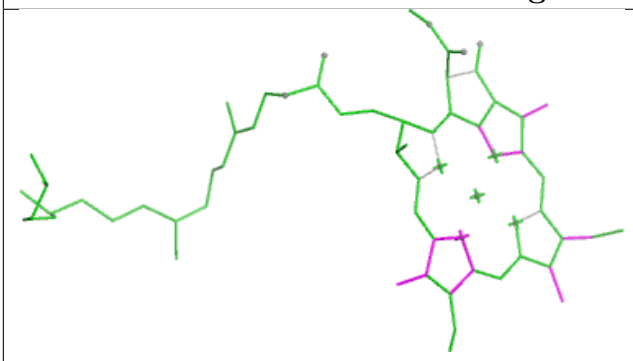


Rings

Ligand CLA 2 810



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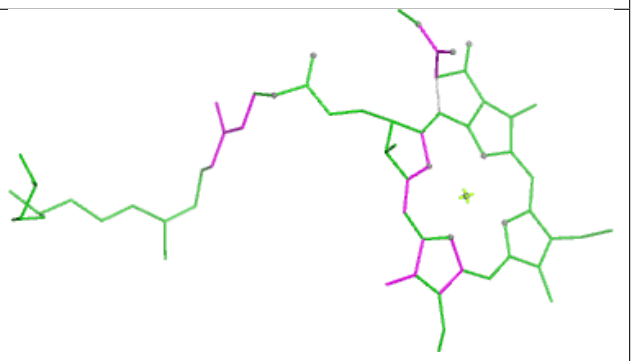
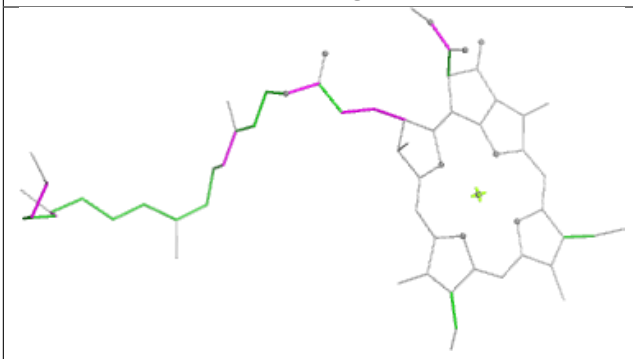


Bond angles



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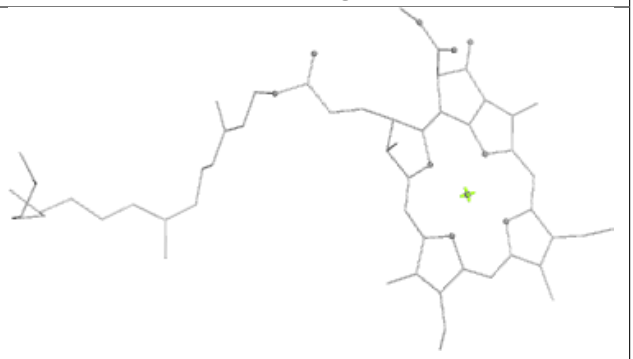
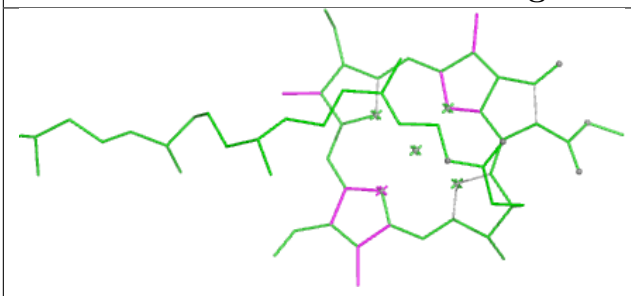
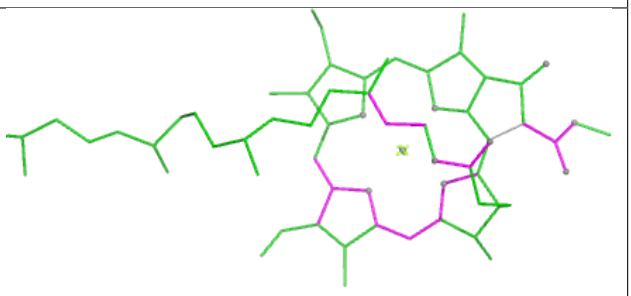
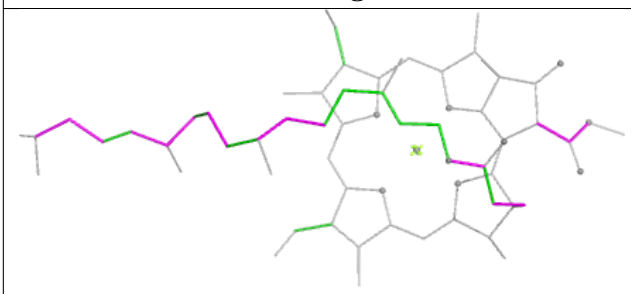
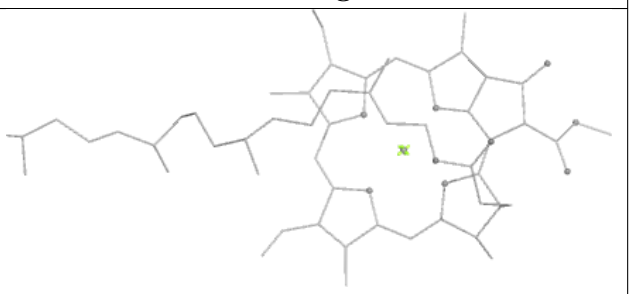
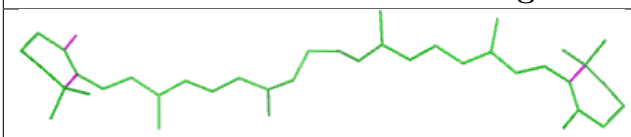
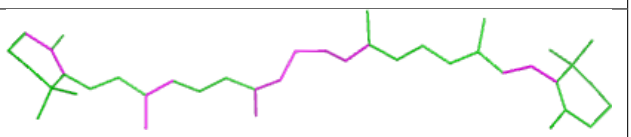
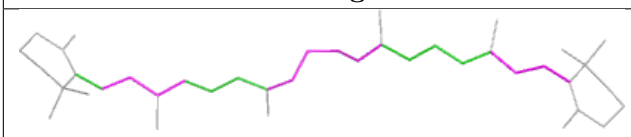
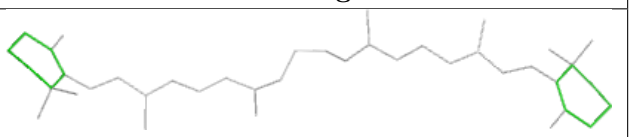
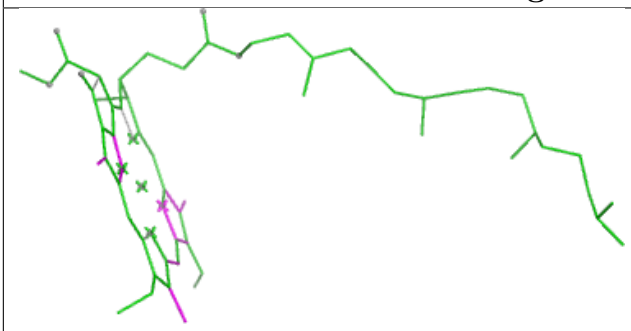


Rings

Ligand CLA a 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 1 1649	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 805



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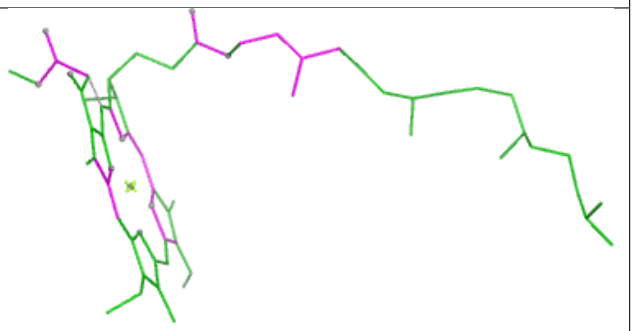
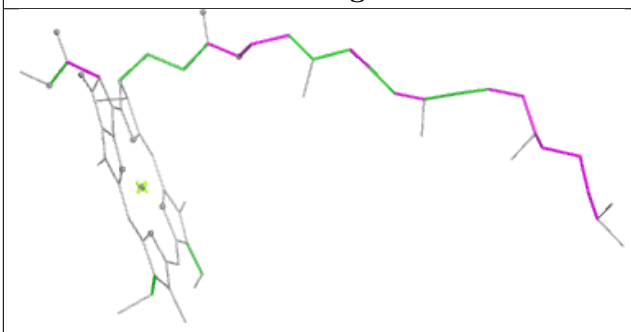


Bond angles

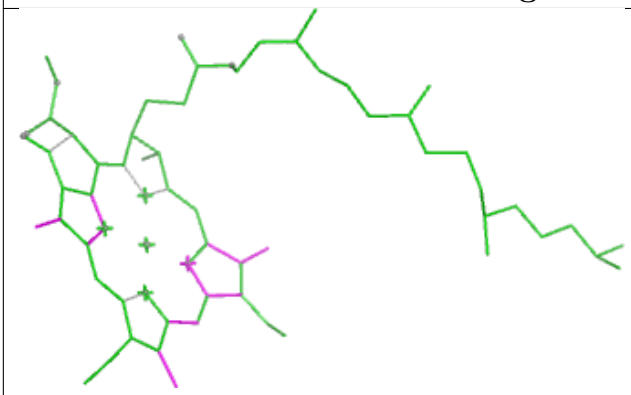


Torsions



Rings

Ligand CLA 1 1618



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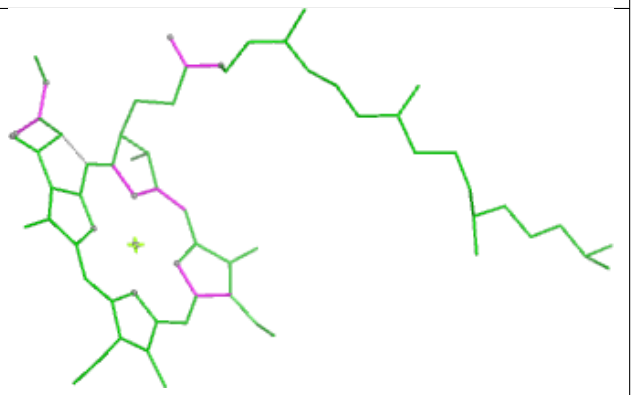
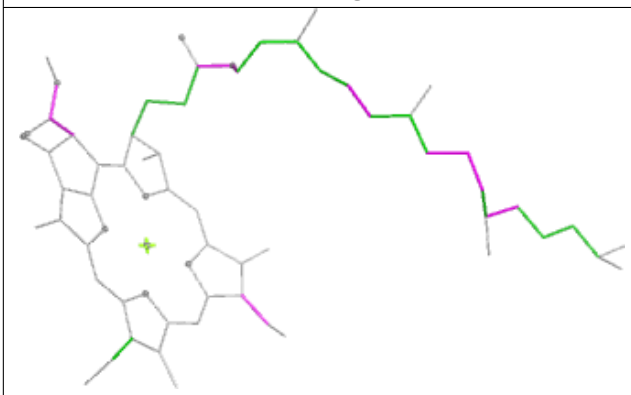


Bond angles

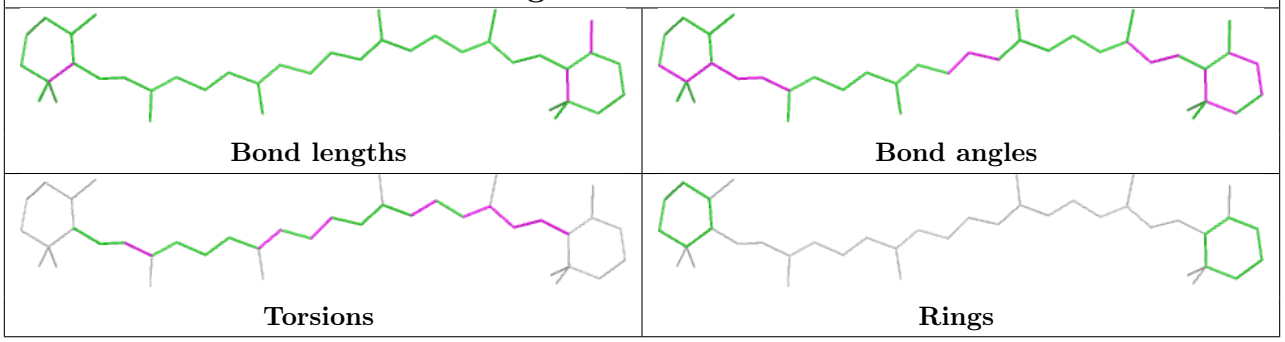


Torsions

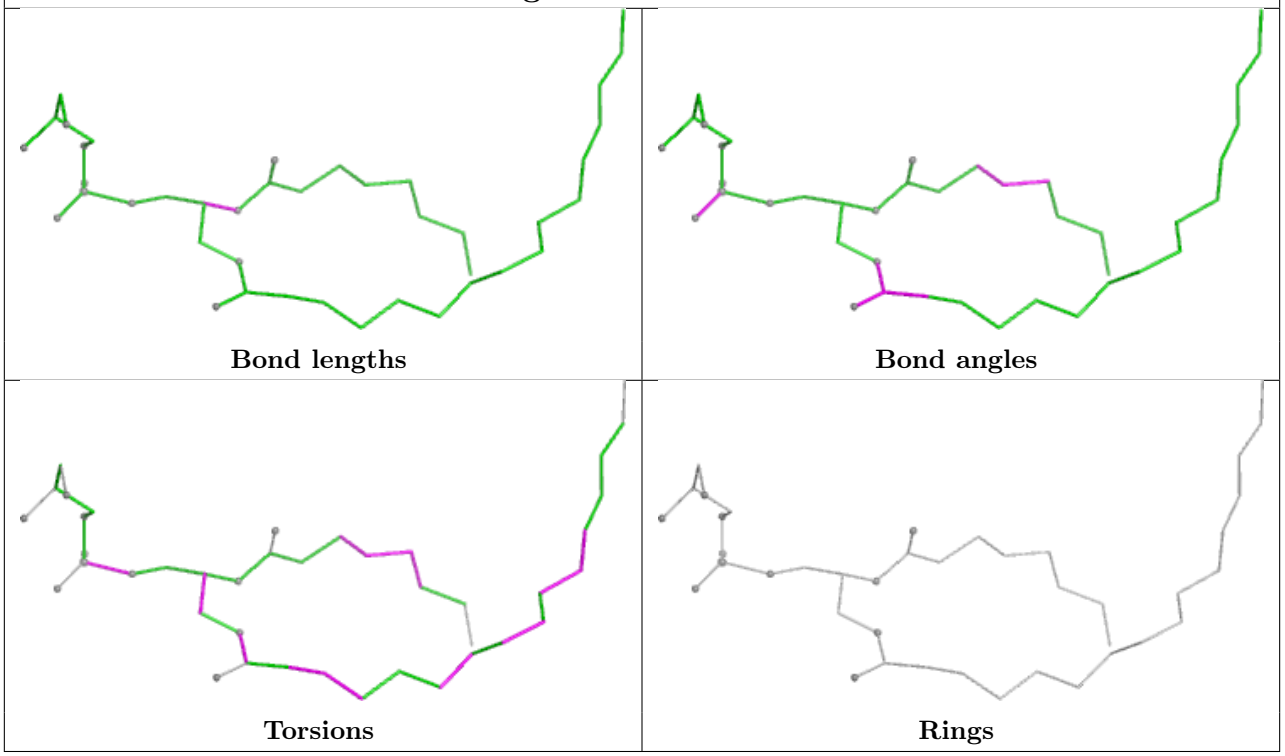


Rings

Ligand BCR 0 208



Ligand LHG A 854



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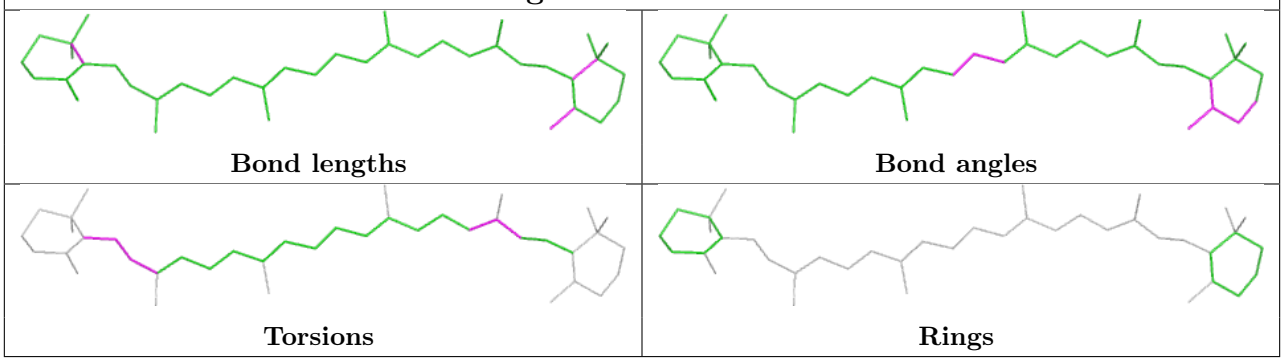

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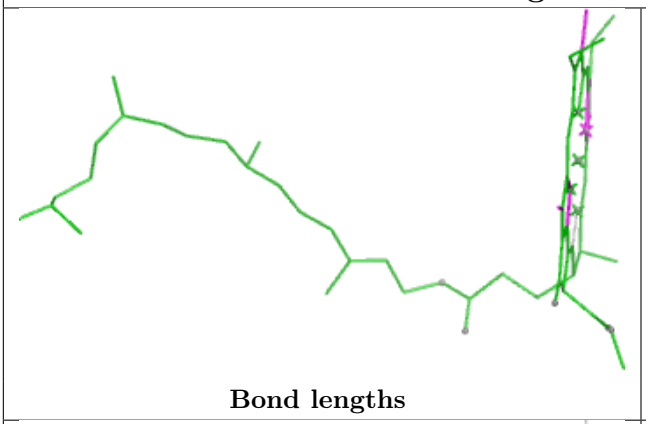

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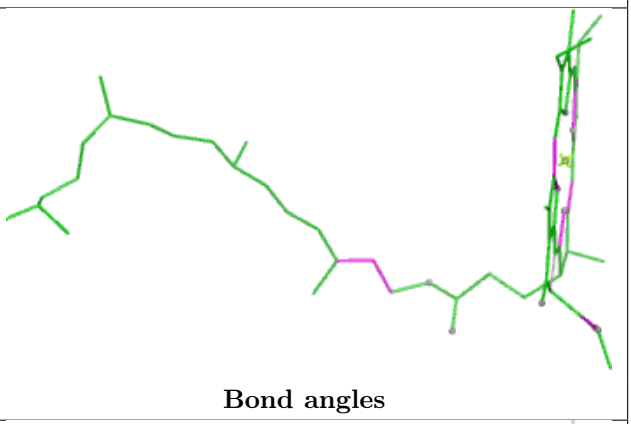
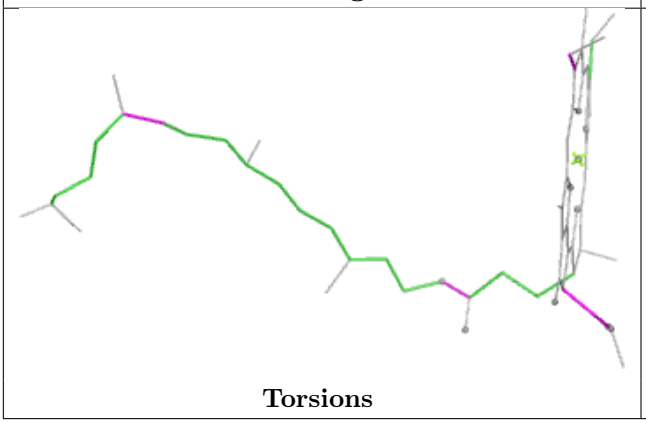


Bond angles



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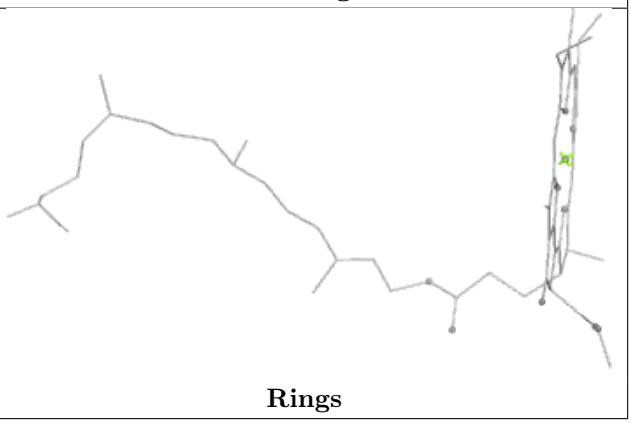
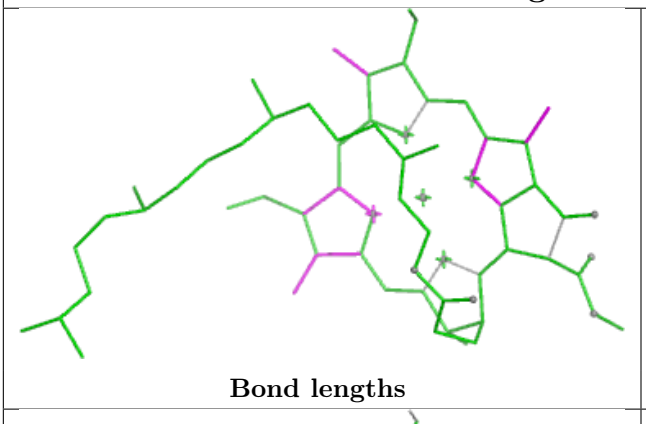


Rings

Ligand CLA 2 808



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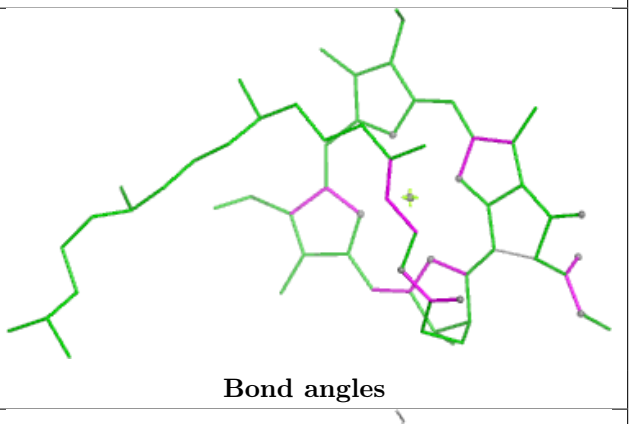
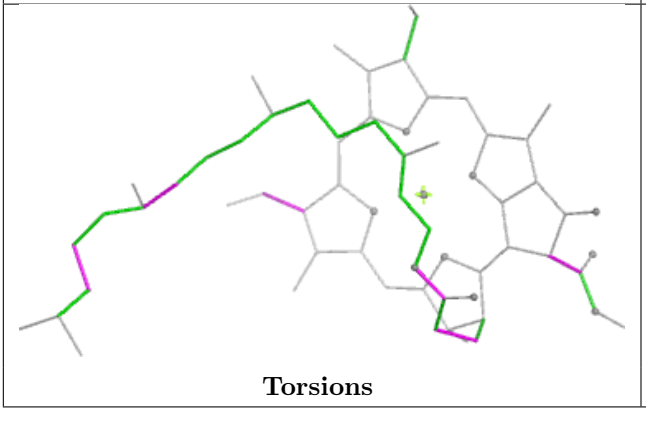


Bond angles



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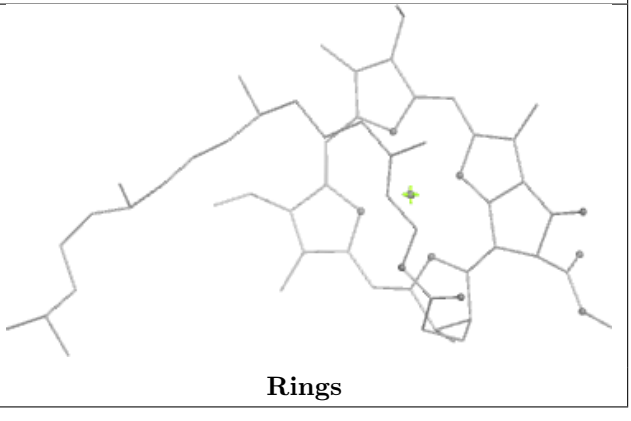
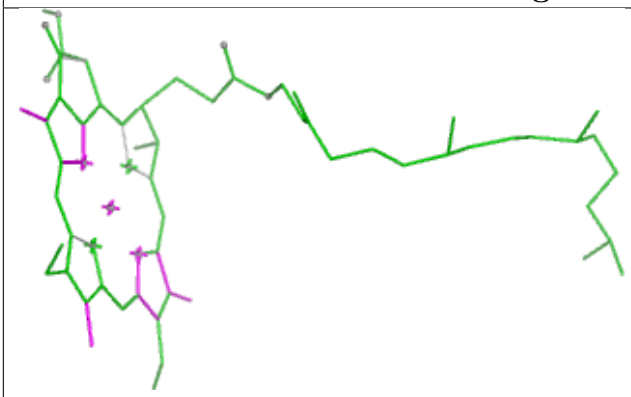


Rings

Ligand CLA l 205



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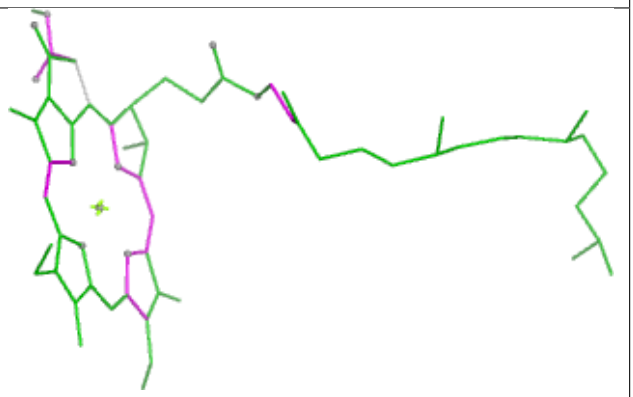
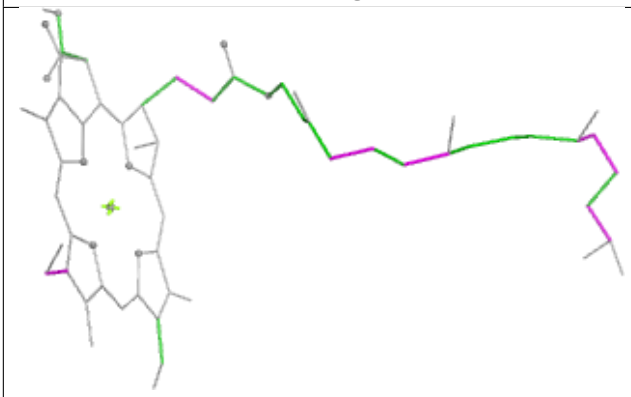


Bond angles

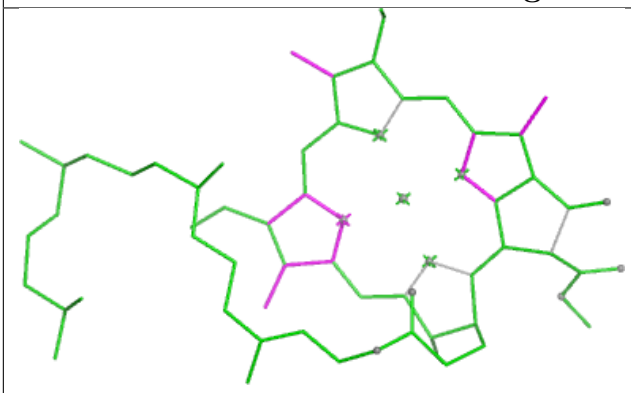


Torsions



Rings

Ligand CLA A 820



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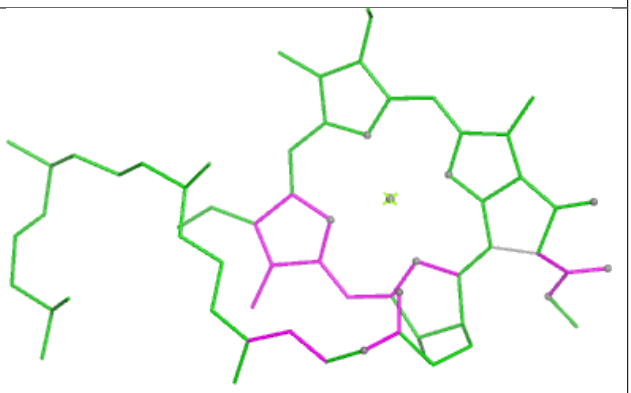
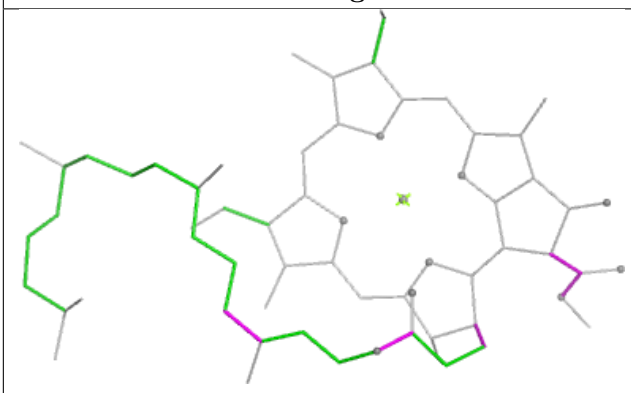


Bond angles



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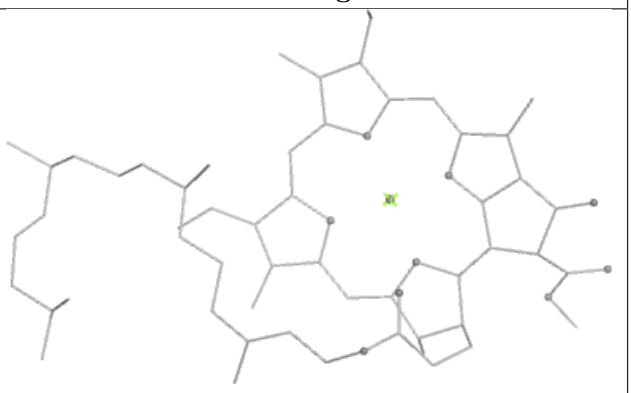
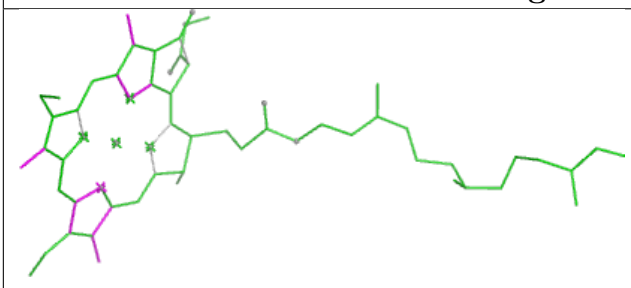


Rings

Ligand CLA a 810



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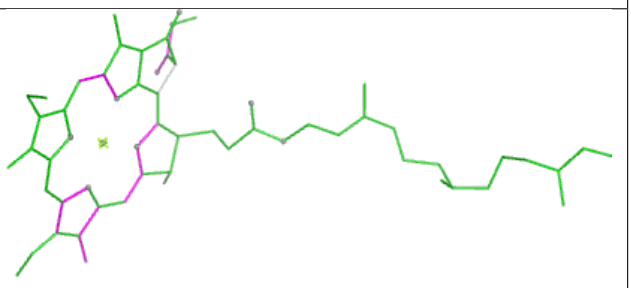
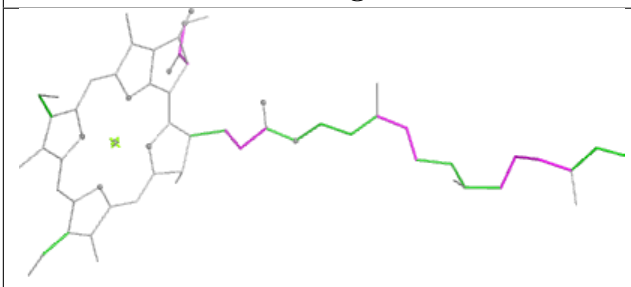


Bond angles



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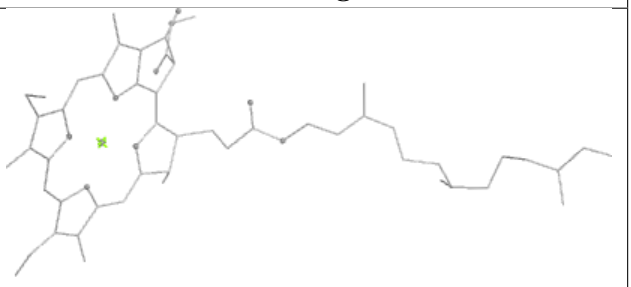
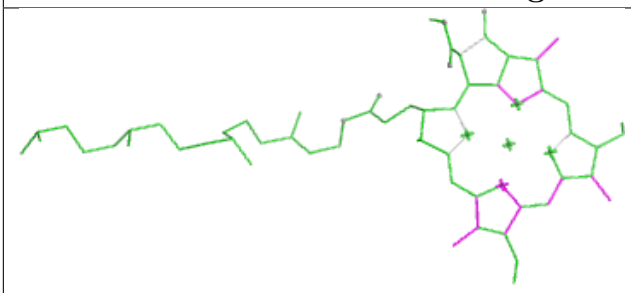


Rings

Ligand CLA b 826



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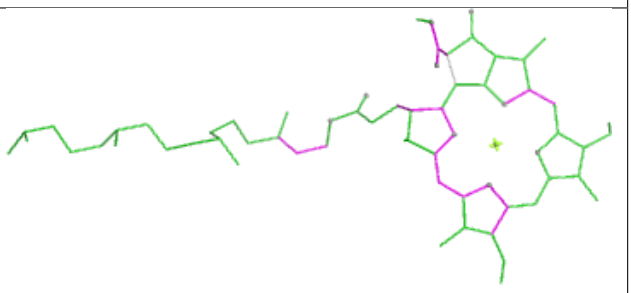
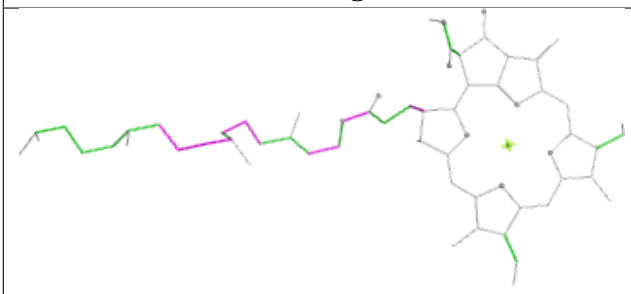


Bond angles



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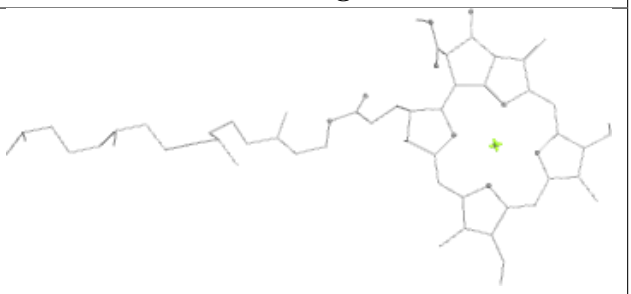
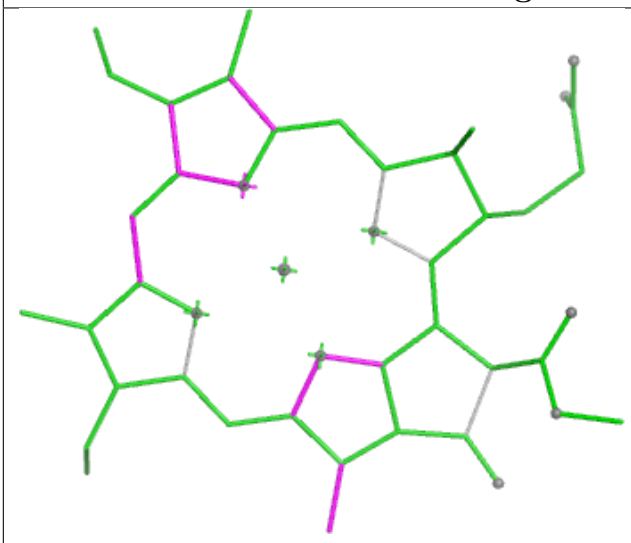


Rings

Ligand CLA X 1701



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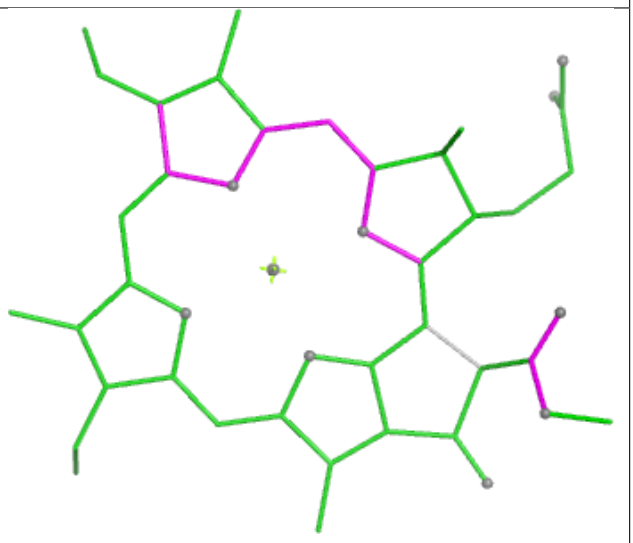
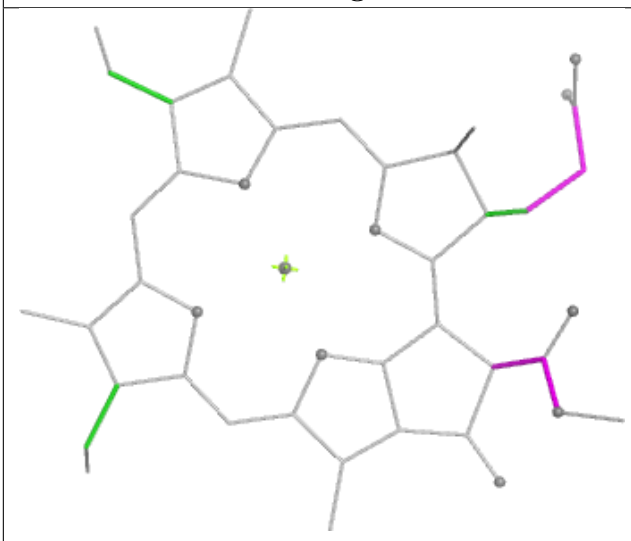


Bond angles



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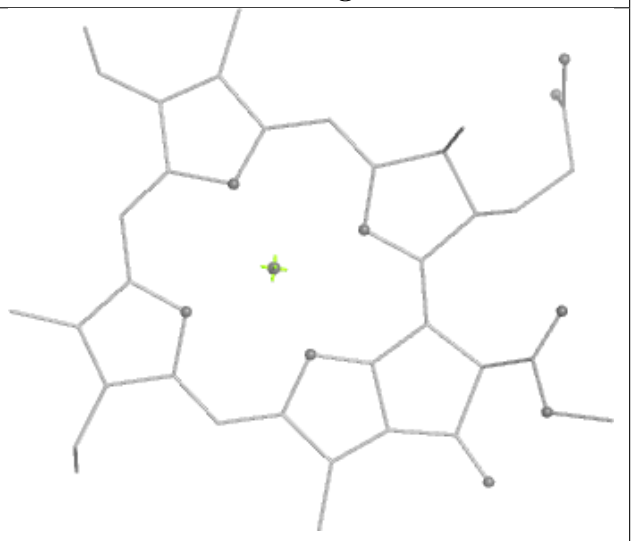
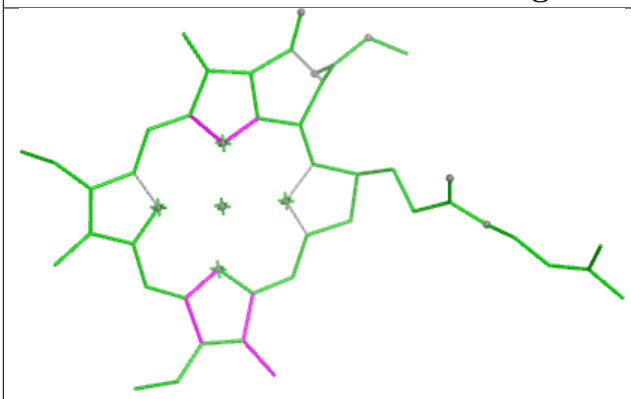


Rings

Ligand CLA f 203



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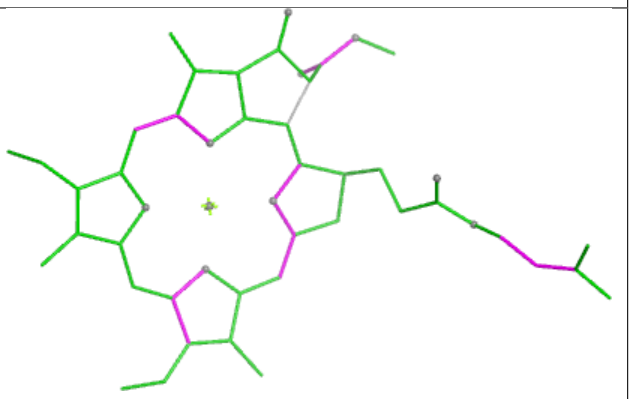
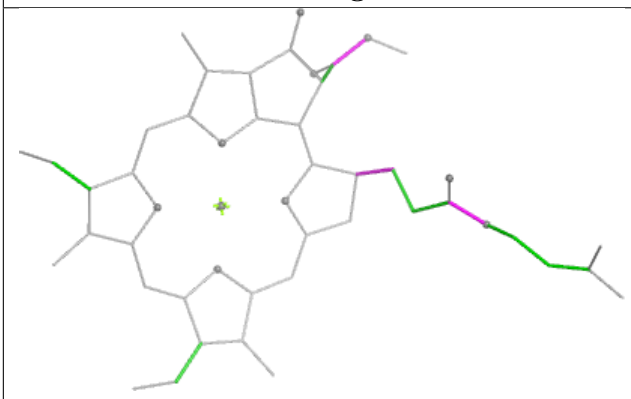


Bond angles



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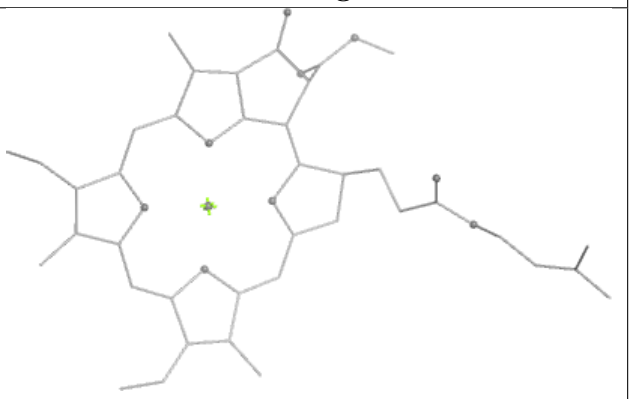
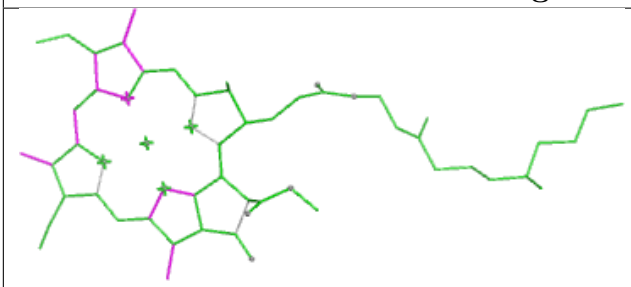


Rings

Ligand CLA f 201



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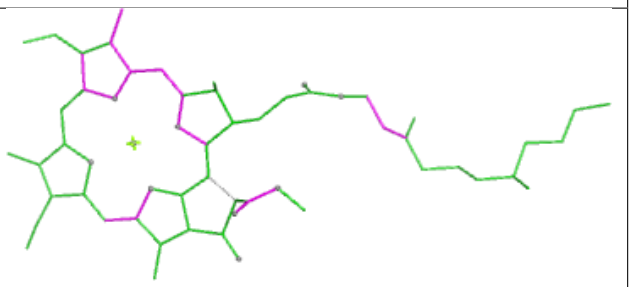
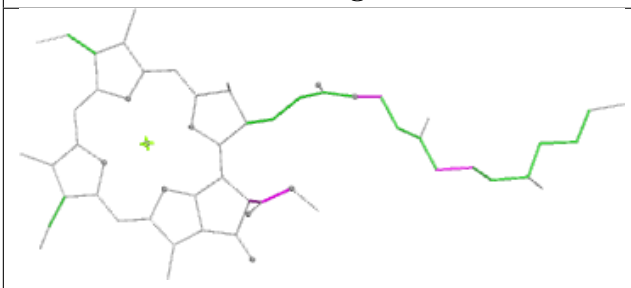
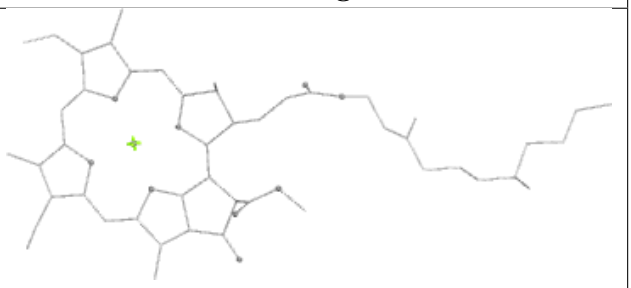


Bond angles

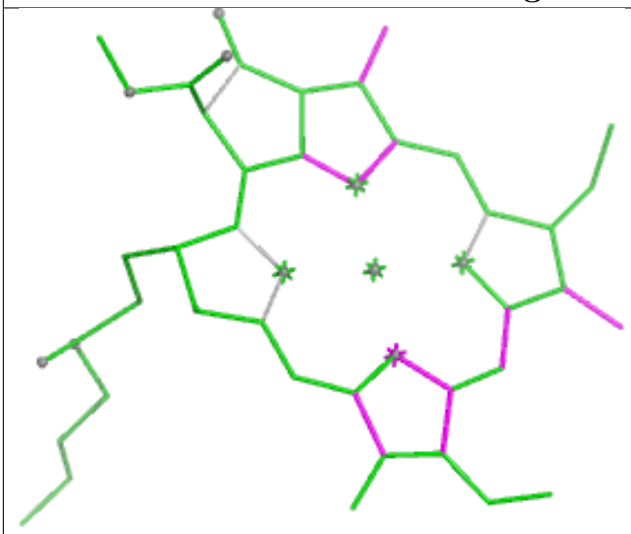


Torsions



Rings

Ligand CLA A 811



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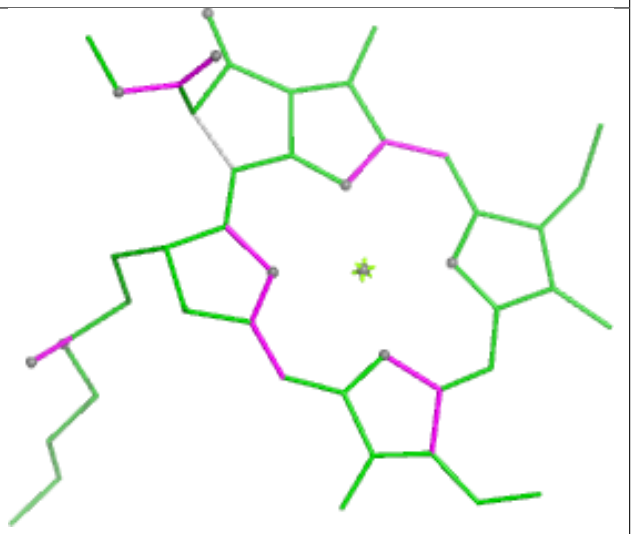

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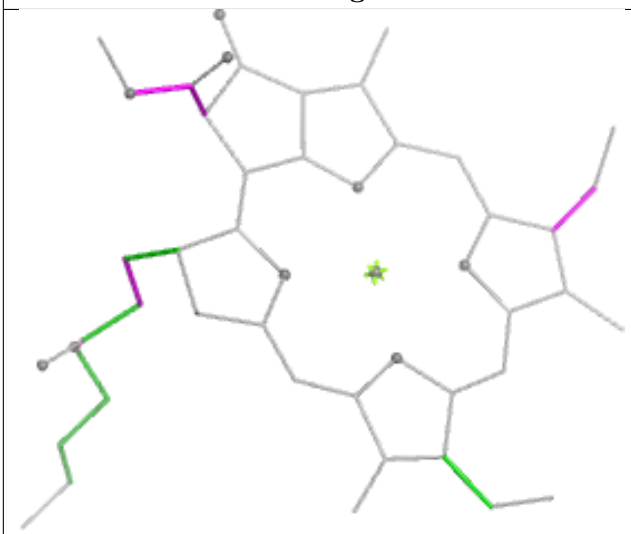

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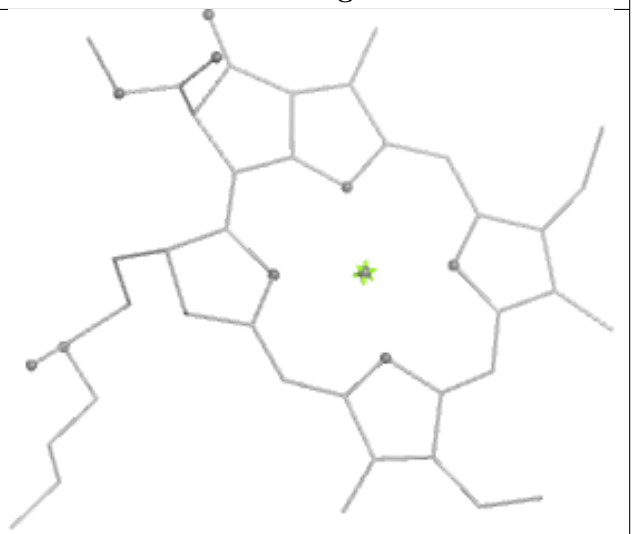


Rings

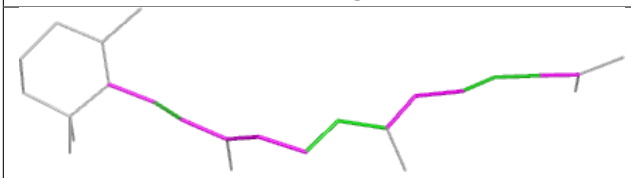
Ligand BCR 1 1653



Bond lengths



Bond angles



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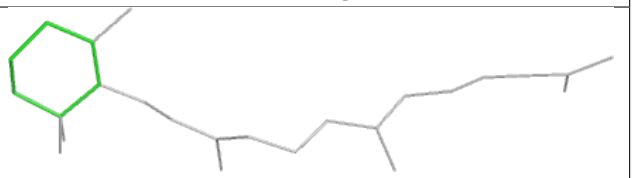
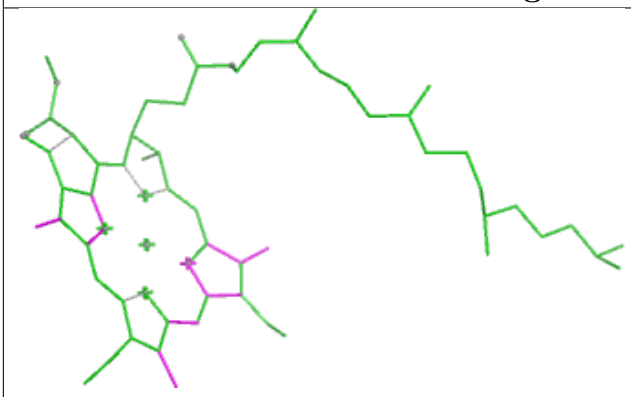


Rings

Ligand CLA A 817



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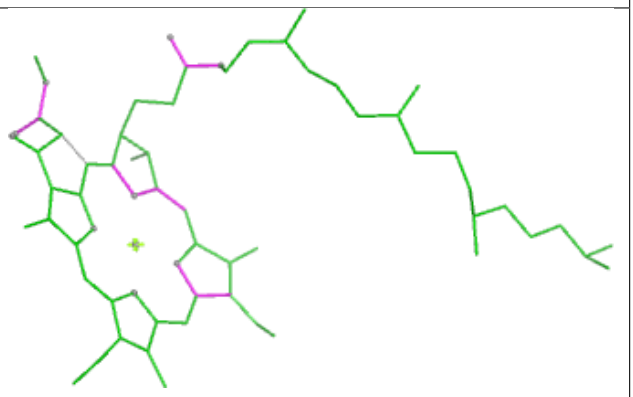

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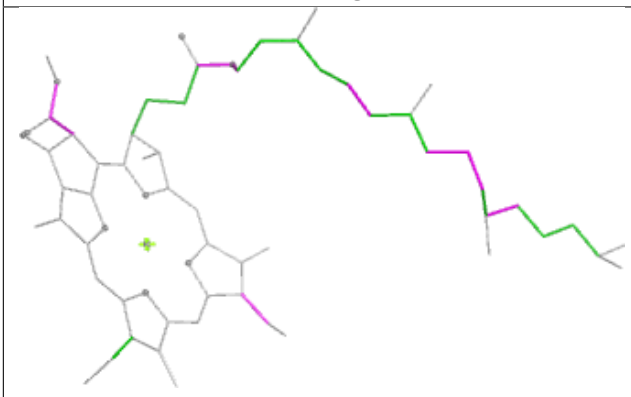

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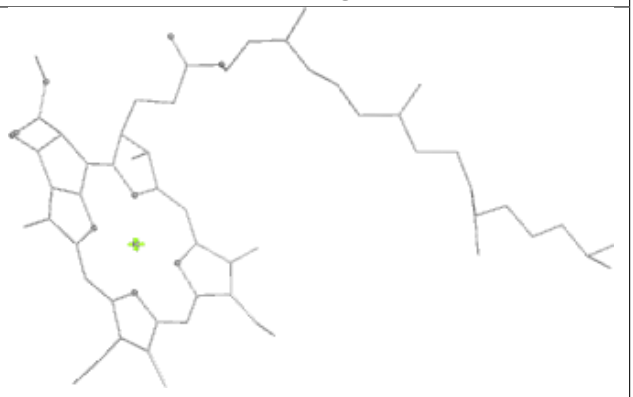
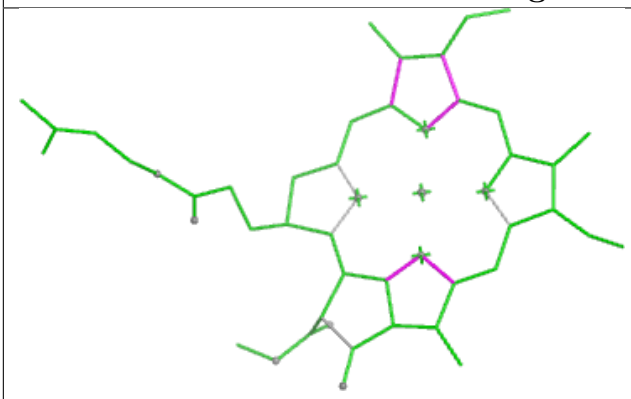


Rings

Ligand CLA 6 203



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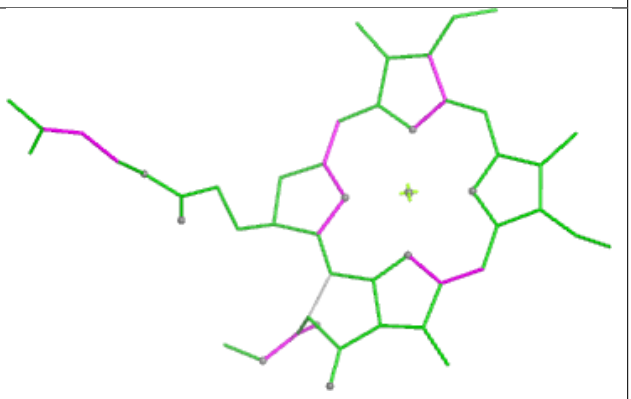
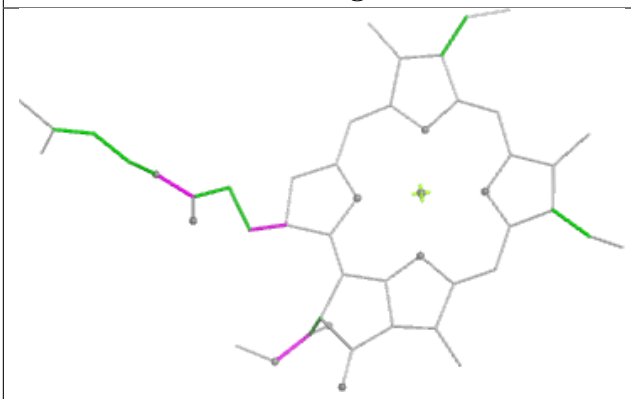


Bond angles



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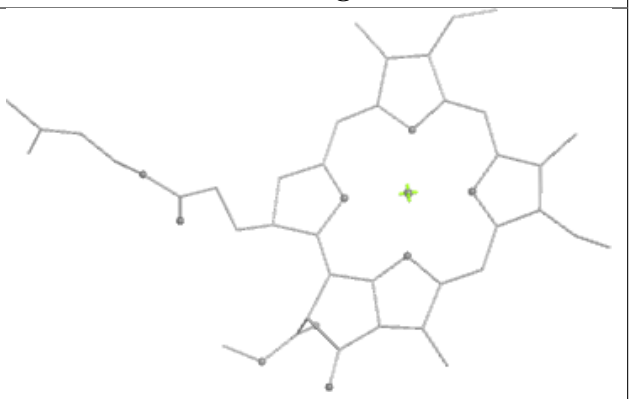
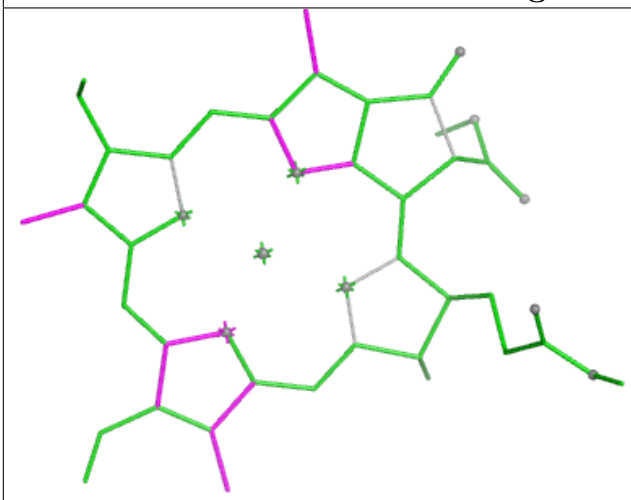


Rings

Ligand CLA 9 101



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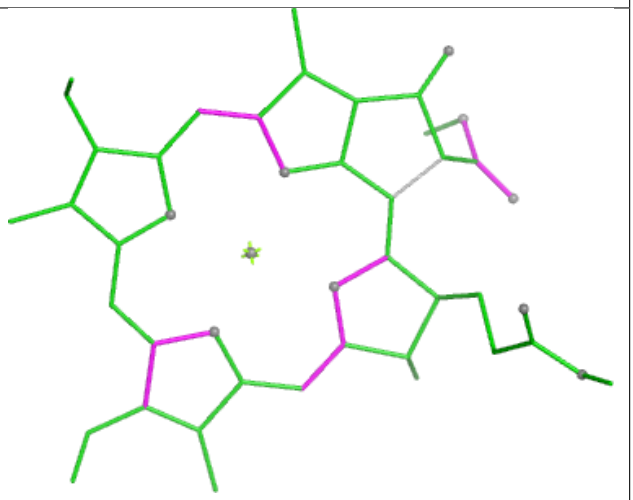

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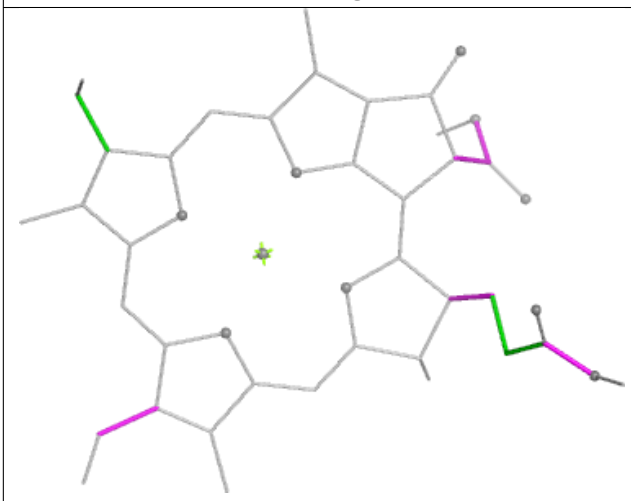

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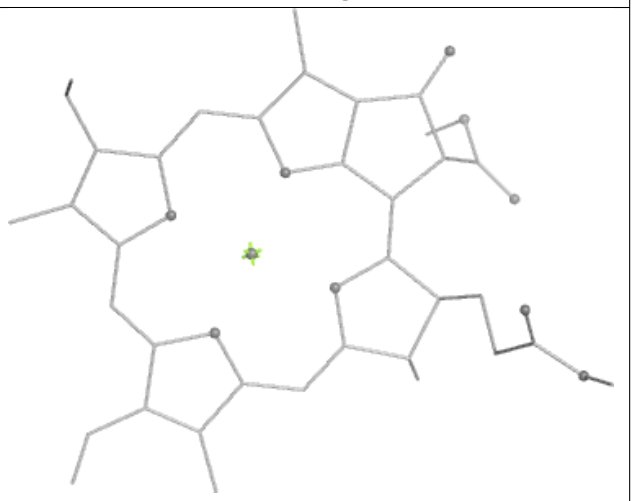
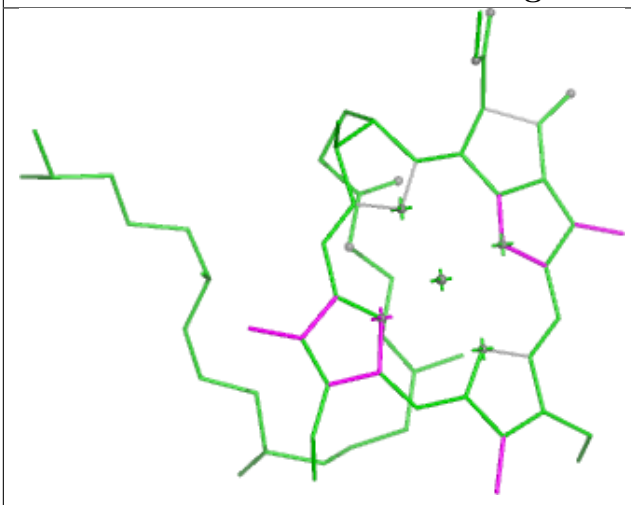


Rings

Ligand CLA B 808



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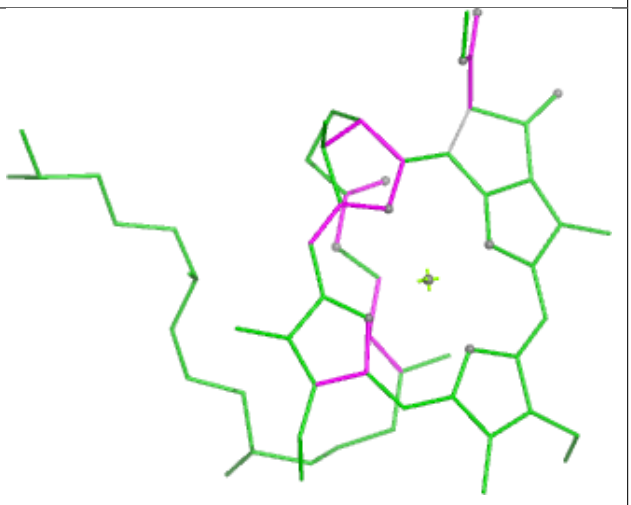

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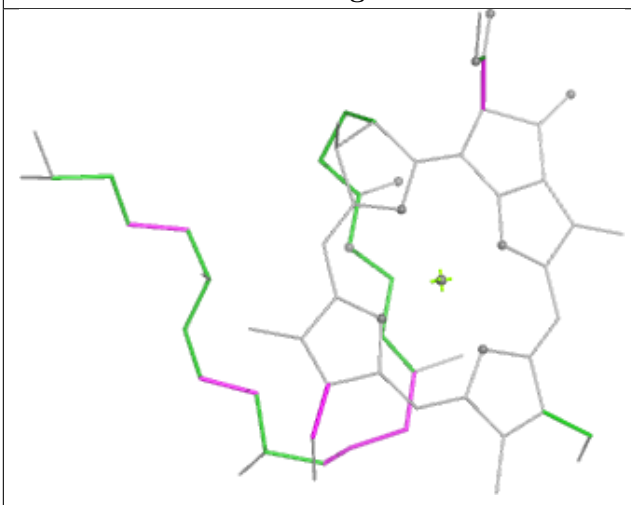

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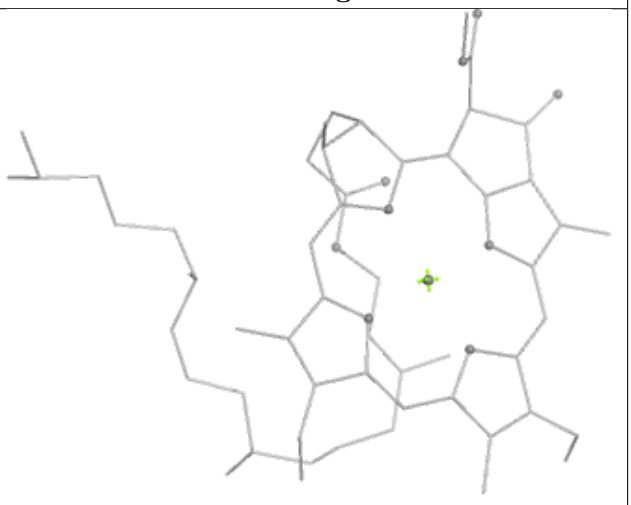
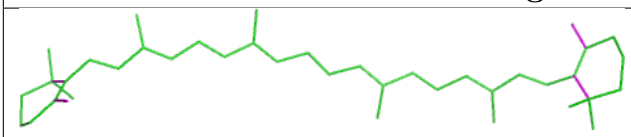


Rings

Ligand BCR 2 849



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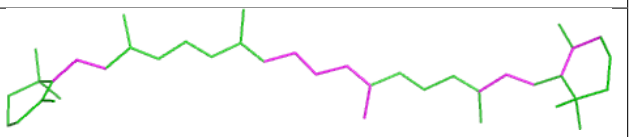
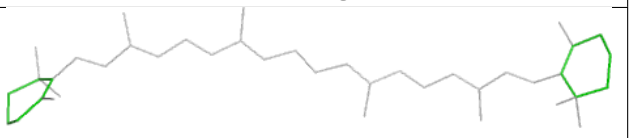


Bond angles

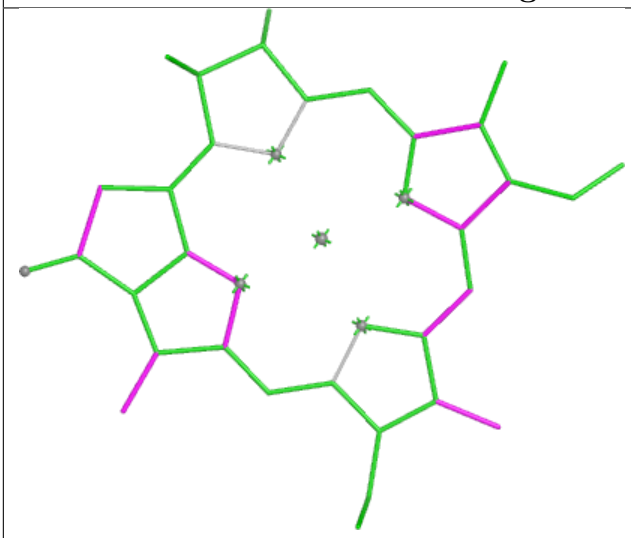


Torsions



Rings

Ligand CLA 8 1303



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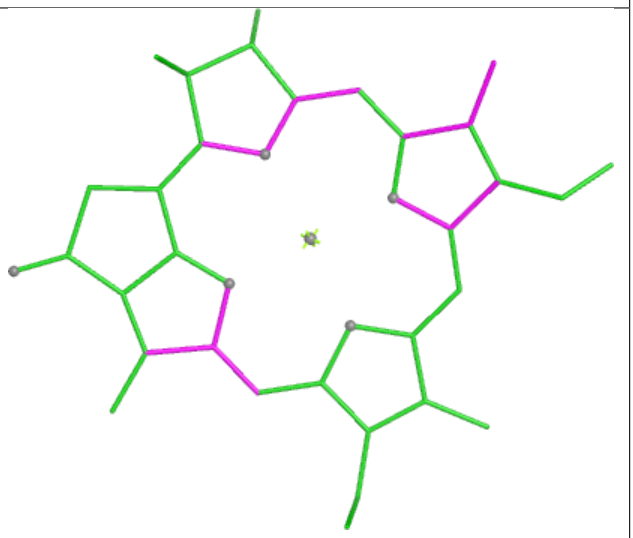

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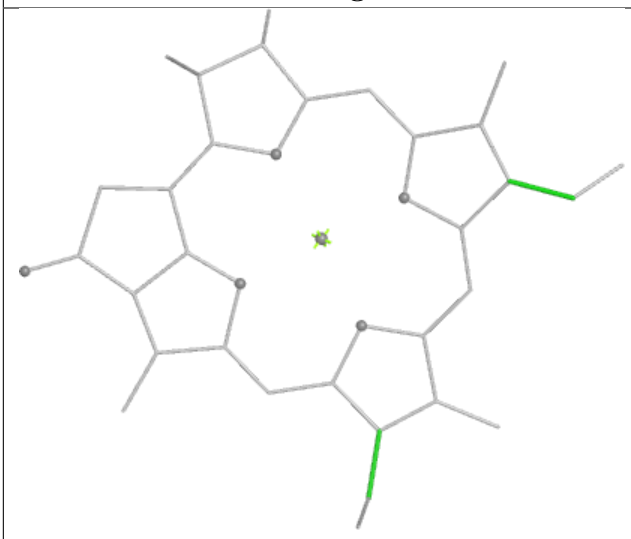

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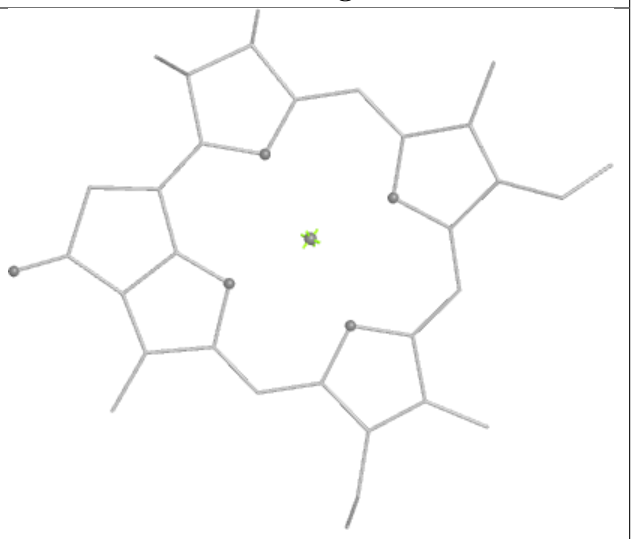
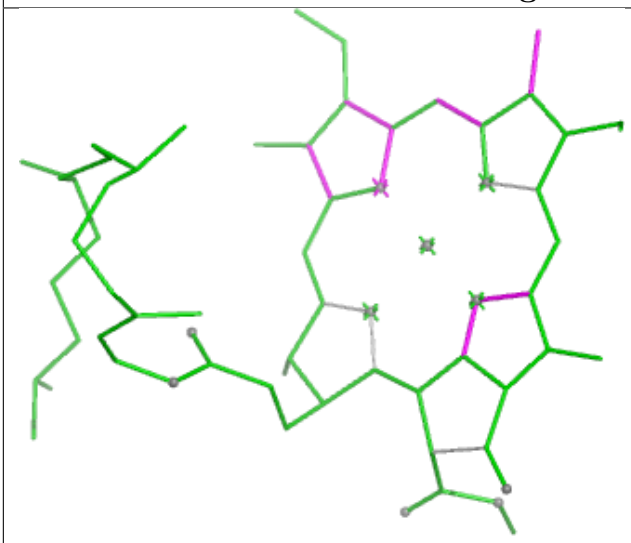


Rings

Ligand CLA 1 1617



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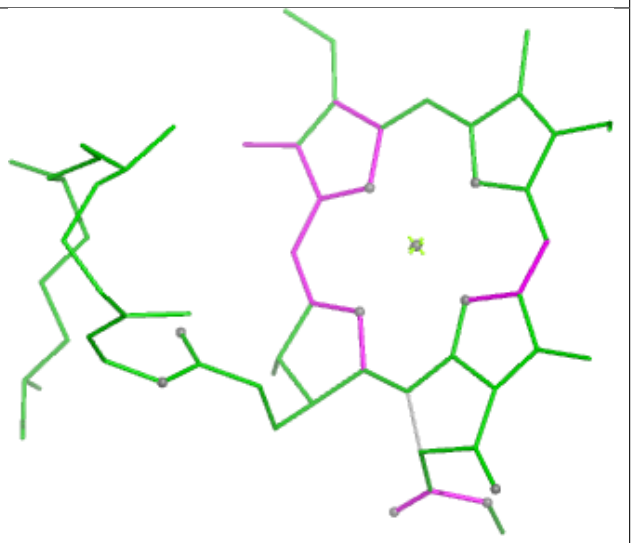

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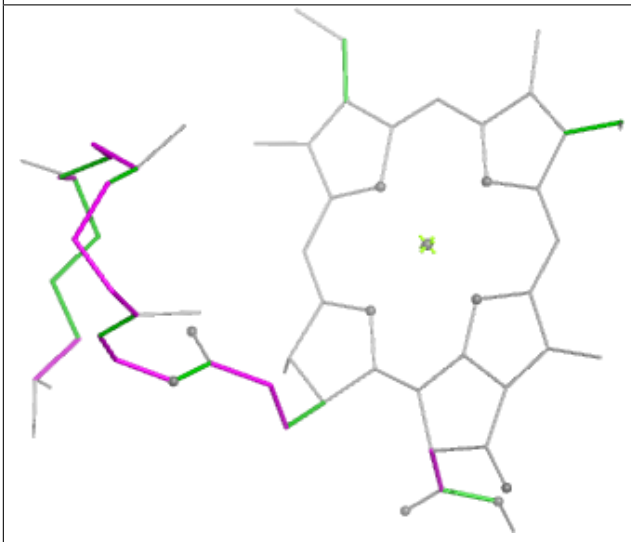

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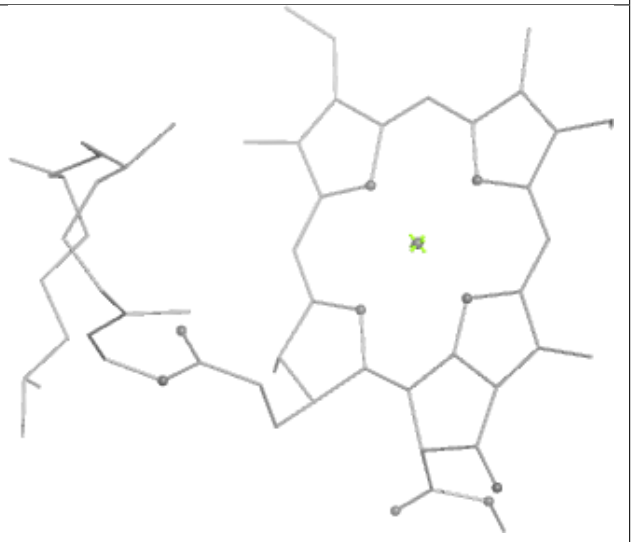
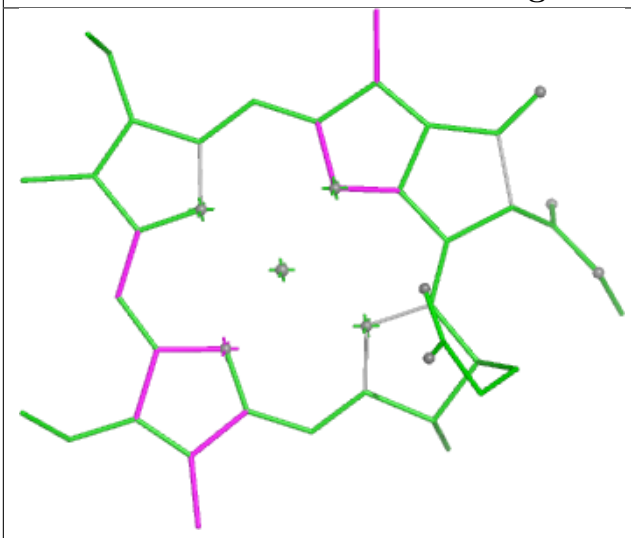


Rings

Ligand CLA a 837



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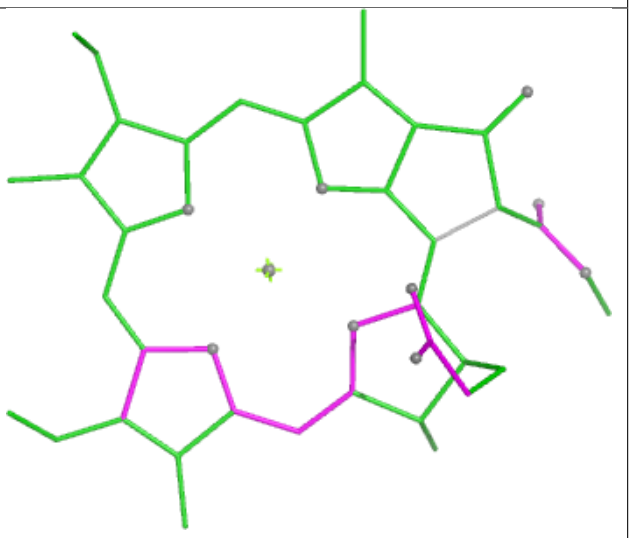

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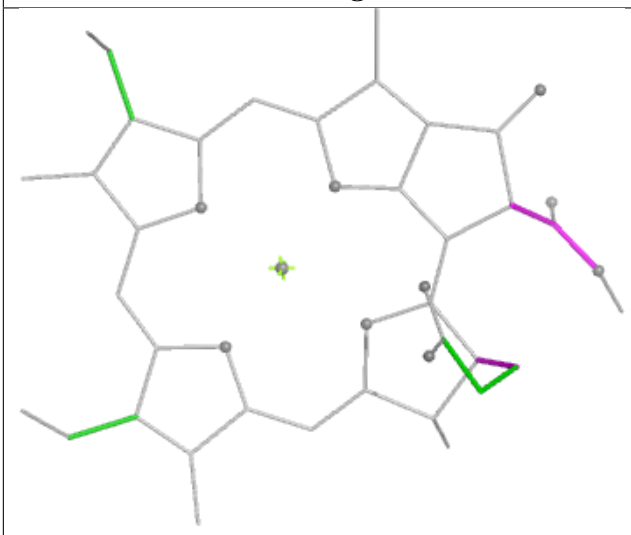

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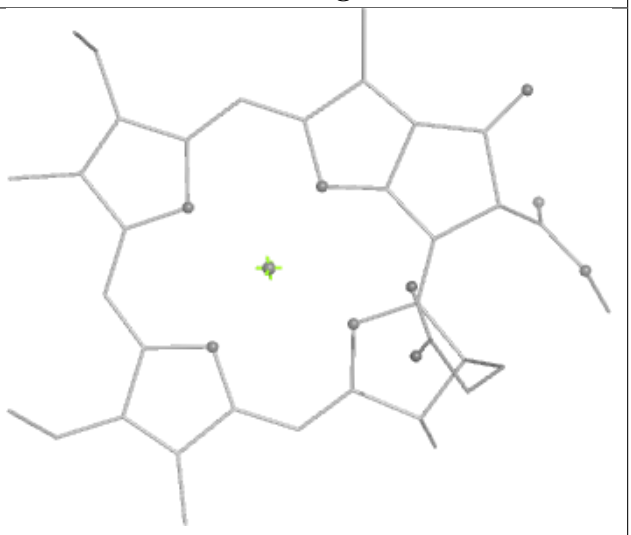
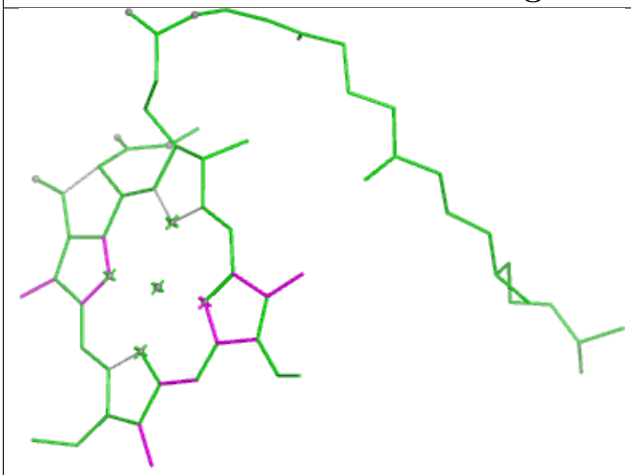


Rings

Ligand CLA B 824



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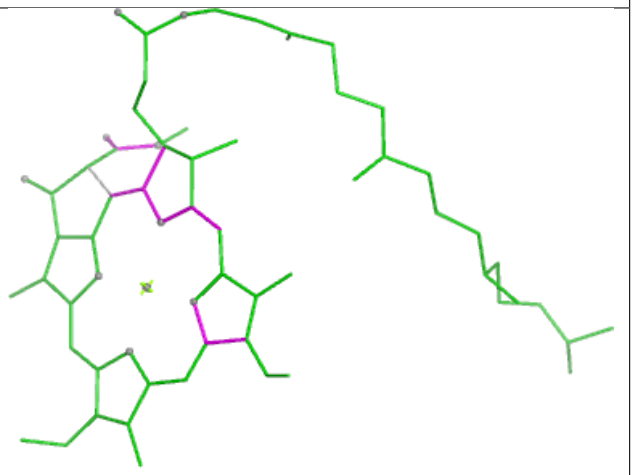

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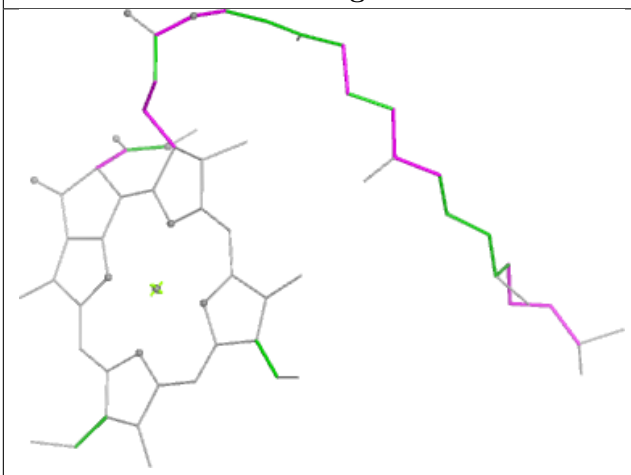

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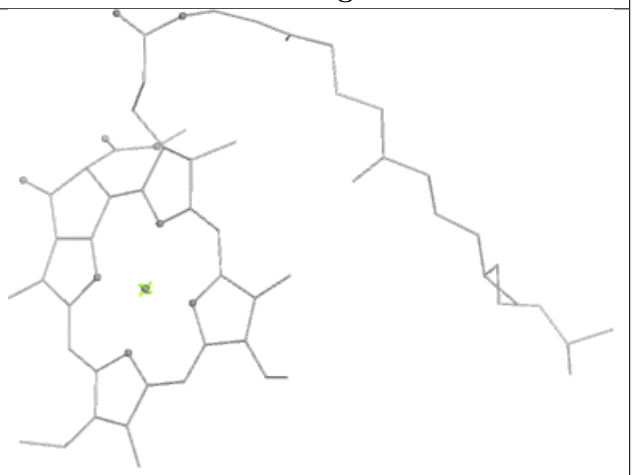
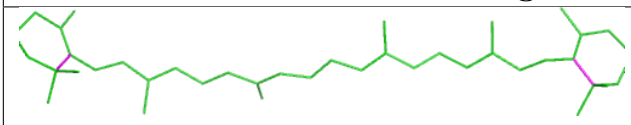


Rings

Ligand BCR 1 1648



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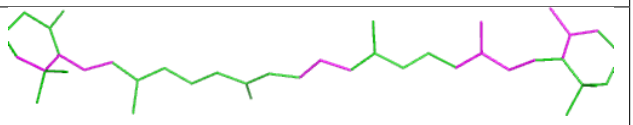
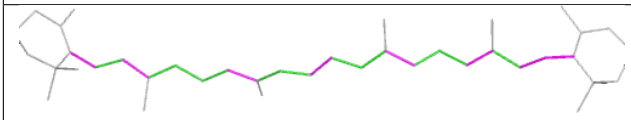


Bond angles



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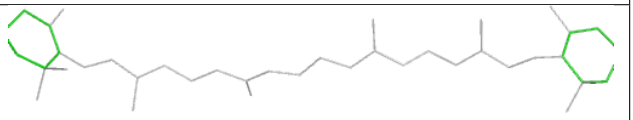
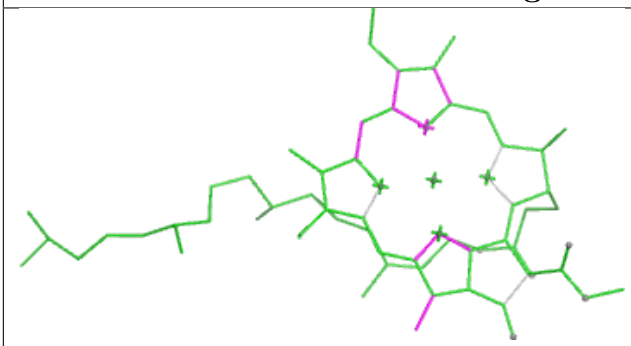


Rings

Ligand CLA A 818



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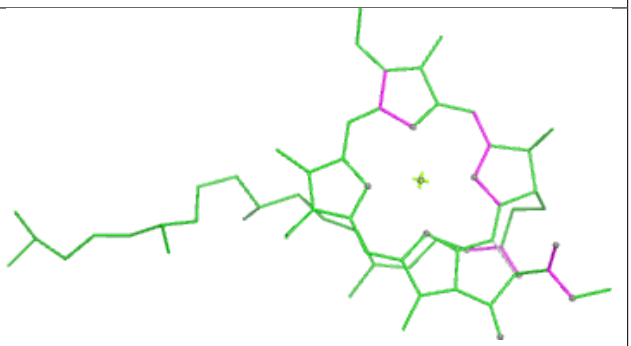
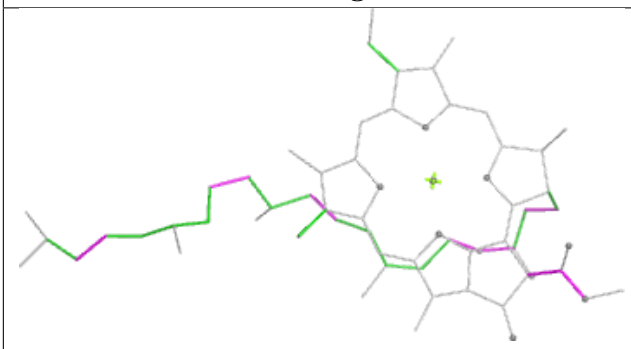


Bond angles



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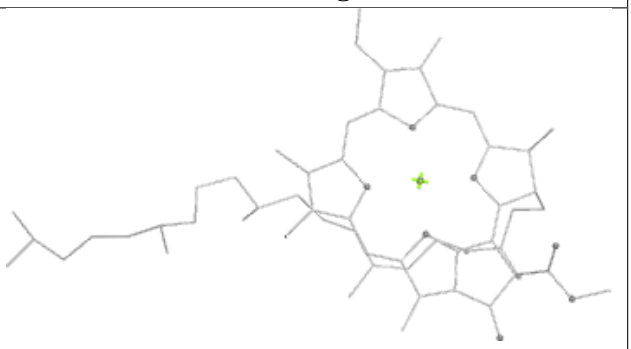
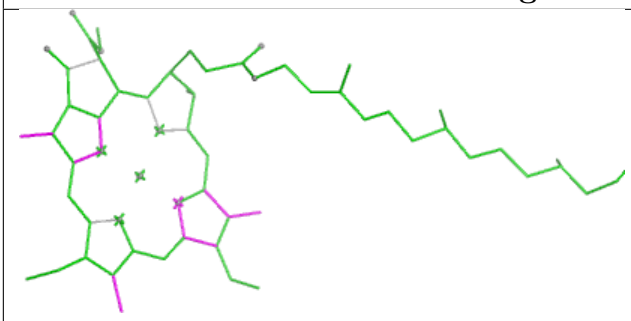


Rings

Ligand CLA 1 1636



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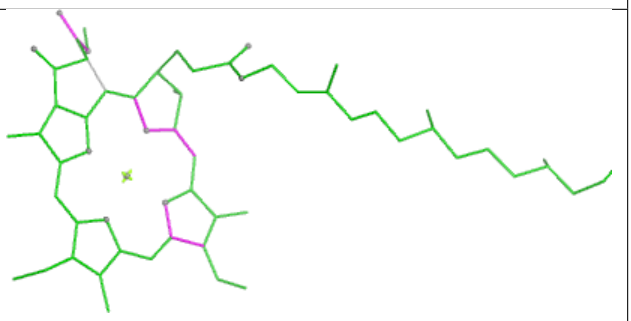
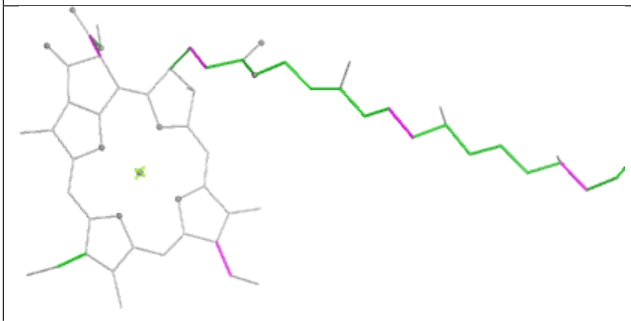


Bond angles



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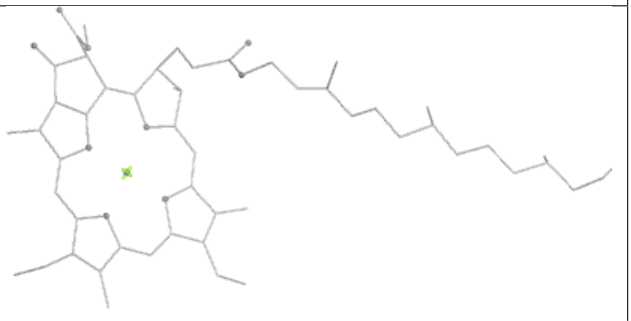
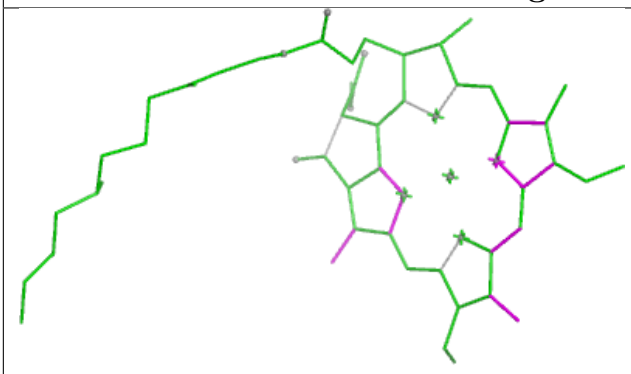


Rings

Ligand CLA 9 103



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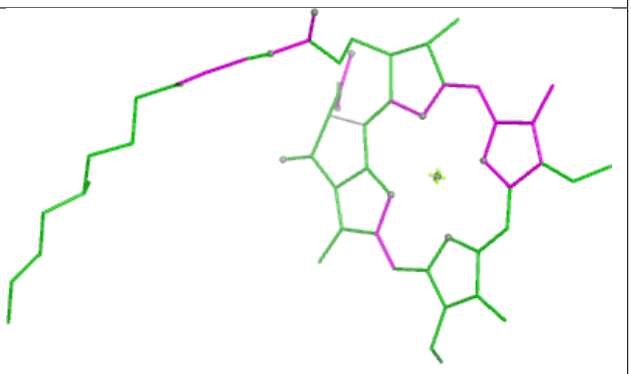
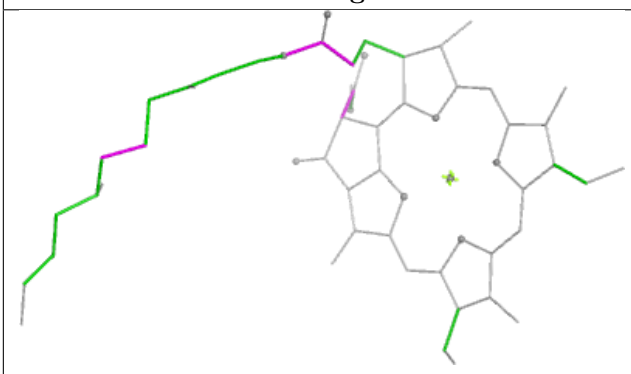
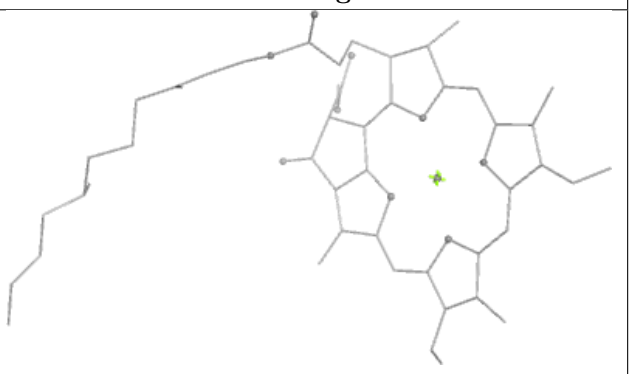


Bond angles

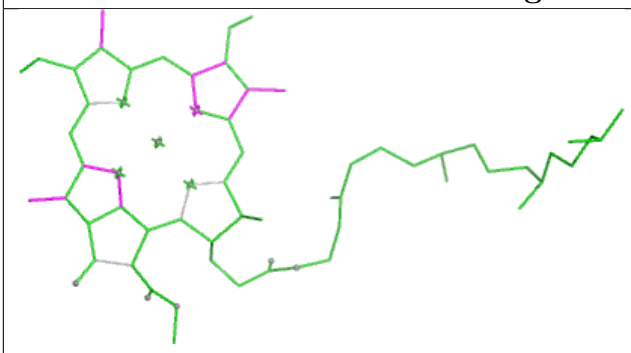


Torsions

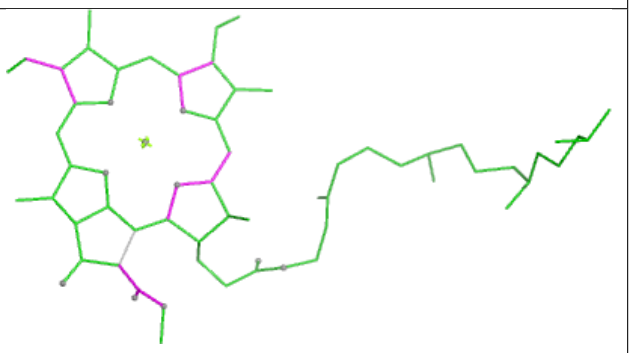


Rings

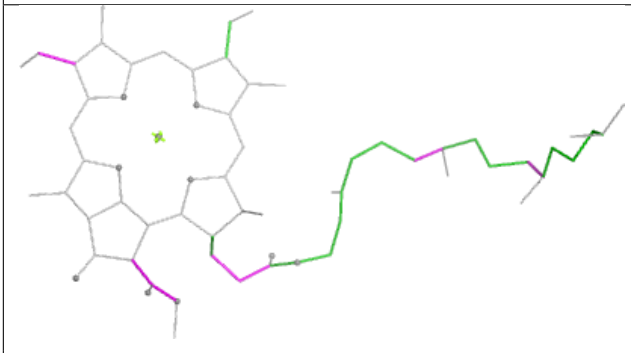
Ligand CLA B 803



Bond lengths



Bond angles

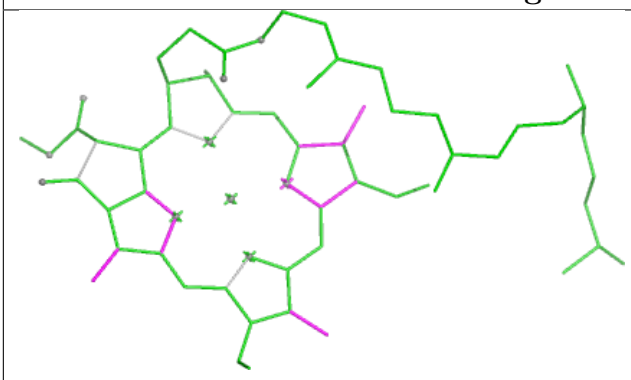


Torsions



Rings

Ligand CLA B 818



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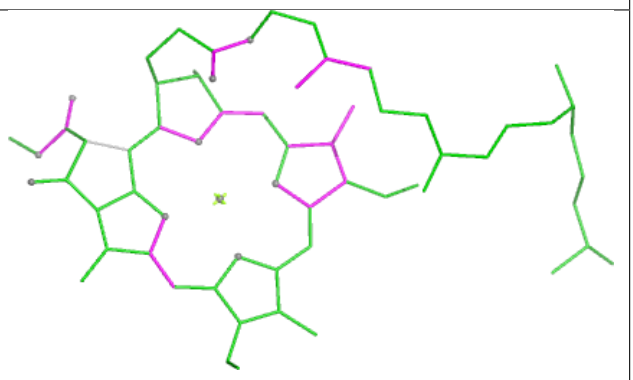
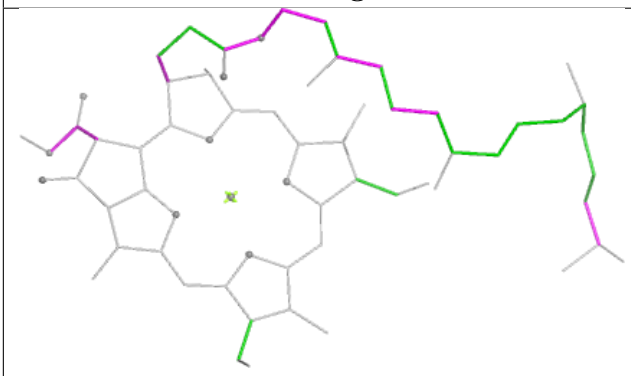


Bond angles



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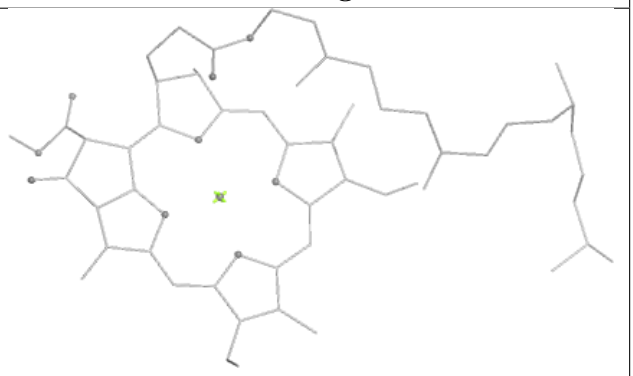
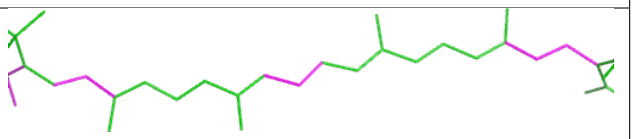


Rings

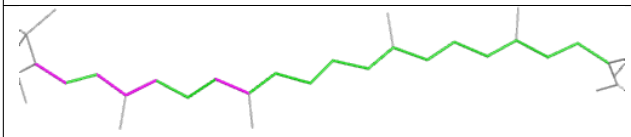
Ligand BCR A 849



Bond lengths



Bond angles



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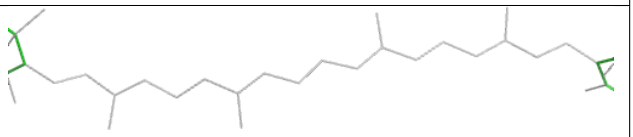
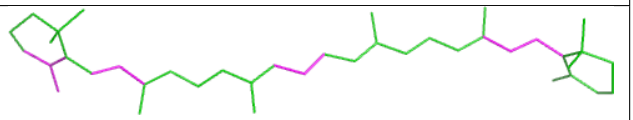


Rings

Ligand BCR a 849



Bond lengths



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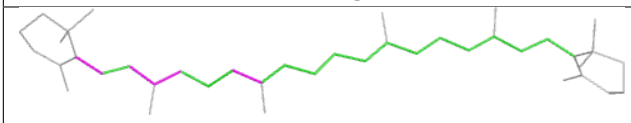

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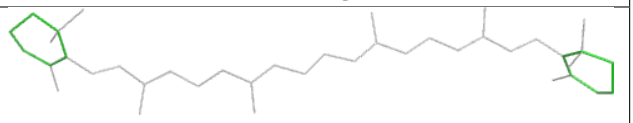
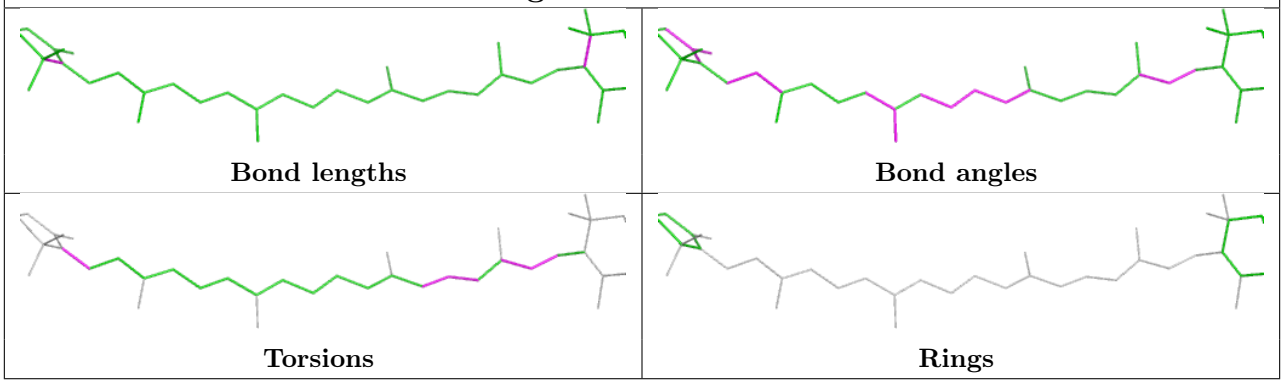
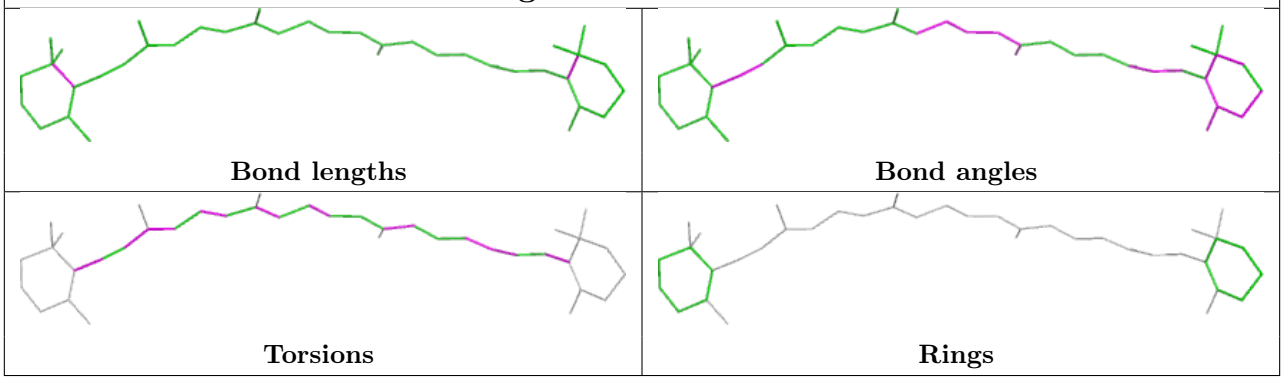


Rings

Ligand BCR k 102



Ligand BCR 8 1305



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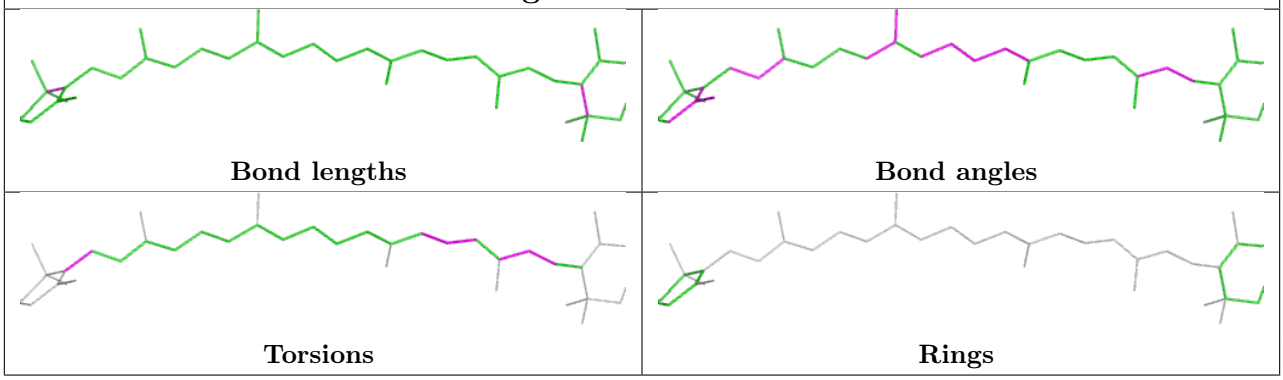

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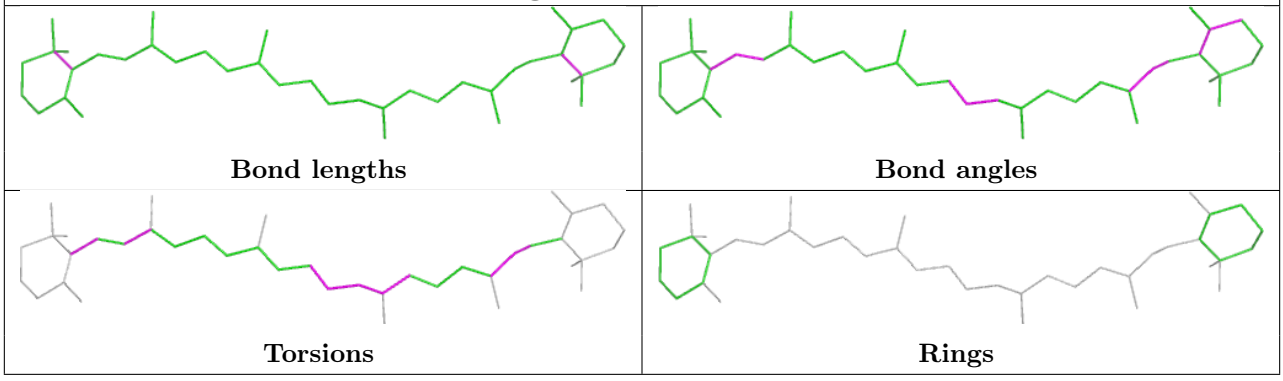

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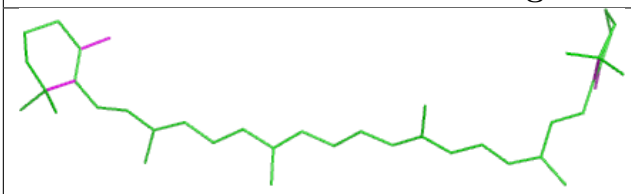
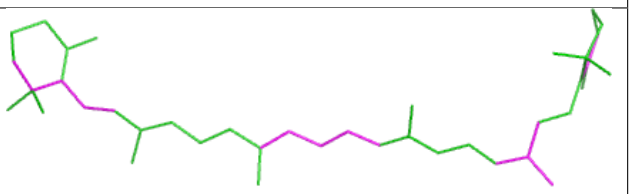
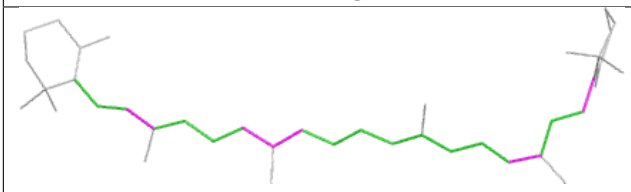


Bond lengths



Bond angles



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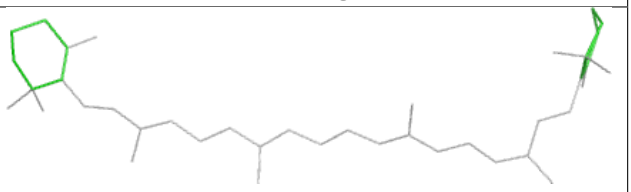
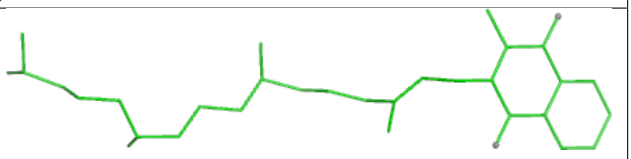


Rings

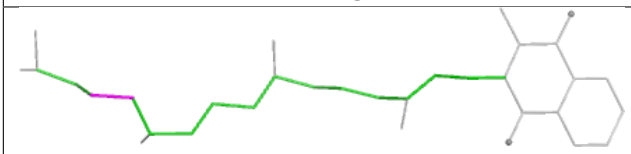
Ligand PQN 1 1646



Bond lengths



Bond angles



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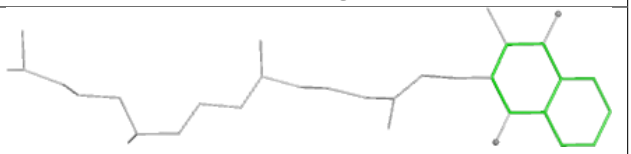
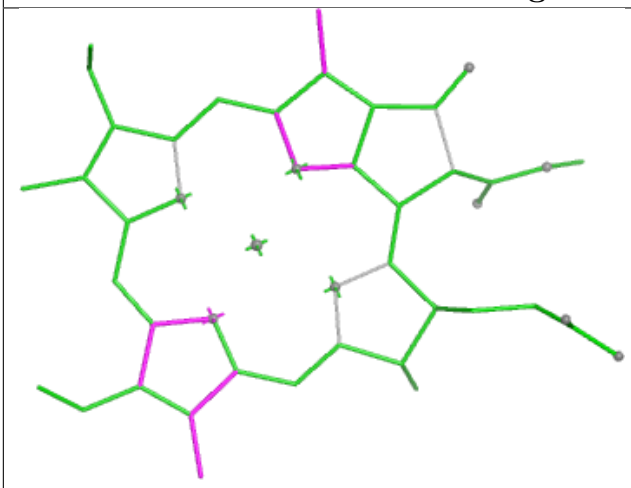


Rings

Ligand CLA 2 837



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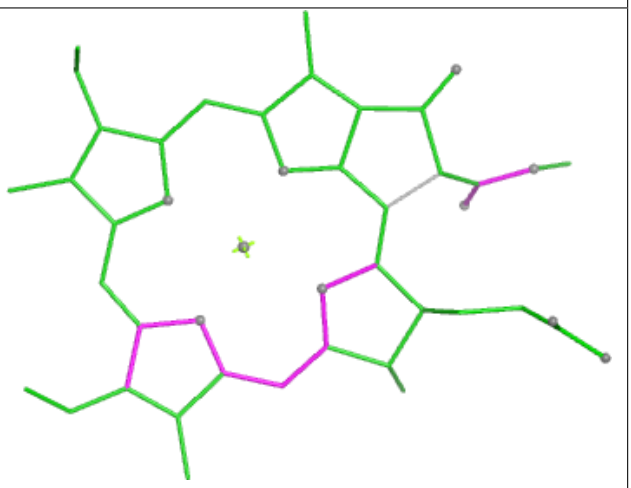
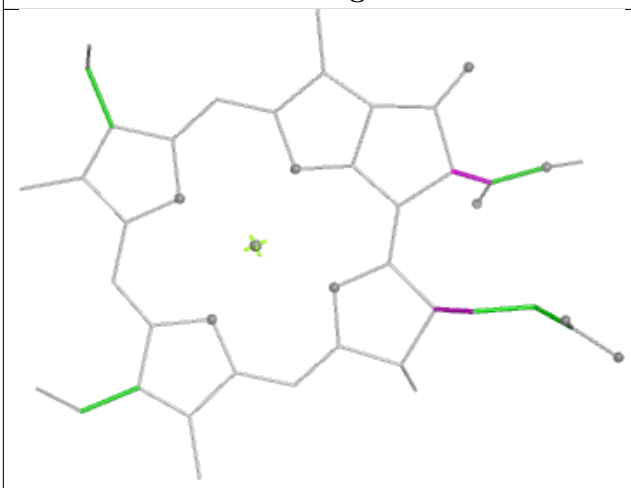


Bond angles



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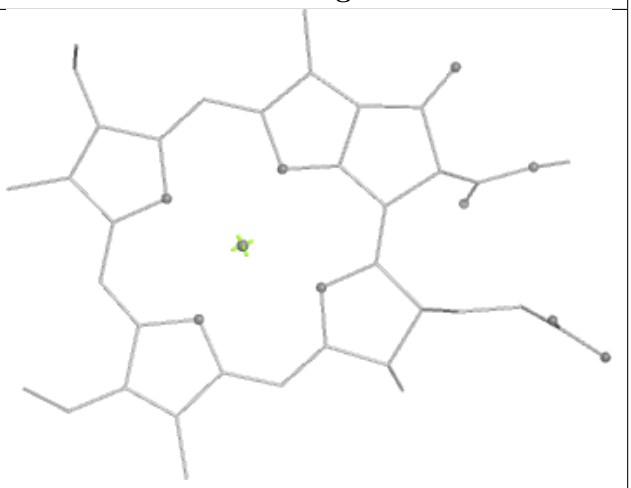
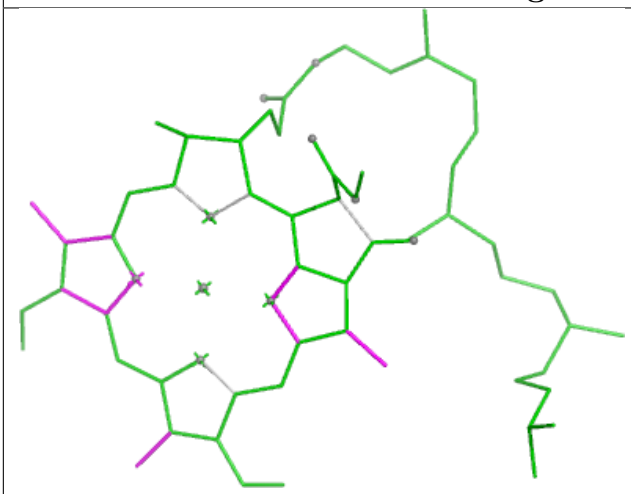


Rings

Ligand CLA b 833



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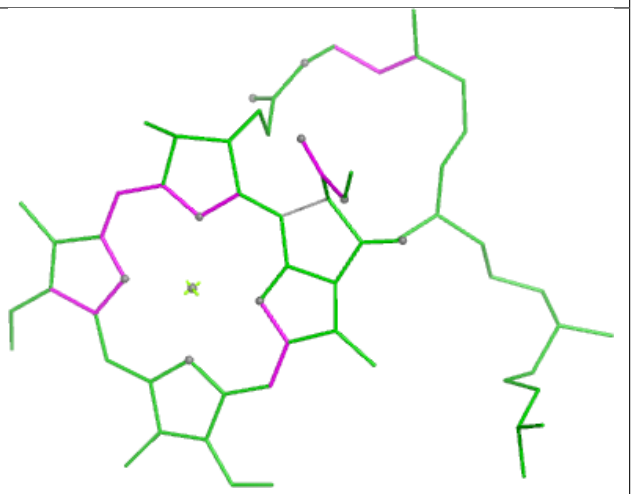
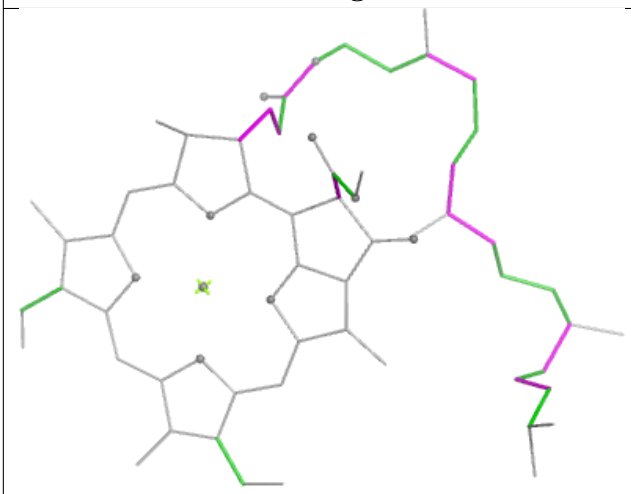


Bond angles



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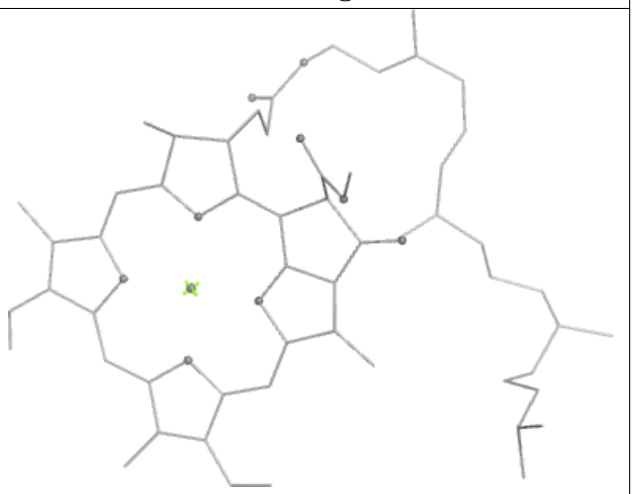
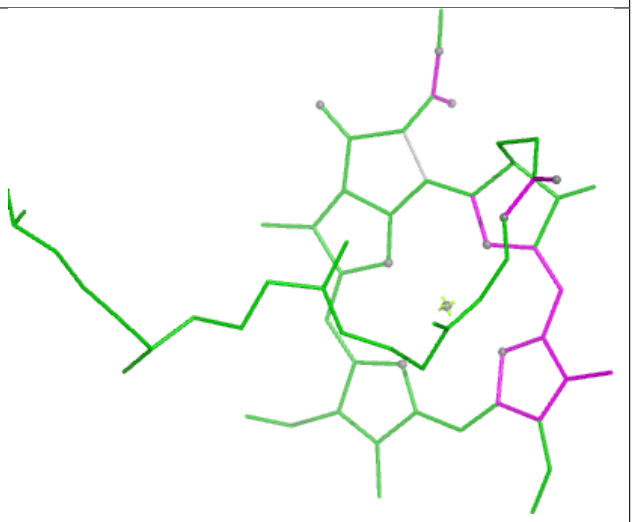


Rings

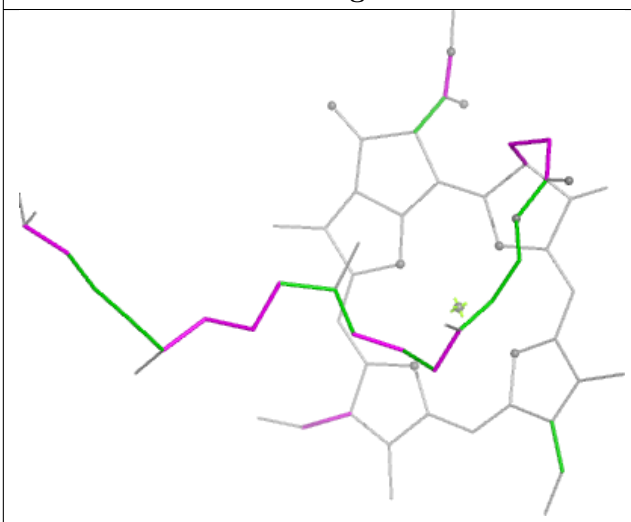
Ligand CLA b 828



Bond lengths



Bond angles



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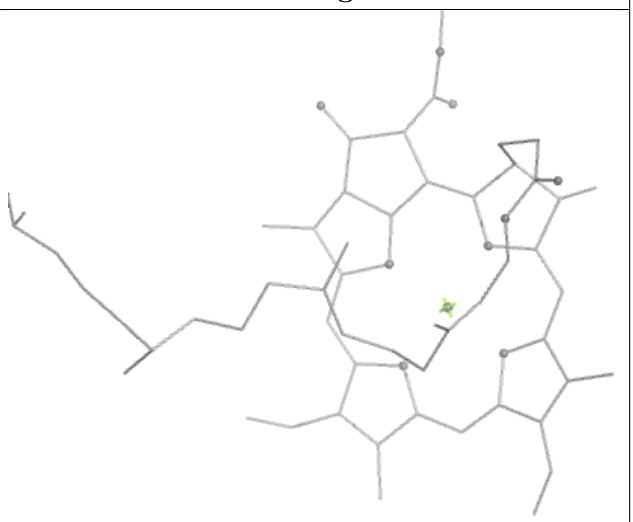
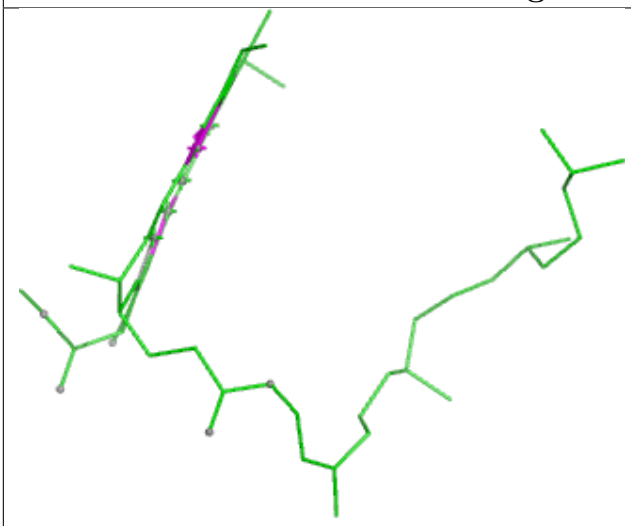


Rings

Ligand CLA b 835



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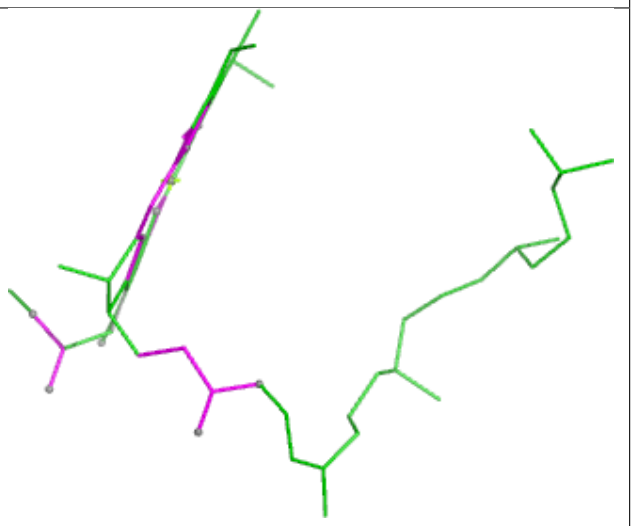
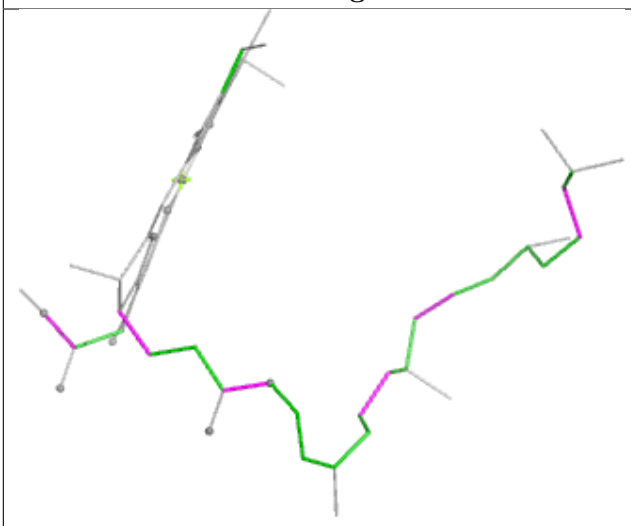


Bond angles



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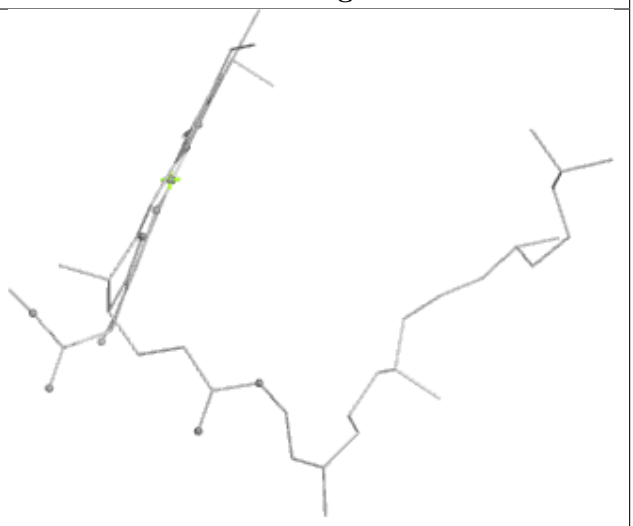
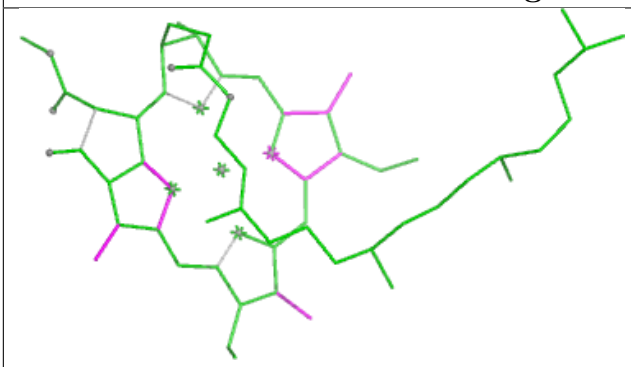


Rings

Ligand CLA B 807



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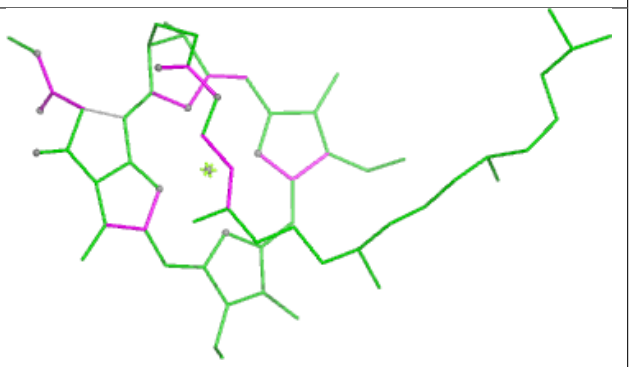
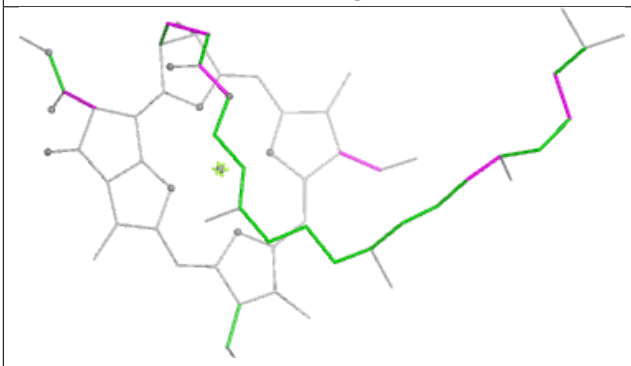


Bond angles



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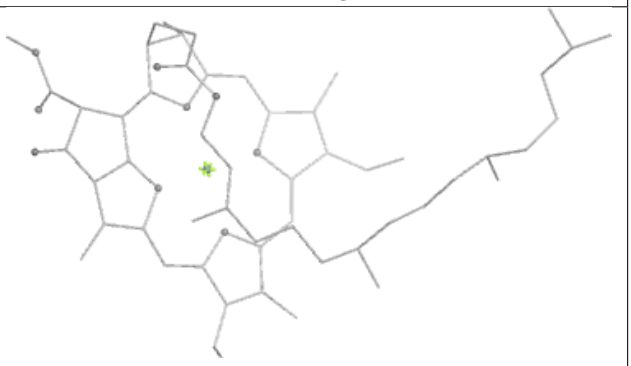
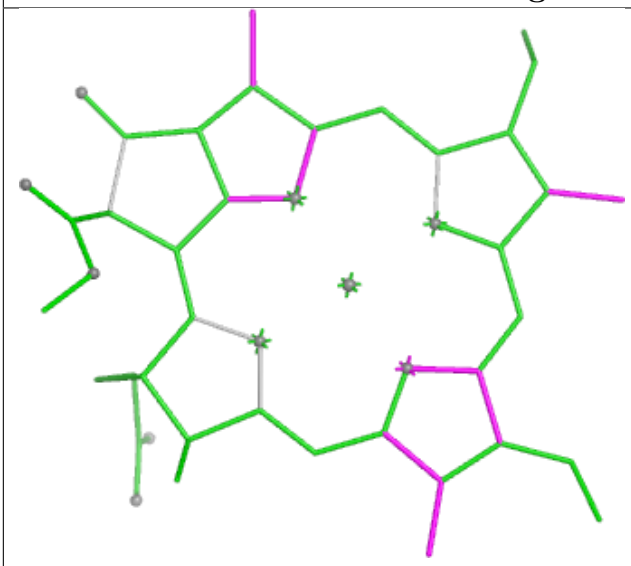


Rings

Ligand CLA 2 822



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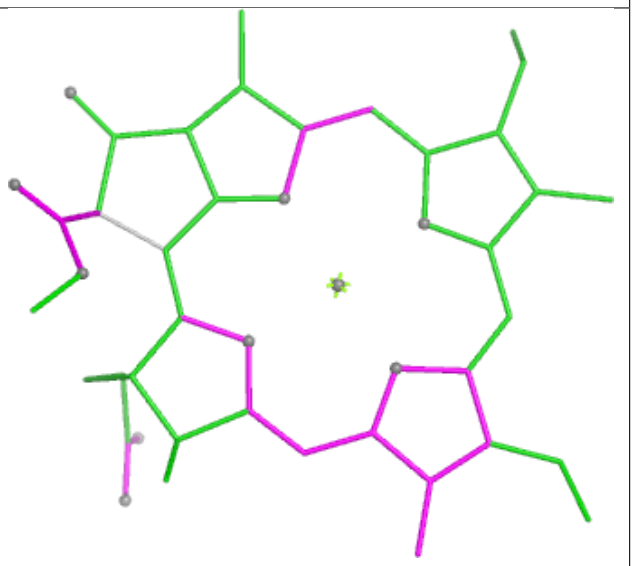
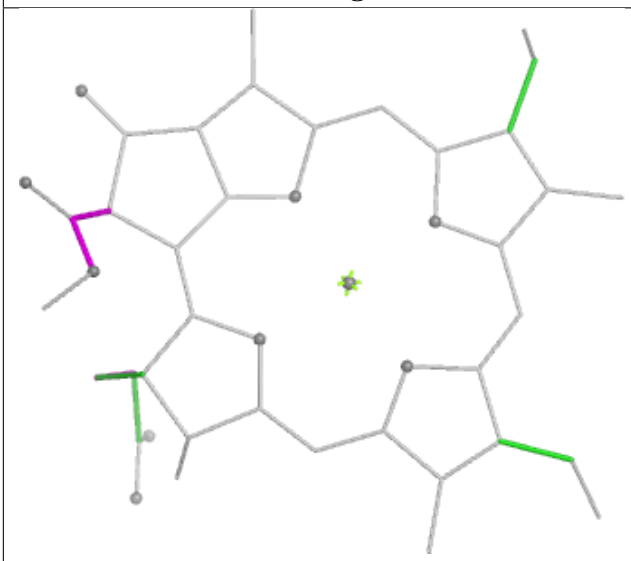


Bond angles



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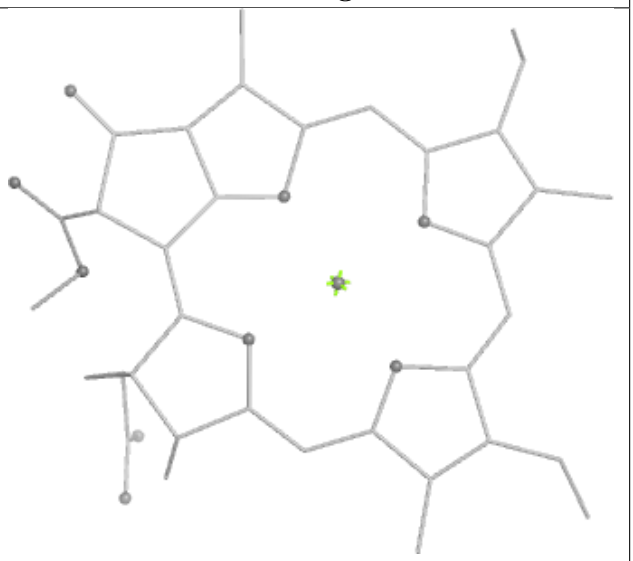
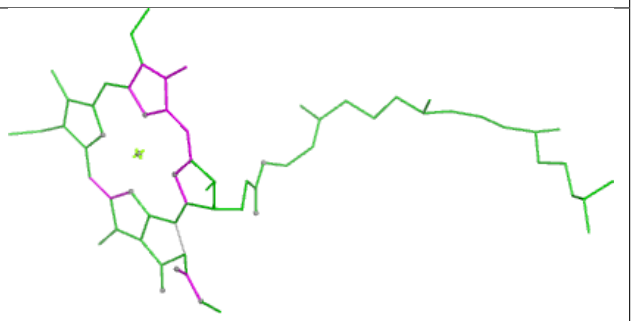


Rings

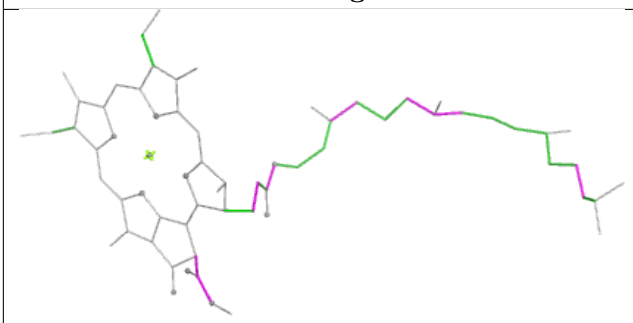
Ligand CLA A 822



Bond lengths



Bond angles



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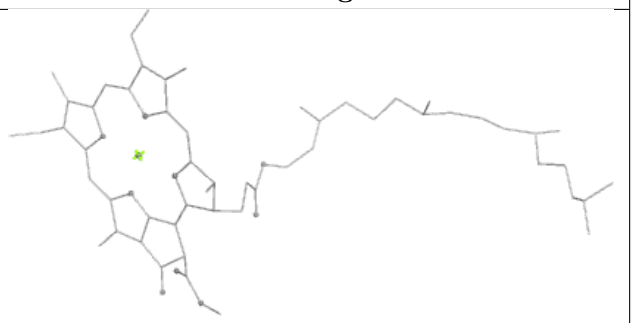
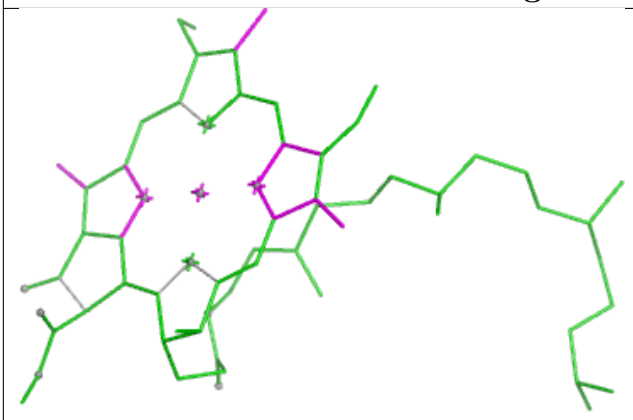


Rings

Ligand CLA A 843



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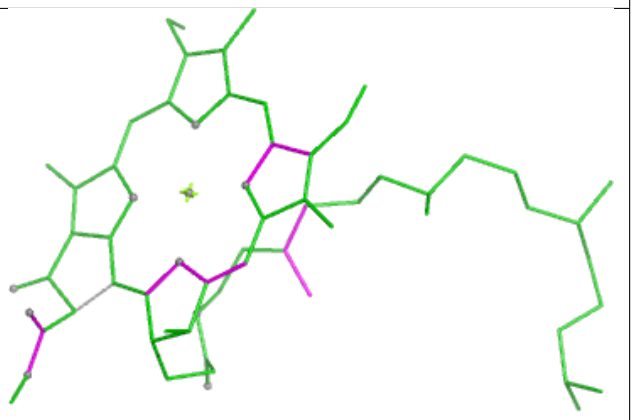
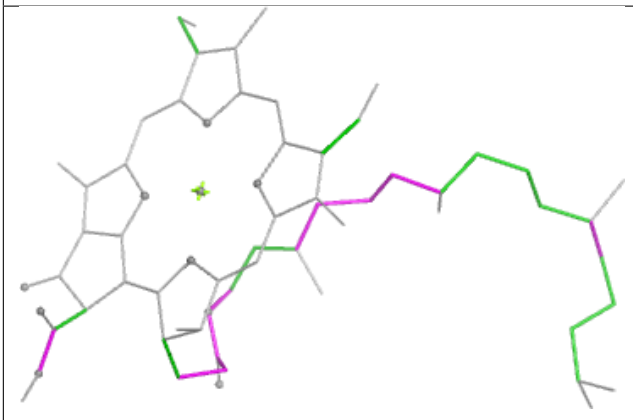


Bond angles



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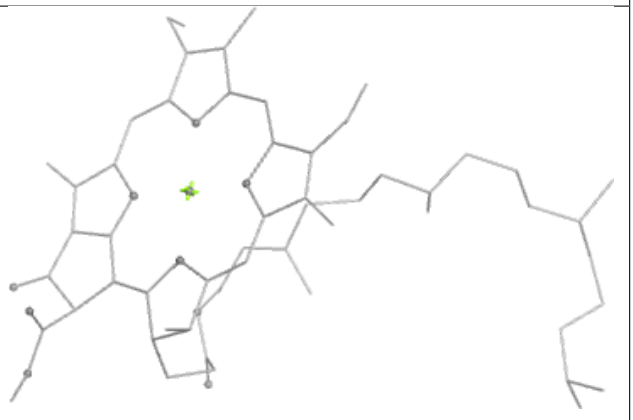
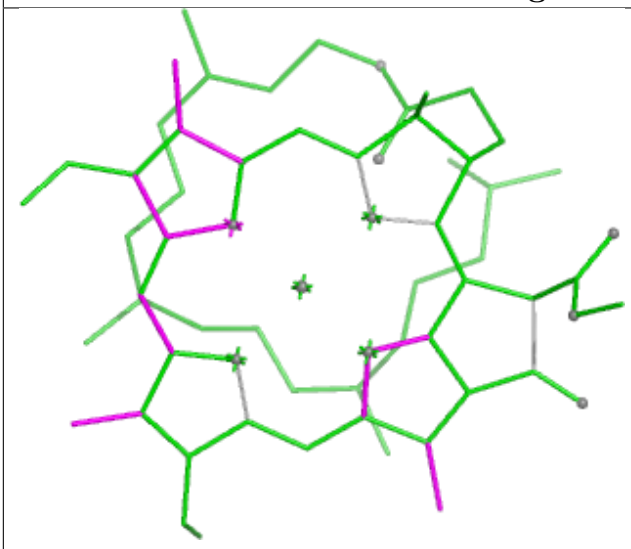


Rings

Ligand CLA 0 205



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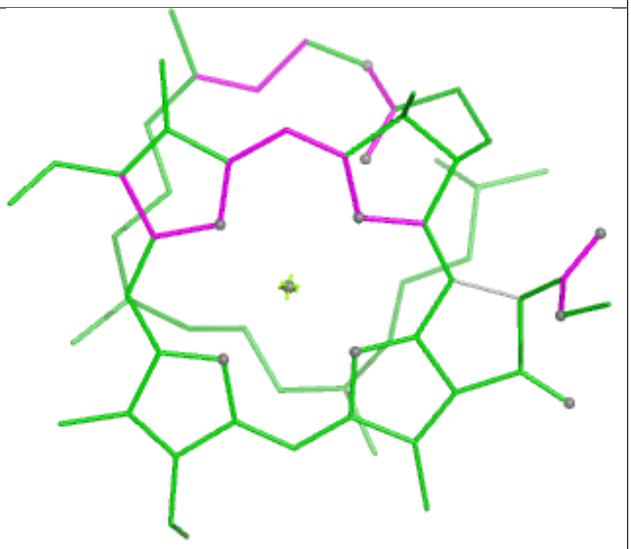
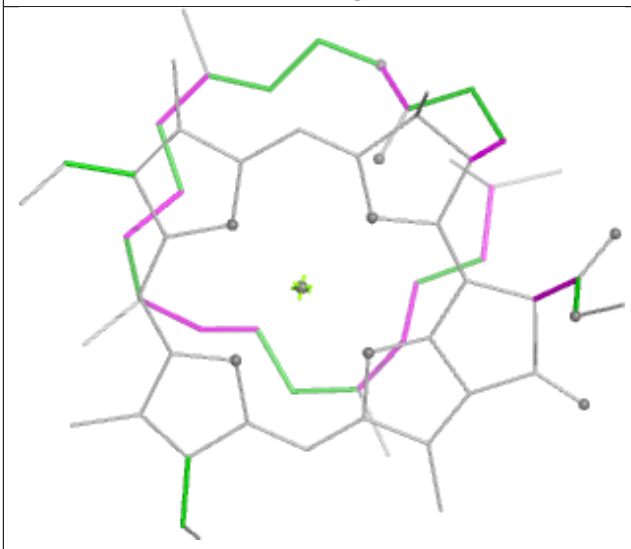
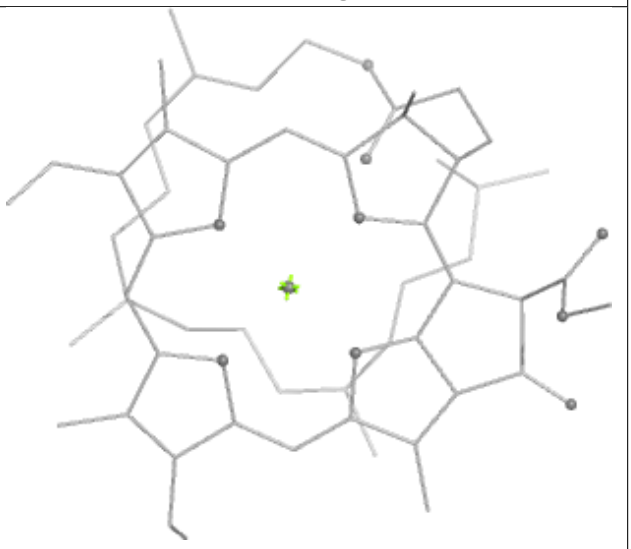


Bond angles

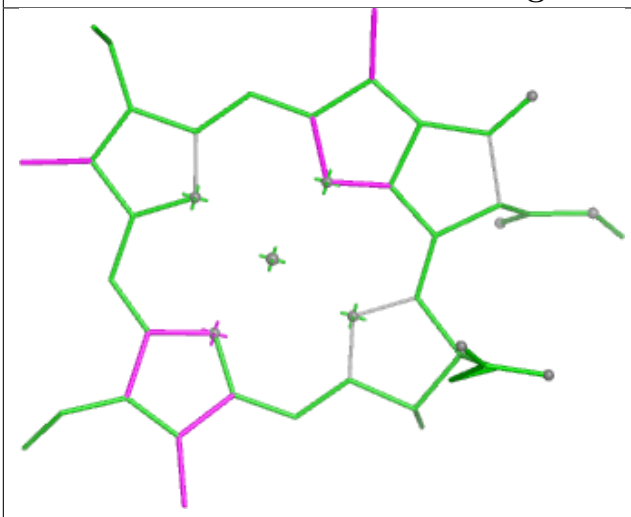


Torsions

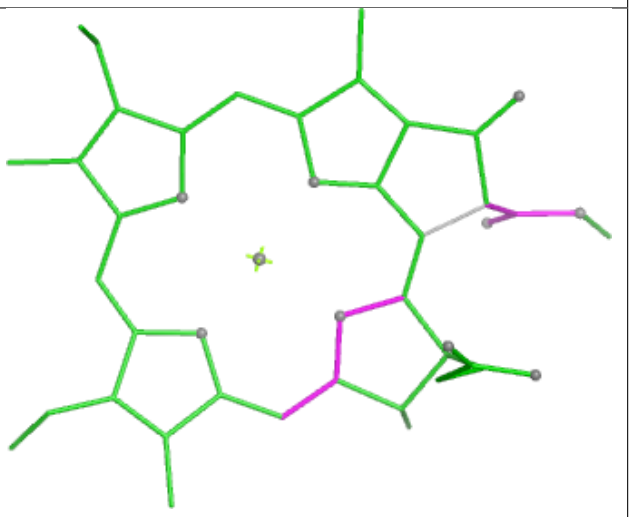


Rings

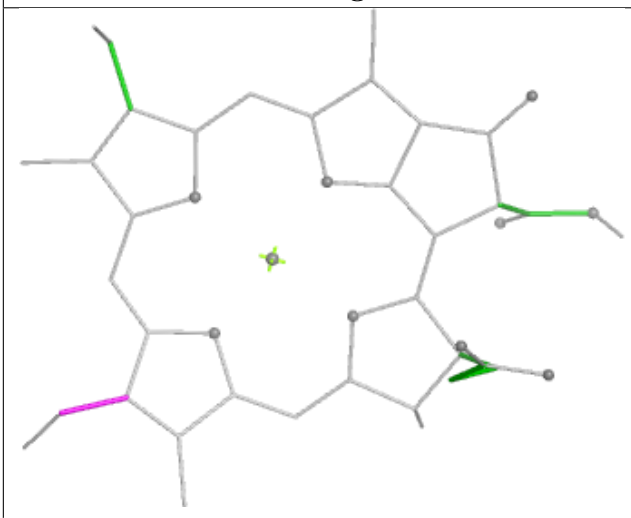
Ligand CLA b 813



Bond lengths



Bond angles



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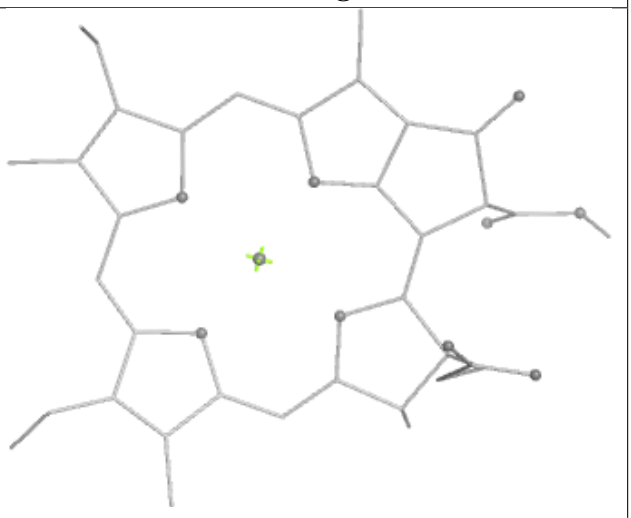


Rings

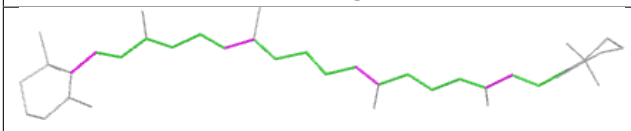
Ligand BCR 0 209



Bond lengths



Bond angles



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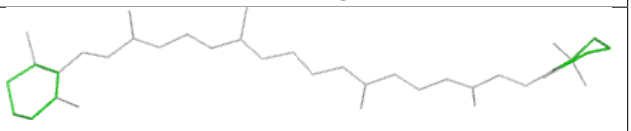
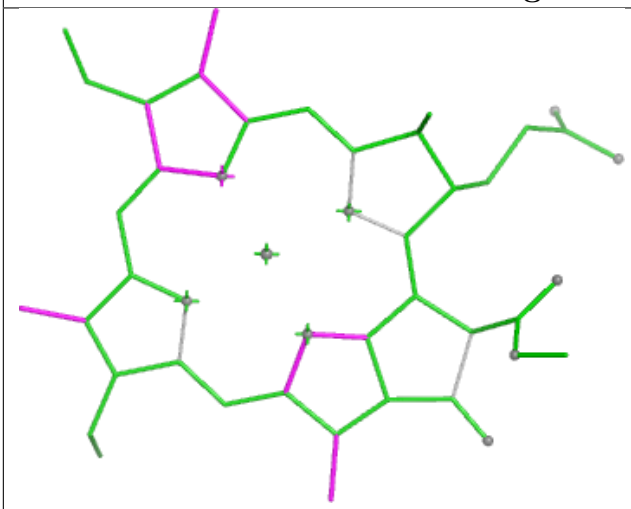
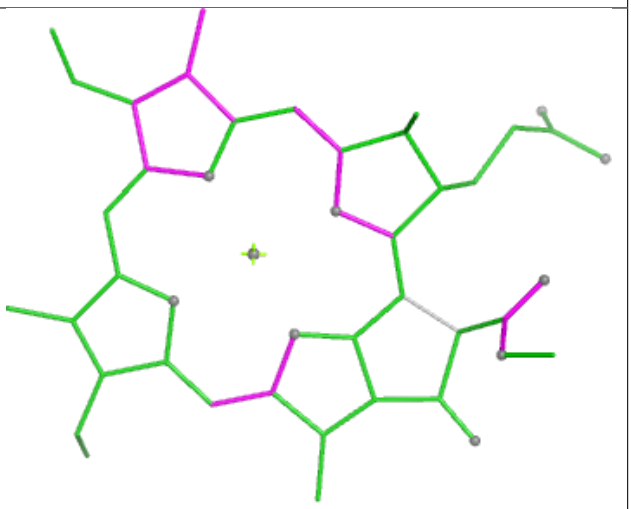


Rings

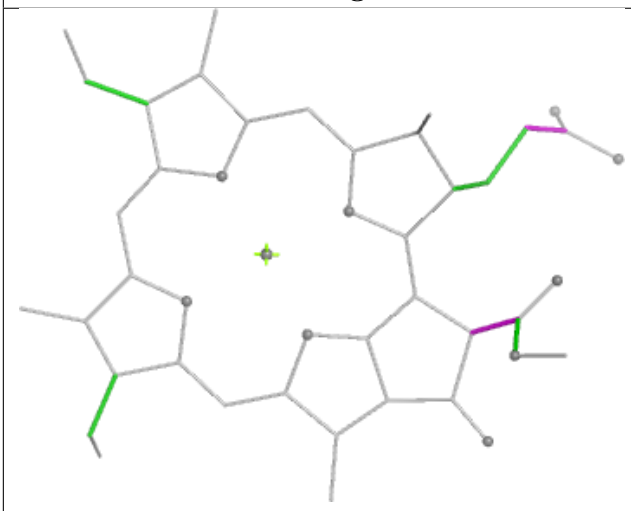
Ligand CLA A 844



Bond lengths



Bond angles



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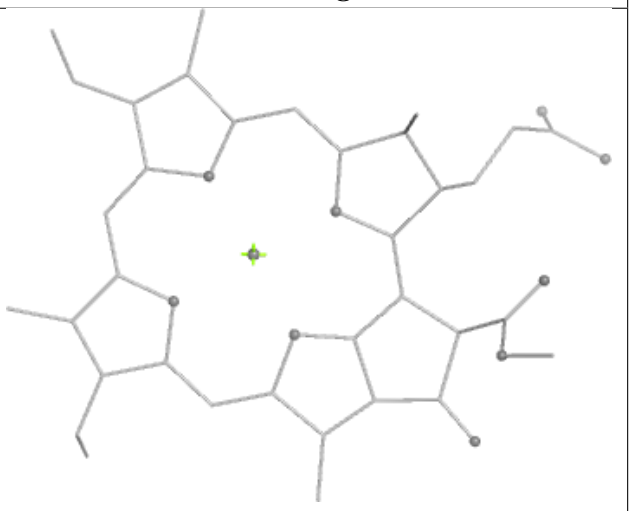
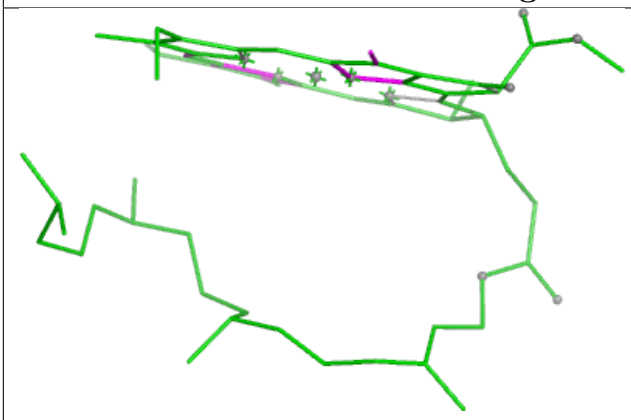


Rings

Ligand CLA 1 1622



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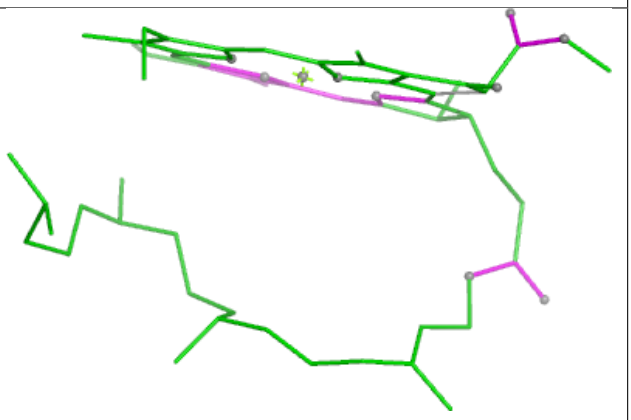

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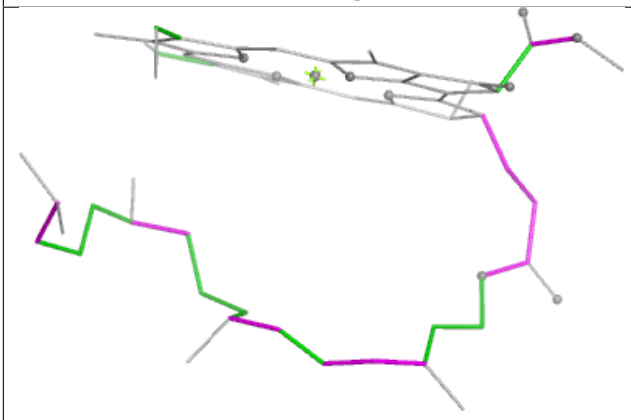
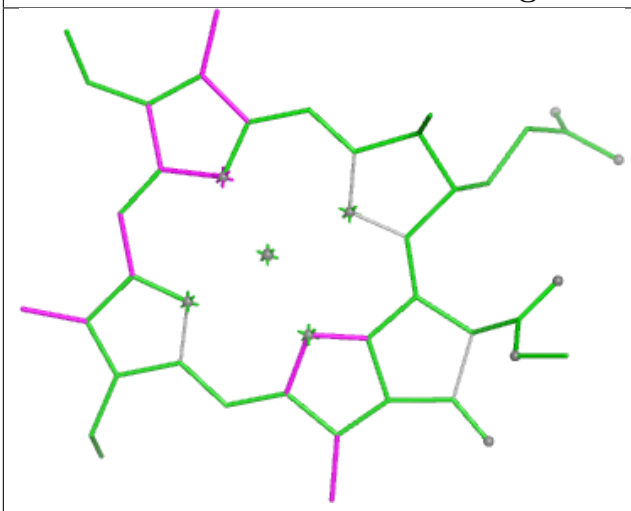


Torsions



Rings

Ligand CLA 1 1645



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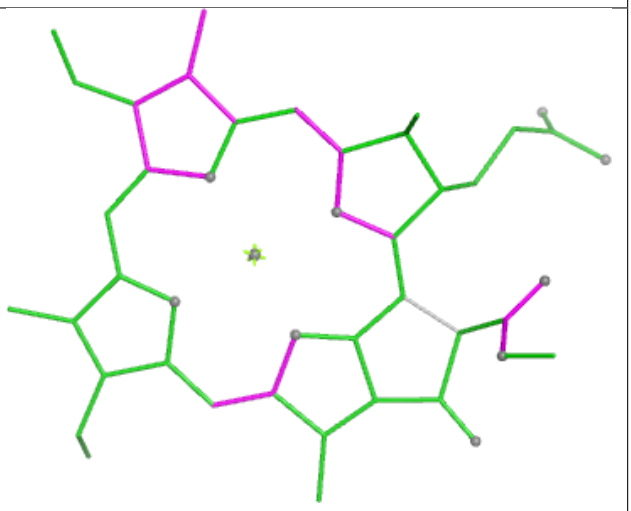
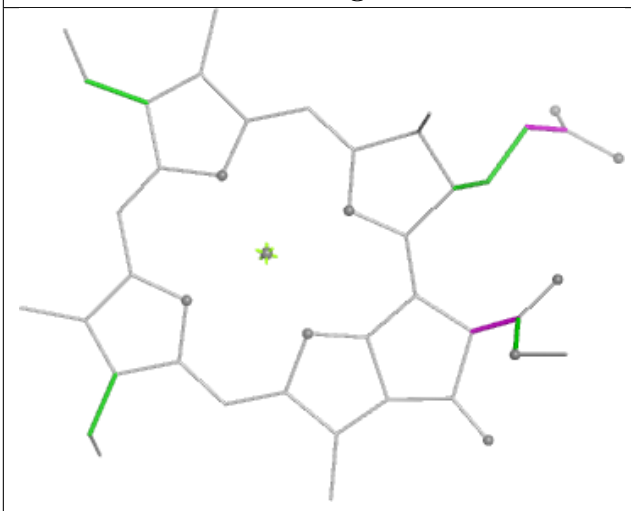


Bond angles



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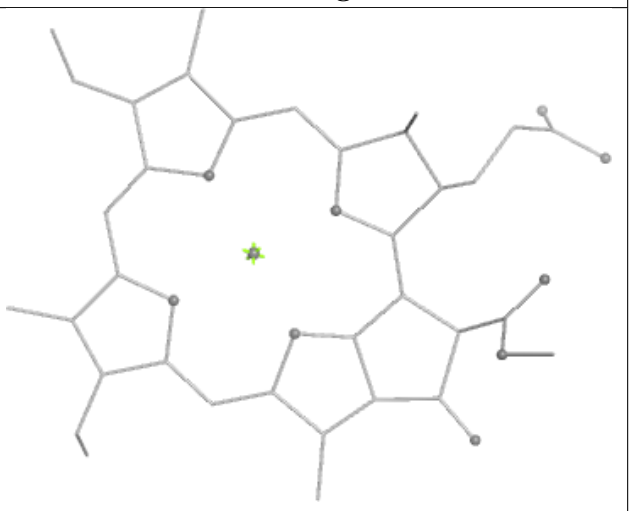
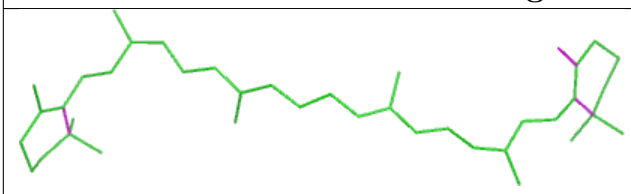


Rings

Ligand BCR 2 846



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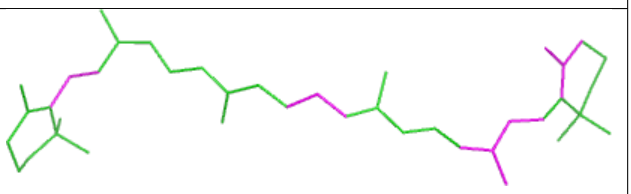
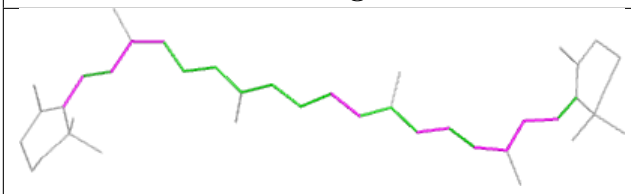


Bond angles



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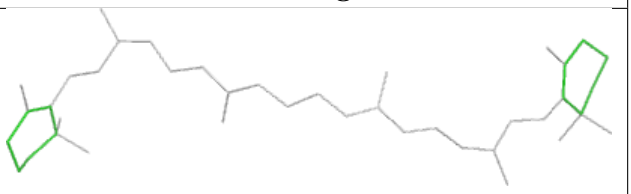
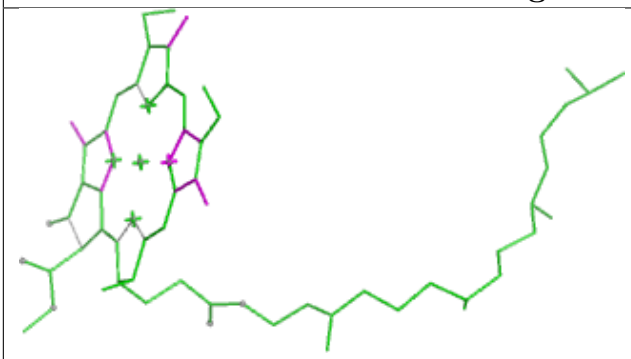


Rings

Ligand CLA a 836



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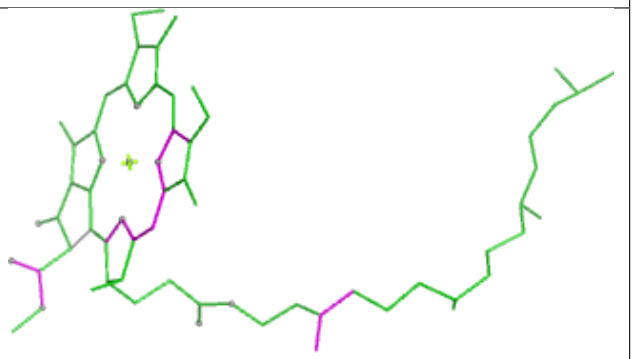
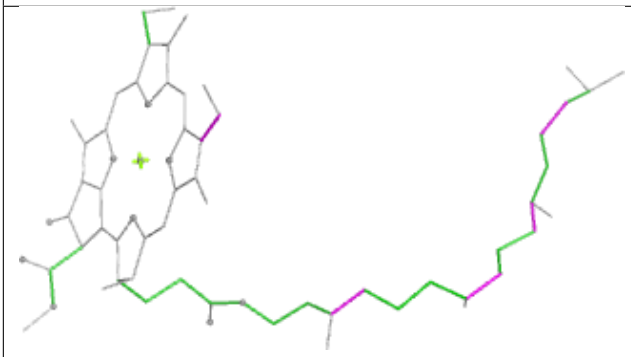


Bond angles



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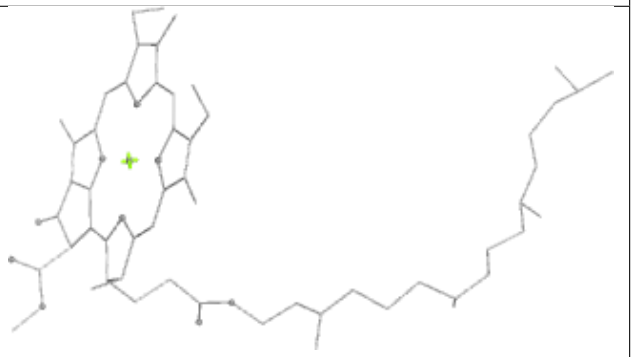
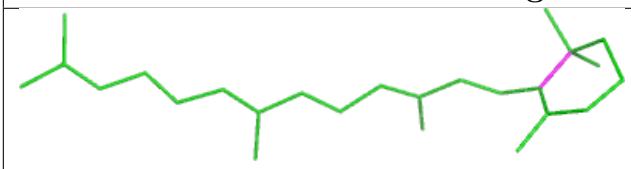


Rings

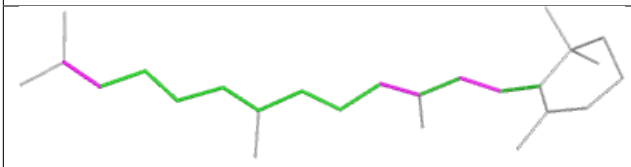
Ligand BCR 9 104



Bond lengths



Bond angles



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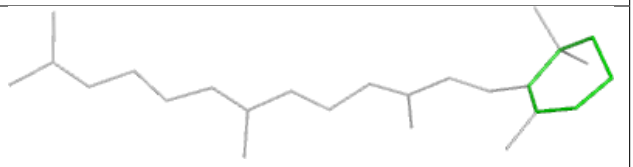
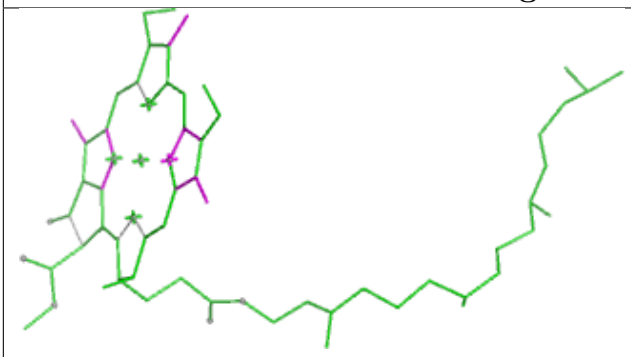


Rings

Ligand CLA 1 1637



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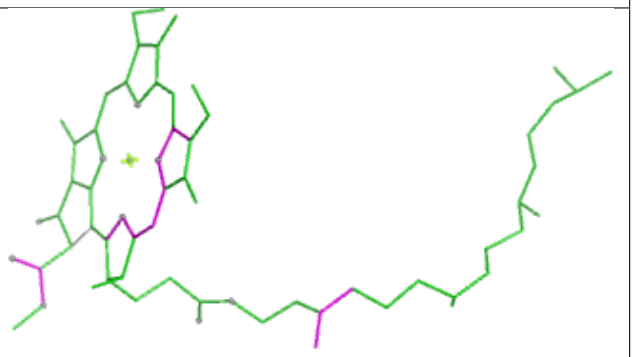
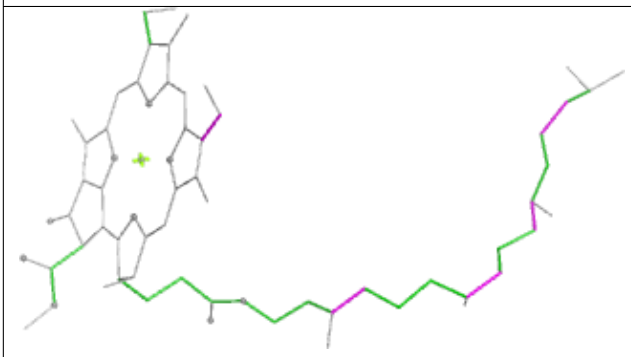


Bond angles



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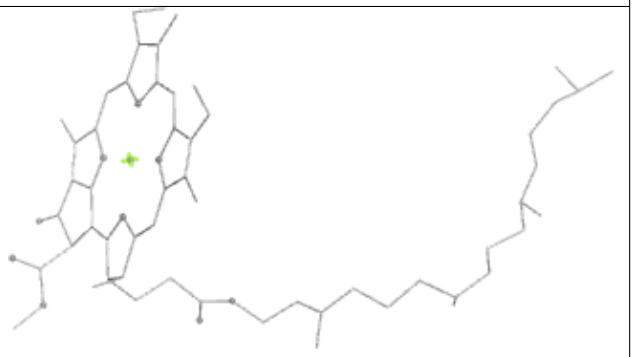
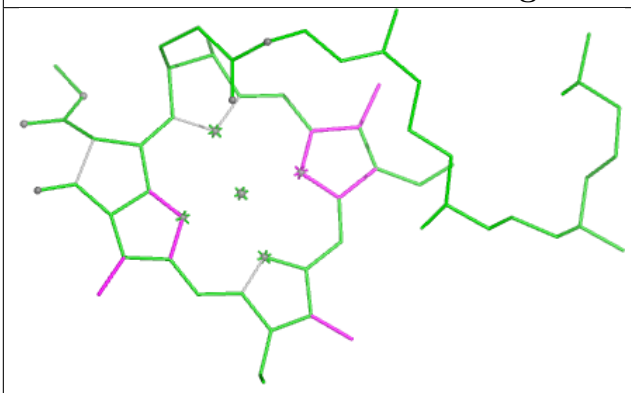


Rings

Ligand CLA 1 1621



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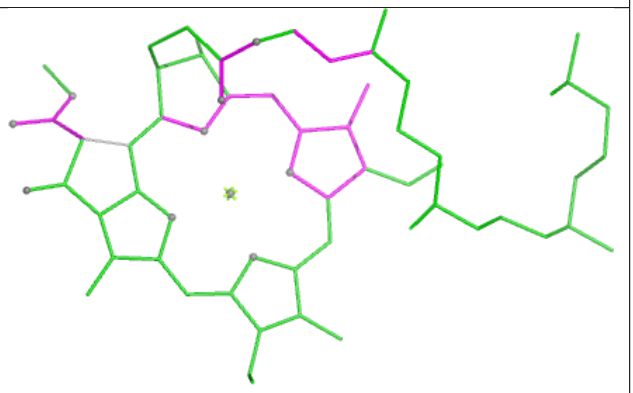
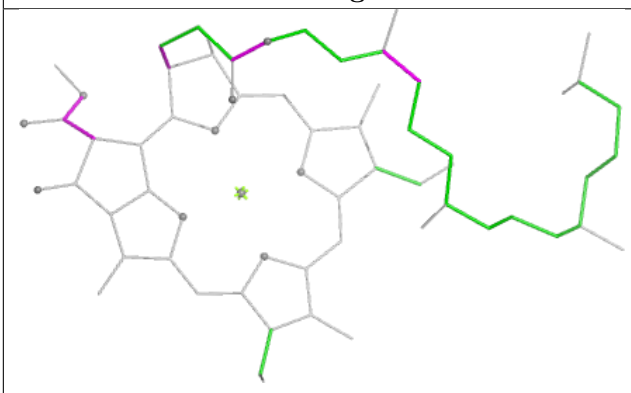


Bond angles



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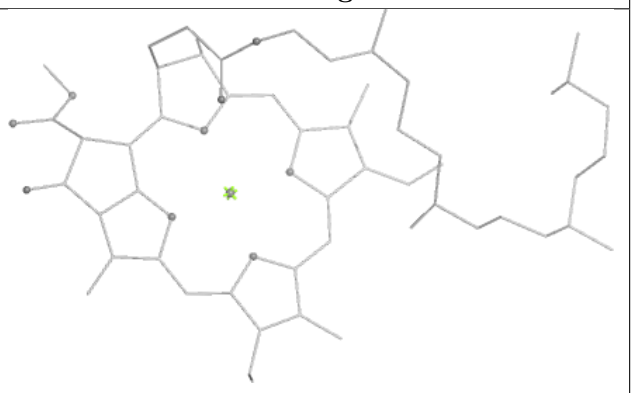
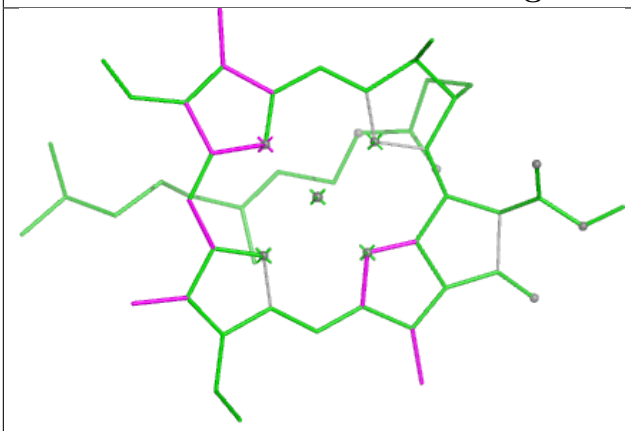


Rings

Ligand CLA B 822



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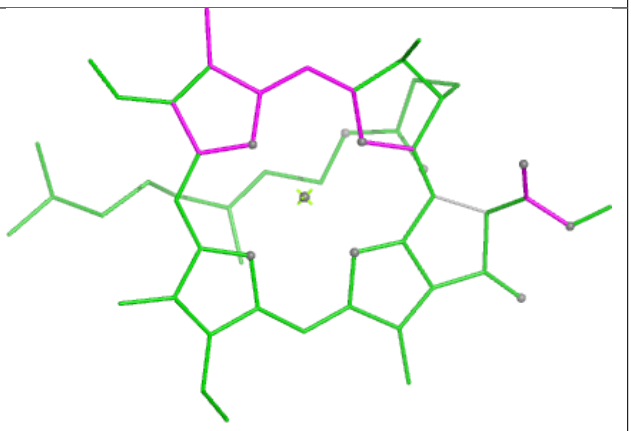
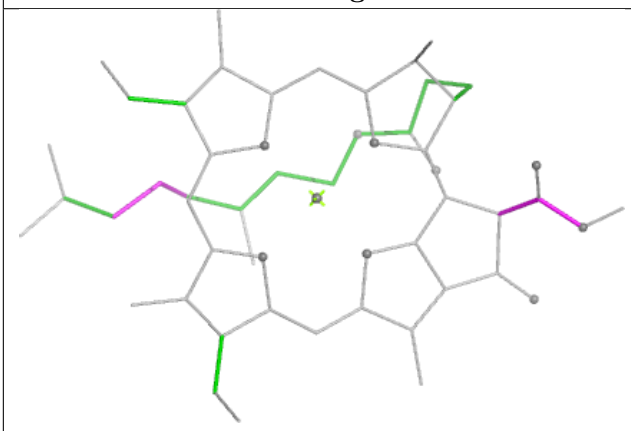


Bond angles



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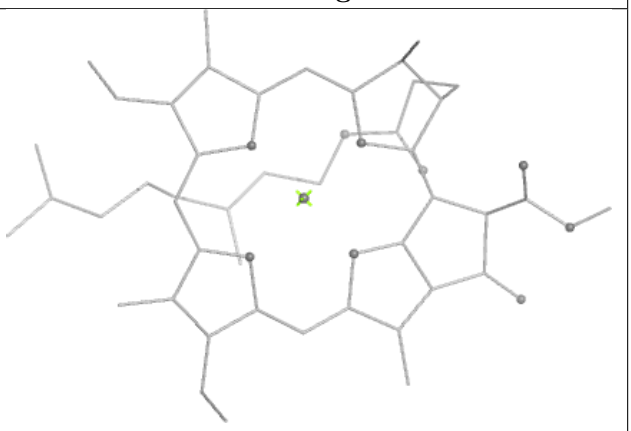
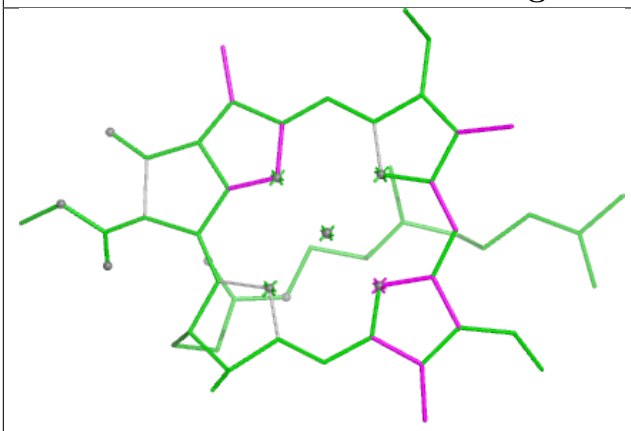


Rings

Ligand CLA 2 823



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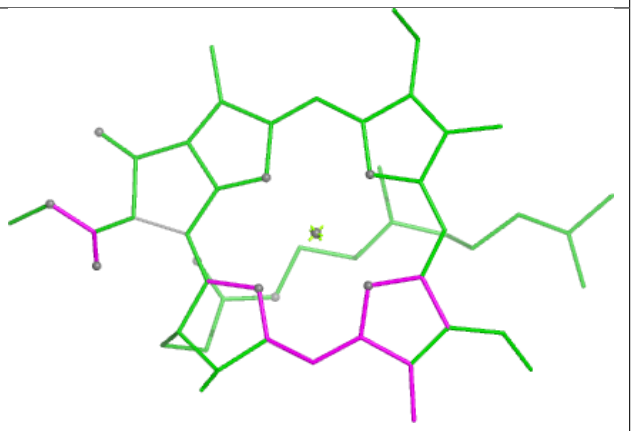
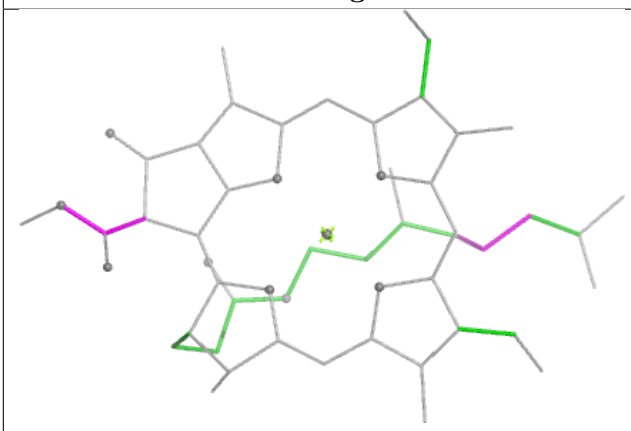


Bond angles



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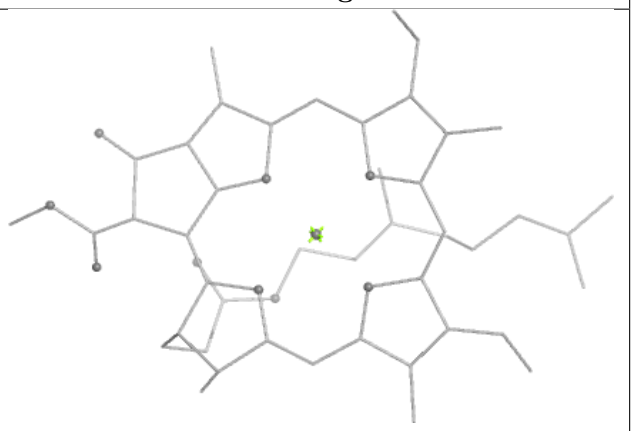
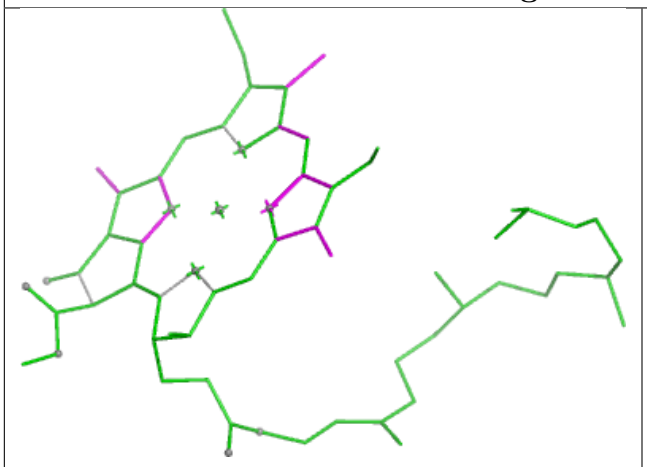


Rings

Ligand CLA 1 1626



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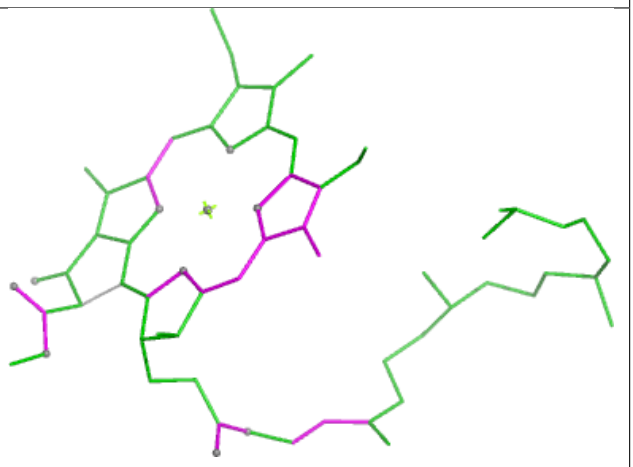
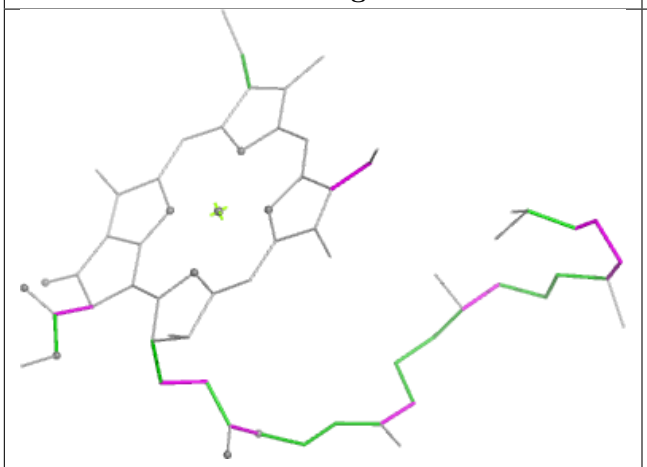


Bond angles



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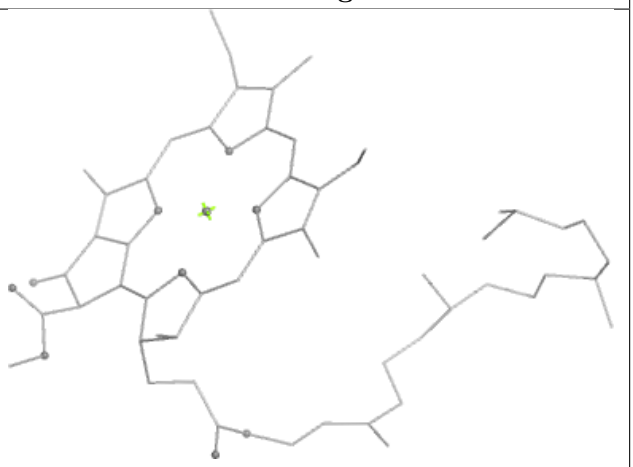
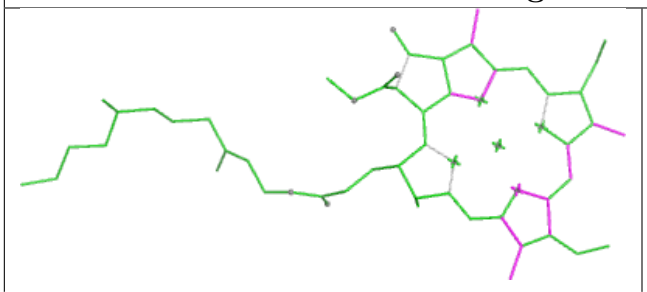


Rings

Ligand CLA F 201



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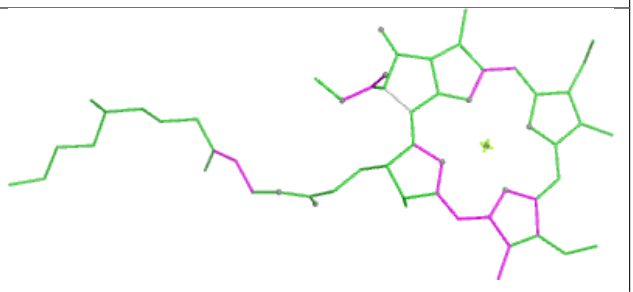
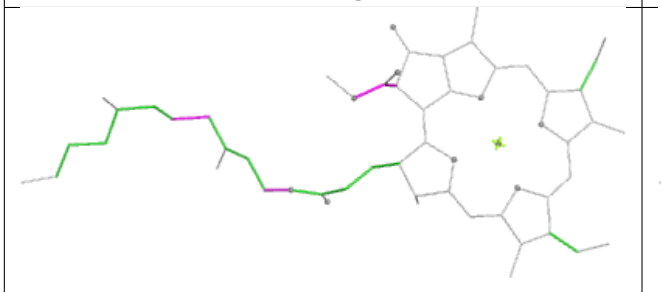


Bond angles



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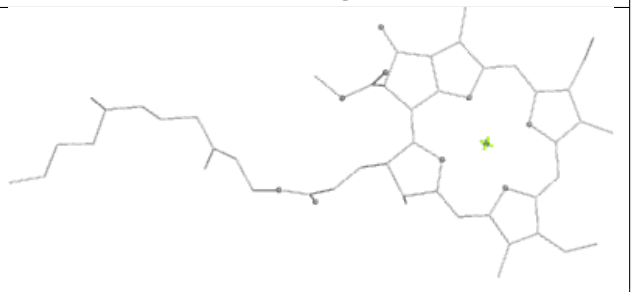
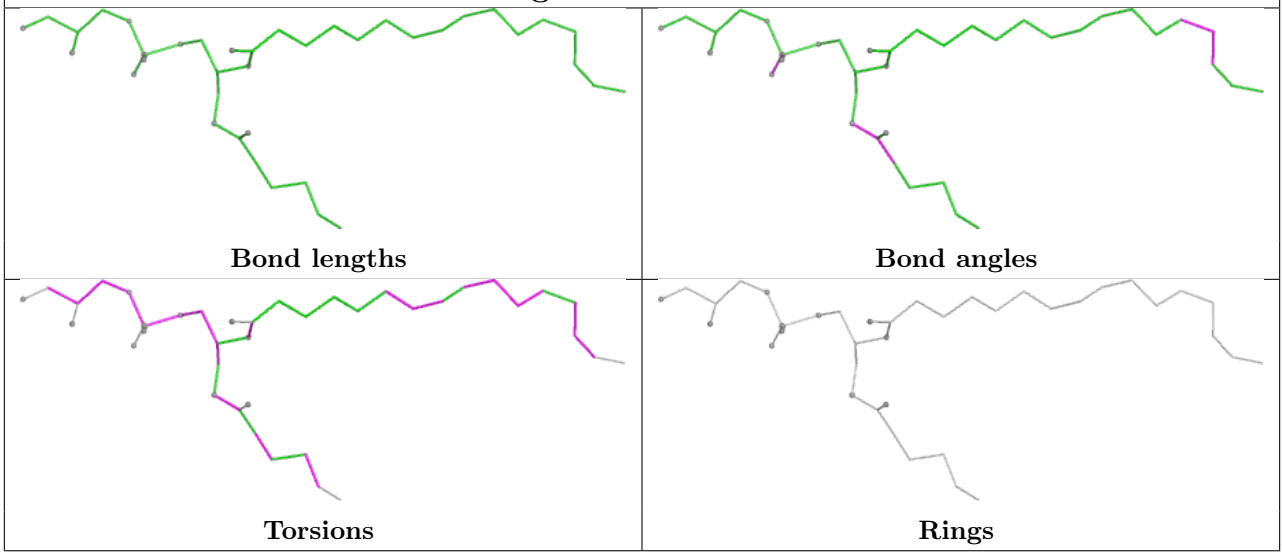
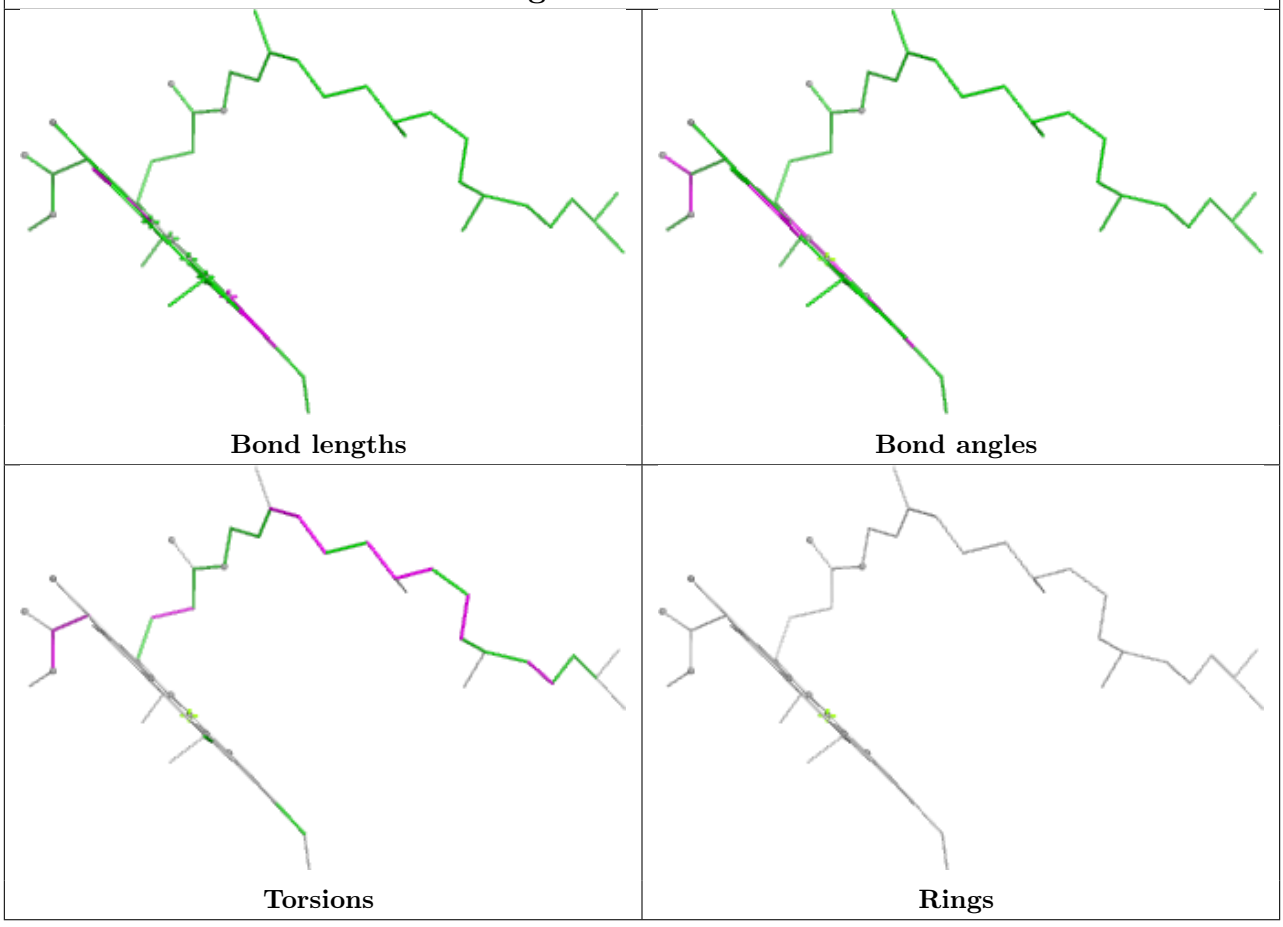


Rings

Ligand LHG l 201



Ligand CLA b 815



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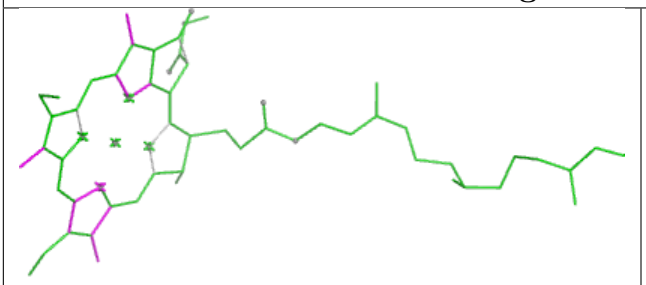
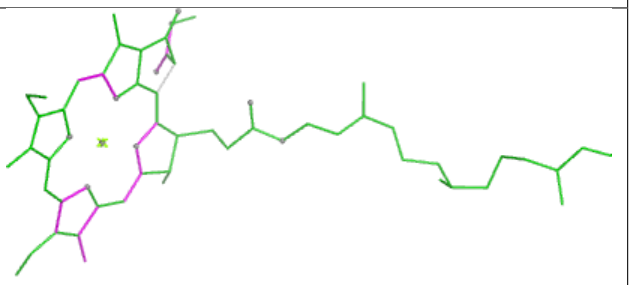
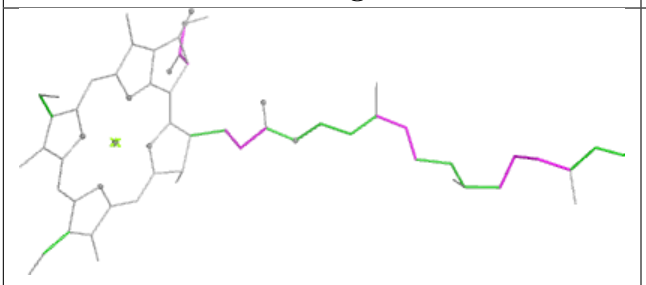


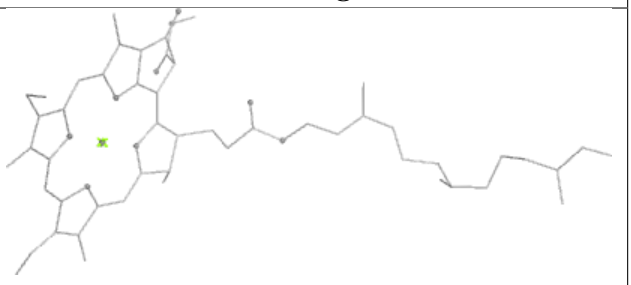
Bond lengths



Bond angles

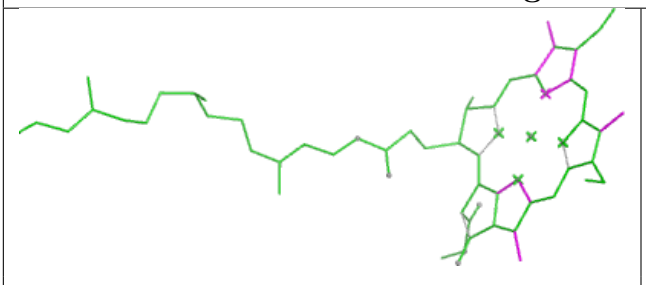


Torsions



Rings

Ligand CLA A 810



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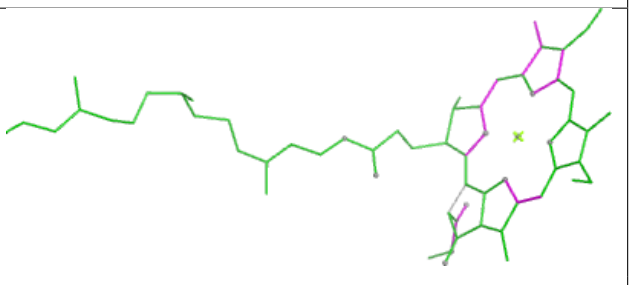
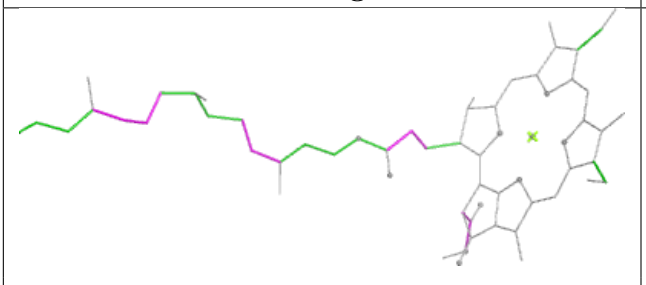


Bond angles



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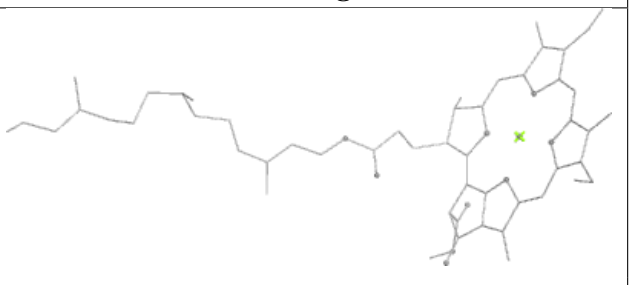
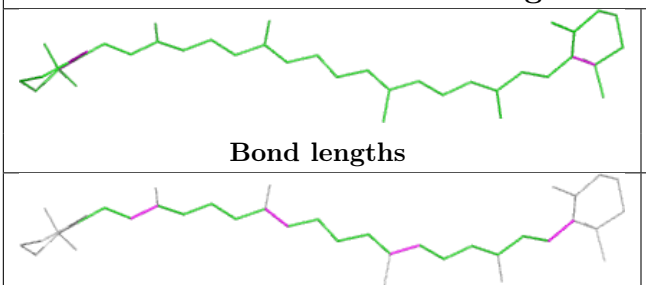


Rings

Ligand BCR L 207



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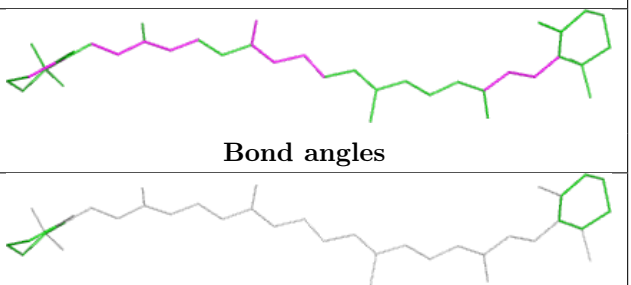
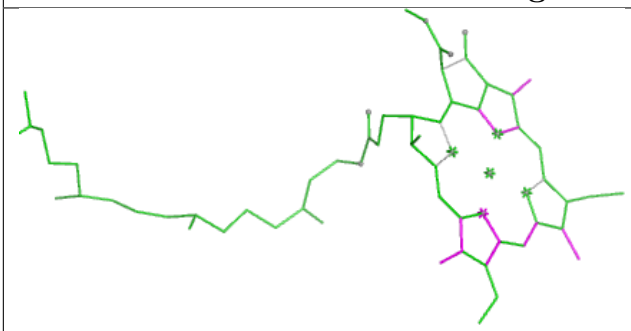


Bond angles

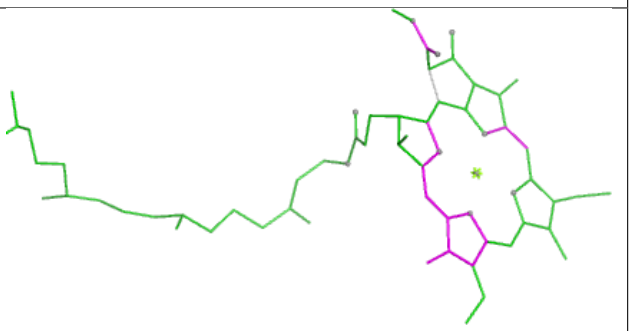
Torsions

Rings

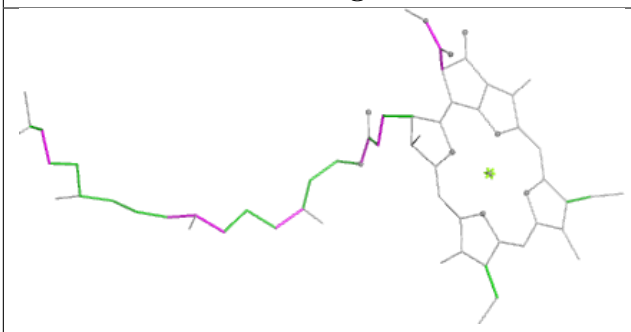
Ligand CLA a 822



Bond lengths



Bond angles



Torsions

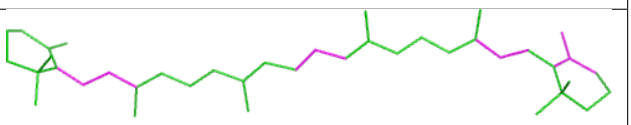


Rings

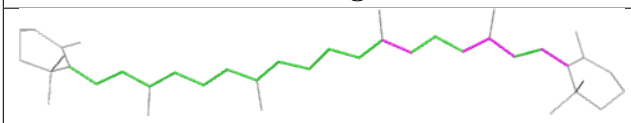
Ligand BCR 1 1650



Bond lengths



Bond angles



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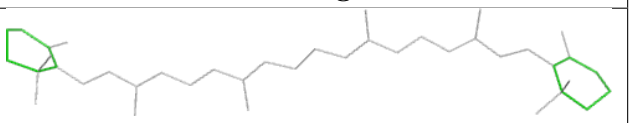
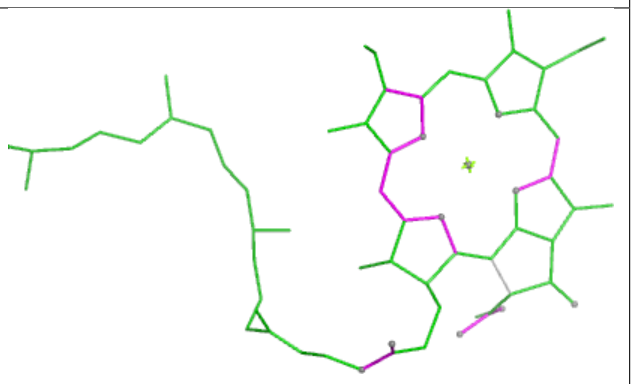


Rings

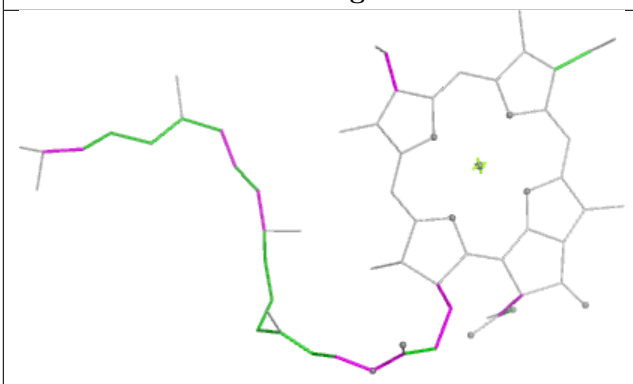
Ligand CLA A 814



Bond lengths



Bond angles



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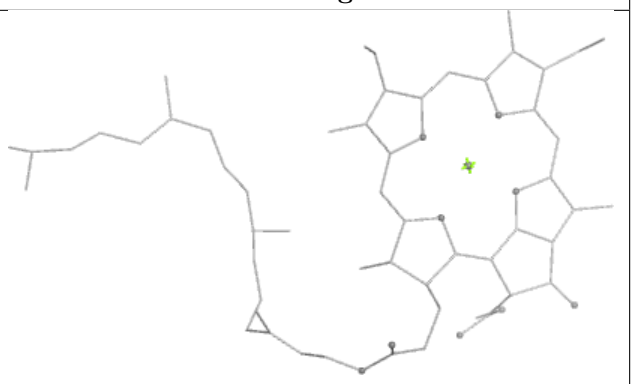
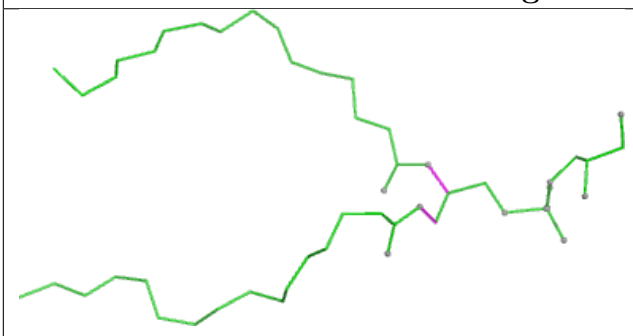
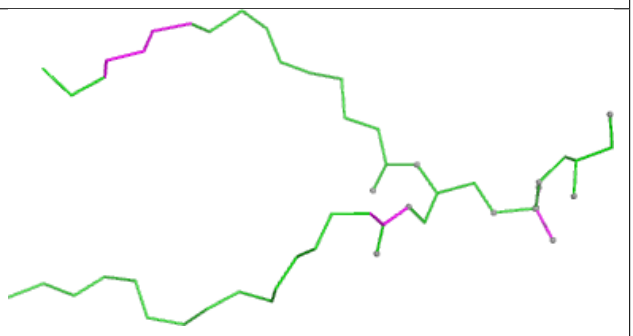


Rings

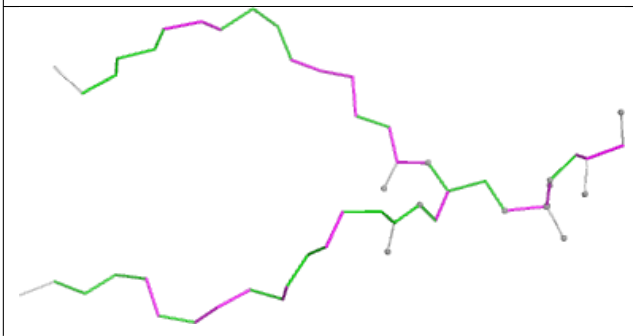
Ligand LHG A 853



Bond lengths



Bond angles



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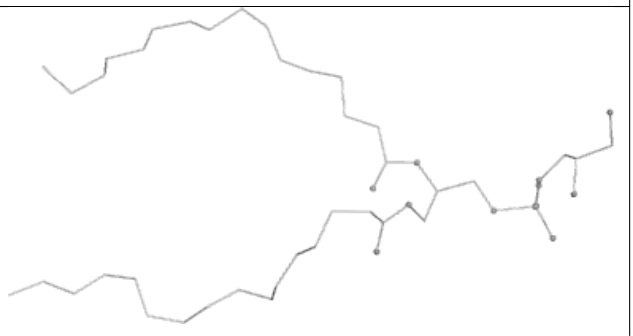
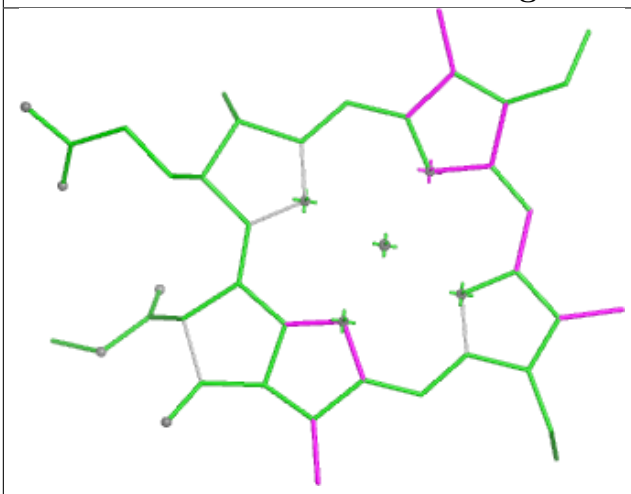


Rings

Ligand CLA 8 1301



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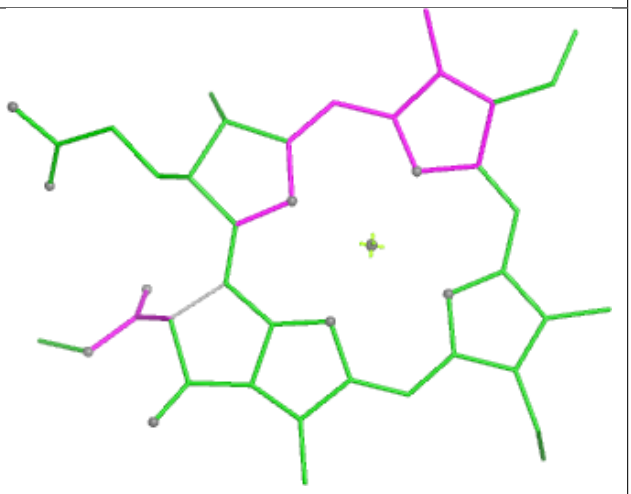
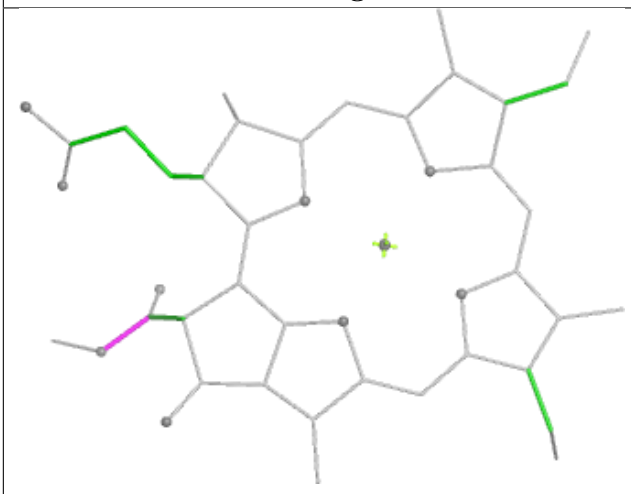


Bond angles



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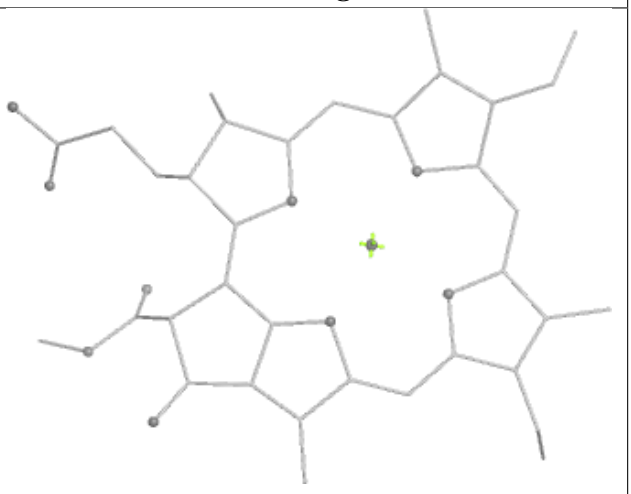
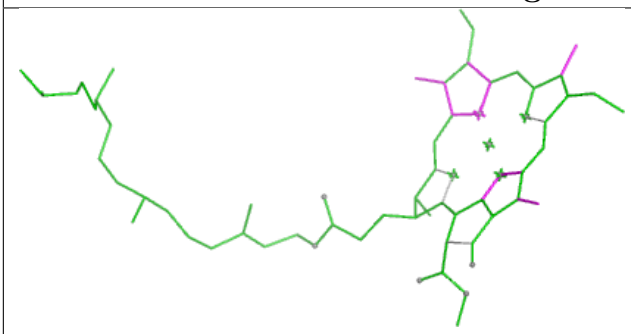


Rings

Ligand CLA A 855



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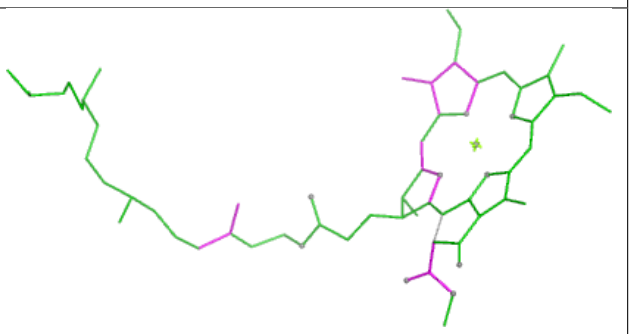
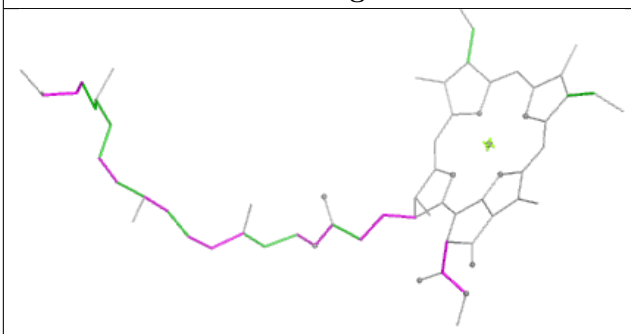


Bond angles



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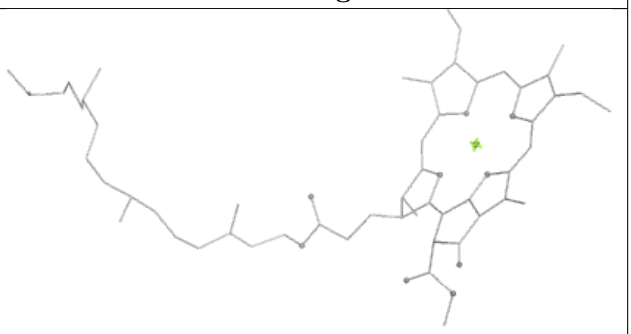
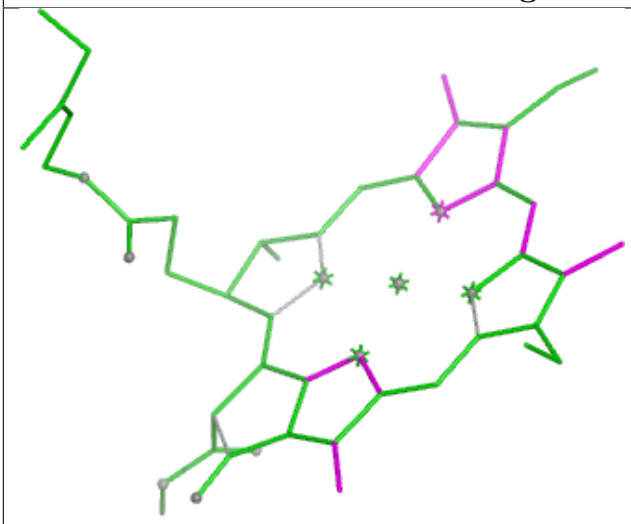


Rings

Ligand CLA 1 1609



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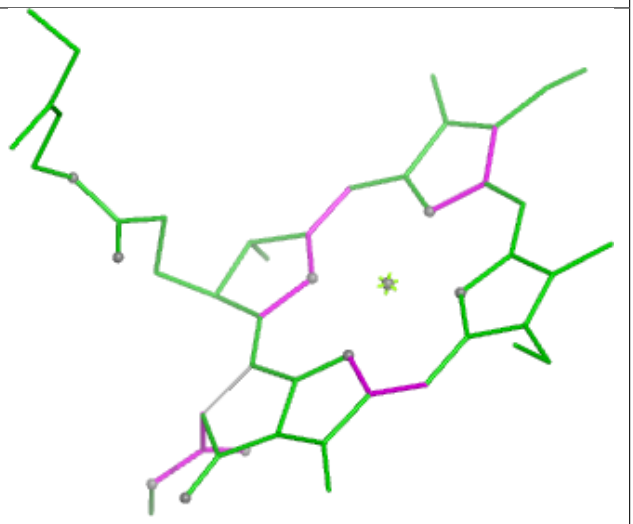
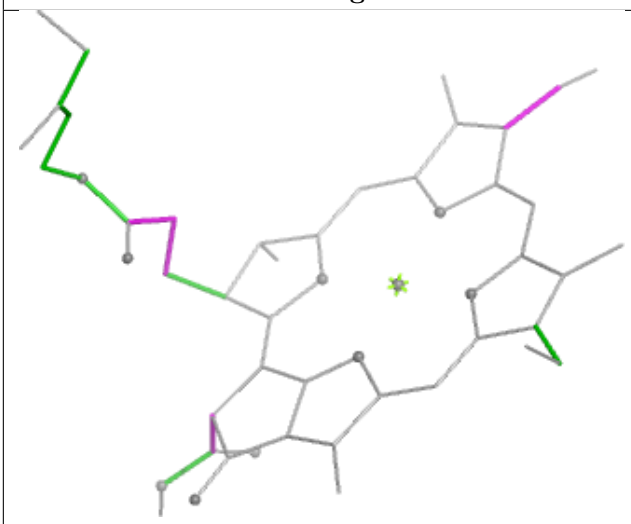


Bond angles

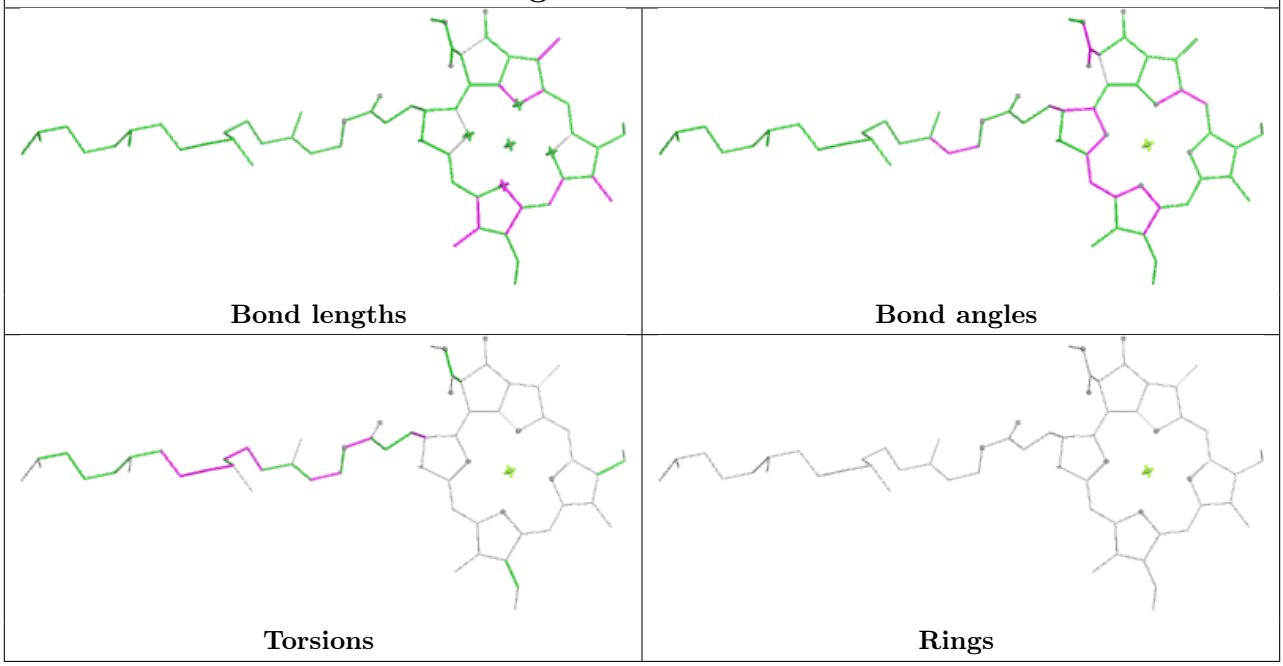


Torsions

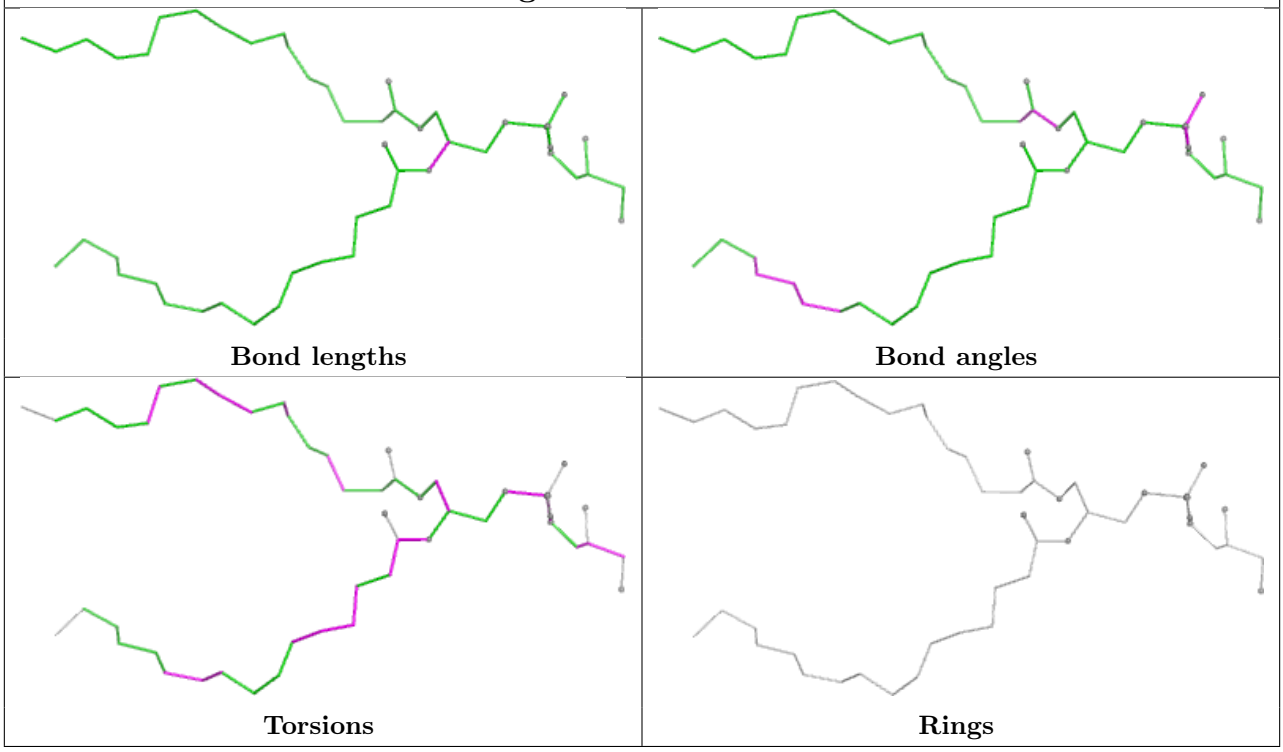


Rings

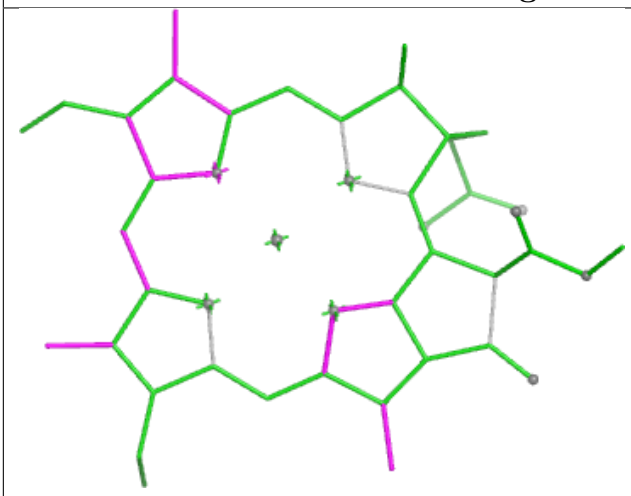
Ligand CLA 2 826



Ligand LHG 1 1654



Ligand CLA 1 1614



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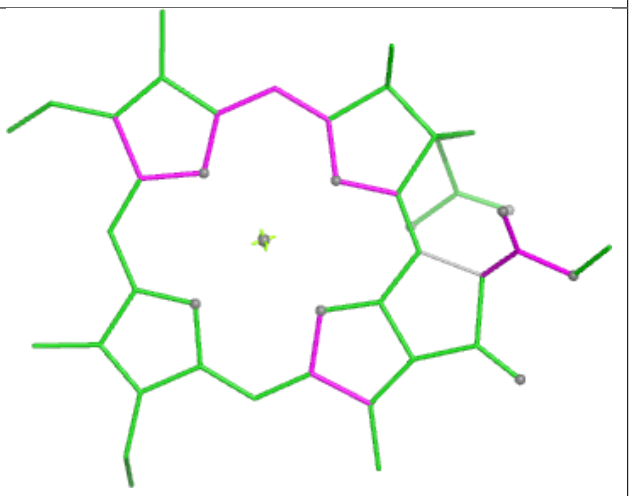
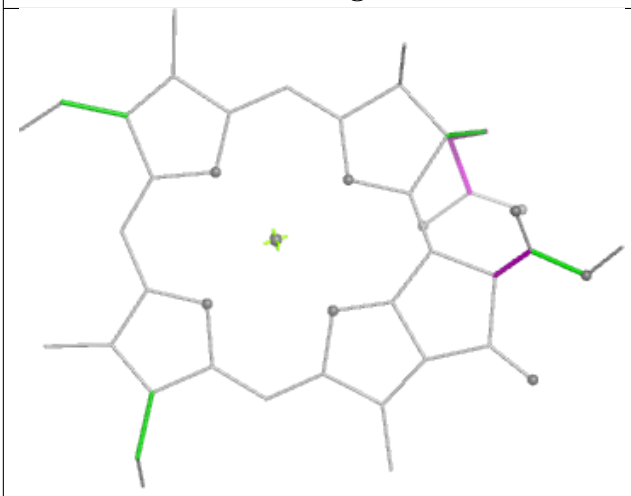


Bond angles



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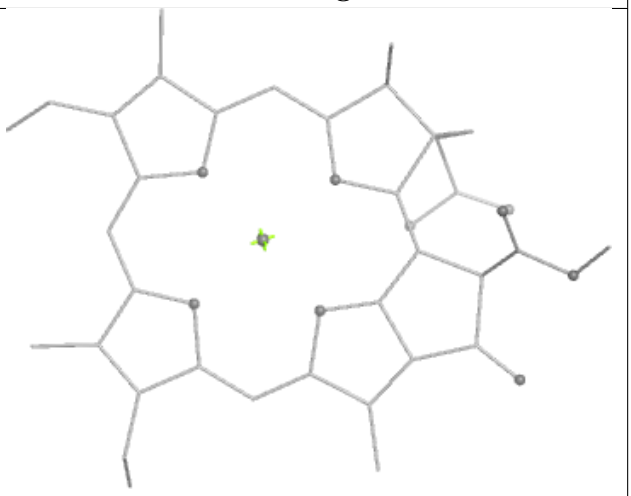
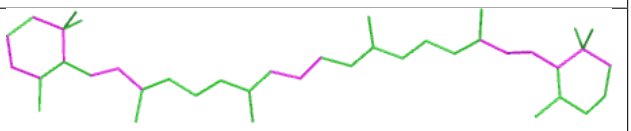


Rings

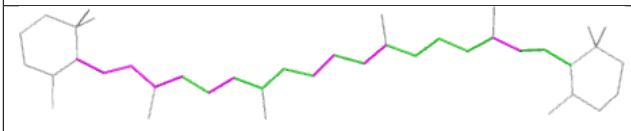
Ligand BCR L 206



Bond lengths



Bond angles



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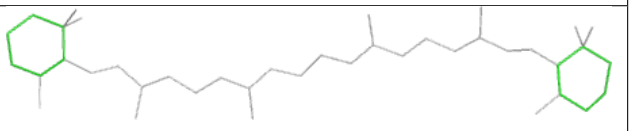
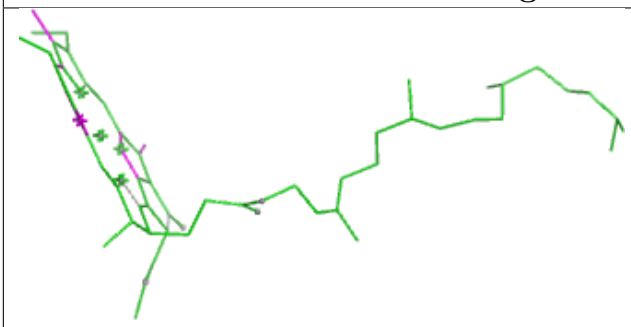


Rings

Ligand CLA 1 1641



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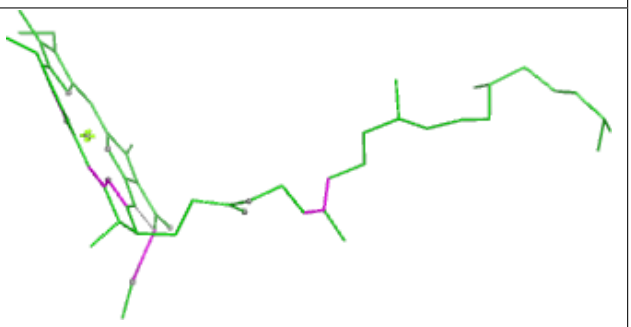
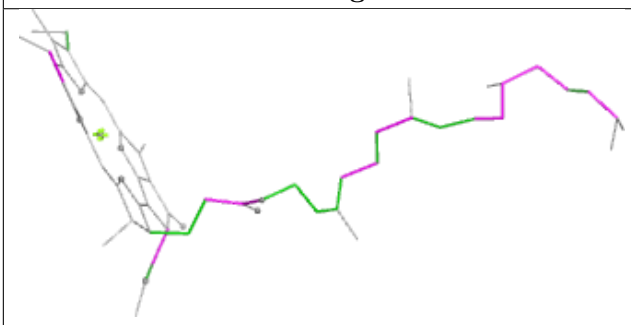
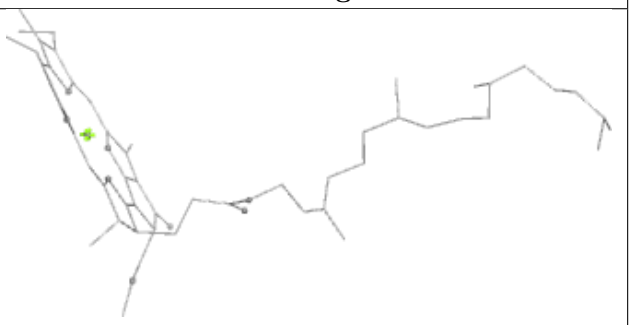


Bond angles



Torsions

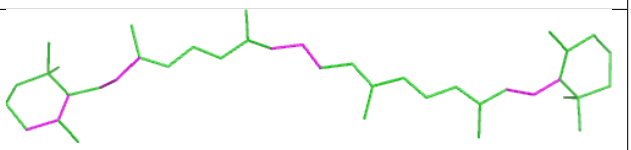


Rings

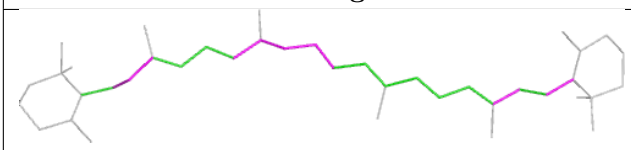
Ligand BCR 2 844



Bond lengths



Bond angles



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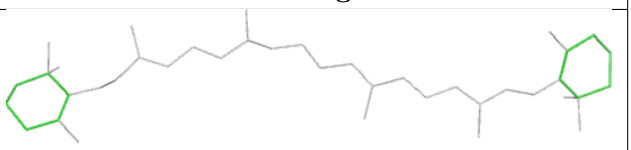
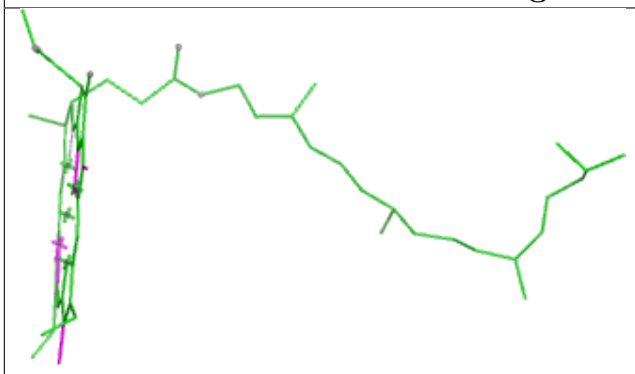
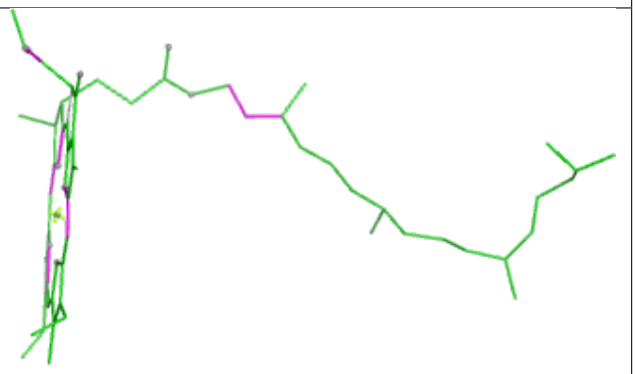


Rings

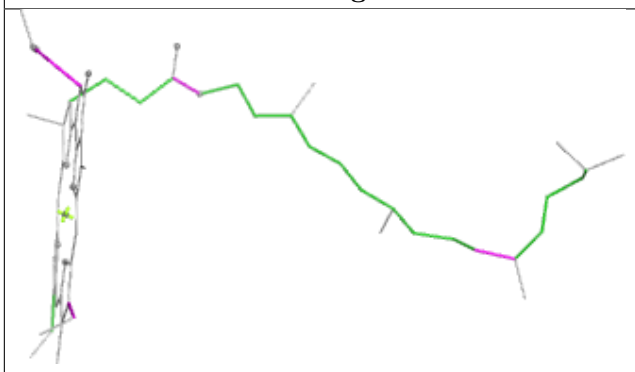
Ligand CLA 2 842



Bond lengths



Bond angles



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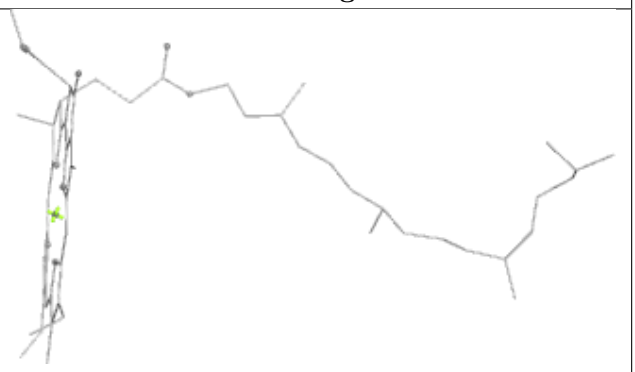
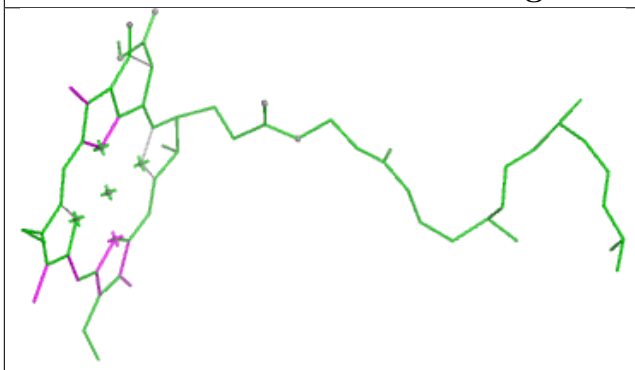
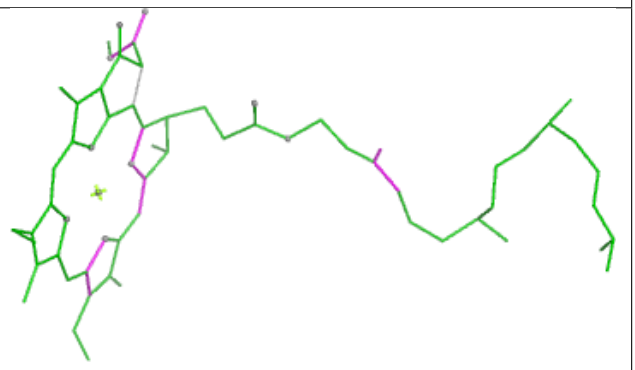


Rings

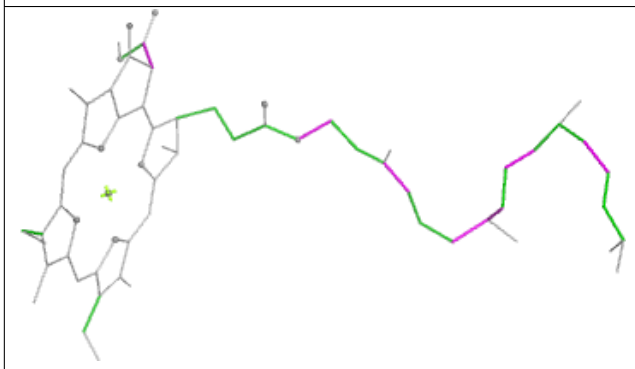
Ligand CLA B 833



Bond lengths



Bond angles



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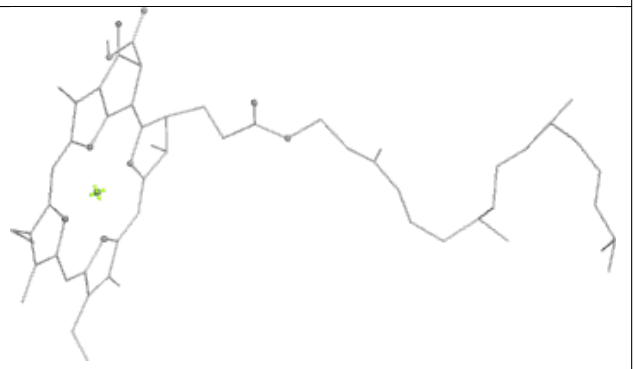
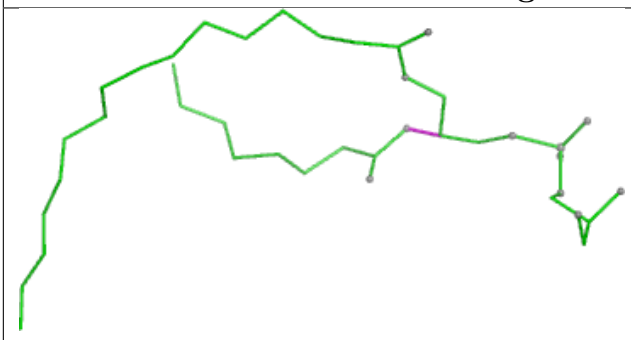


Rings

Ligand LHG 1 1655



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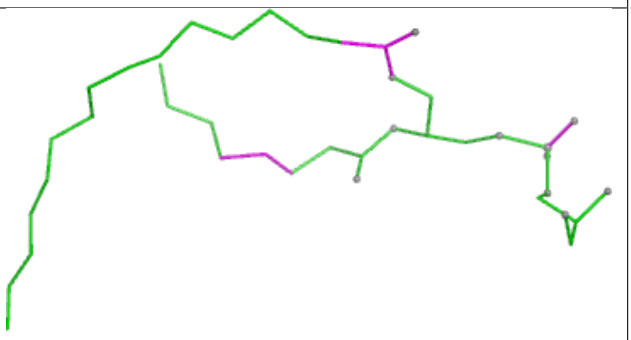
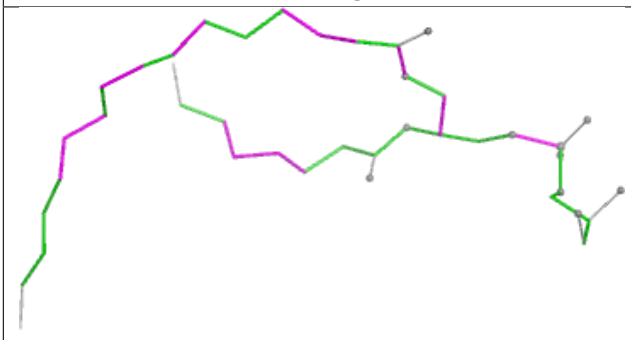


Bond angles

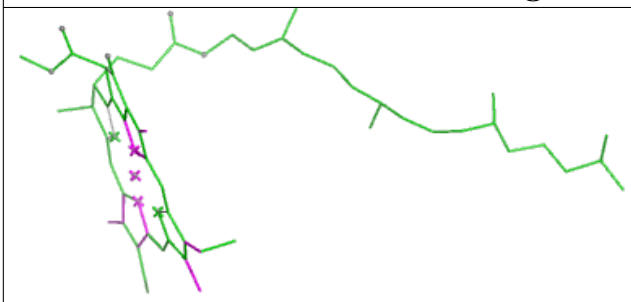


Torsions

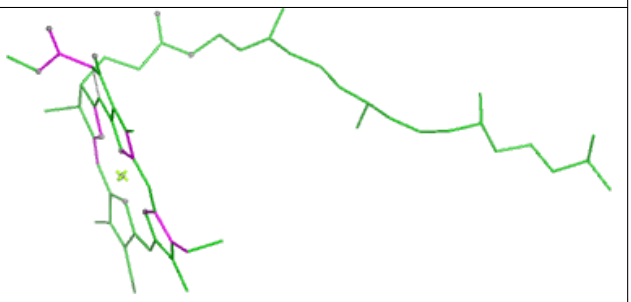


Rings

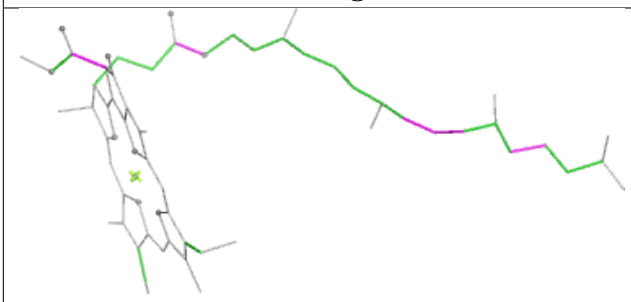
Ligand CLA B 829



Bond lengths



Bond angles

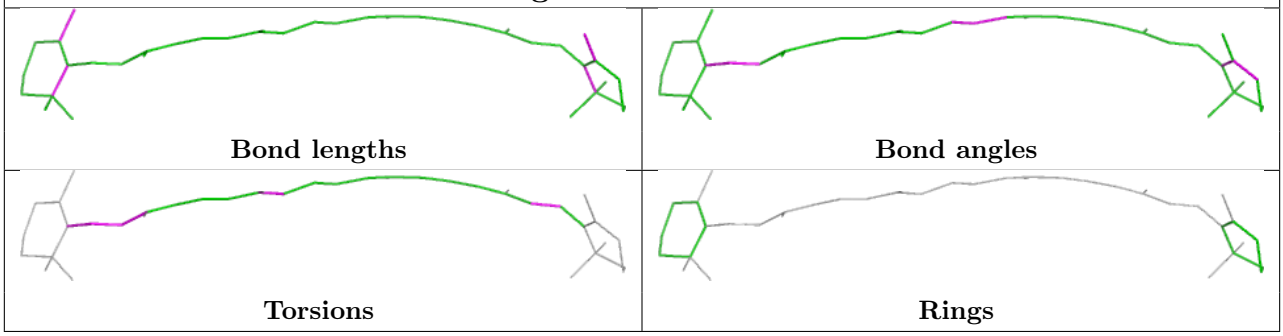


Torsions

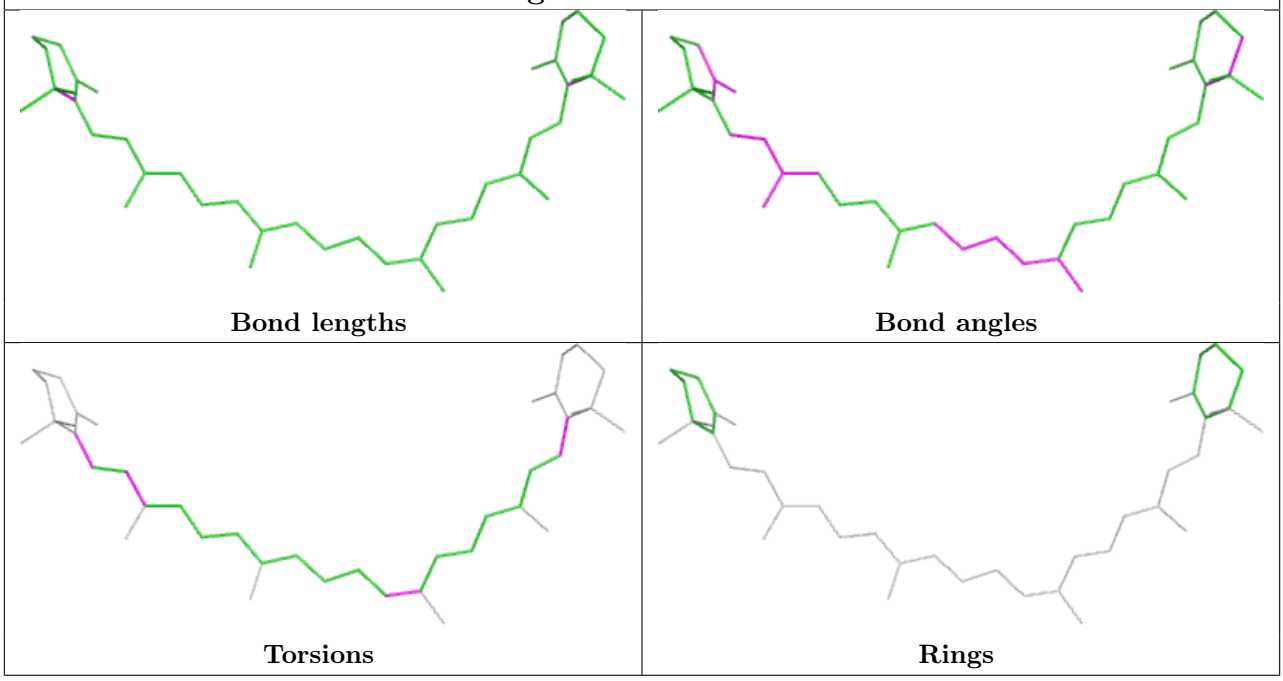


Rings

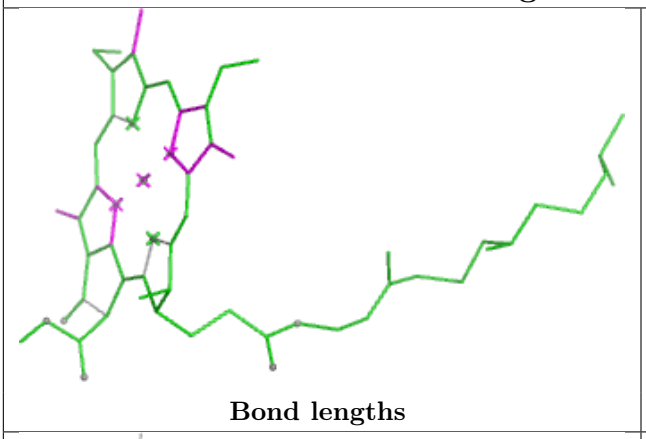
Ligand BCR i 101



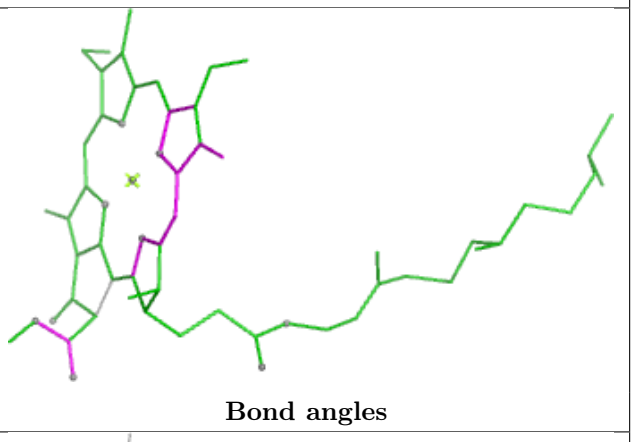
Ligand BCR 6 204



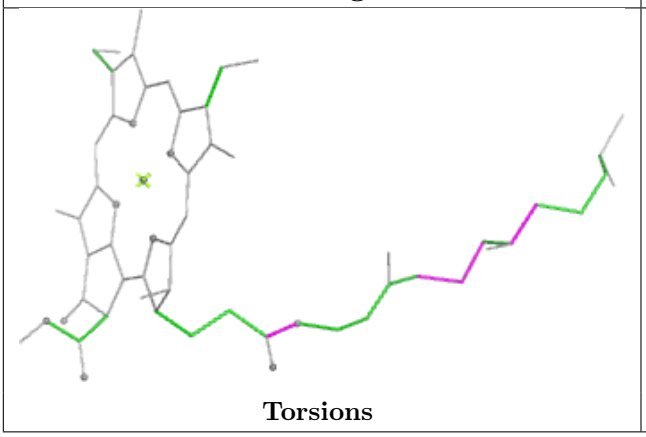
Ligand CLA 1 1633



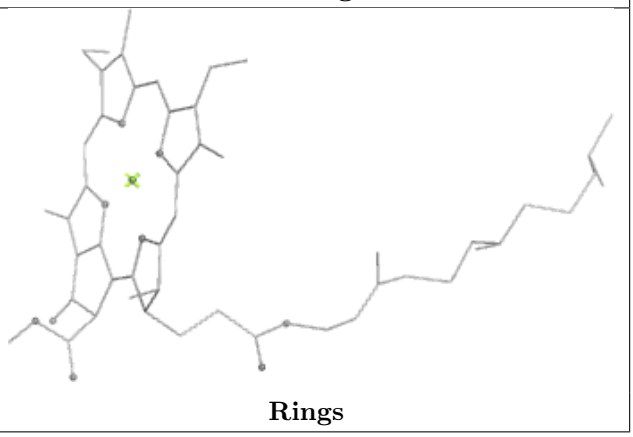
Bond lengths



Bond angles

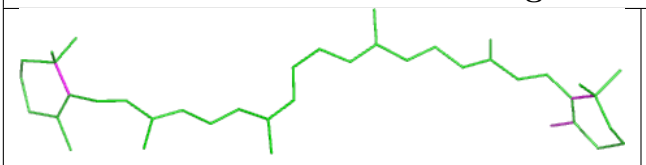


Torsions

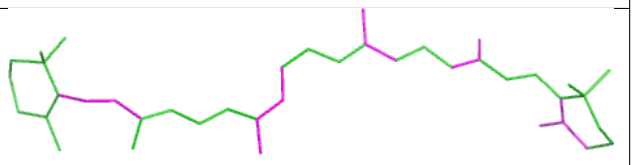


Rings

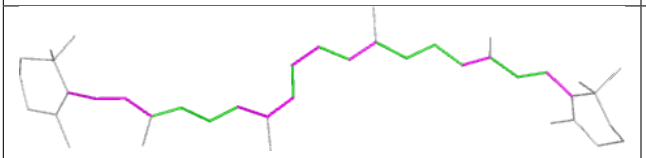
Ligand BCR b 847



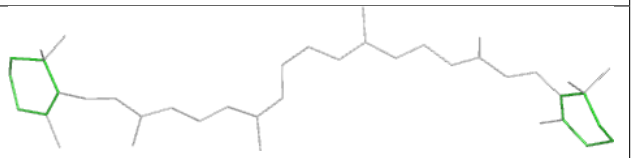
Bond lengths



Bond angles

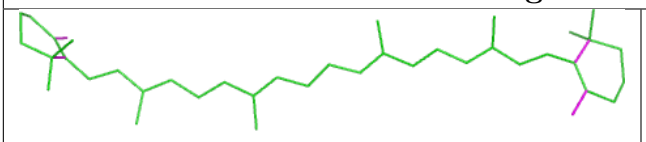


Torsions

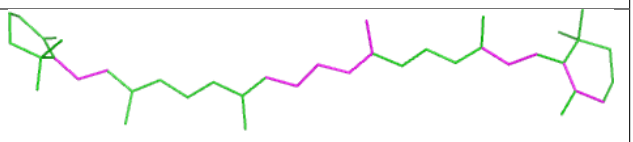


Rings

Ligand BCR b 849



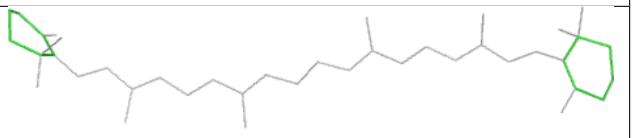
Bond lengths



Bond angles

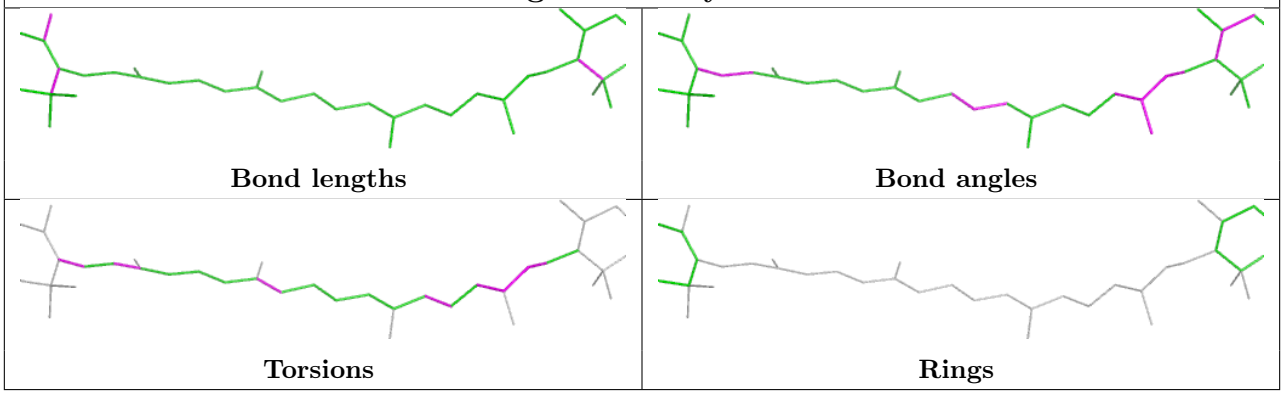


Torsions

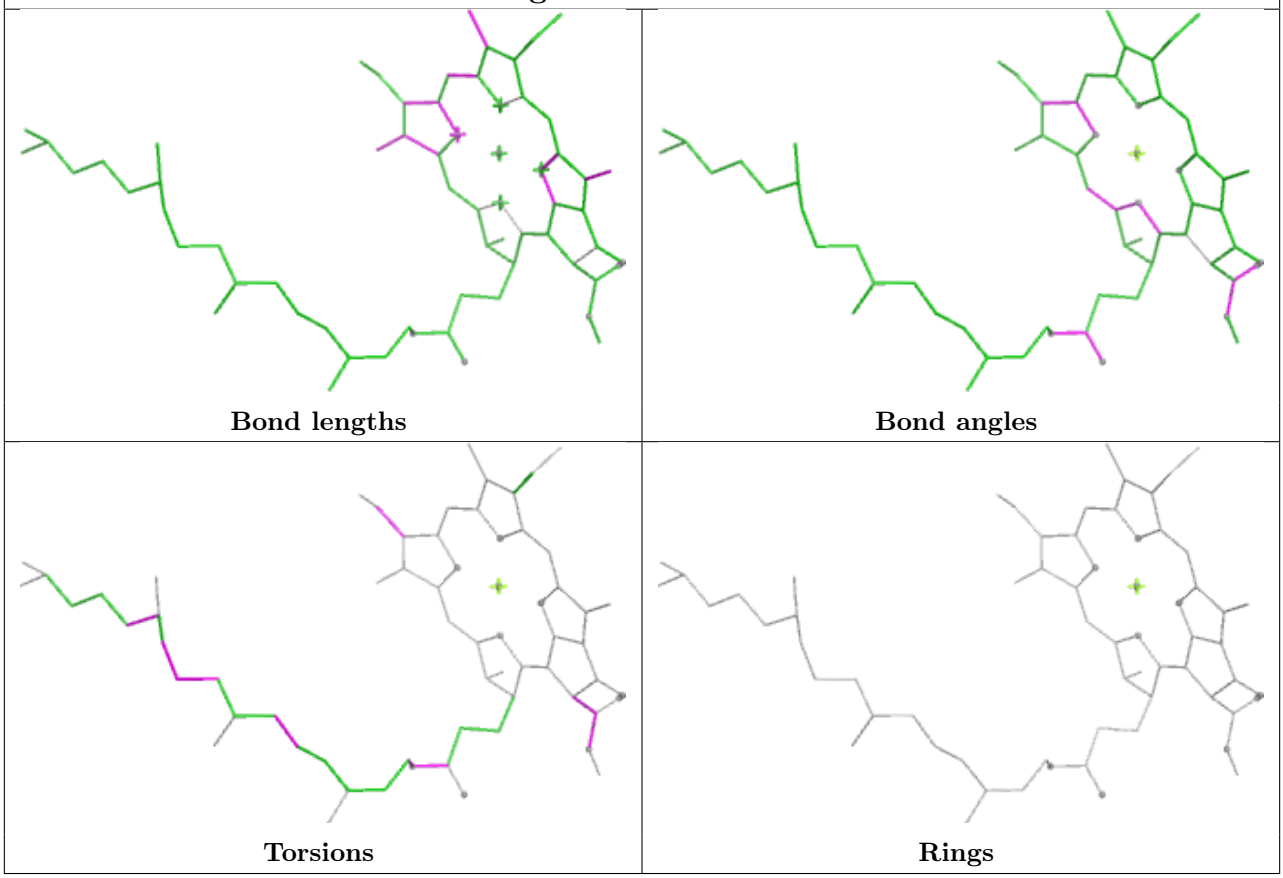


Rings

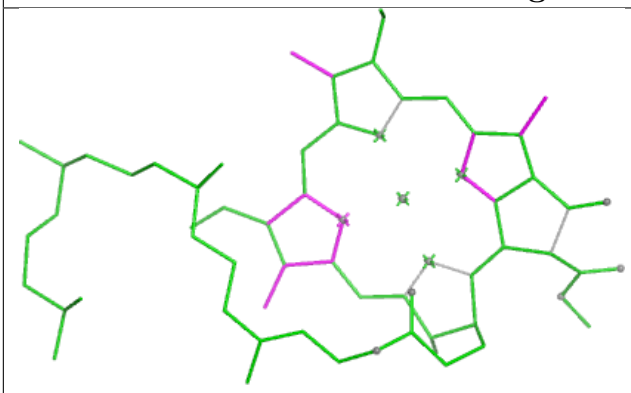
Ligand BCR y 102



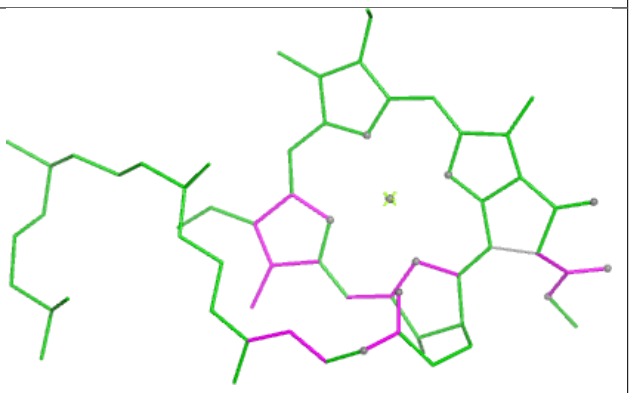
Ligand CLA a 817



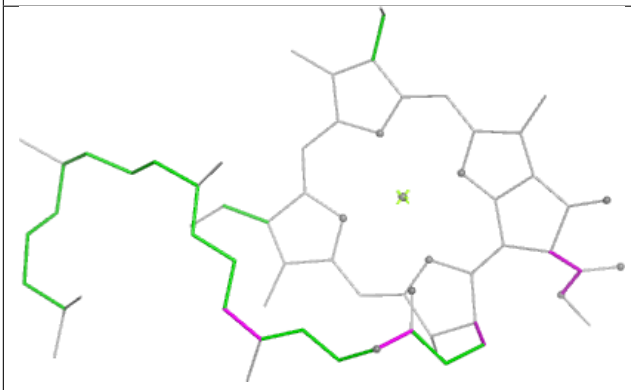
Ligand CLA a 820



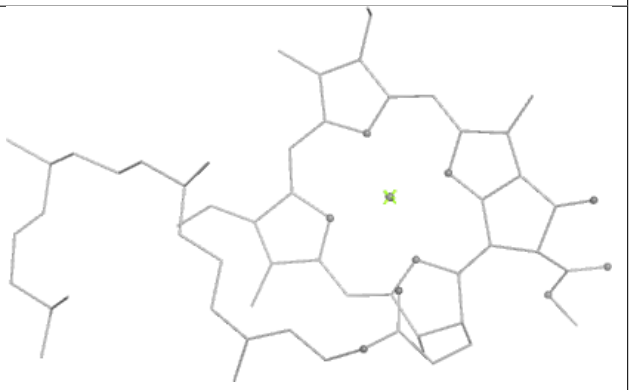
Bond lengths



Bond angles

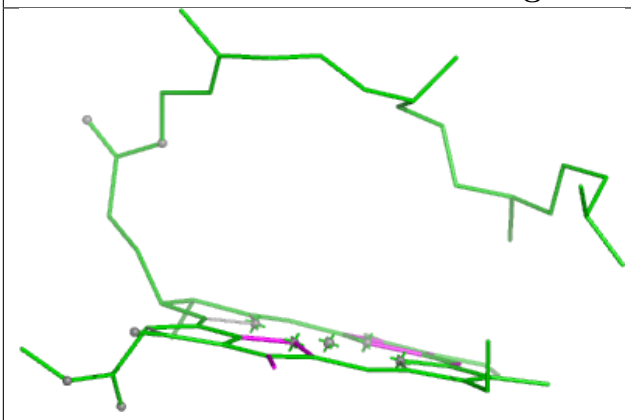


Torsions

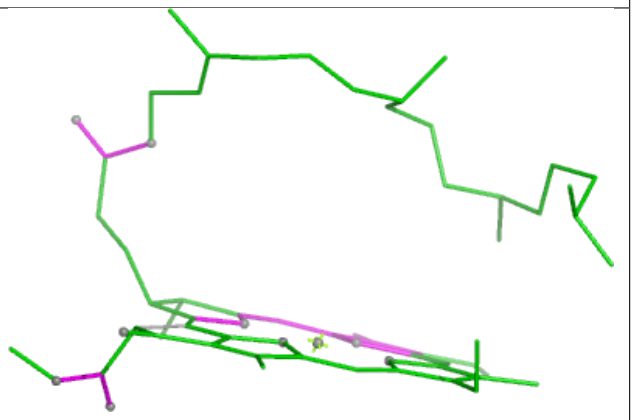


Rings

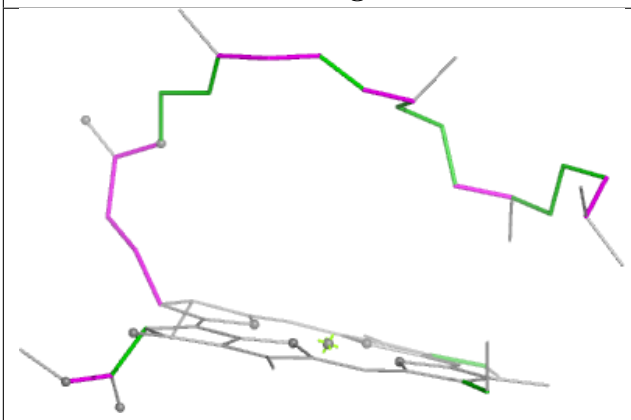
Ligand CLA A 821



Bond lengths



Bond angles

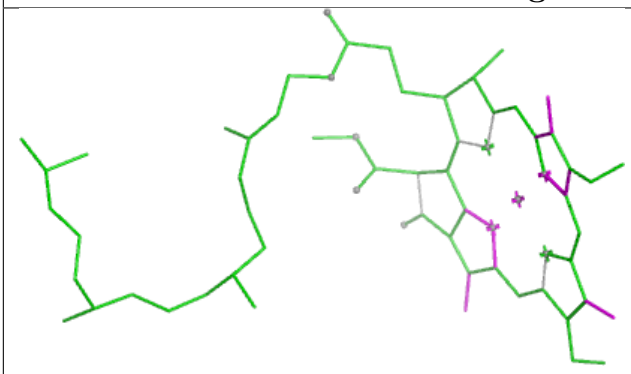


Torsions

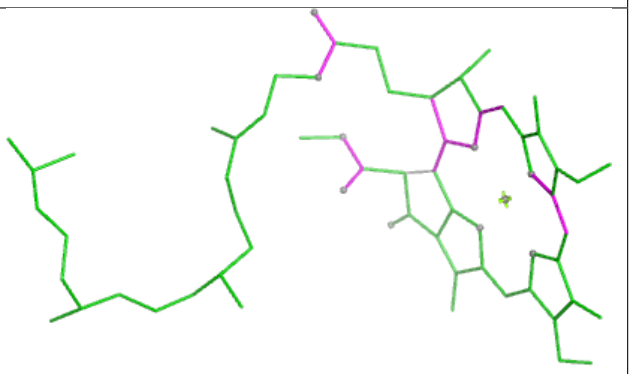


Rings

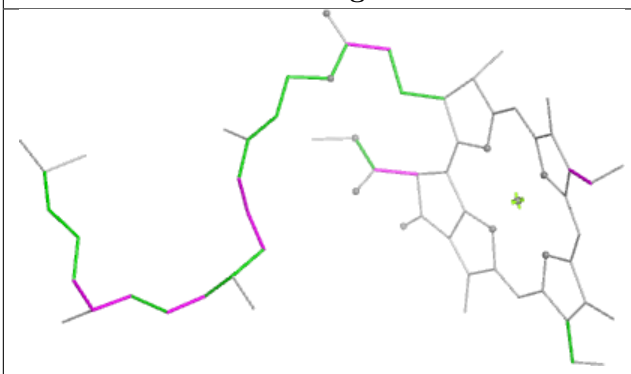
Ligand CL0 A 801



Bond lengths



Bond angles

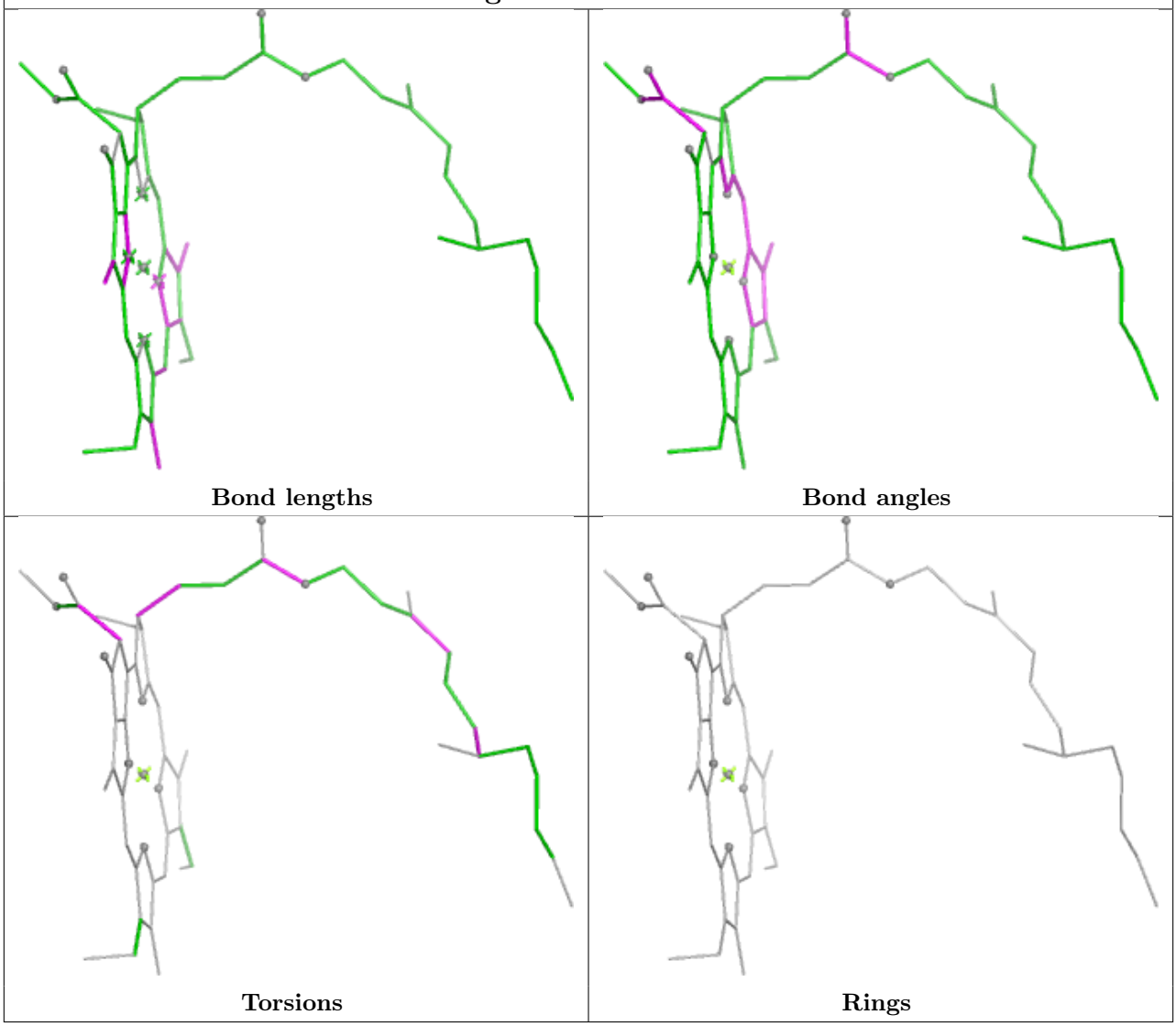


Torsions



Rings

Ligand CLA a 805



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.

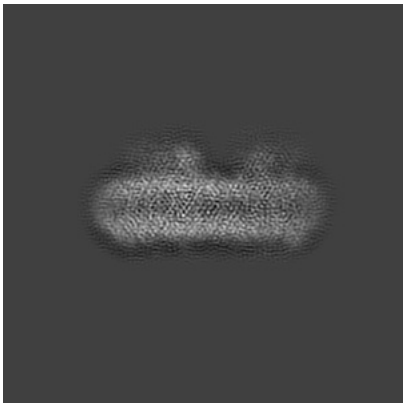
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10559. These allow visual inspection of the internal detail of the map and identification of artifacts.

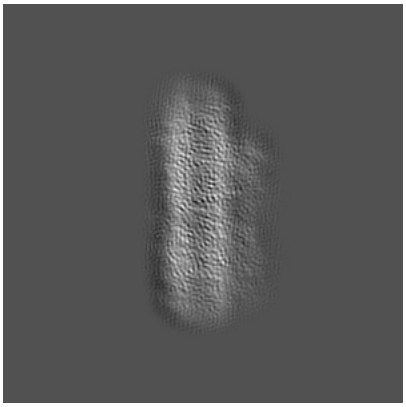
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

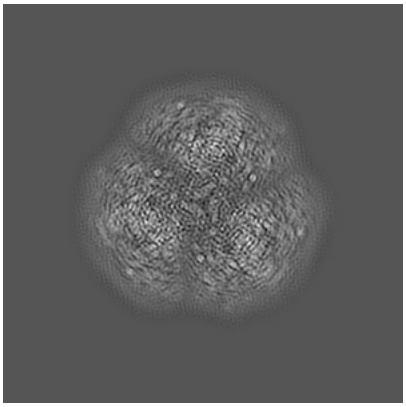
6.1.1 Primary map



X



Y

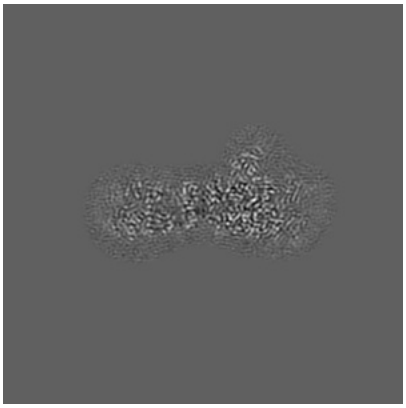


Z

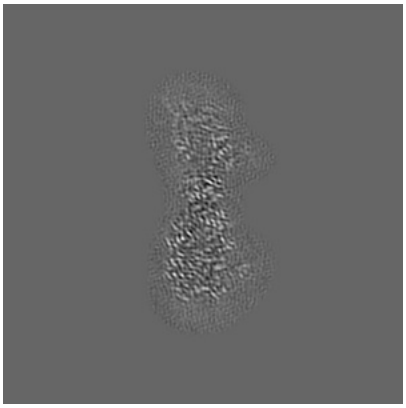
The images above show the map projected in three orthogonal directions.

6.2 Central slices

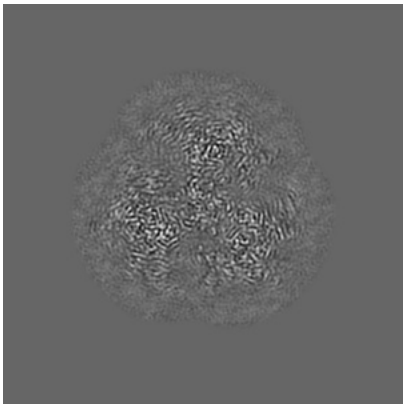
6.2.1 Primary map



X Index: 280



Y Index: 280

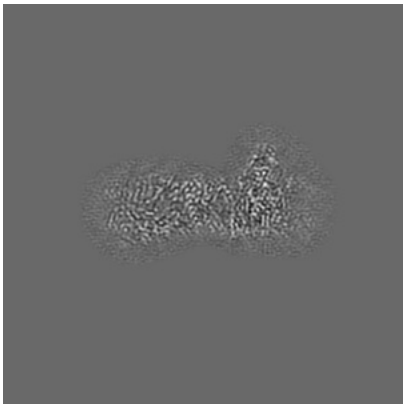


Z Index: 280

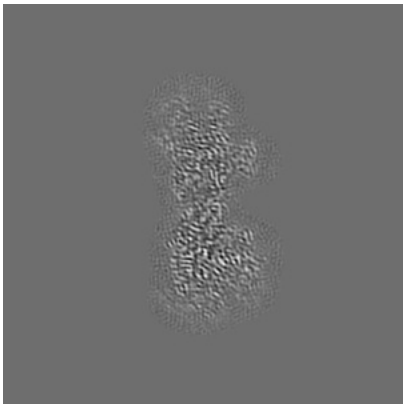
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

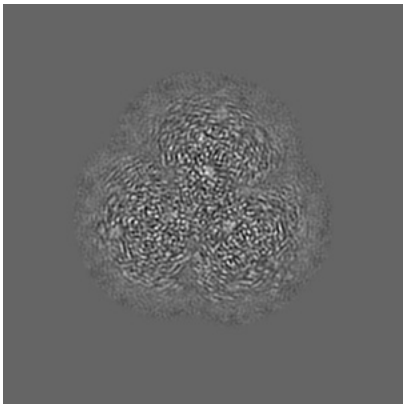
6.3.1 Primary map



X Index: 298



Y Index: 253

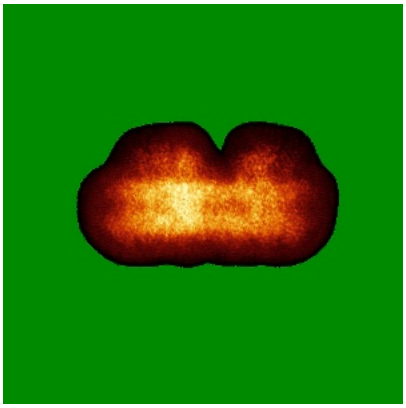


Z Index: 298

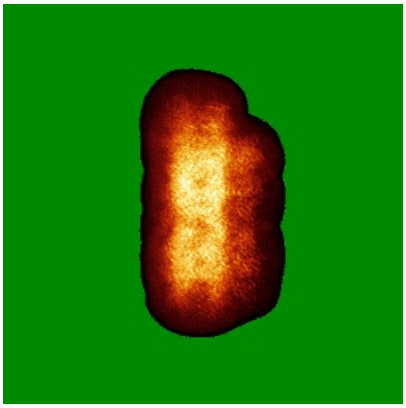
The images above show the largest variance slices of the map in three orthogonal directions.

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

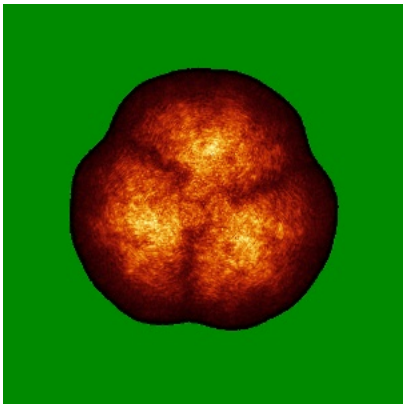
6.4.1 Primary map



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

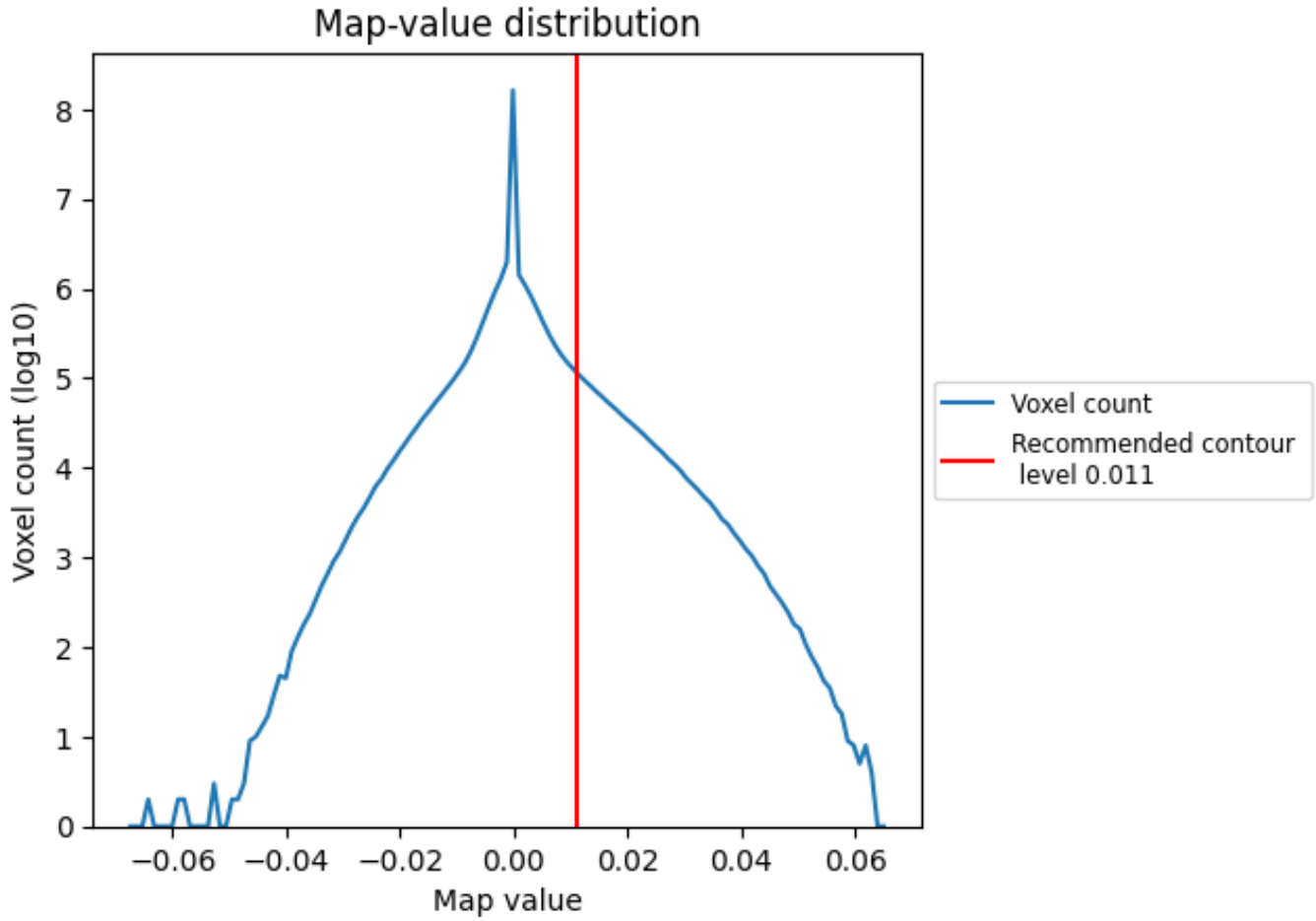
6.6 Mask visualisation (i)

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

7 Map analysis

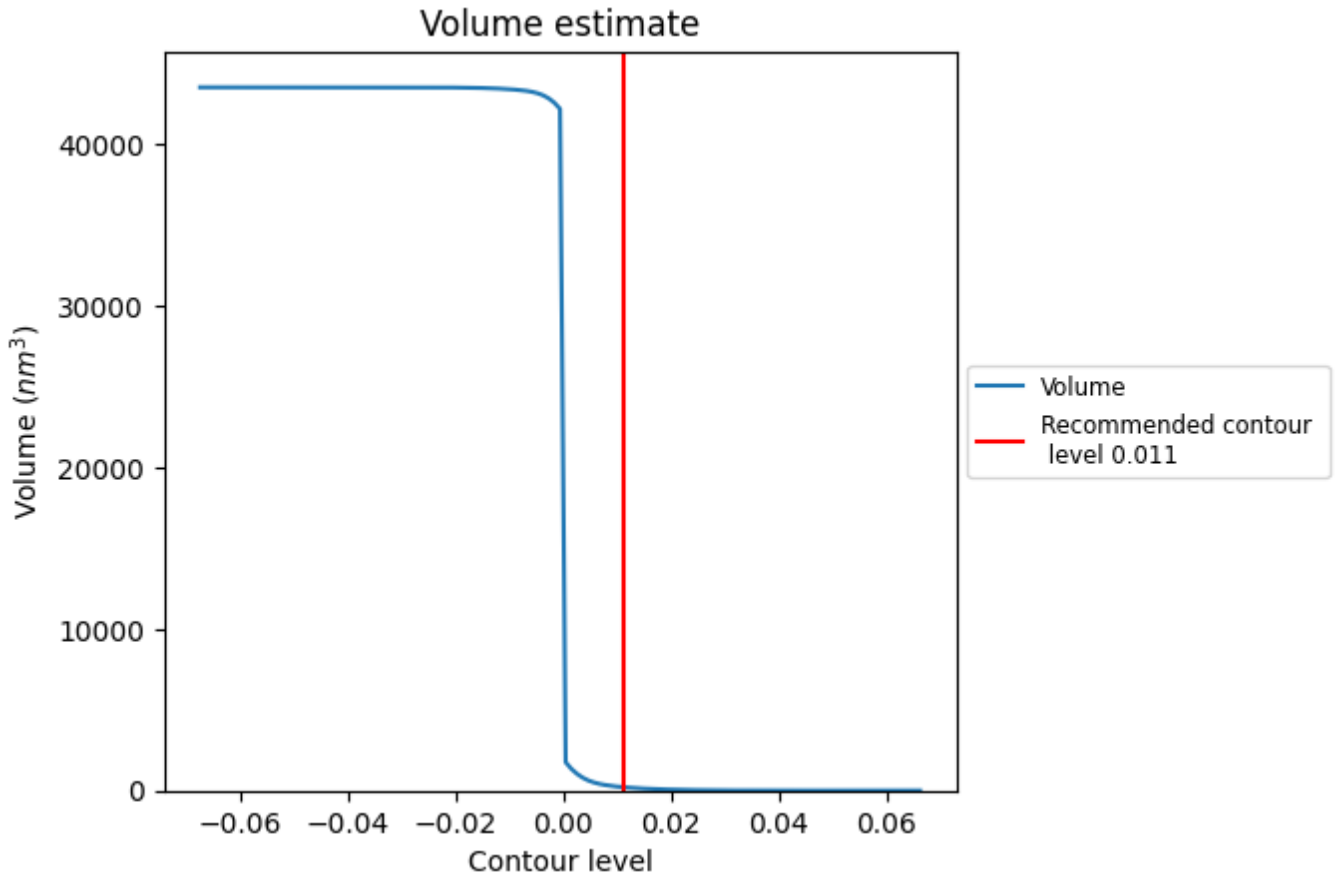
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

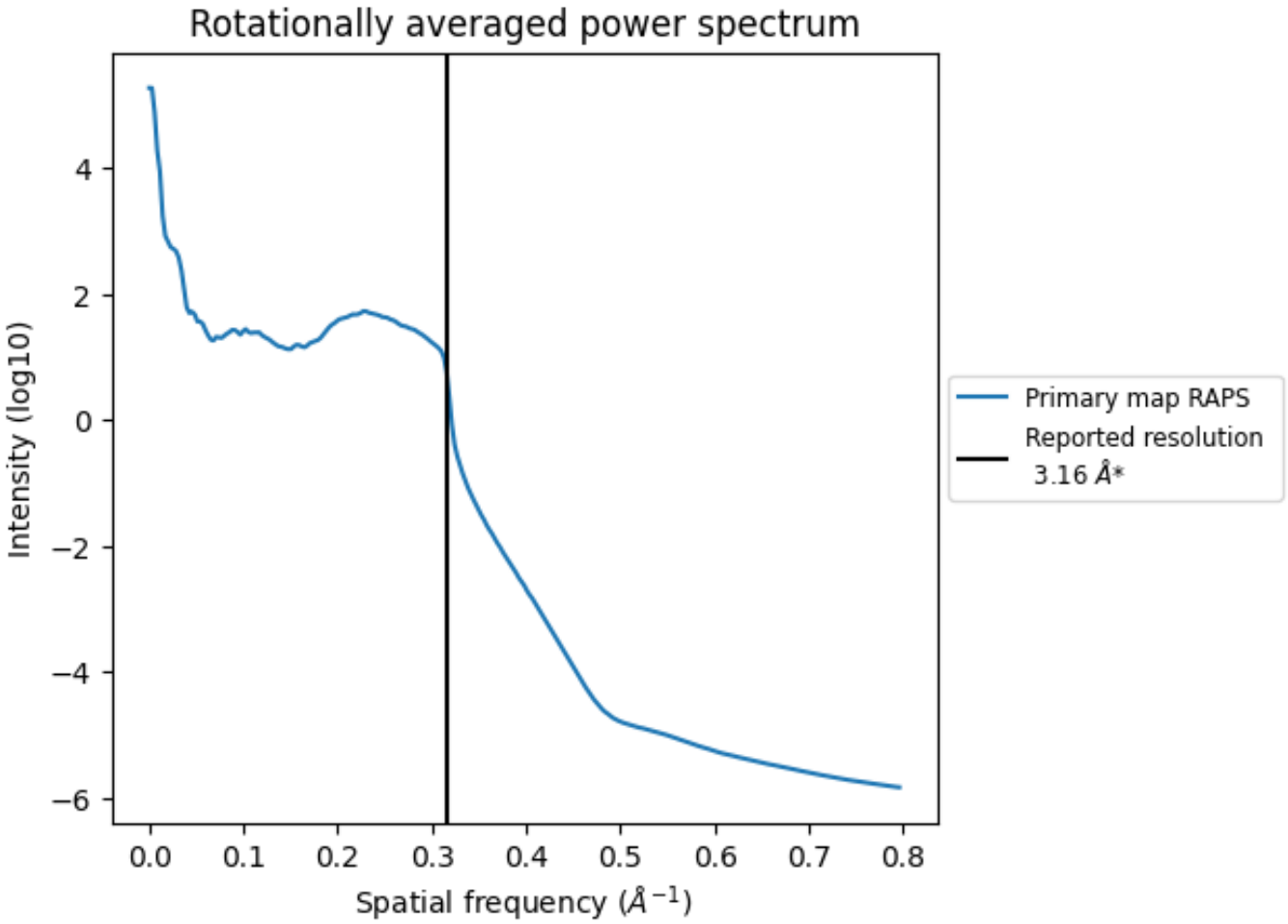
7.2 Volume estimate (i)



The volume at the recommended contour level is 212 nm^3; this corresponds to an approximate mass of 191 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)

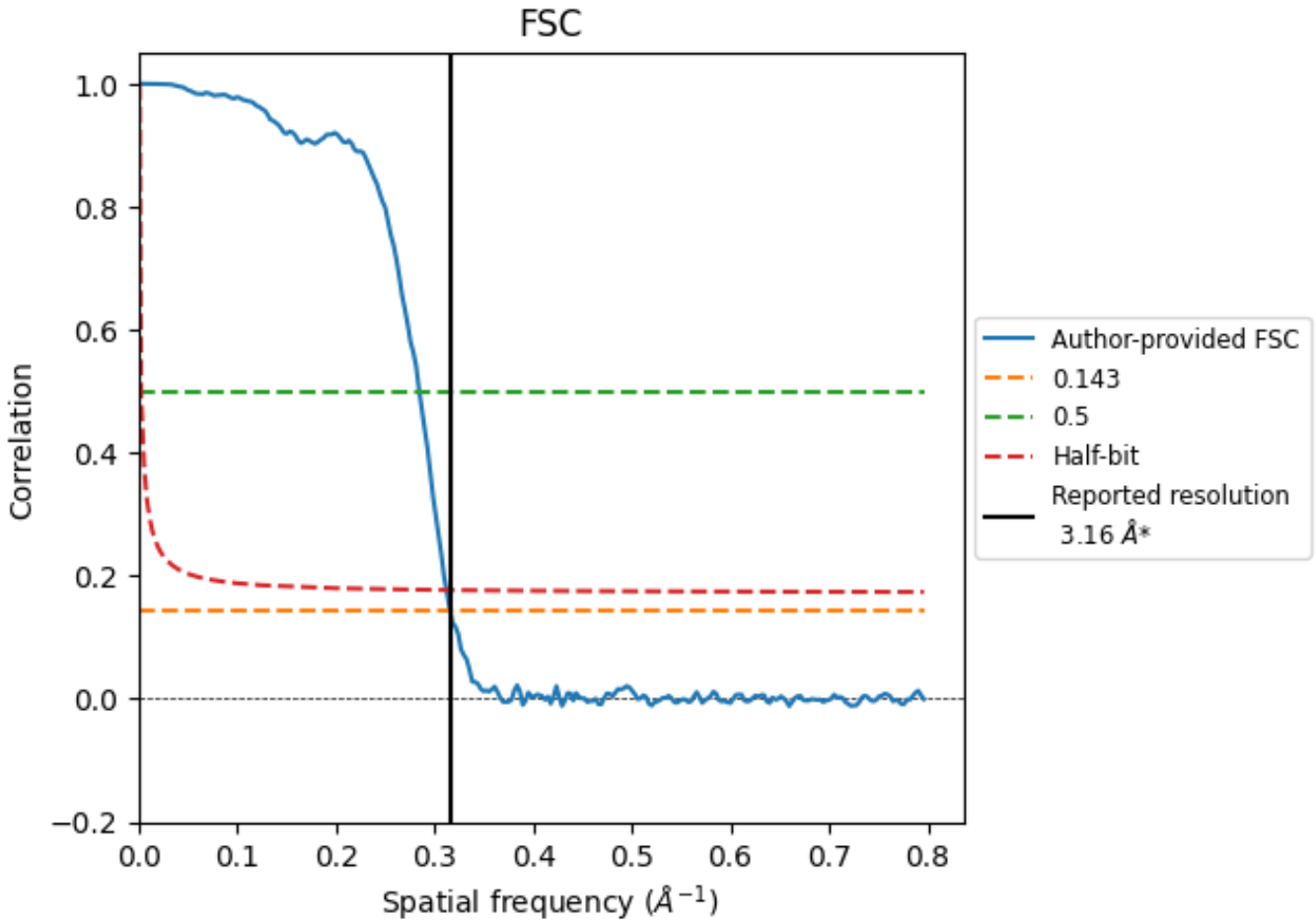


*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

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 0.316 Å^{-1}

8.2 Resolution estimates (i)

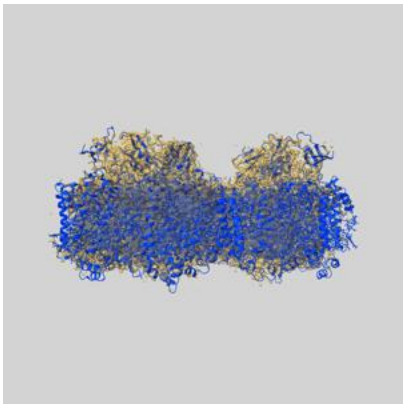
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.17	3.51	3.20
Unmasked-calculated*	-	-	-

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

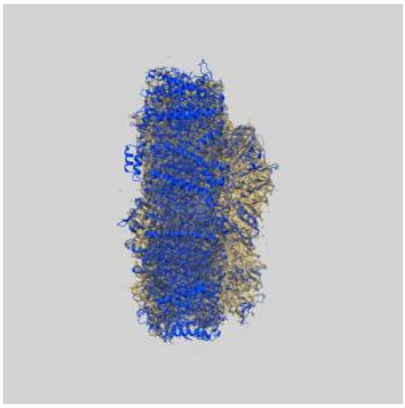
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10559 and PDB model 6TRD. Per-residue inclusion information can be found in section 3 on page 32.

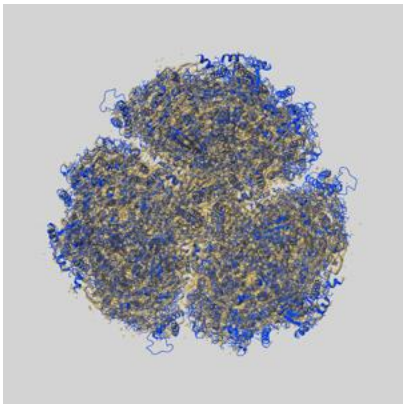
9.1 Map-model overlay



X



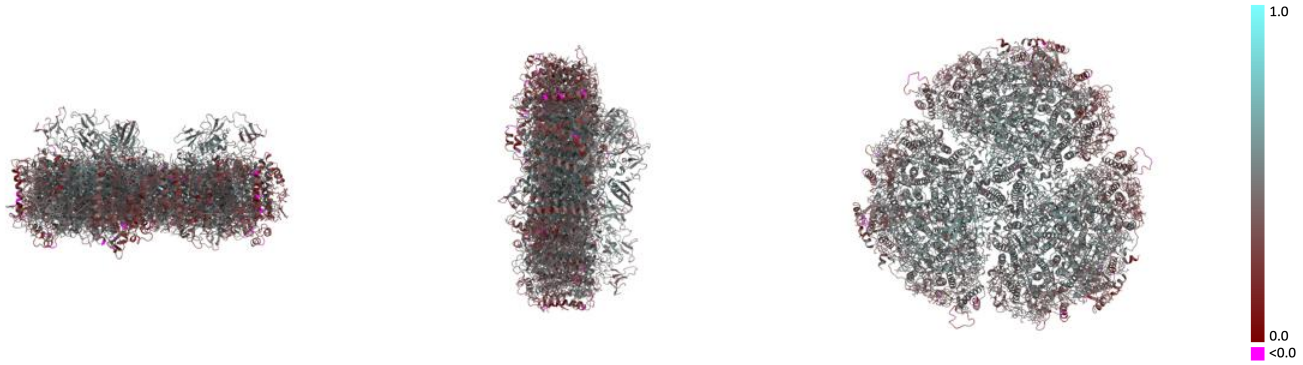
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

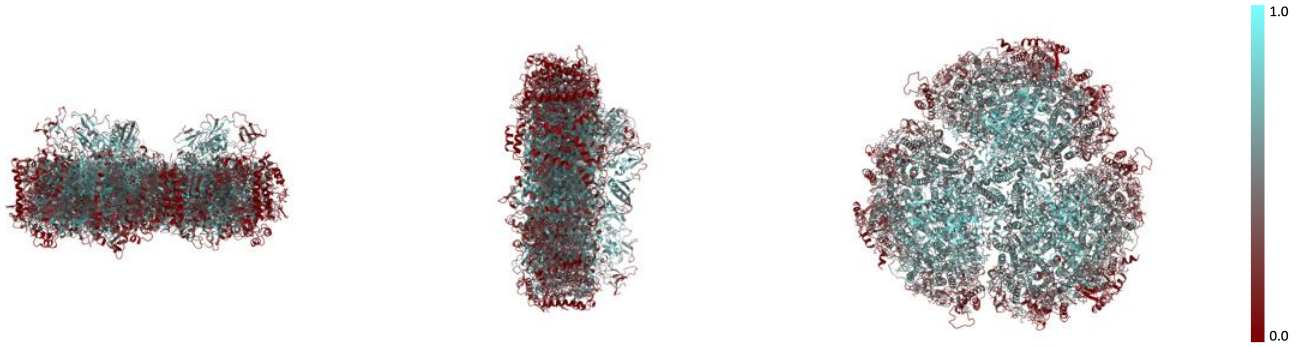
9.2 Q-score mapped to coordinate model



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.

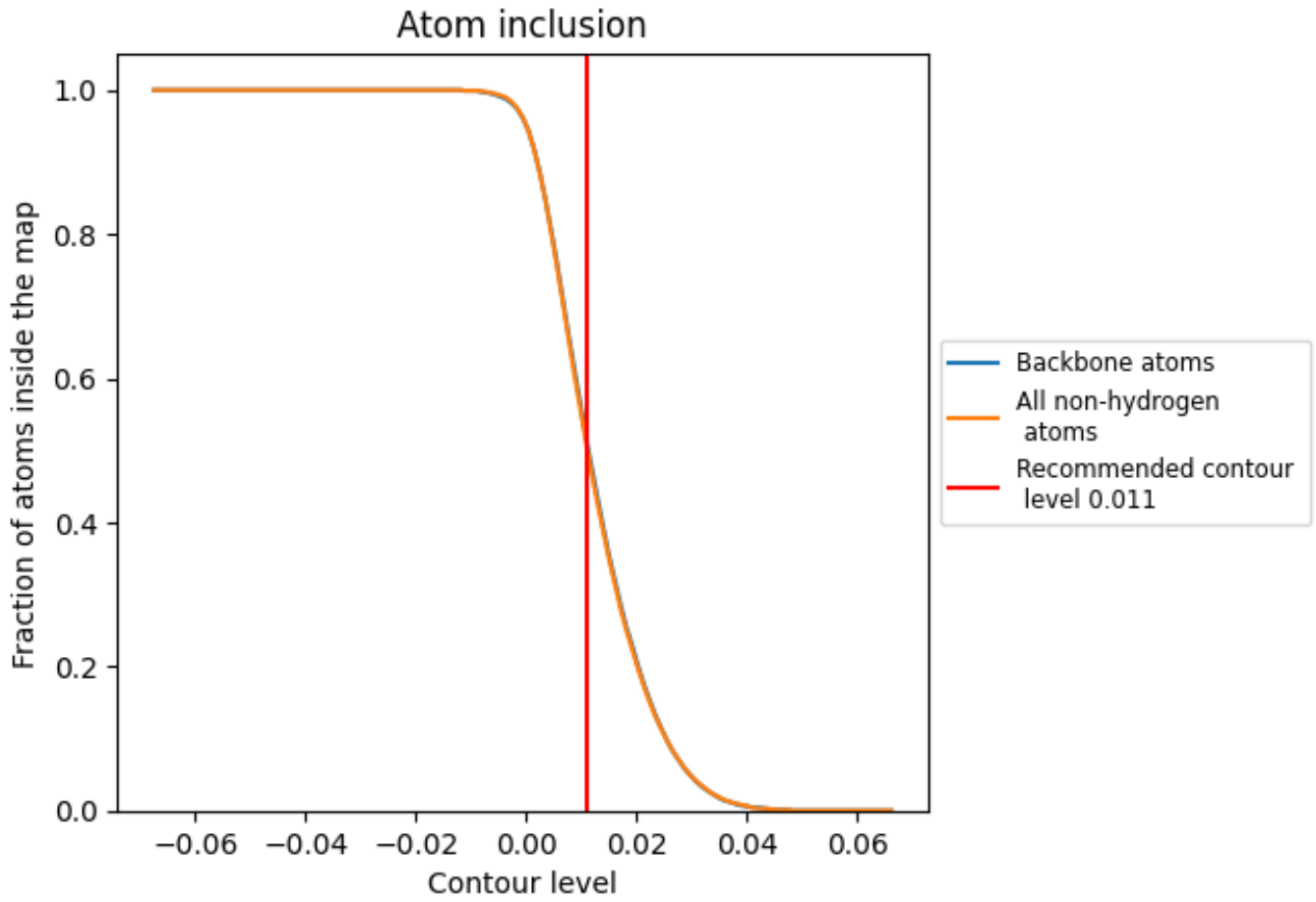
9.3 Atom inclusion mapped to coordinate model



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 50% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5030	0.4500
0	0.6800	0.5210
1	0.5780	0.4730
2	0.5740	0.4770
3	0.6630	0.4830
4	0.5650	0.4700
5	0.3820	0.4120
6	0.2120	0.3470
7	0.6730	0.5060
8	0.1880	0.3310
9	0.1280	0.3720
A	0.5250	0.4540
B	0.5130	0.4490
C	0.6830	0.4970
D	0.5520	0.4870
E	0.3260	0.4300
F	0.1000	0.2840
I	0.6640	0.5280
J	0.1140	0.3370
K	0.1480	0.3590
L	0.6840	0.5250
M	0.4780	0.4820
X	0.0000	0.1740
a	0.5030	0.4360
b	0.5760	0.4770
c	0.6120	0.4930
d	0.5010	0.4630
e	0.3390	0.4240
f	0.1730	0.3380
i	0.7050	0.5110
j	0.1620	0.3670
k	0.0590	0.2860
l	0.6620	0.5180
m	0.5240	0.4520
x	0.0110	0.2250



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Chain	Atom inclusion	Q-score
y	0.5120	0.4820
z	0.0220	0.2350