



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2025 – 12:37 AM JST

PDB ID : 9M4F / pdb_00009m4f
EMDB ID : EMD-63625
Title : Photosystem I from the eukaryotic filamentous algae
Authors : Shao, R.Q.; Pan, X.W.
Deposited on : 2025-03-04
Resolution : 2.82 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

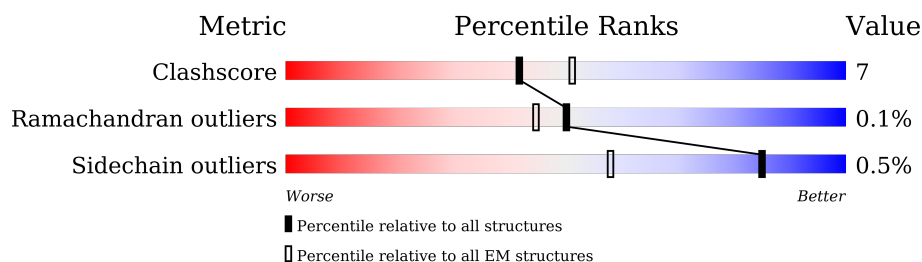
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	220	
2	2	194	
3	3	205	
4	4	231	
5	5	216	
6	6	212	
6	h	212	
7	7	207	
8	8	179	

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Mol	Chain	Length	Quality of chain
9	9	215	
9	k	215	
10	c	210	
11	t	228	
12	A	749	
13	B	734	
14	C	81	
15	D	139	
16	E	61	
17	F	185	
18	I	36	
19	J	42	
20	L	149	
21	M	30	
22	R	87	
23	S	134	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	1	301	X	-	-	-
24	CLA	1	302	X	-	-	-
24	CLA	1	303	X	-	-	-
24	CLA	1	304	X	-	-	-
24	CLA	1	305	X	-	-	-
24	CLA	1	306	X	-	-	-
24	CLA	1	307	X	-	-	-
24	CLA	1	308	X	-	-	-
24	CLA	1	309	X	-	-	-
24	CLA	1	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	2	201	X	-	-	-
24	CLA	2	202	X	-	-	-
24	CLA	2	203	X	-	-	-
24	CLA	2	204	X	-	-	-
24	CLA	2	206	X	-	-	-
24	CLA	2	207	X	-	-	-
24	CLA	2	208	X	-	-	-
24	CLA	2	209	X	-	-	-
24	CLA	3	302	X	-	-	-
24	CLA	3	303	X	-	-	-
24	CLA	3	304	X	-	-	-
24	CLA	3	305	X	-	-	-
24	CLA	3	306	X	-	-	-
24	CLA	3	307	X	-	-	-
24	CLA	3	308	X	-	-	-
24	CLA	3	309	X	-	-	-
24	CLA	4	601	X	-	-	-
24	CLA	4	602	X	-	-	-
24	CLA	4	603	X	-	-	-
24	CLA	4	604	X	-	-	-
24	CLA	4	605	X	-	-	-
24	CLA	4	606	X	-	-	-
24	CLA	4	607	X	-	-	-
24	CLA	4	608	X	-	-	-
24	CLA	4	609	X	-	-	-
24	CLA	4	610	X	-	-	-
24	CLA	4	611	X	-	-	-
24	CLA	4	612	X	-	-	-
24	CLA	4	613	X	-	-	-
24	CLA	5	601	X	-	-	-
24	CLA	5	602	X	-	-	-
24	CLA	5	603	X	-	-	-
24	CLA	5	604	X	-	-	-
24	CLA	5	605	X	-	-	-
24	CLA	5	606	X	-	-	-
24	CLA	5	607	X	-	-	-
24	CLA	6	601	X	-	-	-
24	CLA	6	602	X	-	-	-
24	CLA	6	603	X	-	-	-
24	CLA	6	604	X	-	-	-
24	CLA	6	606	X	-	-	-
24	CLA	6	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	6	608	X	-	-	-
24	CLA	6	609	X	-	-	-
24	CLA	6	610	X	-	-	-
24	CLA	6	611	X	-	-	-
24	CLA	6	612	X	-	-	-
24	CLA	7	601	X	-	-	-
24	CLA	7	602	X	-	-	-
24	CLA	7	603	X	-	-	-
24	CLA	7	604	X	-	-	-
24	CLA	7	605	X	-	-	-
24	CLA	7	606	X	-	-	-
24	CLA	7	607	X	-	-	-
24	CLA	7	608	X	-	-	-
24	CLA	7	609	X	-	-	-
24	CLA	7	610	X	-	-	-
24	CLA	7	611	X	-	-	-
24	CLA	7	612	X	-	-	-
24	CLA	8	201	X	-	-	-
24	CLA	8	202	X	-	-	-
24	CLA	8	203	X	-	-	-
24	CLA	8	204	X	-	-	-
24	CLA	8	205	X	-	-	-
24	CLA	8	206	X	-	-	-
24	CLA	8	207	X	-	-	-
24	CLA	8	208	X	-	-	-
24	CLA	8	209	X	-	-	-
24	CLA	9	301	X	-	-	-
24	CLA	9	302	X	-	-	-
24	CLA	9	303	X	-	-	-
24	CLA	9	304	X	-	-	-
24	CLA	9	306	X	-	-	-
24	CLA	9	307	X	-	-	-
24	CLA	9	308	X	-	-	-
24	CLA	9	309	X	-	-	-
24	CLA	9	310	X	-	-	-
24	CLA	9	311	X	-	-	-
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	806	X	-	-	-
24	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	814	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	818	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	847	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	A	857	X	-	-	-
24	CLA	A	860	X	-	-	-
24	CLA	B	801	X	-	-	-
24	CLA	B	802	X	-	-	-
24	CLA	B	803	X	-	-	-
24	CLA	B	804	X	-	-	-
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	817	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	819	X	-	-	-
24	CLA	B	820	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-
24	CLA	B	827	X	-	-	-
24	CLA	B	828	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	846	X	-	-	-
24	CLA	B	847	X	-	-	-
24	CLA	B	848	X	-	-	-
24	CLA	F	201	X	-	-	-
24	CLA	F	202	X	-	-	-
24	CLA	F	203	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	205	X	-	-	-
24	CLA	R	103	X	-	-	-
24	CLA	R	104	X	-	-	-
24	CLA	c	601	X	-	-	-
24	CLA	c	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	603	X	-	-	-
24	CLA	c	604	X	-	-	-
24	CLA	c	605	X	-	-	-
24	CLA	c	606	X	-	-	-
24	CLA	c	607	X	-	-	-
24	CLA	c	608	X	-	-	-
24	CLA	c	609	X	-	-	-
24	CLA	c	610	X	-	-	-
24	CLA	c	611	X	-	-	-
24	CLA	h	601	X	-	-	-
24	CLA	h	602	X	-	-	-
24	CLA	h	603	X	-	-	-
24	CLA	h	604	X	-	-	-
24	CLA	h	605	X	-	-	-
24	CLA	h	606	X	-	-	-
24	CLA	h	607	X	-	-	-
24	CLA	h	608	X	-	-	-
24	CLA	h	609	X	-	-	-
24	CLA	h	610	X	-	-	-
24	CLA	h	612	X	-	-	-
24	CLA	k	301	X	-	-	-
24	CLA	k	302	X	-	-	-
24	CLA	k	304	X	-	-	-
24	CLA	k	305	X	-	-	-
24	CLA	k	306	X	-	-	-
24	CLA	k	307	X	-	-	-
24	CLA	k	308	X	-	-	-
24	CLA	k	309	X	-	-	-
24	CLA	k	310	X	-	-	-
24	CLA	k	311	X	-	-	-
24	CLA	t	301	X	-	-	-
24	CLA	t	302	X	-	-	-
24	CLA	t	303	X	-	-	-
24	CLA	t	304	X	-	-	-
24	CLA	t	305	X	-	-	-
24	CLA	t	306	X	-	-	-
24	CLA	t	307	X	-	-	-
24	CLA	t	308	X	-	-	-
24	CLA	t	309	X	-	-	-
24	CLA	t	310	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 50344 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 Light-harvesting protein XLH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	176	Total	C	N	O	S	0	0
			1328	865	221	237	5		

- Molecule 2 is a protein called light-harvesting protein XLH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	137	Total	C	N	O	S	0	0
			1080	695	187	191	7		

- Molecule 3 is a protein called light-harvesting protein XLH3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	158	Total	C	N	O	S	0	0
			1206	775	204	221	6		

- Molecule 4 is a protein called light-harvesting protein XLH4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	188	Total	C	N	O	S	0	0
			1396	894	240	251	11		

- Molecule 5 is a protein called light-harvesting protein XLH5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	167	Total	C	N	O	S	0	0
			1249	798	210	234	7		

- Molecule 6 is a protein called light-harvesting protein XLH6/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	163	Total	C	N	O	S	0	0
			1228	790	206	226	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	165	Total	C	N	O	S	0	0
			1244	801	209	228	6		

- Molecule 7 is a protein called light-harvesting protein XLH7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	166	Total	C	N	O	S	0	0
			1268	816	210	230	12		

- Molecule 8 is a protein called light-harvesting protein XLH8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	161	Total	C	N	O	S	0	0
			1240	794	208	229	9		

- Molecule 9 is a protein called light-harvesting protein XLH9/13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	149	Total	C	N	O	S	0	0
			1171	761	195	206	9		
9	k	154	Total	C	N	O	S	0	0
			1201	777	200	215	9		

- Molecule 10 is a protein called light-harvesting protein XLH11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	165	Total	C	N	O	S	0	0
			1231	787	209	225	10		

- Molecule 11 is a protein called light-harvesting protein XLH12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	t	159	Total	C	N	O	S	0	0
			1253	799	212	235	7		

- Molecule 12 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	741	Total	C	N	O	S	0	0
			5835	3825	992	996	22		

- Molecule 13 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	733	Total	C	N	O	S	0	0
			5822	3830	976	997	19		

- Molecule 14 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	80	Total	C	N	O	S	0	0
			592	363	103	115	11		

- Molecule 15 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	132	Total	C	N	O	S	0	0
			1030	668	171	188	3		

- Molecule 16 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	60	Total	C	N	O	S	0	0
			484	307	82	94	1		

- Molecule 17 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	161	Total	C	N	O	S	0	0
			1267	818	215	230	4		

- Molecule 18 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	33	Total	C	N	O	S	0	0
			252	174	34	43	1		

- Molecule 19 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	40	Total	C	N	O	S	0	0
			320	217	47	55	1		

- Molecule 20 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	137	Total	C	N	O	S	0	0
			1027	674	165	186	2		

- Molecule 21 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	30	Total	C	N	O	S	0	0
			227	153	35	38	1		

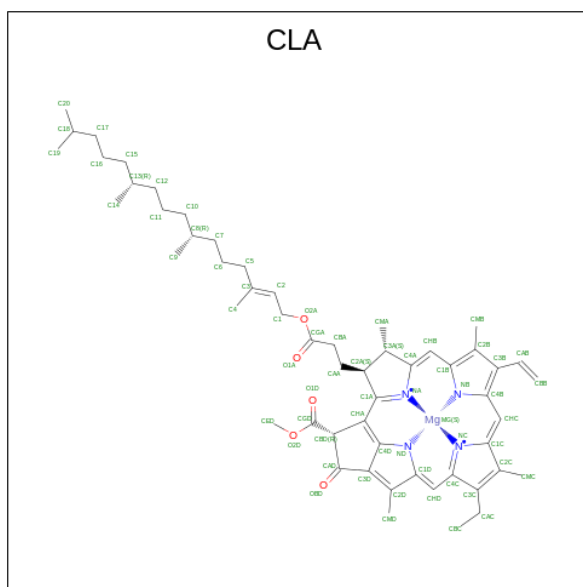
- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	81	Total	C	N	O	S	0	0
			608	397	99	111	1		

- Molecule 23 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	82	Total	C	N	O		0	0
			410	246	82	82			

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	c	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	c	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	k	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 54	C 44	Mg 1	N 4	O 5	0

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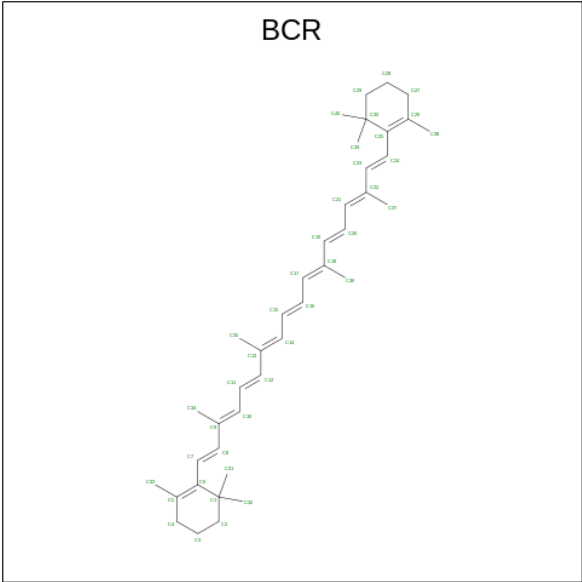
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
24	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	1	1	Total	C	0
			40	40	
25	2	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	7	1	Total	C	0
			40	40	
25	9	1	Total	C	0
			40	40	
25	c	1	Total	C	0
			40	40	
25	t	1	Total	C	0
			40	40	
25	k	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			39	39	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	R	1	Total C 40 40	0
25	R	1	Total C 40 40	0

- Molecule 26 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



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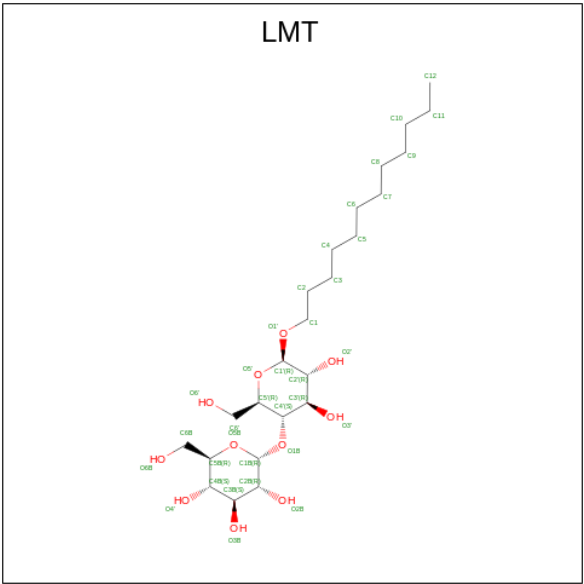
Mol	Chain	Residues	Atoms			AltConf
26	6	1	Total 43	C 40	O 3	0
26	6	1	Total 43	C 40	O 3	0
26	6	1	Total 43	C 40	O 3	0
26	6	1	Total 43	C 40	O 3	0
26	6	1	Total 43	C 40	O 3	0
26	7	1	Total 43	C 40	O 3	0
26	7	1	Total 43	C 40	O 3	0
26	7	1	Total 43	C 40	O 3	0
26	7	1	Total 43	C 40	O 3	0
26	8	1	Total 43	C 40	O 3	0
26	8	1	Total 43	C 40	O 3	0
26	8	1	Total 43	C 40	O 3	0
26	9	1	Total 43	C 40	O 3	0
26	9	1	Total 43	C 40	O 3	0
26	9	1	Total 43	C 40	O 3	0
26	9	1	Total 43	C 40	O 3	0
26	h	1	Total 43	C 40	O 3	0
26	h	1	Total 43	C 40	O 3	0
26	h	1	Total 43	C 40	O 3	0
26	h	1	Total 43	C 40	O 3	0
26	c	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	c	1	43	40	3	0
26	c	1	43	40	3	0
26	t	1	43	40	3	0
26	t	1	43	40	3	0
26	k	1	43	40	3	0
26	k	1	43	40	3	0
26	k	1	43	40	3	0
26	A	1	43	40	3	0
26	J	1	43	40	3	0
26	R	1	43	40	3	0

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



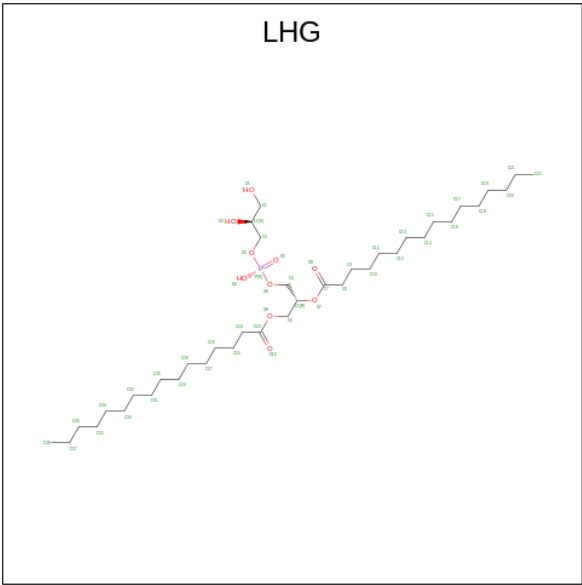
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	1	1	35	24	11	0

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Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			35	24	11	
27	3	1	Total	C	O	0
			30	19	11	
27	h	1	Total	C	O	0
			28	17	11	
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			25	14	11	
27	A	1	Total	C	O	0
			35	24	11	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



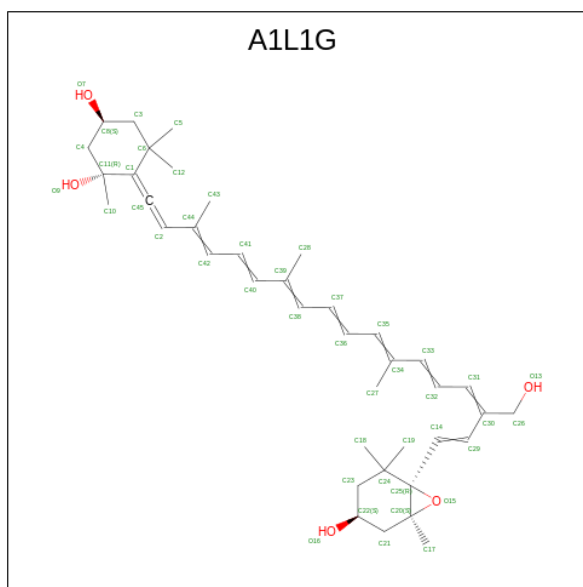
Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			43	32	10	1	
28	2	1	Total	C	O	P	0
			31	20	10	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	4	1	Total	C	O	P	0
			39	28	10	1	
28	8	1	Total	C	O	P	0
			31	20	10	1	

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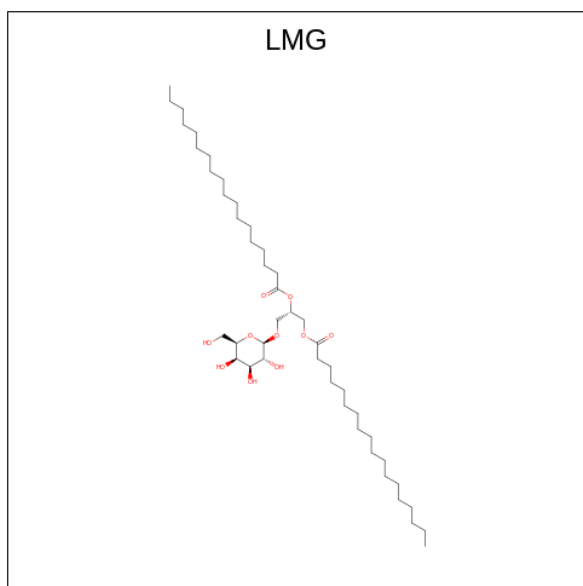
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	A	1	Total 48	37	10	1	0
28	A	1	Total 42	31	10	1	0
28	A	1	Total 41	30	10	1	0
28	A	1	Total 37	26	10	1	0
28	B	1	Total 49	38	10	1	0
28	B	1	Total 41	30	10	1	0
28	I	1	Total 40	29	10	1	0
28	J	1	Total 38	27	10	1	0
28	L	1	Total 29	18	10	1	0

- Molecule 29 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



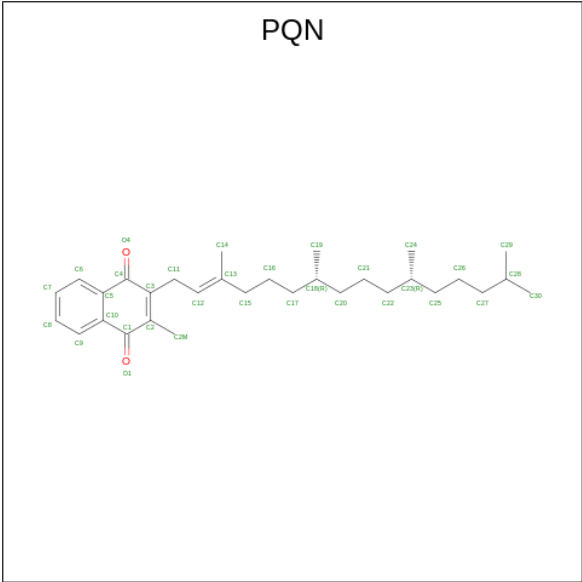
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			45	40	5	
29	3	1	Total	C	O	0
			45	40	5	
29	7	1	Total	C	O	0
			45	40	5	
29	9	1	Total	C	O	0
			45	40	5	
29	k	1	Total	C	O	0
			45	40	5	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



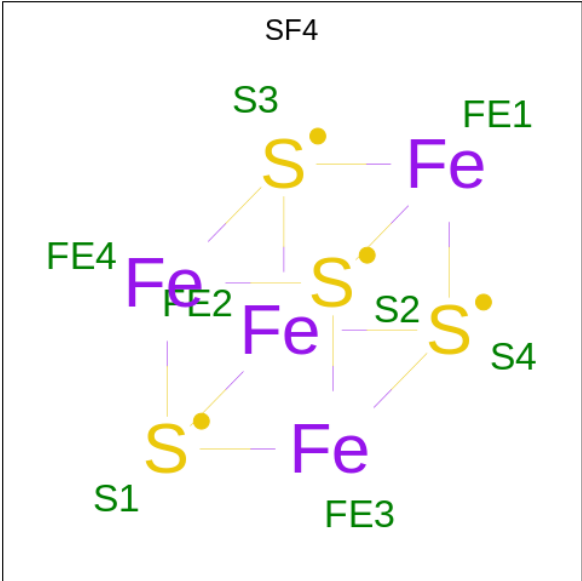
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			45	35	10	
30	t	1	Total	C	O	0
			34	24	10	
30	A	1	Total	C	O	0
			38	28	10	

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



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

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

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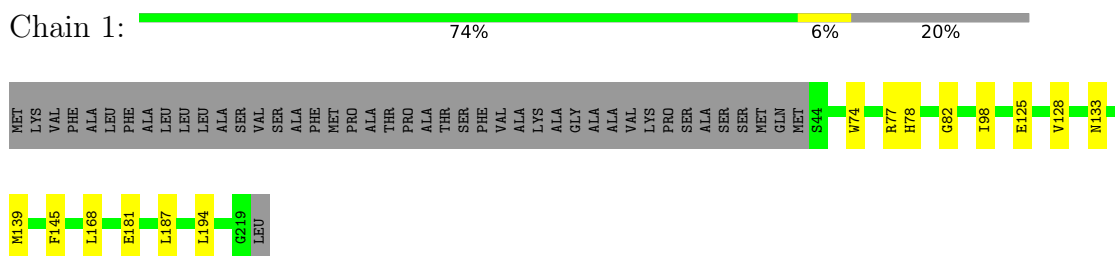
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Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

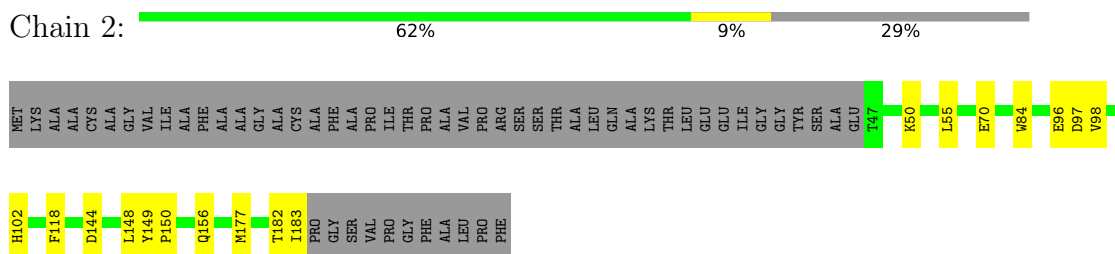
3 Residue-property plots [i](#)

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. 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. 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.

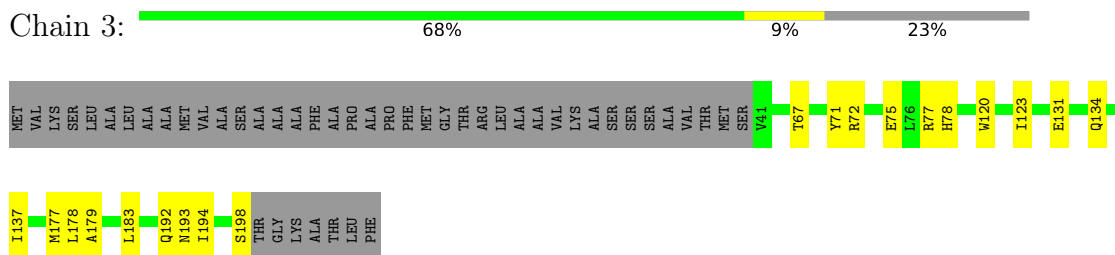
- Molecule 1: Light-harvesting protein XLH1



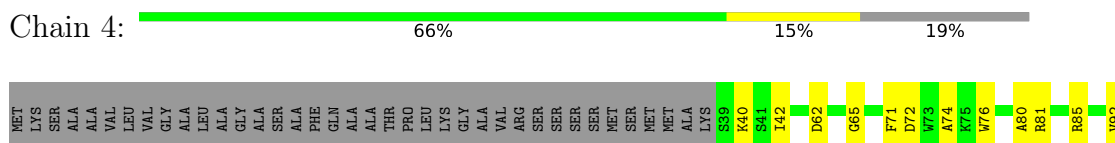
- Molecule 2: light-harvesting protein XLH2



- Molecule 3: light-harvesting protein XLH3



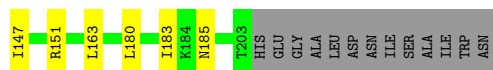
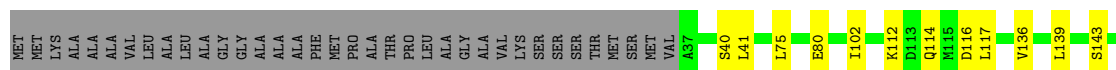
- Molecule 4: light-harvesting protein XLH4





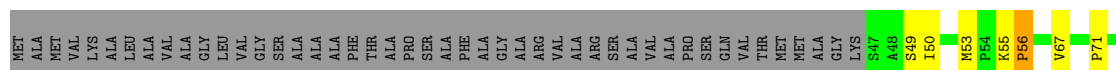
- Molecule 5: light-harvesting protein XLH5

Chain 5: 69% 8% 23%



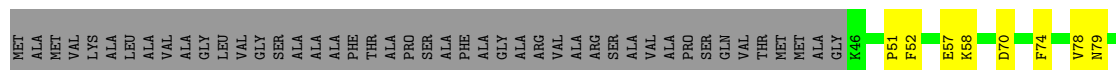
- Molecule 6: light-harvesting protein XLH6/10

Chain 6: 64% 11% 23%



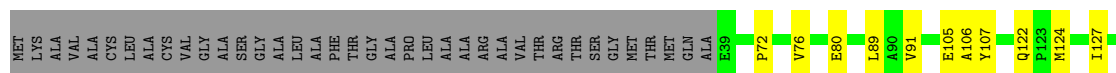
- Molecule 6: light-harvesting protein XLH6/10

Chain h: 67% 10% 22%



- Molecule 7: light-harvesting protein XLH7

Chain 7: 68% 13% 20%



- Molecule 8: light-harvesting protein XLH8

Chain 8: 77% 13% 10%



- Molecule 9: light-harvesting protein XLH9/13

Chain 9:  56% 13% 31%

ALA PRO PRO GLY ALA PRO GLN PRO GLN ARG ARG MET LYS ALA ALA ALA CYS SER LEU ALA ALA LEU LEU ALA ALA GLY ALA SER PHE VAL ALA PRO SER SER PHE GLY SER GLN LEU ALA ARG VAL THR SER ALA LYS M200 I201 ALA LEU SER MET GLU PHE ALA GLY LEU GLY ILE GLY

ALA ASP GLY PRO GLU P66 K69 N70 F71 D72 Y85 L95 A96 M97 Y116 V119 S120 H125 V129 G132 P133 L138 M164 M155 R160 M189 G190 R191 L192 A193 M194 S198 G199 M200 I201 L206 F211 P212 Y213 L214 TYR

- Molecule 9: light-harvesting protein XLH9/13

Chain k:  56% 16% 28%

ALA PRO PRO ALA THR GLN PRO GLN ARG ARG MET LYS ALA ALA ALA CYS SER LEU LEU LEU ALA ALA GLY ALA SER PHE VAL ALA PRO SER SER PHE ALA GLY SER GLN LEU ARG VAL THR SER ALA LYS SER ALA LEU SER MET GLU PHE ALA GLY LEU ILE GLY

G63 P64 K69 D72 R86 E89 L90 R94 P106 R110 L111 I115 Y116 Q117 G118 V119 M128 K131 G132 P133 Q136 W140 L141 T148 A149 P150 L151 T152 W153 N154 F165 R191 M194 F197 P212 Y213 LEU TYR

- Molecule 10: light-harvesting protein XLH11

Chain c:  70% 8% 21%

MET LYS VAL SER ALA VAL ALA ALA GLY VAL MET ALA SER GLY VAL ALA ALA PHE VAL GLN PRO THR ALA PHE ALA GLY SER LYS LEU ALA VAL ALA VAL ALA ALA SER GLY SER THR MET GLN MET ALA ALA ALA GLU R45 S46 K47 S48 I49 V66 D69 P70 L71 G72 D150 D151

D154 A155 K158 Q183 A194 M198 H207 P208 L209 PRO

- Molecule 11: light-harvesting protein XLH12

Chain t:  60% 10% 30%

THR ALA LEU ARG HIS PRO HIS SER LYS MET LYS ALA ALA THR VAL ALA ALA LEU ALA VAL VAL SER VAL SER PHE ALA ALA PRO ASN ALA ALA PHE THR LYS GLY ALA LEU SER THR ALA THR VAL LYS SER THR SER ALA LEU MET GLN MET VAL ASP PHE SER GLY LEU VAL GLY LYS

PRO PHE GLY ALA G65 S66 S67 A75 T76 I95 A97 M98 I101 M104 A105 V106 F110 I130 Y134 E149 T156 Y157 K158 P159 E160 V164 Y167 E202 A209 A216 Q219 R223 GLY ASN GLN VAL PHE

- Molecule 12: PsaA

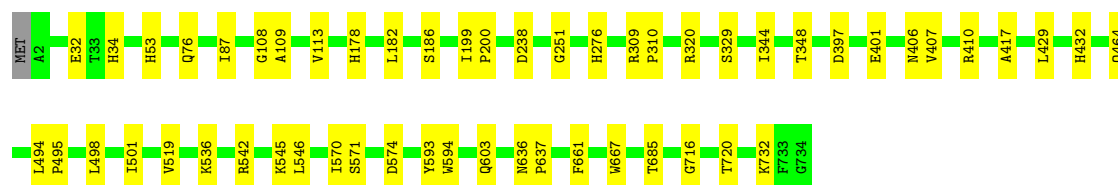
Chain A:  92% 7%

MET SER SER LYS GLN ALA T8 K69 V80 G92 S96 I118 V119 N125 Y157 I161 E192 H197 E233 F254 G257 V259 P260 I315 E321 F330 T331 E340 T344 N353 M356 I357 G358 H367 G395 G396


A403 L423 R426 R429 H448 L452 Q485 G515 S516 R569 C581 W595 M596 L600 L604 E693 E696 H702 V707 T737 S747 V748 GLY

- Molecule 13: PsaB

Chain B:  93% 7%




• Molecule 14: PsaC

Chain C:  89% 10%




• Molecule 15: PsaD

Chain D:  84% 11% 5%




• Molecule 16: PsaE

Chain E:  87% 11%




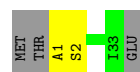
• Molecule 17: PsaF

Chain F:  77% 9% 13%



• Molecule 18: PsaI

Chain I:  86% 6% 8%



• Molecule 19: PsaJ

Chain J:  76% 19% 5%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, PQN, LMG, DD6, CLA, A1L1G, LHG, BCR, SF4

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	0.18	0/1363	0.30	0/1859
2	2	0.36	0/1109	0.60	0/1504
3	3	0.16	0/1238	0.31	0/1677
4	4	0.24	0/1427	0.38	0/1934
5	5	0.23	0/1274	0.43	0/1722
6	6	0.39	0/1257	0.64	0/1704
6	h	0.27	0/1274	0.46	0/1727
7	7	0.18	0/1298	0.36	0/1752
8	8	0.22	0/1276	0.41	0/1730
9	9	0.31	0/1200	0.48	0/1622
9	k	0.38	0/1231	0.57	0/1666
10	c	0.16	0/1255	0.32	0/1697
11	t	0.20	0/1285	0.37	0/1741
12	A	0.19	0/6030	0.33	0/8219
13	B	0.18	0/6034	0.31	0/8236
14	C	0.28	0/602	0.55	0/816
15	D	0.19	0/1059	0.36	0/1432
16	E	0.29	0/492	0.48	0/662
17	F	0.25	0/1297	0.44	0/1761
18	I	0.21	0/258	0.32	0/353
19	J	0.31	0/331	0.49	0/453
20	L	0.30	0/1051	0.45	0/1428
21	M	0.26	0/228	0.44	0/310
22	R	0.15	0/627	0.27	0/864
All	All	0.24	0/34496	0.40	0/46869

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1328	0	1344	24	0
2	2	1080	0	1061	16	0
3	3	1206	0	1171	18	0
4	4	1396	0	1415	32	0
5	5	1249	0	1255	15	0
6	6	1228	0	1215	41	0
6	h	1244	0	1236	16	0
7	7	1268	0	1265	27	0
8	8	1240	0	1195	17	0
9	9	1171	0	1187	28	0
9	k	1201	0	1207	30	0
10	c	1231	0	1259	12	0
11	t	1253	0	1213	15	0
12	A	5835	0	5718	48	0
13	B	5822	0	5629	43	0
14	C	592	0	569	5	0
15	D	1030	0	1028	11	0
16	E	484	0	486	5	0
17	F	1267	0	1290	14	0
18	I	252	0	272	1	0
19	J	320	0	313	9	0
20	L	1027	0	1037	27	0
21	M	227	0	262	5	0
22	R	608	0	612	5	0
23	S	410	0	86	3	0
24	1	507	0	427	16	0
24	2	440	0	345	13	0
24	3	468	0	413	8	0
24	4	607	0	454	27	0
24	5	328	0	247	7	0
24	6	554	0	401	12	0
24	7	564	0	428	23	0
24	8	409	0	299	9	0
24	9	505	0	363	18	0
24	A	2651	0	2720	33	0
24	B	2471	0	2526	59	0
24	F	161	0	144	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	42	0	31	1	0
24	L	166	0	154	6	0
24	R	110	0	105	1	0
24	c	548	0	460	7	0
24	h	553	0	405	5	0
24	k	513	0	387	10	0
24	t	477	0	369	8	0
25	1	80	0	112	7	0
25	2	40	0	56	4	0
25	4	40	0	56	7	0
25	7	40	0	56	2	0
25	9	40	0	56	9	0
25	A	199	0	277	8	0
25	B	200	0	280	11	0
25	F	40	0	56	2	0
25	I	80	0	112	3	0
25	J	80	0	112	5	0
25	L	80	0	112	2	0
25	M	40	0	56	2	0
25	R	80	0	112	2	0
25	c	40	0	56	7	0
25	k	40	0	56	2	0
25	t	40	0	56	2	0
26	1	129	0	0	7	0
26	2	86	0	0	2	0
26	3	129	0	0	1	0
26	4	172	0	0	2	0
26	5	86	0	0	3	0
26	6	215	0	0	2	0
26	7	172	0	0	3	0
26	8	129	0	0	2	0
26	9	172	0	0	6	0
26	A	43	0	0	0	0
26	J	43	0	0	0	0
26	R	43	0	0	0	0
26	c	129	0	0	3	0
26	h	172	0	0	1	0
26	k	129	0	0	4	0
26	t	86	0	0	0	0
27	1	70	0	92	2	0
27	3	30	0	33	1	0
27	A	95	0	115	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	h	28	0	29	1	0
28	1	43	0	56	2	0
28	2	31	0	32	0	0
28	3	43	0	59	1	0
28	4	39	0	48	1	0
28	8	31	0	32	1	0
28	A	168	0	222	2	0
28	B	90	0	129	0	0
28	I	40	0	50	1	0
28	J	38	0	46	1	0
28	L	29	0	28	4	0
29	2	45	0	0	0	0
29	3	45	0	0	2	0
29	7	45	0	0	0	0
29	9	45	0	0	1	0
29	k	45	0	0	2	0
30	2	45	0	60	1	0
30	A	38	0	46	0	0
30	t	34	0	38	0	0
31	A	33	0	46	1	0
31	B	33	0	46	0	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
All	All	50344	0	46831	640	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 7.

The worst 5 of 640 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)
20:L:147:LEU:HD23	24:L:205:CLA:C1	1.56	1.33
3:3:194:ILE:HD13	3:3:198:SER:OG	1.43	1.16
1:1:98:ILE:HG23	1:1:128:VAL:HG11	1.21	1.15
20:L:147:LEU:CD2	24:L:205:CLA:C1	2.31	1.07
6:6:50:ILE:HG21	6:6:53:MET:HG3	1.37	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	174/220 (79%)	169 (97%)	5 (3%)	0	100	100
2	2	135/194 (70%)	121 (90%)	13 (10%)	1 (1%)	19	46
3	3	156/205 (76%)	147 (94%)	9 (6%)	0	100	100
4	4	186/231 (80%)	172 (92%)	14 (8%)	0	100	100
5	5	165/216 (76%)	153 (93%)	12 (7%)	0	100	100
6	6	161/212 (76%)	148 (92%)	12 (8%)	1 (1%)	22	49
6	h	163/212 (77%)	154 (94%)	8 (5%)	1 (1%)	22	49
7	7	164/207 (79%)	149 (91%)	15 (9%)	0	100	100
8	8	159/179 (89%)	146 (92%)	13 (8%)	0	100	100
9	9	147/215 (68%)	142 (97%)	5 (3%)	0	100	100
9	k	152/215 (71%)	144 (95%)	7 (5%)	1 (1%)	19	46
10	c	163/210 (78%)	154 (94%)	9 (6%)	0	100	100
11	t	157/228 (69%)	143 (91%)	14 (9%)	0	100	100
12	A	739/749 (99%)	715 (97%)	24 (3%)	0	100	100
13	B	731/734 (100%)	706 (97%)	25 (3%)	0	100	100
14	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
15	D	130/139 (94%)	120 (92%)	10 (8%)	0	100	100
16	E	58/61 (95%)	56 (97%)	1 (2%)	1 (2%)	7	24
17	F	159/185 (86%)	153 (96%)	5 (3%)	1 (1%)	22	49
18	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
19	J	38/42 (90%)	38 (100%)	0	0	100	100
20	L	133/149 (89%)	130 (98%)	3 (2%)	0	100	100
21	M	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
22	R	79/87 (91%)	77 (98%)	2 (2%)	0	100	100
All	All	4286/5037 (85%)	4069 (95%)	211 (5%)	6 (0%)	50	76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	6	56	PRO
16	E	31	ILE
9	k	119	VAL
6	h	117	VAL
17	F	26	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	137/169 (81%)	137 (100%)	0	100	100
2	2	112/149 (75%)	110 (98%)	2 (2%)	54	82
3	3	121/152 (80%)	121 (100%)	0	100	100
4	4	143/173 (83%)	142 (99%)	1 (1%)	81	94
5	5	130/162 (80%)	130 (100%)	0	100	100
6	6	129/159 (81%)	125 (97%)	4 (3%)	35	68
6	h	131/159 (82%)	131 (100%)	0	100	100
7	7	137/163 (84%)	135 (98%)	2 (2%)	60	85
8	8	127/141 (90%)	126 (99%)	1 (1%)	79	93
9	9	125/168 (74%)	124 (99%)	1 (1%)	79	93
9	k	128/168 (76%)	127 (99%)	1 (1%)	79	93
10	c	129/156 (83%)	128 (99%)	1 (1%)	79	93
11	t	133/178 (75%)	132 (99%)	1 (1%)	79	93
12	A	603/609 (99%)	601 (100%)	2 (0%)	91	97
13	B	597/598 (100%)	597 (100%)	0	100	100
14	C	66/67 (98%)	66 (100%)	0	100	100
15	D	110/117 (94%)	110 (100%)	0	100	100
16	E	55/56 (98%)	55 (100%)	0	100	100
17	F	138/159 (87%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	I	28/31 (90%)	28 (100%)	0	100	100
19	J	32/34 (94%)	32 (100%)	0	100	100
20	L	108/119 (91%)	106 (98%)	2 (2%)	52	81
21	M	25/25 (100%)	25 (100%)	0	100	100
22	R	68/73 (93%)	67 (98%)	1 (2%)	60	85
All	All	3512/3985 (88%)	3493 (100%)	19 (0%)	85	95

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	A	96	SER
20	L	91	LEU
22	R	76	HIS
20	L	16	HIS
7	7	195	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	432	HIS
13	B	598	HIS
22	R	48	ASN
6	h	123	HIS
9	9	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

338 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	L	206	-	41,41,41	0.73	0	56,56,56	2.09	18 (32%)
24	CLA	1	301	1	65,73,73	1.52	6 (9%)	76,113,113	1.25	7 (9%)
25	BCR	B	841	-	41,41,41	0.75	0	56,56,56	2.08	22 (39%)
25	BCR	I	102	-	41,41,41	0.72	0	56,56,56	2.32	26 (46%)
24	CLA	B	804	13	65,73,73	1.54	6 (9%)	76,113,113	1.47	10 (13%)
24	CLA	A	827	12	62,70,73	1.52	5 (8%)	72,109,113	1.31	7 (9%)
29	A1L1G	7	614	-	38,47,47	1.53	8 (21%)	49,71,71	1.10	2 (4%)
26	DD6	c	613	-	39,45,45	1.50	8 (20%)	52,67,67	1.70	8 (15%)
26	DD6	5	608	-	39,45,45	1.53	8 (20%)	52,67,67	1.77	11 (21%)
26	DD6	7	618	-	39,45,45	1.72	6 (15%)	52,67,67	1.72	13 (25%)
24	CLA	k	306	9	46,54,73	1.76	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	1	308	1	46,54,73	1.86	6 (13%)	53,90,113	1.33	7 (13%)
24	CLA	4	602	4	60,68,73	1.54	5 (8%)	70,107,113	1.32	8 (11%)
24	CLA	5	607	5	45,53,73	1.86	8 (17%)	52,89,113	1.56	8 (15%)
24	CLA	4	607	4	46,54,73	1.77	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	B	813	13	46,54,73	1.77	5 (10%)	53,90,113	1.50	8 (15%)
29	A1L1G	3	310	-	38,47,47	1.49	8 (21%)	49,71,71	0.99	3 (6%)
28	LHG	3	315	-	42,42,48	0.99	2 (4%)	45,48,54	1.03	4 (8%)
24	CLA	k	303	-	55,63,73	1.63	5 (9%)	64,101,113	1.55	13 (20%)
24	CLA	A	831	12	65,73,73	1.49	5 (7%)	76,113,113	1.22	7 (9%)
24	CLA	J	103	19	42,50,73	1.86	5 (11%)	48,85,113	1.43	7 (14%)
27	LMT	1	316	-	36,36,36	0.69	0	47,47,47	0.94	2 (4%)
24	CLA	3	305	3	60,68,73	1.57	5 (8%)	70,107,113	1.25	8 (11%)
26	DD6	R	105	-	39,45,45	1.55	10 (25%)	52,67,67	1.87	12 (23%)
24	CLA	B	838	28	65,73,73	1.50	7 (10%)	76,113,113	1.36	9 (11%)
24	CLA	A	807	12	65,73,73	1.48	5 (7%)	76,113,113	1.28	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	824	13	65,73,73	1.55	5 (7%)	76,113,113	1.40	11 (14%)
24	CLA	L	205	-	46,54,73	1.75	6 (13%)	53,90,113	1.39	7 (13%)
26	DD6	4	616	-	39,45,45	1.51	8 (20%)	52,67,67	1.83	13 (25%)
26	DD6	h	614	-	39,45,45	1.53	8 (20%)	52,67,67	1.59	10 (19%)
24	CLA	9	302	9	46,54,73	1.74	6 (13%)	53,90,113	1.56	6 (11%)
24	CLA	8	202	8	46,54,73	1.78	5 (10%)	53,90,113	1.44	7 (13%)
27	LMT	A	850	-	36,36,36	0.68	0	47,47,47	0.64	0
24	CLA	3	301	3	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
24	CLA	A	819	12	45,53,73	1.81	6 (13%)	52,89,113	1.44	8 (15%)
24	CLA	B	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.44	8 (10%)
24	CLA	B	829	13	65,73,73	1.47	7 (10%)	76,113,113	1.50	9 (11%)
24	CLA	A	805	12	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
28	LHG	A	852	-	36,36,48	1.07	2 (5%)	39,42,54	1.02	2 (5%)
24	CLA	B	816	13	65,73,73	1.52	7 (10%)	76,113,113	1.36	9 (11%)
24	CLA	7	605	7	46,54,73	1.81	5 (10%)	53,90,113	1.43	7 (13%)
24	CLA	t	310	-	46,54,73	1.80	5 (10%)	53,90,113	1.41	7 (13%)
24	CLA	2	207	-	46,54,73	1.77	5 (10%)	53,90,113	1.45	7 (13%)
24	CLA	k	310	9	41,49,73	1.92	5 (12%)	47,84,113	1.50	8 (17%)
24	CLA	A	828	12	65,73,73	1.50	6 (9%)	76,113,113	1.26	7 (9%)
24	CLA	k	309	9	45,53,73	1.83	5 (11%)	52,89,113	1.41	8 (15%)
28	LHG	I	103	-	39,39,48	1.03	2 (5%)	42,45,54	1.15	4 (9%)
24	CLA	B	810	13	54,62,73	1.66	7 (12%)	67,100,113	1.47	13 (19%)
26	DD6	A	848	-	39,45,45	1.46	8 (20%)	52,67,67	1.92	10 (19%)
24	CLA	A	817	12	65,73,73	1.49	8 (12%)	76,113,113	1.26	8 (10%)
24	CLA	6	606	6	46,54,73	1.78	5 (10%)	53,90,113	1.34	7 (13%)
24	CLA	3	308	3	46,54,73	1.76	6 (13%)	53,90,113	1.45	8 (15%)
26	DD6	4	617	-	39,45,45	1.50	8 (20%)	52,67,67	1.85	12 (23%)
24	CLA	A	837	12	55,63,73	1.65	5 (9%)	64,101,113	1.38	9 (14%)
24	CLA	c	603	10	46,54,73	1.75	6 (13%)	53,90,113	1.44	8 (15%)
24	CLA	t	304	-	46,54,73	1.77	6 (13%)	53,90,113	1.40	7 (13%)
24	CLA	c	604	-	46,54,73	1.81	6 (13%)	53,90,113	1.37	6 (11%)
24	CLA	A	811	12	46,54,73	1.79	6 (13%)	53,90,113	1.38	7 (13%)
26	DD6	c	614	-	39,45,45	1.50	8 (20%)	52,67,67	2.15	11 (21%)
30	LMG	t	314	-	34,34,55	1.12	2 (5%)	42,42,63	1.21	4 (9%)
24	CLA	2	201	2	45,53,73	1.83	6 (13%)	52,89,113	1.59	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	843	-	41,41,41	0.84	1 (2%)	56,56,56	2.37	20 (35%)
24	CLA	h	605	6	46,54,73	1.81	5 (10%)	53,90,113	1.38	8 (15%)
24	CLA	4	608	-	50,58,73	1.71	5 (10%)	58,95,113	1.51	10 (17%)
28	LHG	B	845	24	40,40,48	1.02	2 (5%)	43,46,54	0.97	1 (2%)
24	CLA	A	856	-	65,73,73	1.53	7 (10%)	76,113,113	1.31	6 (7%)
24	CLA	A	812	12	65,73,73	1.51	7 (10%)	76,113,113	1.31	8 (10%)
24	CLA	B	820	13	55,63,73	1.64	6 (10%)	64,101,113	1.37	9 (14%)
24	CLA	5	606	-	46,54,73	1.81	5 (10%)	53,90,113	1.42	7 (13%)
24	CLA	3	304	3	46,54,73	1.79	5 (10%)	53,90,113	1.66	8 (15%)
24	CLA	2	206	2	46,54,73	1.78	6 (13%)	53,90,113	1.44	8 (15%)
26	DD6	k	315	-	39,45,45	1.50	8 (20%)	52,67,67	2.04	12 (23%)
25	BCR	k	316	-	41,41,41	0.73	0	56,56,56	2.32	20 (35%)
24	CLA	A	826	12	65,73,73	1.48	5 (7%)	76,113,113	1.36	10 (13%)
28	LHG	J	105	-	37,37,48	1.05	2 (5%)	40,43,54	1.11	3 (7%)
24	CLA	B	817	13	65,73,73	1.52	5 (7%)	76,113,113	1.29	8 (10%)
26	DD6	1	313	-	39,45,45	1.52	8 (20%)	52,67,67	1.56	8 (15%)
24	CLA	7	612	7	46,54,73	1.82	5 (10%)	53,90,113	1.41	7 (13%)
24	CLA	B	833	13	58,66,73	1.57	5 (8%)	67,104,113	1.45	9 (13%)
24	CLA	h	603	6	44,53,73	1.81	5 (11%)	50,89,113	1.44	7 (14%)
24	CLA	c	602	10	65,73,73	1.48	5 (7%)	76,113,113	1.28	9 (11%)
24	CLA	t	302	11	46,54,73	1.81	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	1	309	1	44,53,73	1.83	6 (13%)	50,89,113	1.40	7 (14%)
24	CLA	9	307	9	46,54,73	1.74	7 (15%)	53,90,113	1.54	8 (15%)
26	DD6	6	615	-	39,45,45	1.45	8 (20%)	52,67,67	1.88	15 (28%)
29	A1L1G	9	312	-	38,47,47	1.54	8 (21%)	49,71,71	1.24	6 (12%)
25	BCR	1	314	-	41,41,41	0.74	0	56,56,56	2.16	18 (32%)
24	CLA	B	830	13	58,66,73	1.63	6 (10%)	67,104,113	1.33	8 (11%)
24	CLA	A	804	12	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
26	DD6	6	617	-	39,45,45	1.55	9 (23%)	52,67,67	1.63	9 (17%)
24	CLA	A	801	12	65,73,73	1.51	6 (9%)	76,113,113	1.44	10 (13%)
25	BCR	7	617	-	41,41,41	0.77	0	56,56,56	1.98	21 (37%)
25	BCR	B	840	-	41,41,41	0.79	0	56,56,56	2.01	23 (41%)
28	LHG	2	215	-	30,30,48	1.16	2 (6%)	33,36,54	1.13	3 (9%)
25	BCR	1	310	-	41,41,41	0.76	0	56,56,56	2.17	21 (37%)
24	CLA	B	818	-	65,73,73	1.52	6 (9%)	76,113,113	1.24	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	848	13	65,73,73	1.49	5 (7%)	76,113,113	1.26	7 (9%)
24	CLA	1	305	1	45,53,73	1.80	8 (17%)	52,89,113	1.83	8 (15%)
24	CLA	A	802	-	65,73,73	1.47	7 (10%)	76,113,113	1.47	7 (9%)
24	CLA	9	305	-	46,54,73	1.74	5 (10%)	53,90,113	1.60	8 (15%)
26	DD6	5	609	-	39,45,45	1.50	8 (20%)	52,67,67	1.77	9 (17%)
25	BCR	R	101	-	41,41,41	0.79	1 (2%)	56,56,56	2.02	22 (39%)
24	CLA	6	603	6	46,54,73	1.79	5 (10%)	53,90,113	1.35	7 (13%)
26	DD6	3	313	-	39,45,45	1.54	8 (20%)	52,67,67	1.61	10 (19%)
24	CLA	7	609	7	46,54,73	1.80	5 (10%)	53,90,113	1.43	7 (13%)
24	CLA	4	610	4	41,49,73	1.90	5 (12%)	47,84,113	1.46	6 (12%)
24	CLA	A	808	12	65,73,73	1.53	5 (7%)	76,113,113	1.26	7 (9%)
24	CLA	8	204	8	45,53,73	1.84	7 (15%)	52,89,113	1.48	8 (15%)
26	DD6	9	313	-	39,45,45	1.56	8 (20%)	52,67,67	1.61	8 (15%)
25	BCR	F	204	-	41,41,41	0.75	0	56,56,56	2.01	16 (28%)
24	CLA	A	824	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	7 (9%)
24	CLA	1	302	1	45,53,73	1.78	8 (17%)	52,89,113	1.41	8 (15%)
26	DD6	h	615	-	39,45,45	1.50	8 (20%)	52,67,67	1.71	10 (19%)
24	CLA	3	309	3	41,49,73	1.87	5 (12%)	47,84,113	1.51	7 (14%)
24	CLA	2	204	2	60,68,73	1.56	6 (10%)	70,107,113	1.32	7 (10%)
24	CLA	B	828	13	50,58,73	1.75	7 (14%)	58,95,113	1.36	8 (13%)
24	CLA	6	608	6	46,54,73	1.77	5 (10%)	53,90,113	1.36	7 (13%)
32	SF4	C	102	14	0,12,12	-	-	-	-	-
24	CLA	F	201	-	65,73,73	1.52	5 (7%)	76,113,113	1.26	8 (10%)
24	CLA	5	602	5	55,63,73	1.66	5 (9%)	64,101,113	1.42	9 (14%)
25	BCR	R	102	-	41,41,41	0.75	0	56,56,56	2.15	21 (37%)
27	LMT	3	314	-	31,31,36	0.70	0	42,42,47	1.19	3 (7%)
24	CLA	9	301	9	46,54,73	1.80	6 (13%)	53,90,113	1.55	7 (13%)
25	BCR	B	849	-	41,41,41	0.64	0	56,56,56	2.24	20 (35%)
24	CLA	B	847	13	65,73,73	1.54	7 (10%)	76,113,113	1.22	8 (10%)
29	A1L1G	2	213	-	38,47,47	1.51	8 (21%)	49,71,71	1.03	5 (10%)
24	CLA	6	601	6	45,53,73	1.84	5 (11%)	52,89,113	1.44	8 (15%)
24	CLA	7	606	7	60,68,73	1.56	5 (8%)	70,107,113	1.45	7 (10%)
24	CLA	7	607	7	45,53,73	1.82	5 (11%)	52,89,113	1.51	8 (15%)
31	PQN	B	839	-	34,34,34	0.35	0	42,45,45	0.60	1 (2%)
24	CLA	9	308	-	46,54,73	1.79	6 (13%)	53,90,113	1.39	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	840	28	65,73,73	1.50	5 (7%)	76,113,113	1.31	9 (11%)
24	CLA	t	303	11	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
24	CLA	B	846	13	55,63,73	1.63	6 (10%)	64,101,113	1.30	8 (12%)
28	LHG	L	201	-	28,28,48	1.22	2 (7%)	31,34,54	1.13	2 (6%)
24	CLA	A	816	12	65,73,73	1.49	5 (7%)	76,113,113	1.28	9 (11%)
24	CLA	1	304	26	55,63,73	1.63	7 (12%)	64,101,113	1.23	7 (10%)
24	CLA	8	203	-	50,58,73	1.74	7 (14%)	58,95,113	1.44	10 (17%)
24	CLA	c	605	10	46,54,73	1.82	5 (10%)	53,90,113	1.40	6 (11%)
25	BCR	2	211	-	41,41,41	0.76	0	56,56,56	2.12	22 (39%)
24	CLA	c	609	-	60,68,73	1.59	5 (8%)	70,107,113	1.44	10 (14%)
24	CLA	A	823	12	65,73,73	1.52	7 (10%)	76,113,113	1.20	8 (10%)
27	LMT	1	315	-	36,36,36	0.67	0	47,47,47	0.79	1 (2%)
25	BCR	A	846	-	41,41,41	0.74	1 (2%)	56,56,56	2.38	27 (48%)
24	CLA	A	806	12	65,73,73	1.53	5 (7%)	76,113,113	1.24	8 (10%)
24	CLA	B	832	-	45,53,73	1.84	6 (13%)	52,89,113	1.33	6 (11%)
24	CLA	c	610	10	43,52,73	1.89	6 (13%)	49,88,113	1.40	8 (16%)
24	CLA	h	607	6	46,54,73	1.79	6 (13%)	53,90,113	1.30	7 (13%)
26	DD6	t	311	-	39,45,45	1.56	8 (20%)	52,67,67	1.54	7 (13%)
25	BCR	A	843	-	41,41,41	0.72	0	56,56,56	2.34	21 (37%)
28	LHG	A	849	-	40,40,48	1.03	2 (5%)	43,46,54	1.05	2 (4%)
24	CLA	h	611	6	41,49,73	1.80	6 (14%)	47,84,113	1.82	8 (17%)
24	CLA	9	304	9	46,54,73	1.74	6 (13%)	53,90,113	1.61	7 (13%)
24	CLA	B	835	13	47,55,73	1.75	5 (10%)	54,91,113	1.55	7 (12%)
24	CLA	t	306	11	45,53,73	1.82	5 (11%)	52,89,113	1.45	7 (13%)
24	CLA	B	825	13	55,63,73	1.61	5 (9%)	64,101,113	1.35	7 (10%)
24	CLA	5	601	5	45,53,73	1.82	5 (11%)	52,89,113	1.40	8 (15%)
24	CLA	3	302	3	45,53,73	1.79	6 (13%)	52,89,113	1.49	8 (15%)
24	CLA	8	207	-	45,53,73	1.86	5 (11%)	52,89,113	1.42	7 (13%)
24	CLA	6	604	-	46,54,73	1.79	6 (13%)	53,90,113	1.36	7 (13%)
24	CLA	4	601	4	41,50,73	1.89	6 (14%)	46,85,113	1.30	7 (15%)
24	CLA	c	607	10	46,54,73	1.70	7 (15%)	53,90,113	1.47	8 (15%)
24	CLA	4	604	-	46,54,73	1.85	6 (13%)	53,90,113	1.37	6 (11%)
26	DD6	7	616	-	39,45,45	1.63	8 (20%)	52,67,67	1.71	8 (15%)
30	LMG	2	214	-	45,45,55	0.95	2 (4%)	53,53,63	1.37	5 (9%)
26	DD6	4	615	-	39,45,45	1.56	9 (23%)	52,67,67	1.60	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	6	610	6	46,54,73	1.83	6 (13%)	53,90,113	1.30	6 (11%)
24	CLA	7	608	-	45,53,73	1.82	5 (11%)	52,89,113	1.59	7 (13%)
24	CLA	h	609	-	46,54,73	1.81	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	h	610	6	46,54,73	1.84	5 (10%)	53,90,113	1.36	8 (15%)
24	CLA	1	317	-	65,73,73	1.53	6 (9%)	76,113,113	1.22	8 (10%)
24	CLA	k	302	9	46,54,73	1.78	5 (10%)	53,90,113	1.53	7 (13%)
24	CLA	A	833	12	65,73,73	1.53	6 (9%)	76,113,113	1.28	9 (11%)
29	A1L1G	k	312	-	38,47,47	1.48	8 (21%)	49,71,71	1.08	4 (8%)
24	CLA	1	307	1	45,53,73	1.84	5 (11%)	52,89,113	1.39	6 (11%)
24	CLA	A	836	12	65,73,73	1.54	6 (9%)	76,113,113	1.19	8 (10%)
26	DD6	9	317	-	39,45,45	1.48	8 (20%)	52,67,67	2.09	16 (30%)
24	CLA	B	814	13	50,58,73	1.73	7 (14%)	58,95,113	1.45	9 (15%)
25	BCR	L	202	-	41,41,41	0.68	0	56,56,56	2.28	24 (42%)
24	CLA	B	806	13	65,73,73	1.50	5 (7%)	76,113,113	1.29	7 (9%)
24	CLA	4	611	-	46,54,73	1.79	5 (10%)	53,90,113	1.40	7 (13%)
25	BCR	J	104	-	41,41,41	0.69	0	56,56,56	2.28	23 (41%)
24	CLA	A	803	12	55,63,73	1.63	6 (10%)	64,101,113	1.42	9 (14%)
26	DD6	k	313	-	39,45,45	1.48	8 (20%)	52,67,67	1.70	11 (21%)
26	DD6	h	616	-	39,45,45	1.56	8 (20%)	52,67,67	1.72	9 (17%)
24	CLA	8	205	8	45,53,73	1.80	5 (11%)	52,89,113	1.37	8 (15%)
24	CLA	8	209	-	41,49,73	1.89	5 (12%)	47,84,113	1.49	7 (14%)
24	CLA	h	608	6	46,54,73	1.80	6 (13%)	53,90,113	1.34	6 (11%)
24	CLA	B	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
25	BCR	t	312	-	41,41,41	0.76	0	56,56,56	1.79	9 (16%)
24	CLA	6	612	-	46,54,73	1.79	5 (10%)	53,90,113	1.40	7 (13%)
25	BCR	J	101	-	41,41,41	0.88	0	56,56,56	2.37	19 (33%)
24	CLA	A	860	12	65,73,73	1.45	7 (10%)	76,113,113	1.51	11 (14%)
27	LMT	h	617	-	29,29,36	0.74	0	40,40,47	0.85	2 (5%)
24	CLA	B	815	13	55,63,73	1.63	5 (9%)	64,101,113	1.38	9 (14%)
24	CLA	B	809	13	65,73,73	1.50	6 (9%)	76,113,113	1.32	9 (11%)
24	CLA	B	834	13	65,73,73	1.52	5 (7%)	76,113,113	1.24	8 (10%)
24	CLA	6	602	6	47,55,73	1.77	6 (12%)	54,91,113	1.38	8 (14%)
24	CLA	A	820	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
24	CLA	h	612	-	45,53,73	1.83	7 (15%)	52,89,113	1.46	8 (15%)
24	CLA	A	832	12	65,73,73	1.51	6 (9%)	76,113,113	1.26	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	2	210	-	39,45,45	1.50	8 (20%)	52,67,67	1.73	8 (15%)
24	CLA	5	604	5	46,54,73	1.80	5 (10%)	53,90,113	1.33	7 (13%)
24	CLA	L	204	20	65,73,73	1.53	6 (9%)	76,113,113	1.25	9 (11%)
24	CLA	B	827	13	65,73,73	1.51	6 (9%)	76,113,113	1.29	9 (11%)
24	CLA	t	305	11	46,54,73	1.78	5 (10%)	53,90,113	1.45	7 (13%)
24	CLA	k	305	9	46,54,73	1.80	5 (10%)	53,90,113	1.39	6 (11%)
24	CLA	h	606	6	46,54,73	1.77	6 (13%)	53,90,113	1.39	7 (13%)
24	CLA	7	611	7	46,54,73	1.80	6 (13%)	53,90,113	1.44	7 (13%)
24	CLA	2	203	-	50,58,73	1.71	5 (10%)	58,95,113	1.39	8 (13%)
24	CLA	A	838	12	65,73,73	1.52	6 (9%)	76,113,113	1.26	8 (10%)
24	CLA	L	203	20	55,63,73	1.60	5 (9%)	64,101,113	1.45	10 (15%)
26	DD6	1	311	24	39,45,45	1.59	8 (20%)	52,67,67	1.61	12 (23%)
24	CLA	1	303	1	46,54,73	1.77	5 (10%)	53,90,113	1.39	7 (13%)
26	DD6	3	312	-	39,45,45	1.47	8 (20%)	52,67,67	1.84	9 (17%)
28	LHG	B	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	A	822	12	55,63,73	1.66	6 (10%)	64,101,113	1.31	8 (12%)
24	CLA	B	805	13	65,73,73	1.48	5 (7%)	76,113,113	1.32	7 (9%)
24	CLA	c	601	10	43,51,73	1.87	6 (13%)	49,86,113	1.40	8 (16%)
26	DD6	c	612	-	39,45,45	1.48	8 (20%)	52,67,67	2.07	11 (21%)
24	CLA	7	610	7	45,53,73	1.82	5 (11%)	52,89,113	1.39	7 (13%)
24	CLA	9	306	9	46,54,73	1.81	6 (13%)	53,90,113	1.50	8 (15%)
24	CLA	A	853	12	55,63,73	1.61	6 (10%)	64,101,113	1.43	8 (12%)
26	DD6	2	212	-	39,45,45	1.53	8 (20%)	52,67,67	1.67	8 (15%)
24	CLA	8	208	8	45,53,73	1.78	6 (13%)	52,89,113	1.58	6 (11%)
24	CLA	A	829	12	65,73,73	1.52	6 (9%)	76,113,113	1.30	9 (11%)
24	CLA	A	847	-	55,63,73	1.65	5 (9%)	64,101,113	1.43	8 (12%)
25	BCR	I	101	-	41,41,41	0.78	1 (2%)	56,56,56	2.28	25 (44%)
24	CLA	B	802	13	65,73,73	1.49	6 (9%)	76,113,113	1.17	7 (9%)
24	CLA	B	811	13	55,63,73	1.65	7 (12%)	64,101,113	1.38	10 (15%)
24	CLA	c	608	10	65,73,73	1.51	6 (9%)	76,113,113	1.23	8 (10%)
24	CLA	c	606	10	46,54,73	1.80	5 (10%)	53,90,113	1.41	6 (11%)
32	SF4	C	101	14	0,12,12	-	-	-	-	-
24	CLA	4	609	4	46,54,73	1.79	6 (13%)	53,90,113	1.39	8 (15%)
24	CLA	A	830	12	55,63,73	1.66	8 (14%)	64,101,113	1.89	13 (20%)
24	CLA	9	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.52	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	c	615	-	41,41,41	0.71	0	56,56,56	2.64	21 (37%)
24	CLA	9	303	-	46,54,73	1.79	8 (17%)	53,90,113	1.51	7 (13%)
24	CLA	A	810	12	62,70,73	1.55	6 (9%)	72,109,113	1.24	8 (11%)
24	CLA	2	208	-	46,54,73	1.81	5 (10%)	53,90,113	1.37	6 (11%)
25	BCR	A	859	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
24	CLA	h	602	6	55,63,73	1.62	6 (10%)	64,101,113	2.06	13 (20%)
24	CLA	h	604	-	46,54,73	1.78	5 (10%)	53,90,113	1.38	7 (13%)
24	CLA	B	819	13	46,54,73	1.80	5 (10%)	53,90,113	1.38	7 (13%)
28	LHG	4	619	-	38,38,48	1.05	2 (5%)	41,44,54	0.99	2 (4%)
24	CLA	2	202	2	55,63,73	1.67	5 (9%)	64,101,113	1.35	8 (12%)
24	CLA	2	205	2	46,54,73	1.76	5 (10%)	53,90,113	1.46	6 (11%)
24	CLA	2	209	-	46,54,73	1.80	5 (10%)	53,90,113	1.38	7 (13%)
26	DD6	h	613	-	39,45,45	1.50	8 (20%)	52,67,67	1.56	9 (17%)
25	BCR	B	842	-	41,41,41	0.75	0	56,56,56	2.12	14 (25%)
24	CLA	R	104	22	45,53,73	1.76	7 (15%)	52,89,113	1.61	7 (13%)
24	CLA	t	301	11	45,53,73	1.80	5 (11%)	52,89,113	1.69	8 (15%)
24	CLA	A	818	12	65,73,73	1.50	5 (7%)	76,113,113	1.31	10 (13%)
24	CLA	k	301	9	46,54,73	1.77	5 (10%)	53,90,113	1.42	7 (13%)
26	DD6	9	314	-	39,45,45	1.65	7 (17%)	52,67,67	2.20	11 (21%)
24	CLA	5	603	5	45,53,73	1.83	5 (11%)	52,89,113	1.45	8 (15%)
24	CLA	6	609	-	50,58,73	1.74	8 (16%)	58,95,113	1.39	8 (13%)
24	CLA	6	611	6	43,52,73	1.83	7 (16%)	49,88,113	1.55	6 (12%)
24	CLA	c	611	10	41,49,73	1.88	5 (12%)	47,84,113	1.50	7 (14%)
24	CLA	5	605	5	46,54,73	1.78	5 (10%)	53,90,113	1.40	7 (13%)
24	CLA	9	310	9	46,54,73	1.79	6 (13%)	53,90,113	1.52	6 (11%)
24	CLA	B	808	13	65,73,73	1.52	9 (13%)	76,113,113	1.25	10 (13%)
24	CLA	k	304	9	46,54,73	1.82	6 (13%)	53,90,113	1.51	6 (11%)
26	DD6	k	314	-	39,45,45	1.53	9 (23%)	52,67,67	1.75	7 (13%)
24	CLA	R	103	22	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
27	LMT	A	851	-	26,26,36	0.82	0	37,37,47	1.05	5 (13%)
24	CLA	9	309	9	46,54,73	1.75	5 (10%)	53,90,113	1.48	7 (13%)
24	CLA	B	831	-	65,73,73	1.53	6 (9%)	76,113,113	1.24	8 (10%)
24	CLA	t	308	11	46,54,73	1.85	6 (13%)	53,90,113	1.31	7 (13%)
24	CLA	k	308	-	41,49,73	1.89	5 (12%)	47,84,113	1.78	7 (14%)
27	LMT	A	854	-	36,36,36	0.68	0	47,47,47	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	6	607	6	46,54,73	1.80	5 (10%)	53,90,113	1.35	7 (13%)
25	BCR	A	845	-	40,40,41	0.81	0	52,54,56	2.22	18 (34%)
24	CLA	A	815	-	45,53,73	1.83	5 (11%)	52,89,113	1.40	8 (15%)
24	CLA	3	303	-	55,63,73	1.64	5 (9%)	64,101,113	1.38	9 (14%)
25	BCR	A	844	-	41,41,41	0.84	0	56,56,56	2.12	18 (32%)
24	CLA	A	814	12	50,58,73	1.72	5 (10%)	58,95,113	1.43	8 (13%)
30	LMG	A	855	-	38,38,55	1.07	2 (5%)	46,46,63	1.08	2 (4%)
24	CLA	4	603	4	46,54,73	1.80	6 (13%)	53,90,113	1.40	7 (13%)
24	CLA	7	602	7	50,58,73	1.72	5 (10%)	58,95,113	1.67	12 (20%)
26	DD6	6	616	-	39,45,45	1.54	8 (20%)	52,67,67	2.05	12 (23%)
32	SF4	A	858	12,13	0,12,12	-	-	-	-	-
28	LHG	A	842	24	41,41,48	1.09	2 (4%)	44,47,54	1.28	5 (11%)
26	DD6	9	315	-	39,45,45	1.58	9 (23%)	52,67,67	1.74	10 (19%)
26	DD6	J	102	-	39,45,45	1.53	8 (20%)	52,67,67	1.65	11 (21%)
26	DD6	3	311	-	39,45,45	1.51	8 (20%)	52,67,67	1.63	10 (19%)
28	LHG	1	318	-	42,42,48	0.97	3 (7%)	45,48,54	1.39	4 (8%)
24	CLA	h	601	6	45,53,73	1.83	5 (11%)	52,89,113	1.51	8 (15%)
24	CLA	A	809	12	46,54,73	1.76	5 (10%)	53,90,113	1.40	7 (13%)
25	BCR	9	316	-	41,41,41	0.76	0	56,56,56	2.36	18 (32%)
26	DD6	4	614	-	39,45,45	1.52	8 (20%)	52,67,67	1.80	11 (21%)
28	LHG	A	841	-	47,47,48	0.93	2 (4%)	50,53,54	0.98	3 (6%)
24	CLA	4	605	4	46,54,73	1.76	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	B	837	13	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
24	CLA	F	203	17	50,58,73	1.71	5 (10%)	58,95,113	1.44	7 (12%)
31	PQN	A	839	-	34,34,34	0.35	0	42,45,45	0.61	1 (2%)
24	CLA	A	857	12	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
24	CLA	A	835	12	51,59,73	1.70	6 (11%)	59,96,113	1.40	9 (15%)
24	CLA	4	612	4	46,54,73	1.75	6 (13%)	53,90,113	1.51	6 (11%)
26	DD6	1	312	-	39,45,45	1.57	9 (23%)	52,67,67	1.51	7 (13%)
28	LHG	8	213	-	30,30,48	1.19	2 (6%)	33,36,54	1.47	4 (12%)
24	CLA	1	306	1	50,58,73	1.71	5 (10%)	58,95,113	1.43	10 (17%)
26	DD6	t	313	-	39,45,45	1.46	8 (20%)	52,67,67	1.72	11 (21%)
26	DD6	6	614	-	39,45,45	1.61	8 (20%)	52,67,67	1.46	6 (11%)
24	CLA	6	605	6	46,54,73	1.80	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	7	603	7	45,53,73	1.82	5 (11%)	52,89,113	1.45	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	11 (14%)
24	CLA	8	206	8	46,54,73	1.80	5 (10%)	53,90,113	1.45	7 (13%)
24	CLA	B	807	13	65,73,73	1.50	5 (7%)	76,113,113	1.29	8 (10%)
26	DD6	8	211	-	39,45,45	1.51	8 (20%)	52,67,67	1.78	9 (17%)
24	CLA	A	834	12	45,53,73	1.83	5 (11%)	52,89,113	1.47	8 (15%)
26	DD6	8	212	-	39,45,45	1.50	8 (20%)	52,67,67	1.64	10 (19%)
26	DD6	8	210	-	39,45,45	1.68	8 (20%)	52,67,67	2.09	12 (23%)
24	CLA	A	825	-	65,73,73	1.48	5 (7%)	76,113,113	1.28	8 (10%)
24	CLA	7	601	7	45,53,73	1.84	7 (15%)	52,89,113	1.42	8 (15%)
24	CLA	8	201	8	46,54,73	1.81	5 (10%)	53,90,113	1.36	7 (13%)
24	CLA	B	812	13	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)
26	DD6	7	615	-	39,45,45	1.49	8 (20%)	52,67,67	1.82	12 (23%)
24	CLA	t	307	-	46,54,73	1.80	5 (10%)	53,90,113	1.35	6 (11%)
24	CLA	k	307	9	46,54,73	1.81	6 (13%)	53,90,113	1.33	6 (11%)
24	CLA	3	307	-	45,53,73	1.81	6 (13%)	52,89,113	1.48	7 (13%)
24	CLA	B	821	13	53,61,73	1.65	6 (11%)	61,98,113	1.39	11 (18%)
24	CLA	t	309	-	46,54,73	1.81	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	B	826	13	65,73,73	1.55	7 (10%)	76,113,113	1.22	8 (10%)
24	CLA	3	306	3	65,73,73	1.51	6 (9%)	76,113,113	1.24	8 (10%)
24	CLA	4	613	4	46,54,73	1.82	6 (13%)	53,90,113	1.38	7 (13%)
25	BCR	M	101	-	41,41,41	0.74	0	56,56,56	2.14	16 (28%)
26	DD6	6	613	-	39,45,45	1.52	8 (20%)	52,67,67	1.66	8 (15%)
24	CLA	A	813	12	65,73,73	1.51	6 (9%)	76,113,113	1.23	9 (11%)
24	CLA	B	836	-	65,73,73	1.53	6 (9%)	76,113,113	1.21	7 (9%)
24	CLA	F	202	-	46,54,73	1.80	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	7	604	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
24	CLA	B	823	-	64,72,73	1.50	6 (9%)	74,111,113	1.30	9 (12%)
25	BCR	4	618	-	41,41,41	0.79	0	56,56,56	2.38	20 (35%)
24	CLA	A	821	12	49,57,73	1.72	5 (10%)	55,93,113	1.41	7 (12%)
24	CLA	k	311	-	55,63,73	1.64	5 (9%)	64,101,113	1.40	7 (10%)
24	CLA	4	606	4	46,54,73	1.77	5 (10%)	53,90,113	1.38	8 (15%)
26	DD6	7	613	-	39,45,45	1.48	8 (20%)	52,67,67	1.86	11 (21%)

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
25	BCR	L	206	-	-	4/29/63/63	0/2/2/2
24	CLA	1	301	1	1/1/15/20	11/37/115/115	-
25	BCR	B	841	-	-	2/29/63/63	0/2/2/2
25	BCR	I	102	-	-	0/29/63/63	0/2/2/2
24	CLA	B	804	13	1/1/15/20	13/37/115/115	-
24	CLA	A	827	12	1/1/14/20	11/34/112/115	-
29	A1L1G	7	614	-	-	12/29/85/85	0/3/3/3
26	DD6	c	613	-	-	0/26/80/80	0/3/3/3
26	DD6	5	608	-	-	4/26/80/80	0/3/3/3
26	DD6	7	618	-	-	3/26/80/80	0/3/3/3
24	CLA	k	306	9	1/1/11/20	5/15/93/115	-
24	CLA	1	308	1	1/1/11/20	5/15/93/115	-
24	CLA	4	602	4	1/1/14/20	11/31/109/115	-
24	CLA	5	607	5	1/1/11/20	5/13/91/115	-
24	CLA	4	607	4	1/1/11/20	8/15/93/115	-
24	CLA	B	813	13	1/1/11/20	8/15/93/115	-
29	A1L1G	3	310	-	-	16/29/85/85	0/3/3/3
28	LHG	3	315	-	-	26/47/47/53	-
24	CLA	A	831	12	1/1/15/20	12/37/115/115	-
24	CLA	J	103	19	1/1/10/20	6/10/88/115	-
24	CLA	k	303	-	-	10/25/103/115	-
27	LMT	1	316	-	-	8/21/61/61	0/2/2/2
24	CLA	3	305	3	1/1/14/20	8/31/109/115	-
26	DD6	R	105	-	-	6/26/80/80	0/3/3/3
24	CLA	B	838	28	1/1/15/20	7/37/115/115	-
24	CLA	A	807	12	1/1/15/20	16/37/115/115	-
24	CLA	B	824	13	1/1/15/20	9/37/115/115	-
24	CLA	L	205	-	1/1/11/20	6/15/93/115	-
26	DD6	4	616	-	-	4/26/80/80	0/3/3/3
26	DD6	h	614	-	-	4/26/80/80	0/3/3/3
24	CLA	9	302	9	1/1/11/20	7/15/93/115	-
24	CLA	8	202	8	1/1/11/20	9/15/93/115	-
27	LMT	A	850	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	3	301	3	-	15/37/115/115	-
24	CLA	A	819	12	1/1/11/20	2/13/91/115	-
24	CLA	B	803	-	1/1/15/20	8/37/115/115	-
24	CLA	B	829	13	1/1/15/20	9/37/115/115	-
24	CLA	A	805	12	1/1/15/20	11/37/115/115	-
28	LHG	A	852	-	-	9/41/41/53	-
24	CLA	B	816	13	1/1/15/20	12/37/115/115	-
24	CLA	7	605	7	1/1/11/20	4/15/93/115	-
24	CLA	t	310	-	1/1/11/20	6/15/93/115	-
24	CLA	2	207	-	1/1/11/20	6/15/93/115	-
24	CLA	k	310	9	1/1/10/20	2/8/86/115	-
24	CLA	A	828	12	1/1/15/20	12/37/115/115	-
24	CLA	k	309	9	1/1/11/20	5/13/91/115	-
28	LHG	I	103	-	-	13/44/44/53	-
24	CLA	B	810	13	1/1/13/20	8/25/101/115	-
26	DD6	A	848	-	-	1/26/80/80	0/3/3/3
24	CLA	A	817	12	1/1/15/20	11/37/115/115	-
24	CLA	6	606	6	1/1/11/20	9/15/93/115	-
24	CLA	3	308	3	1/1/11/20	8/15/93/115	-
26	DD6	4	617	-	-	1/26/80/80	0/3/3/3
24	CLA	A	837	12	1/1/13/20	8/25/103/115	-
24	CLA	c	603	10	1/1/11/20	9/15/93/115	-
24	CLA	t	304	-	1/1/11/20	5/15/93/115	-
24	CLA	c	604	-	1/1/11/20	8/15/93/115	-
24	CLA	A	811	12	1/1/11/20	6/15/93/115	-
26	DD6	c	614	-	-	1/26/80/80	0/3/3/3
30	LMG	t	314	-	-	6/29/49/70	0/1/1/1
24	CLA	2	201	2	1/1/11/20	9/13/91/115	-
25	BCR	B	843	-	-	4/29/63/63	0/2/2/2
24	CLA	h	605	6	1/1/11/20	4/15/93/115	-
24	CLA	4	608	-	1/1/12/20	7/19/97/115	-
28	LHG	B	845	24	-	9/45/45/53	-
24	CLA	A	856	-	-	11/37/115/115	-
24	CLA	A	812	12	1/1/15/20	13/37/115/115	-
24	CLA	B	820	13	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	5	606	-	1/1/11/20	6/15/93/115	-
24	CLA	3	304	3	1/1/11/20	6/15/93/115	-
24	CLA	2	206	2	1/1/11/20	5/15/93/115	-
26	DD6	k	315	-	-	3/26/80/80	0/3/3/3
25	BCR	k	316	-	-	3/29/63/63	0/2/2/2
24	CLA	A	826	12	1/1/15/20	11/37/115/115	-
28	LHG	J	105	-	-	12/42/42/53	-
24	CLA	B	817	13	1/1/15/20	18/37/115/115	-
26	DD6	1	313	-	-	1/26/80/80	0/3/3/3
24	CLA	7	612	7	1/1/11/20	8/15/93/115	-
24	CLA	B	833	13	1/1/13/20	6/29/107/115	-
24	CLA	h	603	6	1/1/11/20	4/13/91/115	-
24	CLA	c	602	10	1/1/15/20	12/37/115/115	-
24	CLA	t	302	11	1/1/11/20	12/15/93/115	-
24	CLA	1	309	1	1/1/11/20	2/13/91/115	-
24	CLA	9	307	9	1/1/11/20	7/15/93/115	-
26	DD6	6	615	-	-	4/26/80/80	0/3/3/3
29	A1L1G	9	312	-	-	13/29/85/85	0/3/3/3
25	BCR	1	314	-	-	8/29/63/63	0/2/2/2
24	CLA	B	830	13	1/1/13/20	8/29/107/115	-
24	CLA	A	804	12	1/1/15/20	15/37/115/115	-
26	DD6	6	617	-	-	1/26/80/80	0/3/3/3
24	CLA	A	801	12	1/1/15/20	16/37/115/115	-
25	BCR	7	617	-	-	2/29/63/63	0/2/2/2
25	BCR	B	840	-	-	4/29/63/63	0/2/2/2
28	LHG	2	215	-	-	9/35/35/53	-
25	BCR	1	310	-	-	3/29/63/63	0/2/2/2
24	CLA	B	818	-	1/1/15/20	12/37/115/115	-
24	CLA	B	848	13	1/1/15/20	10/37/115/115	-
24	CLA	1	305	1	1/1/11/20	7/13/91/115	-
24	CLA	A	802	-	1/1/15/20	6/37/115/115	-
24	CLA	9	305	-	-	10/15/93/115	-
26	DD6	5	609	-	-	1/26/80/80	0/3/3/3
25	BCR	R	101	-	-	4/29/63/63	0/2/2/2
24	CLA	6	603	6	1/1/11/20	8/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	3	313	-	-	3/26/80/80	0/3/3/3
24	CLA	7	609	7	1/1/11/20	7/15/93/115	-
24	CLA	4	610	4	1/1/10/20	2/8/86/115	-
24	CLA	A	808	12	1/1/15/20	9/37/115/115	-
24	CLA	8	204	8	1/1/11/20	4/13/91/115	-
26	DD6	9	313	-	-	3/26/80/80	0/3/3/3
25	BCR	F	204	-	-	2/29/63/63	0/2/2/2
24	CLA	A	824	-	1/1/15/20	15/37/115/115	-
24	CLA	1	302	1	1/1/11/20	6/13/91/115	-
26	DD6	h	615	-	-	3/26/80/80	0/3/3/3
24	CLA	3	309	3	1/1/10/20	2/8/86/115	-
24	CLA	2	204	2	1/1/14/20	10/31/109/115	-
24	CLA	B	828	13	1/1/12/20	9/19/97/115	-
24	CLA	6	608	6	1/1/11/20	4/15/93/115	-
32	SF4	C	102	14	-	-	0/6/5/5
24	CLA	F	201	-	1/1/15/20	12/37/115/115	-
24	CLA	5	602	5	1/1/13/20	10/25/103/115	-
25	BCR	R	102	-	-	4/29/63/63	0/2/2/2
27	LMT	3	314	-	-	9/16/56/61	0/2/2/2
24	CLA	9	301	9	1/1/11/20	8/15/93/115	-
25	BCR	B	849	-	-	4/29/63/63	0/2/2/2
24	CLA	B	847	13	1/1/15/20	14/37/115/115	-
29	A1L1G	2	213	-	-	19/29/85/85	0/3/3/3
24	CLA	6	601	6	1/1/11/20	6/13/91/115	-
24	CLA	7	606	7	1/1/14/20	12/31/109/115	-
24	CLA	7	607	7	1/1/11/20	3/13/91/115	-
31	PQN	B	839	-	-	10/23/43/43	0/2/2/2
24	CLA	9	308	-	1/1/11/20	8/15/93/115	-
24	CLA	A	840	28	1/1/15/20	11/37/115/115	-
24	CLA	t	303	11	1/1/15/20	15/37/115/115	-
24	CLA	B	846	13	1/1/13/20	8/25/103/115	-
28	LHG	L	201	-	-	15/33/33/53	-
24	CLA	A	816	12	1/1/15/20	13/37/115/115	-
24	CLA	1	304	26	1/1/13/20	11/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	8	203	-	1/1/12/20	8/19/97/115	-
24	CLA	c	605	10	1/1/11/20	10/15/93/115	-
25	BCR	2	211	-	-	4/29/63/63	0/2/2/2
24	CLA	c	609	-	1/1/14/20	11/31/109/115	-
24	CLA	A	823	12	1/1/15/20	19/37/115/115	-
27	LMT	1	315	-	-	12/21/61/61	0/2/2/2
25	BCR	A	846	-	-	2/29/63/63	0/2/2/2
24	CLA	A	806	12	1/1/15/20	10/37/115/115	-
24	CLA	B	832	-	1/1/11/20	9/13/91/115	-
24	CLA	c	610	10	1/1/11/20	3/11/89/115	-
24	CLA	h	607	6	1/1/11/20	4/15/93/115	-
26	DD6	t	311	-	-	2/26/80/80	0/3/3/3
25	BCR	A	843	-	-	4/29/63/63	0/2/2/2
28	LHG	A	849	-	-	13/45/45/53	-
24	CLA	h	611	6	-	4/8/86/115	-
24	CLA	9	304	9	1/1/11/20	6/15/93/115	-
24	CLA	B	835	13	1/1/11/20	7/16/94/115	-
24	CLA	t	306	11	1/1/11/20	8/13/91/115	-
24	CLA	B	825	13	1/1/13/20	8/25/103/115	-
24	CLA	5	601	5	1/1/11/20	3/13/91/115	-
24	CLA	3	302	3	1/1/11/20	3/13/91/115	-
24	CLA	8	207	-	1/1/11/20	7/13/91/115	-
24	CLA	6	604	-	1/1/11/20	4/15/93/115	-
24	CLA	4	601	4	1/1/10/20	3/9/87/115	-
24	CLA	c	607	10	1/1/11/20	3/15/93/115	-
24	CLA	4	604	-	1/1/11/20	8/15/93/115	-
26	DD6	7	616	-	-	2/26/80/80	0/3/3/3
30	LMG	2	214	-	-	8/40/60/70	0/1/1/1
26	DD6	4	615	-	-	1/26/80/80	0/3/3/3
24	CLA	6	610	6	1/1/11/20	4/15/93/115	-
24	CLA	7	608	-	1/1/11/20	6/13/91/115	-
24	CLA	h	609	-	1/1/11/20	5/15/93/115	-
24	CLA	h	610	6	1/1/11/20	7/15/93/115	-
24	CLA	1	317	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	k	302	9	1/1/11/20	9/15/93/115	-
24	CLA	A	833	12	1/1/15/20	5/37/115/115	-
29	A1L1G	k	312	-	-	8/29/85/85	0/3/3/3
24	CLA	1	307	1	1/1/11/20	4/13/91/115	-
24	CLA	A	836	12	1/1/15/20	13/37/115/115	-
26	DD6	9	317	-	-	2/26/80/80	0/3/3/3
24	CLA	B	814	13	1/1/12/20	3/19/97/115	-
25	BCR	L	202	-	-	6/29/63/63	0/2/2/2
24	CLA	B	806	13	1/1/15/20	9/37/115/115	-
24	CLA	4	611	-	1/1/11/20	6/15/93/115	-
25	BCR	J	104	-	-	2/29/63/63	0/2/2/2
24	CLA	A	803	12	-	6/25/103/115	-
26	DD6	k	313	-	-	1/26/80/80	0/3/3/3
26	DD6	h	616	-	-	2/26/80/80	0/3/3/3
24	CLA	8	205	8	1/1/11/20	7/13/91/115	-
24	CLA	8	209	-	1/1/10/20	3/8/86/115	-
24	CLA	h	608	6	1/1/11/20	5/15/93/115	-
24	CLA	B	801	-	1/1/15/20	13/37/115/115	-
25	BCR	t	312	-	-	8/29/63/63	0/2/2/2
24	CLA	6	612	-	1/1/11/20	1/15/93/115	-
25	BCR	J	101	-	-	2/29/63/63	0/2/2/2
24	CLA	A	860	12	1/1/15/20	6/37/115/115	-
27	LMT	h	617	-	-	7/14/54/61	0/2/2/2
24	CLA	B	815	13	1/1/13/20	11/25/103/115	-
24	CLA	B	809	13	1/1/15/20	10/37/115/115	-
24	CLA	B	834	13	1/1/15/20	10/37/115/115	-
24	CLA	6	602	6	1/1/11/20	6/16/94/115	-
24	CLA	A	820	-	1/1/15/20	10/37/115/115	-
24	CLA	h	612	-	1/1/11/20	7/13/91/115	-
24	CLA	A	832	12	-	12/37/115/115	-
26	DD6	2	210	-	-	1/26/80/80	0/3/3/3
24	CLA	5	604	5	1/1/11/20	1/15/93/115	-
24	CLA	L	204	20	-	9/37/115/115	-
24	CLA	B	827	13	1/1/15/20	12/37/115/115	-
24	CLA	t	305	11	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	k	305	9	1/1/11/20	6/15/93/115	-
24	CLA	h	606	6	1/1/11/20	5/15/93/115	-
24	CLA	7	611	7	1/1/11/20	7/15/93/115	-
24	CLA	2	203	-	1/1/12/20	5/19/97/115	-
24	CLA	A	838	12	1/1/15/20	10/37/115/115	-
24	CLA	L	203	20	1/1/13/20	10/25/103/115	-
26	DD6	1	311	24	-	0/26/80/80	0/3/3/3
24	CLA	1	303	1	1/1/11/20	6/15/93/115	-
26	DD6	3	312	-	-	1/26/80/80	0/3/3/3
28	LHG	B	844	-	-	16/53/53/53	-
24	CLA	A	822	12	1/1/13/20	14/25/103/115	-
24	CLA	B	805	13	1/1/15/20	11/37/115/115	-
24	CLA	c	601	10	1/1/10/20	5/11/89/115	-
26	DD6	c	612	-	-	1/26/80/80	0/3/3/3
24	CLA	7	610	7	1/1/11/20	6/13/91/115	-
24	CLA	9	306	9	1/1/11/20	5/15/93/115	-
24	CLA	A	853	12	1/1/13/20	7/25/103/115	-
26	DD6	2	212	-	-	1/26/80/80	0/3/3/3
24	CLA	8	208	8	1/1/11/20	5/13/91/115	-
24	CLA	A	829	12	1/1/15/20	8/37/115/115	-
24	CLA	A	847	-	1/1/13/20	10/25/103/115	-
25	BCR	I	101	-	-	4/29/63/63	0/2/2/2
24	CLA	B	802	13	1/1/15/20	17/37/115/115	-
24	CLA	B	811	13	1/1/13/20	5/25/103/115	-
24	CLA	c	608	10	1/1/15/20	13/37/115/115	-
24	CLA	c	606	10	1/1/11/20	6/15/93/115	-
32	SF4	C	101	14	-	-	0/6/5/5
24	CLA	4	609	4	1/1/11/20	6/15/93/115	-
24	CLA	A	830	12	-	8/25/103/115	-
24	CLA	9	311	-	1/1/11/20	6/13/91/115	-
25	BCR	c	615	-	-	10/29/63/63	0/2/2/2
24	CLA	9	303	-	1/1/11/20	8/15/93/115	-
24	CLA	A	810	12	1/1/14/20	13/34/112/115	-
24	CLA	2	208	-	1/1/11/20	6/15/93/115	-
25	BCR	A	859	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	602	6	1/1/13/20	7/25/103/115	-
24	CLA	h	604	-	1/1/11/20	5/15/93/115	-
24	CLA	B	819	13	1/1/11/20	2/15/93/115	-
28	LHG	4	619	-	-	8/43/43/53	-
24	CLA	2	202	2	1/1/13/20	6/25/103/115	-
24	CLA	2	205	2	-	4/15/93/115	-
24	CLA	2	209	-	1/1/11/20	7/15/93/115	-
26	DD6	h	613	-	-	1/26/80/80	0/3/3/3
25	BCR	B	842	-	-	3/29/63/63	0/2/2/2
24	CLA	R	104	22	1/1/11/20	3/13/91/115	-
24	CLA	t	301	11	1/1/11/20	4/13/91/115	-
24	CLA	A	818	12	1/1/15/20	15/37/115/115	-
24	CLA	k	301	9	1/1/11/20	4/15/93/115	-
26	DD6	9	314	-	-	2/26/80/80	0/3/3/3
24	CLA	5	603	5	1/1/11/20	4/13/91/115	-
24	CLA	6	609	-	1/1/12/20	7/19/97/115	-
24	CLA	6	611	6	1/1/11/20	4/11/89/115	-
24	CLA	c	611	10	1/1/10/20	4/8/86/115	-
24	CLA	5	605	5	1/1/11/20	9/15/93/115	-
24	CLA	9	310	9	1/1/11/20	6/15/93/115	-
24	CLA	B	808	13	1/1/15/20	8/37/115/115	-
24	CLA	k	304	9	1/1/11/20	7/15/93/115	-
26	DD6	k	314	-	-	2/26/80/80	0/3/3/3
24	CLA	R	103	22	1/1/15/20	9/37/115/115	-
27	LMT	A	851	-	-	4/11/51/61	0/2/2/2
24	CLA	9	309	9	1/1/11/20	9/15/93/115	-
24	CLA	B	831	-	1/1/15/20	19/37/115/115	-
24	CLA	t	308	11	1/1/11/20	6/15/93/115	-
24	CLA	k	308	-	1/1/10/20	6/8/86/115	-
27	LMT	A	854	-	-	9/21/61/61	0/2/2/2
24	CLA	6	607	6	1/1/11/20	4/15/93/115	-
25	BCR	A	845	-	-	5/29/60/63	0/2/2/2
24	CLA	A	815	-	1/1/11/20	6/13/91/115	-
24	CLA	3	303	-	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	A	844	-	-	6/29/63/63	0/2/2/2
24	CLA	A	814	12	1/1/12/20	7/19/97/115	-
30	LMG	A	855	-	-	5/33/53/70	0/1/1/1
24	CLA	4	603	4	1/1/11/20	3/15/93/115	-
24	CLA	7	602	7	1/1/12/20	9/19/97/115	-
26	DD6	6	616	-	-	4/26/80/80	0/3/3/3
32	SF4	A	858	12,13	-	-	0/6/5/5
28	LHG	A	842	24	-	10/46/46/53	-
26	DD6	9	315	-	-	4/26/80/80	0/3/3/3
26	DD6	J	102	-	-	2/26/80/80	0/3/3/3
26	DD6	3	311	-	-	1/26/80/80	0/3/3/3
28	LHG	1	318	-	-	15/47/47/53	-
24	CLA	h	601	6	1/1/11/20	5/13/91/115	-
24	CLA	A	809	12	1/1/11/20	6/15/93/115	-
25	BCR	9	316	-	-	2/29/63/63	0/2/2/2
26	DD6	4	614	-	-	1/26/80/80	0/3/3/3
28	LHG	A	841	-	-	19/52/52/53	-
24	CLA	4	605	4	1/1/11/20	4/15/93/115	-
24	CLA	B	837	13	1/1/15/20	15/37/115/115	-
24	CLA	F	203	17	1/1/12/20	7/19/97/115	-
31	PQN	A	839	-	-	5/23/43/43	0/2/2/2
24	CLA	A	857	12	1/1/15/20	9/37/115/115	-
24	CLA	A	835	12	1/1/12/20	5/21/99/115	-
24	CLA	4	612	4	1/1/11/20	5/15/93/115	-
26	DD6	1	312	-	-	0/26/80/80	0/3/3/3
28	LHG	8	213	-	-	17/35/35/53	-
24	CLA	1	306	1	1/1/12/20	4/19/97/115	-
26	DD6	t	313	-	-	0/26/80/80	0/3/3/3
26	DD6	6	614	-	-	1/26/80/80	0/3/3/3
24	CLA	6	605	6	-	2/15/93/115	-
24	CLA	7	603	7	1/1/11/20	2/13/91/115	-
24	CLA	B	822	-	1/1/15/20	12/37/115/115	-
24	CLA	8	206	8	1/1/11/20	8/15/93/115	-
24	CLA	B	807	13	-	7/37/115/115	-
26	DD6	8	211	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	834	12	1/1/11/20	4/13/91/115	-
26	DD6	8	212	-	-	2/26/80/80	0/3/3/3
26	DD6	8	210	-	-	3/26/80/80	0/3/3/3
24	CLA	A	825	-	1/1/15/20	6/37/115/115	-
24	CLA	7	601	7	1/1/11/20	6/13/91/115	-
24	CLA	8	201	8	1/1/11/20	4/15/93/115	-
24	CLA	B	812	13	1/1/15/20	16/37/115/115	-
26	DD6	7	615	-	-	3/26/80/80	0/3/3/3
24	CLA	t	307	-	1/1/11/20	7/15/93/115	-
24	CLA	k	307	9	1/1/11/20	6/15/93/115	-
24	CLA	3	307	-	1/1/11/20	4/13/91/115	-
24	CLA	B	821	13	1/1/12/20	11/23/101/115	-
24	CLA	t	309	-	1/1/11/20	4/15/93/115	-
24	CLA	B	826	13	1/1/15/20	8/37/115/115	-
24	CLA	3	306	3	1/1/15/20	10/37/115/115	-
24	CLA	4	613	4	1/1/11/20	11/15/93/115	-
25	BCR	M	101	-	-	9/29/63/63	0/2/2/2
26	DD6	6	613	-	-	2/26/80/80	0/3/3/3
24	CLA	A	813	12	1/1/15/20	12/37/115/115	-
24	CLA	B	836	-	1/1/15/20	12/37/115/115	-
24	CLA	F	202	-	1/1/11/20	3/15/93/115	-
24	CLA	7	604	-	1/1/11/20	6/13/91/115	-
24	CLA	B	823	-	1/1/14/20	7/36/114/115	-
25	BCR	4	618	-	-	1/29/63/63	0/2/2/2
24	CLA	A	821	12	1/1/11/20	2/18/96/115	-
24	CLA	k	311	-	1/1/13/20	7/25/103/115	-
24	CLA	4	606	4	1/1/11/20	2/15/93/115	-
26	DD6	7	613	-	-	0/26/80/80	0/3/3/3

The worst 5 of 1747 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	308	CLA	C4B-NB	8.30	1.42	1.35
24	B	824	CLA	C4B-NB	8.24	1.42	1.35
24	4	604	CLA	C4B-NB	8.21	1.42	1.35
24	t	308	CLA	C4B-NB	8.18	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	308	CLA	C4B-NB	8.11	1.42	1.35

The worst 5 of 2909 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	830	CLA	C4A-NA-C1A	9.33	110.90	106.71
26	9	314	DD6	C3-C2-C1	-8.92	114.58	127.31
26	8	210	DD6	C14-C13-C11	-8.74	111.97	125.53
25	c	615	BCR	C20-C21-C22	-8.66	114.95	127.31
26	k	315	DD6	C3-C2-C1	-8.60	115.04	127.31

5 of 218 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	301	CLA	ND
24	1	302	CLA	ND
24	1	303	CLA	ND
24	1	304	CLA	ND
24	1	305	CLA	ND

5 of 2325 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	301	CLA	C1A-C2A-CAA-CBA
24	1	301	CLA	C3A-C2A-CAA-CBA
24	1	301	CLA	CBD-CGD-O2D-CED
24	1	303	CLA	CHA-CBD-CGD-O1D
24	1	303	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

205 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	301	CLA	2	0
25	B	841	BCR	2	0
25	I	102	BCR	2	0
24	B	804	CLA	6	0
26	c	613	DD6	1	0
26	5	608	DD6	2	0
26	7	618	DD6	1	0
24	4	602	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	5	607	CLA	2	0
24	4	607	CLA	4	0
29	3	310	A1L1G	2	0
28	3	315	LHG	1	0
24	J	103	CLA	1	0
27	1	316	LMT	2	0
24	3	305	CLA	1	0
24	B	838	CLA	2	0
24	B	824	CLA	2	0
24	L	205	CLA	5	0
26	h	614	DD6	1	0
24	9	302	CLA	2	0
24	A	819	CLA	1	0
24	B	803	CLA	4	0
24	B	829	CLA	4	0
24	A	805	CLA	1	0
24	2	207	CLA	1	0
24	k	309	CLA	1	0
28	I	103	LHG	1	0
24	B	810	CLA	1	0
24	A	817	CLA	2	0
24	6	606	CLA	1	0
24	3	308	CLA	2	0
24	c	603	CLA	1	0
24	2	201	CLA	3	0
25	B	843	BCR	5	0
24	4	608	CLA	4	0
24	A	812	CLA	1	0
24	5	606	CLA	1	0
24	3	304	CLA	5	0
24	2	206	CLA	2	0
26	k	315	DD6	3	0
25	k	316	BCR	2	0
24	A	826	CLA	2	0
28	J	105	LHG	1	0
24	B	817	CLA	2	0
26	1	313	DD6	1	0
24	7	612	CLA	2	0
24	B	833	CLA	2	0
24	c	602	CLA	2	0
24	t	302	CLA	1	0
26	6	615	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	9	312	A1L1G	1	0
25	1	314	BCR	3	0
24	B	830	CLA	7	0
24	A	804	CLA	1	0
24	A	801	CLA	1	0
25	7	617	BCR	2	0
25	B	840	BCR	1	0
25	1	310	BCR	4	0
24	B	848	CLA	1	0
24	1	305	CLA	4	0
24	A	802	CLA	2	0
24	9	305	CLA	3	0
26	5	609	DD6	1	0
24	6	603	CLA	3	0
24	8	204	CLA	2	0
26	9	313	DD6	2	0
25	F	204	BCR	2	0
24	A	824	CLA	1	0
24	1	302	CLA	1	0
24	2	204	CLA	1	0
24	B	828	CLA	1	0
24	6	608	CLA	1	0
25	R	102	BCR	2	0
27	3	314	LMT	1	0
24	9	301	CLA	8	0
25	B	849	BCR	1	0
24	B	847	CLA	1	0
24	6	601	CLA	3	0
24	7	606	CLA	4	0
24	7	607	CLA	4	0
24	9	308	CLA	2	0
24	A	840	CLA	1	0
24	B	846	CLA	1	0
28	L	201	LHG	4	0
24	A	816	CLA	1	0
24	1	304	CLA	3	0
24	8	203	CLA	2	0
25	2	211	BCR	4	0
24	A	823	CLA	1	0
25	A	846	BCR	2	0
24	B	832	CLA	3	0
24	c	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	843	BCR	2	0
24	B	835	CLA	1	0
24	t	306	CLA	1	0
24	B	825	CLA	1	0
24	c	607	CLA	1	0
30	2	214	LMG	1	0
26	4	615	DD6	1	0
24	h	610	CLA	1	0
24	1	317	CLA	2	0
29	k	312	A1L1G	2	0
24	1	307	CLA	2	0
26	9	317	DD6	1	0
25	L	202	BCR	2	0
24	B	806	CLA	1	0
24	4	611	CLA	10	0
25	J	104	BCR	1	0
26	k	313	DD6	1	0
24	8	209	CLA	1	0
24	h	608	CLA	2	0
24	B	801	CLA	1	0
25	t	312	BCR	2	0
25	J	101	BCR	4	0
27	h	617	LMT	1	0
24	B	815	CLA	1	0
24	B	834	CLA	2	0
24	6	602	CLA	2	0
24	h	612	CLA	2	0
24	A	832	CLA	1	0
26	2	210	DD6	1	0
24	5	604	CLA	2	0
24	L	204	CLA	1	0
24	B	827	CLA	1	0
24	t	305	CLA	3	0
24	k	305	CLA	1	0
24	7	611	CLA	2	0
24	A	838	CLA	1	0
26	1	311	DD6	5	0
24	1	303	CLA	1	0
26	3	312	DD6	1	0
24	B	805	CLA	3	0
24	c	601	CLA	2	0
26	c	612	DD6	2	0

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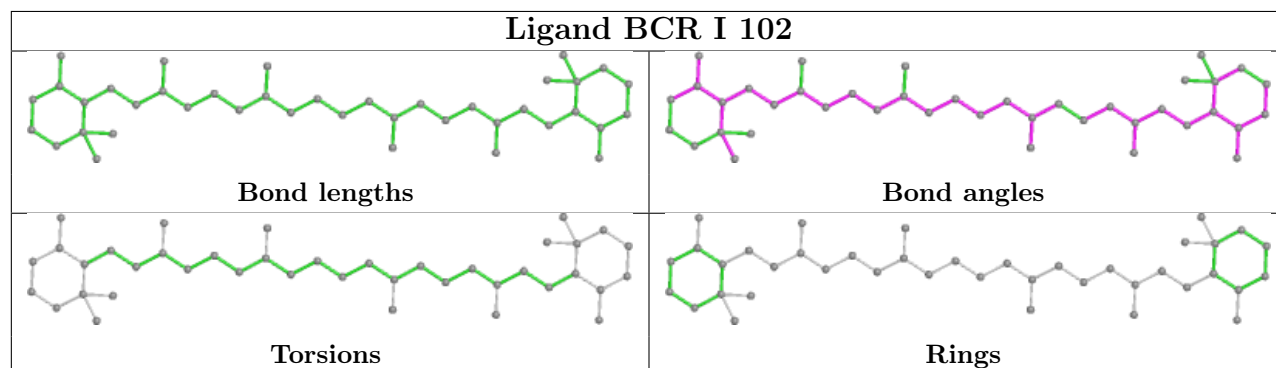
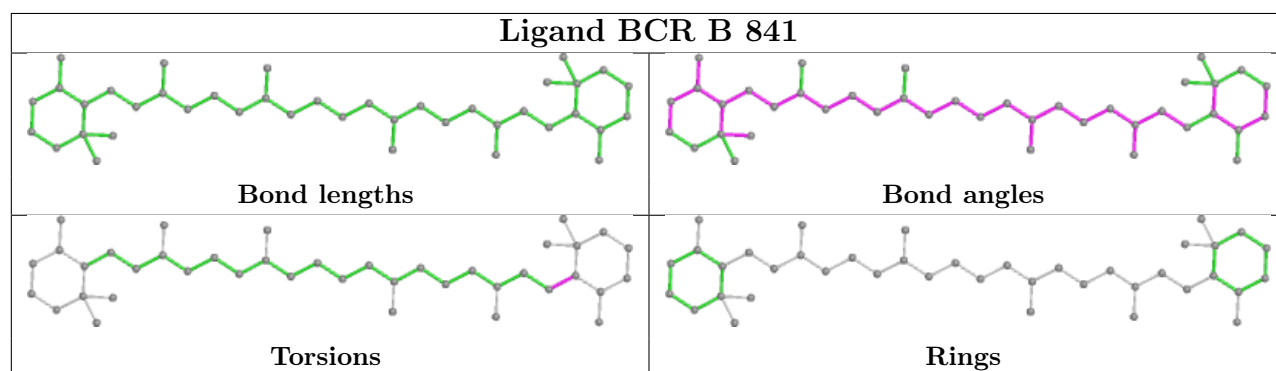
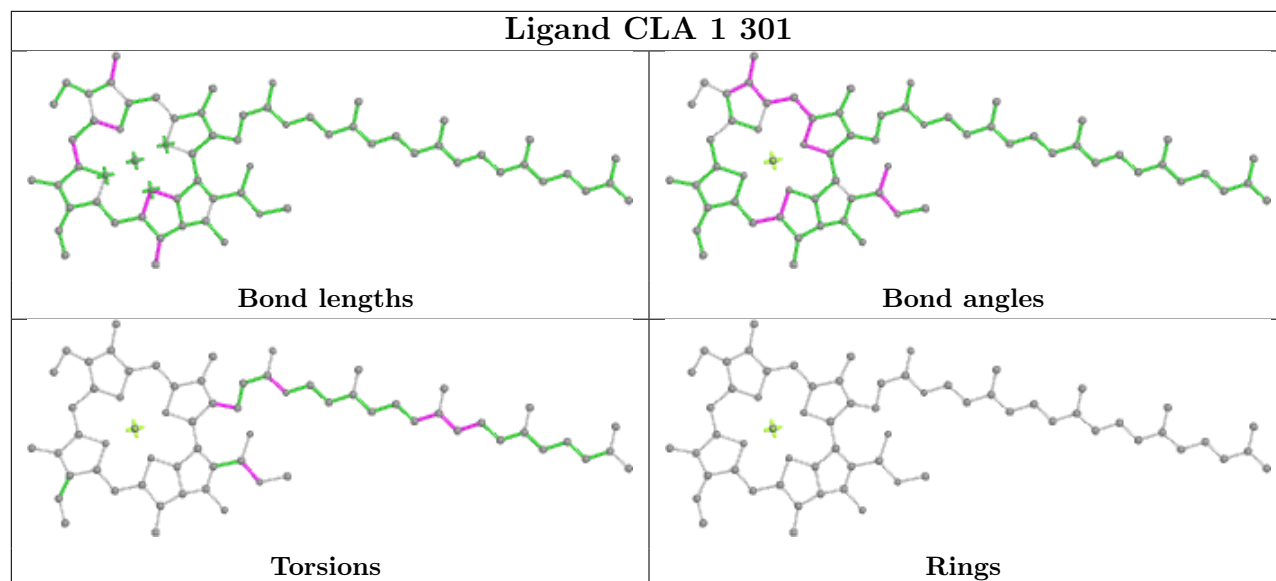
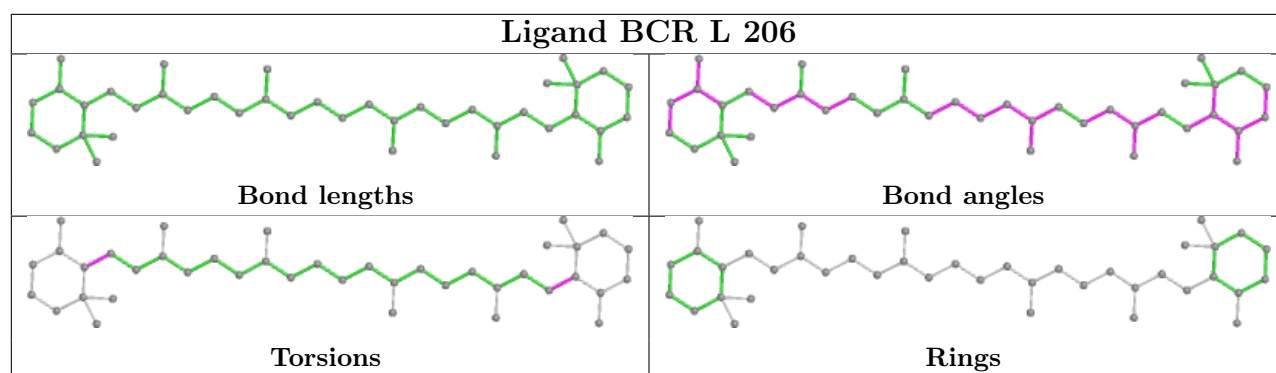
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24	7	610	CLA	2	0
24	A	853	CLA	2	0
26	2	212	DD6	1	0
24	A	829	CLA	2	0
24	A	847	CLA	1	0
25	I	101	BCR	1	0
24	B	802	CLA	2	0
24	B	811	CLA	1	0
24	4	609	CLA	2	0
24	A	830	CLA	6	0
24	9	311	CLA	1	0
25	c	615	BCR	7	0
24	9	303	CLA	1	0
24	A	810	CLA	1	0
25	A	859	BCR	1	0
28	4	619	LHG	1	0
24	2	202	CLA	1	0
24	2	205	CLA	1	0
24	2	209	CLA	4	0
25	B	842	BCR	2	0
24	A	818	CLA	3	0
24	k	301	CLA	4	0
24	6	611	CLA	1	0
24	5	605	CLA	2	0
24	9	310	CLA	2	0
24	B	808	CLA	2	0
24	k	304	CLA	2	0
24	R	103	CLA	1	0
27	A	851	LMT	1	0
24	B	831	CLA	3	0
24	t	308	CLA	1	0
24	k	308	CLA	2	0
27	A	854	LMT	3	0
24	6	607	CLA	2	0
25	A	845	BCR	1	0
25	A	844	BCR	3	0
24	A	814	CLA	1	0
24	7	602	CLA	9	0
28	A	842	LHG	2	0
26	9	315	DD6	3	0
28	1	318	LHG	2	0
25	9	316	BCR	9	0

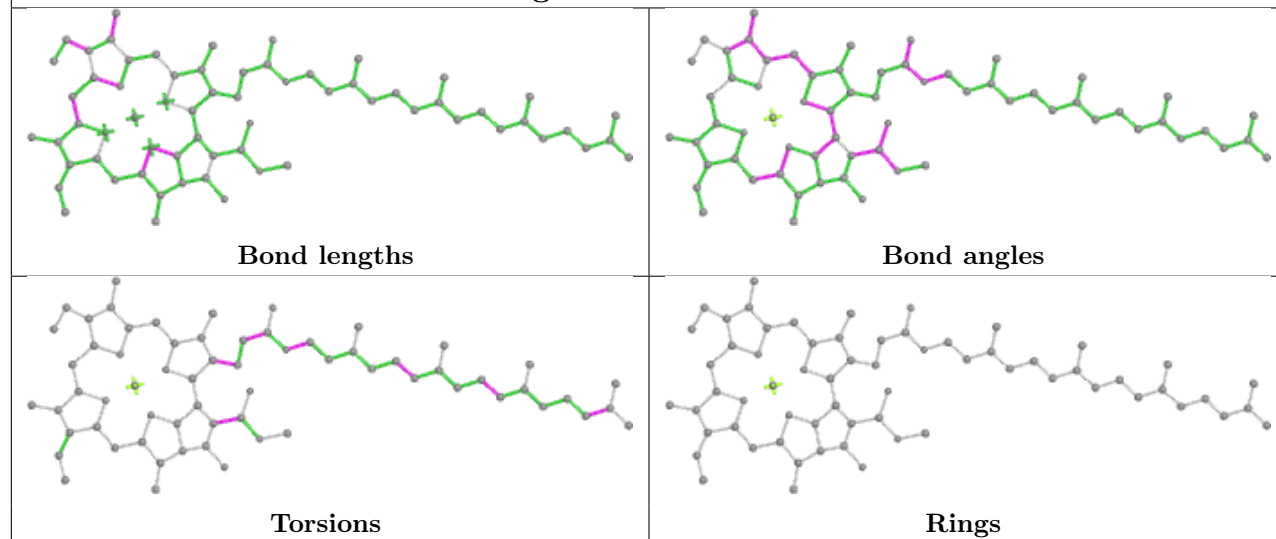
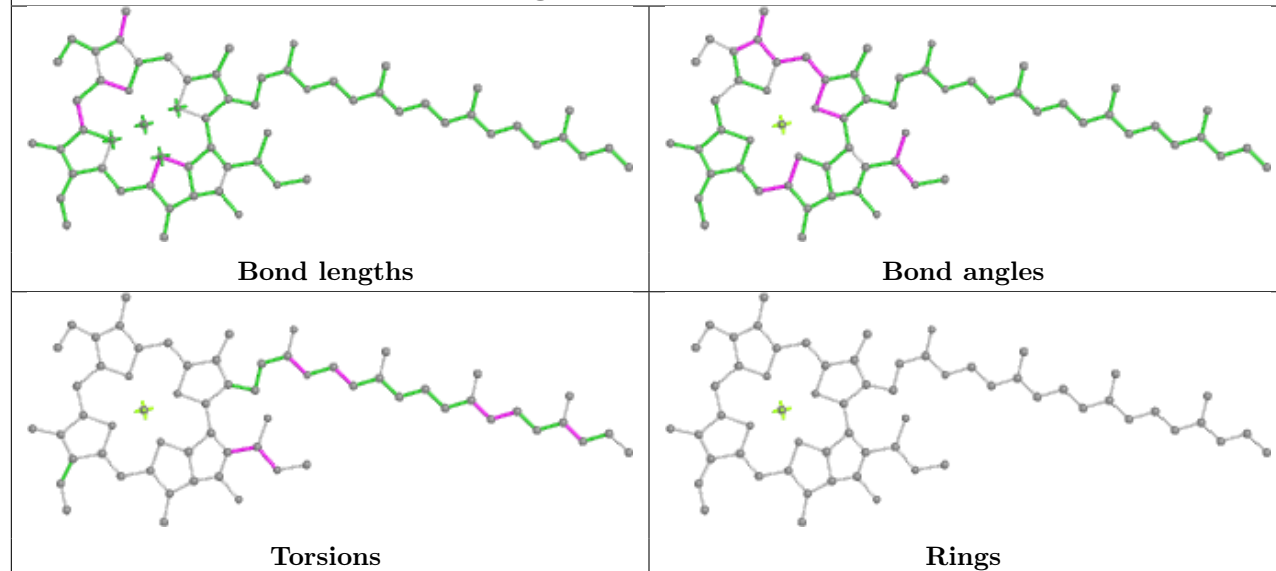
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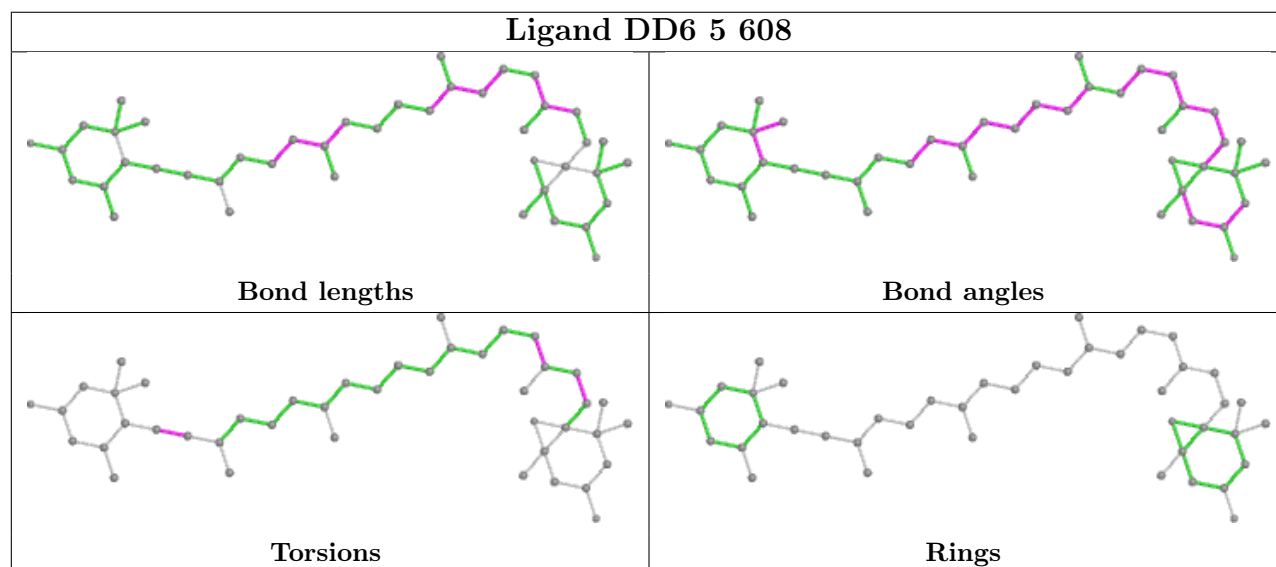
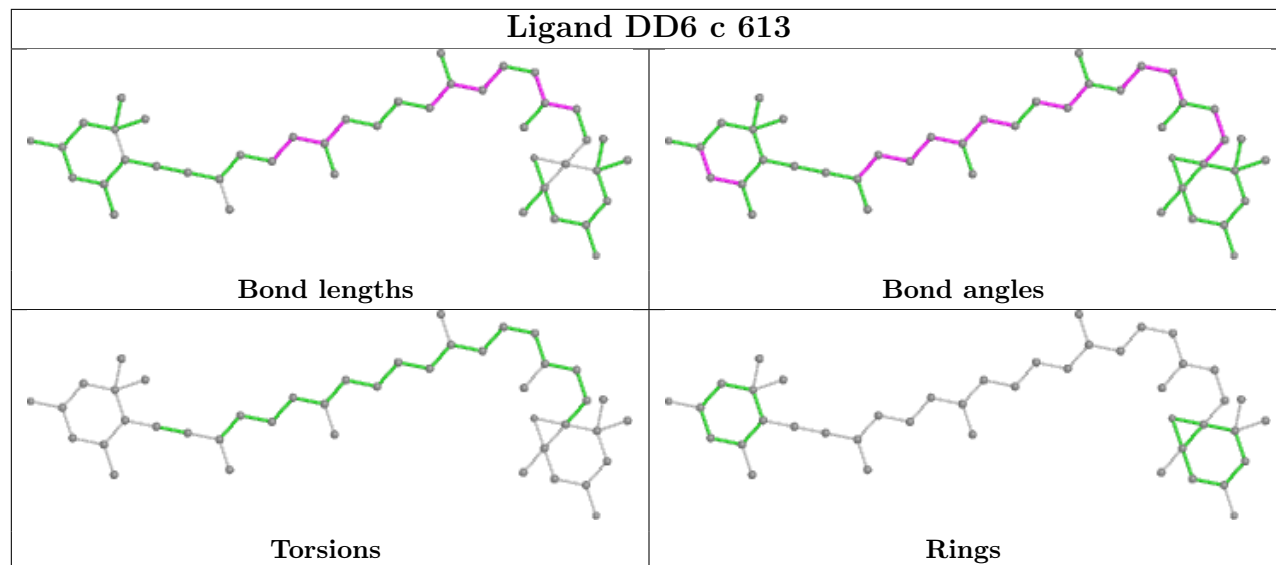
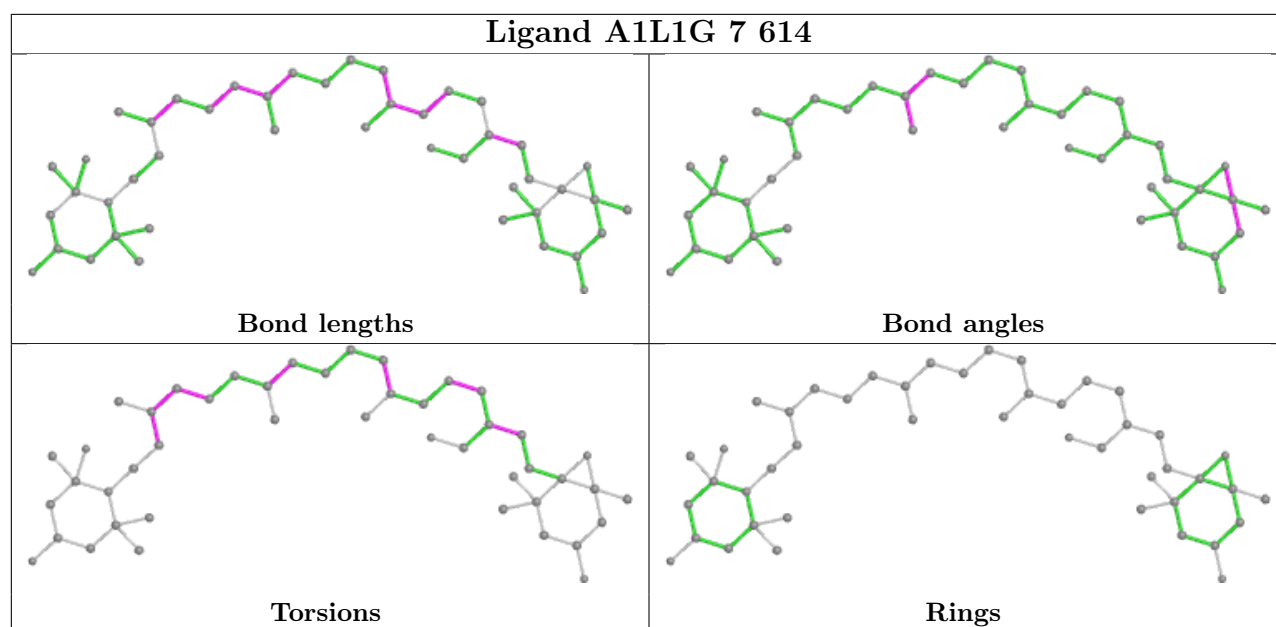
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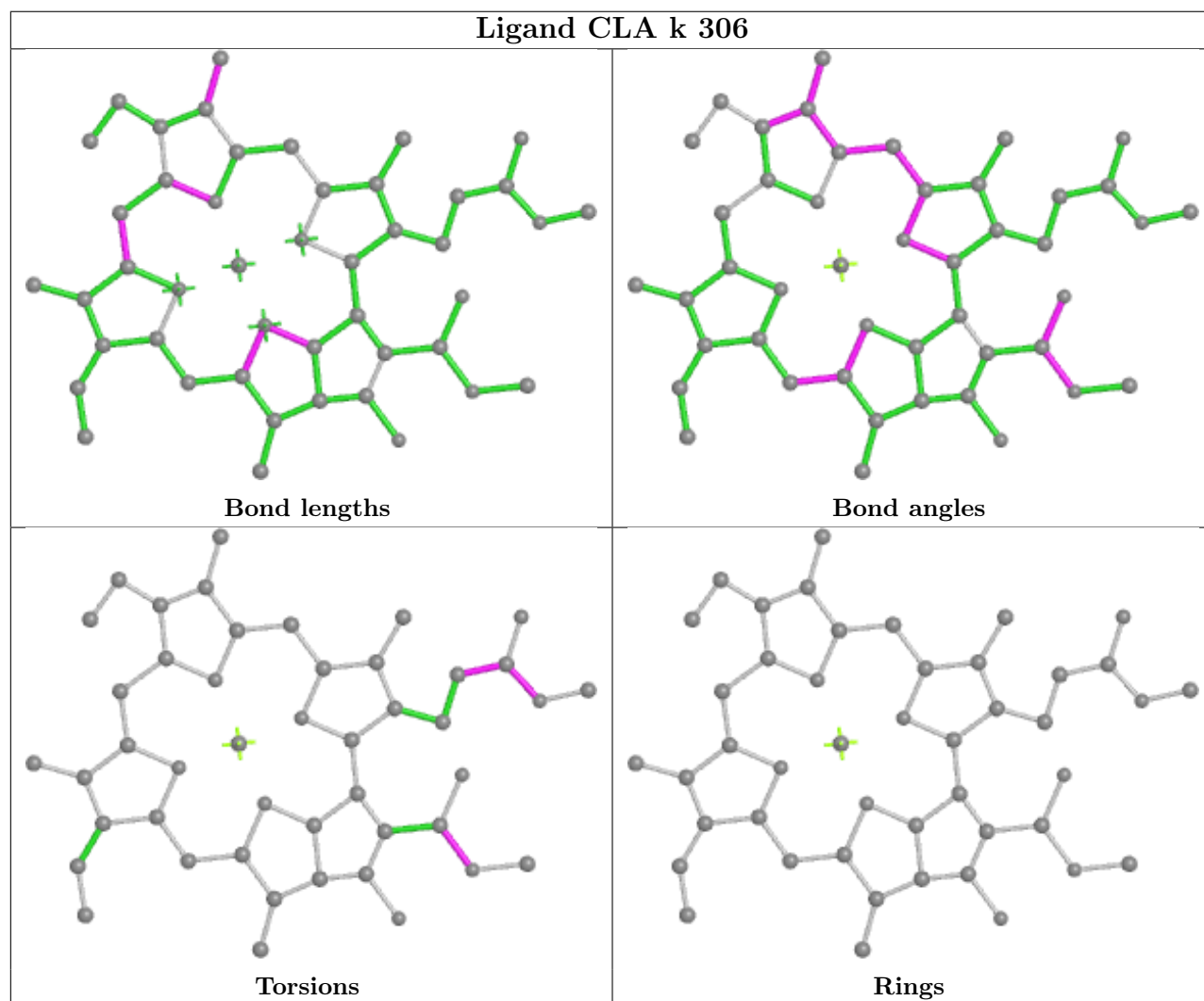
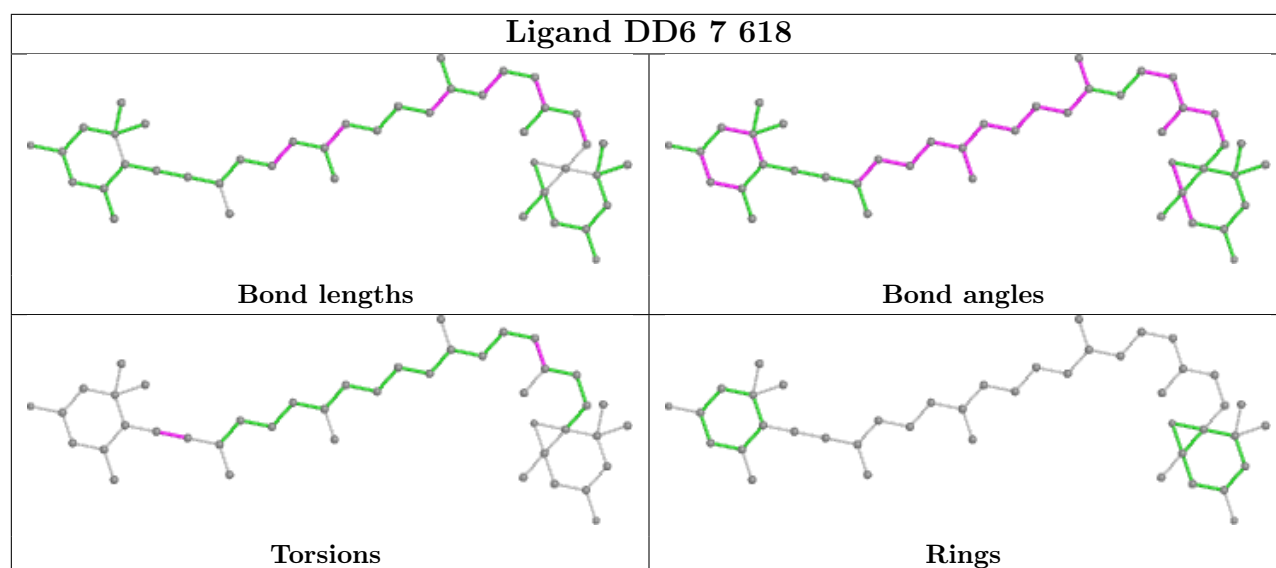
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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24	4	605	CLA	1	0
31	A	839	PQN	1	0
24	A	835	CLA	1	0
24	4	612	CLA	2	0
26	1	312	DD6	1	0
28	8	213	LHG	1	0
24	1	306	CLA	1	0
24	B	822	CLA	1	0
24	8	206	CLA	2	0
24	B	807	CLA	1	0
26	8	211	DD6	1	0
24	A	834	CLA	1	0
26	8	212	DD6	1	0
24	7	601	CLA	1	0
24	8	201	CLA	2	0
24	B	812	CLA	3	0
26	7	615	DD6	1	0
24	t	307	CLA	2	0
24	k	307	CLA	1	0
24	B	821	CLA	1	0
24	4	613	CLA	2	0
25	M	101	BCR	2	0
26	6	613	DD6	1	0
24	F	202	CLA	1	0
24	B	823	CLA	1	0
25	4	618	BCR	7	0
24	4	606	CLA	1	0
26	7	613	DD6	1	0

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

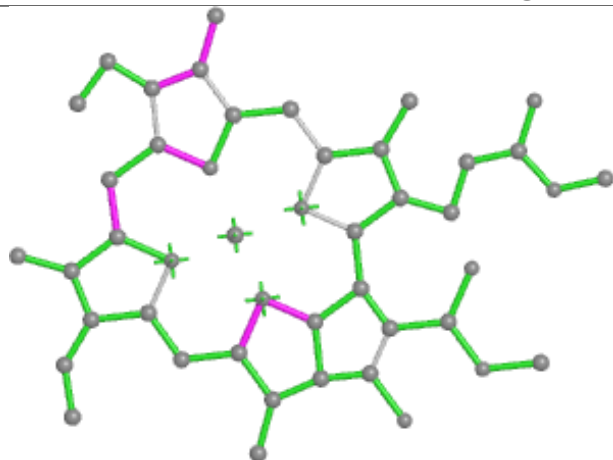


Ligand CLA B 804**Ligand CLA A 827**

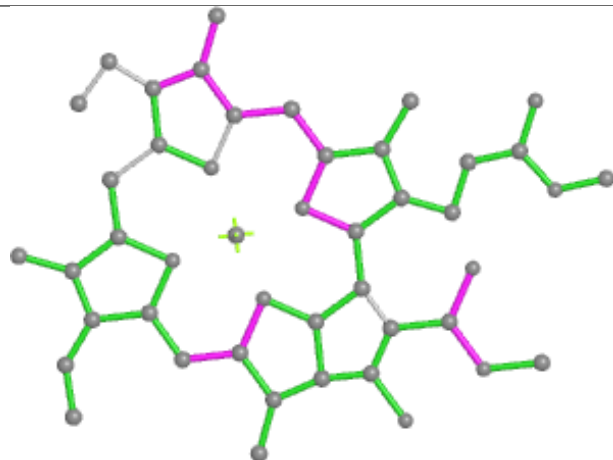




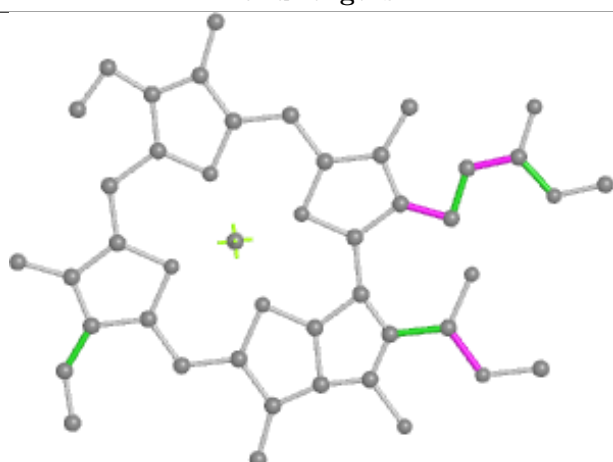
Ligand CLA 1 308



Bond lengths



Bond angles

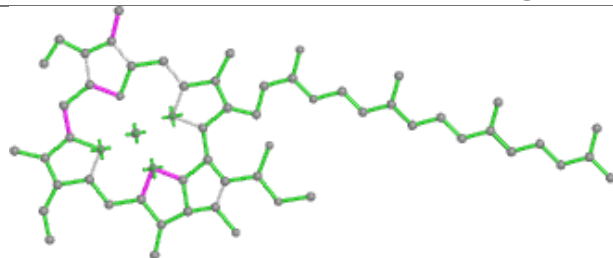


Torsions

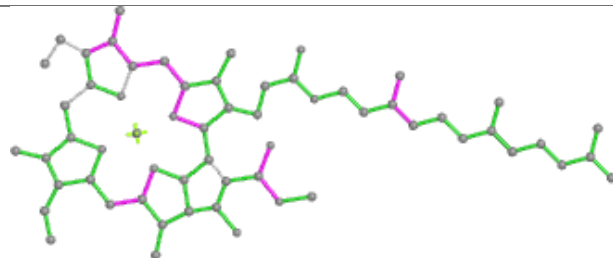


Rings

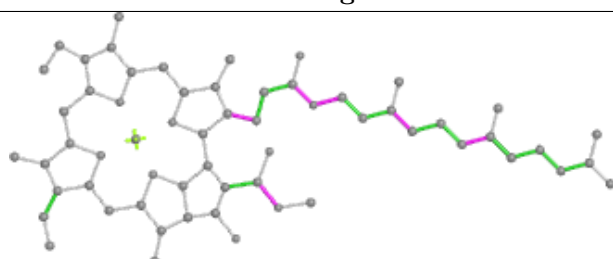
Ligand CLA 4 602



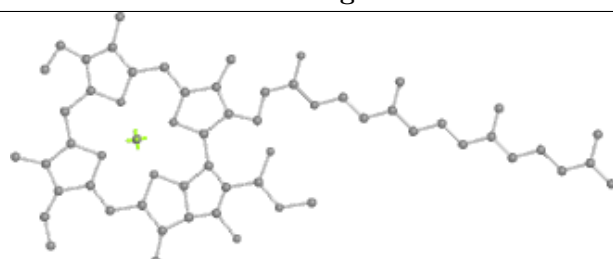
Bond lengths



Bond angles

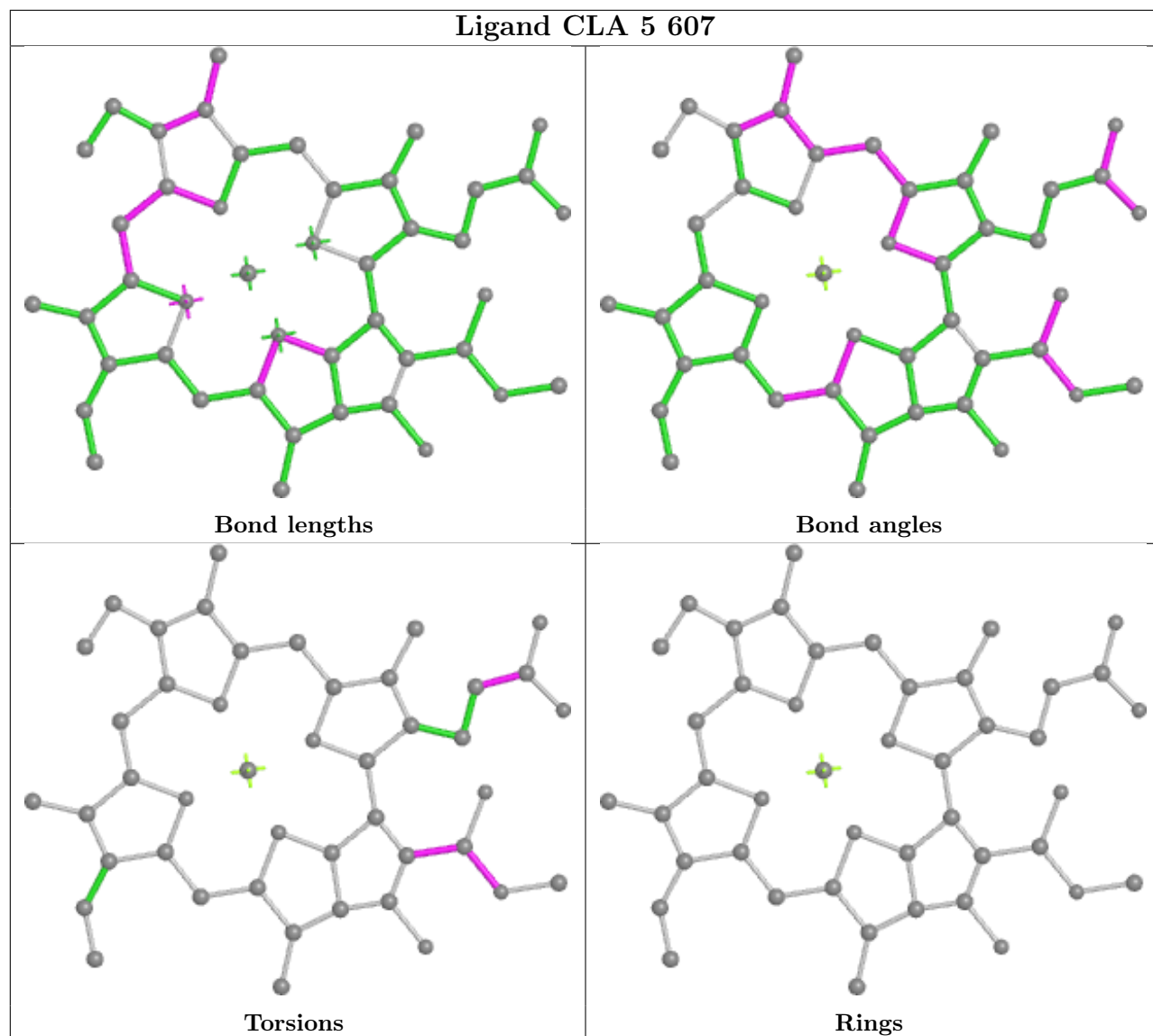


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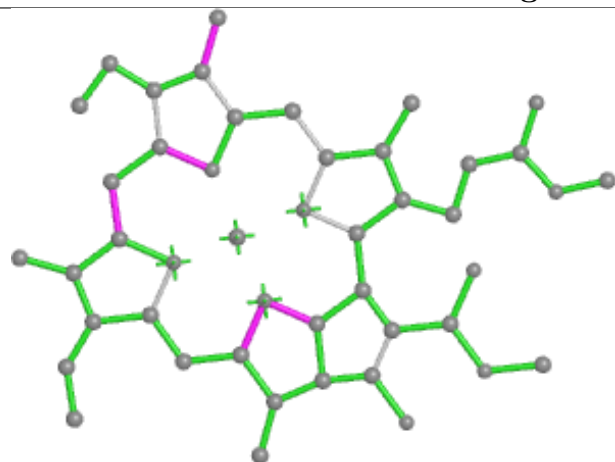


Rings

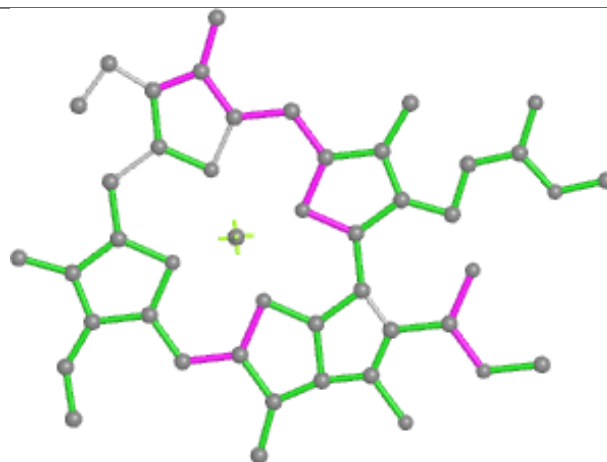
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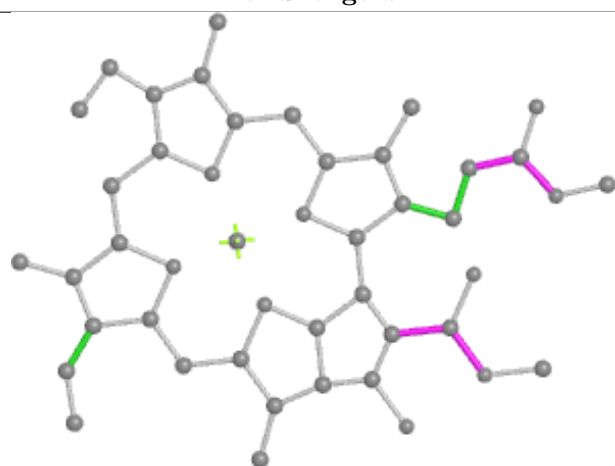
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Bond lengths



Bond angles

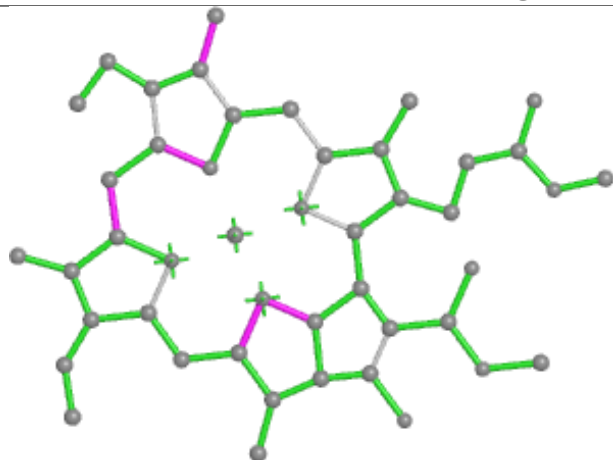


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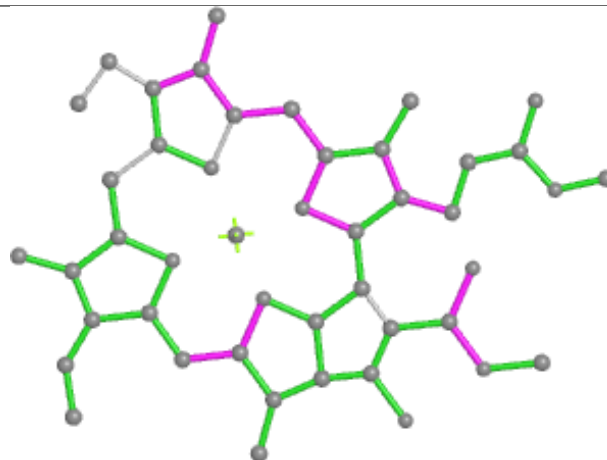


Rings

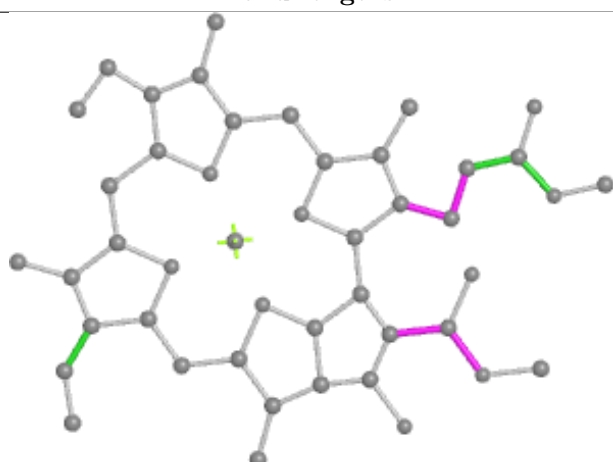
Ligand CLA B 813



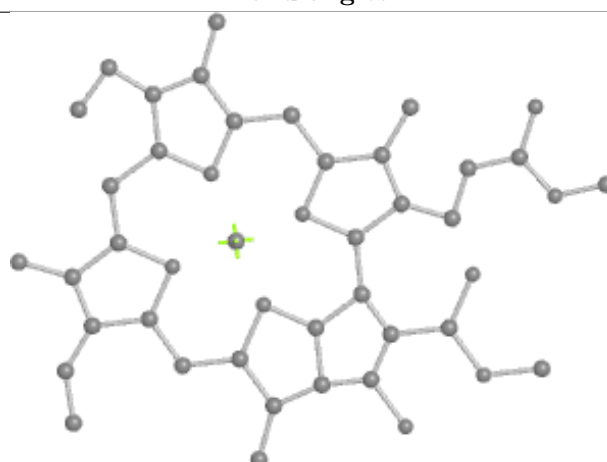
Bond lengths



Bond angles

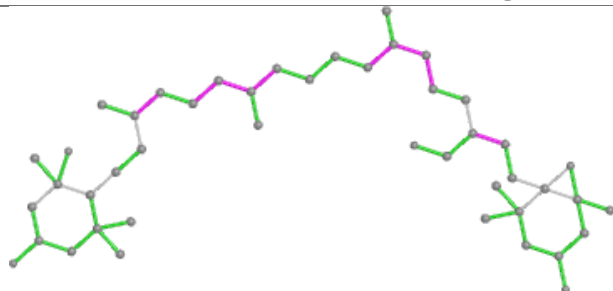


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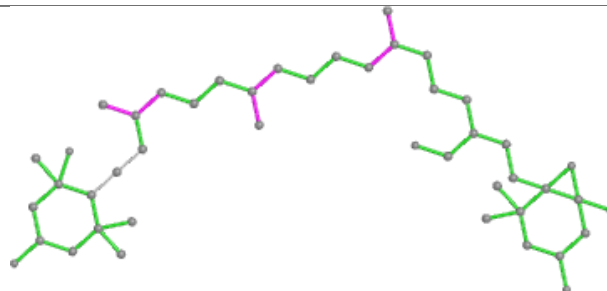


Rings

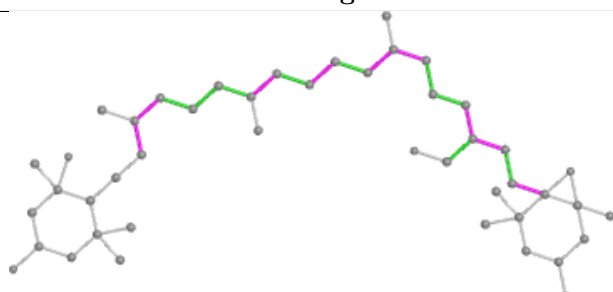
Ligand A1L1G 3 310



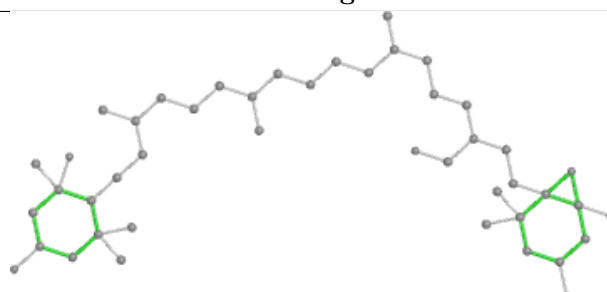
Bond lengths



Bond angles

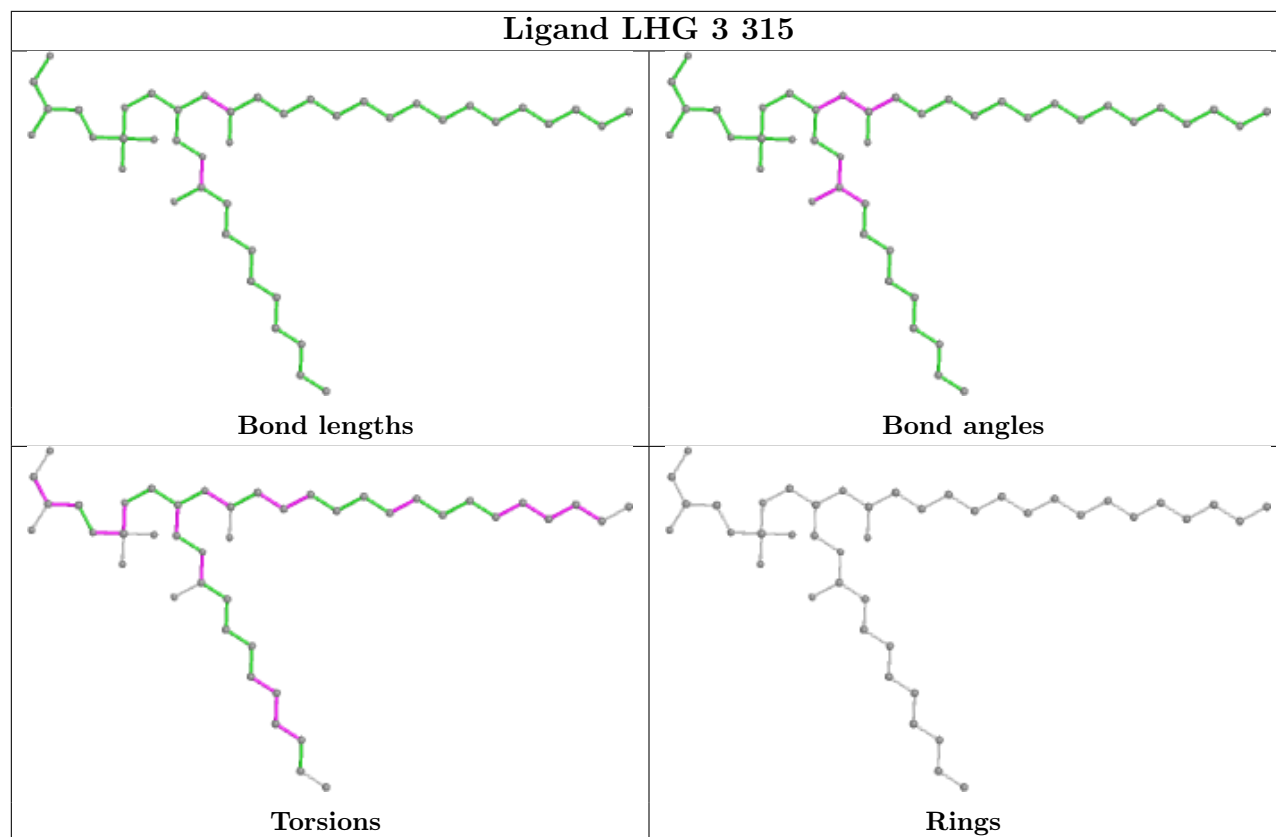


Torsions

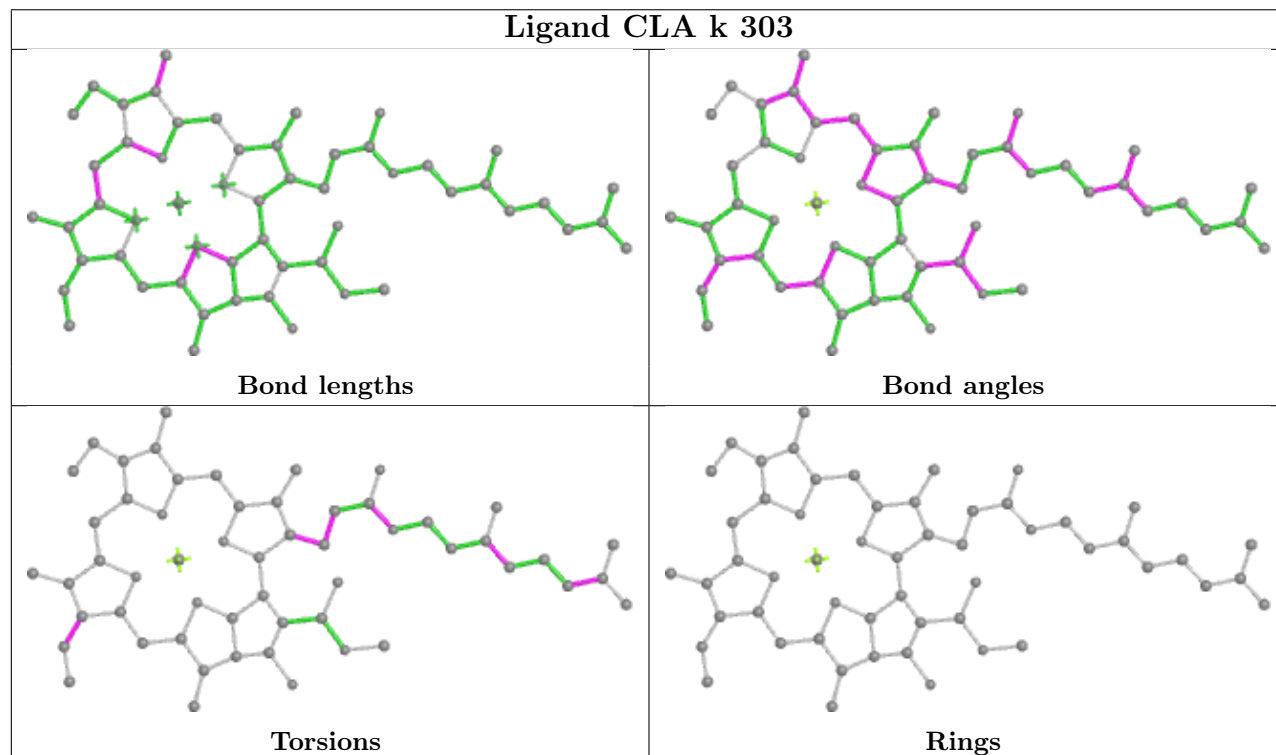


Rings

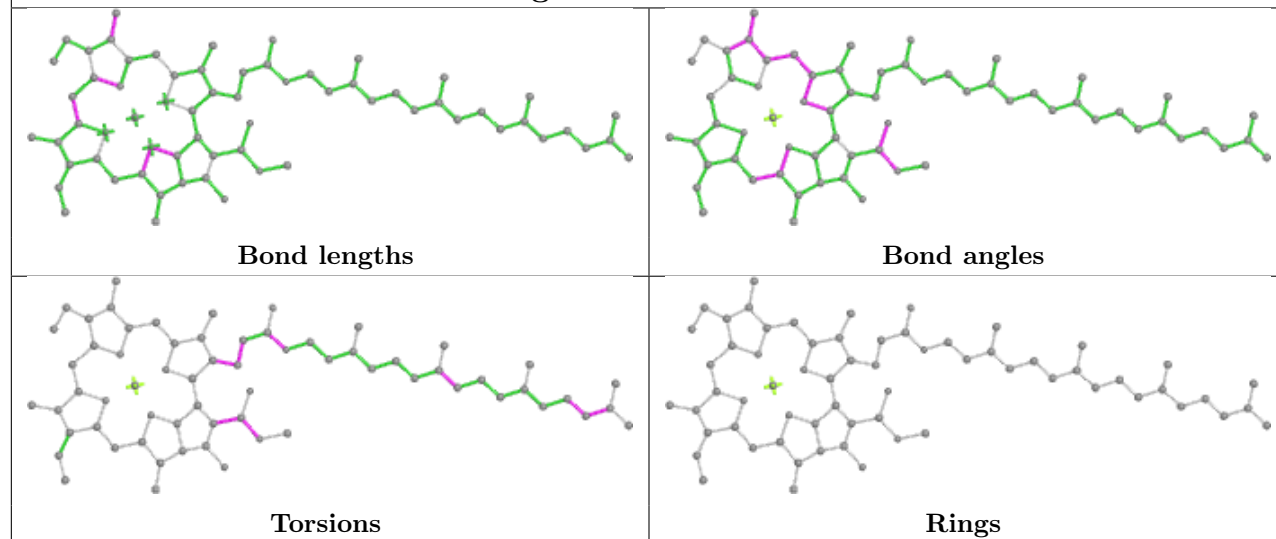
Ligand LHG 3 315



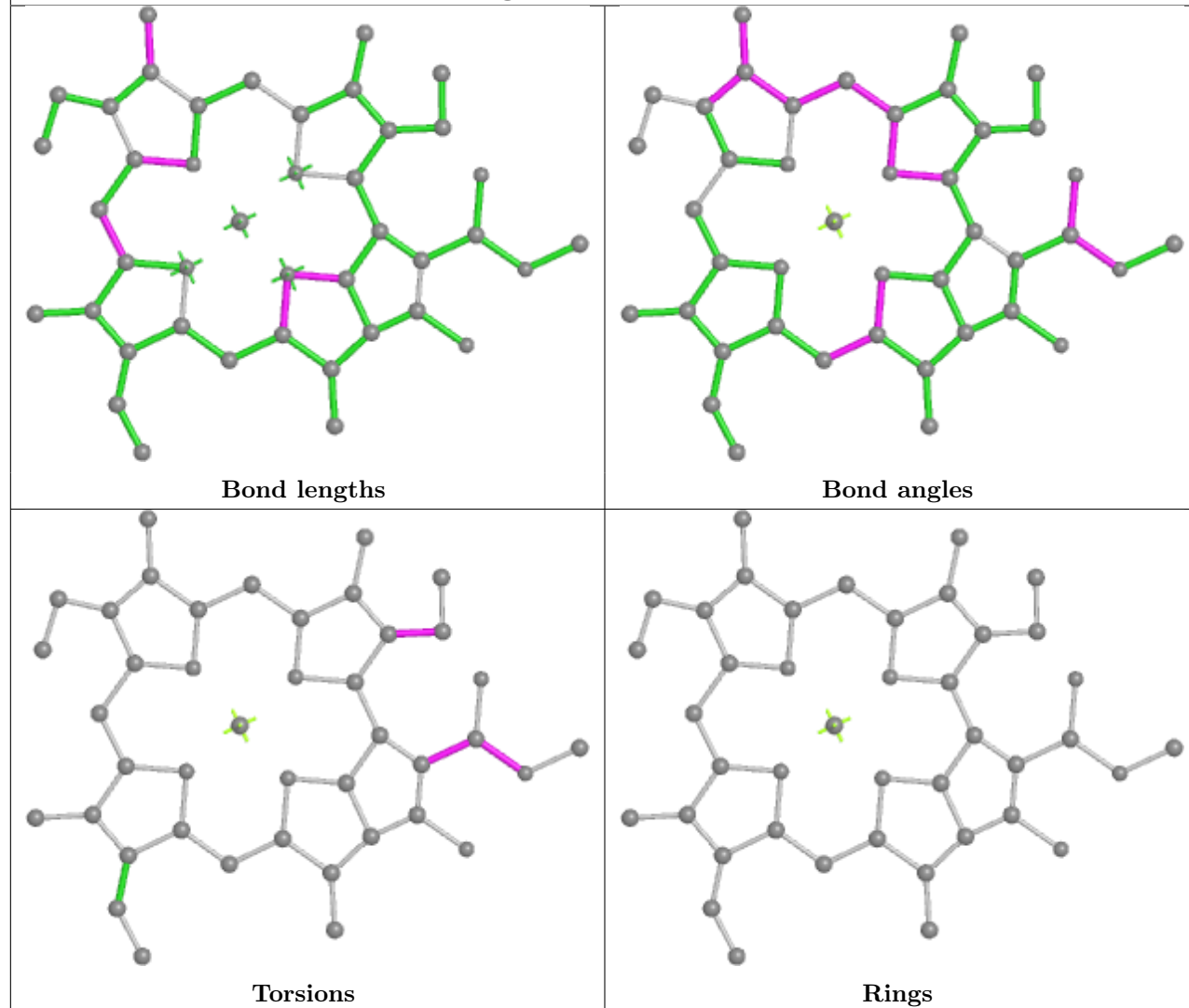
Ligand CLA k 303

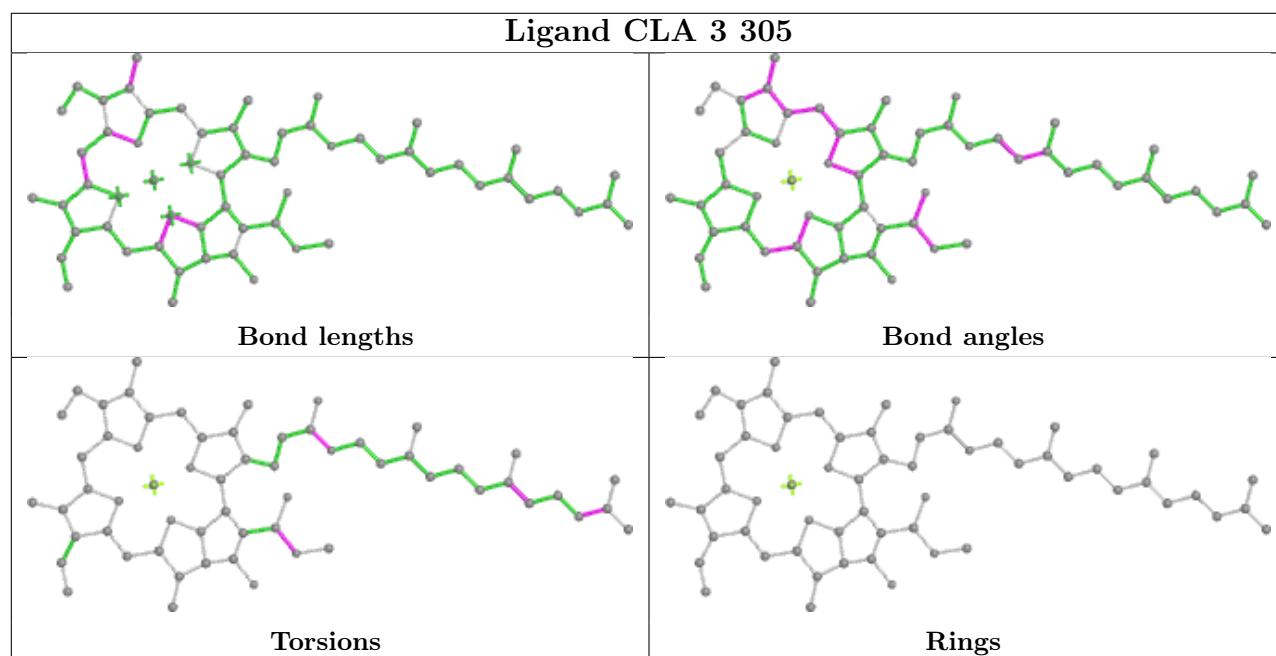
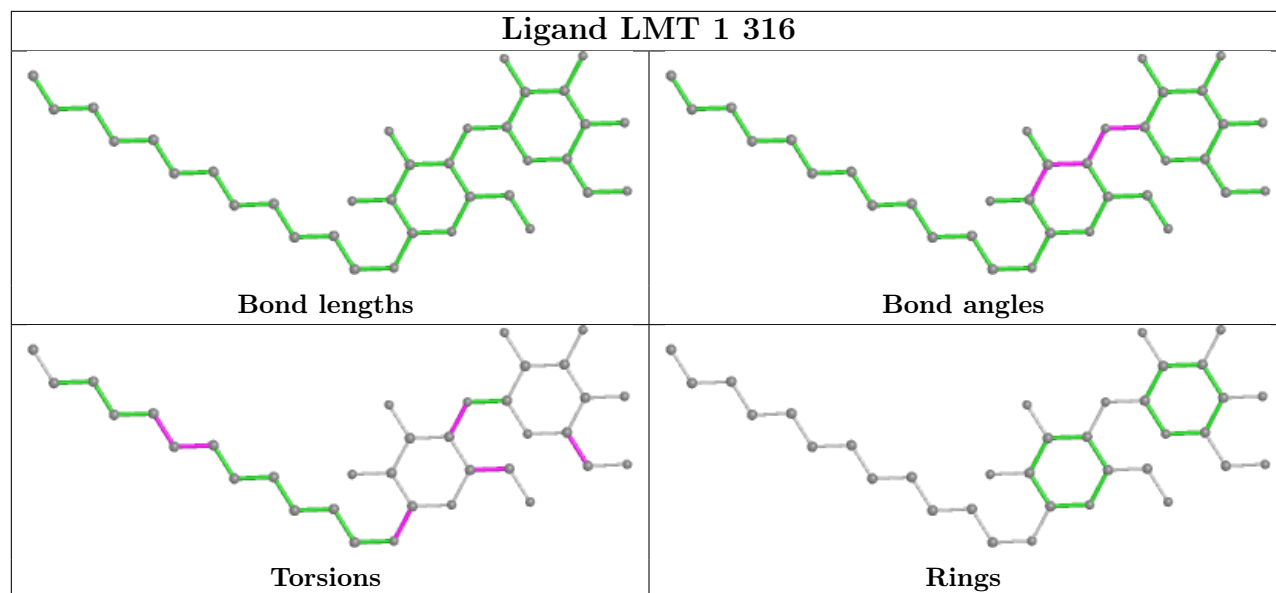


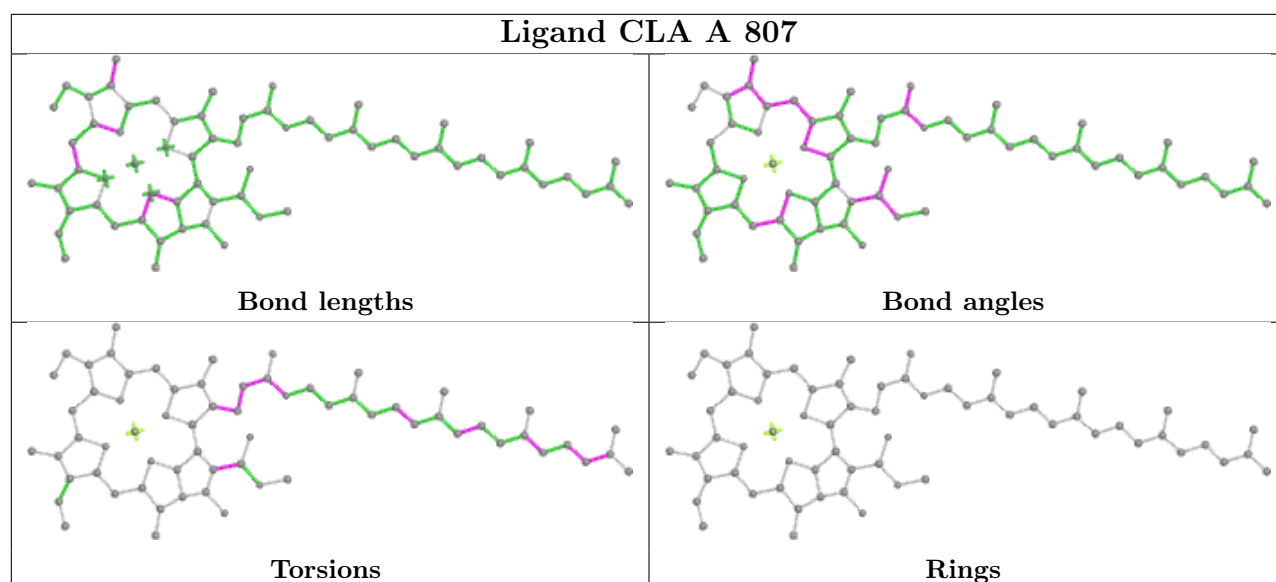
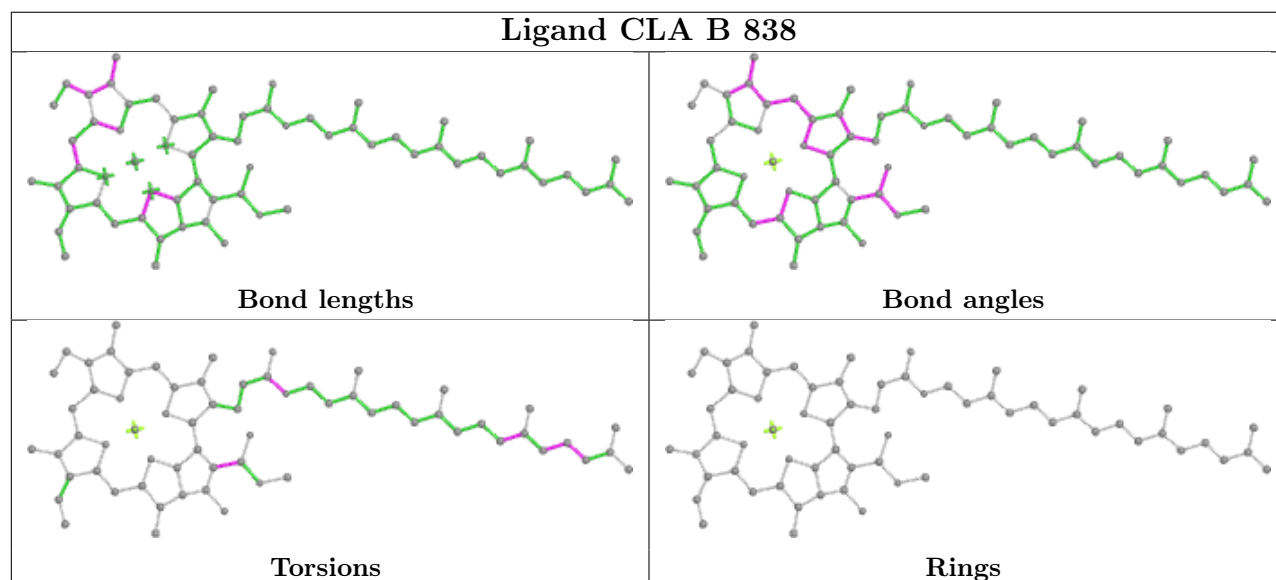
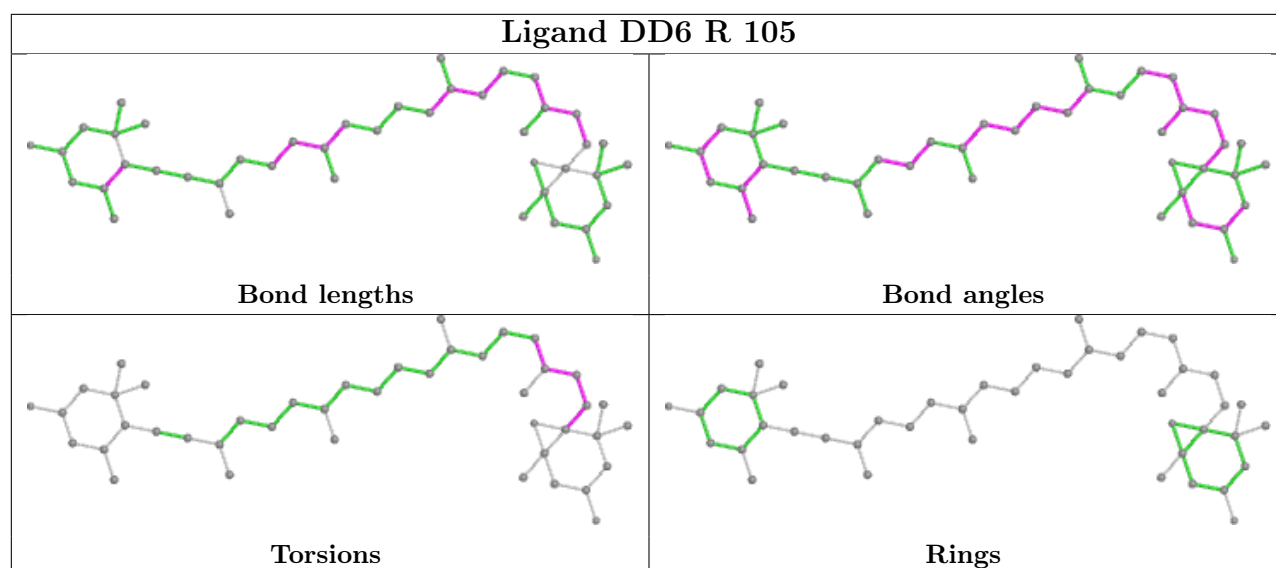
Ligand CLA A 831



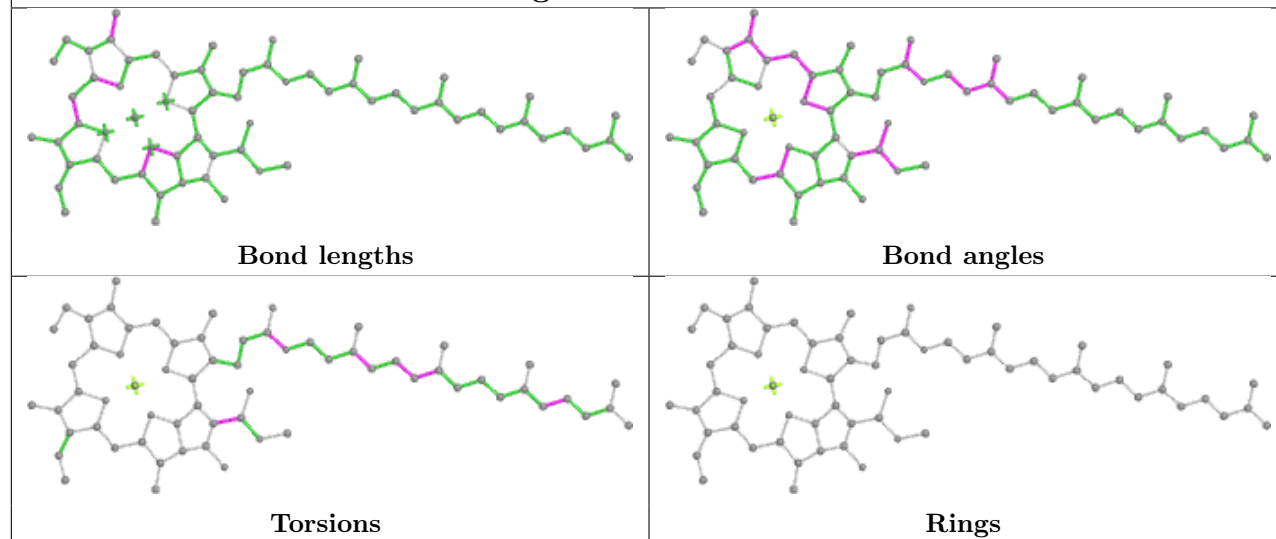
Ligand CLA J 103



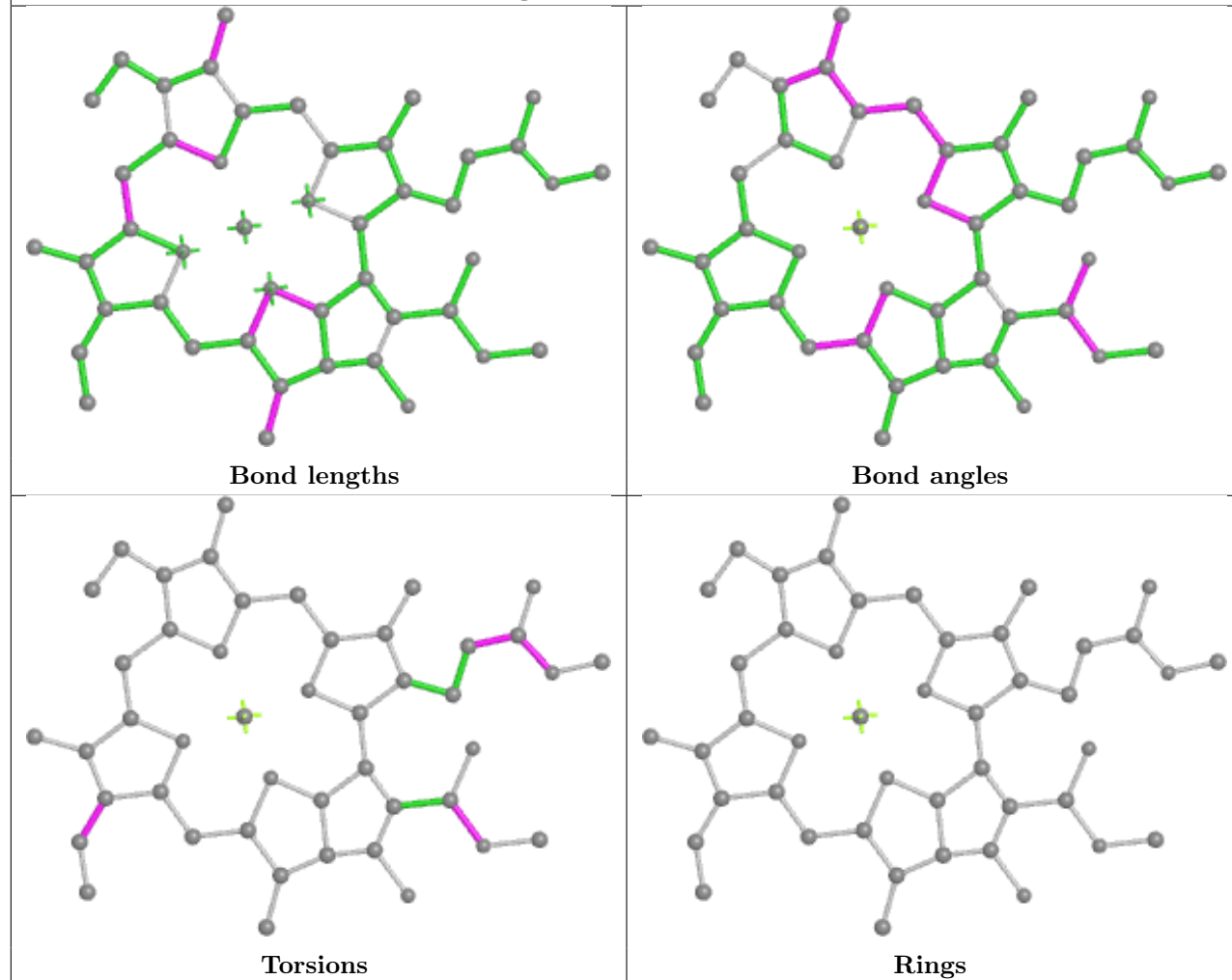


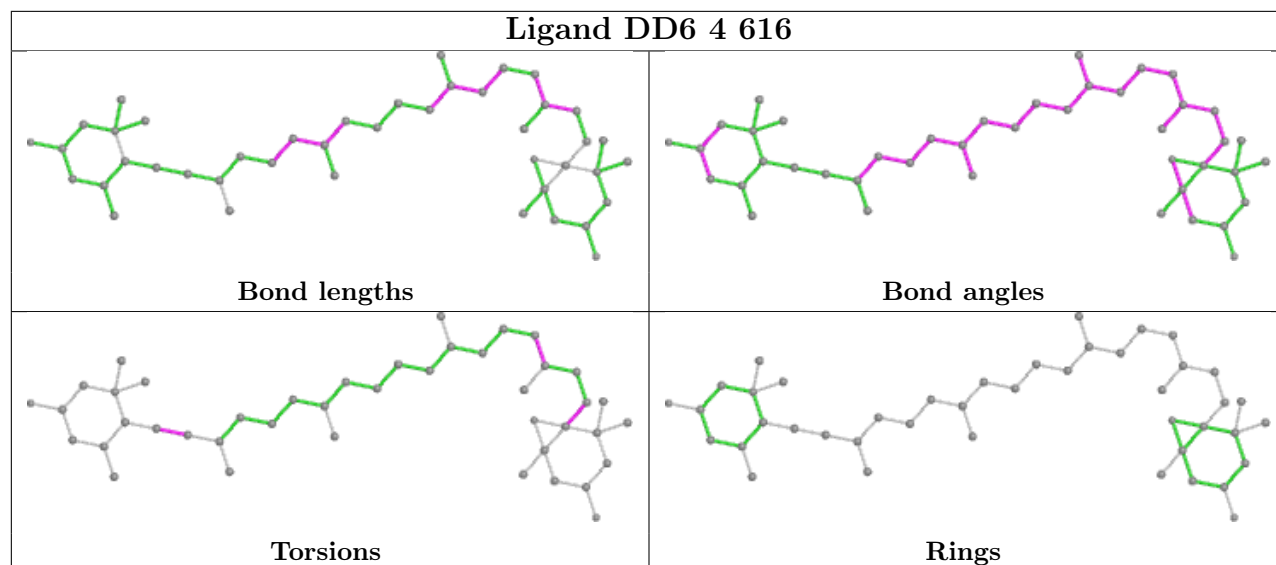
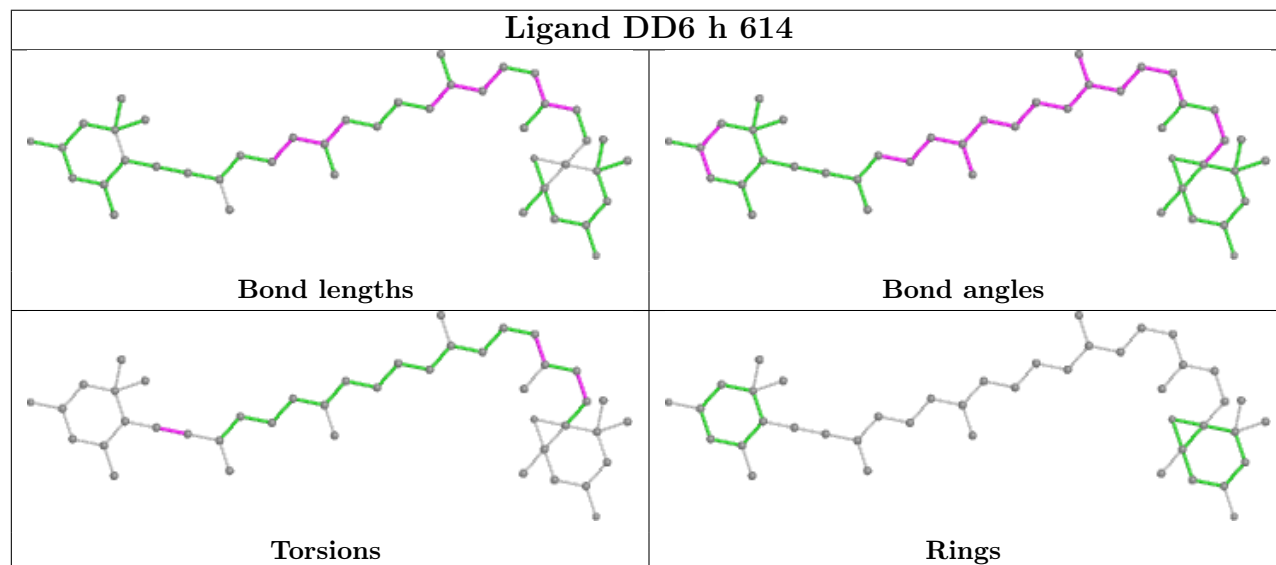


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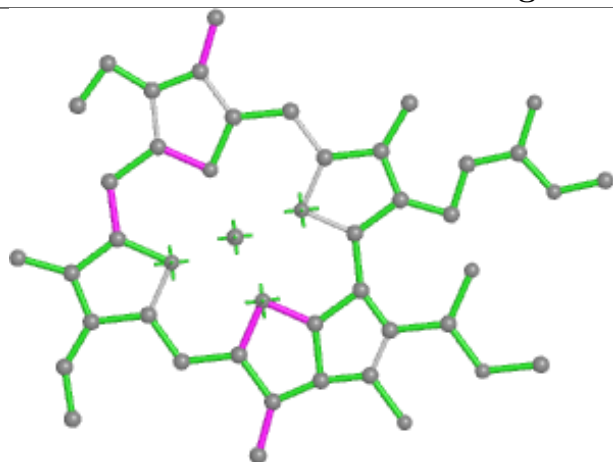


Ligand CLA L 205

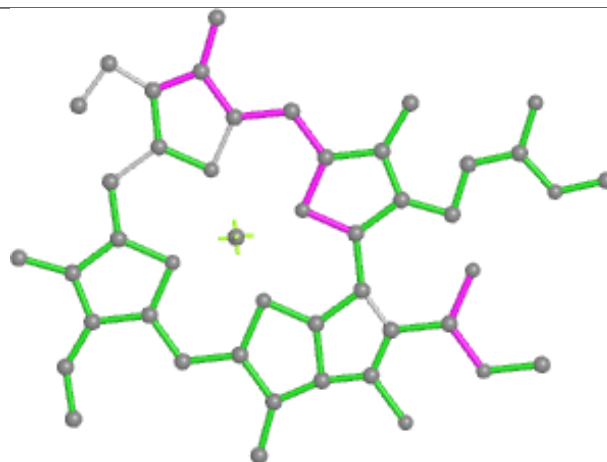


Ligand DD6 4 616**Ligand DD6 h 614**

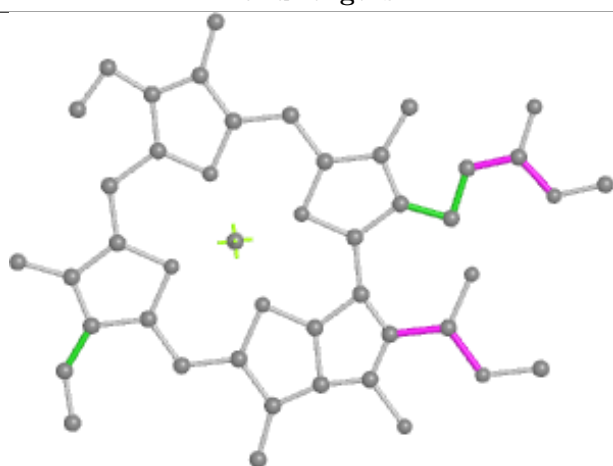
Ligand CLA 9 302



Bond lengths



Bond angles

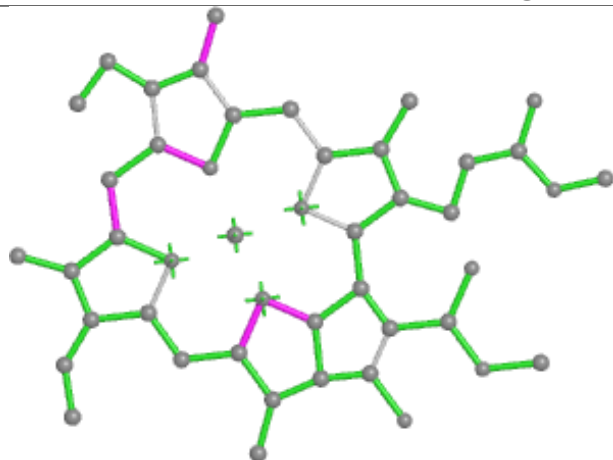


Torsions

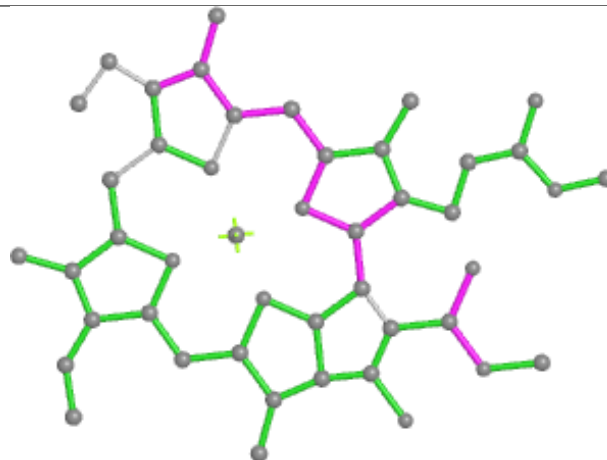


Rings

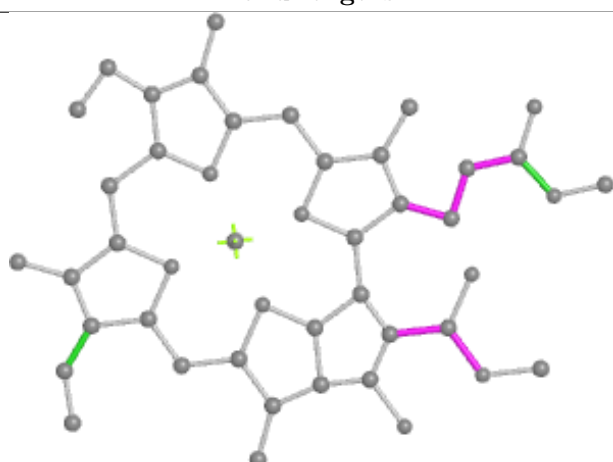
Ligand CLA 8 202



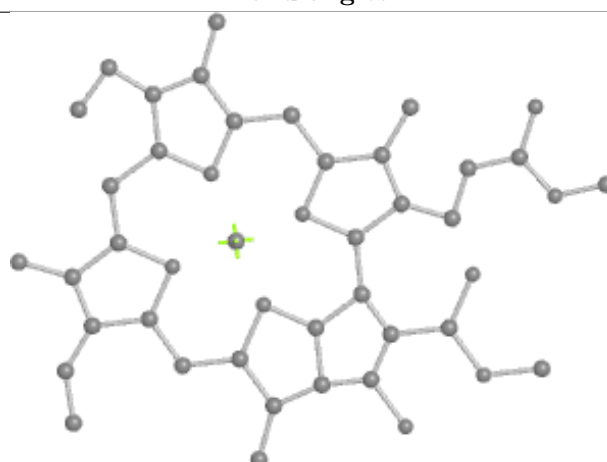
Bond lengths



Bond angles

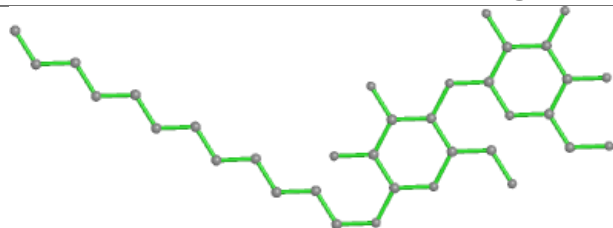


Torsions

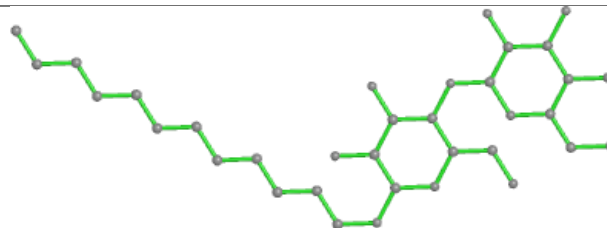


Rings

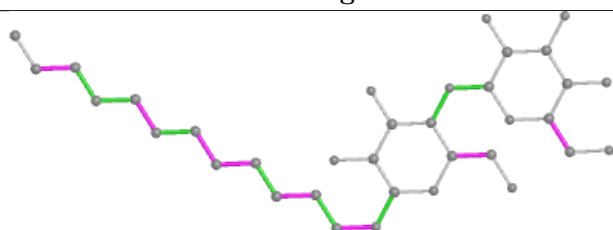
Ligand LMT A 850



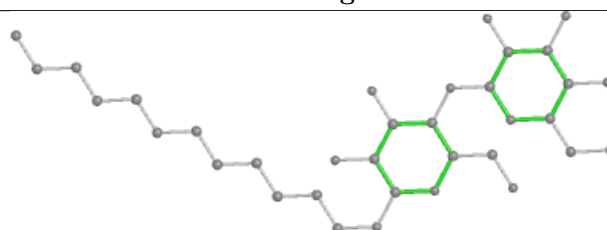
Bond lengths



Bond angles

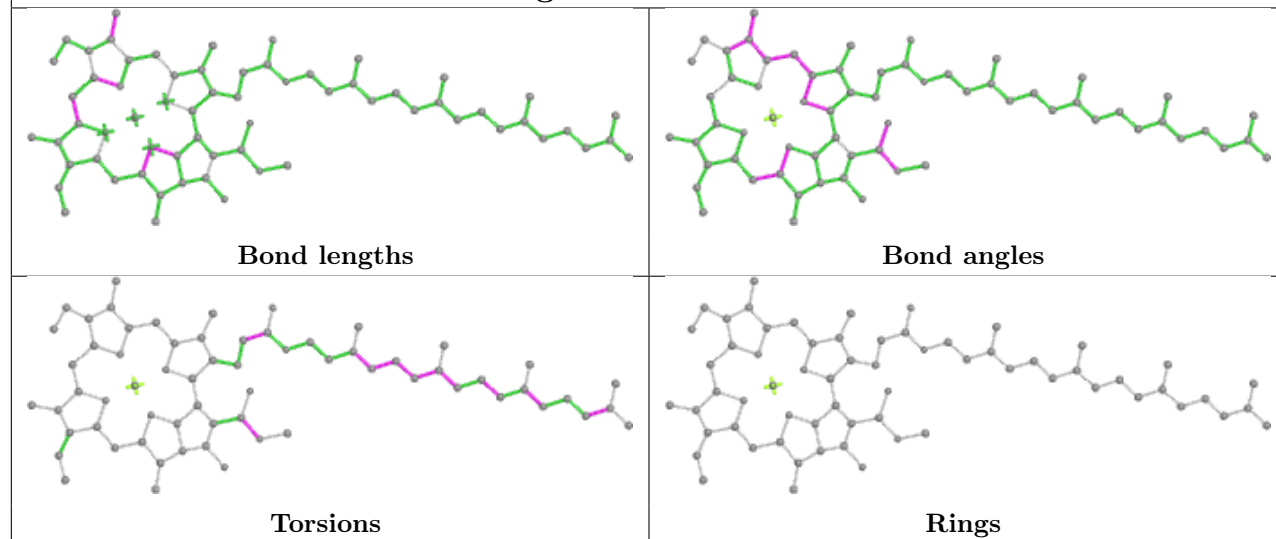


Torsions

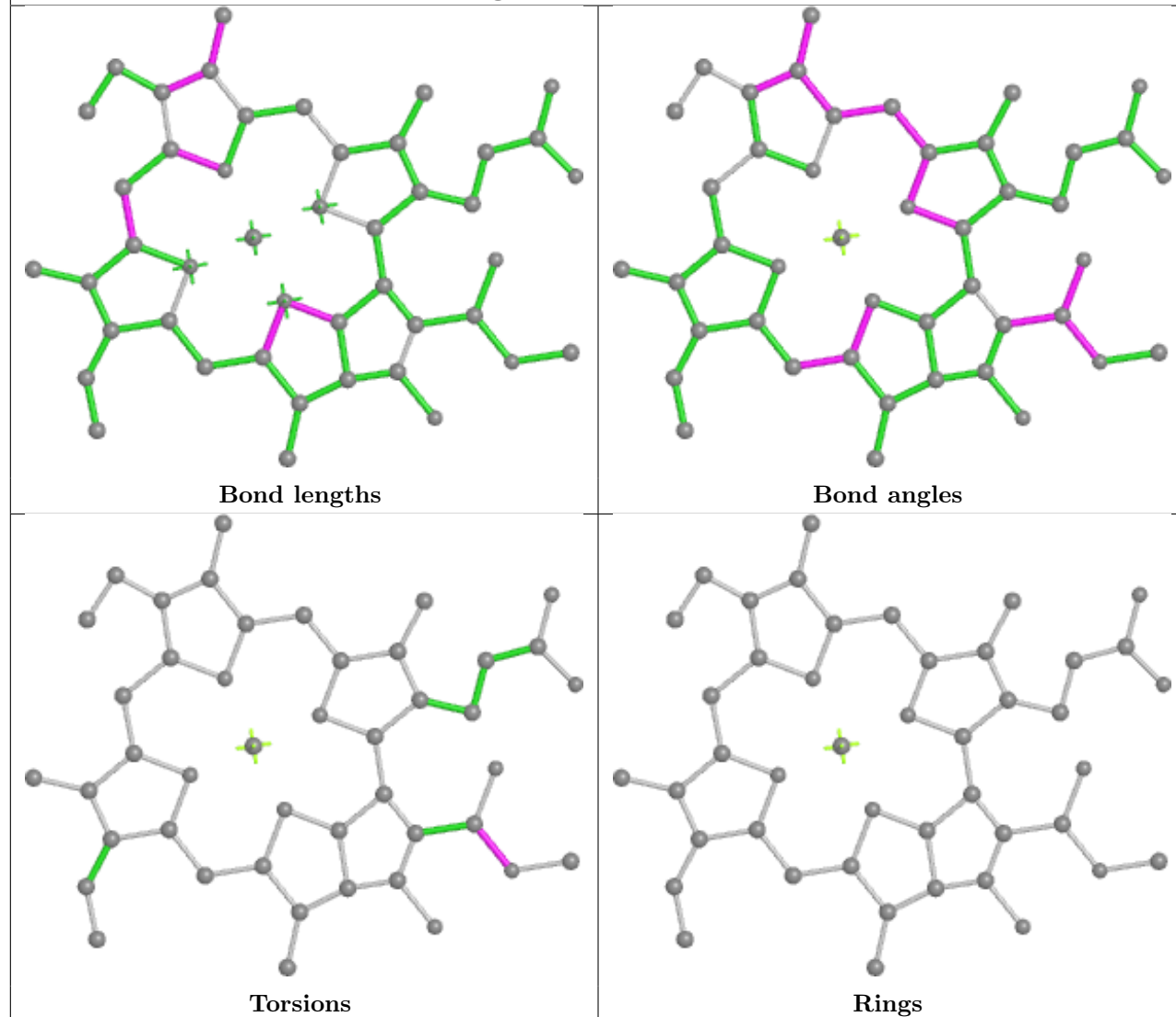


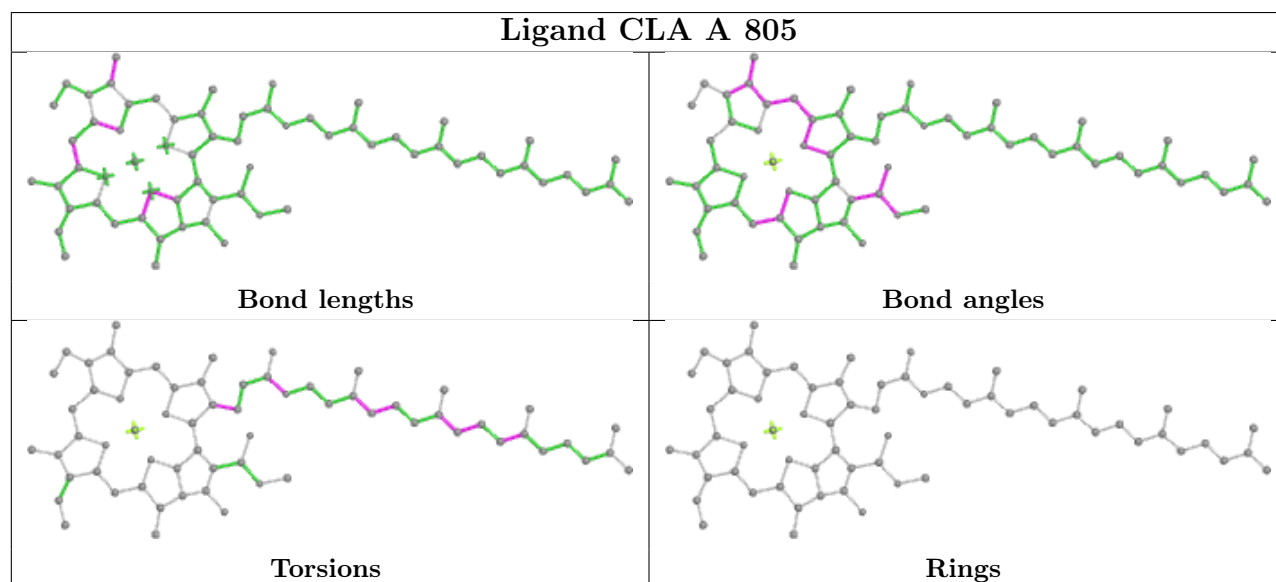
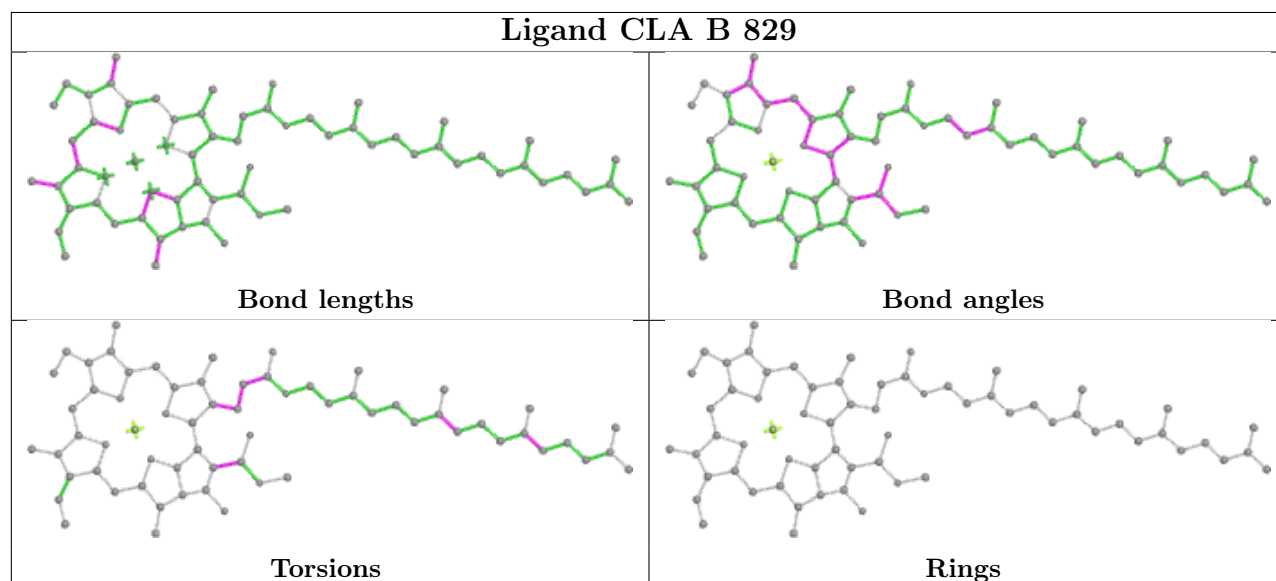
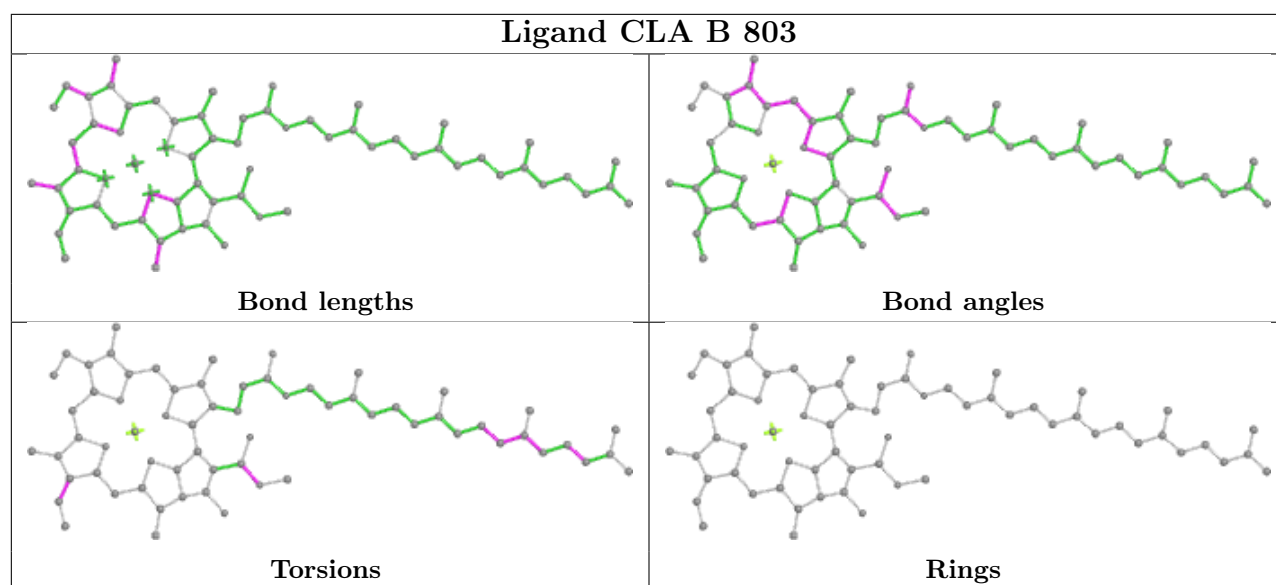
Rings

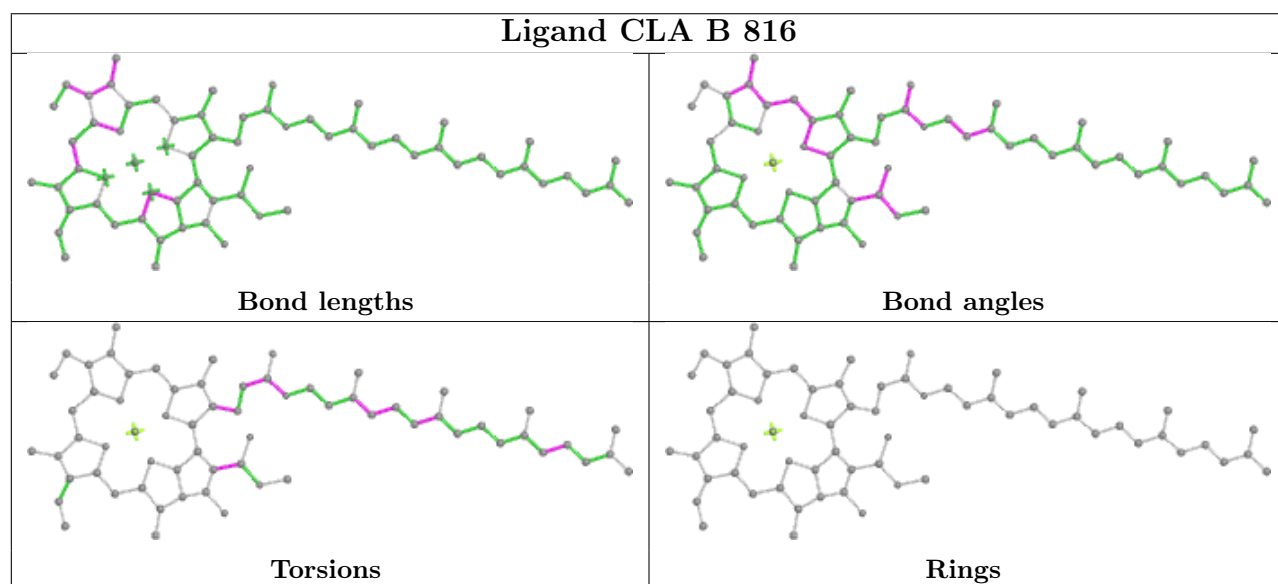
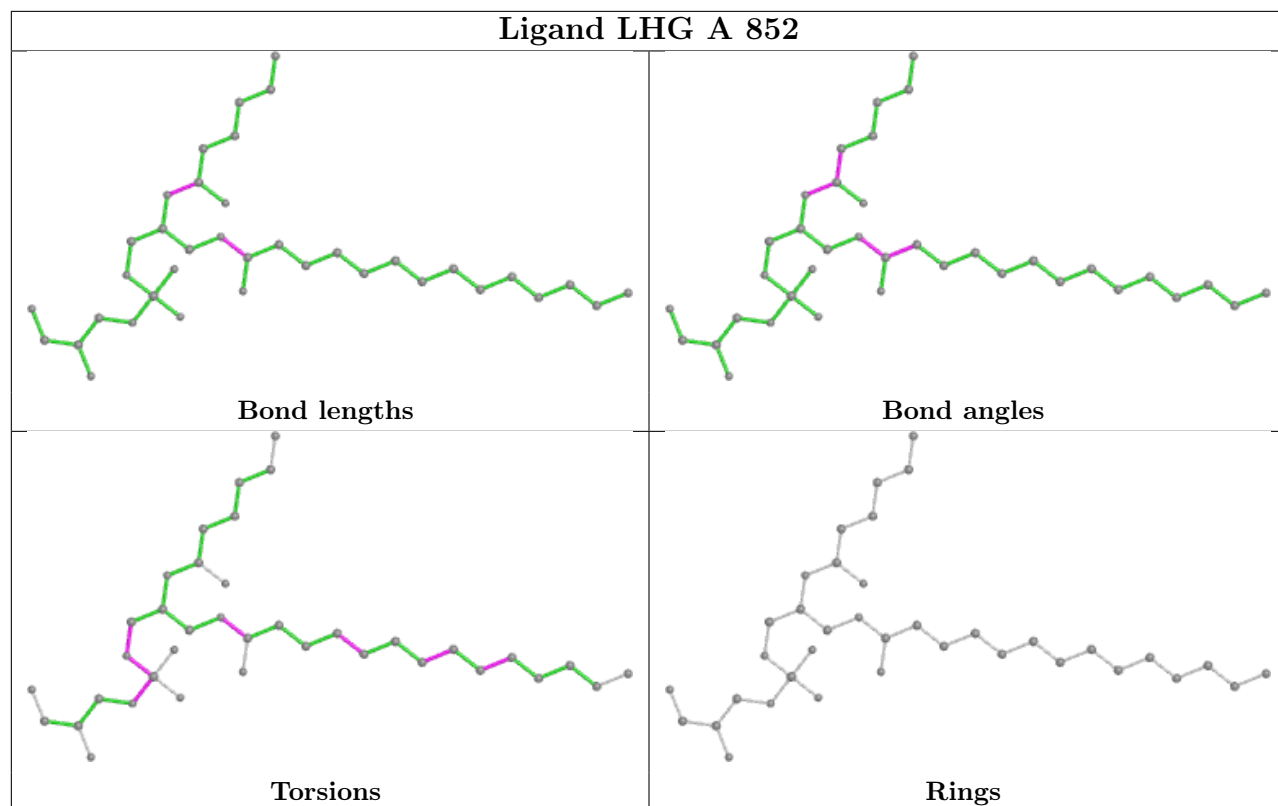
Ligand CLA 3 301



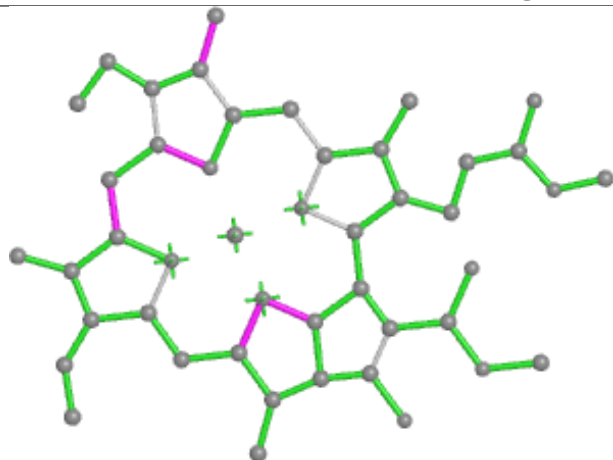
Ligand CLA A 819



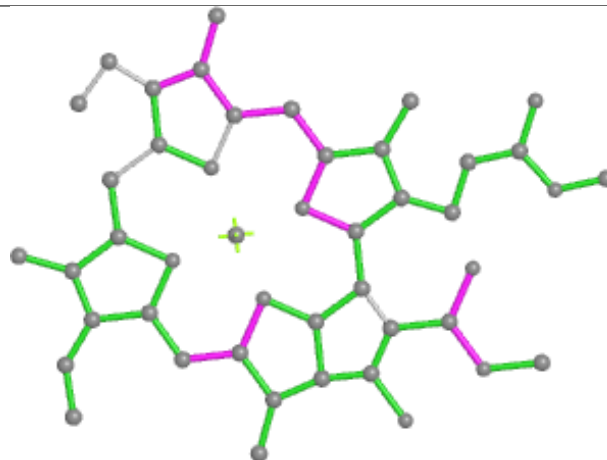




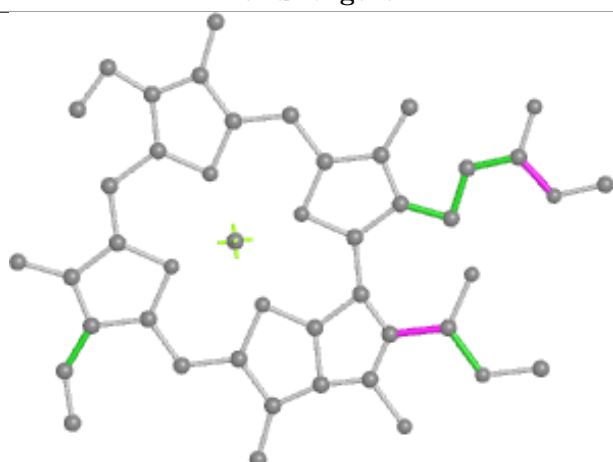
Ligand CLA 7 605



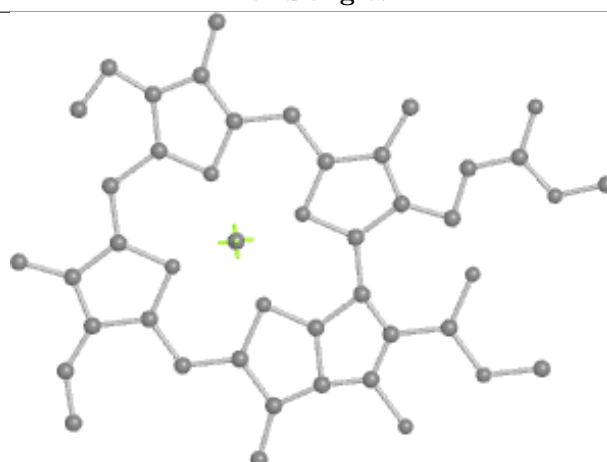
Bond lengths



Bond angles

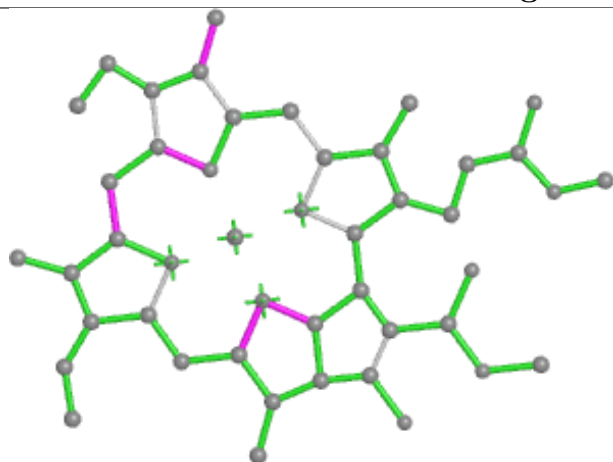


Torsions

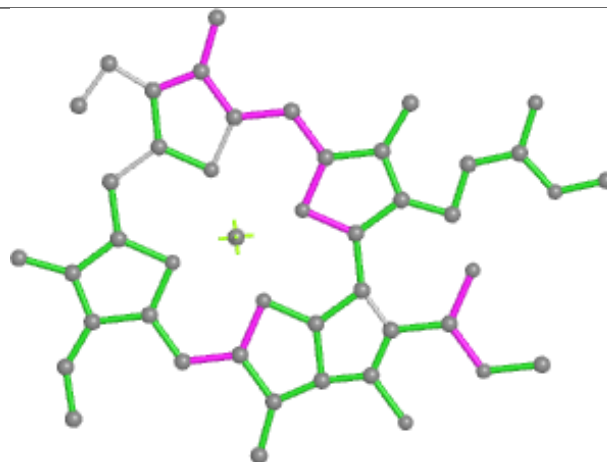


Rings

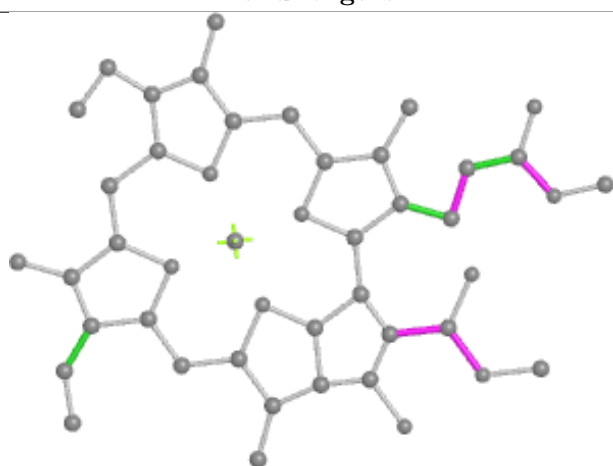
Ligand CLA t 310



Bond lengths



Bond angles

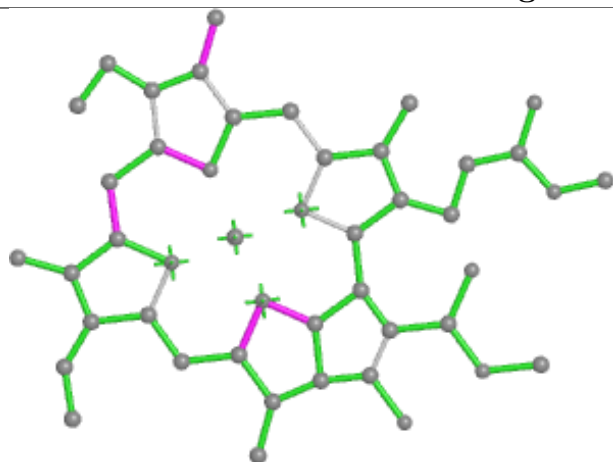


Torsions

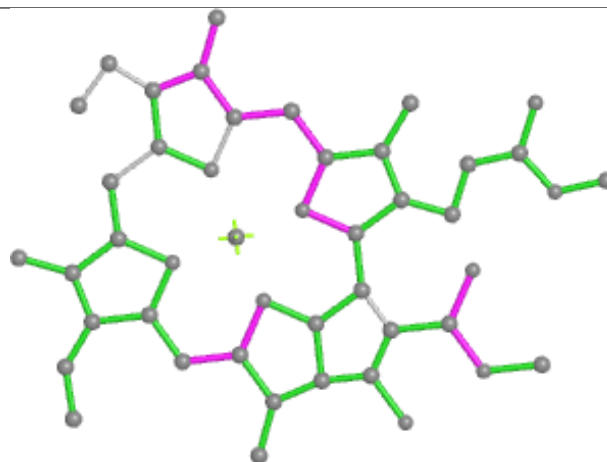


Rings

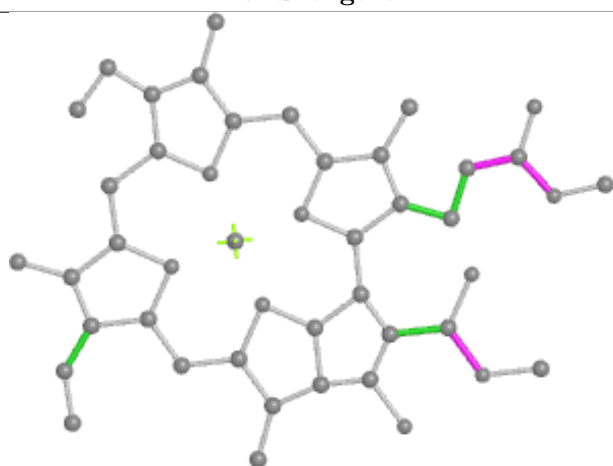
Ligand CLA 2 207



Bond lengths



Bond angles

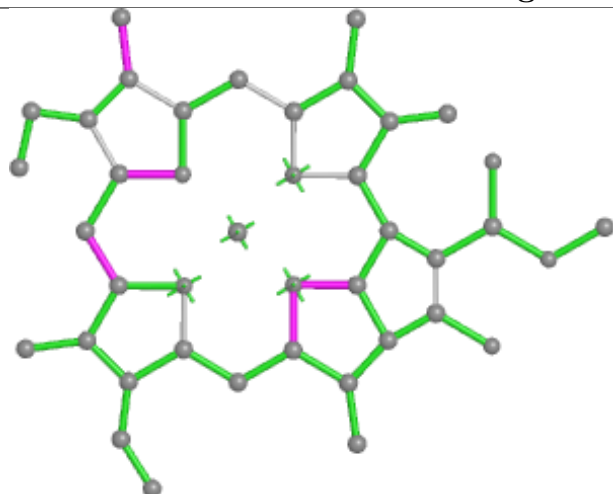


Torsions

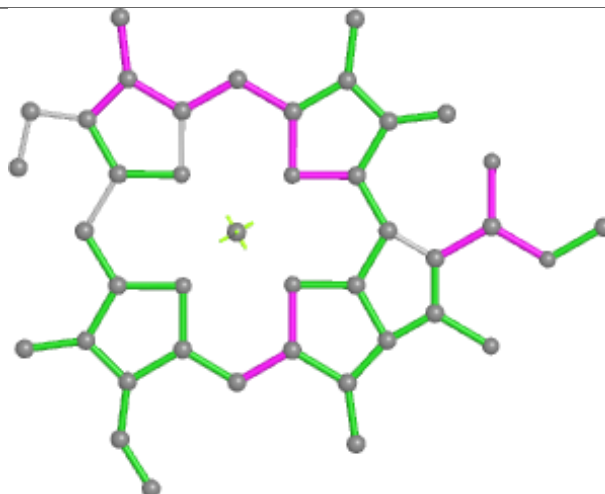


Rings

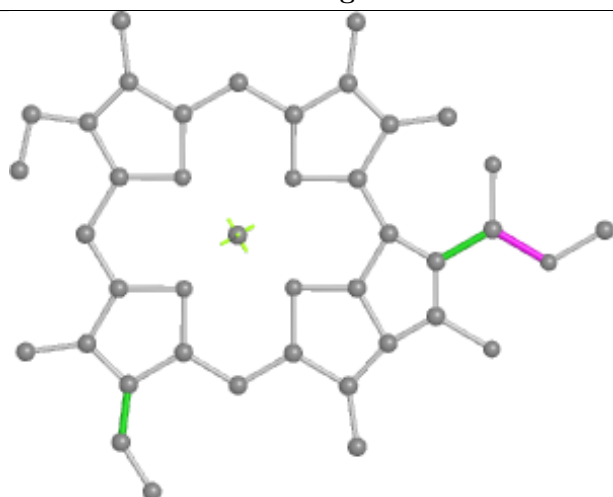
Ligand CLA k 310



Bond lengths



Bond angles

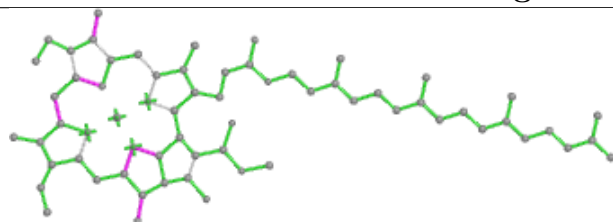


Torsions

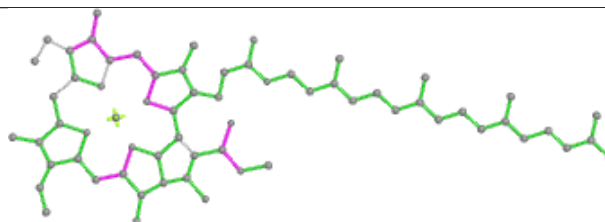


Rings

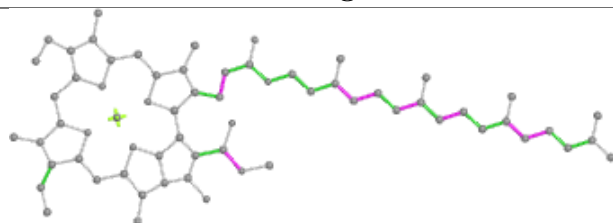
Ligand CLA A 828



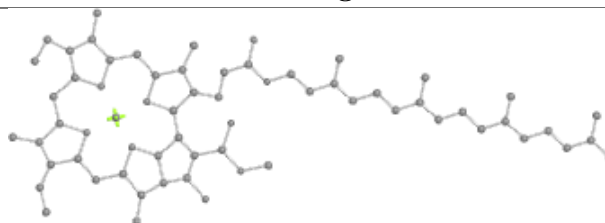
Bond lengths



Bond angles

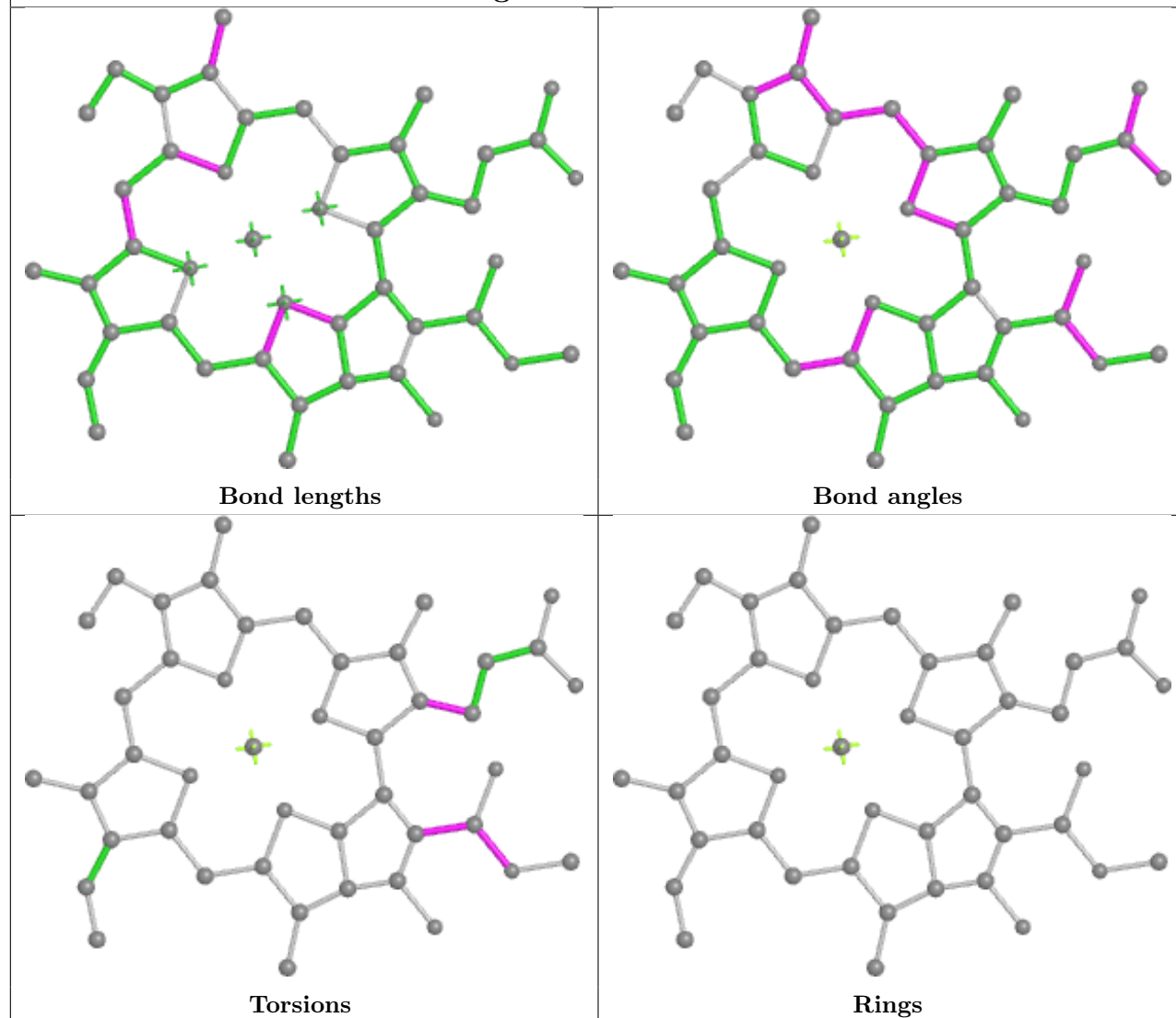


Torsions

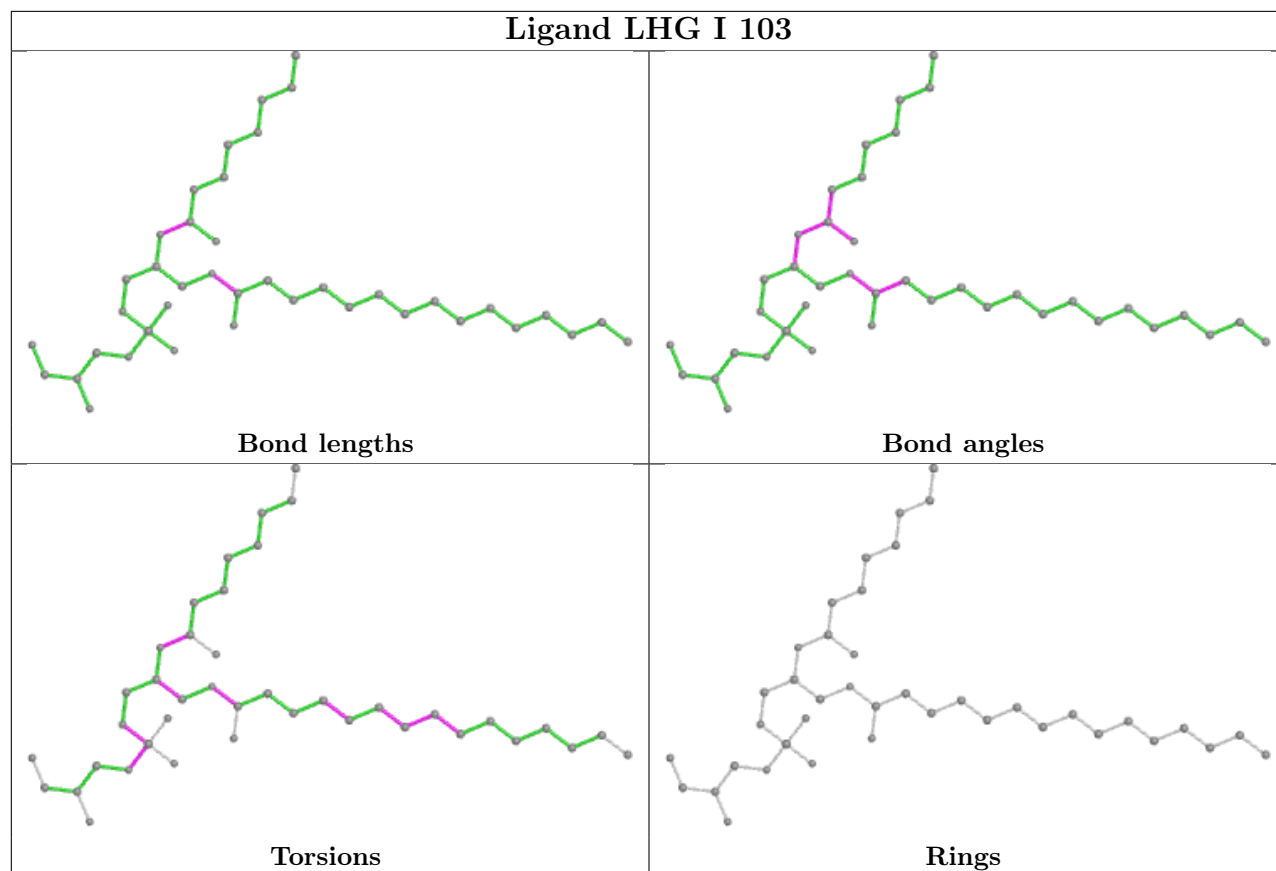


Rings

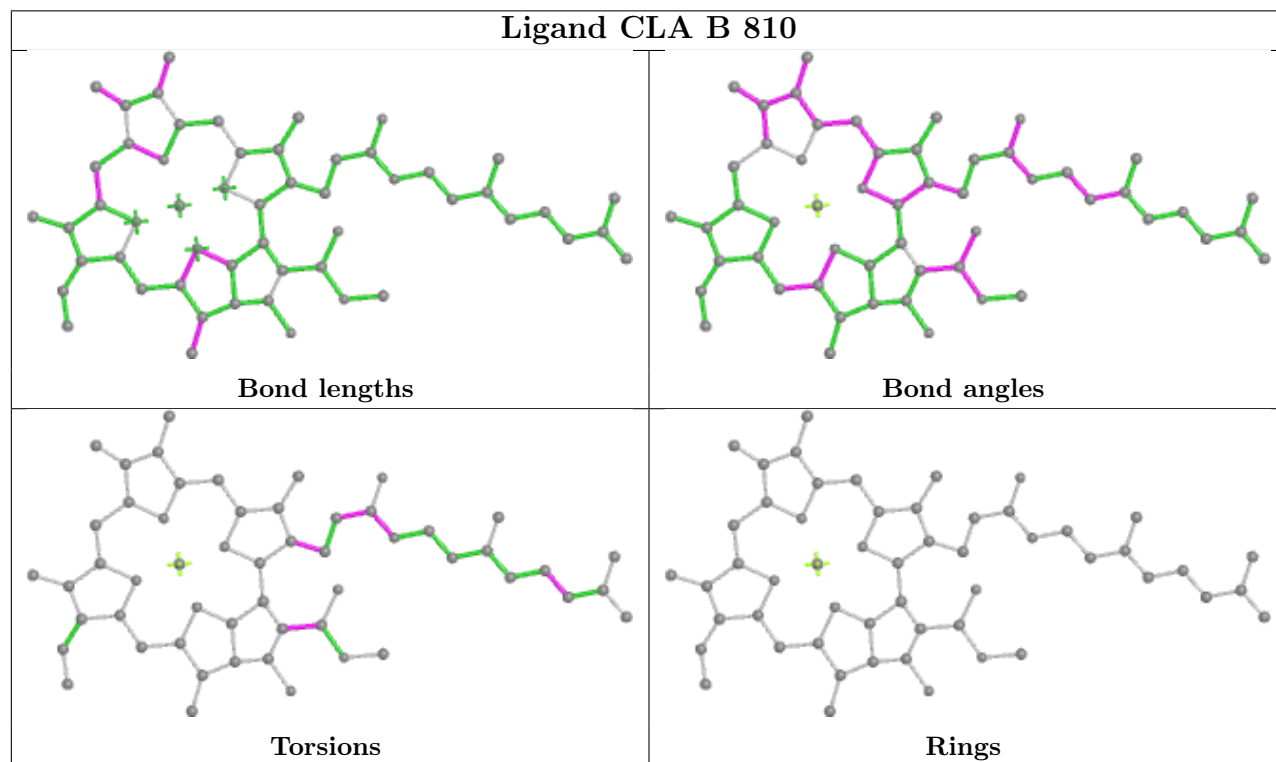
Ligand CLA k 309

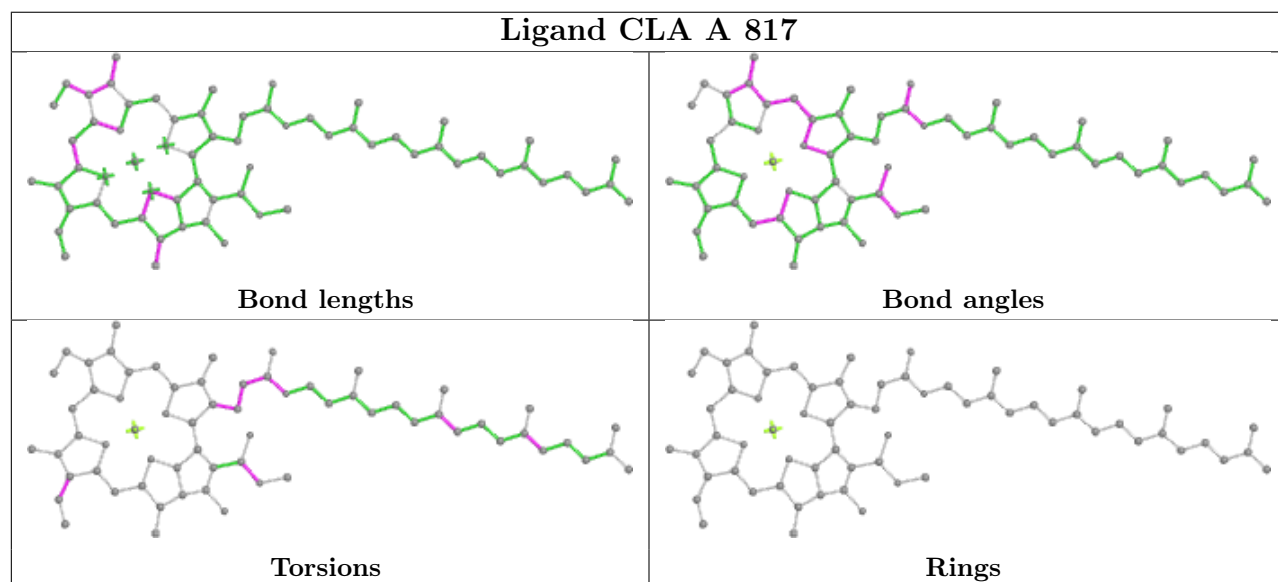
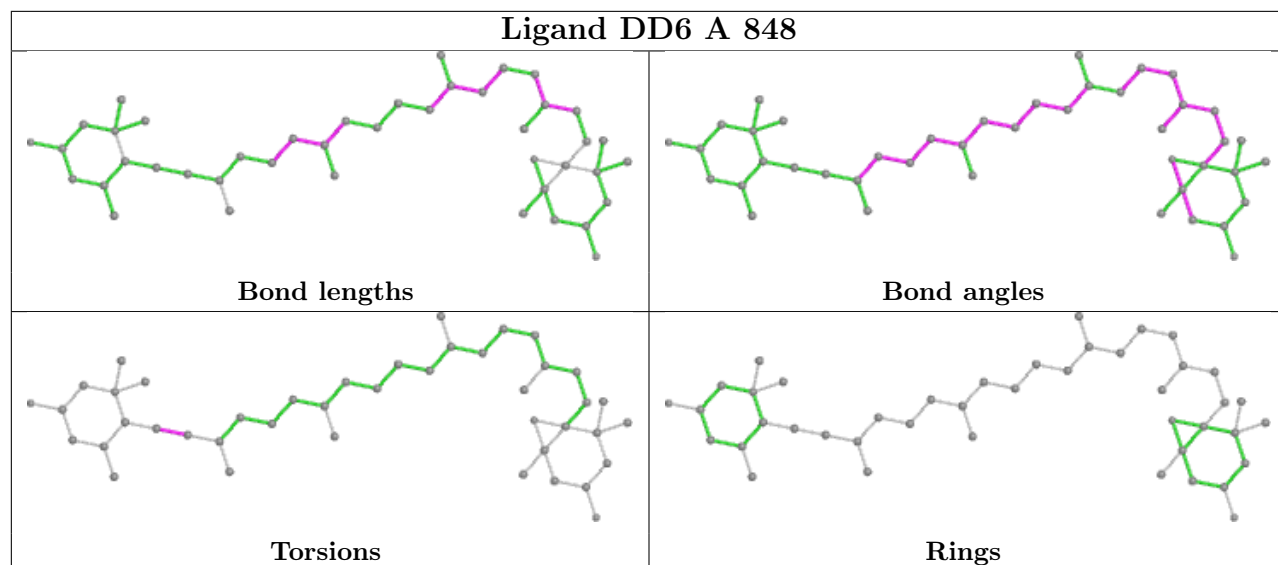


Ligand LHG I 103

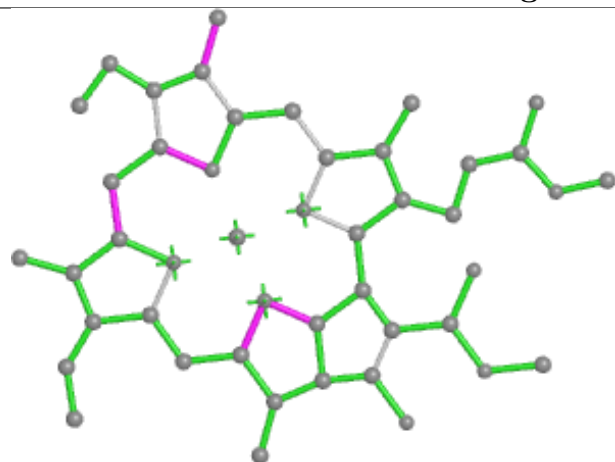


Ligand CLA B 810

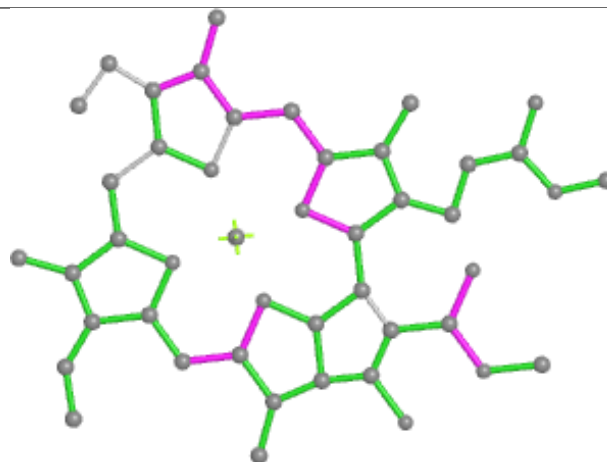




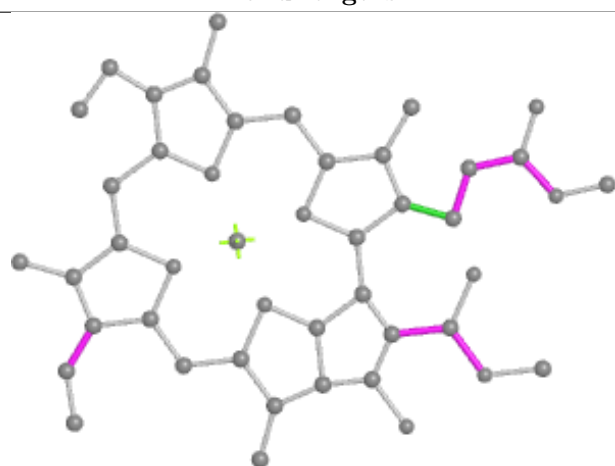
Ligand CLA 6 606



Bond lengths



Bond angles

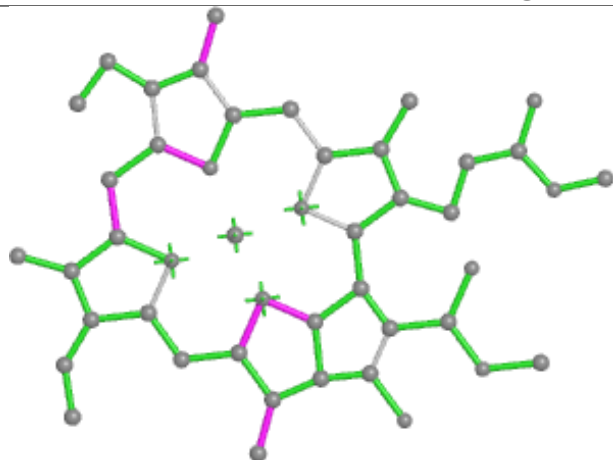


Torsions

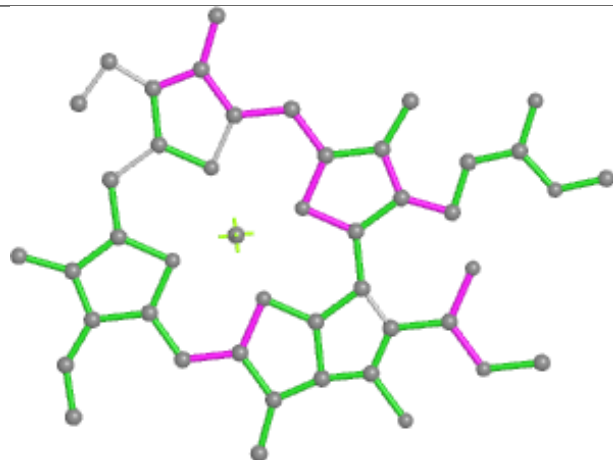


Rings

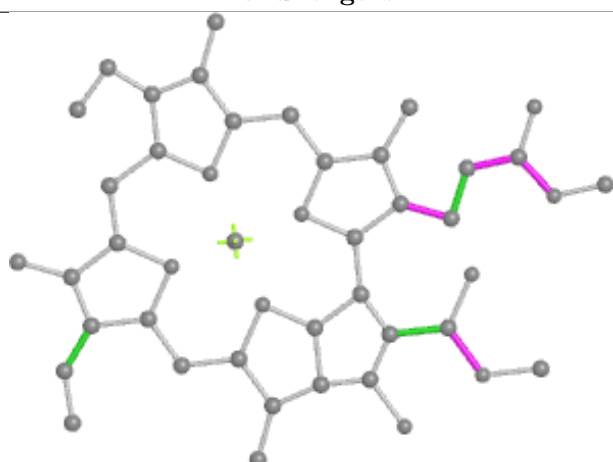
Ligand CLA 3 308



Bond lengths



Bond angles

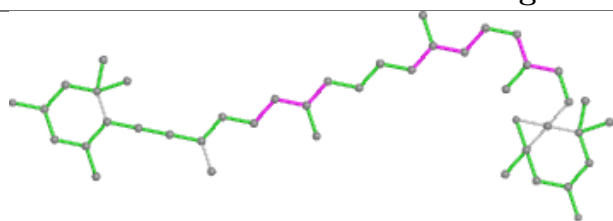


Torsions

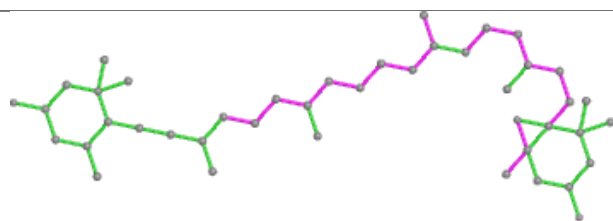


Rings

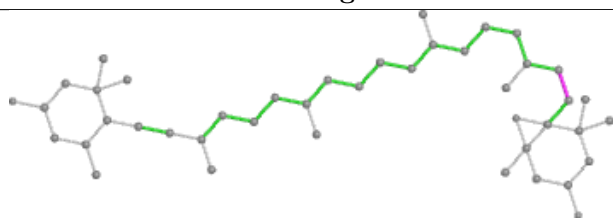
Ligand DD6 4 617



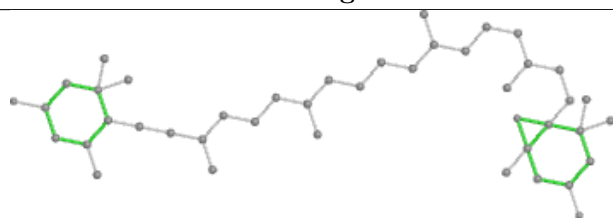
Bond lengths



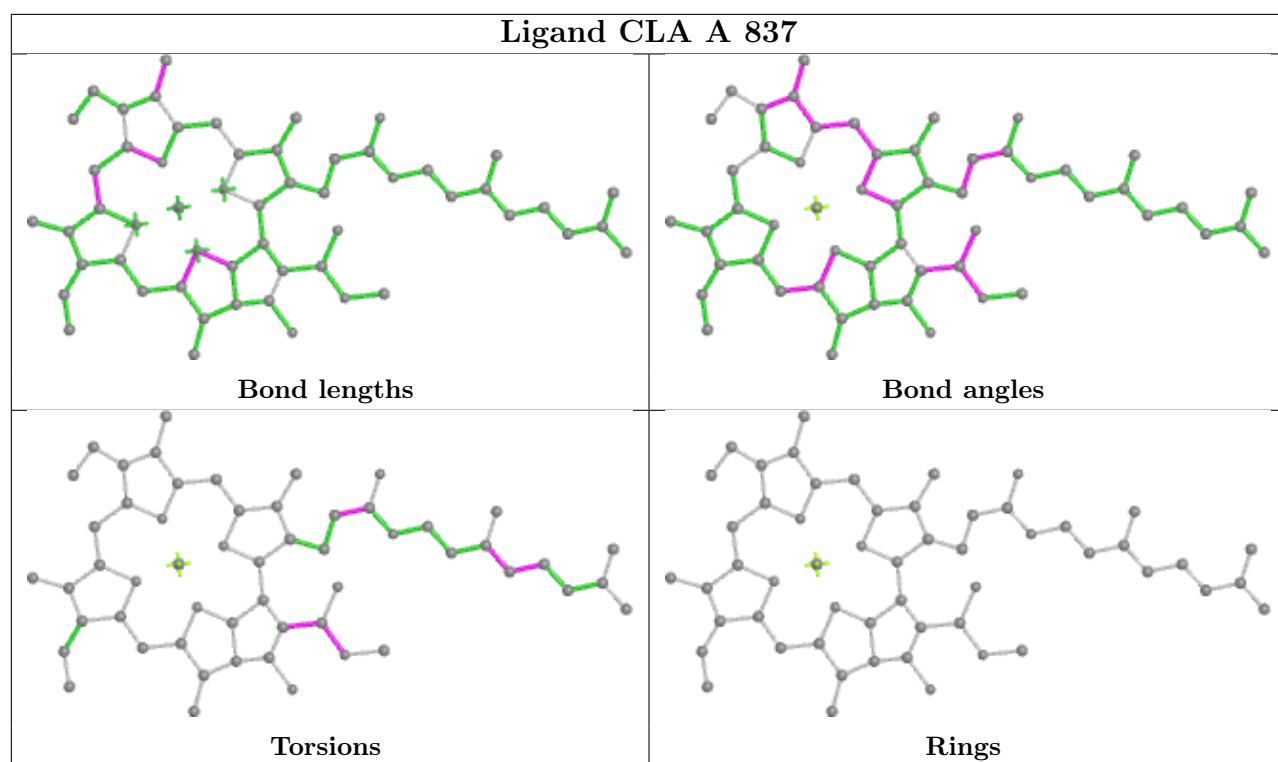
Bond angles



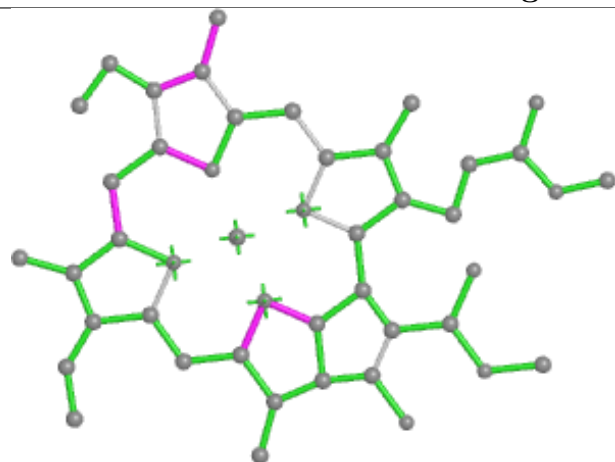
Torsions



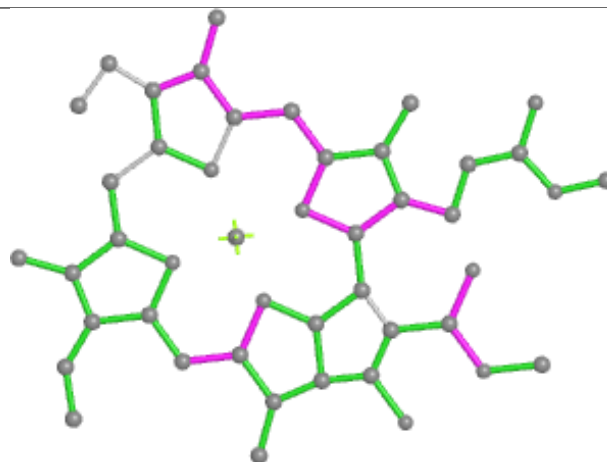
Rings



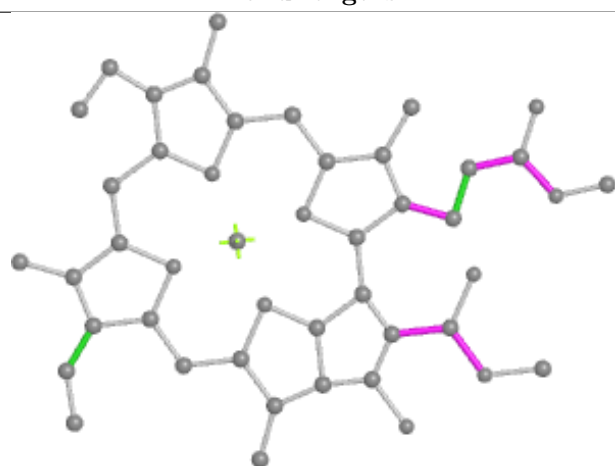
Ligand CLA c 603



Bond lengths



Bond angles

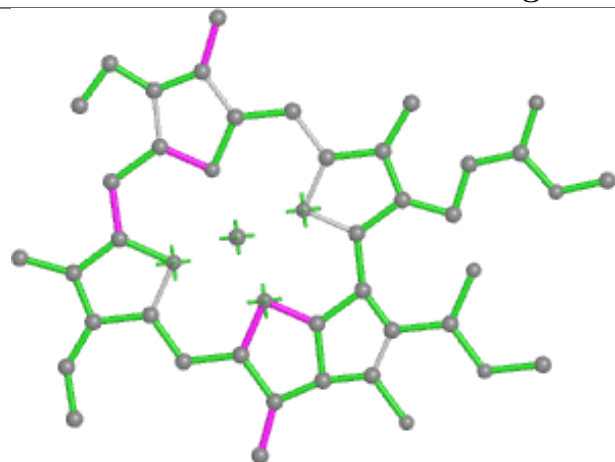


Torsions

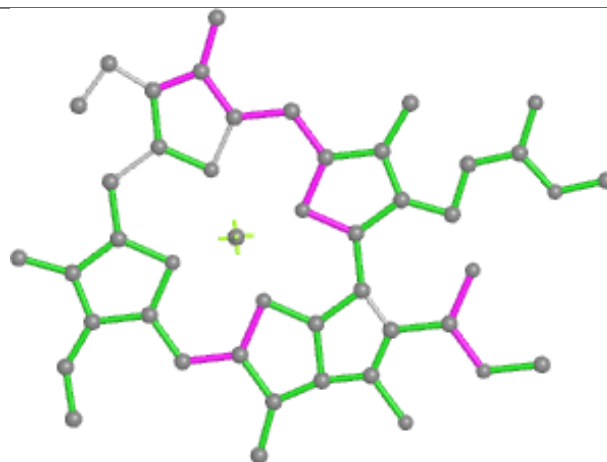


Rings

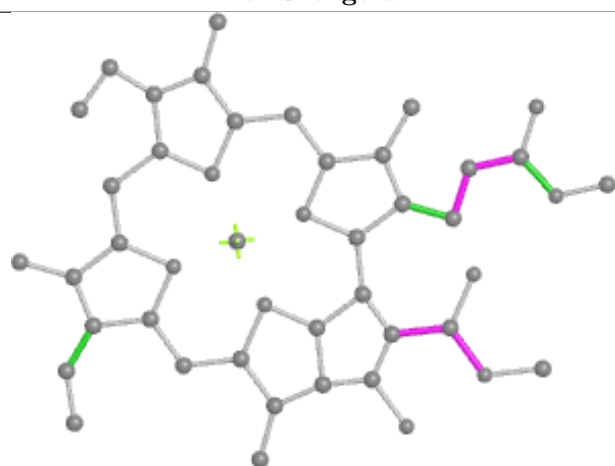
Ligand CLA t 304



Bond lengths



Bond angles

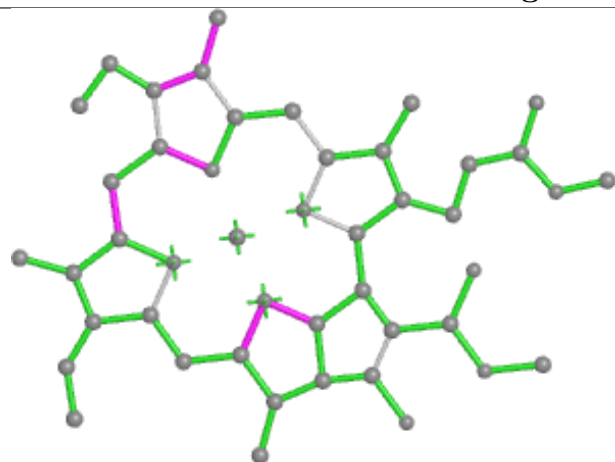


Torsions

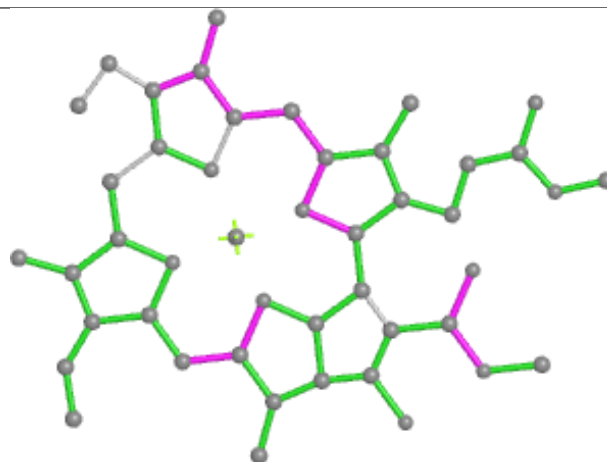


Rings

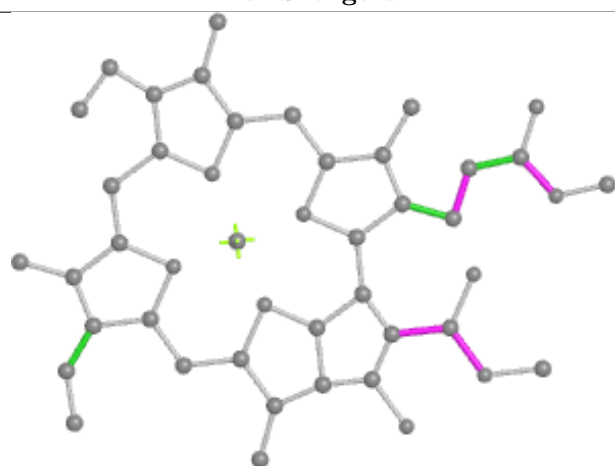
Ligand CLA c 604



Bond lengths



Bond angles

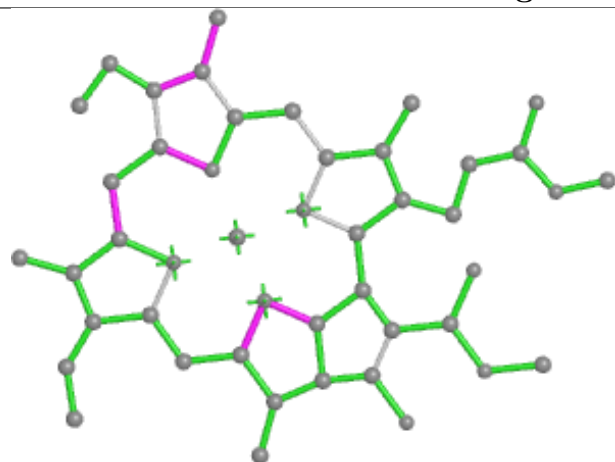


Torsions

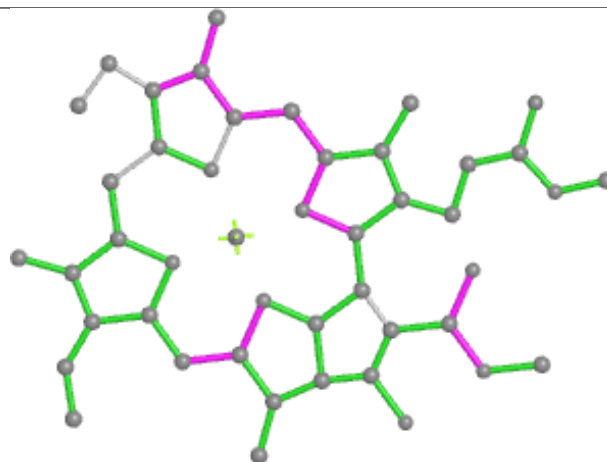


Rings

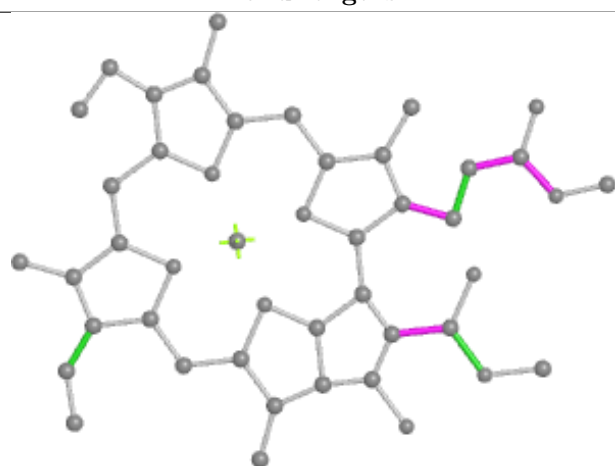
Ligand CLA A 811



Bond lengths



Bond angles

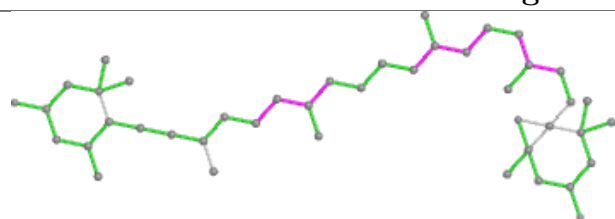


Torsions

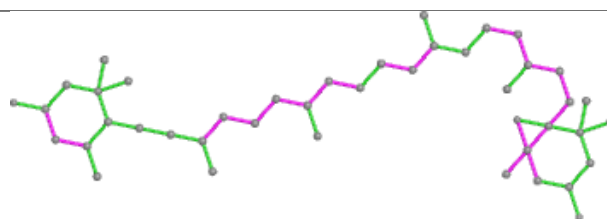


Rings

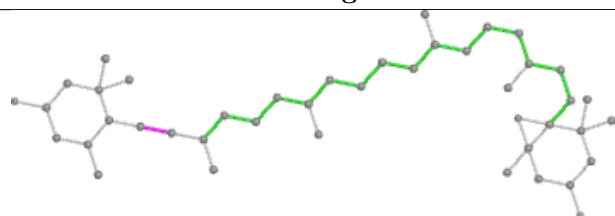
Ligand DD6 c 614



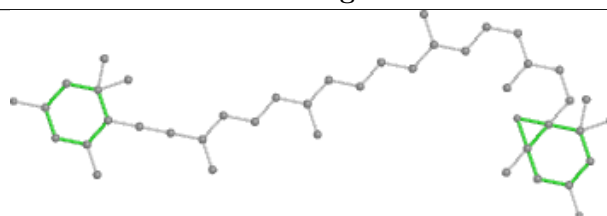
Bond lengths



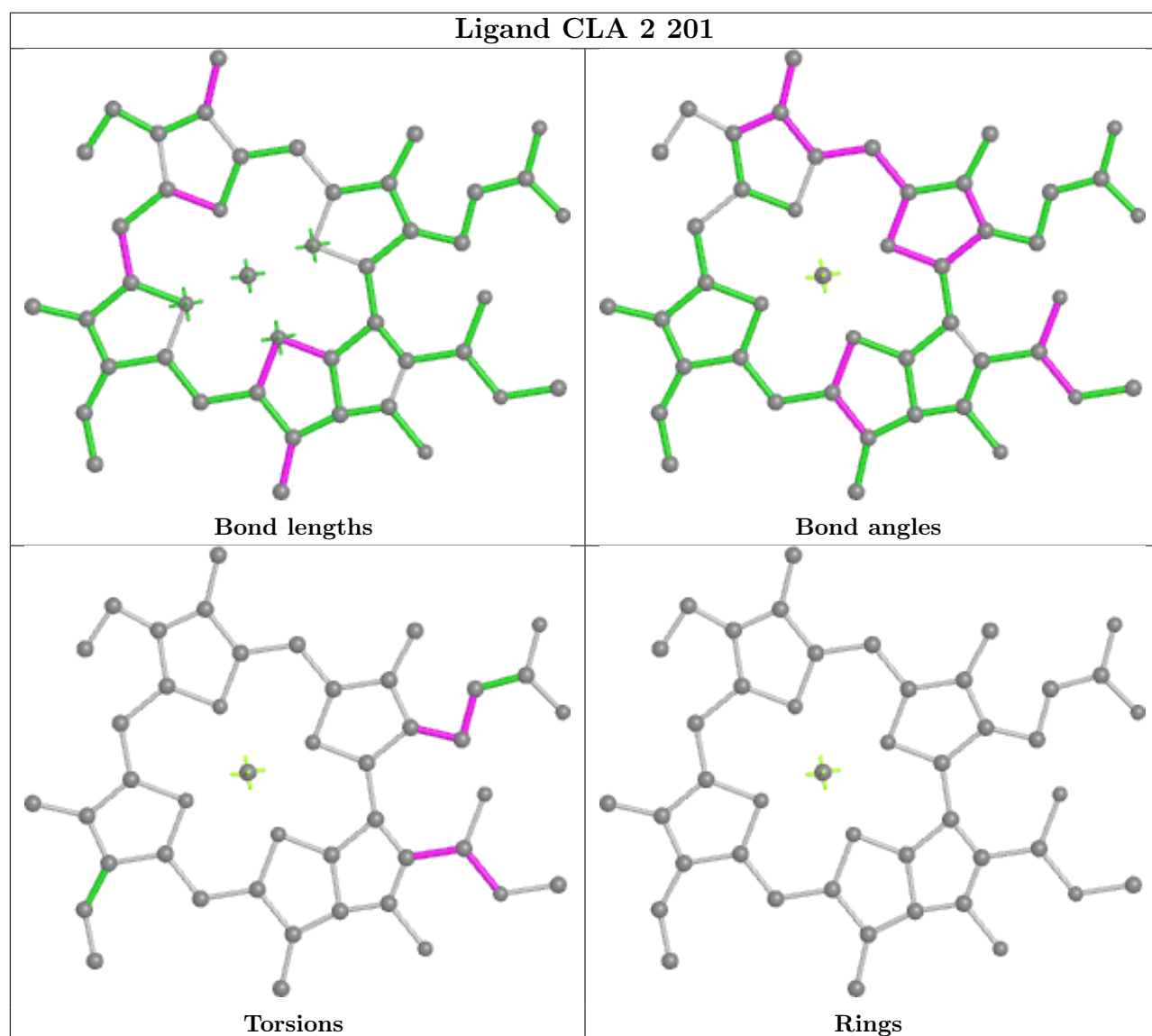
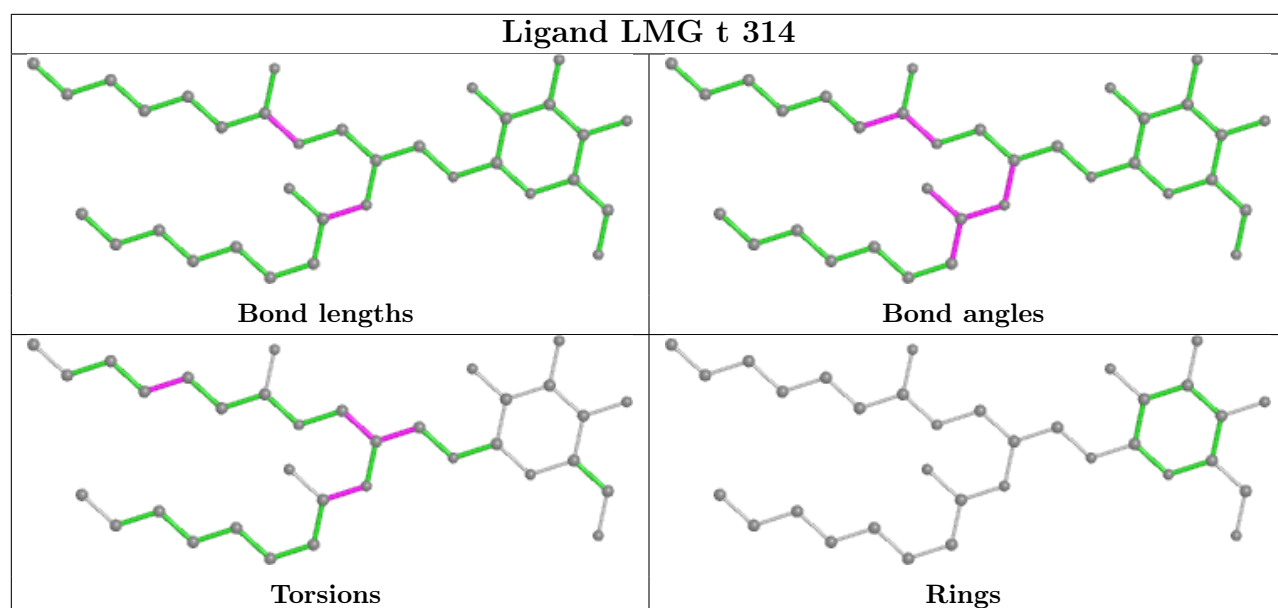
Bond angles

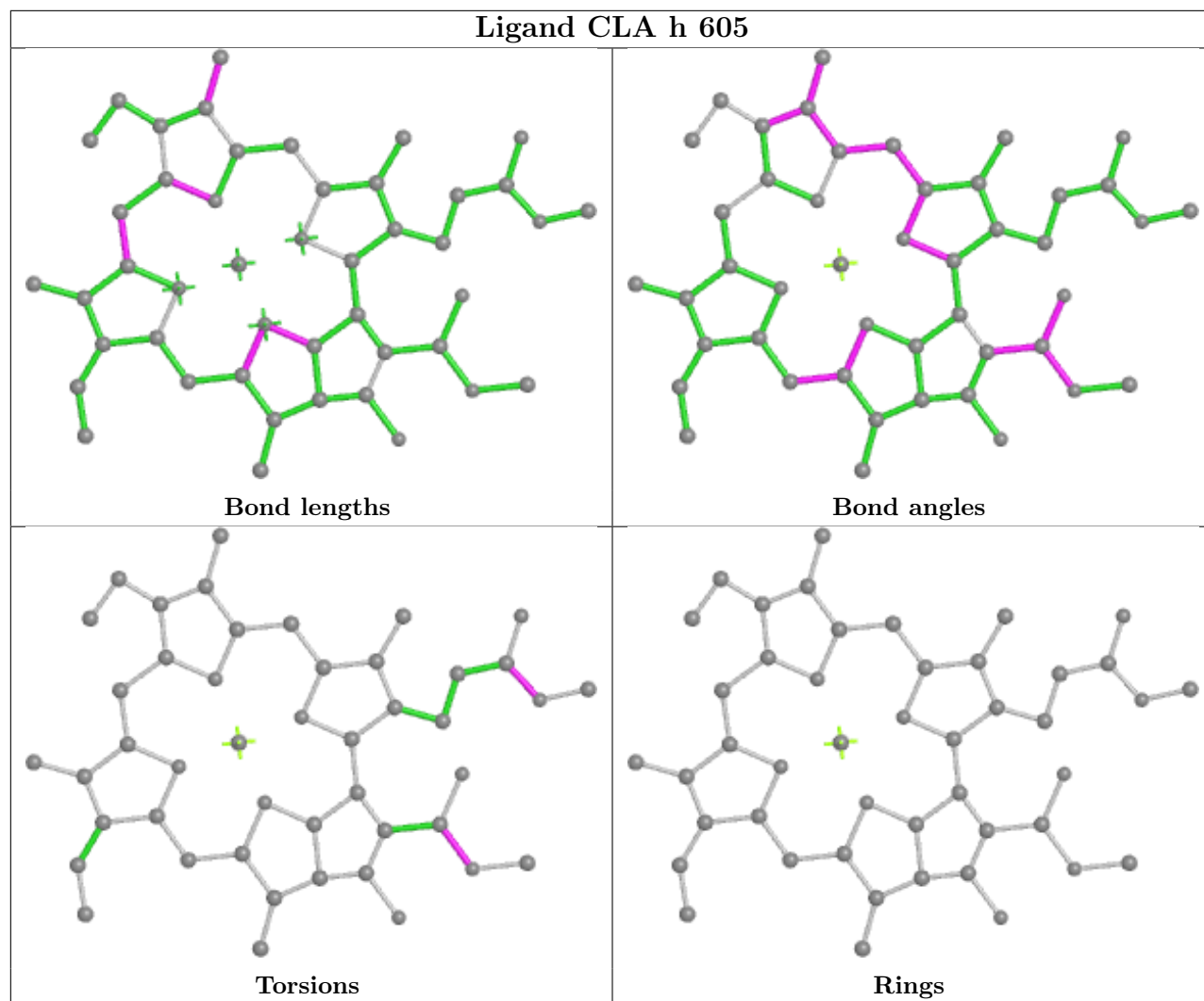
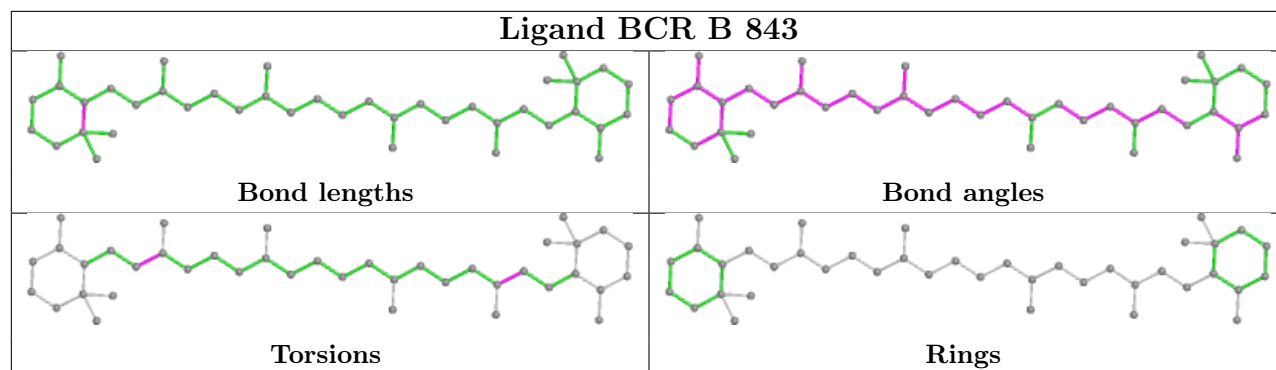


Torsions

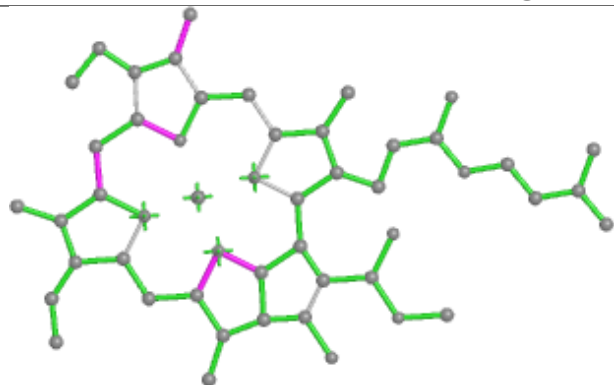


Rings

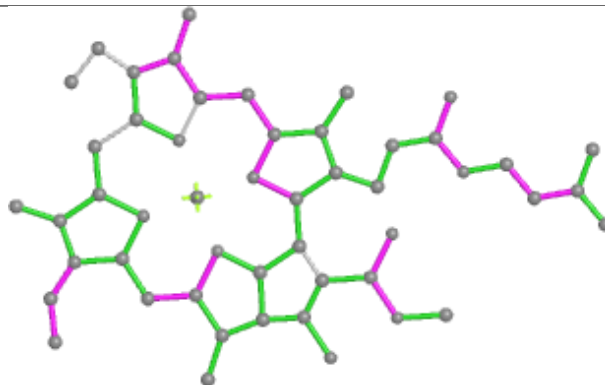




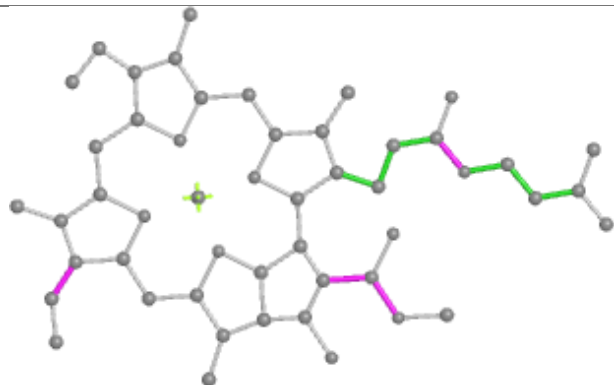
Ligand CLA 4 608



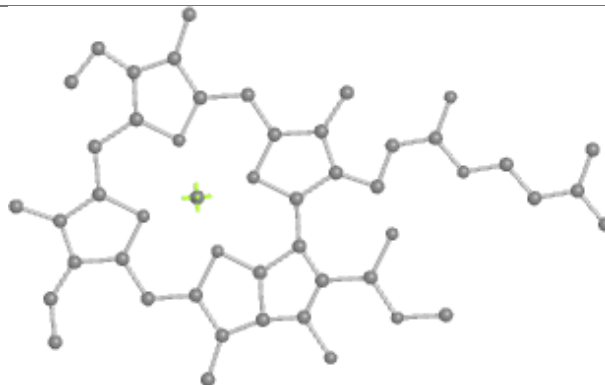
Bond lengths



Bond angles

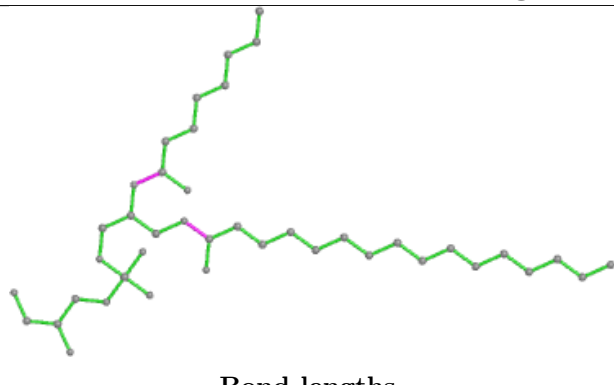


Torsions

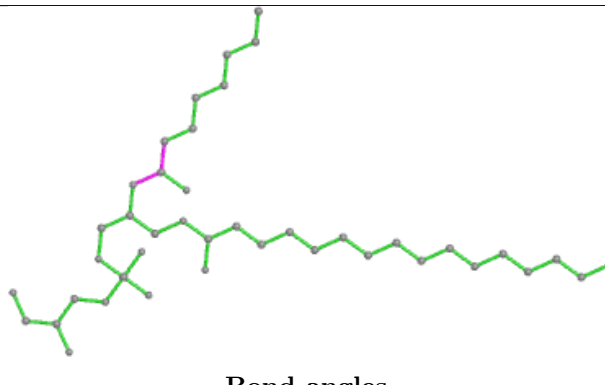


Rings

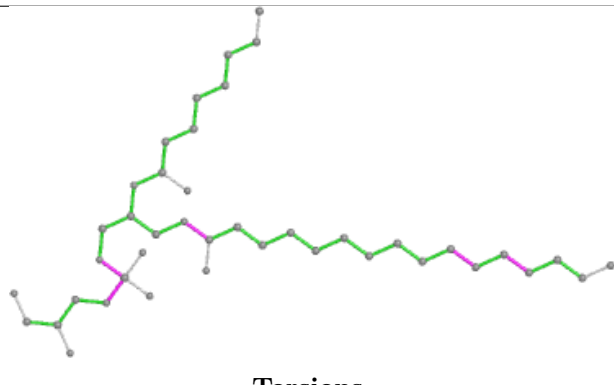
Ligand LHG B 845



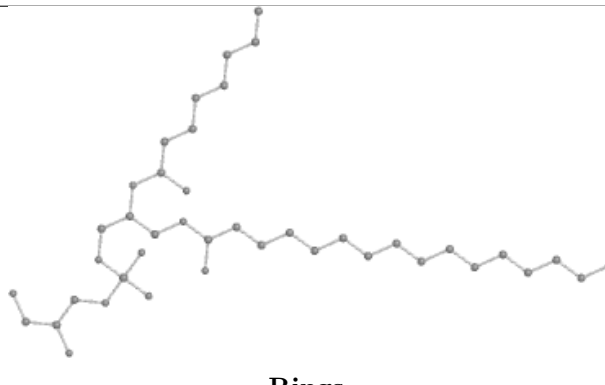
Bond lengths



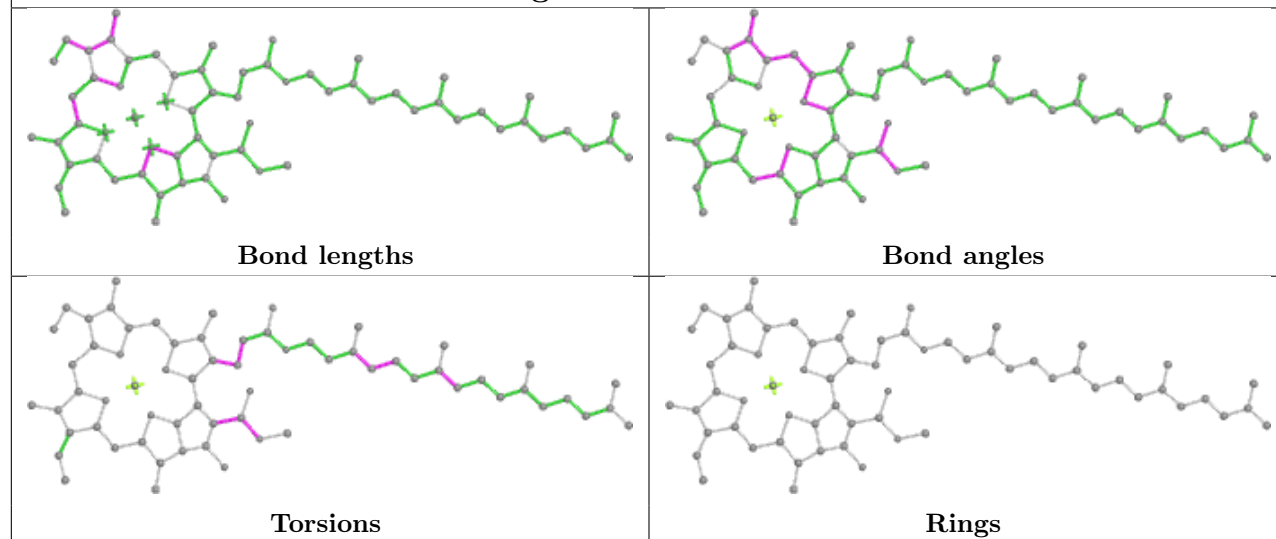
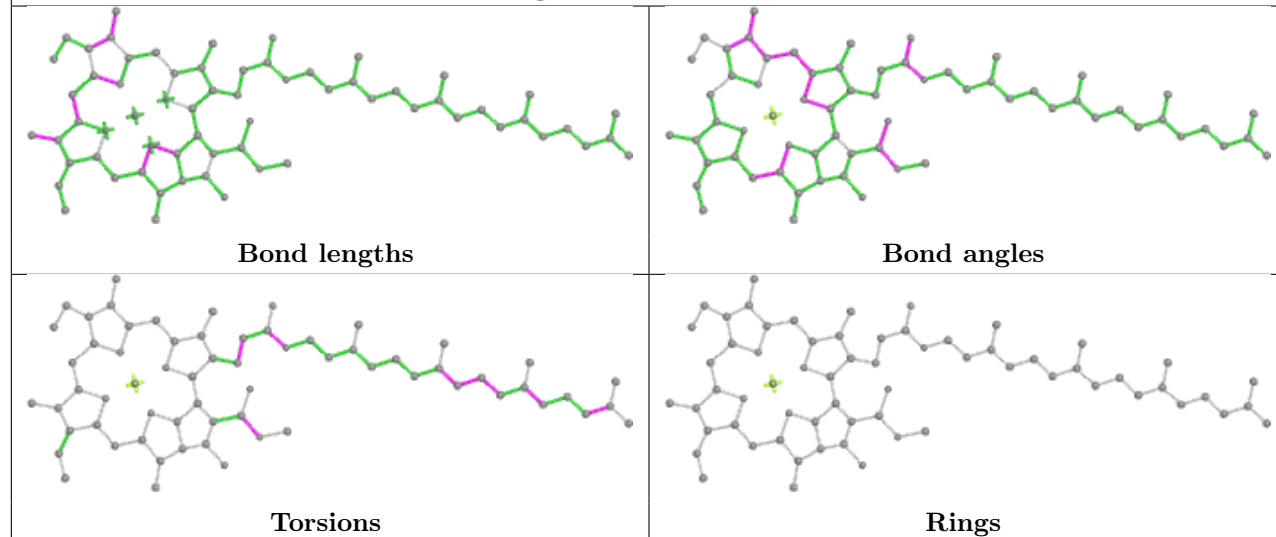
Bond angles

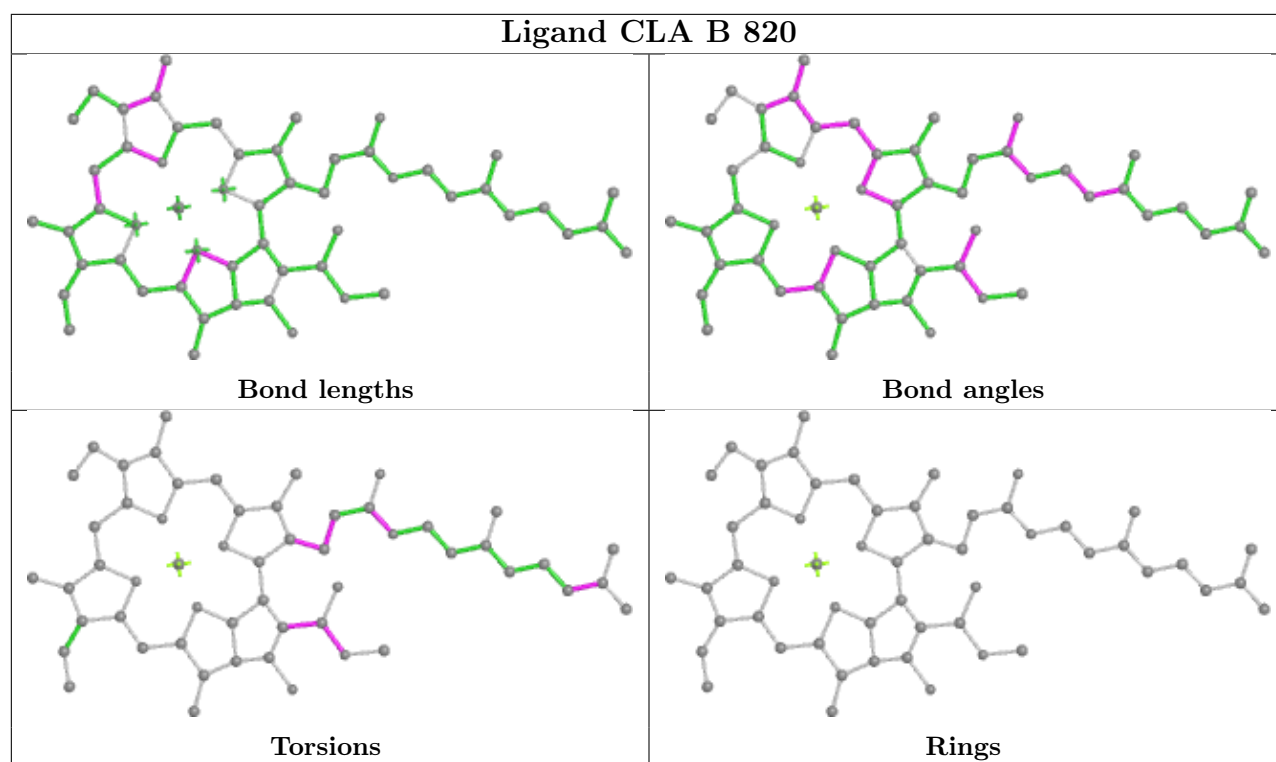


Torsions

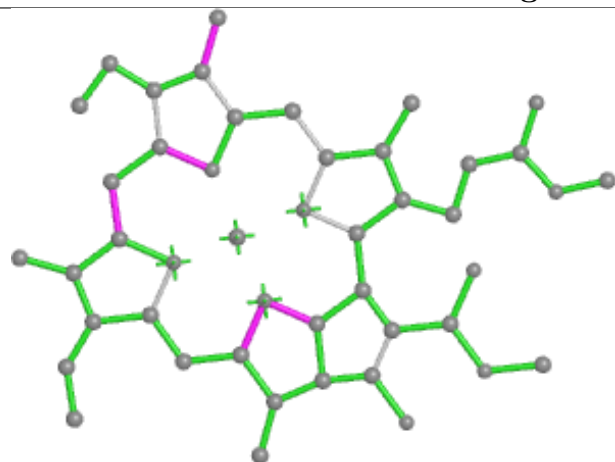


Rings

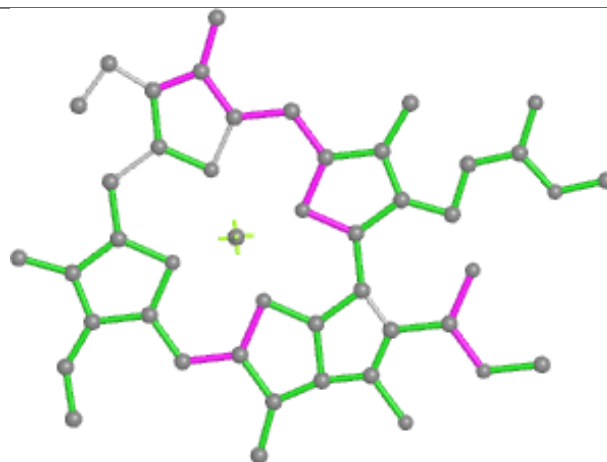
Ligand CLA A 856**Ligand CLA A 812**



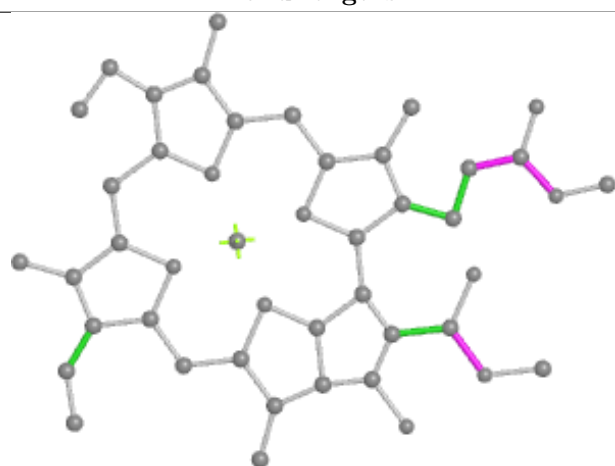
Ligand CLA 5 606



Bond lengths



Bond angles

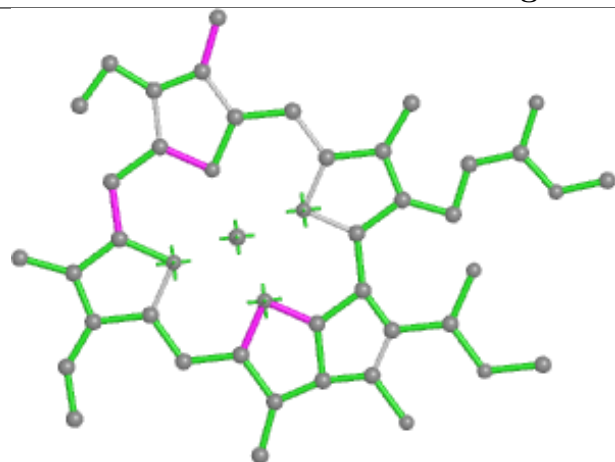


Torsions

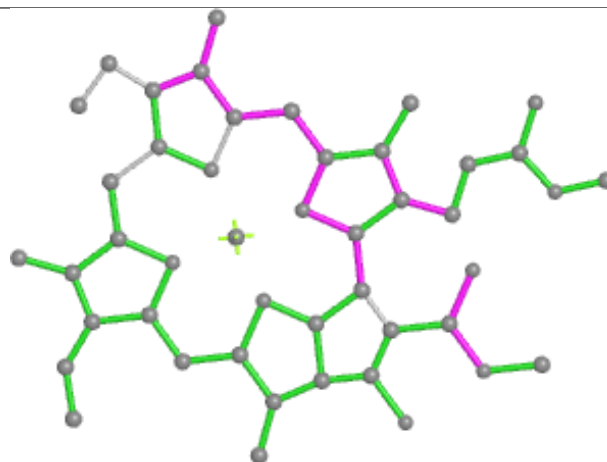


Rings

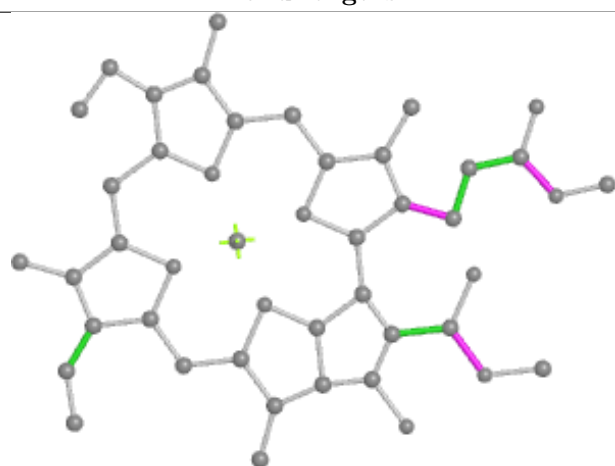
Ligand CLA 3 304



Bond lengths



Bond angles

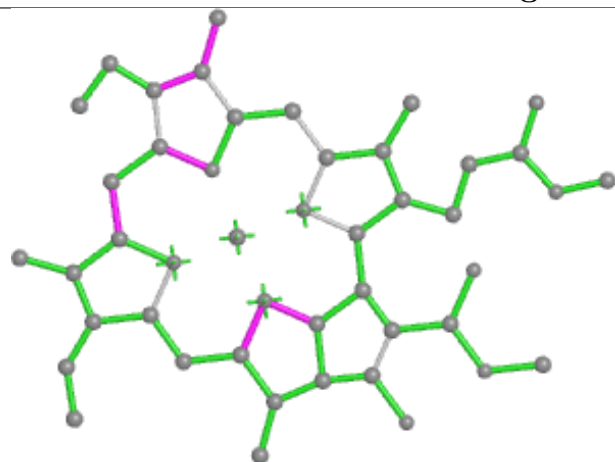


Torsions

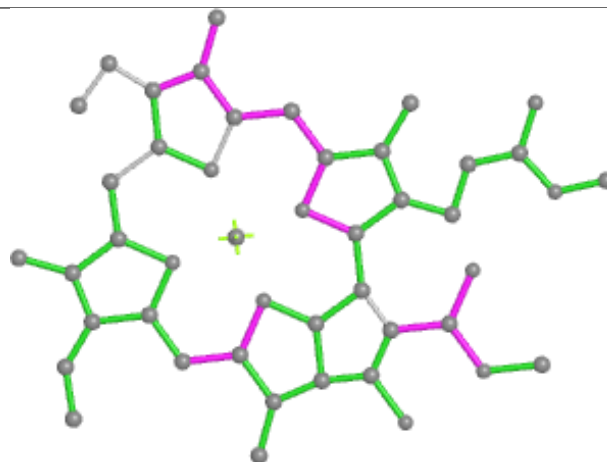


Rings

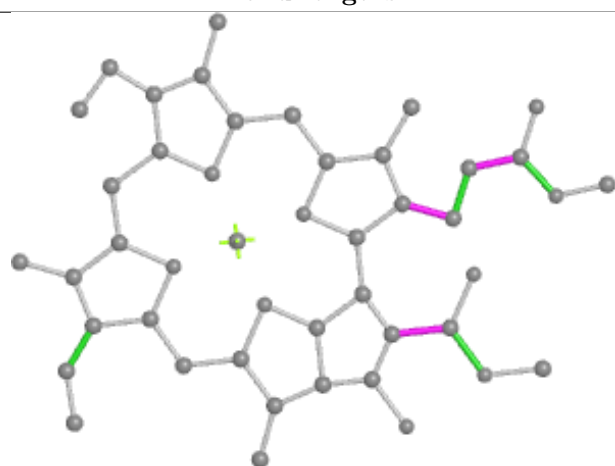
Ligand CLA 2 206



Bond lengths



Bond angles

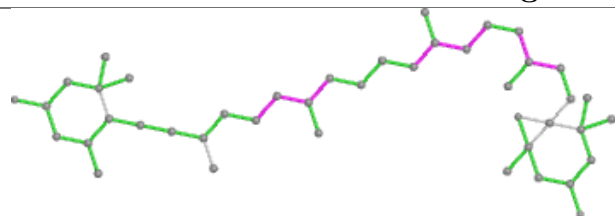


Torsions

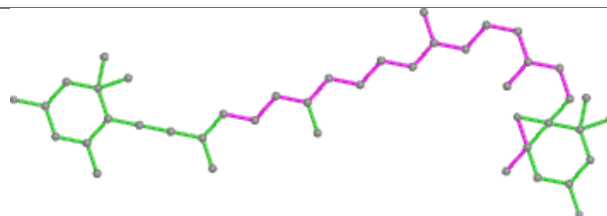


Rings

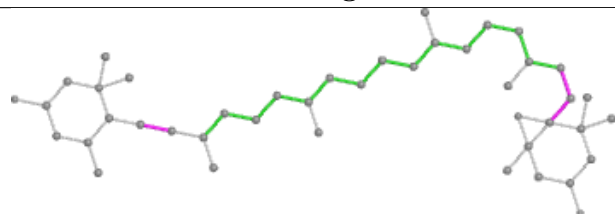
Ligand DD6 k 315



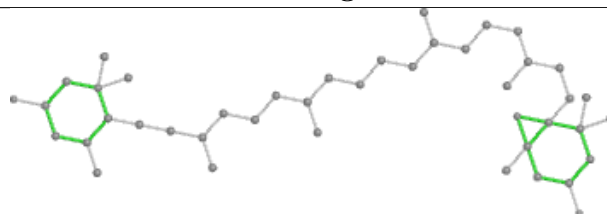
Bond lengths



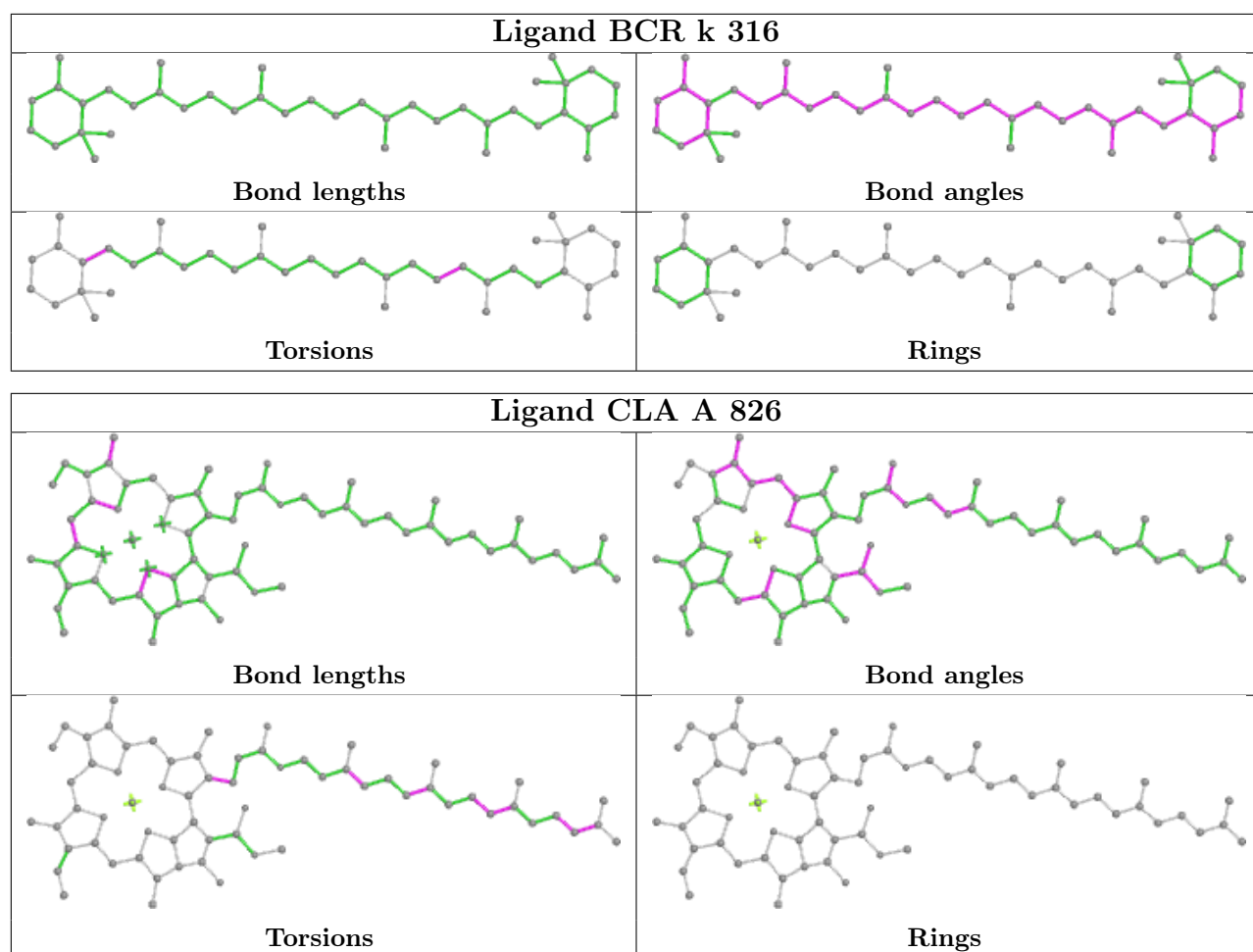
Bond angles

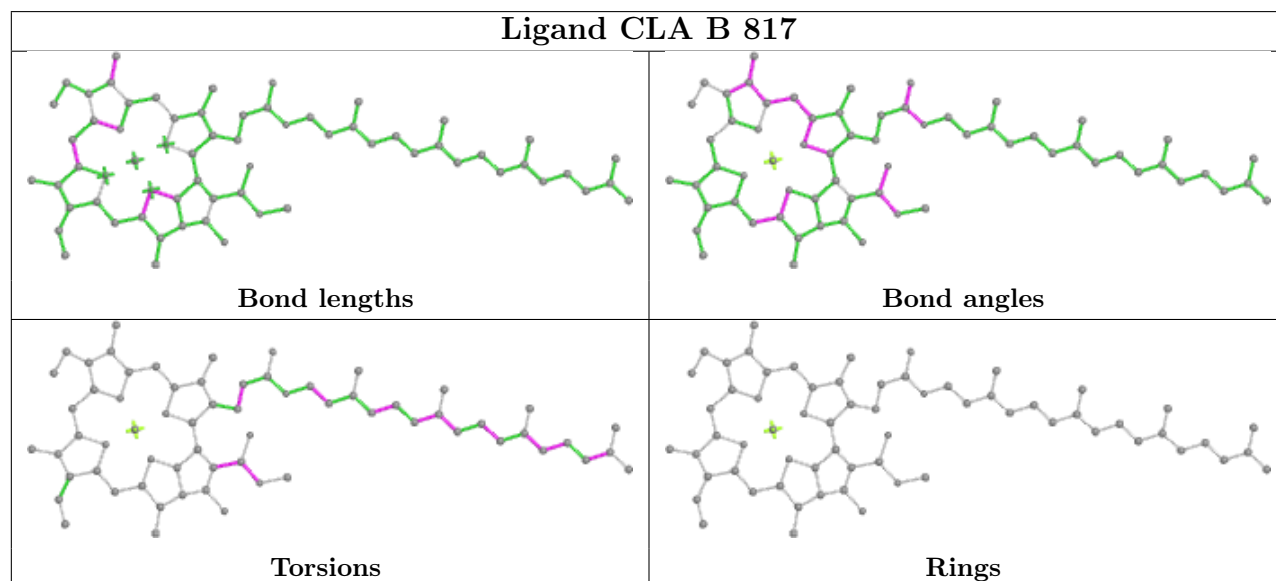
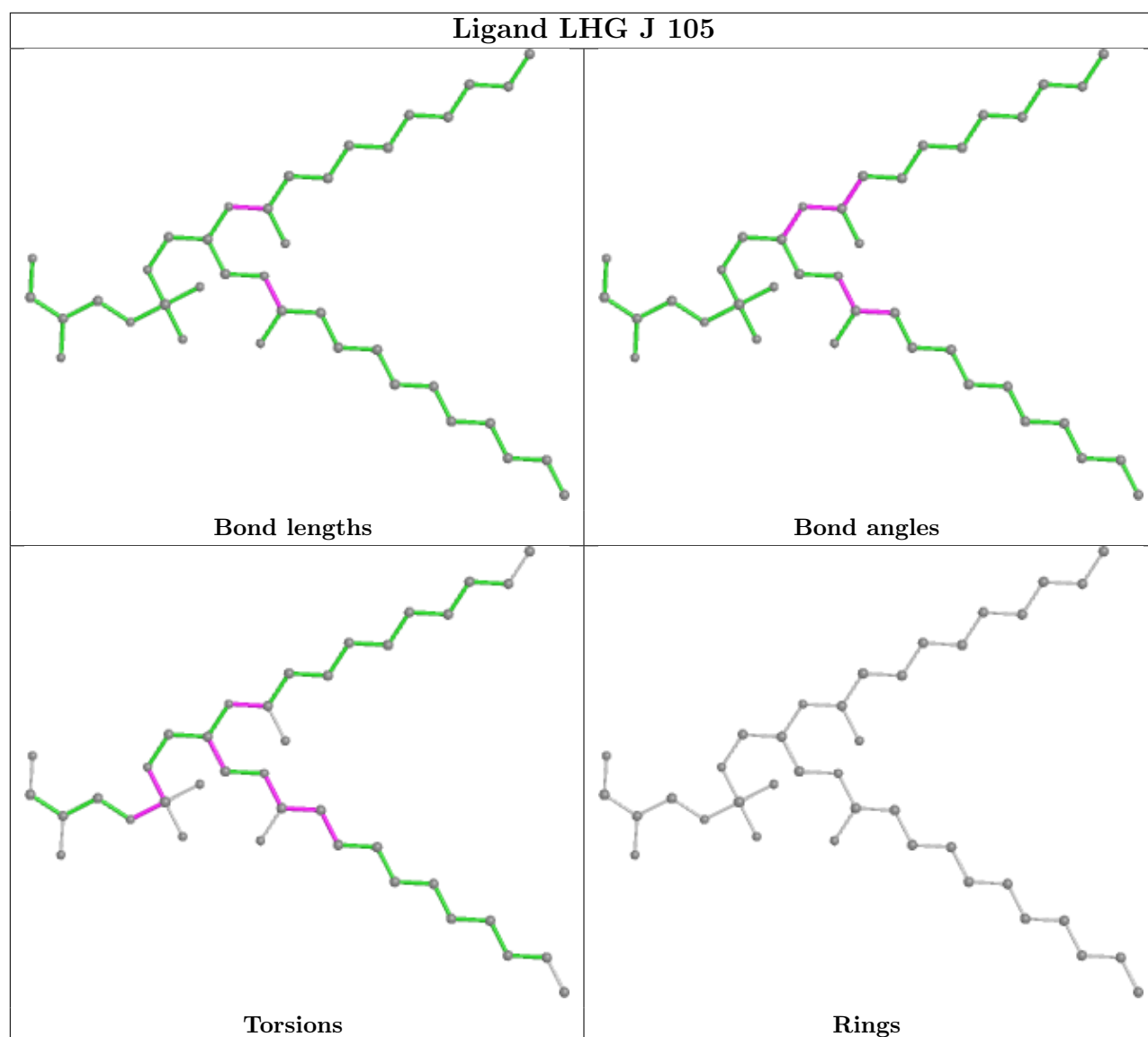


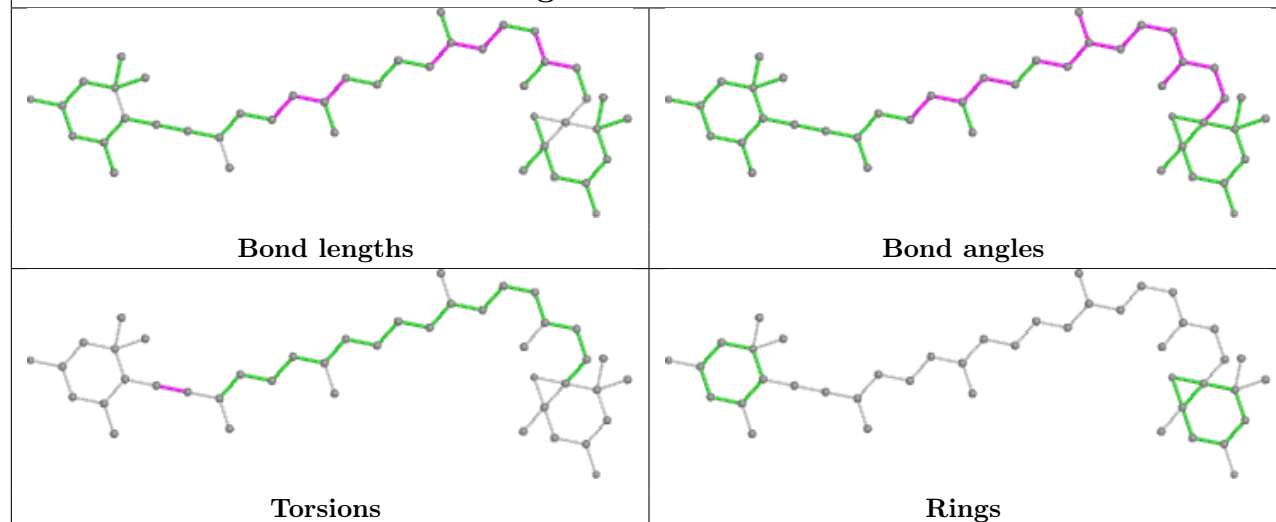
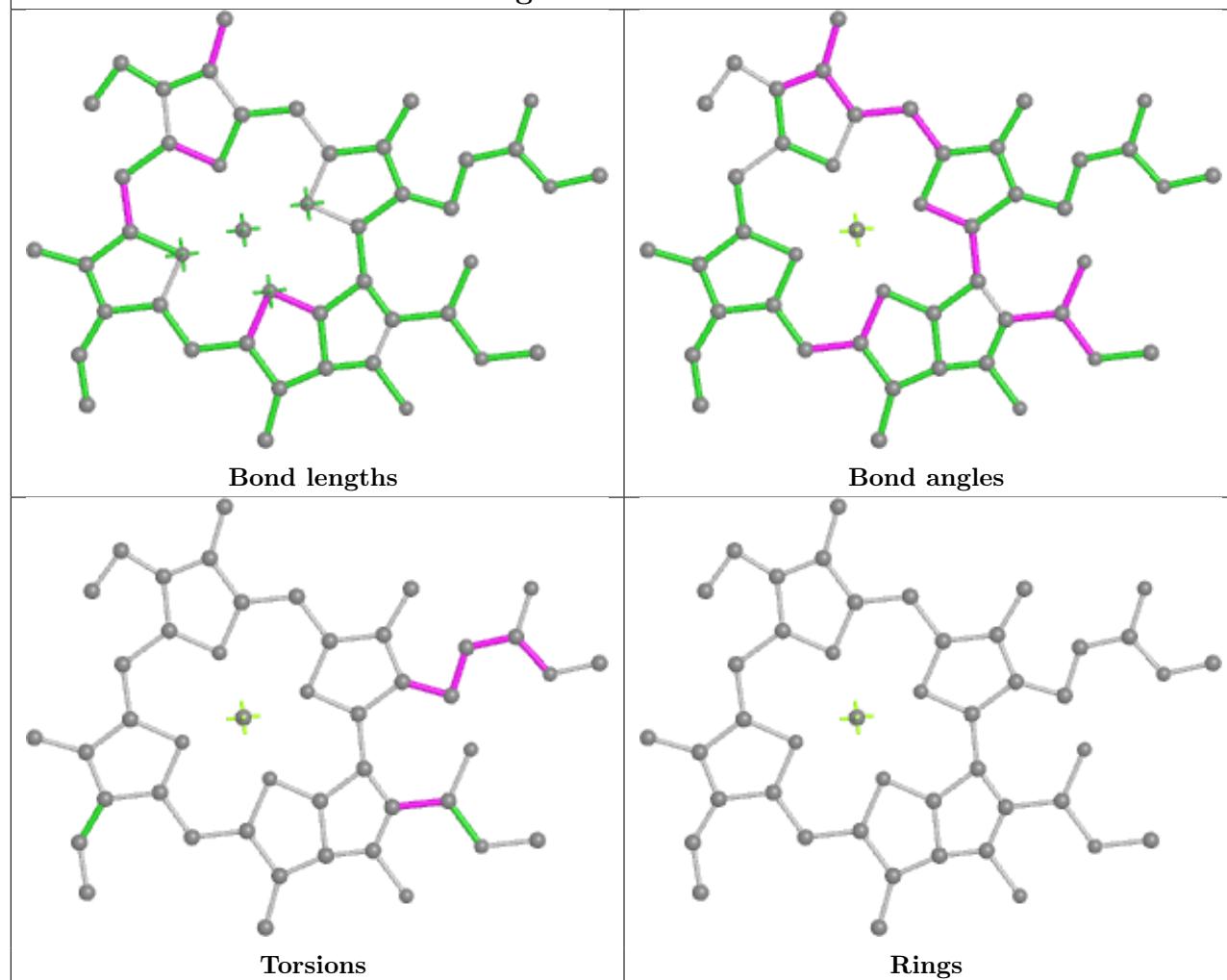
Torsions



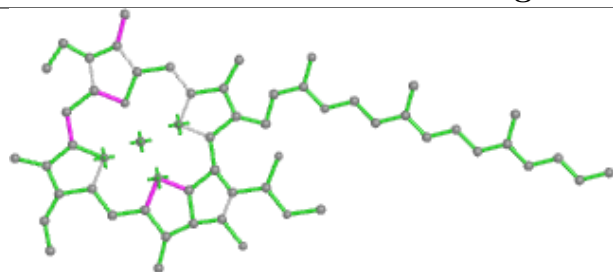
Rings



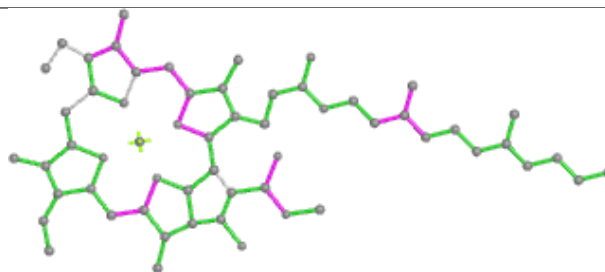


Ligand DD6 1 313**Ligand CLA 7 612**

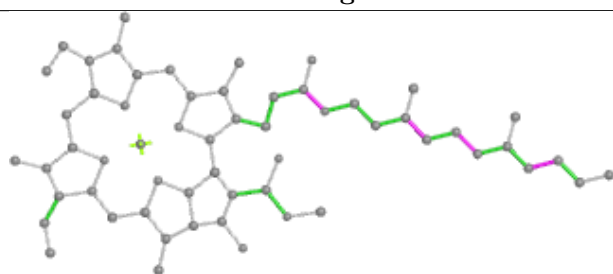
Ligand CLA B 833



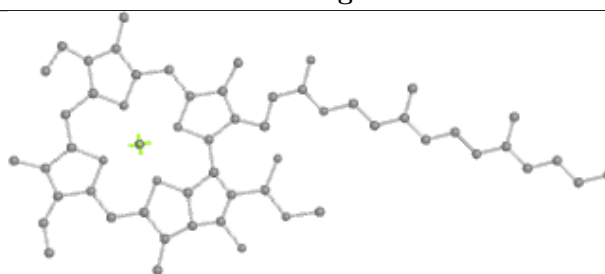
Bond lengths



Bond angles

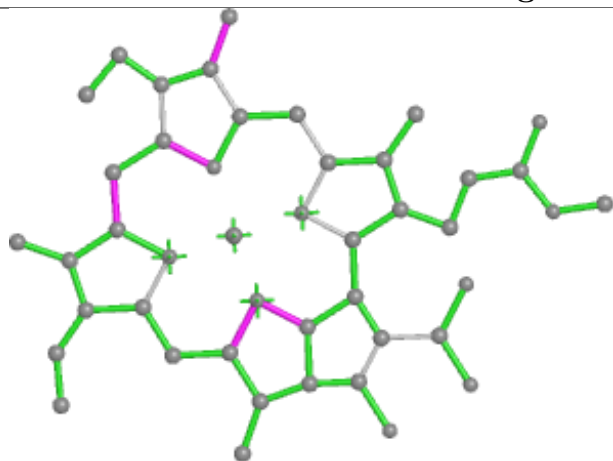


Torsions

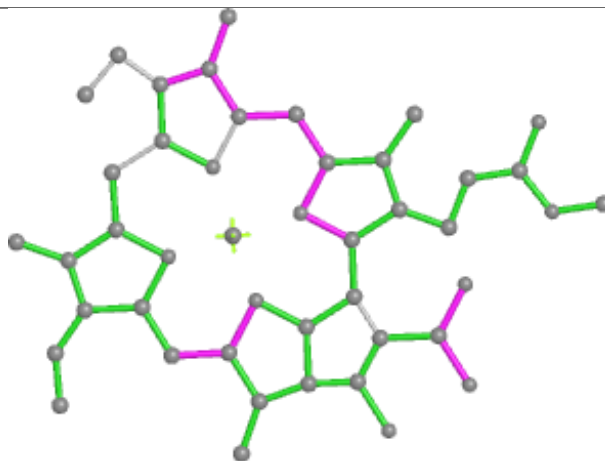


Rings

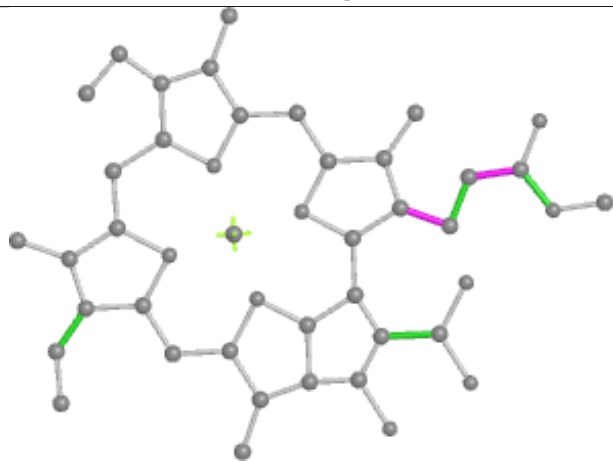
Ligand CLA h 603



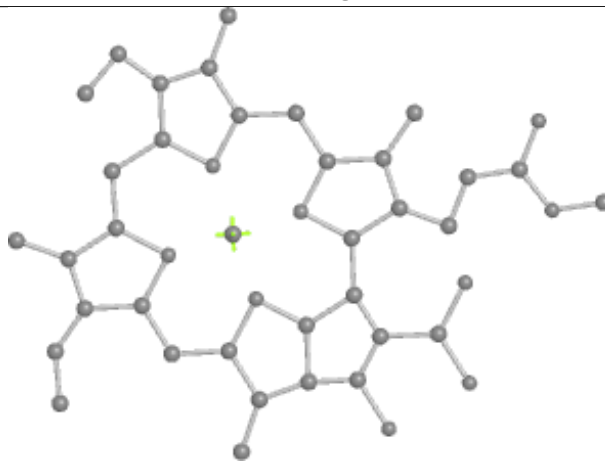
Bond lengths



Bond angles

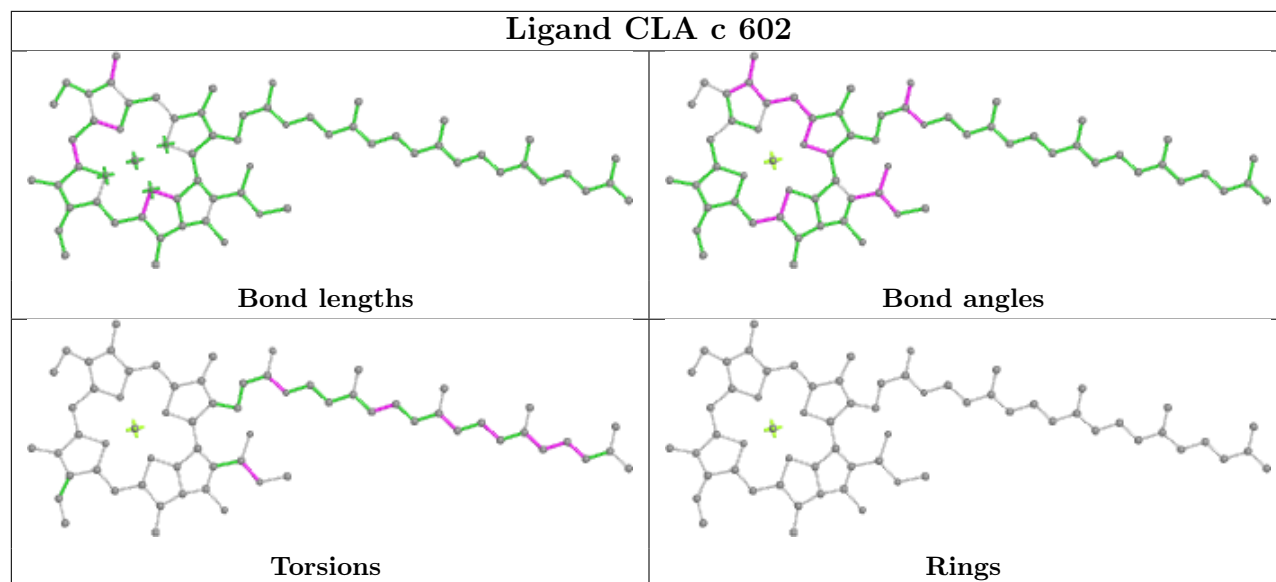


Torsions

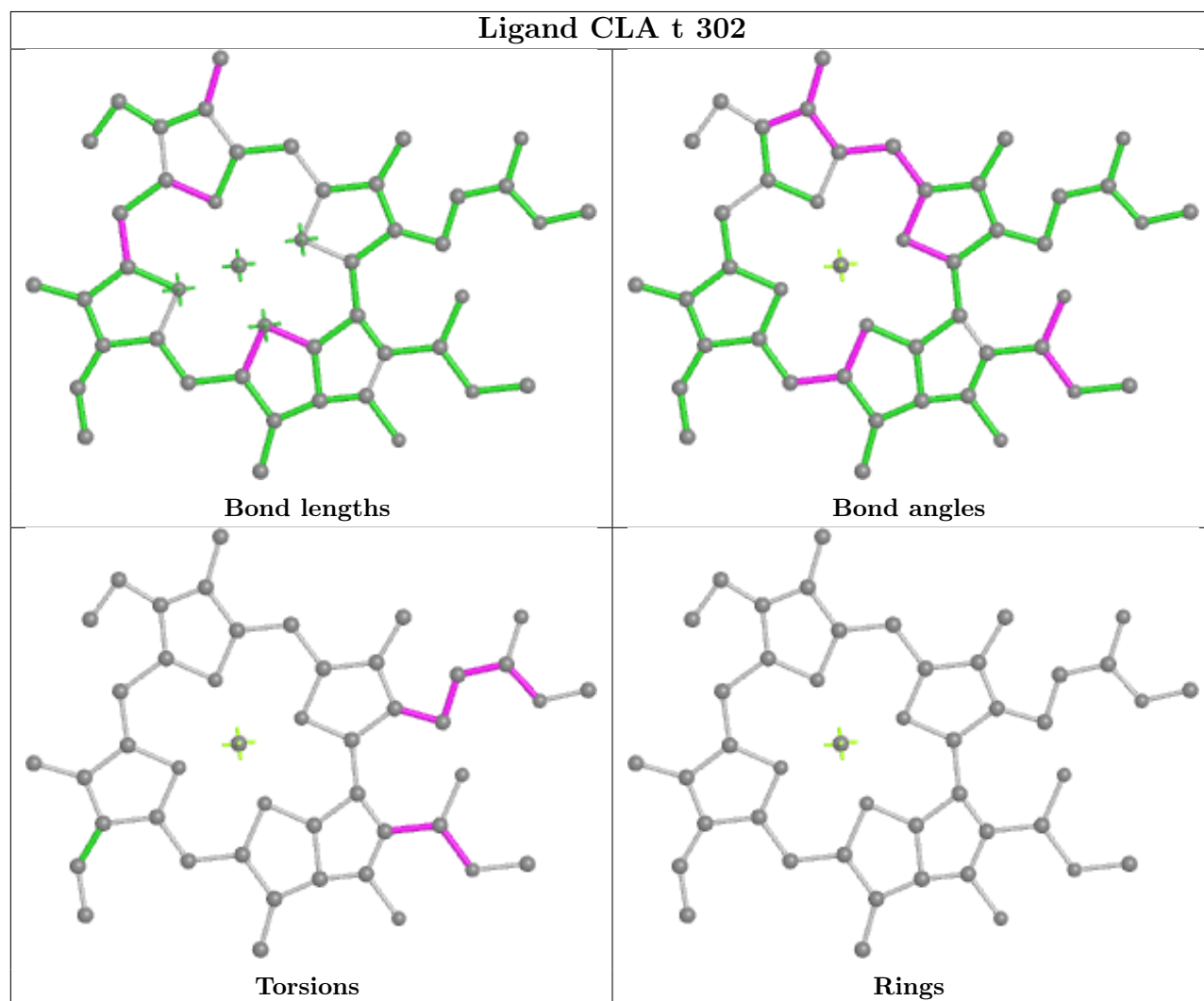


Rings

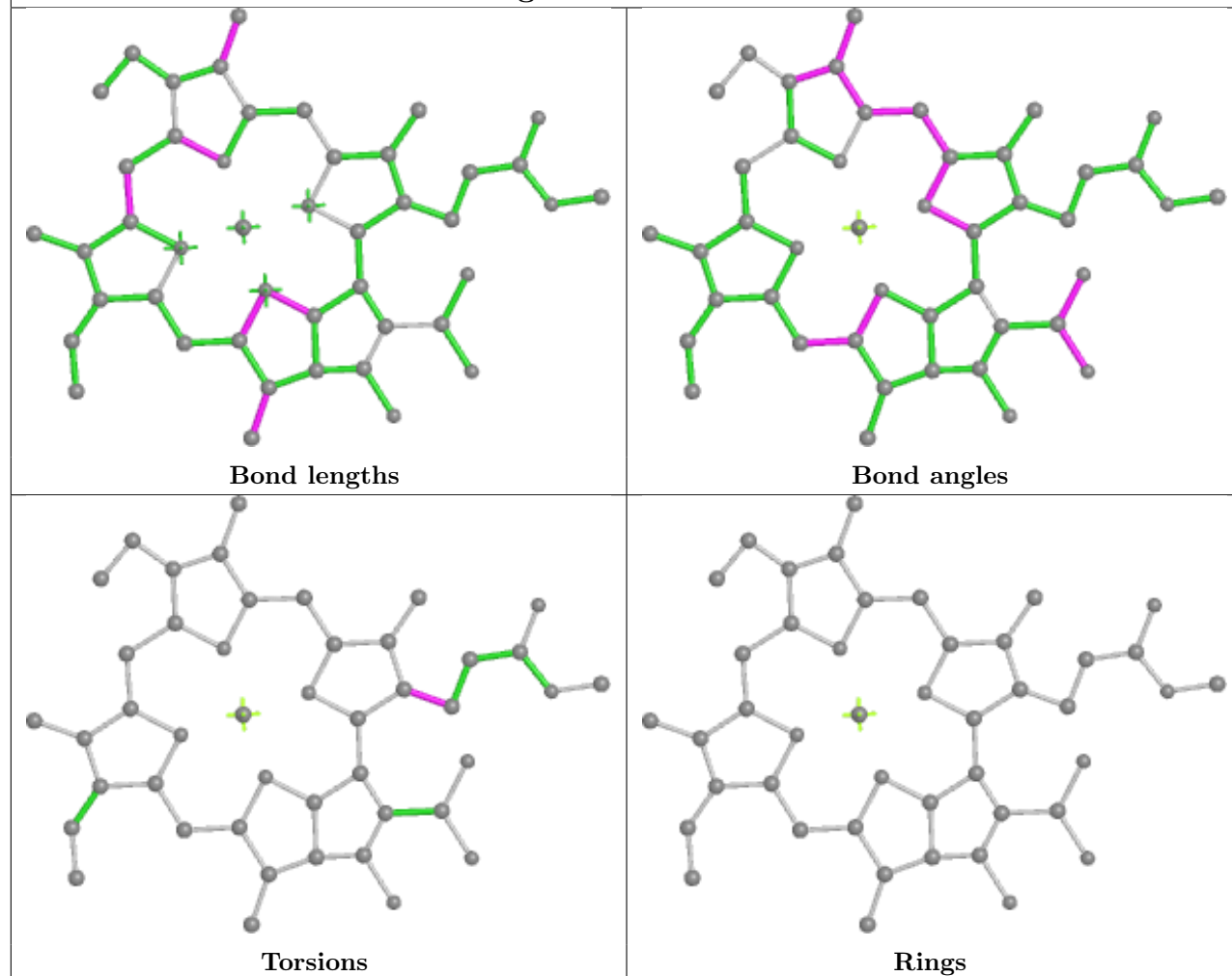
Ligand CLA c 602



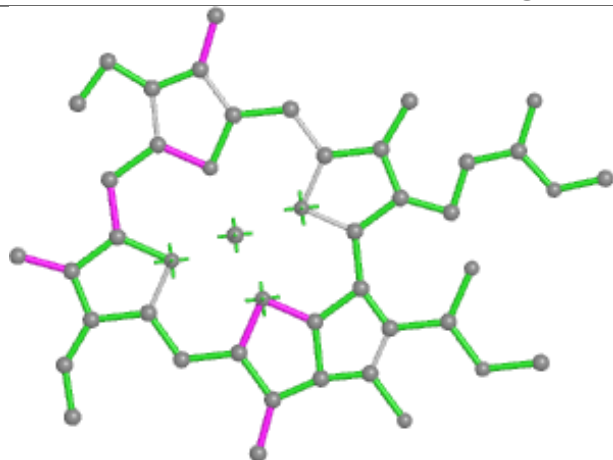
Ligand CLA t 302



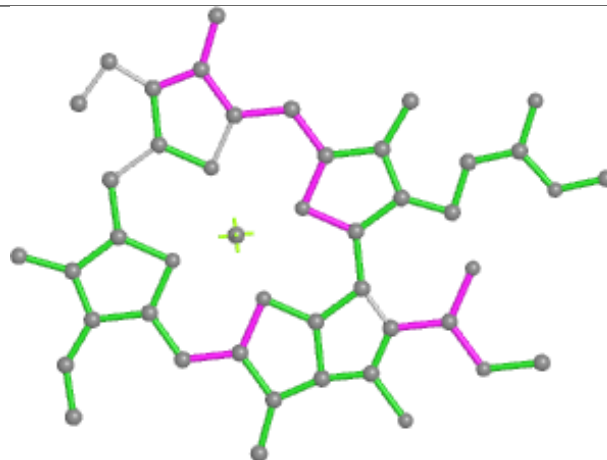
Ligand CLA 1 309



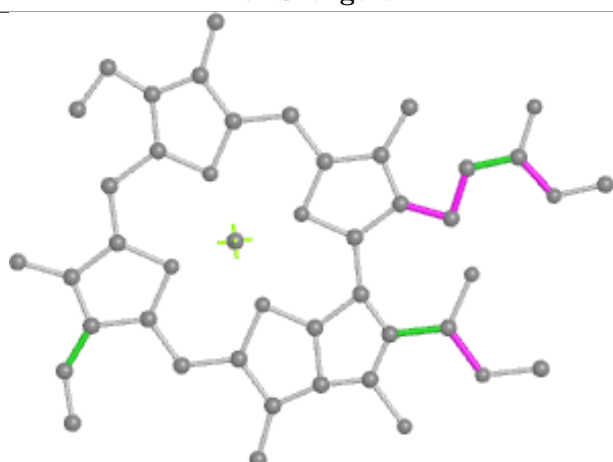
Ligand CLA 9 307



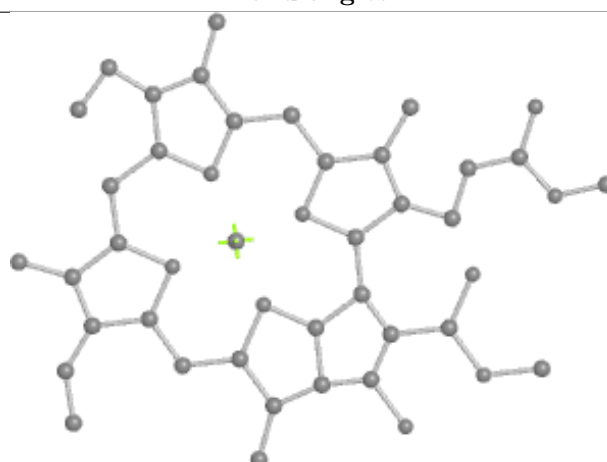
Bond lengths



Bond angles

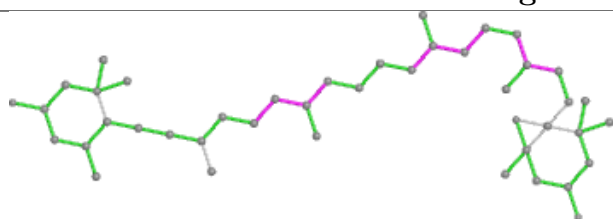


Torsions

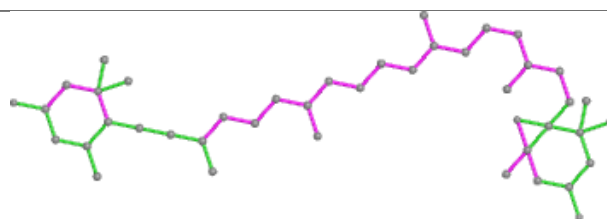


Rings

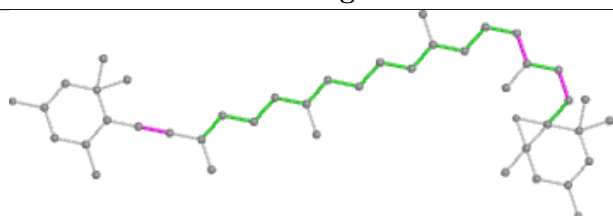
Ligand DD6 6 615



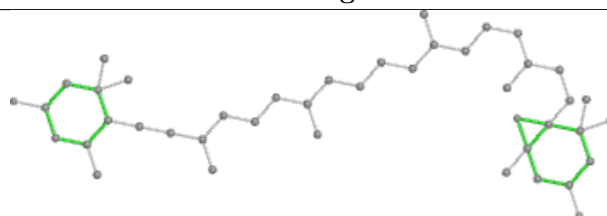
Bond lengths



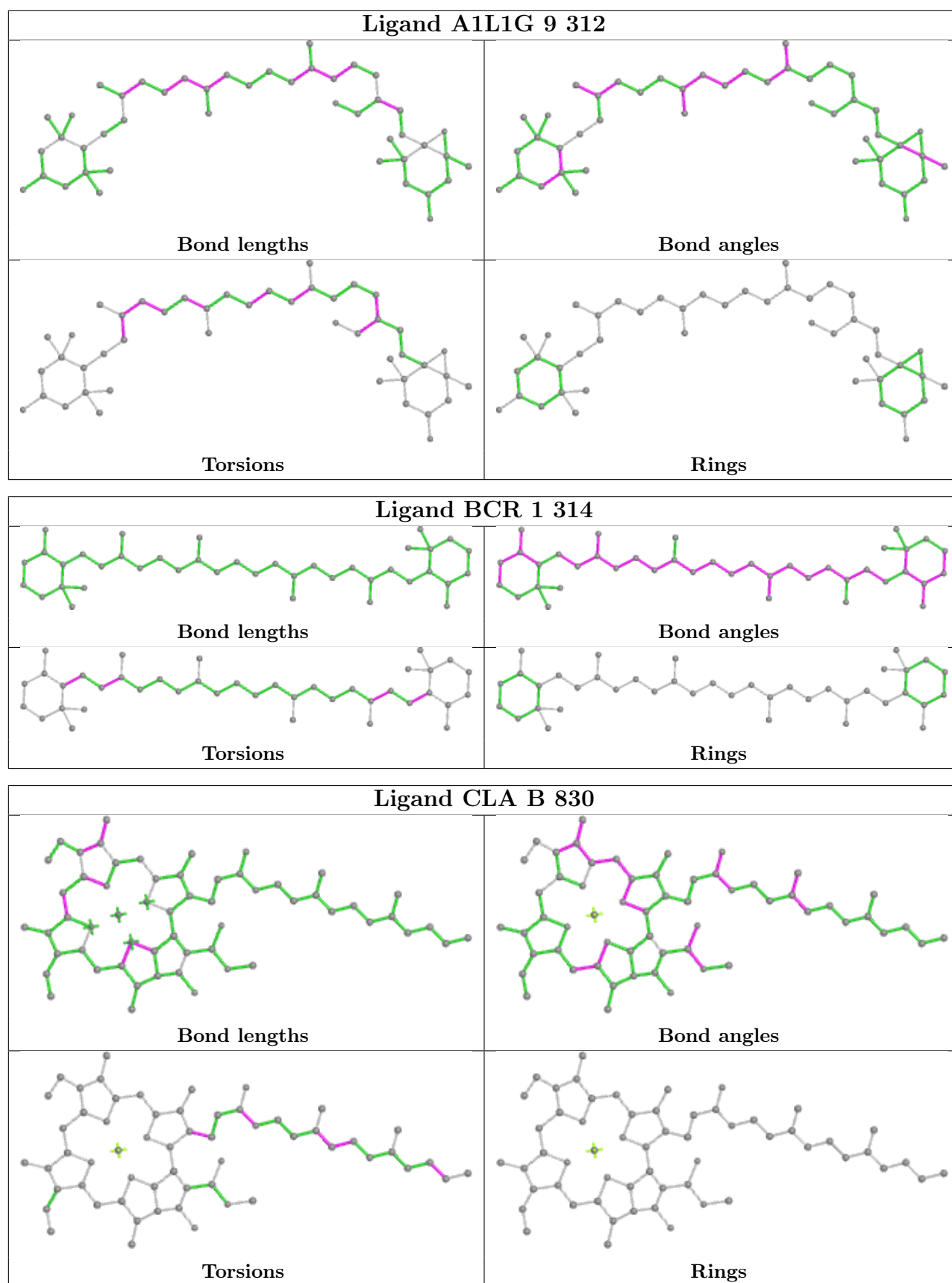
Bond angles

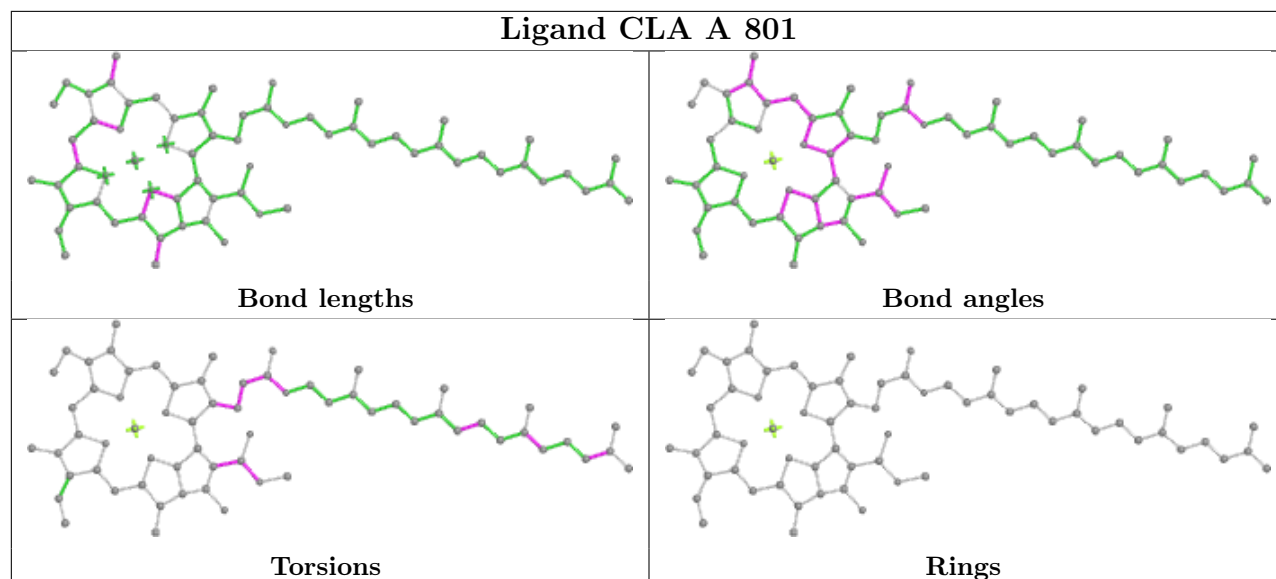
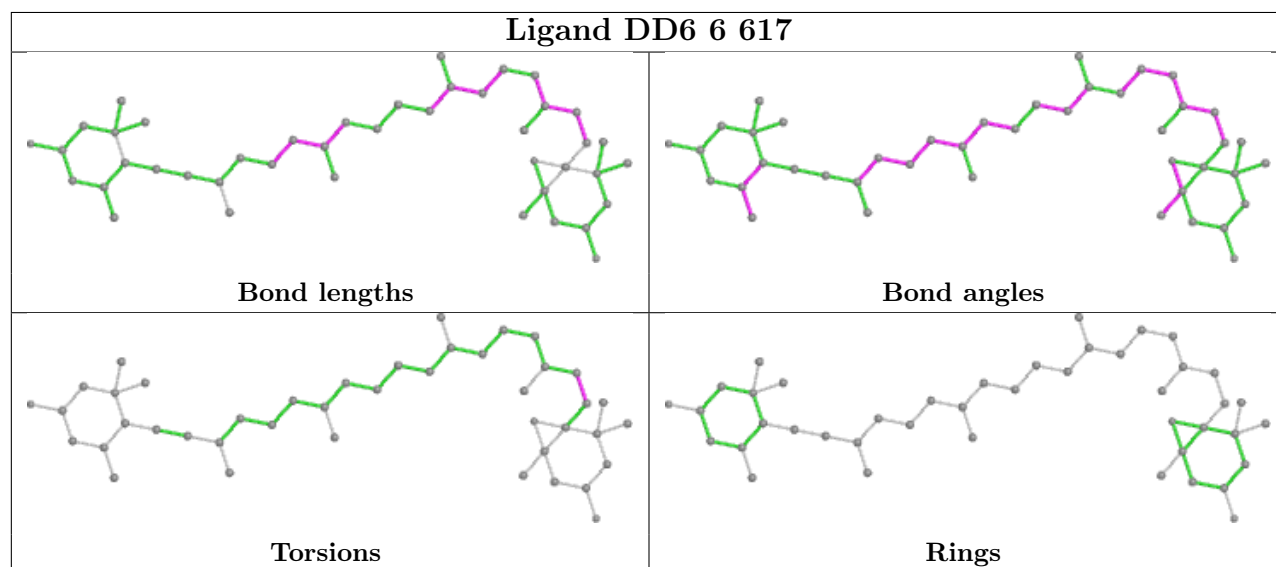
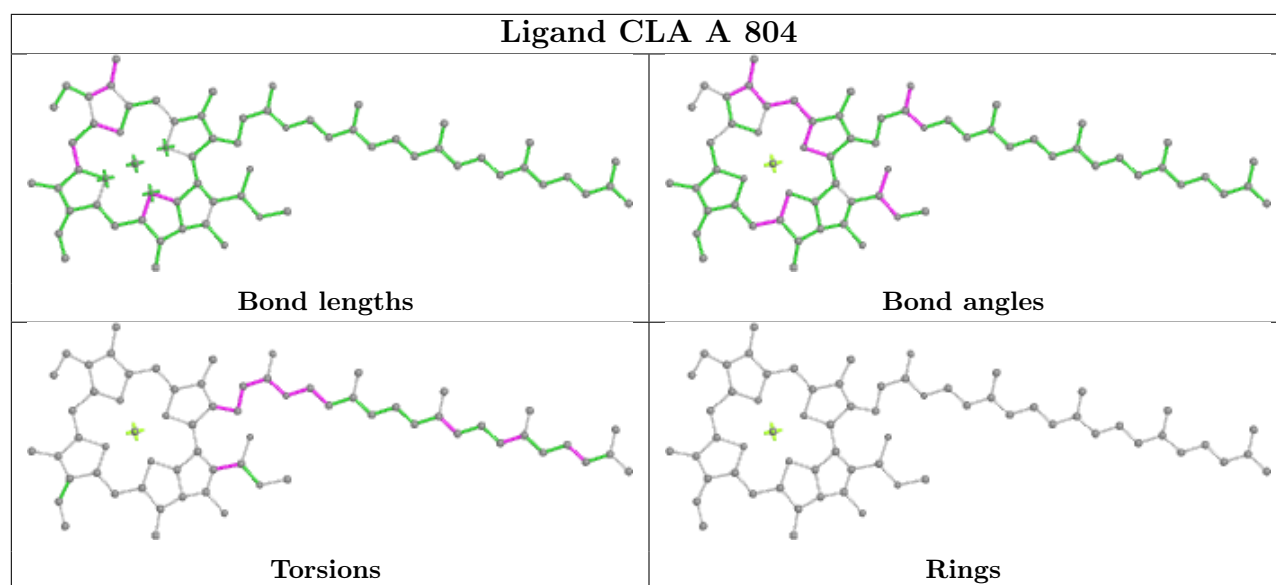


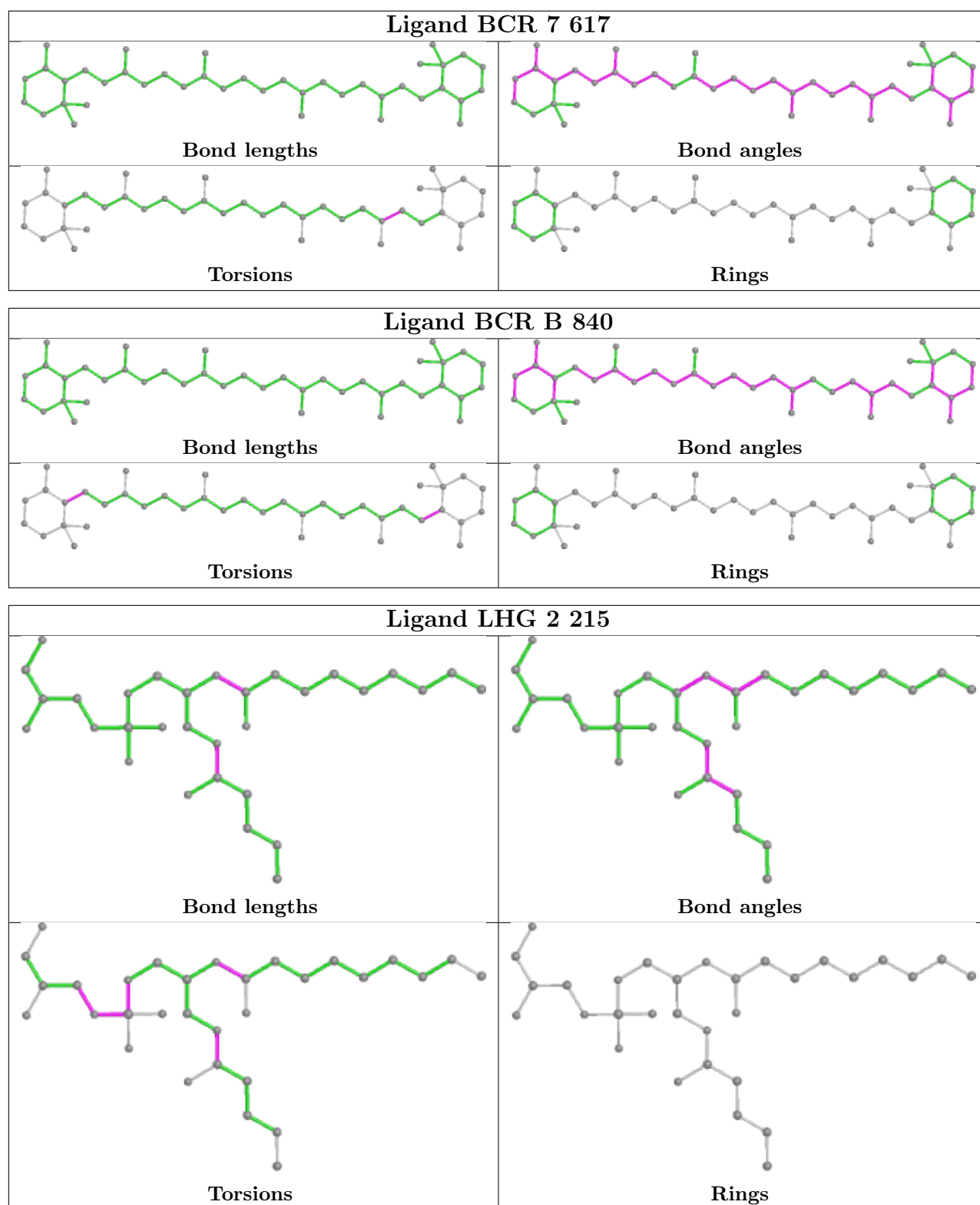
Torsions

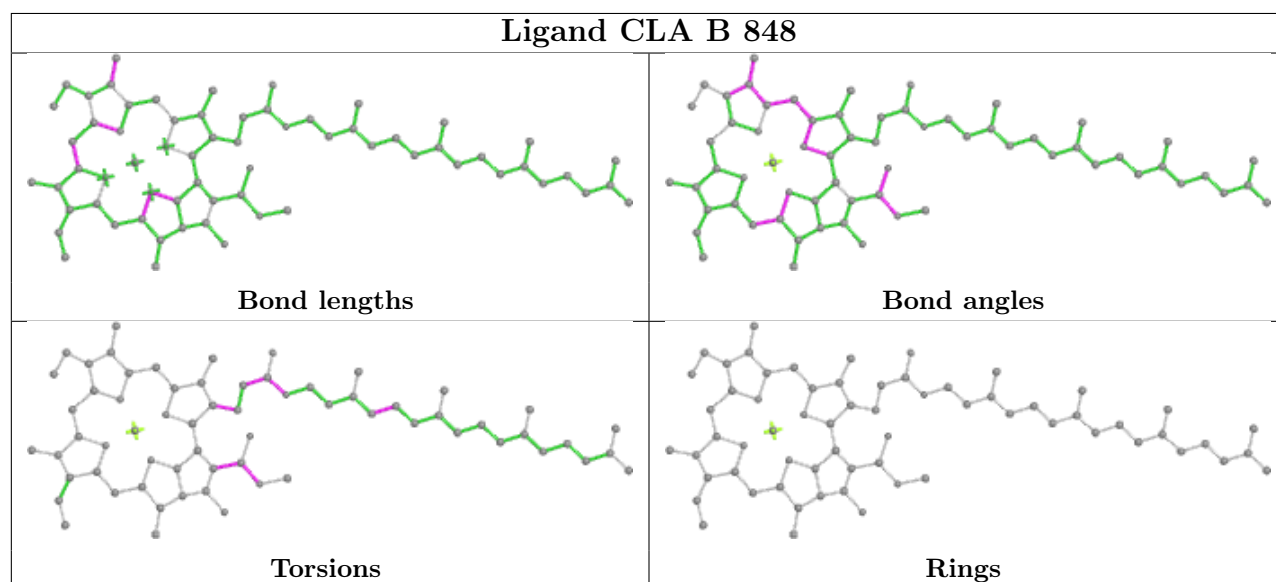
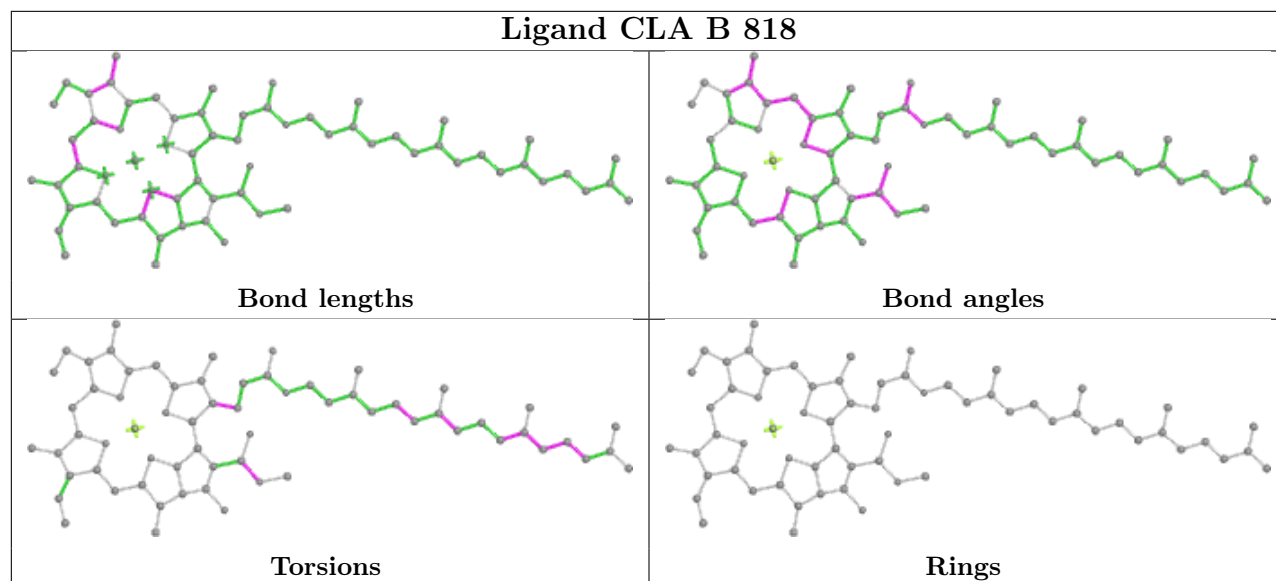
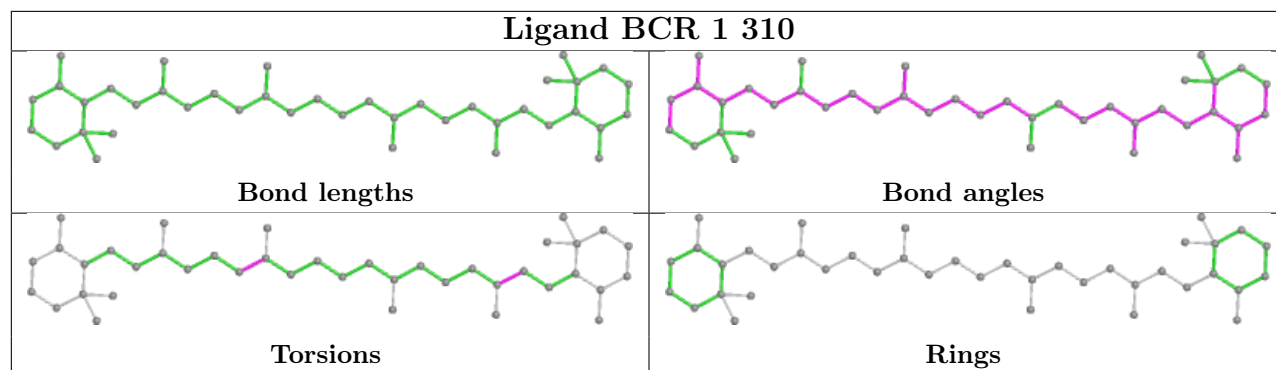


Rings

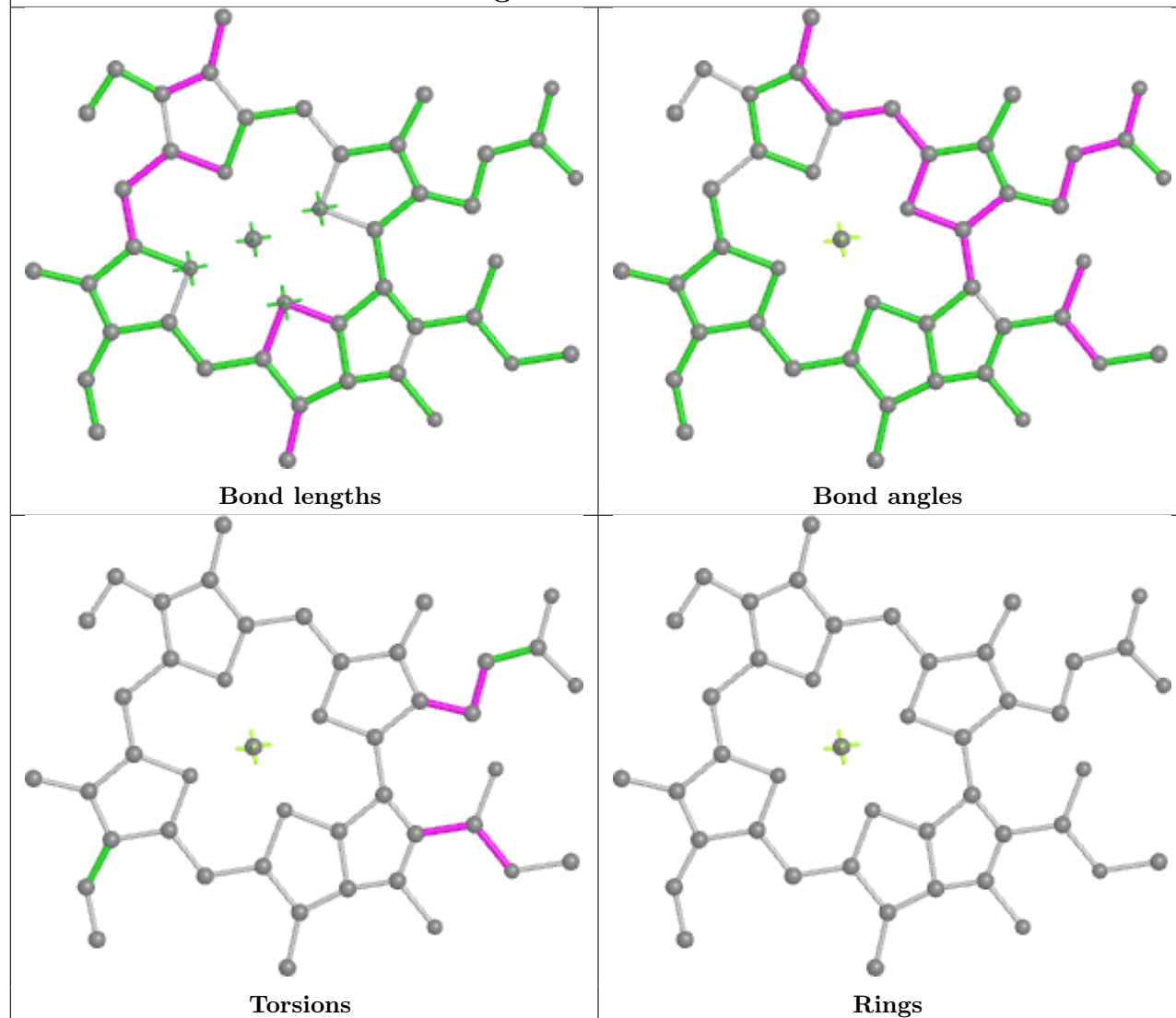




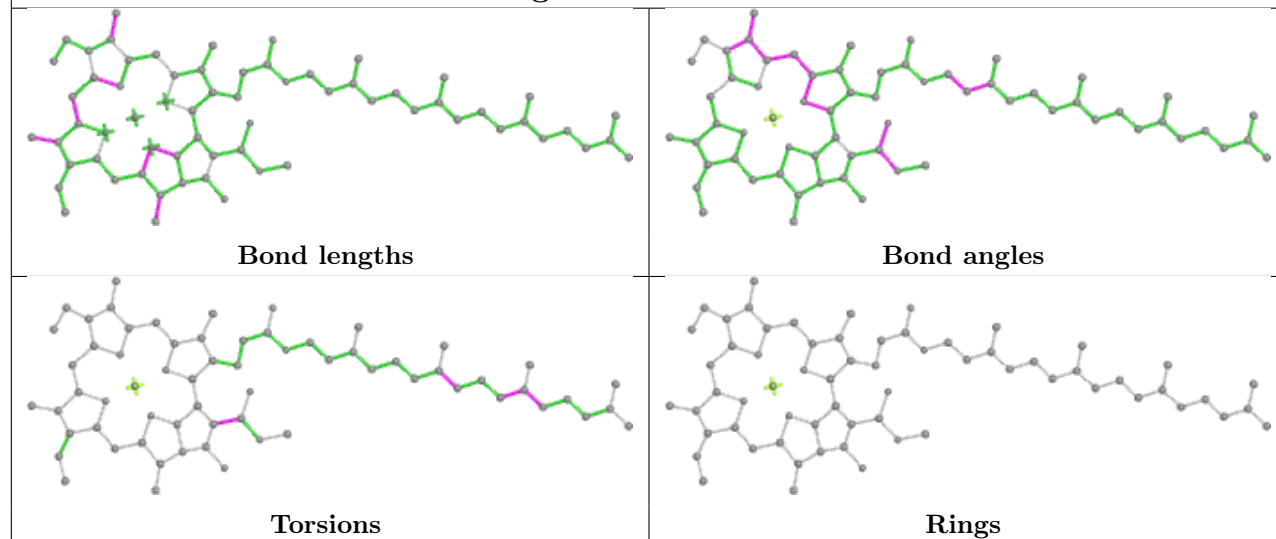




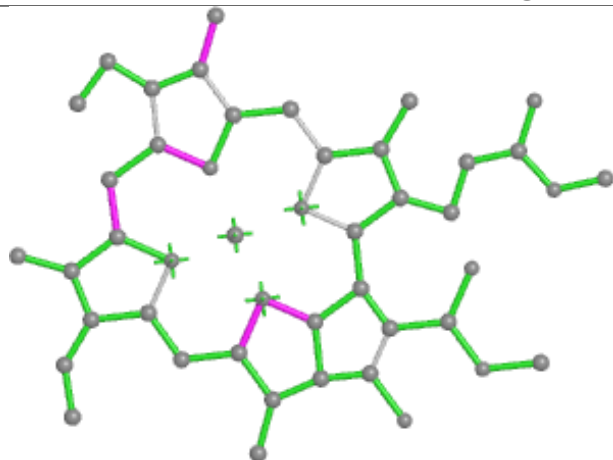
Ligand CLA 1 305



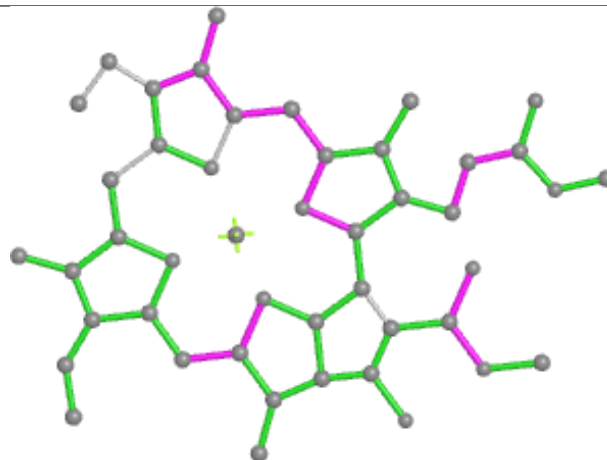
Ligand CLA A 802



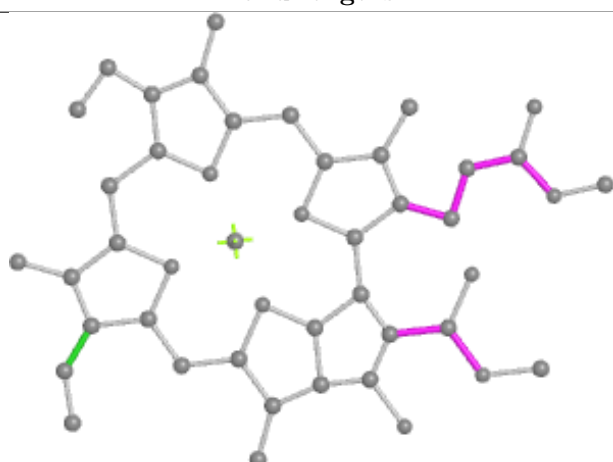
Ligand CLA 9 305



Bond lengths



Bond angles

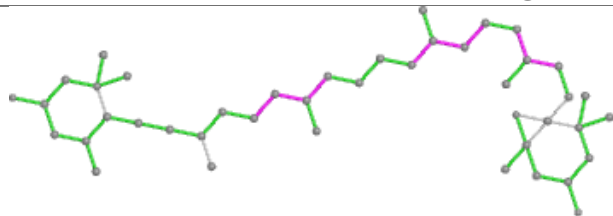


Torsions

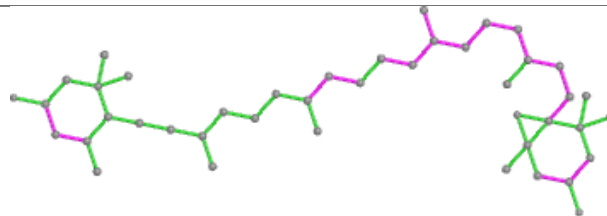


Rings

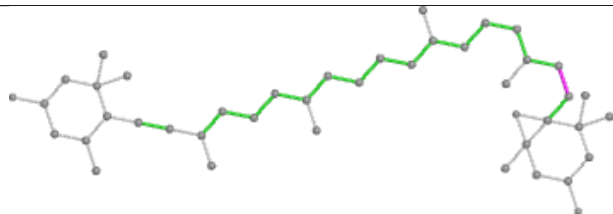
Ligand DD6 5 609



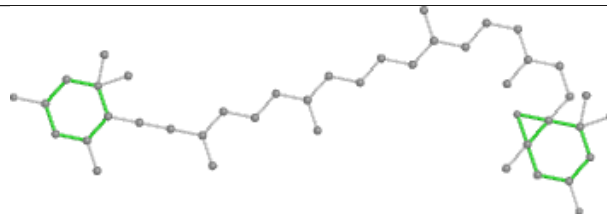
Bond lengths



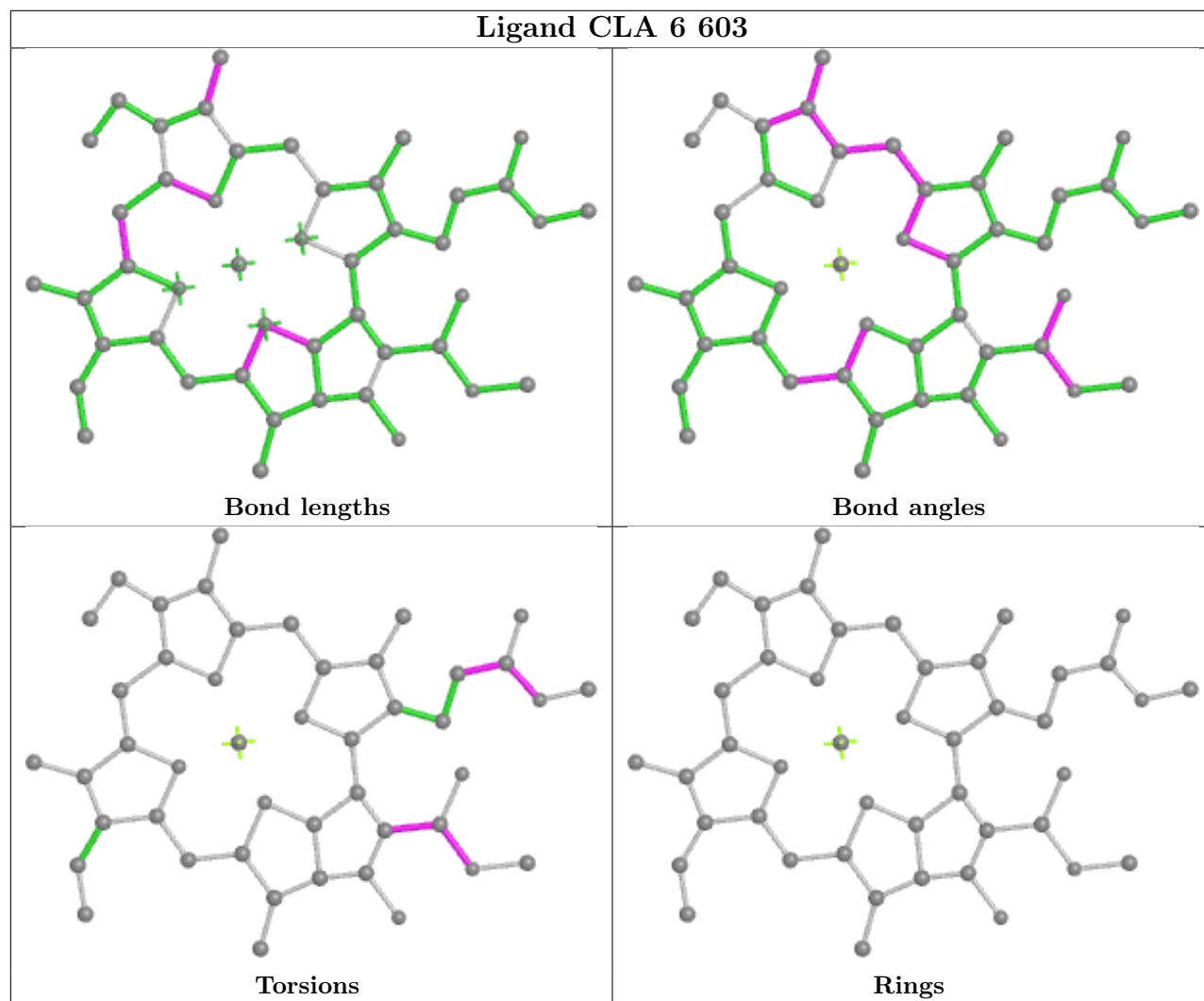
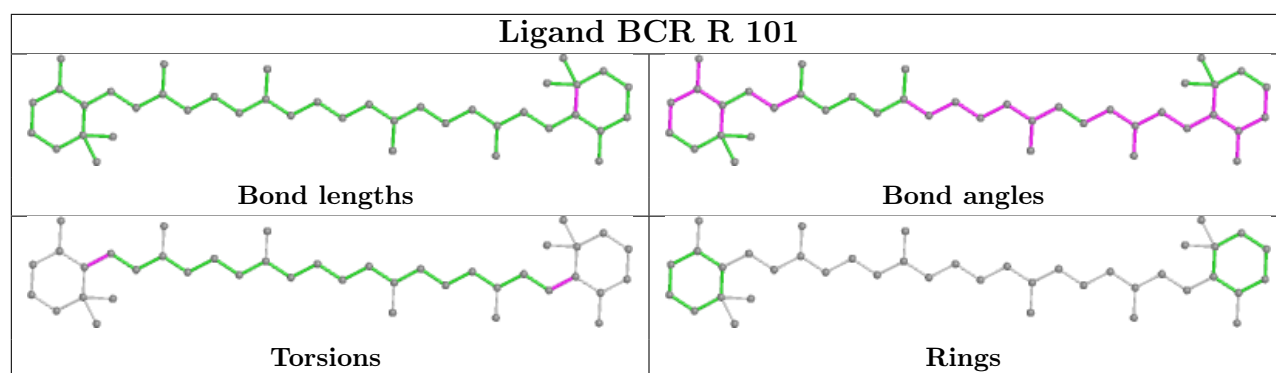
Bond angles

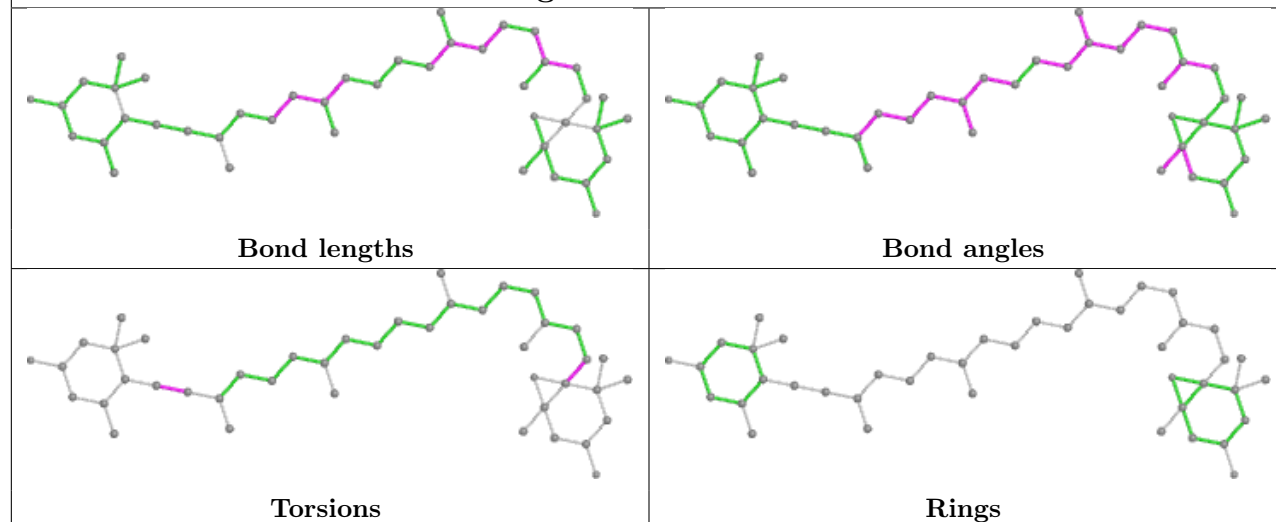
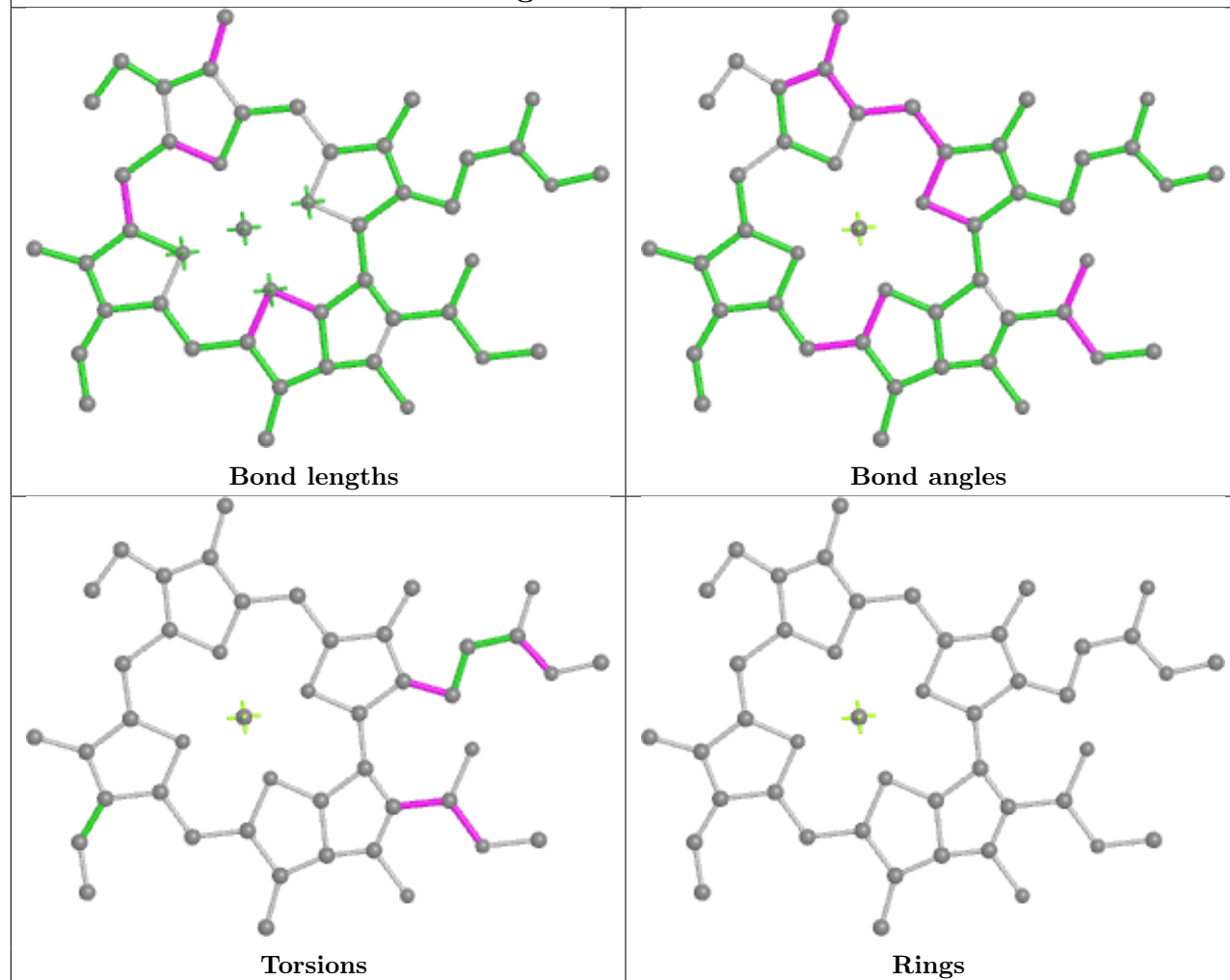


Torsions

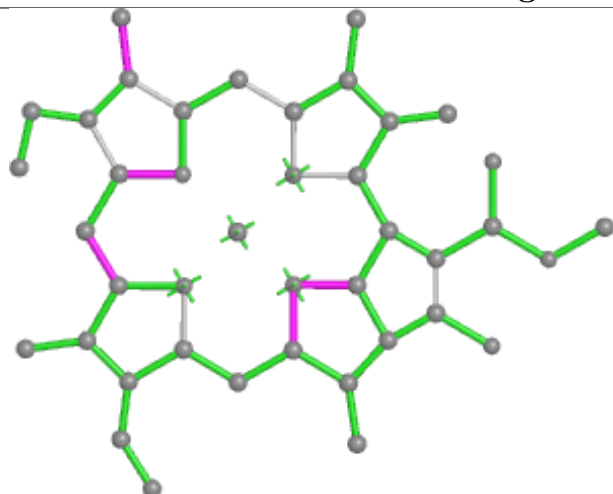


Rings

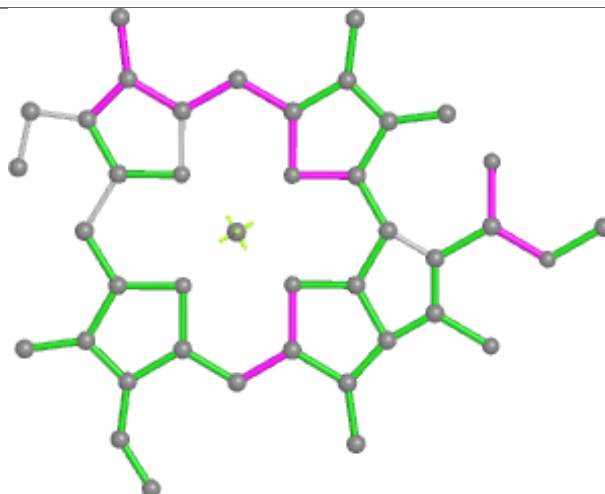


Ligand DD6 3 313**Ligand CLA 7 609**

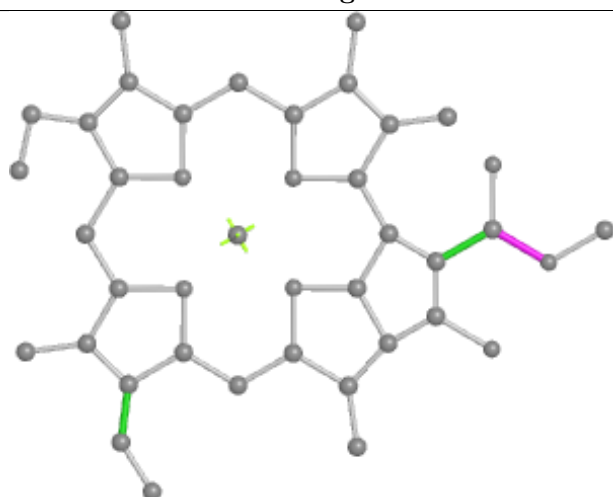
Ligand CLA 4 610



Bond lengths



Bond angles

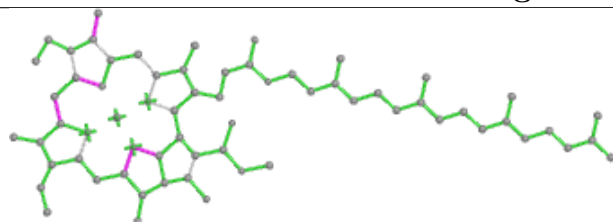


Torsions

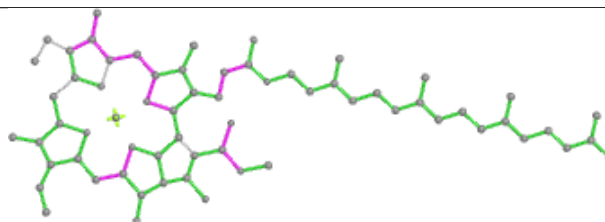


Rings

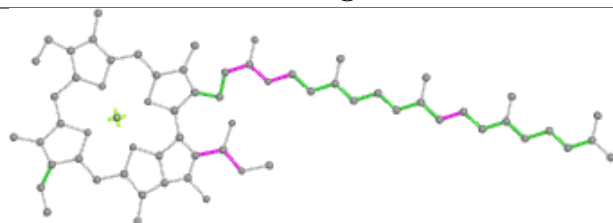
Ligand CLA A 808



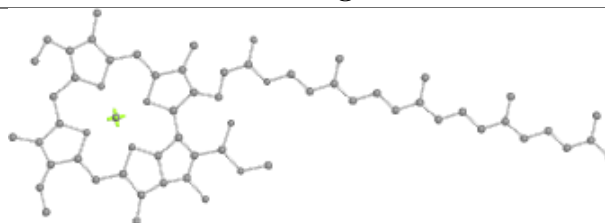
Bond lengths



Bond angles

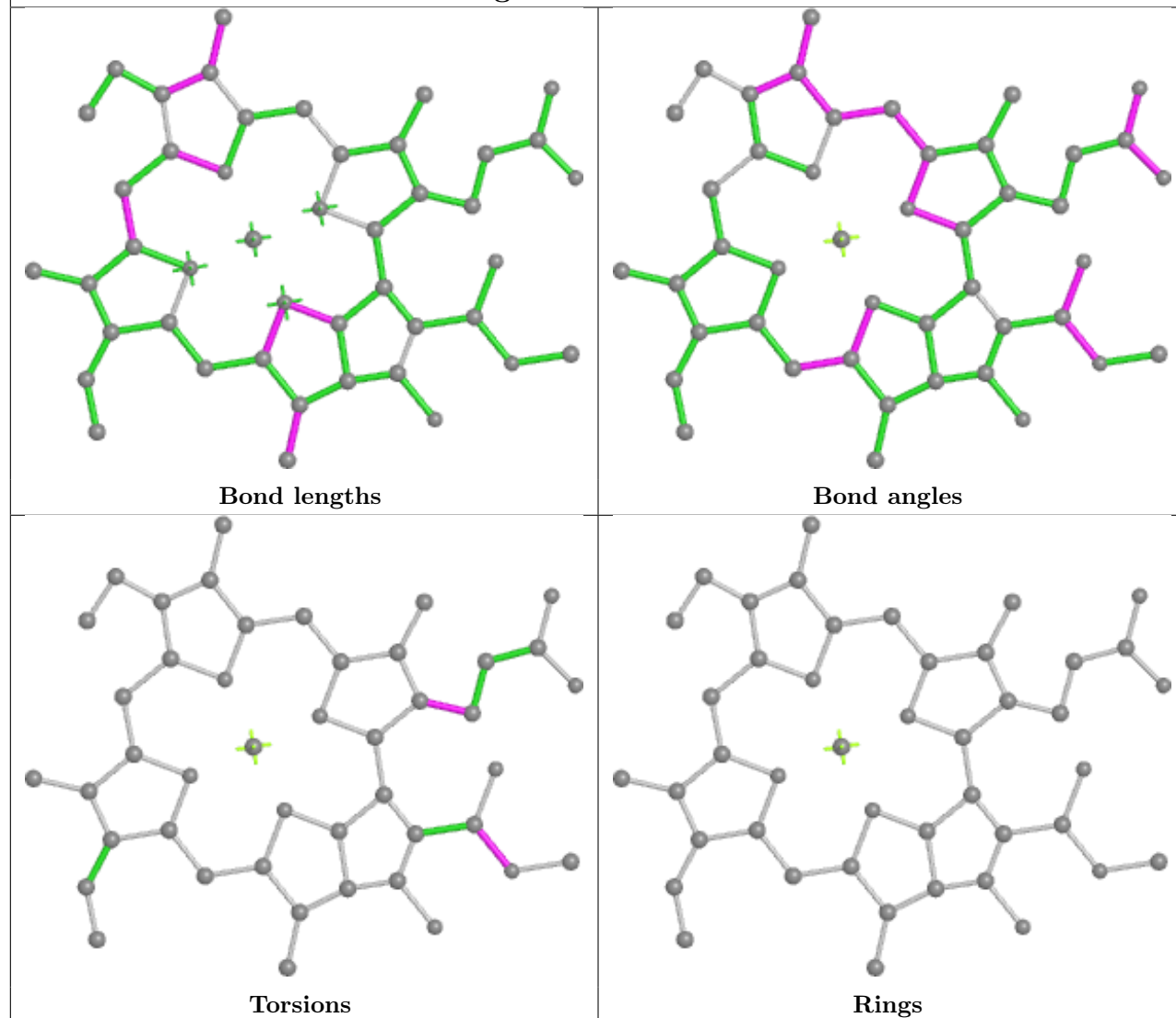


Torsions

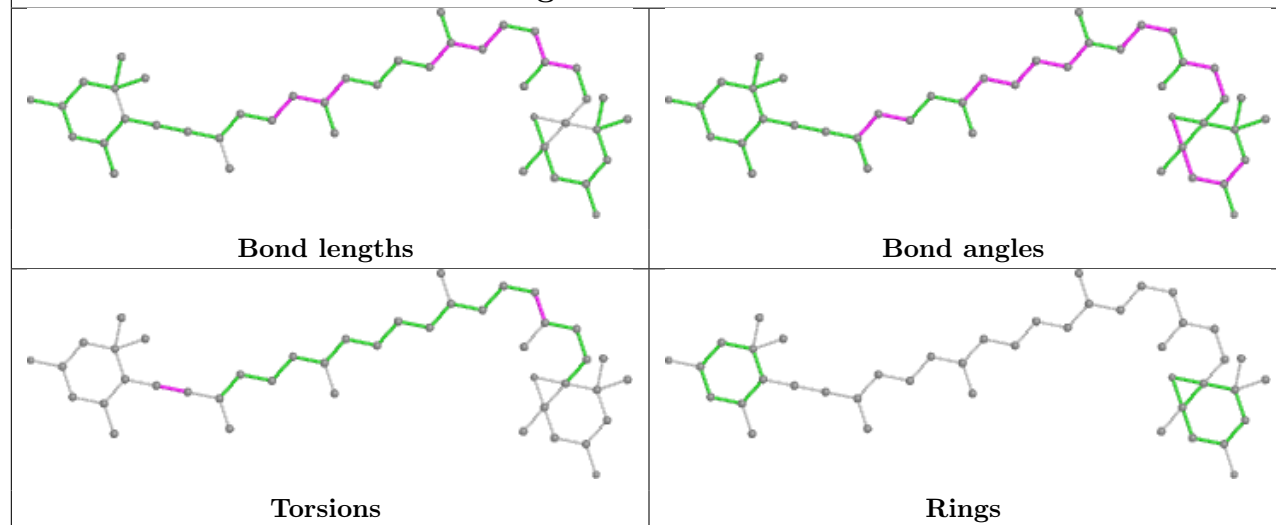


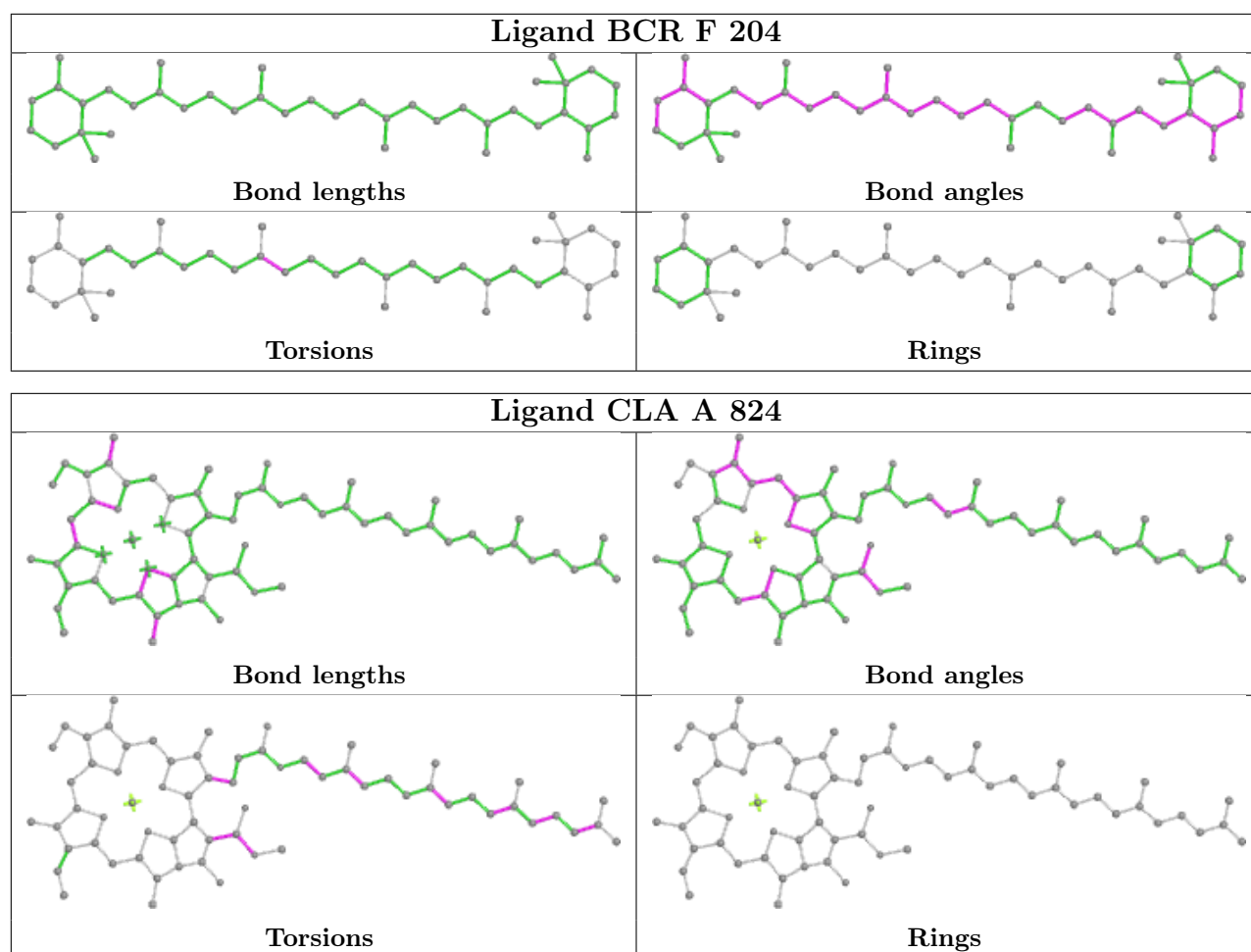
Rings

Ligand CLA 8 204

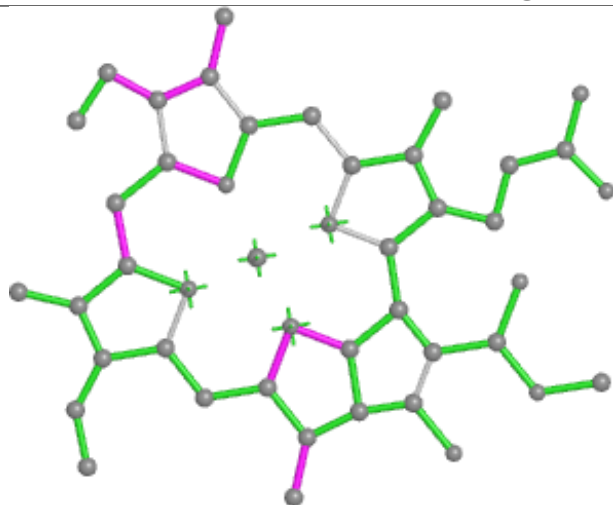


Ligand DD6 9 313

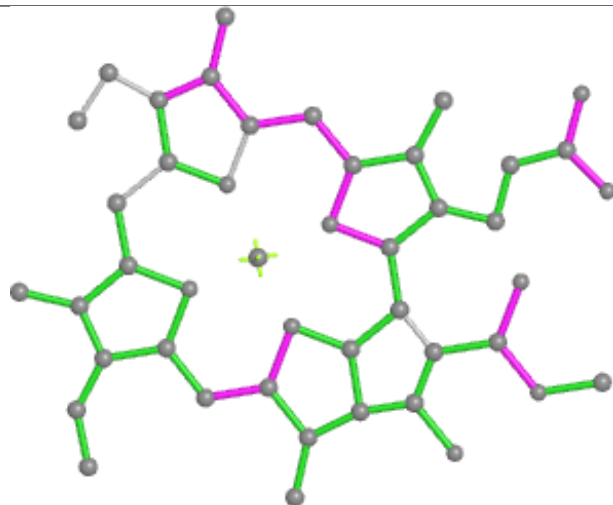




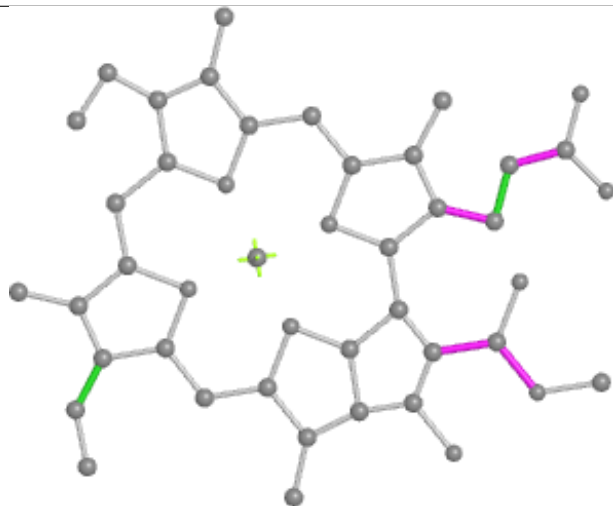
Ligand CLA 1 302



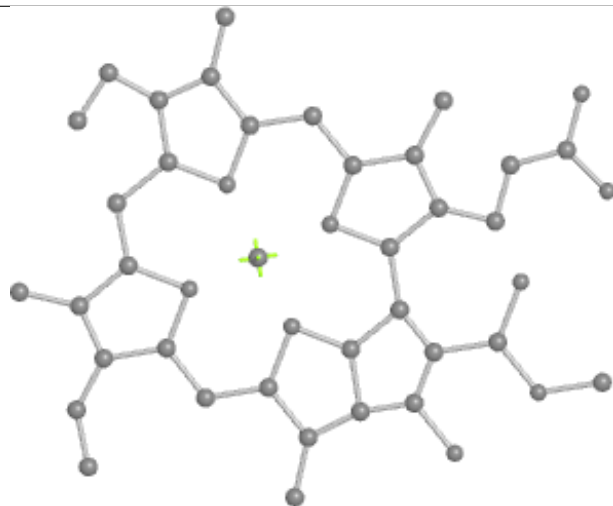
Bond lengths



Bond angles

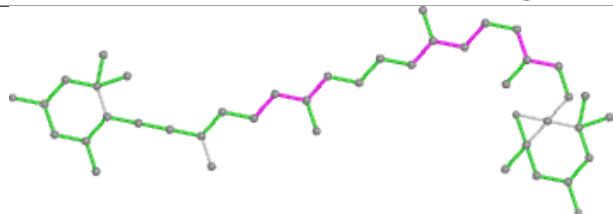


Torsions

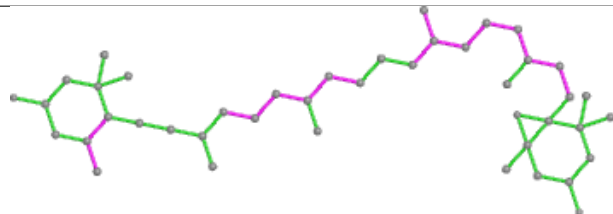


Rings

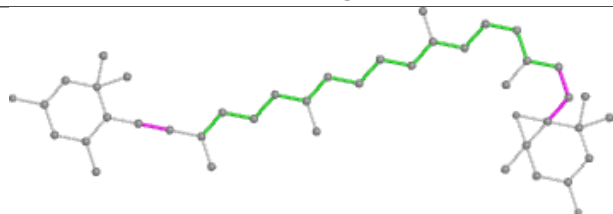
Ligand DD6 h 615



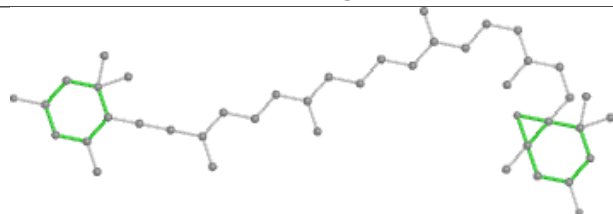
Bond lengths



Bond angles

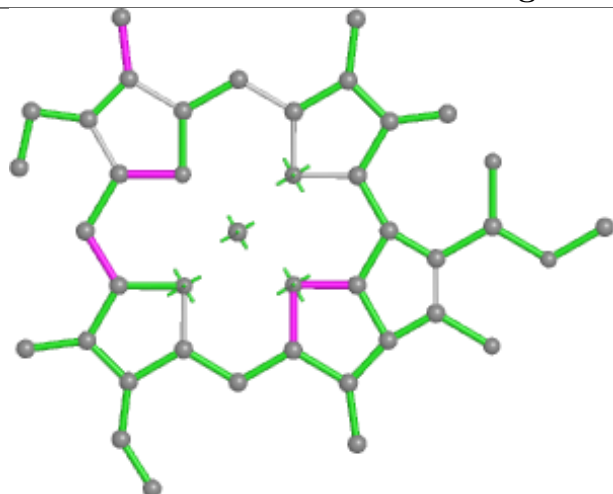


Torsions

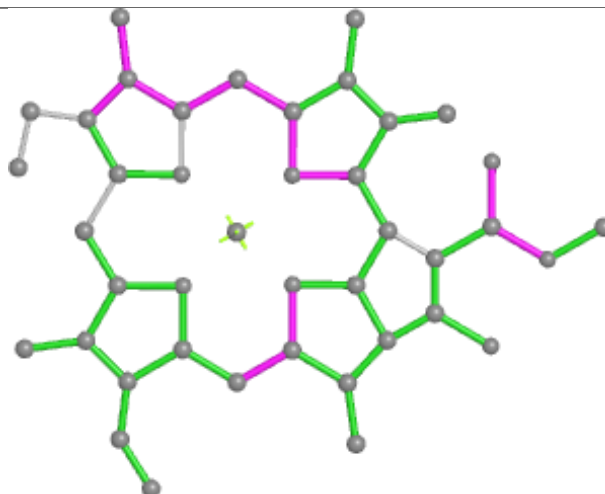


Rings

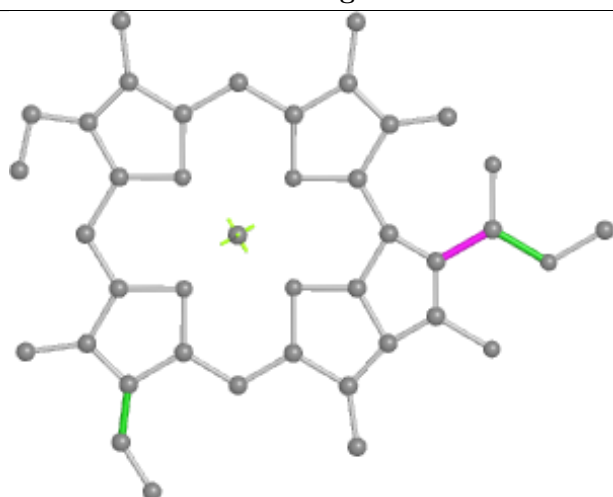
Ligand CLA 3 309



Bond lengths



Bond angles

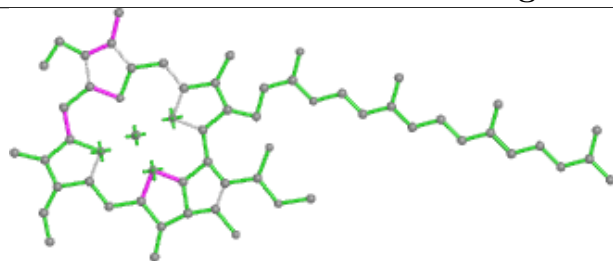


Torsions

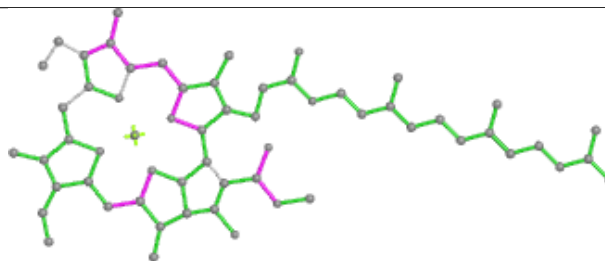


Rings

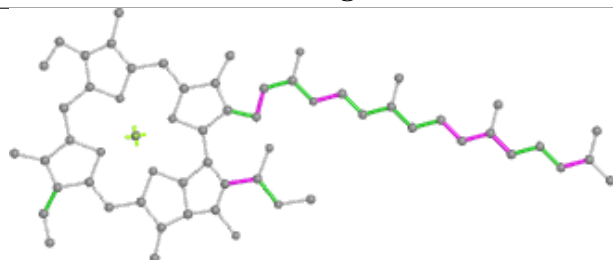
Ligand CLA 2 204



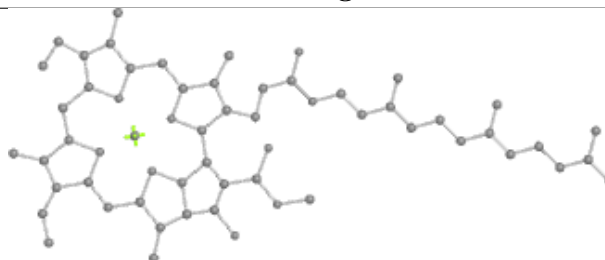
Bond lengths



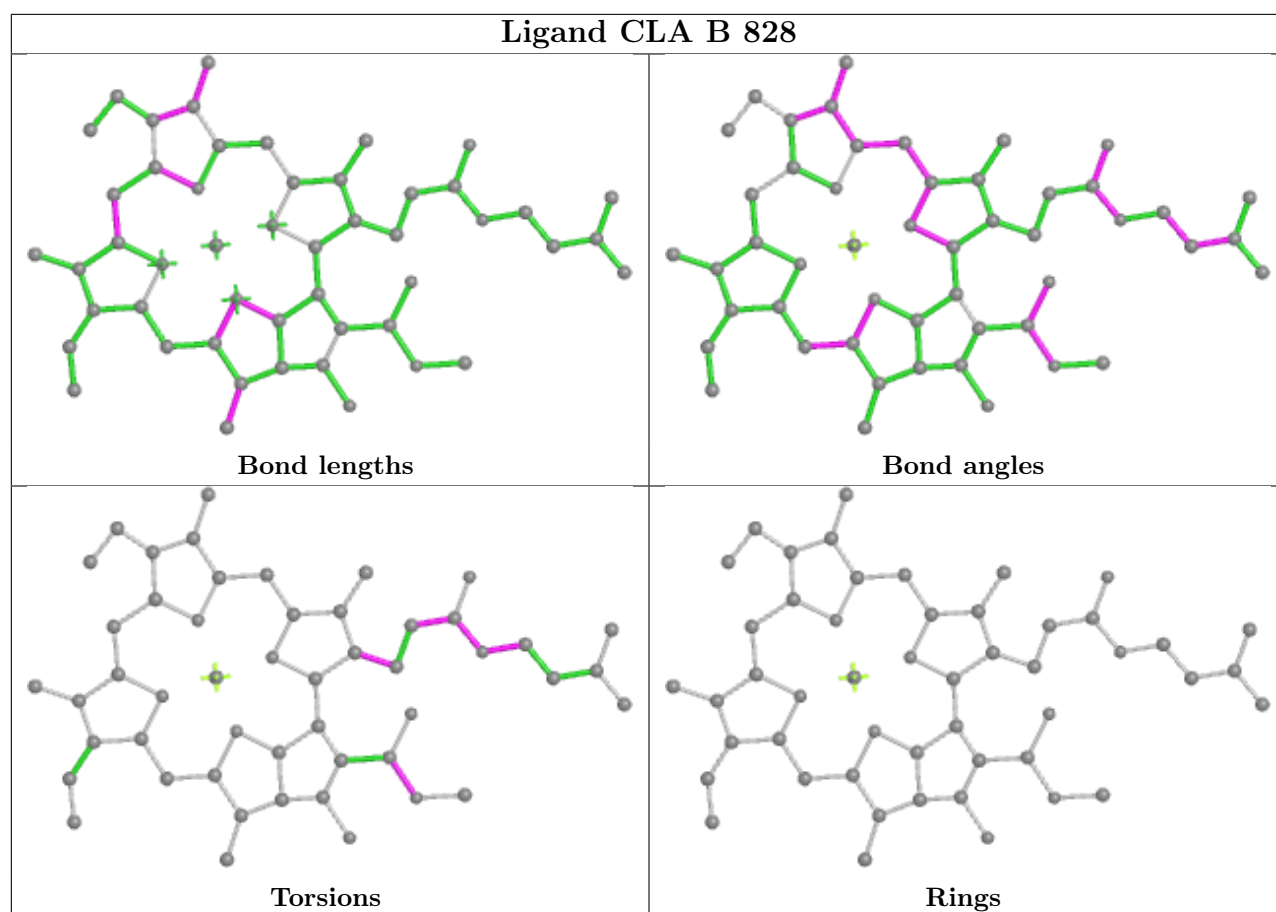
Bond angles



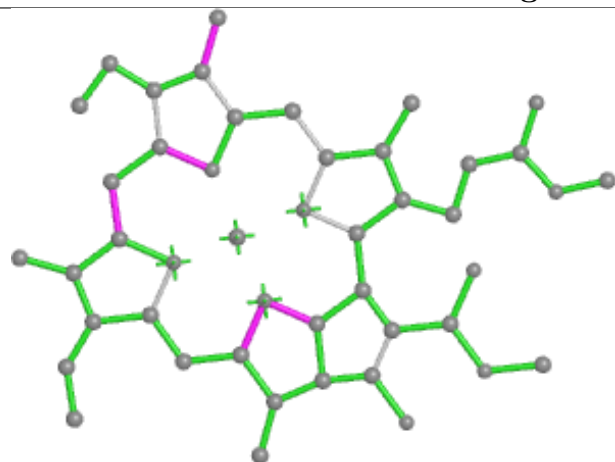
Torsions



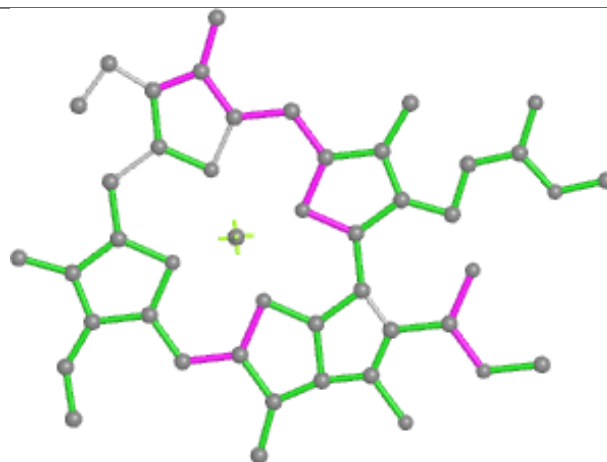
Rings



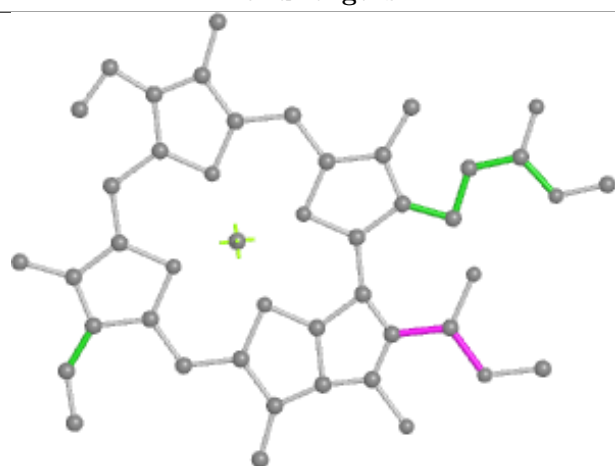
Ligand CLA 6 608



Bond lengths



Bond angles

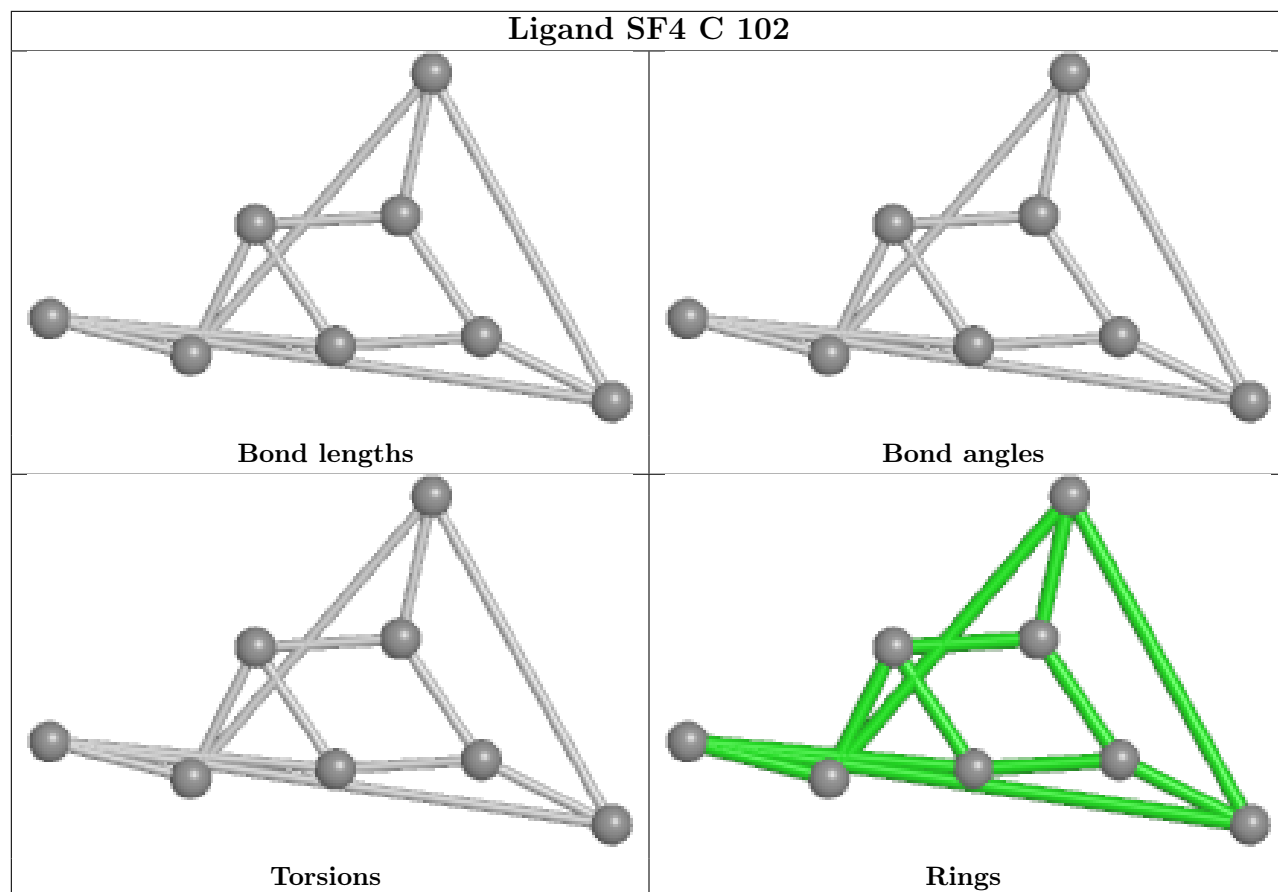


Torsions

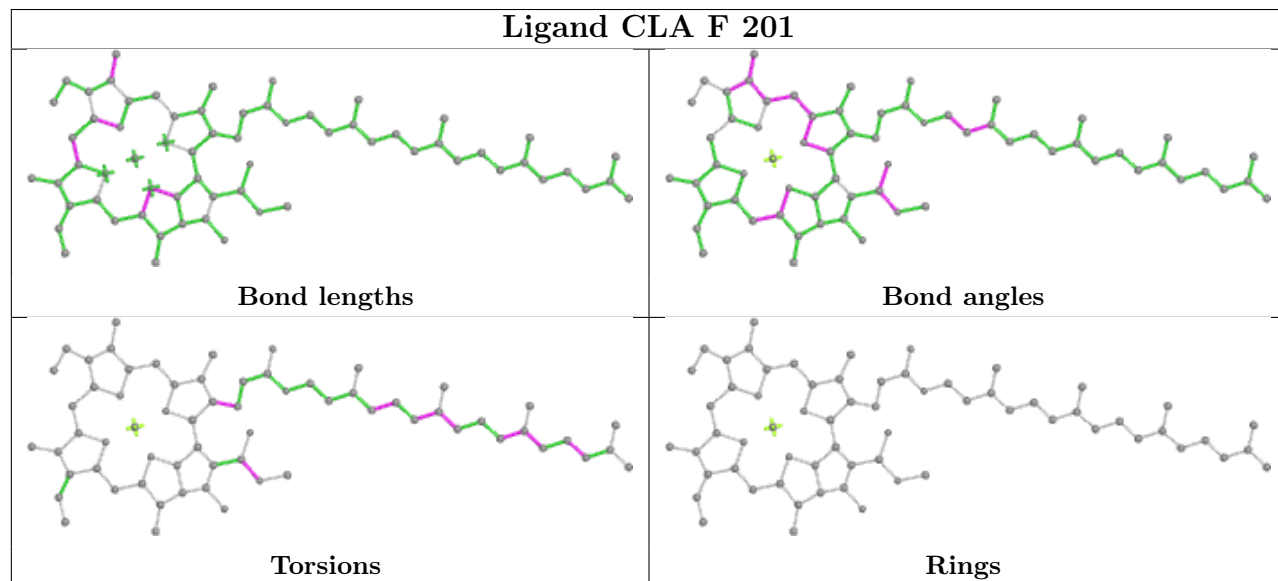


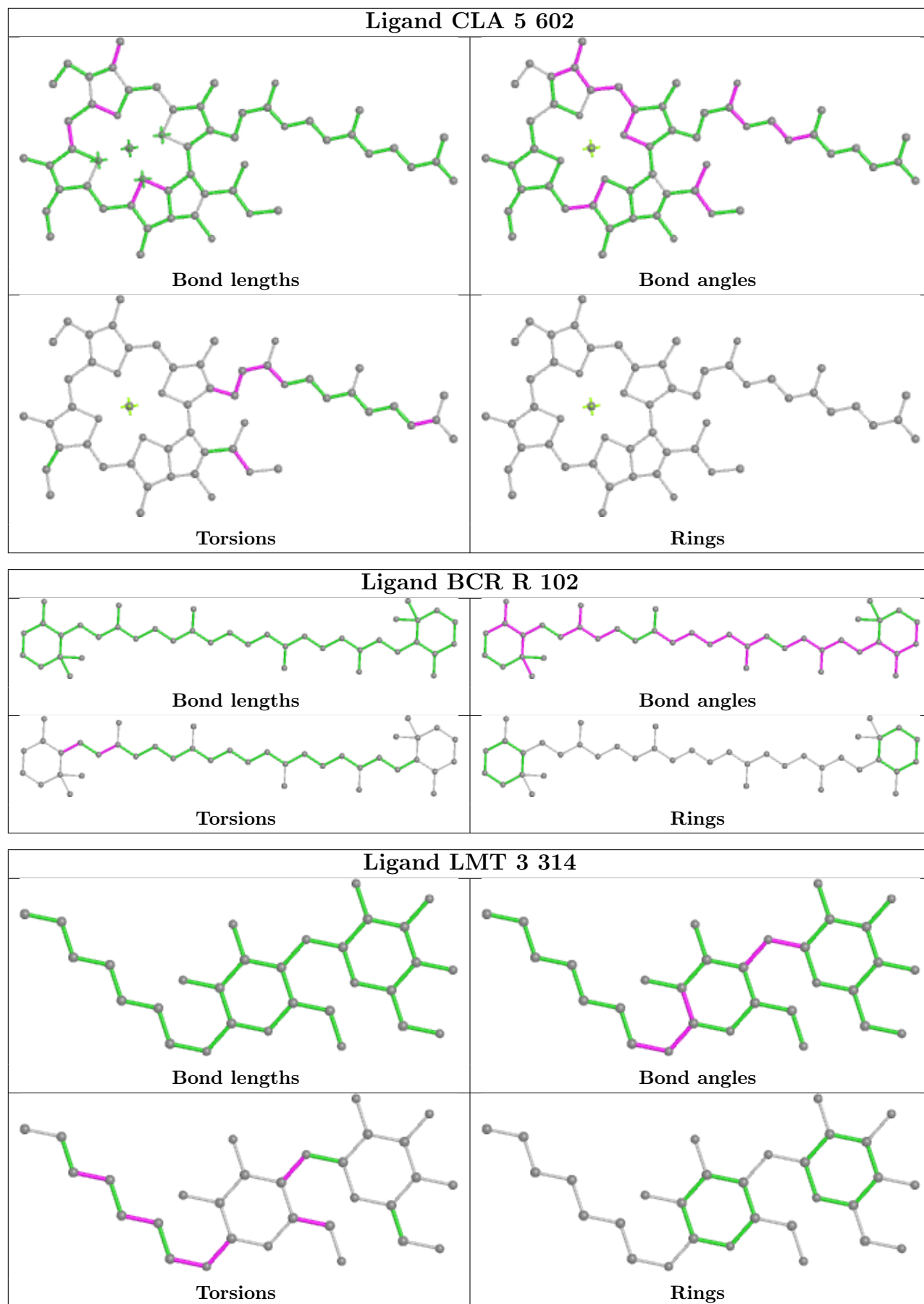
Rings

Ligand SF4 C 102

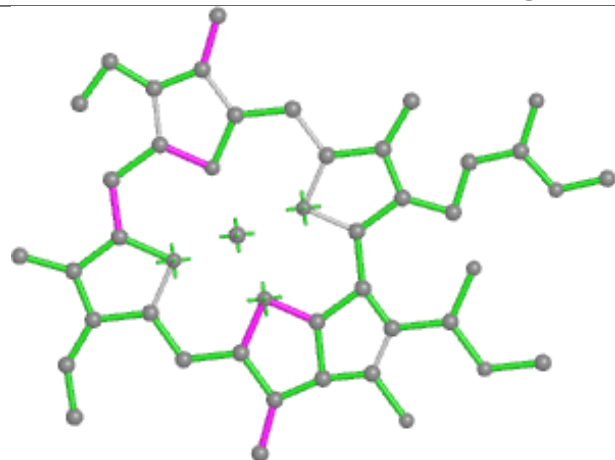


Ligand CLA F 201

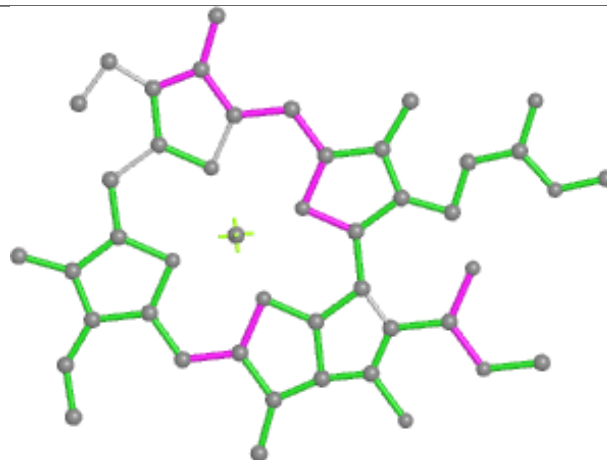




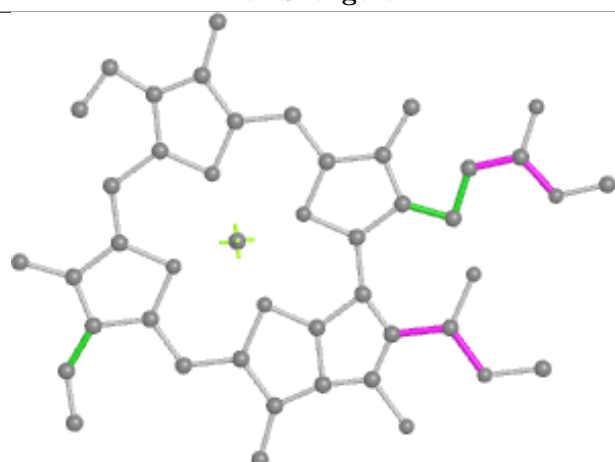
Ligand CLA 9 301



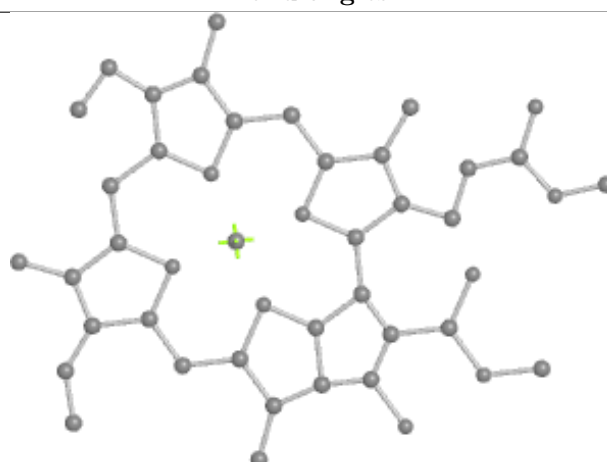
Bond lengths



Bond angles

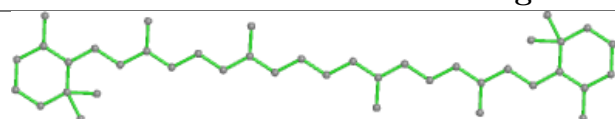


Torsions

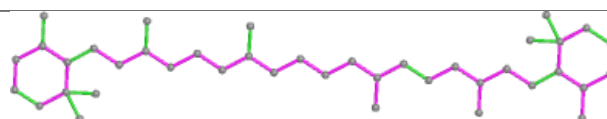


Rings

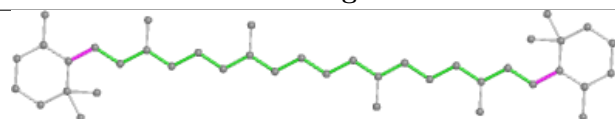
Ligand BCR B 849



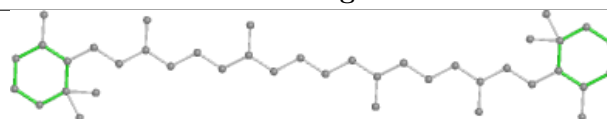
Bond lengths



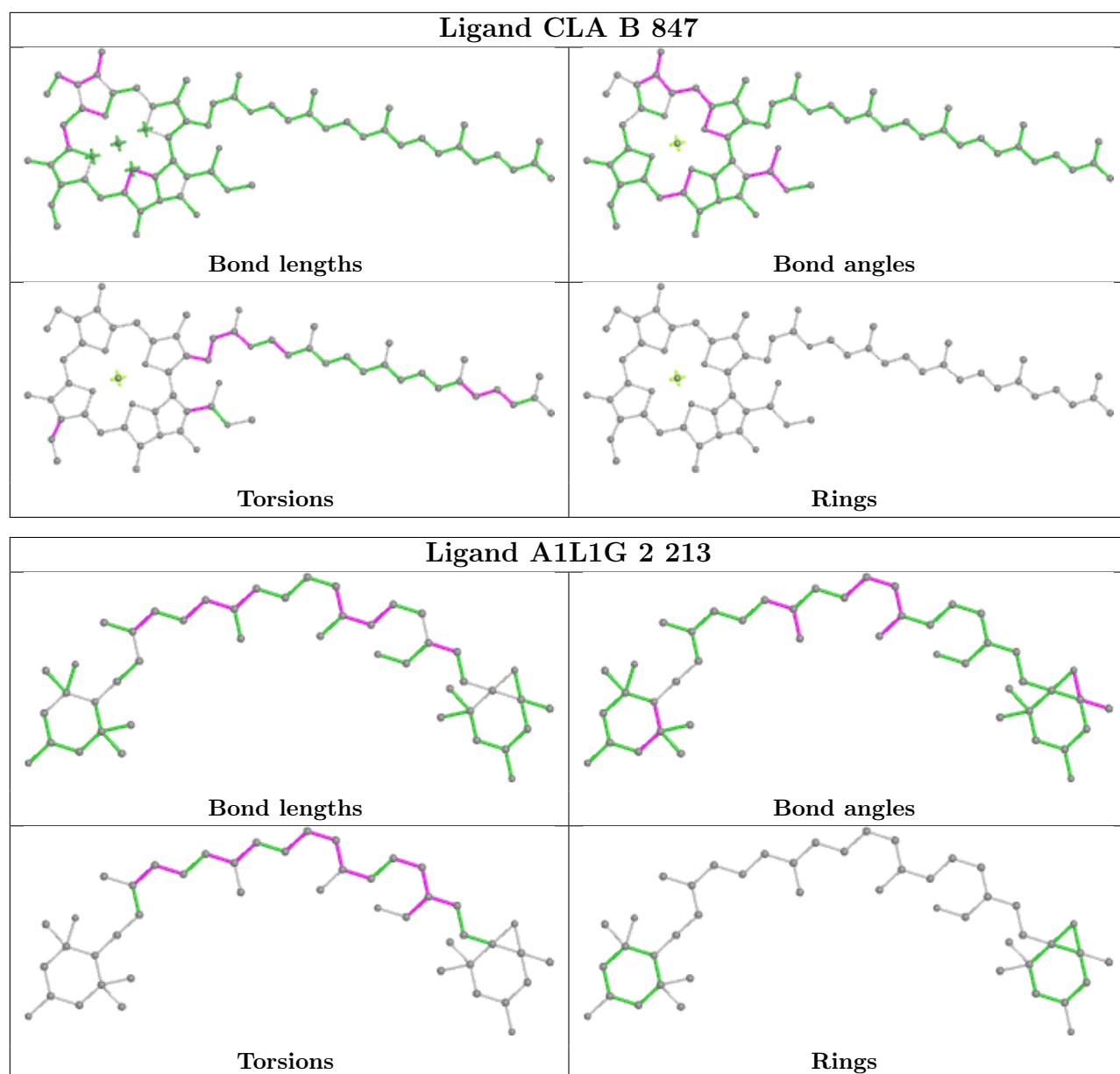
Bond angles



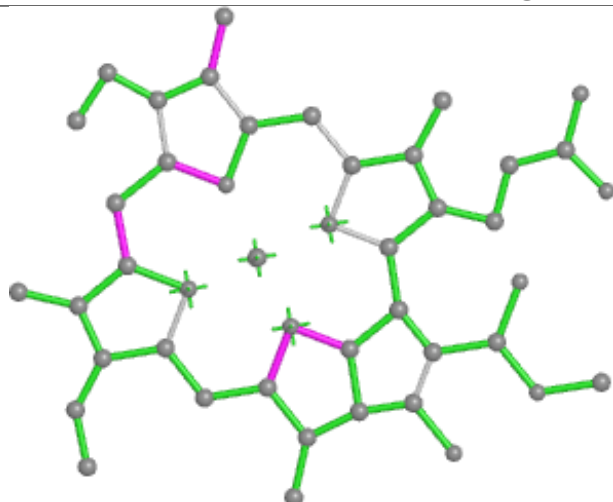
Torsions



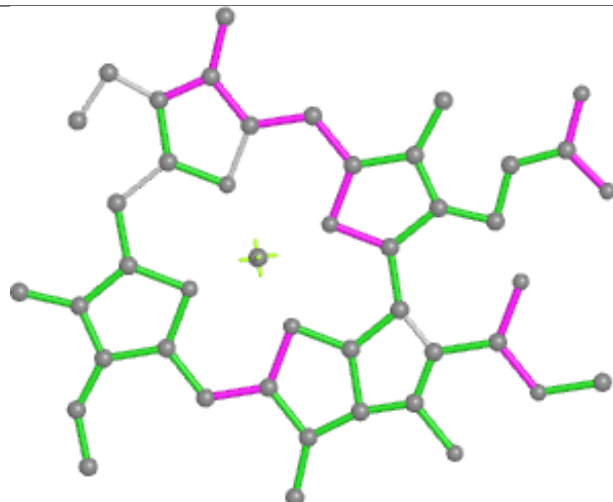
Rings



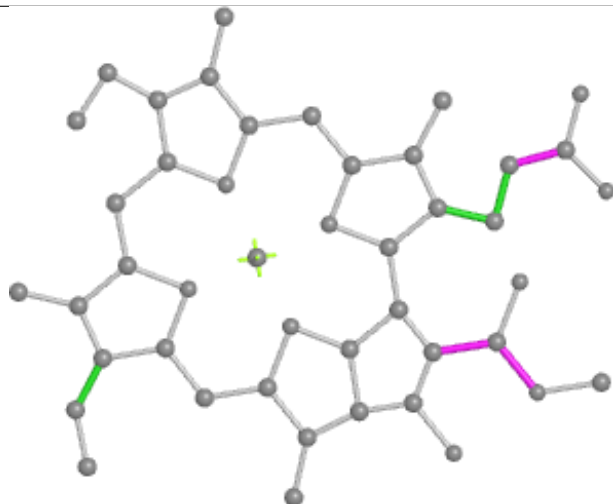
Ligand CLA 6 601



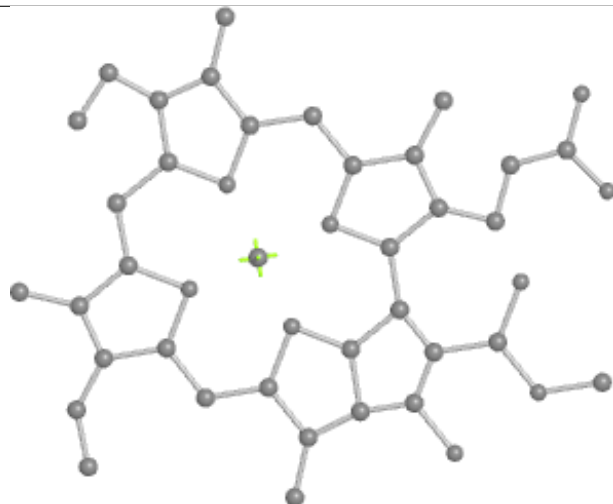
Bond lengths



Bond angles

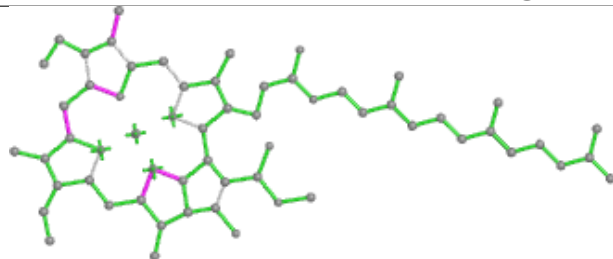


Torsions

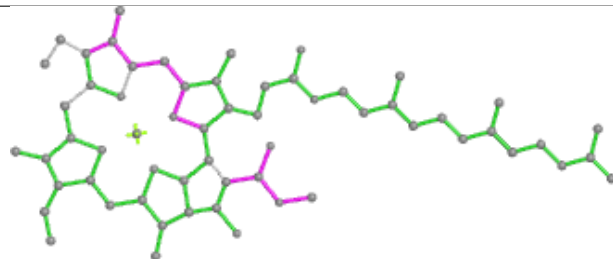


Rings

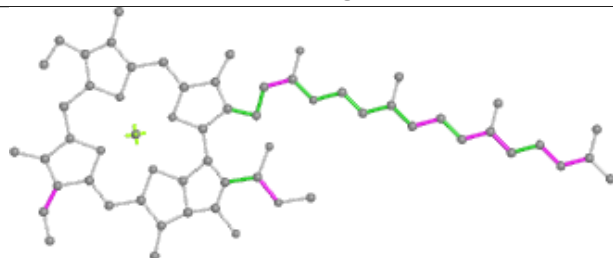
Ligand CLA 7 606



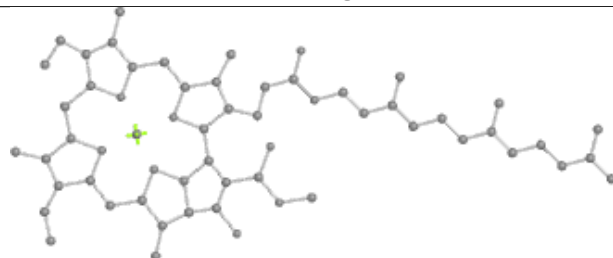
Bond lengths



Bond angles

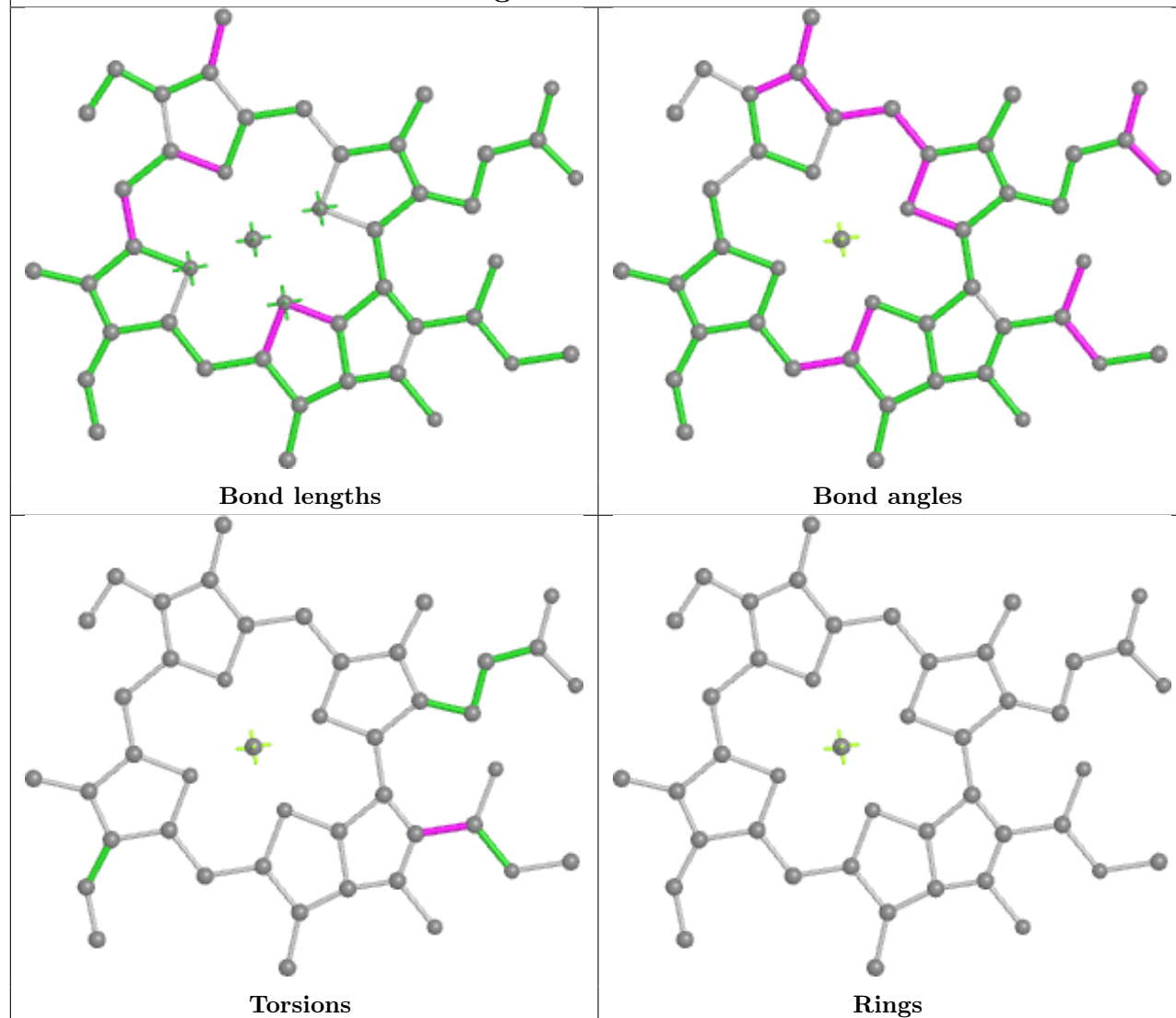


Torsions

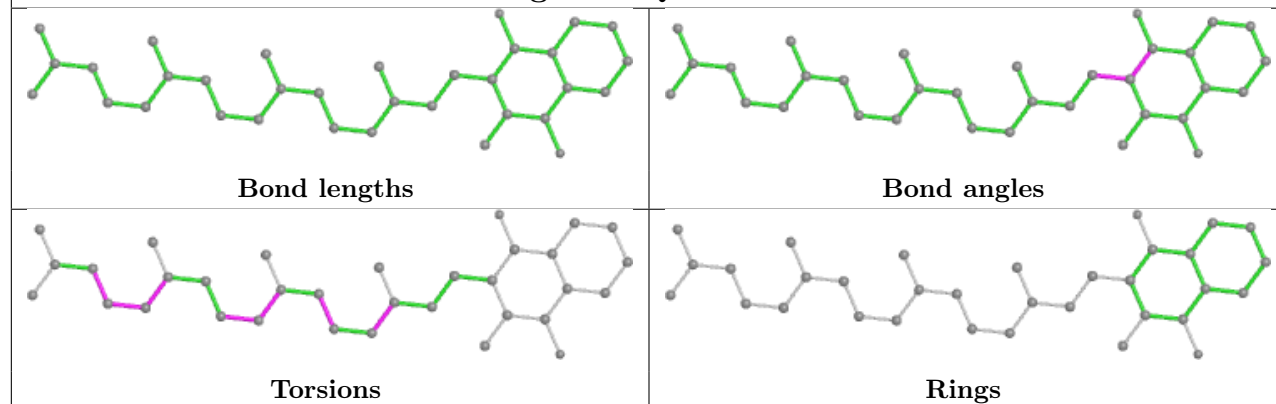


Rings

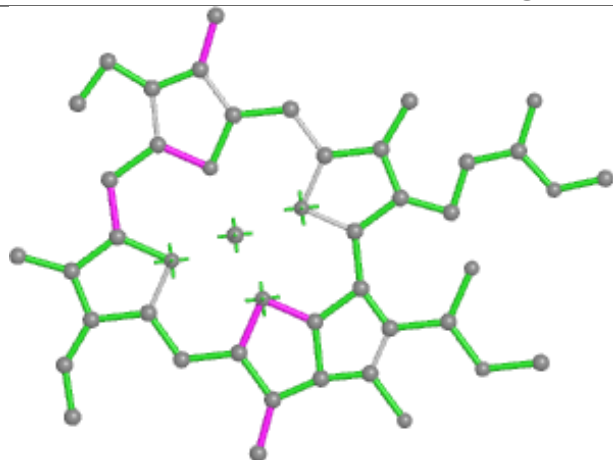
Ligand CLA 7 607



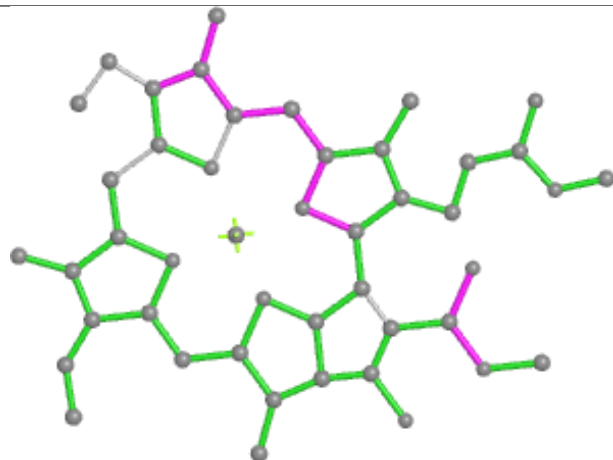
Ligand PQN B 839



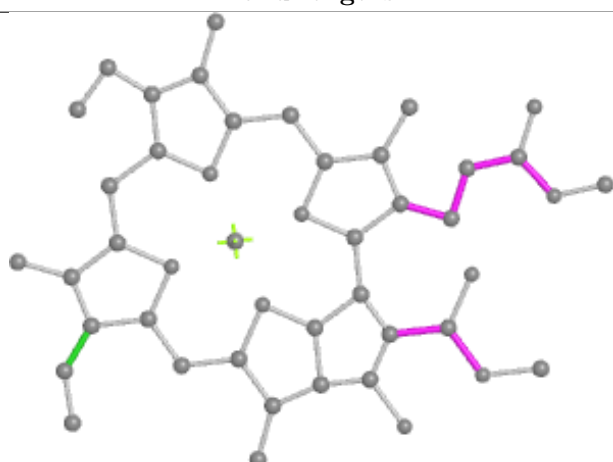
Ligand CLA 9 308



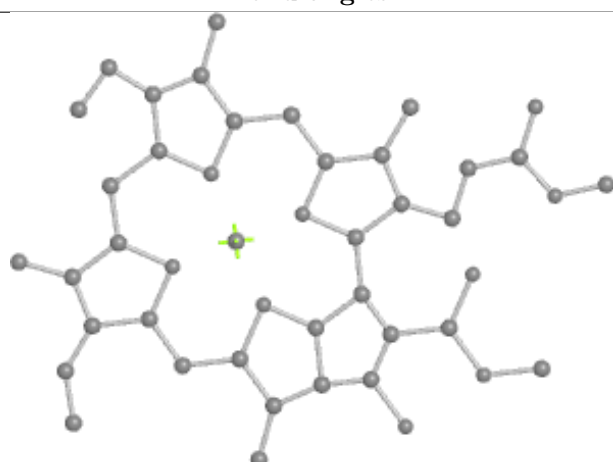
Bond lengths



Bond angles

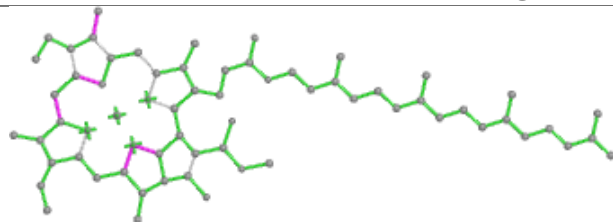


Torsions

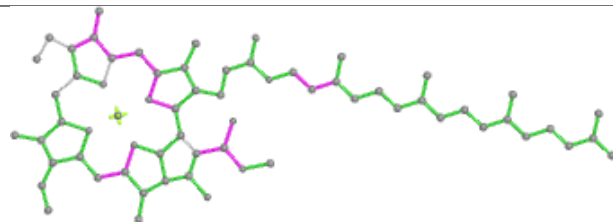


Rings

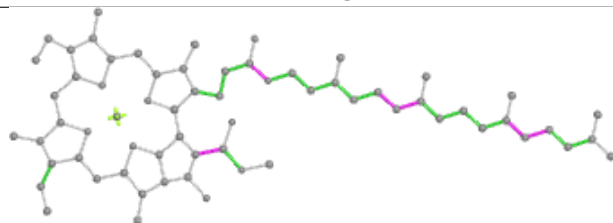
Ligand CLA A 840



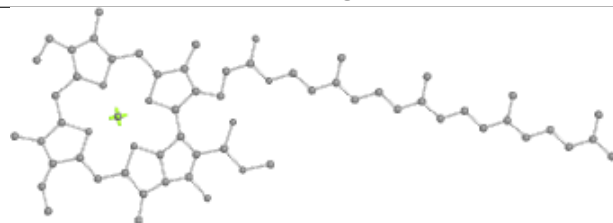
Bond lengths



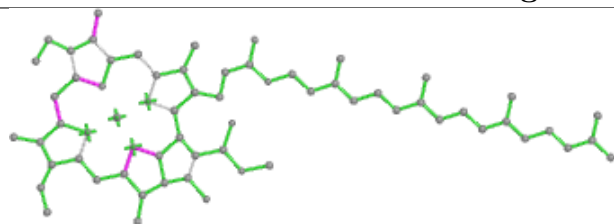
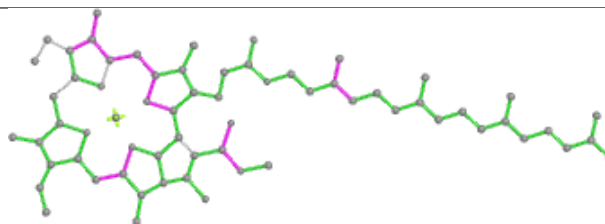
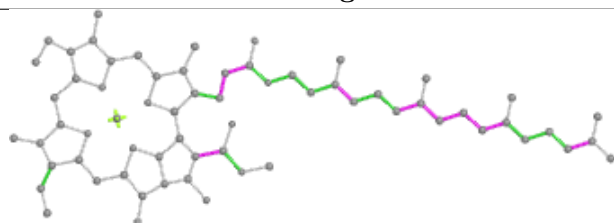
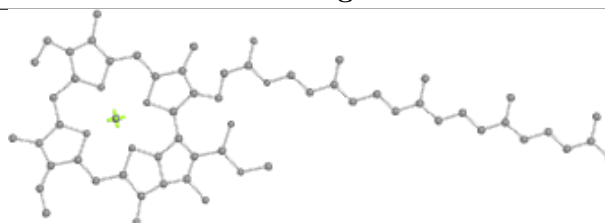
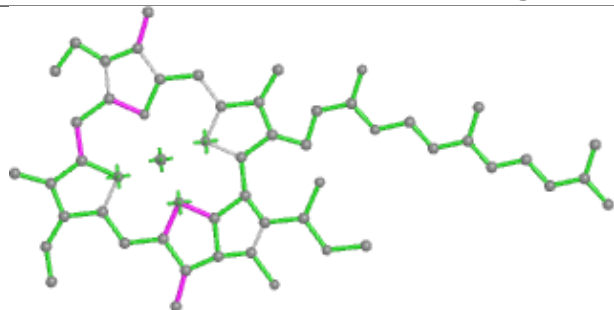
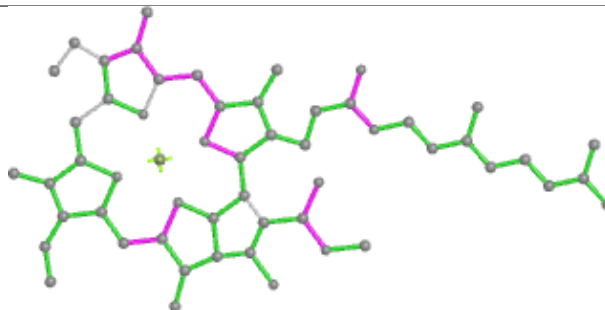
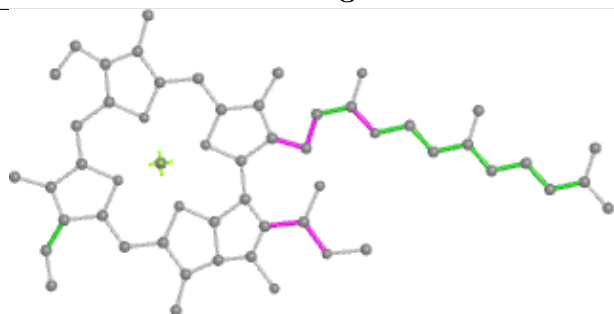
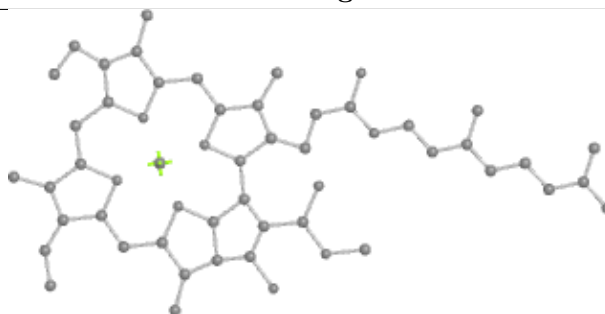
Bond angles

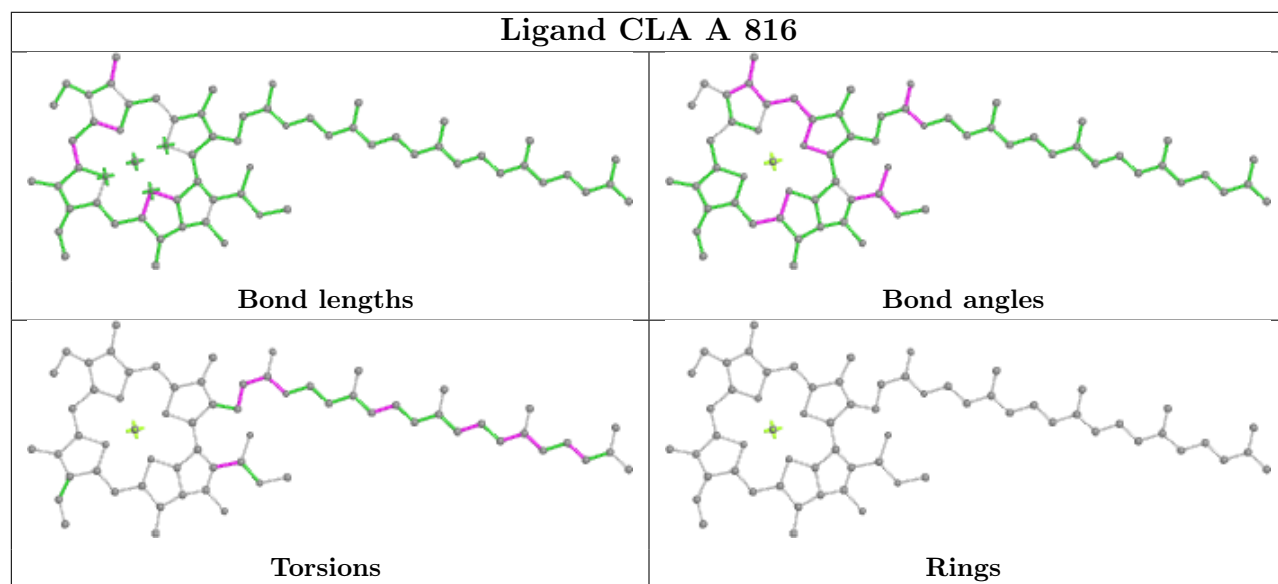
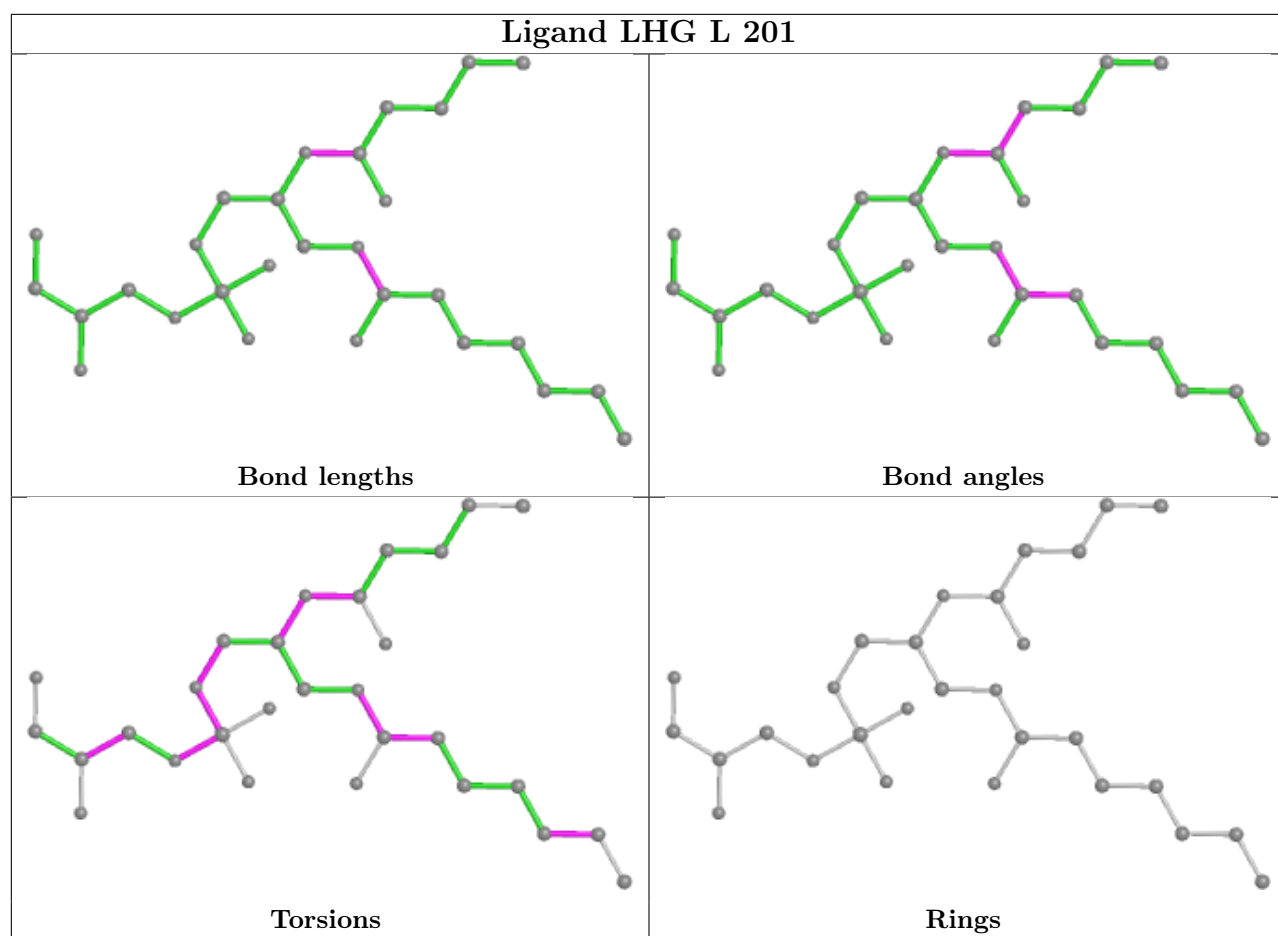


Torsions

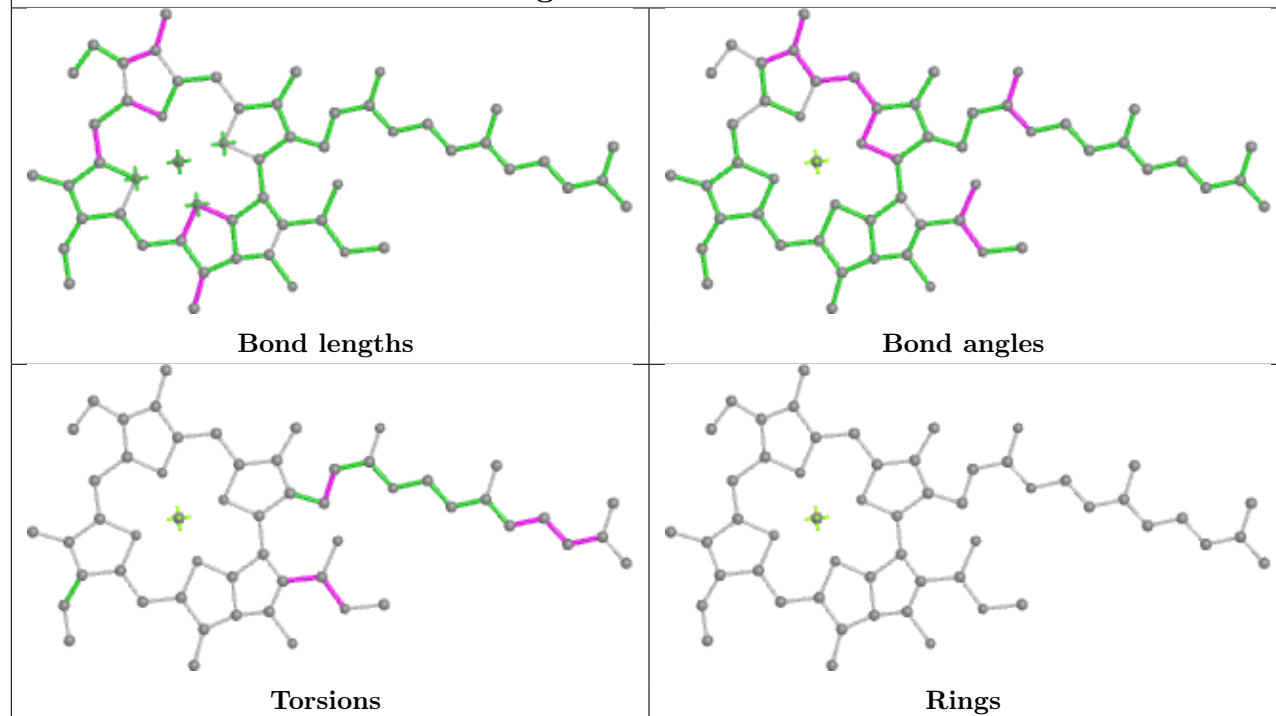


Rings

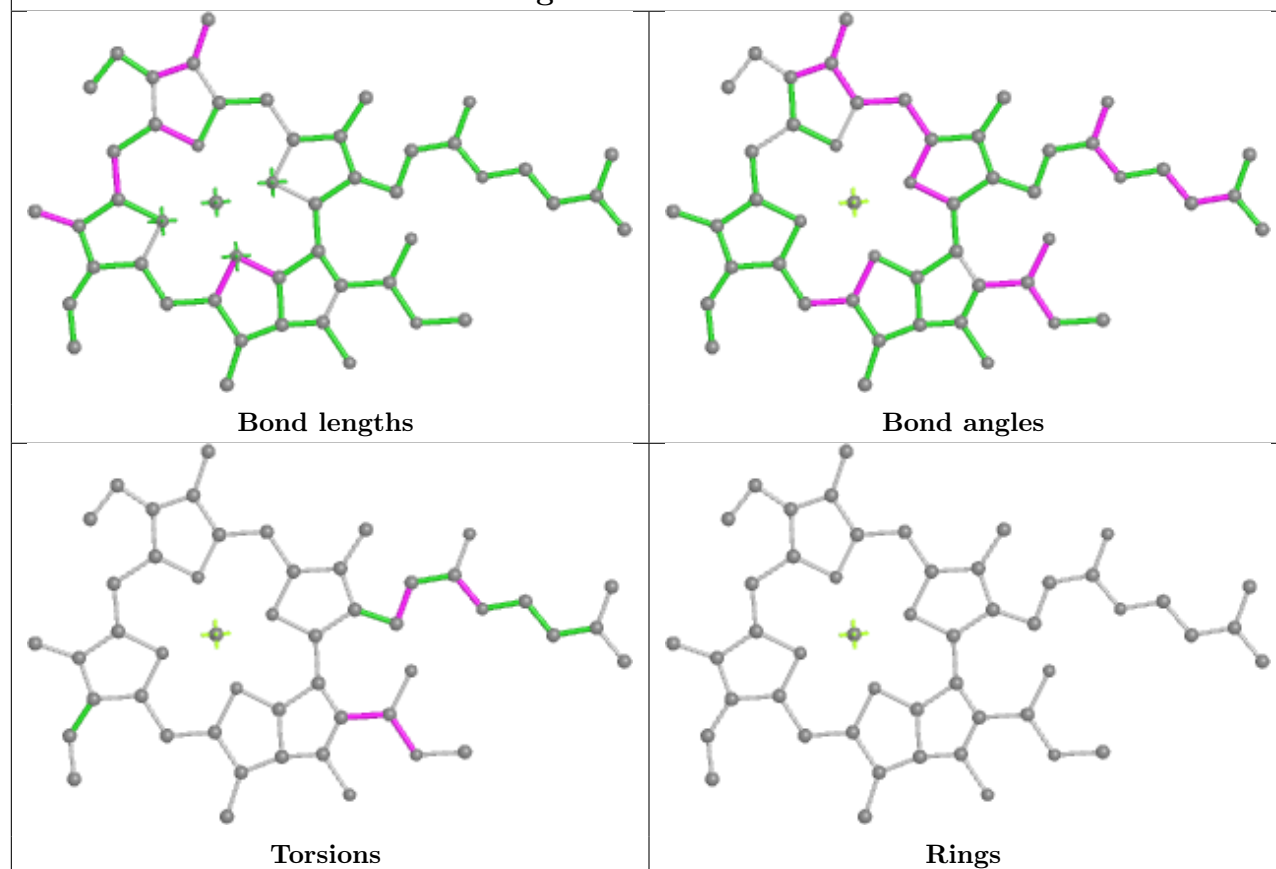
Ligand CLA t 303**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 846****Bond lengths****Bond angles****Torsions****Rings**



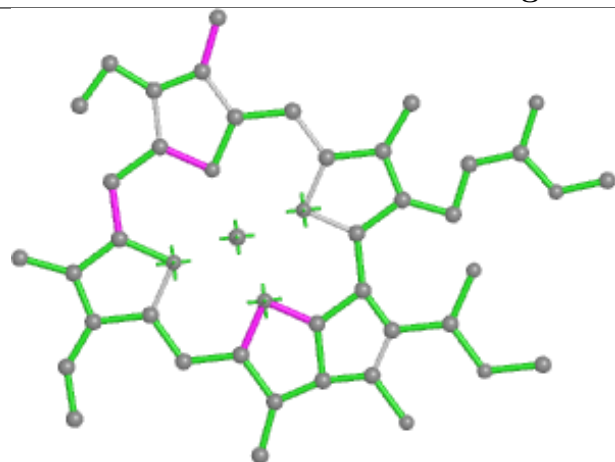
Ligand CLA 1 304



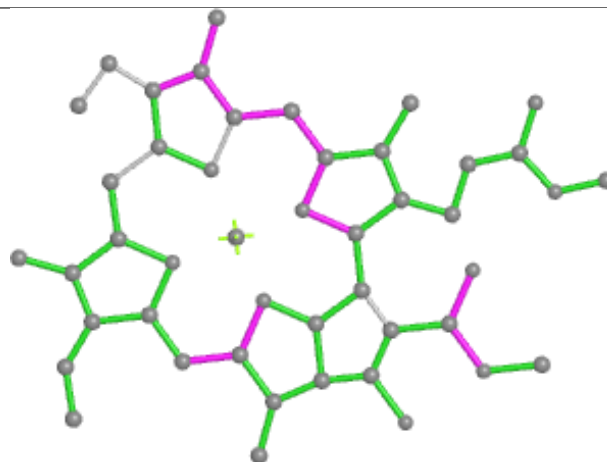
Ligand CLA 8 203



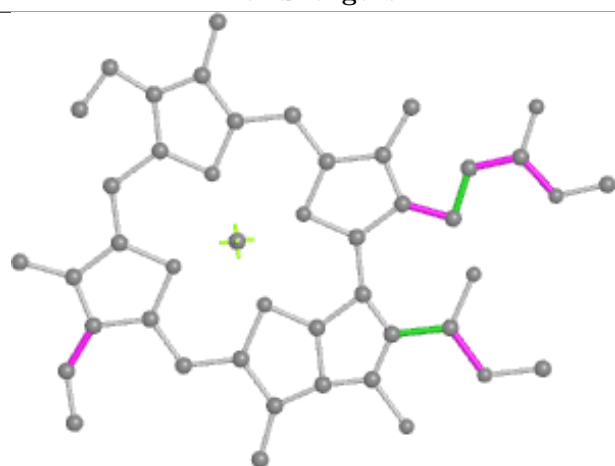
Ligand CLA c 605



Bond lengths



Bond angles

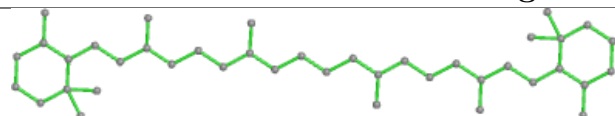


Torsions

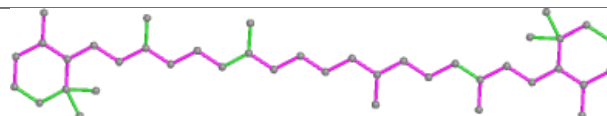


Rings

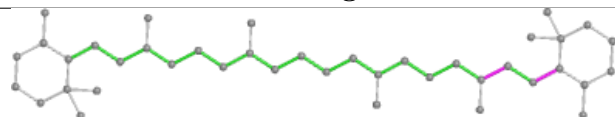
Ligand BCR 2 211



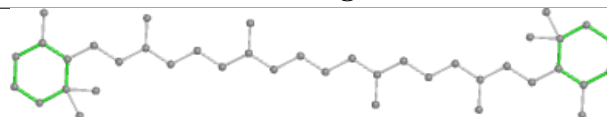
Bond lengths



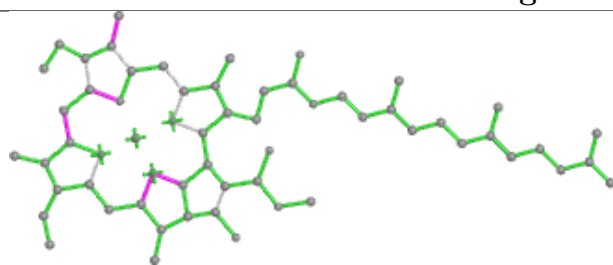
Bond angles



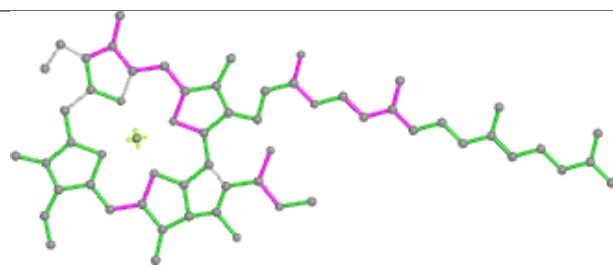
Torsions



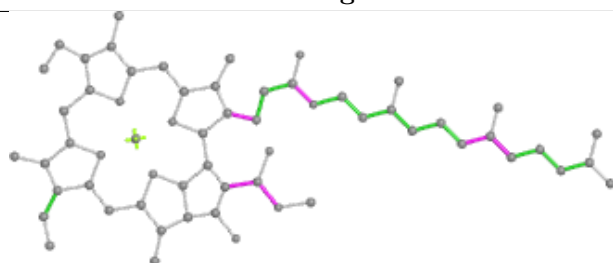
Rings

Ligand CLA c 609

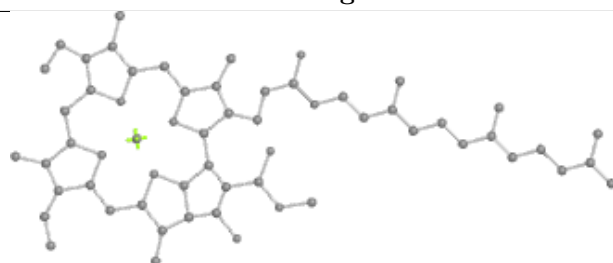
Bond lengths



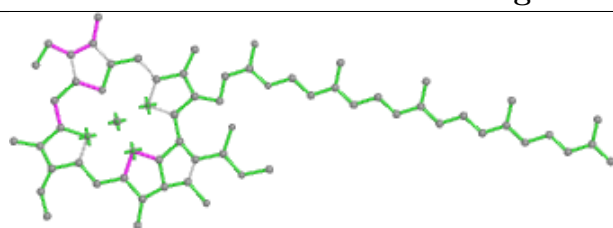
Bond angles



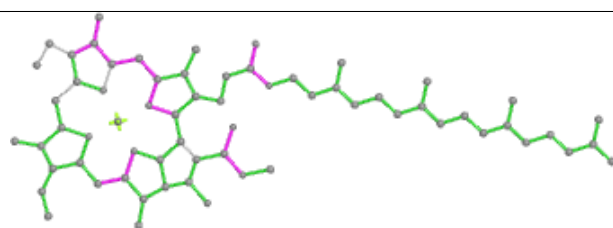
Torsions



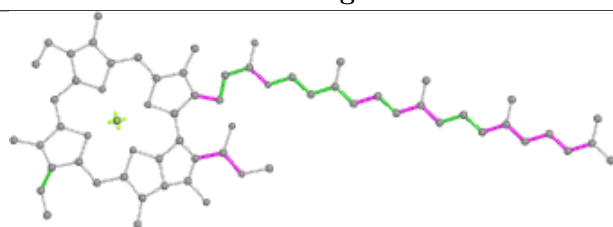
Rings

Ligand CLA A 823

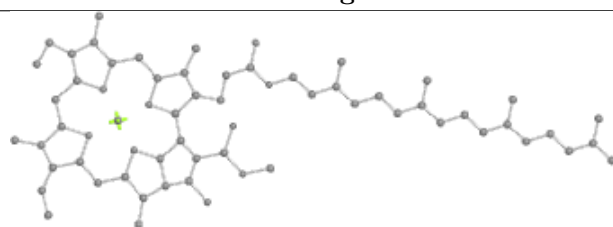
Bond lengths



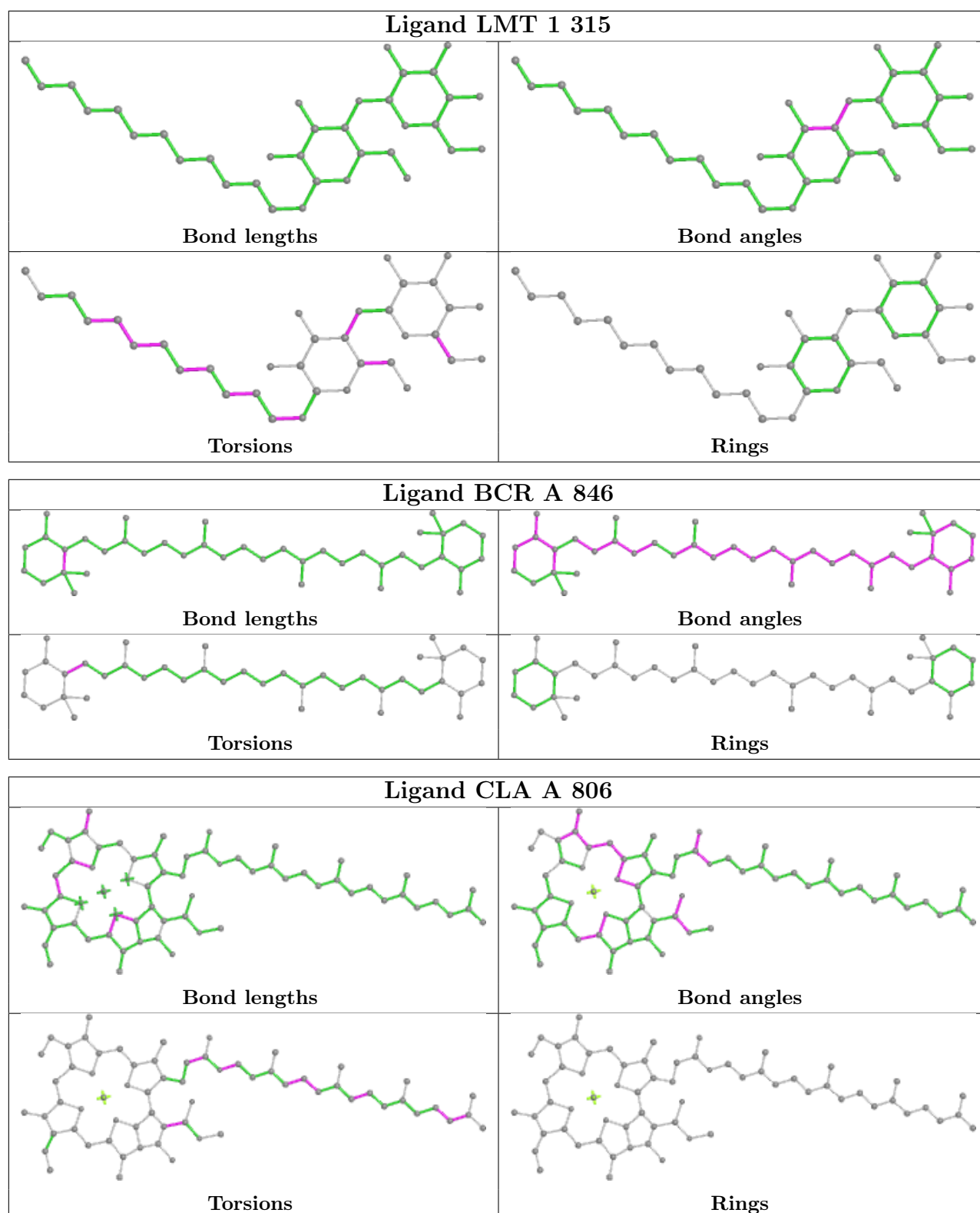
Bond angles



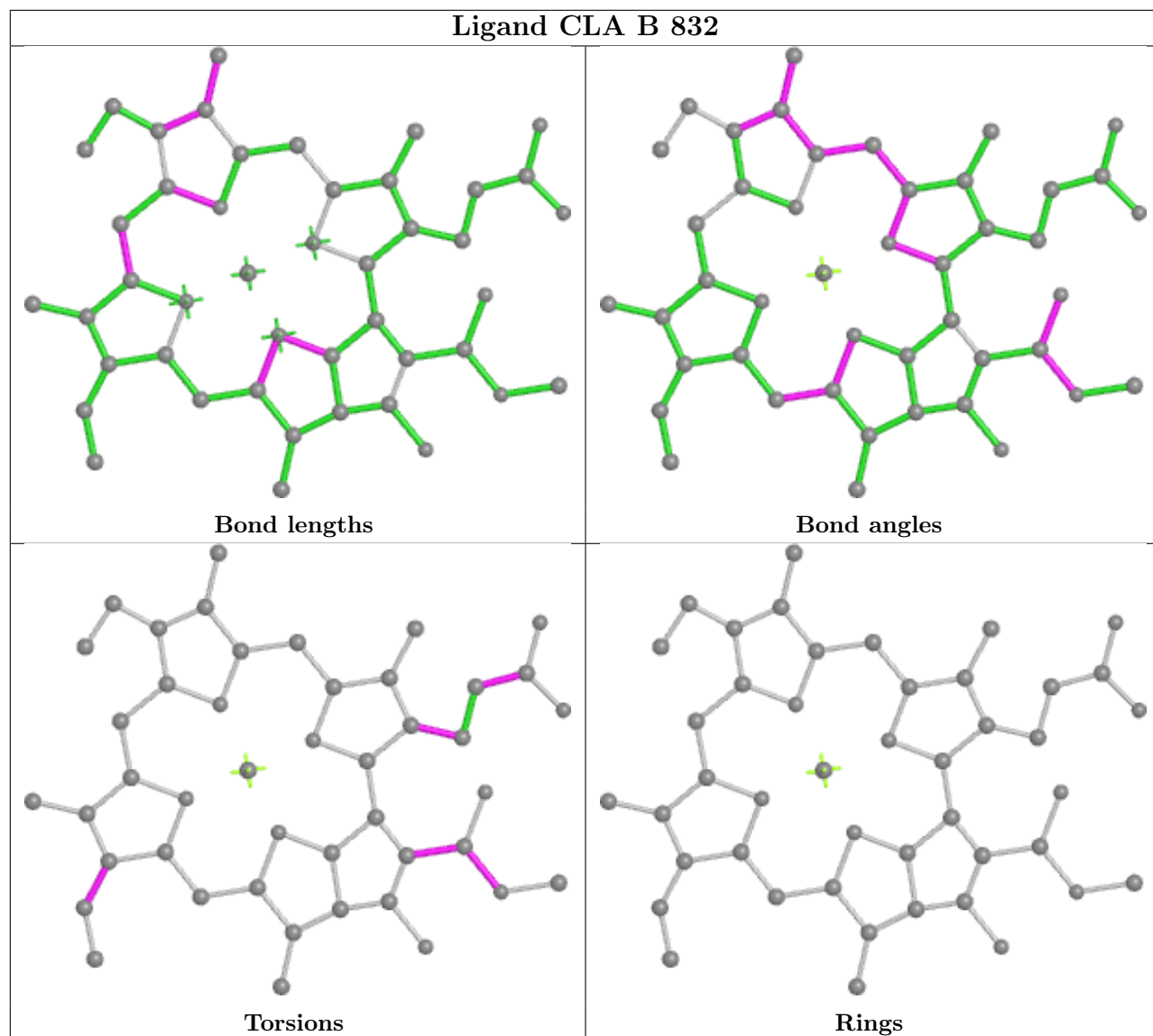
Torsions



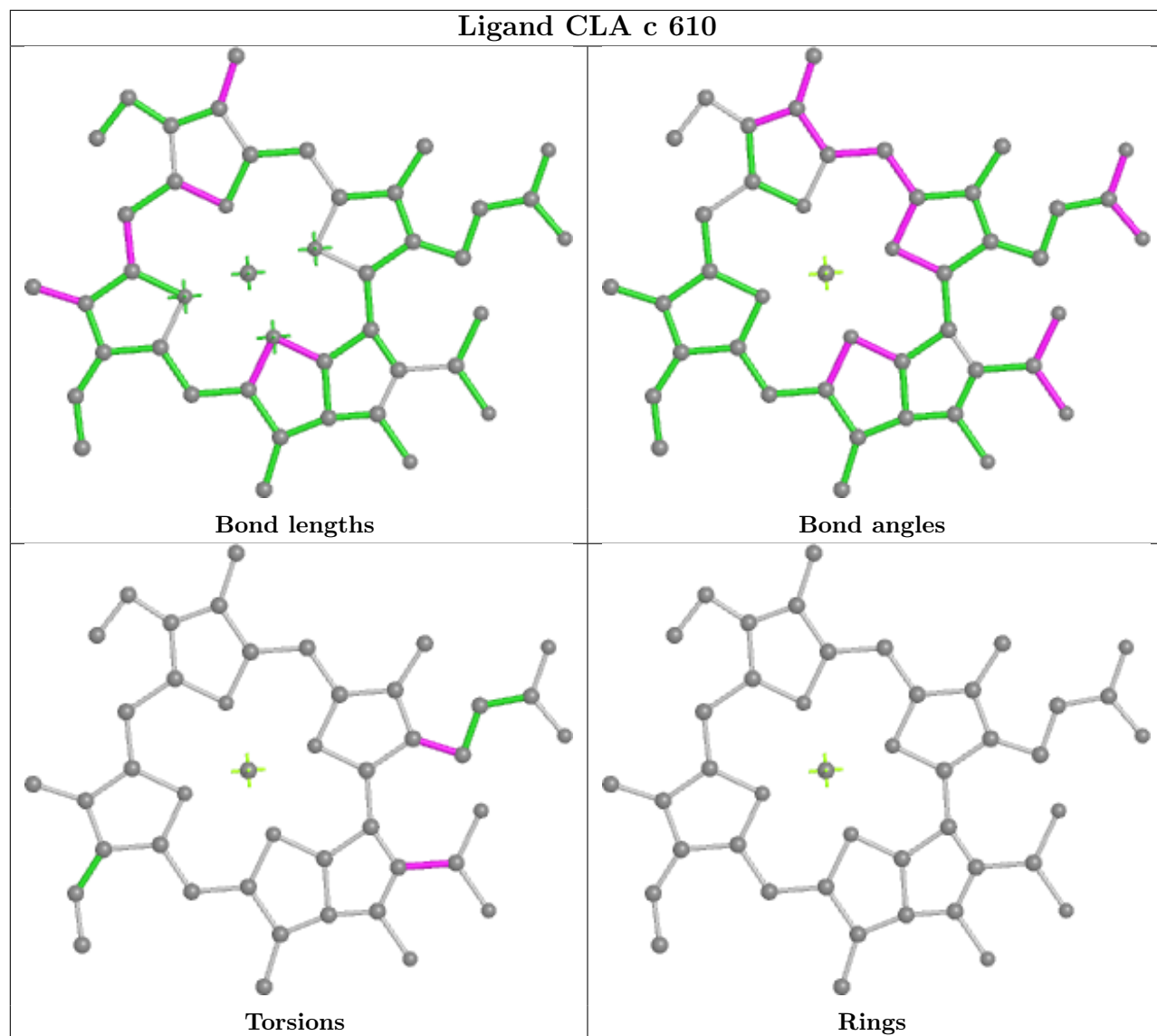
Rings



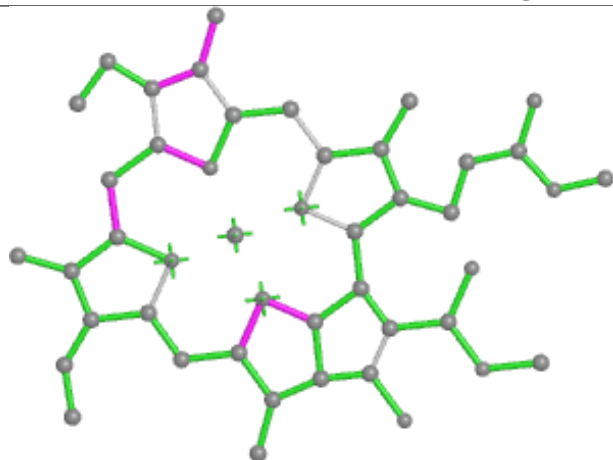
Ligand CLA B 832



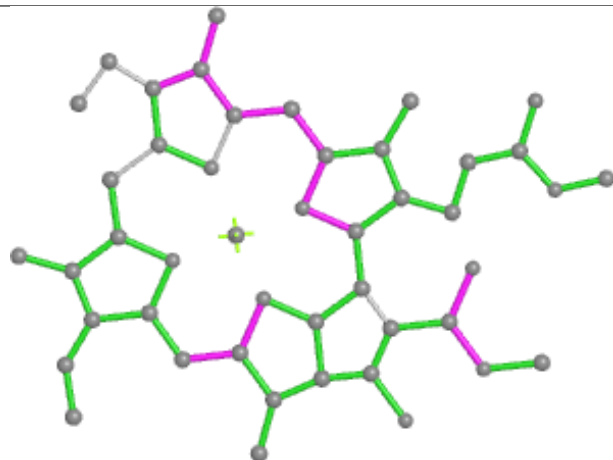
Ligand CLA c 610



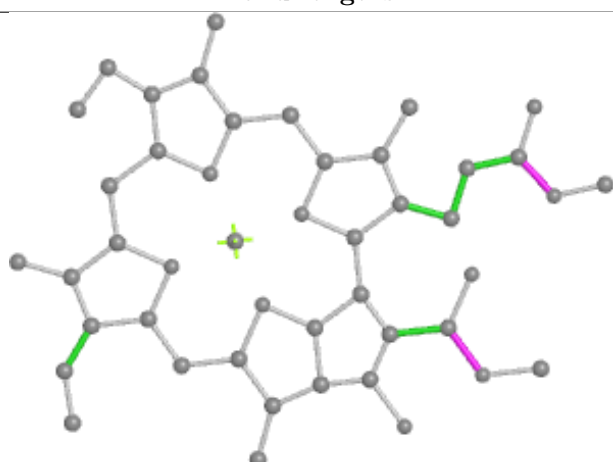
Ligand CLA h 607



Bond lengths



Bond angles

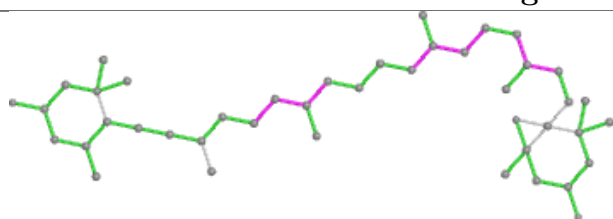


Torsions

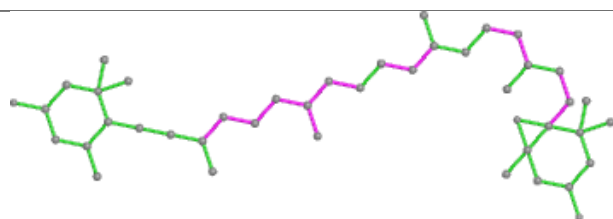


Rings

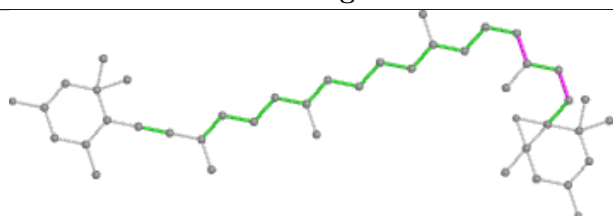
Ligand DD6 t 311



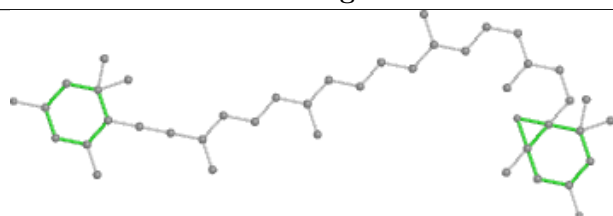
Bond lengths



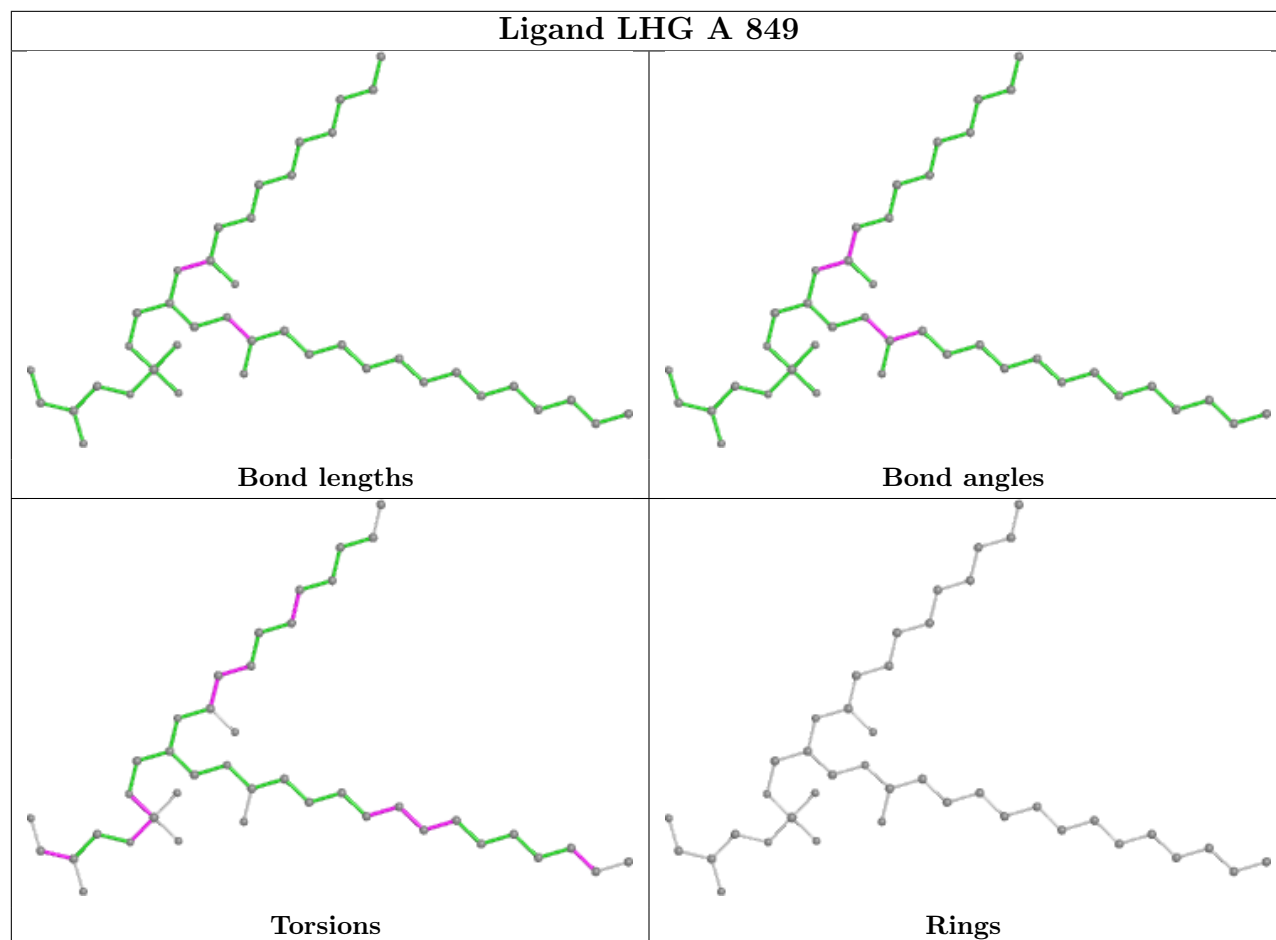
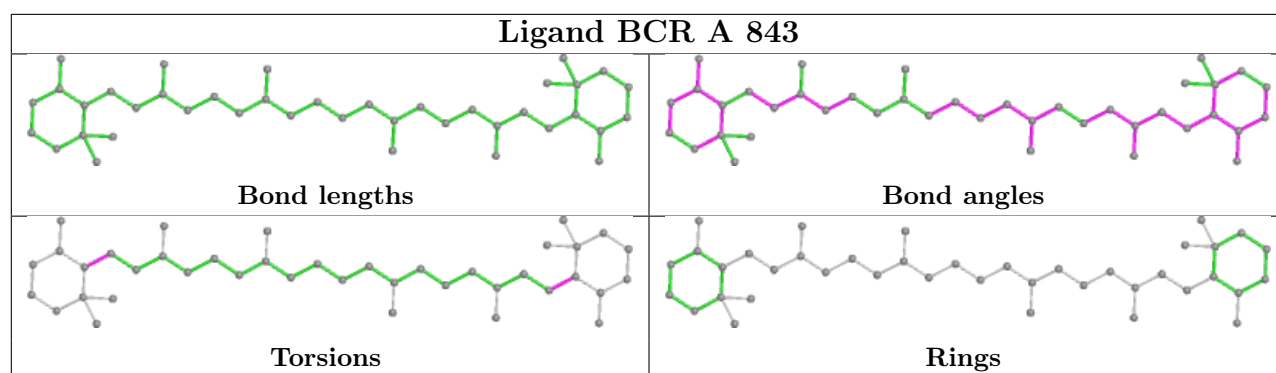
Bond angles



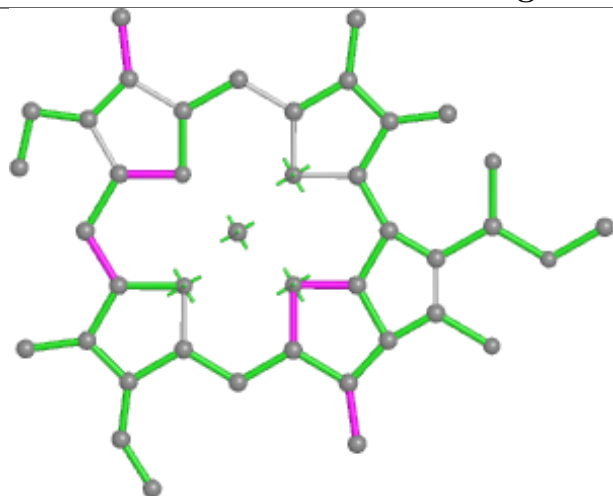
Torsions



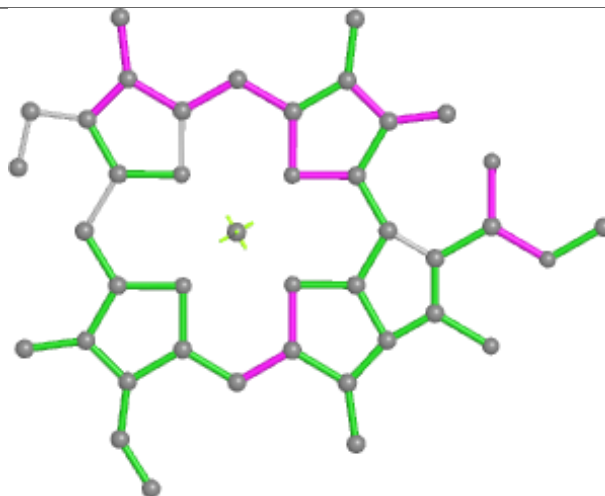
Rings



Ligand CLA h 611



Bond lengths



Bond angles

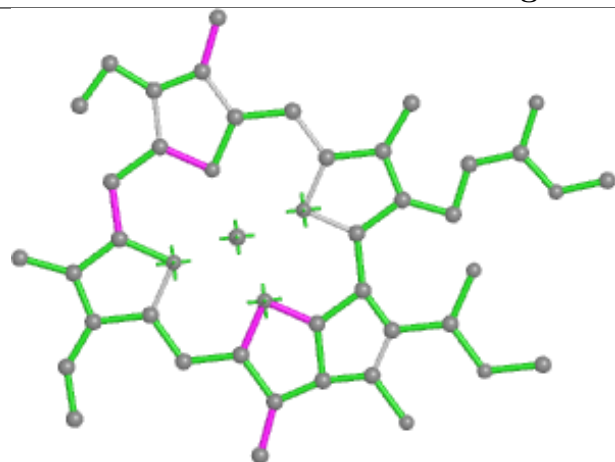


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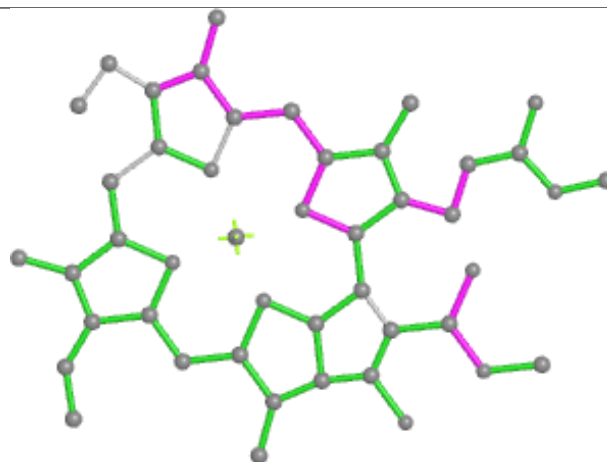


Rings

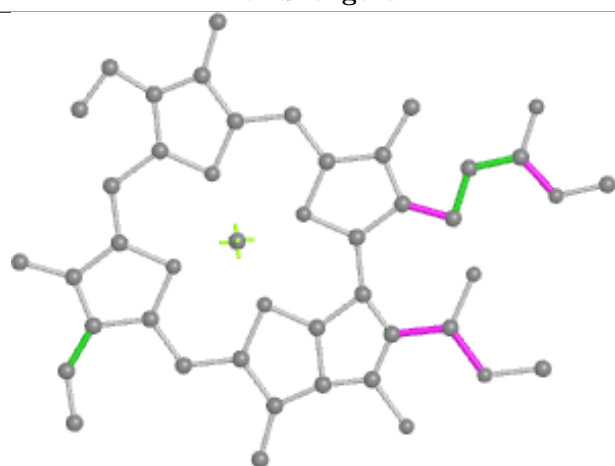
Ligand CLA 9 304



Bond lengths



Bond angles

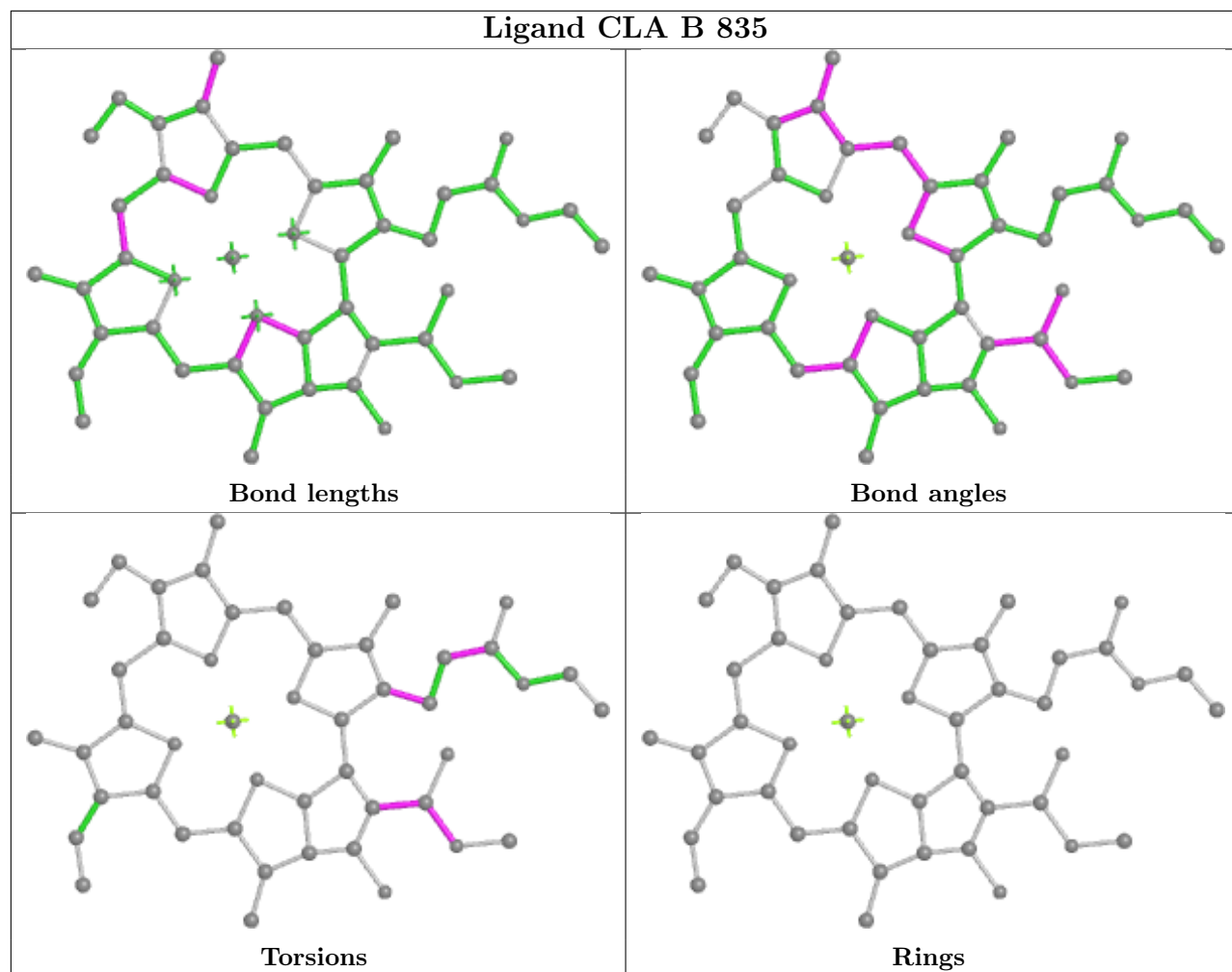


Torsions

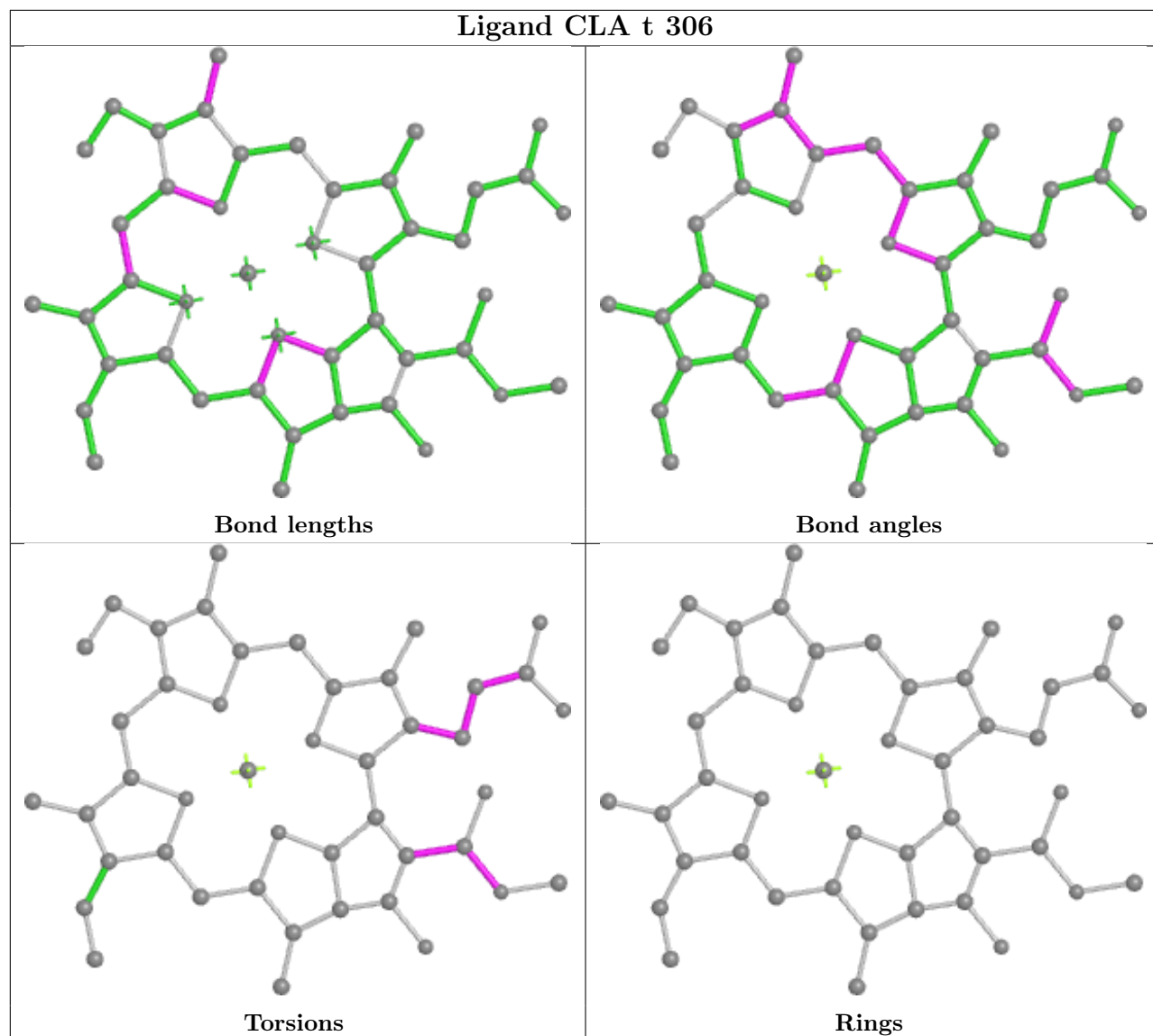


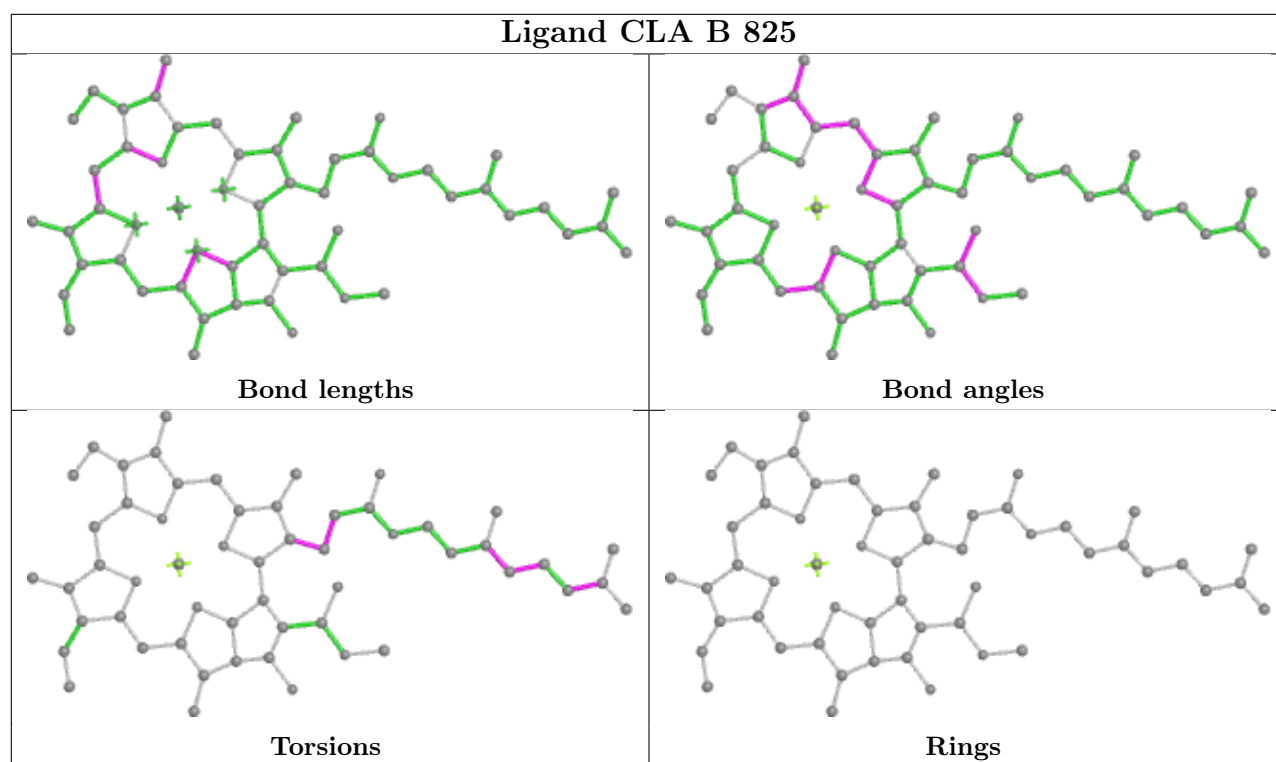
Rings

Ligand CLA B 835

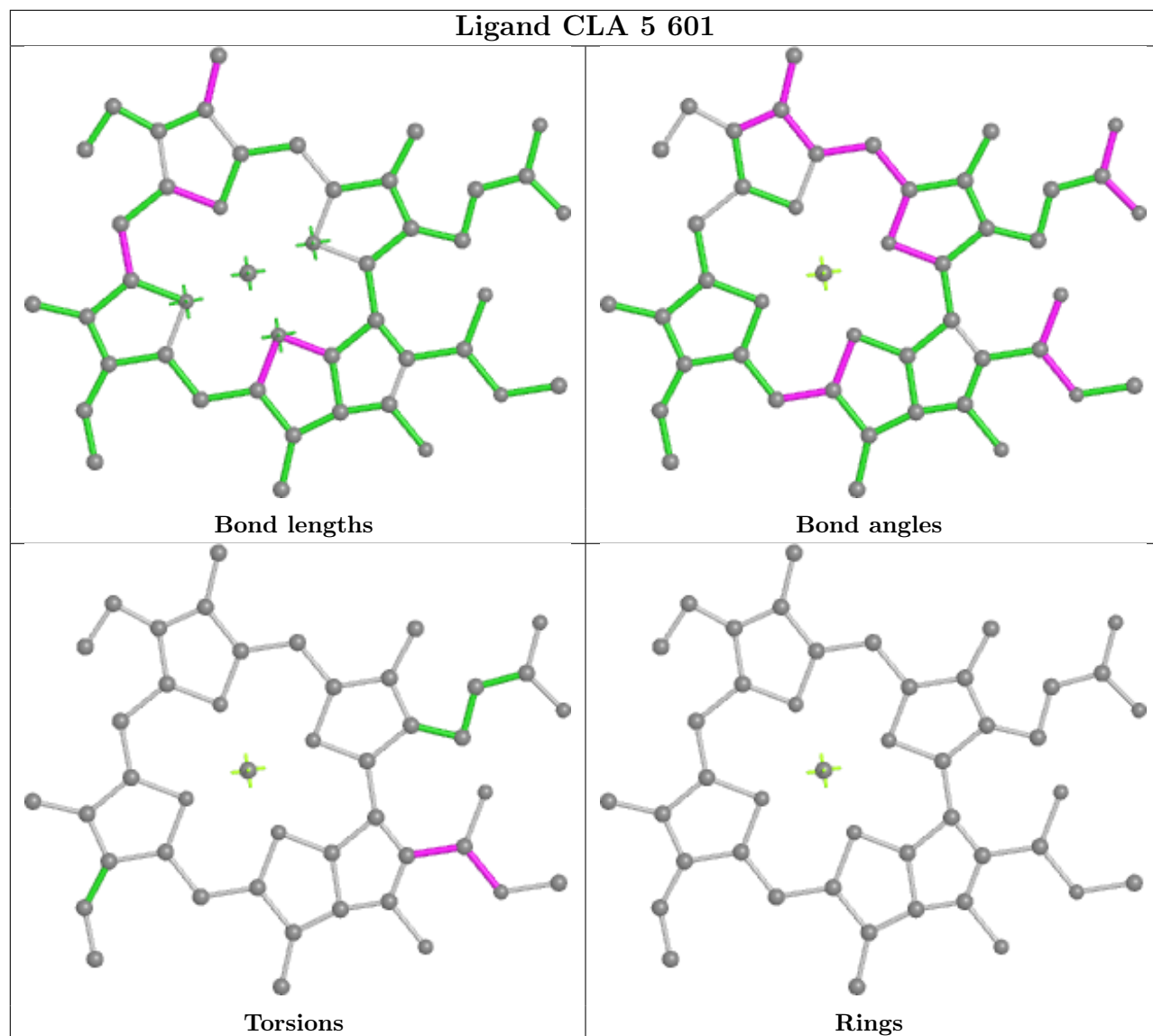


Ligand CLA t 306

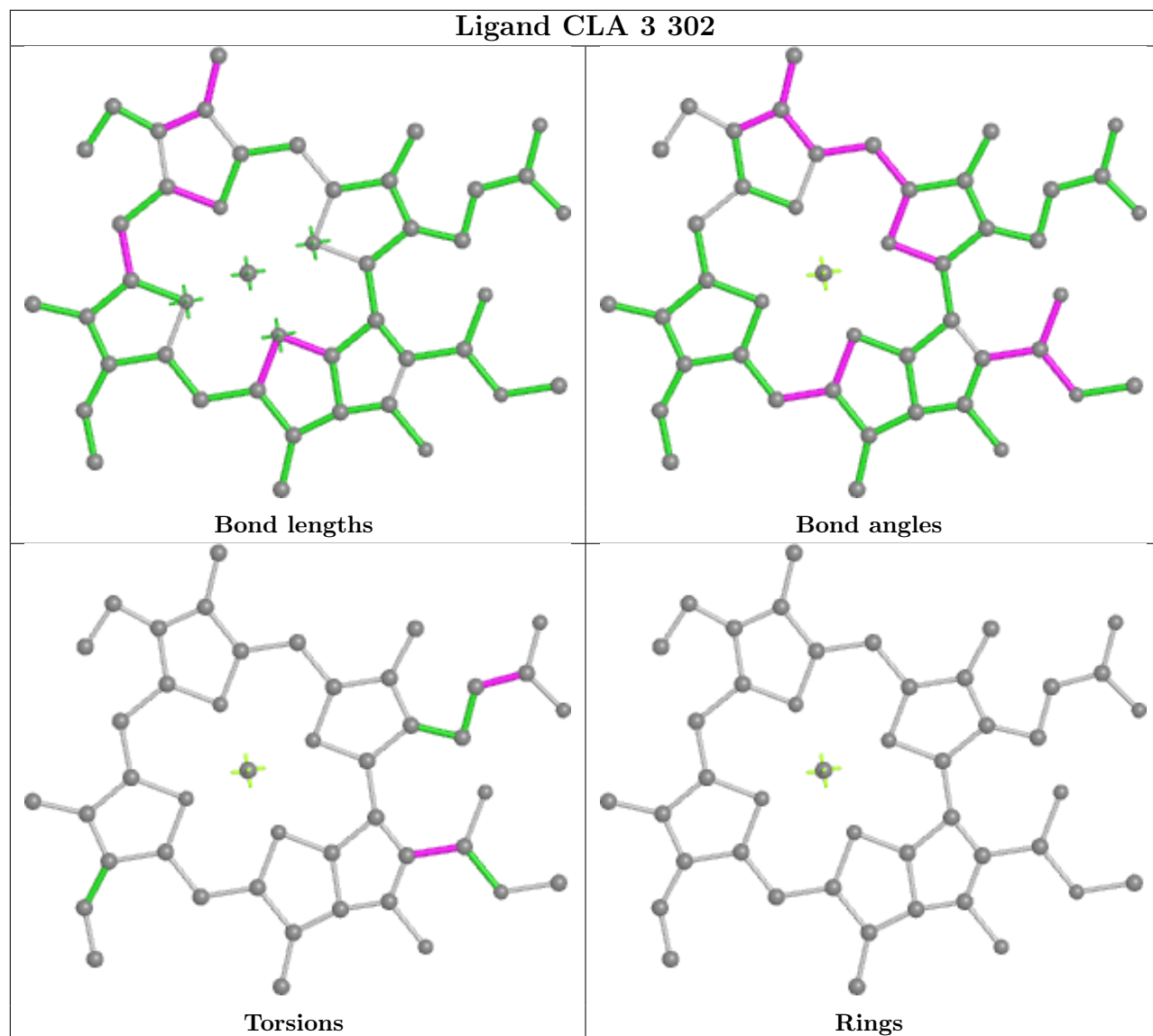




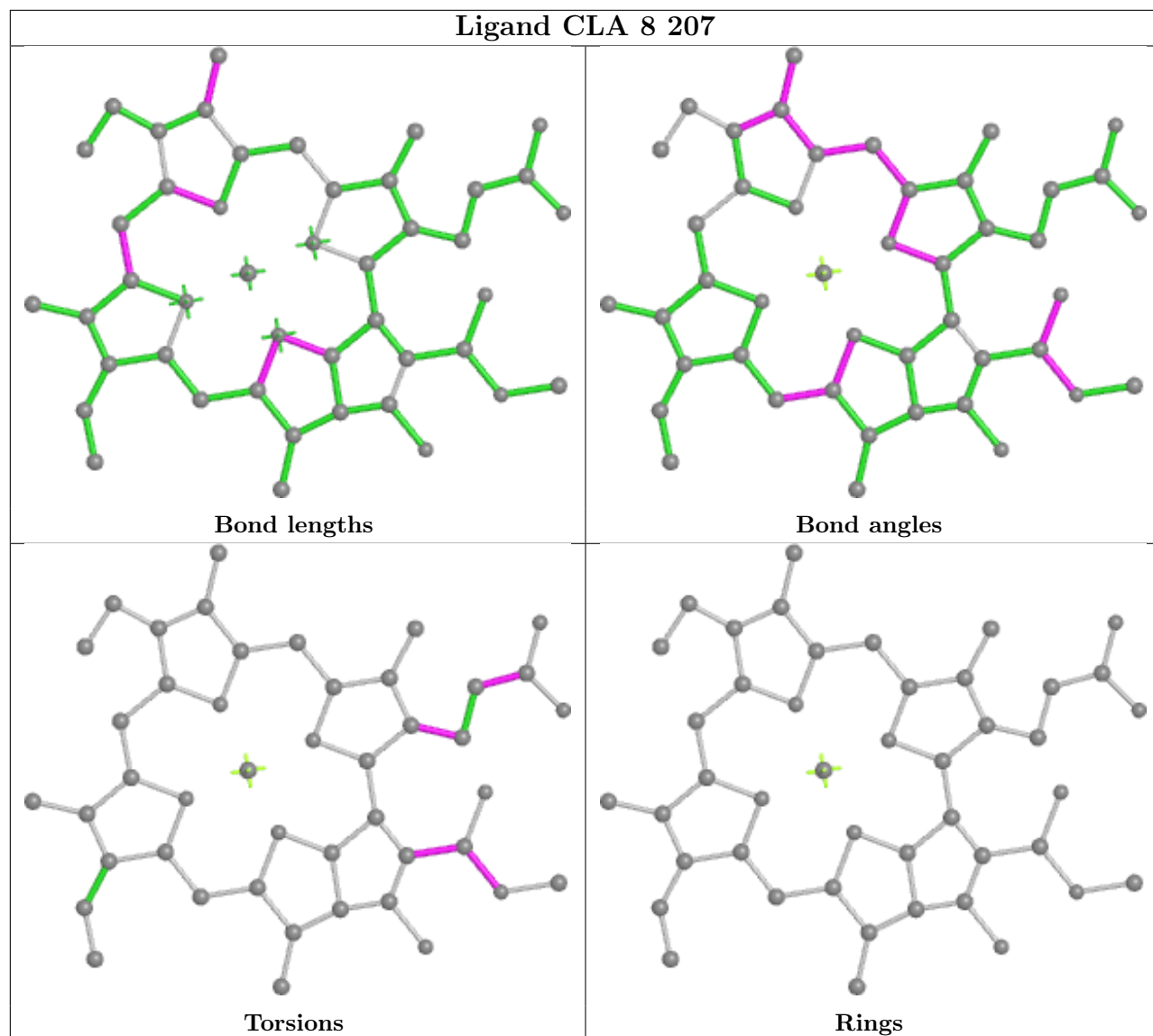
Ligand CLA 5 601



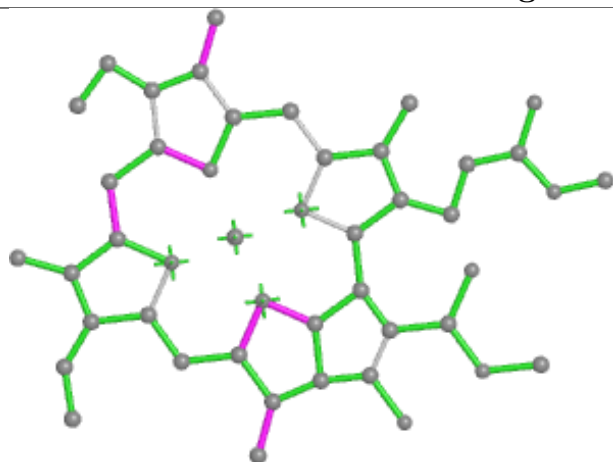
Ligand CLA 3 302



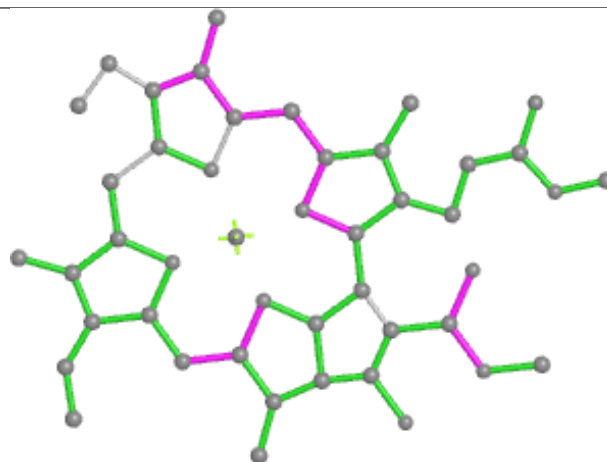
Ligand CLA 8 207



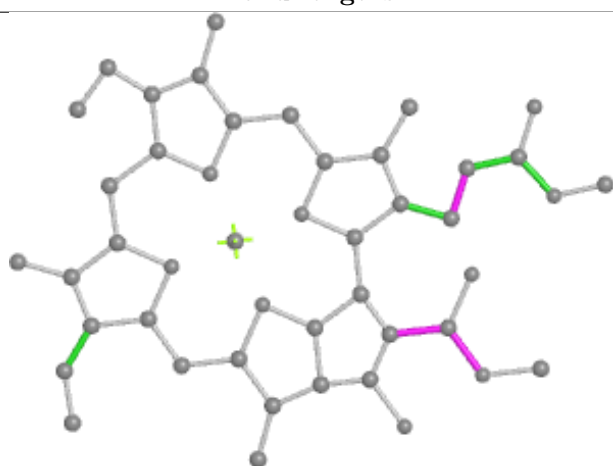
Ligand CLA 6 604



Bond lengths



Bond angles

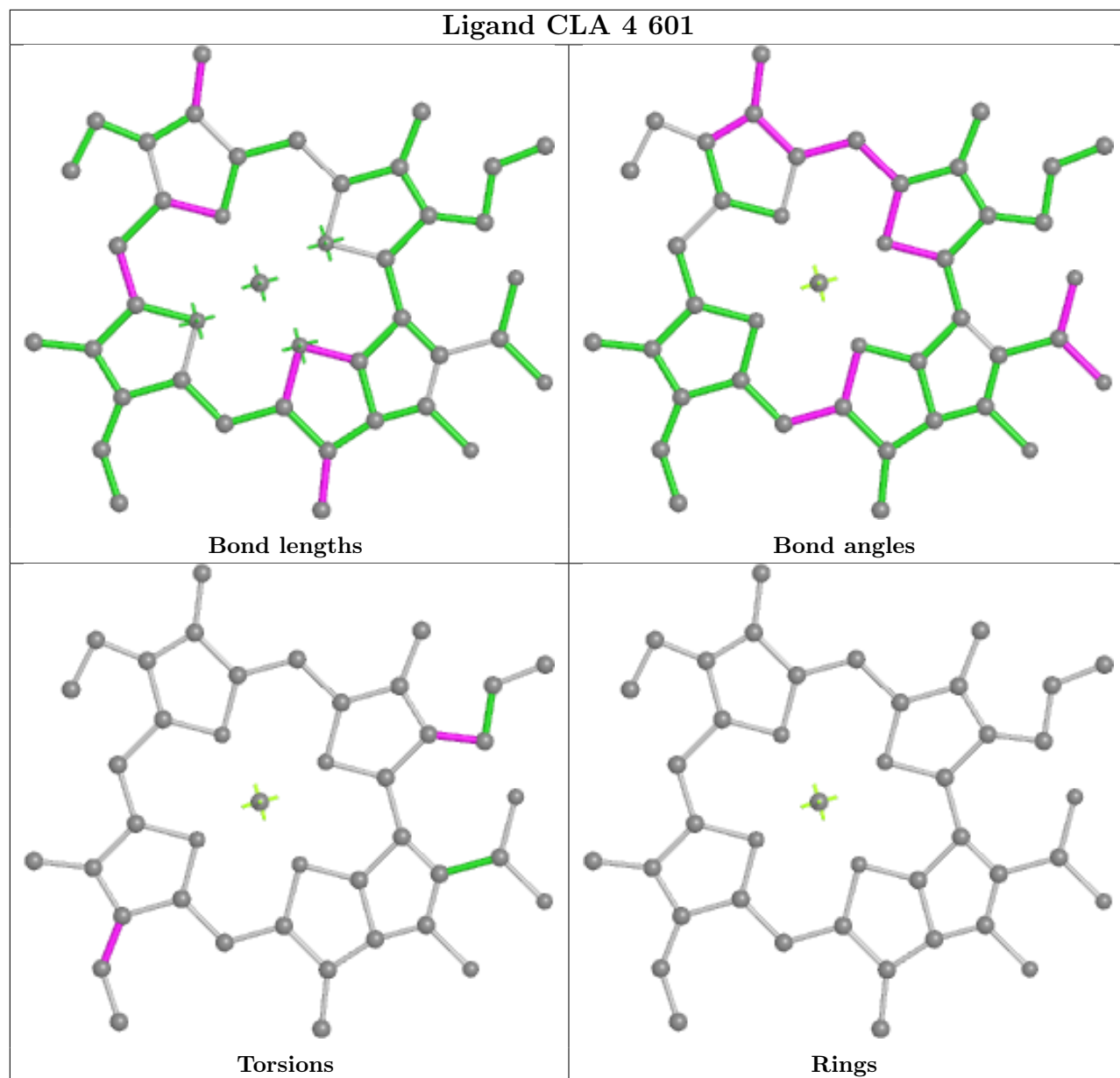


Torsions

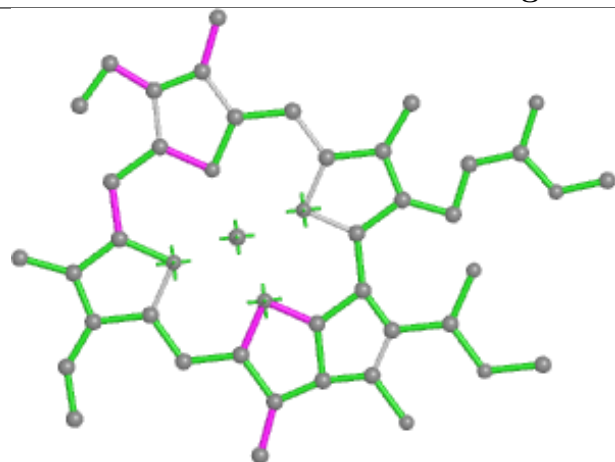


Rings

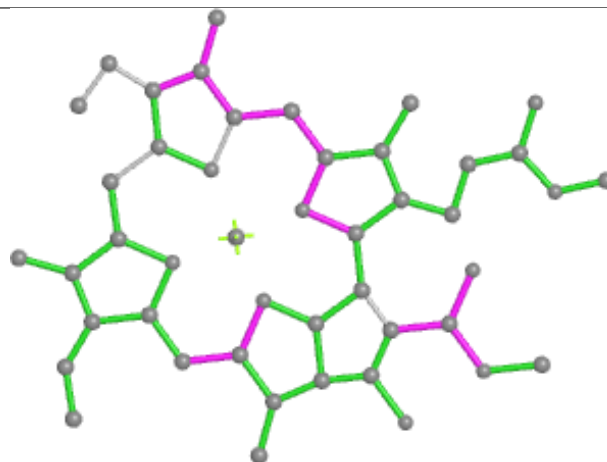
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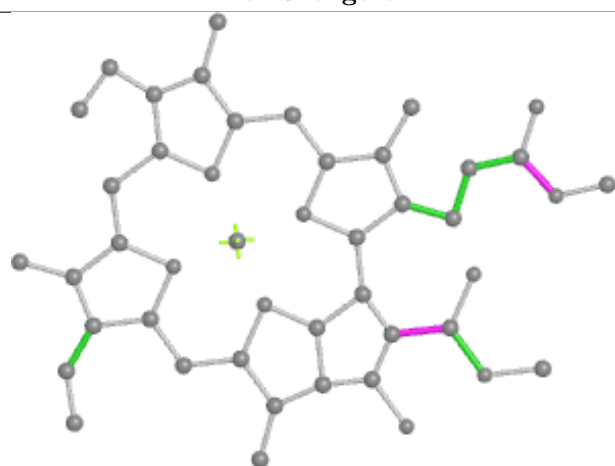
Ligand CLA c 607



Bond lengths



Bond angles

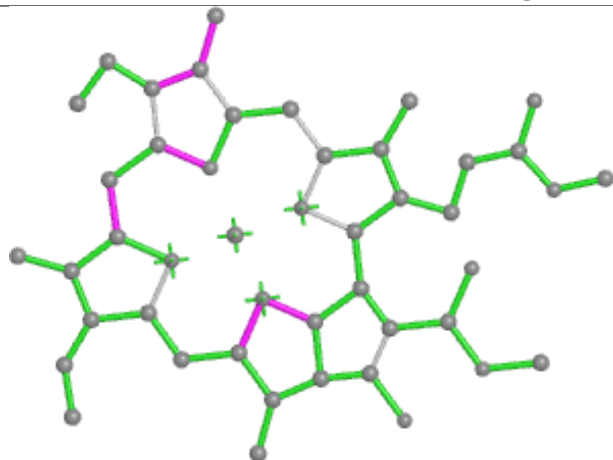


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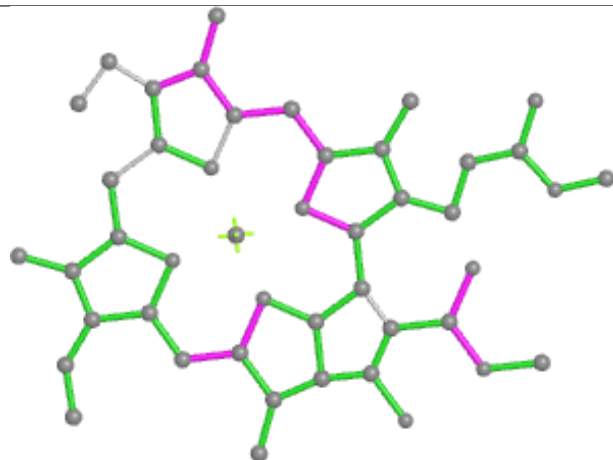


Rings

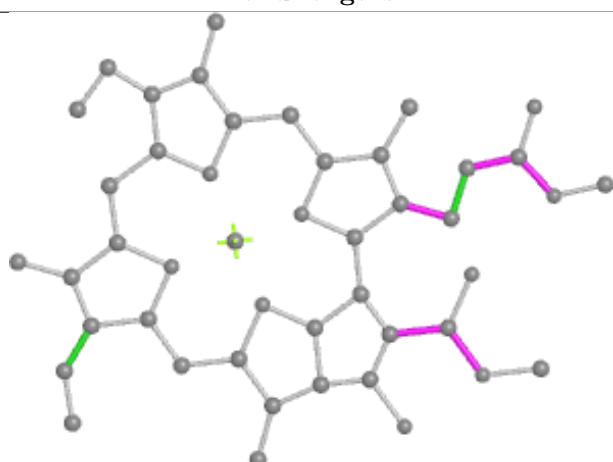
Ligand CLA 4 604



Bond lengths



Bond angles

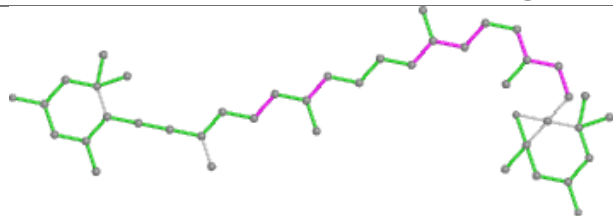


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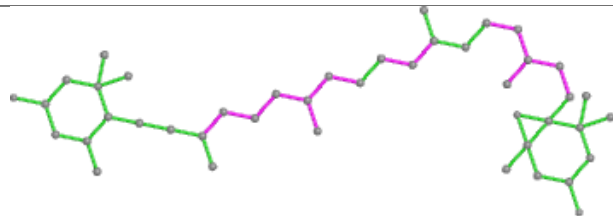


Rings

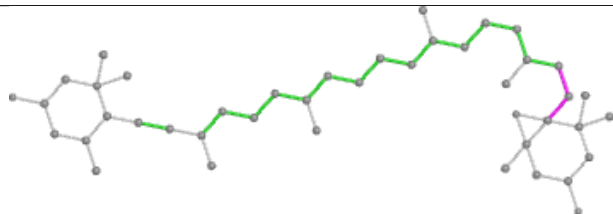
Ligand DD6 7 616



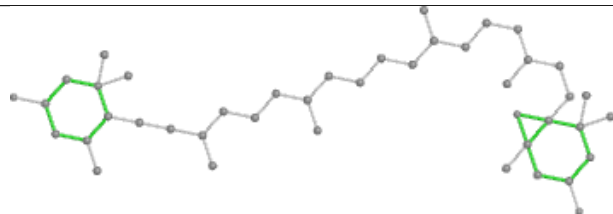
Bond lengths



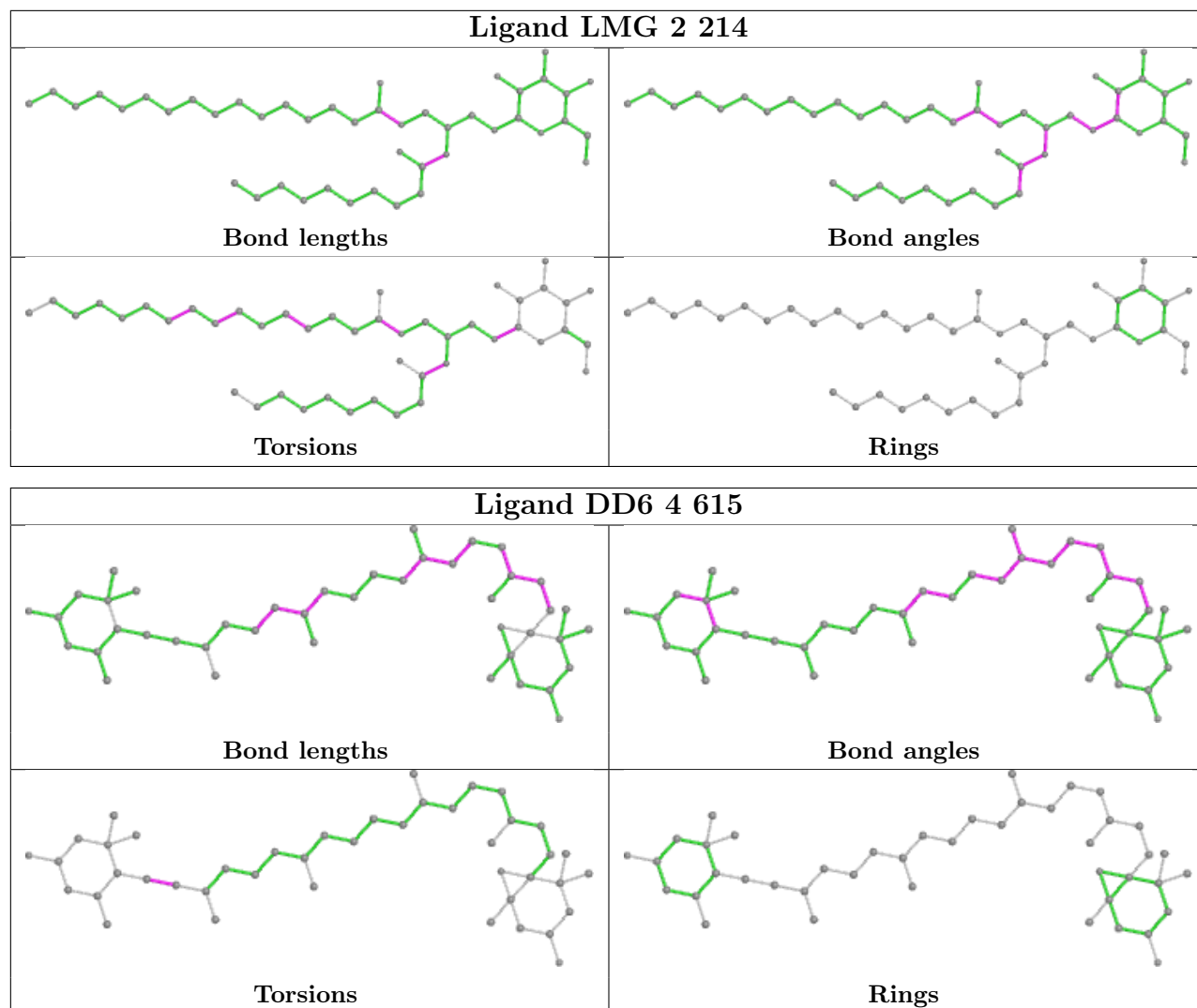
Bond angles



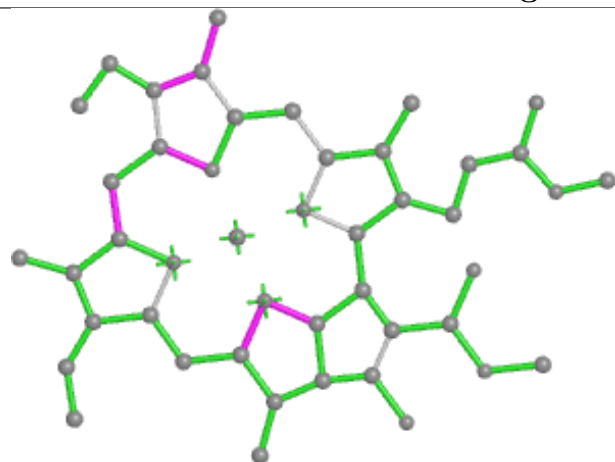
Torsions



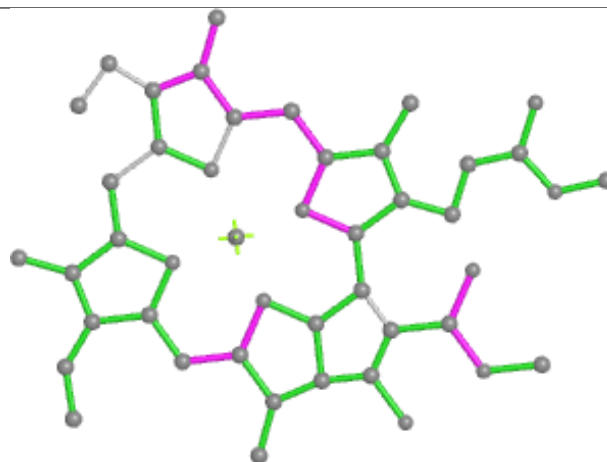
Rings



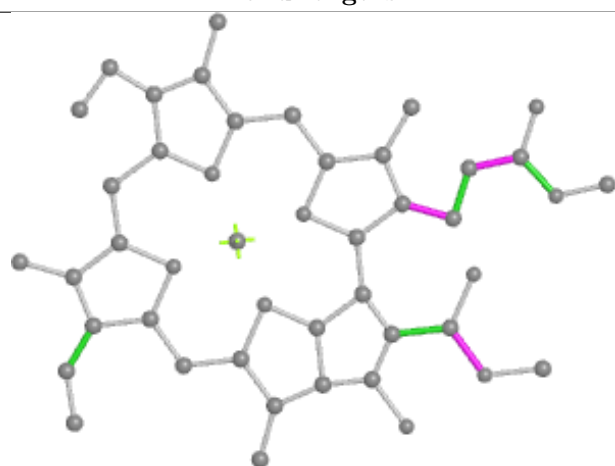
Ligand CLA 6 610



Bond lengths



Bond angles

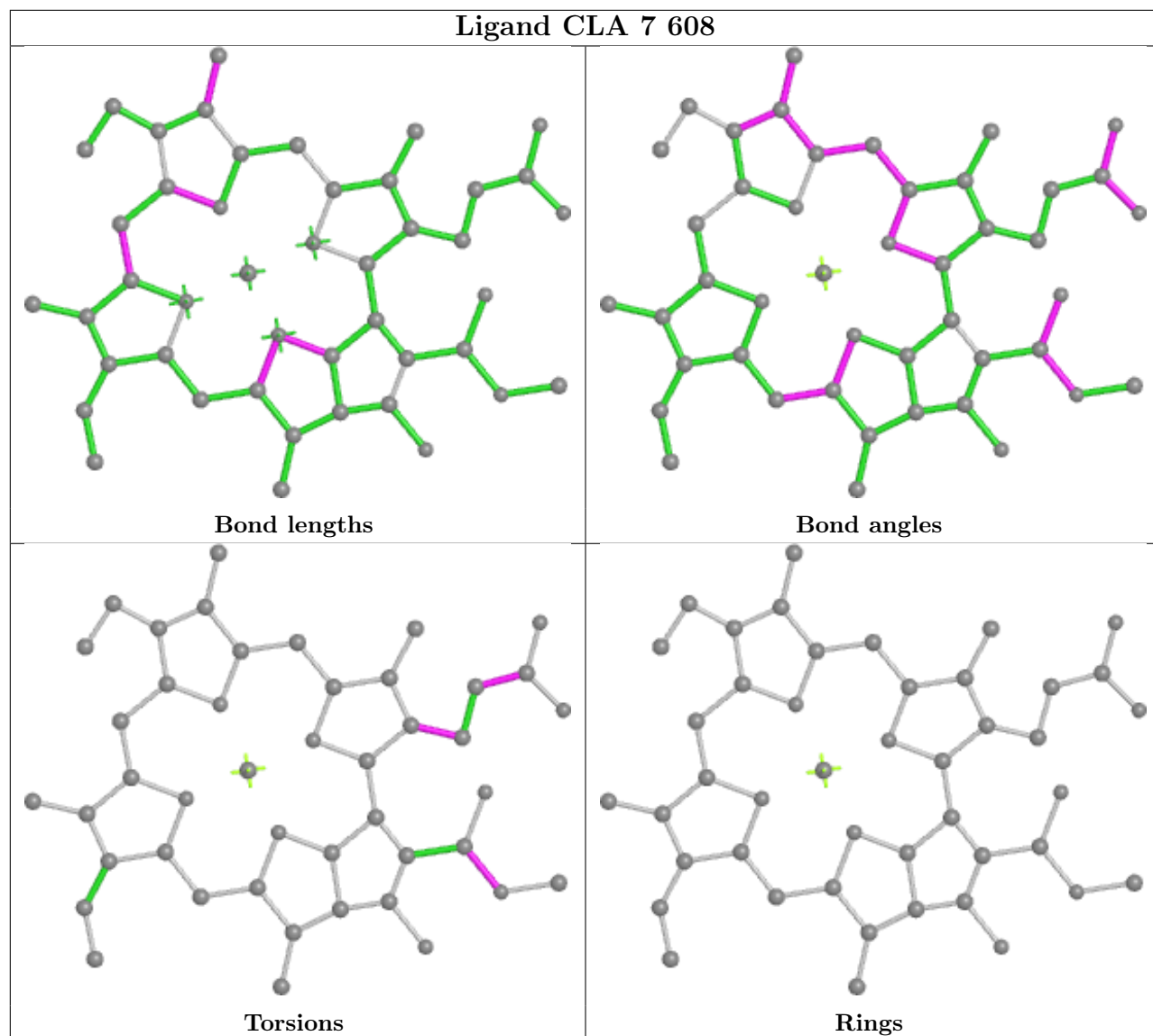


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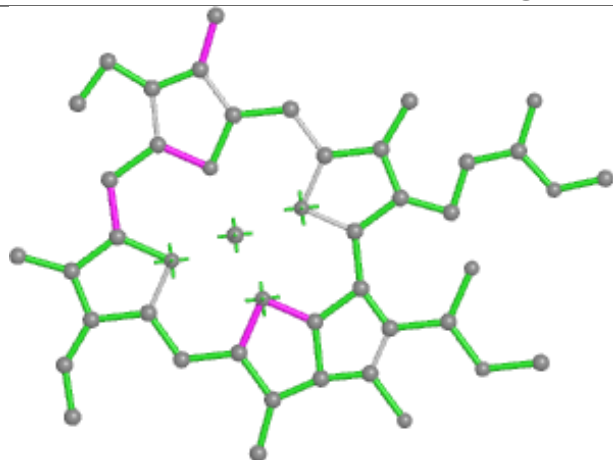


Rings

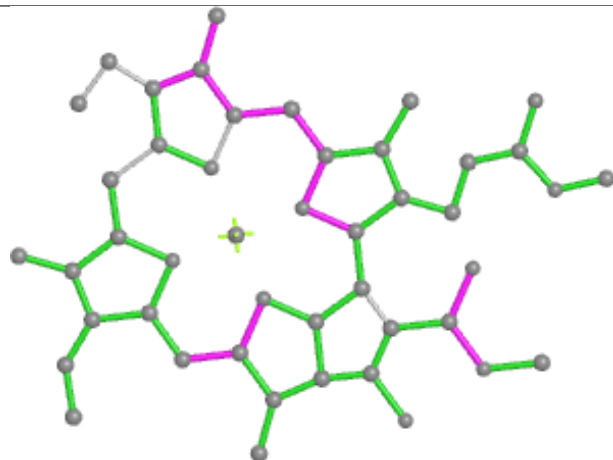
Ligand CLA 7 608



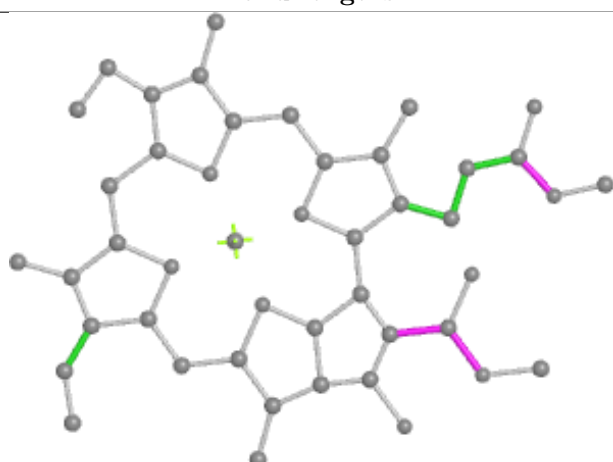
Ligand CLA h 609



Bond lengths



Bond angles

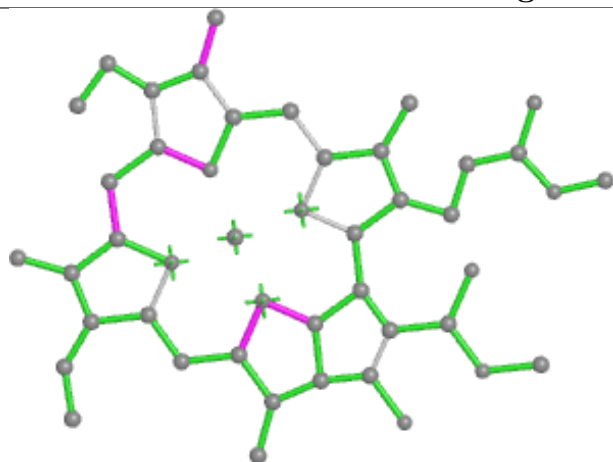


Torsions

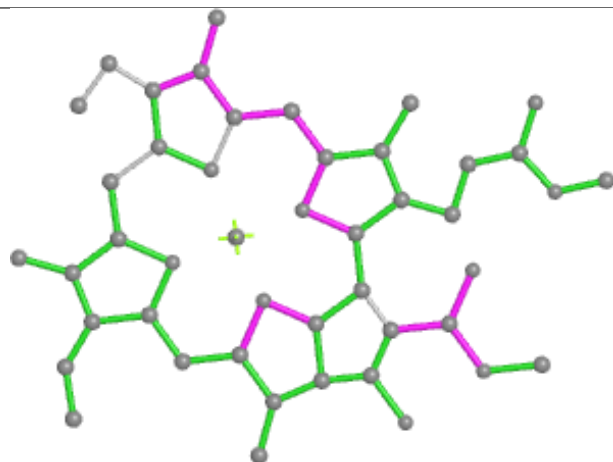


Rings

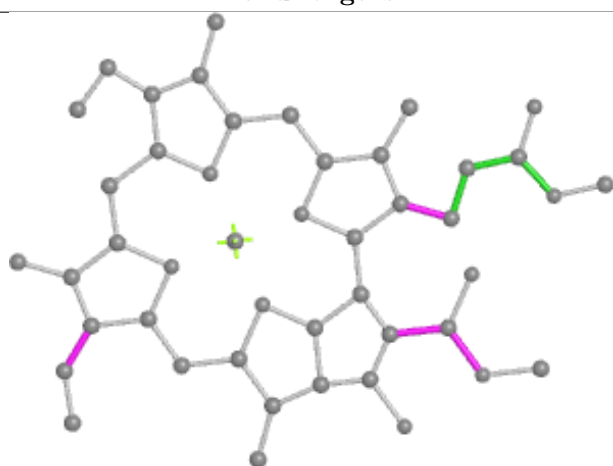
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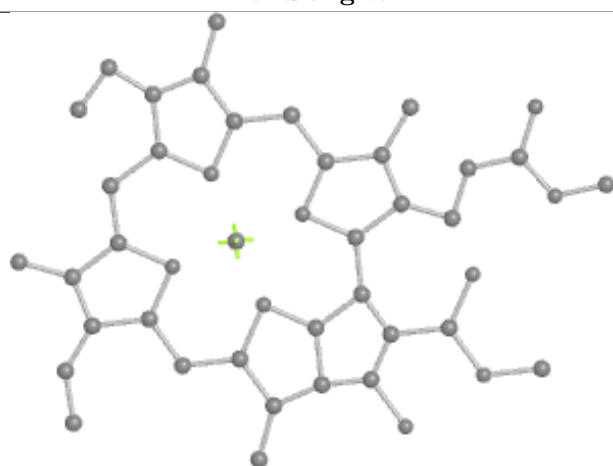
Bond lengths



Bond angles

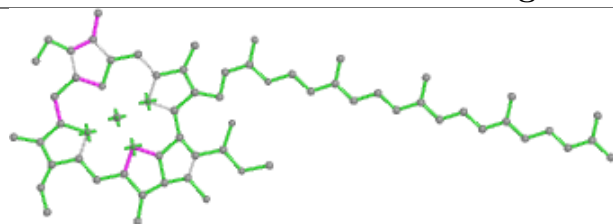


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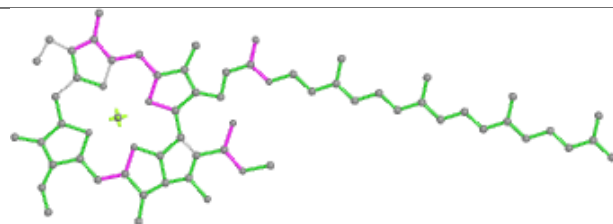


Rings

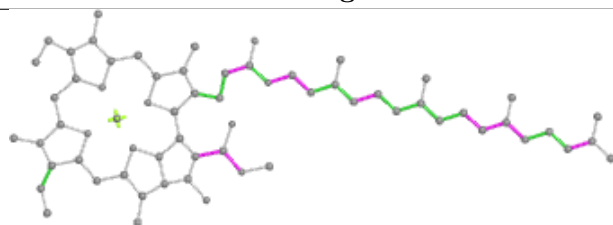
Ligand CLA 1 317



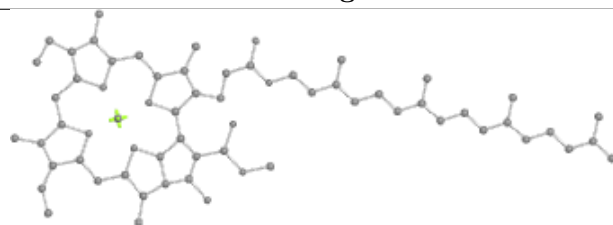
Bond lengths



Bond angles

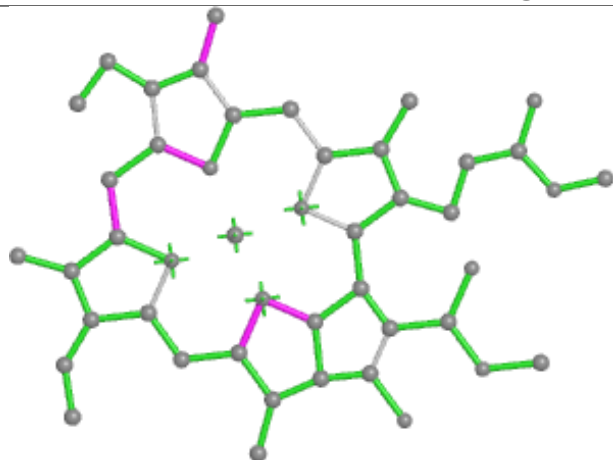


Torsions

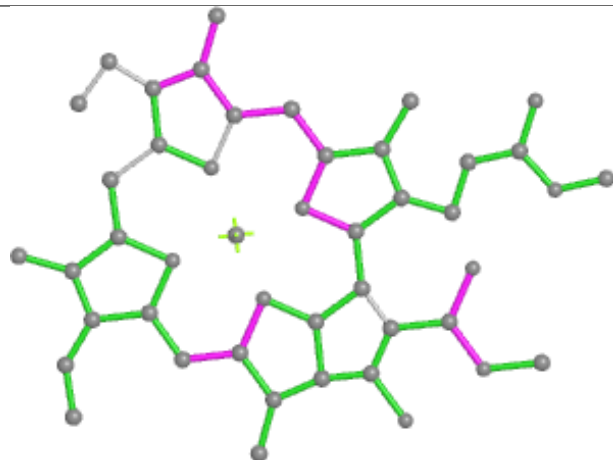


Rings

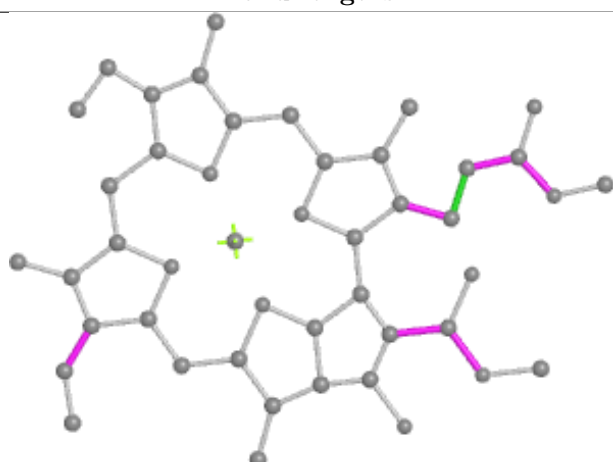
Ligand CLA k 302



Bond lengths



Bond angles

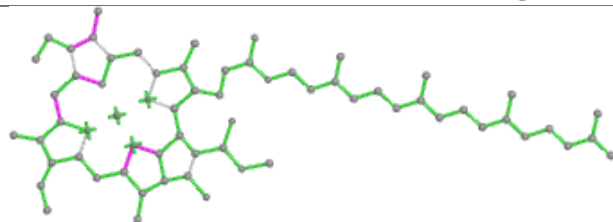


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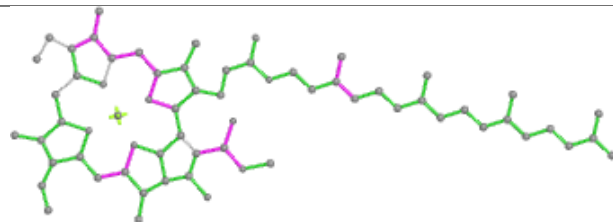


Rings

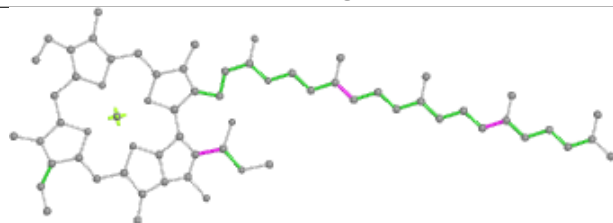
Ligand CLA A 833



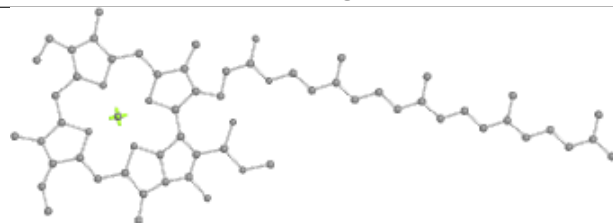
Bond lengths



Bond angles

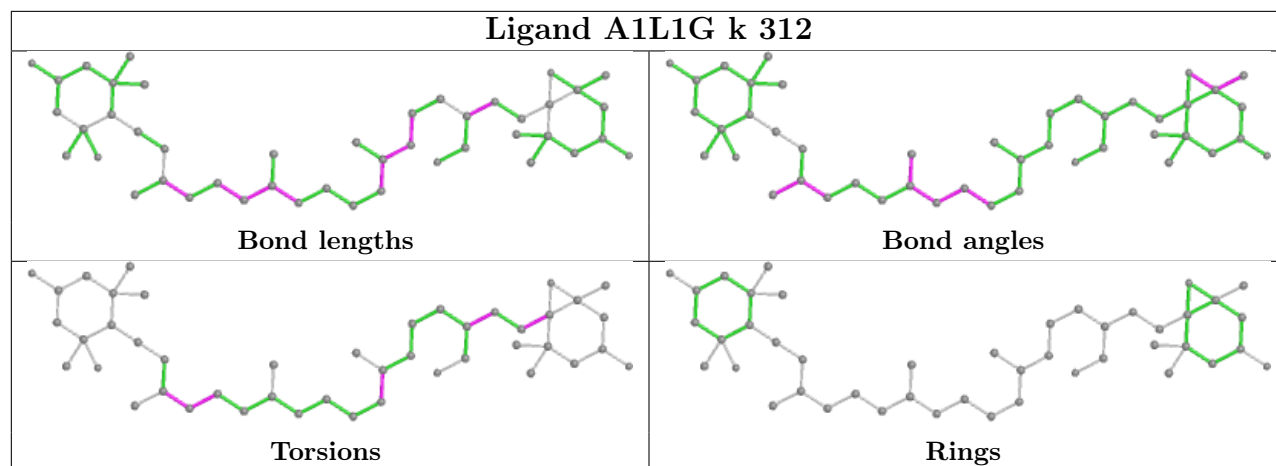


Torsions

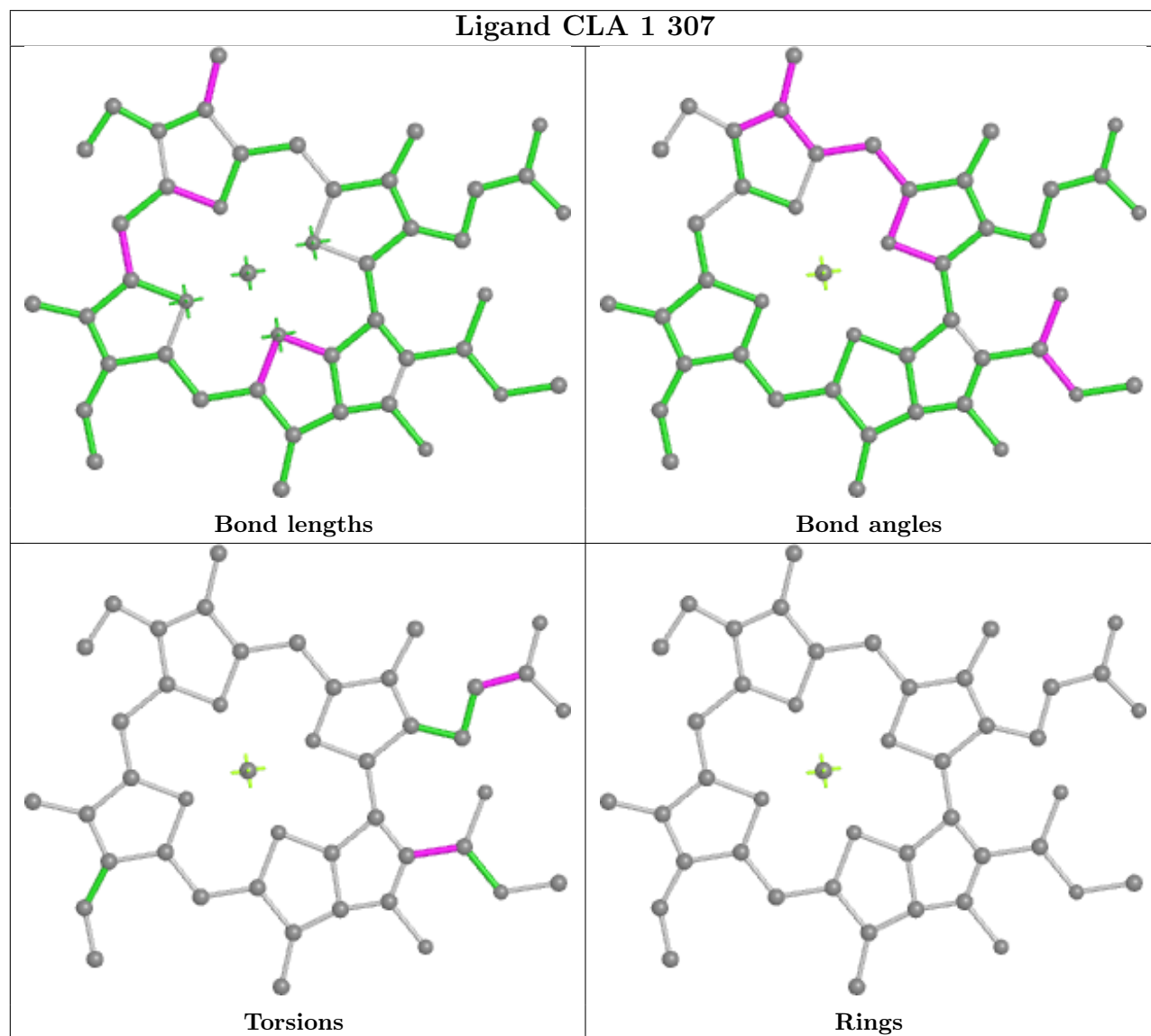


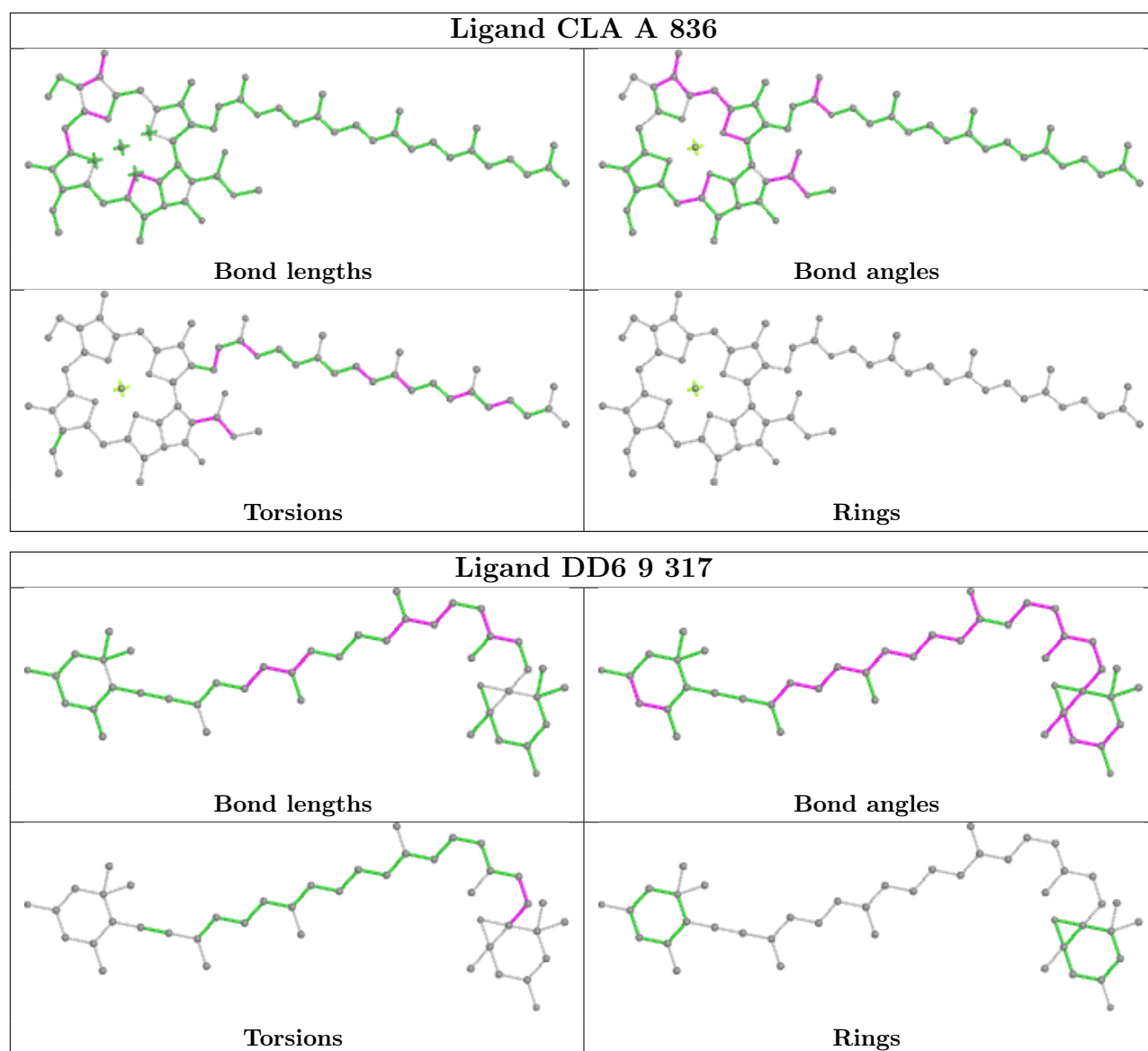
Rings

Ligand A1L1G k 312

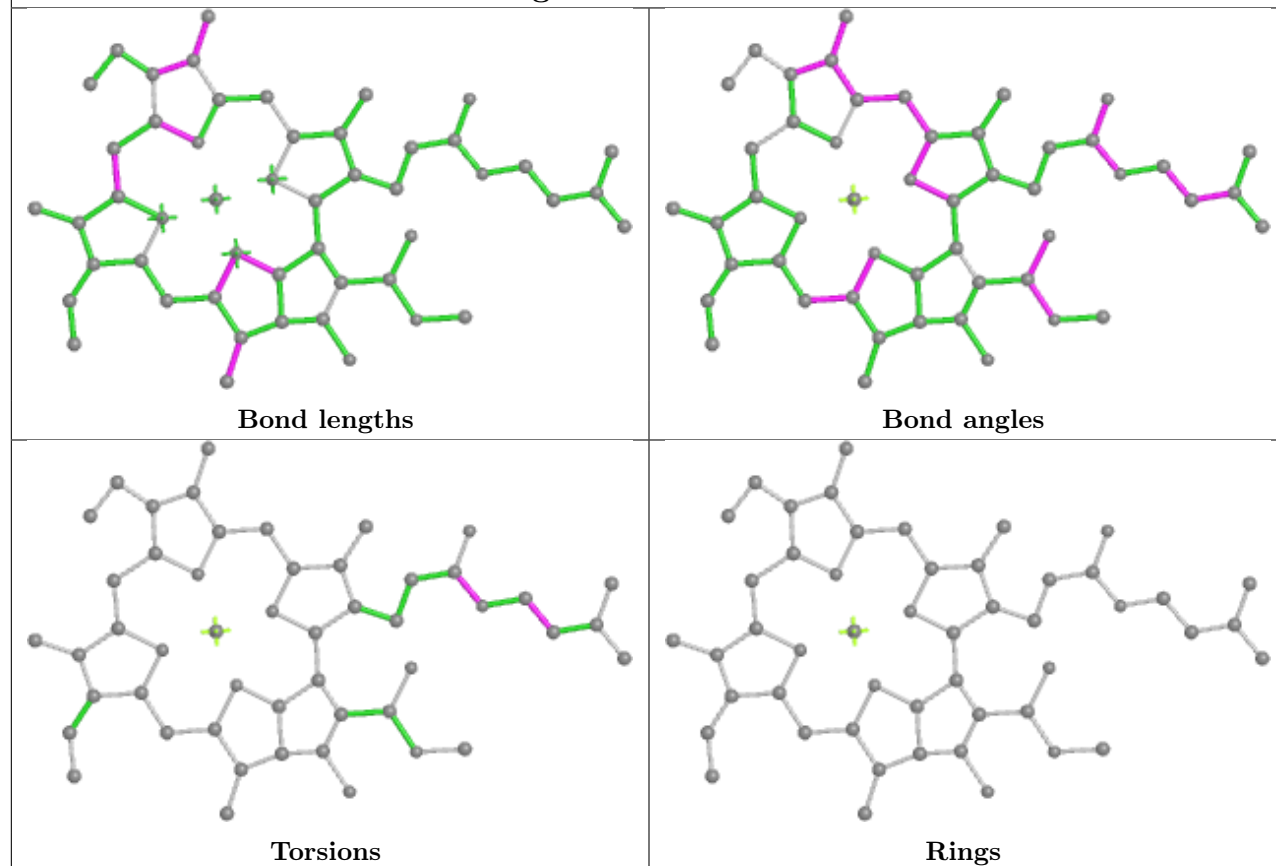


Ligand CLA 1 307

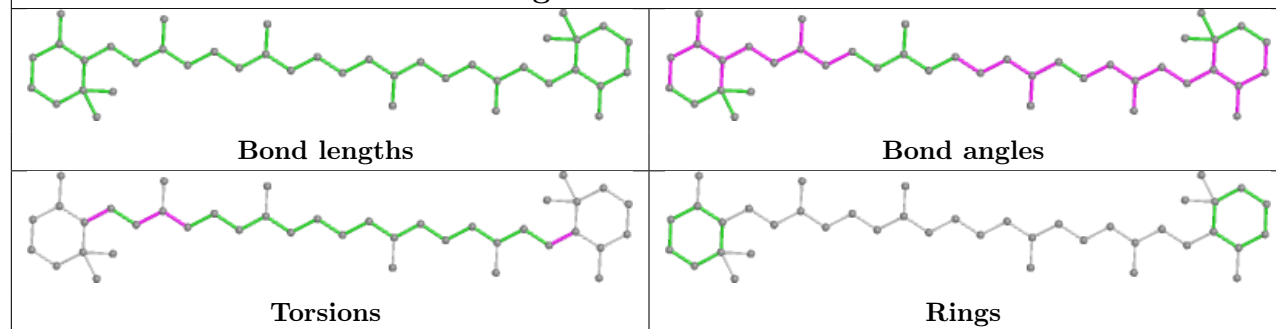




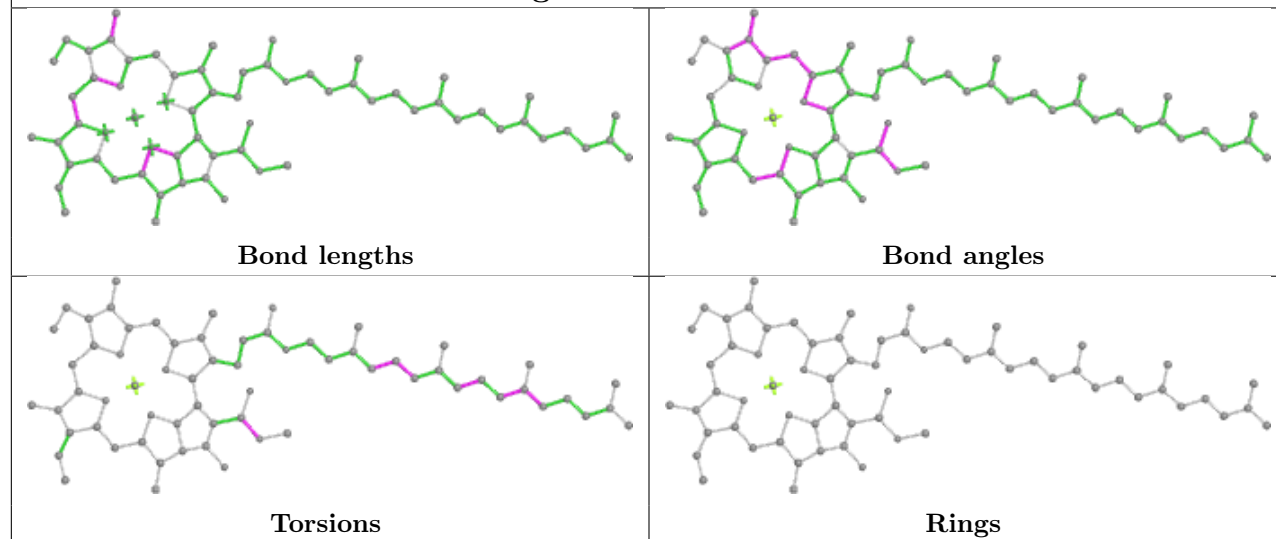
Ligand CLA B 814



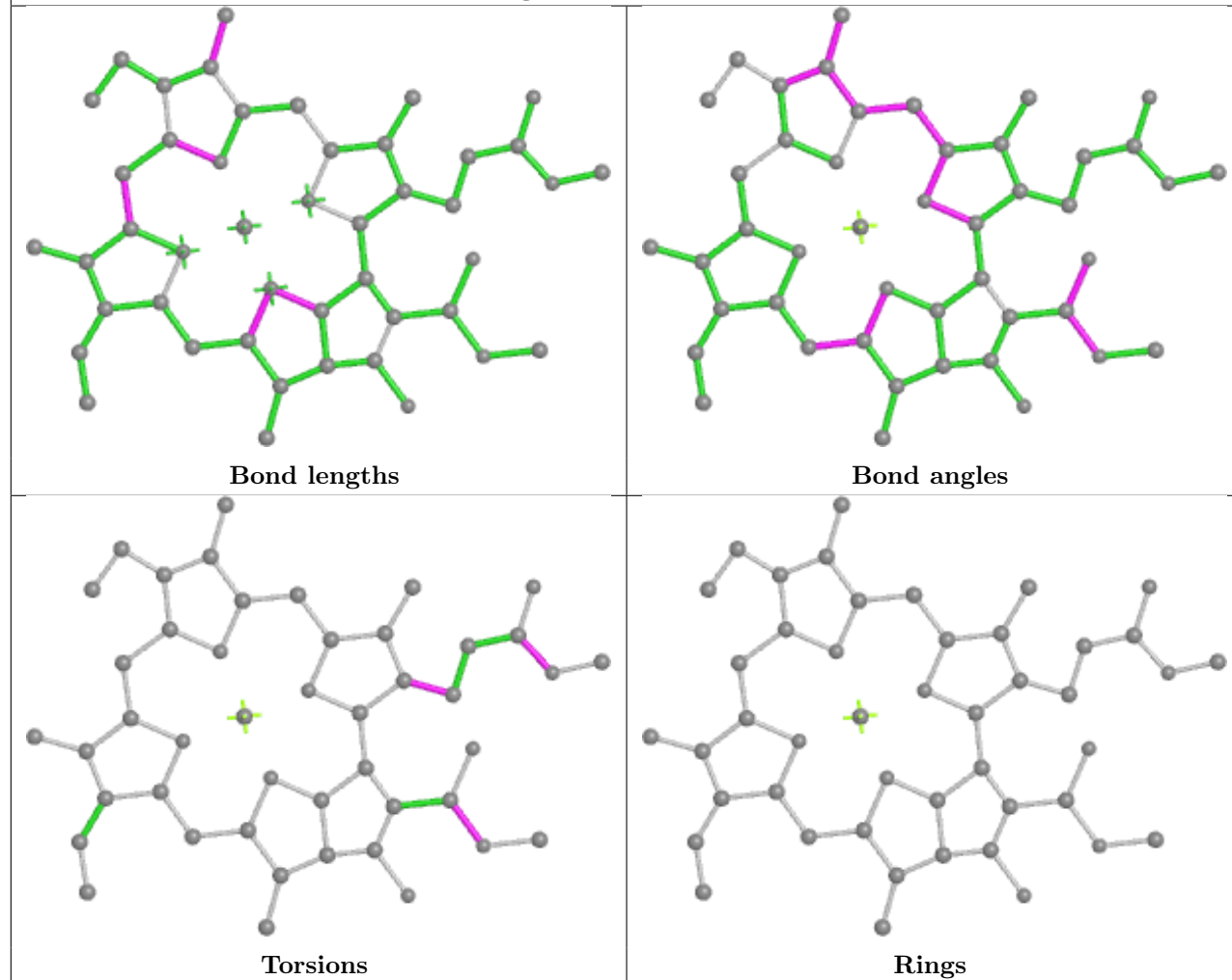
Ligand BCR L 202

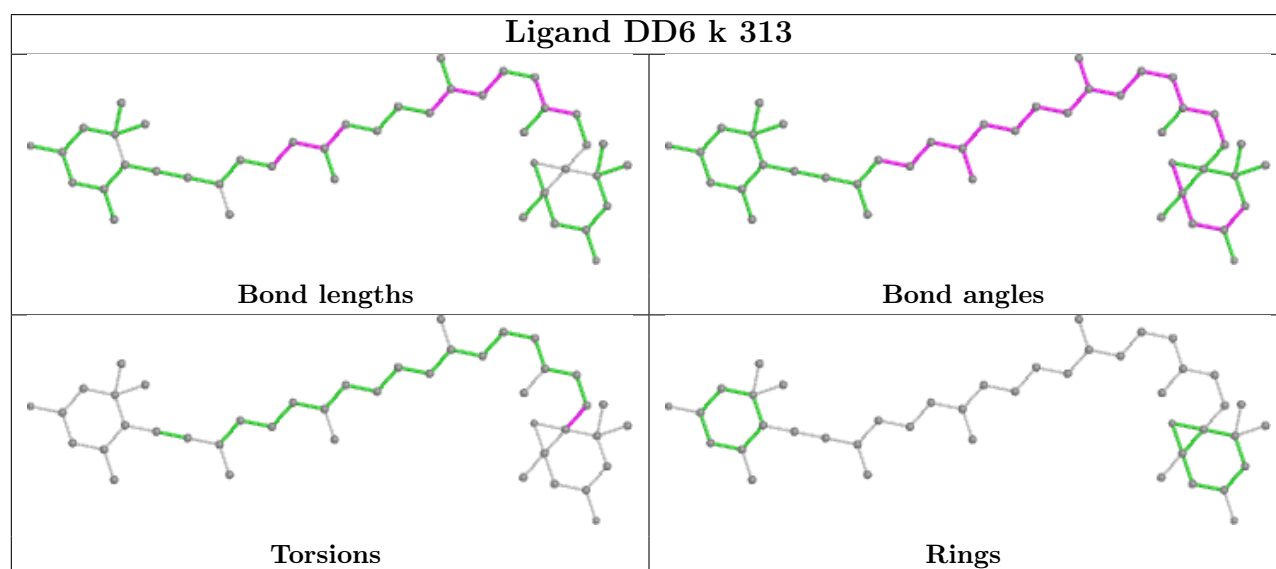
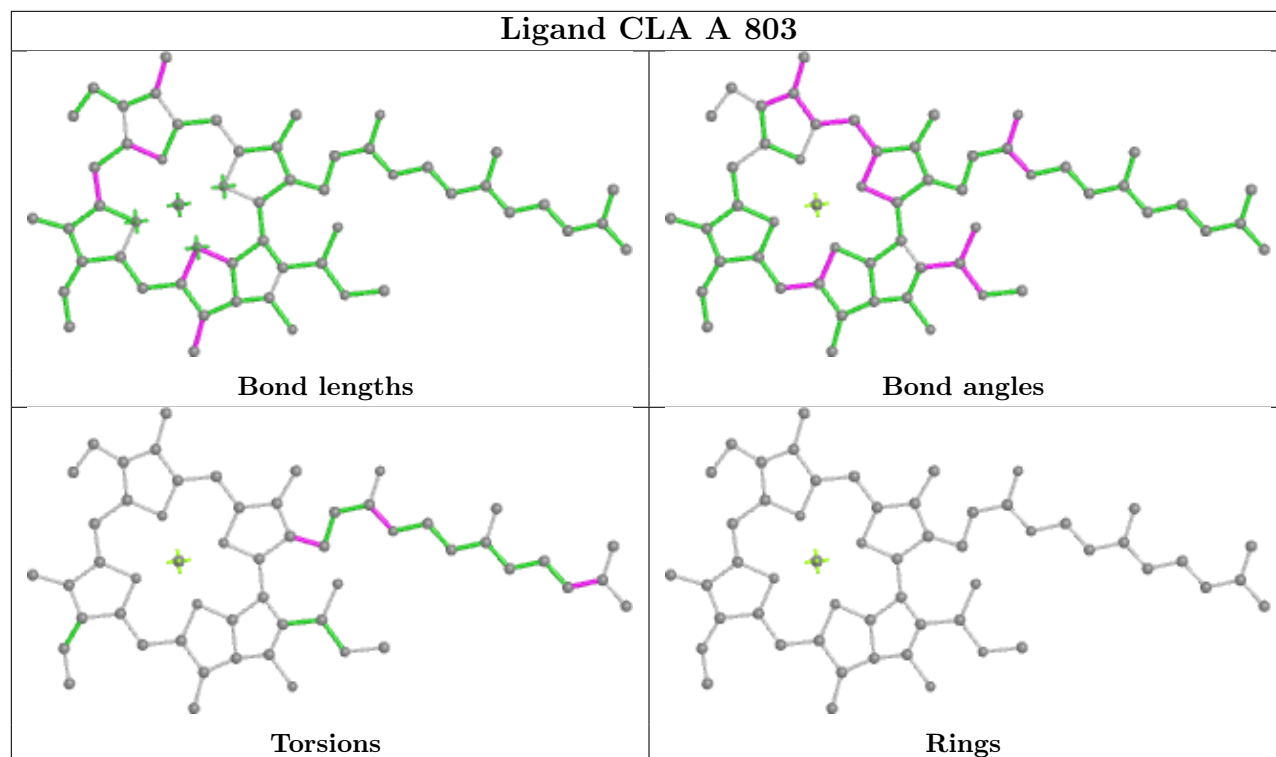
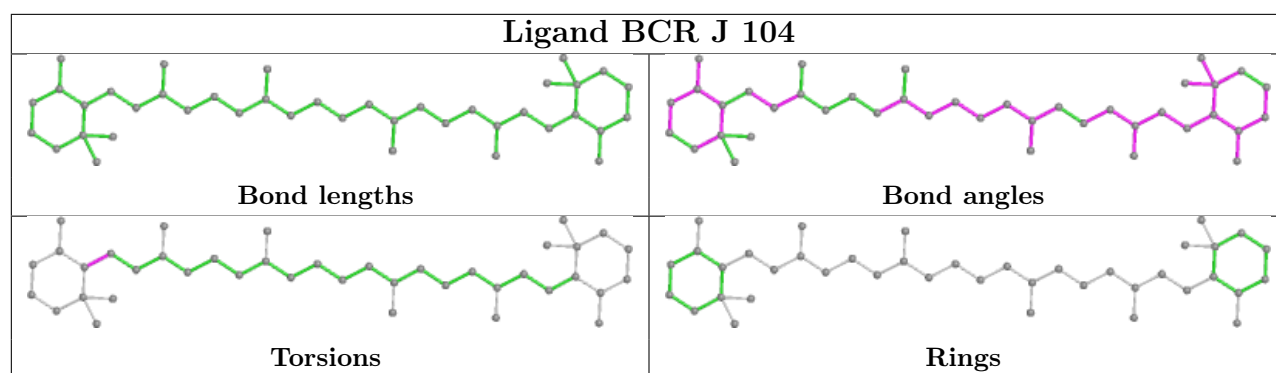


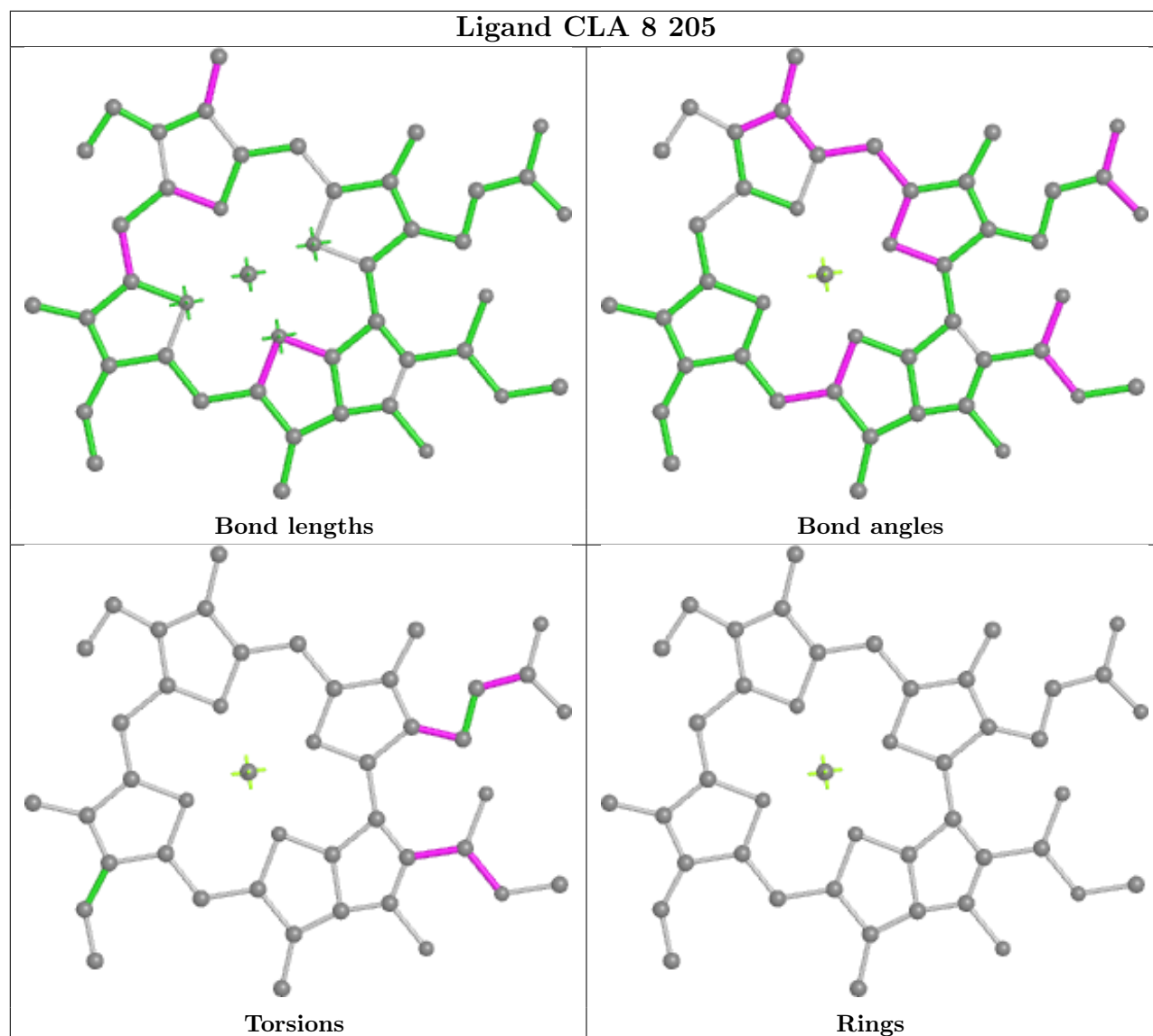
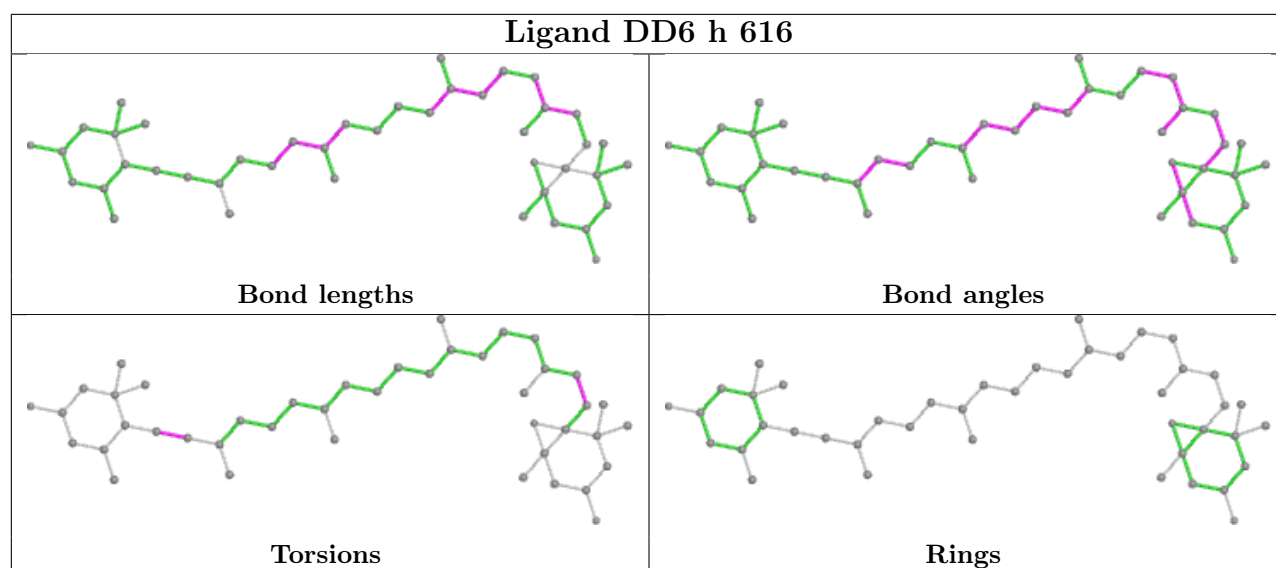
Ligand CLA B 806



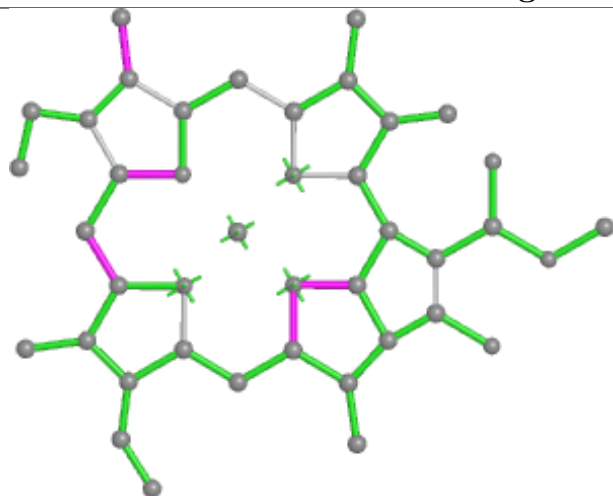
Ligand CLA 4 611



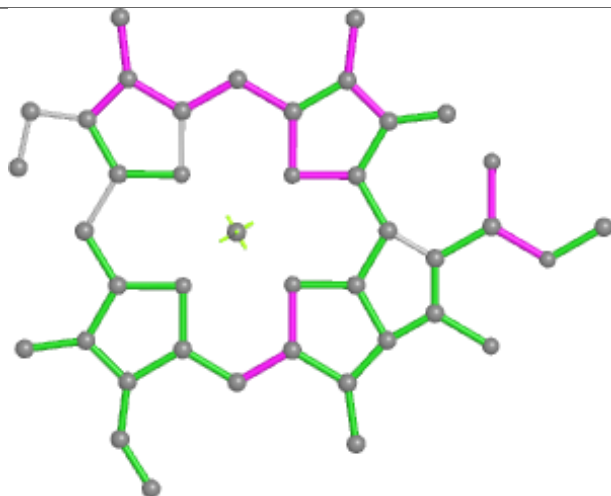




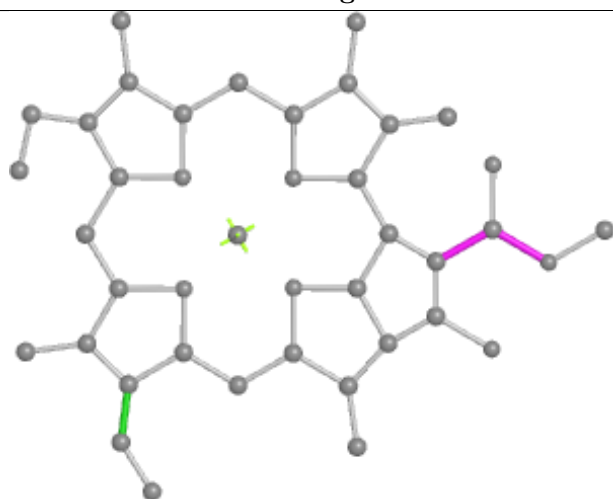
Ligand CLA 8 209



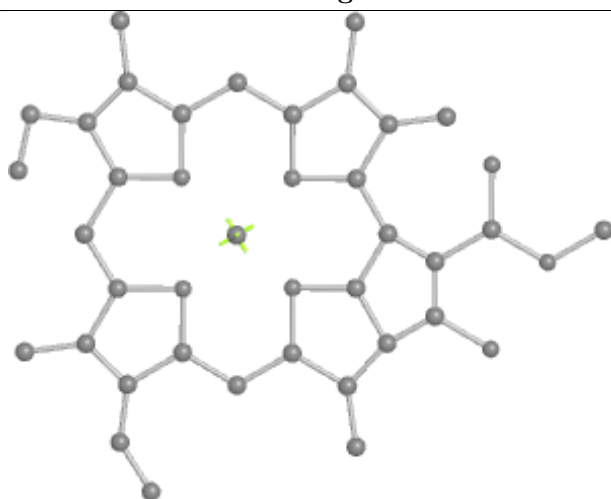
Bond lengths



Bond angles

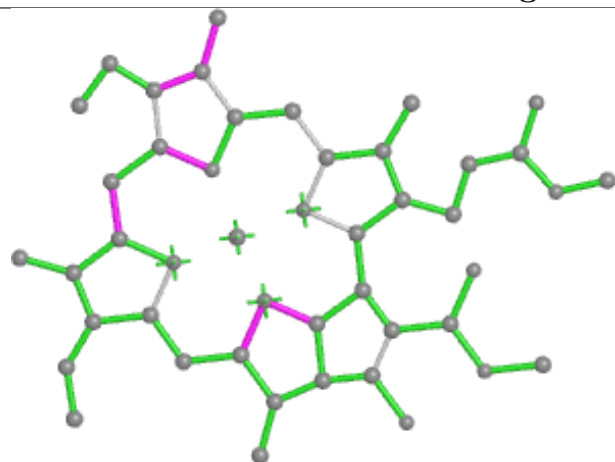


Torsions

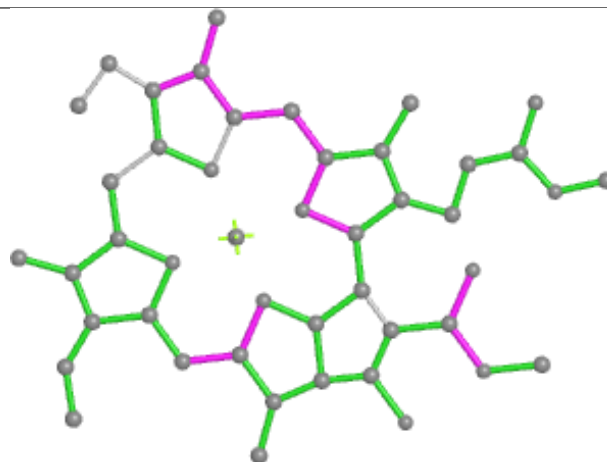


Rings

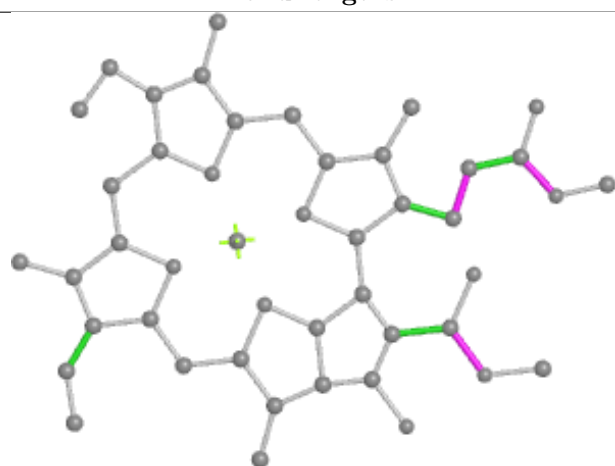
Ligand CLA h 608



Bond lengths



Bond angles

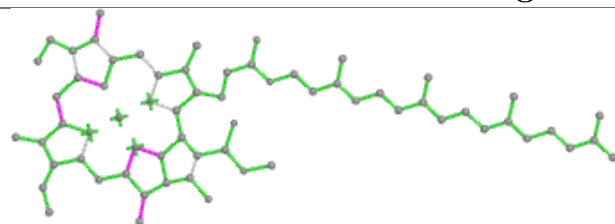


Torsions

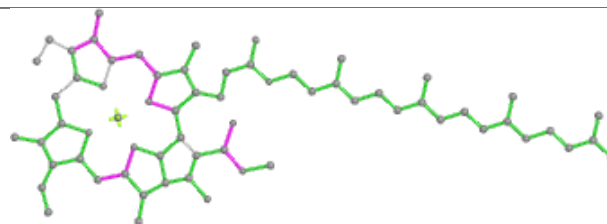


Rings

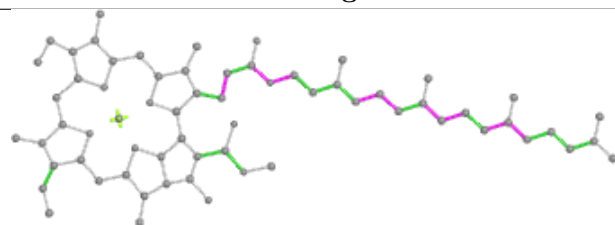
Ligand CLA B 801



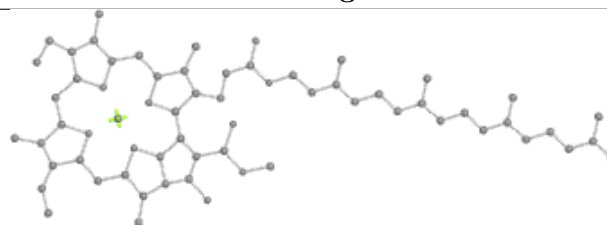
Bond lengths



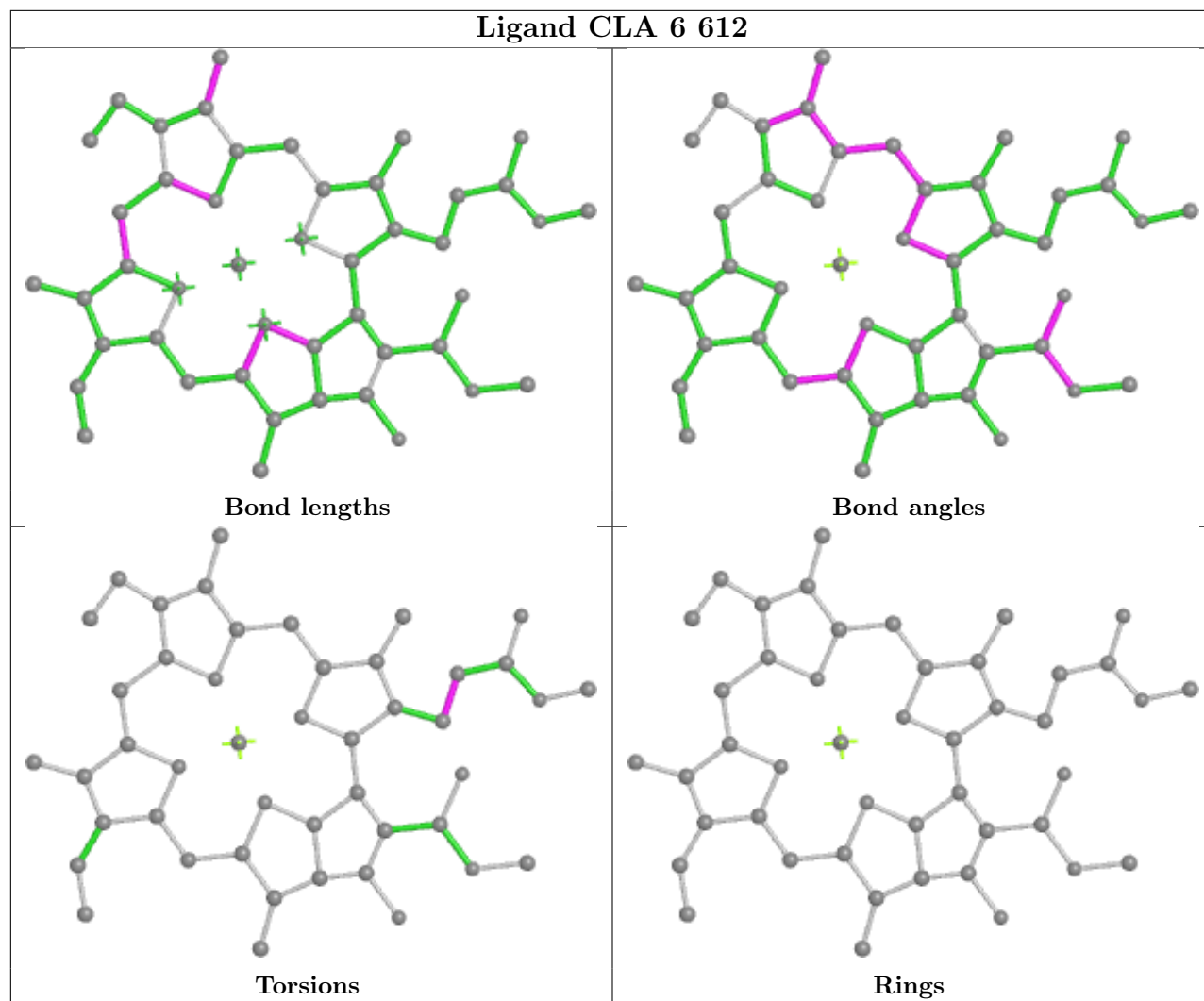
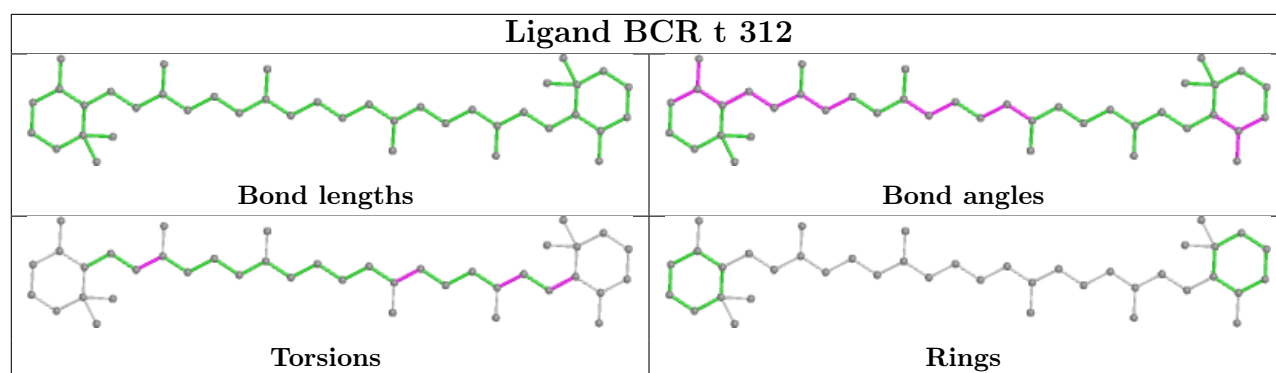
Bond angles

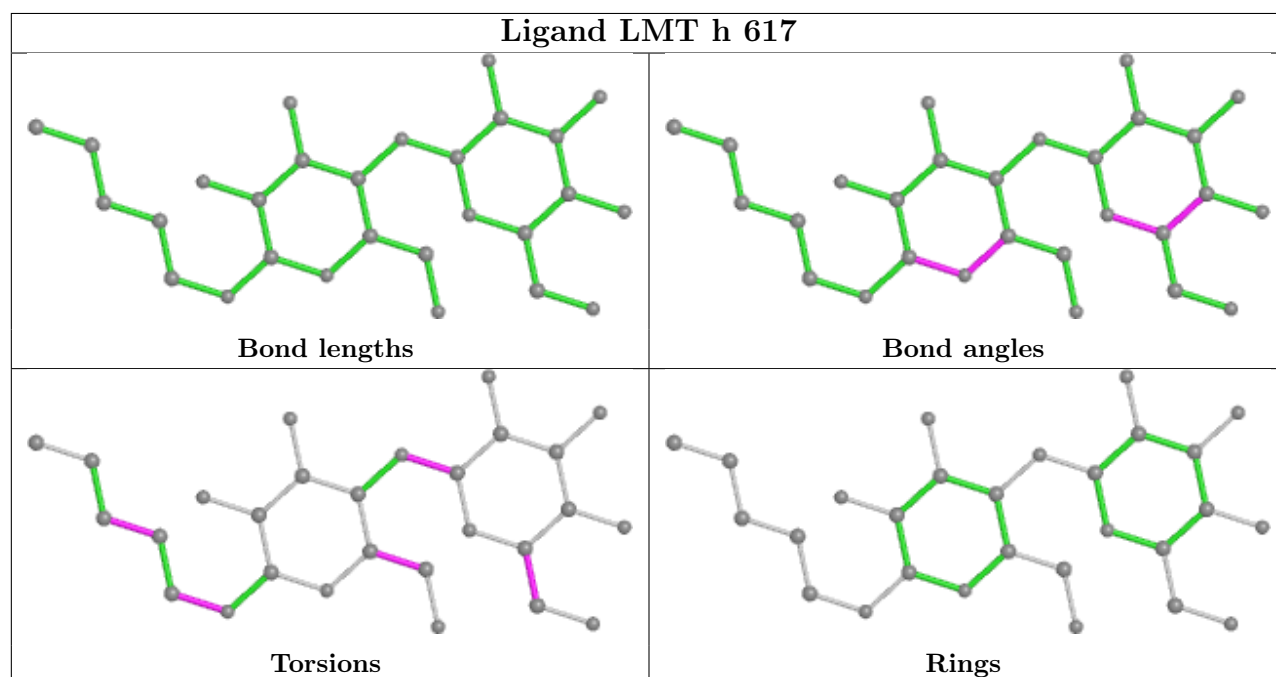
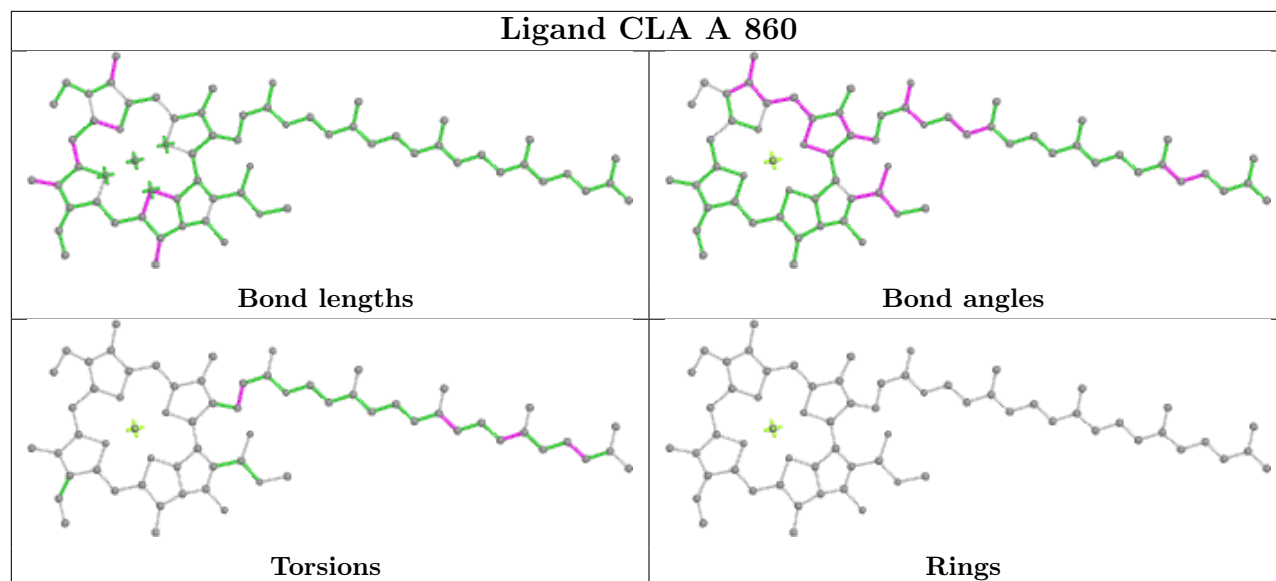
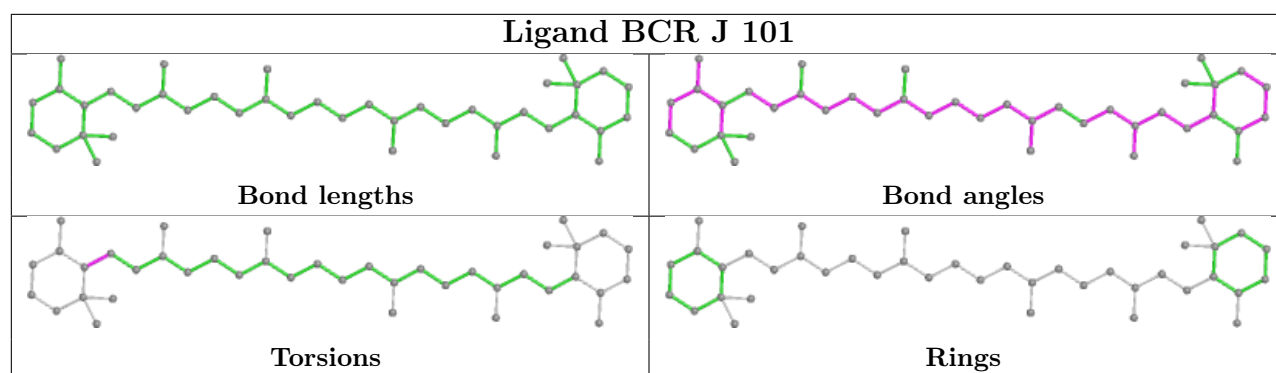


Torsions

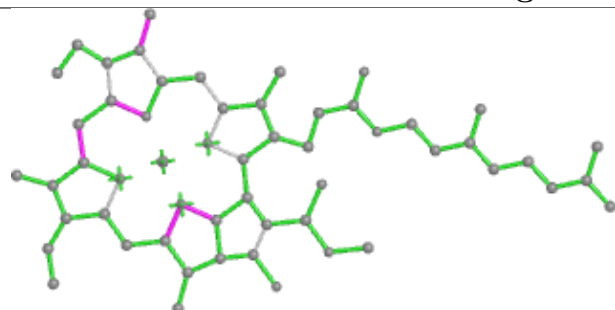


Rings

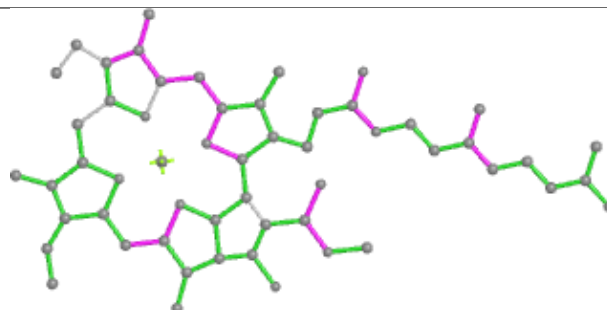




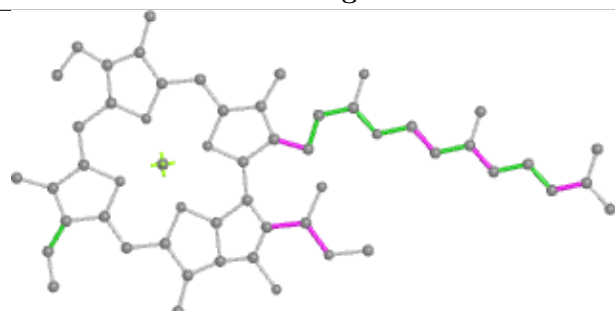
Ligand CLA B 815



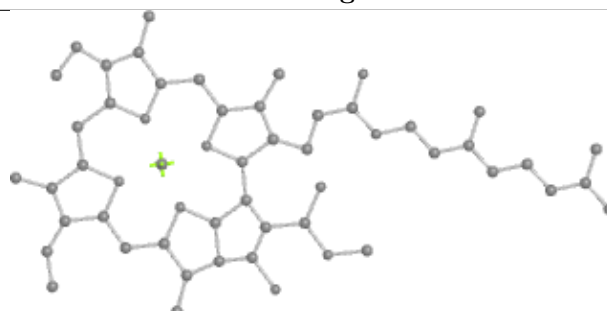
Bond lengths



Bond angles

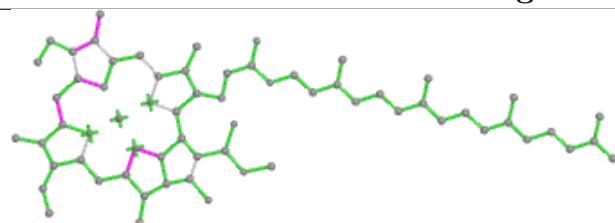


Torsions

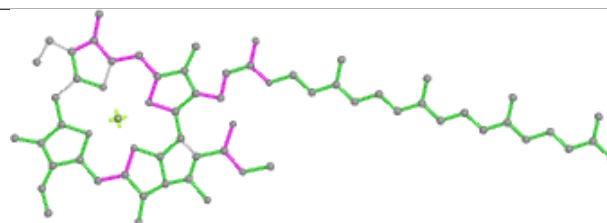


Rings

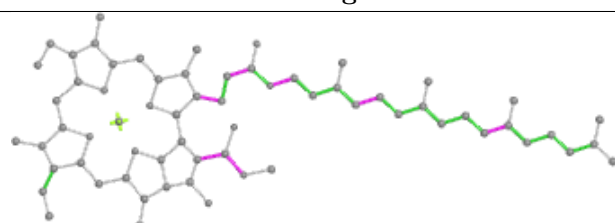
Ligand CLA B 809



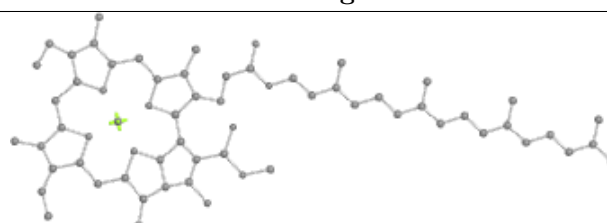
Bond lengths



Bond angles

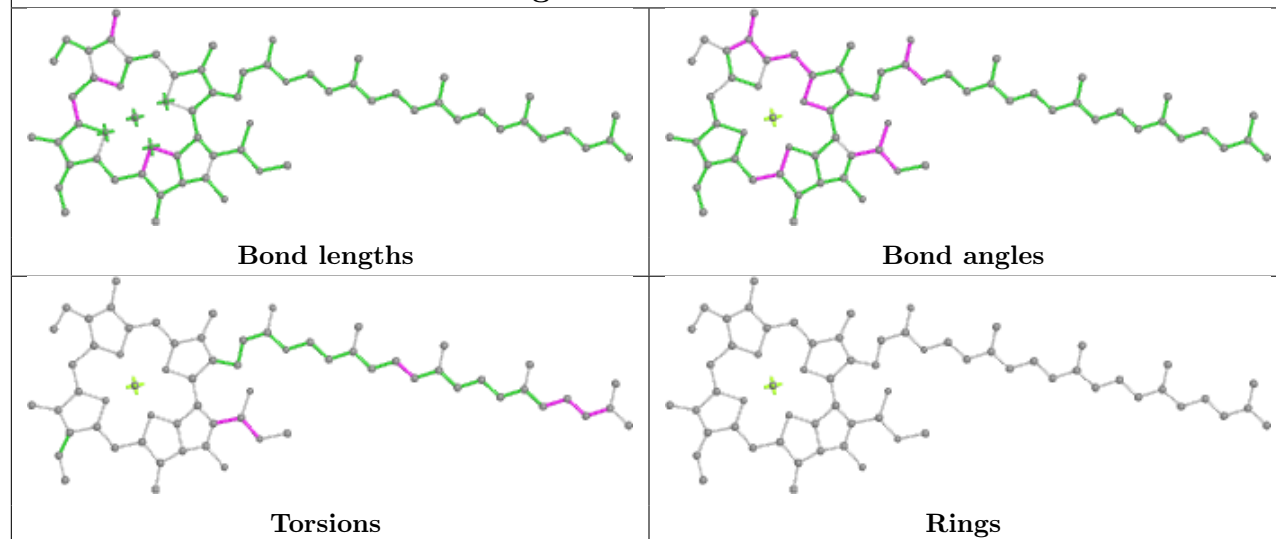


Torsions

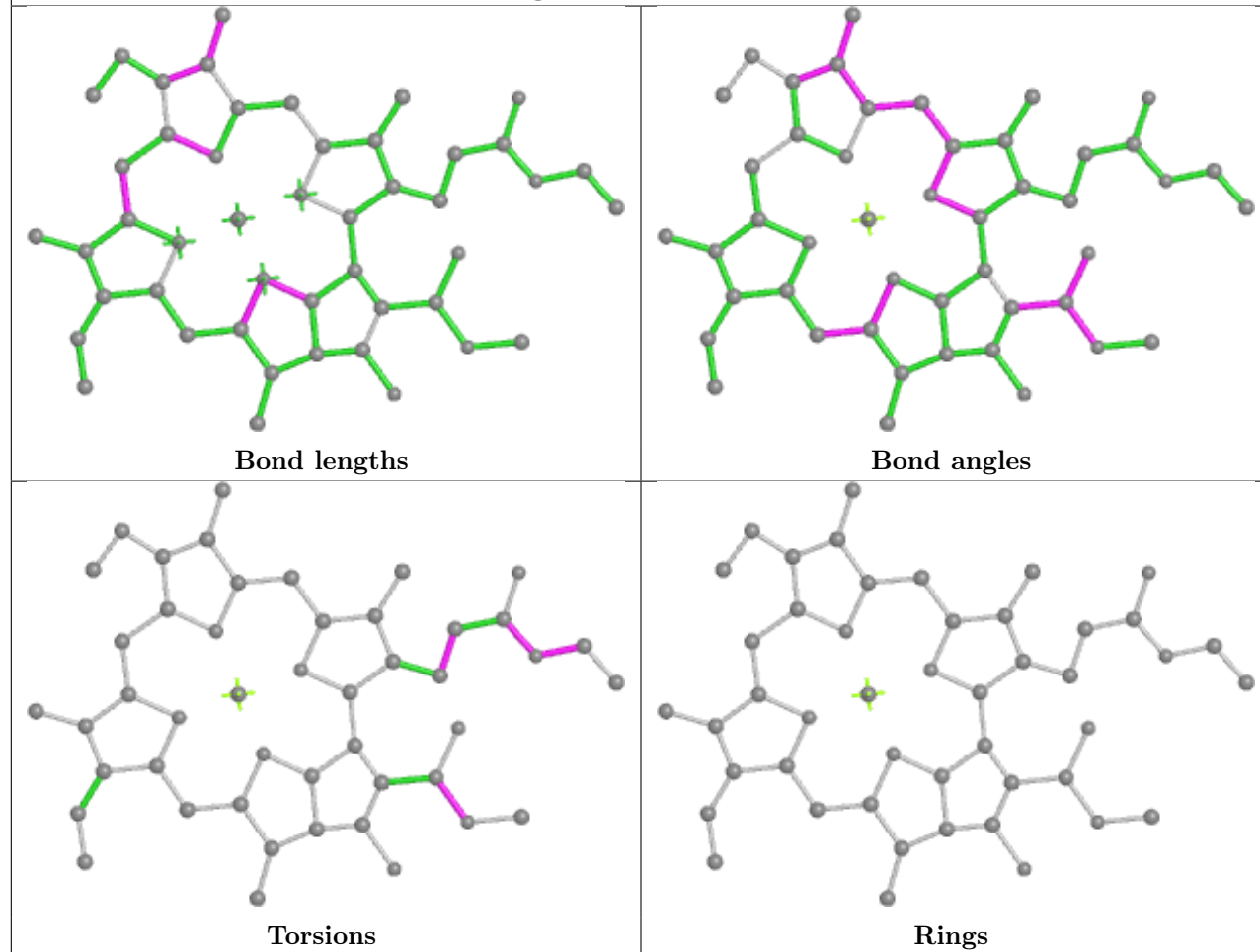


Rings

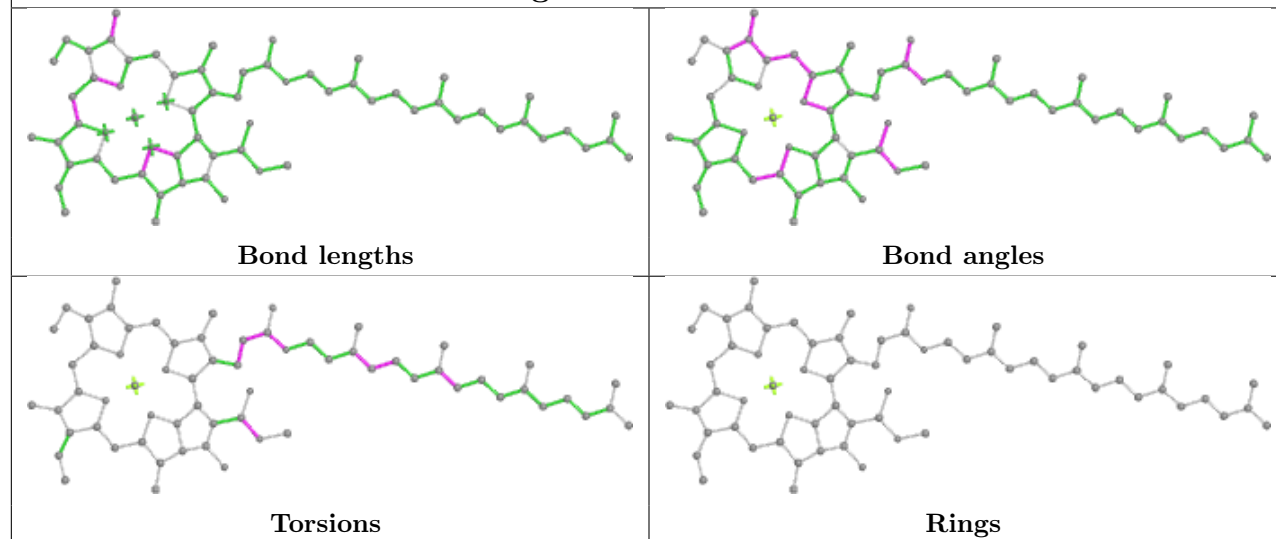
Ligand CLA B 834



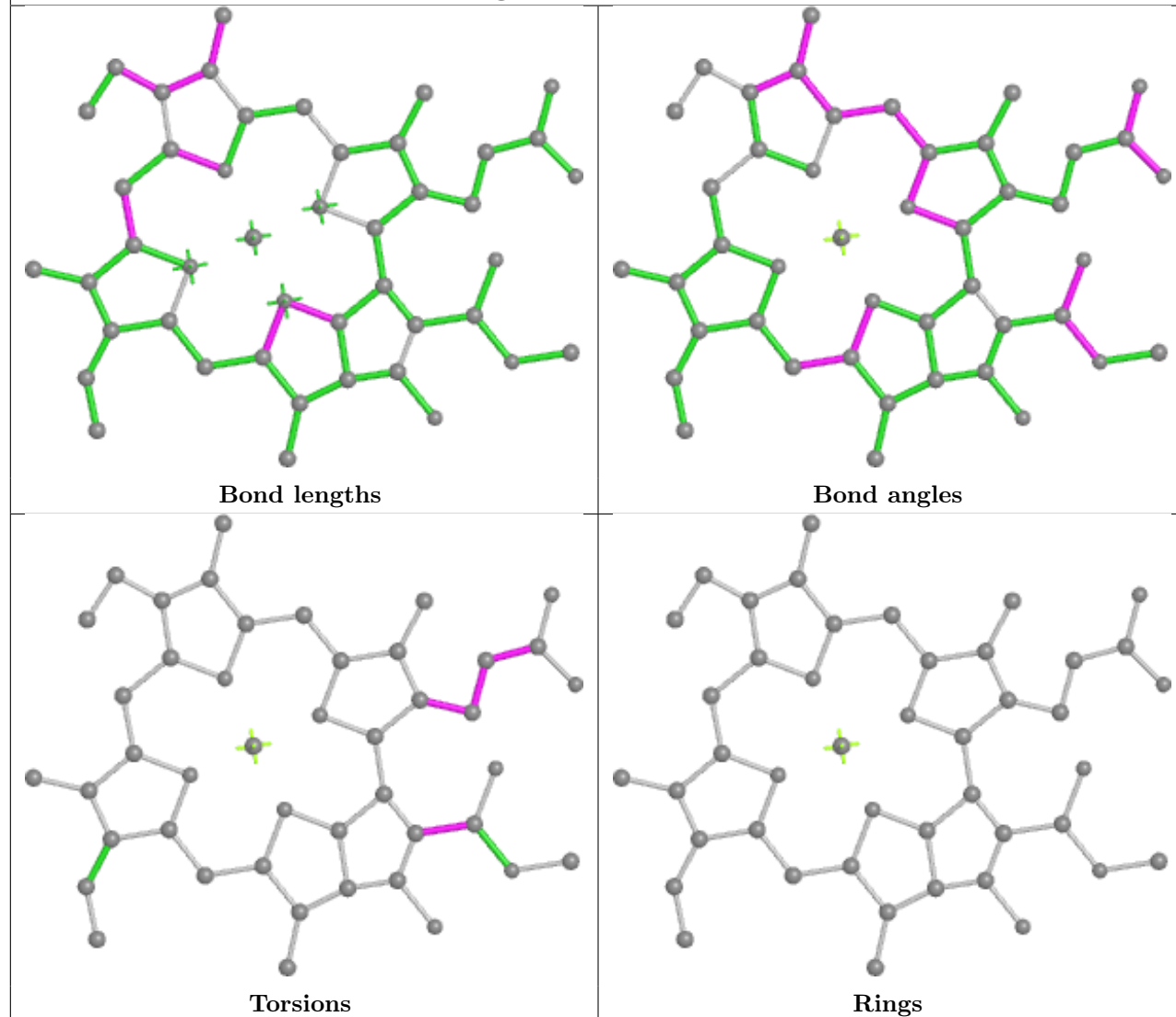
Ligand CLA 6 602

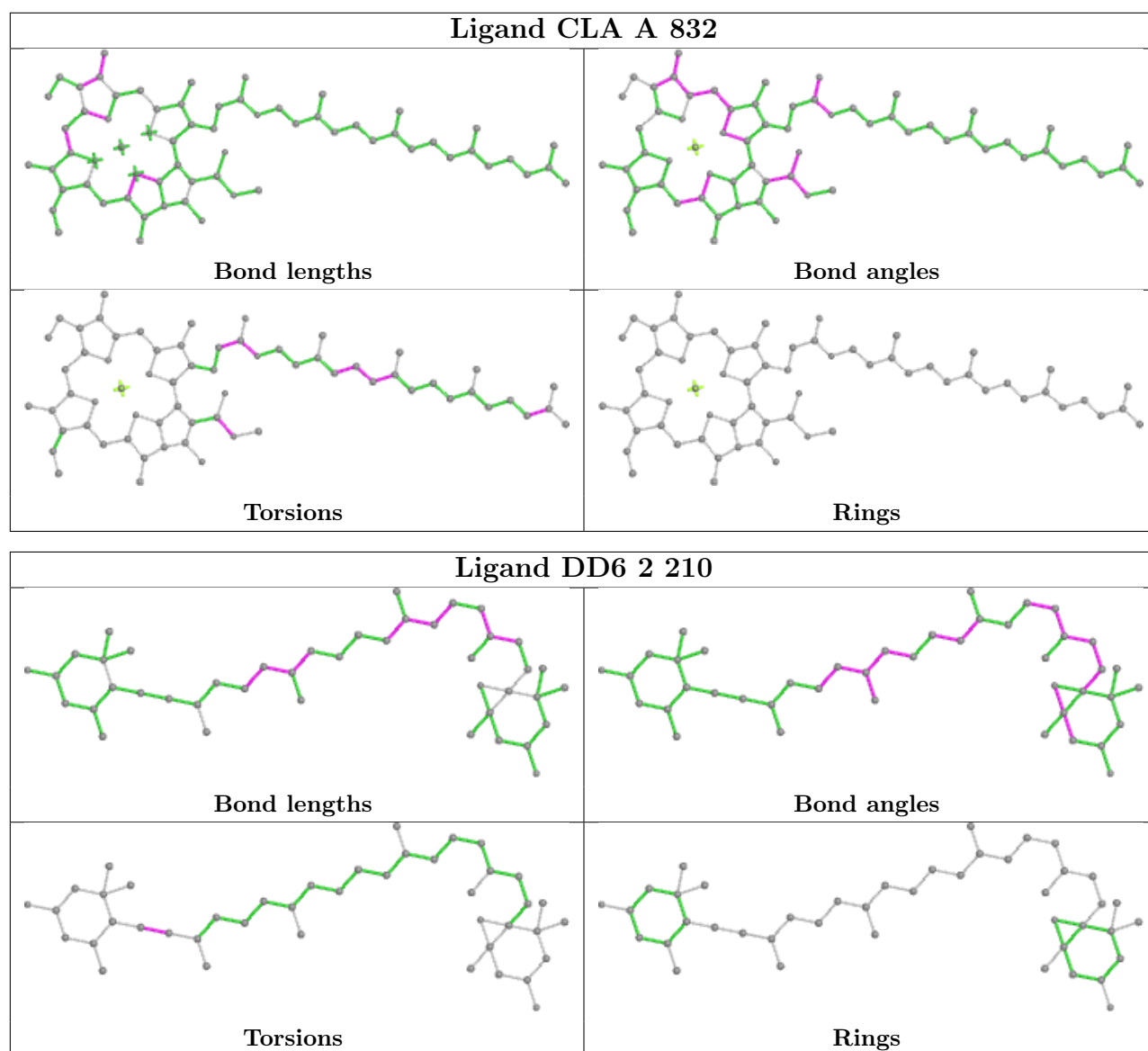


Ligand CLA A 820

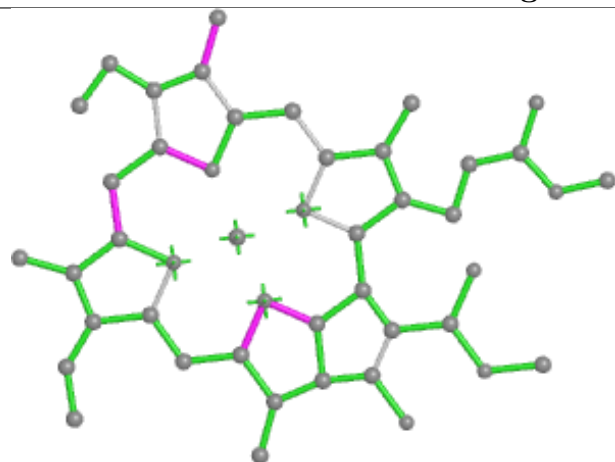


Ligand CLA h 612

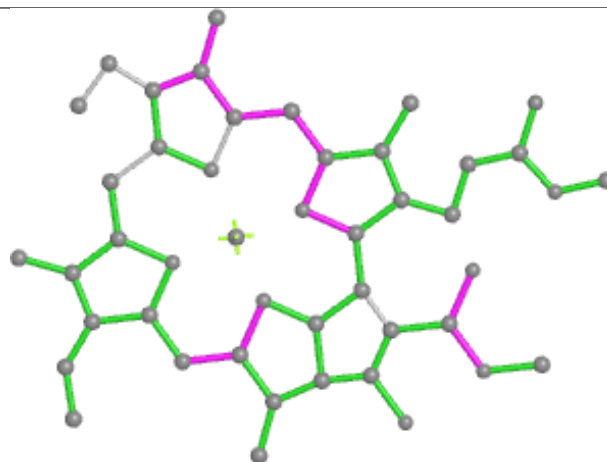




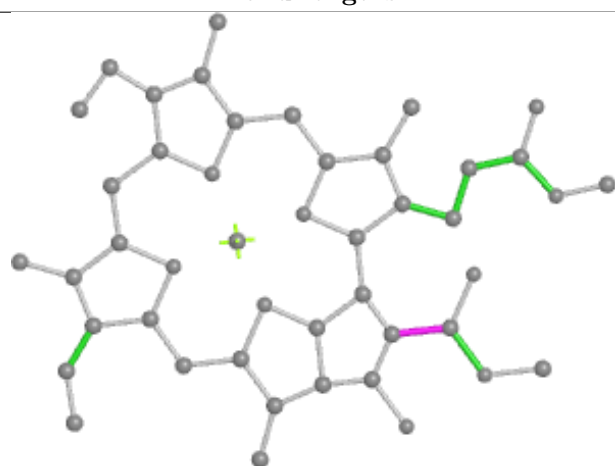
Ligand CLA 5 604



Bond lengths



Bond angles

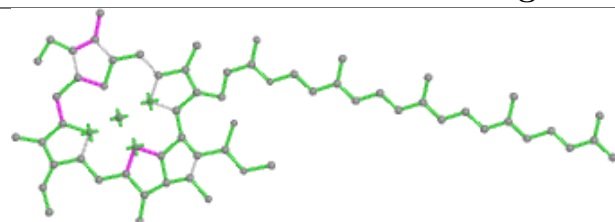


Torsions

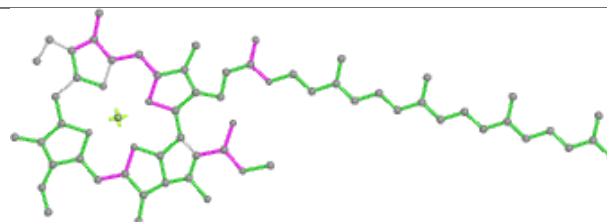


Rings

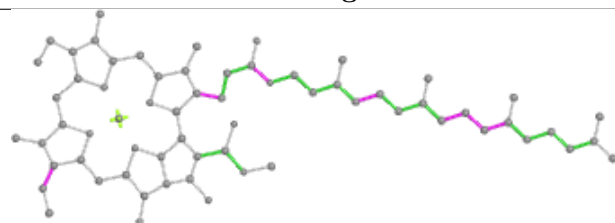
Ligand CLA L 204



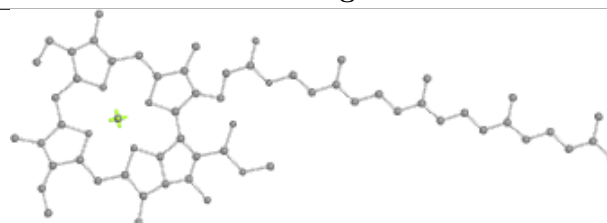
Bond lengths



Bond angles

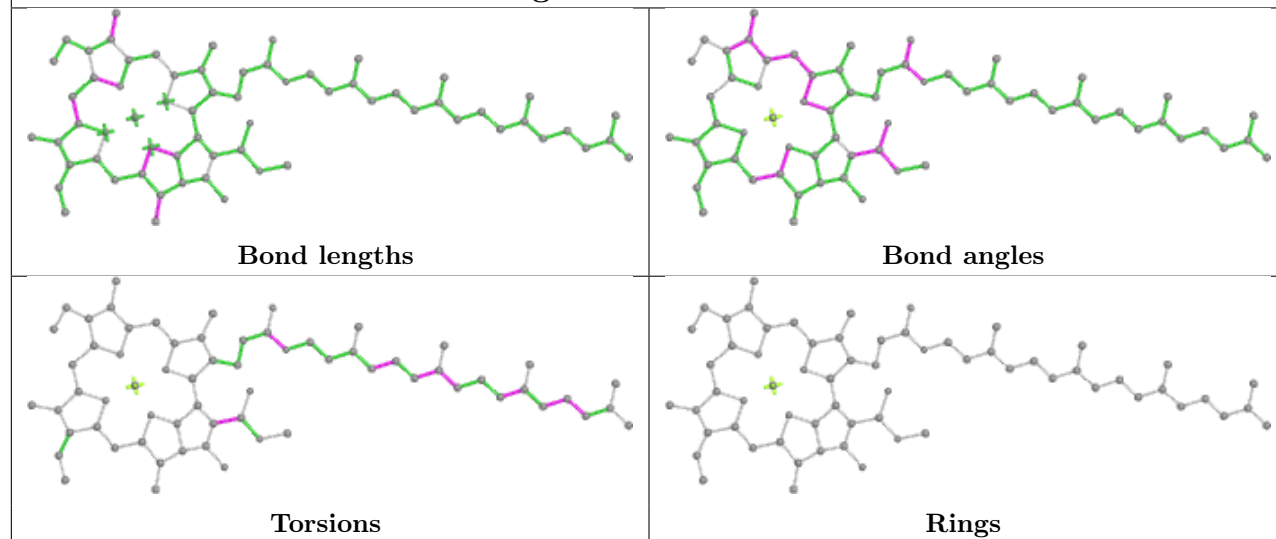


Torsions

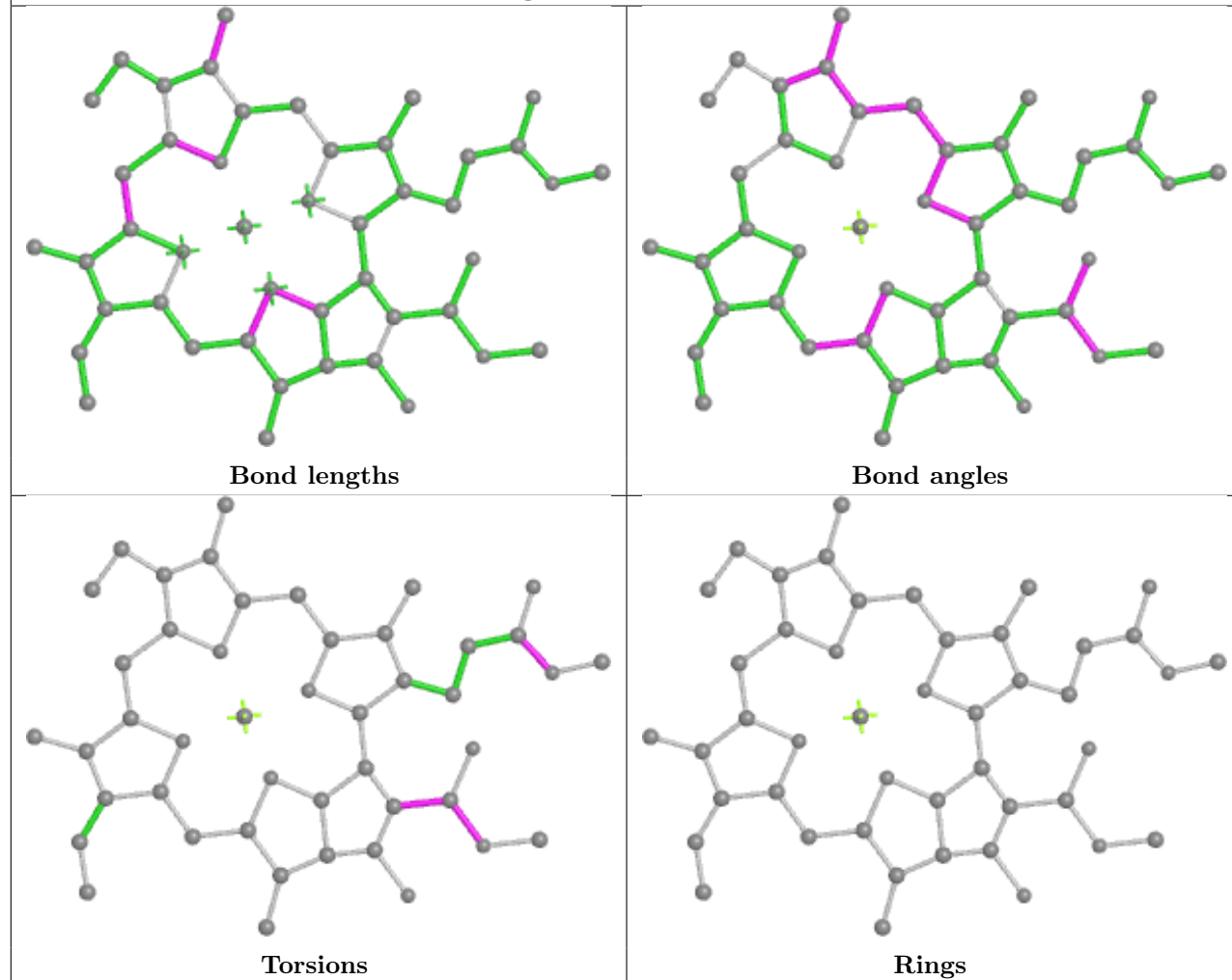


Rings

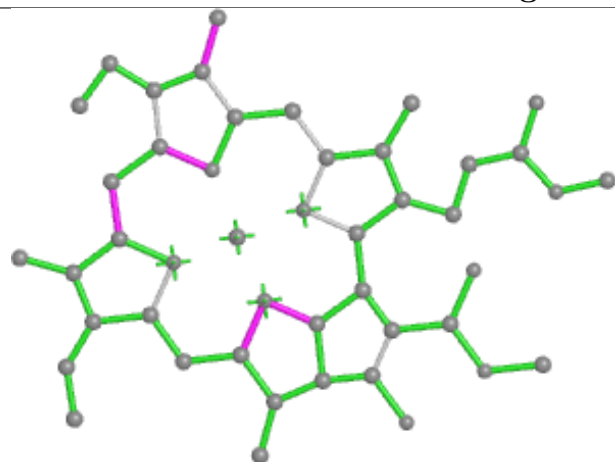
Ligand CLA B 827



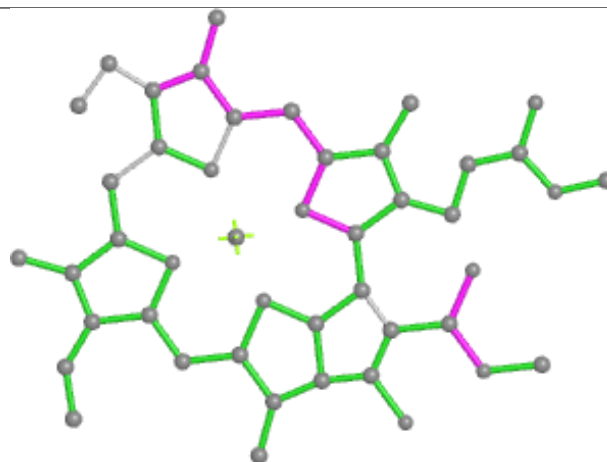
Ligand CLA t 305



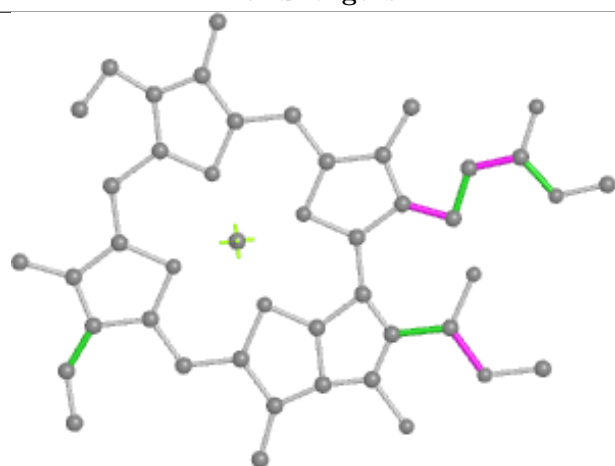
Ligand CLA k 305



Bond lengths



Bond angles

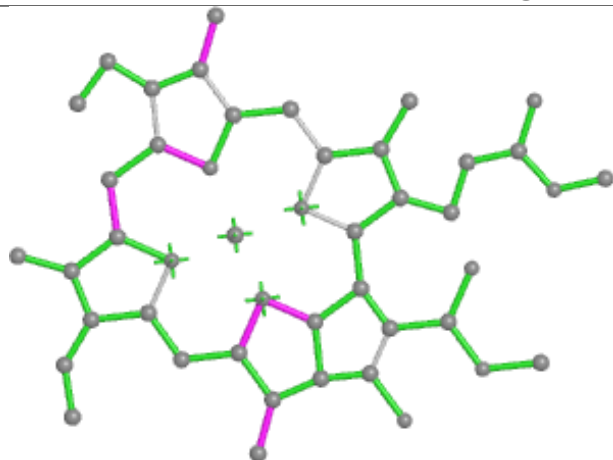


Torsions

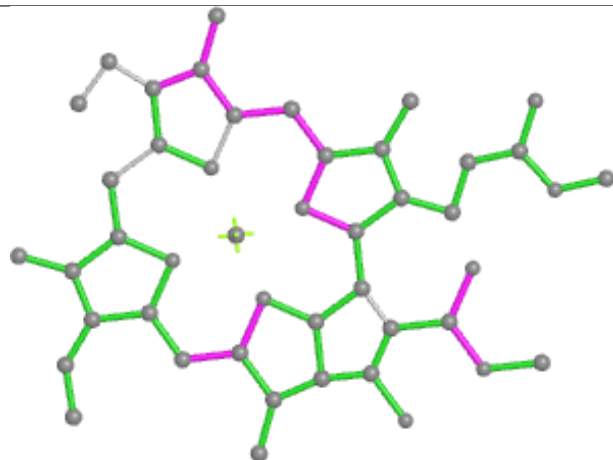


Rings

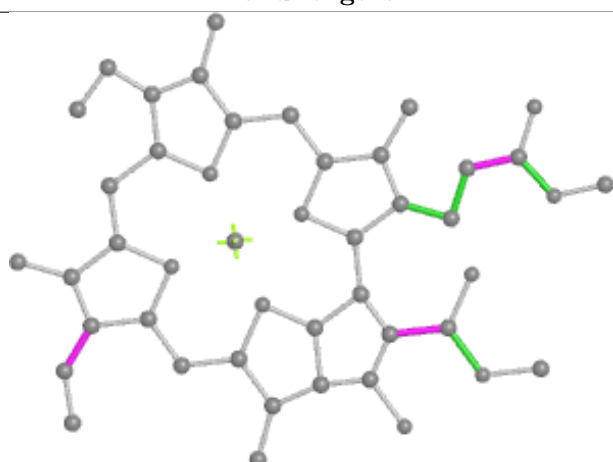
Ligand CLA h 606



Bond lengths



Bond angles

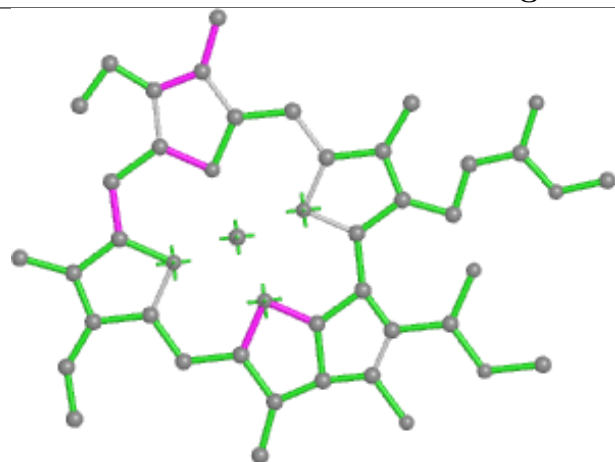


Torsions

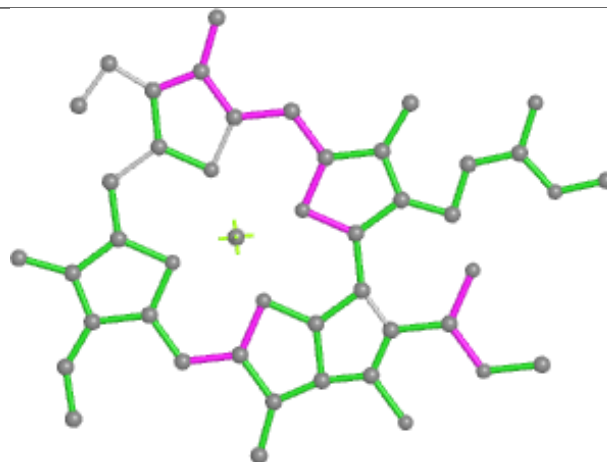


Rings

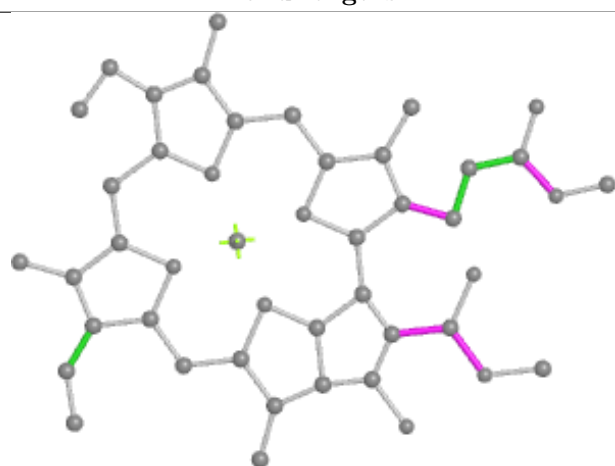
Ligand CLA 7 611



Bond lengths



Bond angles

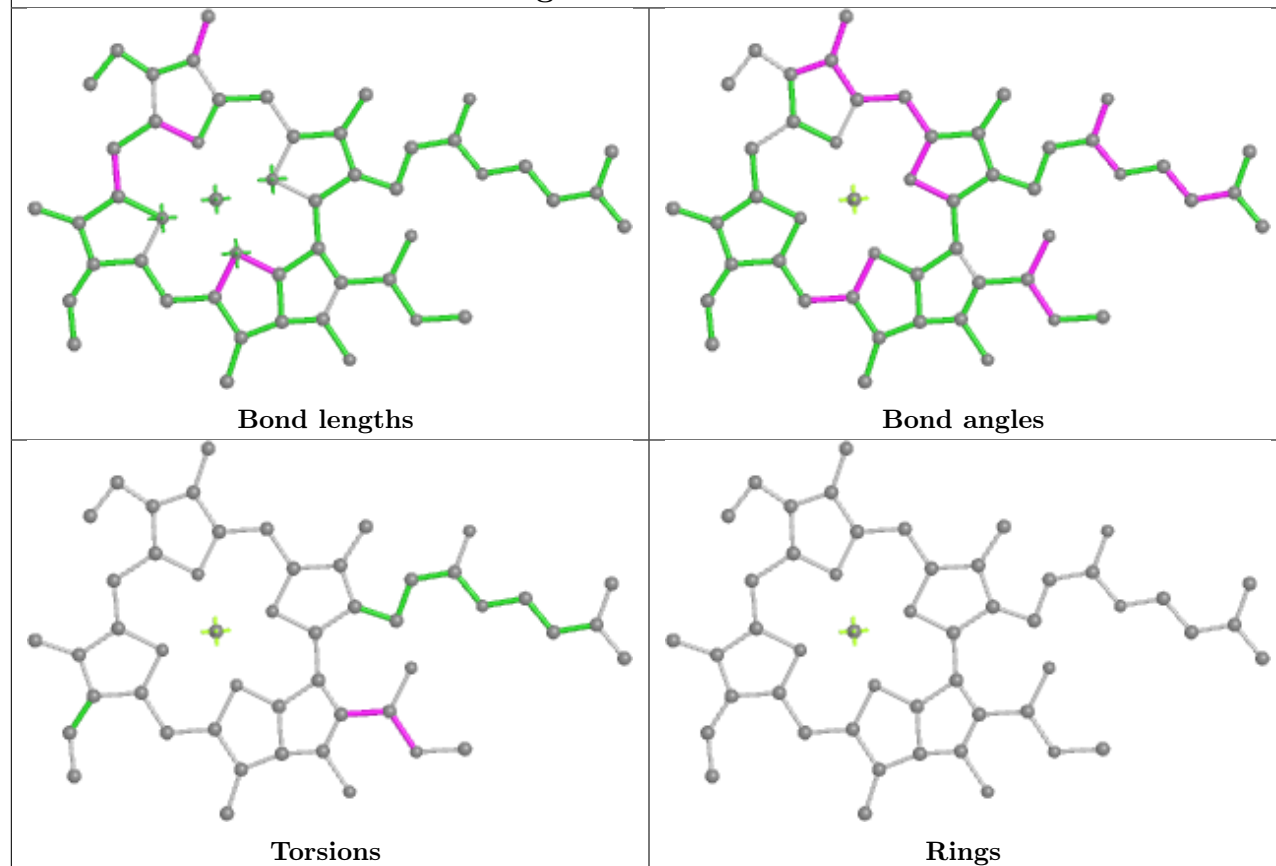


Torsions

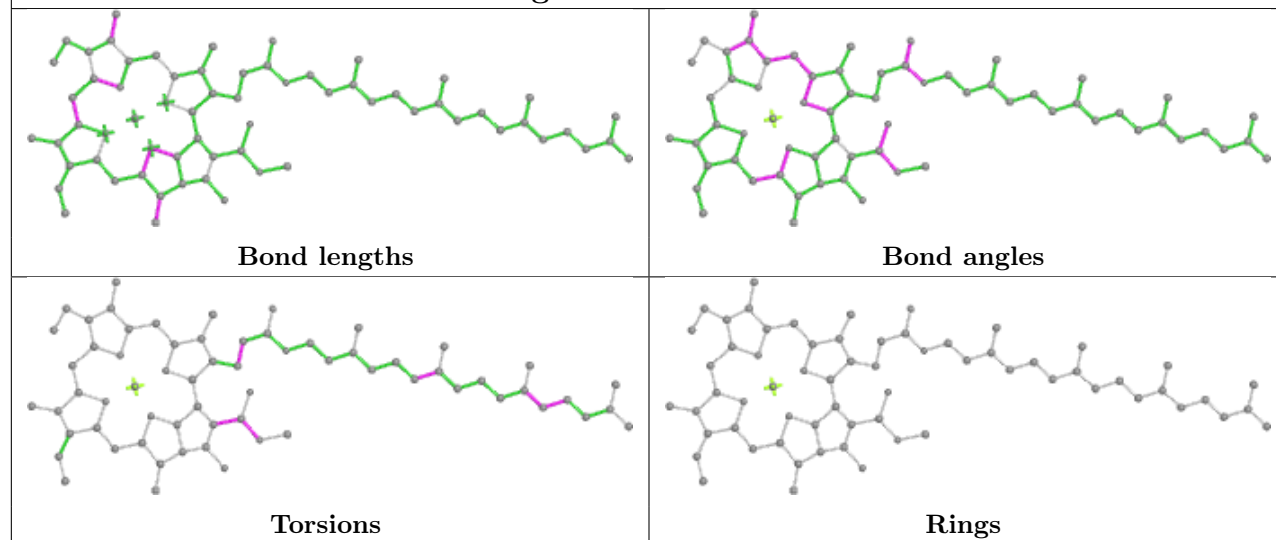


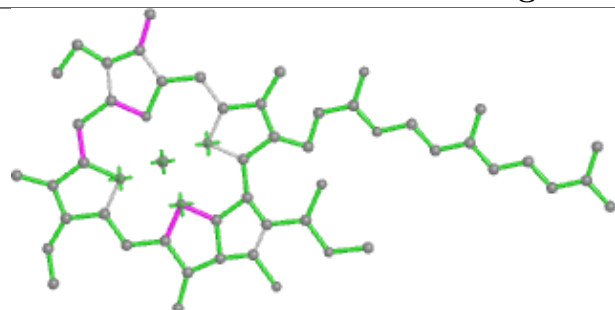
Rings

Ligand CLA 2 203

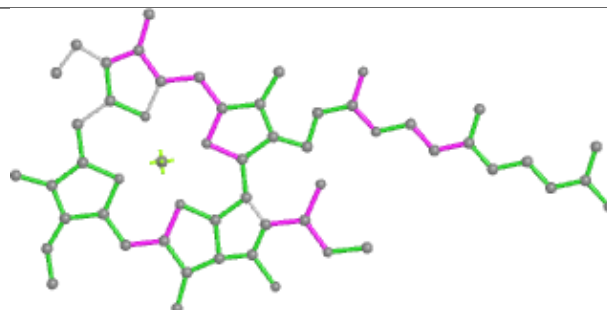


Ligand CLA A 838

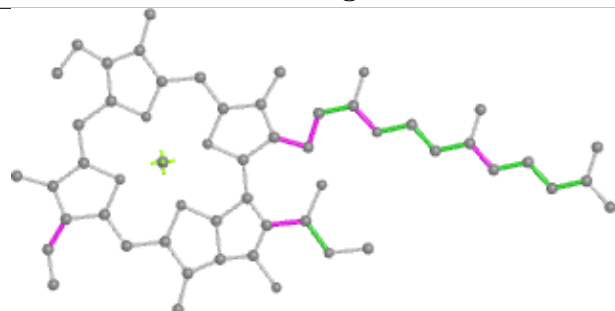


Ligand CLA L 203

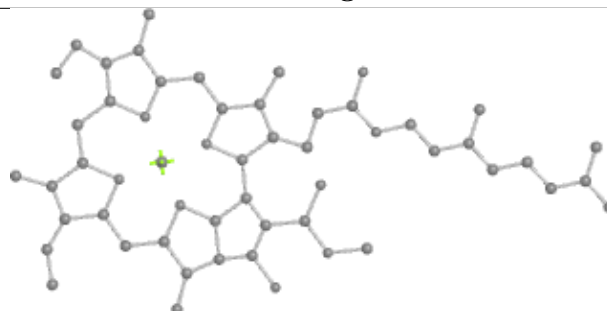
Bond lengths



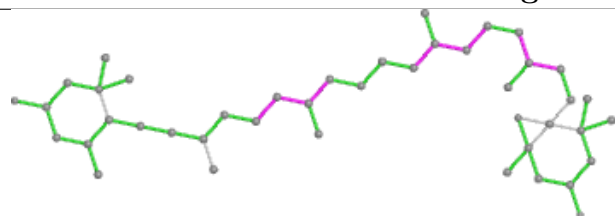
Bond angles



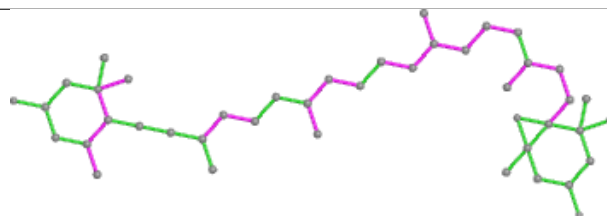
Torsions



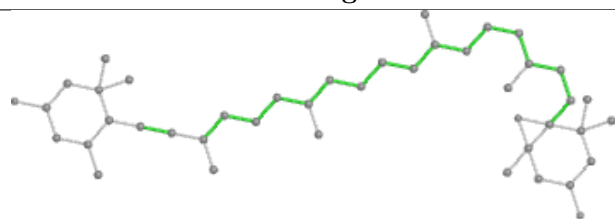
Rings

Ligand DD6 1 311

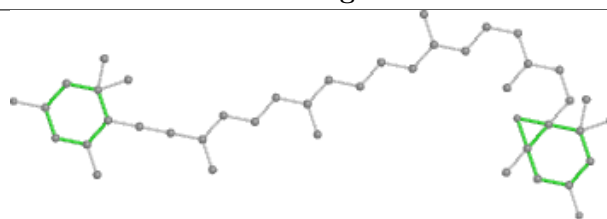
Bond lengths



Bond angles

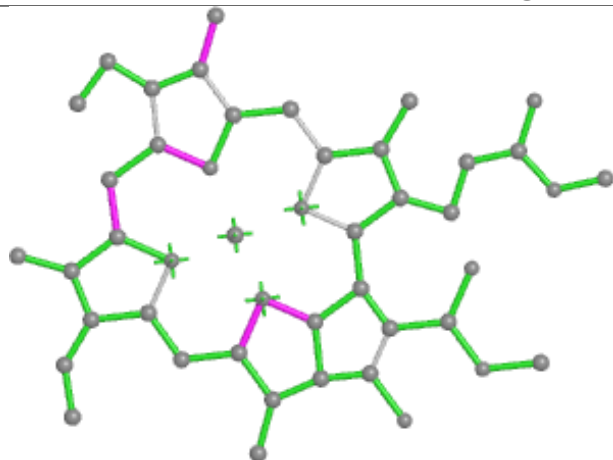


Torsions

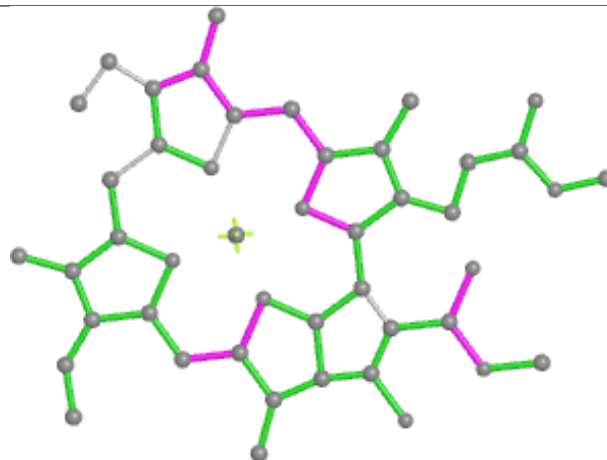


Rings

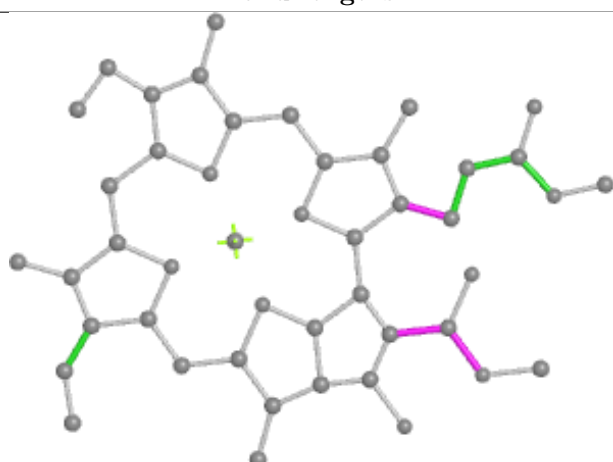
Ligand CLA 1 303



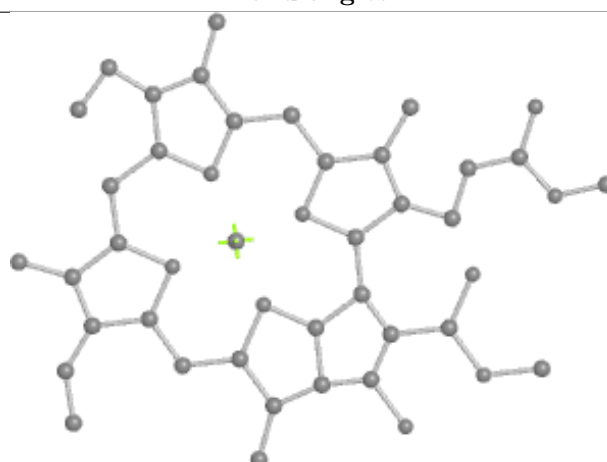
Bond lengths



Bond angles

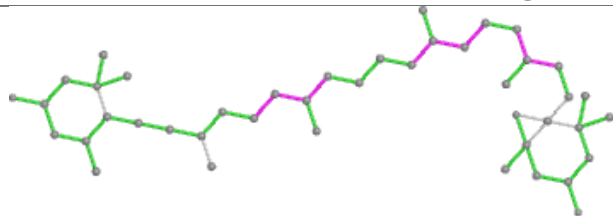


Torsions

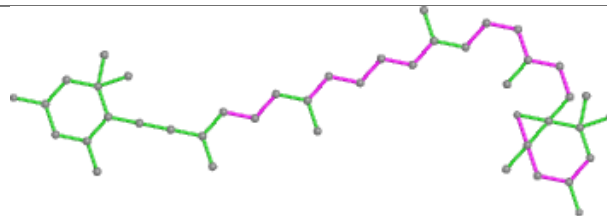


Rings

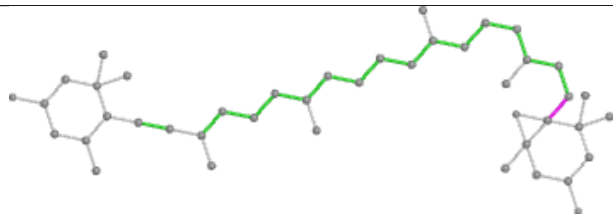
Ligand DD6 3 312



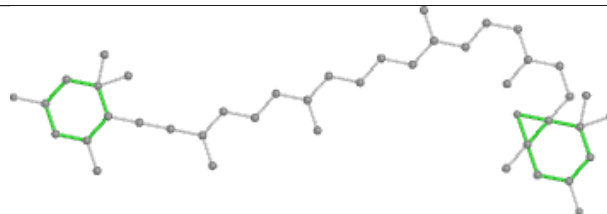
Bond lengths



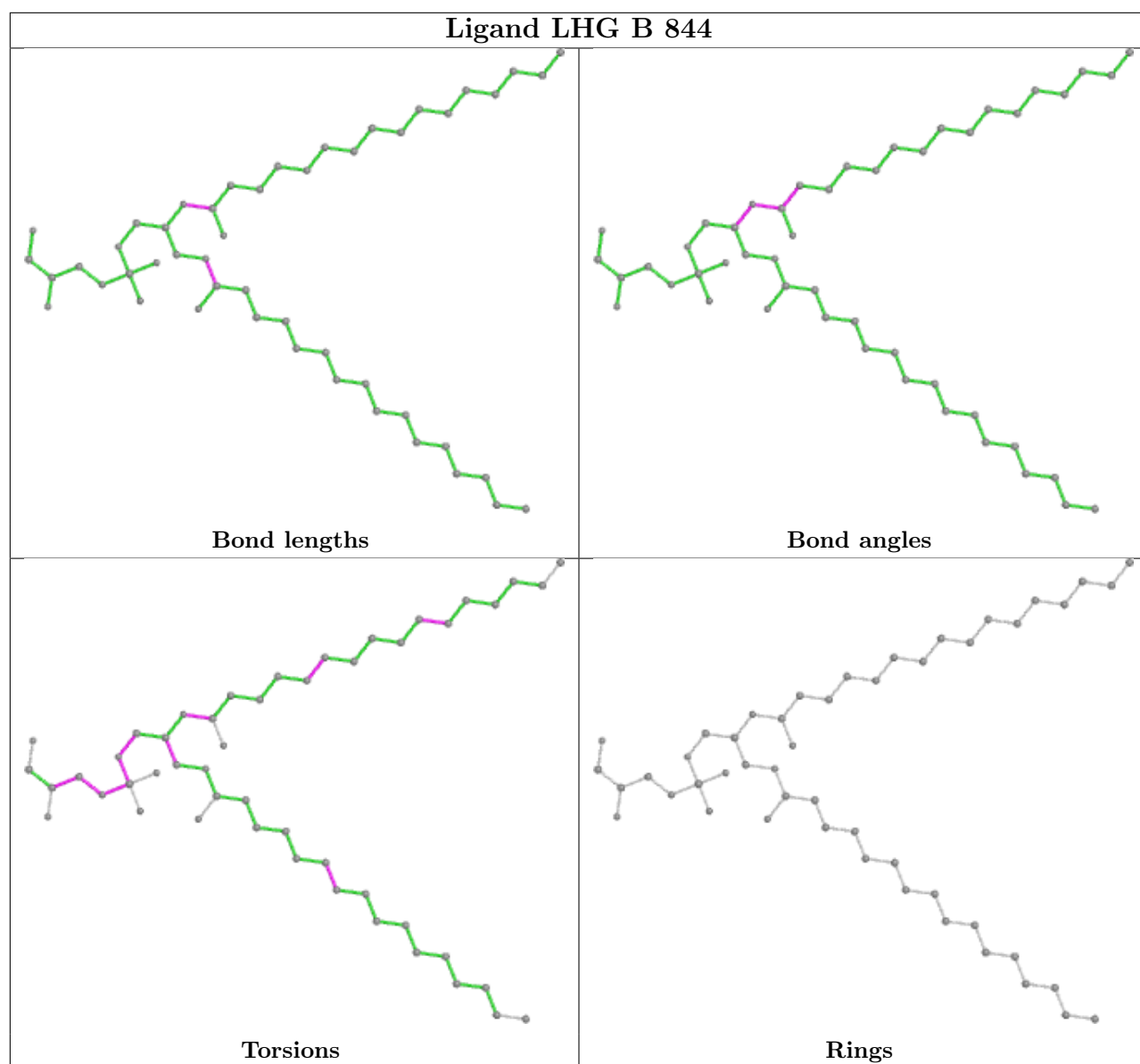
Bond angles

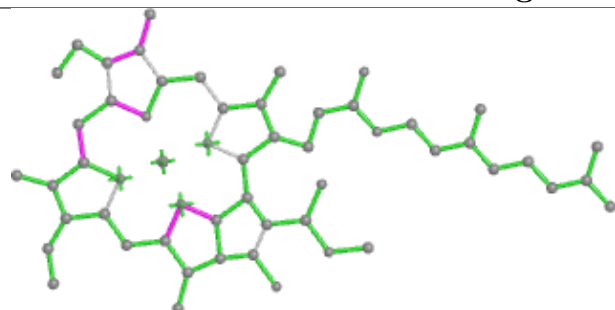


Torsions

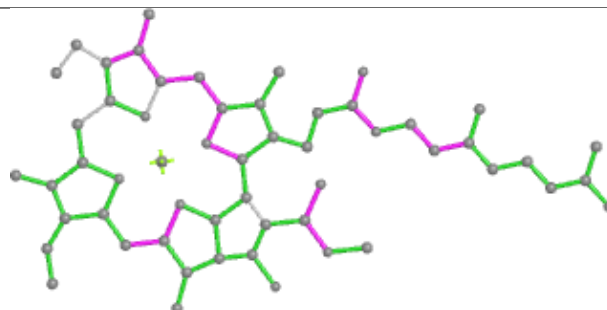


Rings

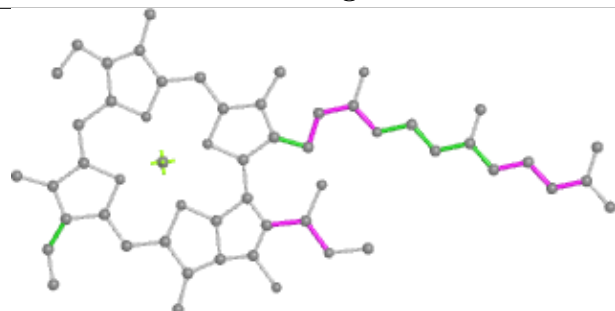


Ligand CLA A 822

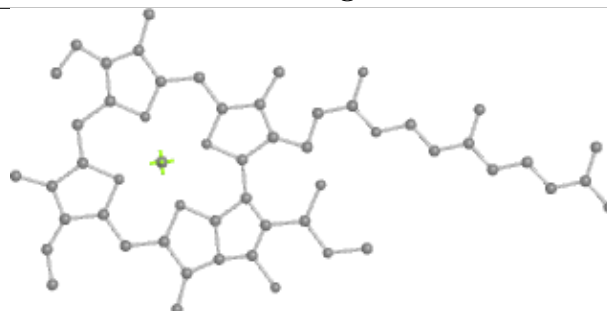
Bond lengths



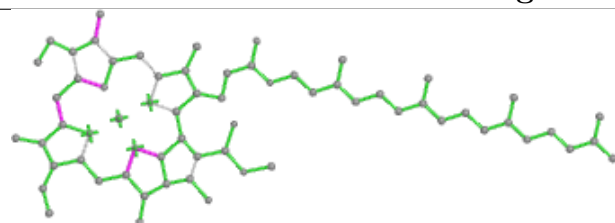
Bond angles



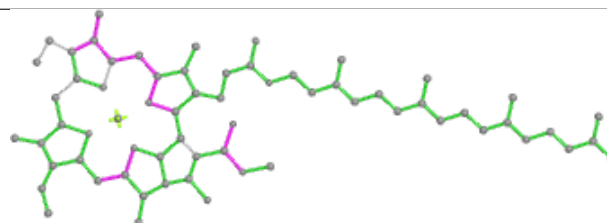
Torsions



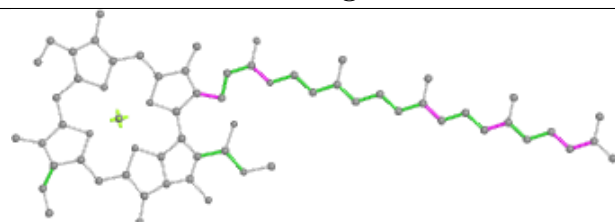
Rings

Ligand CLA B 805

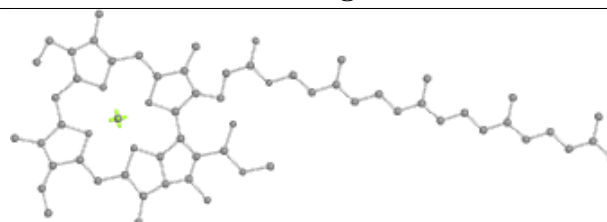
Bond lengths



Bond angles

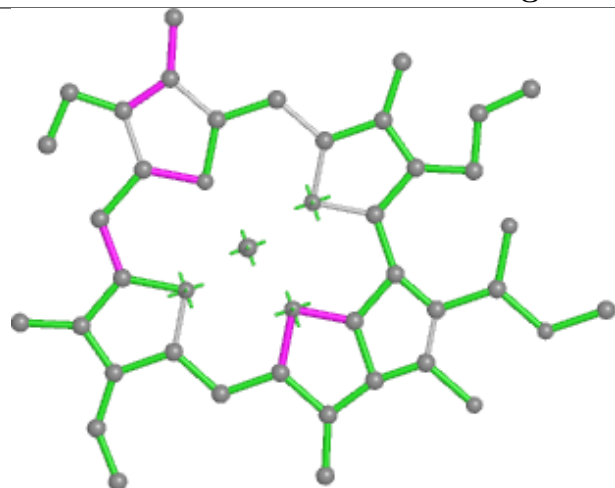


Torsions

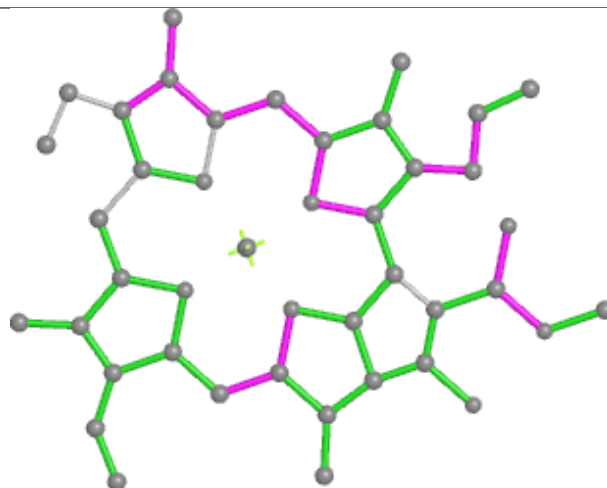


Rings

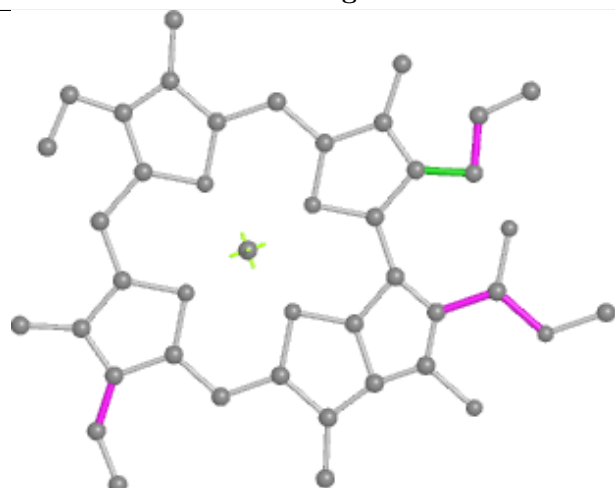
Ligand CLA c 601



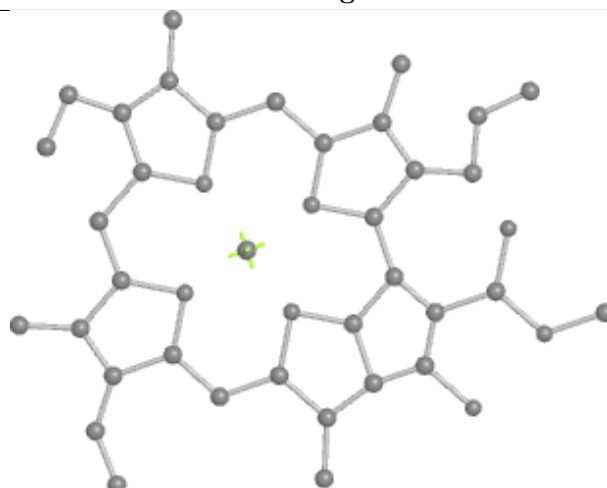
Bond lengths



Bond angles

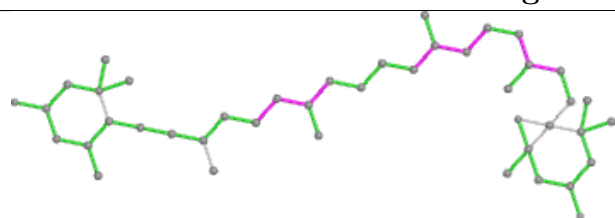


Torsions

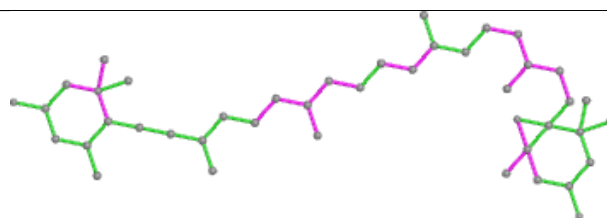


Rings

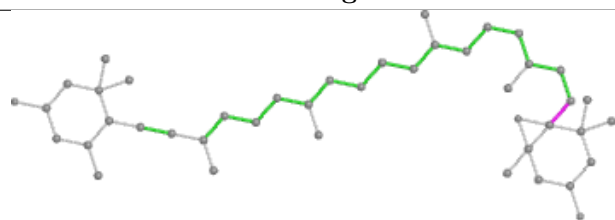
Ligand DD6 c 612



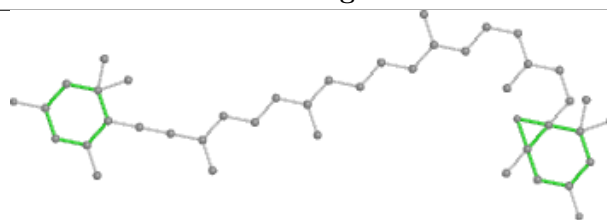
Bond lengths



Bond angles

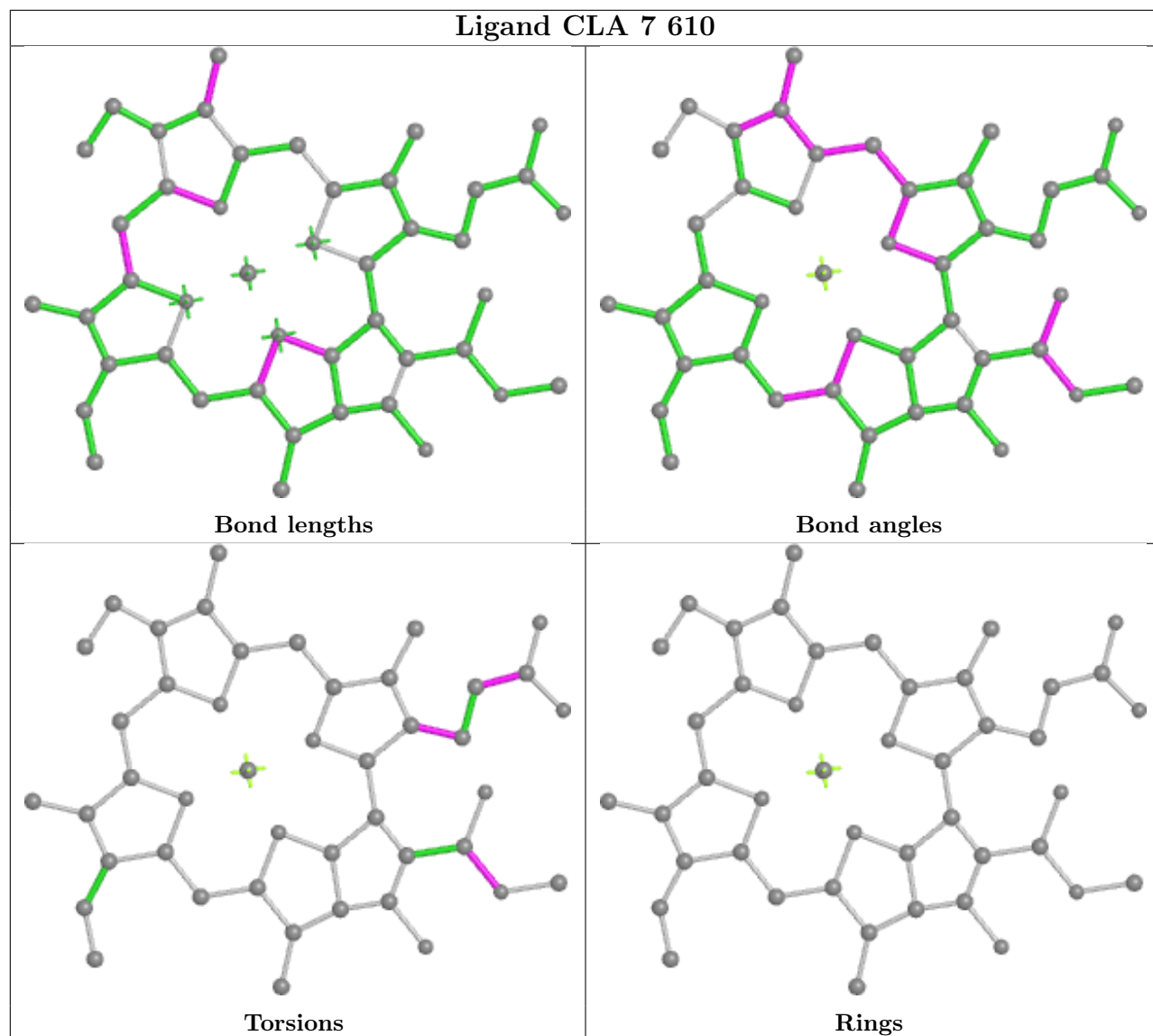


Torsions

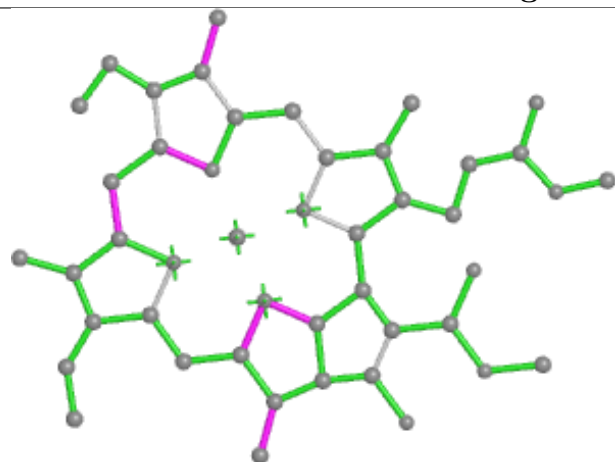


Rings

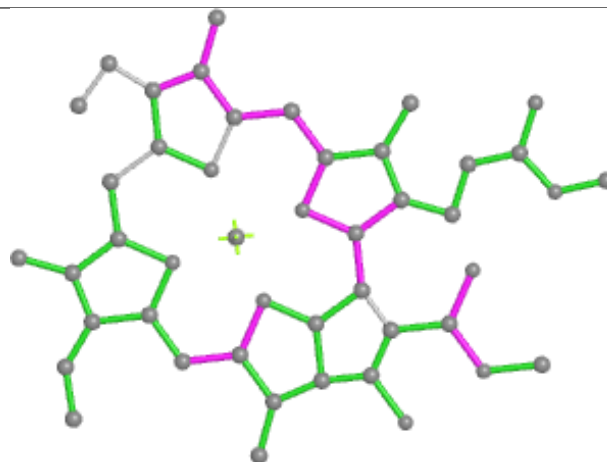
Ligand CLA 7 610



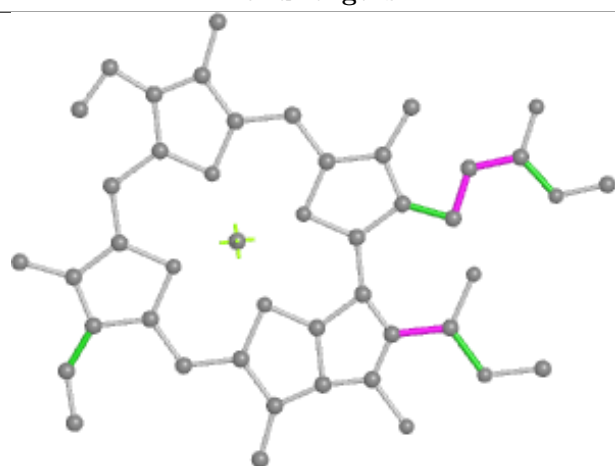
Ligand CLA 9 306



Bond lengths



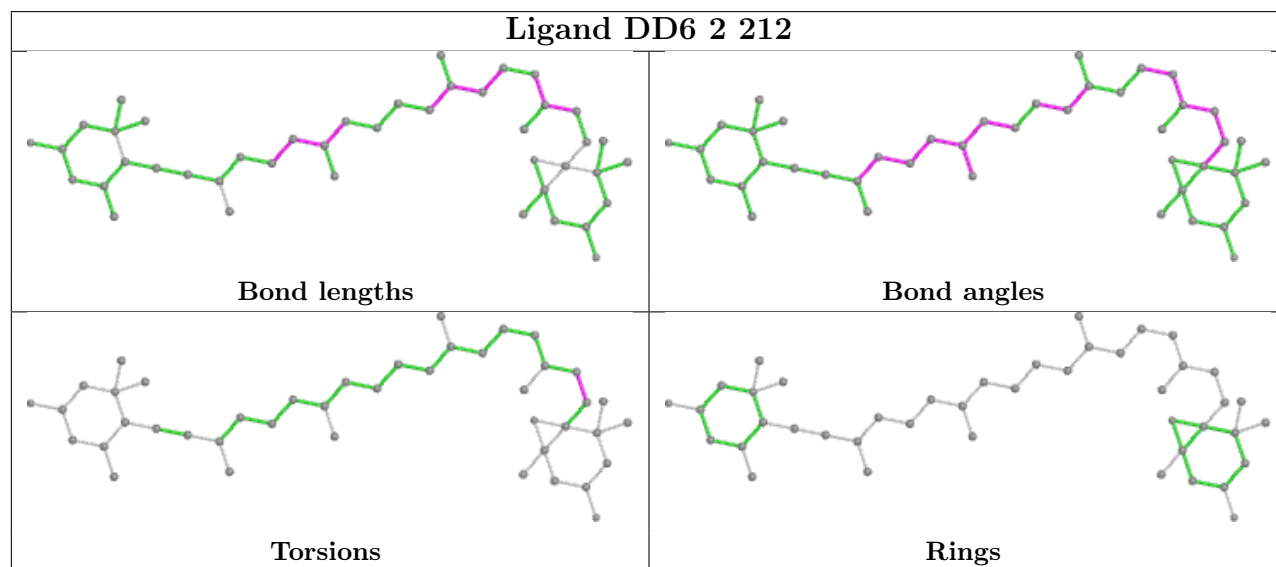
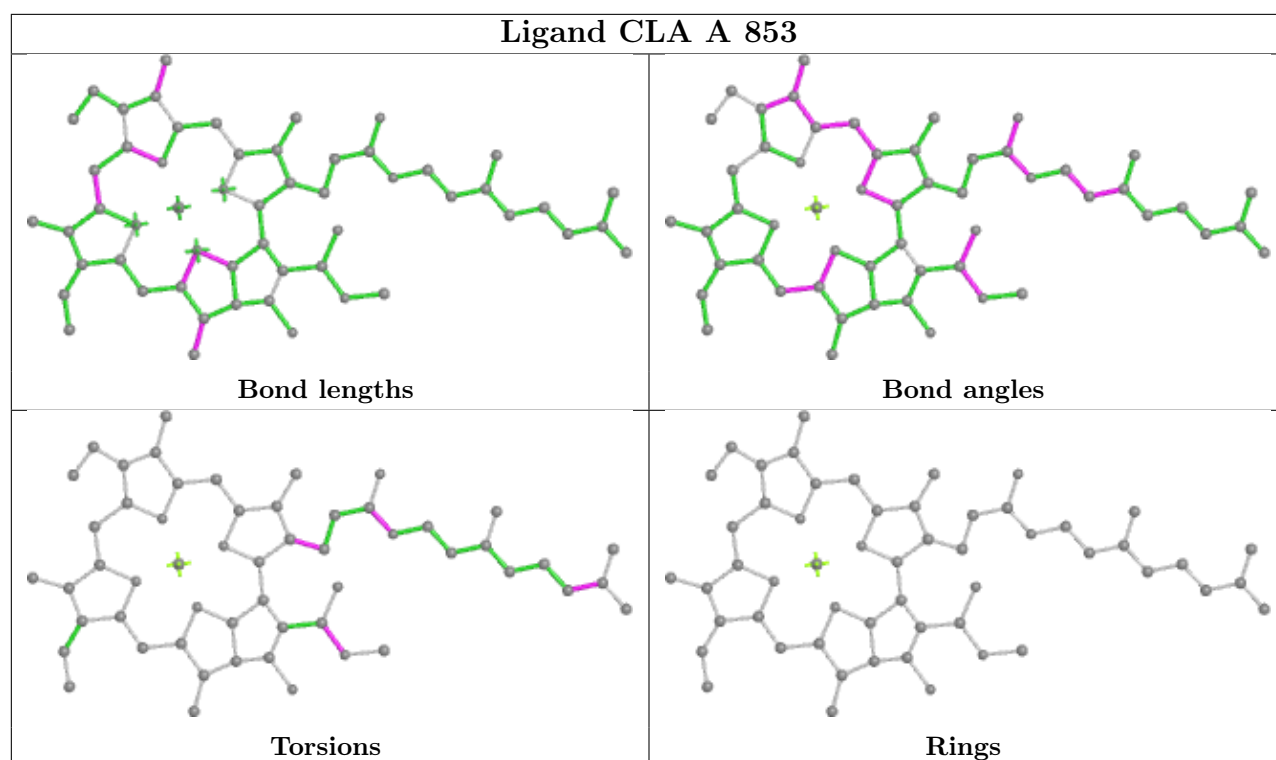
Bond angles



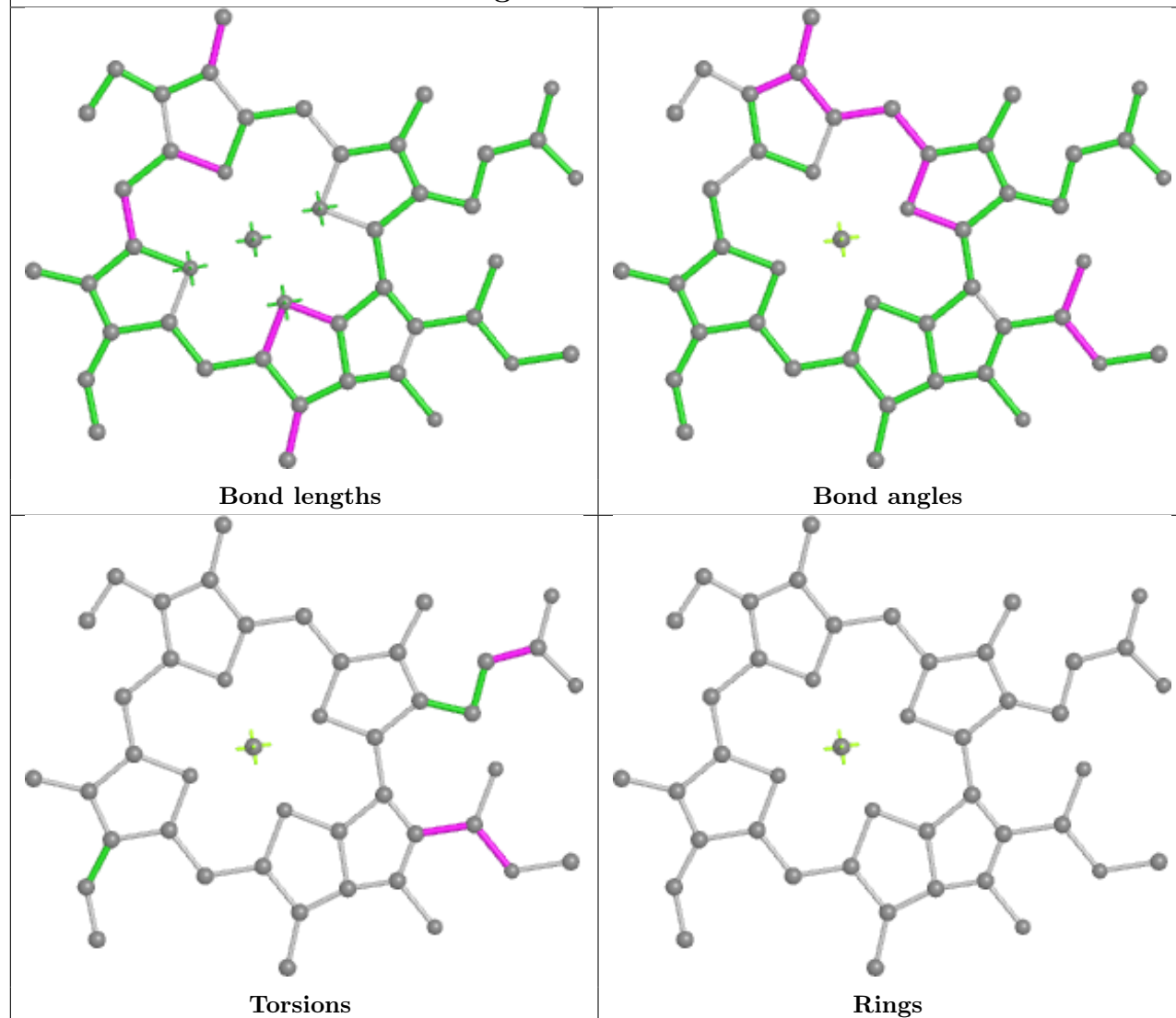
Torsions



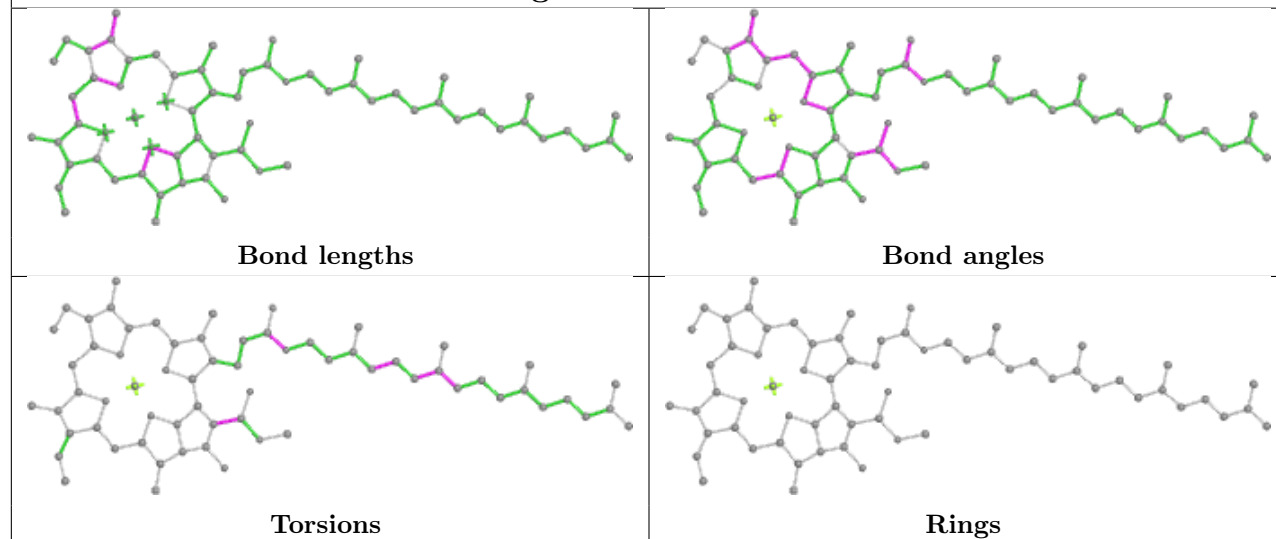
Rings

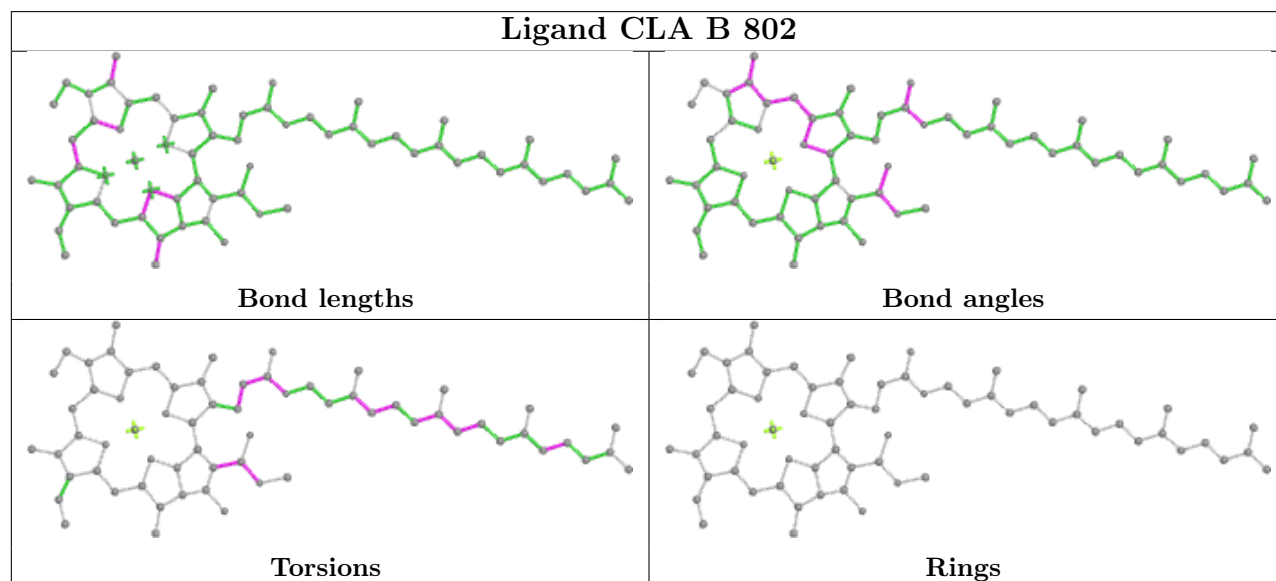
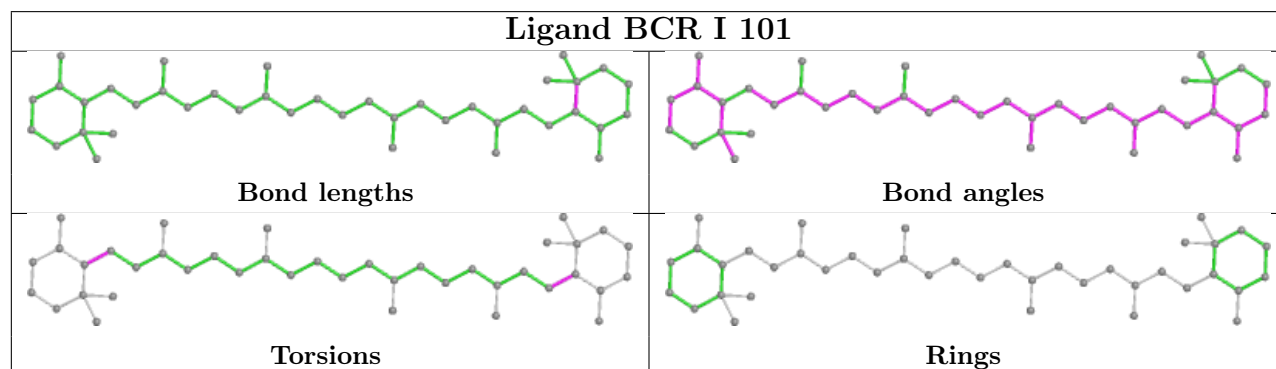
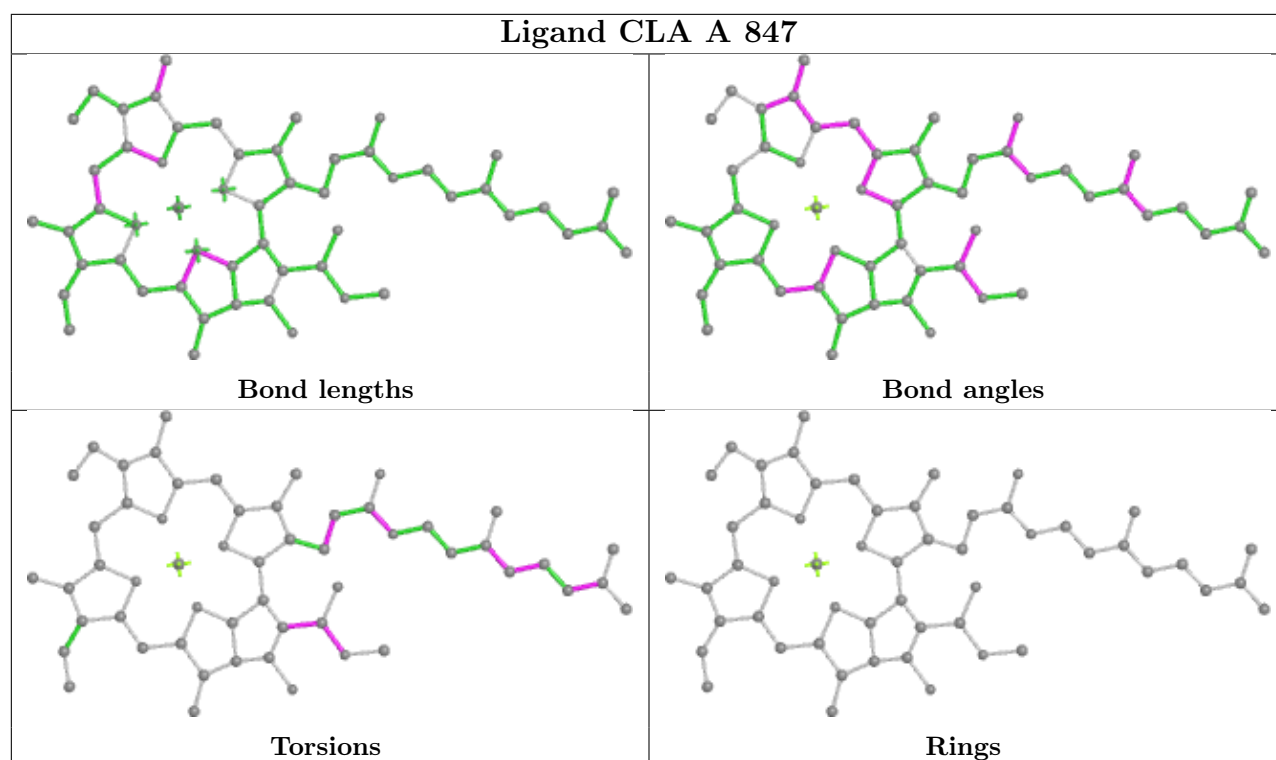


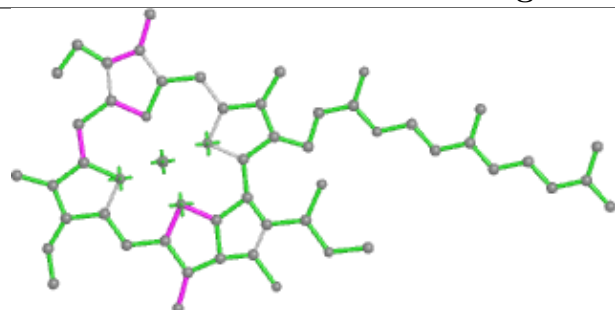
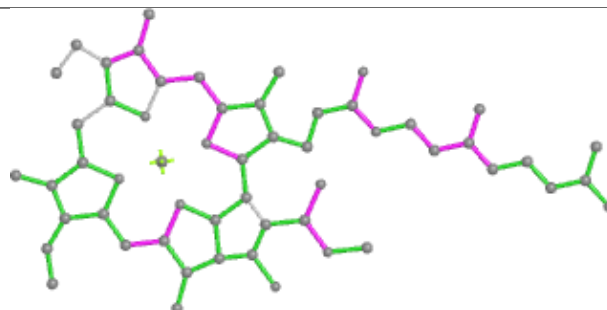
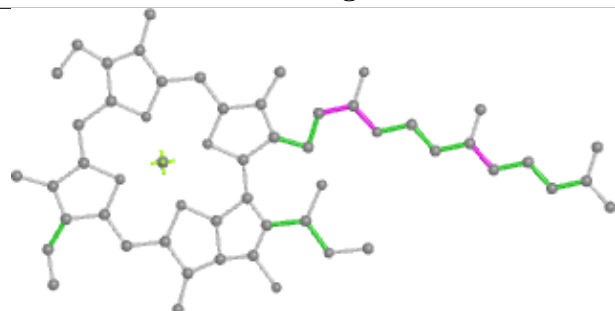
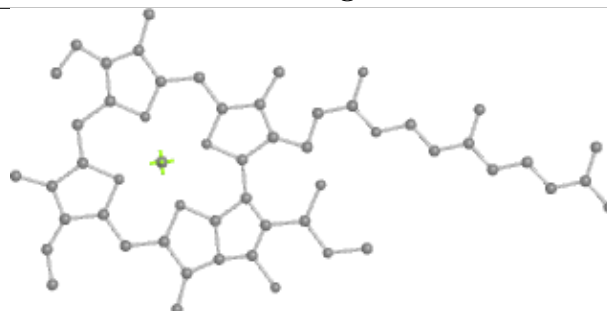
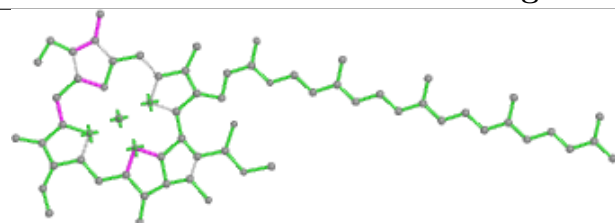
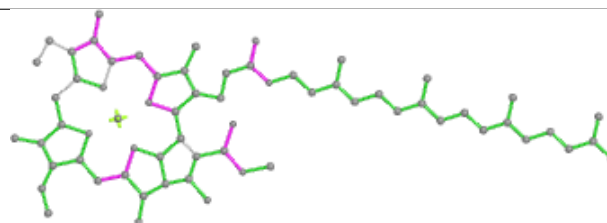
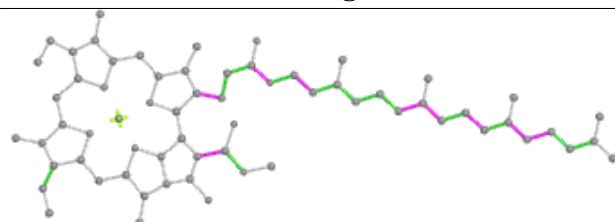
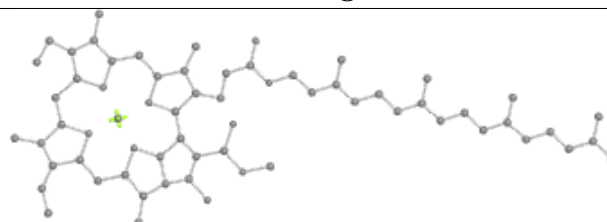
Ligand CLA 8 208



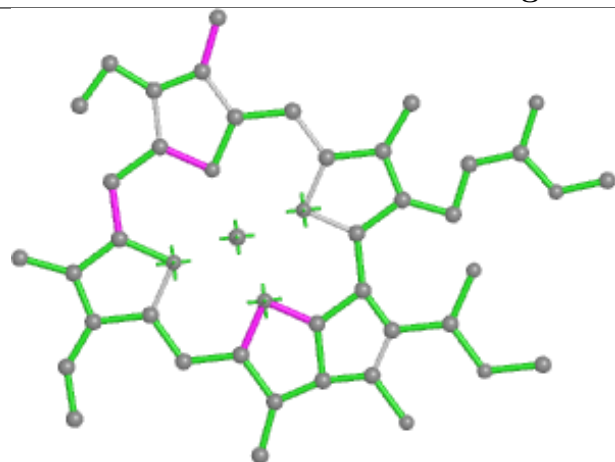
Ligand CLA A 829



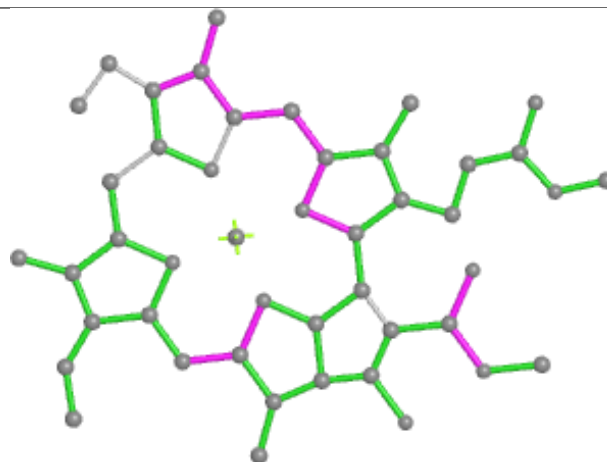


Ligand CLA B 811**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA c 608****Bond lengths****Bond angles****Torsions****Rings**

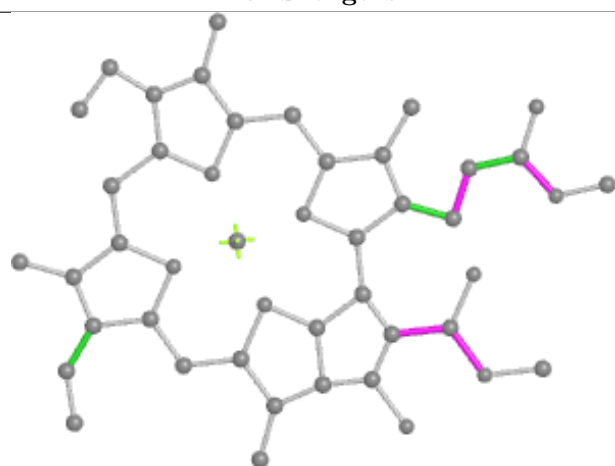
Ligand CLA c 606



Bond lengths



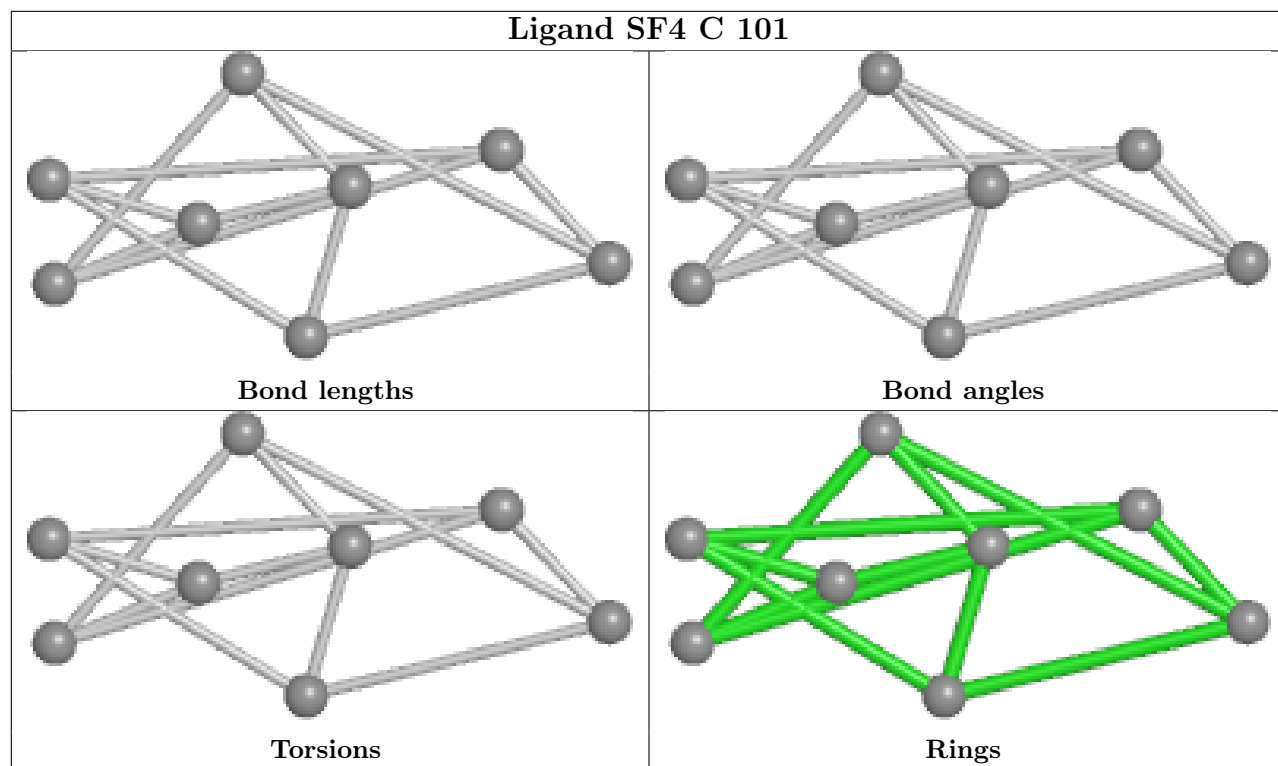
Bond angles



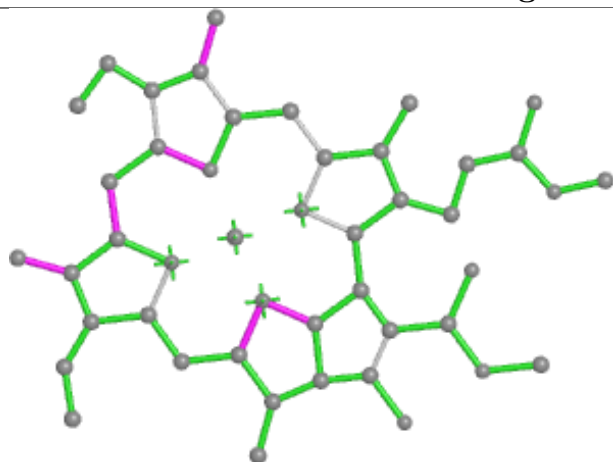
Torsions



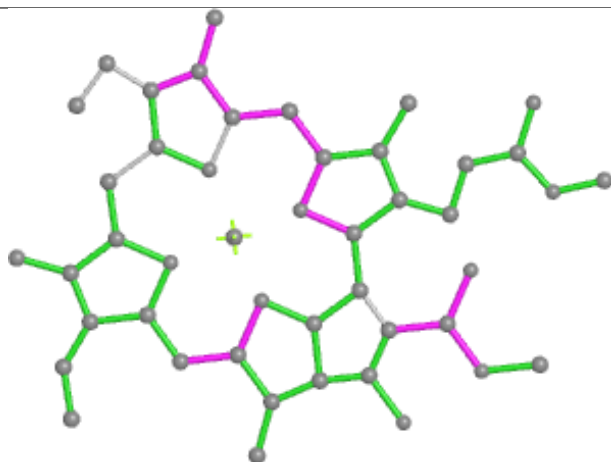
Rings



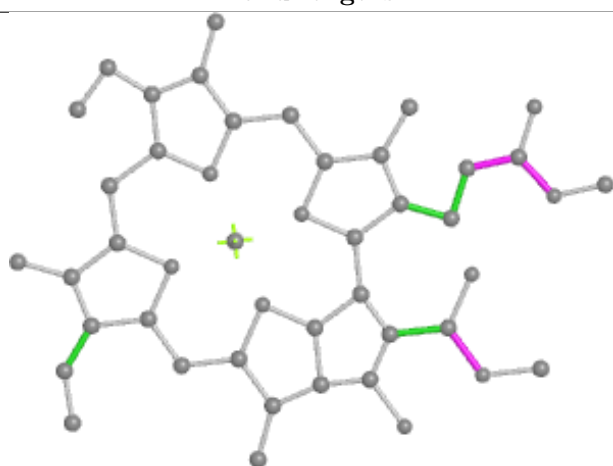
Ligand CLA 4 609



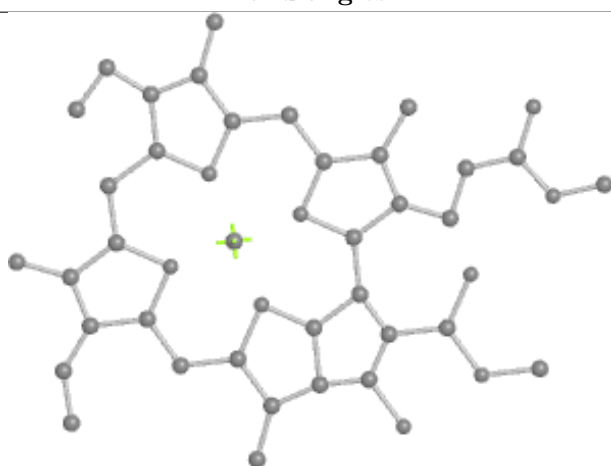
Bond lengths



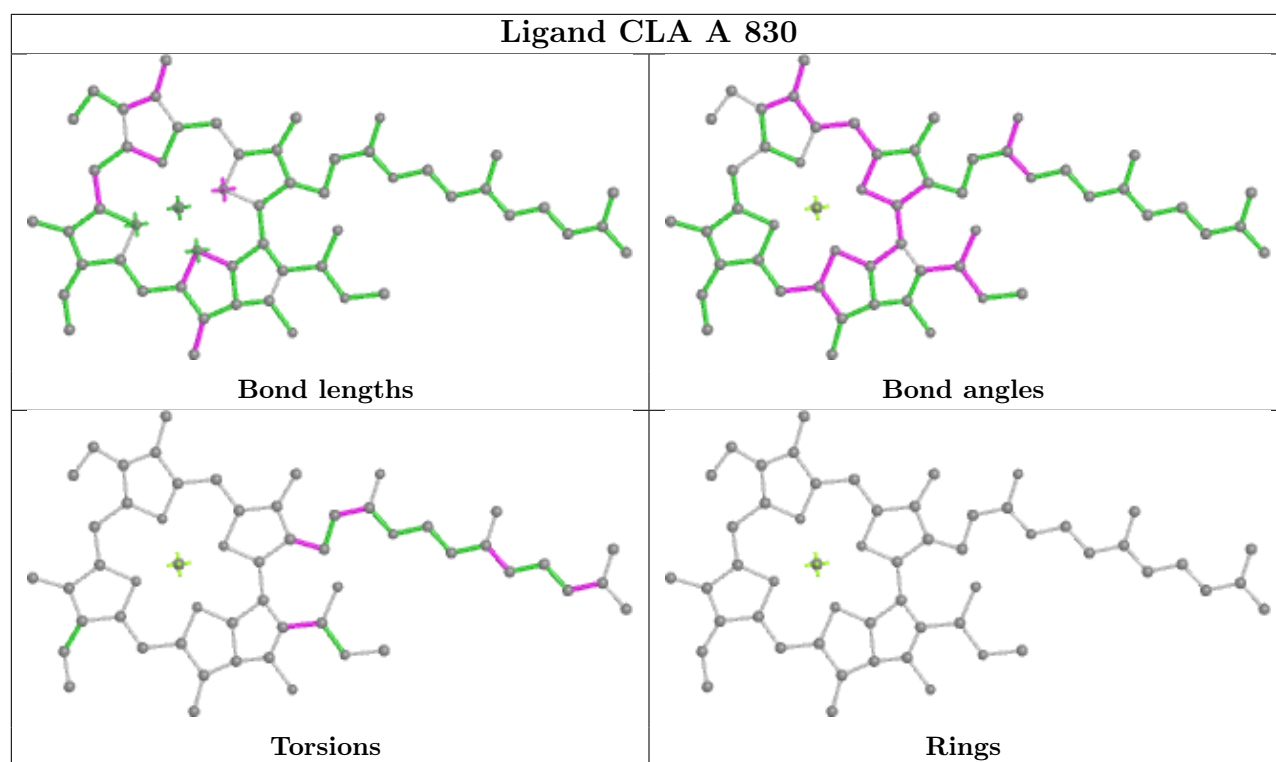
Bond angles



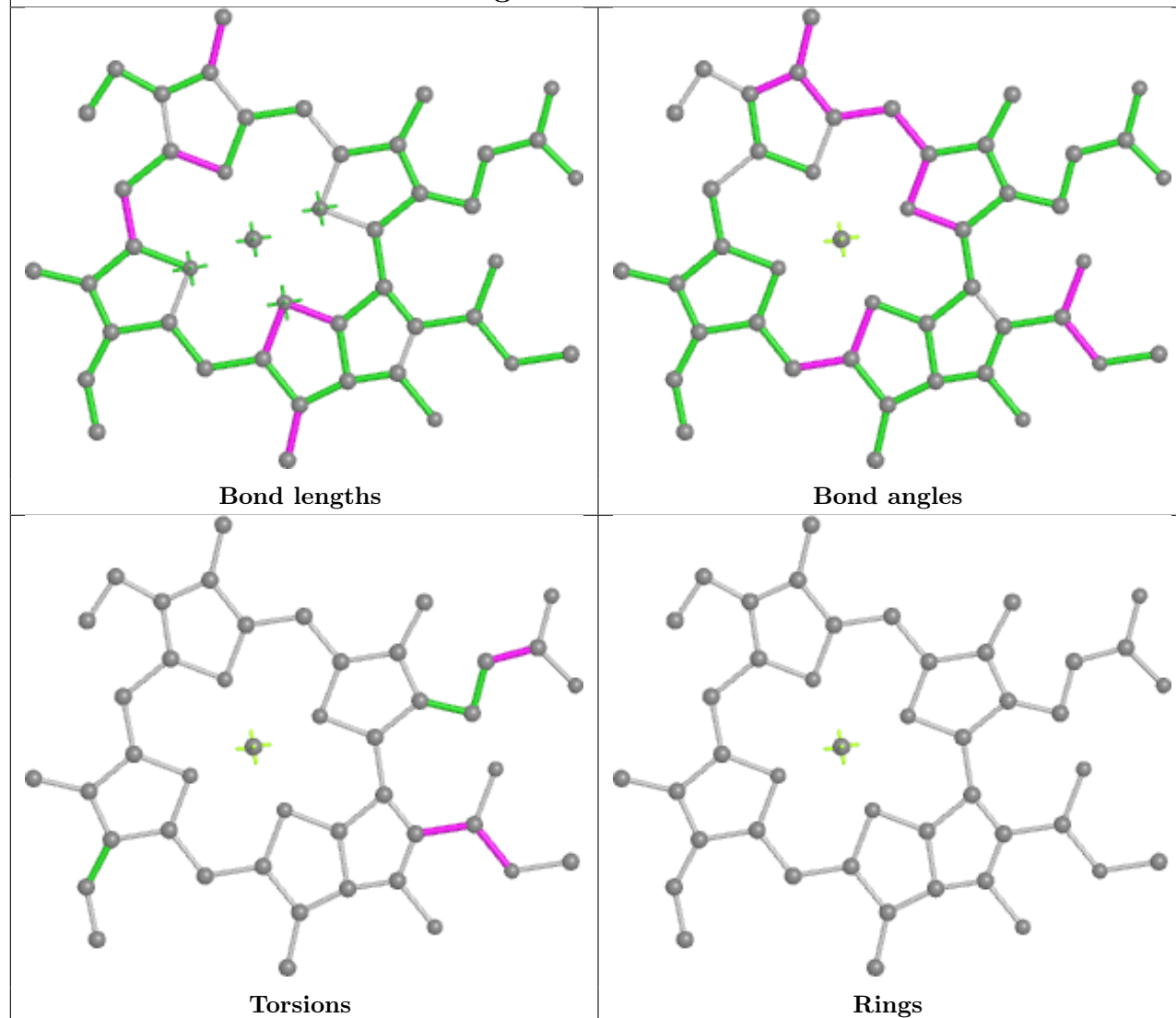
Torsions



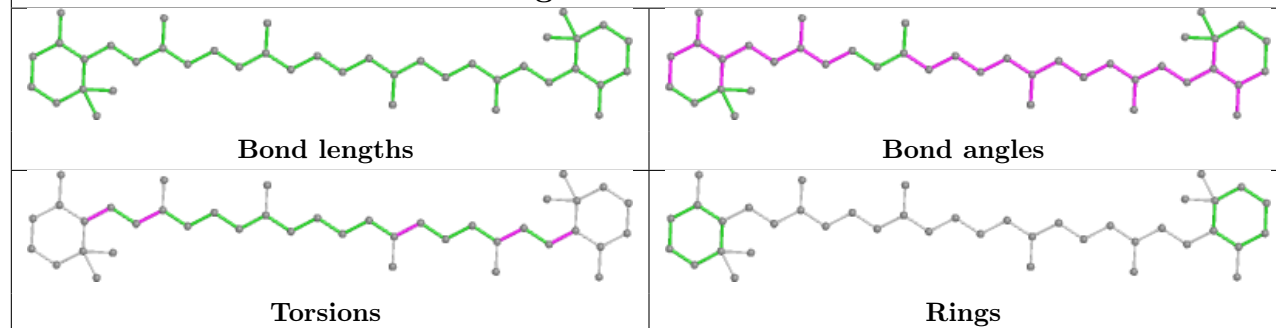
Rings



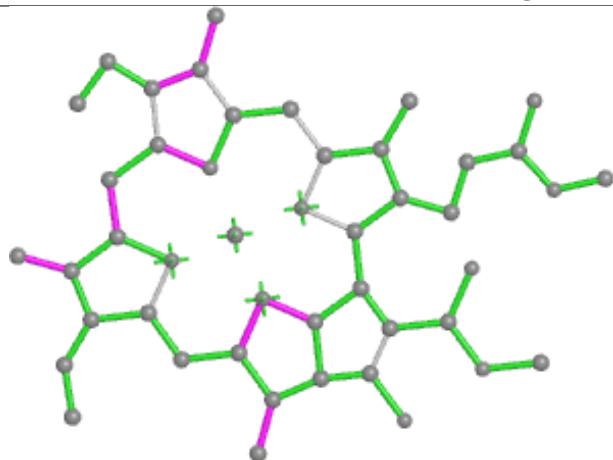
Ligand CLA 9 311



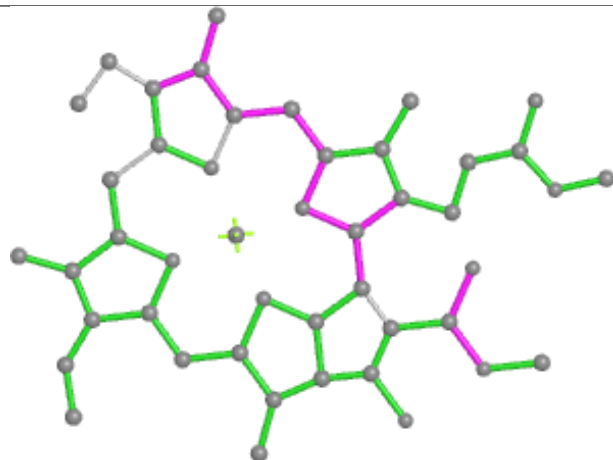
Ligand BCR c 615



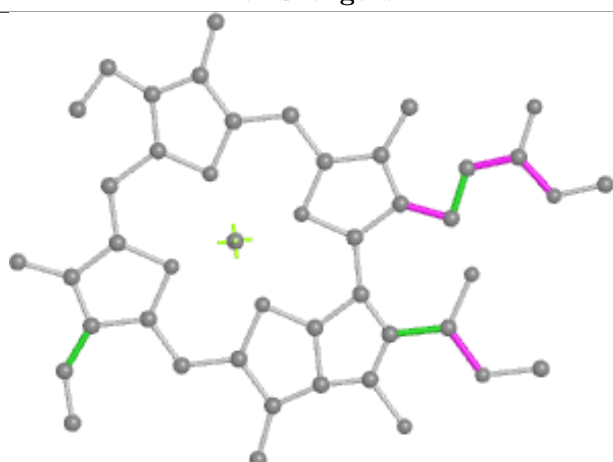
Ligand CLA 9 303



Bond lengths



Bond angles

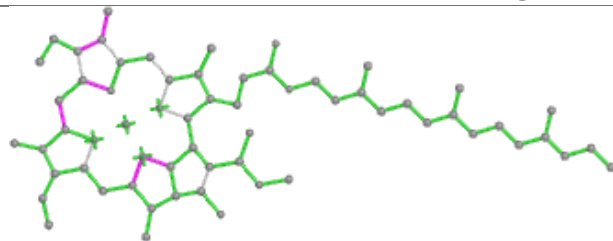


Torsions

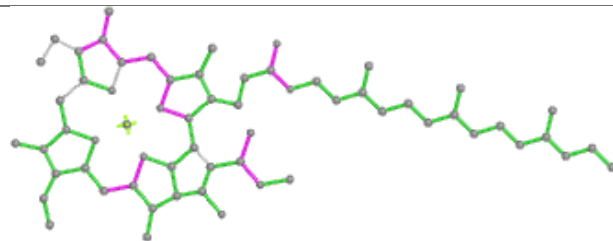


Rings

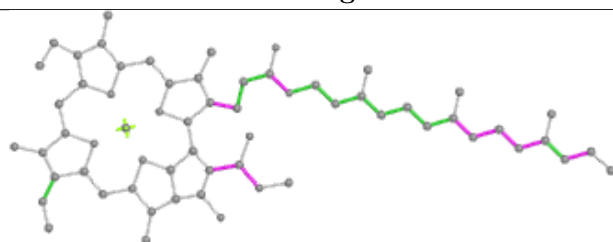
Ligand CLA A 810



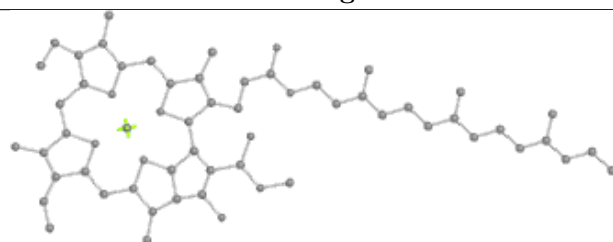
Bond lengths



Bond angles

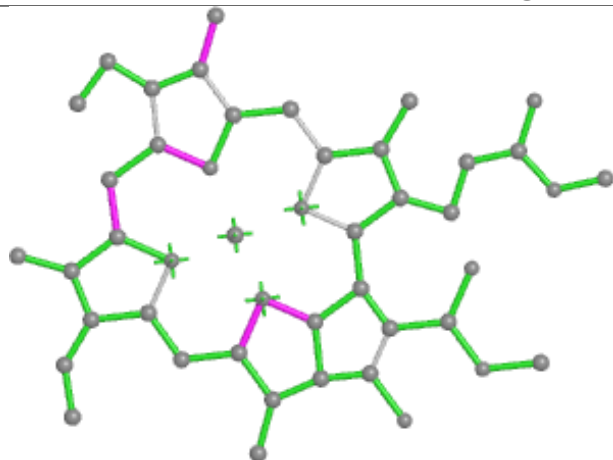


Torsions

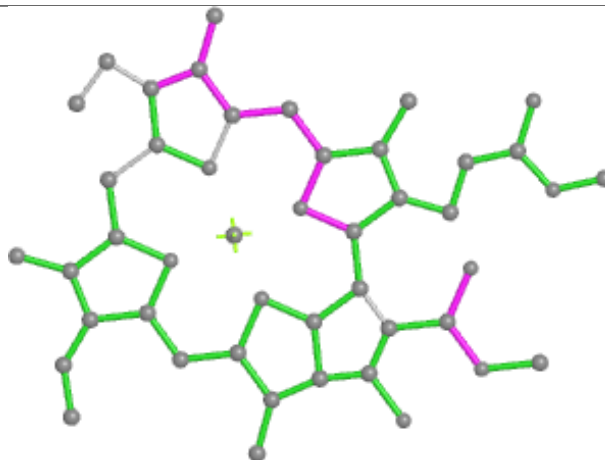


Rings

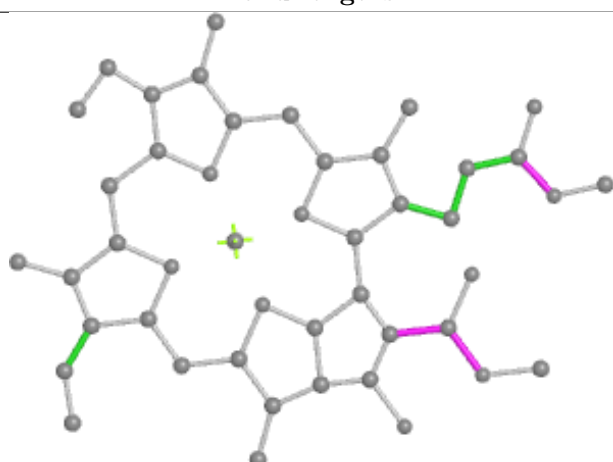
Ligand CLA 2 208



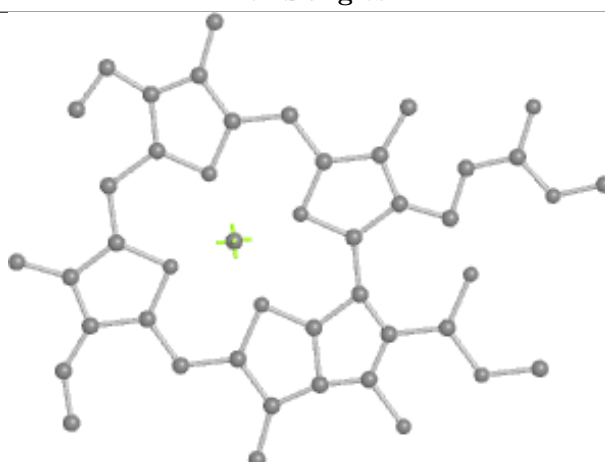
Bond lengths



Bond angles

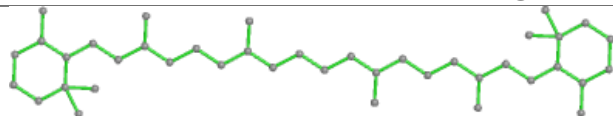


Torsions

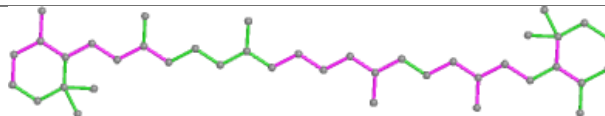


Rings

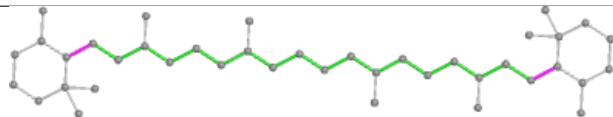
Ligand BCR A 859



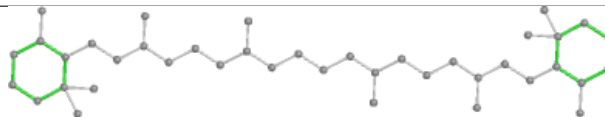
Bond lengths



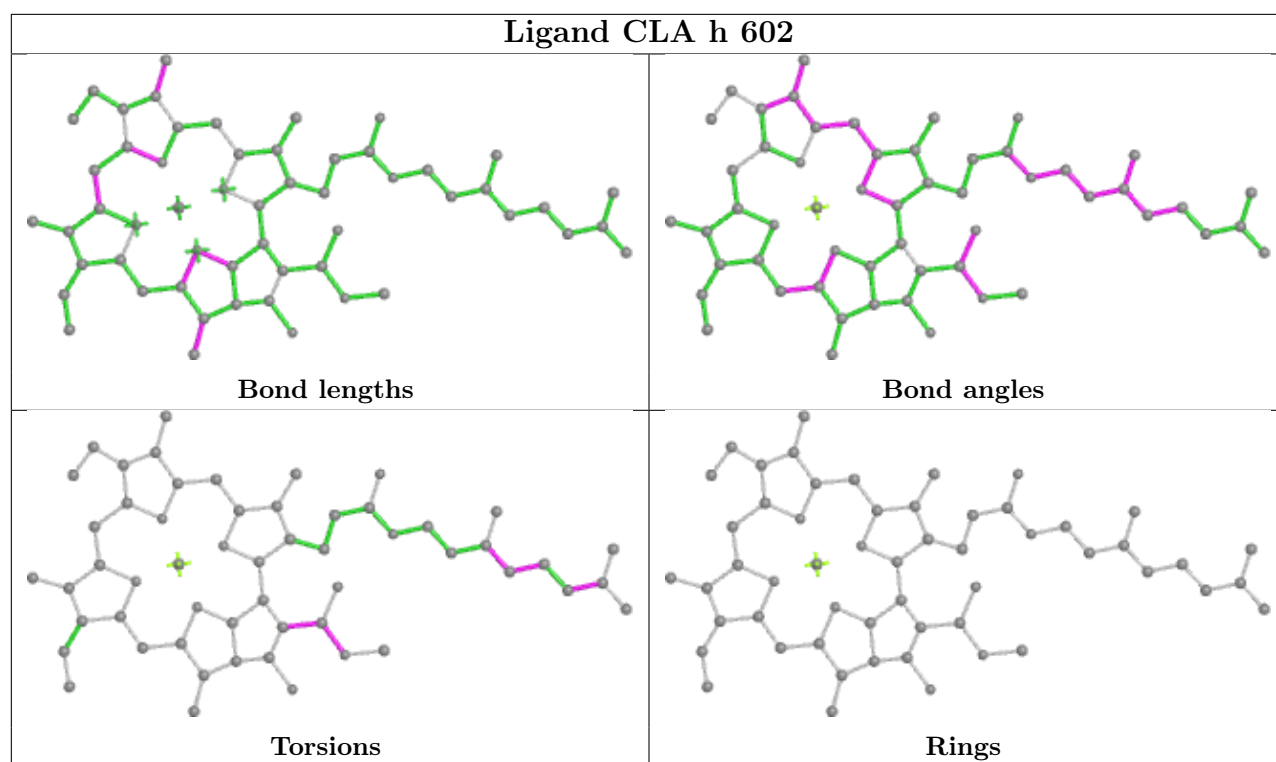
Bond angles



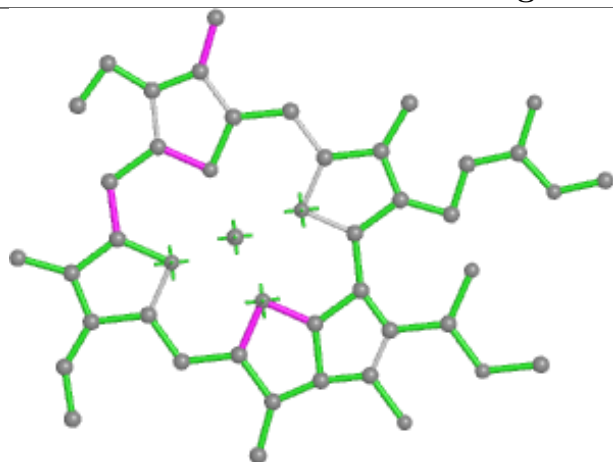
Torsions



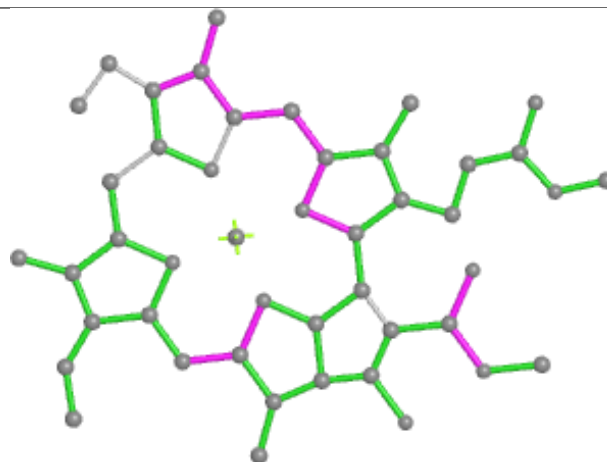
Rings



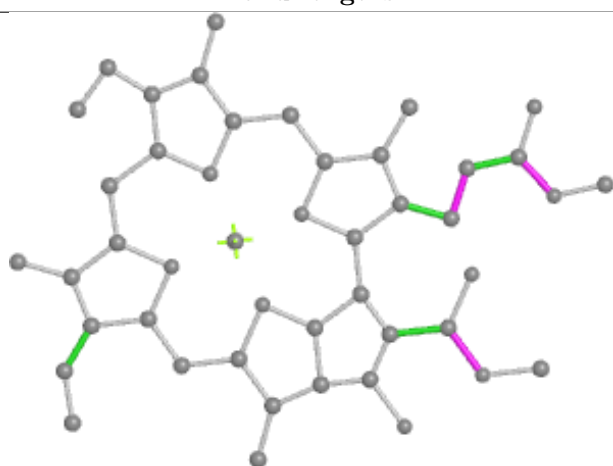
Ligand CLA h 604



Bond lengths



Bond angles

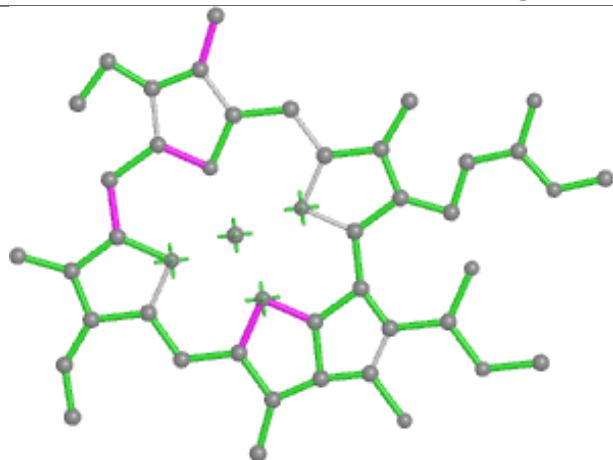


Torsions

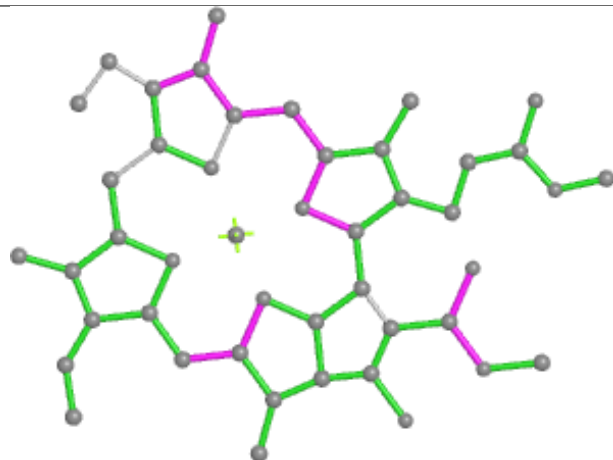


Rings

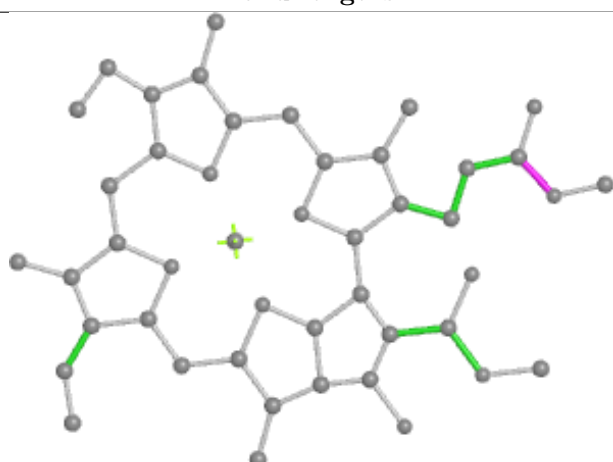
Ligand CLA B 819



Bond lengths



Bond angles

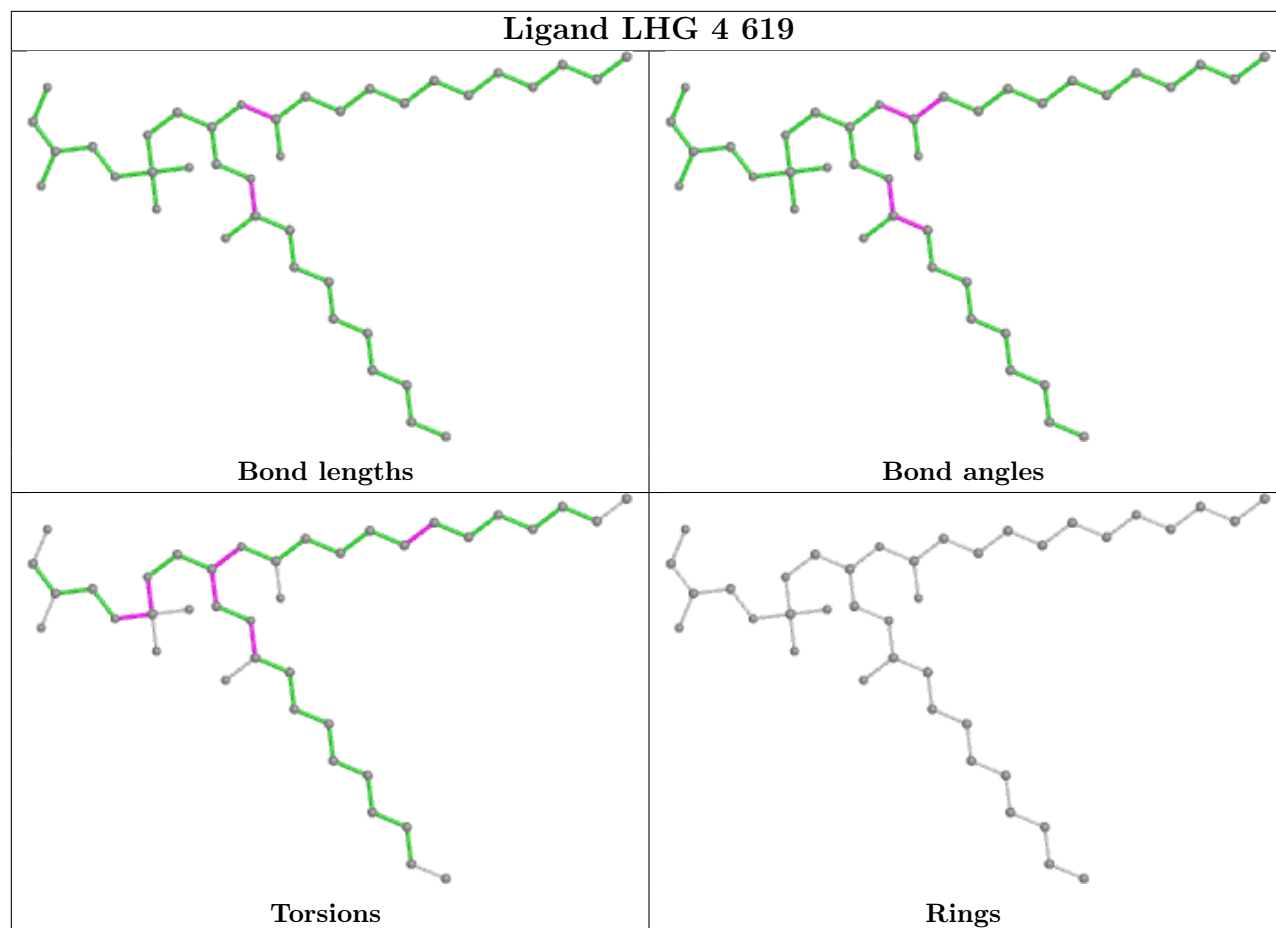


Torsions

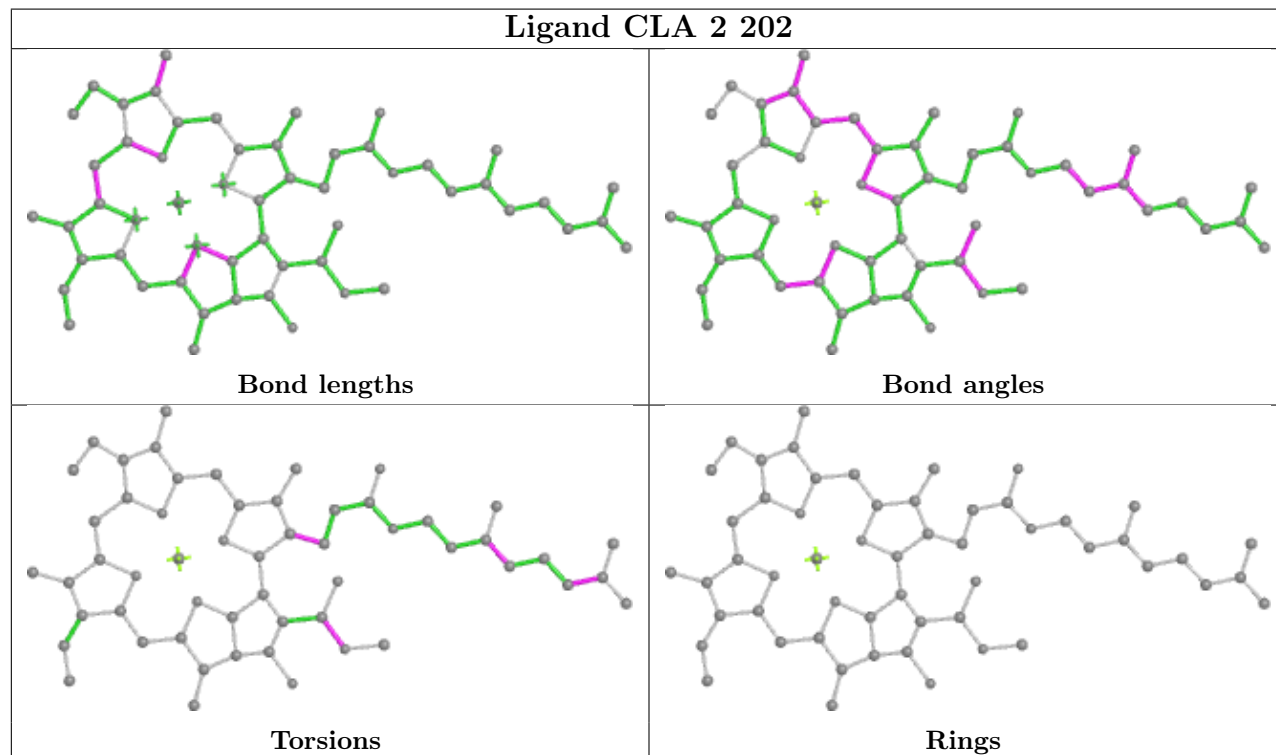


Rings

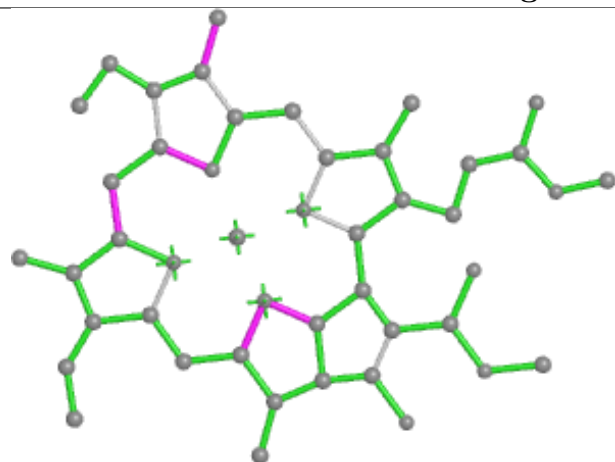
Ligand LHG 4 619



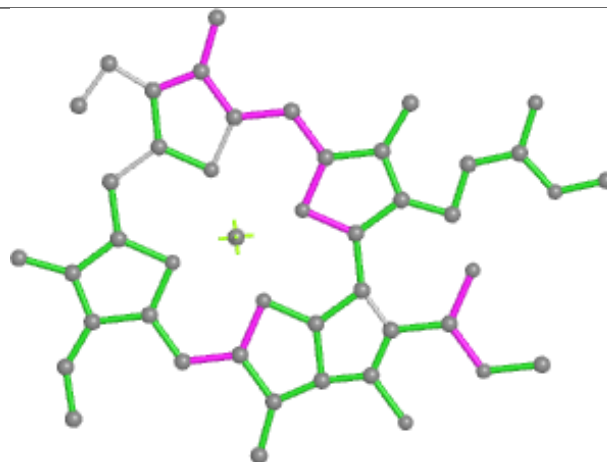
Ligand CLA 2 202



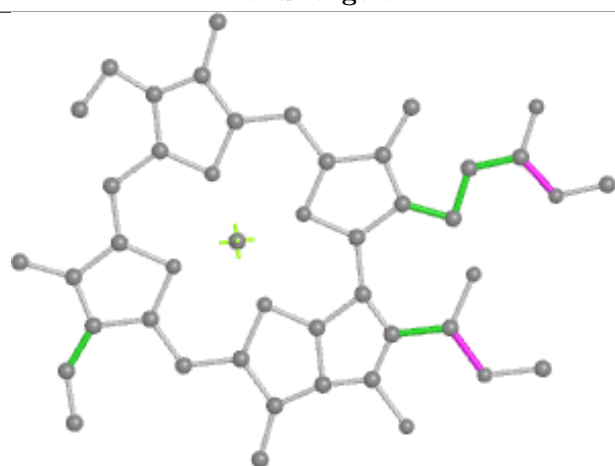
Ligand CLA 2 205



Bond lengths



Bond angles

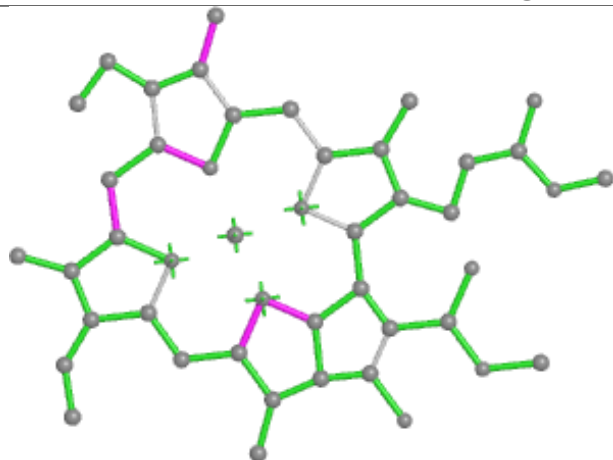


Torsions

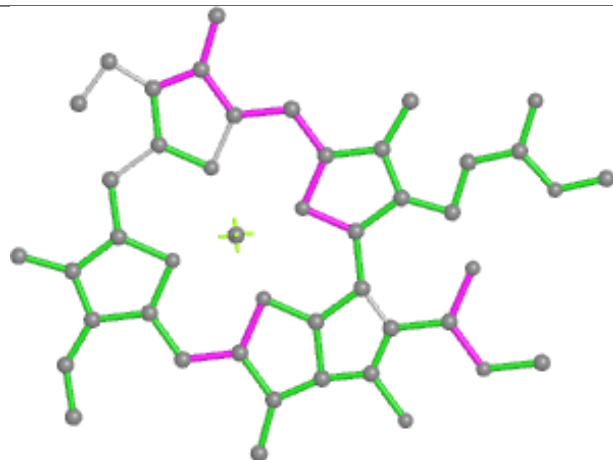


Rings

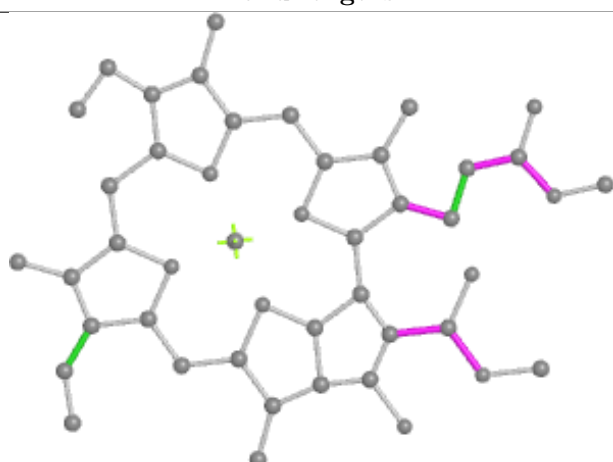
Ligand CLA 2 209



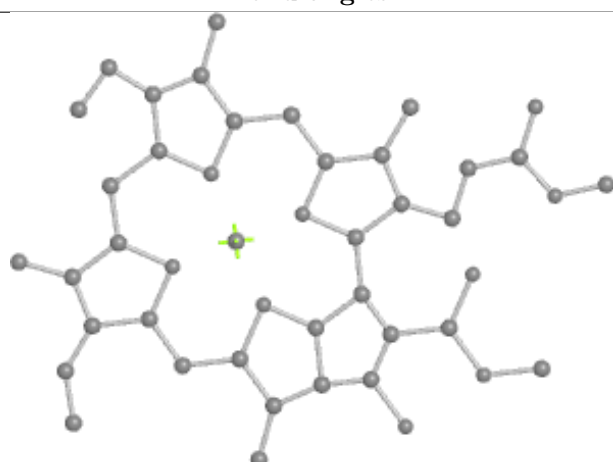
Bond lengths



Bond angles

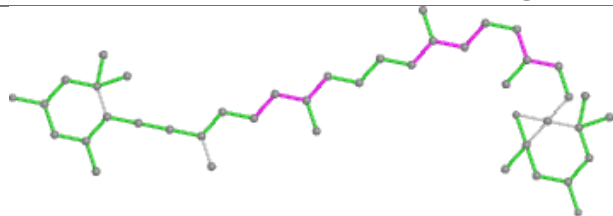


Torsions

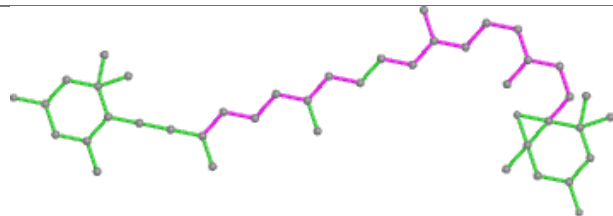


Rings

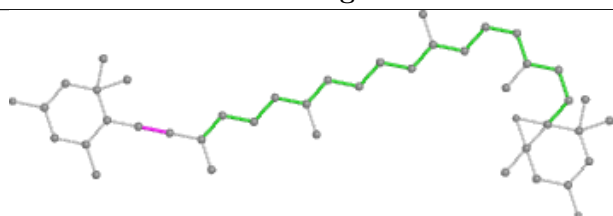
Ligand DD6 h 613



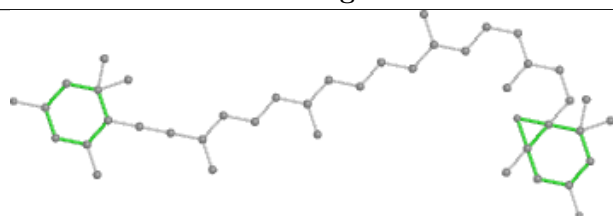
Bond lengths



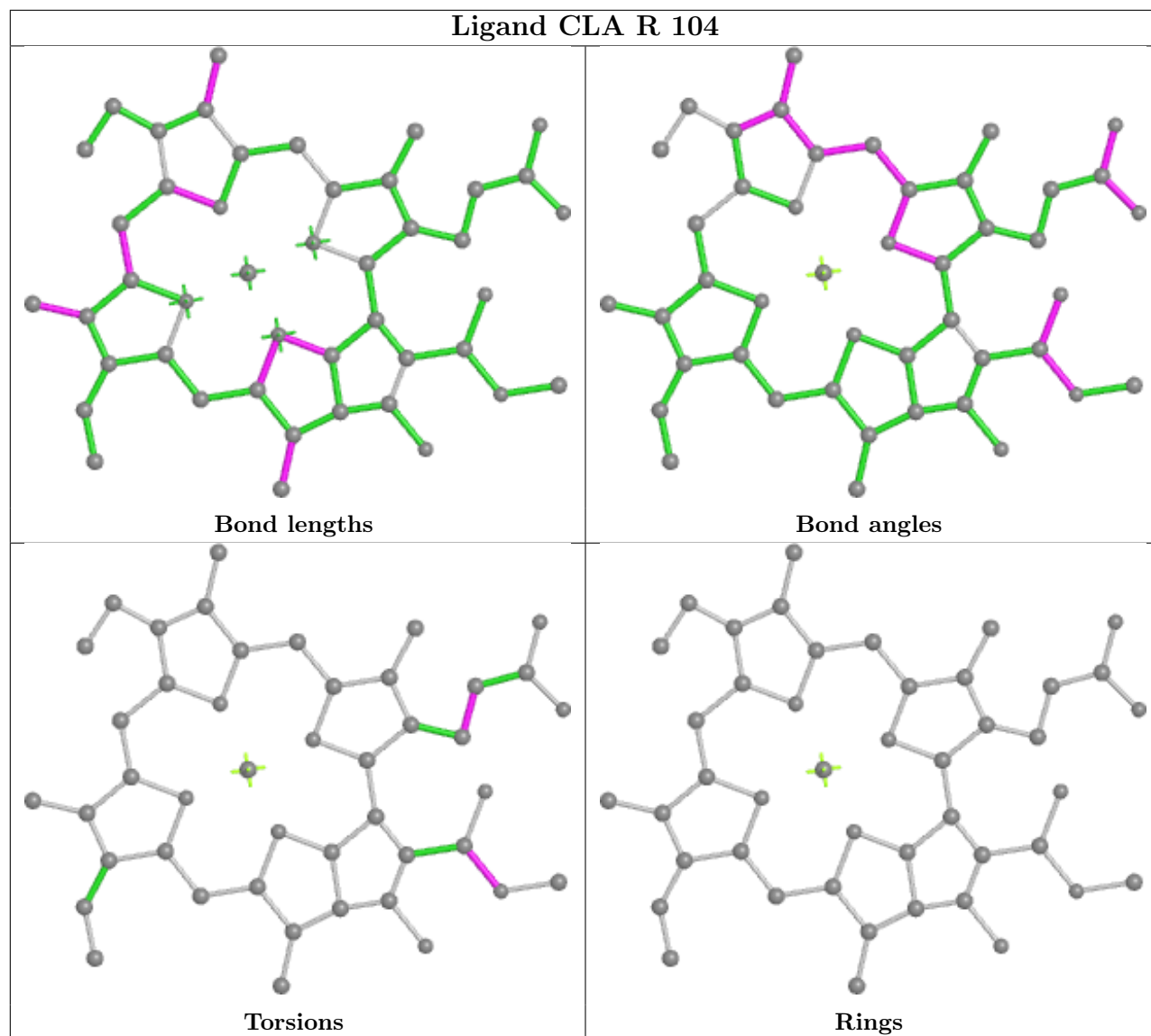
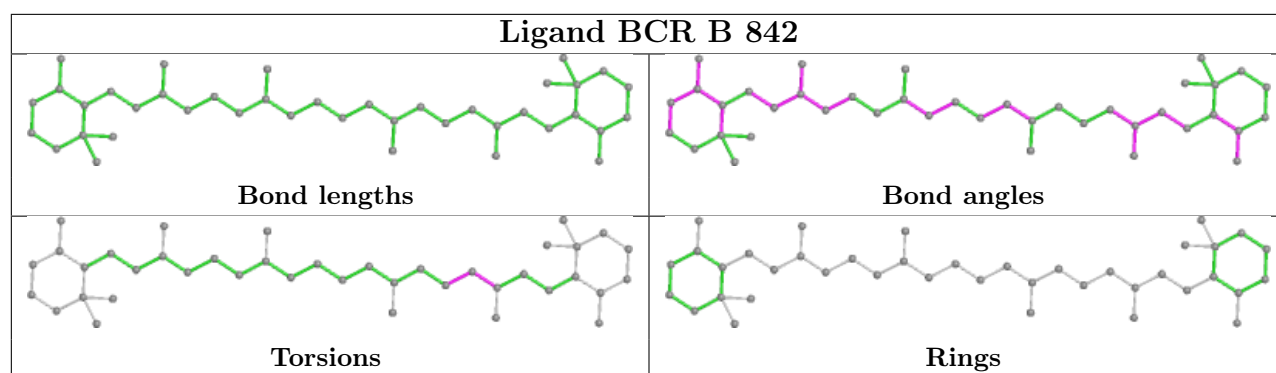
Bond angles



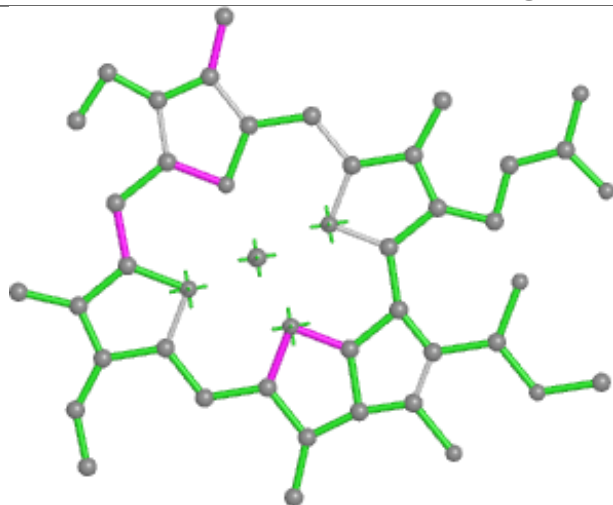
Torsions



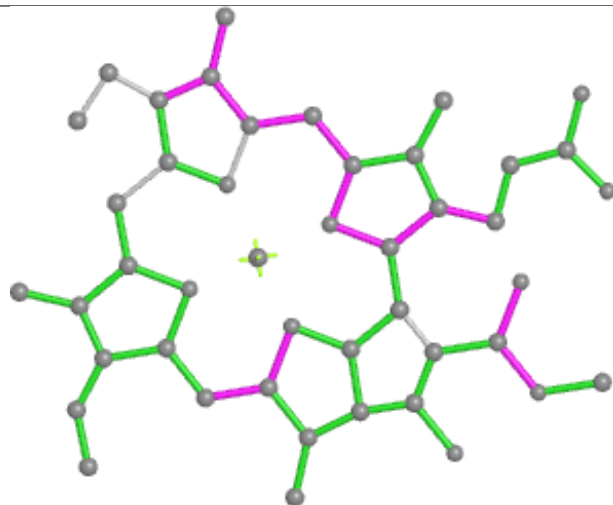
Rings



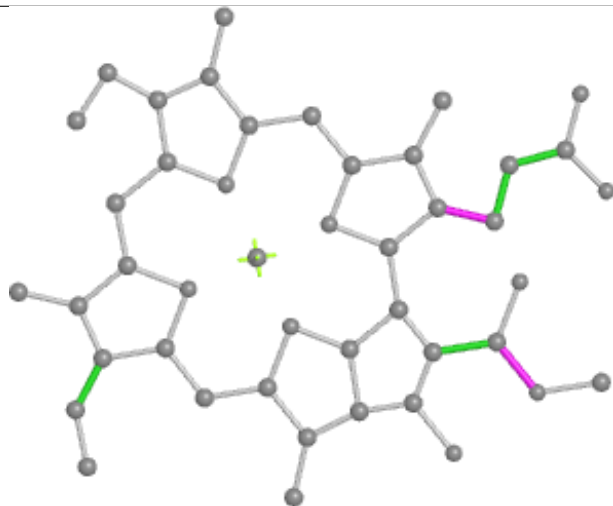
Ligand CLA t 301



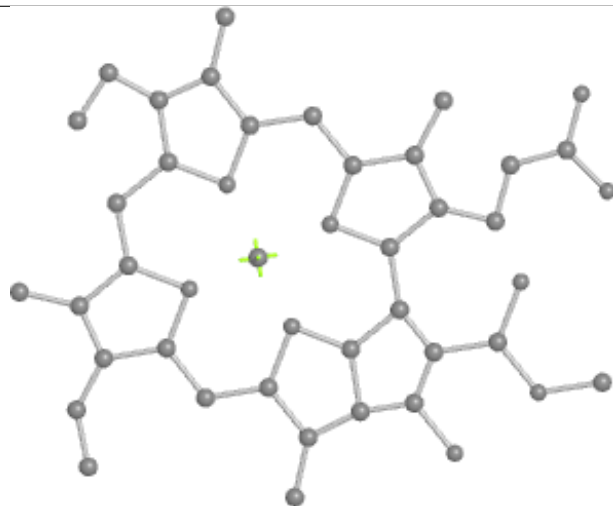
Bond lengths



Bond angles

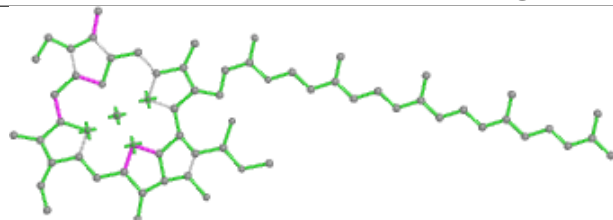


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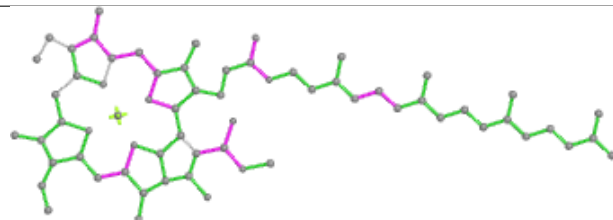


Rings

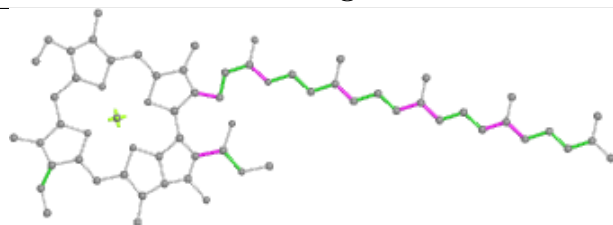
Ligand CLA A 818



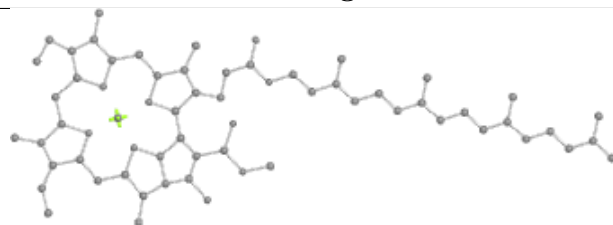
Bond lengths



Bond angles

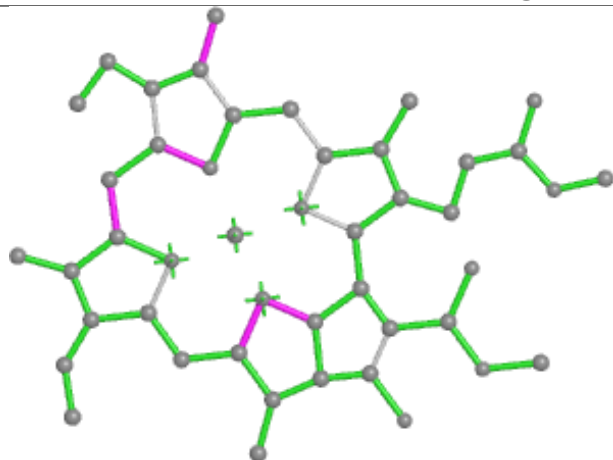


Torsions

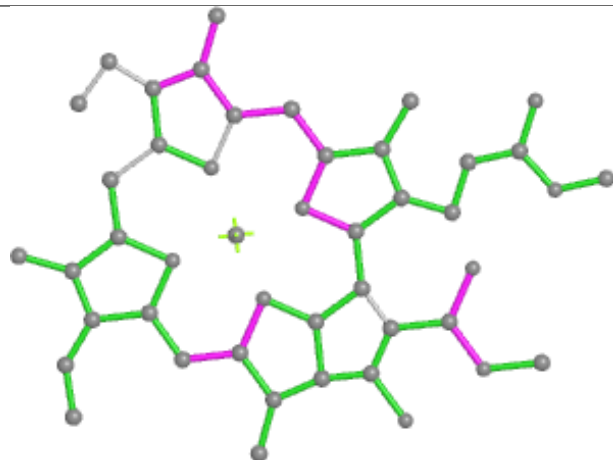


Rings

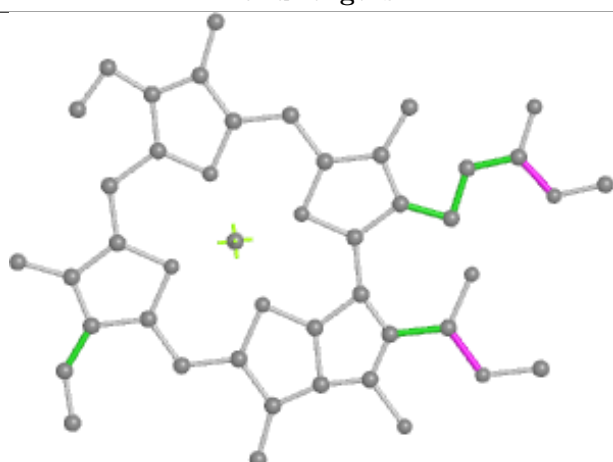
Ligand CLA k 301



Bond lengths



Bond angles

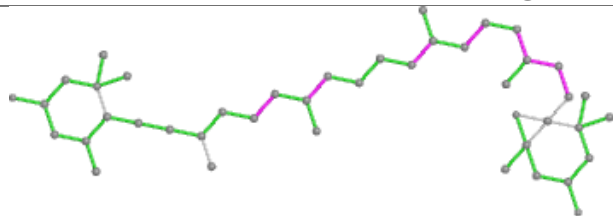


Torsions

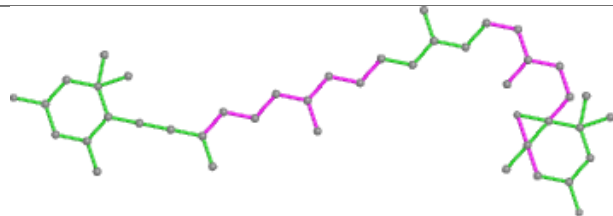


Rings

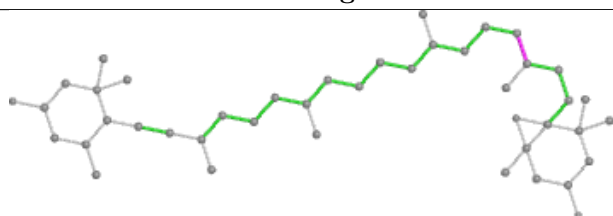
Ligand DD6 9 314



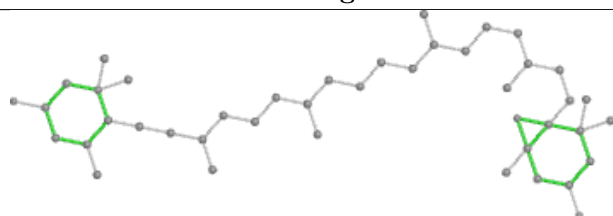
Bond lengths



Bond angles

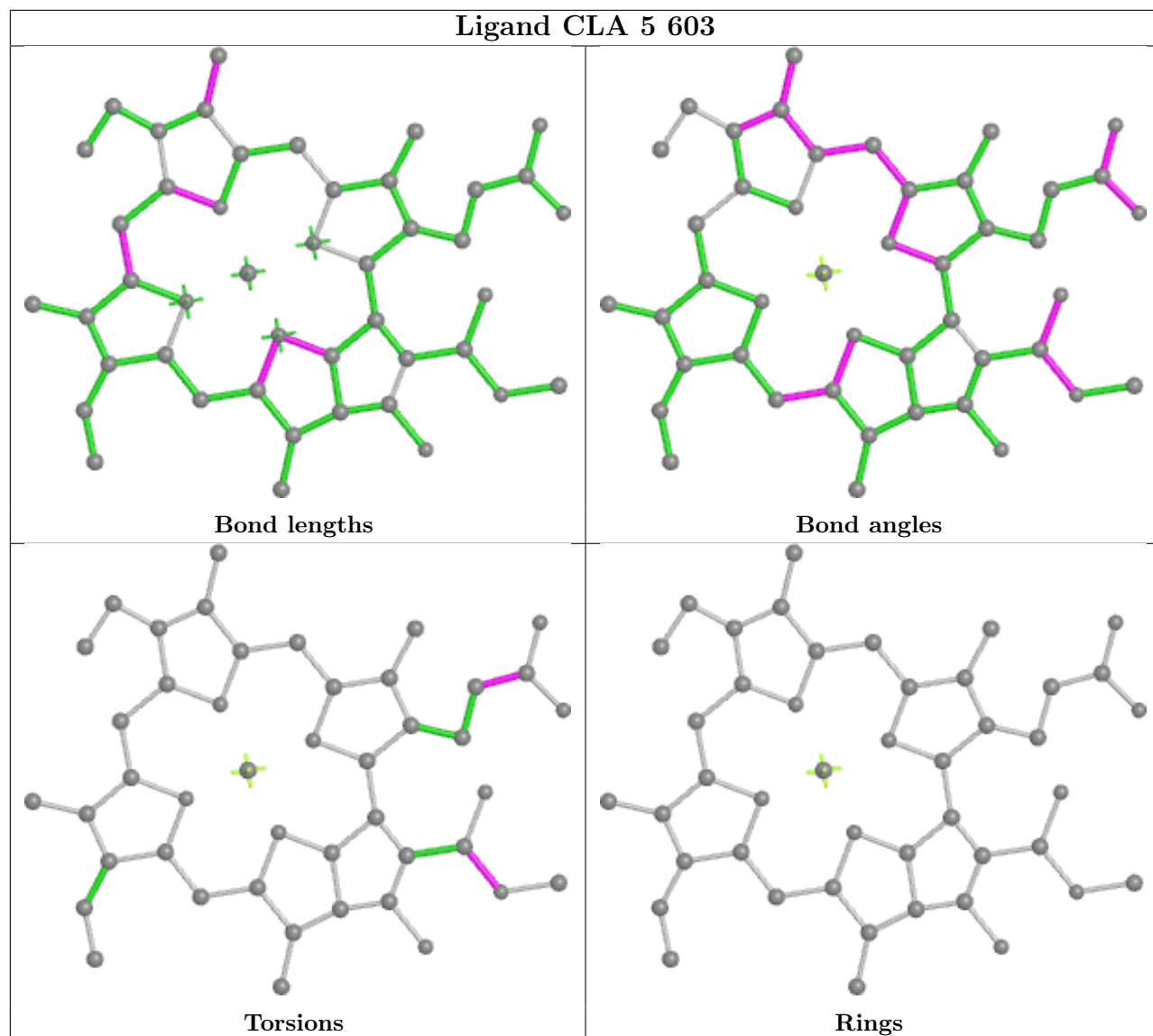


Torsions

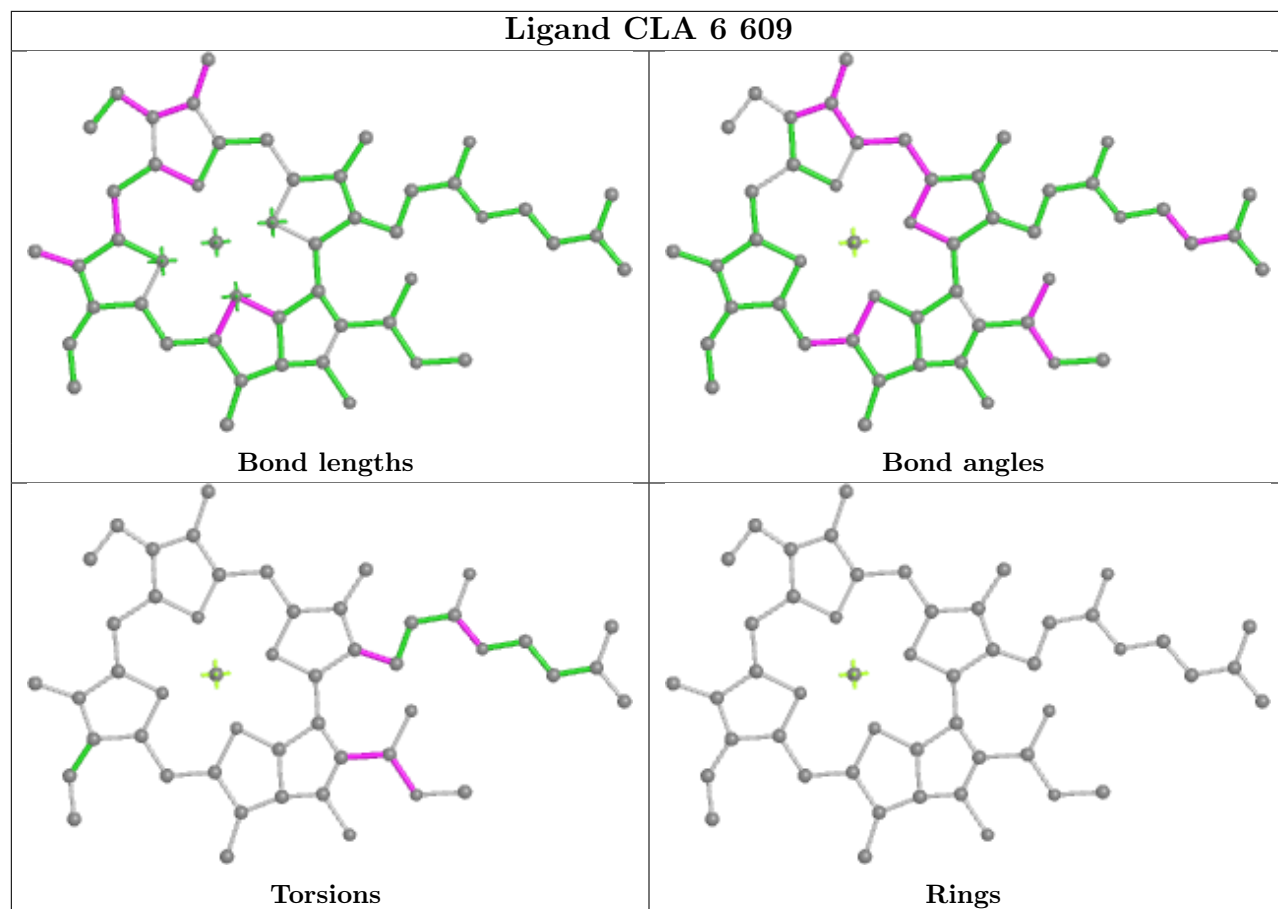


Rings

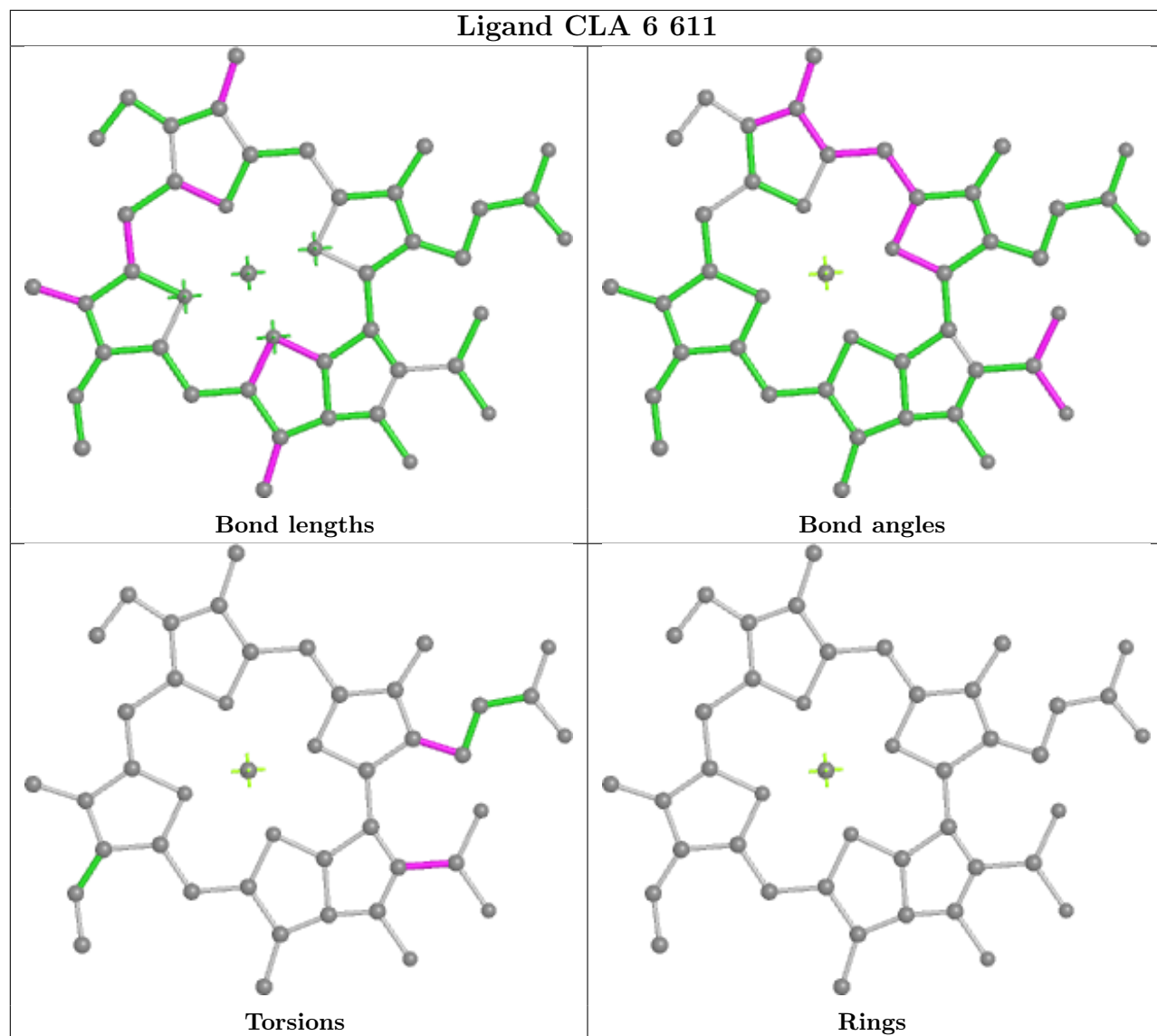
Ligand CLA 5 603



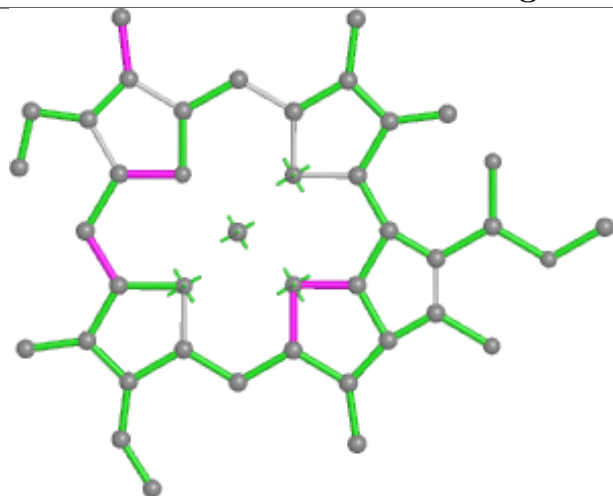
Ligand CLA 6 609



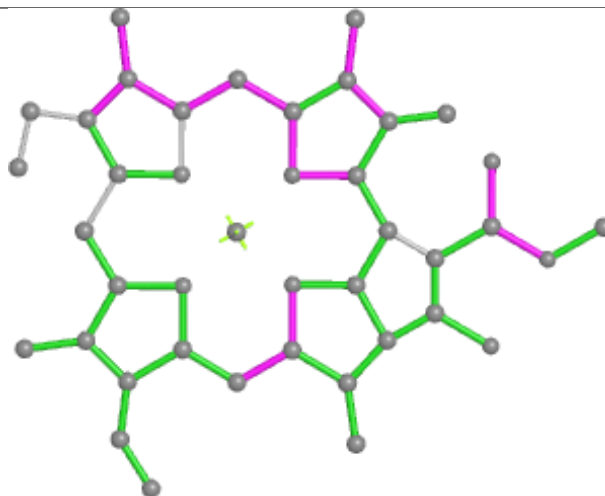
Ligand CLA 6 611



Ligand CLA c 611



Bond lengths



Bond angles

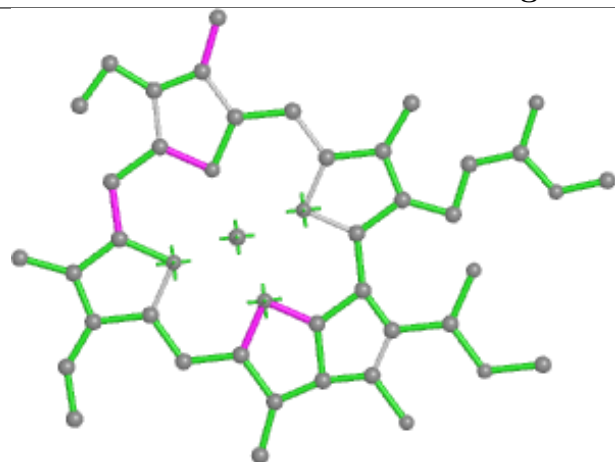


Torsions

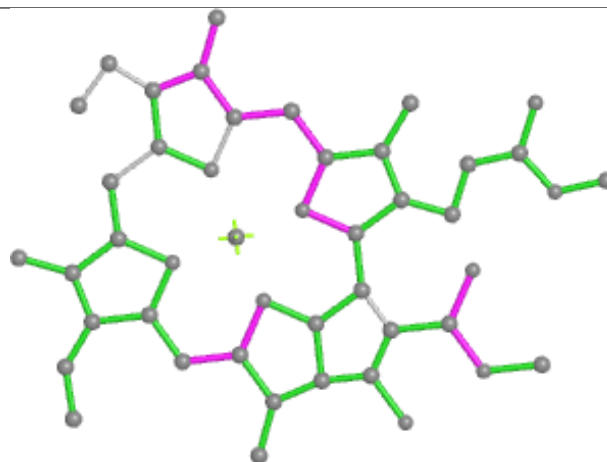


Rings

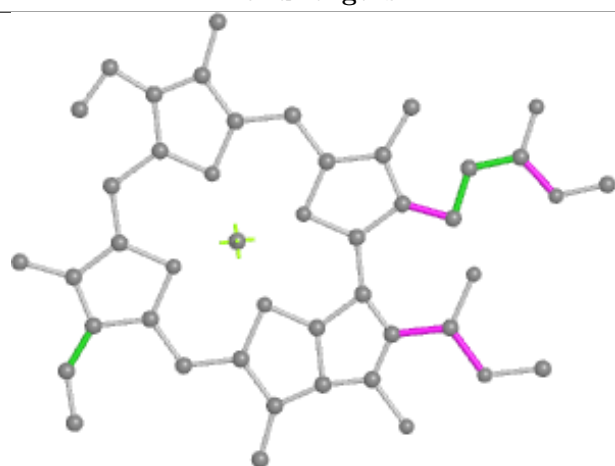
Ligand CLA 5 605



Bond lengths



Bond angles

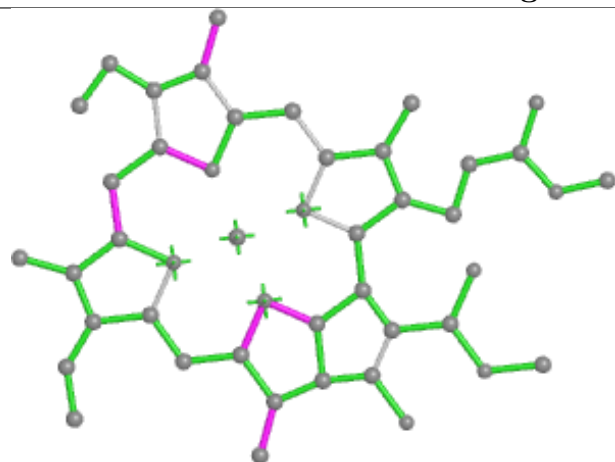


Torsions

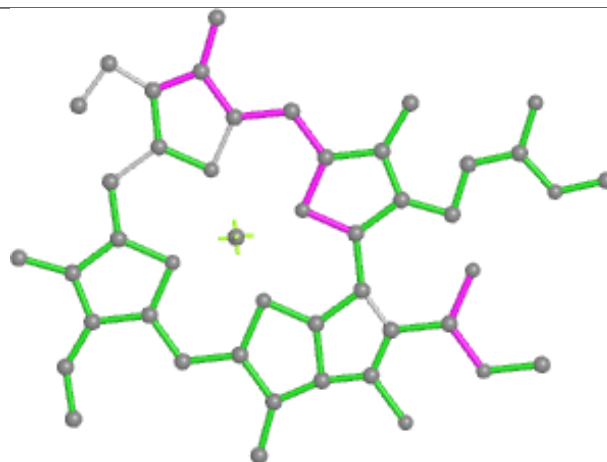


Rings

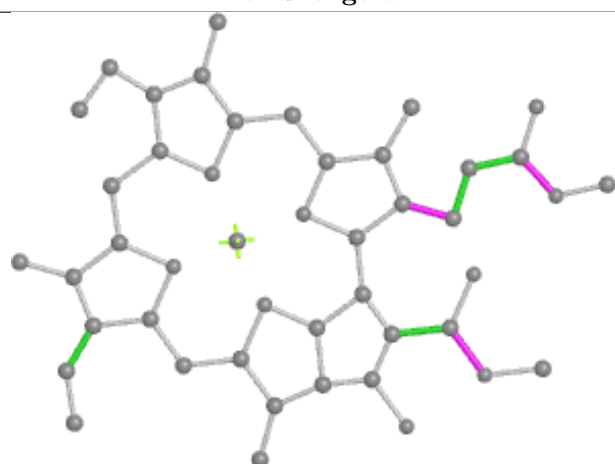
Ligand CLA 9 310



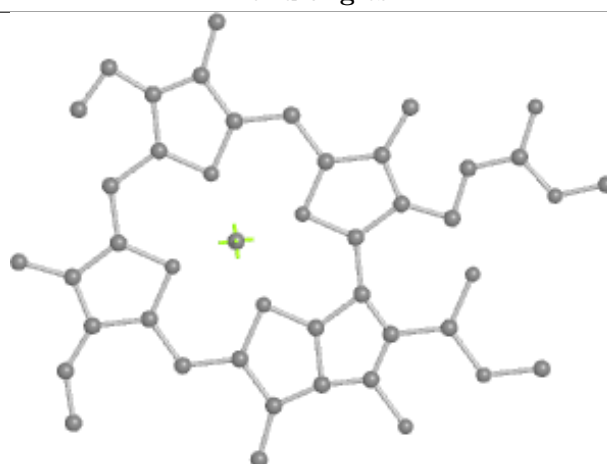
Bond lengths



Bond angles

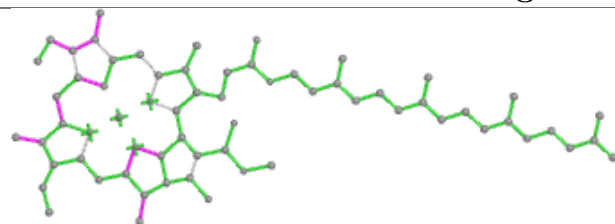


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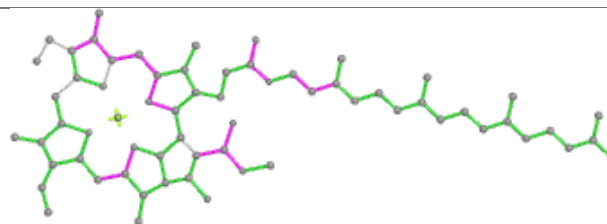


Rings

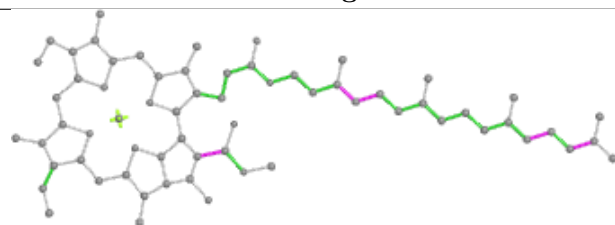
Ligand CLA B 808



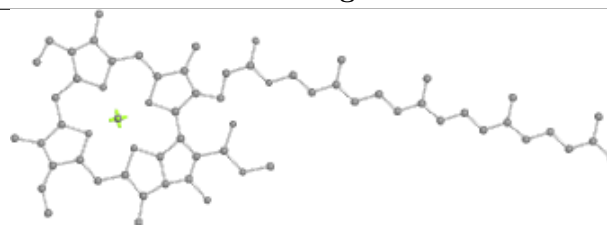
Bond lengths



Bond angles

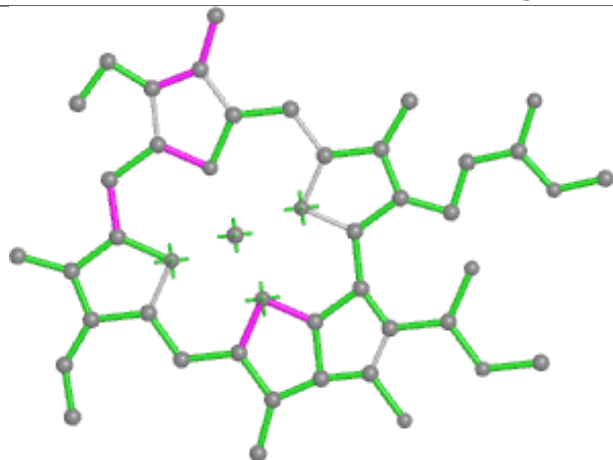


Torsions

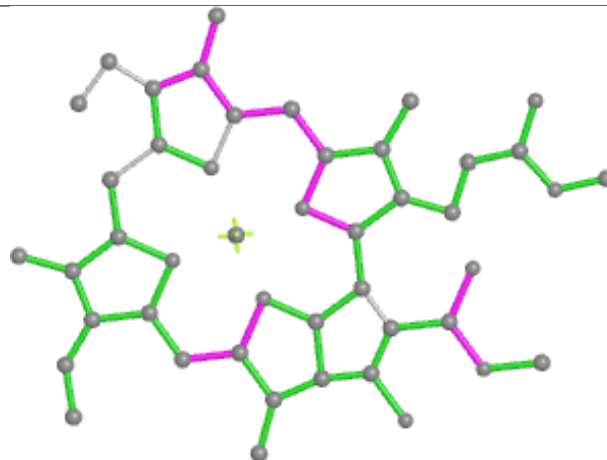


Rings

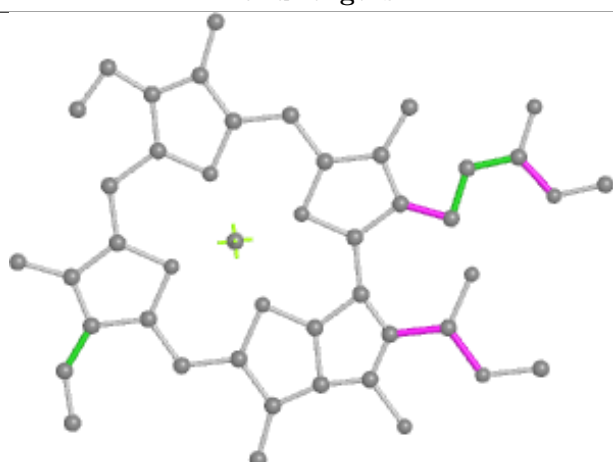
Ligand CLA k 304



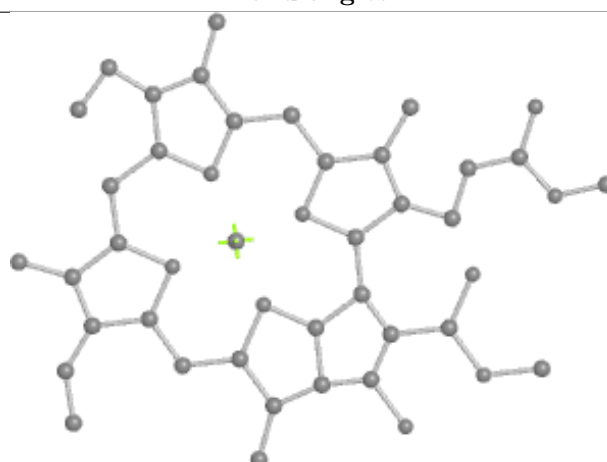
Bond lengths



Bond angles

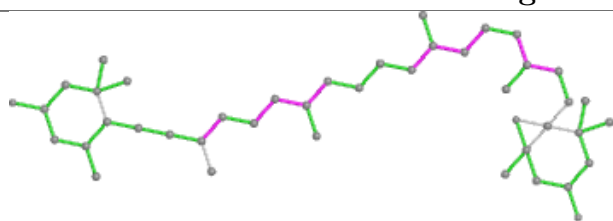


Torsions

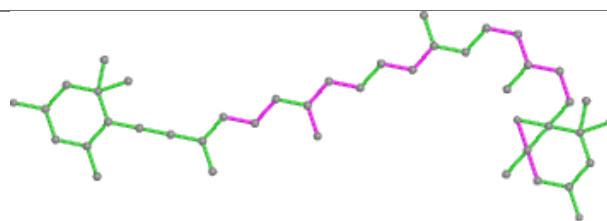


Rings

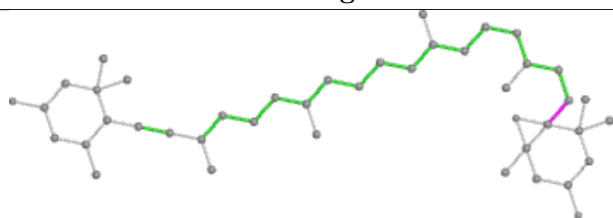
Ligand DD6 k 314



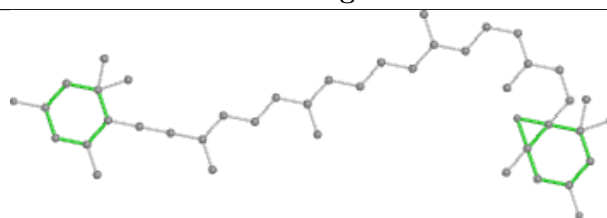
Bond lengths



Bond angles

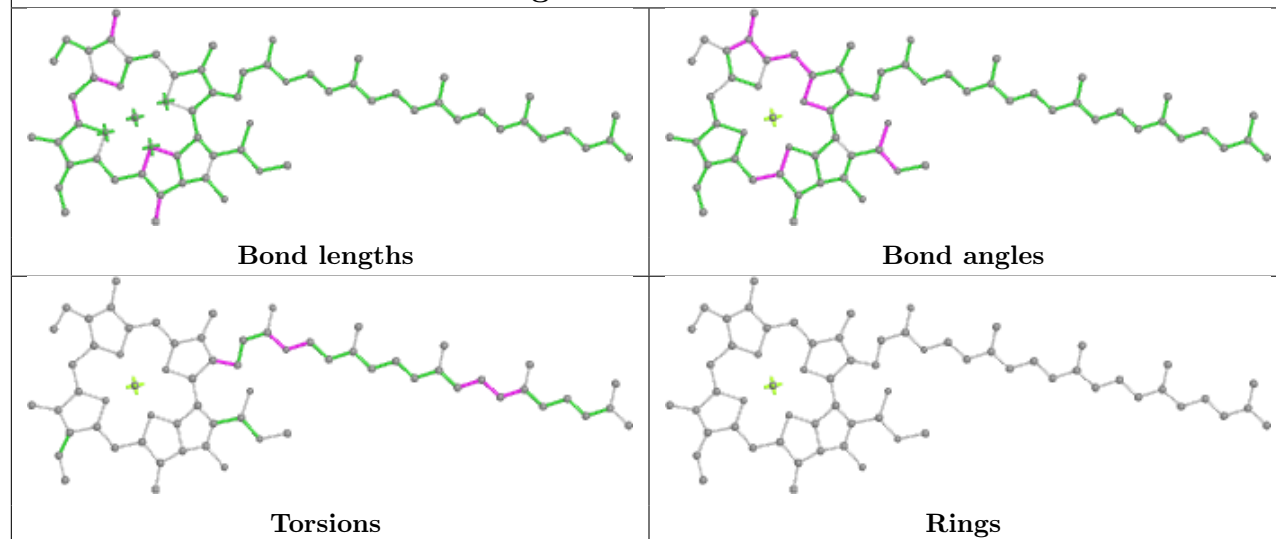


Torsions

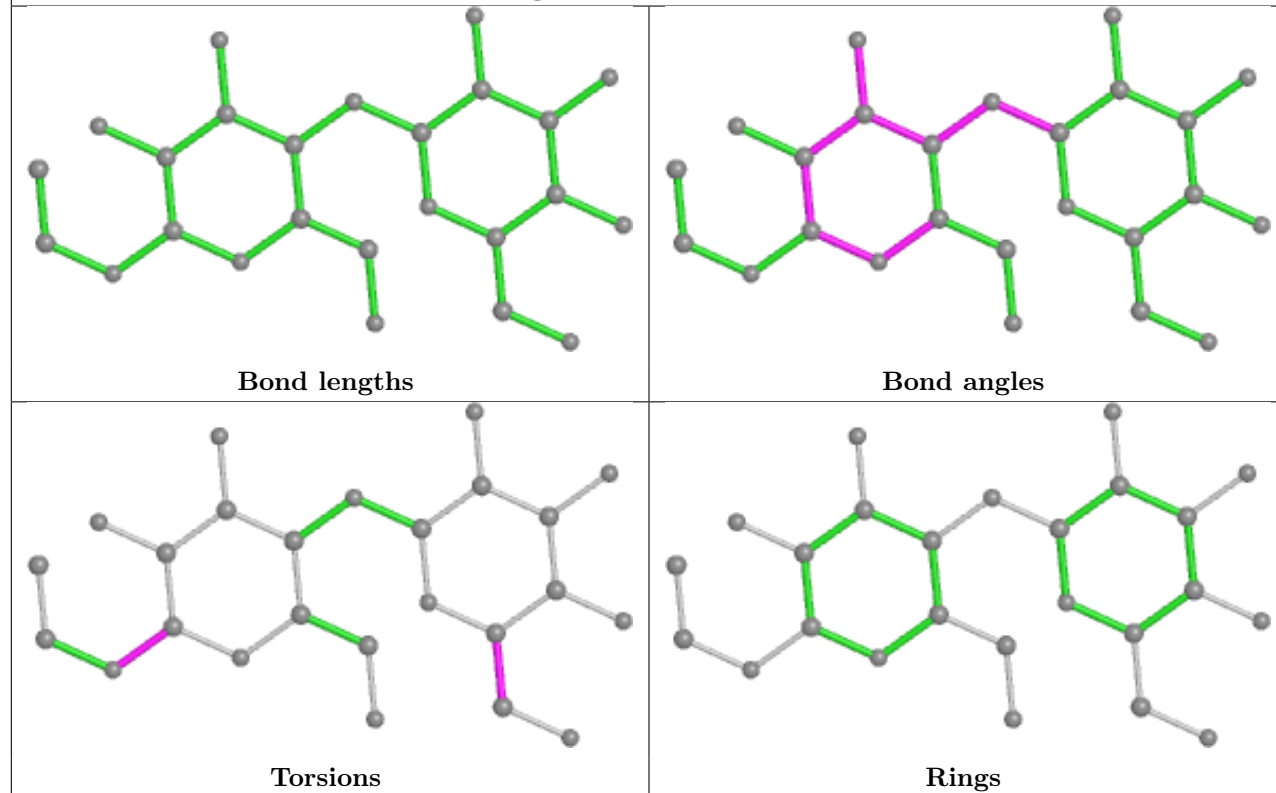


Rings

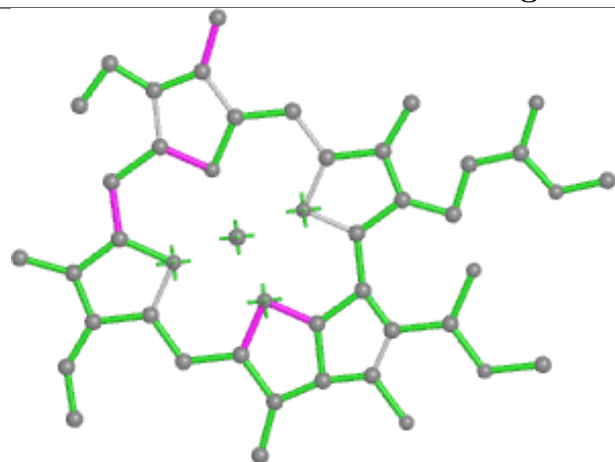
Ligand CLA R 103



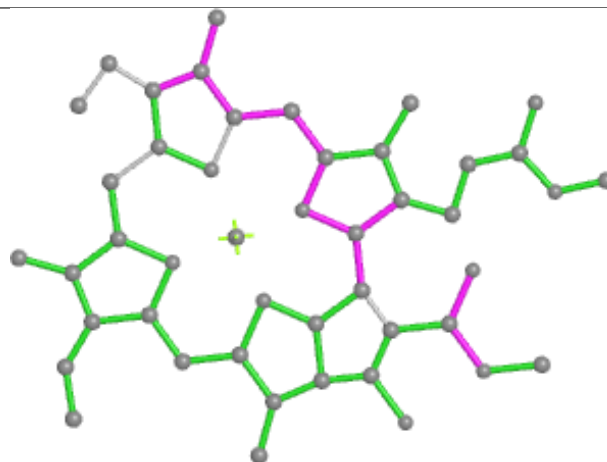
Ligand LMT A 851



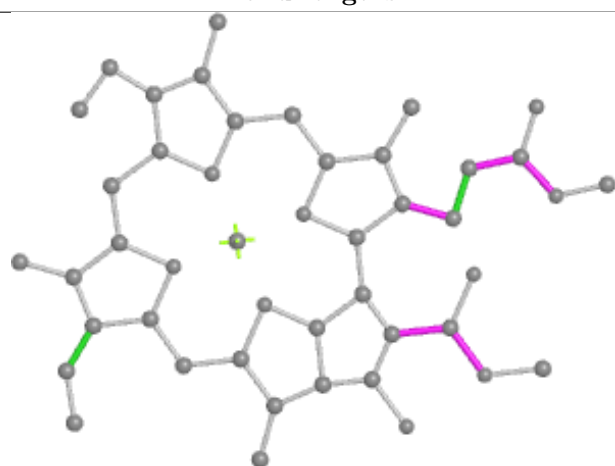
Ligand CLA 9 309



Bond lengths



Bond angles

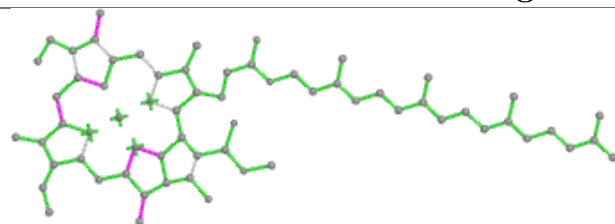


Torsions

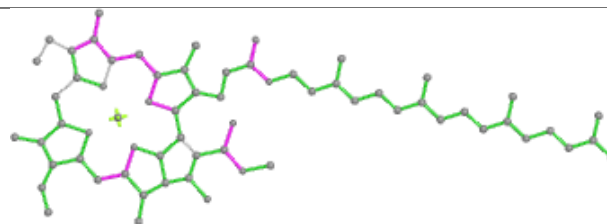


Rings

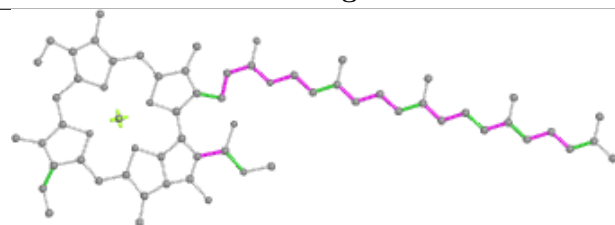
Ligand CLA B 831



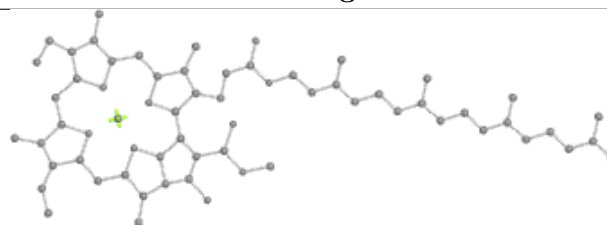
Bond lengths



Bond angles

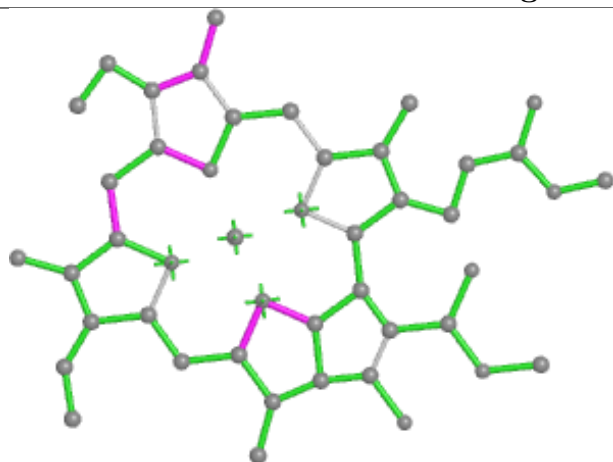


Torsions

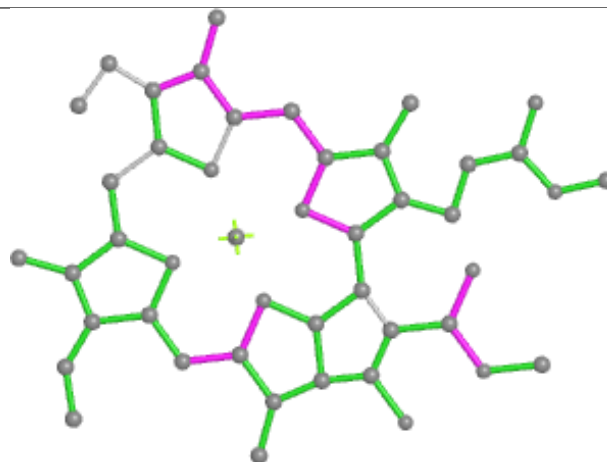


Rings

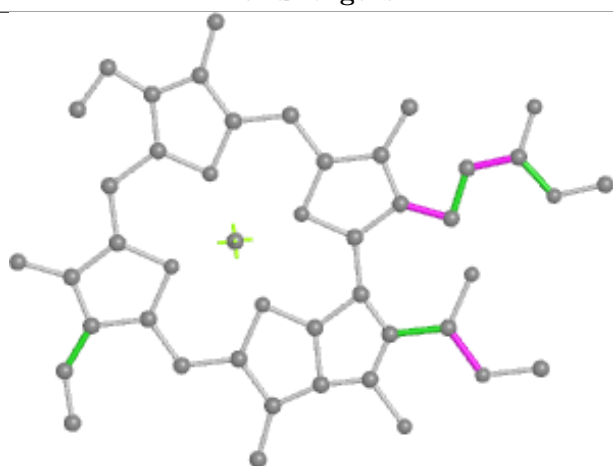
Ligand CLA t 308



Bond lengths



Bond angles

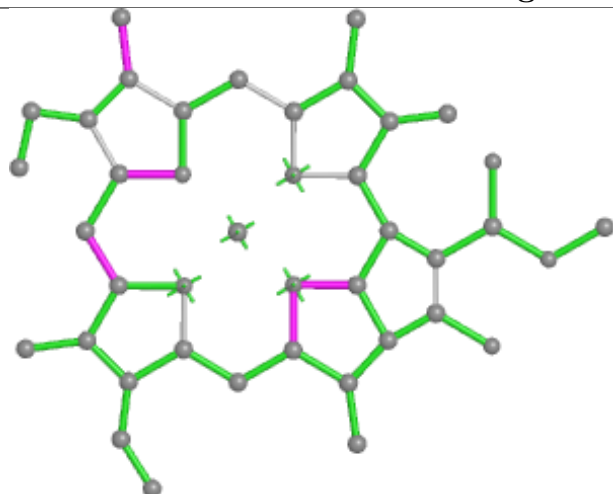


Torsions

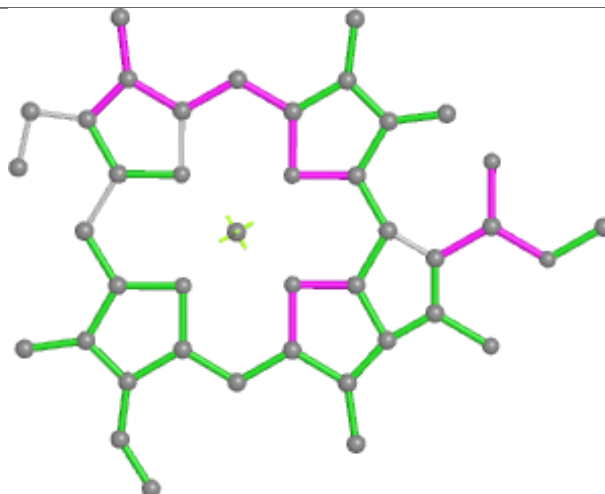


Rings

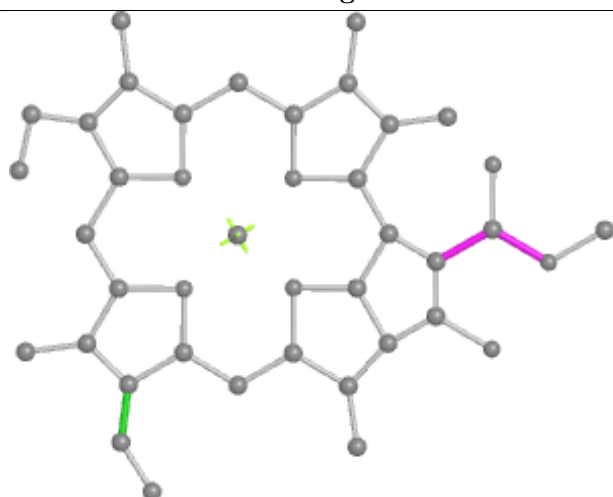
Ligand CLA k 308



Bond lengths



Bond angles

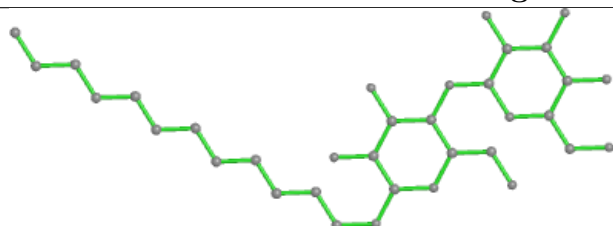


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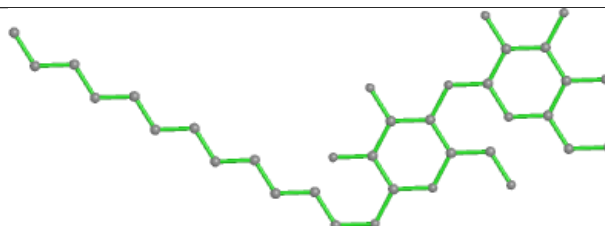


Rings

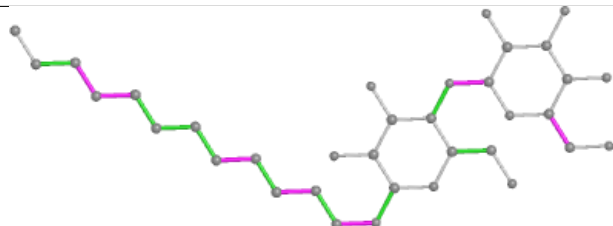
Ligand LMT A 854



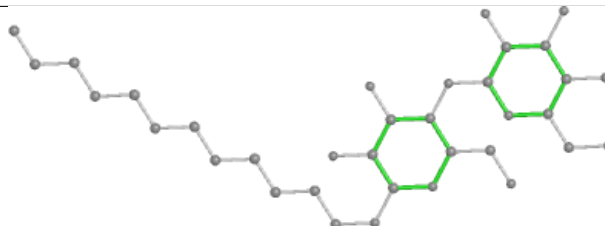
Bond lengths



Bond angles

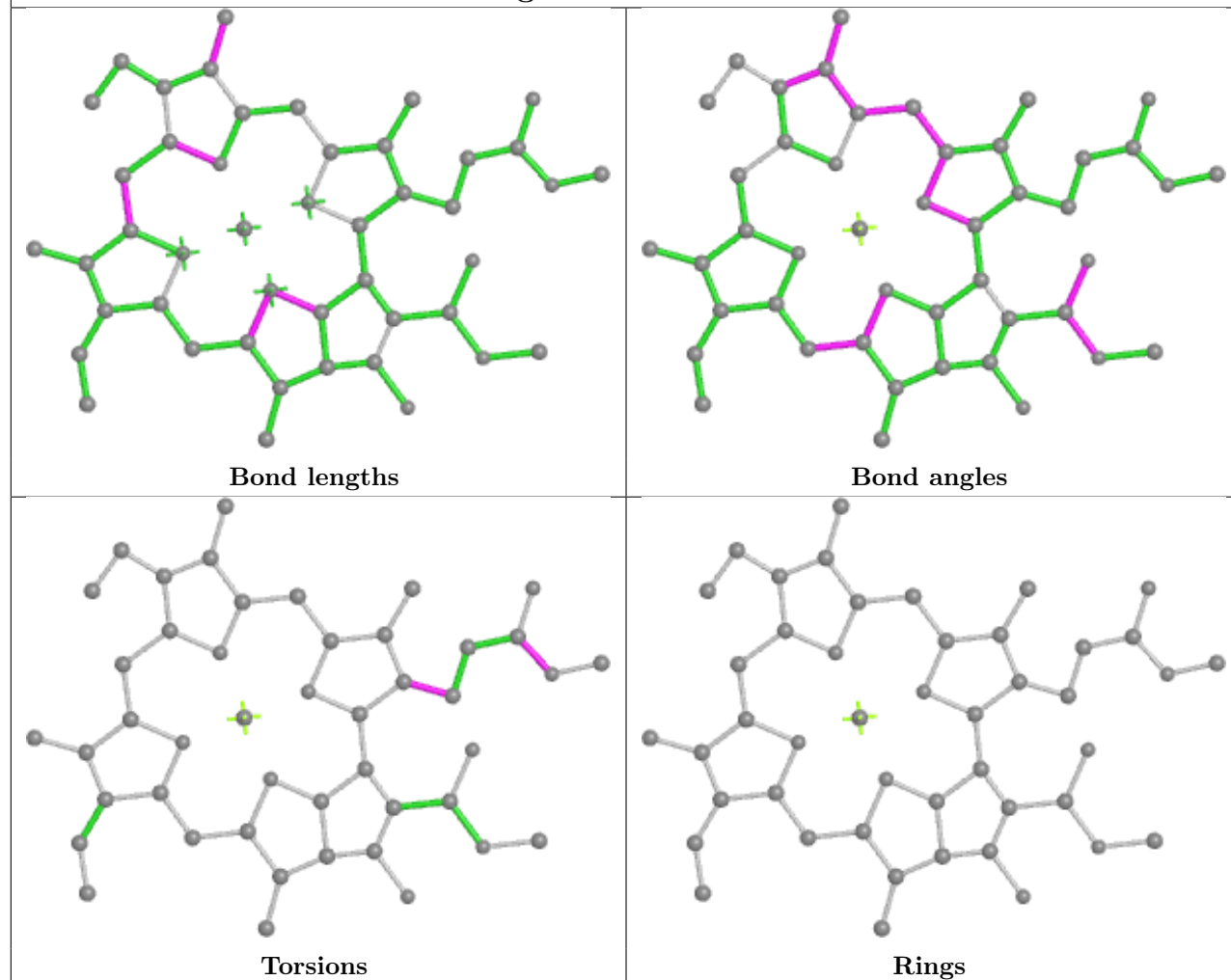


Torsions

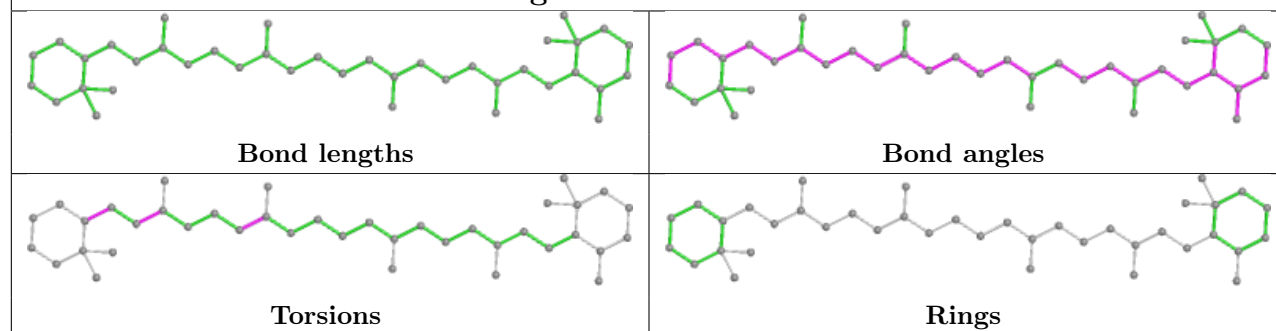


Rings

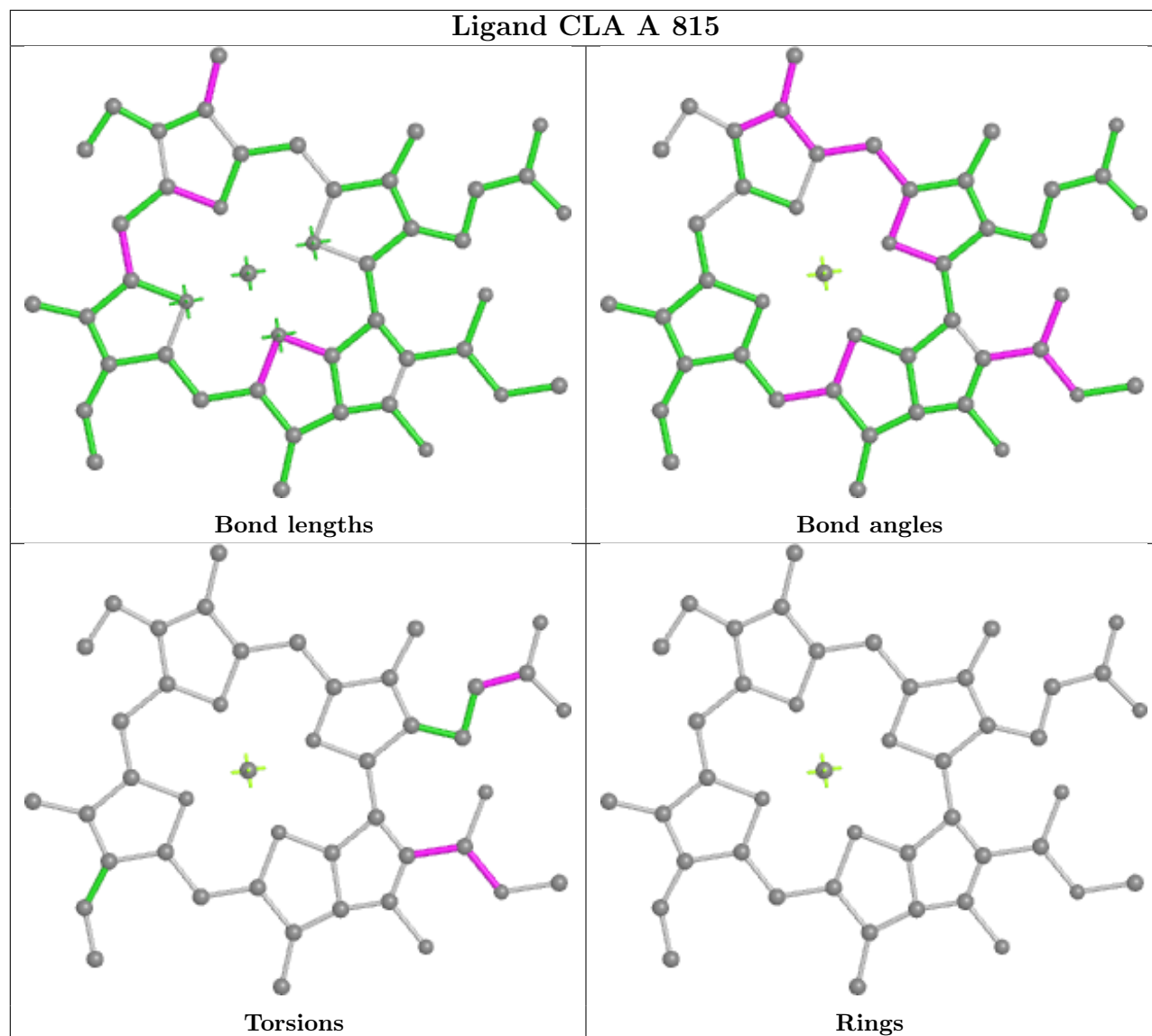
Ligand CLA 6 607

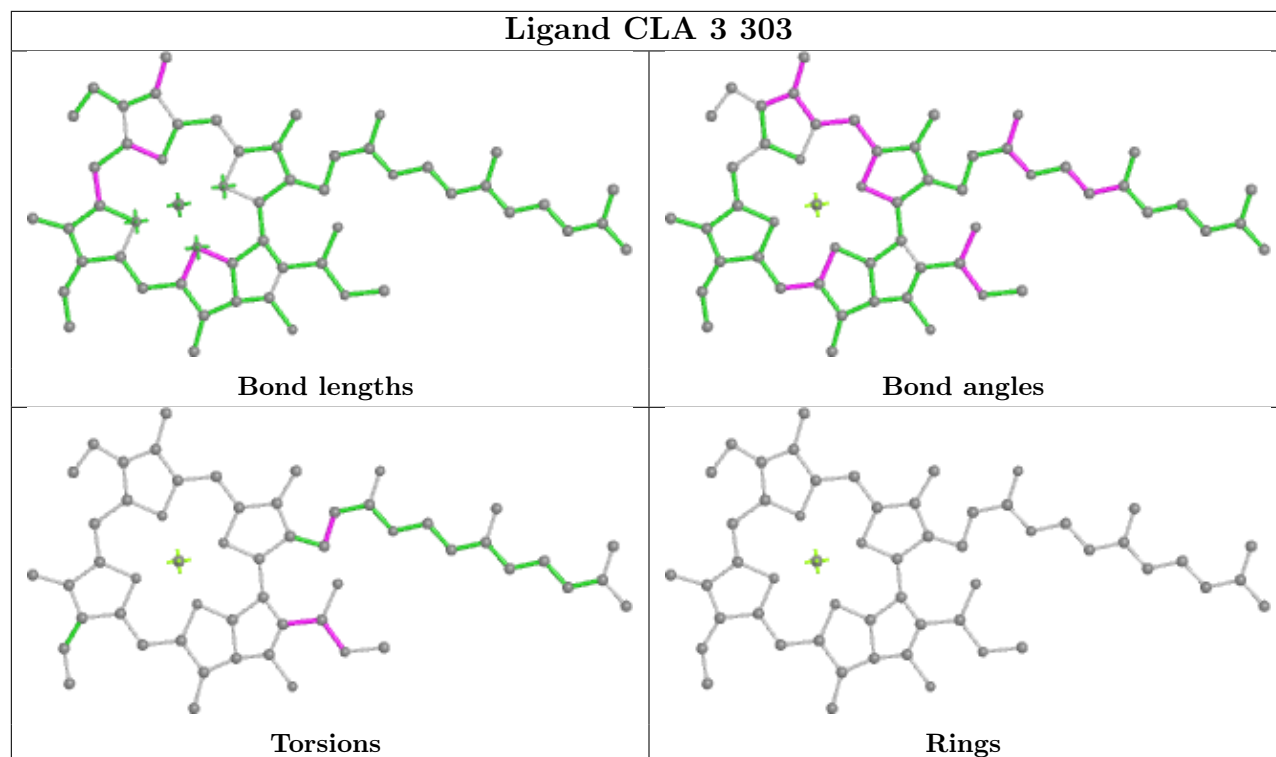
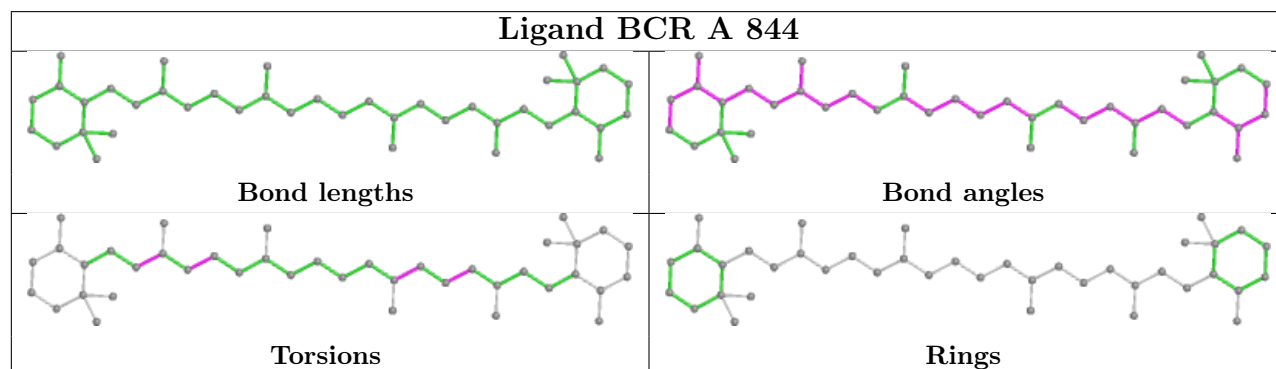


Ligand BCR A 845

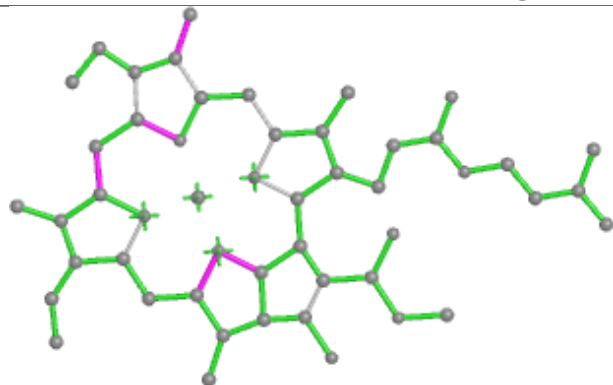


Ligand CLA A 815

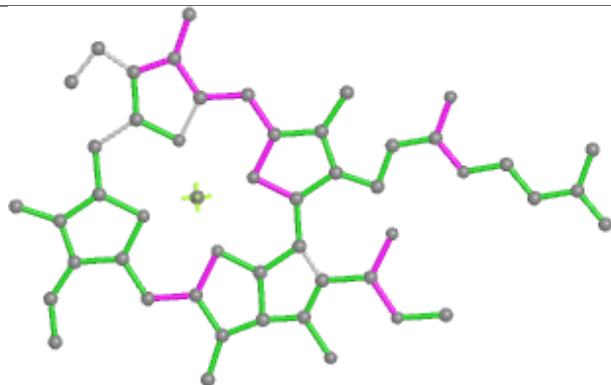


Ligand CLA 3 303**Ligand BCR A 844**

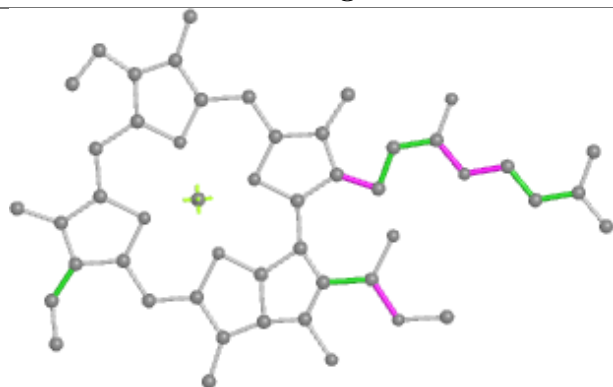
Ligand CLA A 814



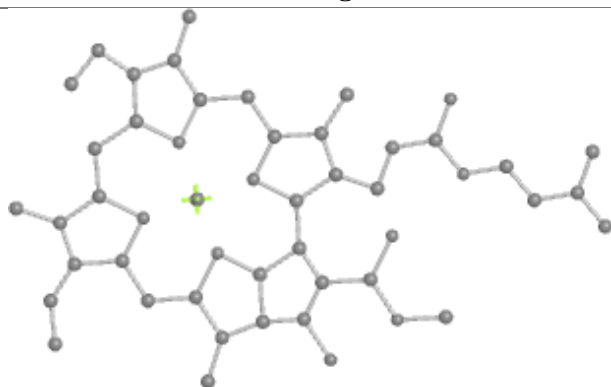
Bond lengths



Bond angles

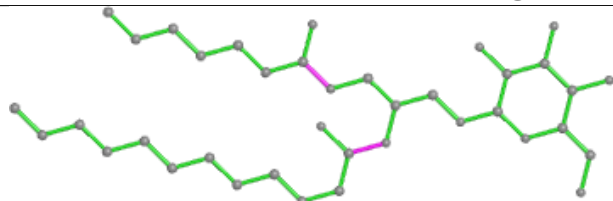


Torsions

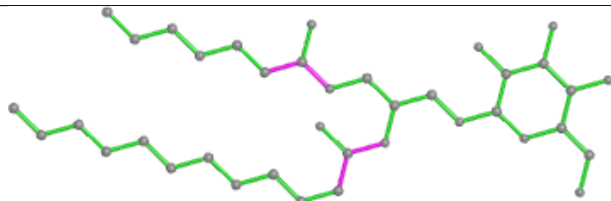


Rings

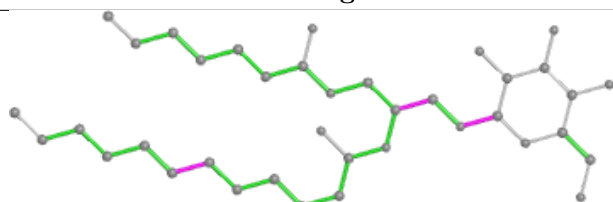
Ligand LMG A 855



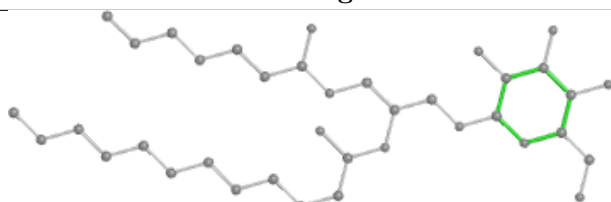
Bond lengths



Bond angles

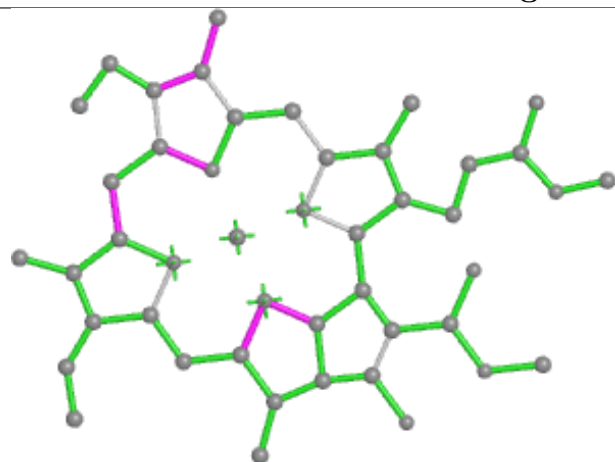


Torsions

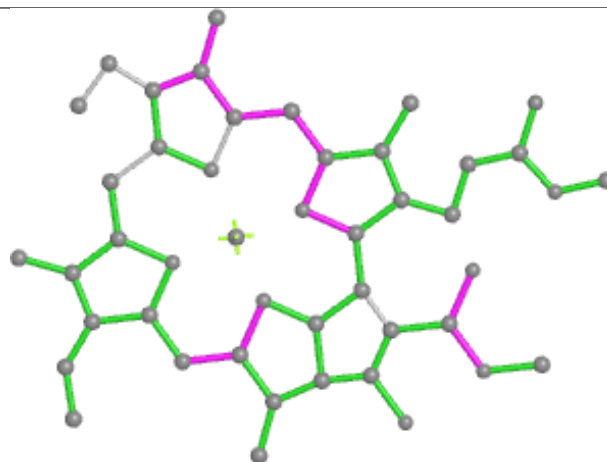


Rings

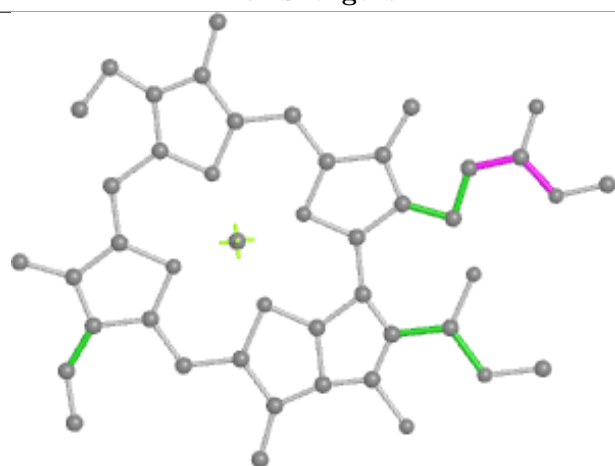
Ligand CLA 4 603



Bond lengths



Bond angles

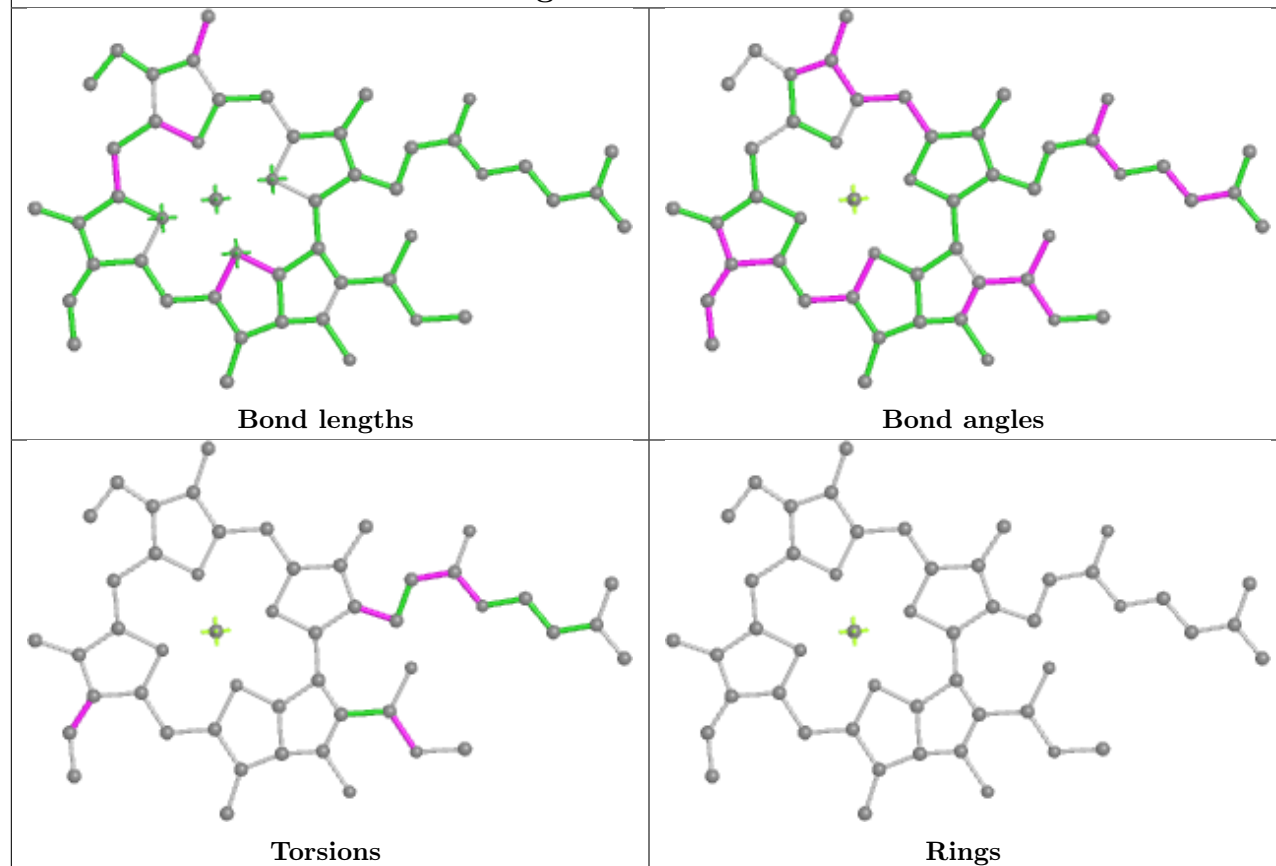


Torsions

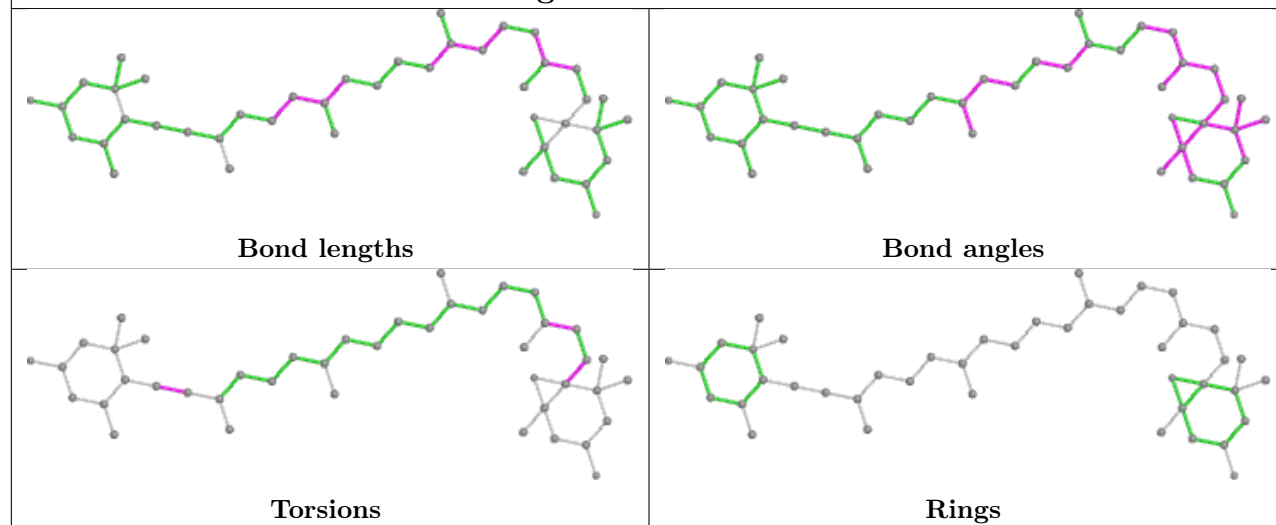


Rings

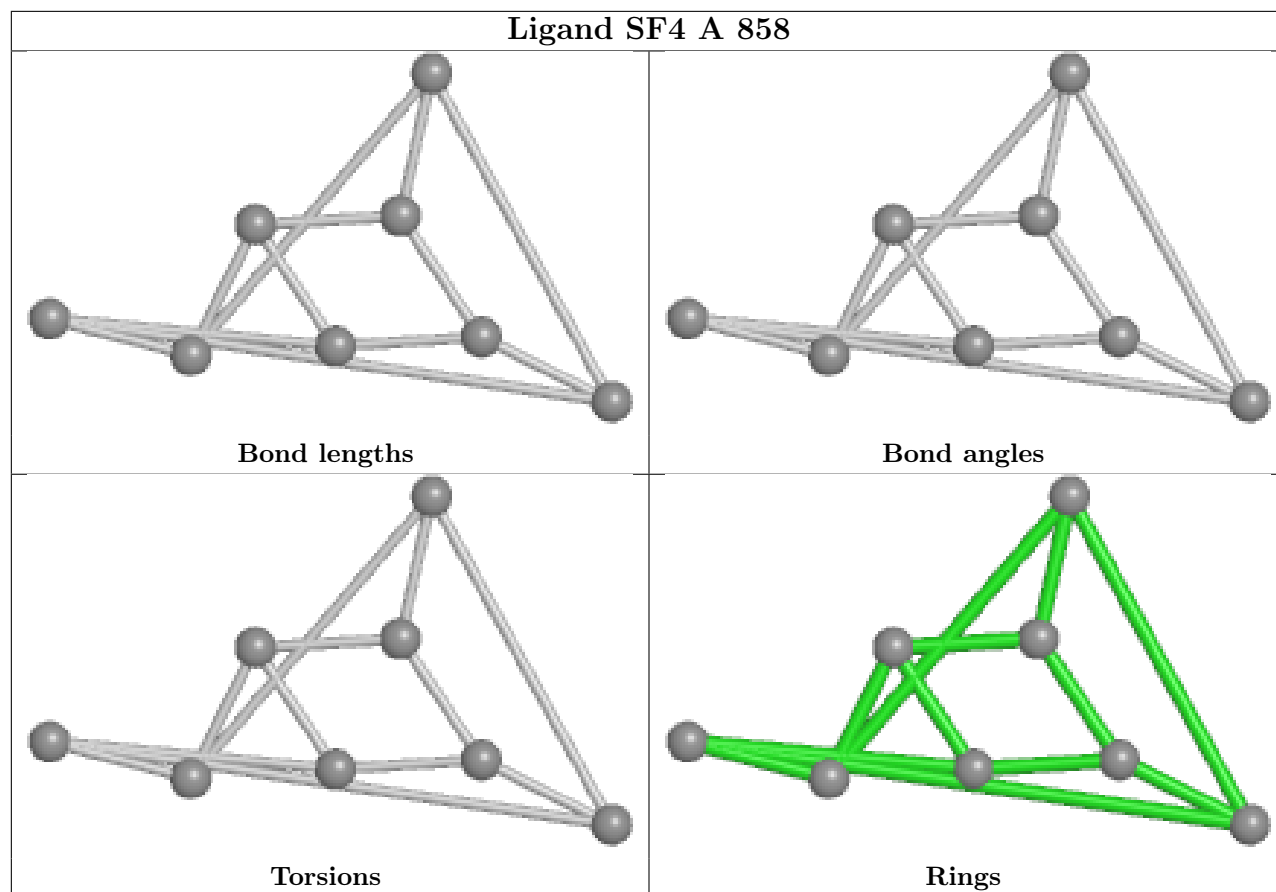
Ligand CLA 7 602



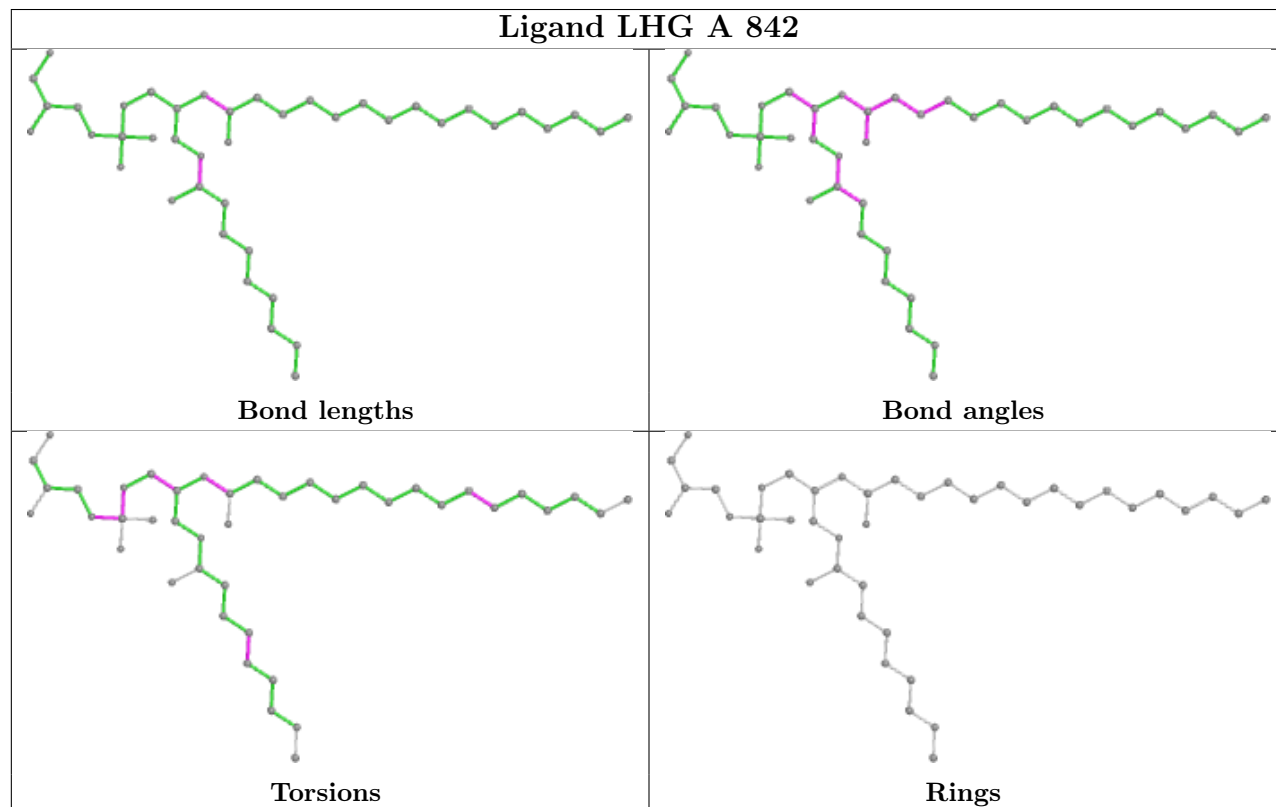
Ligand DD6 6 616

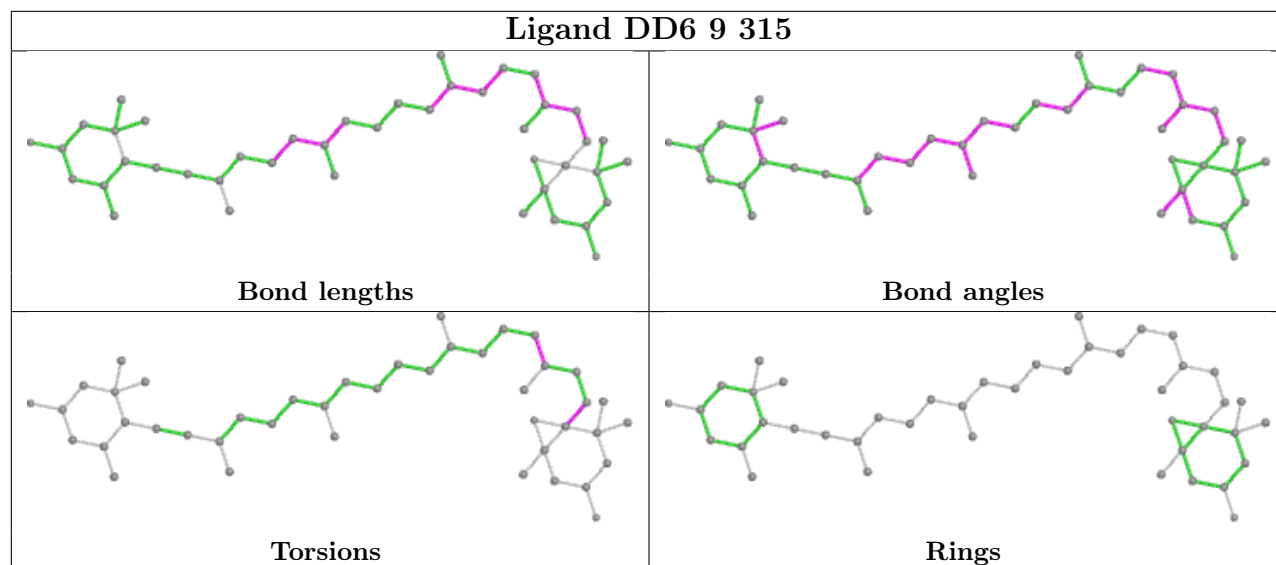
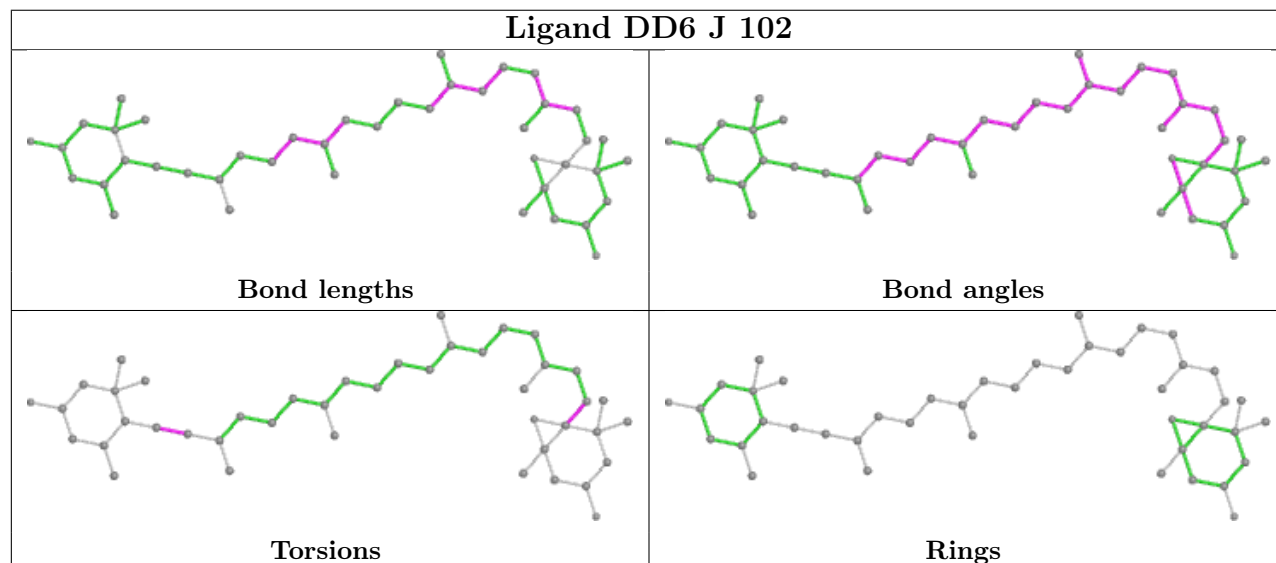
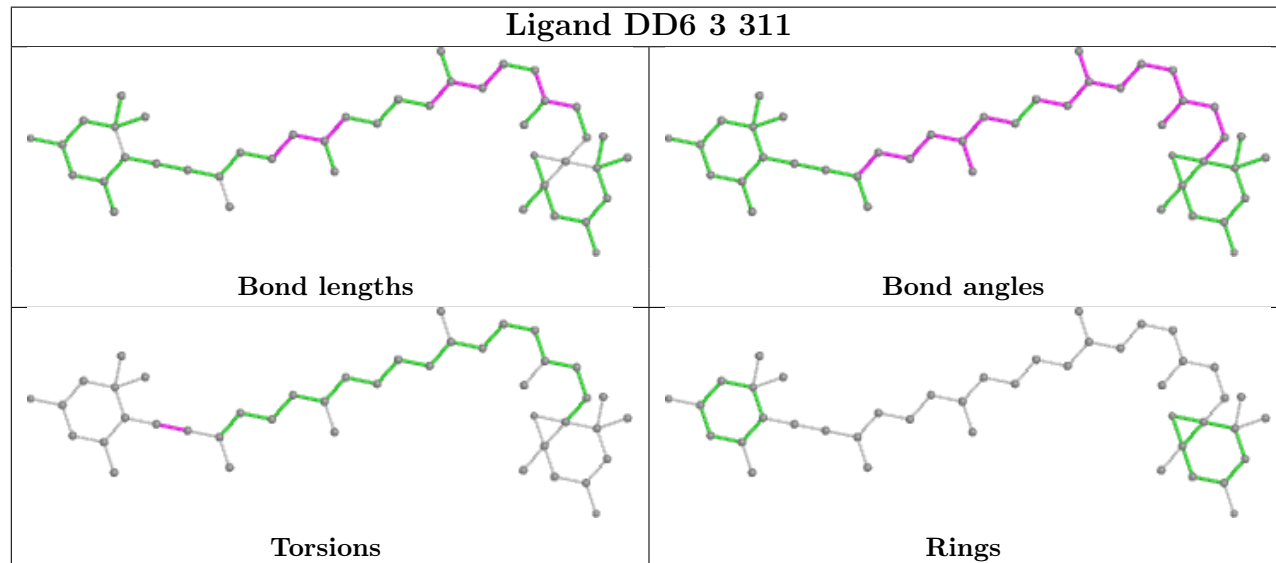


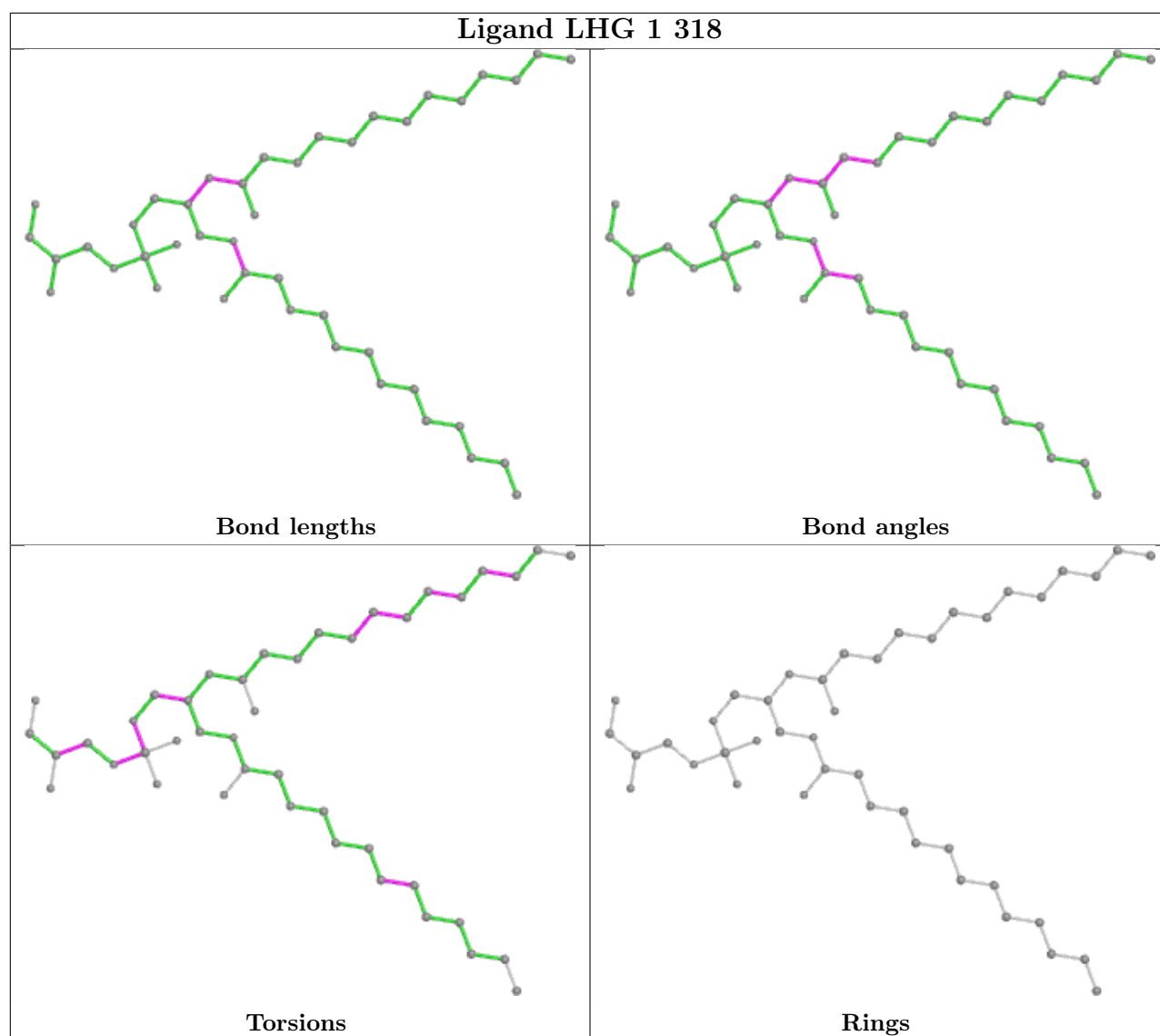
Ligand SF4 A 858



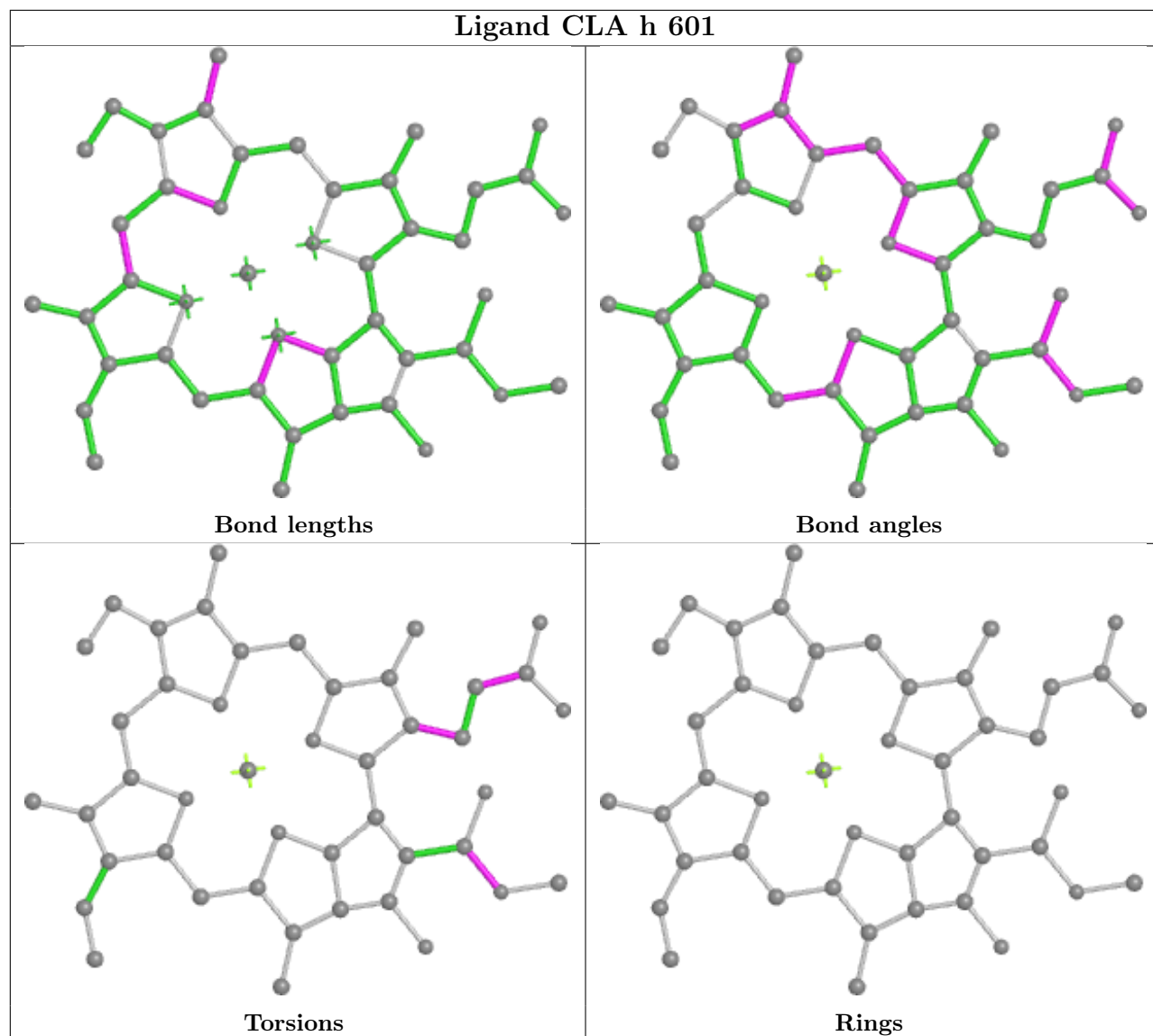
Ligand LHG A 842



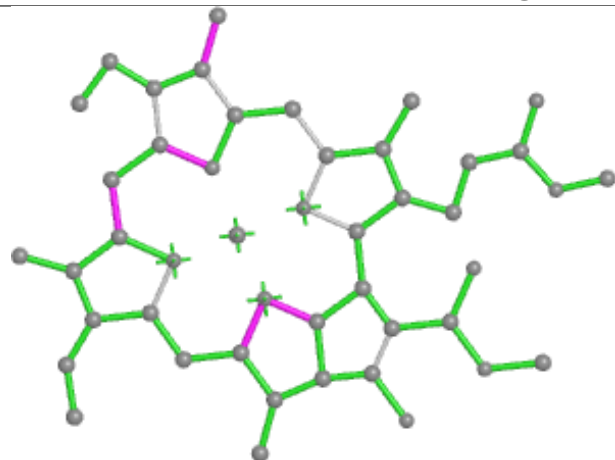
Ligand DD6 9 315**Ligand DD6 J 102****Ligand DD6 3 311**



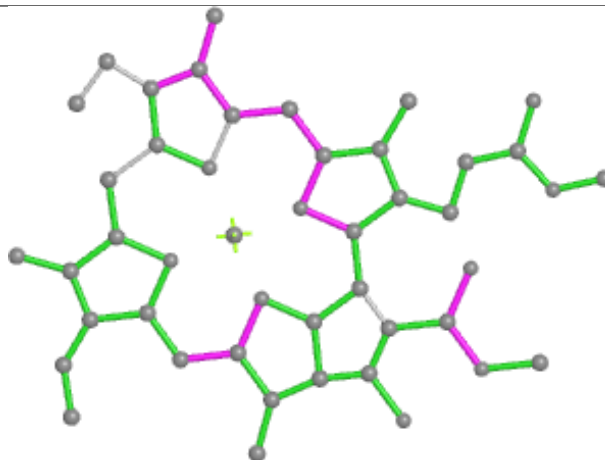
Ligand CLA h 601



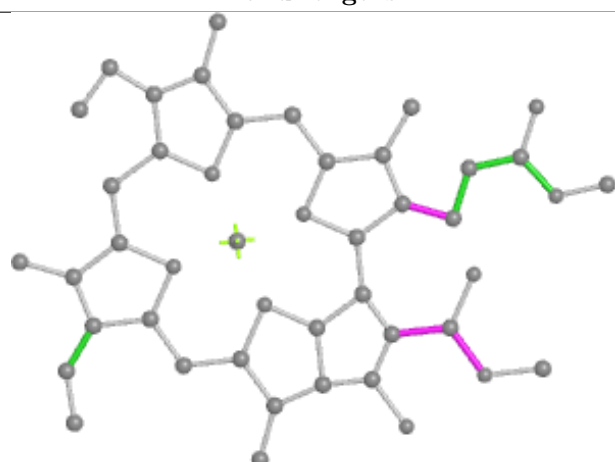
Ligand CLA A 809



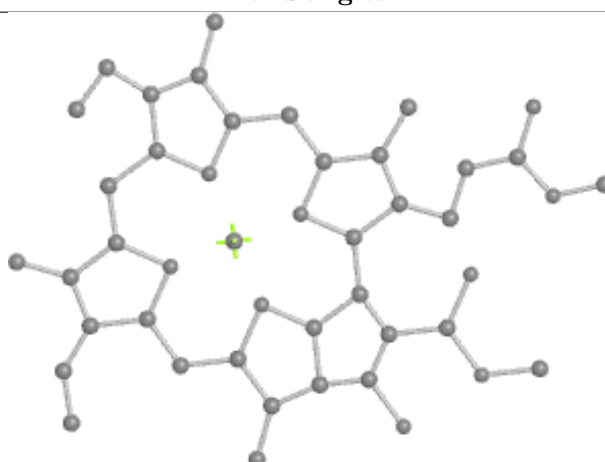
Bond lengths



Bond angles

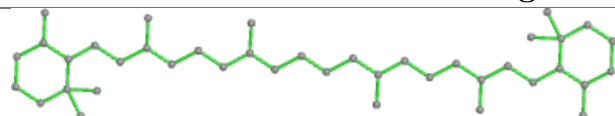


Torsions

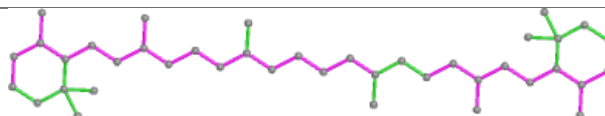


Rings

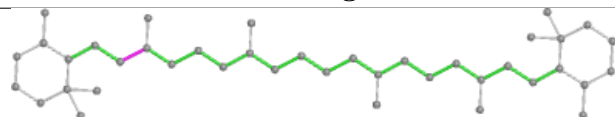
Ligand BCR 9 316



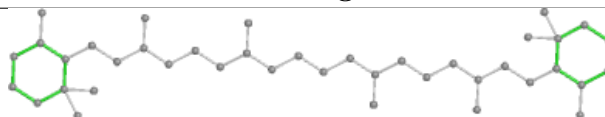
Bond lengths



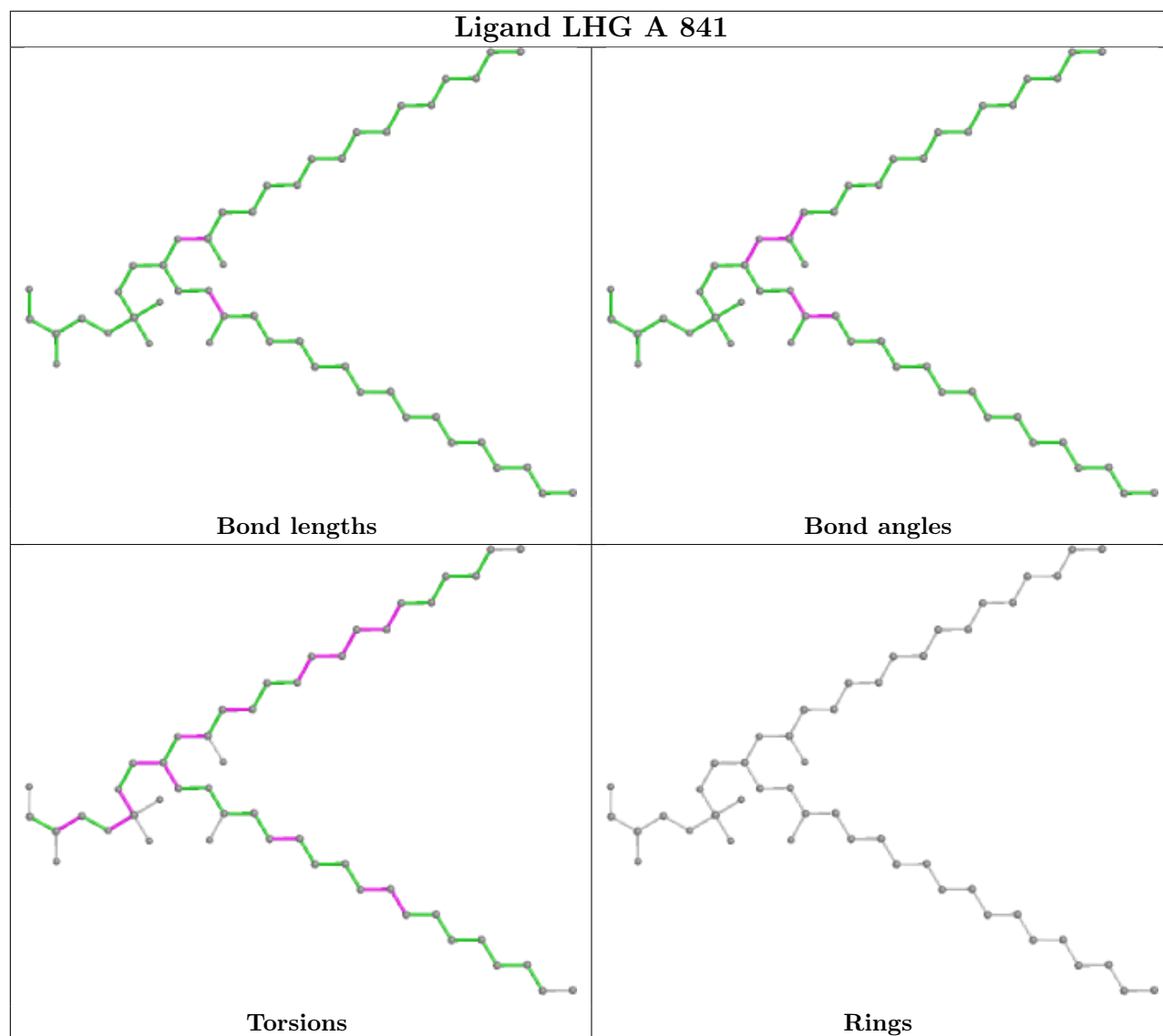
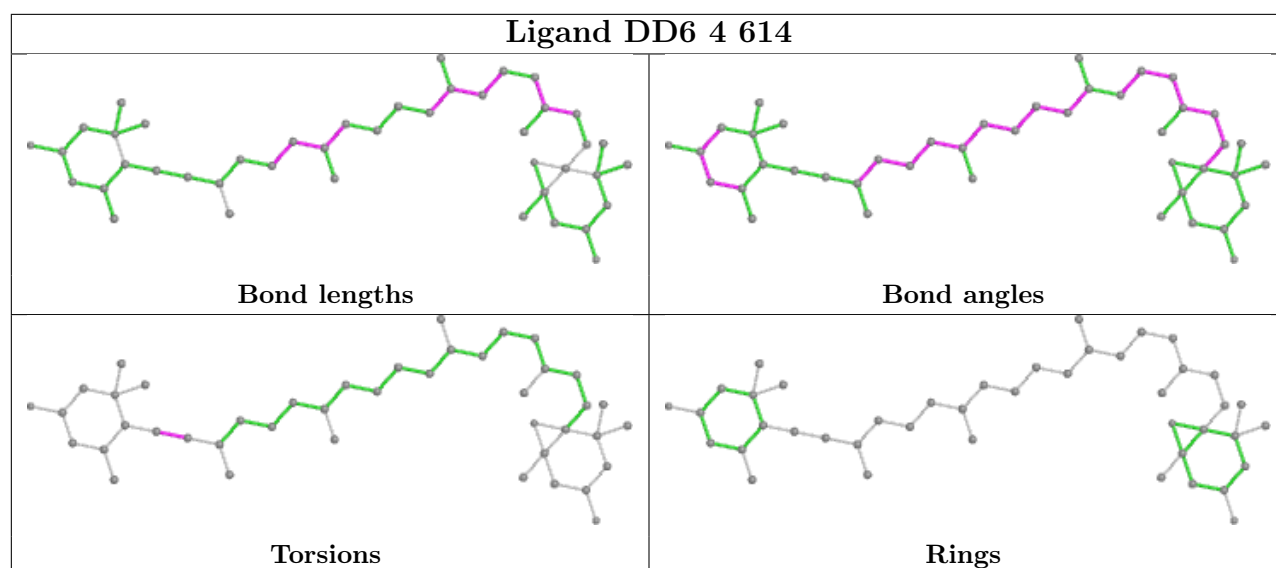
Bond angles



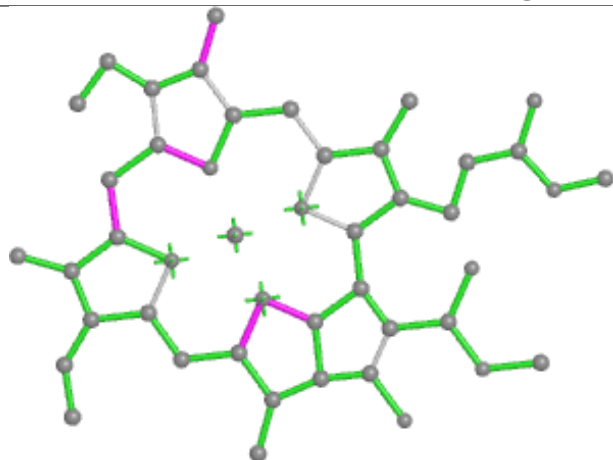
Torsions



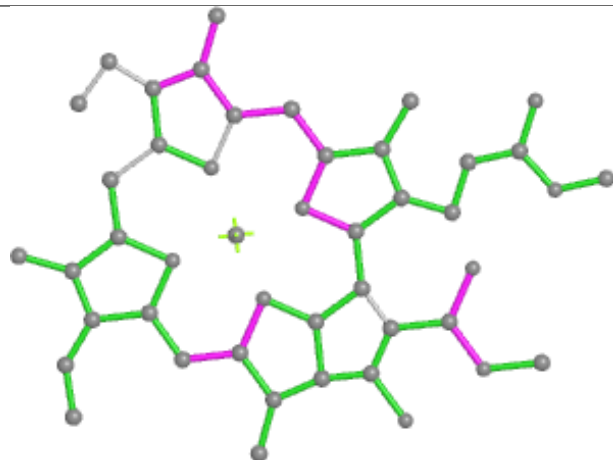
Rings



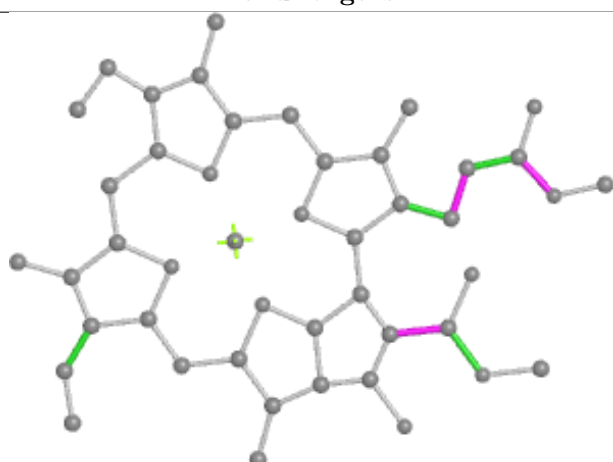
Ligand CLA 4 605



Bond lengths



Bond angles

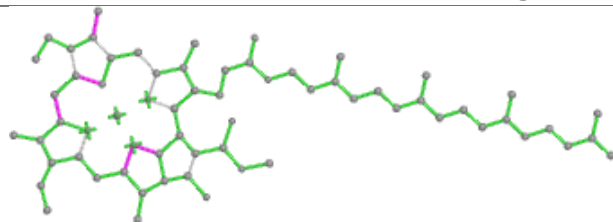


Torsions

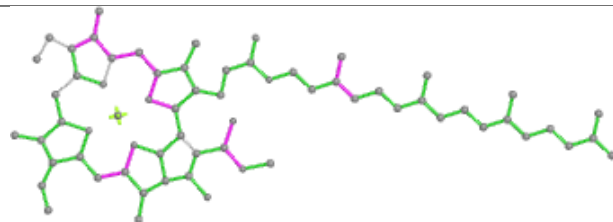


Rings

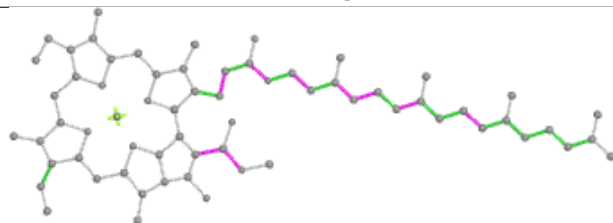
Ligand CLA B 837



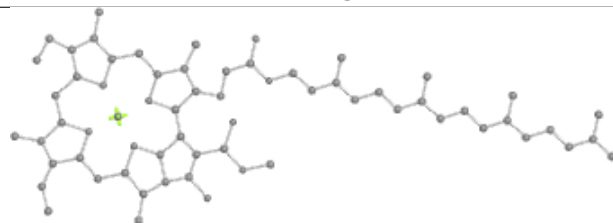
Bond lengths



Bond angles

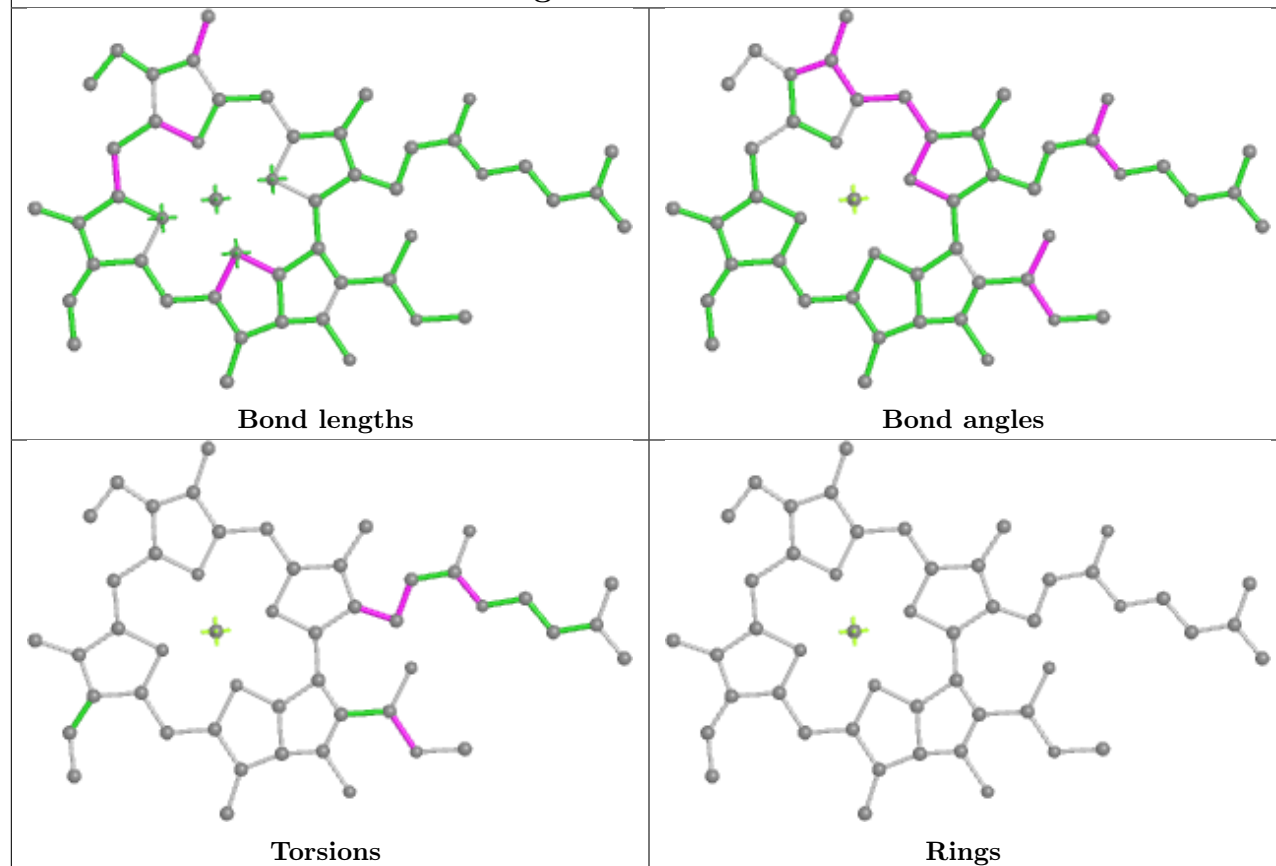


Torsions

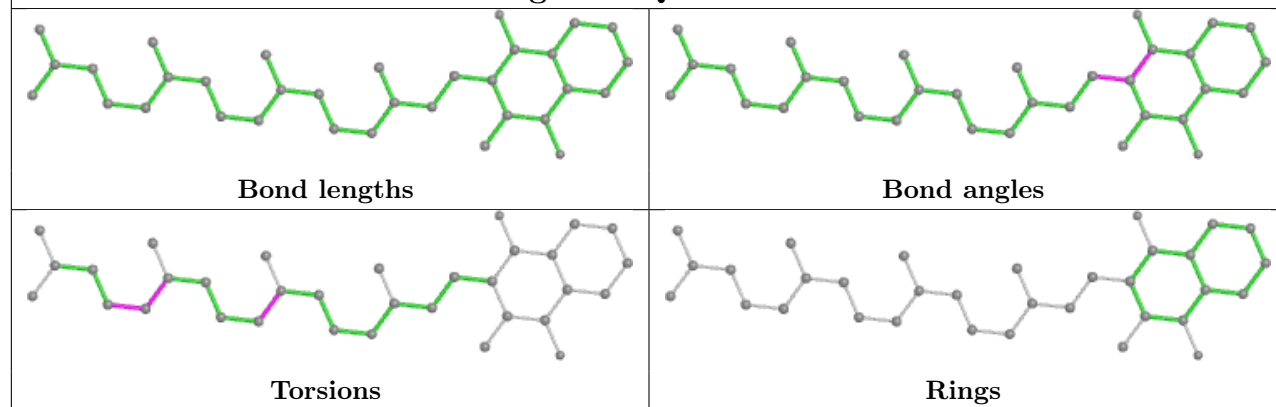


Rings

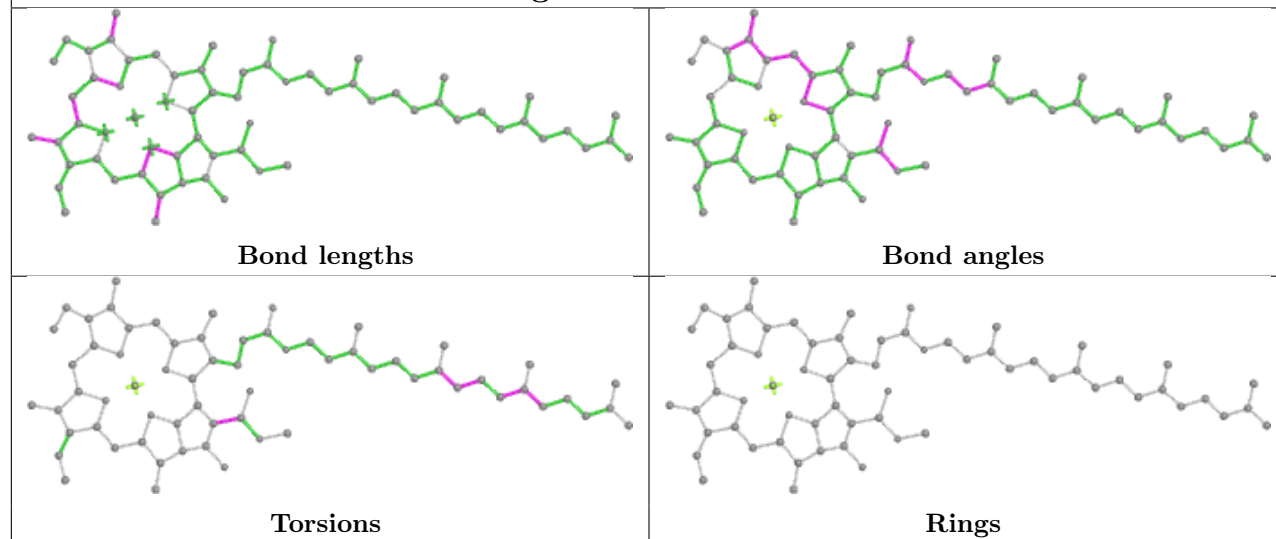
Ligand CLA F 203



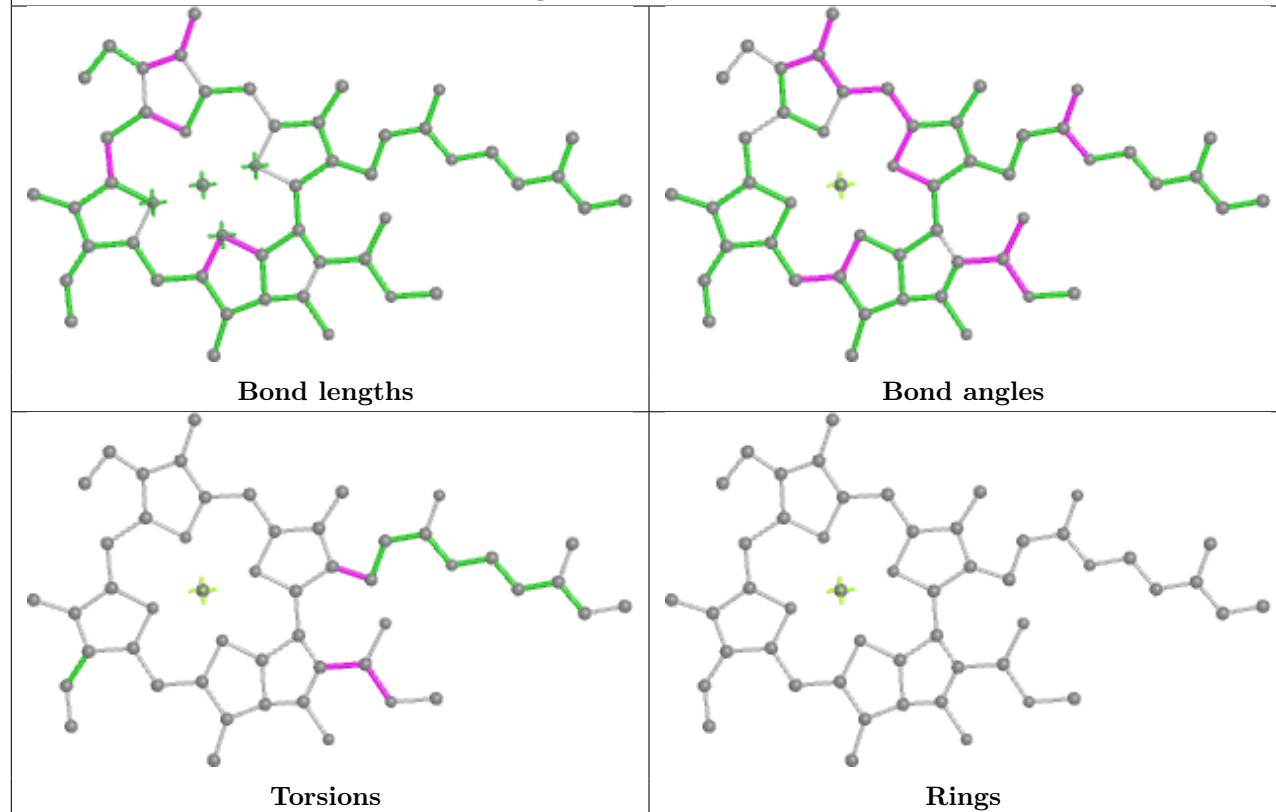
Ligand PQN A 839



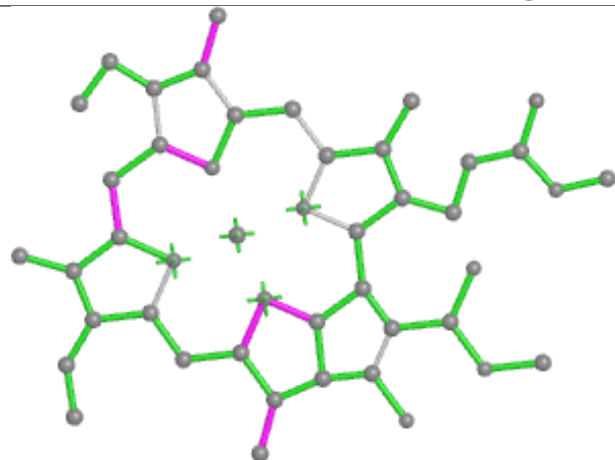
Ligand CLA A 857



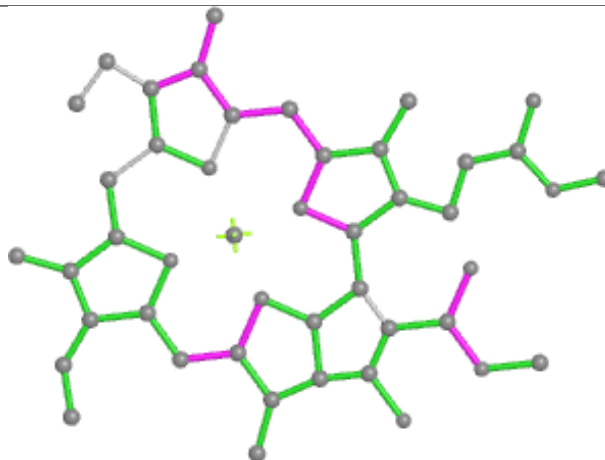
Ligand CLA A 835



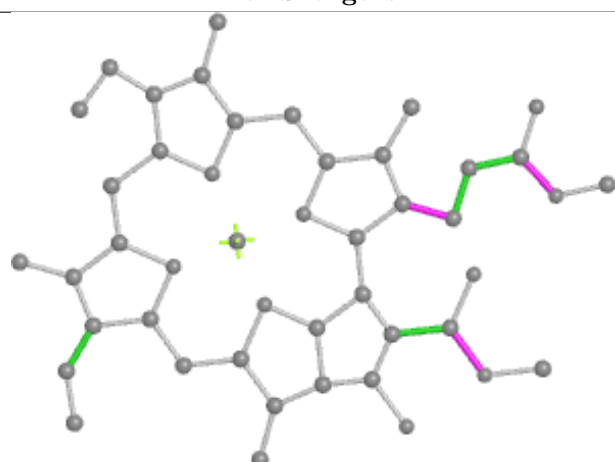
Ligand CLA 4 612



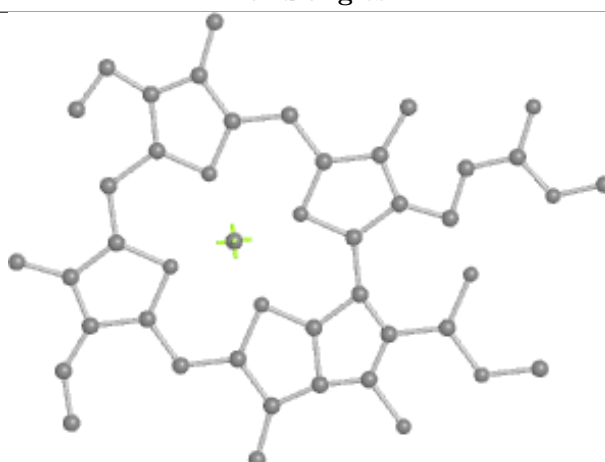
Bond lengths



Bond angles

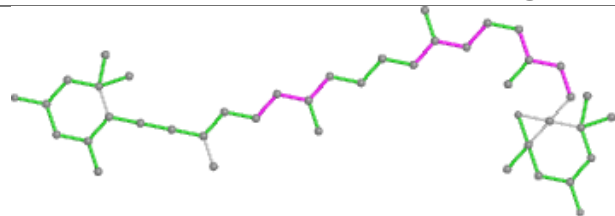


Torsions

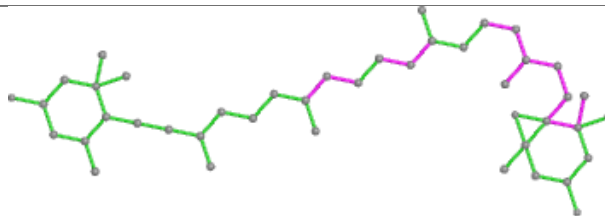


Rings

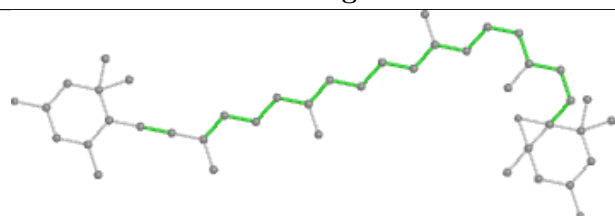
Ligand DD6 1 312



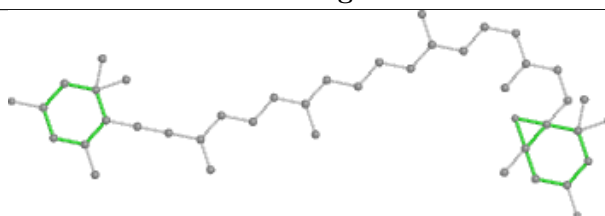
Bond lengths



Bond angles

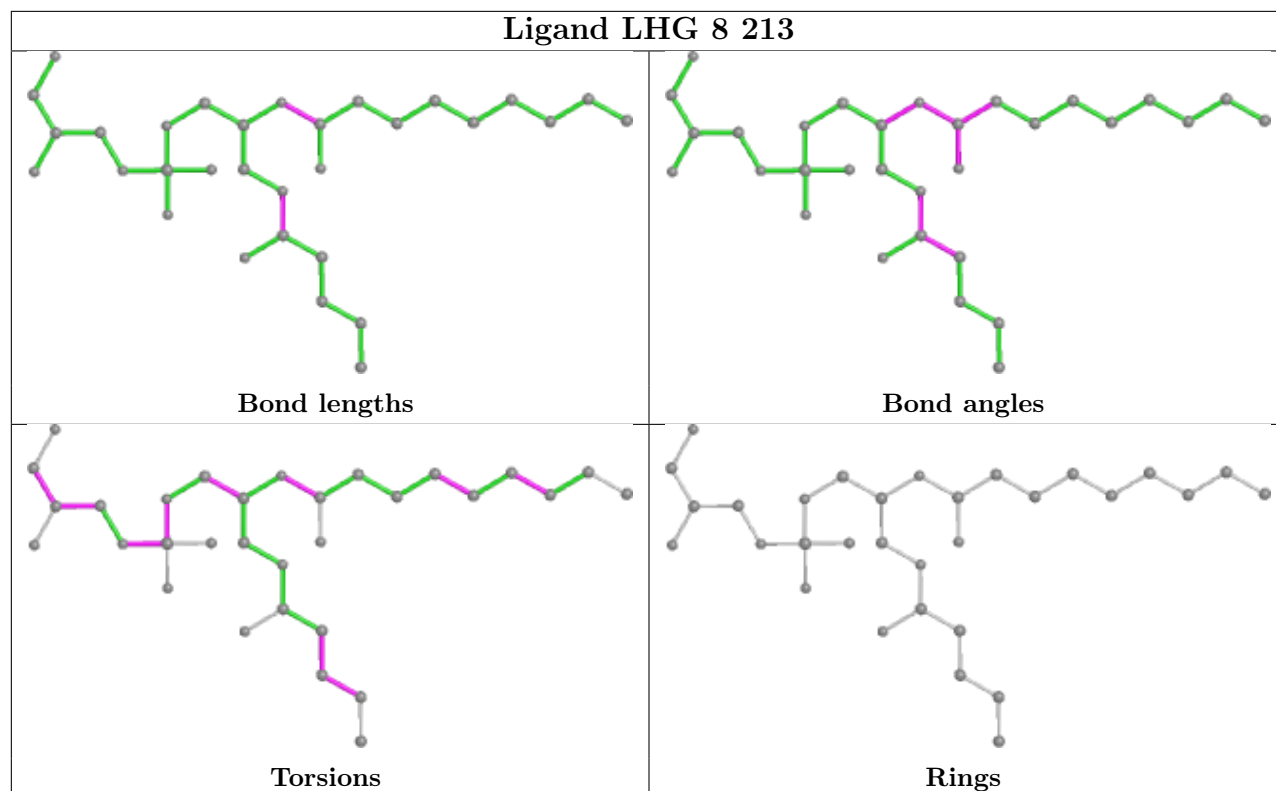


Torsions

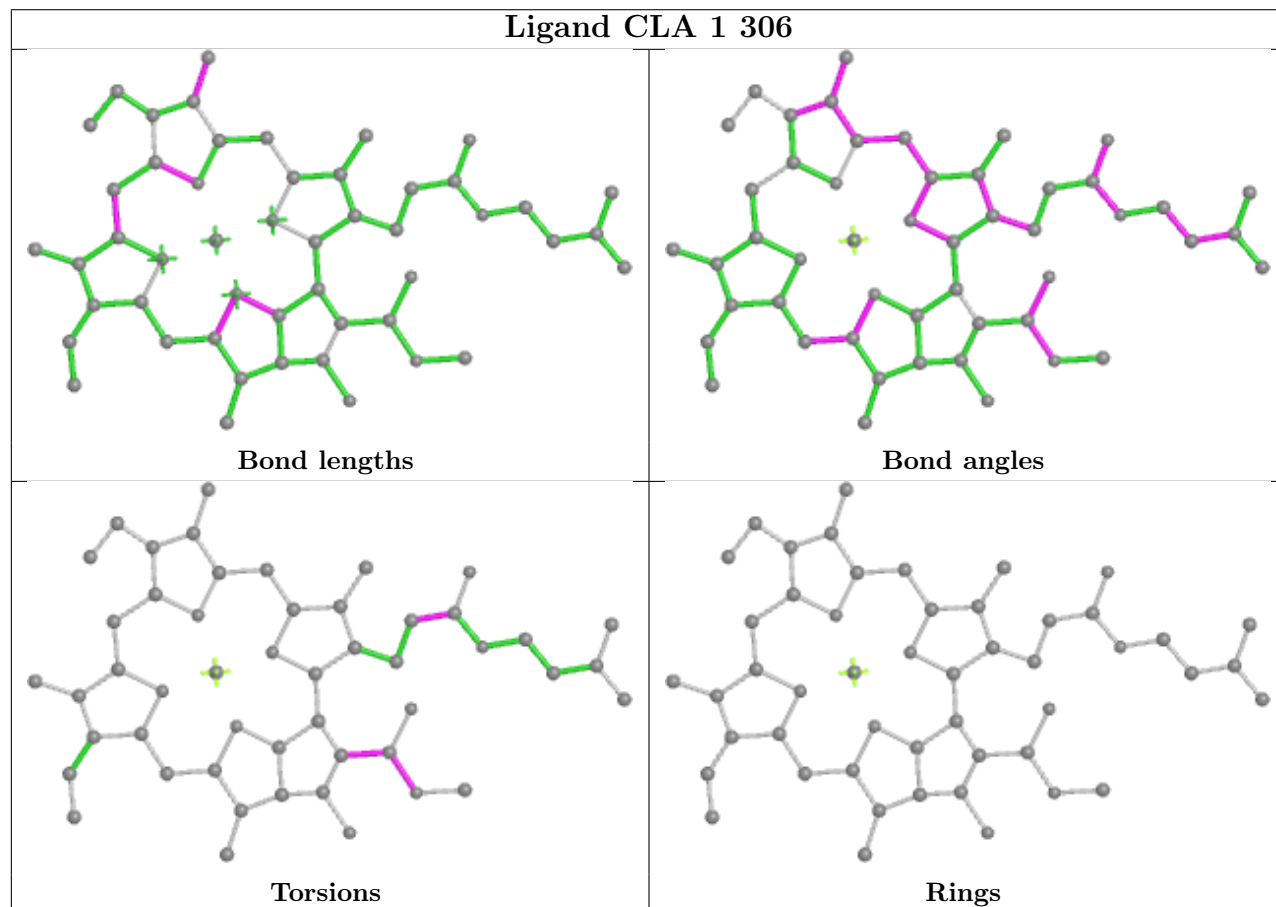


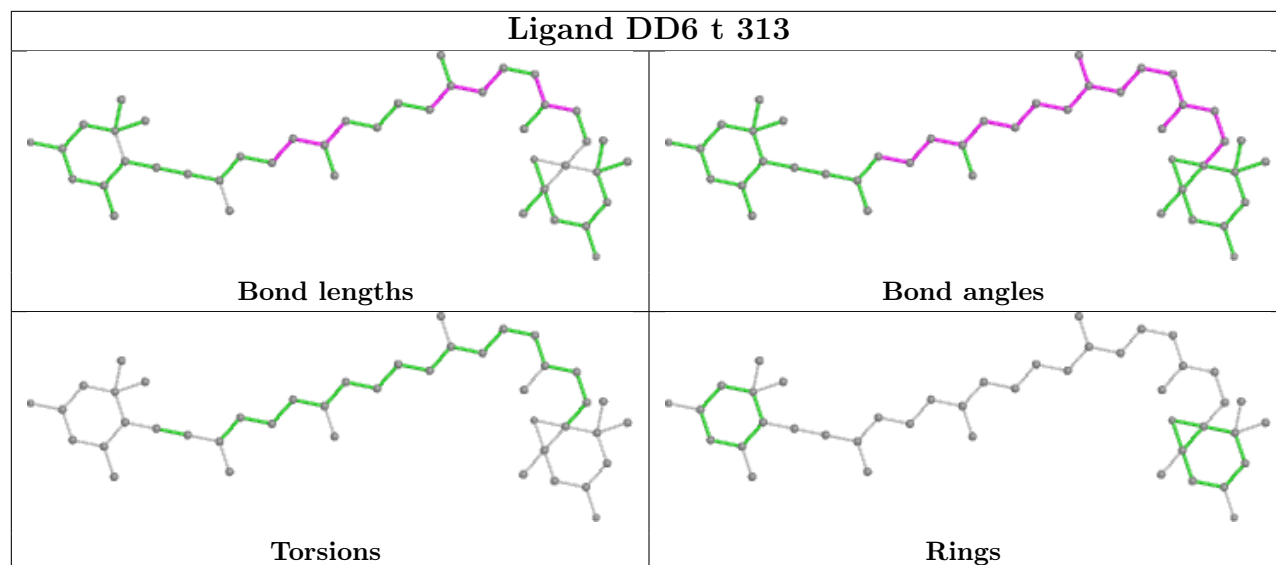
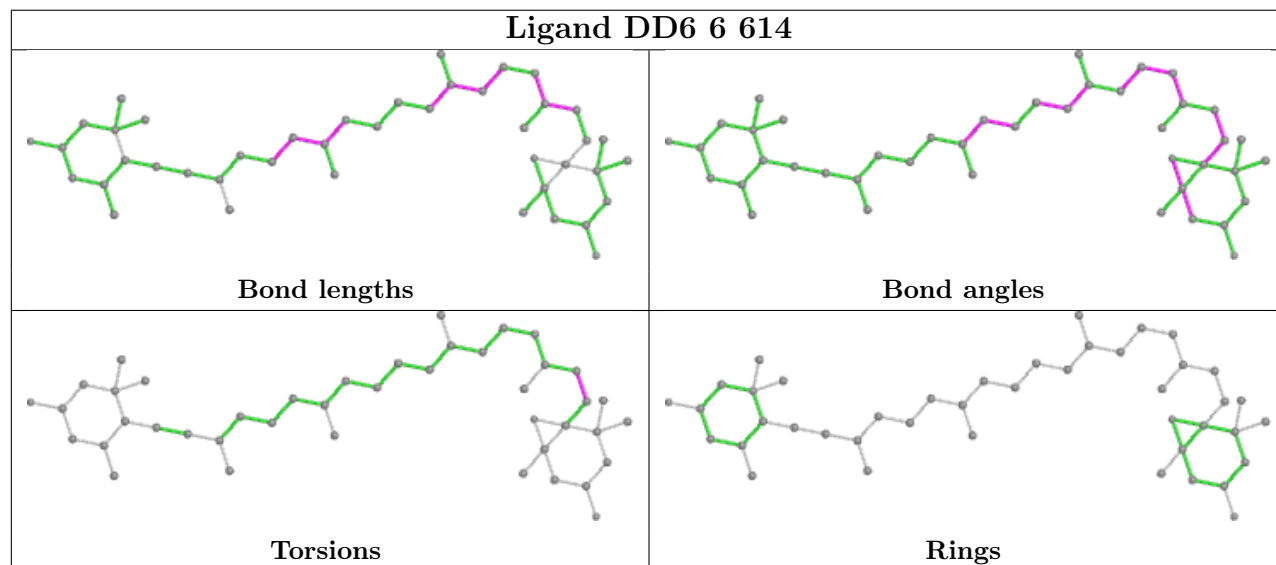
Rings

Ligand LHG 8 213

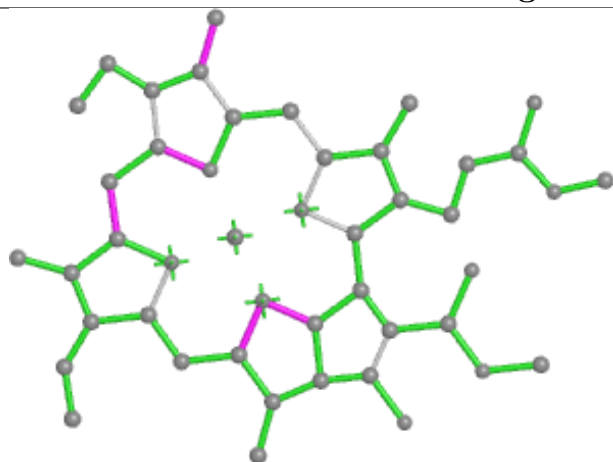


Ligand CLA 1 306

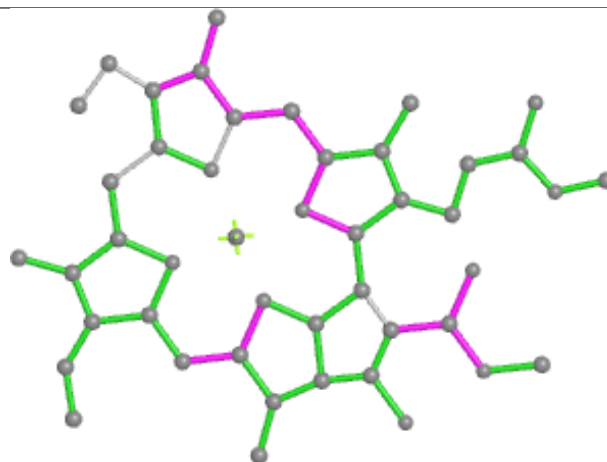


Ligand DD6 t 313**Ligand DD6 6 614**

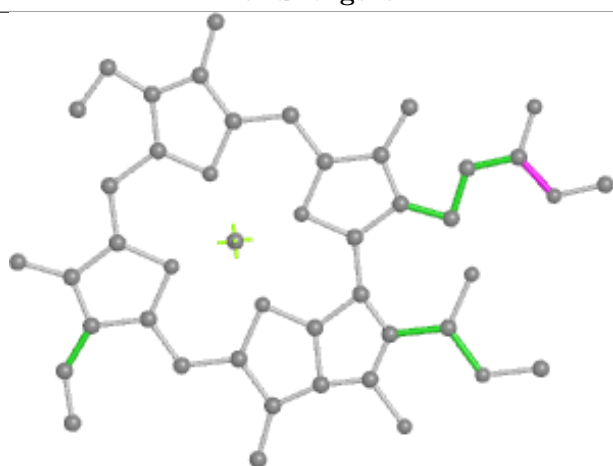
Ligand CLA 6 605



Bond lengths



Bond angles

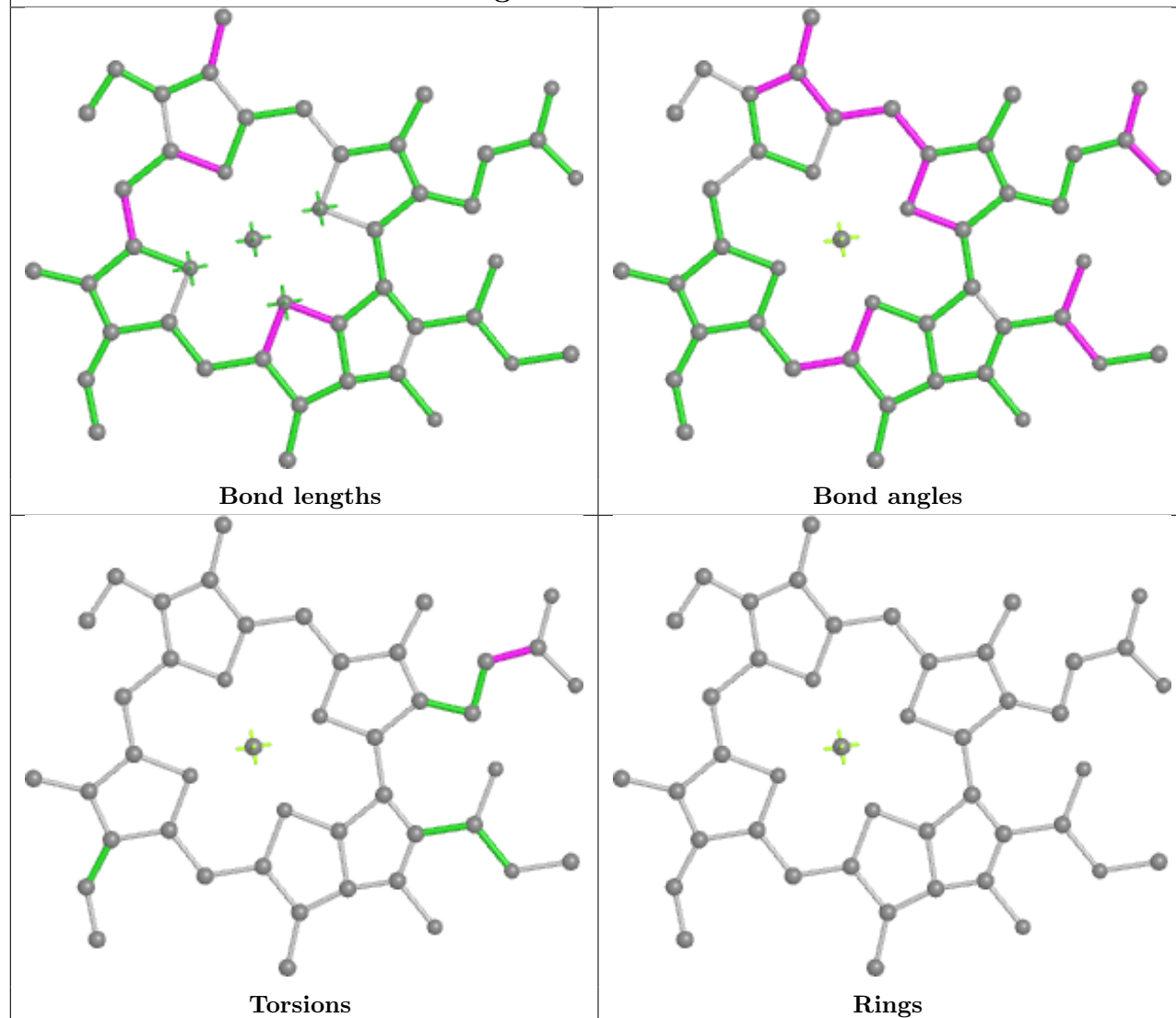


Torsions

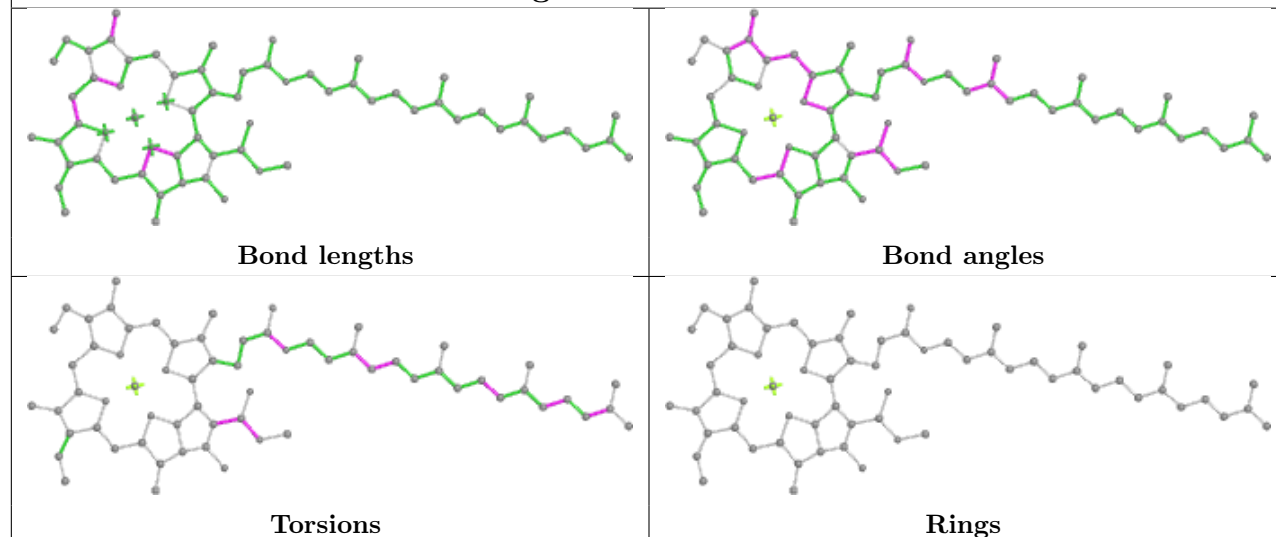


Rings

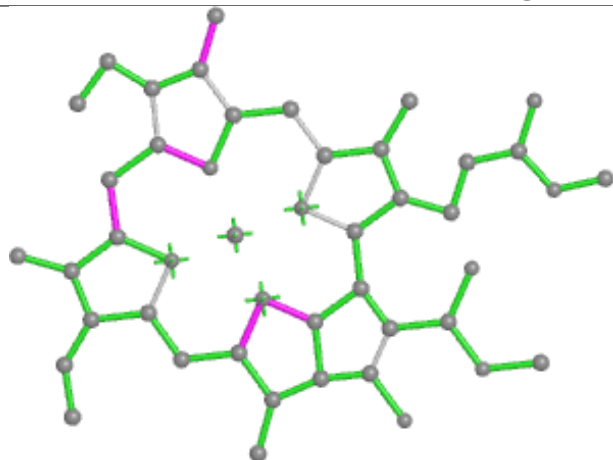
Ligand CLA 7 603



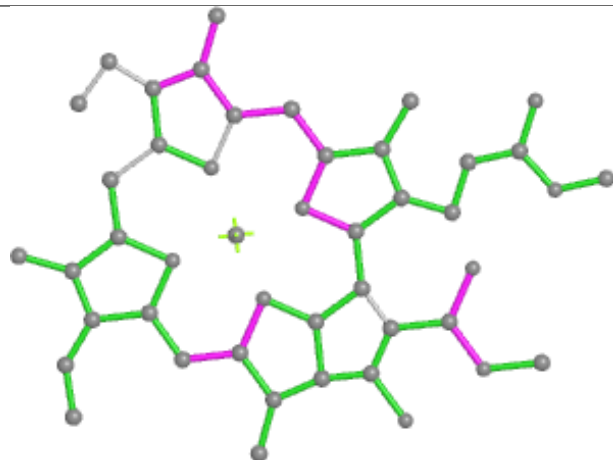
Ligand CLA B 822



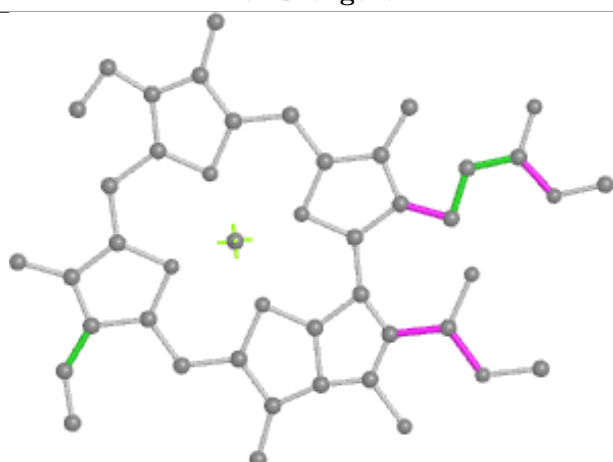
Ligand CLA 8 206



Bond lengths



Bond angles

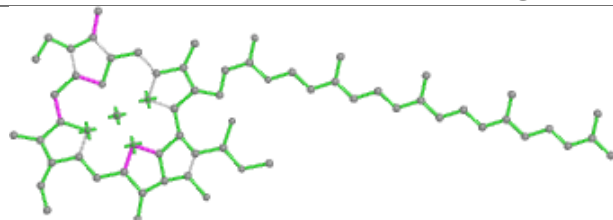


Torsions

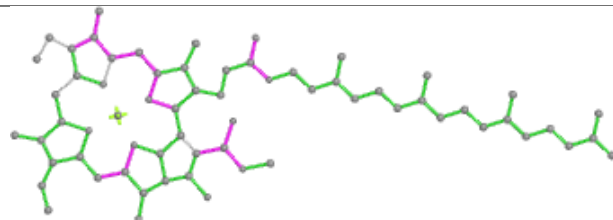


Rings

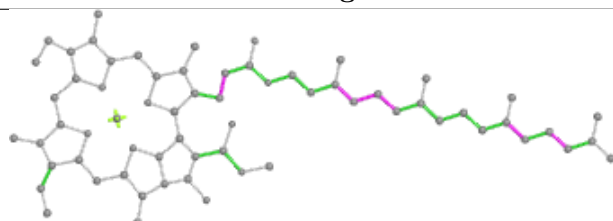
Ligand CLA B 807



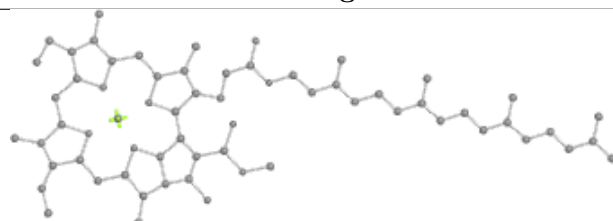
Bond lengths



Bond angles

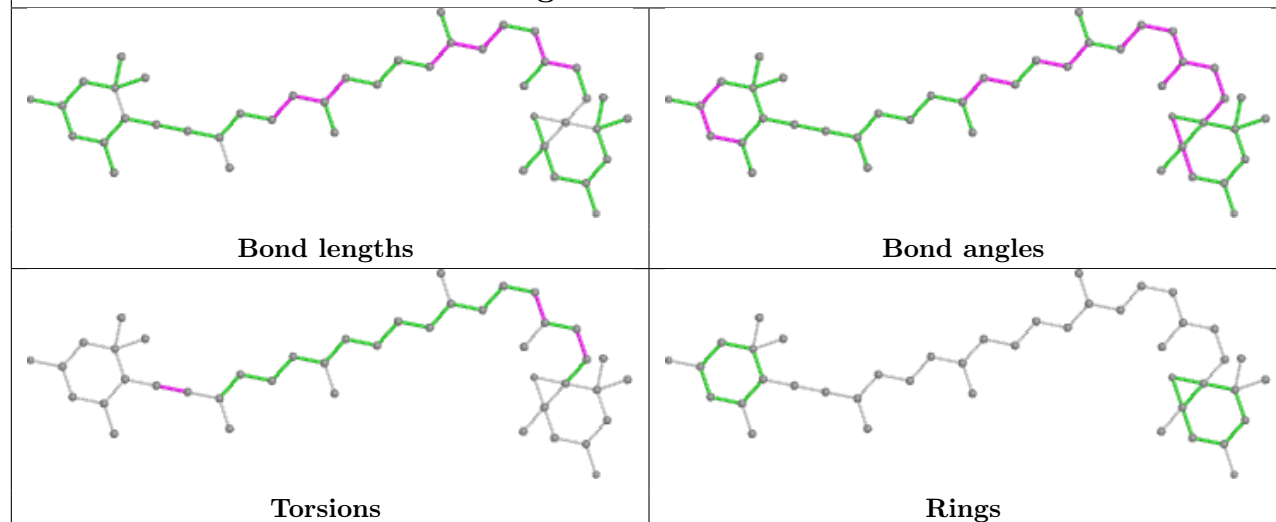


Torsions

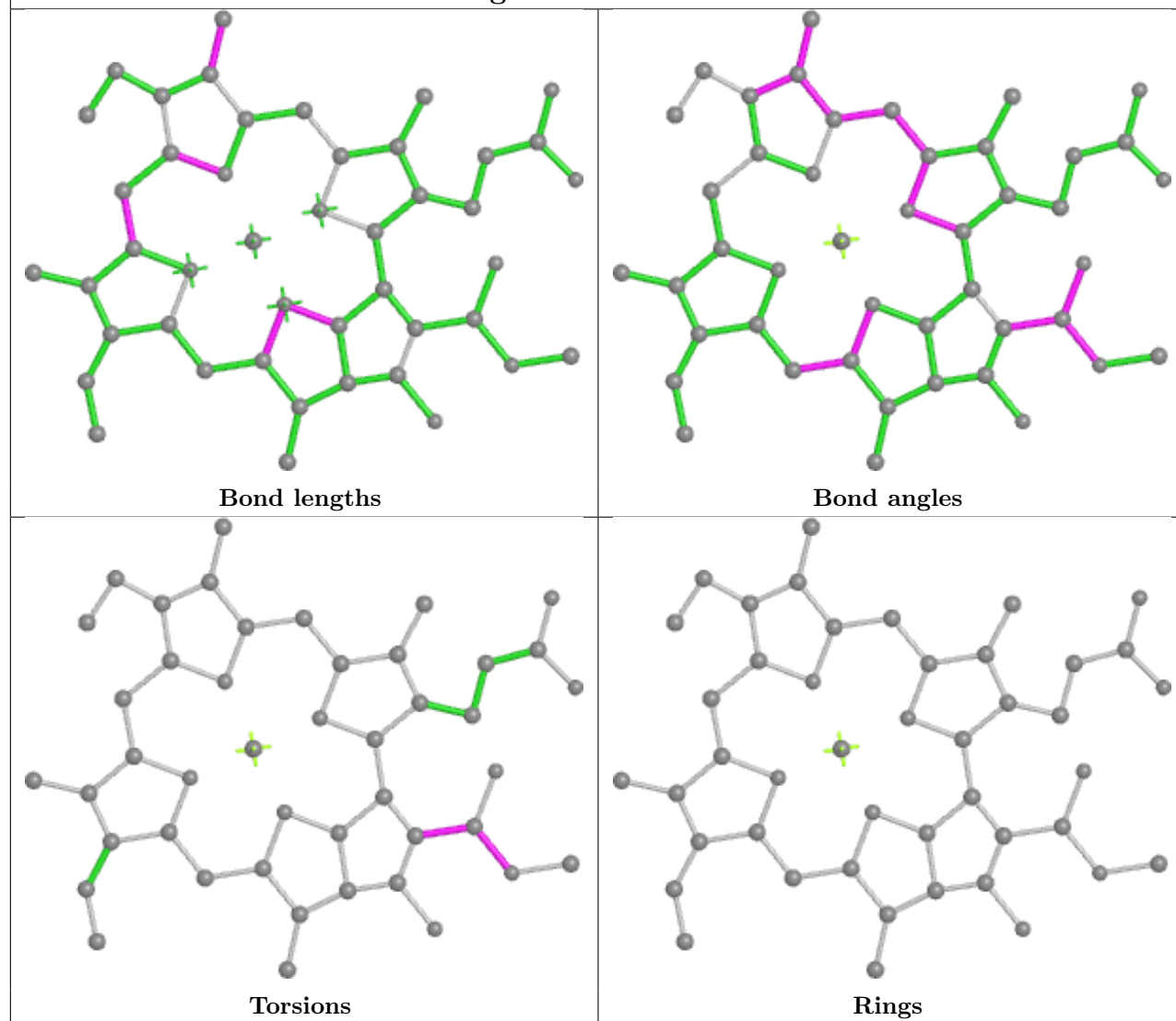


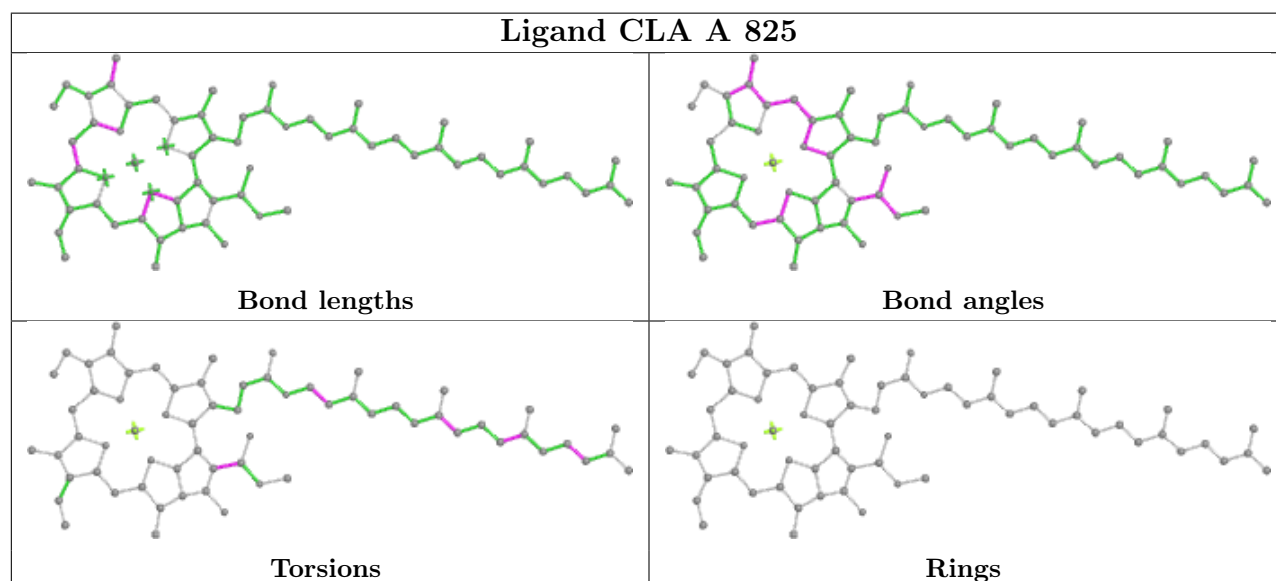
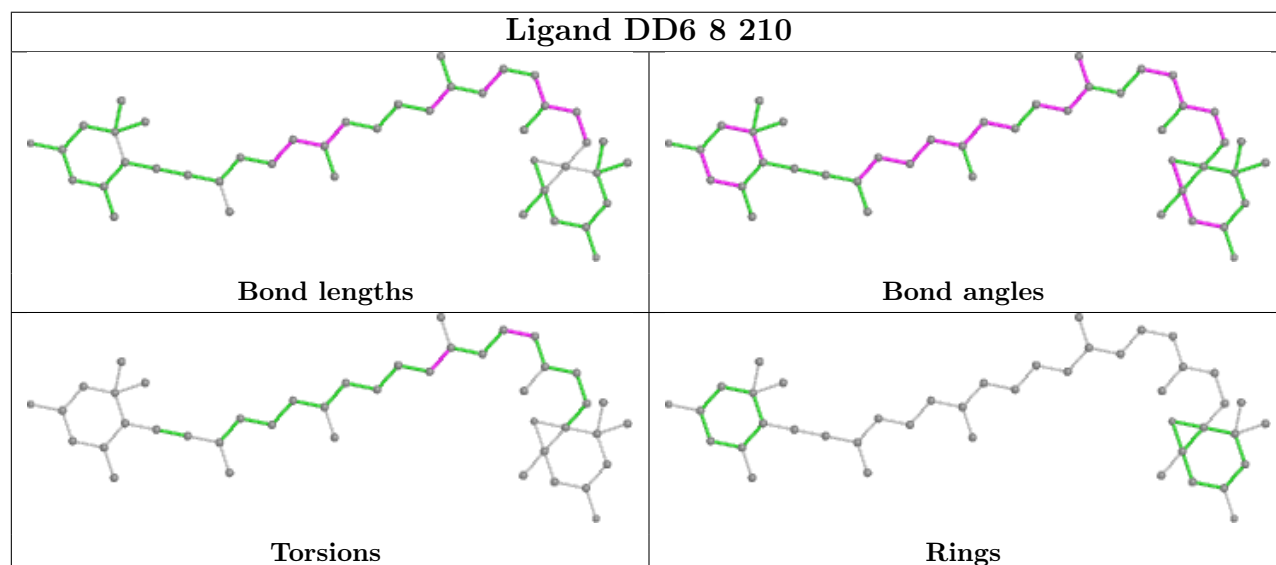
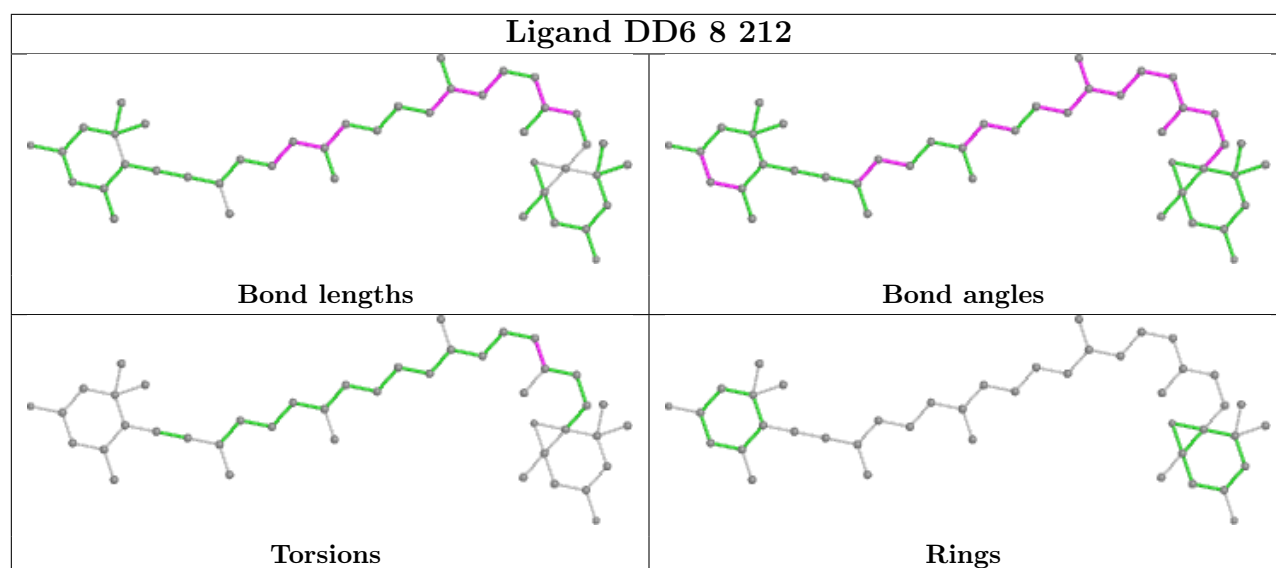
Rings

Ligand DD6 8 211

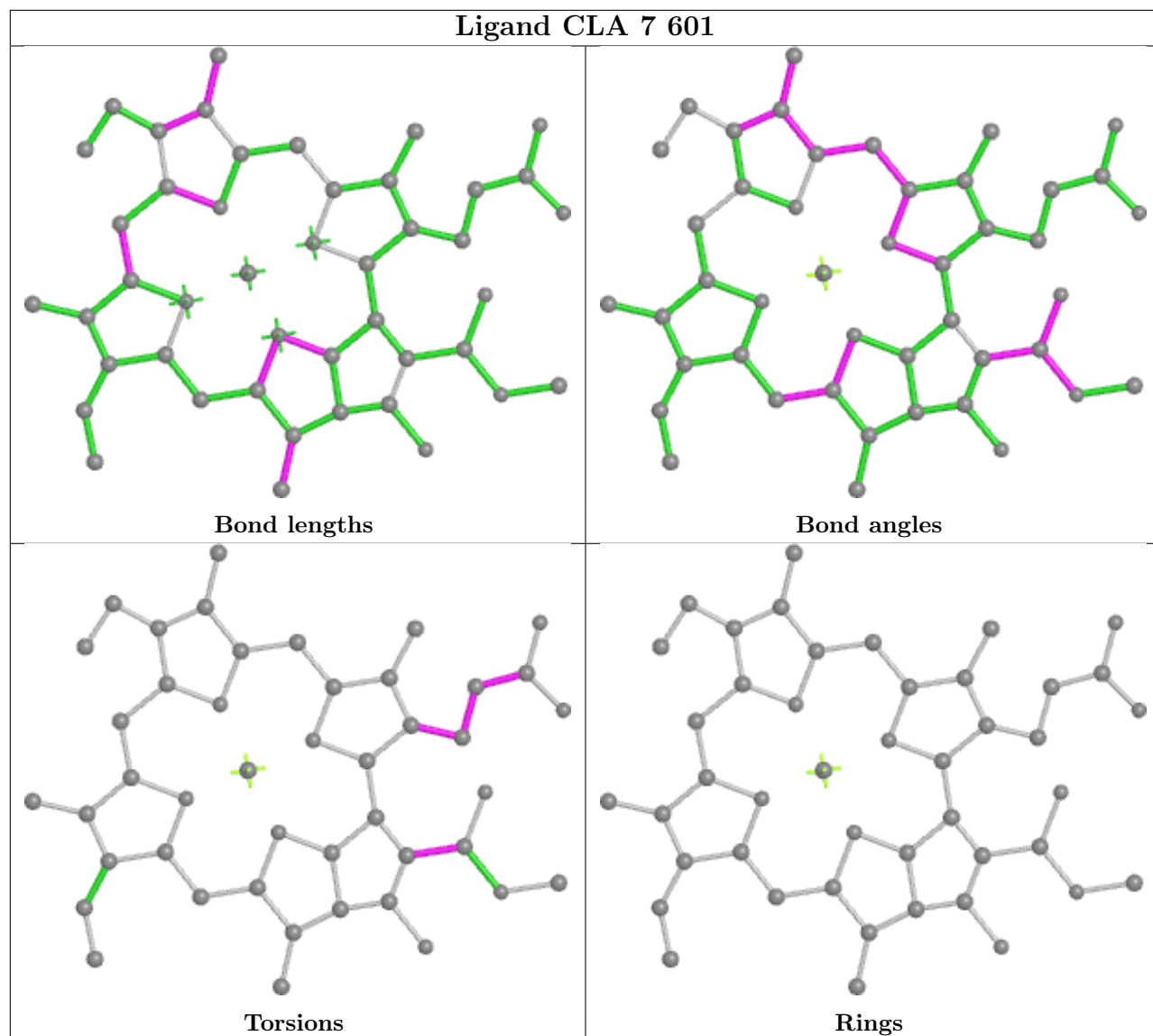


Ligand CLA A 834

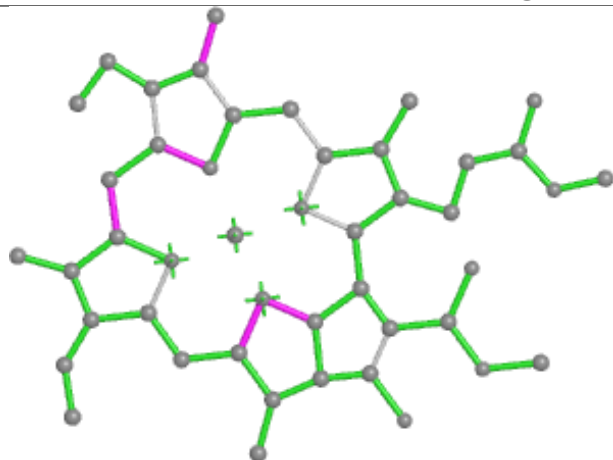




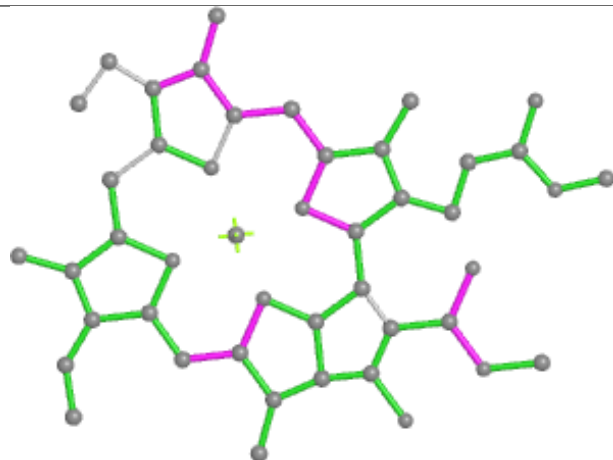
Ligand CLA 7 601



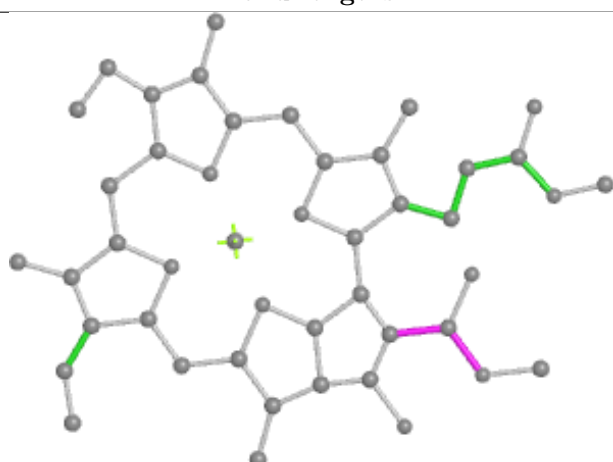
Ligand CLA 8 201



Bond lengths



Bond angles

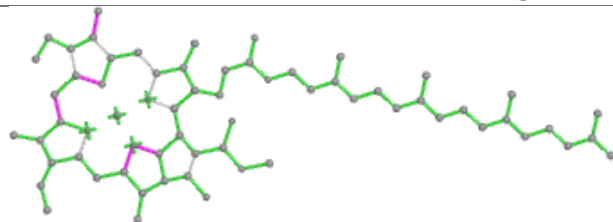


Torsions

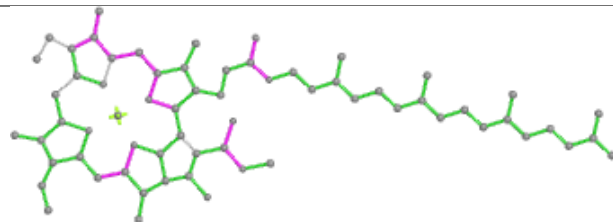


Rings

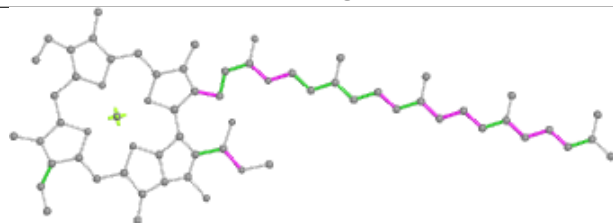
Ligand CLA B 812



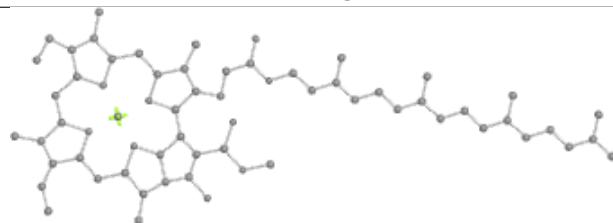
Bond lengths



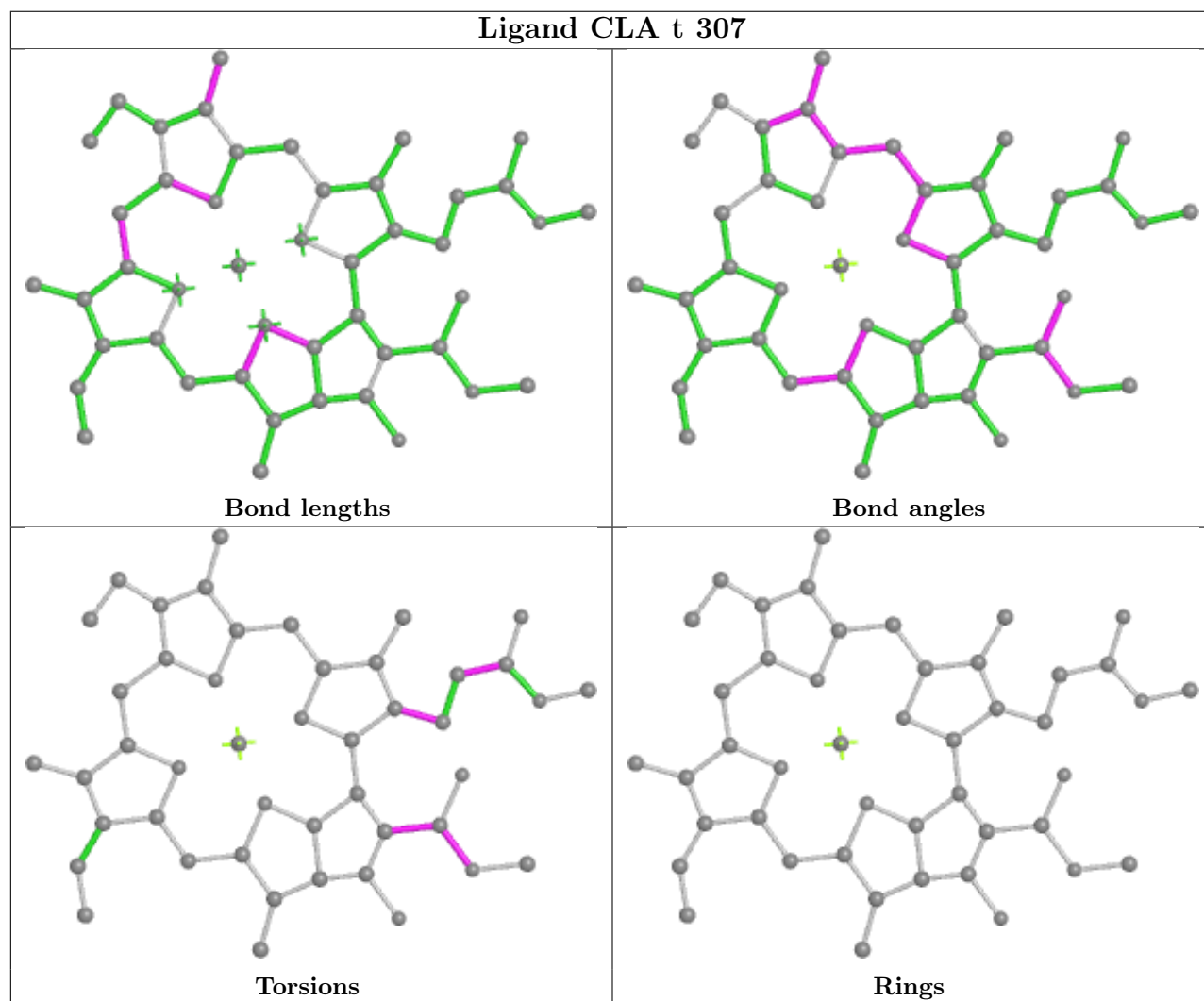
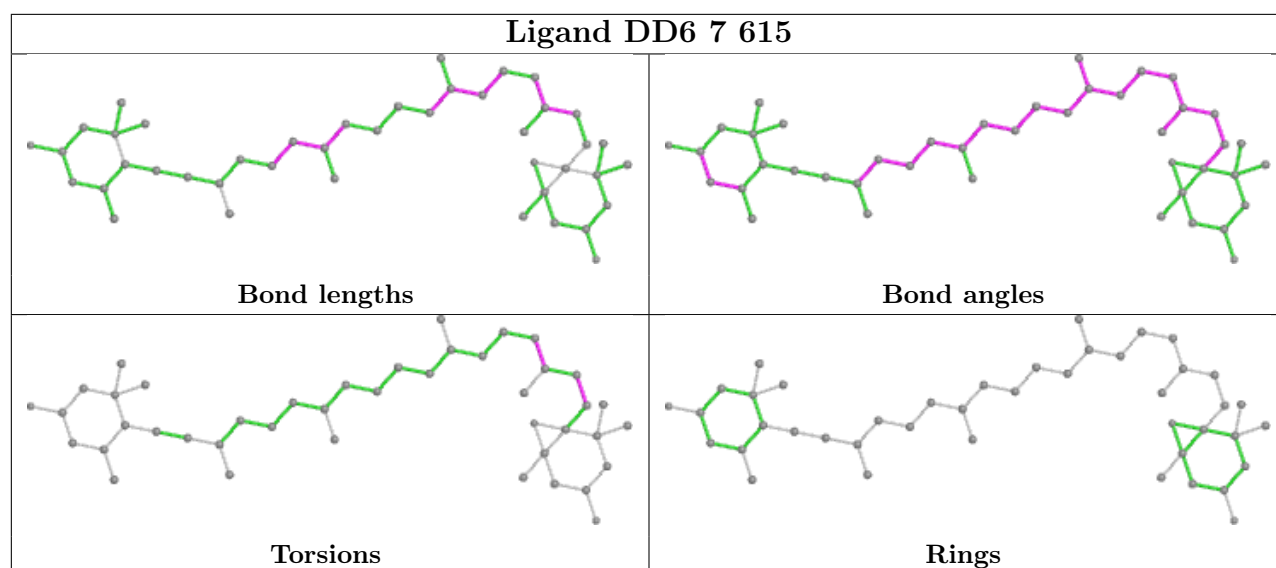
Bond angles



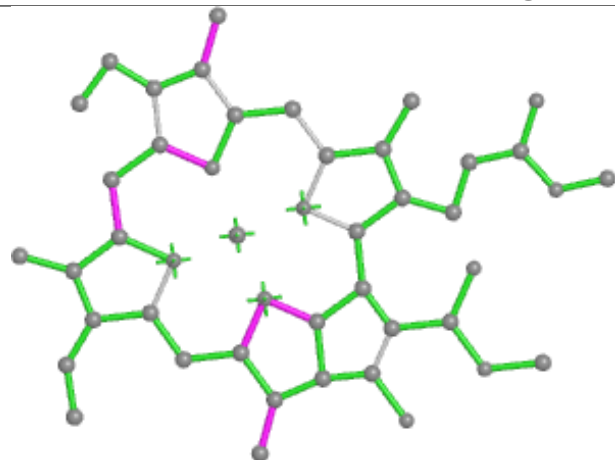
Torsions



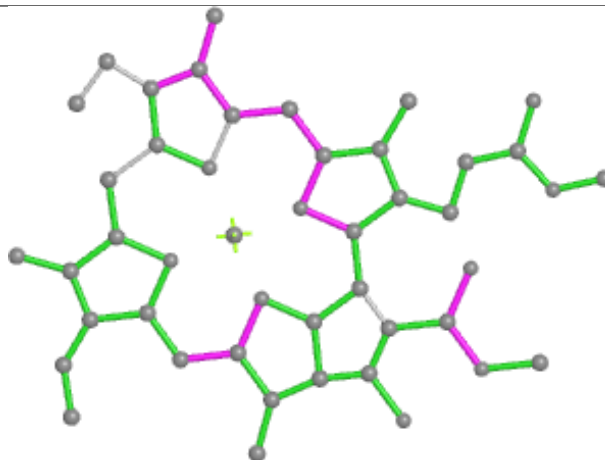
Rings



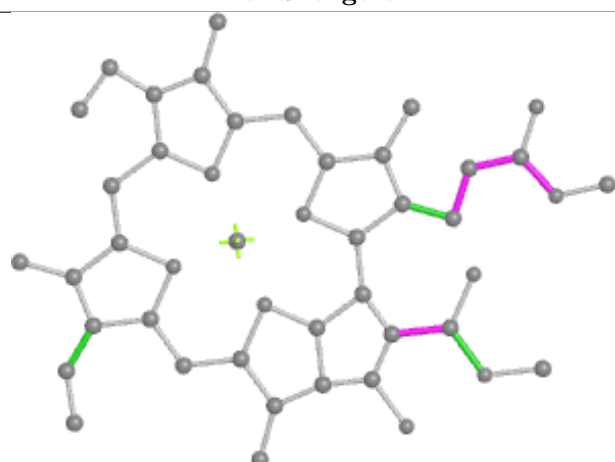
Ligand CLA k 307



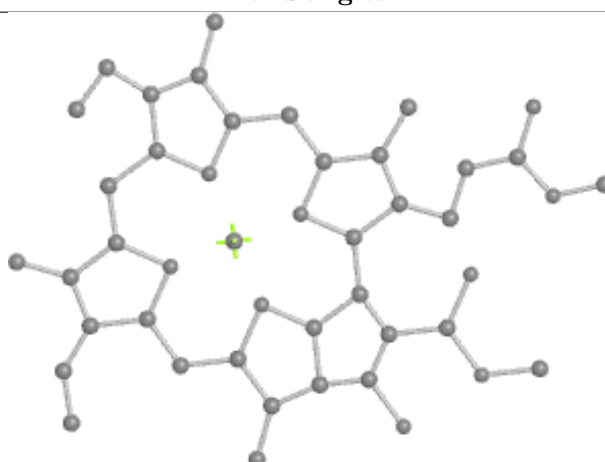
Bond lengths



Bond angles

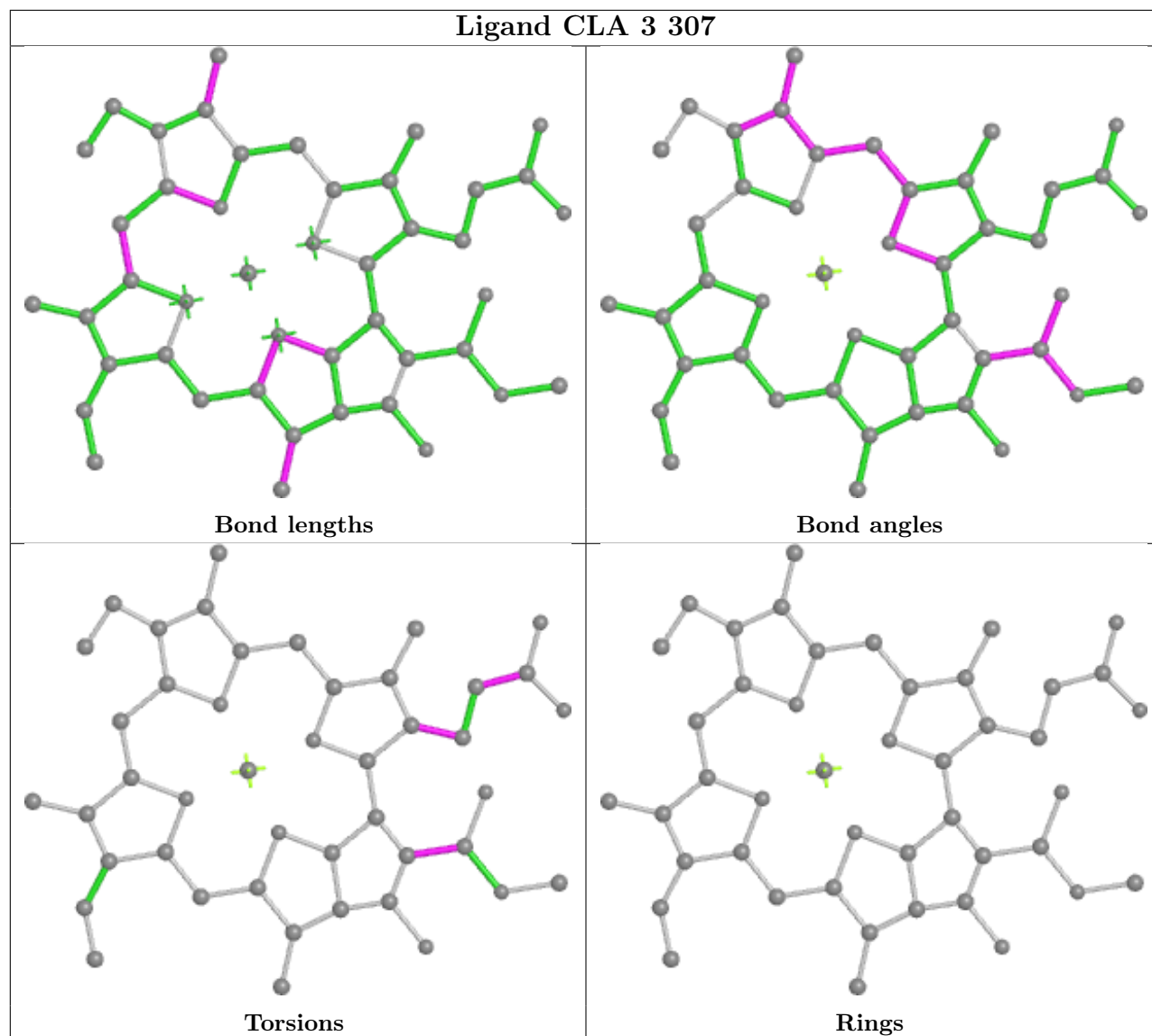


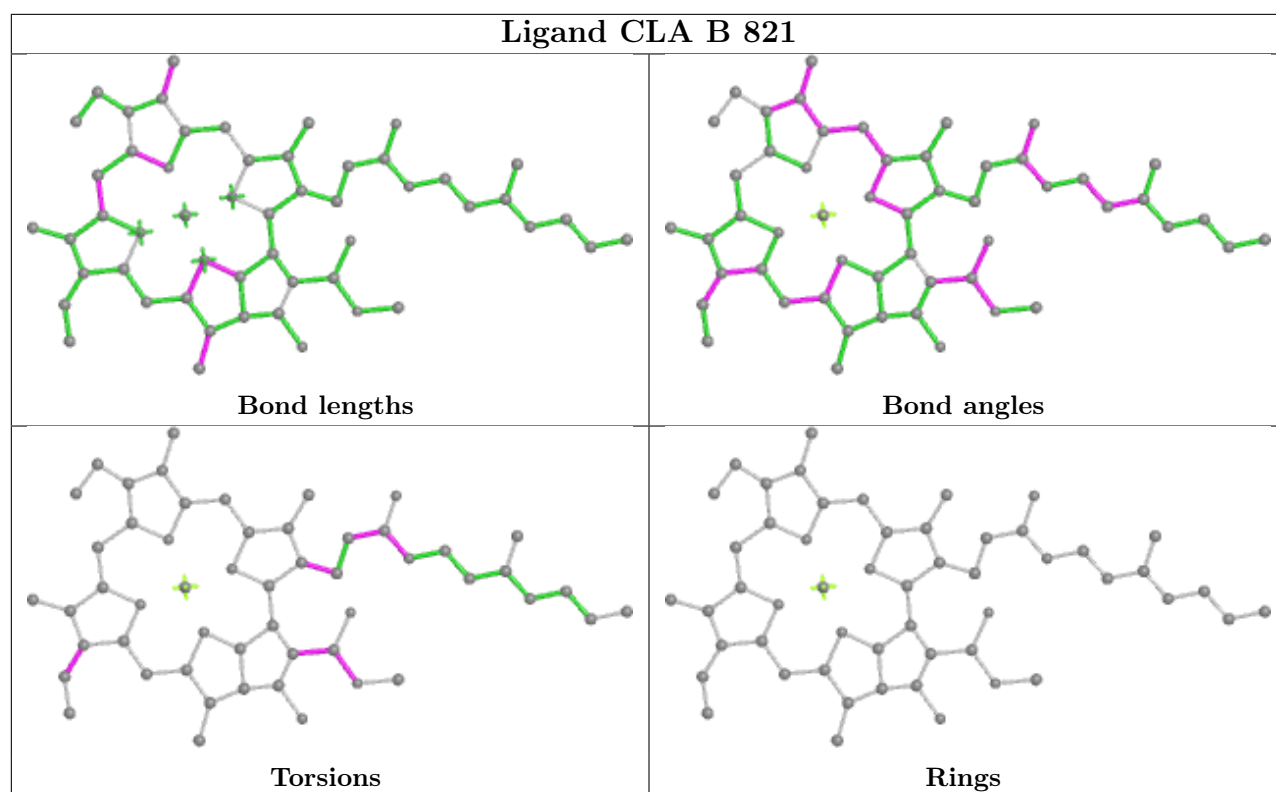
Torsions



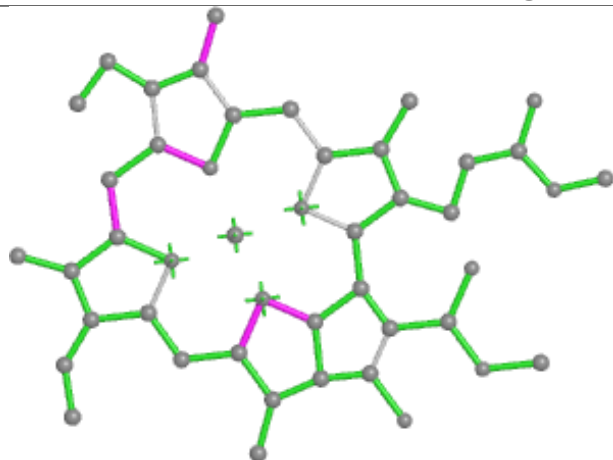
Rings

Ligand CLA 3 307

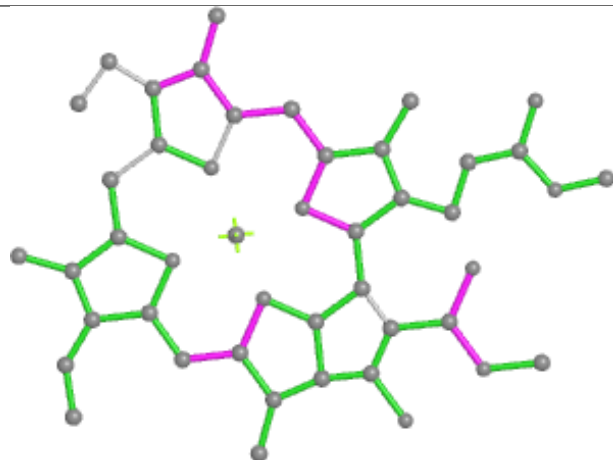




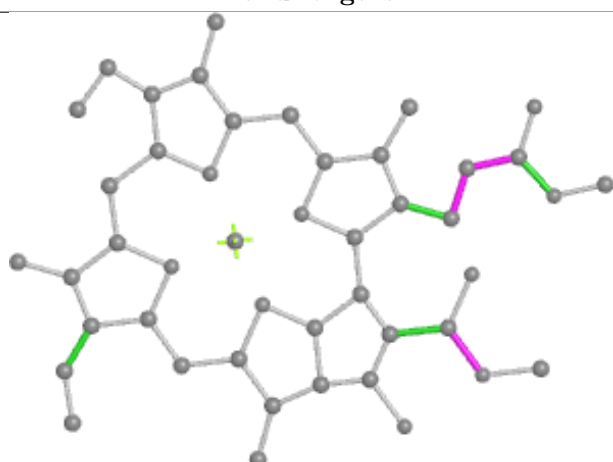
Ligand CLA t 309



Bond lengths



Bond angles

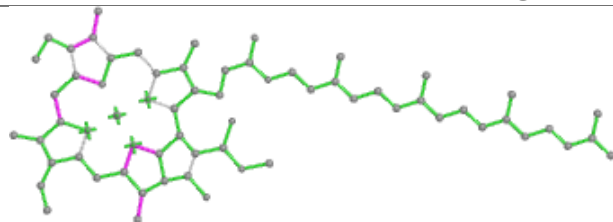


Torsions

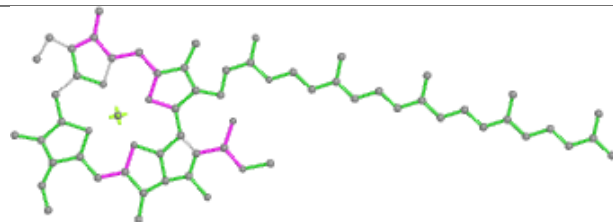


Rings

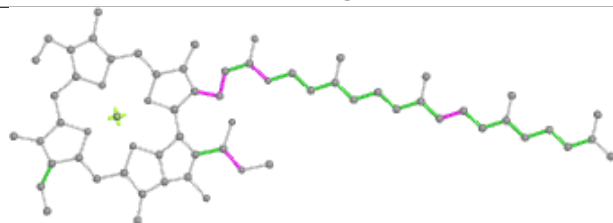
Ligand CLA B 826



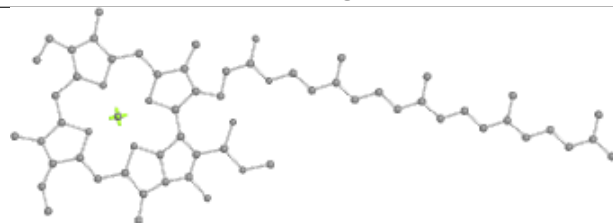
Bond lengths



Bond angles

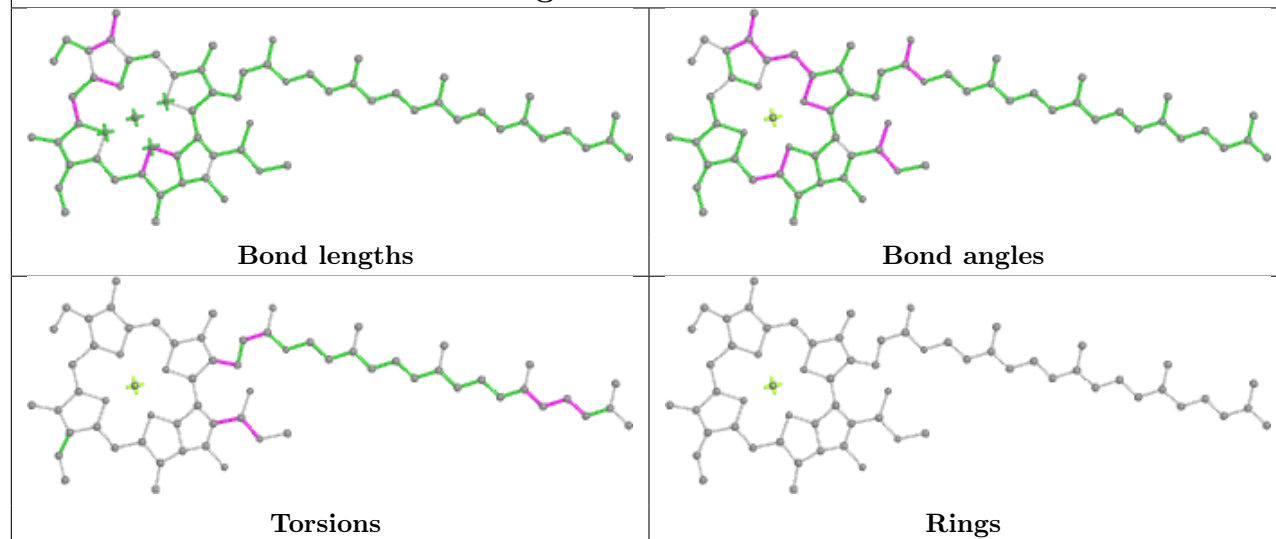


Torsions

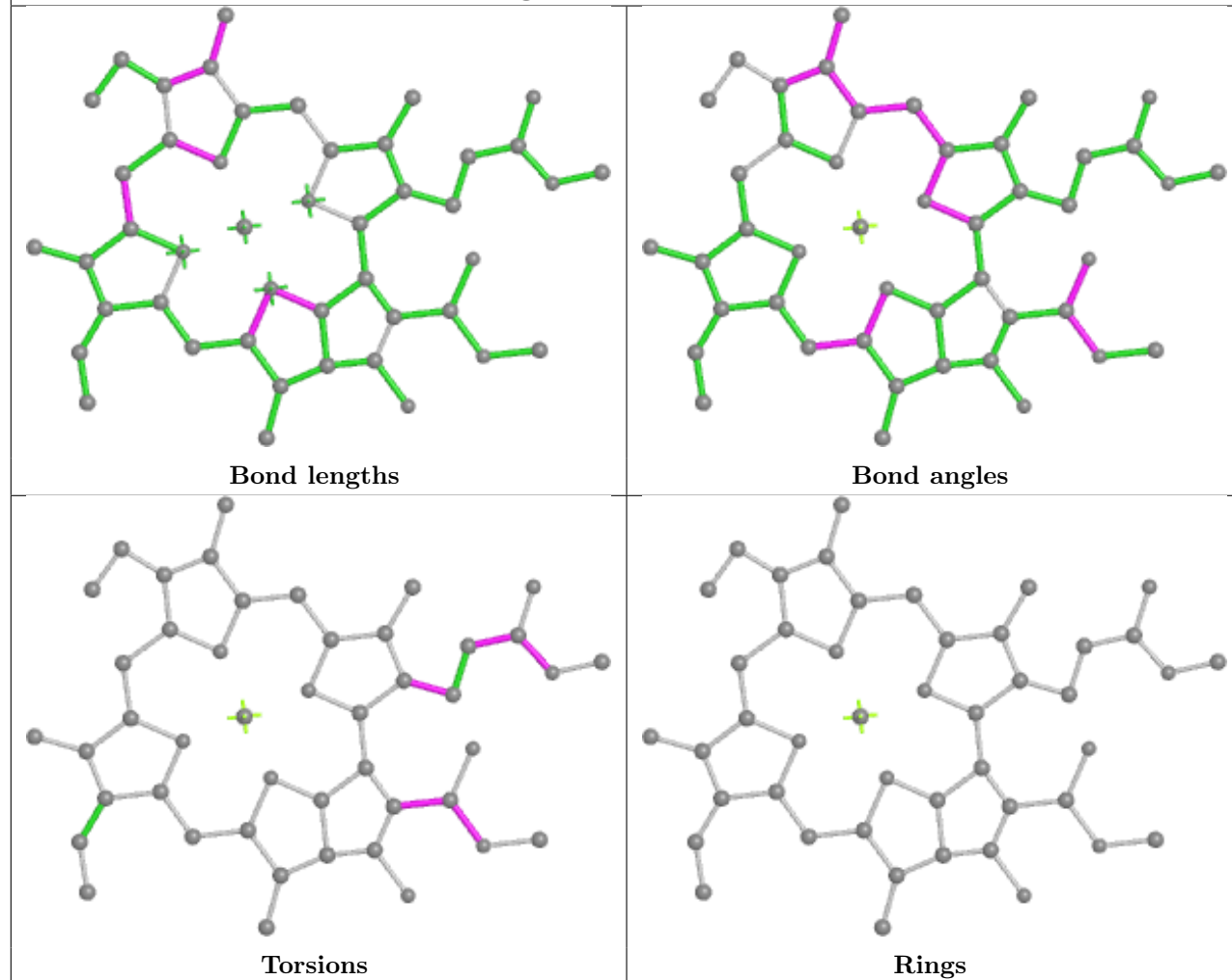


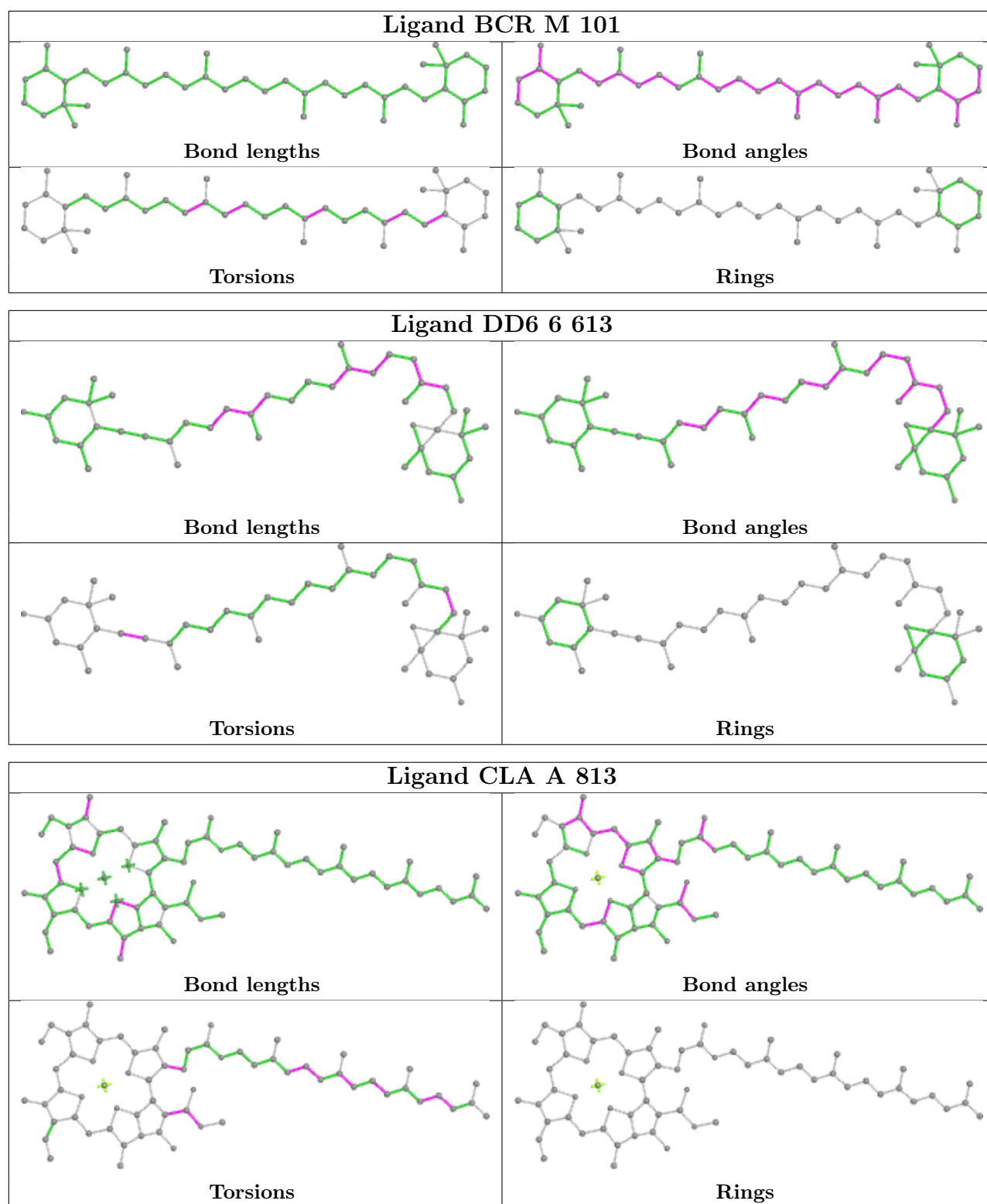
Rings

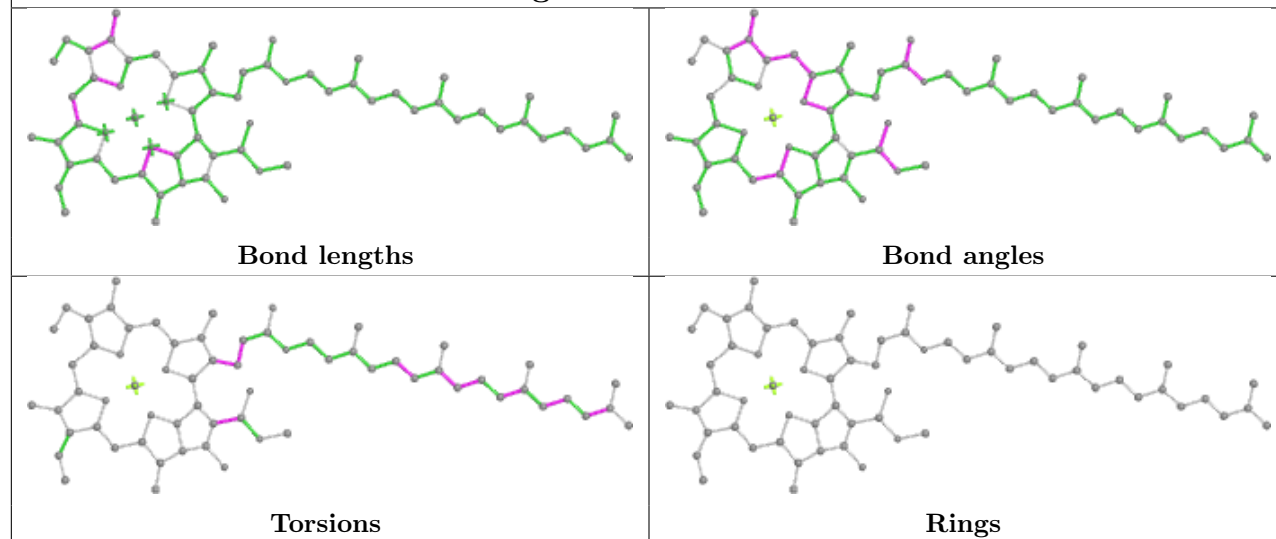
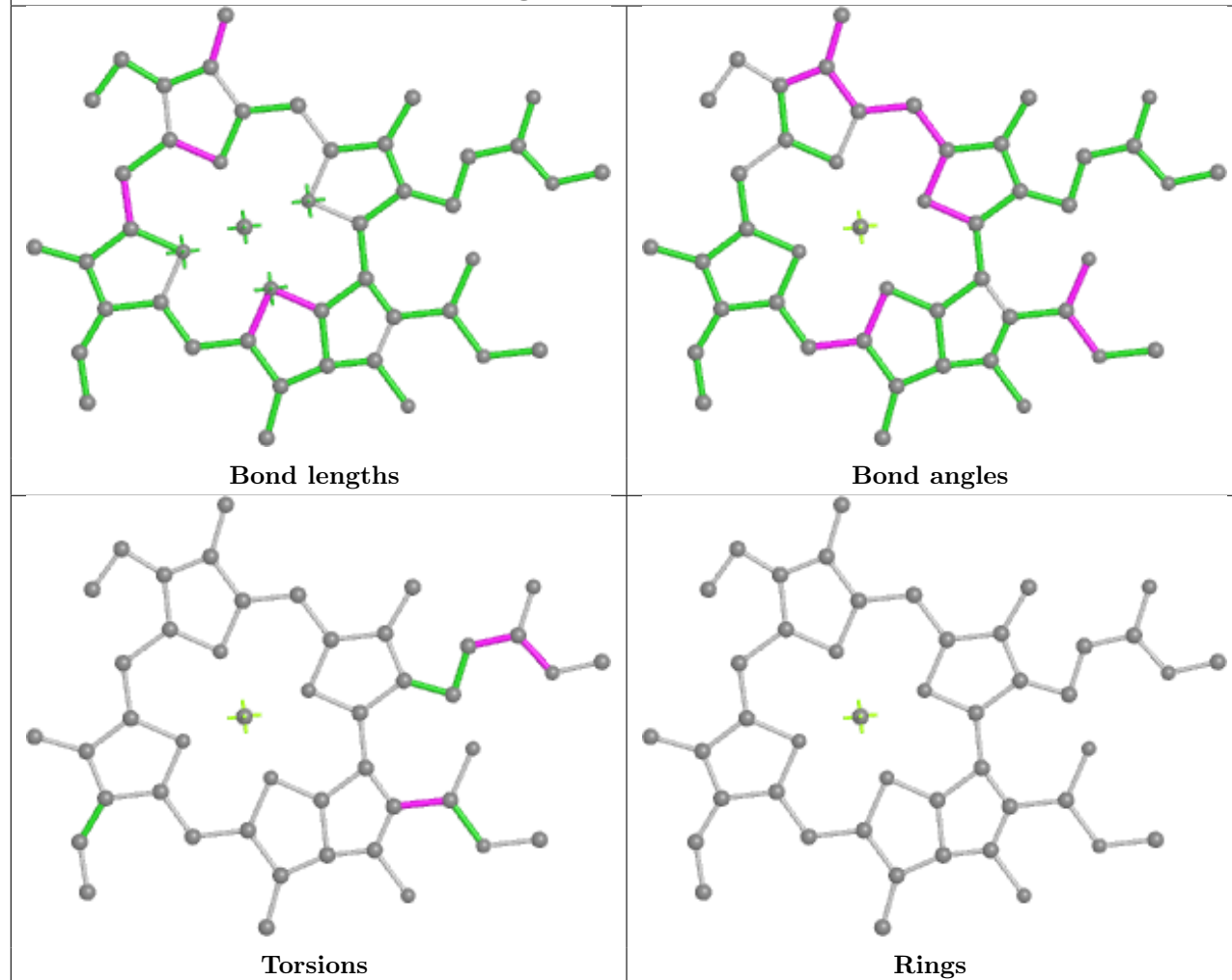
Ligand CLA 3 306



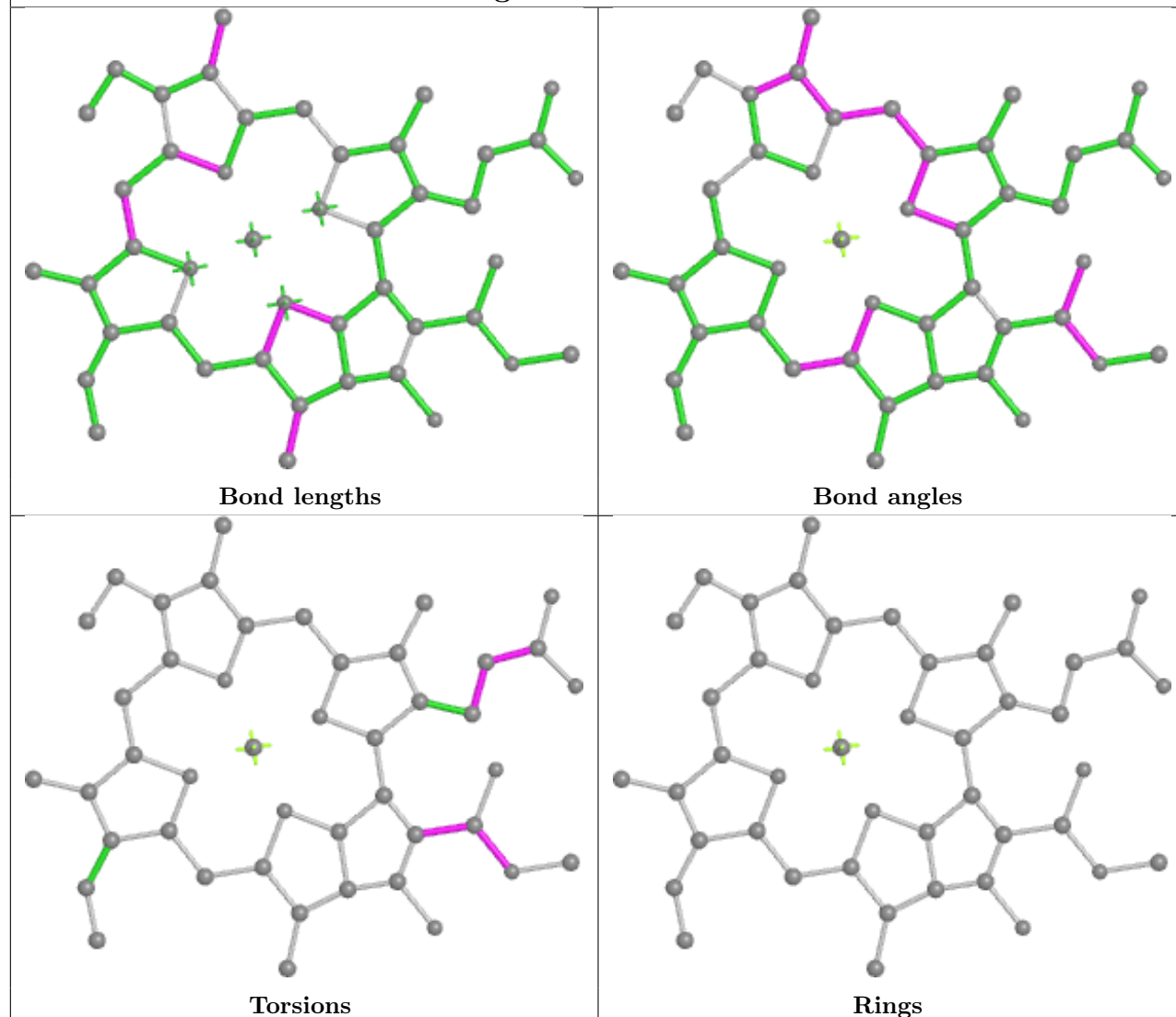
Ligand CLA 4 613



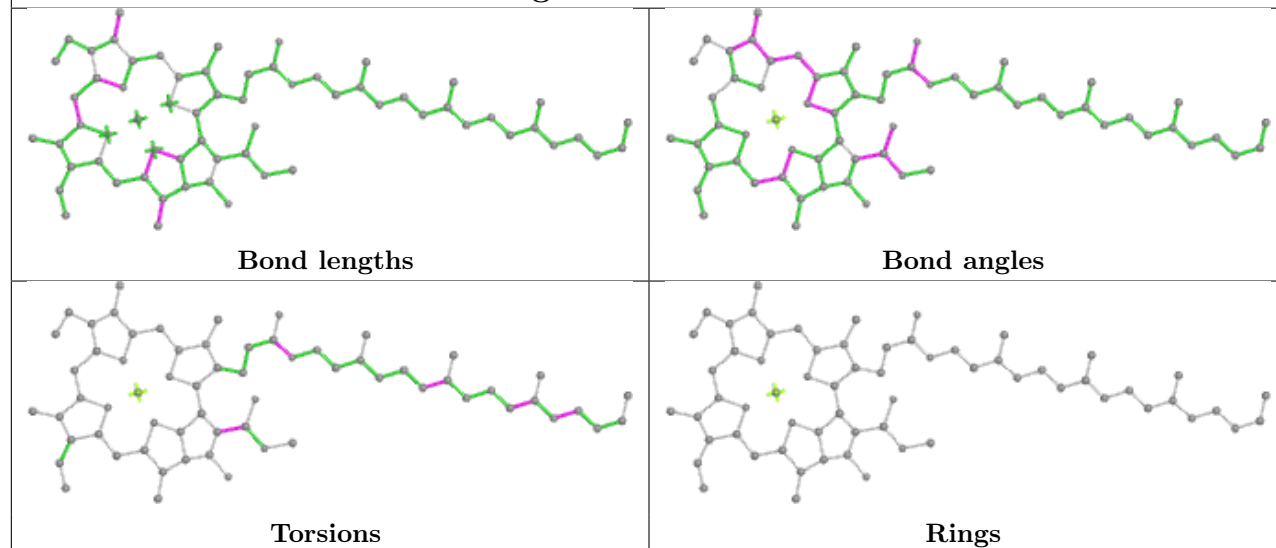


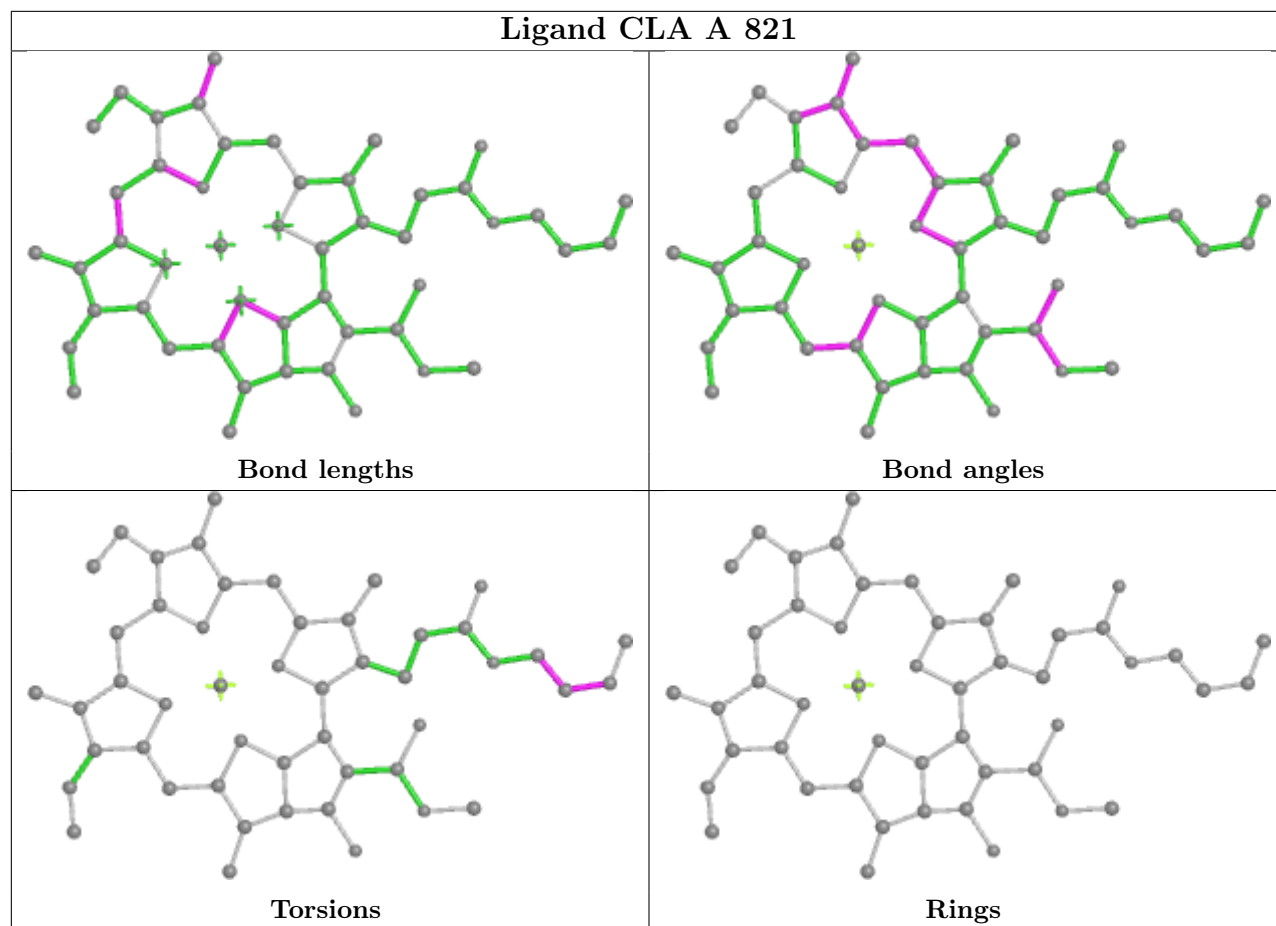
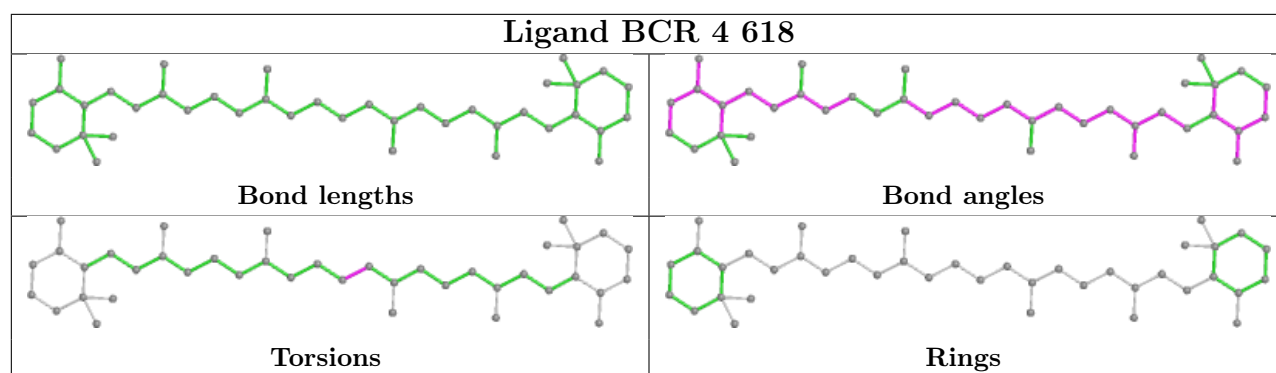
Ligand CLA B 836**Ligand CLA F 202**

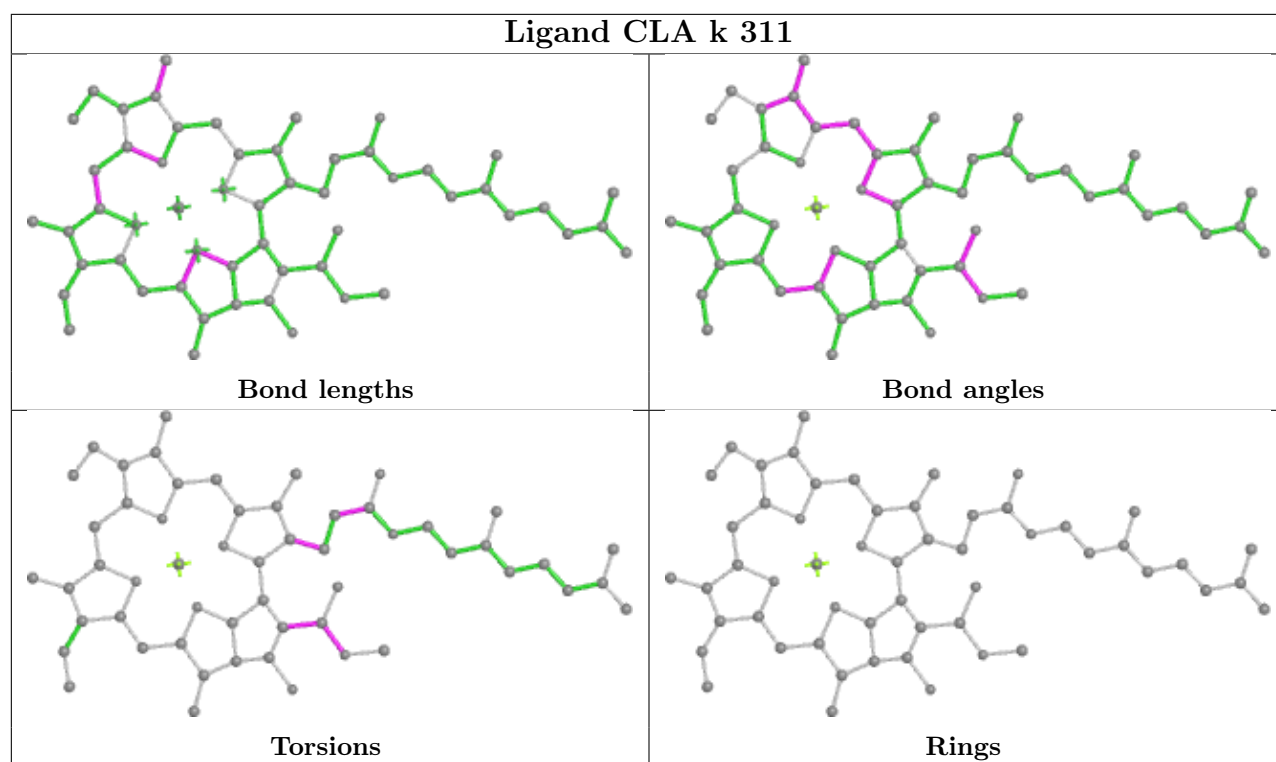
Ligand CLA 7 604



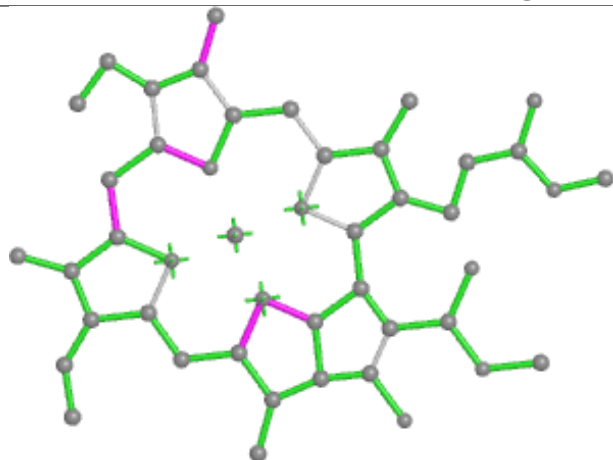
Ligand CLA B 823



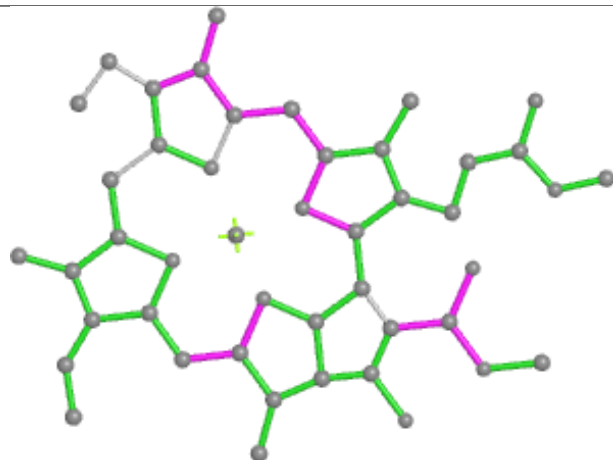




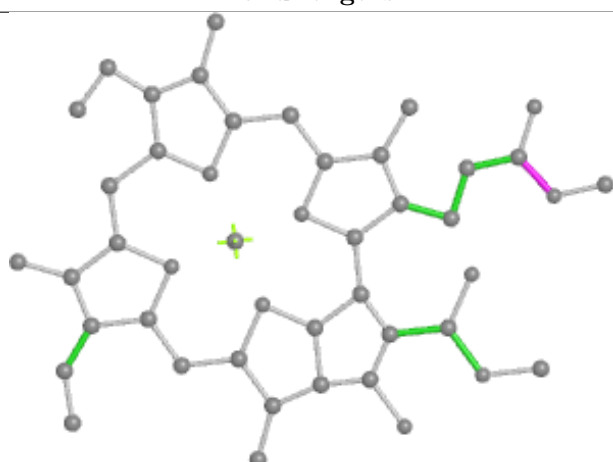
Ligand CLA 4 606



Bond lengths



Bond angles

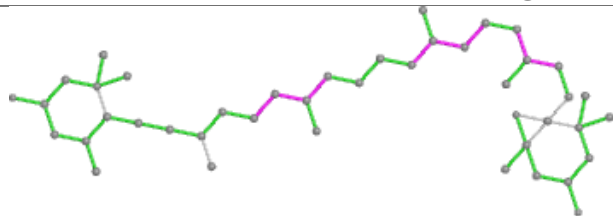


Torsions

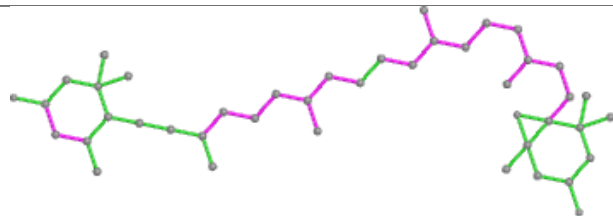


Rings

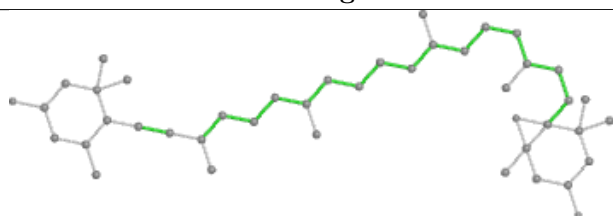
Ligand DD6 7 613



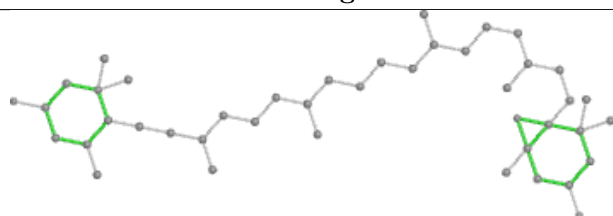
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.