



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:16 AM UTC

PDB ID : 8JJR / pdb_00008jjr
EMDB ID : EMD-36366
Title : Cryo-EM structure of Symbiodinium photosystem I
Authors : Zhao, L.S.; Wang, N.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2023-05-31
Resolution : 2.80 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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

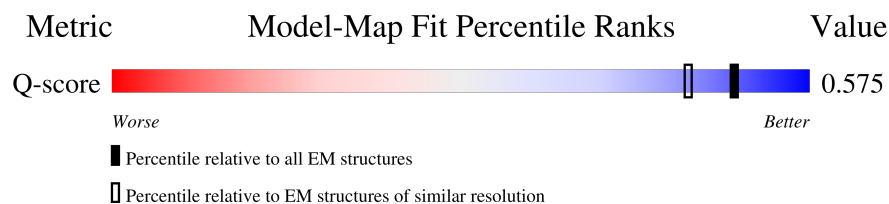
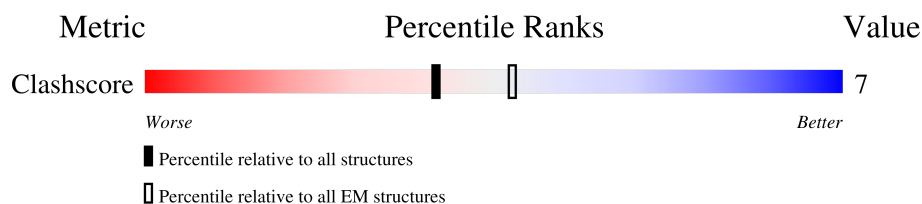
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

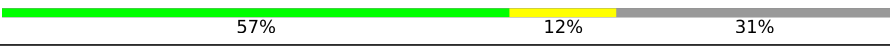
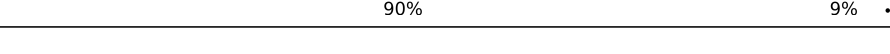
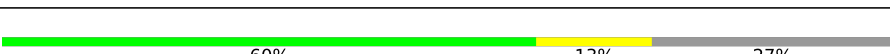
The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



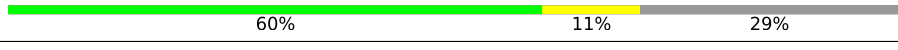
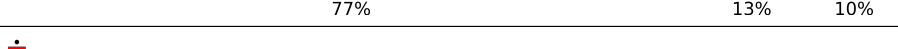
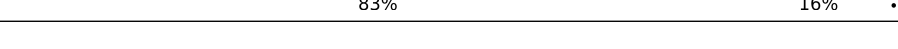
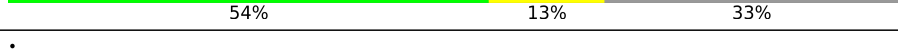
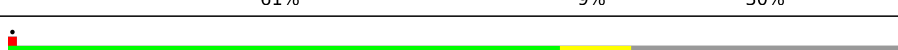
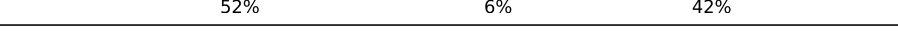
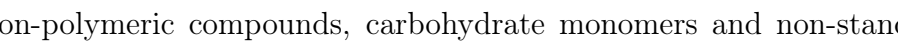
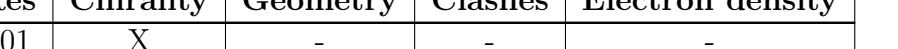
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	11806 (2.30 - 3.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	256	
2	B	269	
3	C	193	
4	D	177	
5	E	253	
6	F	286	

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Mol	Chain	Length	Quality of chain
7	G	228	
8	H	271	
9	I	246	
10	J	203	
11	K	226	
12	T	206	
13	U	137	
14	a	687	
15	b	669	
16	c	161	
17	d	295	
18	e	121	
19	f	279	
20	i	179	
21	j	141	
22	l	361	
23	m	142	
24	r	152	
25	x	121	
26	y	223	

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
27	CLA	A	601	X	-	-	-
27	CLA	A	602	X	-	-	-
27	CLA	A	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	604	X	-	-	-
27	CLA	A	605	X	-	-	-
27	CLA	A	606	X	-	-	-
27	CLA	A	607	X	-	-	-
27	CLA	A	609	X	-	-	-
27	CLA	A	610	X	-	-	-
27	CLA	A	611	X	-	-	-
27	CLA	A	612	X	-	-	-
27	CLA	B	601	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	C	201	X	-	-	-
27	CLA	C	202	X	-	-	-
27	CLA	C	203	X	-	-	-
27	CLA	C	204	X	-	-	-
27	CLA	C	205	X	-	-	-
27	CLA	C	206	X	-	-	-
27	CLA	C	207	X	-	-	-
27	CLA	C	208	X	-	-	-
27	CLA	C	209	X	-	-	-
27	CLA	C	211	X	-	-	-
27	CLA	C	212	X	-	-	-
27	CLA	D	601	X	-	-	-
27	CLA	D	602	X	-	-	-
27	CLA	D	603	X	-	-	-
27	CLA	D	604	X	-	-	-
27	CLA	D	605	X	-	-	-
27	CLA	D	606	X	-	-	-
27	CLA	D	607	X	-	-	-
27	CLA	D	608	X	-	-	-
27	CLA	D	609	X	-	-	-
27	CLA	D	610	X	-	-	-
27	CLA	D	611	X	-	-	-
27	CLA	D	612	X	-	-	-
27	CLA	E	602	X	-	-	-
27	CLA	E	603	X	-	-	-
27	CLA	E	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	E	605	X	-	-	-
27	CLA	E	606	X	-	-	-
27	CLA	E	607	X	-	-	-
27	CLA	E	608	X	-	-	-
27	CLA	E	609	X	-	-	-
27	CLA	E	611	X	-	-	-
27	CLA	E	612	X	-	-	-
27	CLA	F	601	X	-	-	-
27	CLA	F	602	X	-	-	-
27	CLA	F	603	X	-	-	-
27	CLA	F	604	X	-	-	-
27	CLA	F	605	X	-	-	-
27	CLA	F	606	X	-	-	-
27	CLA	F	607	X	-	-	-
27	CLA	F	608	X	-	-	-
27	CLA	F	610	X	-	-	-
27	CLA	F	617	X	-	-	-
27	CLA	F	619	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	605	X	-	-	-
27	CLA	G	606	X	-	-	-
27	CLA	G	607	X	-	-	-
27	CLA	G	608	X	-	-	-
27	CLA	G	609	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	H	303	X	-	-	-
27	CLA	H	304	X	-	-	-
27	CLA	H	305	X	-	-	-
27	CLA	H	306	X	-	-	-
27	CLA	H	307	X	-	-	-
27	CLA	H	308	X	-	-	-
27	CLA	H	309	X	-	-	-
27	CLA	H	310	X	-	-	-
27	CLA	H	312	X	-	-	-
27	CLA	H	313	X	-	-	-
27	CLA	H	319	X	-	-	-
27	CLA	I	601	X	-	-	-
27	CLA	I	602	X	-	-	-
27	CLA	I	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	I	605	X	-	-	-
27	CLA	I	606	X	-	-	-
27	CLA	I	607	X	-	-	-
27	CLA	I	608	X	-	-	-
27	CLA	I	609	X	-	-	-
27	CLA	I	610	X	-	-	-
27	CLA	I	611	X	-	-	-
27	CLA	I	616	X	-	-	-
27	CLA	J	601	X	-	-	-
27	CLA	J	603	X	-	-	-
27	CLA	J	605	X	-	-	-
27	CLA	J	607	X	-	-	-
27	CLA	J	609	X	-	-	-
27	CLA	K	601	X	-	-	-
27	CLA	K	602	X	-	-	-
27	CLA	K	603	X	-	-	-
27	CLA	K	604	X	-	-	-
27	CLA	K	605	X	-	-	-
27	CLA	K	606	X	-	-	-
27	CLA	K	608	X	-	-	-
27	CLA	T	601	X	-	-	-
27	CLA	T	602	X	-	-	-
27	CLA	T	603	X	-	-	-
27	CLA	T	604	X	-	-	-
27	CLA	T	605	X	-	-	-
27	CLA	T	606	X	-	-	-
27	CLA	T	607	X	-	-	-
27	CLA	T	609	X	-	-	-
27	CLA	U	601	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	605	X	-	-	-
27	CLA	U	606	X	-	-	-
27	CLA	a	801	X	-	-	-
27	CLA	a	802	X	-	-	-
27	CLA	a	803	X	-	-	-
27	CLA	a	804	X	-	-	-
27	CLA	a	805	X	-	-	-
27	CLA	a	806	X	-	-	-
27	CLA	a	807	X	-	-	-
27	CLA	a	808	X	-	-	-
27	CLA	a	809	X	-	-	-
27	CLA	a	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	a	811	X	-	-	-
27	CLA	a	812	X	-	-	-
27	CLA	a	813	X	-	-	-
27	CLA	a	814	X	-	-	-
27	CLA	a	815	X	-	-	-
27	CLA	a	816	X	-	-	-
27	CLA	a	817	X	-	-	-
27	CLA	a	818	X	-	-	-
27	CLA	a	819	X	-	-	-
27	CLA	a	820	X	-	-	-
27	CLA	a	821	X	-	-	-
27	CLA	a	822	X	-	-	-
27	CLA	a	823	X	-	-	-
27	CLA	a	824	X	-	-	-
27	CLA	a	825	X	-	-	-
27	CLA	a	826	X	-	-	-
27	CLA	a	827	X	-	-	-
27	CLA	a	828	X	-	-	-
27	CLA	a	829	X	-	-	-
27	CLA	a	830	X	-	-	-
27	CLA	a	831	X	-	-	-
27	CLA	a	837	X	-	-	-
27	CLA	a	839	X	-	-	-
27	CLA	b	701	X	-	-	-
27	CLA	b	702	X	-	-	-
27	CLA	b	703	X	-	-	-
27	CLA	b	704	X	-	-	-
27	CLA	b	705	X	-	-	-
27	CLA	b	706	X	-	-	-
27	CLA	b	707	X	-	-	-
27	CLA	b	708	X	-	-	-
27	CLA	b	709	X	-	-	-
27	CLA	b	710	X	-	-	-
27	CLA	b	711	X	-	-	-
27	CLA	b	712	X	-	-	-
27	CLA	b	713	X	-	-	-
27	CLA	b	714	X	-	-	-
27	CLA	b	715	X	-	-	-
27	CLA	b	716	X	-	-	-
27	CLA	b	717	X	-	-	-
27	CLA	b	718	X	-	-	-
27	CLA	b	719	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	720	X	-	-	-
27	CLA	b	721	X	-	-	-
27	CLA	b	722	X	-	-	-
27	CLA	b	723	X	-	-	-
27	CLA	b	724	X	-	-	-
27	CLA	b	725	X	-	-	-
27	CLA	b	726	X	-	-	-
27	CLA	b	727	X	-	-	-
27	CLA	b	728	X	-	-	-
27	CLA	f	302	X	-	-	-
27	CLA	f	303	X	-	-	-
27	CLA	j	202	X	-	-	-
27	CLA	l	402	X	-	-	-
27	CLA	l	403	X	-	-	-
27	CLA	l	404	X	-	-	-
27	CLA	l	405	X	-	-	-
27	CLA	l	406	X	-	-	-
27	CLA	l	407	X	-	-	-
27	CLA	l	408	X	-	-	-
27	CLA	l	409	X	-	-	-
27	CLA	l	410	X	-	-	-
27	CLA	l	411	X	-	-	-
27	CLA	l	412	X	-	-	-
27	CLA	r	203	X	-	-	-
27	CLA	r	204	X	-	-	-
30	DD6	D	613	X	-	-	-
38	BCR	a	834	-	-	X	-
38	BCR	a	836	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55980 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 PCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total	C	N	O	S	0	0
			1461	941	239	274	7		

- Molecule 2 is a protein called PCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	185	Total	C	N	O	S	0	0
			1412	900	237	264	11		

- Molecule 3 is a protein called PCP-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	192	Total	C	N	O	S	0	0
			1518	990	244	273	11		

- Molecule 4 is a protein called PCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1375	893	226	245	11		

- Molecule 5 is a protein called PCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	184	Total	C	N	O	S	0	0
			1444	940	241	256	7		

- Molecule 6 is a protein called PCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1731	1118	282	314	17		

- Molecule 7 is a protein called PCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	173	Total	C	N	O	S	0	0
			1329	861	220	238	10		

- Molecule 8 is a protein called PCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1458	948	241	261	8		

- Molecule 9 is a protein called PCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	221	Total	C	N	O	S	0	0
			1736	1138	272	315	11		

- Molecule 10 is a protein called PCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	173	Total	C	N	O	S	0	0
			1322	849	220	244	9		

- Molecule 11 is a protein called PCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	154	Total	C	N	O	S	0	0
			1134	718	194	211	11		

- Molecule 12 is a protein called PCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	140	Total	C	N	O	S	0	0
			1065	681	180	196	8		

- Molecule 13 is a protein called PCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	104	Total	C	N	O	S	0	0
			828	535	144	142	7		

- Molecule 14 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	665	Total	C	N	O	S	0	0
			5250	3443	877	904	26		

- Molecule 15 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	659	Total	C	N	O	S	0	0
			5220	3437	845	918	20		

- Molecule 16 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	86	Total	C	N	O	S	0	0
			651	402	109	131	9		

- Molecule 17 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	216	Total	C	N	O	S	0	0
			1765	1123	308	321	13		

- Molecule 18 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	e	73	Total	C	N	O	0	0
			590	386	101	103		

- Molecule 19 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1349	859	238	246	6		

- Molecule 20 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	120	Total	C	N	O	S	0	0
			971	627	165	177	2		

- Molecule 21 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	99	Total	C	N	O	S	0	0
			791	507	130	153	1		

- Molecule 22 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	253	Total	C	N	O	S	0	0
			1974	1290	319	356	9		

- Molecule 23 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	79	Total	C	N	O	S	0	0
			598	391	102	104	1		

- Molecule 24 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	131	Total	C	N	O	S	0	0
			1082	714	168	194	6		

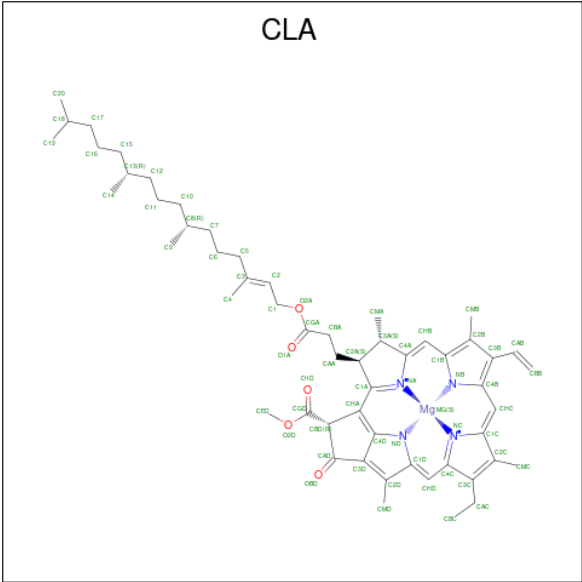
- Molecule 25 is a protein called PsaT.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	79	Total	C	N	O	S	0	0
			642	411	107	123	1		

- Molecule 26 is a protein called PsaU.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	130	Total	C	N	O	S	0	0
			1085	690	184	208	3		

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	I	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	J	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	J	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	K	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	U	1	Total 43	C 35	Mg 1	N 4	O 3	0
27	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	U	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	f	1	Total 48	C 38	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	j	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 28 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

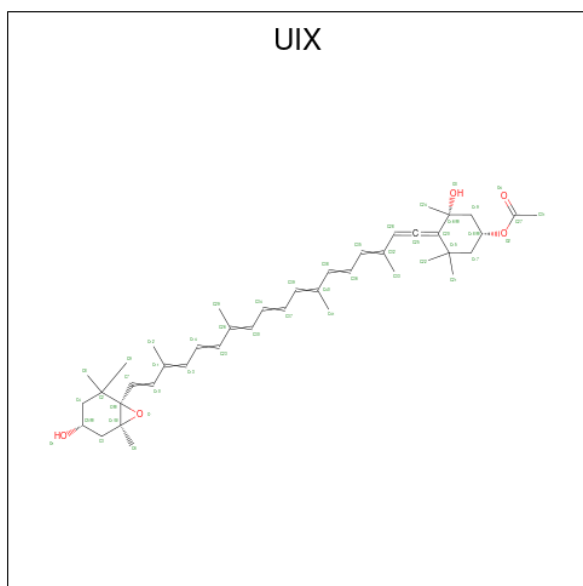


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Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-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]cyclohexyl] ethanoate (CCD ID: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



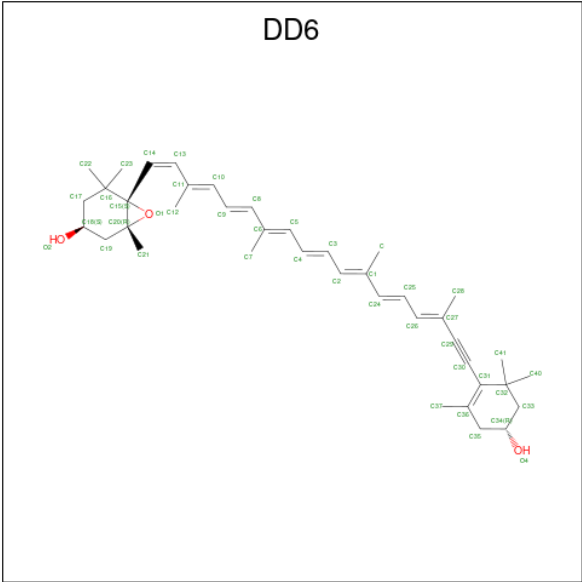
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O		0
			47	42	5		
29	A	1	Total	C	O		0
			47	42	5		
29	B	1	Total	C	O		0
			47	42	5		

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Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			47	42	5	
29	C	1	Total	C	O	0
			47	42	5	
29	C	1	Total	C	O	0
			47	42	5	
29	D	1	Total	C	O	0
			47	42	5	
29	E	1	Total	C	O	0
			47	42	5	
29	F	1	Total	C	O	0
			47	42	5	
29	G	1	Total	C	O	0
			47	42	5	
29	H	1	Total	C	O	0
			47	42	5	
29	H	1	Total	C	O	0
			47	42	5	
29	I	1	Total	C	O	0
			47	42	5	
29	J	1	Total	C	O	0
			47	42	5	
29	T	1	Total	C	O	0
			47	42	5	
29	j	1	Total	C	O	0
			47	42	5	

- Molecule 30 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).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	C	1	Total	C	O	0
			43	40	3	
30	C	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	E	1	Total	C	O	0
			43	40	3	

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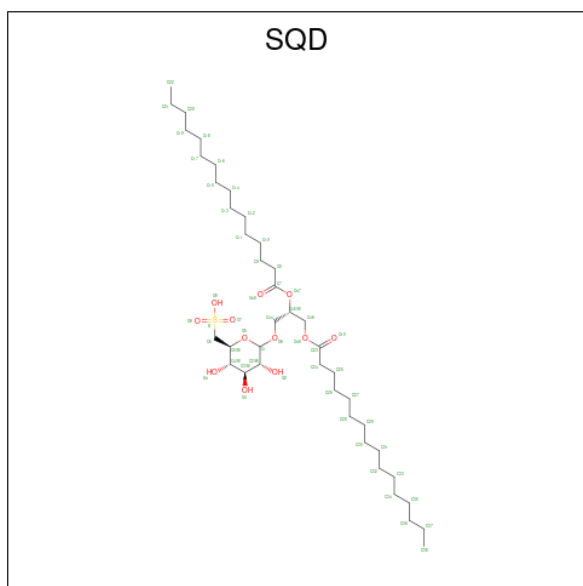
Mol	Chain	Residues	Atoms			AltConf
30	E	1	Total 43	C 40	O 3	0
30	E	1	Total 43	C 40	O 3	0
30	E	1	Total 43	C 40	O 3	0
30	F	1	Total 43	C 40	O 3	0
30	F	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	I	1	Total 43	C 40	O 3	0
30	I	1	Total 43	C 40	O 3	0
30	J	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	T	1	Total 43	C 40	O 3	0
30	T	1	Total 43	C 40	O 3	0

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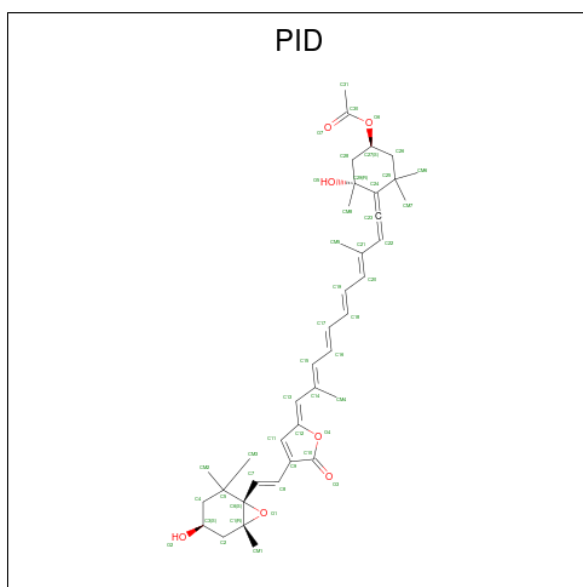
Mol	Chain	Residues	Atoms			AltConf
30	U	1	Total	C	O	0
			43	40	3	
30	b	1	Total	C	O	0
			43	40	3	
30	i	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



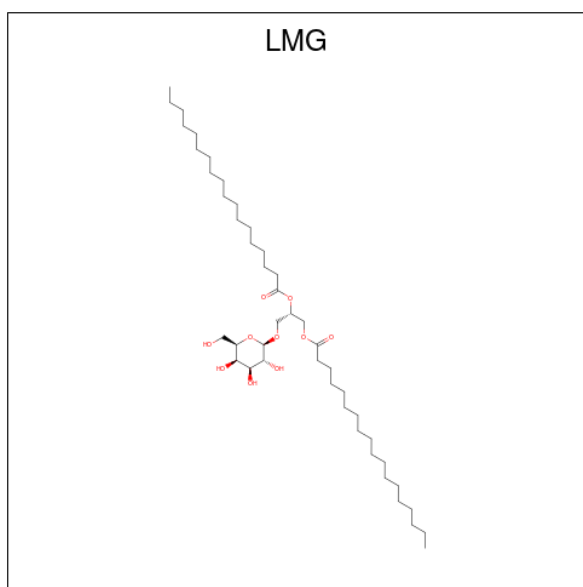
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			28	15	12	1	
31	H	1	Total	C	O	S	0
			46	33	12	1	
31	y	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 32 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



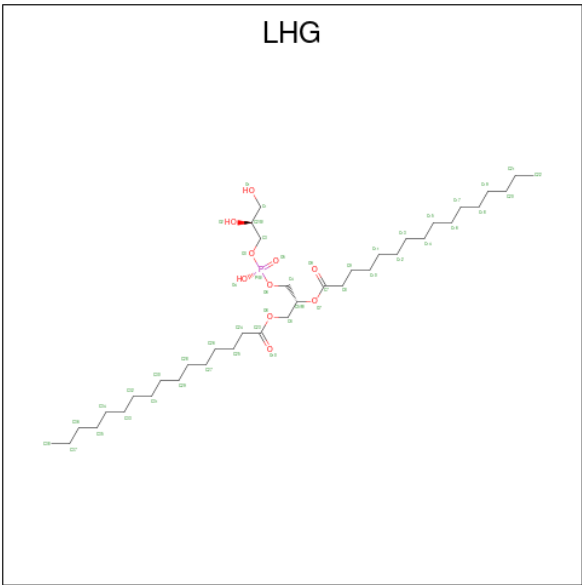
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	I	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	K	1	Total	C	O	0
			46	39	7	
32	U	1	Total	C	O	0
			46	39	7	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



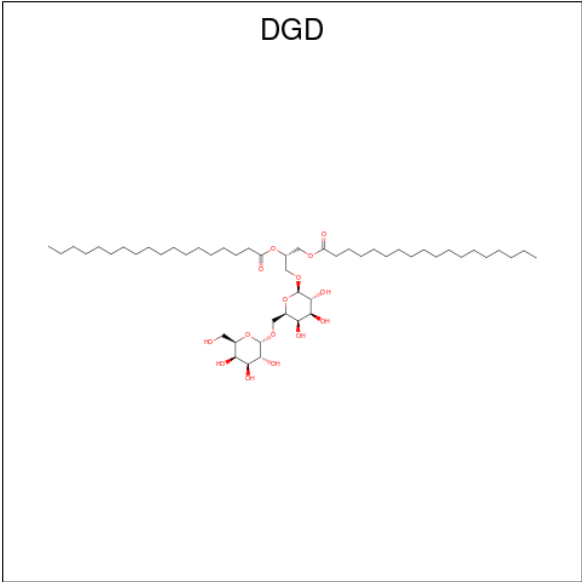
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			34	24	10	
33	D	1	Total	C	O	0
			35	25	10	
33	D	1	Total	C	O	0
			46	36	10	
33	F	1	Total	C	O	0
			46	36	10	
33	K	1	Total	C	O	0
			42	32	10	
33	b	1	Total	C	O	0
			55	45	10	
33	l	1	Total	C	O	0
			50	40	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



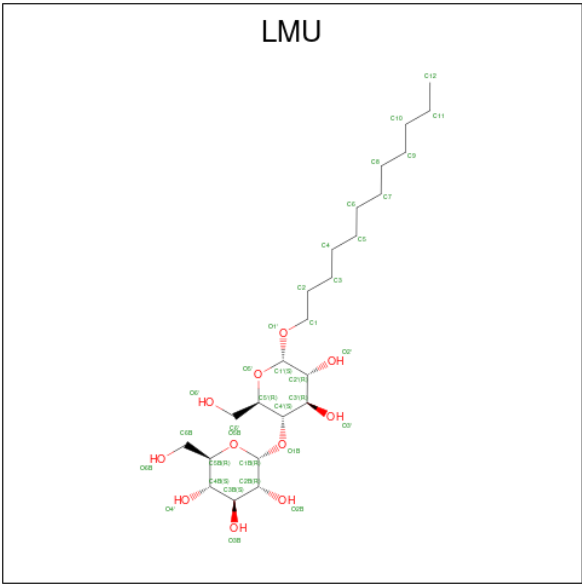
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			46	35	10	1	
34	F	1	Total	C	O	P	0
			37	26	10	1	
34	G	1	Total	C	O	P	0
			34	23	10	1	
34	a	1	Total	C	O	P	0
			48	37	10	1	
34	j	1	Total	C	O	P	0
			37	26	10	1	
34	l	1	Total	C	O	P	0
			46	35	10	1	
34	r	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



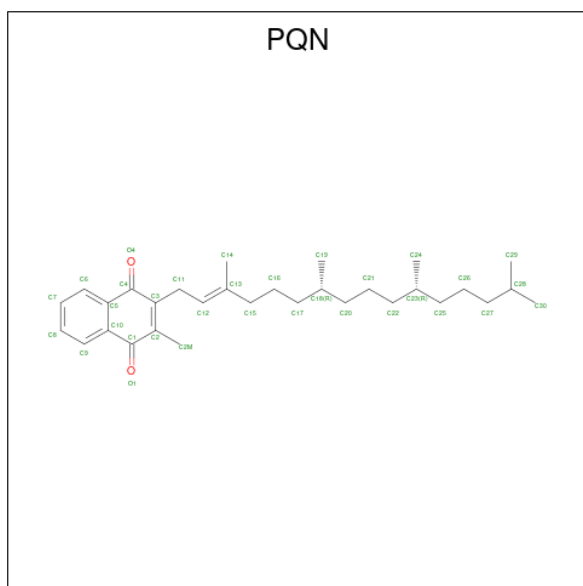
Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total	C	O	0
			47	32	15	
35	f	1	Total	C	O	0
			52	37	15	
35	j	1	Total	C	O	0
			60	45	15	
35	l	1	Total	C	O	0
			55	40	15	

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



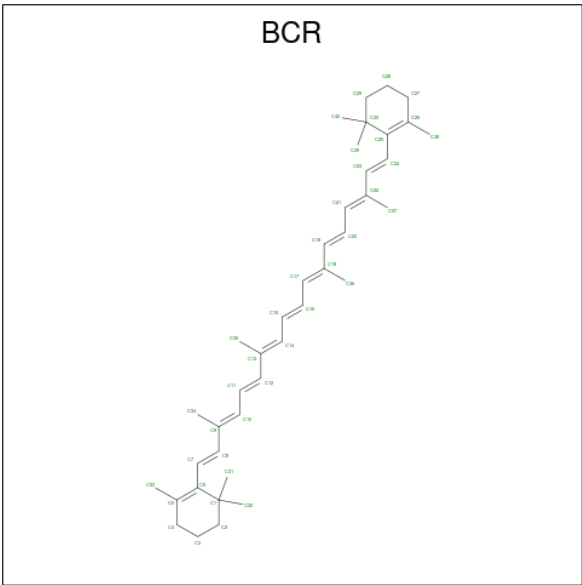
Mol	Chain	Residues	Atoms			AltConf
36	T	1	Total	C	O	0
			35	24	11	

- Molecule 37 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	a	1	Total	C	O	0
			33	31	2	
37	b	1	Total	C	O	0
			33	31	2	

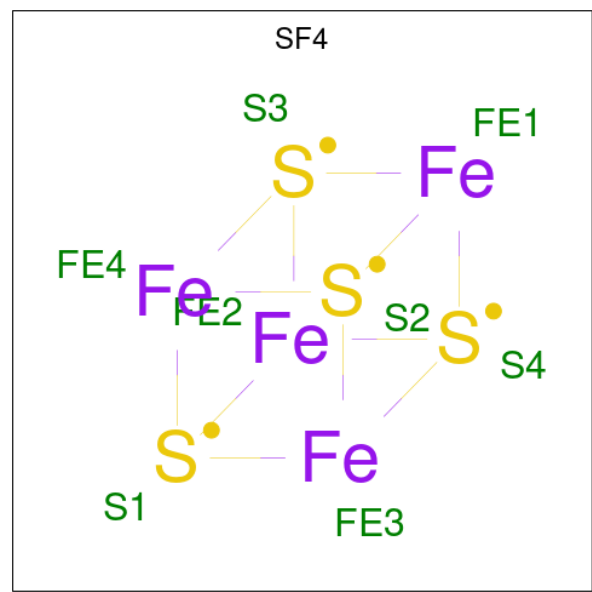
- Molecule 38 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	i	1	Total C 40 40	0
38	j	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	m	1	Total C 40 40	0

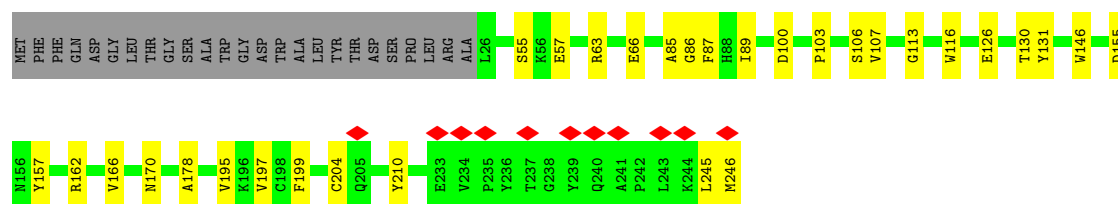
- Molecule 39 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as

"Ligand of Interest" by depositor).



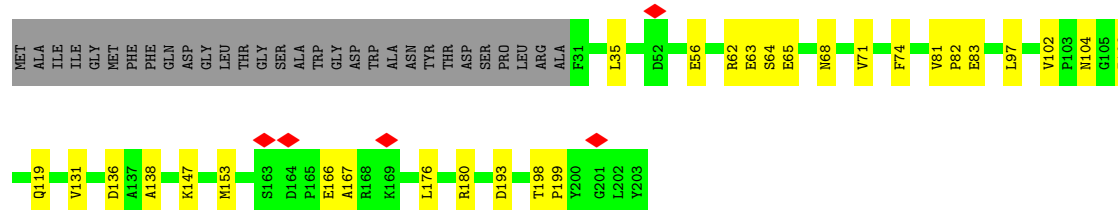
Mol	Chain	Residues	Atoms			AltConf
39	a	1	Total	Fe	S	0
			8	4	4	
39	c	1	Total	Fe	S	0
			8	4	4	
39	c	1	Total	Fe	S	0
			8	4	4	

Chain I: 

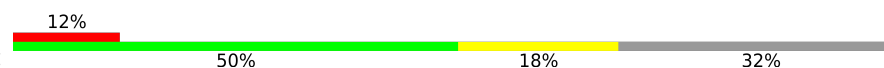


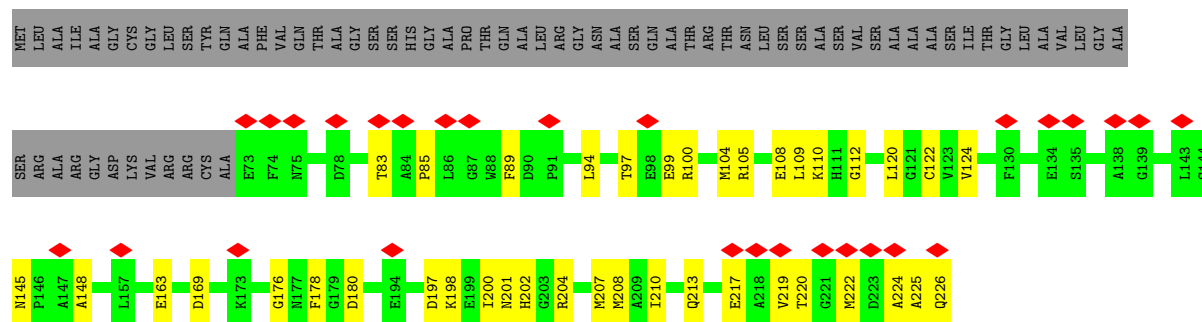
• Molecule 10: PCPI-9

Chain J: 



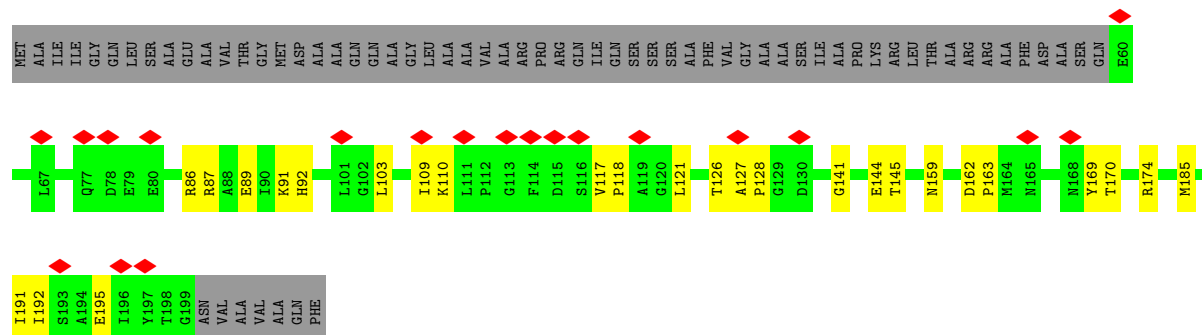
• Molecule 11: PCPI-13

Chain K: 

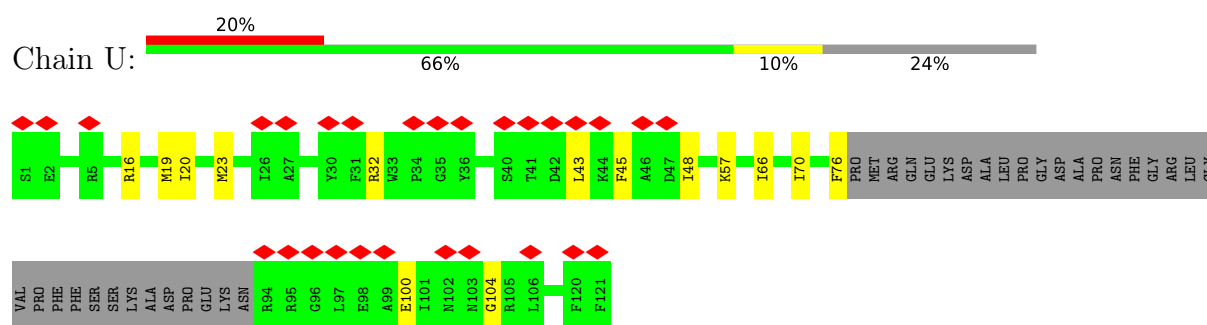


• Molecule 12: PCPI-12

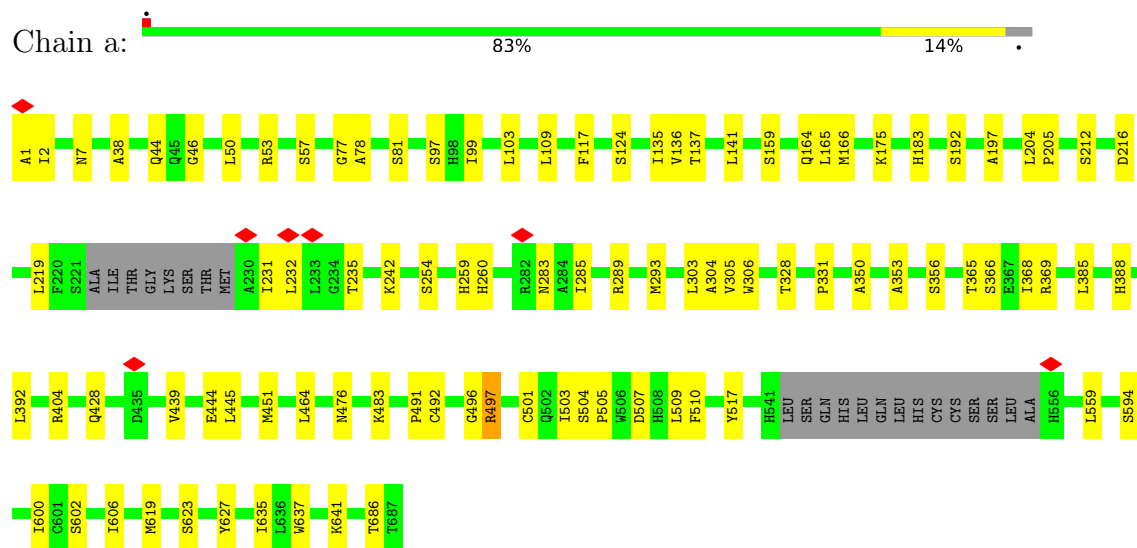
Chain T: 



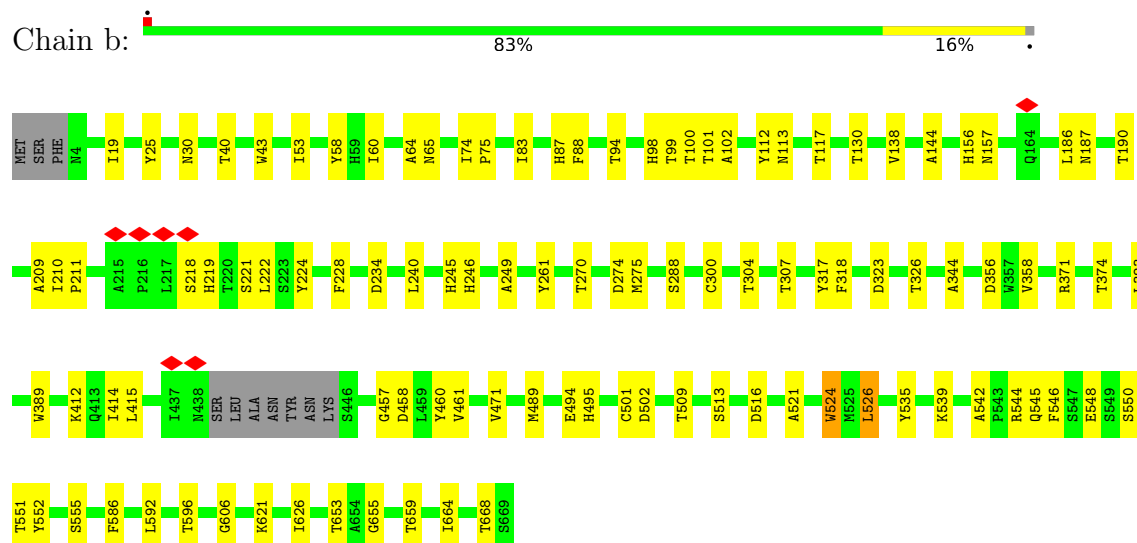
• Molecule 13: PCPI-2



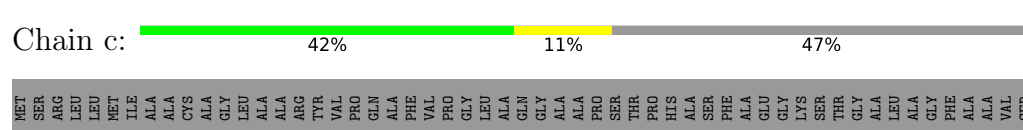
- Molecule 14: PsaA

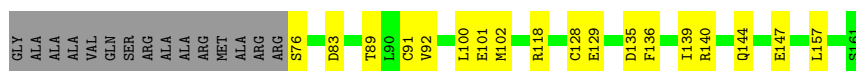


- Molecule 15: PsaB



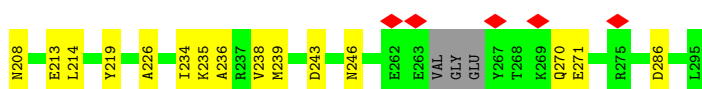
- Molecule 16: PsaC





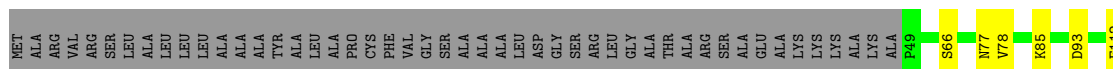
• Molecule 17: PsaD

Chain d: 60% 13% 27%



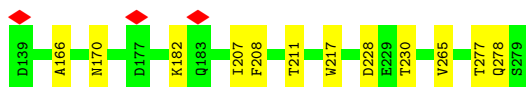
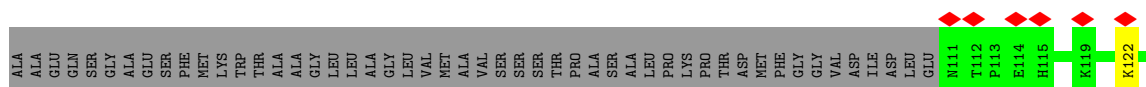
• Molecule 18: PsaE

Chain e: 55% 5% 40%



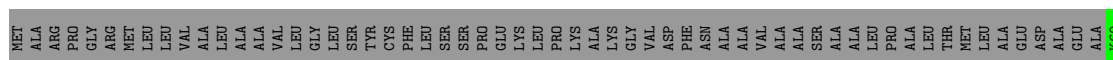
• Molecule 19: PsaF

Chain f: 56% 5% 39%

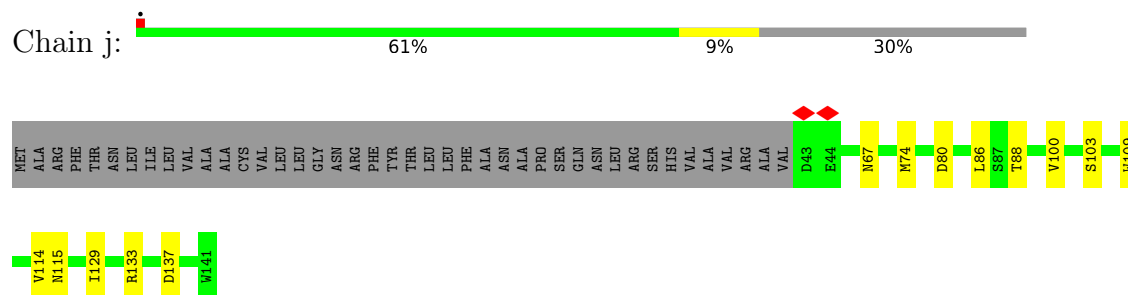


• Molecule 20: PsaI

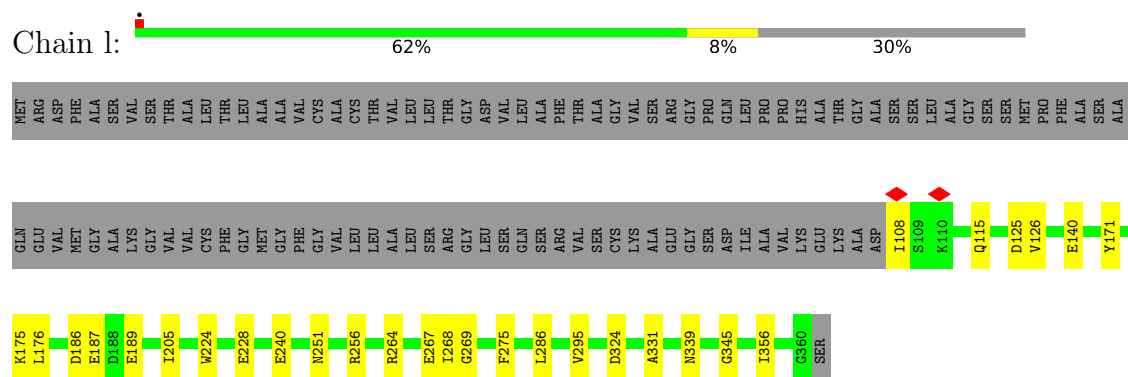
Chain i: 54% 13% 33%



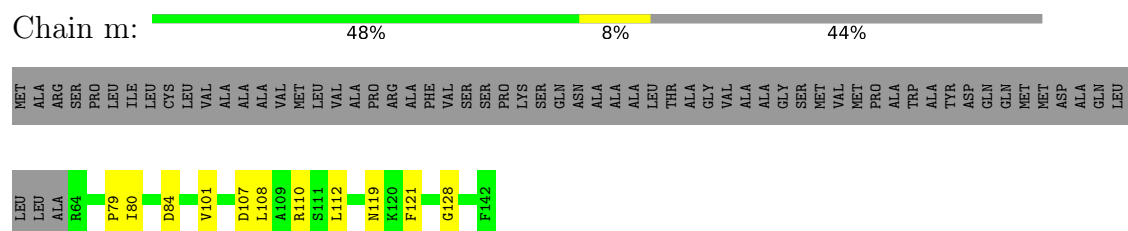
• Molecule 21: PsaJ



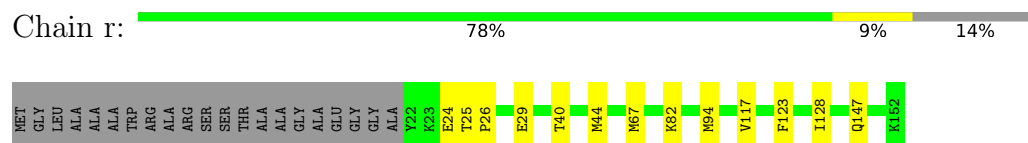
● Molecule 22: PsaL



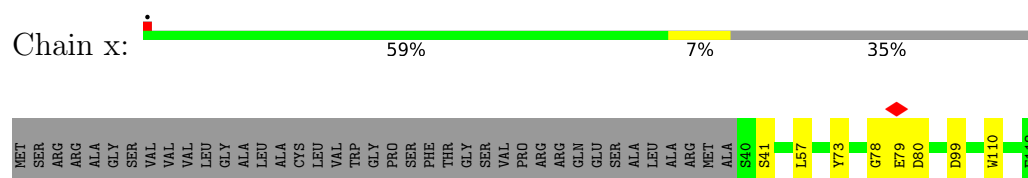
● Molecule 23: PsaM



● Molecule 24: PsaR



● Molecule 25: PsaT



● Molecule 26: PsaU



MET
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ARG
SER
LEU
SER
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VAL
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ALA
THR
PRO
ALA
PRO
GLY
P94
E97
V108
E114
F148
Y170
P171
I172
R173
I180
Q184
D187
L188
R189
A190
K191
M192
K193
E194

Y196
I196
G197
R198
E199
E202
I203
R204
D208
Y209
D210
R213
Y216
H219
N220
G221
Y222
Y223

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.960	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, UIX, LHG, DGD, SQD, PID, SF4, PQN, LMU, KC2, CLA, DD6, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/1501	0.28	0/2037
2	B	0.28	0/1443	0.38	0/1954
3	C	0.14	0/1562	0.26	0/2114
4	D	0.15	0/1413	0.27	0/1912
5	E	0.19	0/1484	0.39	1/2006 (0.0%)
6	F	0.15	0/1785	0.31	1/2426 (0.0%)
7	G	0.32	0/1365	0.37	1/1841 (0.1%)
8	H	0.13	0/1499	0.29	0/2030
9	I	0.35	0/1794	0.42	1/2454 (0.0%)
10	J	0.25	0/1355	0.35	1/1835 (0.1%)
11	K	0.47	0/1162	0.52	0/1565
12	T	0.35	0/1090	0.39	0/1477
13	U	0.24	0/847	0.36	0/1140
14	a	0.19	0/5412	0.30	1/7363 (0.0%)
15	b	0.51	4/5390 (0.1%)	0.44	4/7368 (0.1%)
16	c	0.36	0/661	0.42	0/901
17	d	0.14	0/1803	0.29	0/2419
18	e	0.11	0/611	0.24	0/836
19	f	0.49	1/1384 (0.1%)	0.35	0/1873
20	i	0.14	0/1001	0.28	0/1357
21	j	0.14	0/808	0.26	0/1104
22	l	0.21	0/2031	0.31	0/2755
23	m	0.33	0/608	0.33	0/820
24	r	0.27	0/1118	0.33	0/1513
25	x	0.13	0/667	0.26	0/908
26	y	0.21	0/1119	0.40	1/1515 (0.1%)
All	All	0.30	5/40913 (0.0%)	0.35	11/55523 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	246	HIS	CA-C	-5.75	1.45	1.52
15	b	521	ALA	CA-C	-5.64	1.44	1.52
19	f	217	TRP	CA-C	-5.40	1.46	1.52
15	b	157	ASN	CA-C	-5.39	1.45	1.52
15	b	526	LEU	CA-C	-5.12	1.46	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	228	PHE	N-CA-C	-9.21	97.63	110.35
26	y	108	VAL	N-CA-C	8.17	119.16	111.48
5	E	77	ASN	N-CA-C	-8.16	98.39	110.23
9	I	89	ILE	N-CA-C	7.05	117.84	110.72
10	J	153	MET	CB-CA-C	-6.26	101.06	110.88

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	A	1461	0	1420	18	0
2	B	1412	0	1384	22	0
3	C	1518	0	1491	16	0
4	D	1375	0	1359	19	0
5	E	1444	0	1418	24	0
6	F	1731	0	1691	24	0
7	G	1329	0	1301	23	0
8	H	1458	0	1426	20	0
9	I	1736	0	1687	25	0
10	J	1322	0	1296	19	0
11	K	1134	0	1085	49	0
12	T	1065	0	1042	19	0
13	U	828	0	828	13	0
14	a	5250	0	5201	86	0
15	b	5220	0	5122	94	0
16	c	651	0	634	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	d	1765	0	1785	40	0
18	e	590	0	582	7	0
19	f	1349	0	1334	8	0
20	i	971	0	951	21	0
21	j	791	0	783	13	0
22	l	1974	0	1950	29	0
23	m	598	0	641	14	0
24	r	1082	0	1041	12	0
25	x	642	0	594	6	0
26	y	1085	0	1025	11	0
27	A	543	0	441	4	0
27	B	454	0	437	1	0
27	C	565	0	489	5	0
27	D	624	0	532	8	0
27	E	537	0	481	2	0
27	F	575	0	500	10	0
27	G	529	0	463	4	0
27	H	602	0	559	9	0
27	I	623	0	596	6	0
27	J	248	0	211	4	0
27	K	360	0	309	14	0
27	T	354	0	258	5	0
27	U	198	0	164	8	0
27	a	1927	0	1885	50	0
27	b	1717	0	1790	43	0
27	f	96	0	72	1	0
27	j	56	0	51	1	0
27	l	627	0	600	7	0
27	r	108	0	95	1	0
28	A	45	0	0	0	0
28	B	90	0	0	0	0
28	C	45	0	0	0	0
28	E	90	0	0	0	0
28	F	45	0	0	0	0
28	G	45	0	0	0	0
28	H	90	0	0	0	0
28	I	45	0	0	1	0
28	J	225	0	0	6	0
28	K	45	0	0	6	0
28	T	45	0	0	0	0
28	U	90	0	0	0	0
29	A	94	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	94	0	0	0	0
29	C	94	0	0	1	0
29	D	47	0	0	0	0
29	E	47	0	0	0	0
29	F	47	0	0	0	0
29	G	47	0	0	0	0
29	H	94	0	0	1	0
29	I	47	0	0	2	0
29	J	47	0	0	0	0
29	T	47	0	0	0	0
29	j	47	0	0	2	0
30	A	129	0	0	2	0
30	B	129	0	0	1	0
30	C	86	0	0	2	0
30	D	215	0	0	3	0
30	E	172	0	0	1	0
30	F	86	0	0	1	0
30	G	172	0	0	2	0
30	H	172	0	0	3	0
30	I	86	0	0	0	0
30	J	43	0	0	0	0
30	K	129	0	0	2	0
30	T	86	0	0	0	0
30	U	43	0	0	0	0
30	b	43	0	0	1	0
30	i	43	0	0	1	0
30	r	129	0	0	0	0
31	A	28	0	20	0	0
31	H	46	0	56	0	0
31	y	46	0	56	0	0
32	B	46	0	50	1	0
32	F	92	0	100	9	0
32	I	46	0	50	4	0
32	J	184	0	200	21	0
32	K	46	0	50	12	0
32	U	46	0	50	0	0
33	C	34	0	38	1	0
33	D	81	0	105	1	0
33	F	46	0	65	0	0
33	K	42	0	57	1	0
33	b	55	0	86	0	0
33	l	50	0	73	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D	46	0	65	0	0
34	F	37	0	44	0	0
34	G	34	0	38	0	0
34	a	48	0	69	0	0
34	j	37	0	44	0	0
34	l	46	0	65	1	0
34	r	46	0	65	1	0
35	K	47	0	52	3	0
35	f	52	0	62	0	0
35	j	60	0	81	1	0
35	l	55	0	71	3	0
36	T	35	0	46	1	0
37	a	33	0	46	0	0
37	b	33	0	46	0	0
38	a	120	0	168	44	0
38	b	80	0	112	2	0
38	f	80	0	112	6	0
38	i	40	0	56	5	0
38	j	40	0	56	0	0
38	l	120	0	168	13	0
38	m	40	0	56	1	0
39	a	8	0	0	0	0
39	c	16	0	0	0	0
All	All	55980	0	51582	736	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 736 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)
38:a:834:BCR:H362	38:a:836:BCR:C21	1.13	1.61
38:a:834:BCR:C36	38:a:836:BCR:H21C	0.99	1.45
3:C:12:THR:HG22	17:d:286:ASP:OD2	1.33	1.28
15:b:245:HIS:CD2	27:b:714:CLA:CBB	2.15	1.28
38:a:834:BCR:H372	38:a:836:BCR:C39	1.63	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

323 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	$\# Z > 2$
38	BCR	f	304	-	41,41,41	0.29	0	56,56,56	0.52	0
32	PID	J	615	-	43,49,49	1.60	7 (16%)	52,76,76	3.79	20 (38%)
38	BCR	f	301	-	41,41,41	0.30	0	56,56,56	0.73	0
27	CLA	T	604	12	45,49,73	2.17	10 (22%)	54,84,113	1.62	8 (14%)
27	CLA	l	405	22	65,69,73	1.77	9 (13%)	77,108,113	1.34	8 (10%)
27	CLA	a	806	-	59,63,73	1.84	9 (15%)	70,101,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	609	-	51,55,73	2.00	9 (17%)	60,91,113	1.48	8 (13%)
27	CLA	b	703	-	69,73,73	1.71	9 (13%)	82,113,113	1.31	11 (13%)
27	CLA	C	202	3	49,53,73	2.04	9 (18%)	58,89,113	1.54	8 (13%)
30	DD6	r	201	-	40,45,45	0.16	0	51,67,67	0.93	4 (7%)
30	DD6	C	216	-	40,45,45	0.15	0	51,67,67	0.77	2 (3%)
27	CLA	T	601	12	51,55,73	2.04	9 (17%)	60,91,113	1.55	8 (13%)
27	CLA	a	805	-	69,73,73	1.71	9 (13%)	82,113,113	1.30	8 (9%)
27	CLA	K	605	11	64,68,73	1.76	9 (14%)	76,107,113	1.32	7 (9%)
28	KC2	B	608	2	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	C	205	-	59,63,73	1.92	9 (15%)	70,101,113	1.58	8 (11%)
32	PID	J	611	-	43,49,49	1.64	7 (16%)	52,76,76	4.16	21 (40%)
27	CLA	K	601	11	61,65,73	1.83	9 (14%)	72,103,113	1.41	6 (8%)
30	DD6	F	612	-	40,45,45	0.16	0	51,67,67	0.52	0
33	LMG	K	613	-	42,42,55	0.54	0	50,50,63	0.65	0
27	CLA	T	606	12	49,53,73	2.05	9 (18%)	58,89,113	1.51	6 (10%)
27	CLA	l	409	-	69,73,73	1.69	9 (13%)	82,113,113	1.30	8 (9%)
27	CLA	D	610	4	51,55,73	1.99	9 (17%)	60,91,113	1.47	9 (15%)
33	LMG	D	619	-	46,46,55	0.53	0	54,54,63	0.70	1 (1%)
38	BCR	b	732	-	41,41,41	0.31	0	56,56,56	0.75	1 (1%)
30	DD6	i	202	-	40,45,45	0.19	0	51,67,67	0.81	2 (3%)
27	CLA	D	606	-	49,53,73	2.02	9 (18%)	58,89,113	1.51	8 (13%)
29	UIX	I	612	-	43,49,49	1.44	4 (9%)	53,74,74	2.15	19 (35%)
28	KC2	K	607	-	49,53,53	1.83	4 (8%)	60,89,89	1.16	4 (6%)
33	LMG	b	733	-	55,55,55	0.48	0	63,63,63	0.56	0
38	BCR	j	203	-	41,41,41	0.31	0	56,56,56	0.57	0
27	CLA	G	607	7	49,53,73	2.03	9 (18%)	58,89,113	1.60	8 (13%)
30	DD6	I	615	-	40,45,45	0.17	0	51,67,67	0.63	1 (1%)
27	CLA	I	605	9	59,63,73	1.82	9 (15%)	70,101,113	1.35	8 (11%)
27	CLA	B	601	-	64,68,73	1.76	9 (14%)	76,107,113	1.39	8 (10%)
27	CLA	A	607	-	49,53,73	2.05	9 (18%)	58,89,113	1.52	8 (13%)
27	CLA	A	605	1	59,63,73	1.84	9 (15%)	70,101,113	1.39	8 (11%)
27	CLA	a	814	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	8 (11%)
28	KC2	T	608	-	49,53,53	1.83	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	U	603	-	54,58,73	2.00	9 (16%)	64,95,113	1.55	8 (12%)
28	KC2	G	601	-	49,53,53	1.81	4 (8%)	60,89,89	1.18	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	609	2	69,73,73	1.71	9 (13%)	82,113,113	1.28	9 (10%)
30	DD6	E	615	-	40,45,45	0.18	0	51,67,67	0.60	1 (1%)
27	CLA	b	704	-	69,73,73	1.69	9 (13%)	82,113,113	1.28	8 (9%)
32	PID	B	613	-	43,49,49	1.66	7 (16%)	52,76,76	3.65	23 (44%)
27	CLA	G	603	-	54,58,73	1.92	9 (16%)	64,95,113	1.46	9 (14%)
27	CLA	b	718	-	69,73,73	1.72	9 (13%)	82,113,113	1.41	10 (12%)
30	DD6	E	613	-	40,45,45	0.17	0	51,67,67	0.78	2 (3%)
29	UIX	C	213	-	43,49,49	1.36	5 (11%)	53,74,74	1.90	14 (26%)
27	CLA	B	603	-	69,73,73	1.76	9 (13%)	82,113,113	1.39	8 (9%)
27	CLA	a	802	-	59,63,73	1.84	9 (15%)	70,101,113	1.36	8 (11%)
38	BCR	a	836	-	41,41,41	0.82	2 (4%)	56,56,56	2.19	19 (33%)
27	CLA	C	212	-	51,55,73	2.02	9 (17%)	60,91,113	1.50	8 (13%)
27	CLA	D	612	-	59,63,73	1.87	9 (15%)	70,101,113	1.40	8 (11%)
30	DD6	G	613	-	40,45,45	0.16	0	51,67,67	0.70	2 (3%)
32	PID	J	613	-	43,49,49	1.75	8 (18%)	52,76,76	4.27	21 (40%)
27	CLA	l	404	-	59,63,73	1.85	9 (15%)	70,101,113	1.42	8 (11%)
27	CLA	T	607	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	C	209	-	49,53,73	2.06	9 (18%)	58,89,113	1.54	9 (15%)
27	CLA	b	707	-	69,73,73	1.70	9 (13%)	82,113,113	1.33	8 (9%)
27	CLA	r	204	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	8 (10%)
27	CLA	a	822	-	64,68,73	1.78	9 (14%)	76,107,113	1.36	9 (11%)
30	DD6	K	610	-	40,45,45	0.17	0	51,67,67	0.77	2 (3%)
27	CLA	B	607	-	64,68,73	1.77	9 (14%)	76,107,113	1.32	9 (11%)
30	DD6	b	730	-	40,45,45	0.17	0	51,67,67	0.58	1 (1%)
28	KC2	J	608	-	49,53,53	1.83	4 (8%)	60,89,89	1.15	4 (6%)
34	LHG	D	620	-	45,45,48	0.53	0	48,51,54	0.51	0
27	CLA	l	411	22	52,56,73	1.97	9 (17%)	61,92,113	1.52	8 (13%)
27	CLA	l	403	-	69,73,73	1.72	9 (13%)	82,113,113	1.25	8 (9%)
30	DD6	D	621	-	40,45,45	0.18	0	51,67,67	0.77	2 (3%)
28	KC2	J	610	-	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
30	DD6	C	214	-	40,45,45	0.19	0	51,67,67	0.68	3 (5%)
27	CLA	F	602	-	60,64,73	1.87	9 (15%)	71,102,113	1.39	9 (12%)
27	CLA	a	826	-	59,63,73	1.83	9 (15%)	70,101,113	1.37	8 (11%)
32	PID	I	614	-	43,49,49	1.70	7 (16%)	52,76,76	3.91	24 (46%)
29	UIX	E	616	-	43,49,49	1.38	5 (11%)	53,74,74	1.99	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PQN	b	729	-	34,34,34	0.37	0	43,45,45	0.65	1 (2%)
27	CLA	a	803	27	54,58,73	1.93	9 (16%)	64,95,113	1.52	6 (9%)
35	DGD	j	201	-	61,61,67	0.92	4 (6%)	75,75,81	1.44	13 (17%)
29	UIX	F	613	-	43,49,49	1.33	4 (9%)	53,74,74	2.02	15 (28%)
33	LMG	D	618	-	35,35,55	0.55	0	43,43,63	0.77	1 (2%)
27	CLA	D	608	4	59,63,73	1.85	9 (15%)	70,101,113	1.43	8 (11%)
27	CLA	B	610	-	51,55,73	1.97	9 (17%)	60,91,113	1.52	8 (13%)
27	CLA	E	602	5	59,63,73	1.85	9 (15%)	70,101,113	1.41	9 (12%)
35	DGD	K	614	-	48,48,67	0.99	4 (8%)	62,62,81	1.42	10 (16%)
27	CLA	l	410	-	52,56,73	2.03	9 (17%)	61,92,113	1.54	8 (13%)
27	CLA	b	701	-	69,73,73	1.70	9 (13%)	82,113,113	1.27	8 (9%)
30	DD6	D	614	-	40,45,45	0.15	0	51,67,67	0.63	2 (3%)
30	DD6	J	612	-	40,45,45	0.18	0	51,67,67	0.59	1 (1%)
27	CLA	I	611	-	46,50,73	2.18	9 (19%)	53,85,113	1.69	9 (16%)
27	CLA	K	602	-	59,63,73	1.87	9 (15%)	70,101,113	1.39	8 (11%)
27	CLA	F	605	6	49,53,73	2.03	9 (18%)	58,89,113	1.56	9 (15%)
32	PID	J	614	-	43,49,49	1.63	6 (13%)	52,76,76	3.49	18 (34%)
28	KC2	A	608	-	49,53,53	1.81	4 (8%)	60,89,89	1.19	5 (8%)
27	CLA	C	203	3	69,73,73	1.71	9 (13%)	82,113,113	1.35	8 (9%)
27	CLA	E	605	5	49,53,73	2.08	9 (18%)	58,89,113	1.58	9 (15%)
27	CLA	F	601	6	64,68,73	1.79	9 (14%)	76,107,113	1.35	7 (9%)
27	CLA	H	310	-	49,53,73	2.10	9 (18%)	58,89,113	1.61	8 (13%)
30	DD6	H	316	-	40,45,45	0.20	0	51,67,67	0.73	2 (3%)
27	CLA	I	616	-	69,73,73	1.73	9 (13%)	82,113,113	1.25	9 (10%)
27	CLA	j	202	27	60,64,73	1.86	9 (15%)	71,102,113	1.32	8 (11%)
27	CLA	f	302	-	52,56,73	1.96	9 (17%)	61,92,113	1.47	9 (14%)
34	LHG	F	618	-	36,36,48	0.58	0	39,42,54	0.57	0
27	CLA	K	608	-	49,53,73	2.11	9 (18%)	58,89,113	1.52	9 (15%)
27	CLA	a	801	-	69,73,73	1.67	8 (11%)	82,113,113	1.20	9 (10%)
28	KC2	B	602	-	49,53,53	1.81	4 (8%)	60,89,89	1.11	4 (6%)
27	CLA	T	609	-	45,49,73	2.22	10 (22%)	54,84,113	1.66	8 (14%)
27	CLA	J	601	-	49,53,73	2.07	9 (18%)	58,89,113	1.60	6 (10%)
27	CLA	a	821	-	69,73,73	1.69	9 (13%)	82,113,113	1.28	8 (9%)
27	CLA	H	303	8	64,68,73	1.74	9 (14%)	76,107,113	1.35	10 (13%)
39	SF4	a	838	14	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	C	211	-	51,55,73	2.01	9 (17%)	60,91,113	1.45	8 (13%)
27	CLA	D	604	-	59,63,73	1.85	9 (15%)	70,101,113	1.43	8 (11%)
35	DGD	l	416	-	56,56,67	0.92	2 (3%)	70,70,81	1.39	8 (11%)
27	CLA	b	714	-	52,56,73	2.01	9 (17%)	61,92,113	1.59	7 (11%)
27	CLA	b	705	-	69,73,73	1.73	9 (13%)	82,113,113	1.38	7 (8%)
30	DD6	E	617	-	40,45,45	0.16	0	51,67,67	0.80	2 (3%)
27	CLA	J	607	-	46,50,73	2.12	9 (19%)	53,85,113	1.59	8 (15%)
27	CLA	K	603	-	49,53,73	2.05	9 (18%)	58,89,113	1.57	7 (12%)
30	DD6	A	615	-	40,45,45	0.17	0	51,67,67	0.72	1 (1%)
30	DD6	F	611	-	40,45,45	0.17	0	51,67,67	0.82	3 (5%)
27	CLA	a	817	-	59,63,73	1.86	9 (15%)	70,101,113	1.41	9 (12%)
27	CLA	G	608	-	64,68,73	1.82	9 (14%)	76,107,113	1.41	7 (9%)
27	CLA	a	820	-	69,73,73	1.74	9 (13%)	82,113,113	1.27	8 (9%)
27	CLA	b	723	-	69,73,73	1.71	9 (13%)	82,113,113	1.33	7 (8%)
30	DD6	I	613	-	40,45,45	0.18	0	51,67,67	0.78	2 (3%)
27	CLA	b	726	-	64,68,73	1.77	9 (14%)	76,107,113	1.32	9 (11%)
29	UIX	A	616	-	43,49,49	1.40	5 (11%)	53,74,74	1.98	18 (33%)
27	CLA	F	608	6	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	C	208	-	51,55,73	2.01	9 (17%)	60,91,113	1.49	8 (13%)
30	DD6	G	616	-	40,45,45	0.15	0	51,67,67	0.47	0
29	UIX	B	611	-	43,49,49	1.45	5 (11%)	53,74,74	2.02	21 (39%)
28	KC2	U	604	13	49,53,53	1.81	4 (8%)	60,89,89	1.12	4 (6%)
27	CLA	T	602	-	49,53,73	2.07	9 (18%)	58,89,113	1.52	8 (13%)
27	CLA	l	408	-	51,55,73	2.02	9 (17%)	60,91,113	1.55	7 (11%)
29	UIX	A	613	-	43,49,49	1.36	4 (9%)	53,74,74	1.88	16 (30%)
27	CLA	a	827	-	69,73,73	1.75	9 (13%)	82,113,113	1.42	8 (9%)
27	CLA	A	602	1	64,68,73	1.79	9 (14%)	76,107,113	1.37	9 (11%)
27	CLA	I	603	-	69,73,73	1.70	9 (13%)	82,113,113	1.34	8 (9%)
27	CLA	a	829	27	69,73,73	1.72	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	U	601	-	47,51,73	2.15	9 (19%)	55,86,113	1.72	7 (12%)
27	CLA	b	720	-	52,56,73	1.99	9 (17%)	61,92,113	1.48	8 (13%)
27	CLA	U	605	13	64,68,73	1.79	9 (14%)	76,107,113	1.29	7 (9%)
27	CLA	F	607	6	49,53,73	2.03	9 (18%)	58,89,113	1.57	7 (12%)
27	CLA	J	609	-	45,49,73	2.22	10 (22%)	54,84,113	1.69	8 (14%)
27	CLA	H	309	-	69,73,73	1.72	9 (13%)	82,113,113	1.31	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	716	-	69,73,73	1.73	9 (13%)	82,113,113	1.28	8 (9%)
27	CLA	a	808	14	59,63,73	1.90	9 (15%)	70,101,113	1.43	10 (14%)
30	DD6	K	612	-	40,45,45	0.17	0	51,67,67	0.72	4 (7%)
28	KC2	F	609	6	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
28	KC2	J	606	-	49,53,53	1.82	4 (8%)	60,89,89	1.11	4 (6%)
27	CLA	a	804	-	69,73,73	1.70	9 (13%)	82,113,113	1.37	11 (13%)
30	DD6	G	612	-	40,45,45	0.18	0	51,67,67	0.79	2 (3%)
30	DD6	G	614	-	40,45,45	0.16	0	51,67,67	0.56	1 (1%)
27	CLA	G	605	-	64,68,73	1.82	9 (14%)	76,107,113	1.44	9 (11%)
27	CLA	I	607	-	65,69,73	1.78	9 (13%)	77,108,113	1.33	8 (10%)
27	CLA	D	601	4	49,53,73	2.03	9 (18%)	58,89,113	1.50	8 (13%)
27	CLA	F	603	-	56,60,73	1.90	9 (16%)	65,97,113	1.44	8 (12%)
27	CLA	b	719	-	69,73,73	1.74	9 (13%)	82,113,113	1.27	8 (9%)
27	CLA	H	307	-	49,53,73	2.06	9 (18%)	58,89,113	1.50	8 (13%)
28	KC2	C	210	-	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
27	CLA	J	605	10	64,68,73	1.78	9 (14%)	76,107,113	1.28	7 (9%)
36	LMU	T	613	-	36,36,36	0.42	0	47,47,47	0.96	2 (4%)
35	DGD	f	305	-	53,53,67	0.97	3 (5%)	67,67,81	1.50	11 (16%)
30	DD6	A	614	-	40,45,45	0.16	0	51,67,67	0.72	3 (5%)
38	BCR	a	833	-	41,41,41	0.29	0	56,56,56	0.61	0
29	UIX	D	616	-	43,49,49	1.36	4 (9%)	53,74,74	2.08	17 (32%)
39	SF4	c	202	-	0,12,12	-	-	-	-	-
38	BCR	i	201	-	41,41,41	0.31	0	56,56,56	0.95	1 (1%)
30	DD6	H	301	-	40,45,45	0.19	0	51,67,67	0.72	2 (3%)
27	CLA	K	604	-	61,65,73	1.81	9 (14%)	72,103,113	1.35	7 (9%)
27	CLA	H	306	-	49,53,73	2.01	9 (18%)	58,89,113	1.51	8 (13%)
28	KC2	E	601	27	49,53,53	1.81	4 (8%)	60,89,89	1.16	4 (6%)
29	UIX	H	314	-	43,49,49	1.37	4 (9%)	53,74,74	1.96	20 (37%)
27	CLA	b	727	-	69,73,73	1.72	9 (13%)	82,113,113	1.35	9 (10%)
27	CLA	b	711	-	64,68,73	1.79	9 (14%)	76,107,113	1.36	8 (10%)
28	KC2	J	604	10	49,53,53	1.80	4 (8%)	60,89,89	1.14	4 (6%)
32	PID	F	614	-	43,49,49	1.69	6 (13%)	52,76,76	3.95	19 (36%)
27	CLA	H	305	-	64,68,73	1.80	9 (14%)	76,107,113	1.43	9 (11%)
27	CLA	B	604	2	51,55,73	2.06	9 (17%)	60,91,113	1.54	9 (15%)
27	CLA	E	609	28	49,53,73	2.05	9 (18%)	58,89,113	1.49	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	SF4	c	201	16	0,12,12	-	-	-		
27	CLA	r	203	-	52,56,73	2.02	9 (17%)	61,92,113	1.51	6 (9%)
30	DD6	H	318	28	40,45,45	0.15	0	51,67,67	0.56	2 (3%)
27	CLA	b	715	-	69,73,73	1.72	9 (13%)	82,113,113	1.40	10 (12%)
27	CLA	E	608	5	64,68,73	1.79	9 (14%)	76,107,113	1.36	7 (9%)
34	LHG	r	202	-	45,45,48	0.53	0	48,51,54	0.51	0
38	BCR	b	731	-	41,41,41	0.30	0	56,56,56	0.72	1 (1%)
27	CLA	b	710	-	59,63,73	1.89	9 (15%)	70,101,113	1.44	9 (12%)
27	CLA	a	812	-	54,58,73	2.01	9 (16%)	64,95,113	1.58	10 (15%)
27	CLA	I	610	-	59,63,73	1.88	9 (15%)	70,101,113	1.51	7 (10%)
27	CLA	a	811	-	52,56,73	2.01	9 (17%)	61,92,113	1.49	8 (13%)
27	CLA	H	313	-	64,68,73	1.80	9 (14%)	76,107,113	1.35	9 (11%)
27	CLA	I	606	9	59,63,73	1.86	9 (15%)	70,101,113	1.40	8 (11%)
27	CLA	l	406	-	69,73,73	1.70	9 (13%)	82,113,113	1.26	9 (10%)
27	CLA	C	206	-	51,55,73	1.96	9 (17%)	60,91,113	1.47	8 (13%)
27	CLA	G	610	7	51,55,73	1.99	9 (17%)	60,91,113	1.48	8 (13%)
30	DD6	B	612	-	40,45,45	0.17	0	51,67,67	0.61	2 (3%)
27	CLA	K	606	-	45,49,73	2.25	10 (22%)	54,84,113	1.72	8 (14%)
29	UIX	T	612	-	43,49,49	1.36	5 (11%)	53,74,74	2.03	21 (39%)
27	CLA	U	606	-	49,53,73	2.06	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	F	617	-	64,68,73	1.78	9 (14%)	76,107,113	1.34	8 (10%)
32	PID	K	611	-	43,49,49	1.76	6 (13%)	52,76,76	3.82	21 (40%)
27	CLA	F	610	6	51,55,73	2.03	9 (17%)	60,91,113	1.52	8 (13%)
27	CLA	b	702	-	69,73,73	1.66	9 (13%)	82,113,113	1.20	10 (12%)
29	UIX	J	616	-	43,49,49	1.36	4 (9%)	53,74,74	1.86	14 (26%)
27	CLA	a	831	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	9 (12%)
30	DD6	E	614	-	40,45,45	0.16	0	51,67,67	0.51	0
31	SQD	H	320	-	44,46,54	1.19	3 (6%)	54,57,65	1.06	3 (5%)
27	CLA	A	610	-	59,63,73	1.84	9 (15%)	70,101,113	1.39	8 (11%)
27	CLA	T	605	12	49,53,73	2.00	9 (18%)	58,89,113	1.46	8 (13%)
33	LMG	C	217	-	34,34,55	0.58	0	42,42,63	0.71	1 (2%)
27	CLA	H	319	-	69,73,73	1.70	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	l	412	22	69,73,73	1.71	9 (13%)	82,113,113	1.32	9 (10%)
27	CLA	G	609	7	59,63,73	1.86	9 (15%)	70,101,113	1.39	10 (14%)
27	CLA	D	605	4	51,55,73	1.99	9 (17%)	60,91,113	1.44	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	a	835	-	47,47,48	0.52	0	50,53,54	0.53	0
32	PID	F	615	-	43,49,49	1.63	7 (16%)	52,76,76	3.66	18 (34%)
27	CLA	b	713	-	69,73,73	1.71	9 (13%)	82,113,113	1.38	10 (12%)
28	KC2	H	302	30	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	a	815	-	64,68,73	1.75	9 (14%)	76,107,113	1.34	8 (10%)
27	CLA	f	303	19	52,56,73	2.01	9 (17%)	61,92,113	1.46	8 (13%)
27	CLA	H	312	-	46,50,73	2.09	9 (19%)	53,85,113	1.60	9 (16%)
30	DD6	B	616	-	40,45,45	0.15	0	51,67,67	0.53	0
27	CLA	b	712	-	52,56,73	2.01	9 (17%)	61,92,113	1.53	9 (14%)
30	DD6	D	617	-	40,45,45	0.18	0	51,67,67	0.62	2 (3%)
37	PQN	a	832	-	34,34,34	0.37	0	43,45,45	0.73	0
27	CLA	E	603	-	51,55,73	2.02	9 (17%)	60,91,113	1.49	8 (13%)
27	CLA	a	810	-	54,58,73	1.94	9 (16%)	64,95,113	1.47	9 (14%)
28	KC2	I	604	9	49,53,53	1.81	4 (8%)	60,89,89	1.14	4 (6%)
30	DD6	r	206	-	40,45,45	0.18	0	51,67,67	0.81	3 (5%)
27	CLA	B	606	-	69,73,73	1.74	9 (13%)	82,113,113	1.35	8 (9%)
29	UIX	H	317	-	43,49,49	1.32	5 (11%)	53,74,74	1.92	15 (28%)
38	BCR	l	414	-	41,41,41	0.34	0	56,56,56	0.83	0
27	CLA	b	725	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	9 (10%)
27	CLA	b	708	-	69,73,73	1.67	9 (13%)	82,113,113	1.23	8 (9%)
27	CLA	I	608	9	64,68,73	1.78	9 (14%)	76,107,113	1.30	8 (10%)
27	CLA	C	207	3	64,68,73	1.78	9 (14%)	76,107,113	1.35	9 (11%)
27	CLA	A	611	27	49,53,73	2.04	9 (18%)	58,89,113	1.54	8 (13%)
27	CLA	a	825	-	69,73,73	1.72	9 (13%)	82,113,113	1.28	8 (9%)
27	CLA	a	809	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	7 (11%)
30	DD6	U	607	-	40,45,45	0.14	0	51,67,67	0.63	1 (1%)
27	CLA	D	602	-	59,63,73	1.87	9 (15%)	70,101,113	1.44	8 (11%)
31	SQD	A	618	-	26,28,54	1.42	3 (11%)	36,39,65	1.25	3 (8%)
27	CLA	E	604	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	9 (12%)
31	SQD	y	301	-	44,46,54	1.23	3 (6%)	54,57,65	1.03	3 (5%)
27	CLA	a	819	-	64,68,73	1.77	9 (14%)	76,107,113	1.32	8 (10%)
27	CLA	b	724	-	69,73,73	1.71	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	b	709	15	69,73,73	1.67	9 (13%)	82,113,113	1.25	9 (10%)
27	CLA	b	706	-	69,73,73	1.71	9 (13%)	82,113,113	1.28	9 (10%)
27	CLA	H	304	-	64,68,73	1.79	9 (14%)	76,107,113	1.41	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PID	U	608	-	43,49,49	1.65	8 (18%)	52,76,76	3.74	18 (34%)
27	CLA	D	609	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	a	837	-	69,73,73	1.68	9 (13%)	82,113,113	1.30	7 (8%)
34	LHG	l	401	-	45,45,48	0.52	0	48,51,54	0.47	0
34	LHG	j	205	-	36,36,48	0.58	0	39,42,54	0.54	0
27	CLA	b	721	-	54,58,73	1.97	9 (16%)	64,95,113	1.47	7 (10%)
33	LMG	l	417	-	50,50,55	0.50	0	58,58,63	0.61	0
27	CLA	a	839	-	65,69,73	1.76	9 (13%)	77,108,113	1.30	8 (10%)
27	CLA	l	407	-	52,56,73	2.01	9 (17%)	61,92,113	1.48	8 (13%)
27	CLA	A	603	-	59,63,73	1.85	9 (15%)	70,101,113	1.40	9 (12%)
27	CLA	a	830	-	69,73,73	1.71	9 (13%)	82,113,113	1.29	7 (8%)
27	CLA	D	611	-	64,68,73	1.78	9 (14%)	76,107,113	1.32	9 (11%)
30	DD6	T	611	-	40,45,45	0.18	0	51,67,67	0.65	2 (3%)
27	CLA	B	605	2	49,53,73	2.01	9 (18%)	58,89,113	1.52	9 (15%)
28	KC2	H	311	-	49,53,53	1.82	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	H	308	8	59,63,73	1.82	9 (15%)	70,101,113	1.36	8 (11%)
27	CLA	a	813	-	52,56,73	2.00	9 (17%)	61,92,113	1.49	8 (13%)
27	CLA	G	606	7	69,73,73	1.74	9 (13%)	82,113,113	1.36	9 (10%)
30	DD6	H	315	-	40,45,45	0.17	0	51,67,67	0.61	1 (1%)
30	DD6	B	614	-	40,45,45	0.40	0	51,67,67	0.77	1 (1%)
27	CLA	F	606	6	69,73,73	1.70	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	a	828	-	52,56,73	2.06	9 (17%)	61,92,113	1.59	7 (11%)
28	KC2	E	610	5	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
27	CLA	b	728	-	69,73,73	1.69	9 (13%)	82,113,113	1.27	9 (10%)
27	CLA	I	601	9	69,73,73	1.71	9 (13%)	82,113,113	1.30	7 (8%)
27	CLA	a	807	-	69,73,73	1.71	9 (13%)	82,113,113	1.33	10 (12%)
27	CLA	E	606	-	64,68,73	1.78	9 (14%)	76,107,113	1.36	8 (10%)
34	LHG	G	617	-	33,33,48	0.60	0	36,39,54	0.55	0
27	CLA	I	602	-	59,63,73	1.84	9 (15%)	70,101,113	1.34	8 (11%)
29	UIX	j	204	-	43,49,49	1.41	5 (11%)	53,74,74	2.02	18 (33%)
38	BCR	l	415	-	41,41,41	0.31	0	56,56,56	0.56	0
27	CLA	E	611	5	64,68,73	1.80	9 (14%)	76,107,113	1.39	8 (10%)
30	DD6	A	617	-	40,45,45	0.18	0	51,67,67	0.53	0
27	CLA	E	612	-	49,53,73	2.05	9 (18%)	58,89,113	1.50	8 (13%)
27	CLA	G	602	7	59,63,73	1.85	9 (15%)	70,101,113	1.39	7 (10%)
27	CLA	J	603	-	64,68,73	1.80	9 (14%)	76,107,113	1.35	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	824	-	69,73,73	1.72	9 (13%)	82,113,113	1.31	9 (10%)
30	DD6	D	613	-	40,45,45	0.42	0	51,67,67	0.72	2 (3%)
30	DD6	D	615	-	40,45,45	0.16	0	51,67,67	0.58	1 (1%)
29	UIX	G	615	-	43,49,49	1.38	4 (9%)	53,74,74	1.96	15 (28%)
27	CLA	F	604	-	49,53,73	1.97	9 (18%)	58,89,113	1.50	9 (15%)
30	DD6	K	609	-	40,45,45	0.17	0	51,67,67	0.56	1 (1%)
27	CLA	A	604	-	49,53,73	2.03	9 (18%)	58,89,113	1.52	8 (13%)
27	CLA	F	619	-	59,63,73	1.83	9 (15%)	70,101,113	1.38	8 (11%)
27	CLA	C	201	-	46,50,73	2.13	9 (19%)	53,85,113	1.62	10 (18%)
28	KC2	J	602	10	49,53,53	1.83	4 (8%)	60,89,89	1.13	4 (6%)
27	CLA	G	604	-	51,55,73	2.03	9 (17%)	60,91,113	1.56	6 (10%)
27	CLA	A	601	1	46,50,73	2.09	9 (19%)	53,85,113	1.59	9 (16%)
28	KC2	U	602	-	49,53,53	1.83	4 (8%)	60,89,89	1.14	4 (6%)
29	UIX	C	215	-	43,49,49	1.36	4 (9%)	53,74,74	2.14	22 (41%)
38	BCR	a	834	-	41,41,41	0.27	0	56,56,56	0.53	0
27	CLA	a	823	-	69,73,73	1.74	9 (13%)	82,113,113	1.37	8 (9%)
30	DD6	T	610	-	40,45,45	0.16	0	51,67,67	0.69	2 (3%)
27	CLA	C	204	-	69,73,73	1.73	9 (13%)	82,113,113	1.33	9 (10%)
27	CLA	l	402	-	64,68,73	1.78	9 (14%)	76,107,113	1.38	9 (11%)
38	BCR	m	201	-	41,41,41	0.30	0	56,56,56	0.69	0
27	CLA	D	607	4	64,68,73	1.78	9 (14%)	76,107,113	1.33	7 (9%)
27	CLA	I	609	9	49,53,73	2.05	9 (18%)	58,89,113	1.57	9 (15%)
27	CLA	b	722	-	52,56,73	1.98	9 (17%)	61,92,113	1.51	8 (13%)
29	UIX	B	615	-	43,49,49	1.38	5 (11%)	53,74,74	1.92	17 (32%)
27	CLA	T	603	-	49,53,73	2.03	9 (18%)	58,89,113	1.49	7 (12%)
27	CLA	A	606	1	51,55,73	1.99	9 (17%)	60,91,113	1.51	7 (11%)
27	CLA	D	603	-	59,63,73	1.88	9 (15%)	70,101,113	1.44	8 (11%)
30	DD6	r	205	-	40,45,45	0.19	0	51,67,67	0.79	2 (3%)
33	LMG	F	616	-	46,46,55	0.52	0	54,54,63	0.69	0
38	BCR	l	413	-	41,41,41	0.32	0	56,56,56	0.53	0
27	CLA	G	611	-	49,53,73	2.05	9 (18%)	58,89,113	1.50	8 (13%)
27	CLA	A	612	1	51,55,73	2.06	9 (17%)	60,91,113	1.71	10 (16%)
27	CLA	E	607	5	69,73,73	1.69	9 (13%)	82,113,113	1.22	8 (9%)
27	CLA	a	816	-	64,68,73	1.81	9 (14%)	76,107,113	1.36	8 (10%)
27	CLA	b	717	-	69,73,73	1.67	9 (13%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	818	-	59,63,73	1.85	9 (15%)	70,101,113	1.37	8 (11%)

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
38	BCR	f	304	-	-	3/29/63/63	0/2/2/2
32	PID	J	615	-	-	6/24/93/93	0/4/4/4
38	BCR	f	301	-	-	9/29/63/63	0/2/2/2
27	CLA	T	604	12	1/1/10/20	2/10/86/115	-
27	CLA	l	405	22	1/1/14/20	3/35/111/115	-
27	CLA	a	806	-	1/1/13/20	3/27/103/115	-
27	CLA	A	609	-	1/1/11/20	1/18/94/115	-
27	CLA	b	703	-	1/1/15/20	5/39/115/115	-
27	CLA	C	202	3	1/1/11/20	2/15/91/115	-
30	DD6	r	201	-	-	1/26/80/80	0/3/3/3
30	DD6	C	216	-	-	1/26/80/80	0/3/3/3
27	CLA	T	601	12	1/1/11/20	2/18/94/115	-
27	CLA	a	805	-	1/1/15/20	8/39/115/115	-
27	CLA	K	605	11	1/1/14/20	8/33/109/115	-
28	KC2	B	608	2	-	4/15/71/71	-
27	CLA	C	205	-	1/1/13/20	6/27/103/115	-
32	PID	J	611	-	-	4/24/93/93	0/4/4/4
27	CLA	K	601	11	1/1/13/20	3/30/106/115	-
30	DD6	F	612	-	-	0/26/80/80	0/3/3/3
33	LMG	K	613	-	-	11/37/57/70	0/1/1/1
27	CLA	T	606	12	1/1/11/20	1/15/91/115	-
27	CLA	l	409	-	1/1/15/20	12/39/115/115	-
27	CLA	D	610	4	1/1/11/20	4/18/94/115	-
33	LMG	D	619	-	-	21/41/61/70	0/1/1/1
38	BCR	b	732	-	-	0/29/63/63	0/2/2/2
30	DD6	i	202	-	-	3/26/80/80	0/3/3/3
27	CLA	D	606	-	1/1/11/20	2/15/91/115	-
29	UIX	I	612	-	-	2/31/87/87	1/3/3/3
28	KC2	K	607	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	b	733	-	-	26/50/70/70	0/1/1/1
38	BCR	j	203	-	-	10/29/63/63	0/2/2/2
27	CLA	G	607	7	1/1/11/20	7/15/91/115	-
30	DD6	I	615	-	-	0/26/80/80	0/3/3/3
27	CLA	I	605	9	1/1/13/20	5/27/103/115	-
27	CLA	B	601	-	1/1/14/20	6/33/109/115	-
27	CLA	A	607	-	1/1/11/20	2/15/91/115	-
27	CLA	A	605	1	1/1/13/20	3/27/103/115	-
27	CLA	a	814	-	1/1/13/20	4/27/103/115	-
28	KC2	T	608	-	-	5/15/71/71	-
27	CLA	U	603	-	1/1/12/20	8/21/97/115	-
28	KC2	G	601	-	-	9/15/71/71	-
27	CLA	B	609	2	1/1/15/20	6/39/115/115	-
30	DD6	E	615	-	-	2/26/80/80	0/3/3/3
27	CLA	b	704	-	1/1/15/20	10/39/115/115	-
32	PID	B	613	-	-	3/24/93/93	0/4/4/4
27	CLA	G	603	-	1/1/12/20	4/21/97/115	-
27	CLA	b	718	-	1/1/15/20	7/39/115/115	-
30	DD6	E	613	-	-	1/26/80/80	0/3/3/3
29	UIX	C	213	-	-	2/31/87/87	0/3/3/3
27	CLA	B	603	-	1/1/15/20	8/39/115/115	-
27	CLA	a	802	-	1/1/13/20	1/27/103/115	-
38	BCR	a	836	-	-	14/29/63/63	0/2/2/2
27	CLA	C	212	-	1/1/11/20	2/18/94/115	-
27	CLA	D	612	-	1/1/13/20	6/27/103/115	-
30	DD6	G	613	-	-	2/26/80/80	0/3/3/3
32	PID	J	613	-	-	3/24/93/93	0/4/4/4
27	CLA	l	404	-	1/1/13/20	3/27/103/115	-
27	CLA	T	607	-	1/1/11/20	5/15/91/115	-
27	CLA	C	209	-	1/1/11/20	0/15/91/115	-
27	CLA	b	707	-	1/1/15/20	5/39/115/115	-
27	CLA	r	204	-	1/1/14/20	11/33/109/115	-
27	CLA	a	822	-	1/1/14/20	8/33/109/115	-
30	DD6	K	610	-	-	3/26/80/80	0/3/3/3
27	CLA	B	607	-	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DD6	b	730	-	-	0/26/80/80	0/3/3/3
28	KC2	J	608	-	-	4/15/71/71	-
34	LHG	D	620	-	-	22/50/50/53	-
27	CLA	l	411	22	1/1/11/20	3/19/95/115	-
27	CLA	l	403	-	1/1/15/20	9/39/115/115	-
30	DD6	D	621	-	-	5/26/80/80	0/3/3/3
28	KC2	J	610	-	-	8/15/71/71	-
30	DD6	C	214	-	-	1/26/80/80	0/3/3/3
27	CLA	F	602	-	1/1/13/20	5/29/105/115	-
27	CLA	a	826	-	1/1/13/20	4/27/103/115	-
32	PID	I	614	-	-	5/24/93/93	0/4/4/4
29	UIX	E	616	-	-	3/31/87/87	0/3/3/3
37	PQN	b	729	-	-	10/23/43/43	0/2/2/2
27	CLA	a	803	27	1/1/12/20	2/21/97/115	-
35	DGD	j	201	-	-	16/49/89/95	0/2/2/2
29	UIX	F	613	-	-	4/31/87/87	0/3/3/3
33	LMG	D	618	-	-	17/30/50/70	0/1/1/1
27	CLA	D	608	4	1/1/13/20	0/27/103/115	-
27	CLA	B	610	-	1/1/11/20	5/18/94/115	-
27	CLA	E	602	5	1/1/13/20	0/27/103/115	-
35	DGD	K	614	-	-	19/36/76/95	0/2/2/2
27	CLA	l	410	-	1/1/11/20	5/19/95/115	-
27	CLA	b	701	-	1/1/15/20	7/39/115/115	-
30	DD6	D	614	-	-	0/26/80/80	0/3/3/3
30	DD6	J	612	-	-	1/26/80/80	0/3/3/3
27	CLA	I	611	-	1/1/10/20	4/12/88/115	-
27	CLA	K	602	-	1/1/13/20	8/27/103/115	-
27	CLA	F	605	6	1/1/11/20	5/15/91/115	-
32	PID	J	614	-	-	0/24/93/93	0/4/4/4
28	KC2	A	608	-	-	7/15/71/71	-
27	CLA	C	203	3	1/1/15/20	2/39/115/115	-
27	CLA	E	605	5	1/1/11/20	6/15/91/115	-
27	CLA	F	601	6	1/1/14/20	2/33/109/115	-
27	CLA	H	310	-	1/1/11/20	4/15/91/115	-
30	DD6	H	316	-	-	1/26/80/80	0/3/3/3
27	CLA	I	616	-	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	j	202	27	1/1/13/20	3/29/105/115	-
27	CLA	f	302	-	1/1/11/20	1/19/95/115	-
34	LHG	F	618	-	-	21/41/41/53	-
27	CLA	K	608	-	1/1/11/20	3/15/91/115	-
27	CLA	a	801	-	1/1/15/20	3/39/115/115	-
28	KC2	B	602	-	-	3/15/71/71	-
27	CLA	T	609	-	1/1/10/20	0/10/86/115	-
27	CLA	J	601	-	1/1/11/20	4/15/91/115	-
27	CLA	a	821	-	1/1/15/20	9/39/115/115	-
27	CLA	H	303	8	1/1/14/20	2/33/109/115	-
39	SF4	a	838	14	-	-	0/6/5/5
27	CLA	C	211	-	1/1/11/20	0/18/94/115	-
27	CLA	D	604	-	1/1/13/20	7/27/103/115	-
35	DGD	l	416	-	-	17/44/84/95	0/2/2/2
27	CLA	b	714	-	1/1/11/20	5/19/95/115	-
27	CLA	b	705	-	1/1/15/20	9/39/115/115	-
30	DD6	E	617	-	-	2/26/80/80	0/3/3/3
27	CLA	J	607	-	1/1/10/20	2/12/88/115	-
27	CLA	K	603	-	1/1/11/20	5/15/91/115	-
30	DD6	A	615	-	-	2/26/80/80	0/3/3/3
30	DD6	F	611	-	-	3/26/80/80	0/3/3/3
27	CLA	a	817	-	1/1/13/20	2/27/103/115	-
27	CLA	G	608	-	1/1/14/20	5/33/109/115	-
27	CLA	a	820	-	1/1/15/20	8/39/115/115	-
27	CLA	b	723	-	1/1/15/20	4/39/115/115	-
30	DD6	I	613	-	-	1/26/80/80	0/3/3/3
27	CLA	b	726	-	1/1/14/20	5/33/109/115	-
29	UIX	A	616	-	-	6/31/87/87	0/3/3/3
27	CLA	F	608	6	1/1/11/20	3/15/91/115	-
27	CLA	C	208	-	1/1/11/20	0/18/94/115	-
30	DD6	G	616	-	-	1/26/80/80	0/3/3/3
29	UIX	B	611	-	-	2/31/87/87	0/3/3/3
28	KC2	U	604	13	-	8/15/71/71	-
27	CLA	T	602	-	1/1/11/20	4/15/91/115	-
27	CLA	l	408	-	1/1/11/20	3/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	UIX	A	613	-	-	2/31/87/87	0/3/3/3
27	CLA	a	827	-	1/1/15/20	14/39/115/115	-
27	CLA	A	602	1	1/1/14/20	0/33/109/115	-
27	CLA	I	603	-	1/1/15/20	9/39/115/115	-
27	CLA	a	829	27	1/1/15/20	14/39/115/115	-
27	CLA	U	601	-	1/1/10/20	1/13/89/115	-
27	CLA	b	720	-	1/1/11/20	4/19/95/115	-
27	CLA	U	605	13	1/1/14/20	6/33/109/115	-
27	CLA	F	607	6	1/1/11/20	7/15/91/115	-
27	CLA	J	609	-	1/1/10/20	4/10/86/115	-
27	CLA	H	309	-	1/1/15/20	5/39/115/115	-
27	CLA	b	716	-	1/1/15/20	4/39/115/115	-
27	CLA	a	808	14	1/1/13/20	4/27/103/115	-
30	DD6	K	612	-	-	5/26/80/80	0/3/3/3
28	KC2	F	609	6	-	6/15/71/71	-
28	KC2	J	606	-	-	6/15/71/71	-
27	CLA	a	804	-	1/1/15/20	11/39/115/115	-
30	DD6	G	612	-	-	0/26/80/80	0/3/3/3
30	DD6	G	614	-	-	2/26/80/80	0/3/3/3
27	CLA	G	605	-	1/1/14/20	0/33/109/115	-
27	CLA	I	607	-	1/1/14/20	3/35/111/115	-
27	CLA	D	601	4	1/1/11/20	3/15/91/115	-
27	CLA	F	603	-	1/1/12/20	4/24/100/115	-
27	CLA	b	719	-	1/1/15/20	6/39/115/115	-
27	CLA	H	307	-	1/1/11/20	5/15/91/115	-
28	KC2	C	210	-	-	7/15/71/71	-
27	CLA	J	605	10	1/1/14/20	4/33/109/115	-
36	LMU	T	613	-	-	5/21/61/61	0/2/2/2
35	DGD	f	305	-	-	17/41/81/95	0/2/2/2
30	DD6	A	614	-	-	1/26/80/80	0/3/3/3
38	BCR	a	833	-	-	7/29/63/63	0/2/2/2
29	UIX	D	616	-	-	5/31/87/87	0/3/3/3
39	SF4	c	202	-	-	-	0/6/5/5
38	BCR	i	201	-	-	6/29/63/63	0/2/2/2
30	DD6	H	301	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	K	604	-	1/1/13/20	5/30/106/115	-
27	CLA	H	306	-	1/1/11/20	5/15/91/115	-
28	KC2	E	601	27	-	10/15/71/71	-
29	UIX	H	314	-	-	2/31/87/87	0/3/3/3
27	CLA	b	727	-	1/1/15/20	10/39/115/115	-
27	CLA	b	711	-	1/1/14/20	4/33/109/115	-
28	KC2	J	604	10	-	4/15/71/71	-
32	PID	F	614	-	-	5/24/93/93	0/4/4/4
27	CLA	H	305	-	1/1/14/20	11/33/109/115	-
27	CLA	B	604	2	1/1/11/20	2/18/94/115	-
27	CLA	E	609	28	1/1/11/20	4/15/91/115	-
39	SF4	c	201	16	-	-	0/6/5/5
27	CLA	r	203	-	1/1/11/20	6/19/95/115	-
30	DD6	H	318	28	-	0/26/80/80	0/3/3/3
27	CLA	b	715	-	1/1/15/20	6/39/115/115	-
27	CLA	E	608	5	1/1/14/20	5/33/109/115	-
34	LHG	r	202	-	-	20/50/50/53	-
38	BCR	b	731	-	-	7/29/63/63	0/2/2/2
27	CLA	b	710	-	1/1/13/20	3/27/103/115	-
27	CLA	a	812	-	1/1/12/20	3/21/97/115	-
27	CLA	I	610	-	1/1/13/20	3/27/103/115	-
27	CLA	a	811	-	1/1/11/20	2/19/95/115	-
27	CLA	H	313	-	1/1/14/20	2/33/109/115	-
27	CLA	I	606	9	1/1/13/20	2/27/103/115	-
27	CLA	l	406	-	1/1/15/20	3/39/115/115	-
27	CLA	C	206	-	1/1/11/20	2/18/94/115	-
27	CLA	G	610	7	1/1/11/20	6/18/94/115	-
30	DD6	B	612	-	-	1/26/80/80	0/3/3/3
27	CLA	K	606	-	1/1/10/20	2/10/86/115	-
29	UIX	T	612	-	-	5/31/87/87	0/3/3/3
27	CLA	U	606	-	1/1/11/20	7/15/91/115	-
27	CLA	F	617	-	1/1/14/20	10/33/109/115	-
32	PID	K	611	-	-	6/24/93/93	1/4/4/4
27	CLA	F	610	6	1/1/11/20	5/18/94/115	-
27	CLA	b	702	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	UIX	J	616	-	-	3/31/87/87	0/3/3/3
27	CLA	a	831	-	1/1/13/20	2/27/103/115	-
30	DD6	E	614	-	-	0/26/80/80	0/3/3/3
31	SQD	H	320	-	-	14/41/61/69	0/1/1/1
27	CLA	A	610	-	1/1/13/20	4/27/103/115	-
27	CLA	T	605	12	1/1/11/20	0/15/91/115	-
33	LMG	C	217	-	-	13/29/49/70	0/1/1/1
27	CLA	H	319	-	1/1/15/20	8/39/115/115	-
27	CLA	l	412	22	1/1/15/20	12/39/115/115	-
27	CLA	G	609	7	1/1/13/20	4/27/103/115	-
27	CLA	D	605	4	1/1/11/20	2/18/94/115	-
34	LHG	a	835	-	-	20/52/52/53	-
32	PID	F	615	-	-	4/24/93/93	0/4/4/4
27	CLA	b	713	-	1/1/15/20	6/39/115/115	-
28	KC2	H	302	30	-	8/15/71/71	-
27	CLA	a	815	-	1/1/14/20	5/33/109/115	-
27	CLA	f	303	19	1/1/11/20	0/19/95/115	-
27	CLA	H	312	-	1/1/10/20	4/12/88/115	-
30	DD6	B	616	-	-	3/26/80/80	0/3/3/3
27	CLA	b	712	-	1/1/11/20	3/19/95/115	-
30	DD6	D	617	-	-	0/26/80/80	0/3/3/3
37	PQN	a	832	-	-	6/23/43/43	0/2/2/2
27	CLA	E	603	-	1/1/11/20	0/18/94/115	-
27	CLA	a	810	-	1/1/12/20	2/21/97/115	-
28	KC2	I	604	9	-	3/15/71/71	-
30	DD6	r	206	-	-	3/26/80/80	0/3/3/3
27	CLA	B	606	-	1/1/15/20	6/39/115/115	-
29	UIX	H	317	-	-	4/31/87/87	0/3/3/3
38	BCR	l	414	-	-	5/29/63/63	0/2/2/2
27	CLA	b	725	-	1/1/15/20	6/39/115/115	-
27	CLA	b	708	-	1/1/15/20	10/39/115/115	-
27	CLA	I	608	9	1/1/14/20	4/33/109/115	-
27	CLA	C	207	3	1/1/14/20	4/33/109/115	-
27	CLA	A	611	27	1/1/11/20	3/15/91/115	-
27	CLA	a	825	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	809	-	1/1/11/20	3/18/94/115	-
30	DD6	U	607	-	-	0/26/80/80	0/3/3/3
27	CLA	D	602	-	1/1/13/20	5/27/103/115	-
31	SQD	A	618	-	-	8/22/42/69	0/1/1/1
27	CLA	E	604	-	1/1/13/20	2/27/103/115	-
31	SQD	y	301	-	-	6/41/61/69	0/1/1/1
27	CLA	a	819	-	1/1/14/20	4/33/109/115	-
27	CLA	b	724	-	1/1/15/20	4/39/115/115	-
27	CLA	b	709	15	1/1/15/20	3/39/115/115	-
27	CLA	b	706	-	1/1/15/20	10/39/115/115	-
27	CLA	H	304	-	1/1/14/20	8/33/109/115	-
32	PID	U	608	-	-	4/24/93/93	1/4/4/4
27	CLA	D	609	-	1/1/11/20	2/15/91/115	-
27	CLA	a	837	-	1/1/15/20	3/39/115/115	-
34	LHG	l	401	-	-	22/50/50/53	-
34	LHG	j	205	-	-	15/41/41/53	-
27	CLA	b	721	-	1/1/12/20	2/21/97/115	-
33	LMG	l	417	-	-	21/45/65/70	0/1/1/1
27	CLA	a	839	-	1/1/14/20	5/35/111/115	-
27	CLA	l	407	-	1/1/11/20	3/19/95/115	-
27	CLA	A	603	-	1/1/13/20	2/27/103/115	-
27	CLA	a	830	-	1/1/15/20	11/39/115/115	-
27	CLA	D	611	-	1/1/14/20	4/33/109/115	-
30	DD6	T	611	-	-	2/26/80/80	0/3/3/3
27	CLA	B	605	2	1/1/11/20	5/15/91/115	-
28	KC2	H	311	-	-	10/15/71/71	-
27	CLA	H	308	8	1/1/13/20	2/27/103/115	-
27	CLA	a	813	-	1/1/11/20	5/19/95/115	-
27	CLA	G	606	7	1/1/15/20	7/39/115/115	-
30	DD6	H	315	-	-	0/26/80/80	0/3/3/3
30	DD6	B	614	-	-	5/26/80/80	0/3/3/3
27	CLA	F	606	6	1/1/15/20	13/39/115/115	-
27	CLA	a	828	-	1/1/11/20	4/19/95/115	-
28	KC2	E	610	5	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	728	-	1/1/15/20	8/39/115/115	-
27	CLA	I	601	9	1/1/15/20	7/39/115/115	-
27	CLA	a	807	-	1/1/15/20	10/39/115/115	-
27	CLA	E	606	-	1/1/14/20	7/33/109/115	-
34	LHG	G	617	-	-	22/38/38/53	-
27	CLA	I	602	-	1/1/13/20	6/27/103/115	-
29	UIX	j	204	-	-	6/31/87/87	0/3/3/3
38	BCR	l	415	-	-	13/29/63/63	0/2/2/2
27	CLA	E	611	5	1/1/14/20	4/33/109/115	-
30	DD6	A	617	-	-	4/26/80/80	0/3/3/3
27	CLA	E	612	-	1/1/11/20	2/15/91/115	-
27	CLA	G	602	7	1/1/13/20	4/27/103/115	-
27	CLA	J	603	-	1/1/14/20	5/33/109/115	-
27	CLA	a	824	-	1/1/15/20	8/39/115/115	-
30	DD6	D	613	-	1/1/12/24	2/26/80/80	0/3/3/3
30	DD6	D	615	-	-	2/26/80/80	0/3/3/3
29	UIX	G	615	-	-	4/31/87/87	0/3/3/3
27	CLA	F	604	-	1/1/11/20	4/15/91/115	-
30	DD6	K	609	-	-	4/26/80/80	0/3/3/3
27	CLA	A	604	-	1/1/11/20	2/15/91/115	-
27	CLA	F	619	-	1/1/13/20	3/27/103/115	-
27	CLA	C	201	-	1/1/10/20	4/12/88/115	-
28	KC2	J	602	10	-	5/15/71/71	-
27	CLA	G	604	-	1/1/11/20	2/18/94/115	-
27	CLA	A	601	1	1/1/10/20	4/12/88/115	-
28	KC2	U	602	-	-	4/15/71/71	-
29	UIX	C	215	-	-	3/31/87/87	0/3/3/3
38	BCR	a	834	-	-	5/29/63/63	0/2/2/2
27	CLA	a	823	-	1/1/15/20	12/39/115/115	-
30	DD6	T	610	-	-	3/26/80/80	0/3/3/3
27	CLA	C	204	-	1/1/15/20	4/39/115/115	-
27	CLA	l	402	-	1/1/14/20	3/33/109/115	-
38	BCR	m	201	-	-	10/29/63/63	0/2/2/2
27	CLA	D	607	4	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	I	609	9	1/1/11/20	2/15/91/115	-
27	CLA	b	722	-	1/1/11/20	5/19/95/115	-
29	UIX	B	615	-	-	3/31/87/87	1/3/3/3
27	CLA	T	603	-	1/1/11/20	4/15/91/115	-
27	CLA	A	606	1	1/1/11/20	2/18/94/115	-
27	CLA	D	603	-	1/1/13/20	3/27/103/115	-
30	DD6	r	205	-	-	4/26/80/80	0/3/3/3
33	LMG	F	616	-	-	14/41/61/70	0/1/1/1
38	BCR	l	413	-	-	3/29/63/63	0/2/2/2
27	CLA	G	611	-	1/1/11/20	0/15/91/115	-
27	CLA	A	612	1	1/1/11/20	4/18/94/115	-
27	CLA	E	607	5	1/1/15/20	10/39/115/115	-
27	CLA	a	816	-	1/1/14/20	8/33/109/115	-
27	CLA	b	717	-	1/1/15/20	7/39/115/115	-
27	CLA	a	818	-	1/1/13/20	6/27/103/115	-

The worst 5 of 2012 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	602	KC2	MG-ND	-10.18	1.85	2.05
28	J	606	KC2	MG-ND	-10.15	1.85	2.05
28	J	602	KC2	MG-ND	-10.14	1.85	2.05
28	B	608	KC2	MG-ND	-10.11	1.85	2.05
28	A	608	KC2	MG-ND	-10.11	1.85	2.05

The worst 5 of 2317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	613	PID	O4-C12-C11	17.74	117.47	107.39
32	J	615	PID	O4-C12-C11	17.60	117.39	107.39
32	J	611	PID	O4-C12-C11	17.60	117.39	107.39
32	U	608	PID	O4-C12-C11	17.23	117.17	107.39
32	F	614	PID	O4-C12-C11	17.17	117.14	107.39

5 of 197 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	601	CLA	ND
27	A	602	CLA	ND

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Mol	Chain	Res	Type	Atom
27	A	603	CLA	ND
27	A	604	CLA	ND
27	A	605	CLA	ND

5 of 1685 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	601	CLA	C1A-C2A-CAA-CBA
27	A	601	CLA	C2B-C3B-CAB-CBB
27	A	601	CLA	C4B-C3B-CAB-CBB
27	A	604	CLA	C1A-C2A-CAA-CBA
27	A	606	CLA	C1A-C2A-CAA-CBA

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	K	611	PID	C24-C25-C26-C27-C28-C29
29	B	615	UIX	C15-C16-C17-C18-C19-C20
29	I	612	UIX	C15-C16-C17-C18-C19-C20
32	U	608	PID	C24-C25-C26-C27-C28-C29

158 monomers are involved in 306 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	f	304	BCR	1	0
32	J	615	PID	3	0
38	f	301	BCR	5	0
27	a	806	CLA	2	0
27	A	609	CLA	1	0
27	b	703	CLA	1	0
30	C	216	DD6	2	0
27	K	605	CLA	3	0
27	C	205	CLA	2	0
32	J	611	PID	6	0
27	K	601	CLA	3	0
30	F	612	DD6	1	0
33	K	613	LMG	1	0
27	T	606	CLA	2	0
27	l	409	CLA	1	0
33	D	619	LMG	1	0
30	i	202	DD6	1	0
29	I	612	UIX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	K	607	KC2	6	0
27	I	605	CLA	1	0
27	A	605	CLA	1	0
27	a	814	CLA	1	0
27	U	603	CLA	7	0
27	b	704	CLA	3	0
32	B	613	PID	1	0
27	b	718	CLA	1	0
27	a	802	CLA	1	0
38	a	836	BCR	41	0
27	D	612	CLA	1	0
32	J	613	PID	10	0
30	K	610	DD6	1	0
30	b	730	DD6	1	0
28	J	608	KC2	2	0
27	l	411	CLA	1	0
30	D	621	DD6	1	0
27	F	602	CLA	2	0
27	a	826	CLA	3	0
32	I	614	PID	4	0
35	j	201	DGD	1	0
27	D	608	CLA	1	0
35	K	614	DGD	3	0
27	l	410	CLA	2	0
27	b	701	CLA	4	0
27	K	602	CLA	2	0
27	F	605	CLA	1	0
32	J	614	PID	4	0
27	C	203	CLA	1	0
27	F	601	CLA	1	0
30	H	316	DD6	1	0
27	I	616	CLA	1	0
27	j	202	CLA	1	0
27	f	302	CLA	1	0
27	a	801	CLA	3	0
27	H	303	CLA	1	0
27	D	604	CLA	1	0
35	l	416	DGD	3	0
27	b	714	CLA	12	0
27	b	705	CLA	1	0
27	K	603	CLA	6	0
30	A	615	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	817	CLA	1	0
27	G	608	CLA	1	0
27	a	820	CLA	4	0
27	b	723	CLA	2	0
27	F	608	CLA	1	0
30	G	616	DD6	1	0
29	A	613	UIX	1	0
27	a	827	CLA	3	0
27	I	603	CLA	1	0
27	U	605	CLA	1	0
27	J	609	CLA	2	0
27	b	716	CLA	1	0
27	a	804	CLA	10	0
30	G	614	DD6	1	0
27	G	605	CLA	1	0
27	I	607	CLA	1	0
27	b	719	CLA	3	0
27	J	605	CLA	2	0
36	T	613	LMU	1	0
30	A	614	DD6	1	0
38	a	833	BCR	2	0
38	i	201	BCR	5	0
29	H	314	UIX	1	0
27	b	727	CLA	1	0
27	b	711	CLA	1	0
28	J	604	KC2	4	0
32	F	614	PID	6	0
27	E	609	CLA	1	0
27	r	203	CLA	1	0
30	H	318	DD6	1	0
34	r	202	LHG	1	0
38	b	731	BCR	2	0
27	b	710	CLA	2	0
27	a	812	CLA	1	0
27	I	610	CLA	1	0
27	a	811	CLA	1	0
27	H	313	CLA	1	0
27	I	606	CLA	1	0
27	l	406	CLA	1	0
30	B	612	DD6	1	0
27	F	617	CLA	3	0
32	K	611	PID	12	0

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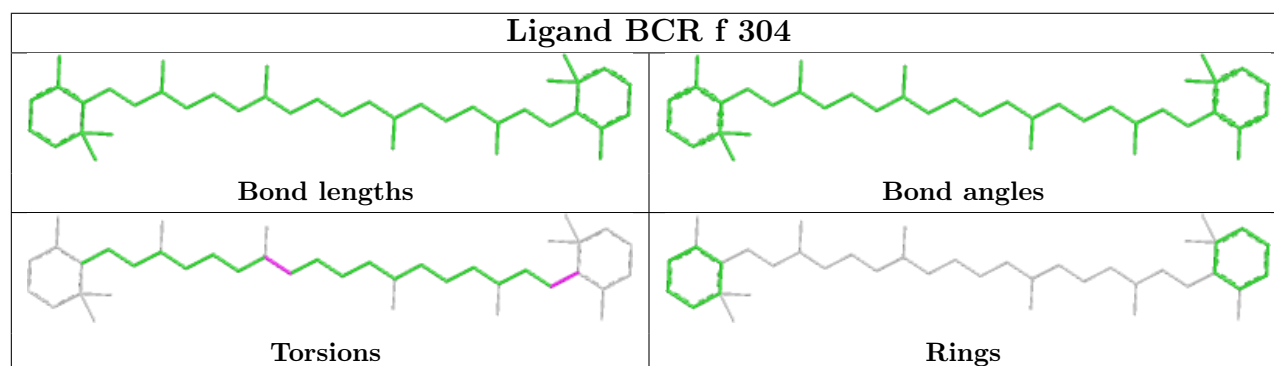
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	702	CLA	3	0
27	a	831	CLA	1	0
30	E	614	DD6	1	0
27	T	605	CLA	2	0
33	C	217	LMG	1	0
27	H	319	CLA	4	0
27	l	412	CLA	1	0
27	D	605	CLA	2	0
32	F	615	PID	3	0
27	b	713	CLA	1	0
27	a	815	CLA	1	0
27	H	312	CLA	1	0
27	a	810	CLA	1	0
28	I	604	KC2	1	0
38	l	414	BCR	4	0
27	b	725	CLA	2	0
27	b	708	CLA	1	0
27	a	825	CLA	1	0
27	D	602	CLA	1	0
27	a	819	CLA	6	0
27	b	709	CLA	2	0
27	H	304	CLA	1	0
27	a	837	CLA	1	0
34	l	401	LHG	1	0
27	a	830	CLA	1	0
27	D	611	CLA	1	0
27	B	605	CLA	1	0
27	H	308	CLA	1	0
27	G	606	CLA	1	0
30	H	315	DD6	1	0
27	b	728	CLA	1	0
27	a	807	CLA	2	0
29	j	204	UIX	2	0
38	l	415	BCR	4	0
27	E	611	CLA	1	0
27	G	602	CLA	1	0
27	a	824	CLA	3	0
30	D	615	DD6	2	0
27	F	604	CLA	1	0
30	K	609	DD6	1	0
27	A	604	CLA	1	0
27	F	619	CLA	1	0

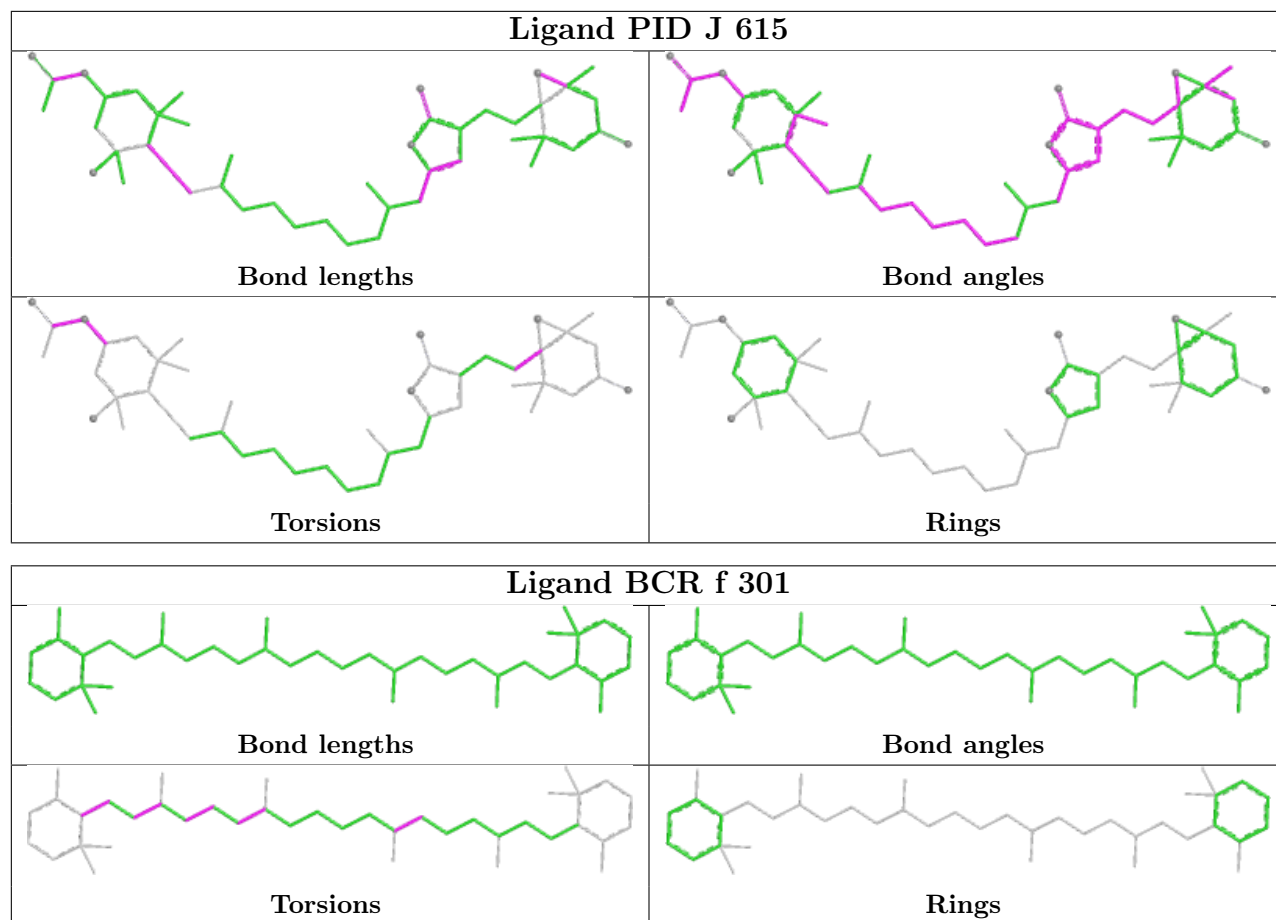
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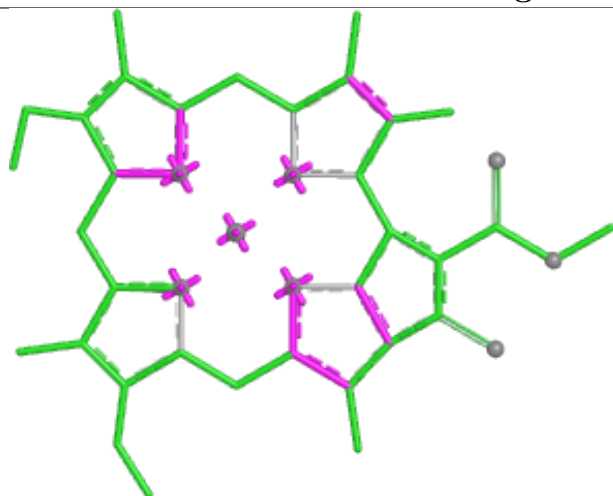
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	201	CLA	1	0
27	A	601	CLA	1	0
29	C	215	UIX	1	0
38	a	834	BCR	22	0
27	a	823	CLA	2	0
27	C	204	CLA	1	0
27	l	402	CLA	1	0
38	m	201	BCR	1	0
27	b	722	CLA	2	0
27	T	603	CLA	1	0
27	D	603	CLA	1	0
38	l	413	BCR	5	0
27	a	816	CLA	3	0
27	a	818	CLA	1	0

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

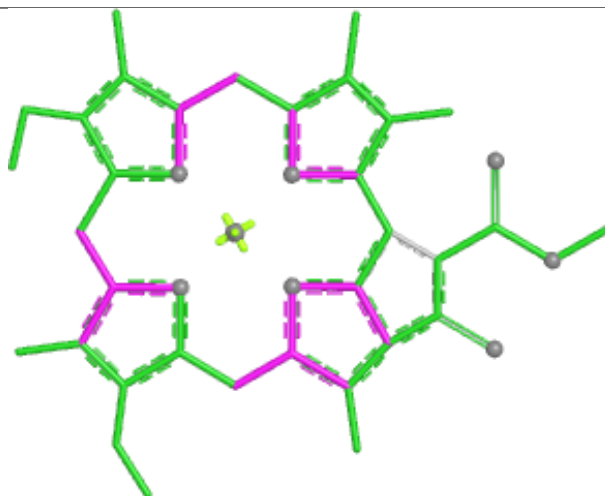




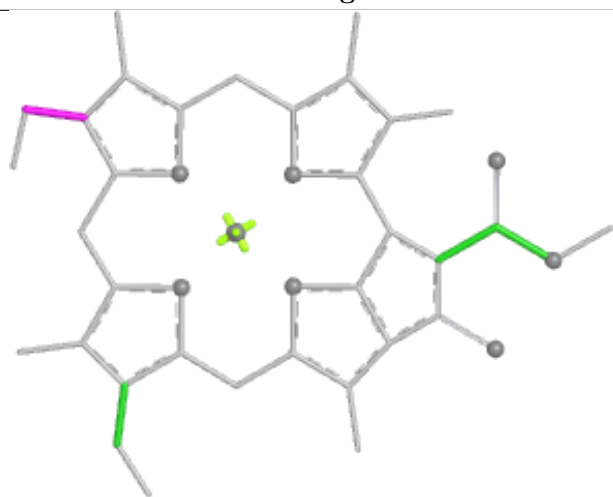
Ligand CLA T 604



Bond lengths



Bond angles

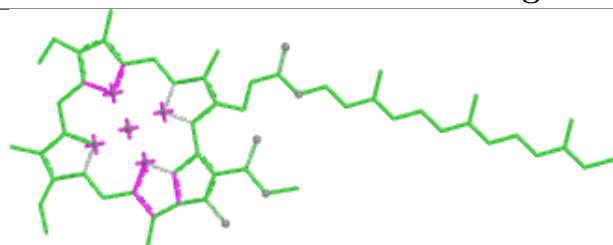


Torsions

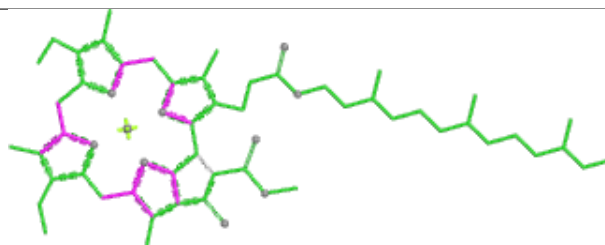


Rings

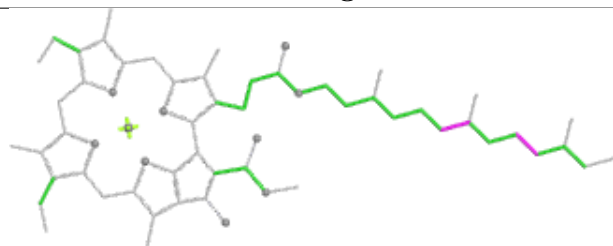
Ligand CLA 1 405



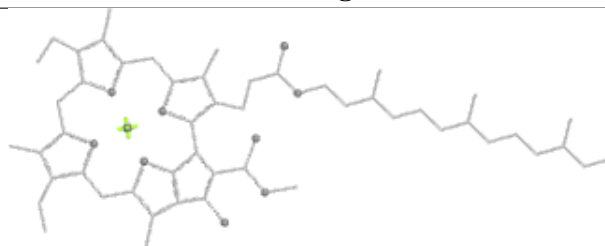
Bond lengths



Bond angles

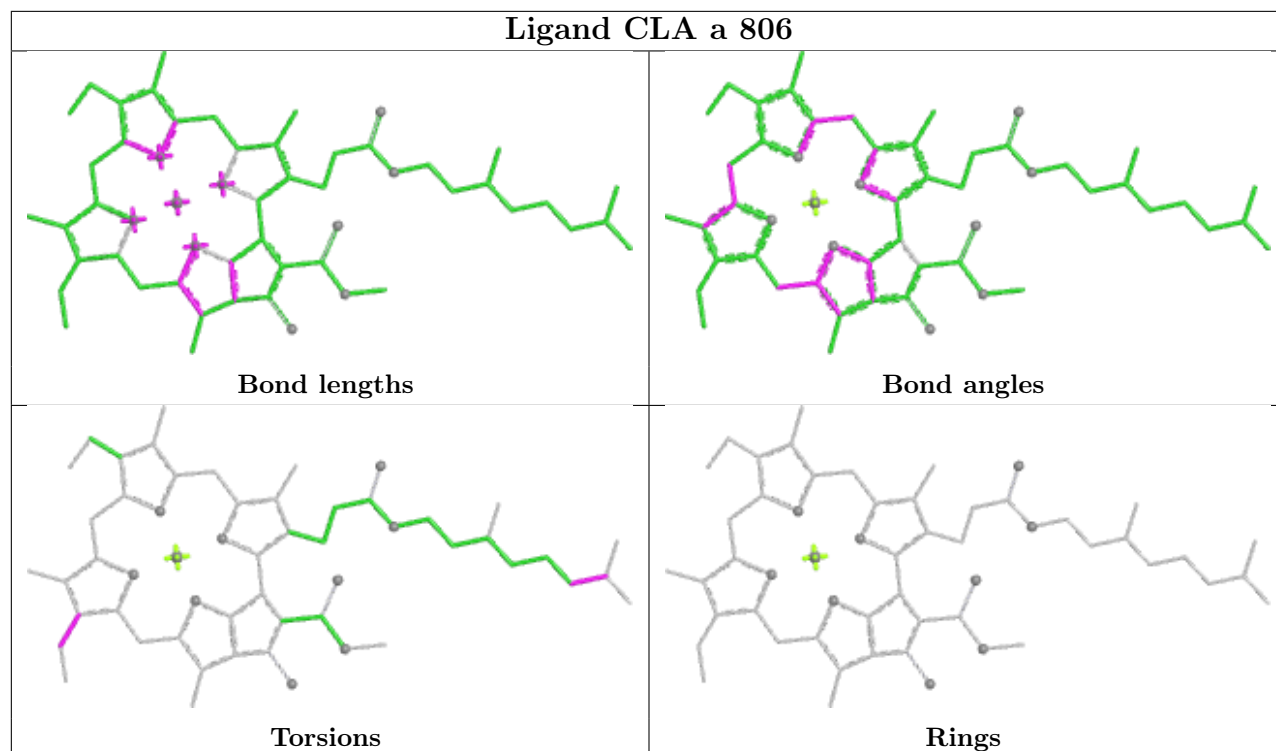


Torsions

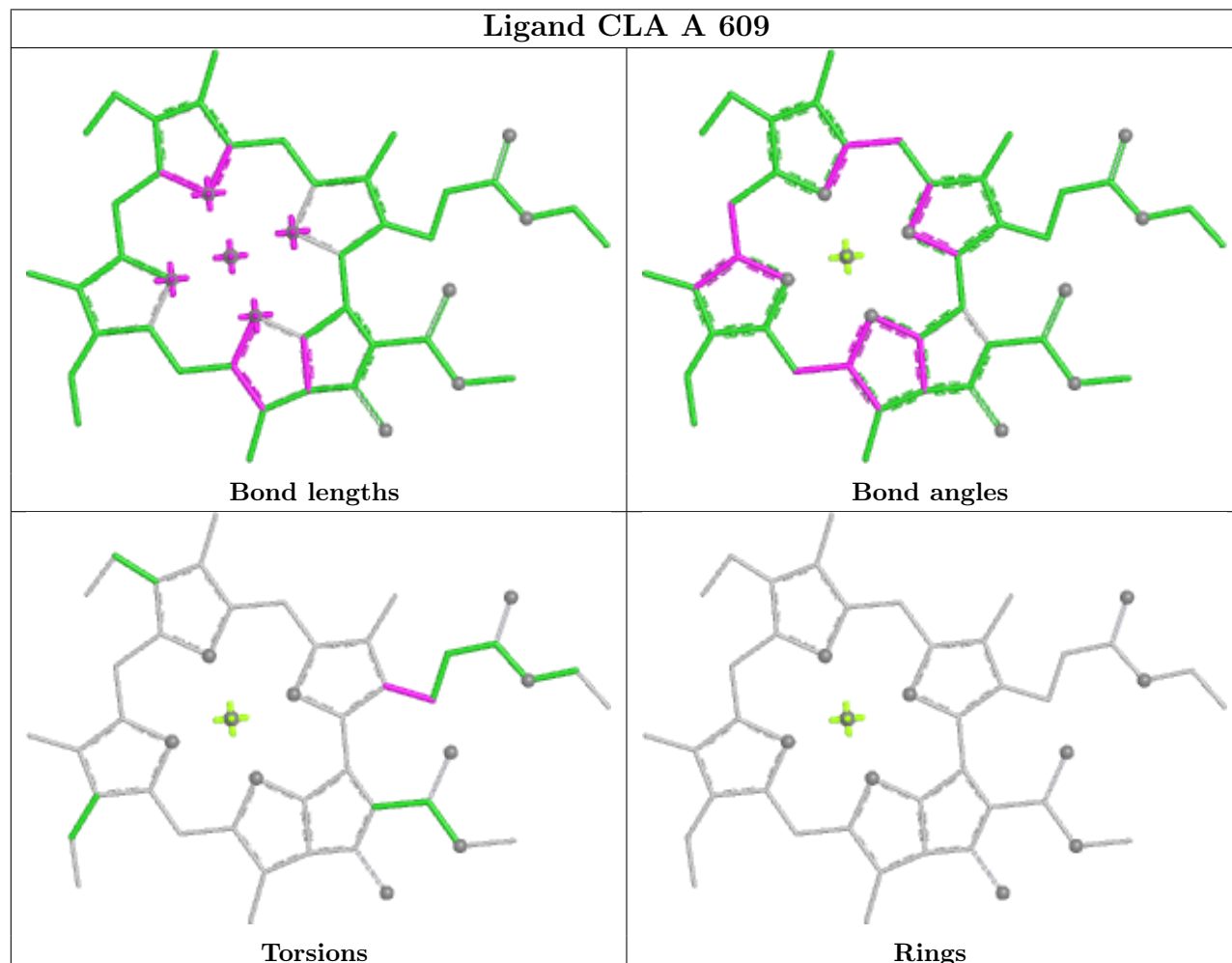


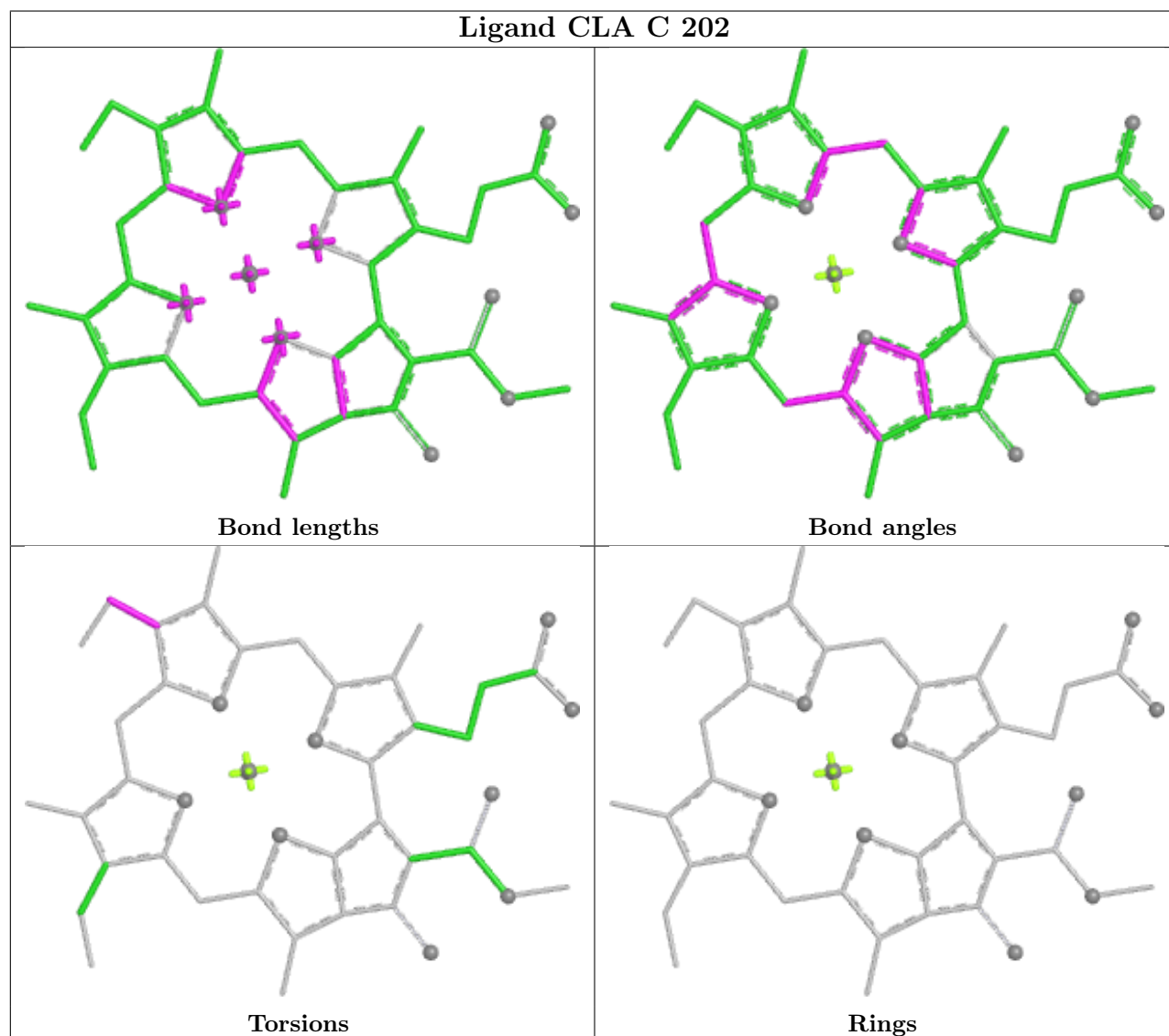
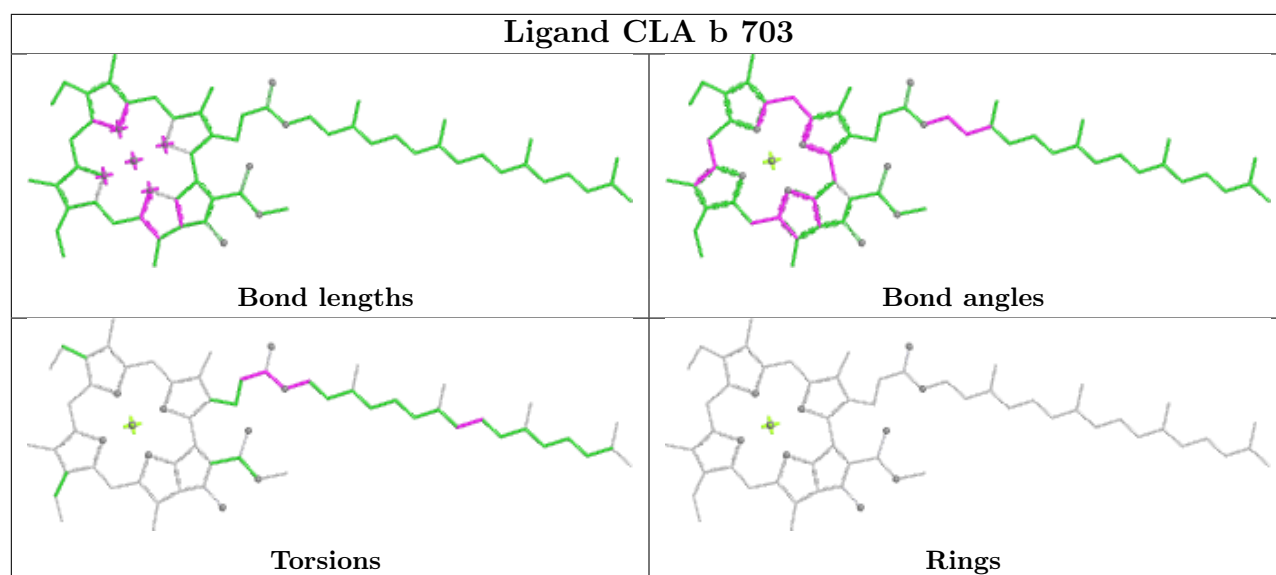
Rings

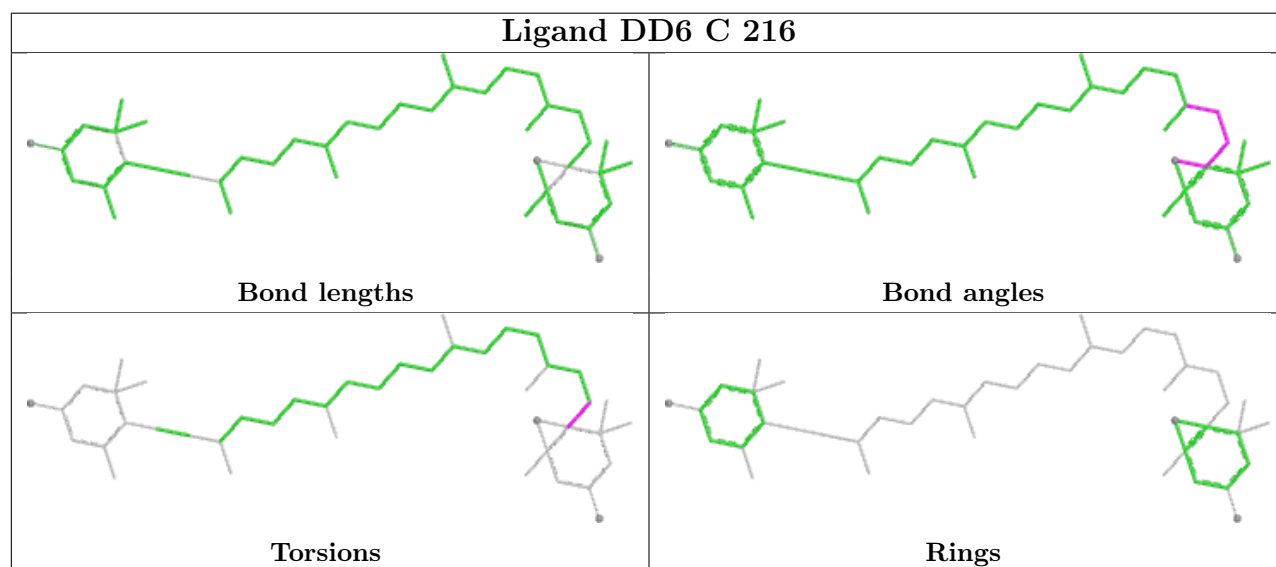
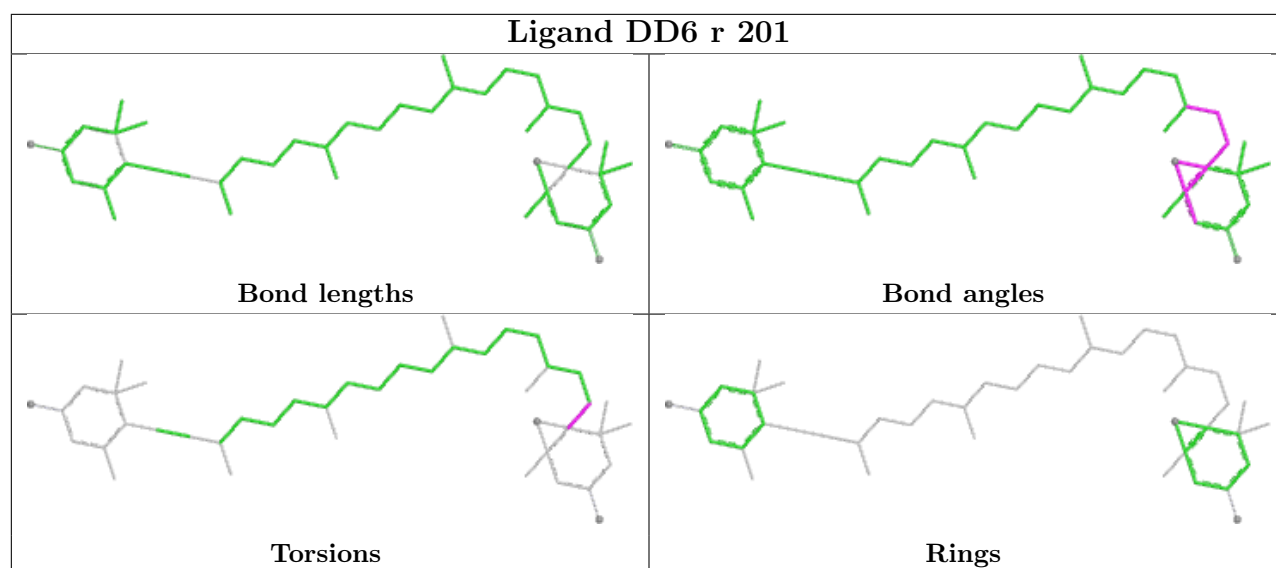
Ligand CLA a 806



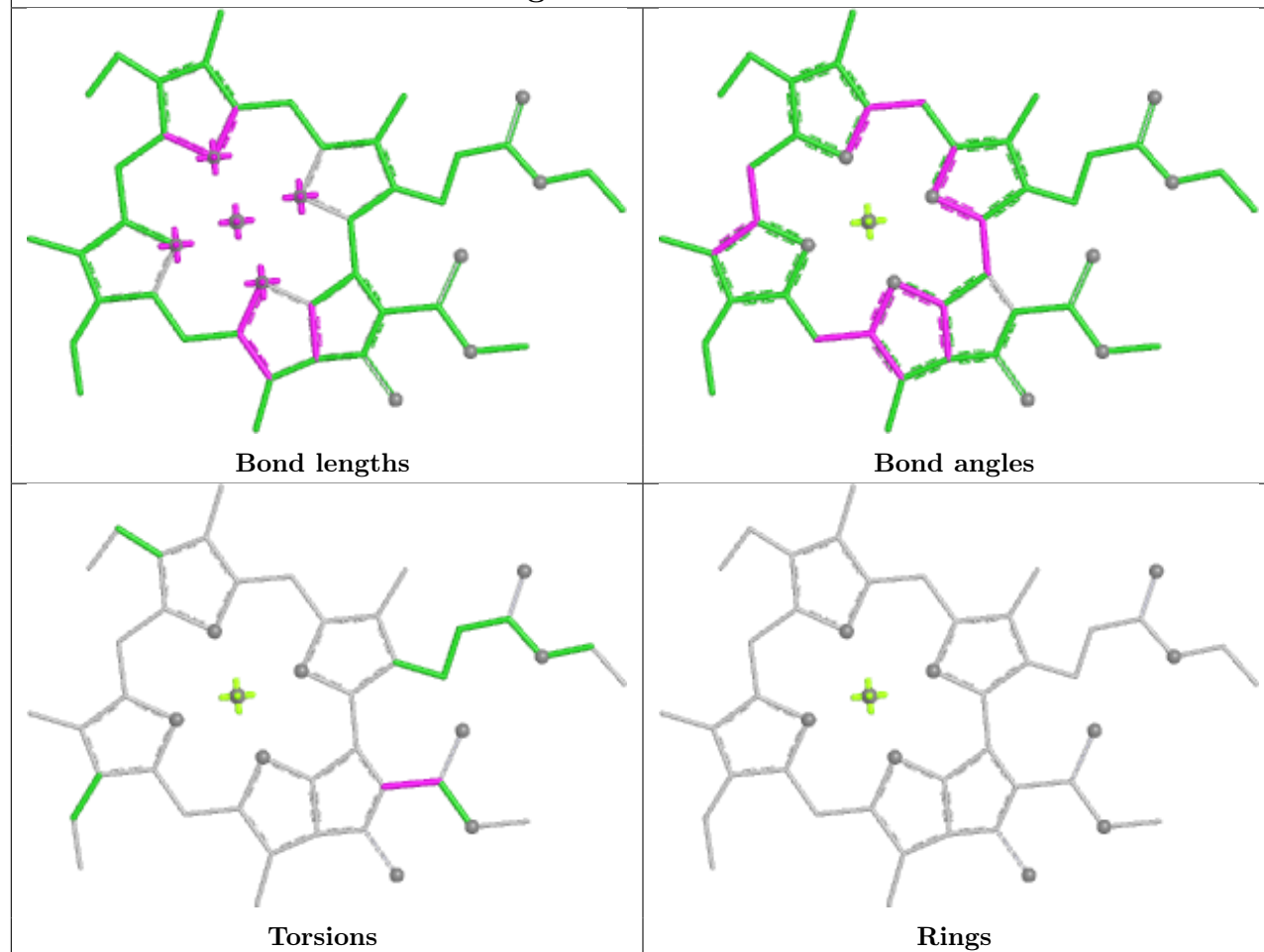
Ligand CLA A 609



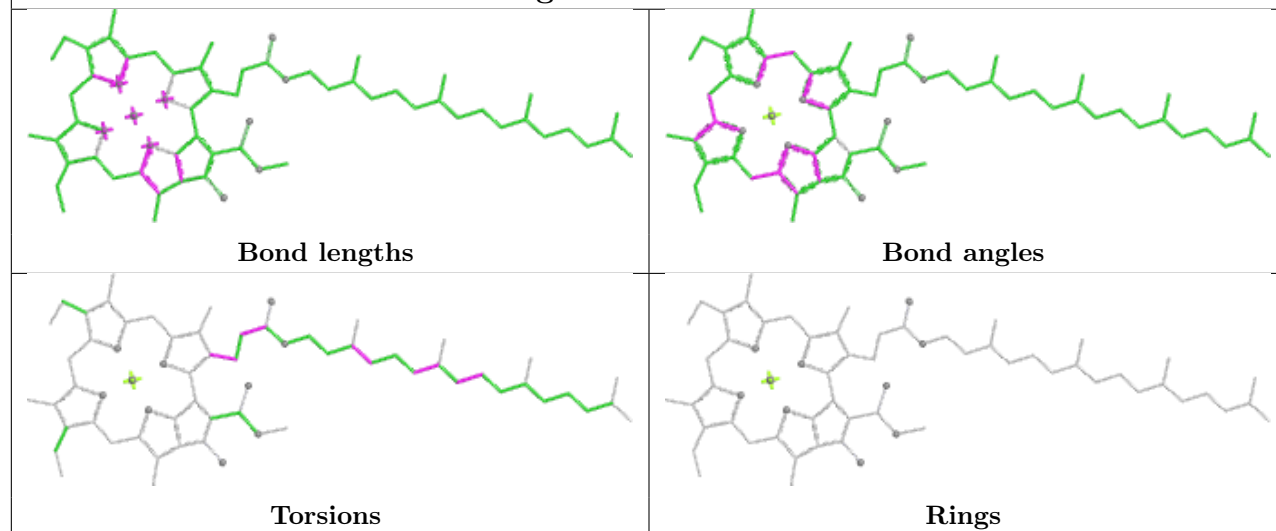


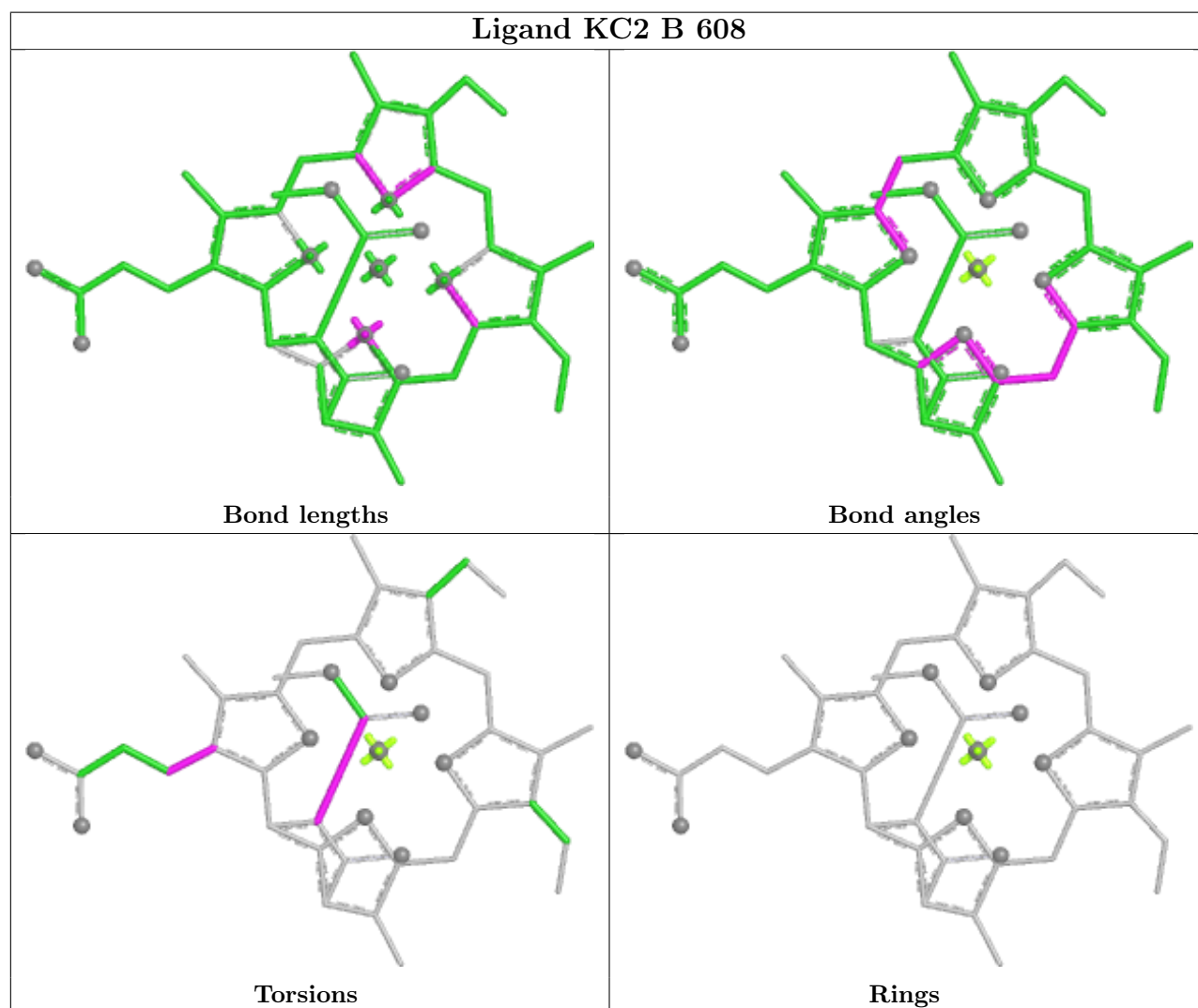
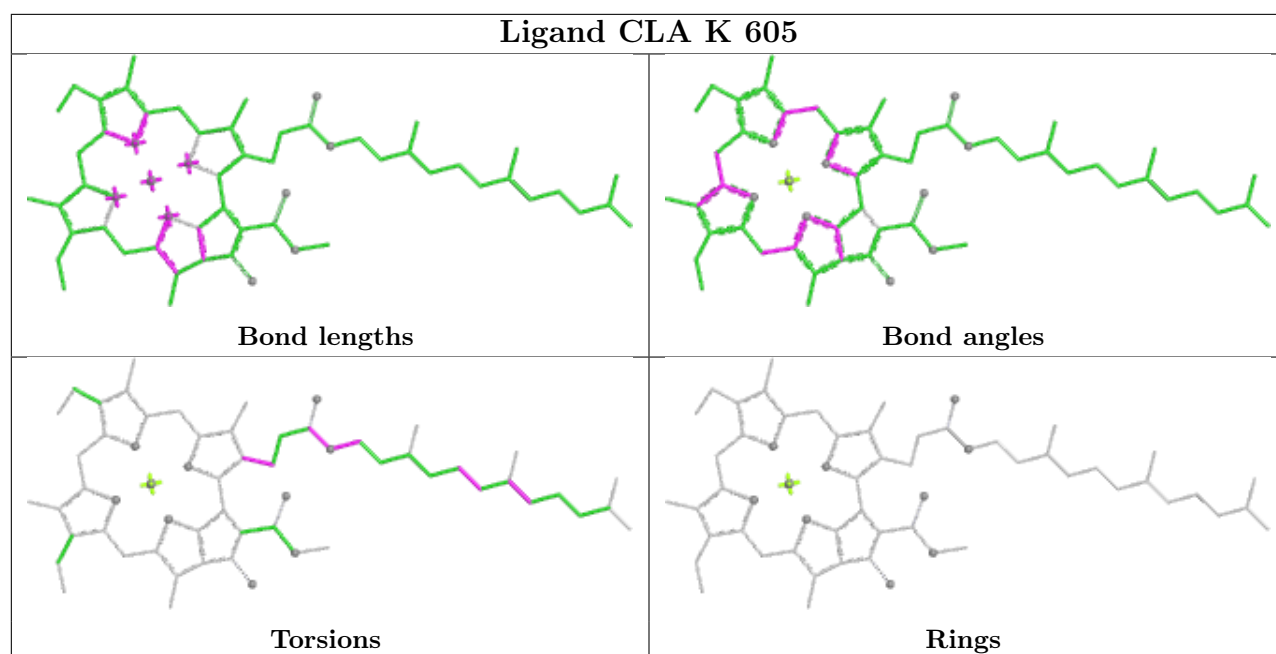


Ligand CLA T 601

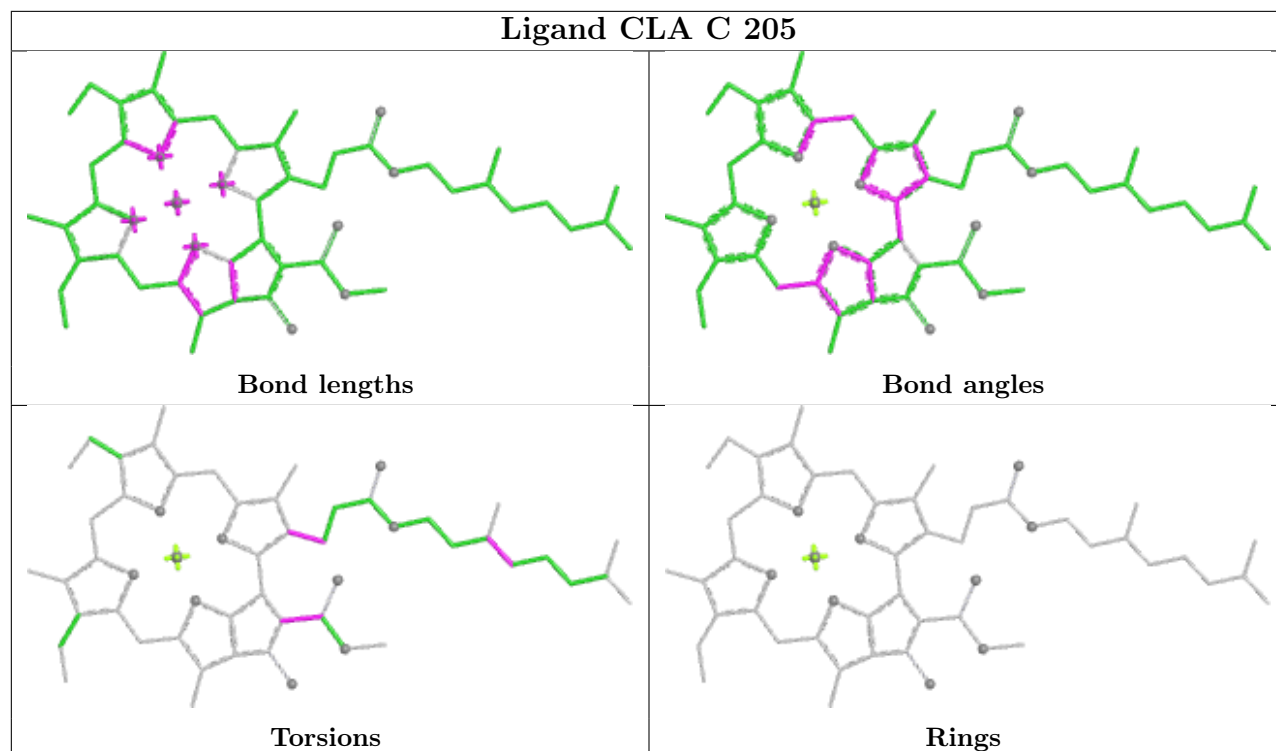


Ligand CLA a 805

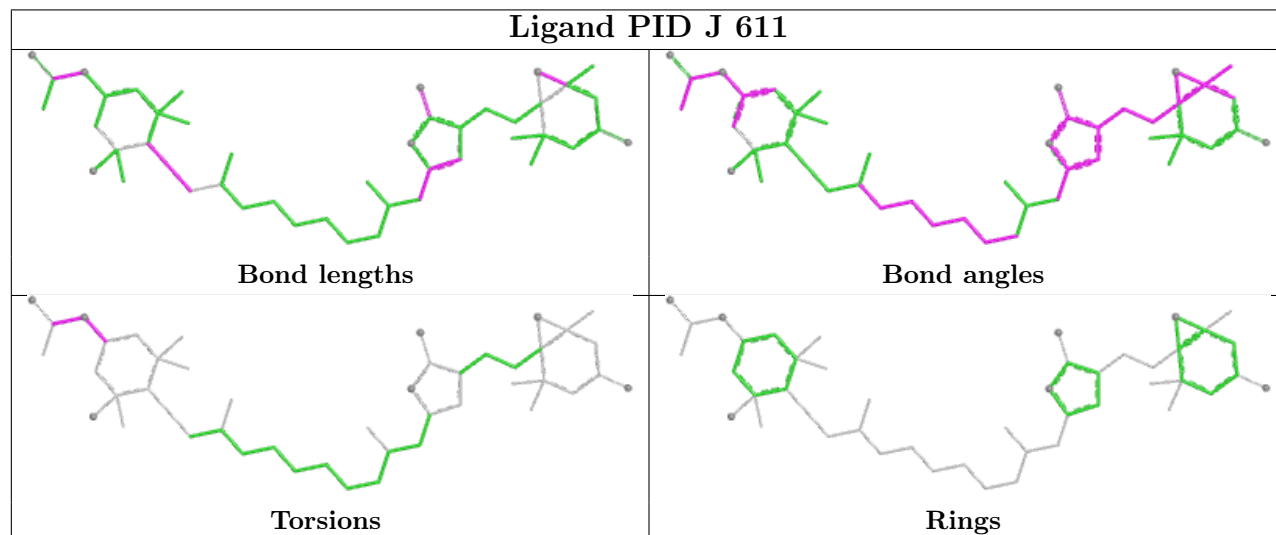


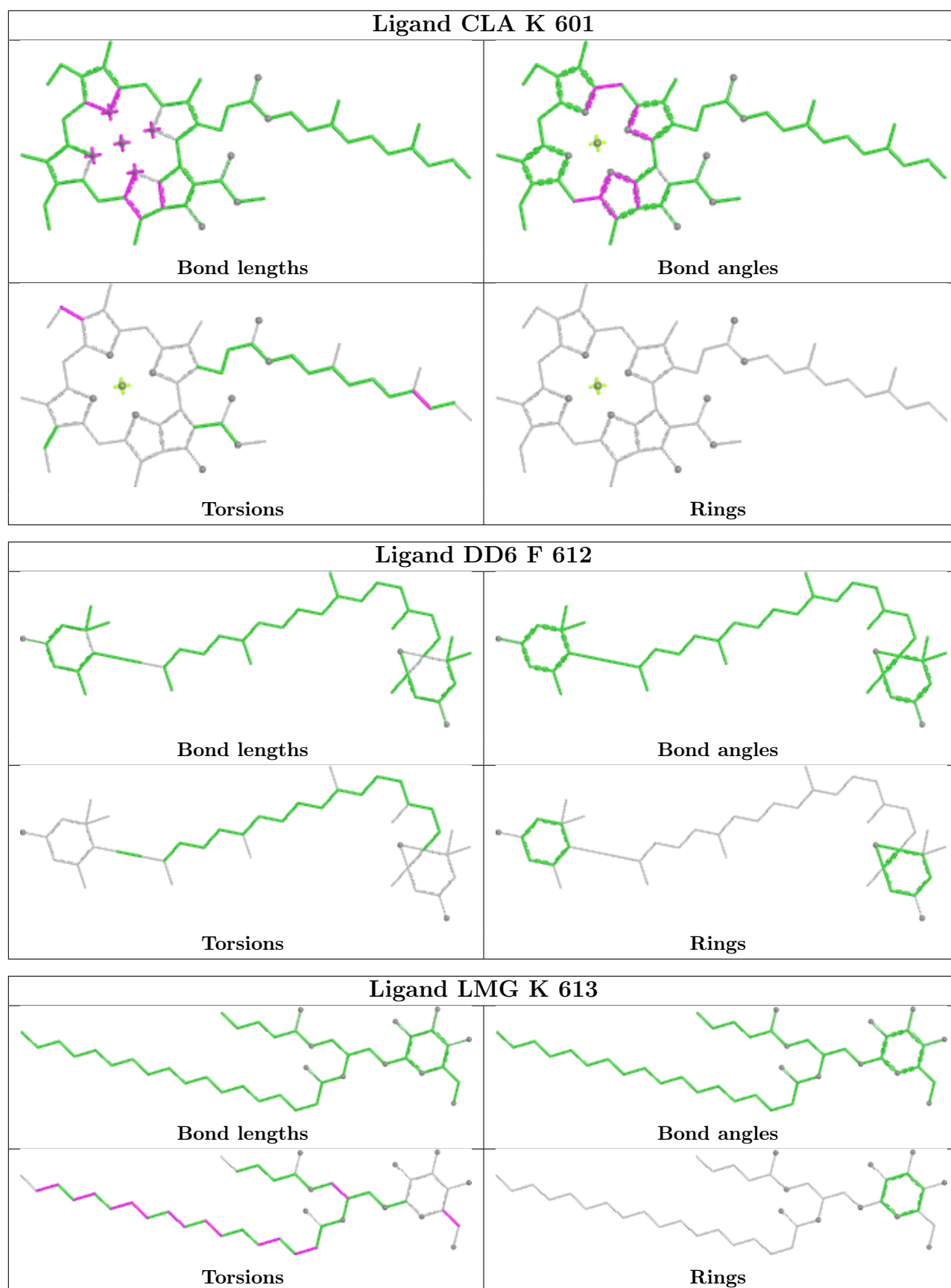


Ligand CLA C 205

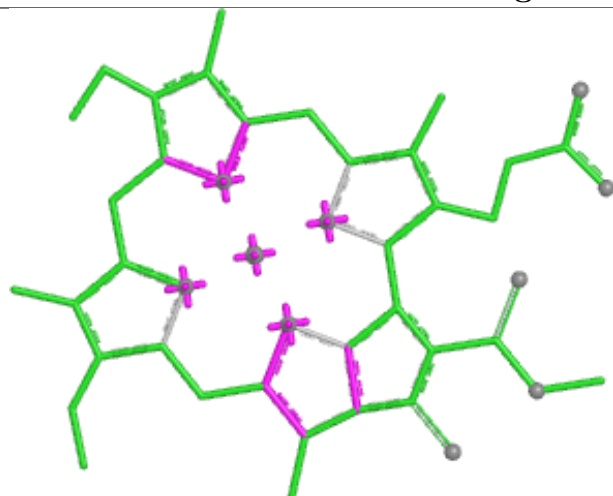


Ligand PID J 611

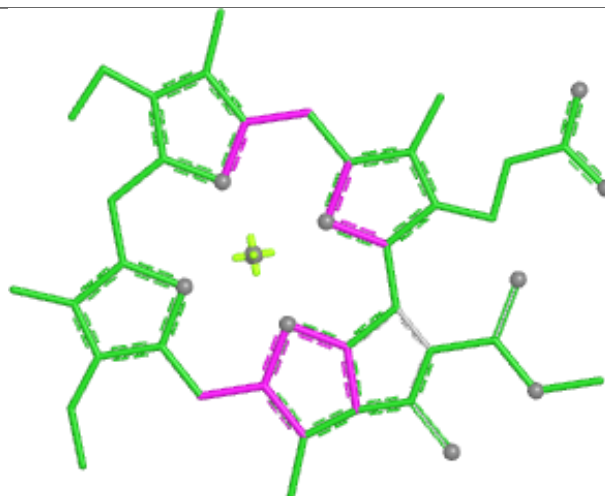




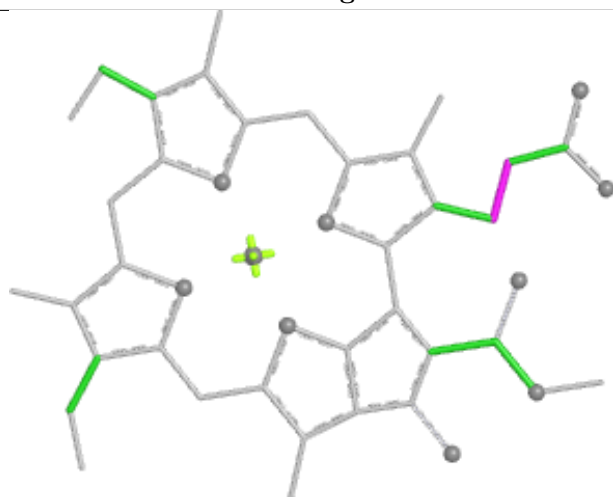
Ligand CLA T 606



Bond lengths



Bond angles

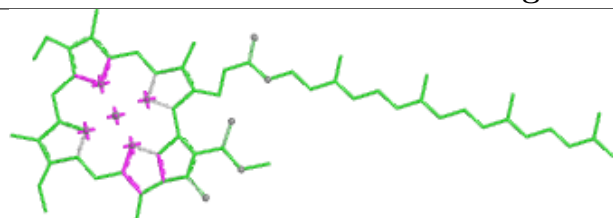


Torsions

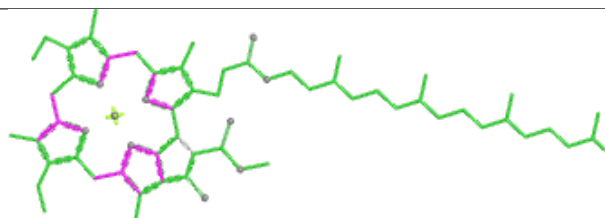


Rings

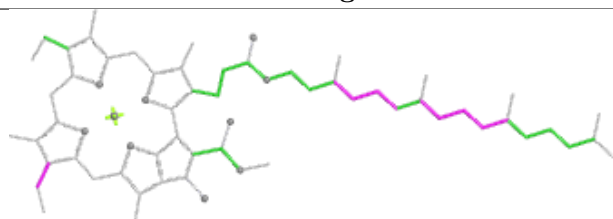
Ligand CLA I 409



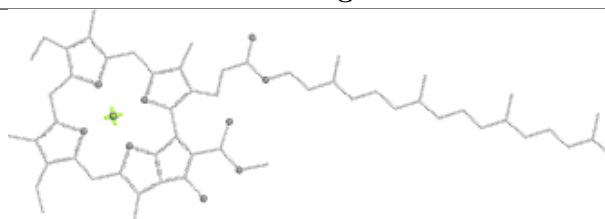
Bond lengths



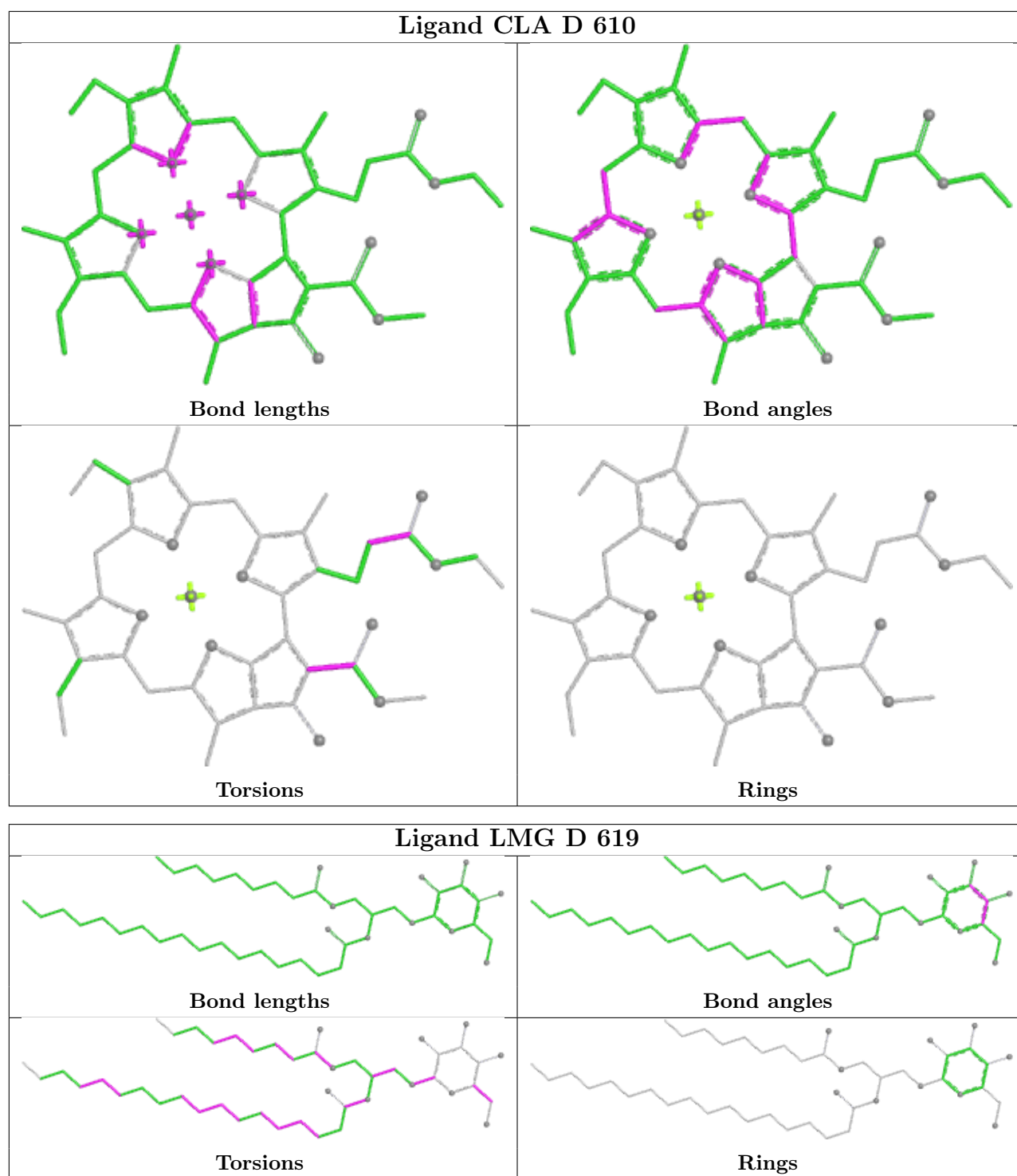
Bond angles

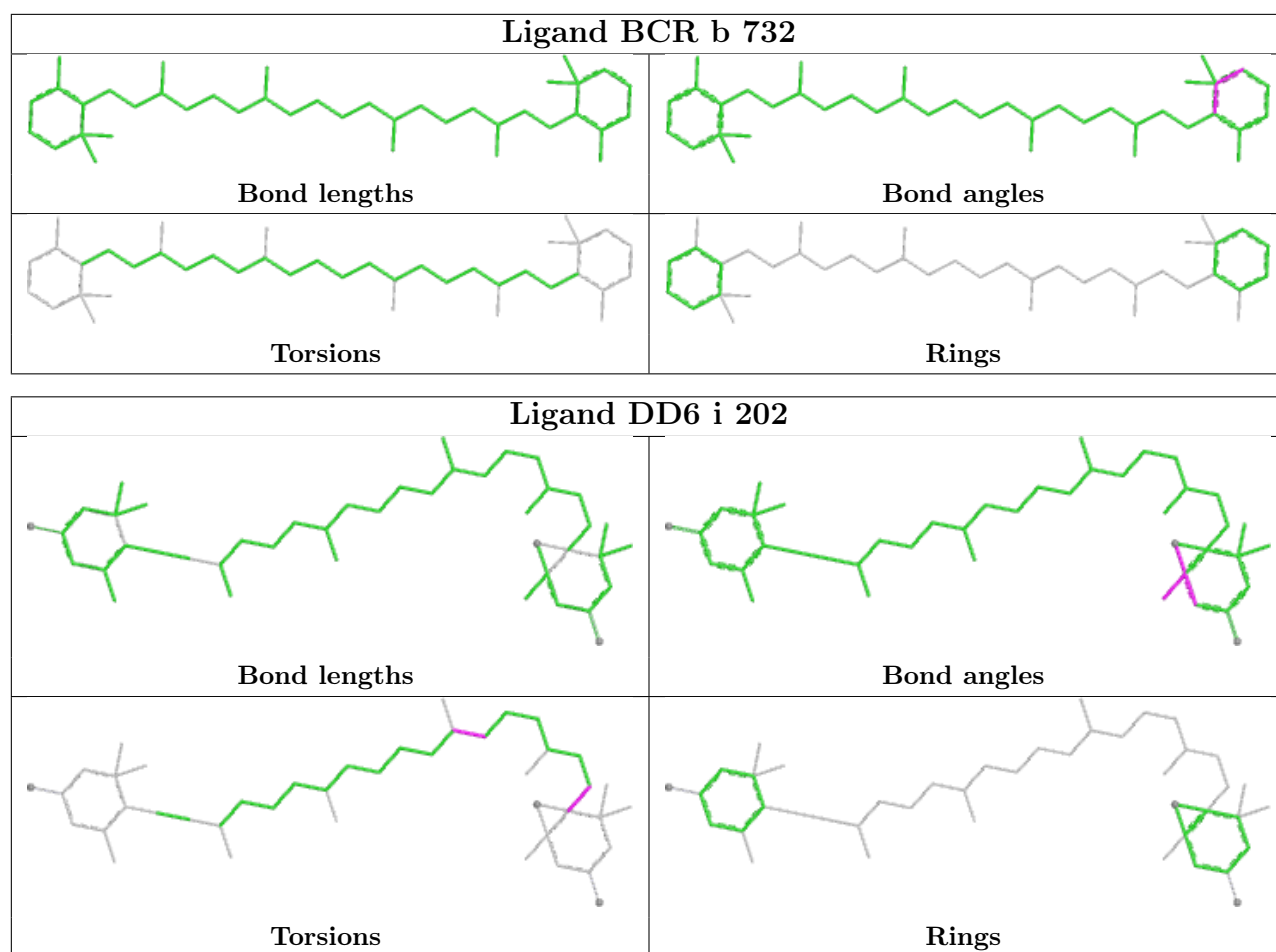


Torsions

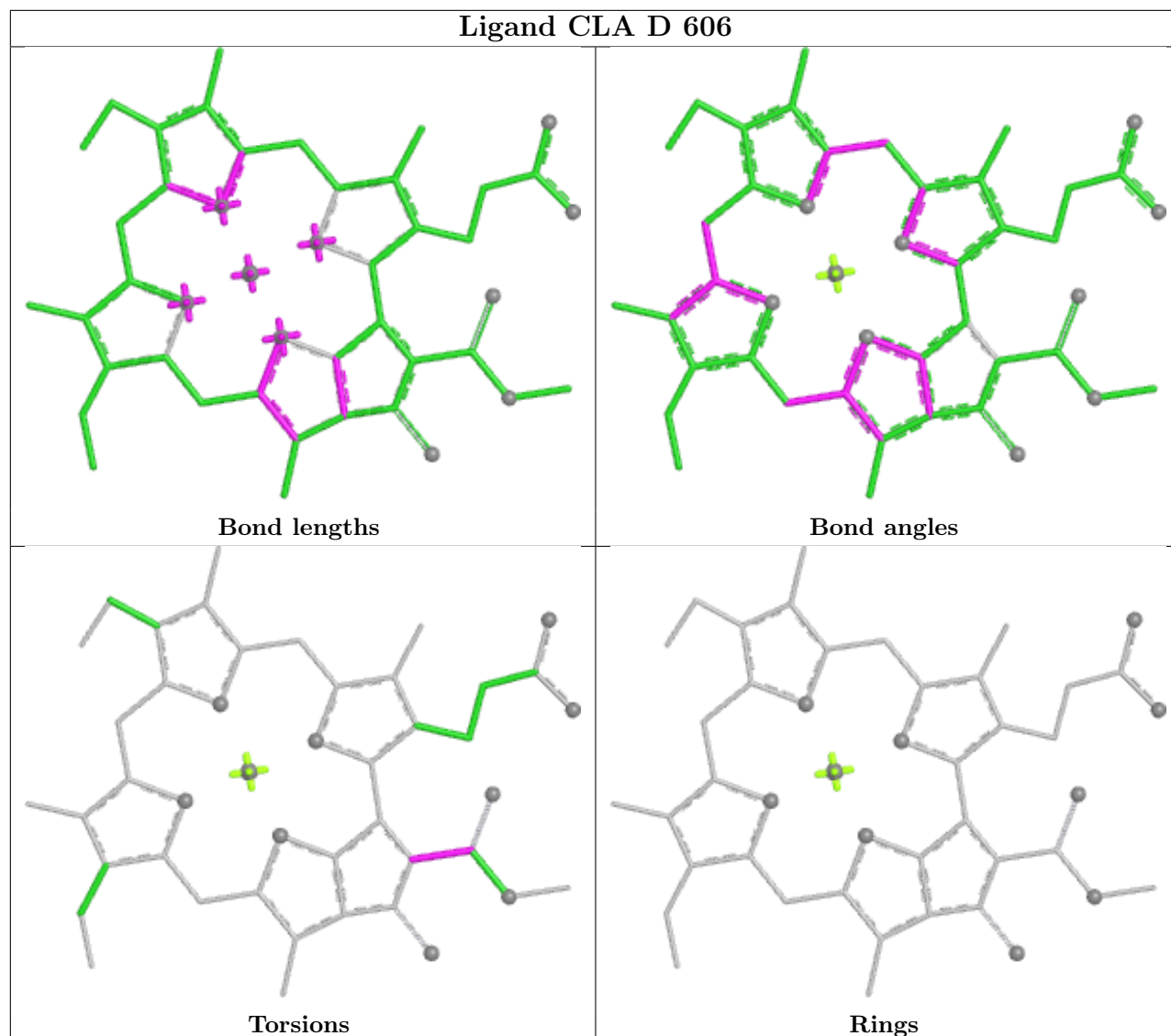


Rings

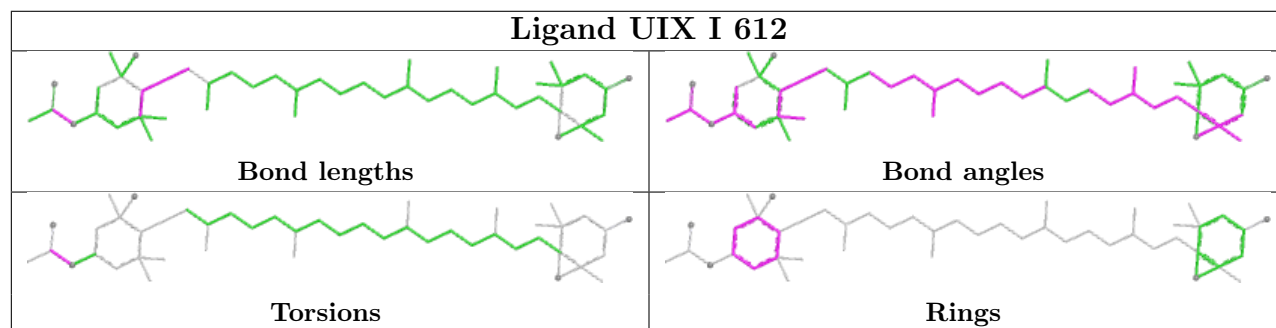




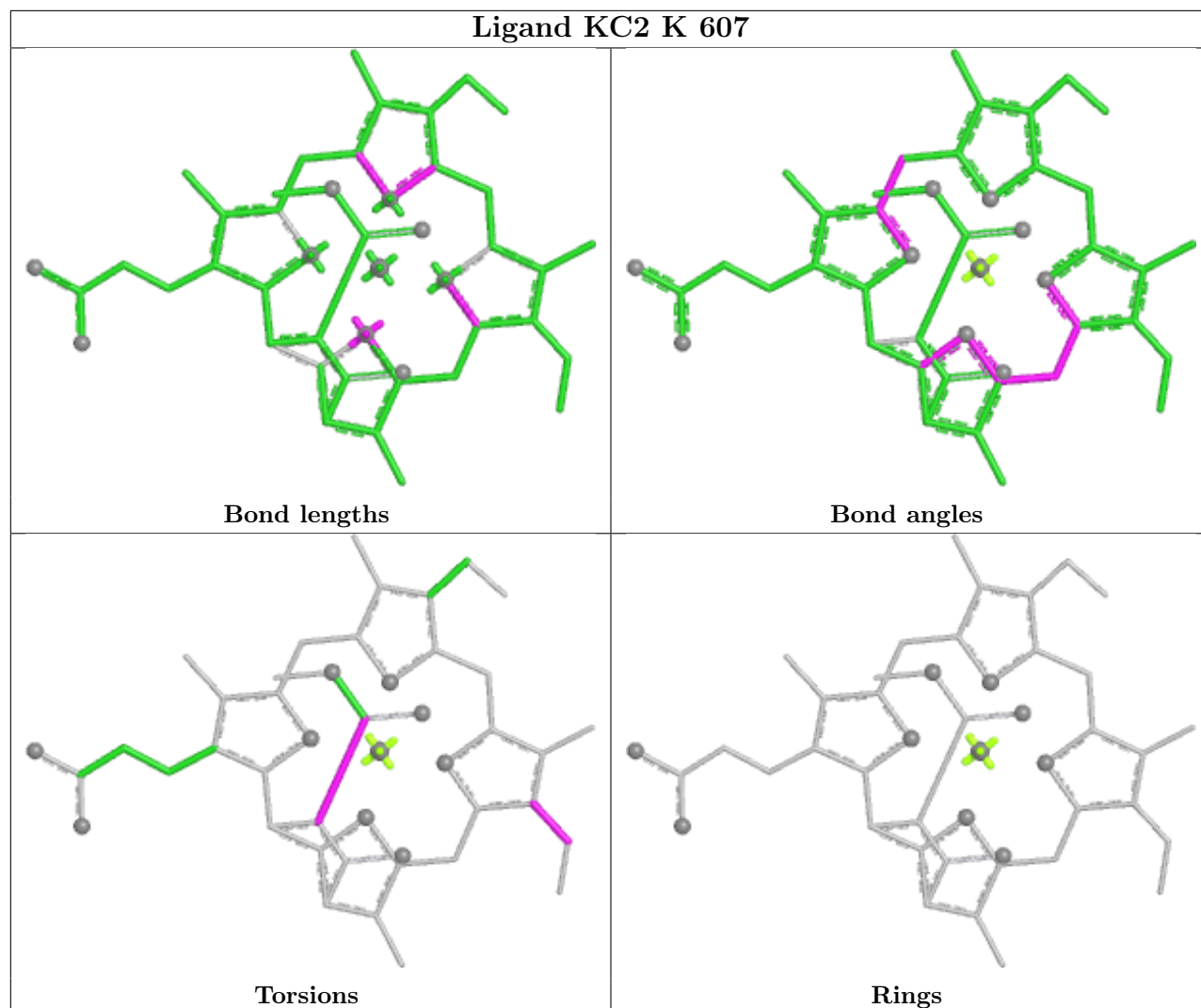
Ligand CLA D 606



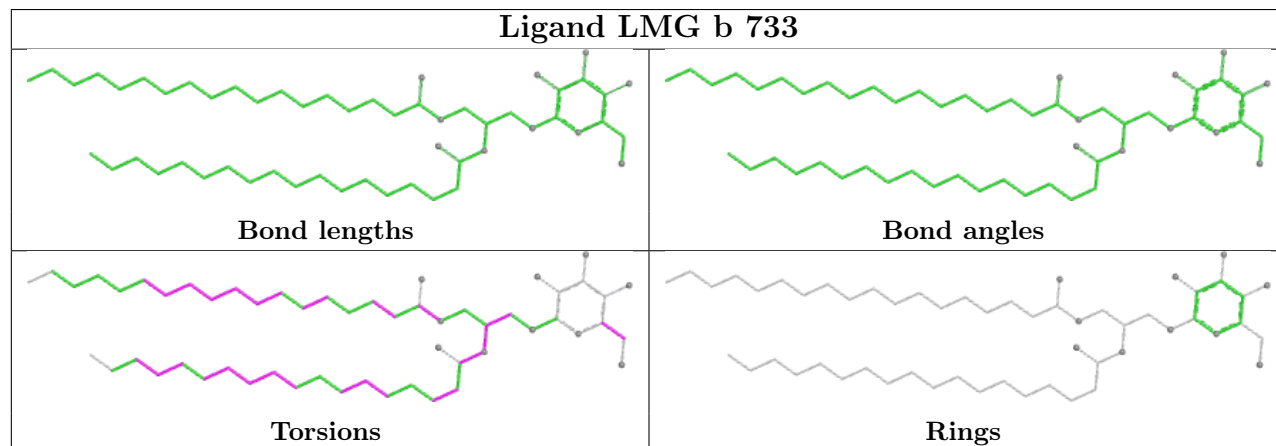
Ligand UIX I 612

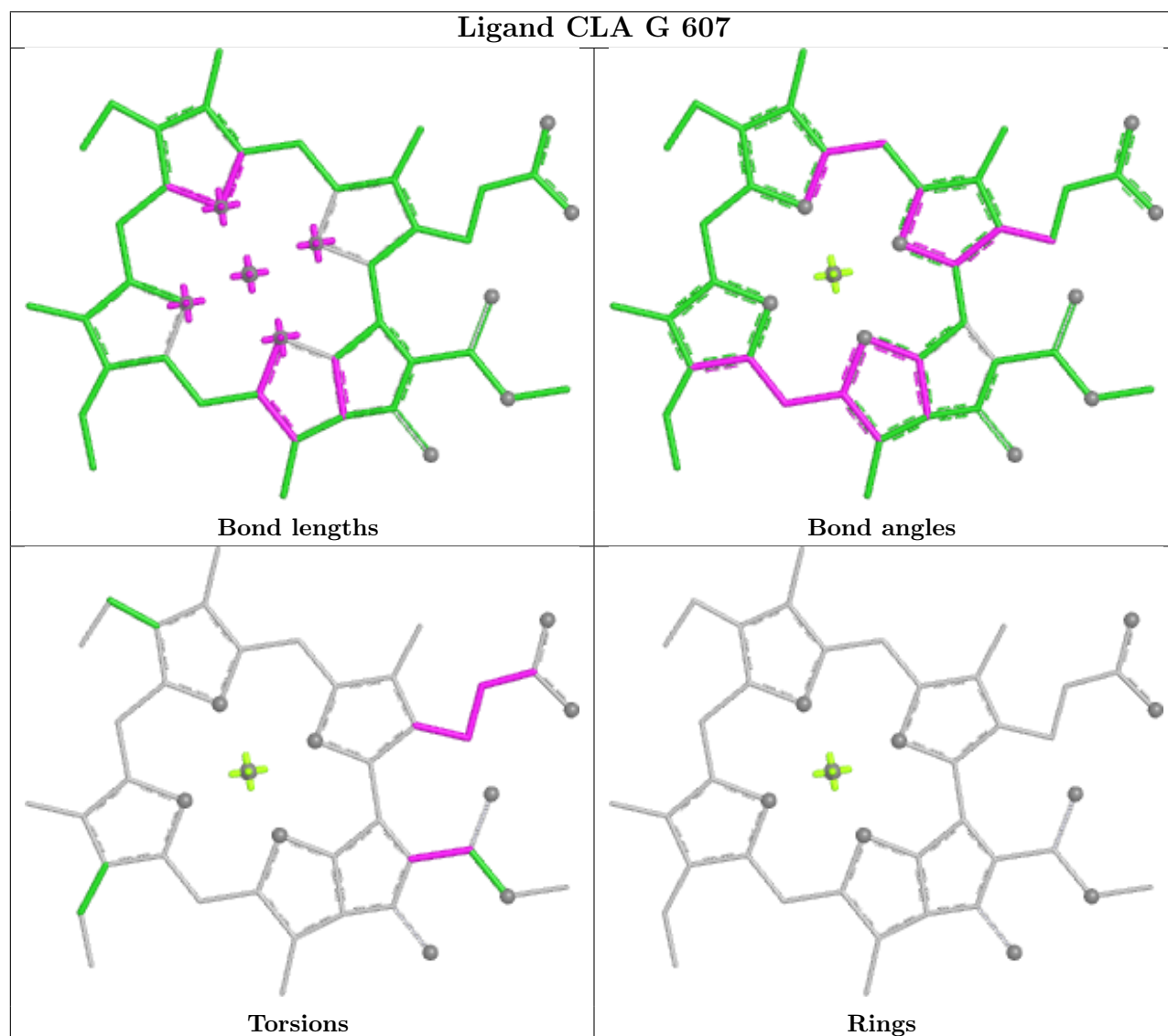
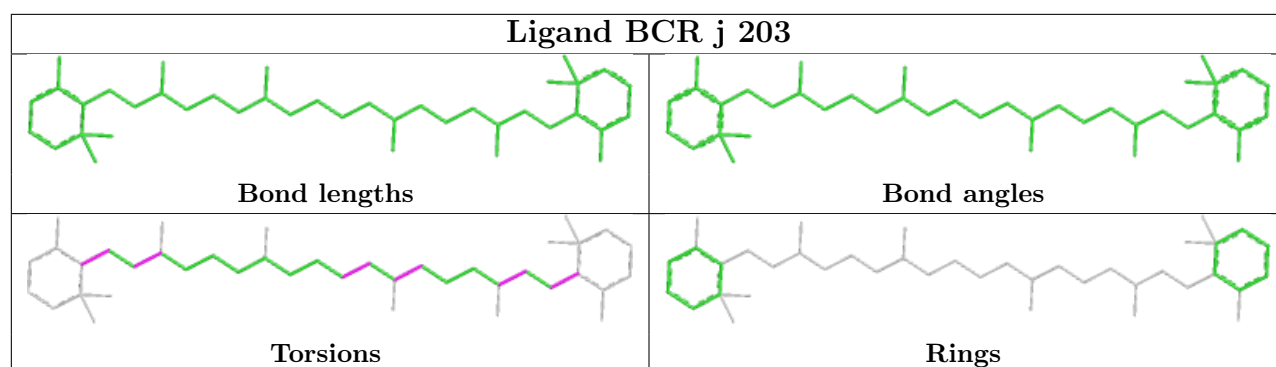


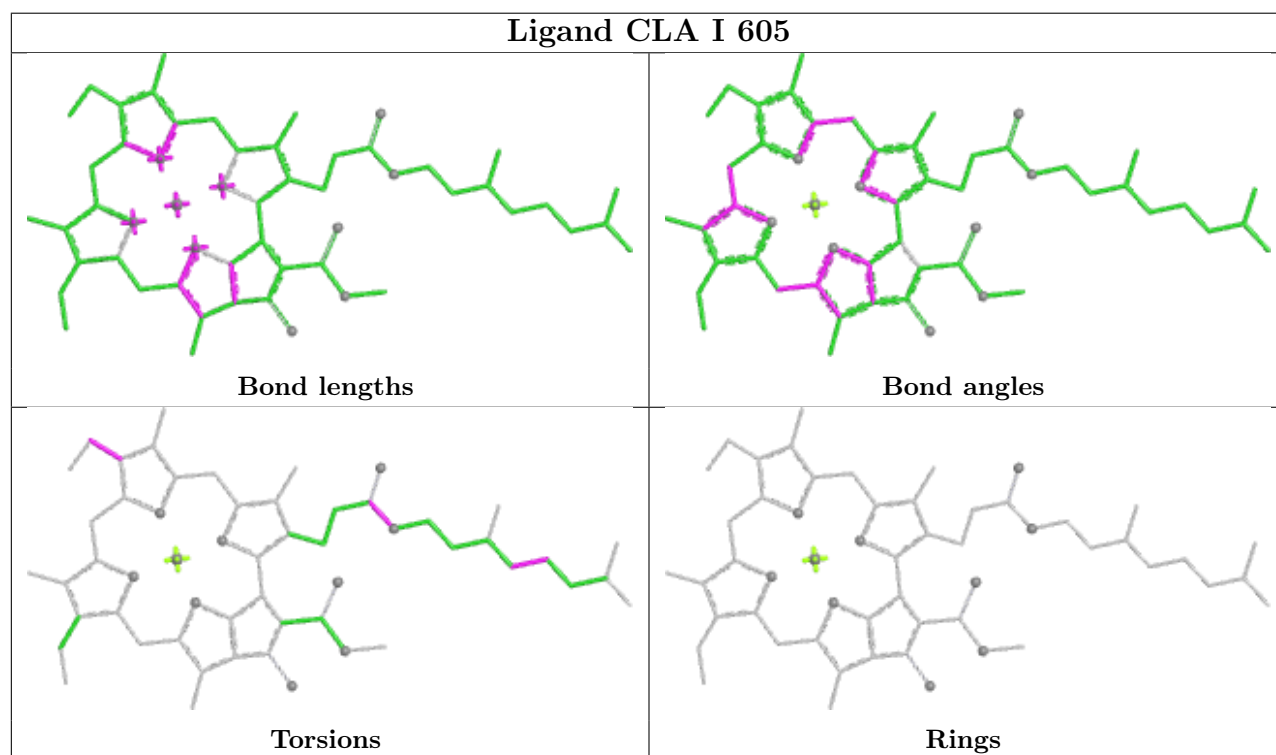
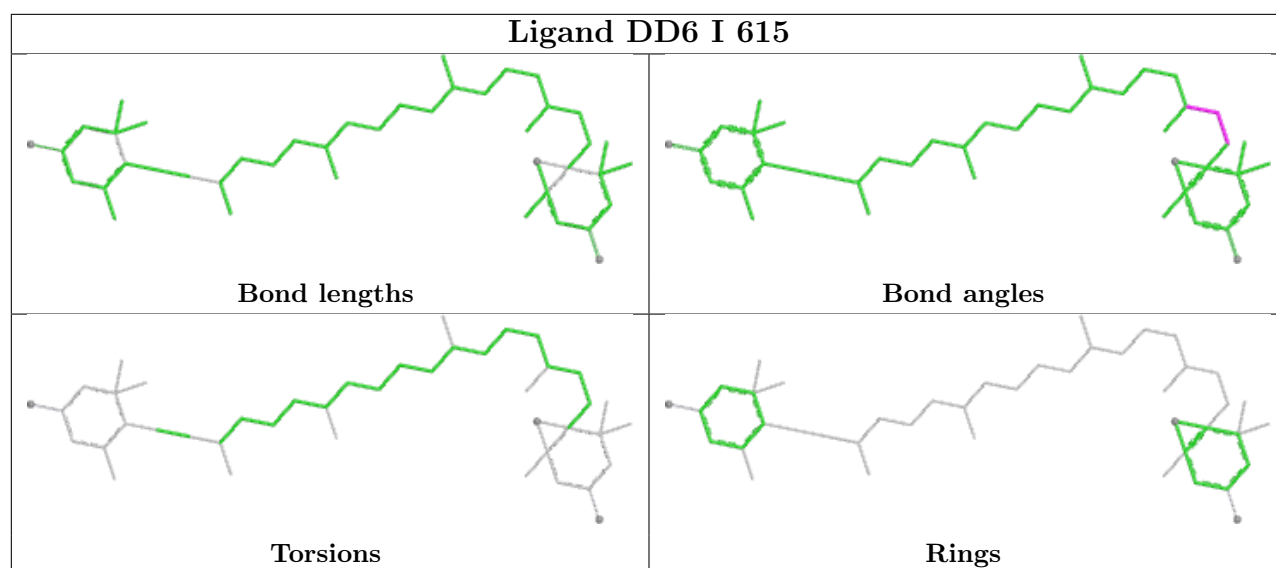
Ligand KC2 K 607

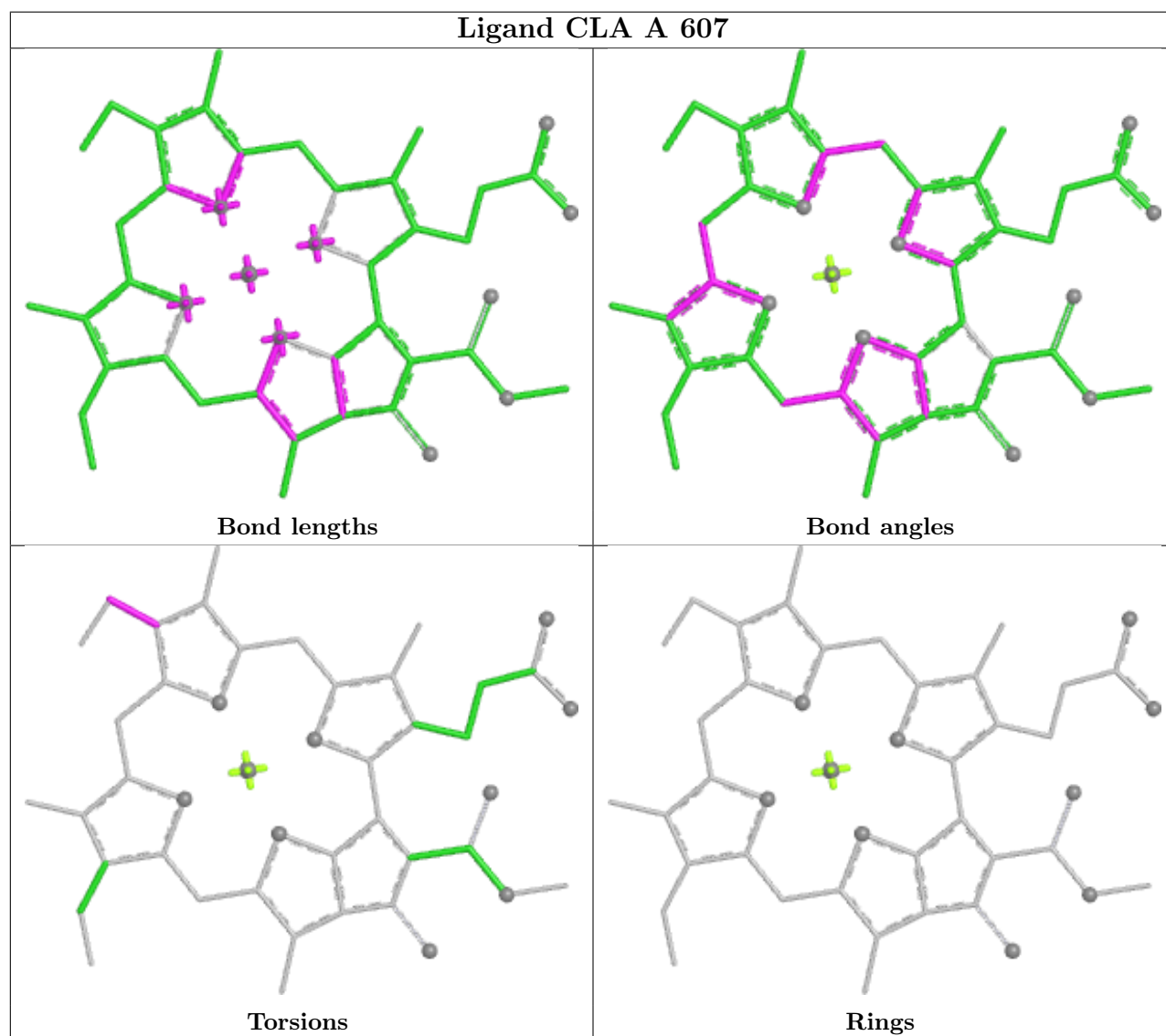
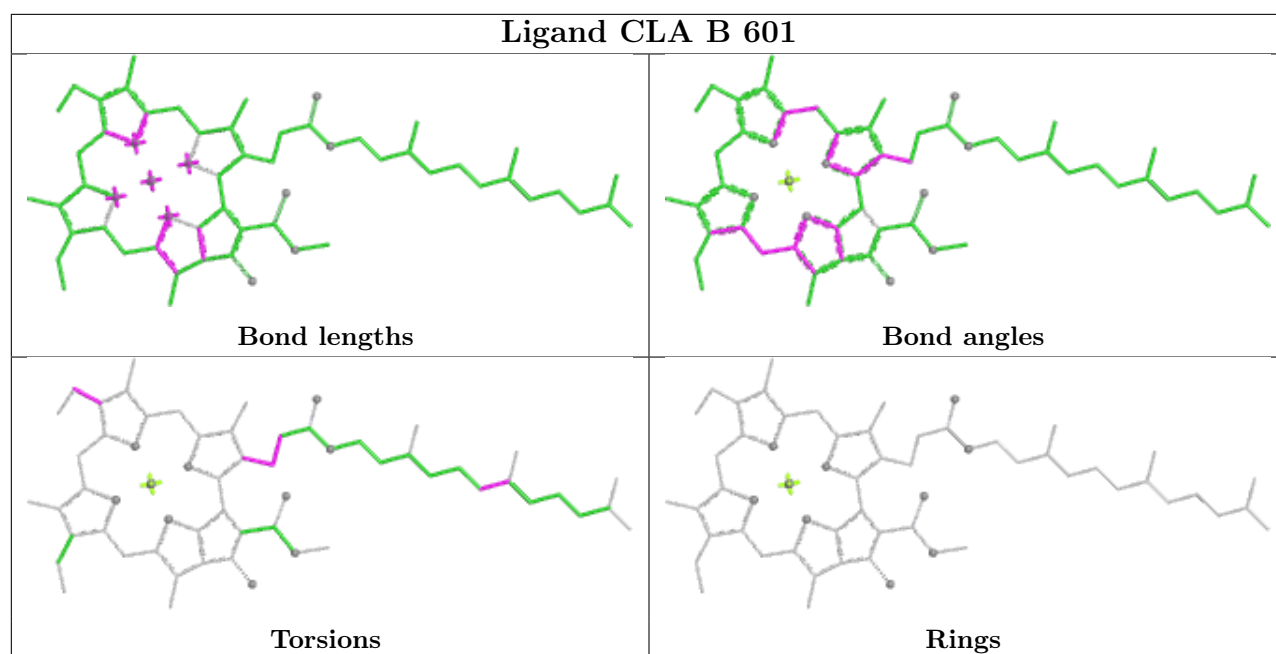


Ligand LMG b 733

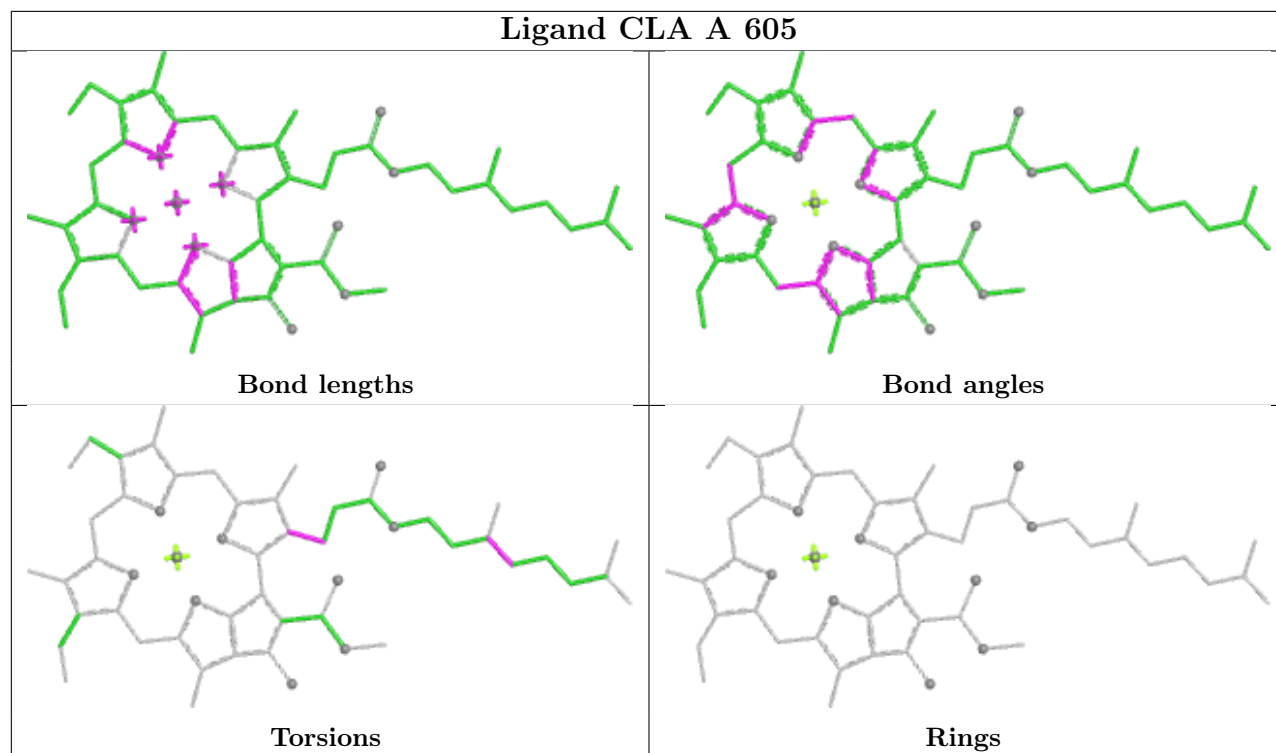




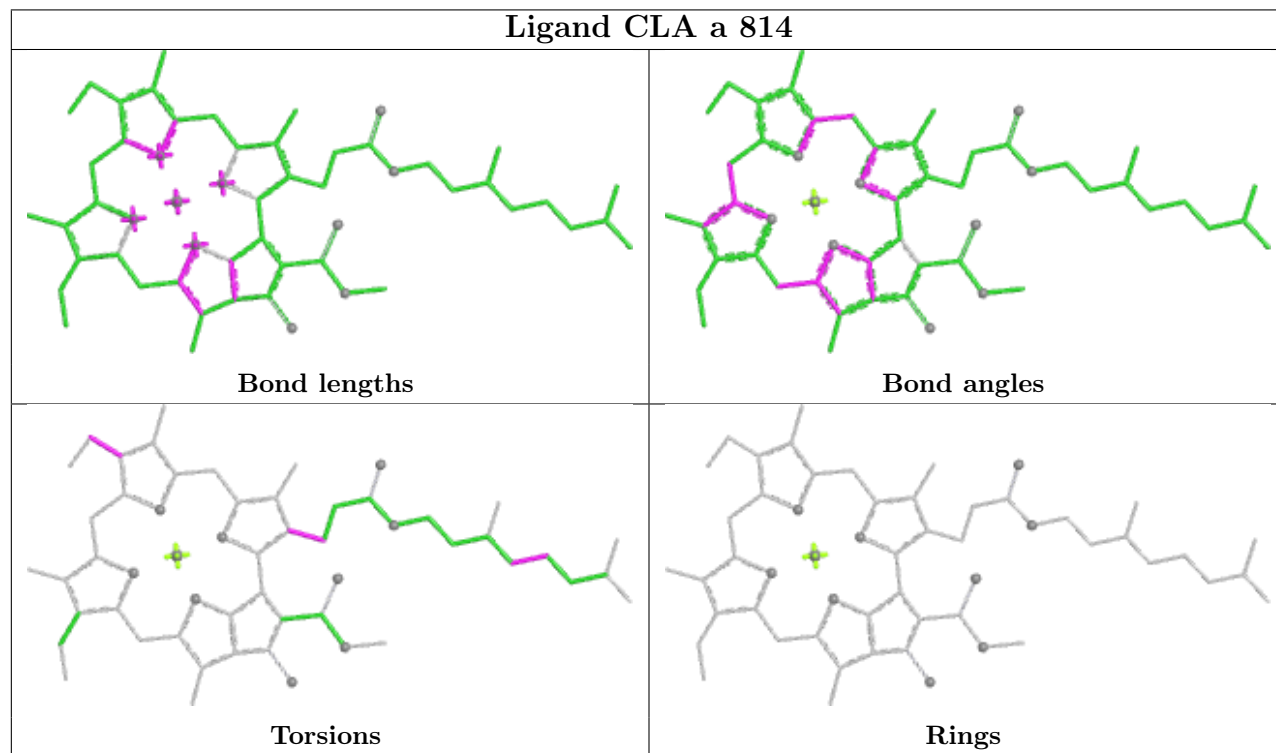




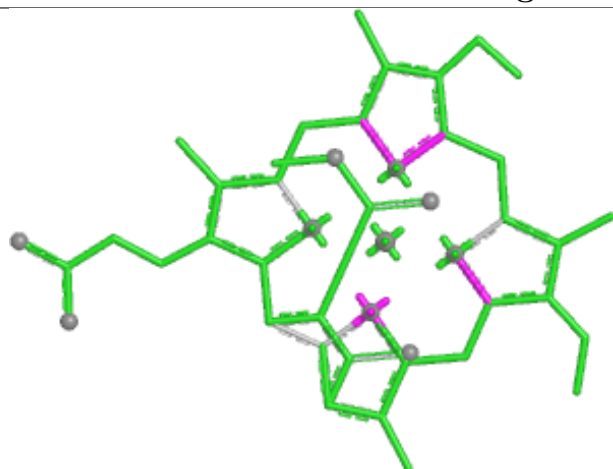
Ligand CLA A 605



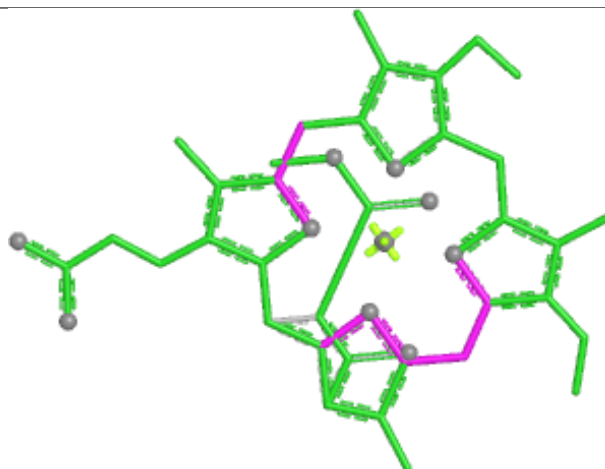
Ligand CLA a 814



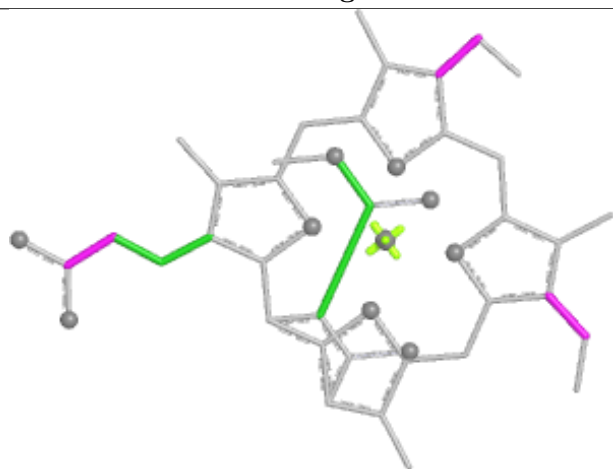
Ligand KC2 T 608



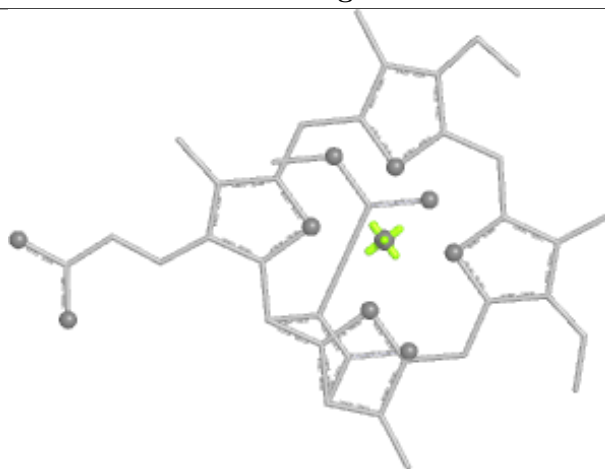
Bond lengths



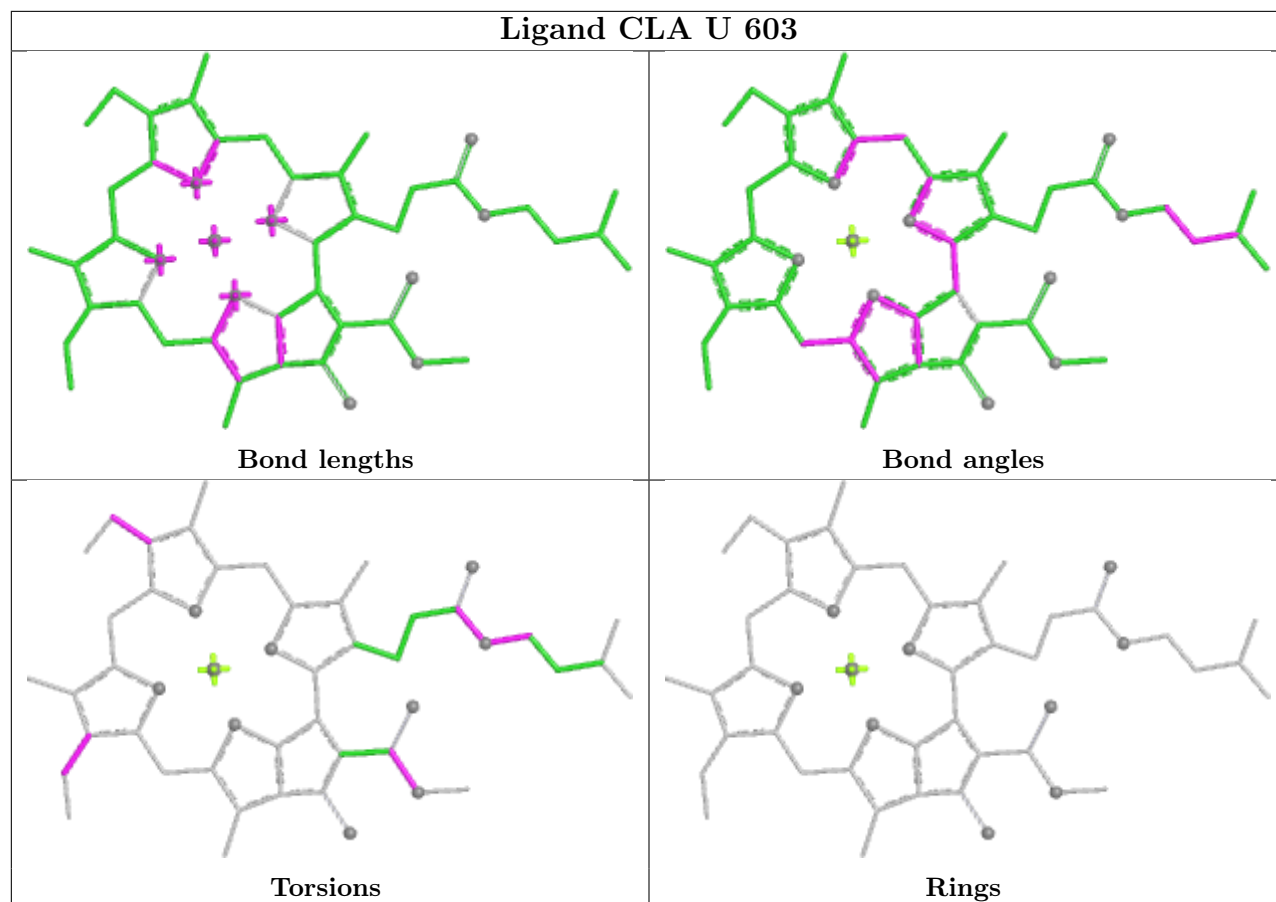
Bond angles



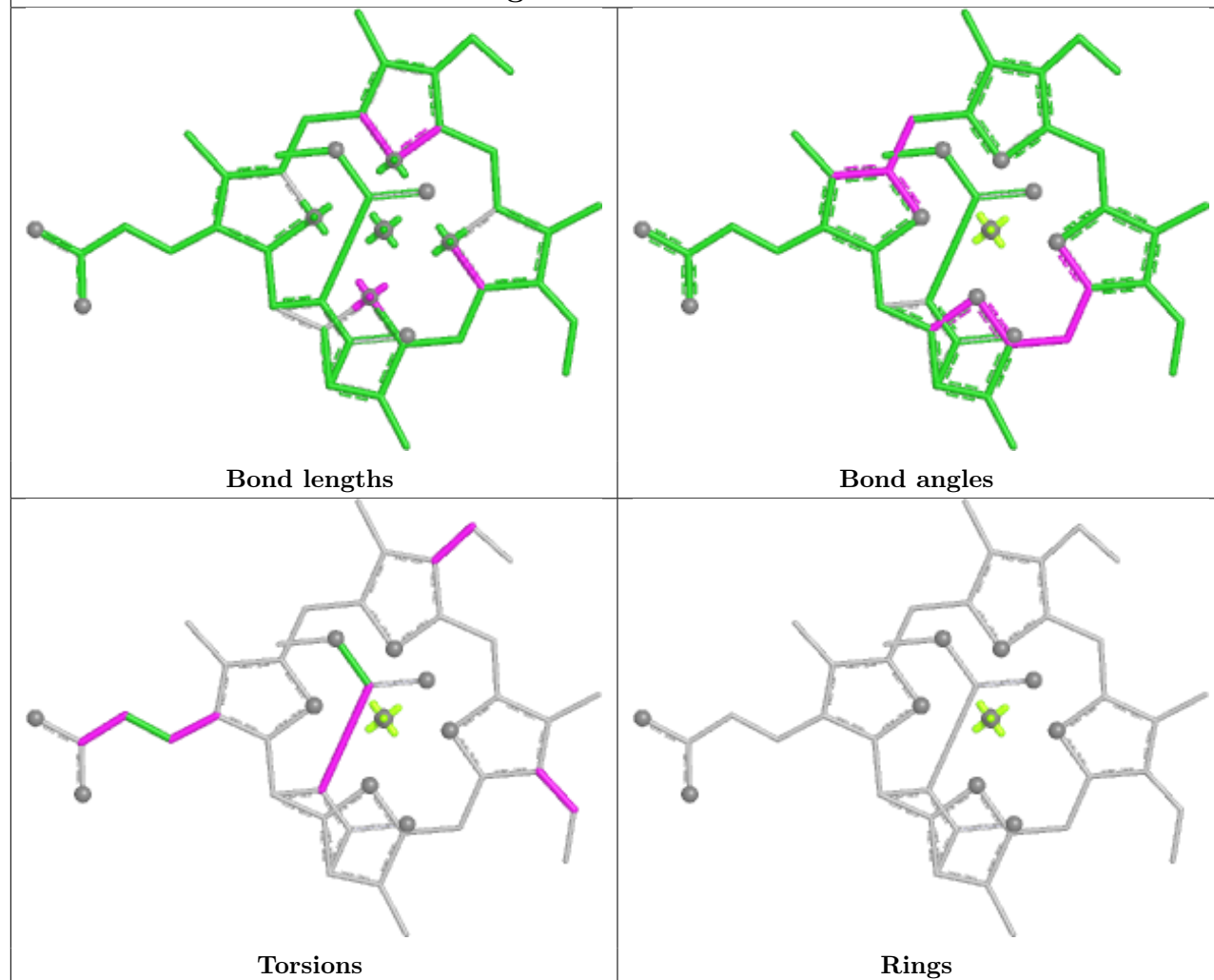
Torsions



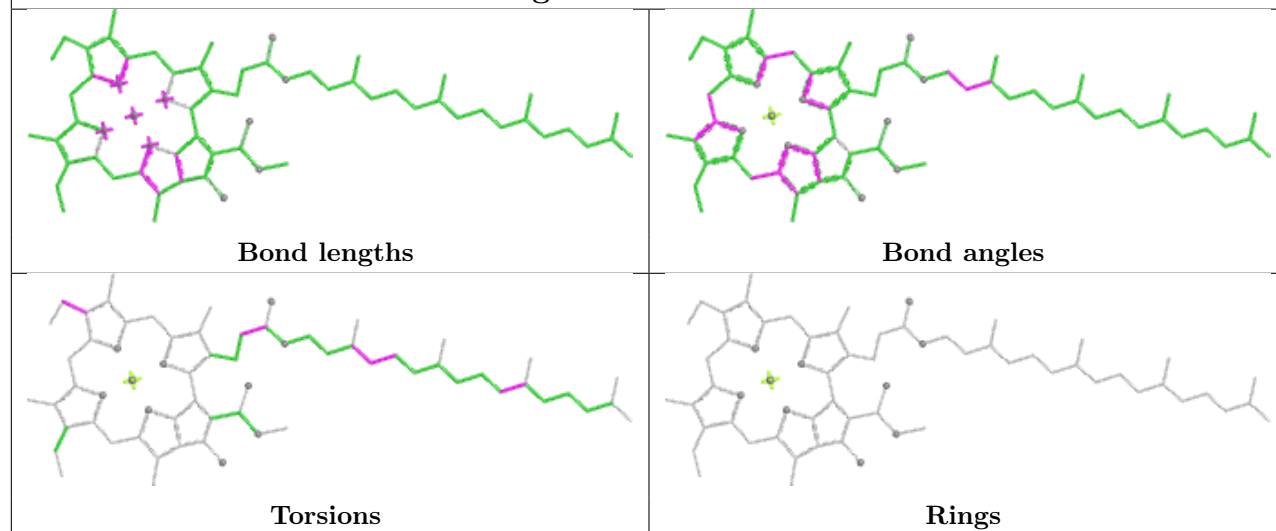
Rings

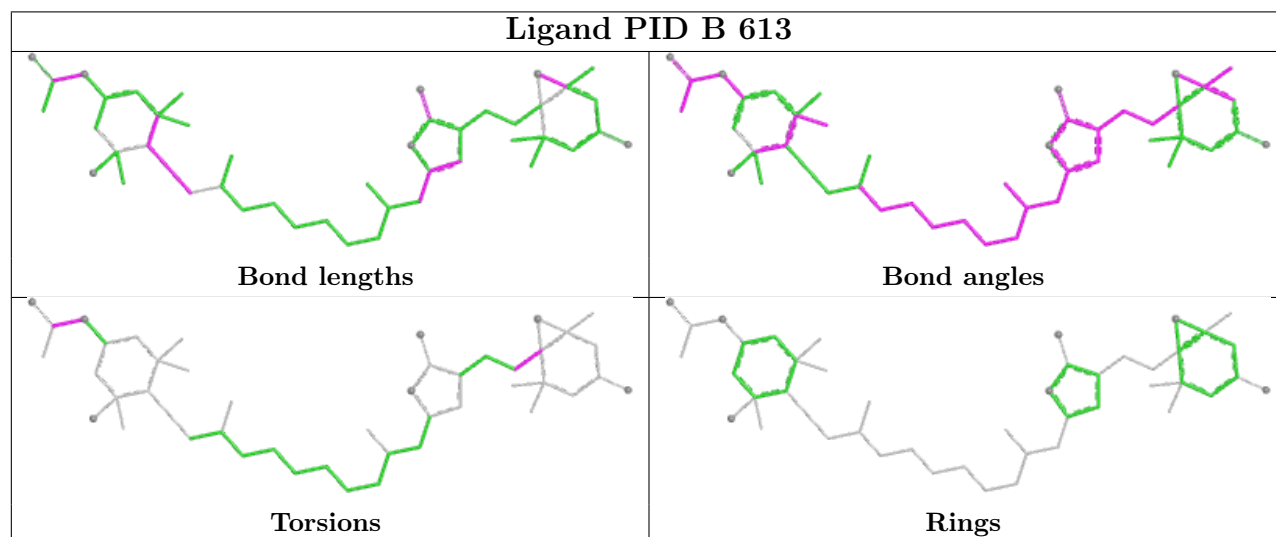
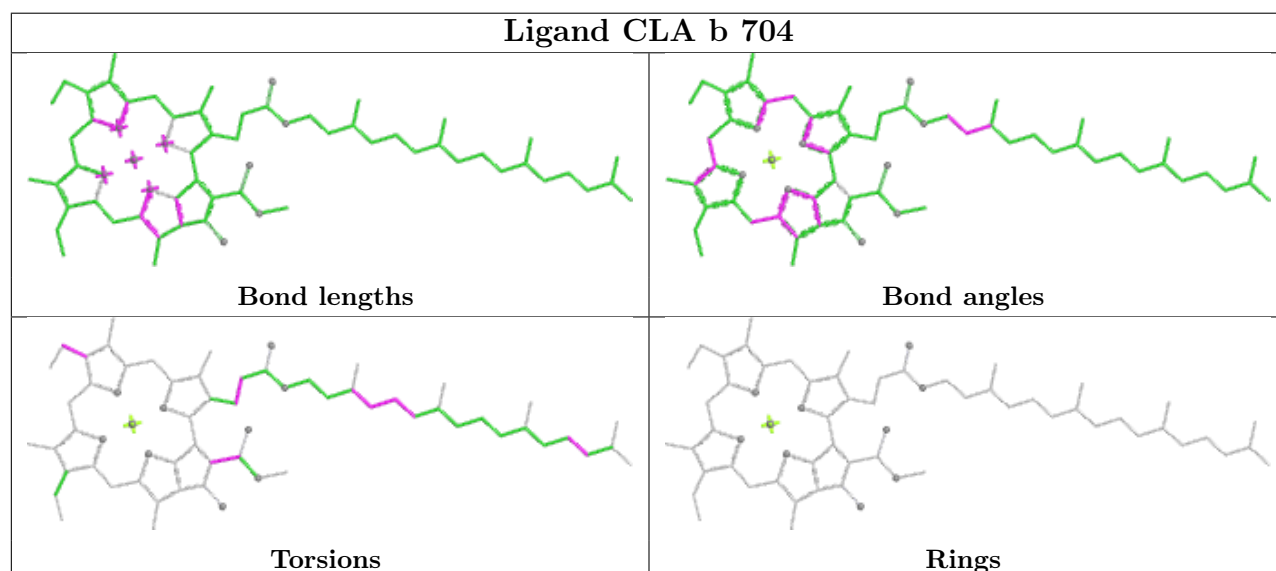
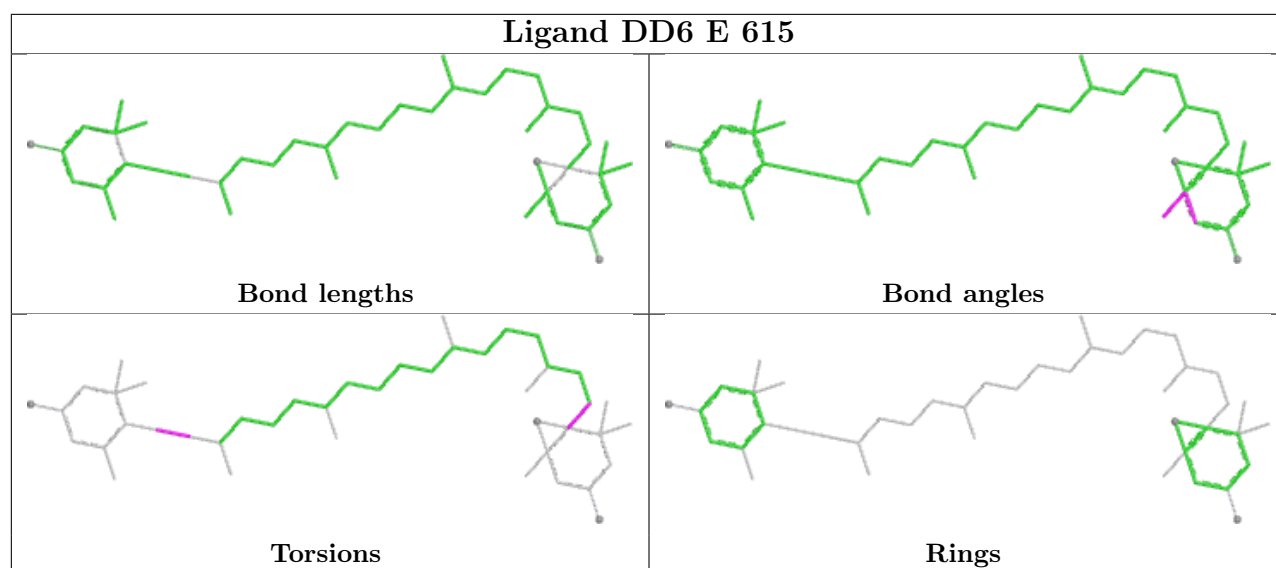


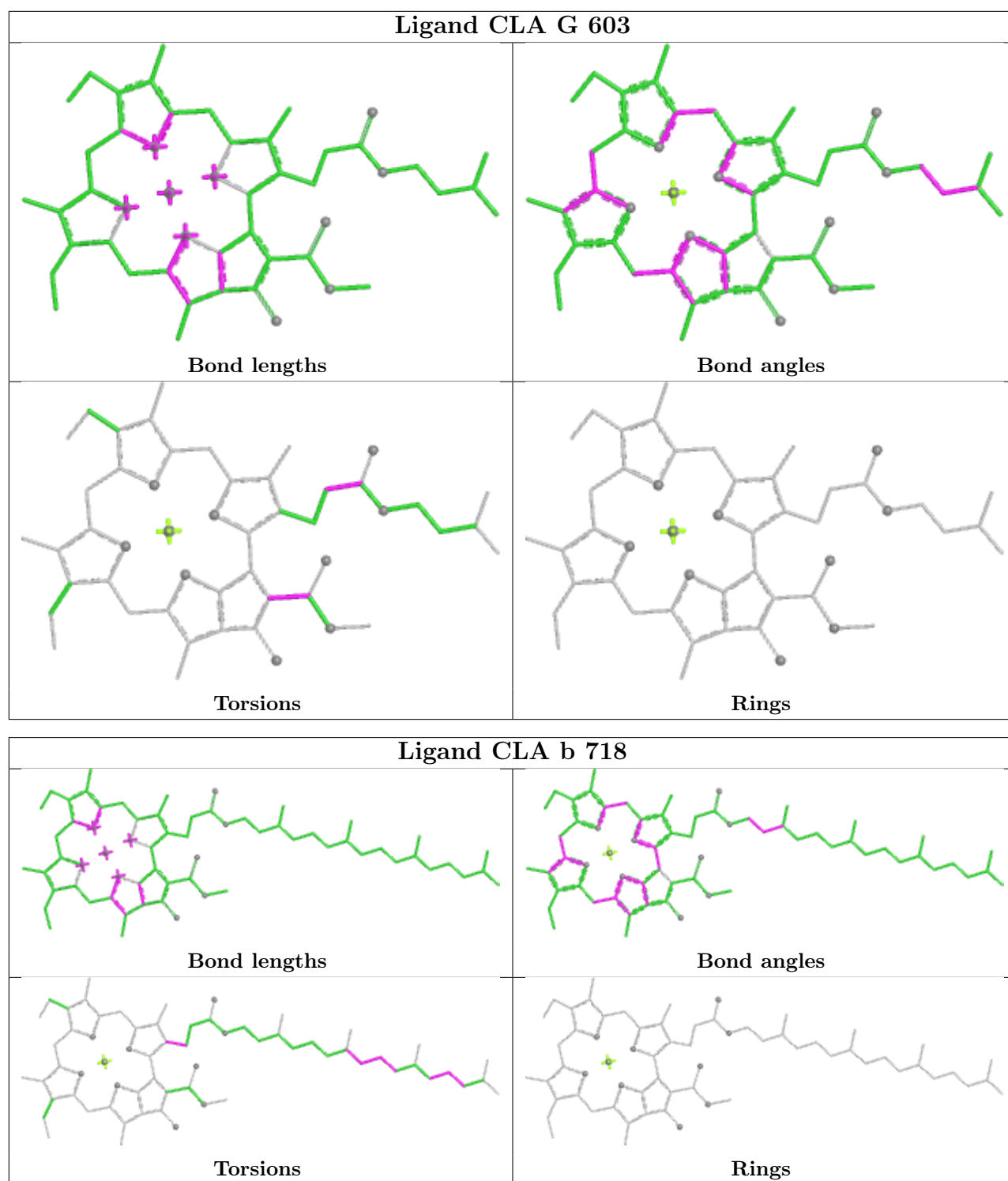
Ligand KC2 G 601

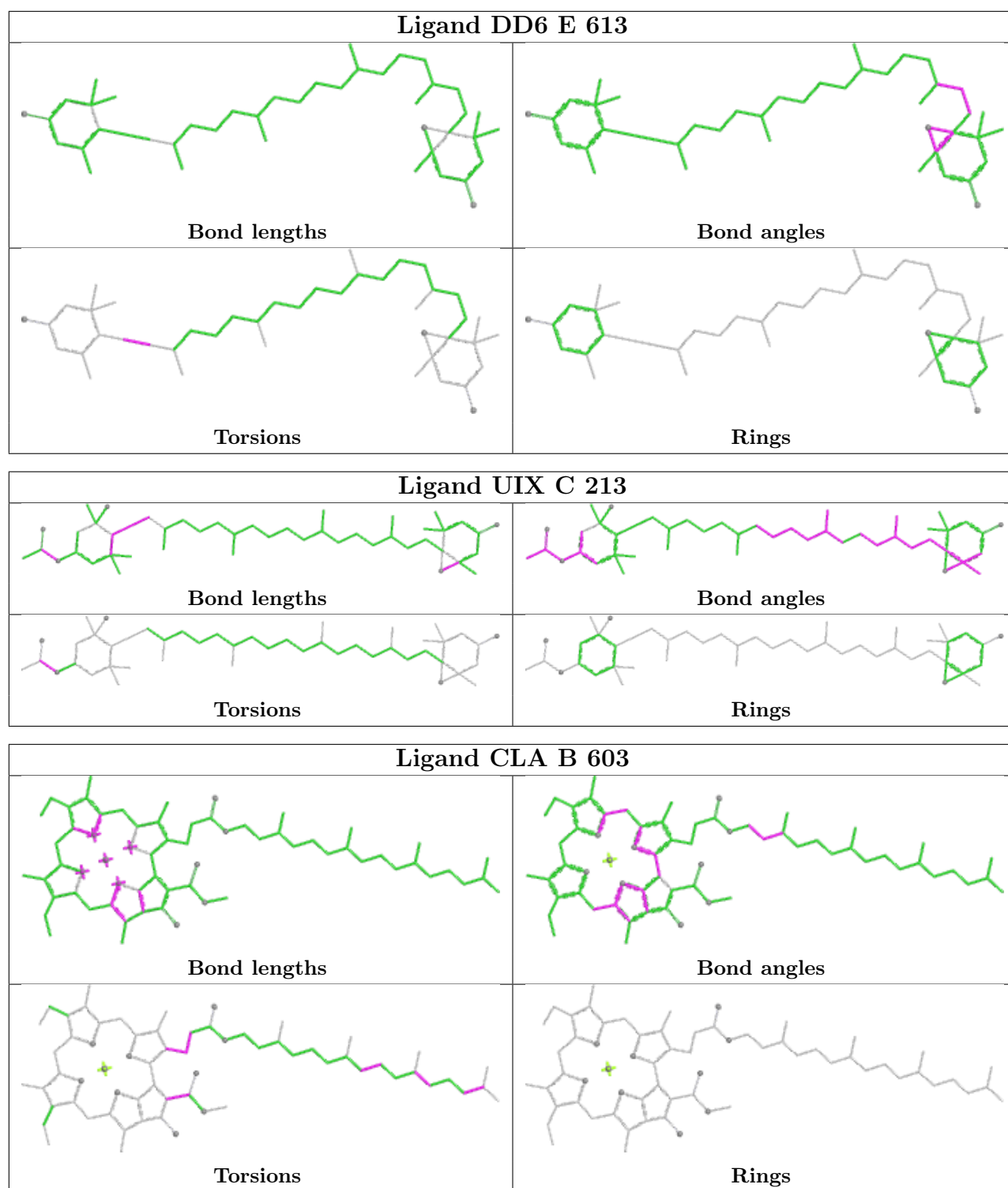


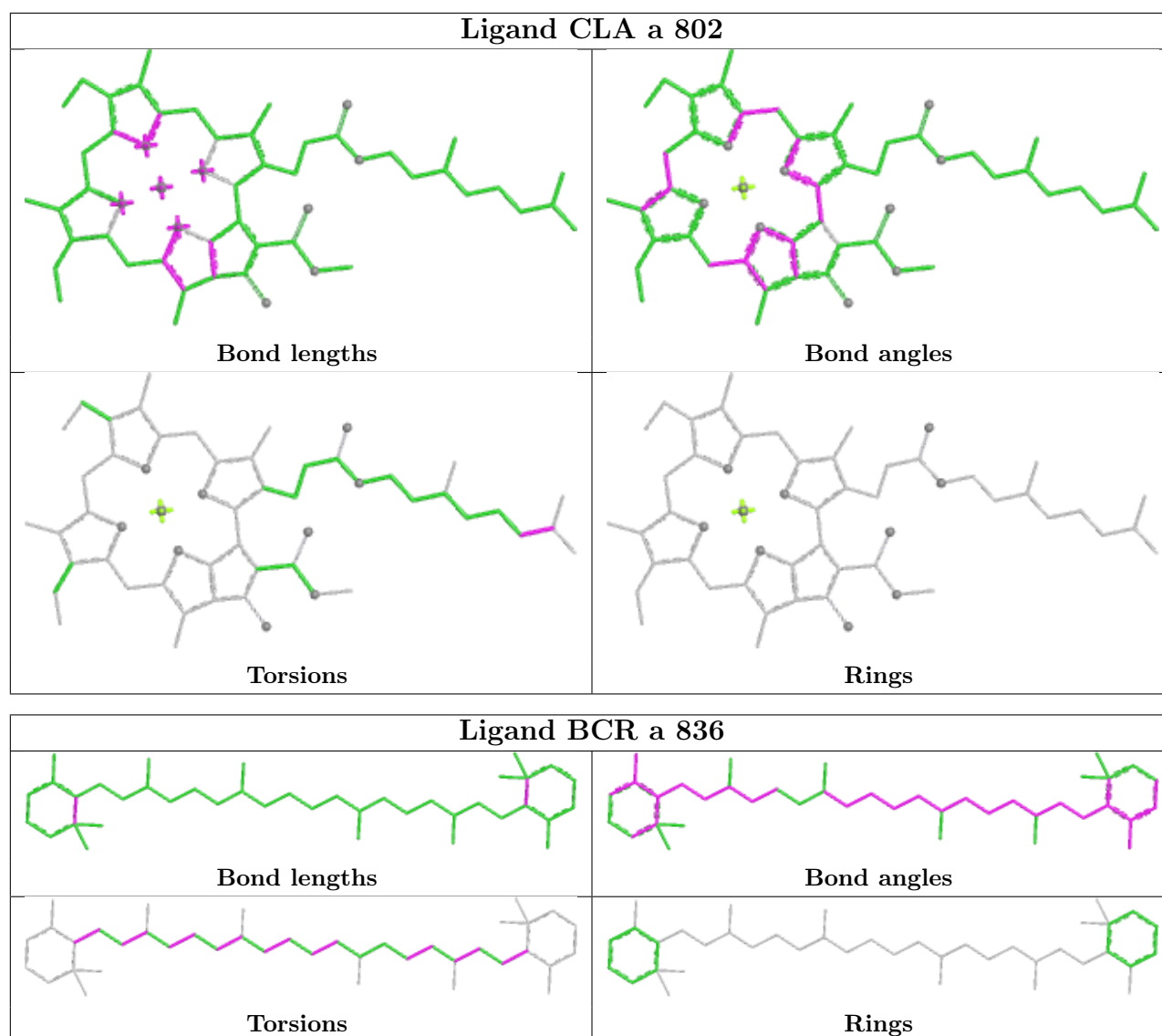
Ligand CLA B 609



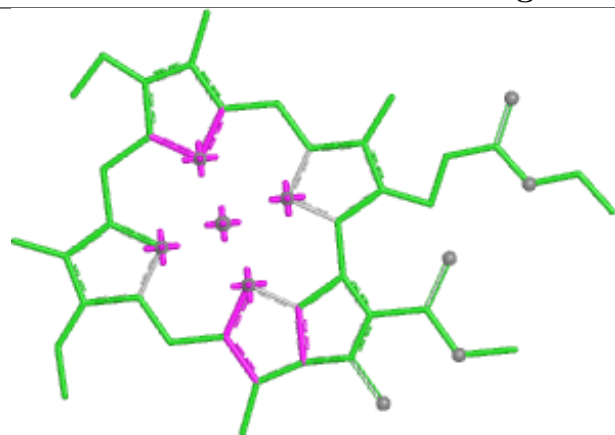




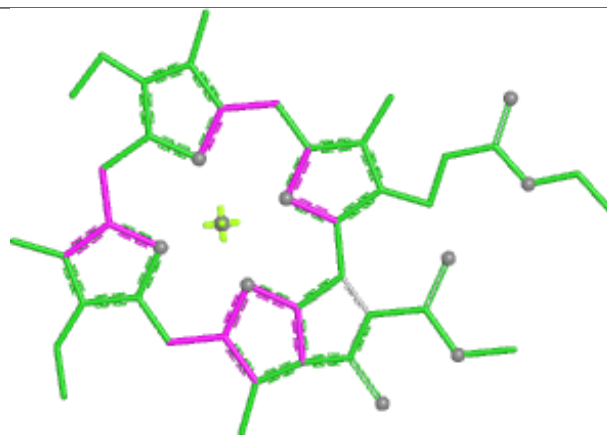




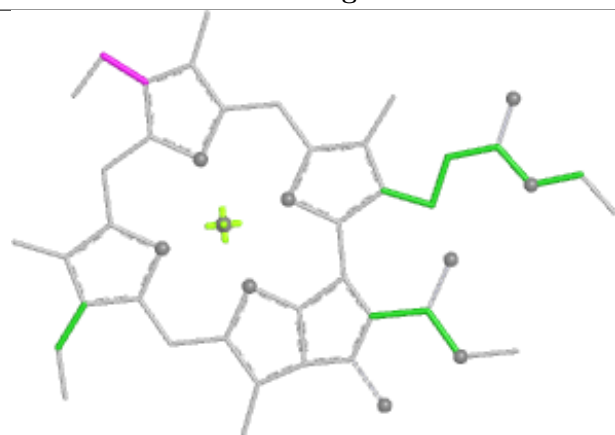
Ligand CLA C 212



Bond lengths



Bond angles

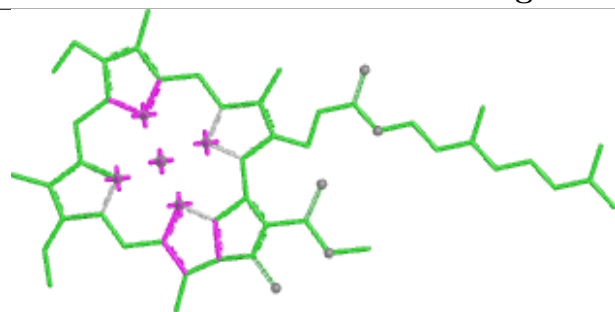


Torsions

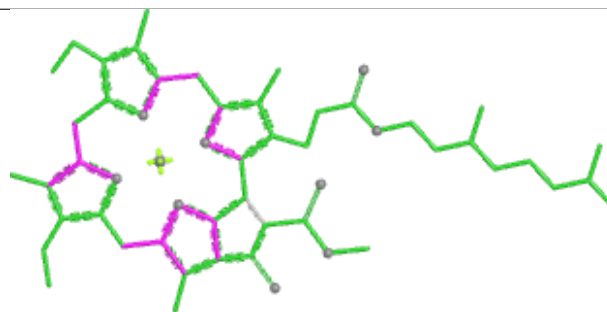


Rings

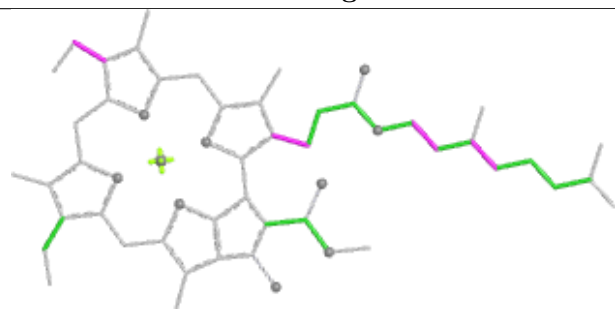
Ligand CLA D 612



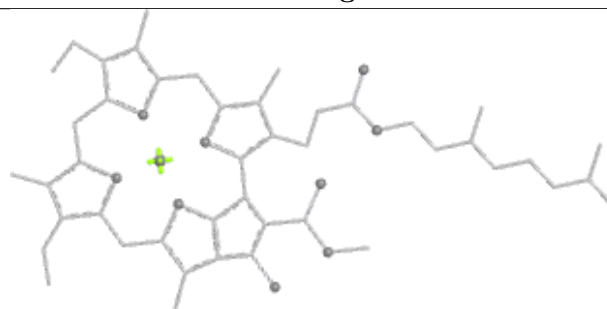
Bond lengths



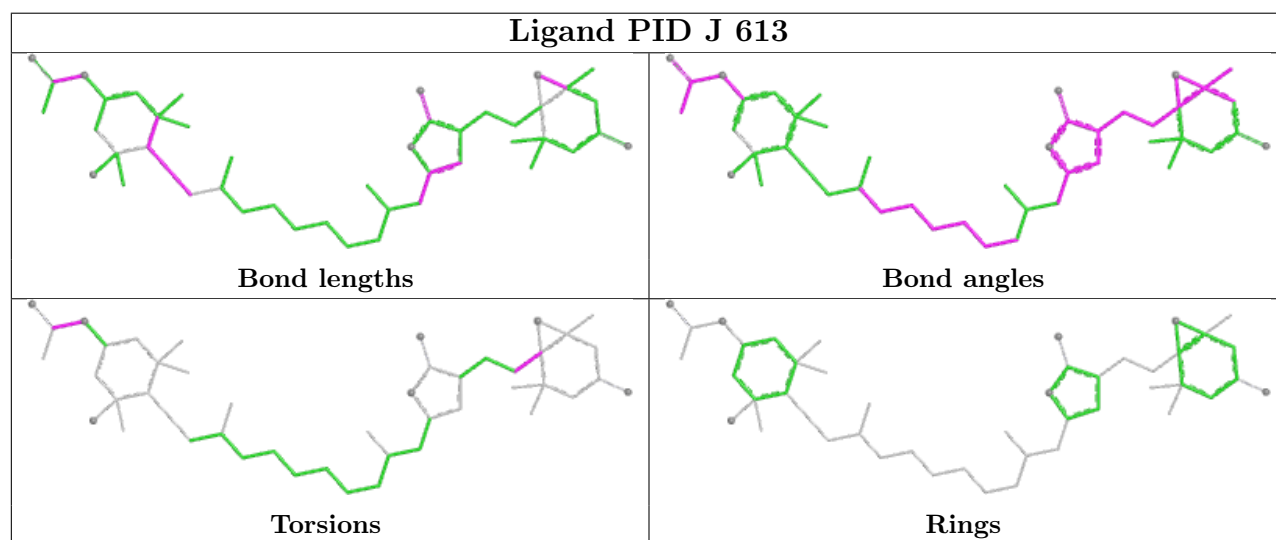
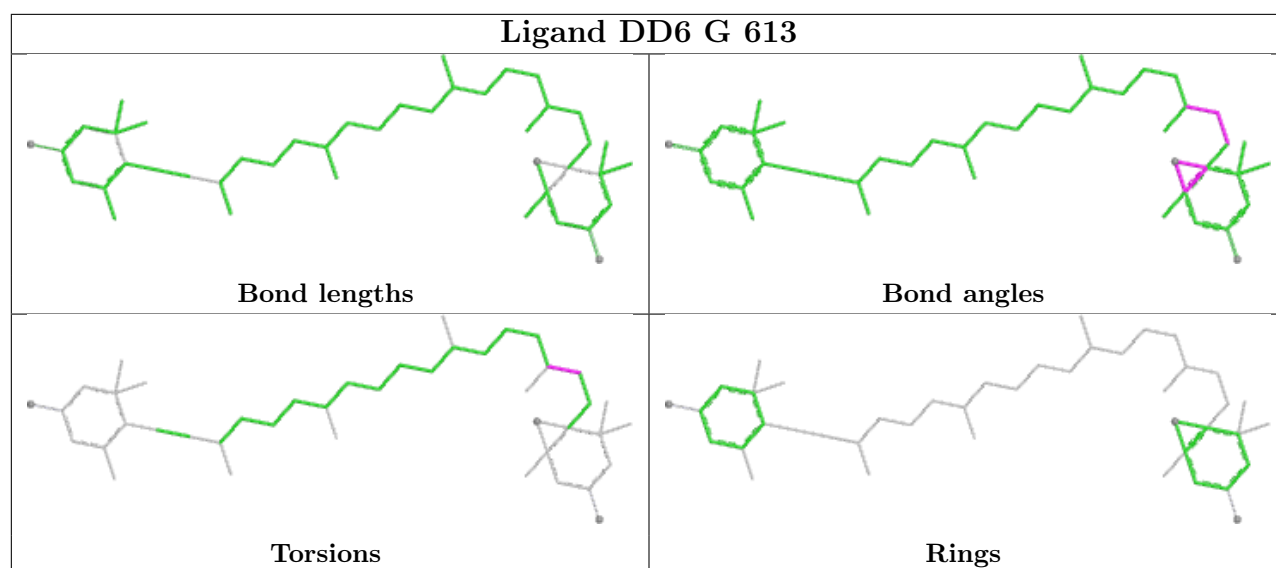
Bond angles

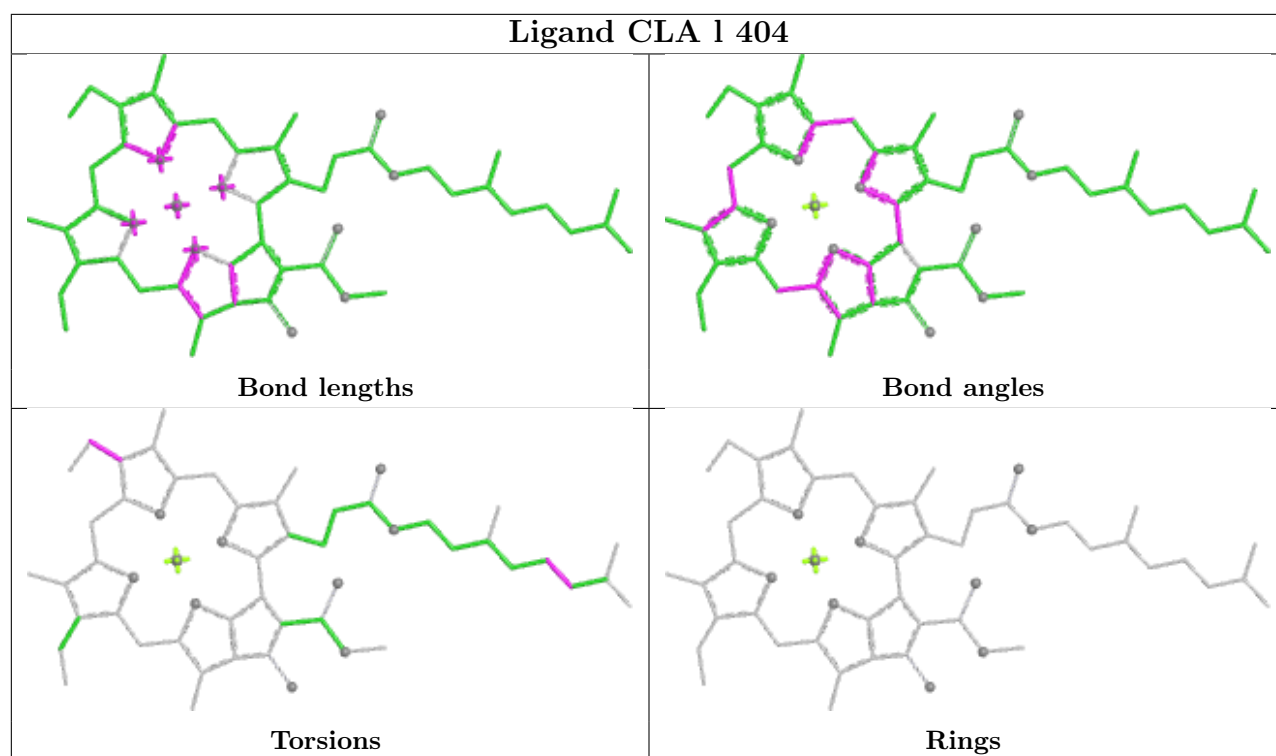


Torsions

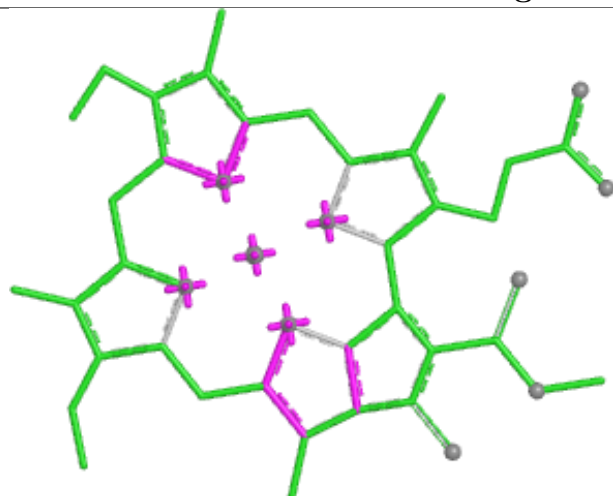


Rings

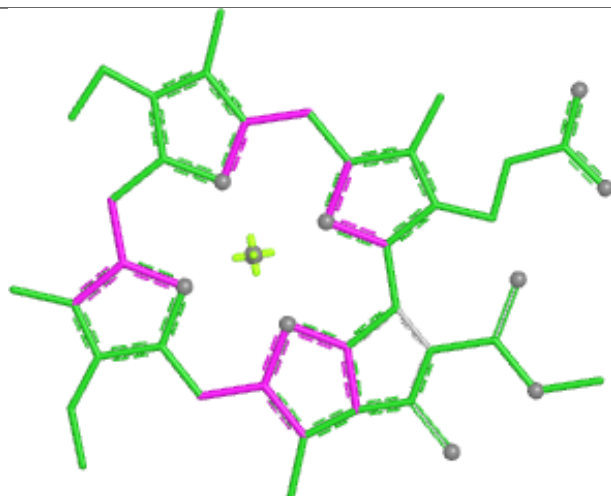




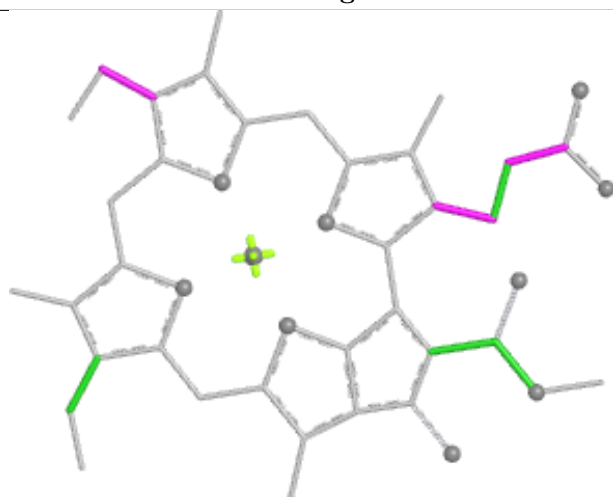
Ligand CLA T 607



Bond lengths



Bond angles

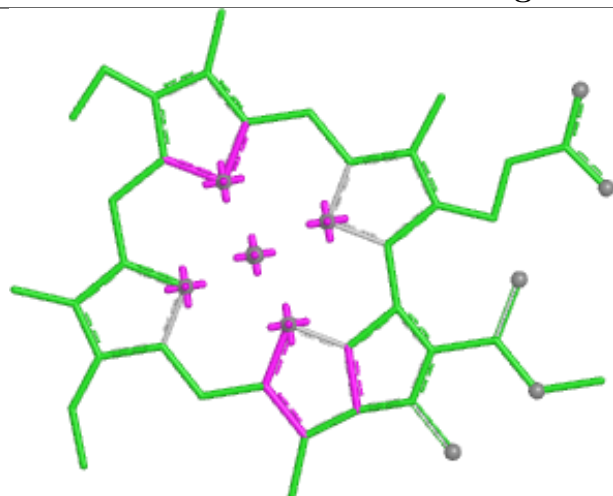


Torsions

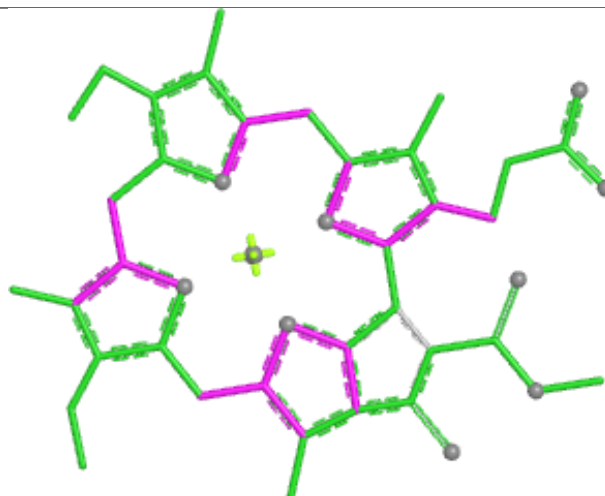


Rings

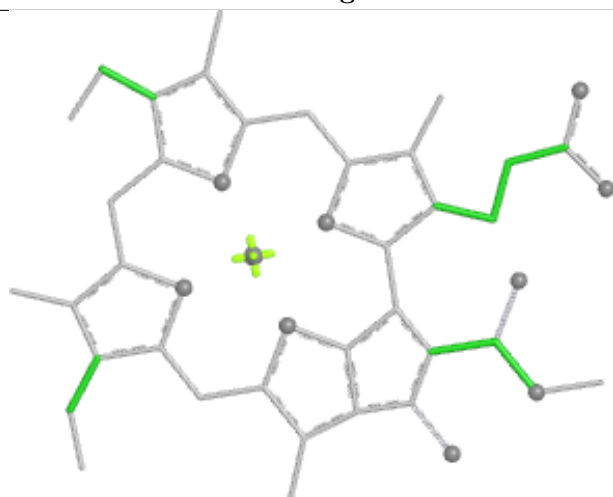
Ligand CLA C 209



Bond lengths



Bond angles

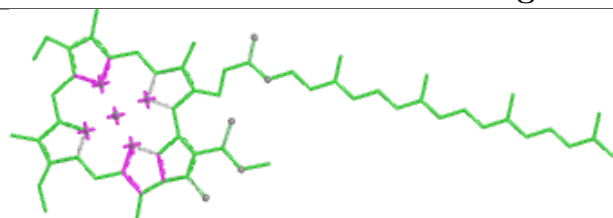


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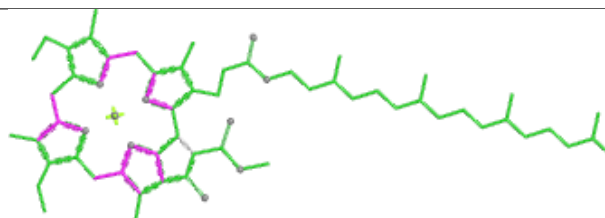


Rings

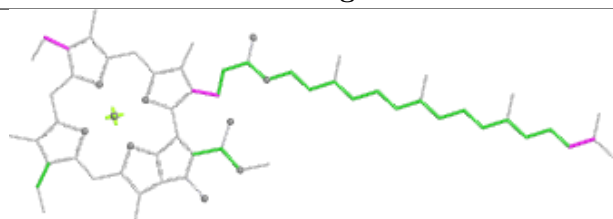
Ligand CLA b 707



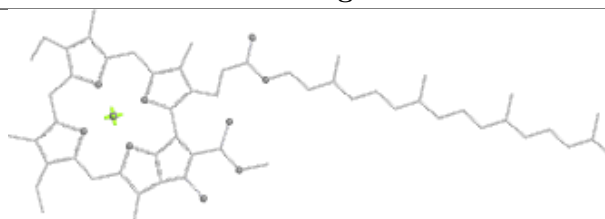
Bond lengths



Bond angles

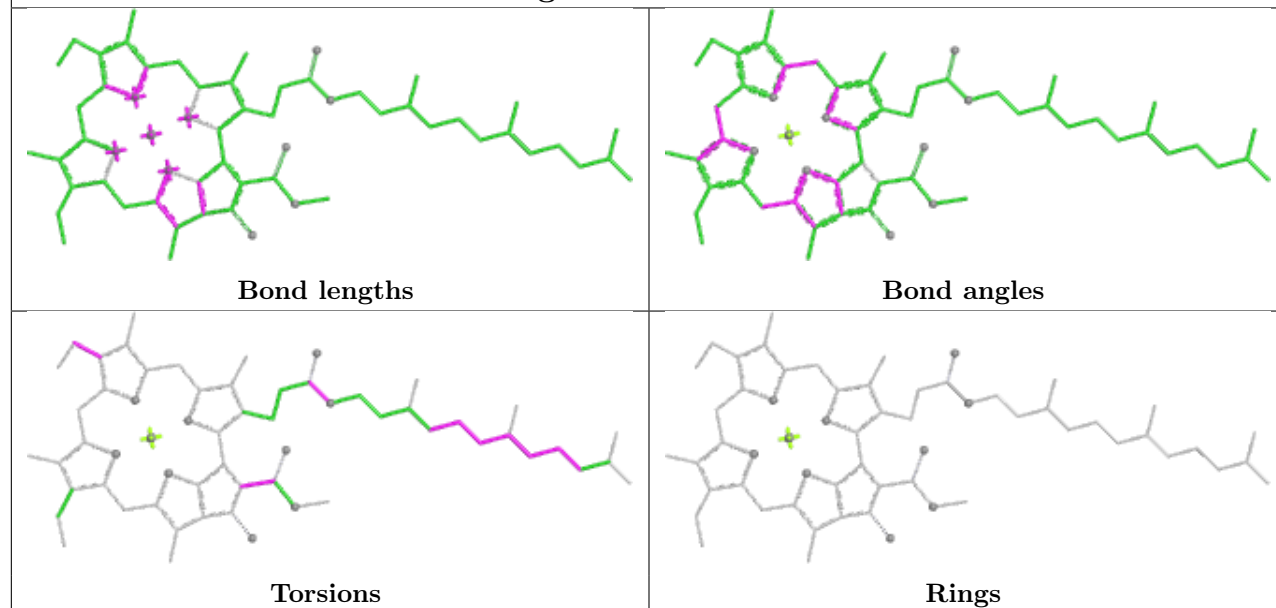


Torsions

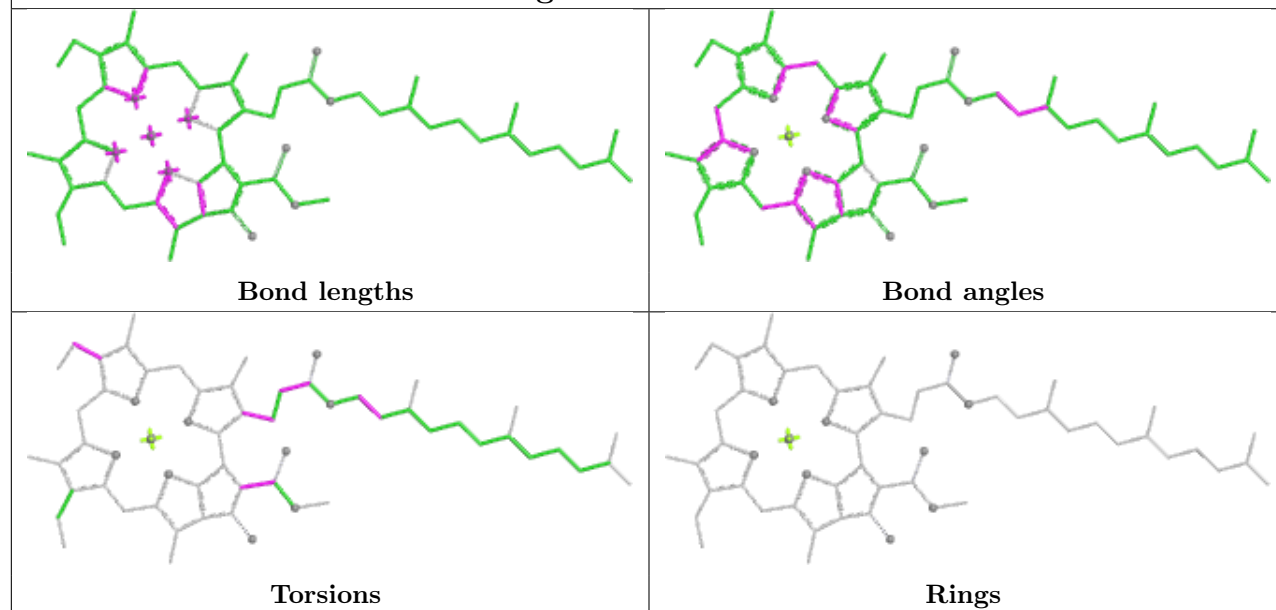


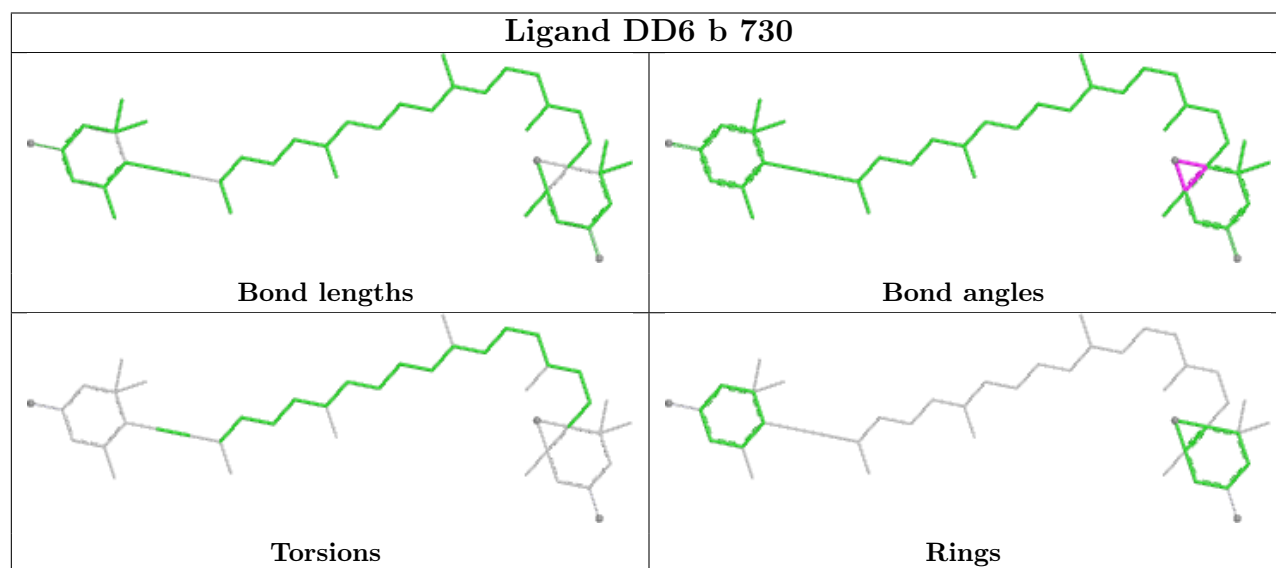
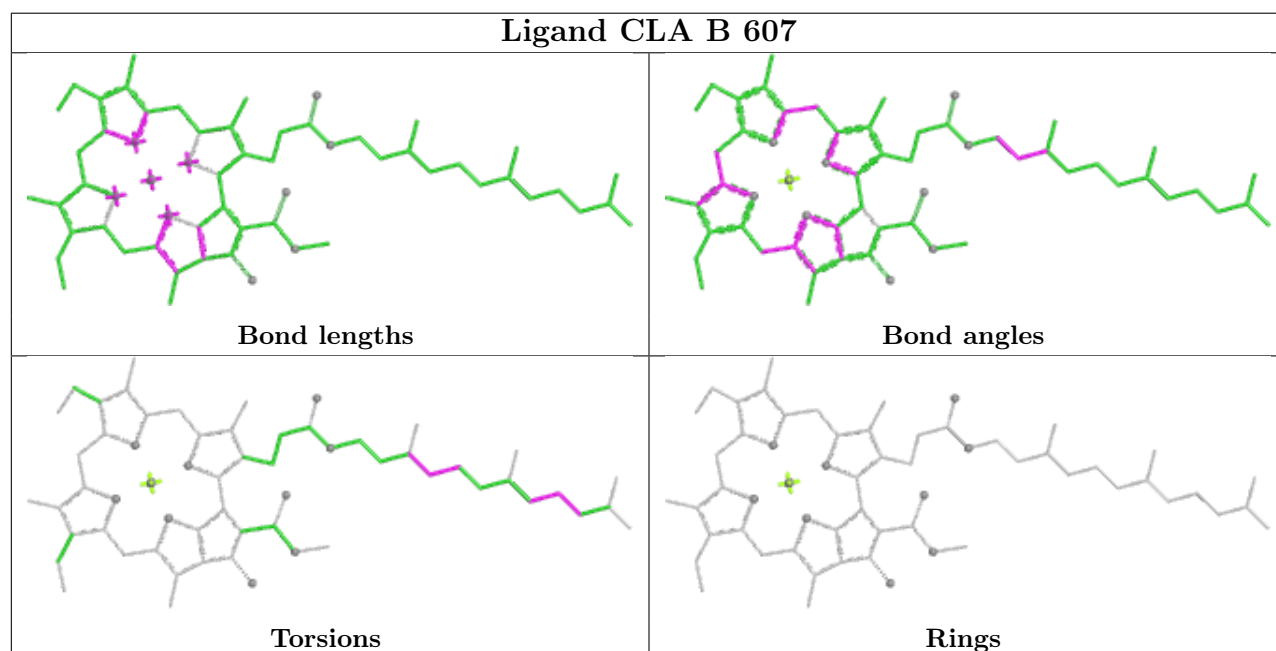
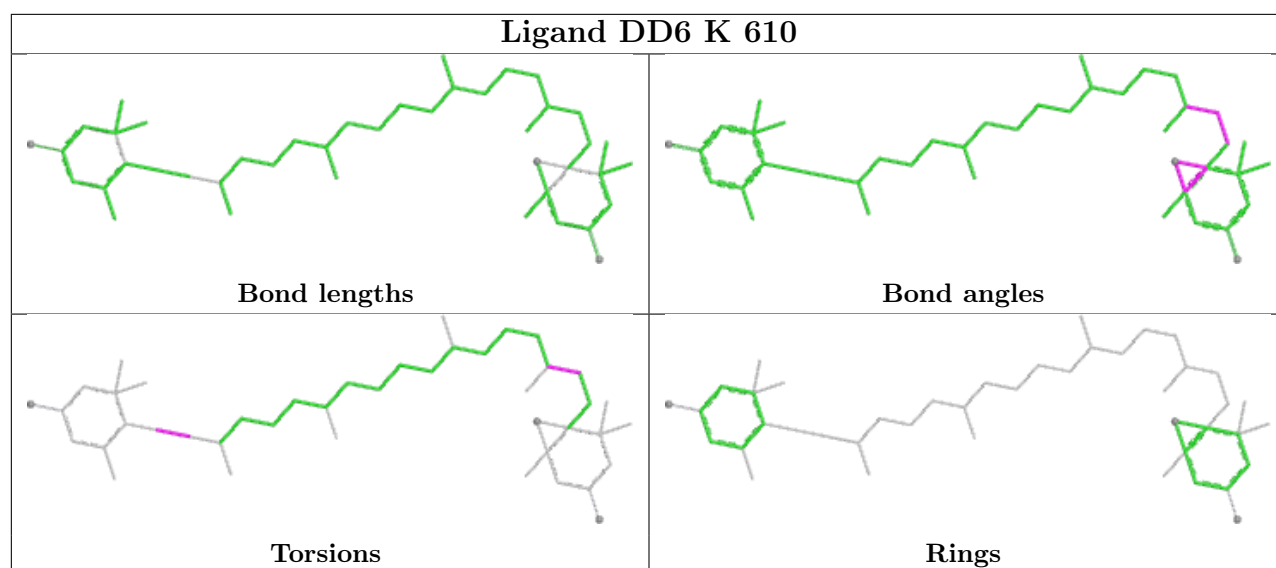
Rings

Ligand CLA r 204

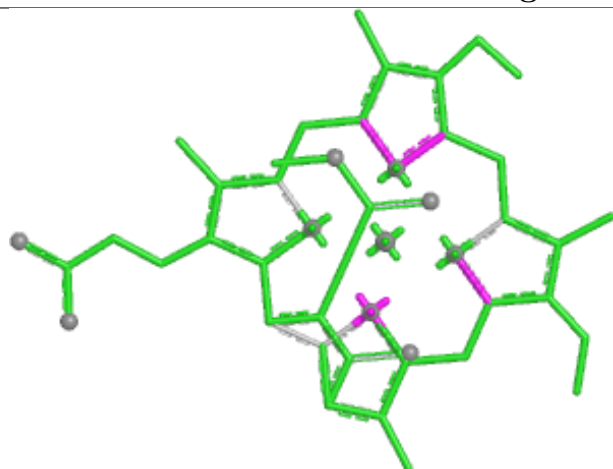


Ligand CLA a 822

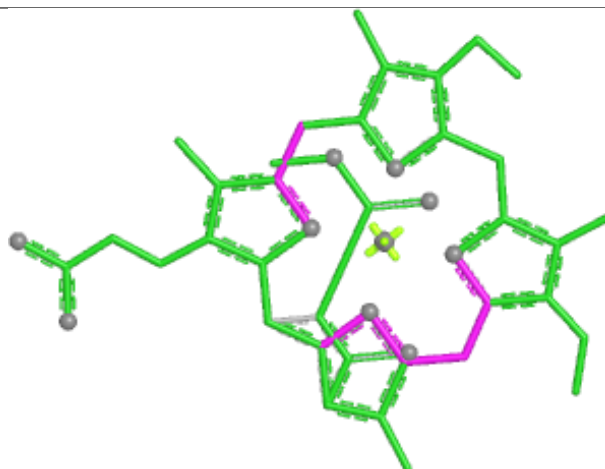




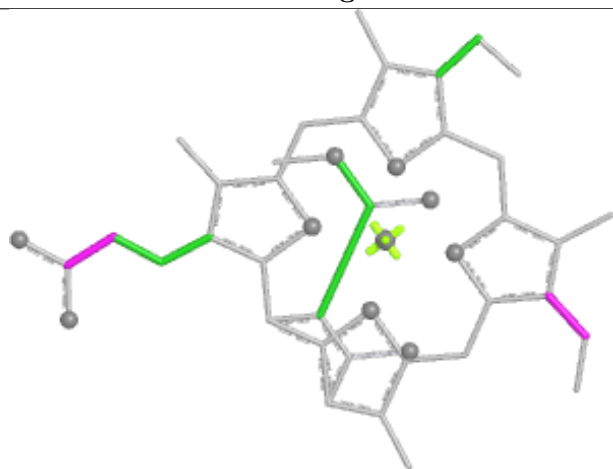
Ligand KC2 J 608



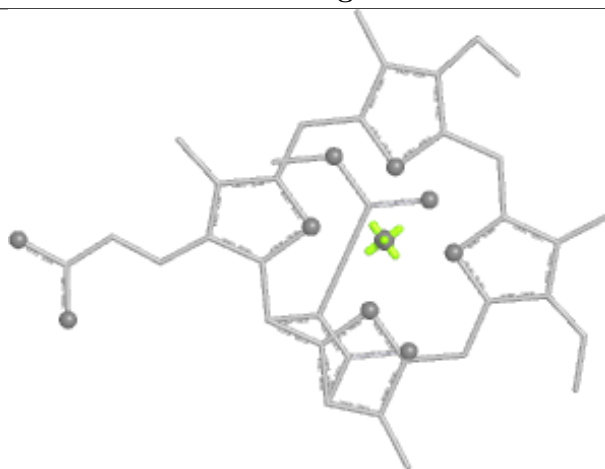
Bond lengths



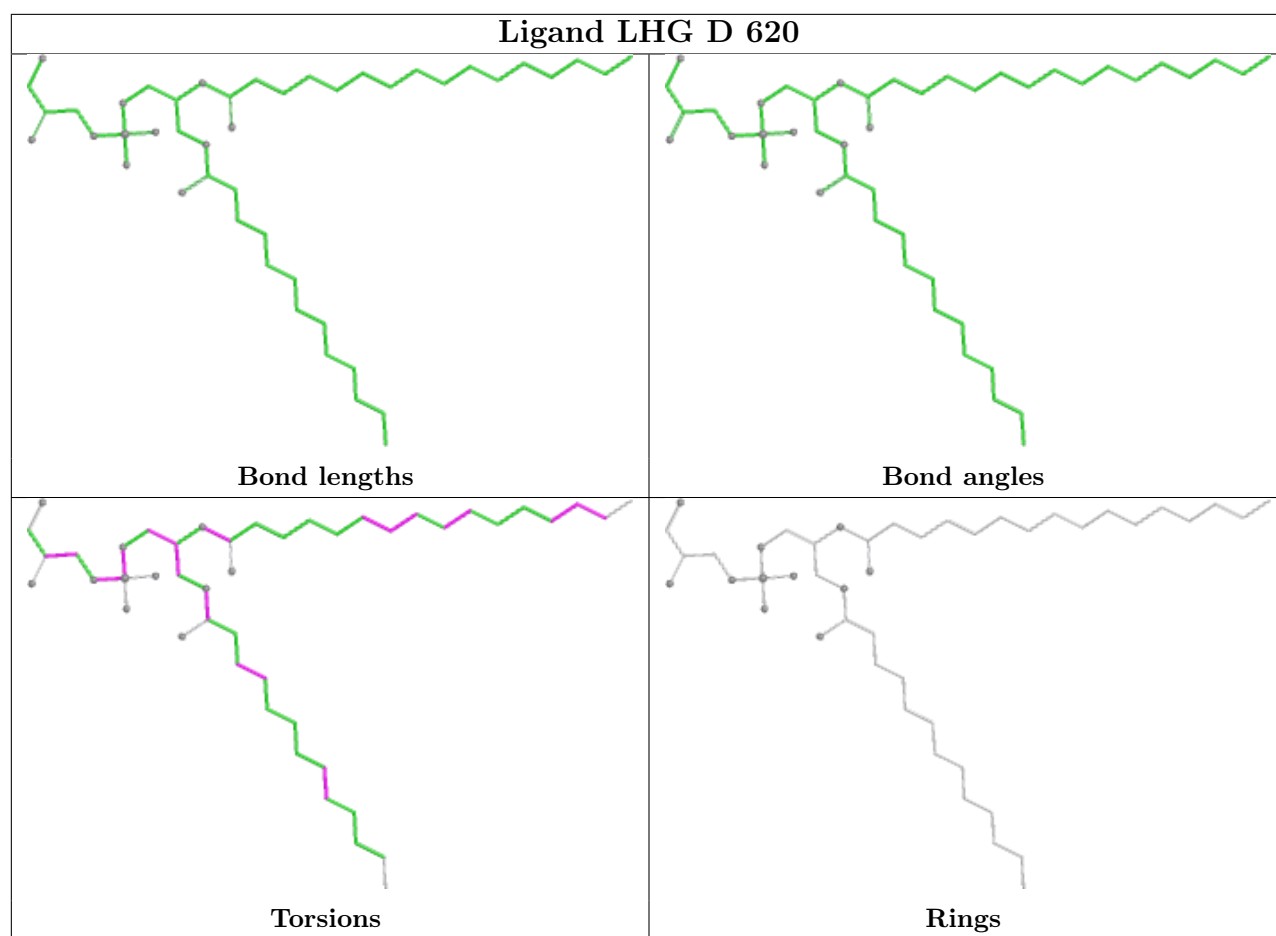
Bond angles



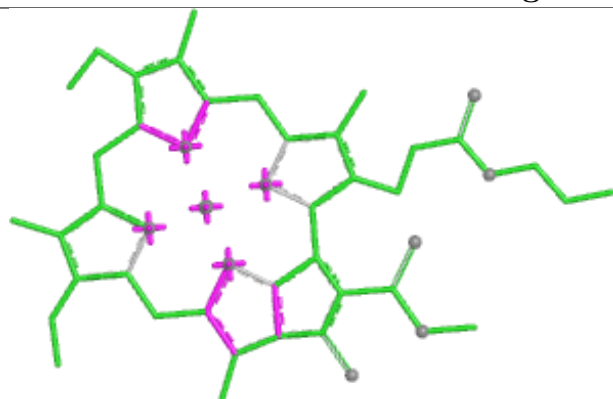
Torsions



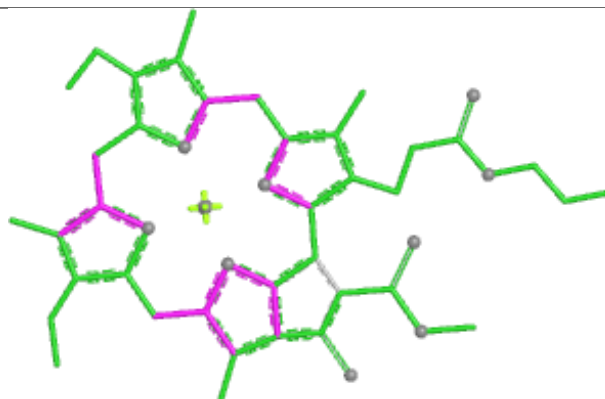
Rings



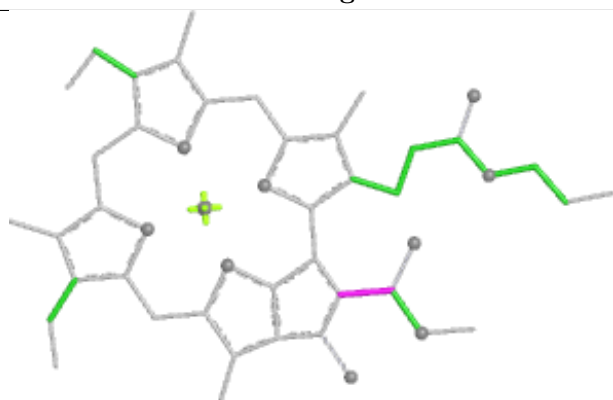
Ligand CLA 1 411



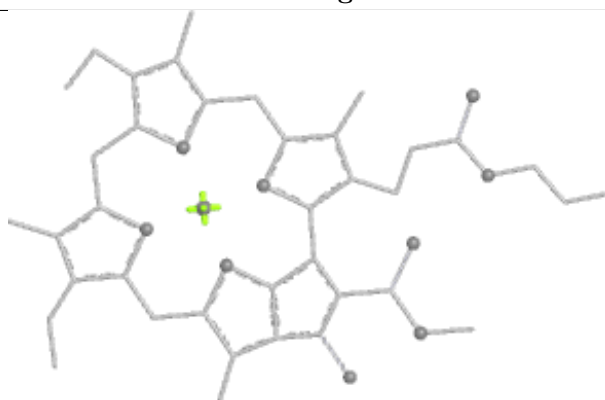
Bond lengths



Bond angles

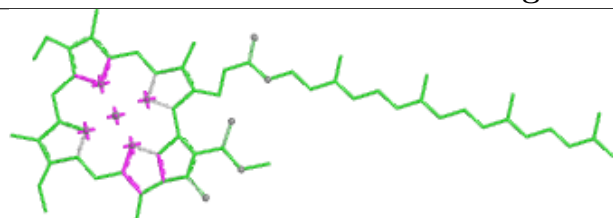


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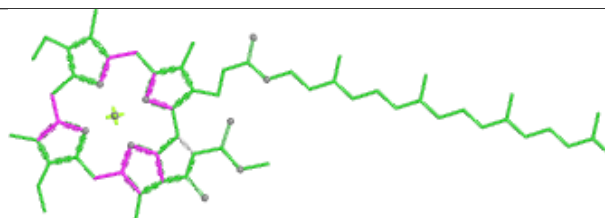


Rings

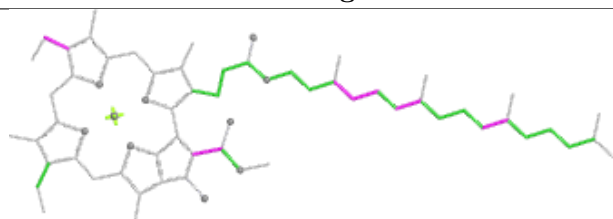
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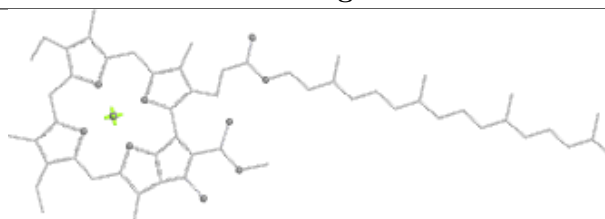
Bond lengths



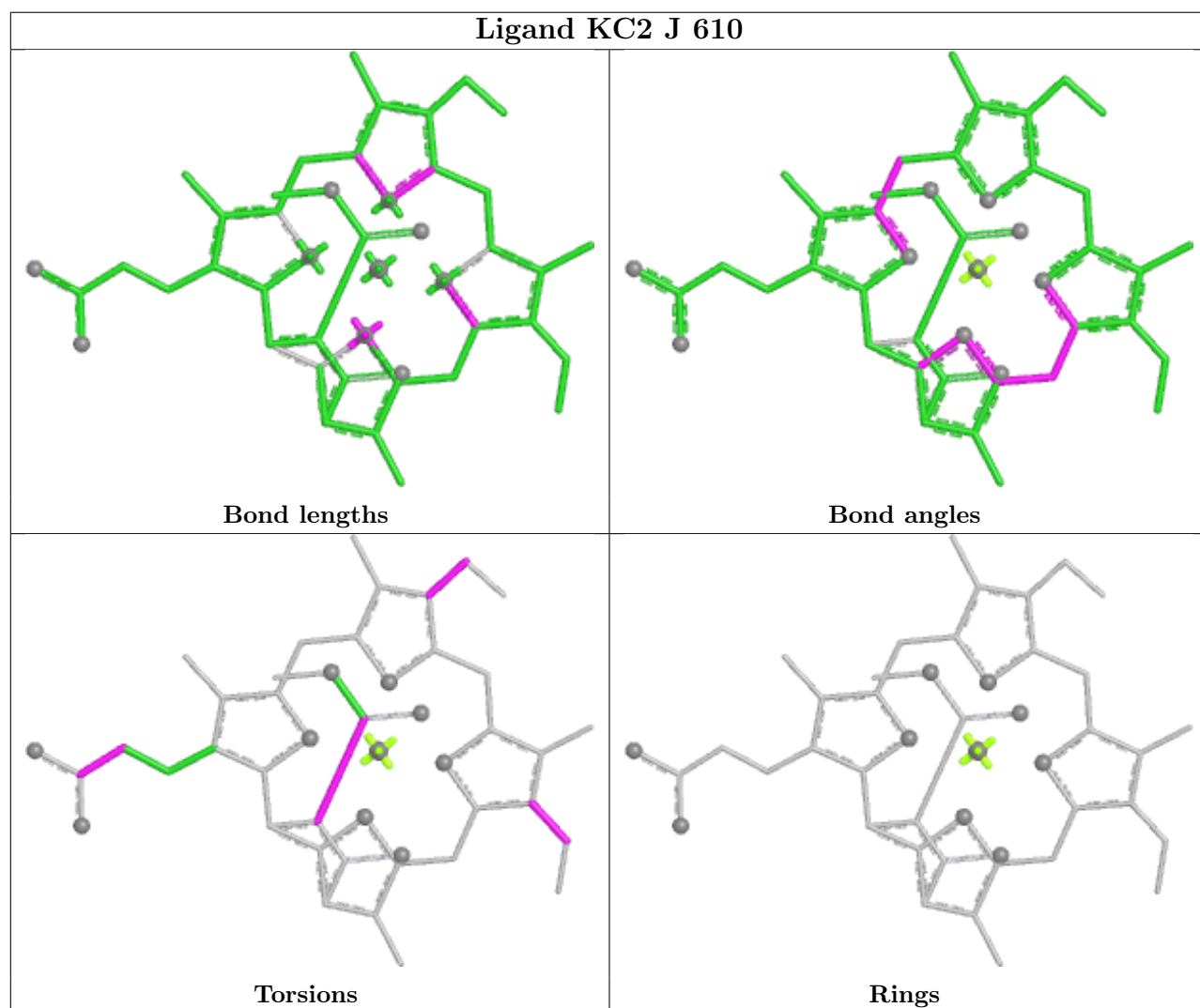
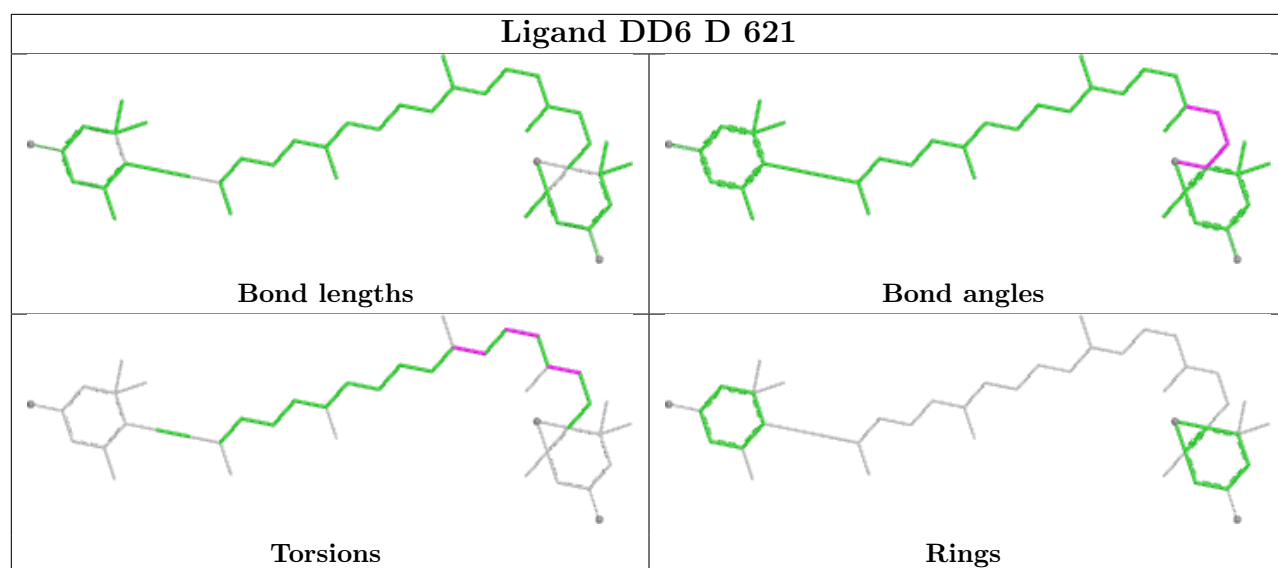
Bond angles

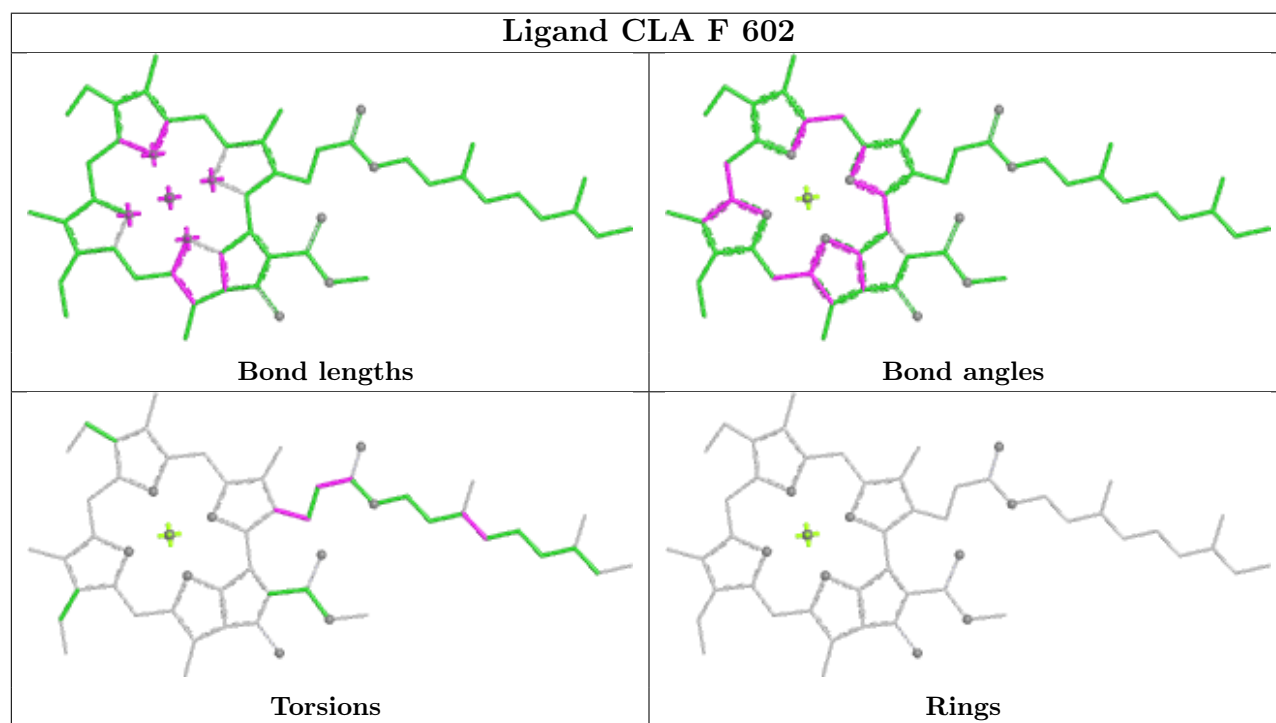
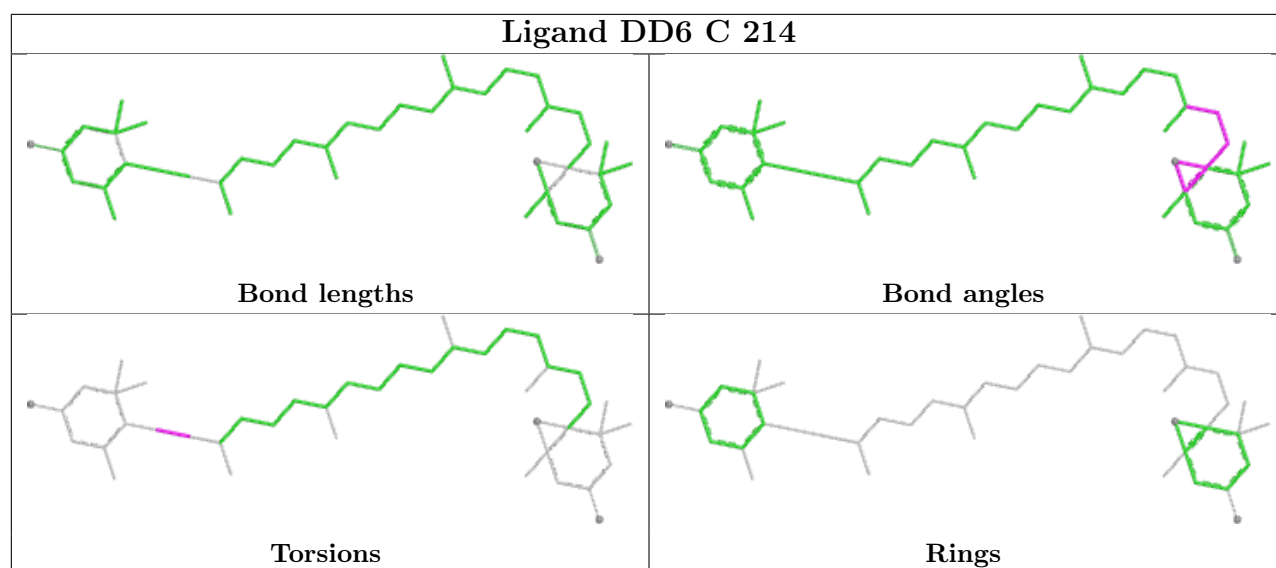


Torsions

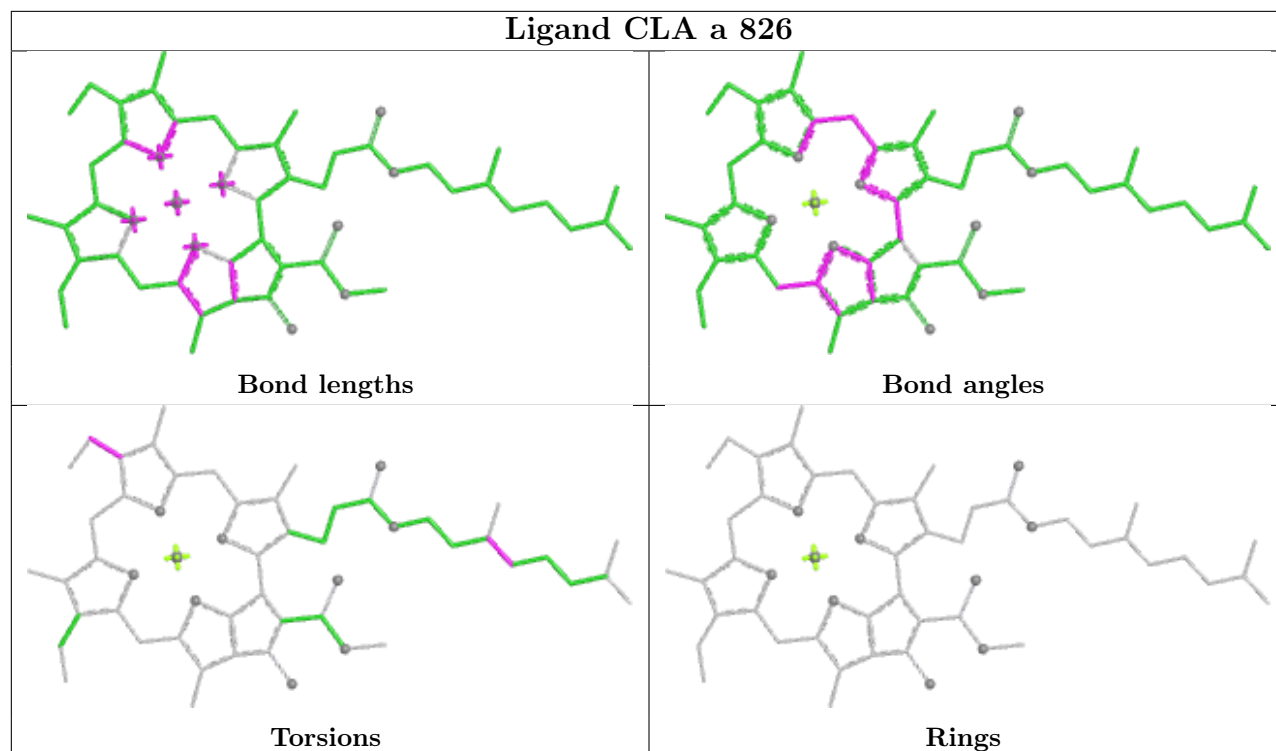


Rings

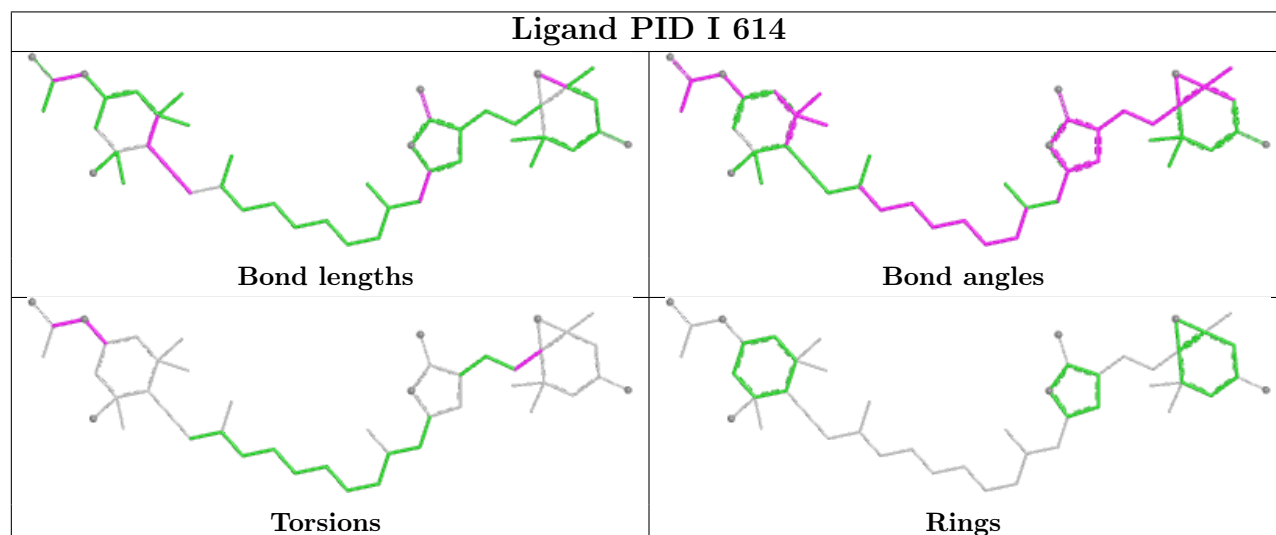




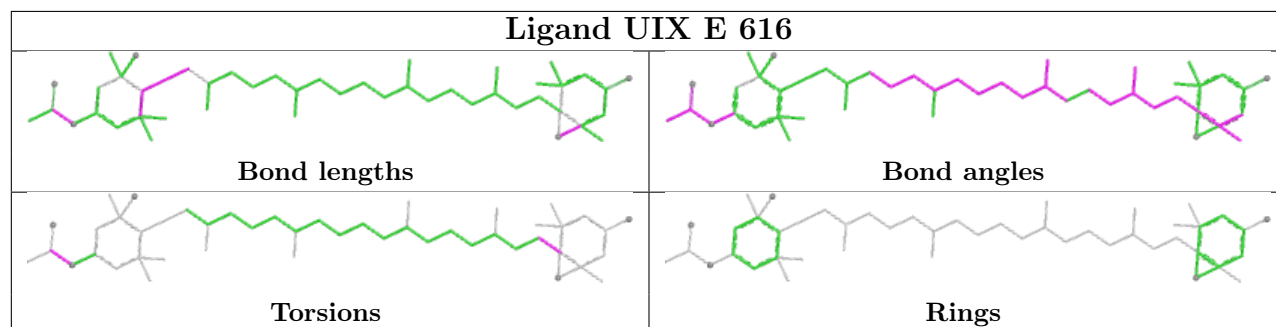
Ligand CLA a 826

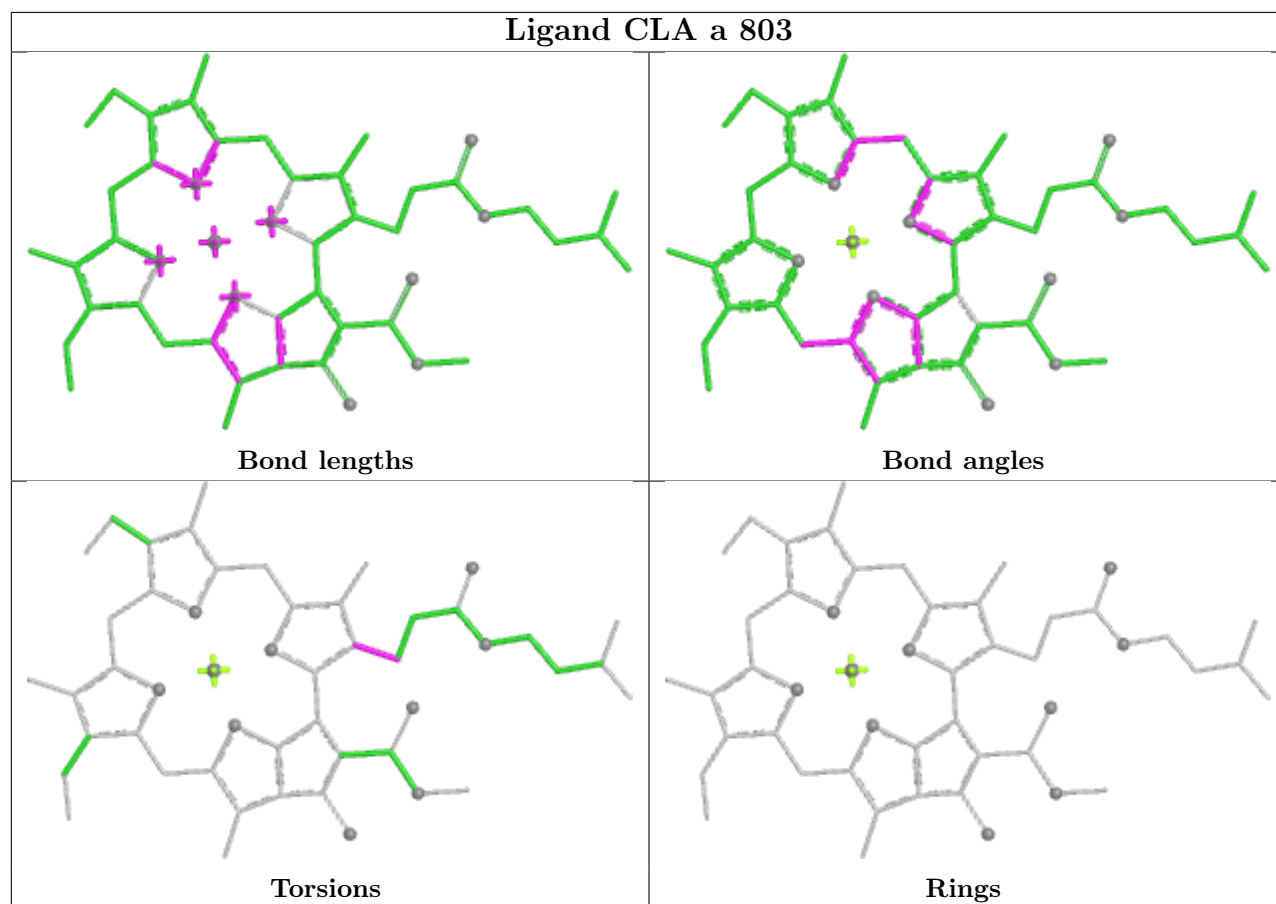
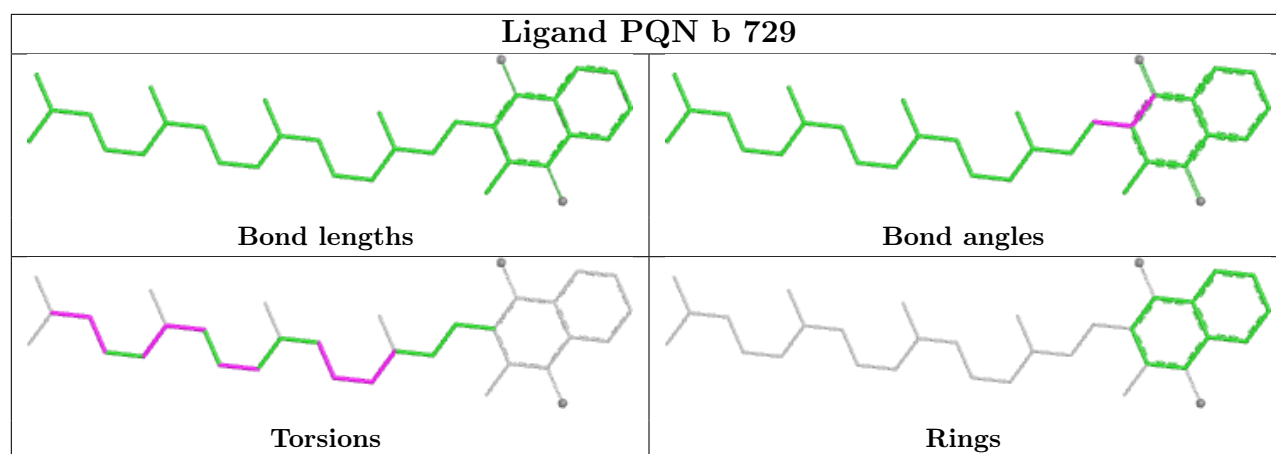


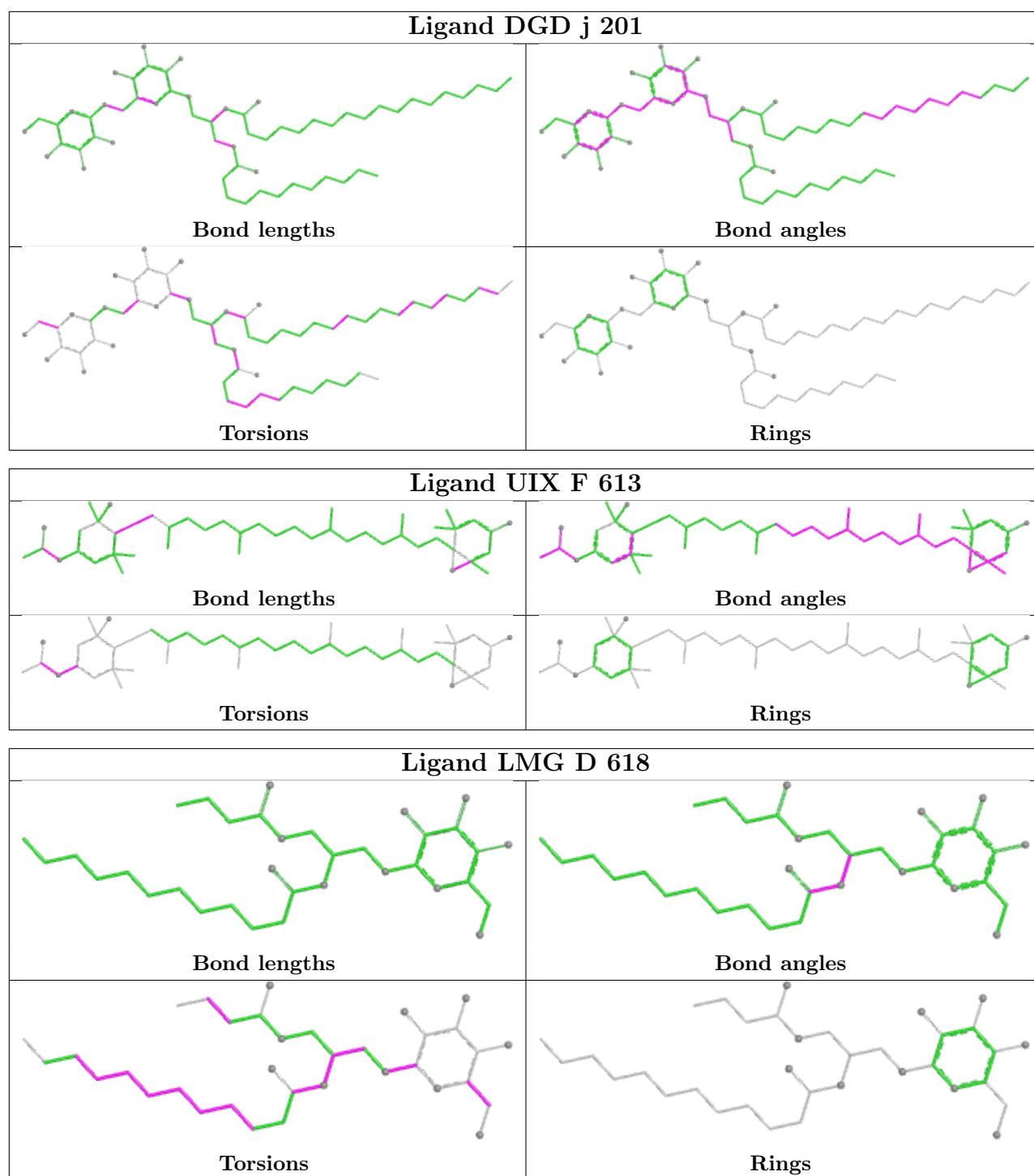
Ligand PID I 614



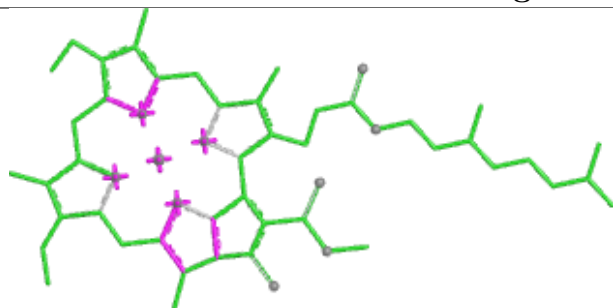
Ligand UIX E 616



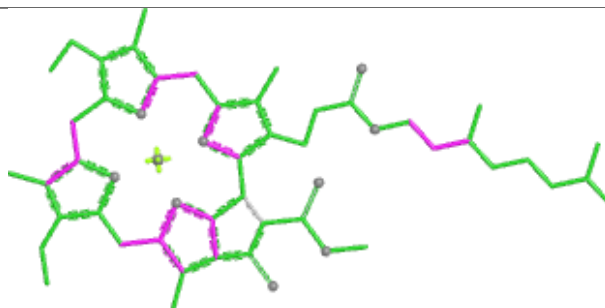




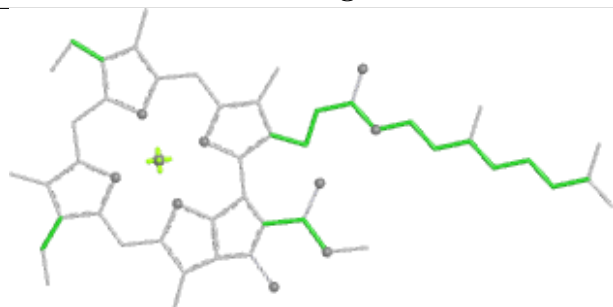
Ligand CLA D 608



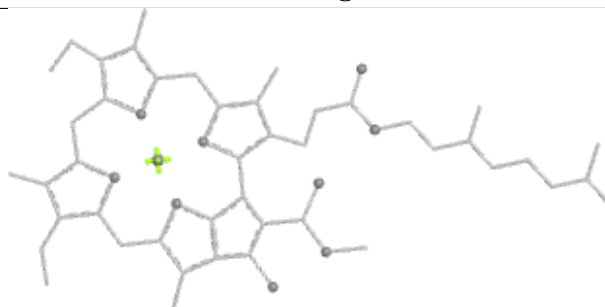
Bond lengths



Bond angles

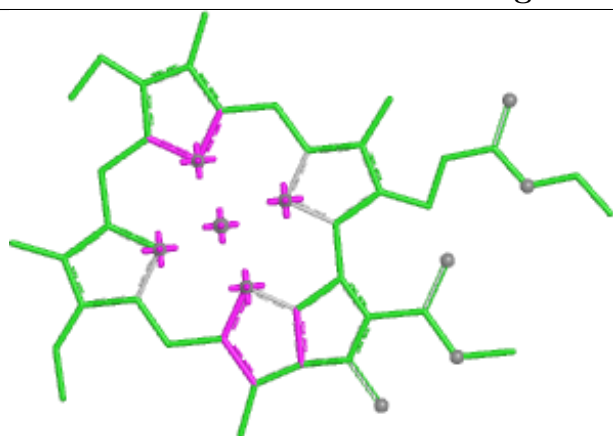


Torsions

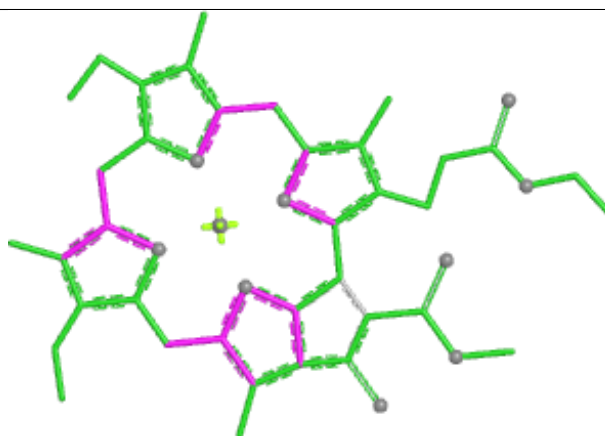


Rings

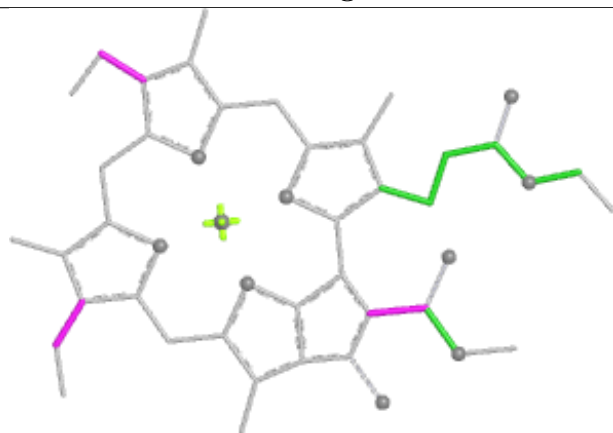
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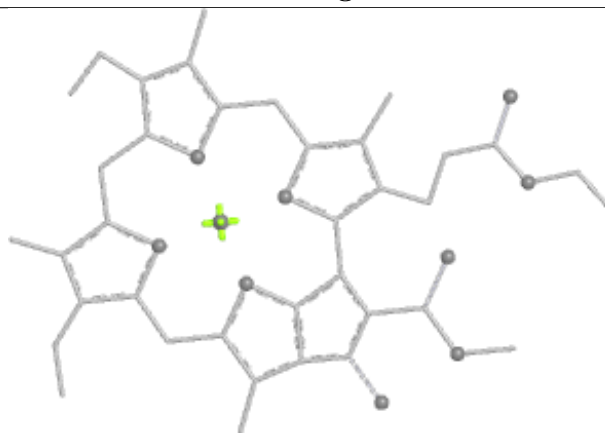
Bond lengths



Bond angles

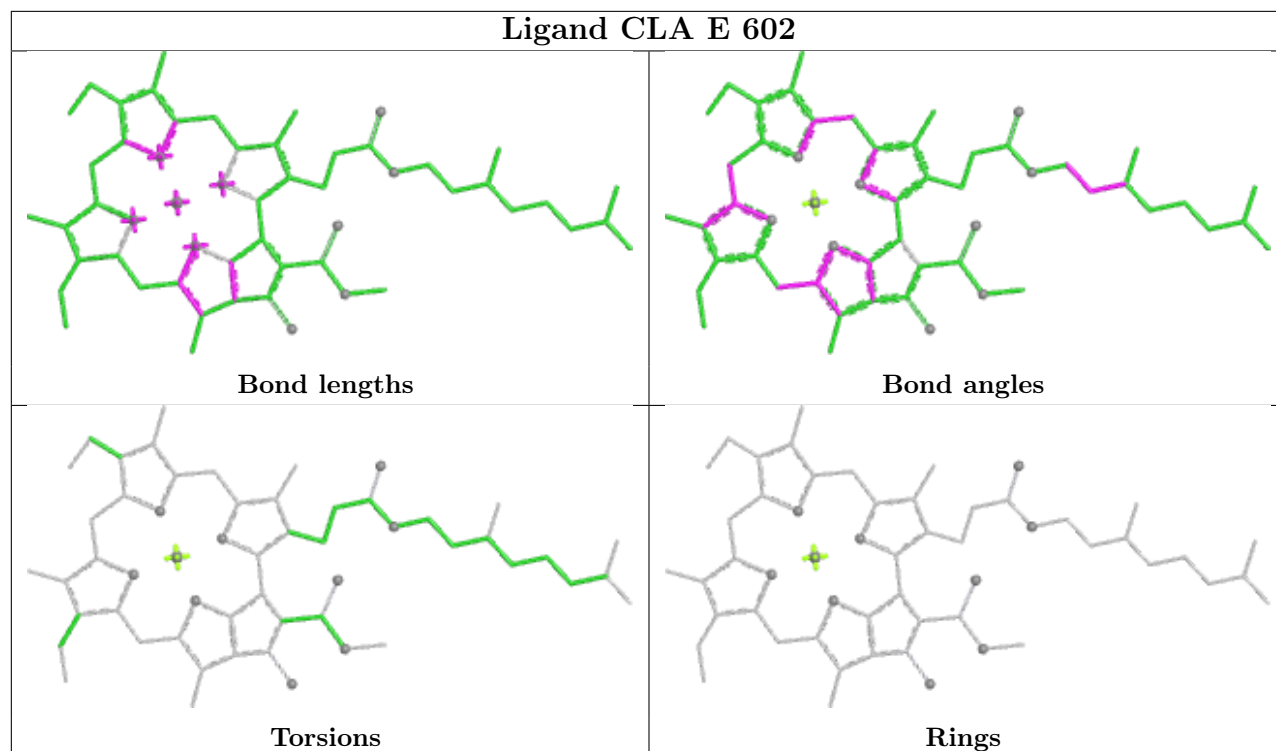


Torsions

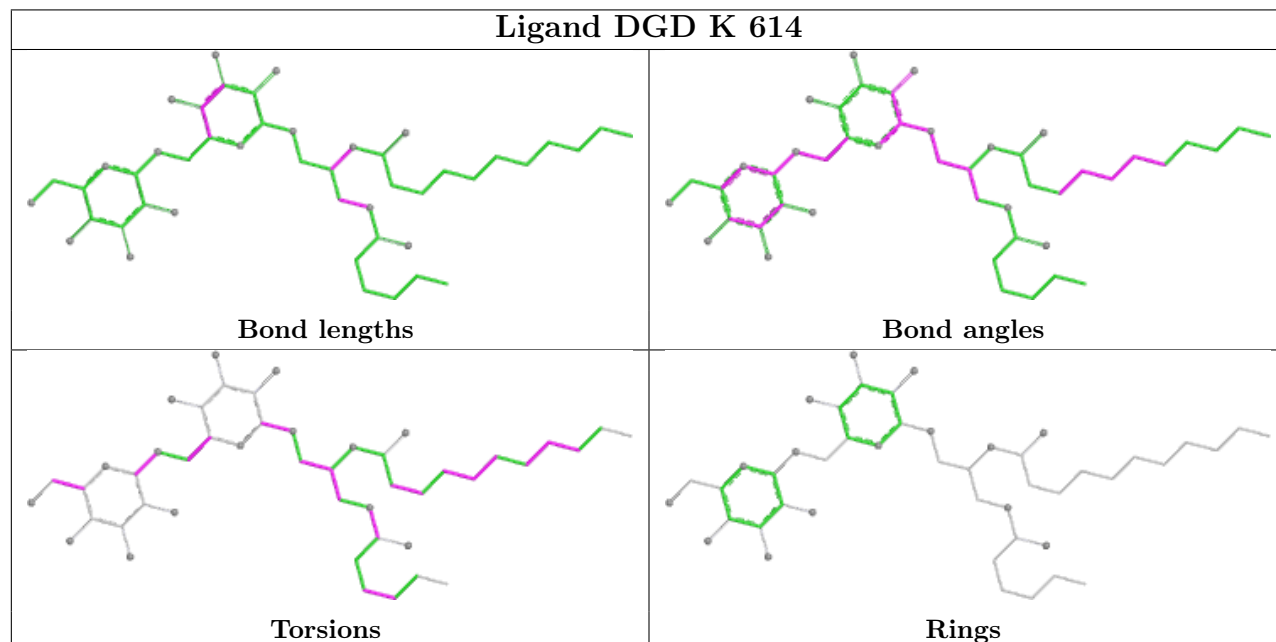


Rings

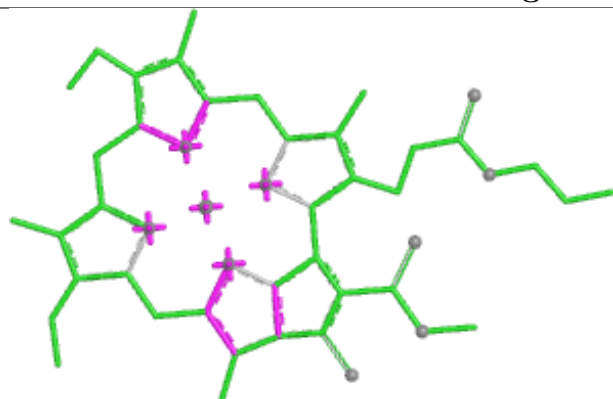
Ligand CLA E 602



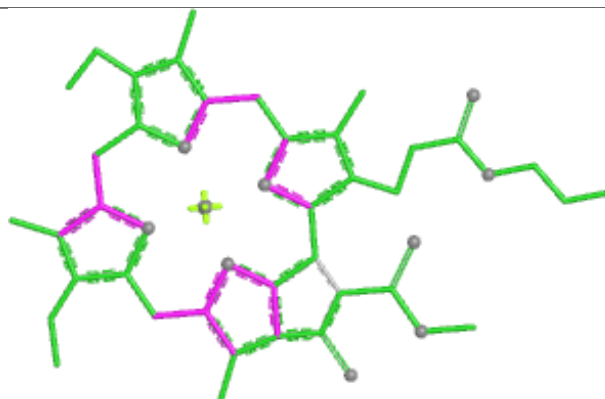
Ligand DGD K 614



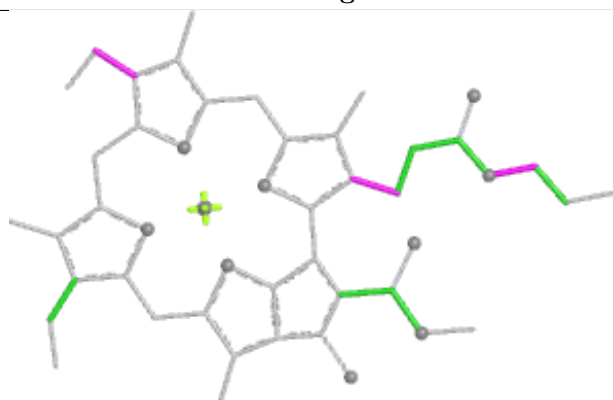
Ligand CLA l 410



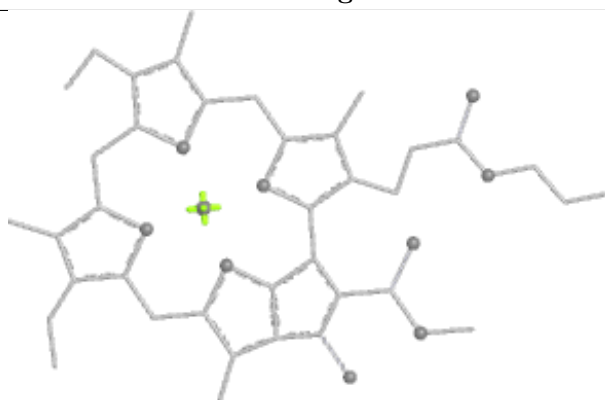
Bond lengths



Bond angles

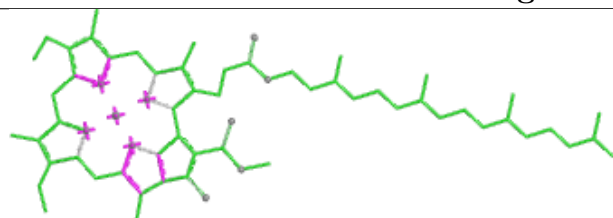


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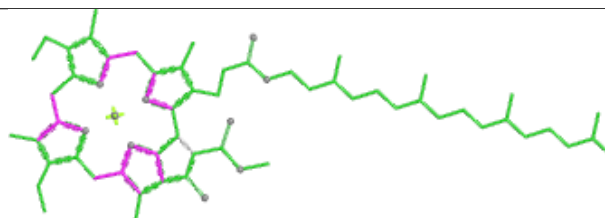


Rings

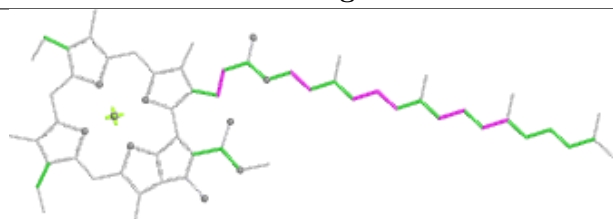
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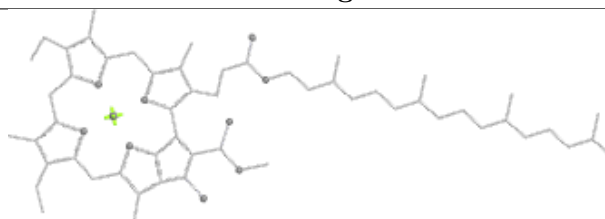
Bond lengths



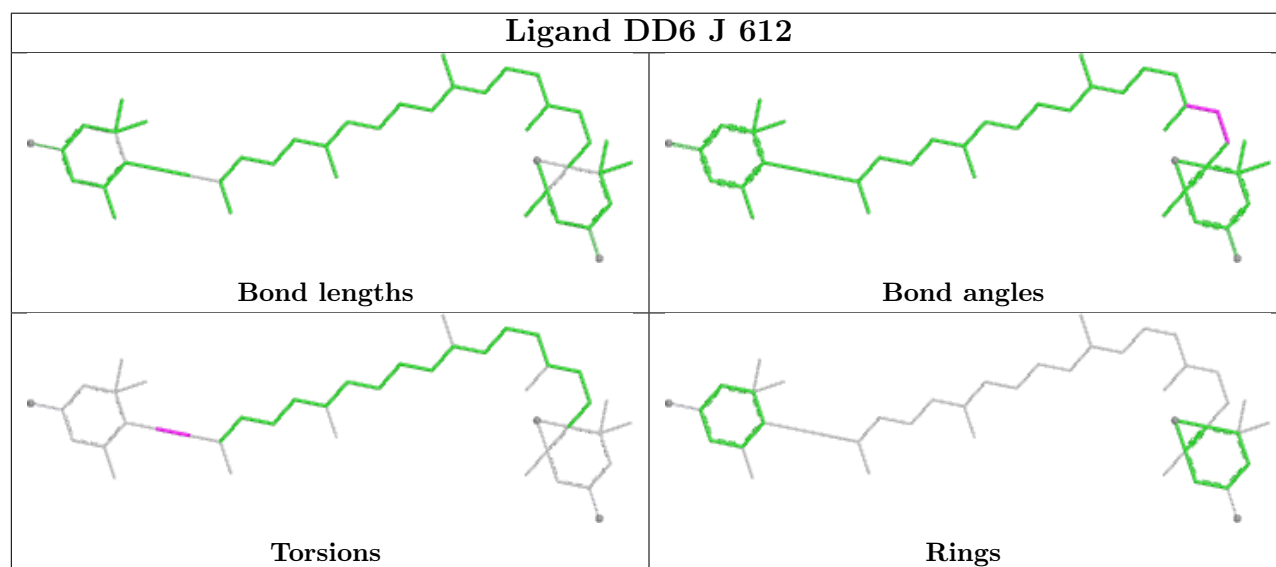
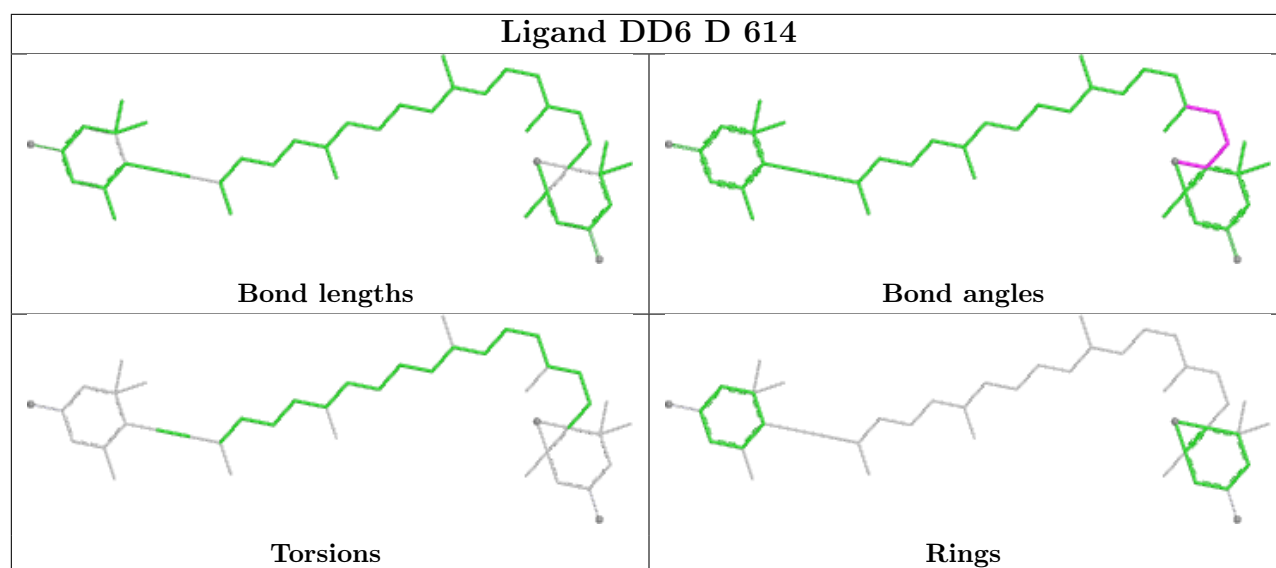
Bond angles



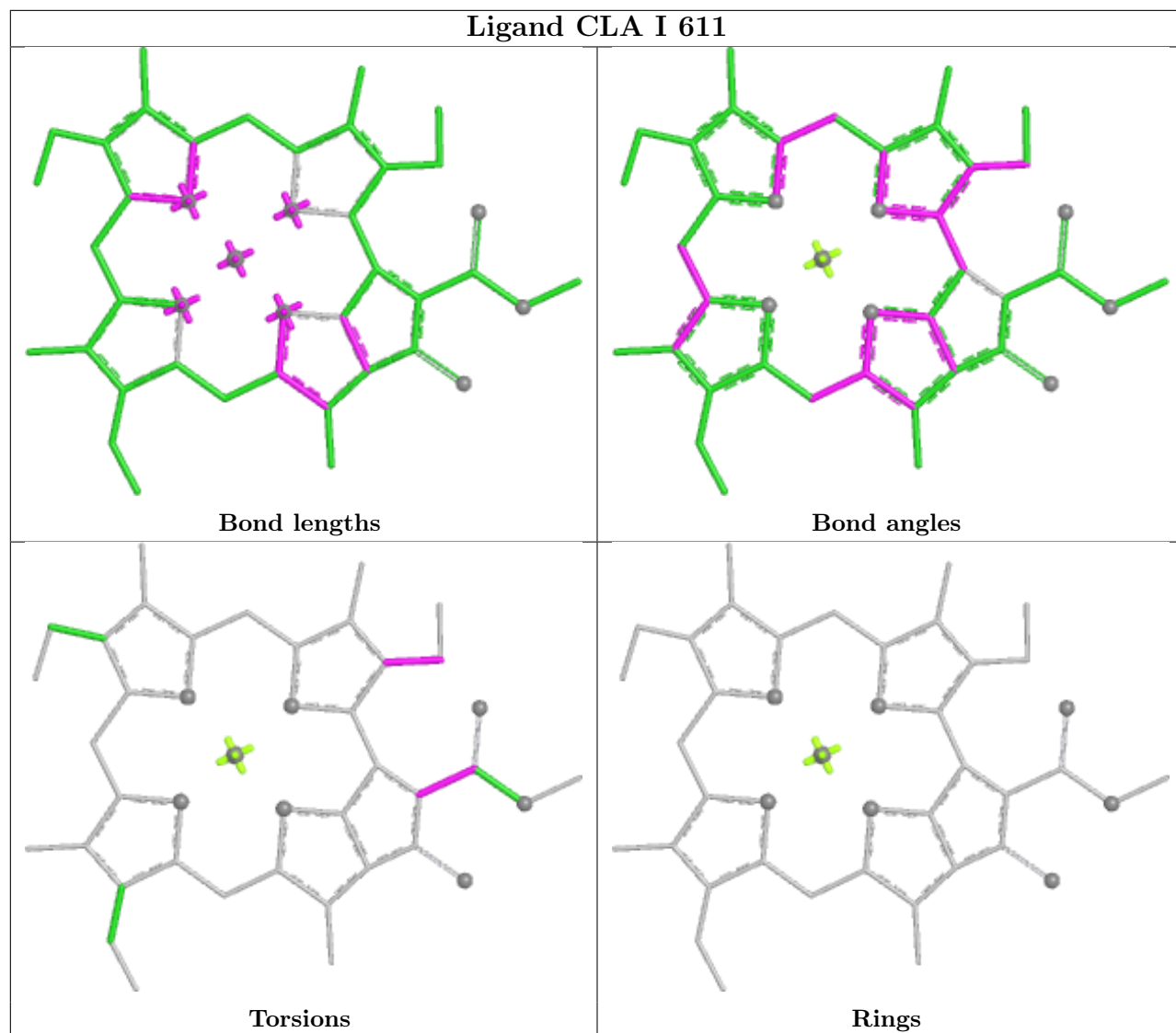
Torsions

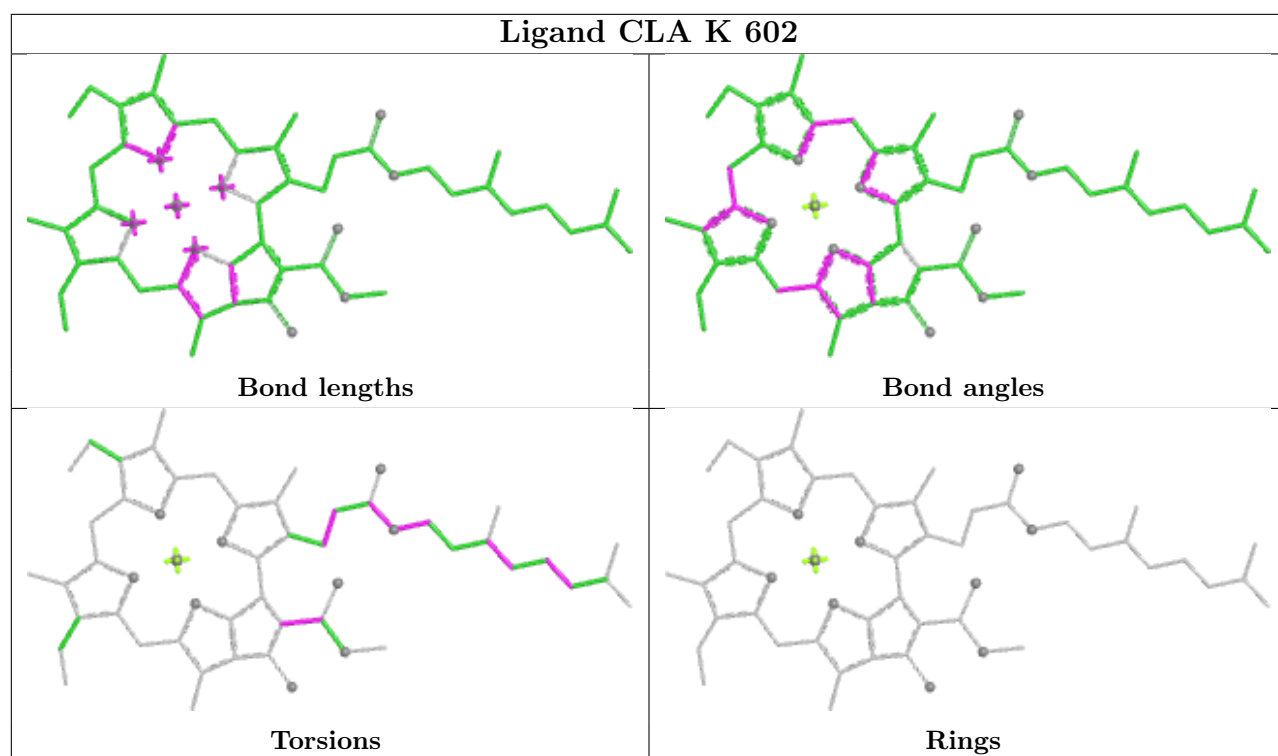


Rings

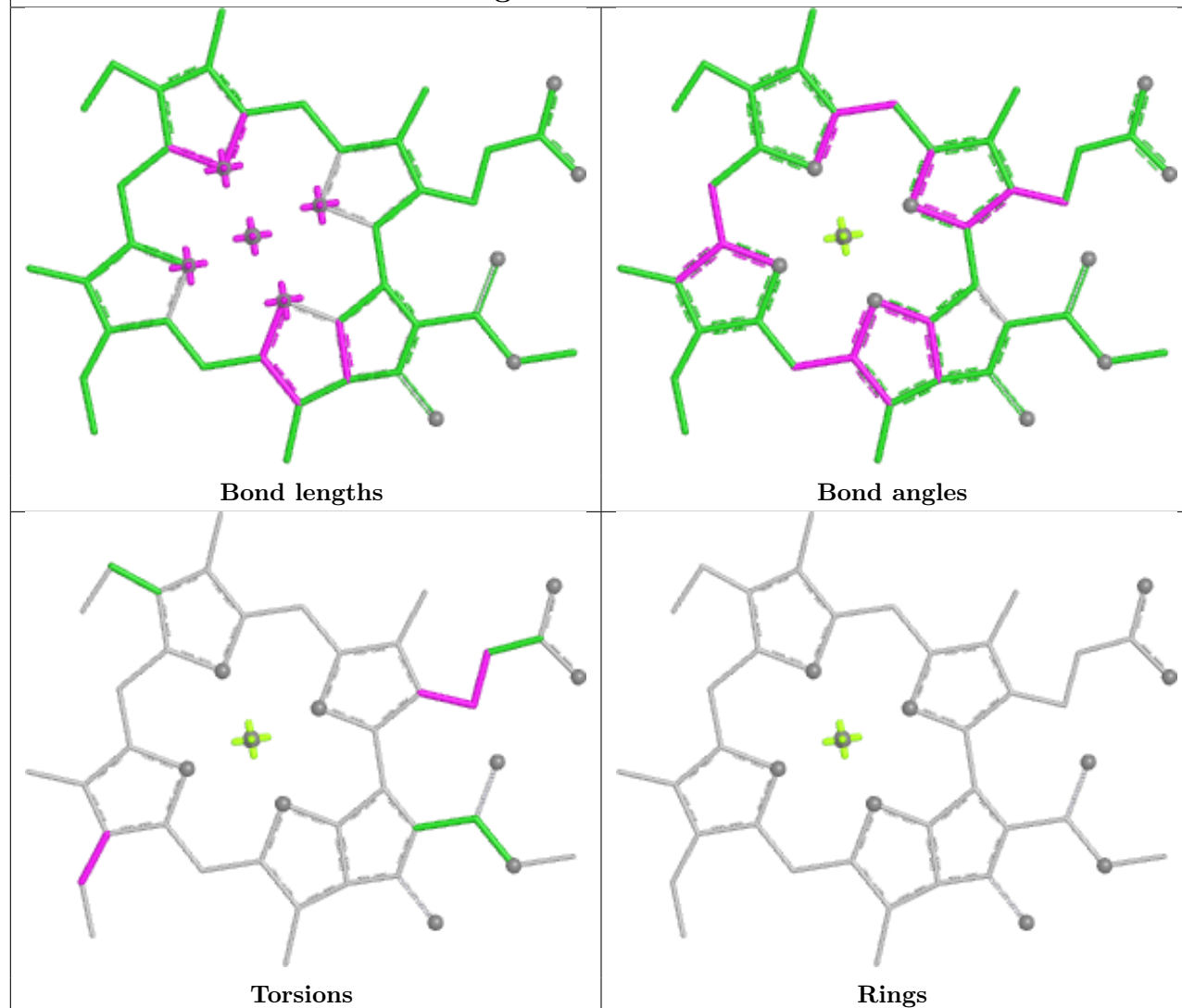


Ligand CLA I 611

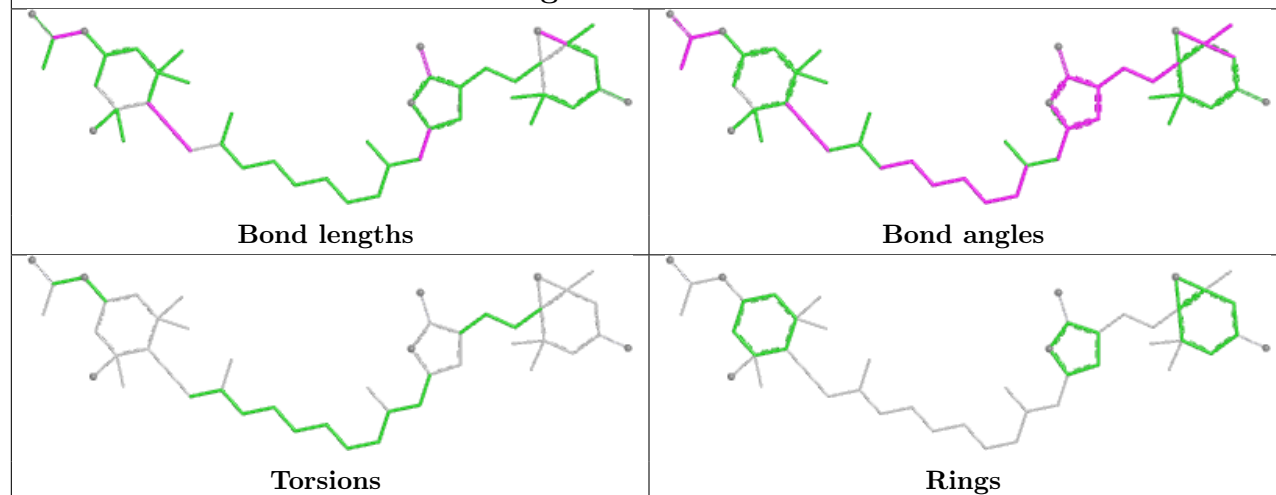




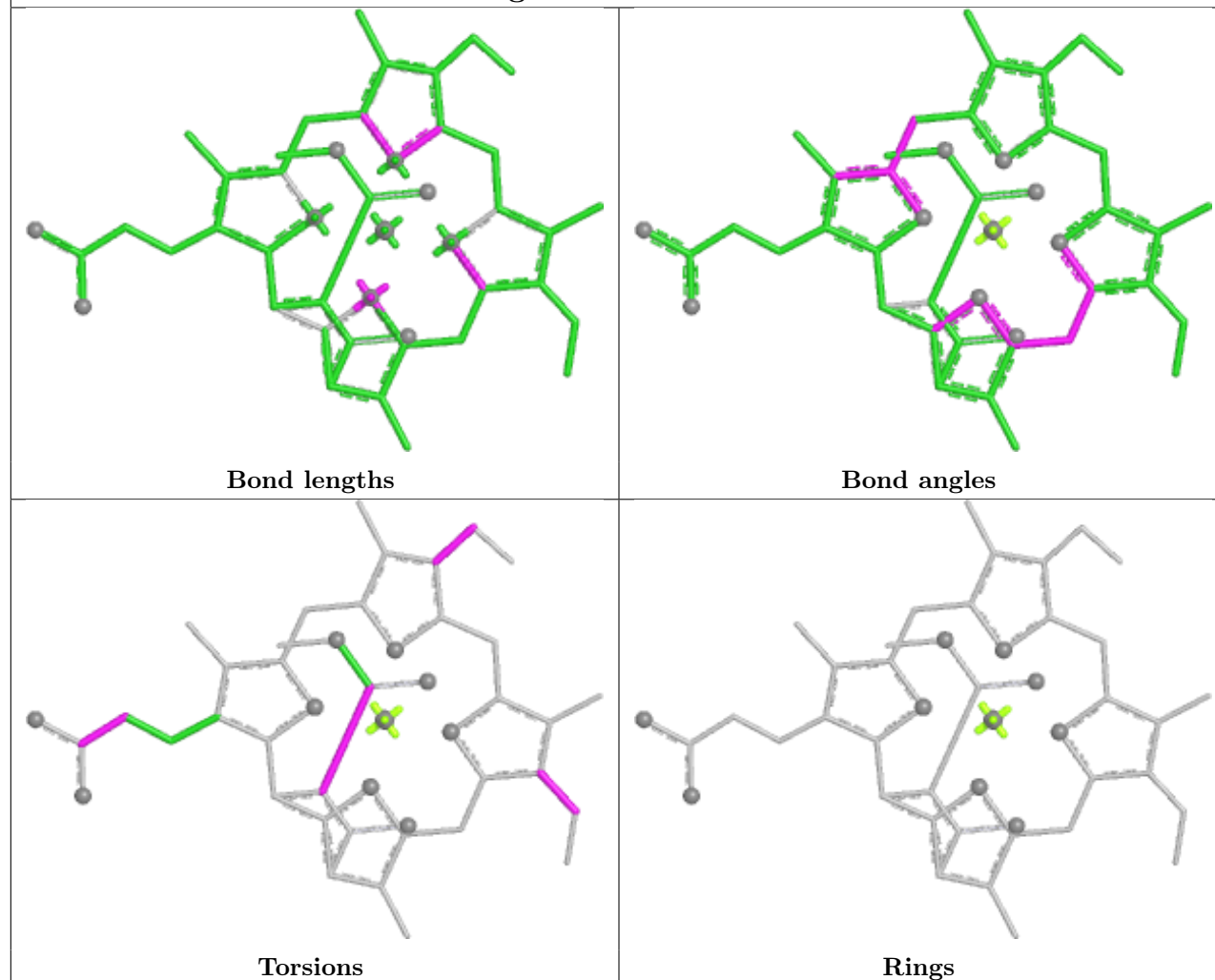
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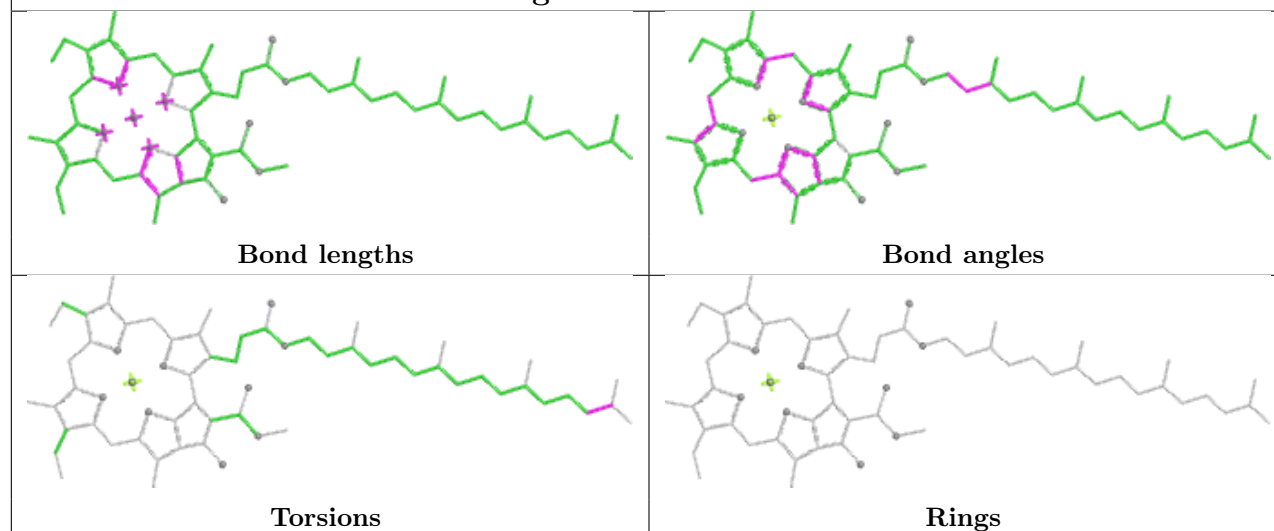
Ligand PID J 614



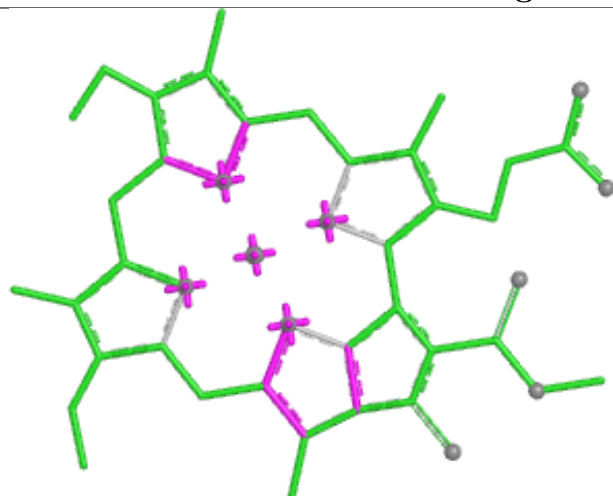
Ligand KC2 A 608



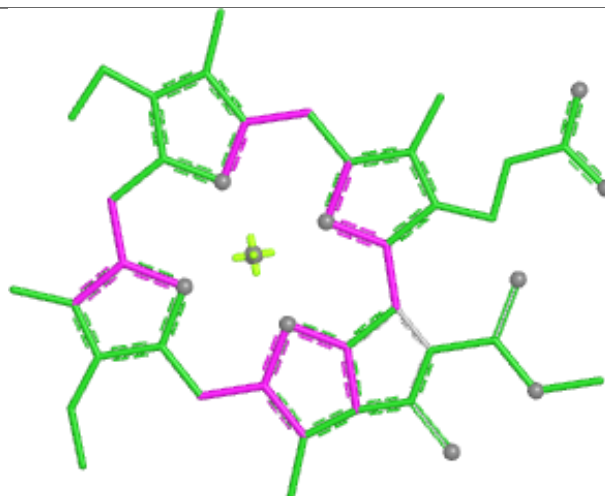
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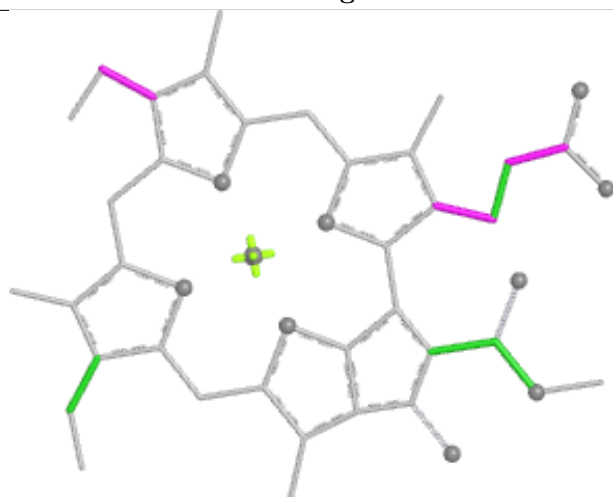
Ligand CLA E 605



Bond lengths



Bond angles

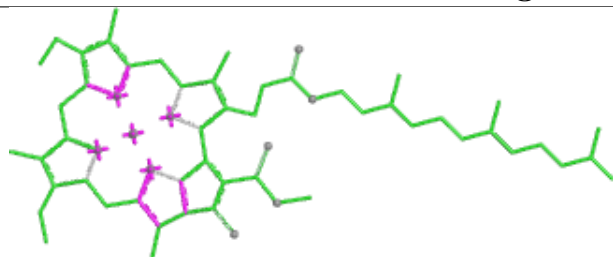


Torsions

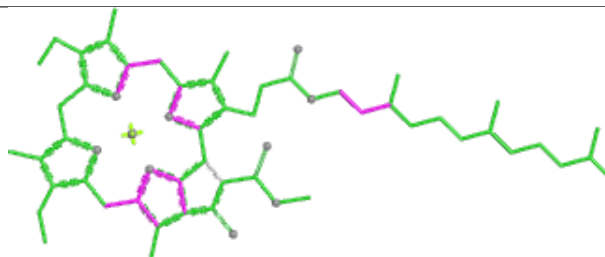


Rings

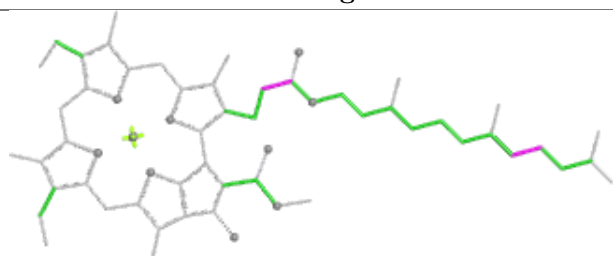
Ligand CLA F 601



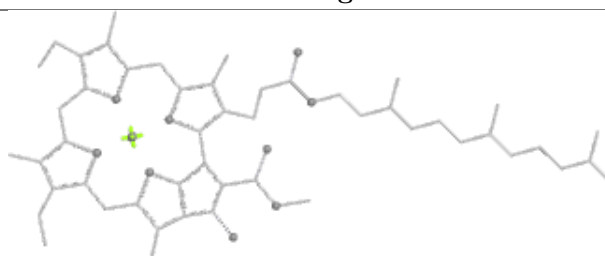
Bond lengths



Bond angles

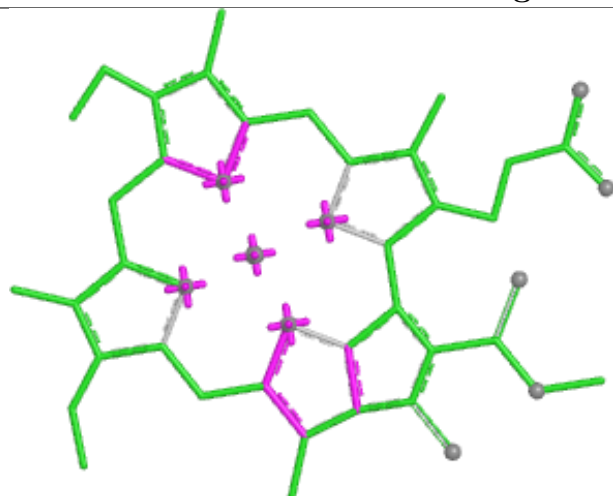


Torsions

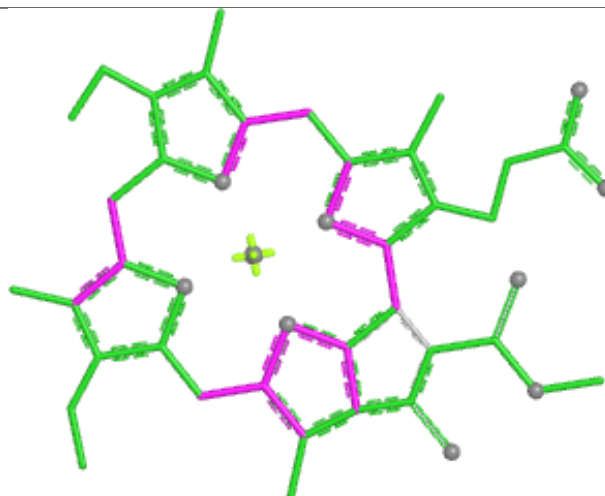


Rings

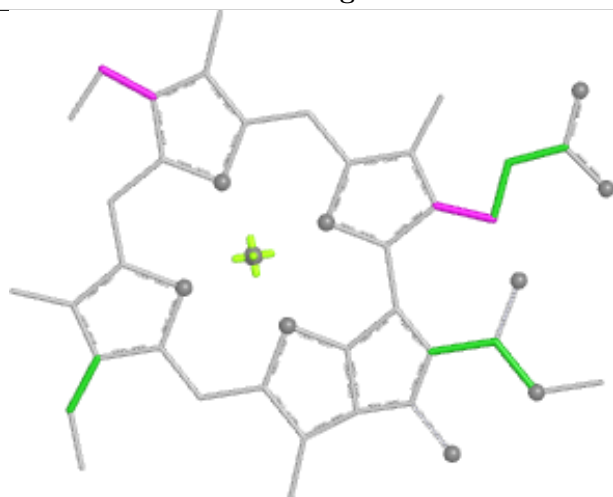
Ligand CLA H 310



Bond lengths



Bond angles

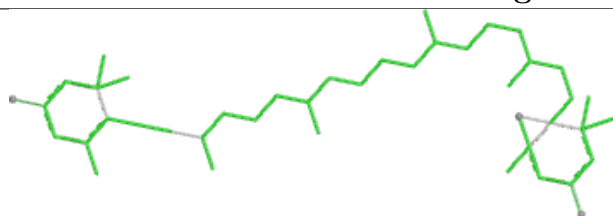


Torsions

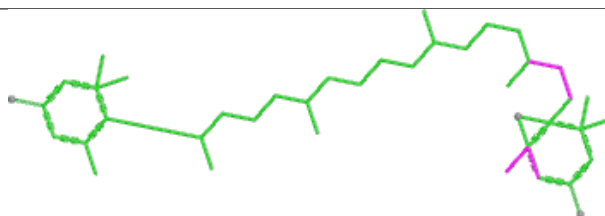


Rings

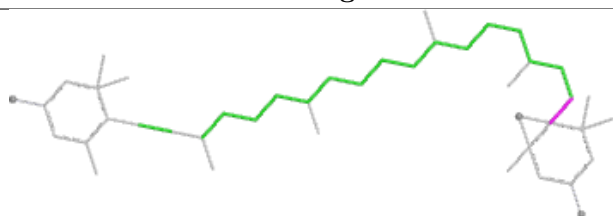
Ligand DD6 H 316



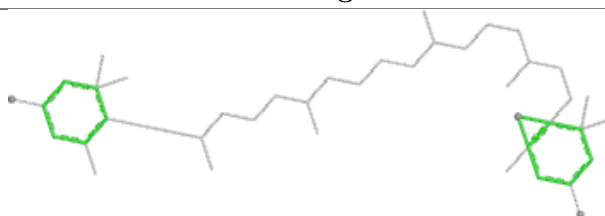
Bond lengths



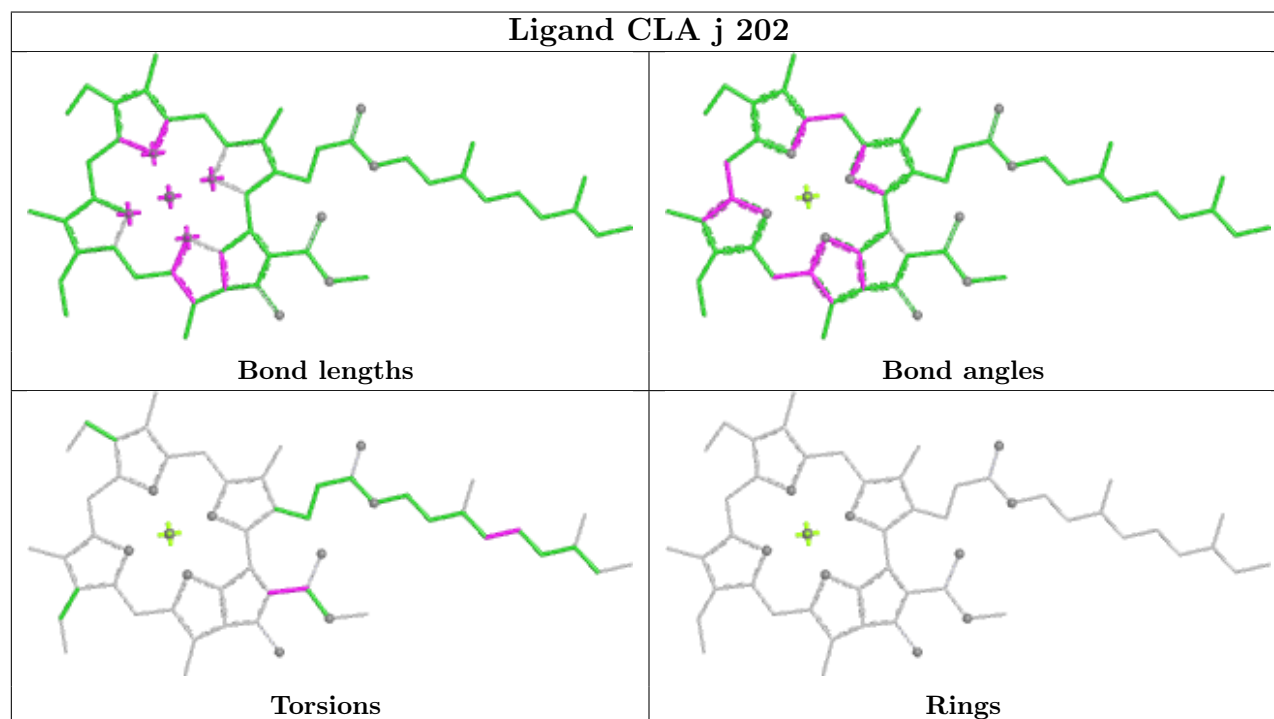
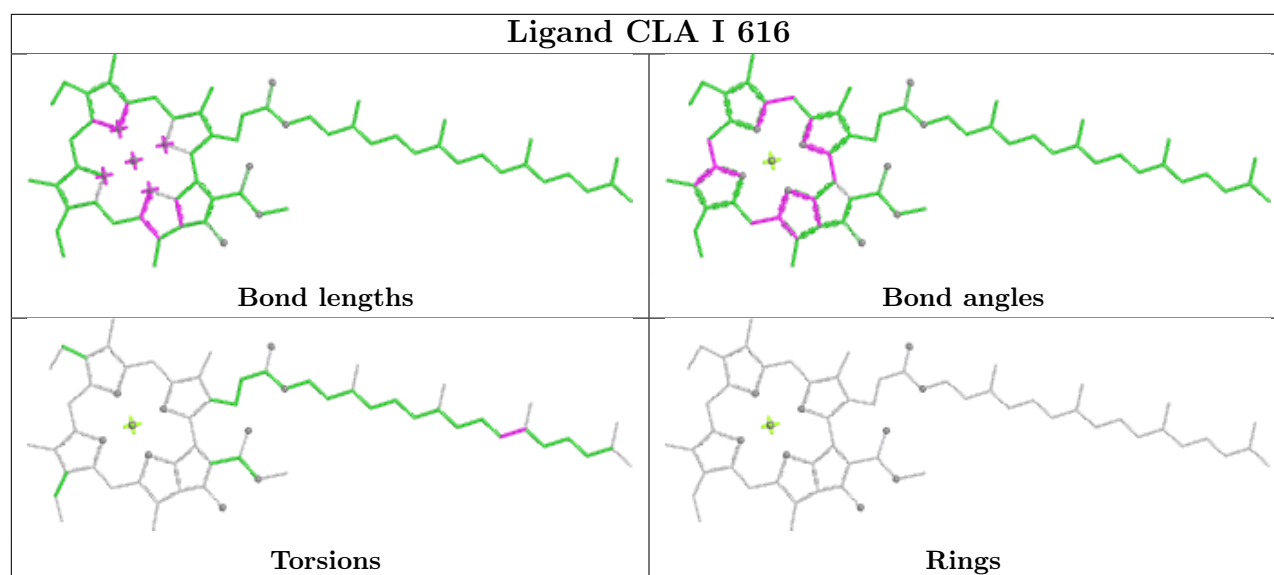
Bond angles

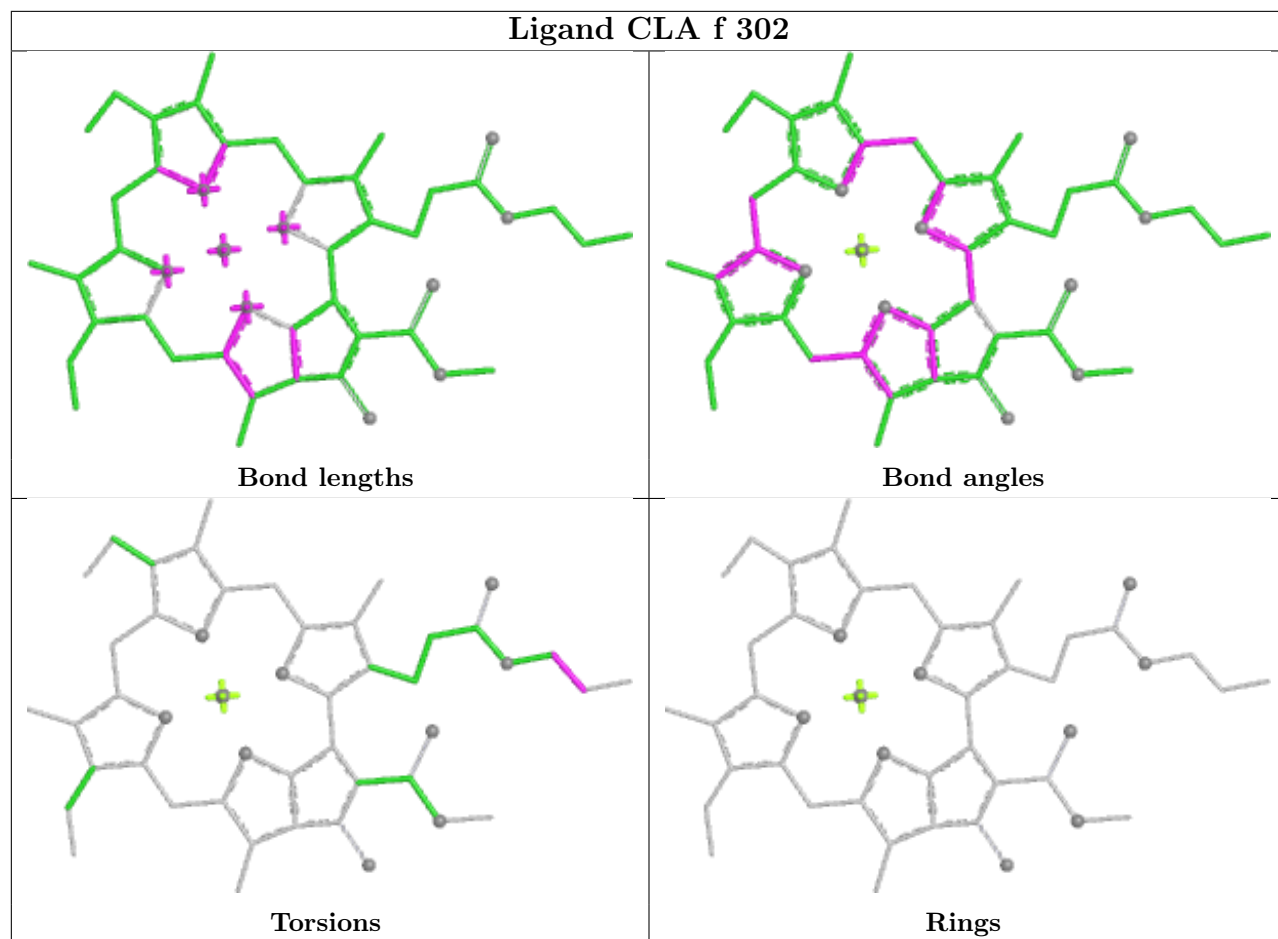


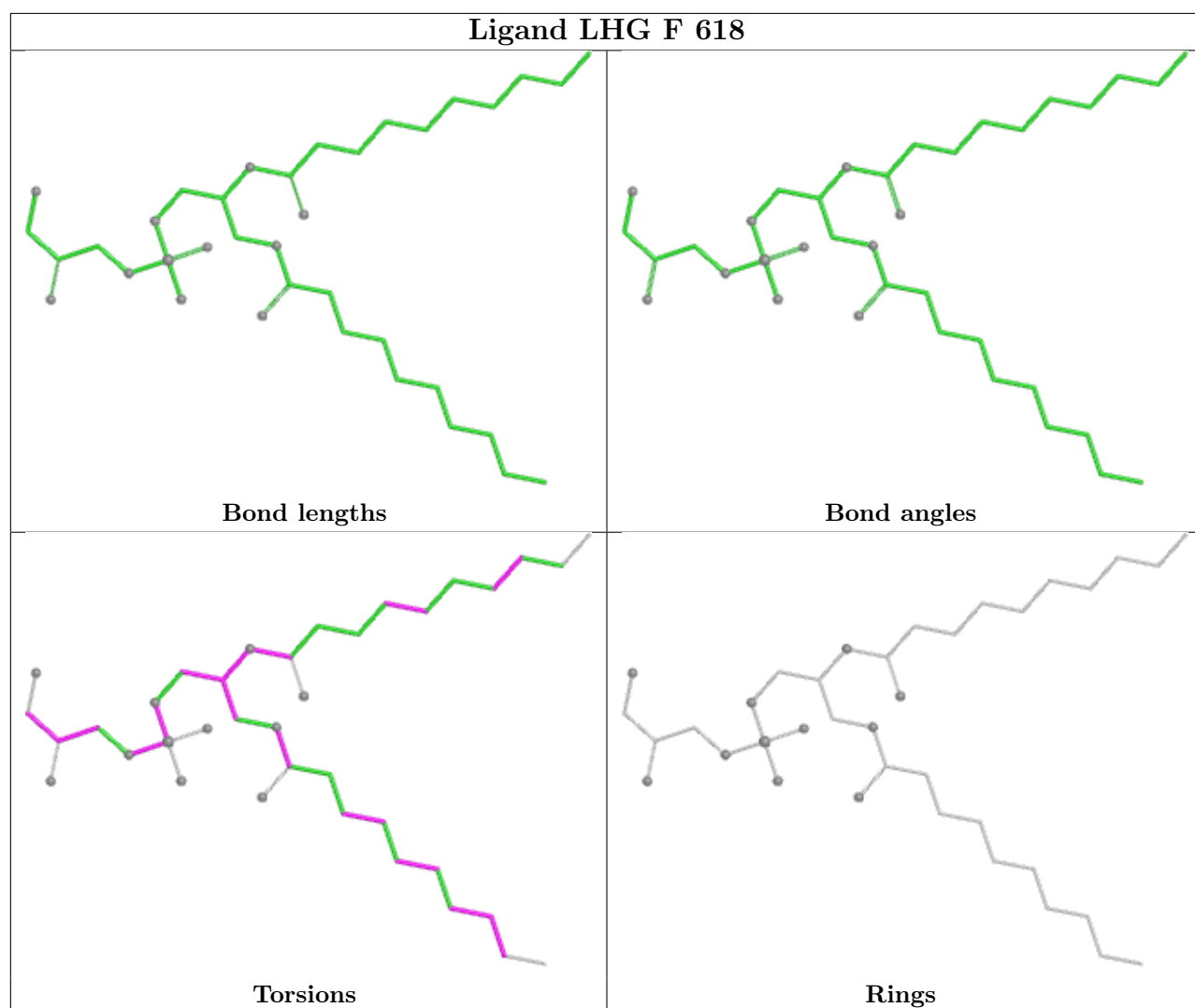
Torsions



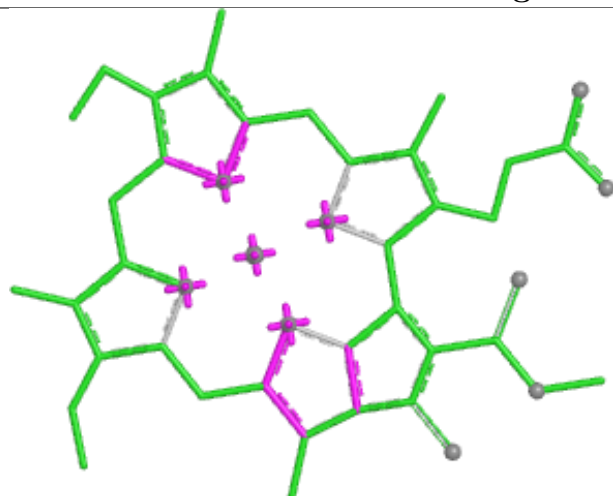
Rings



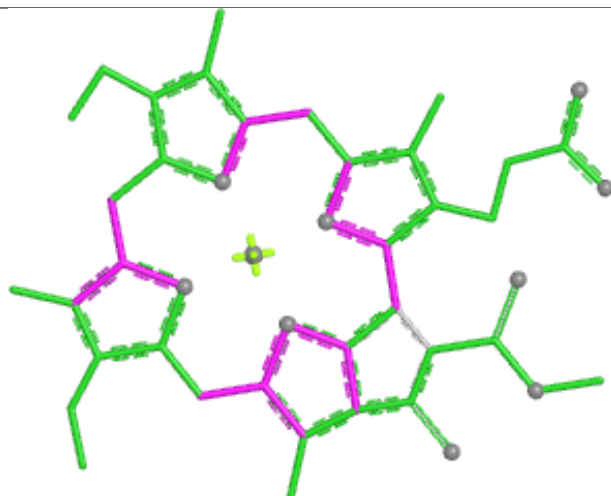




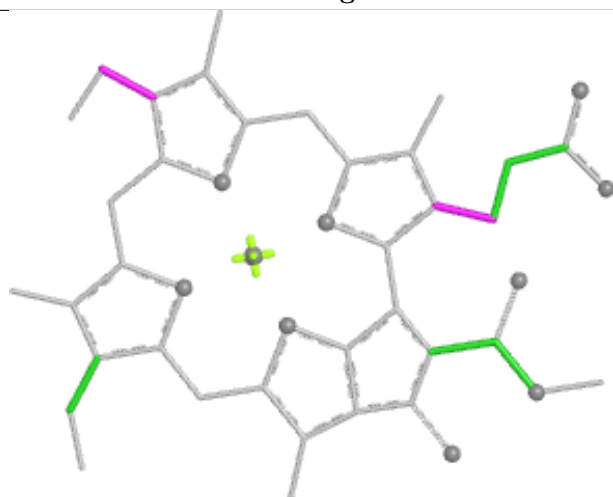
Ligand CLA K 608



Bond lengths



Bond angles

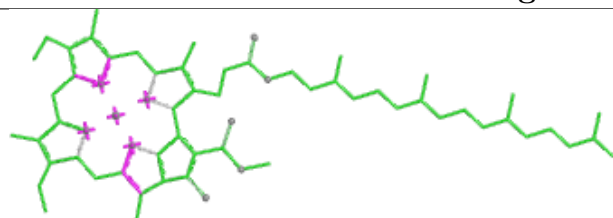


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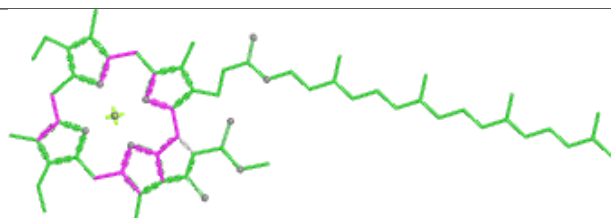


Rings

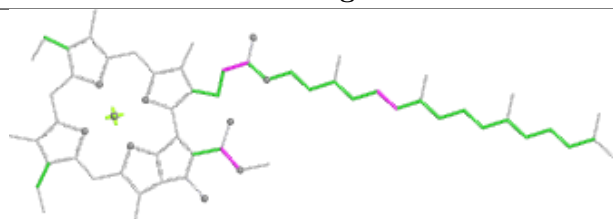
Ligand CLA a 801



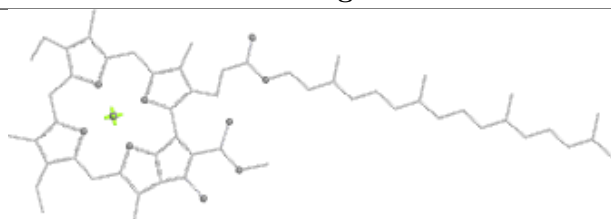
Bond lengths



Bond angles

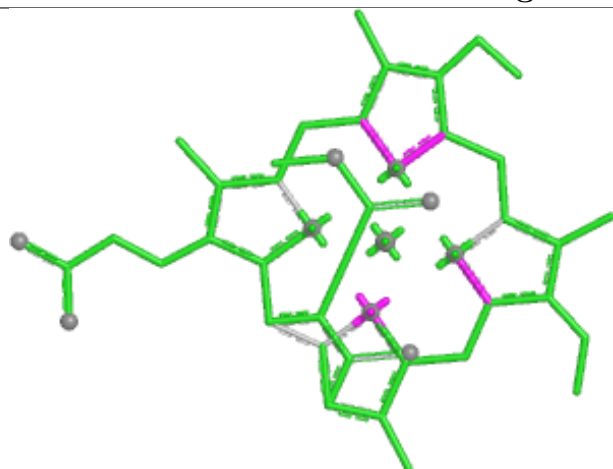


Torsions

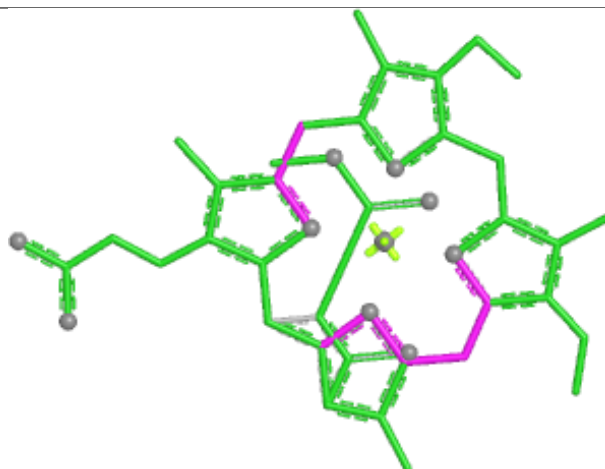


Rings

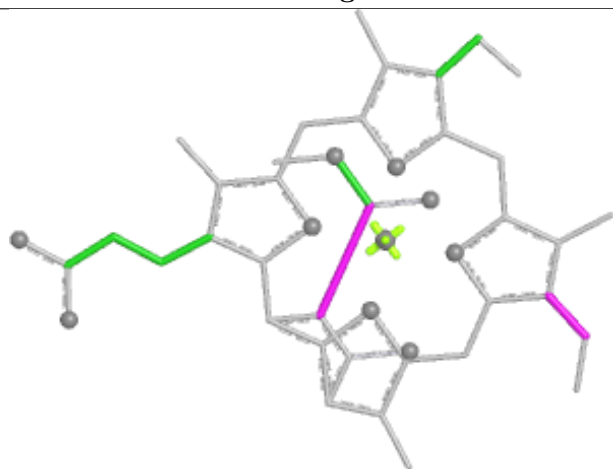
Ligand KC2 B 602



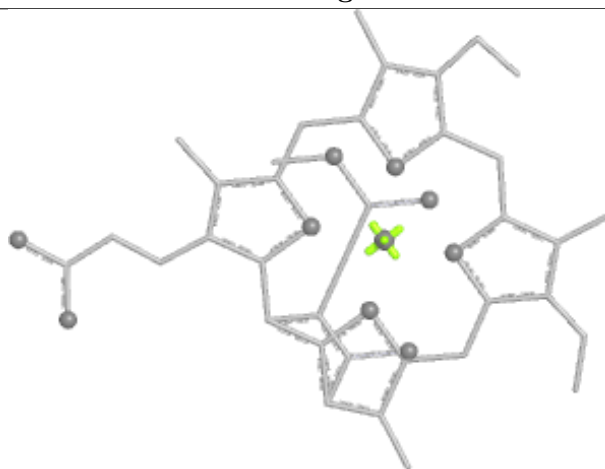
Bond lengths



Bond angles

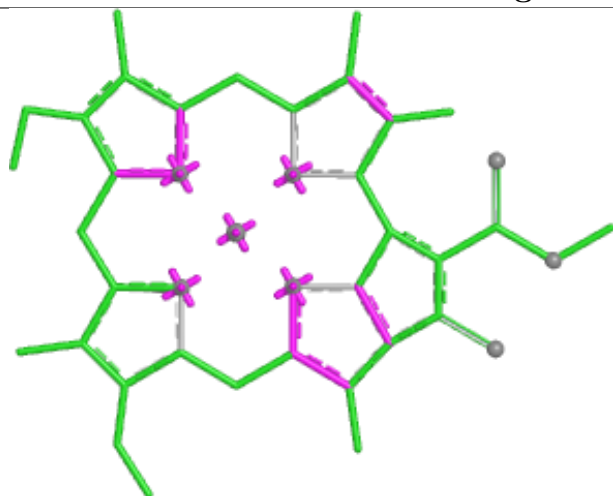


Torsions

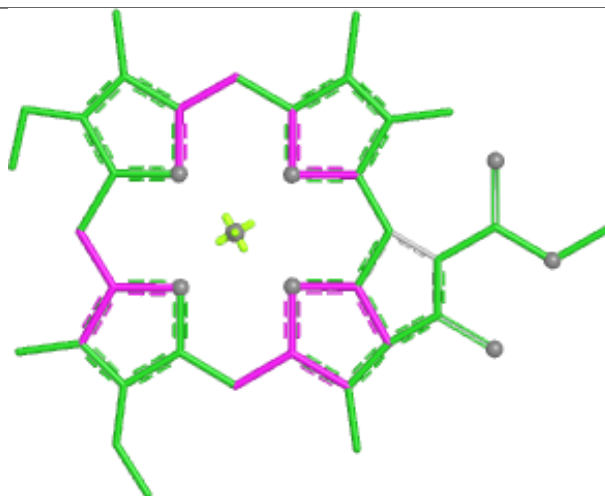


Rings

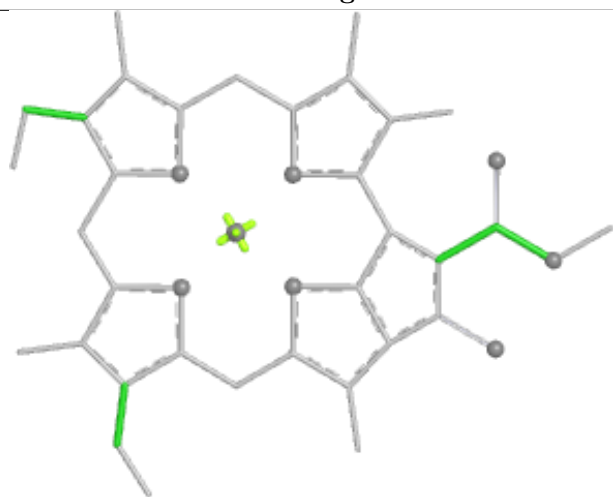
Ligand CLA T 609



Bond lengths



Bond angles

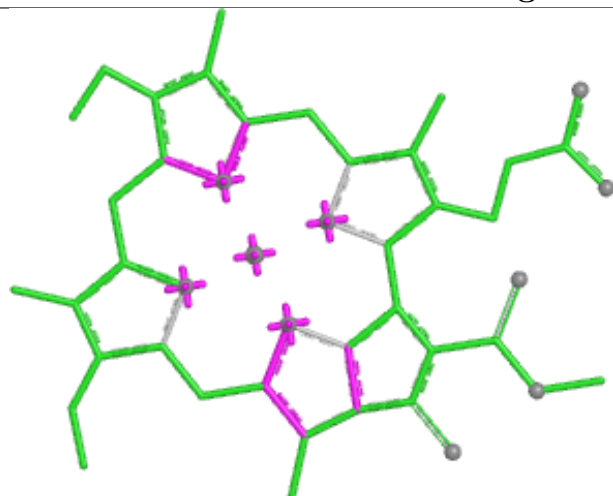


Torsions

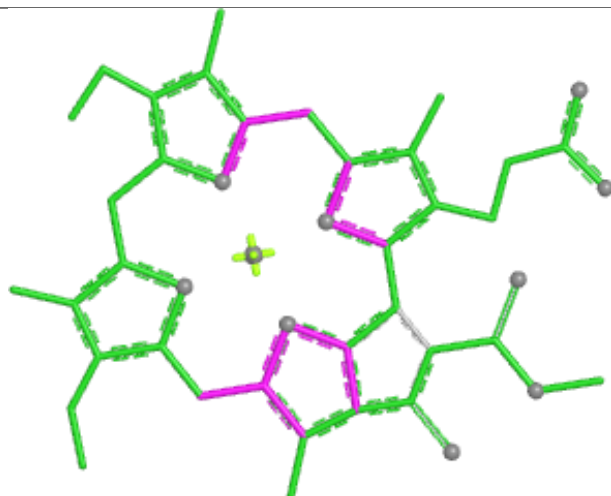


Rings

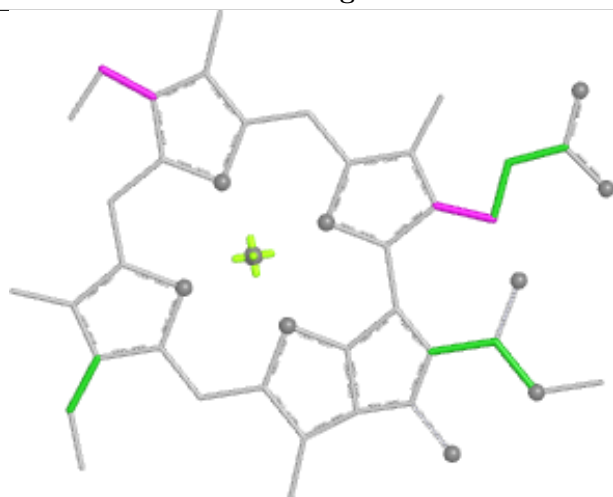
Ligand CLA J 601



Bond lengths



Bond angles

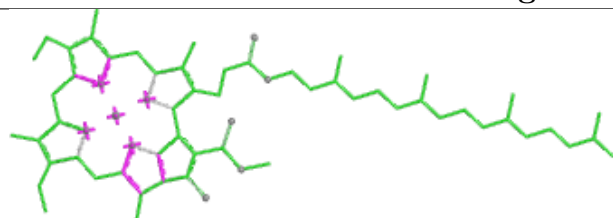


Torsions

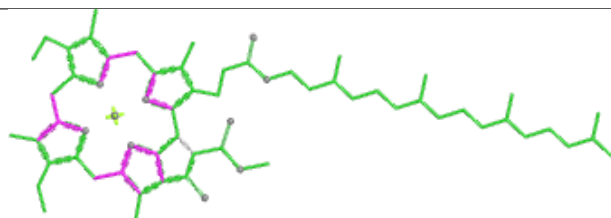


Rings

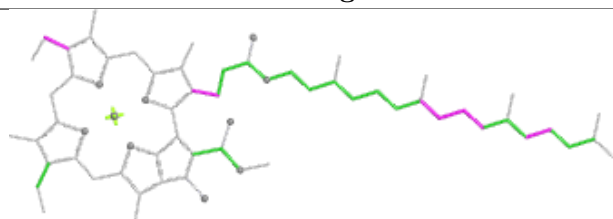
Ligand CLA a 821



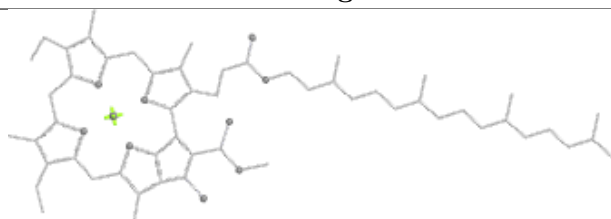
Bond lengths



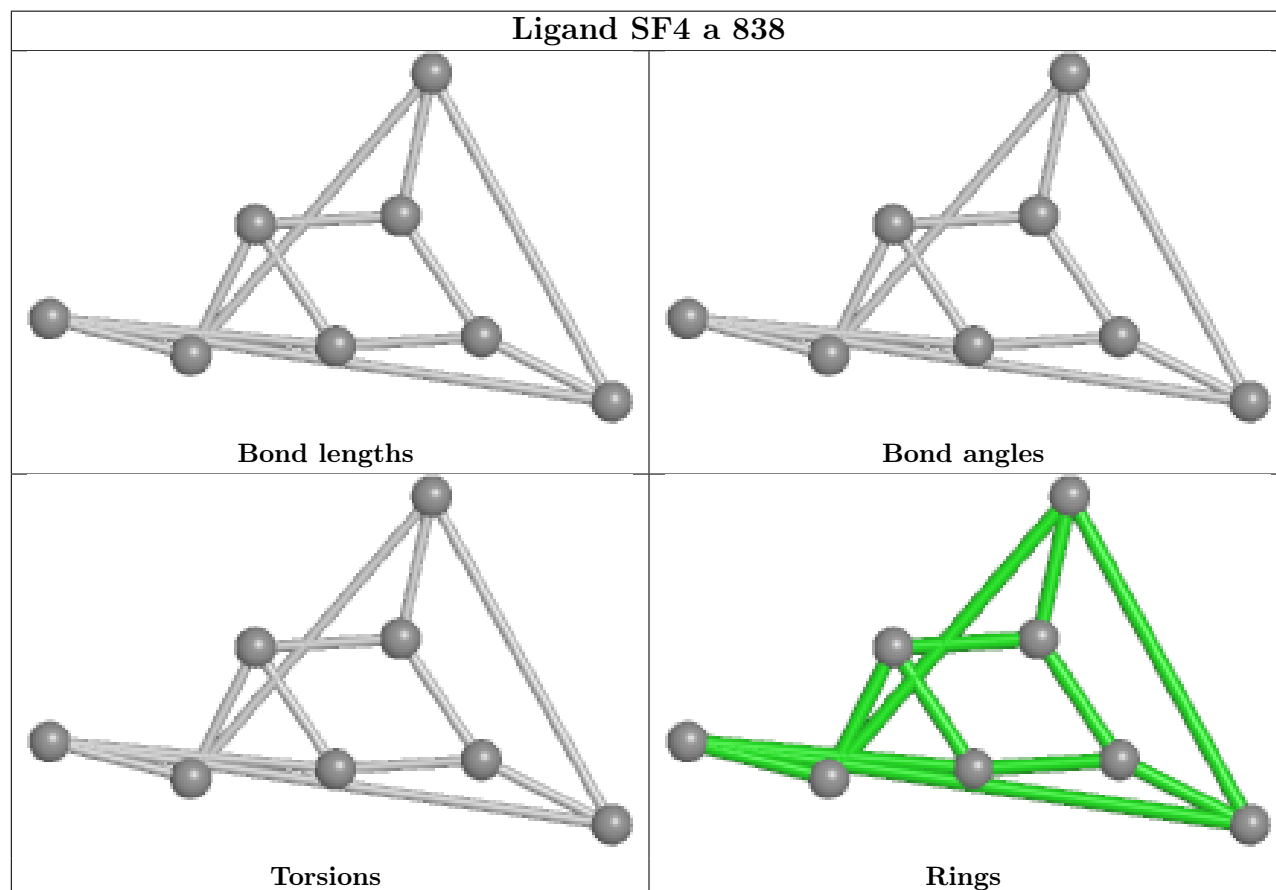
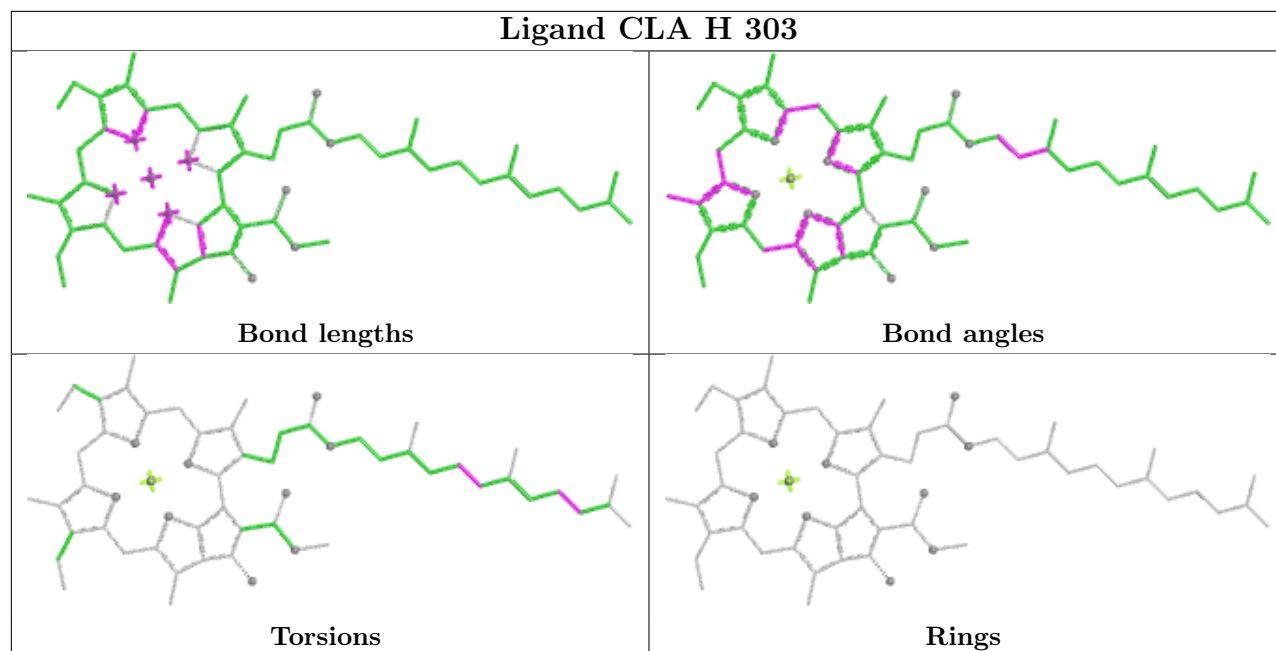
Bond angles



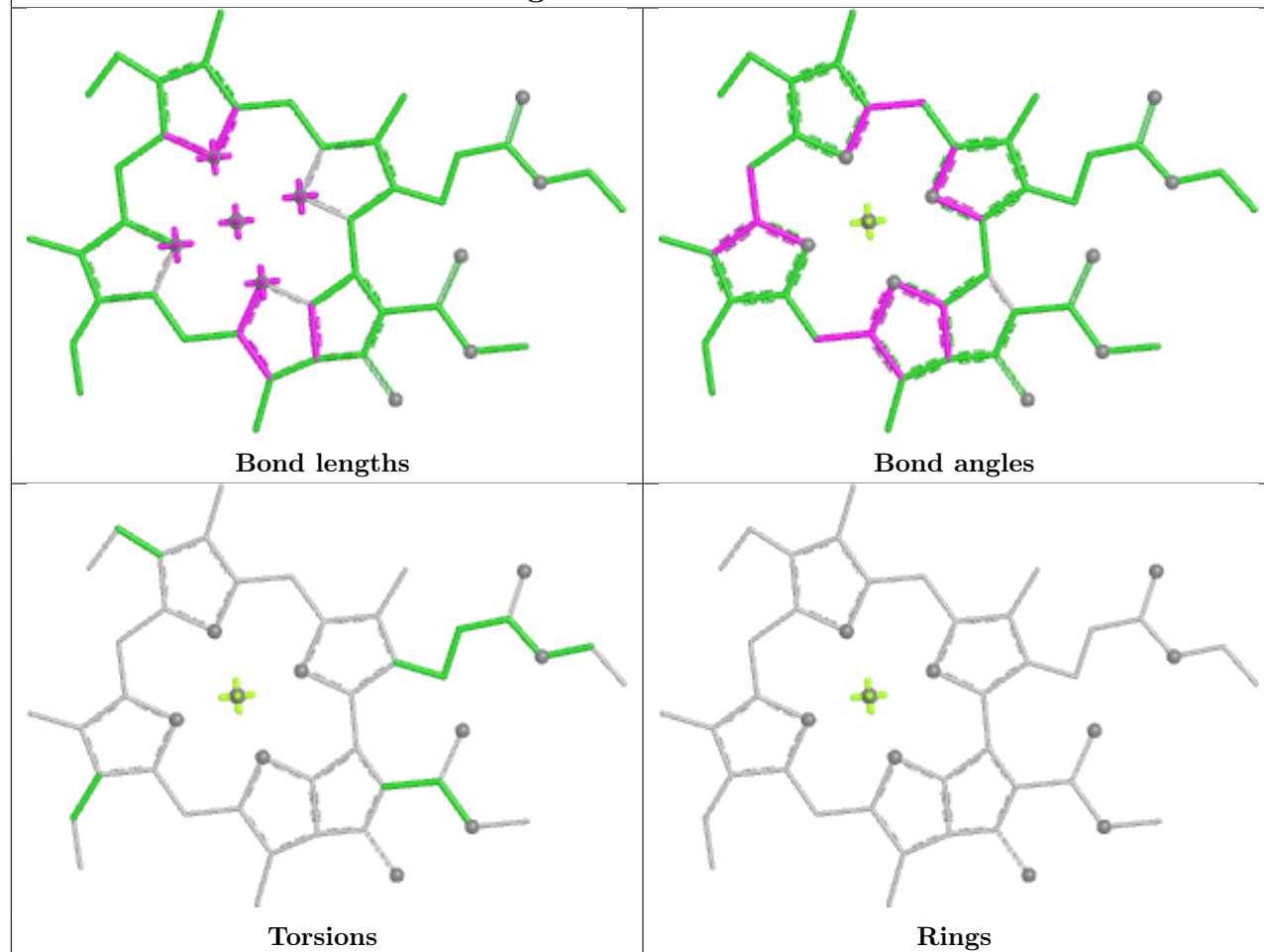
Torsions



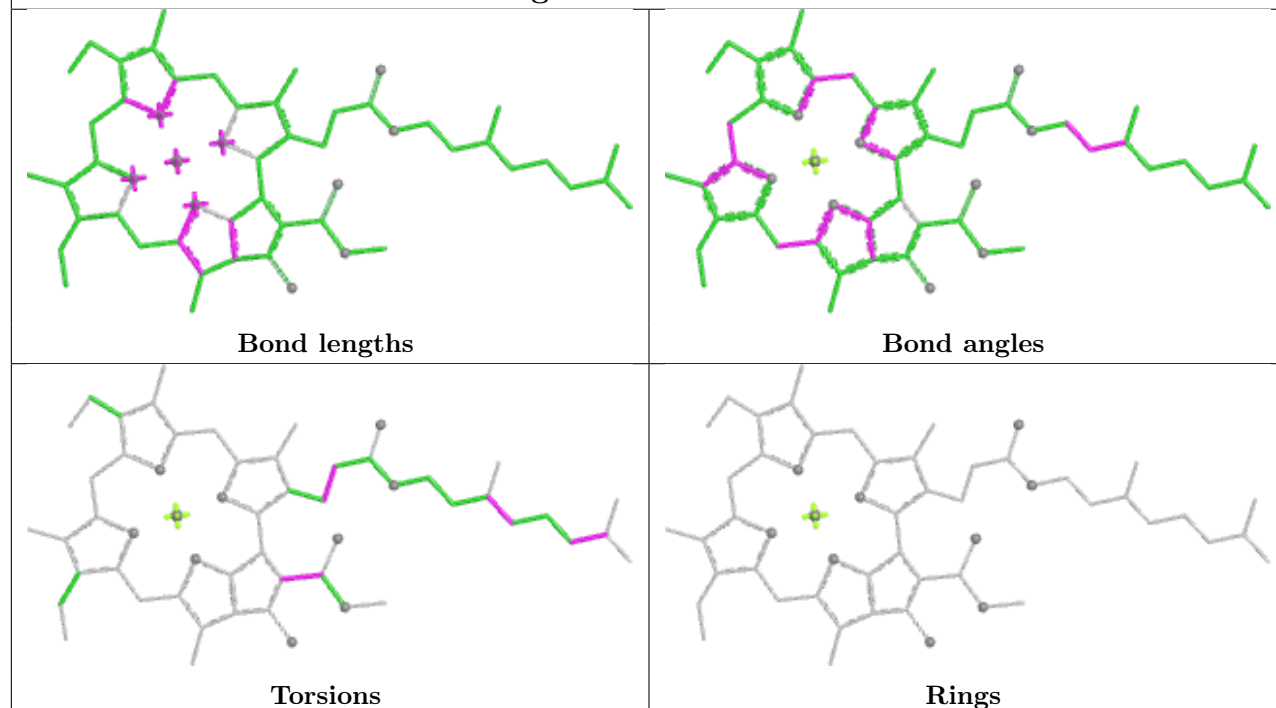
Rings

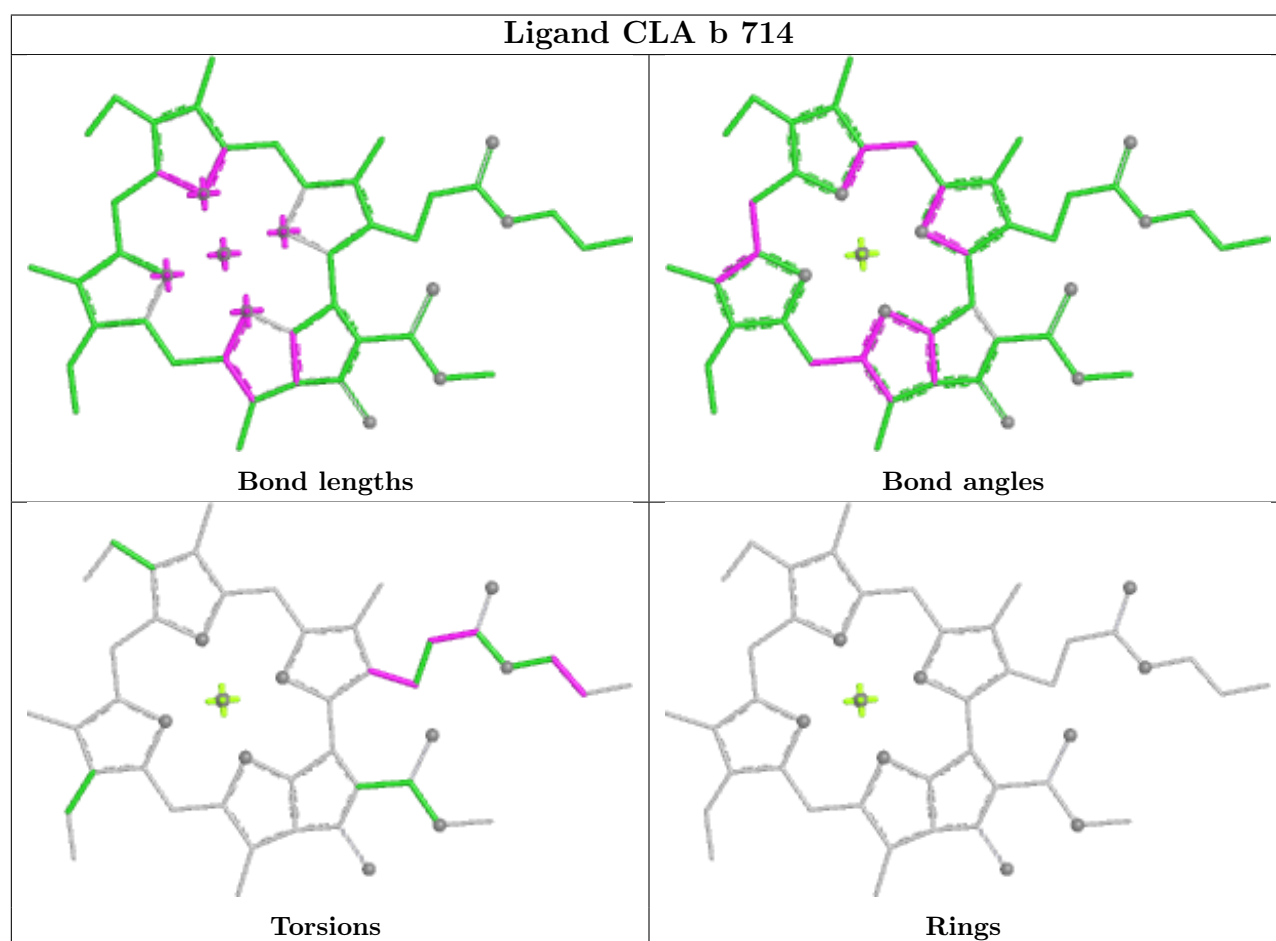
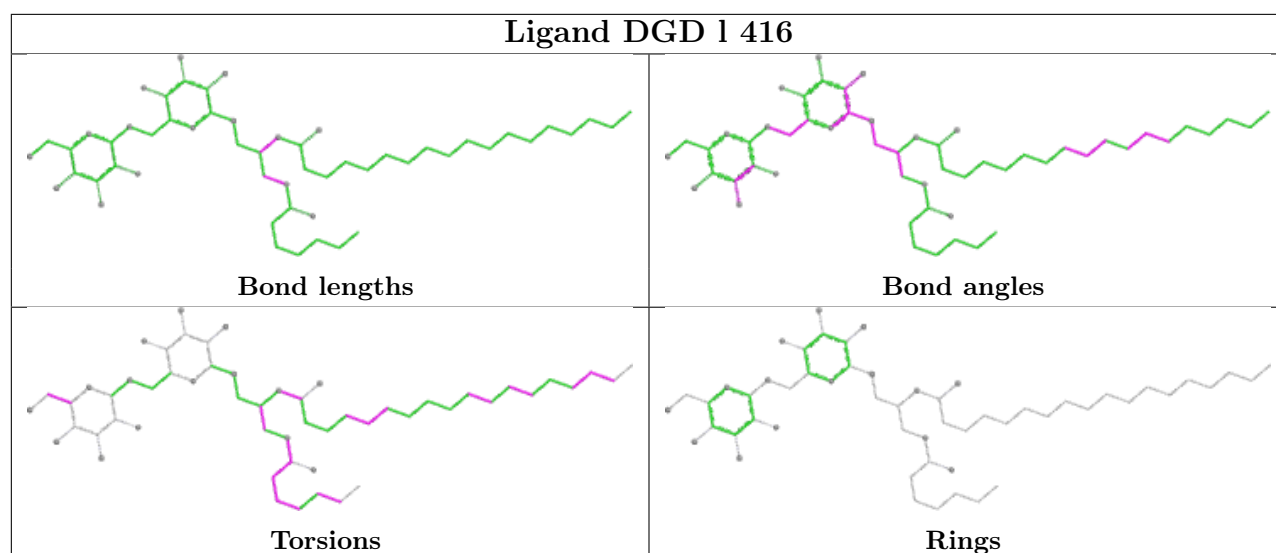


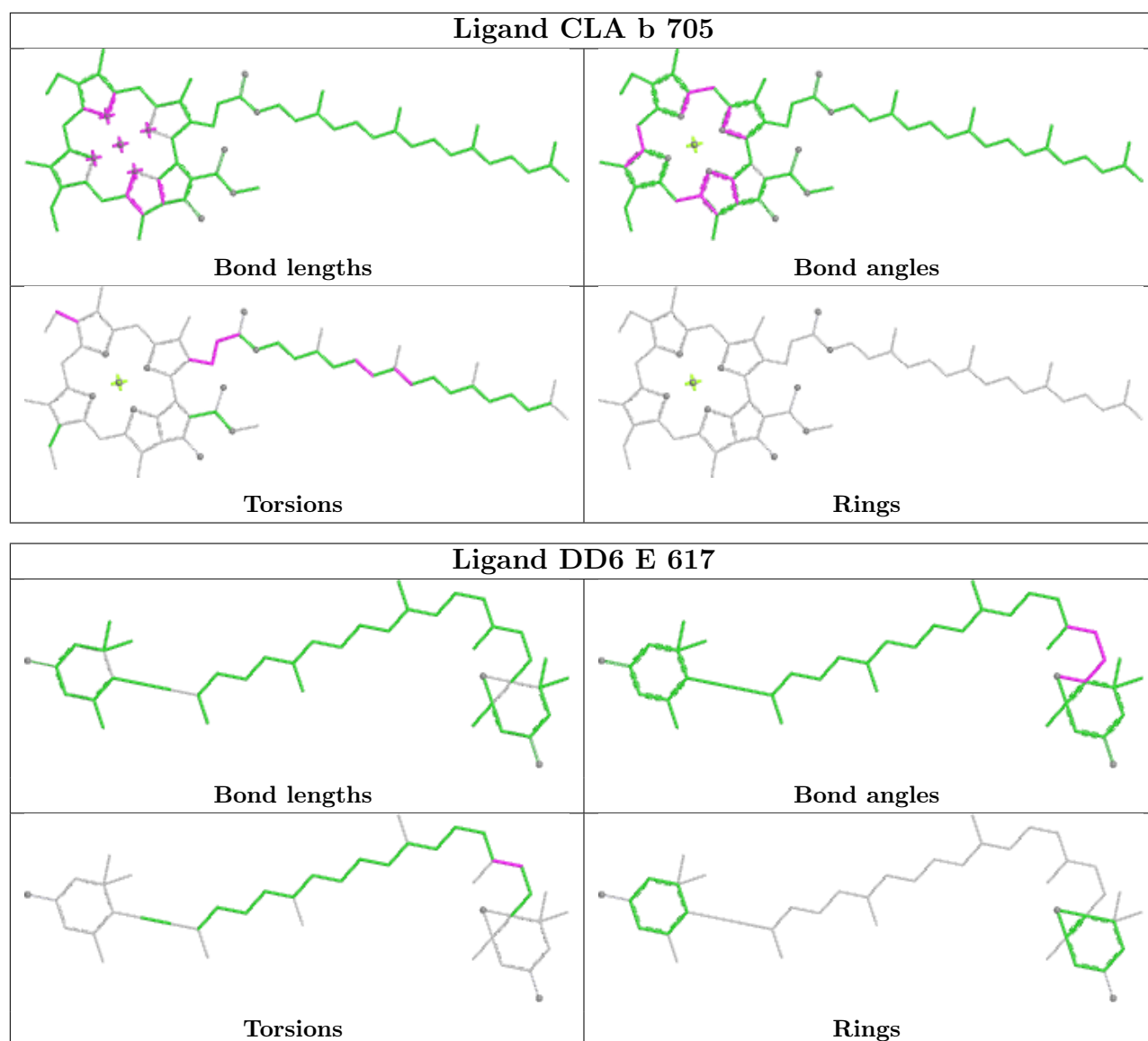
Ligand CLA C 211



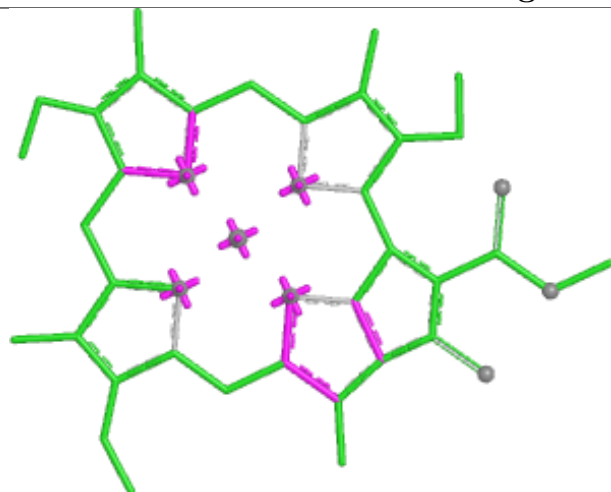
Ligand CLA D 604



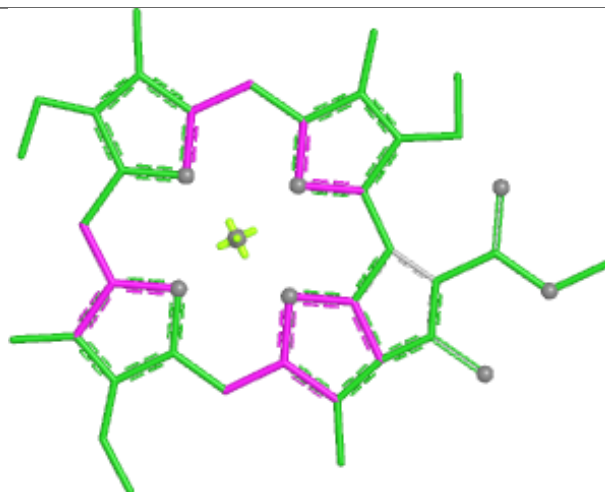




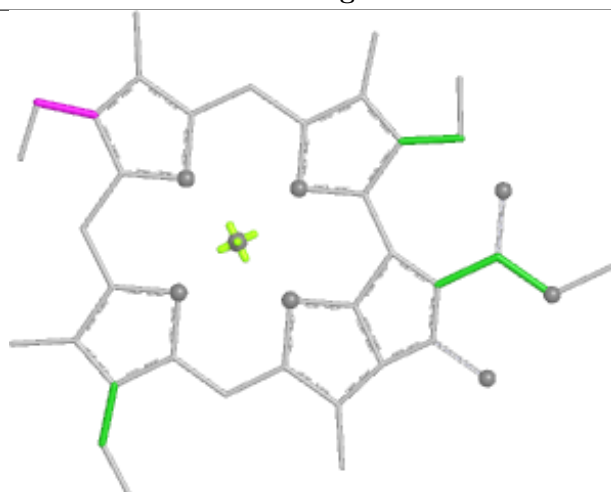
Ligand CLA J 607



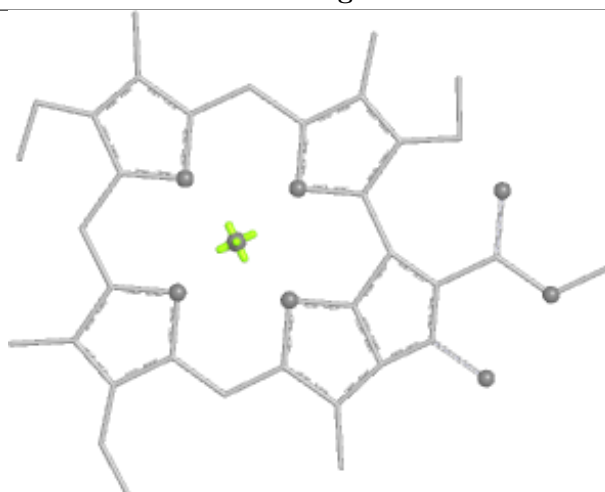
Bond lengths



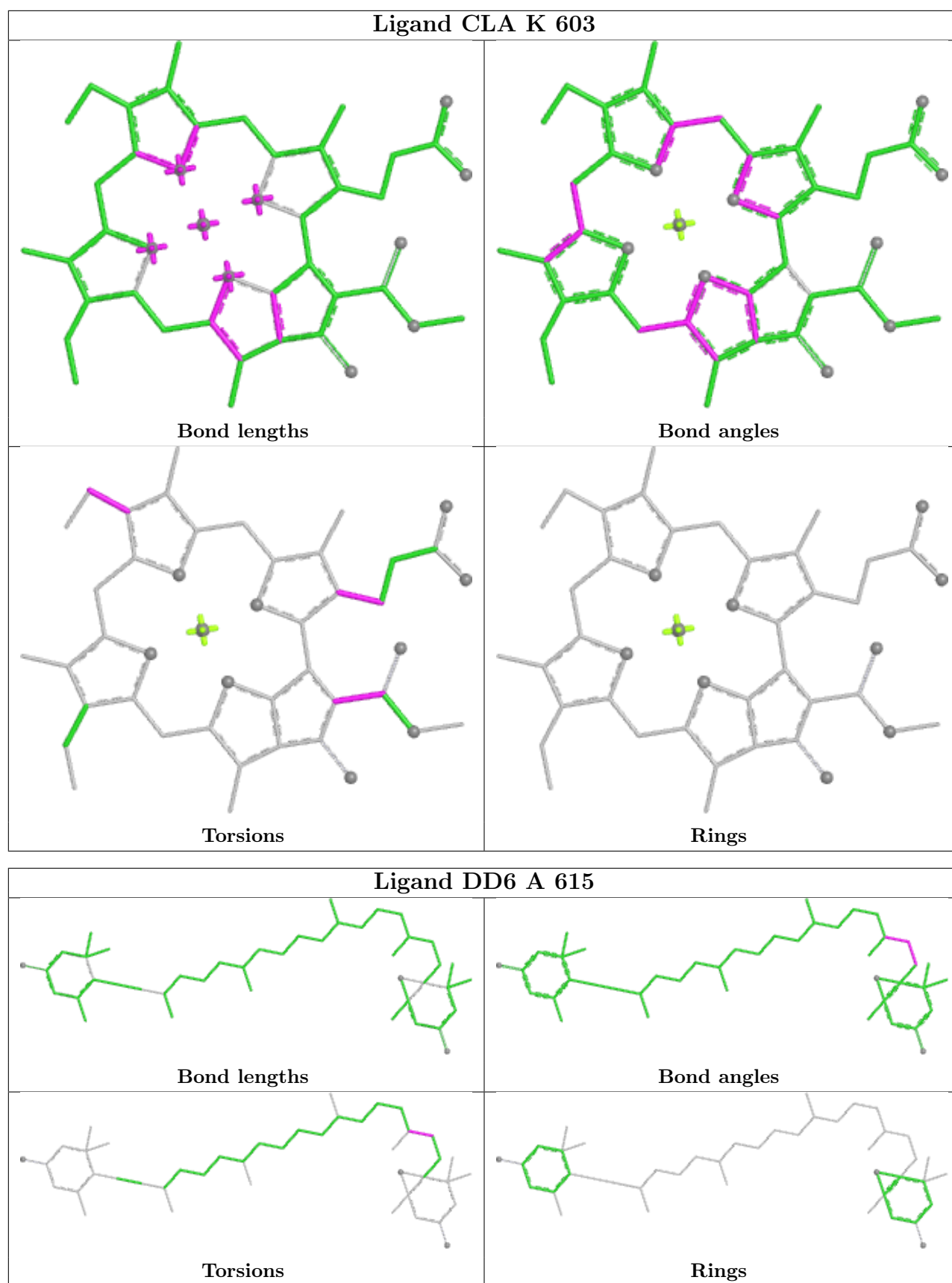
Bond angles

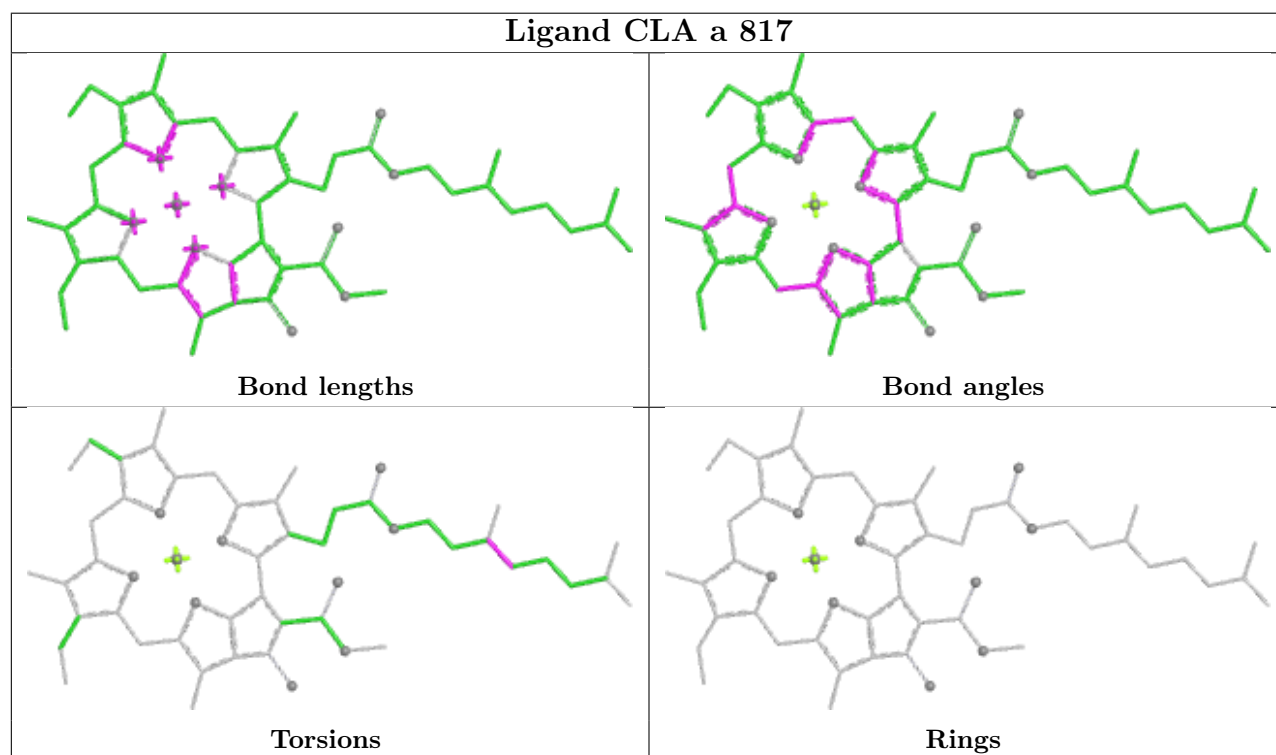
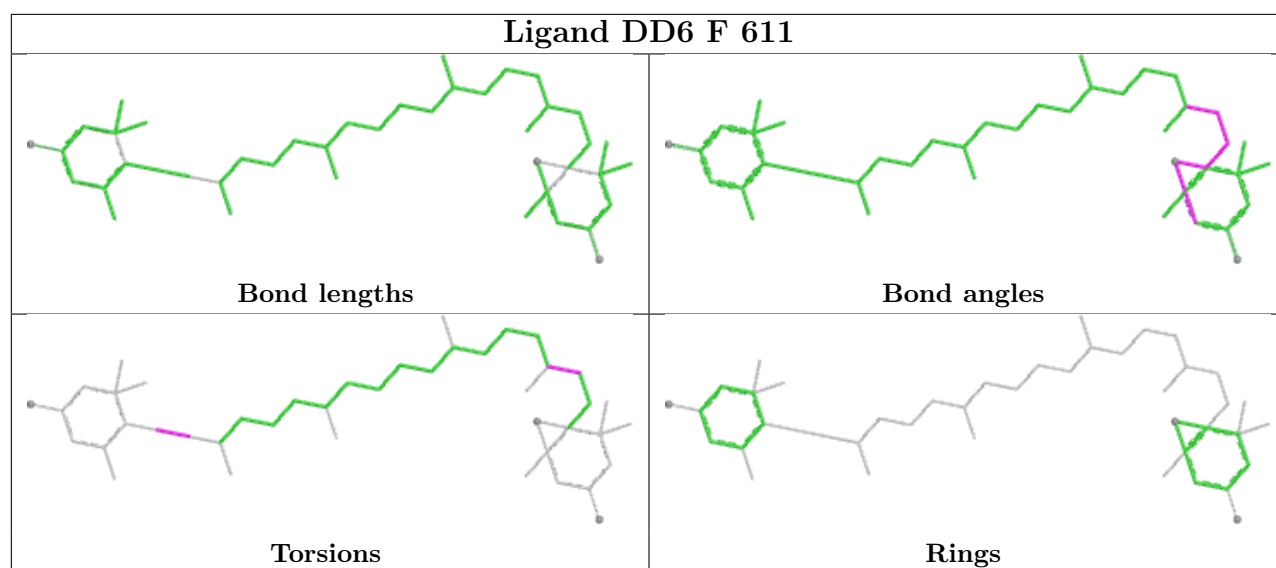


Torsions

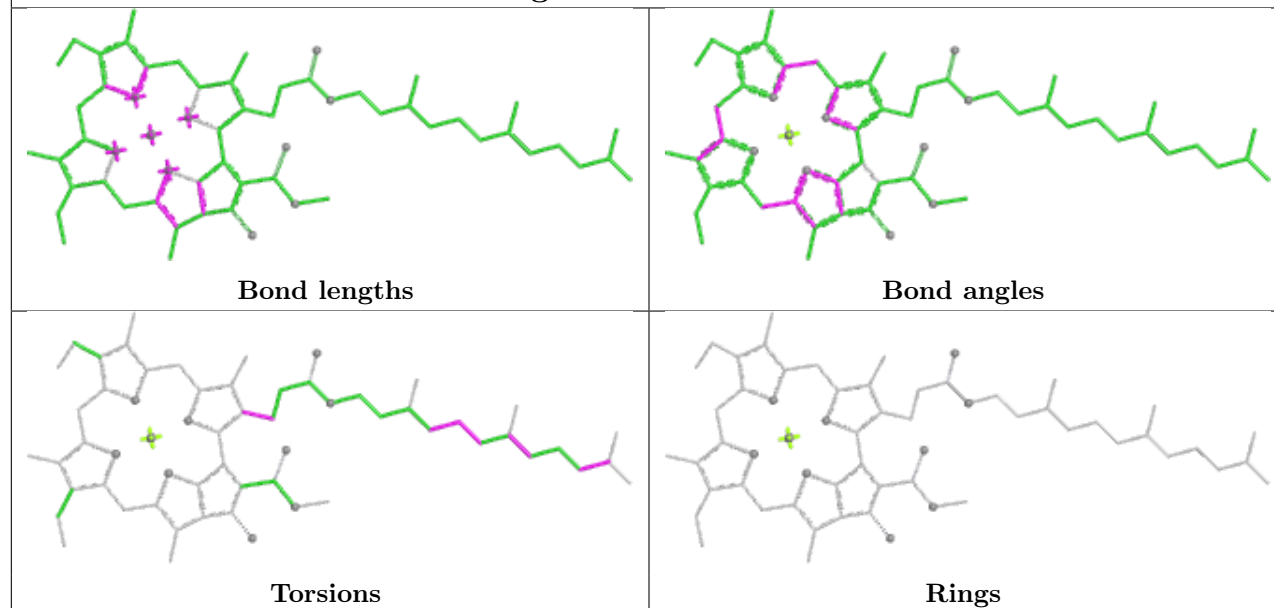


Rings

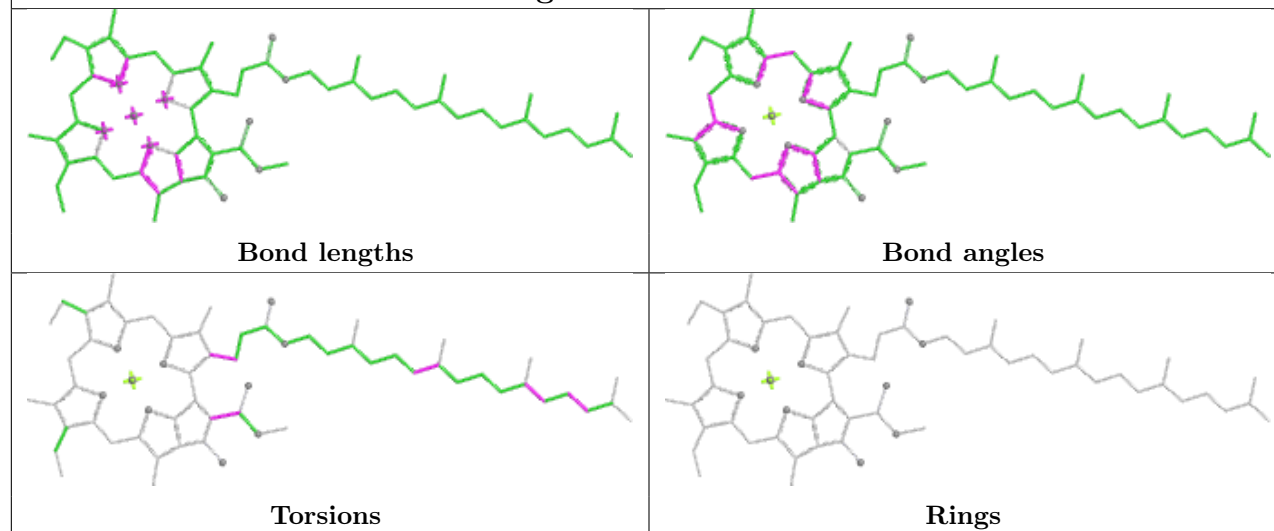


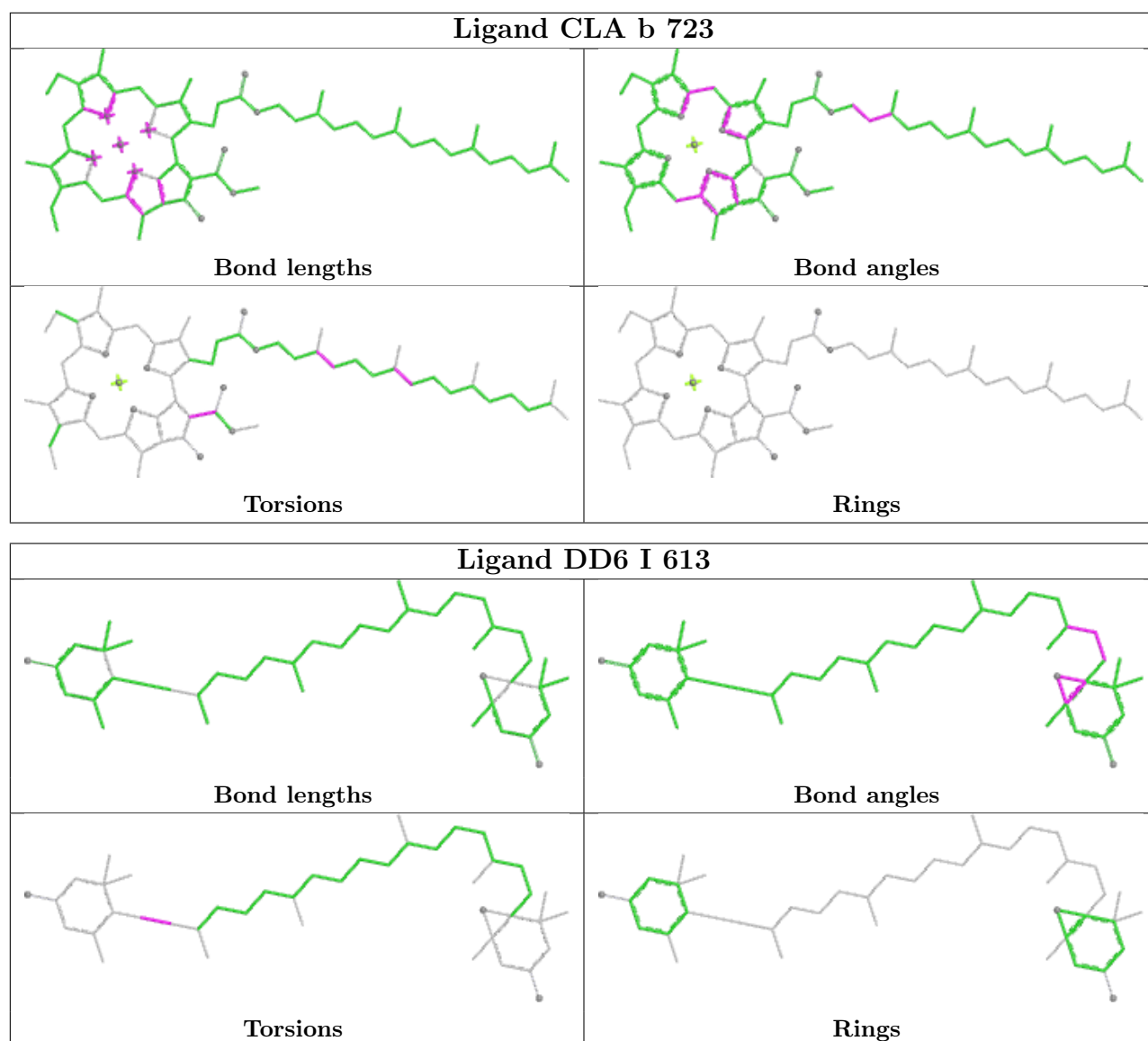


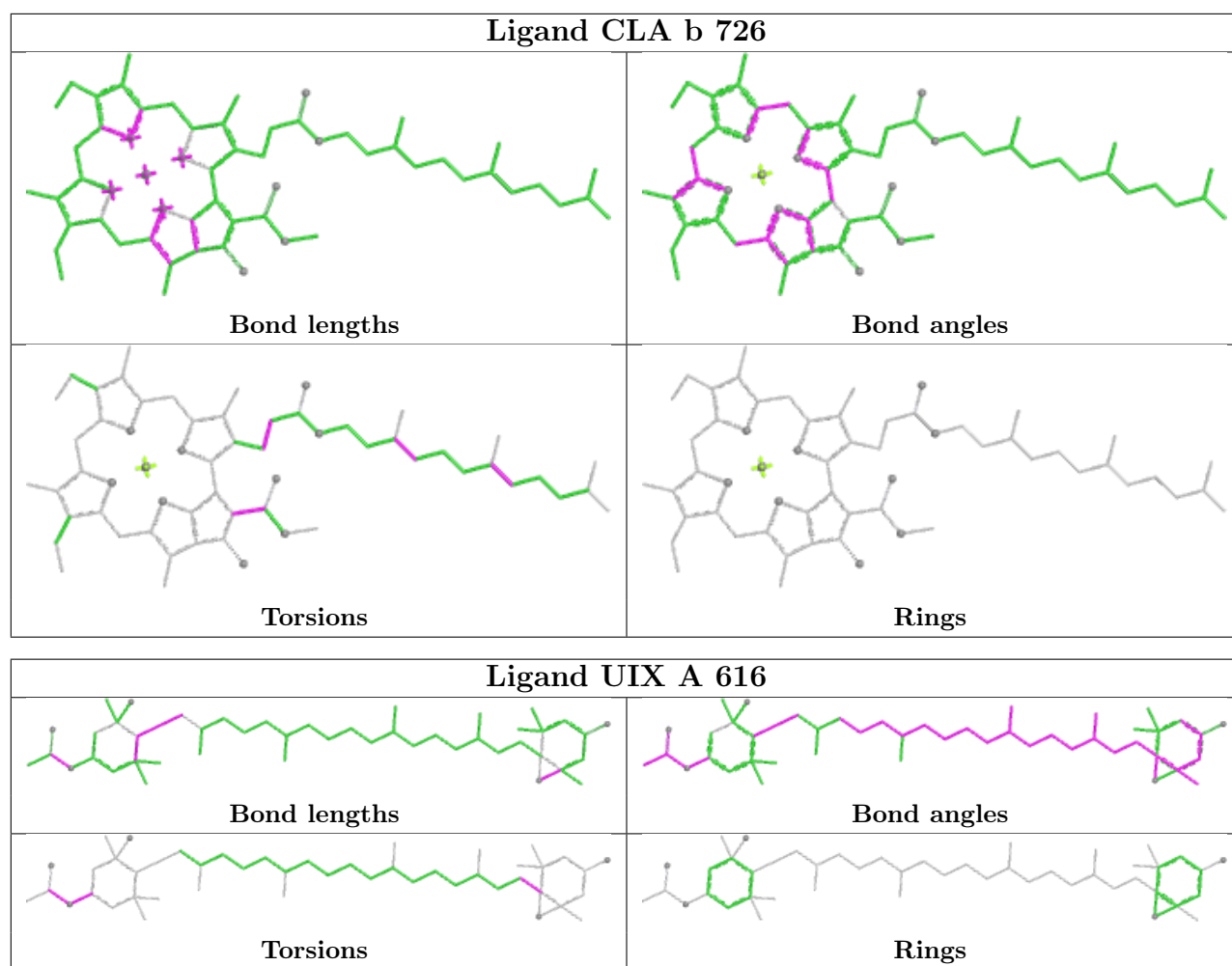
Ligand CLA G 608



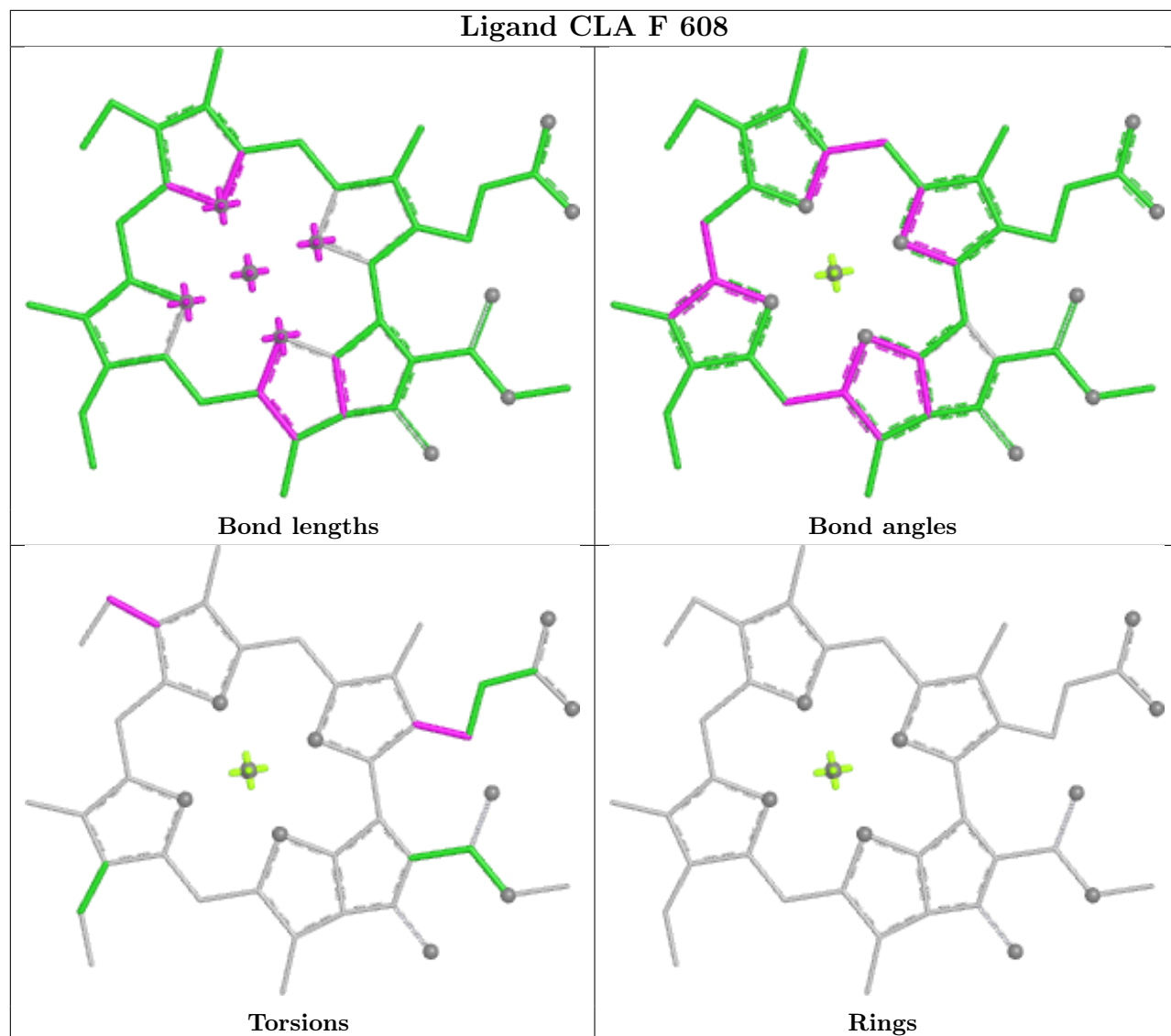
Ligand CLA a 820



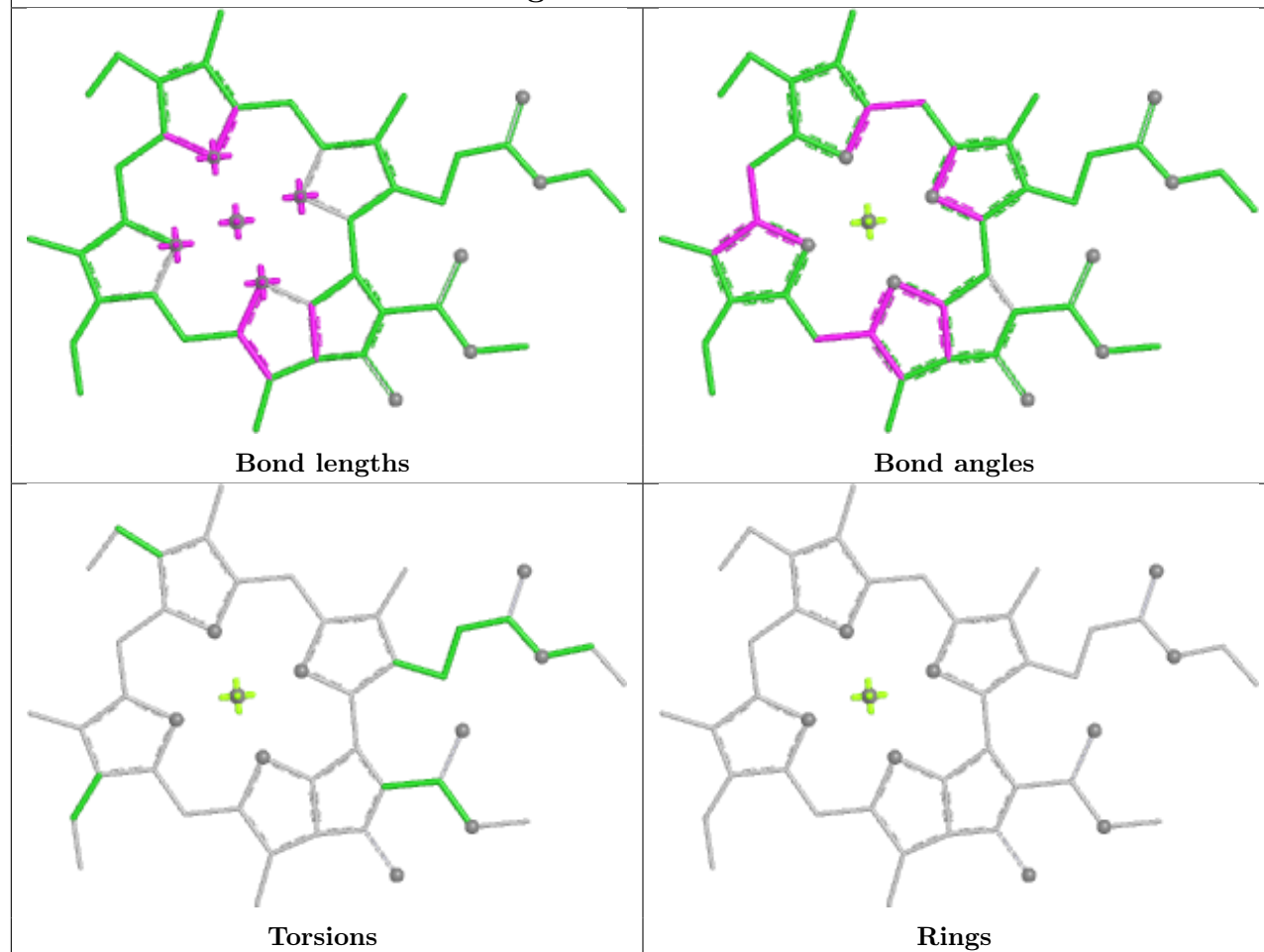




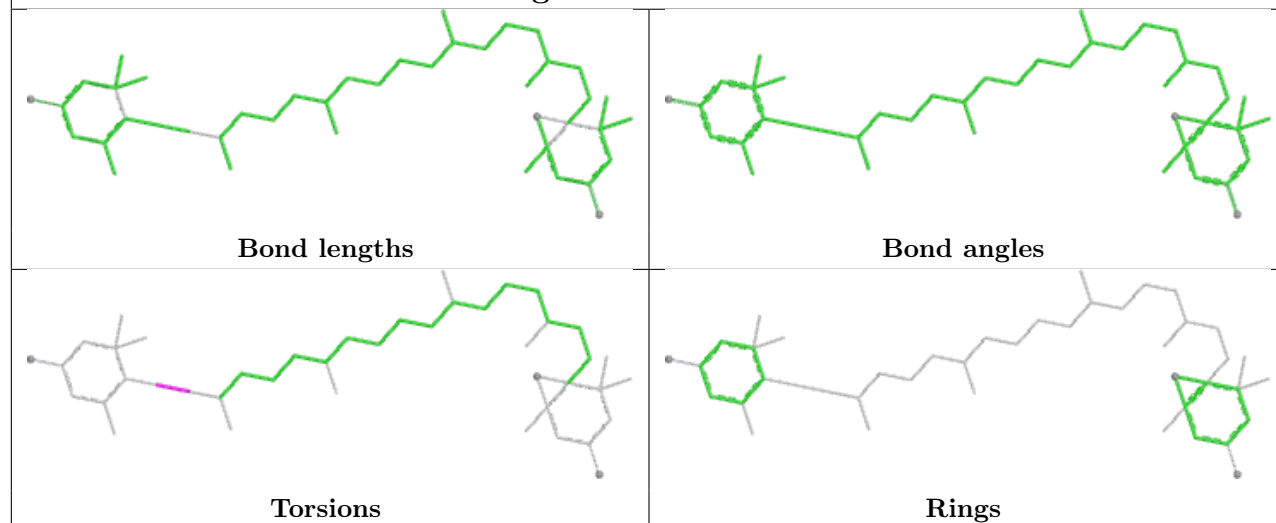
Ligand CLA F 608

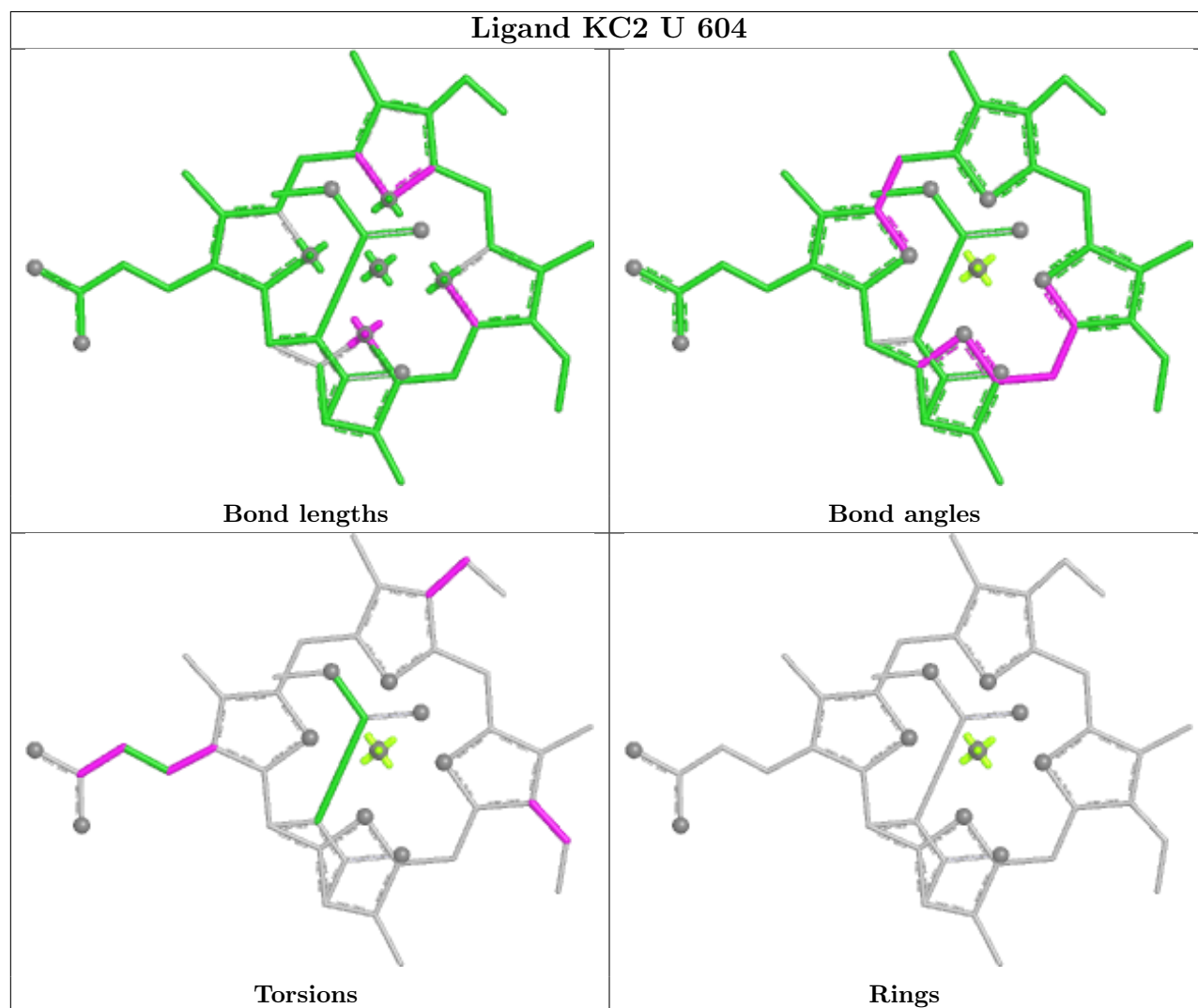
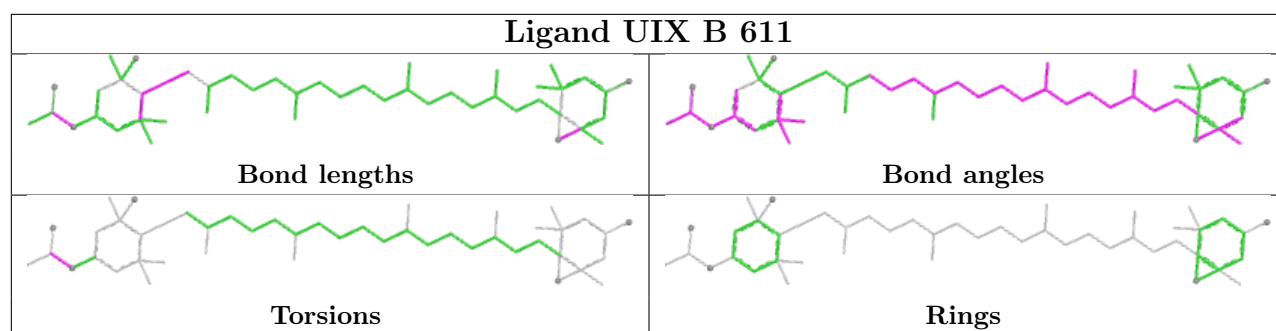


Ligand CLA C 208

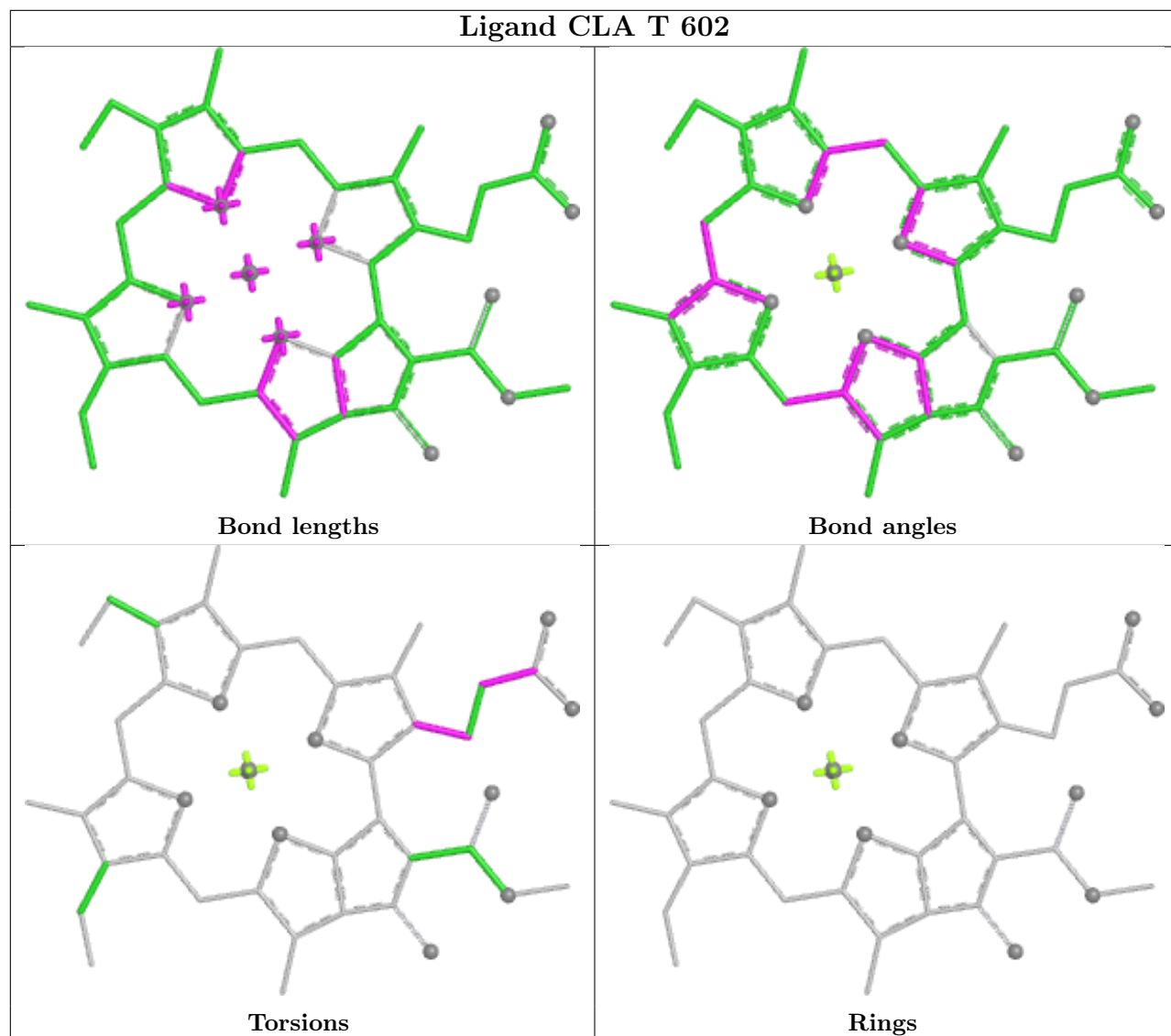


Ligand DD6 G 616

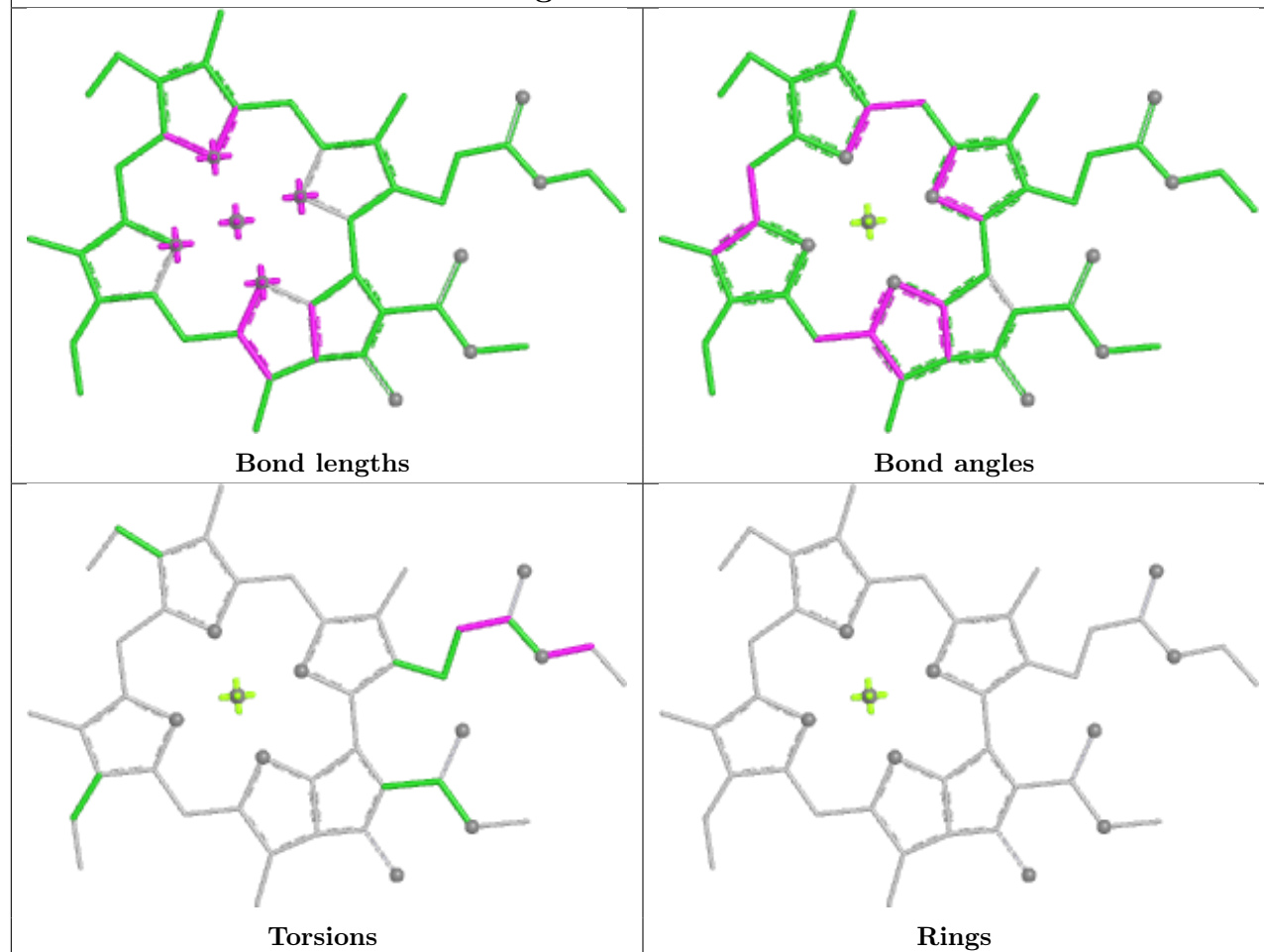




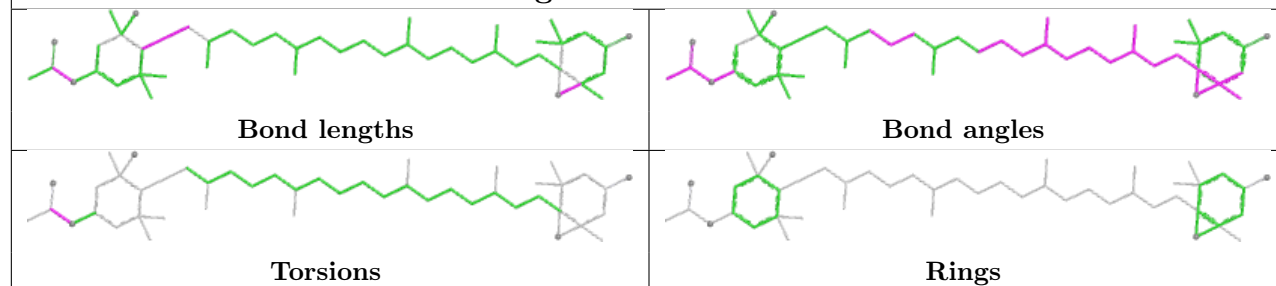
Ligand CLA T 602

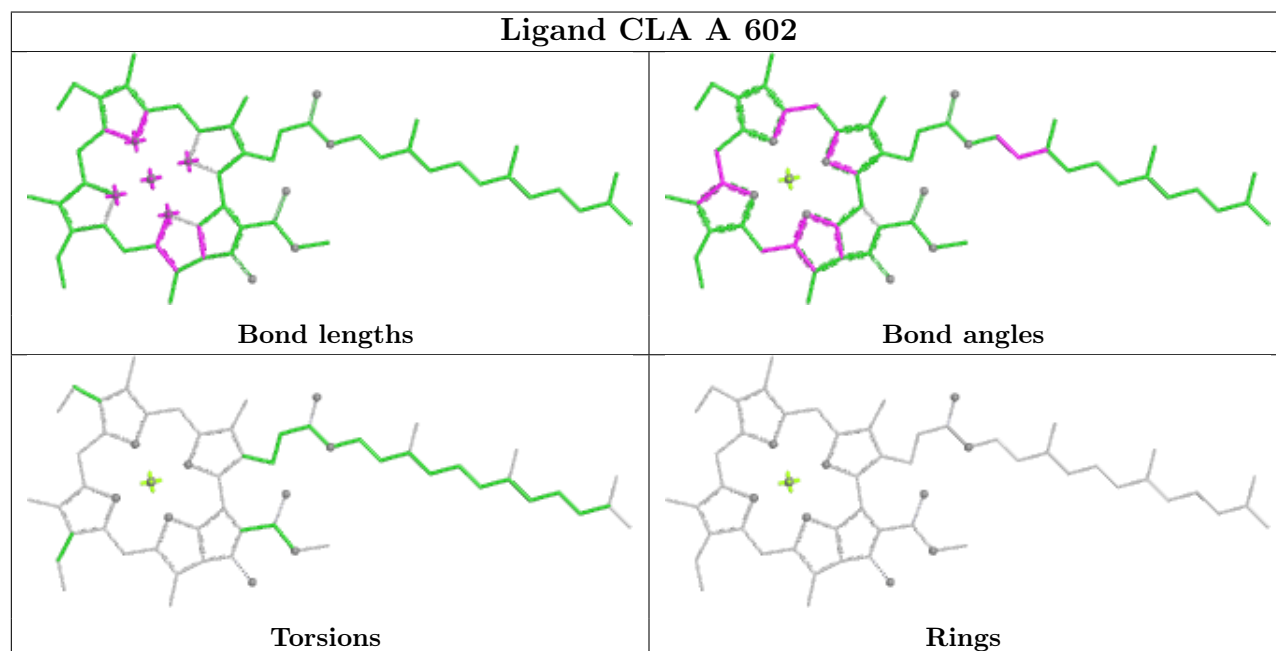
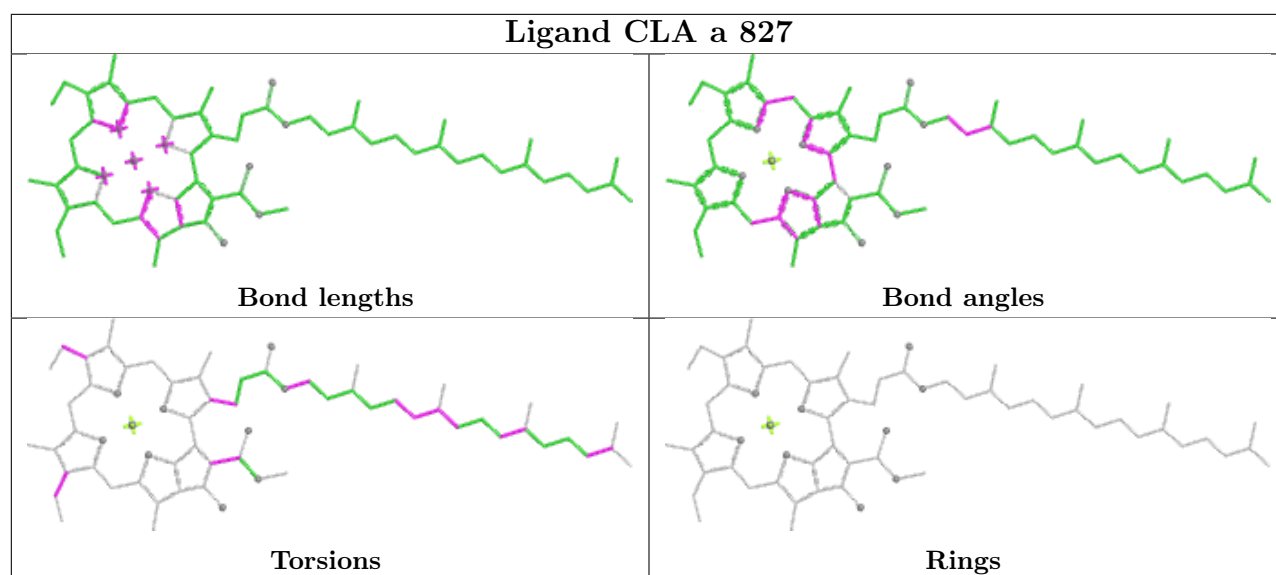


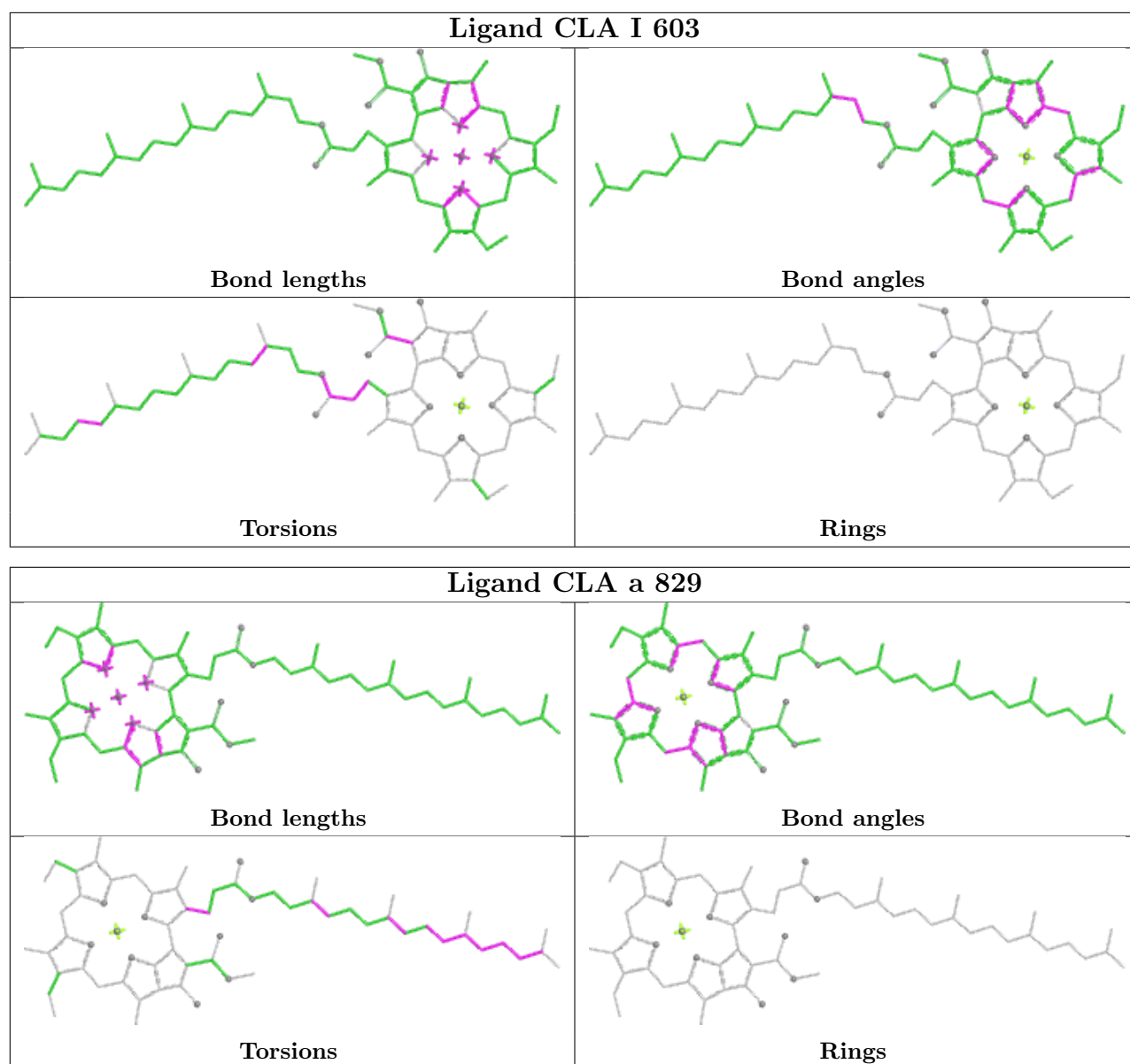
Ligand CLA 1 408

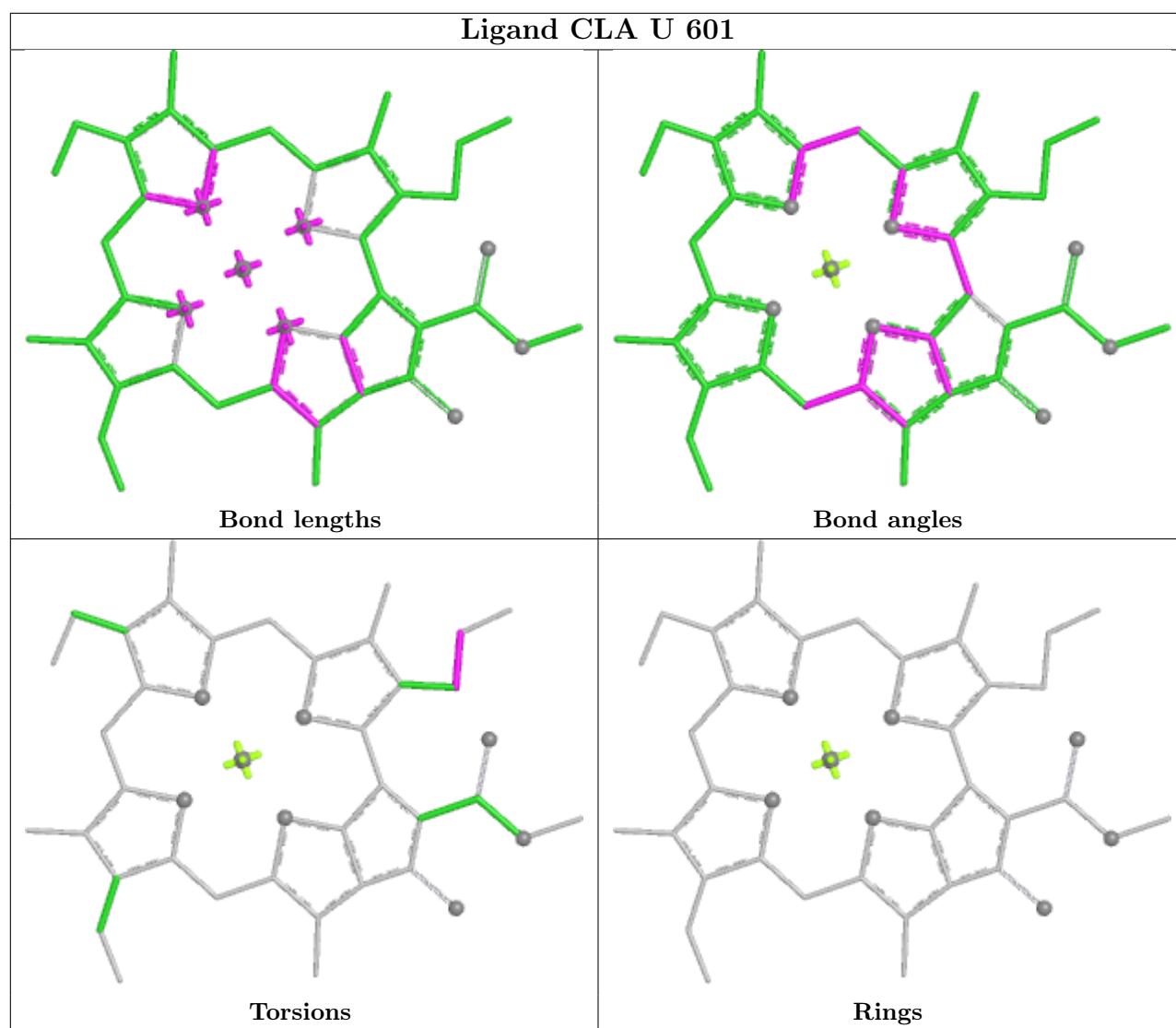


Ligand UIX A 613

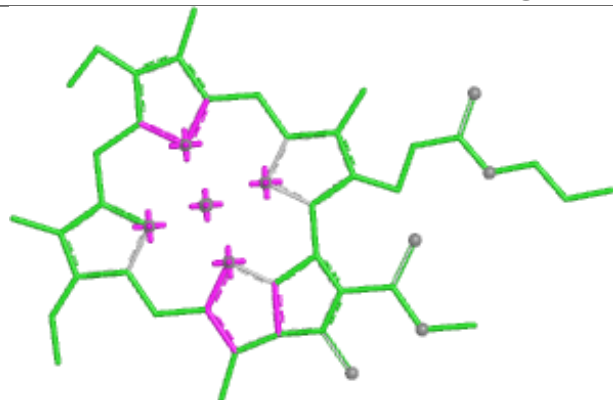




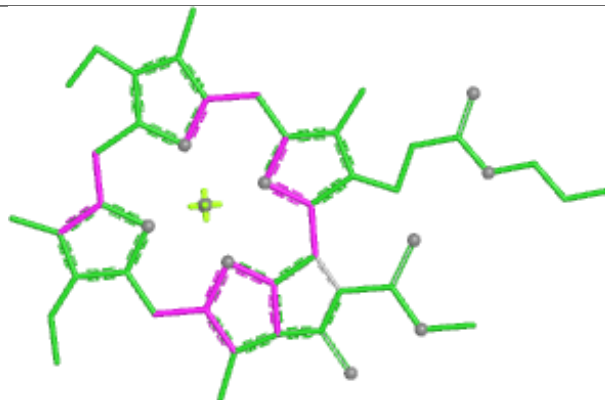




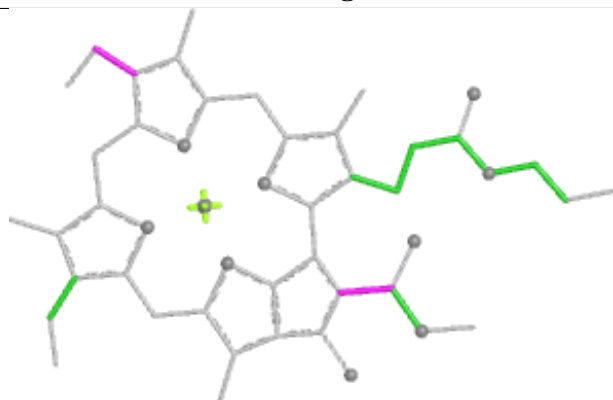
Ligand CLA b 720



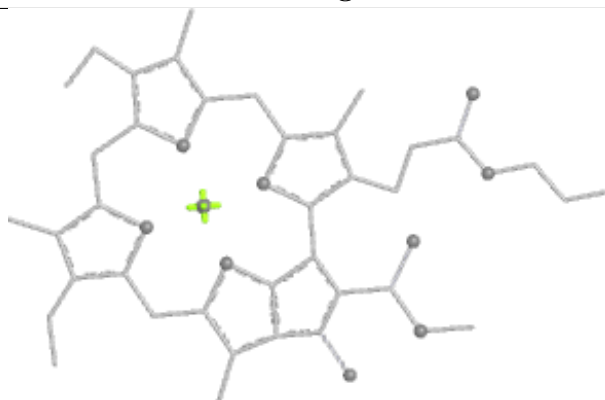
Bond lengths



Bond angles

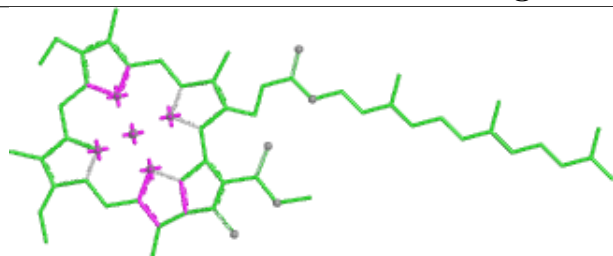


Torsions

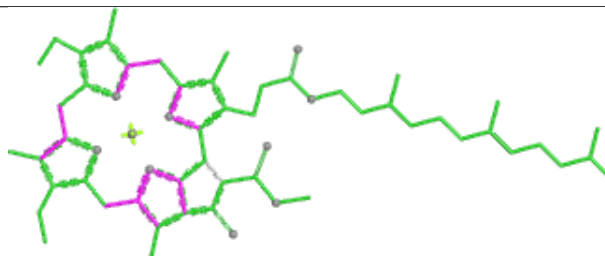


Rings

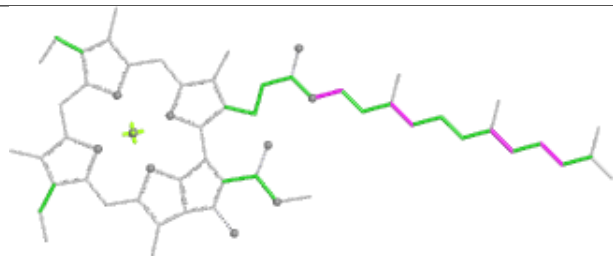
Ligand CLA U 605



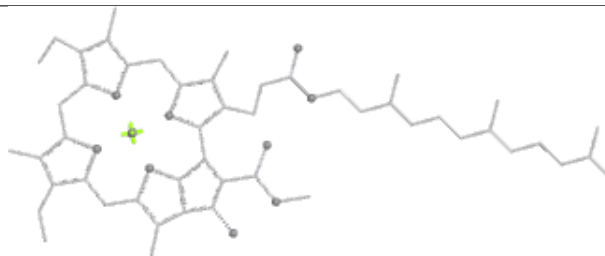
Bond lengths



Bond angles

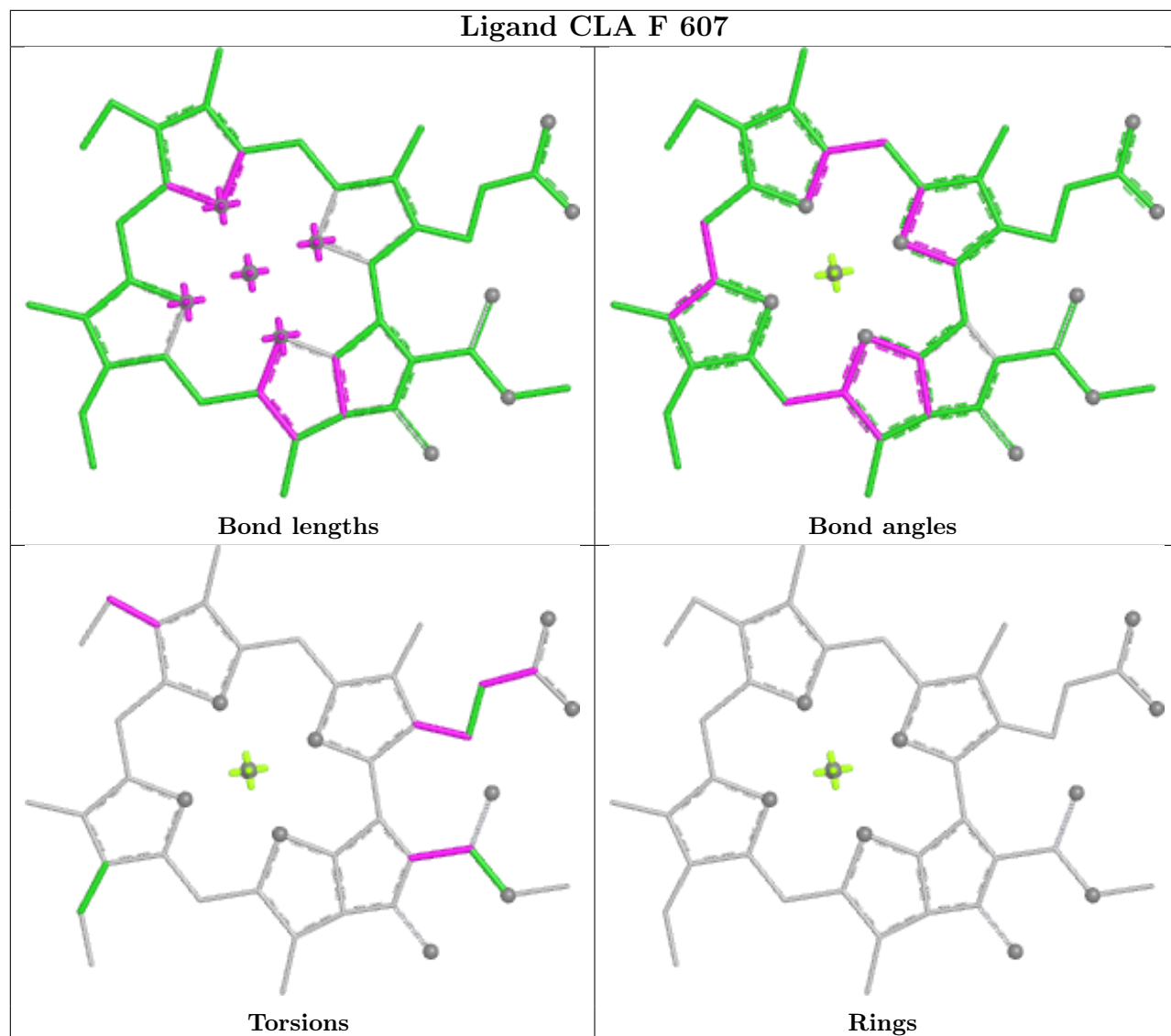


Torsions

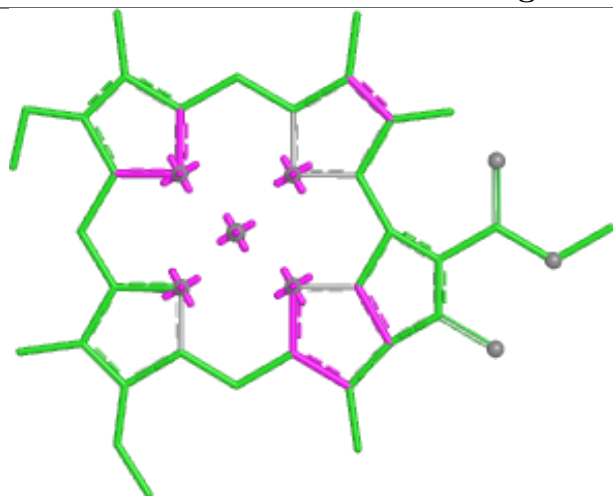


Rings

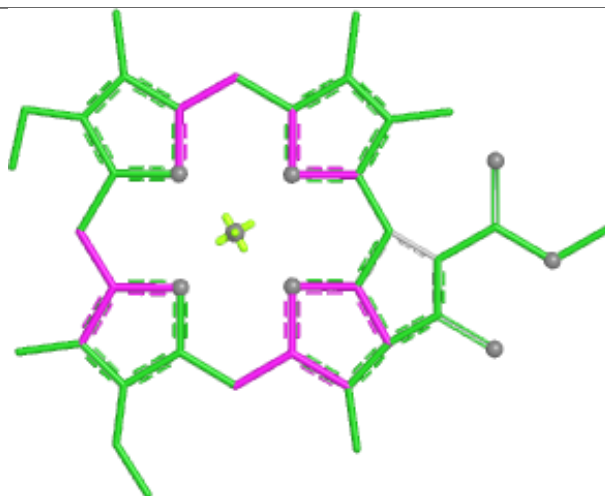
Ligand CLA F 607



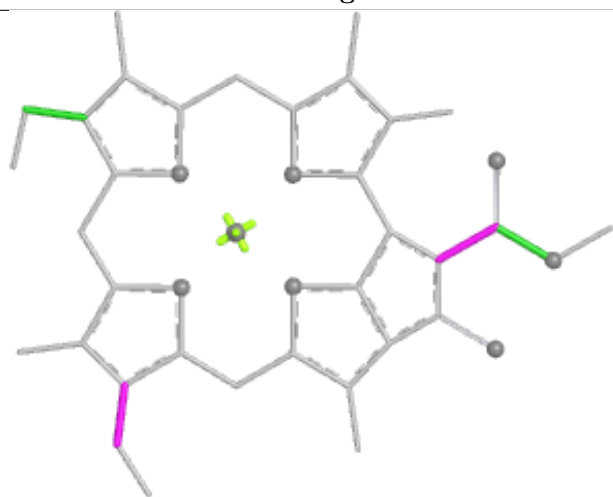
Ligand CLA J 609



Bond lengths



Bond angles

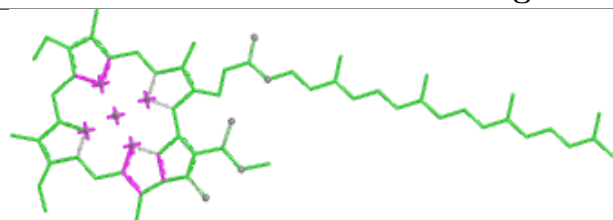


Torsions

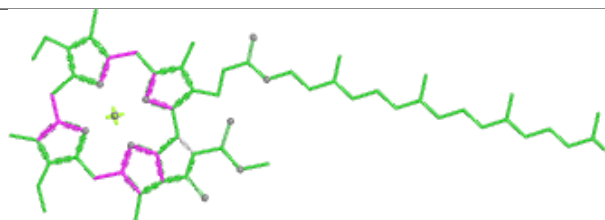


Rings

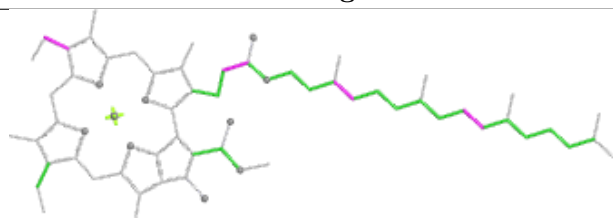
Ligand CLA H 309



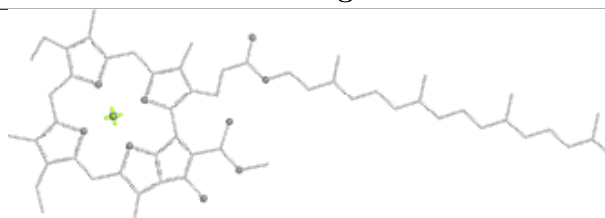
Bond lengths



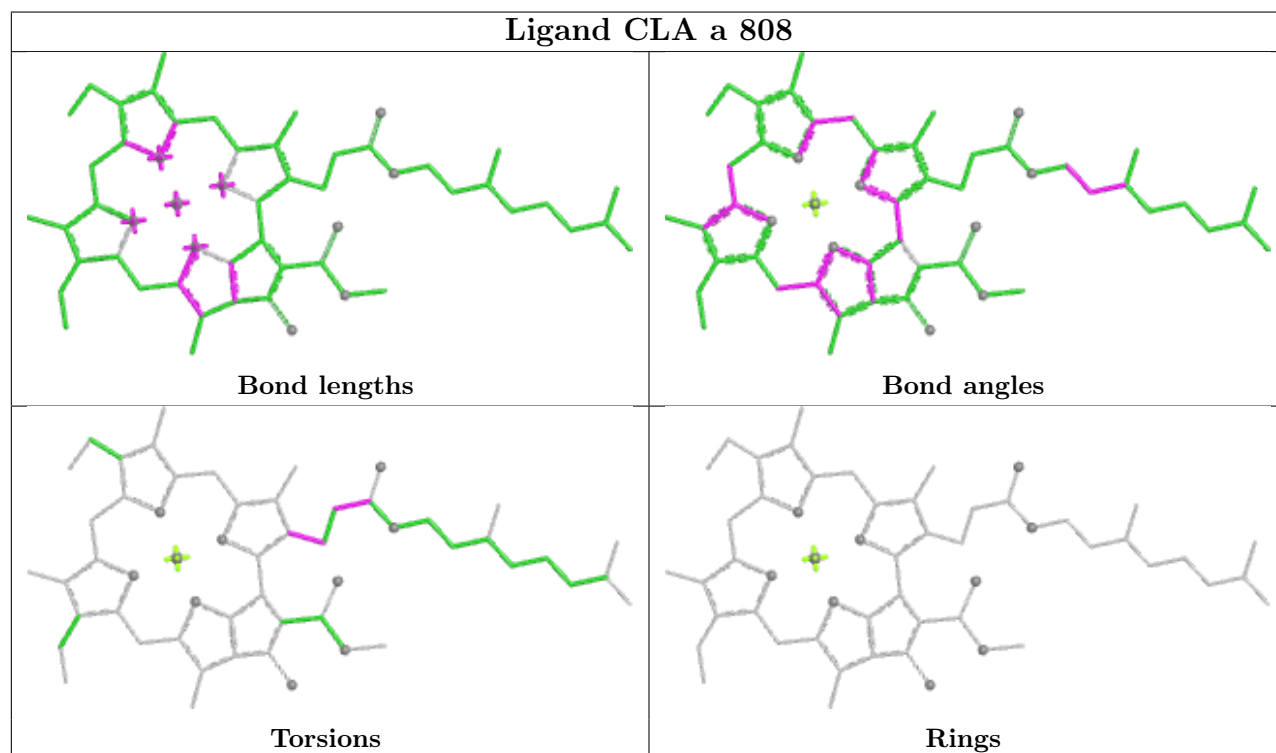
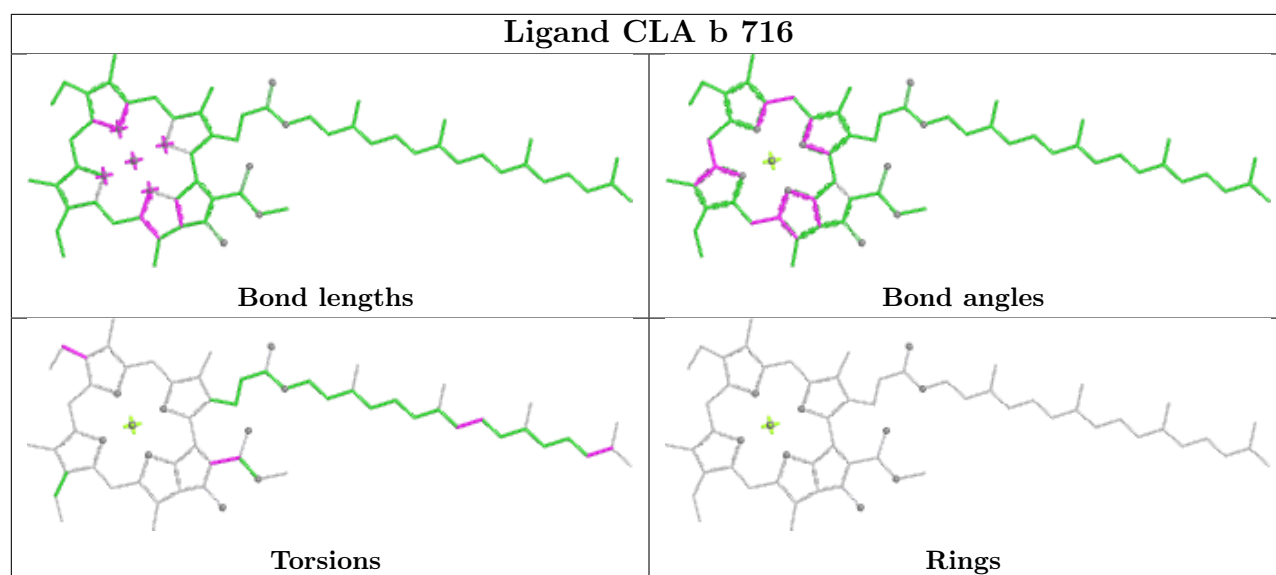
Bond angles

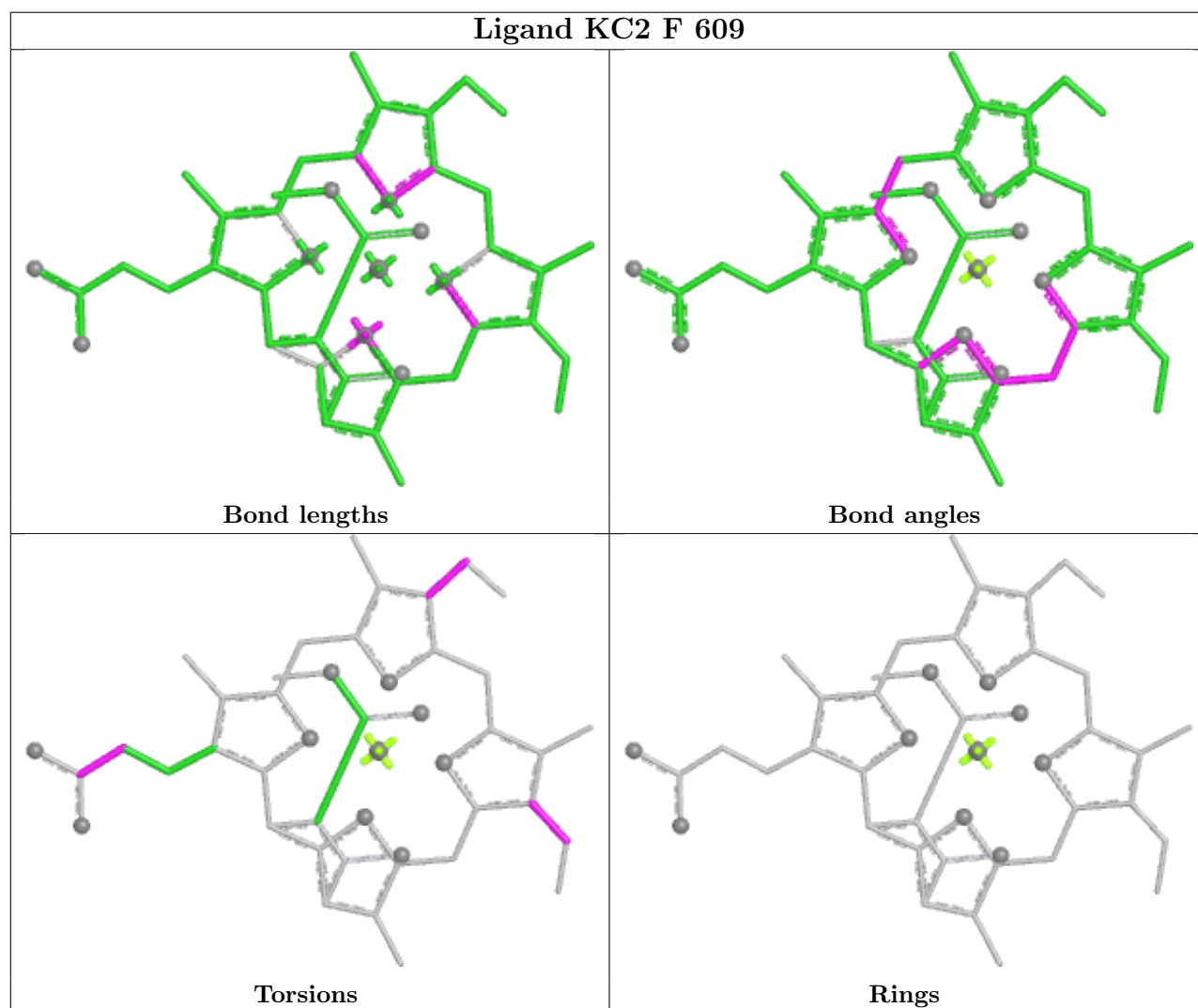
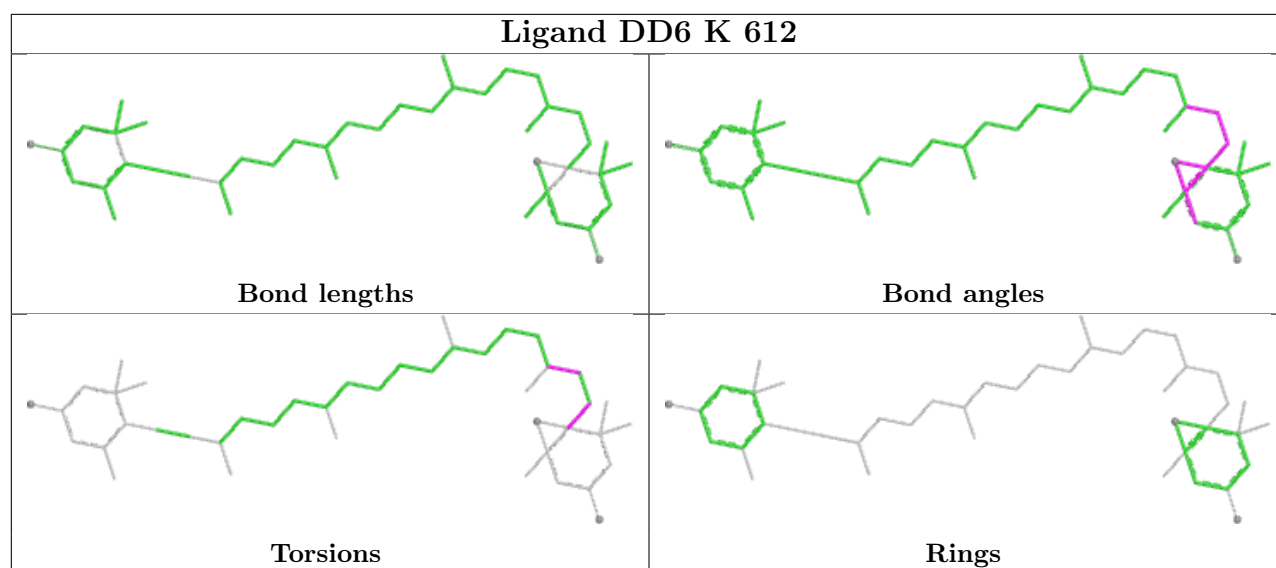


Torsions

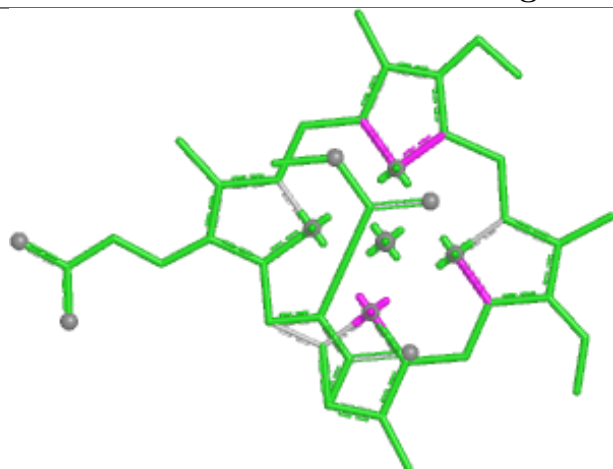


Rings

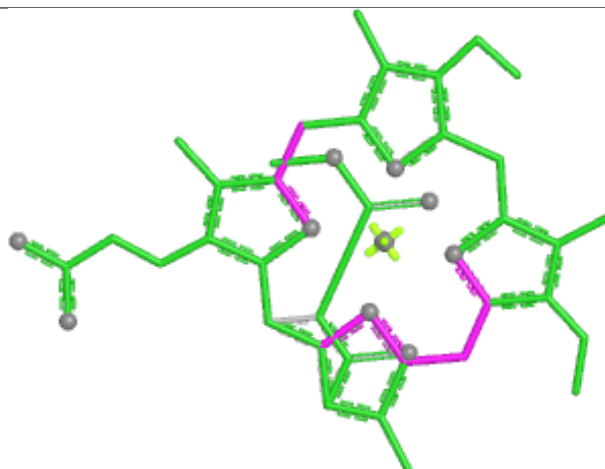




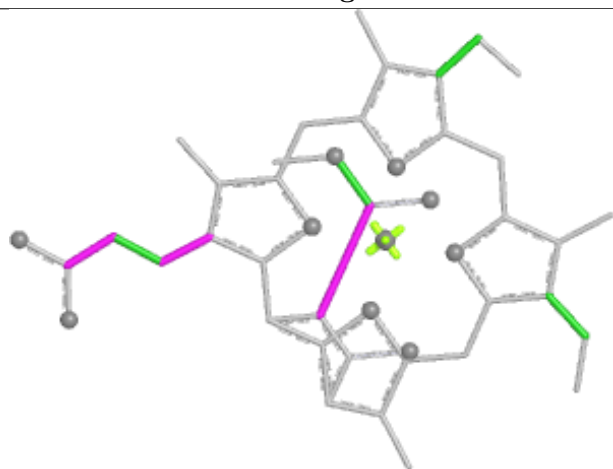
Ligand KC2 J 606



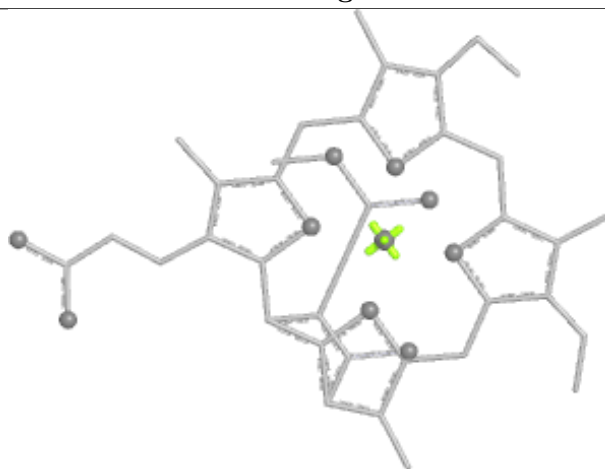
Bond lengths



Bond angles

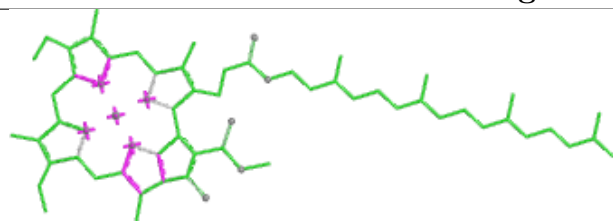


Torsions

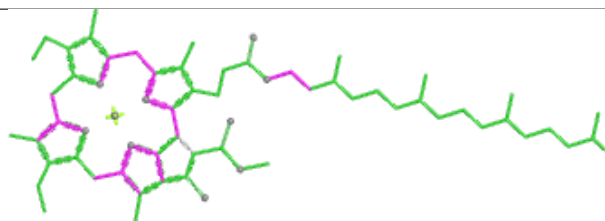


Rings

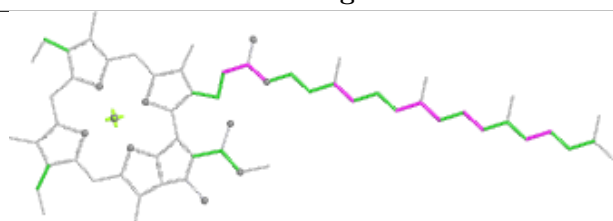
Ligand CLA a 804



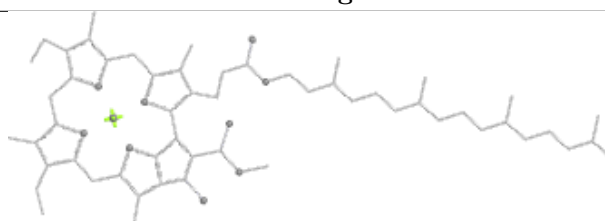
Bond lengths



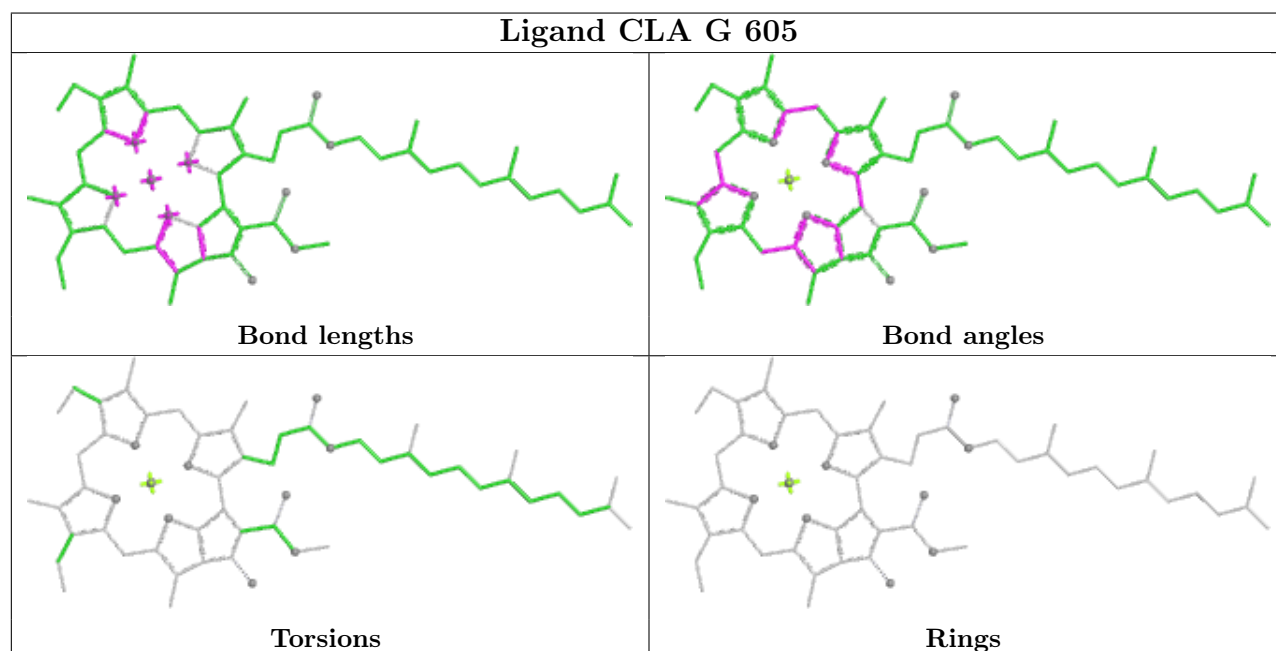
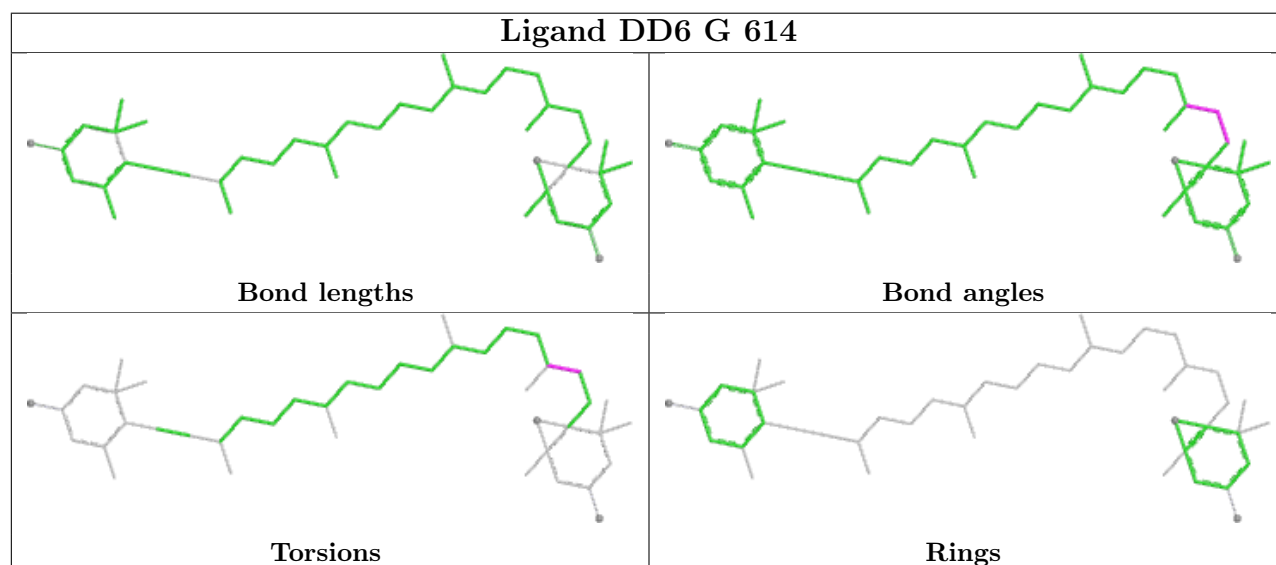
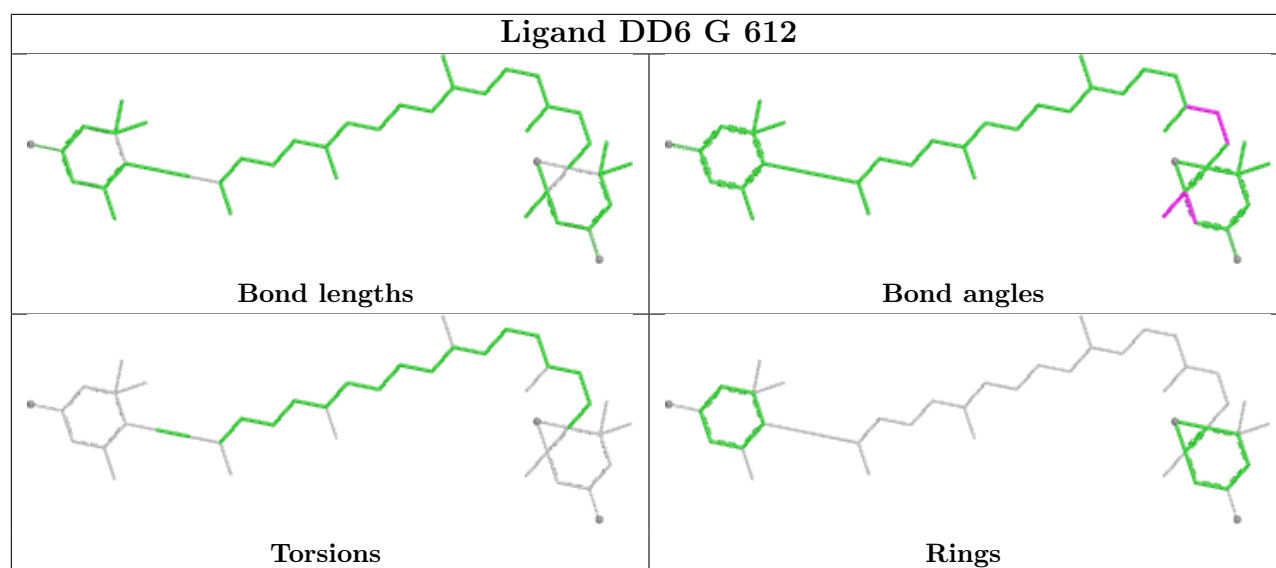
Bond angles



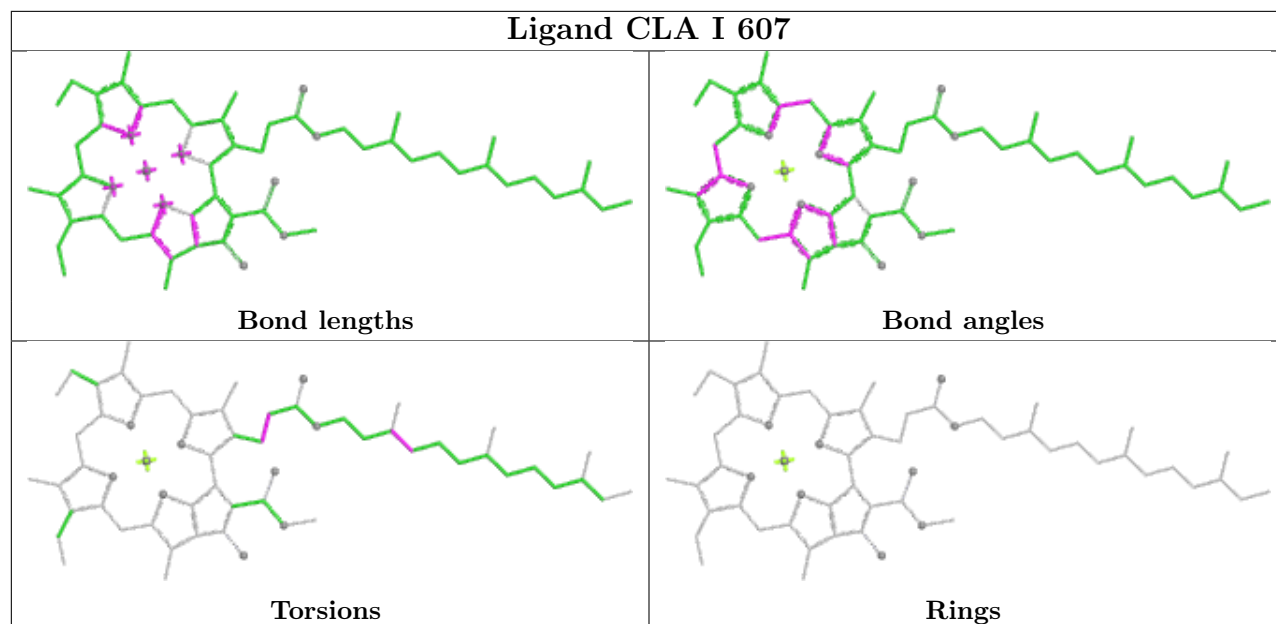
Torsions



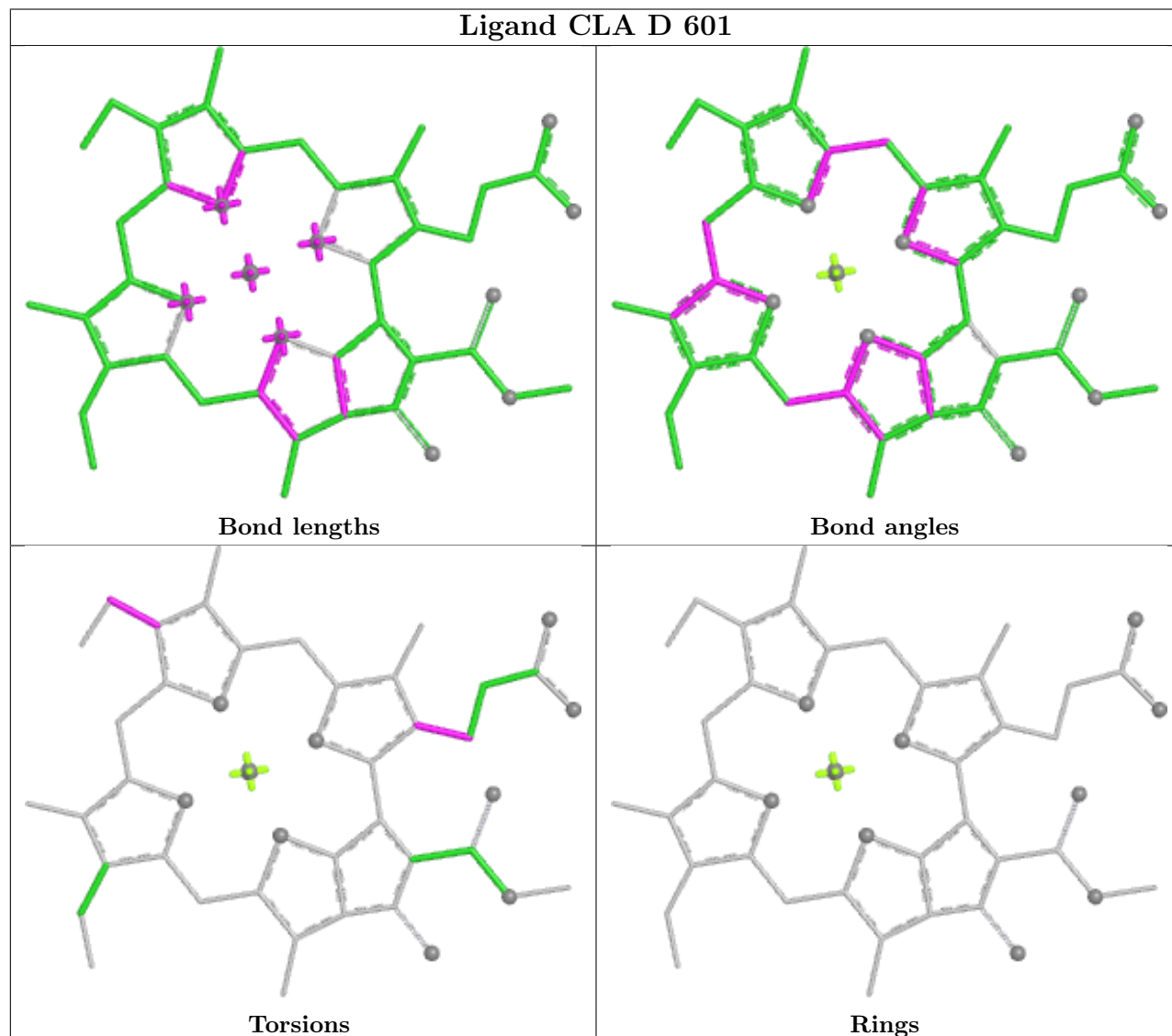
Rings

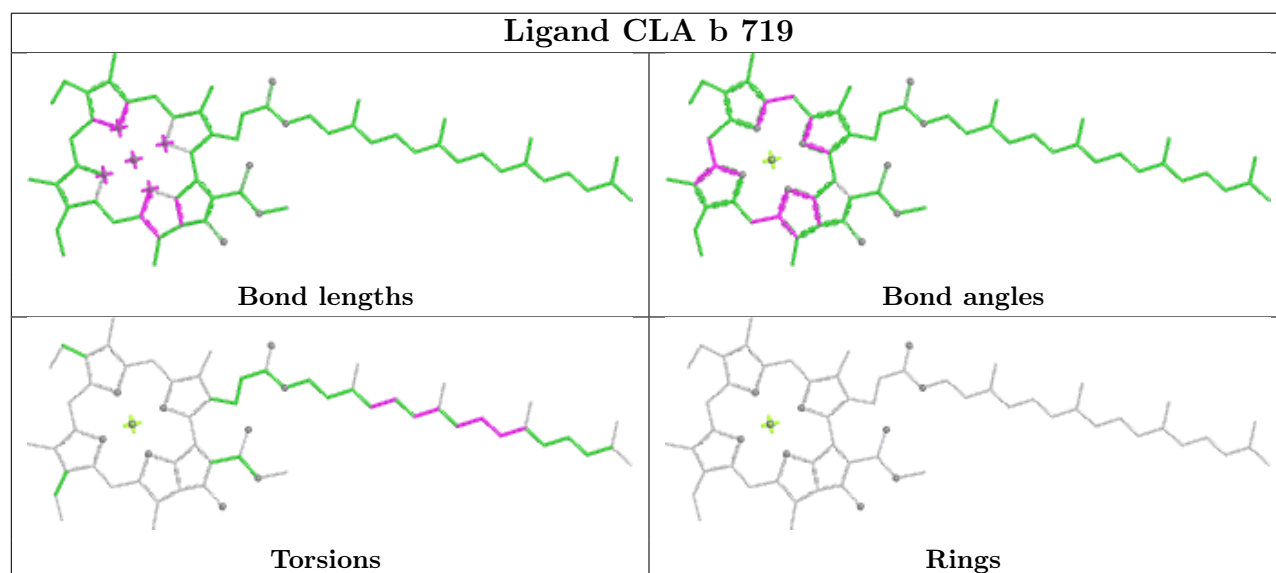
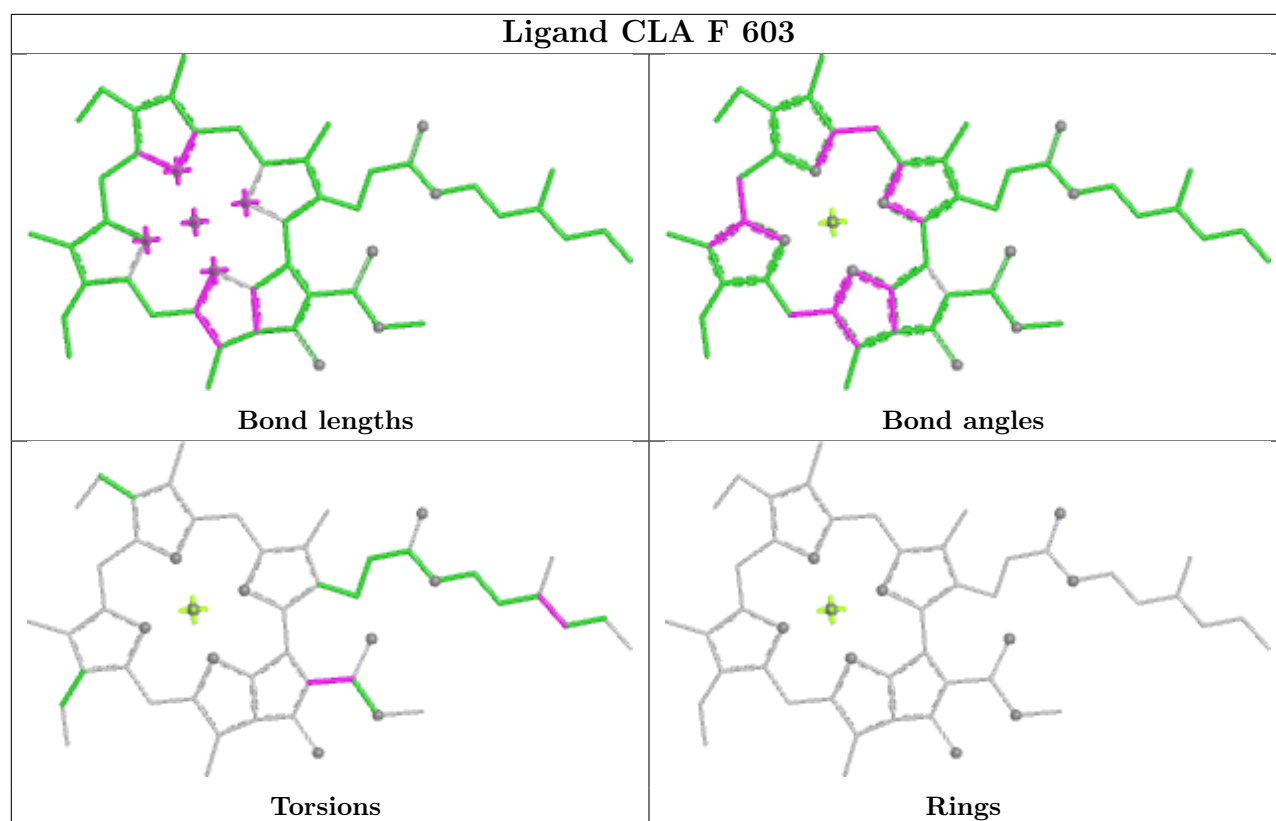


Ligand CLA I 607

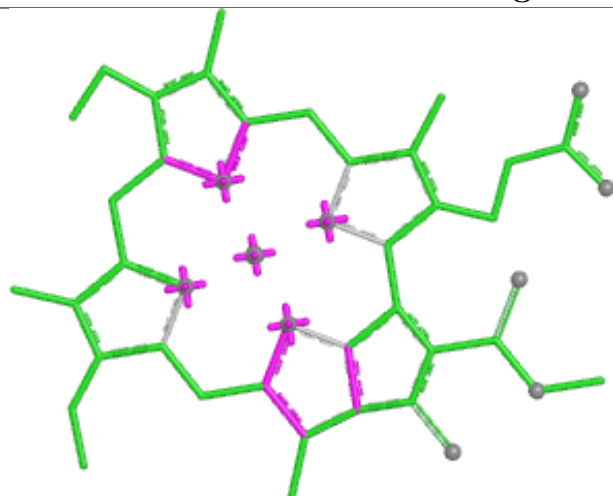


Ligand CLA D 601

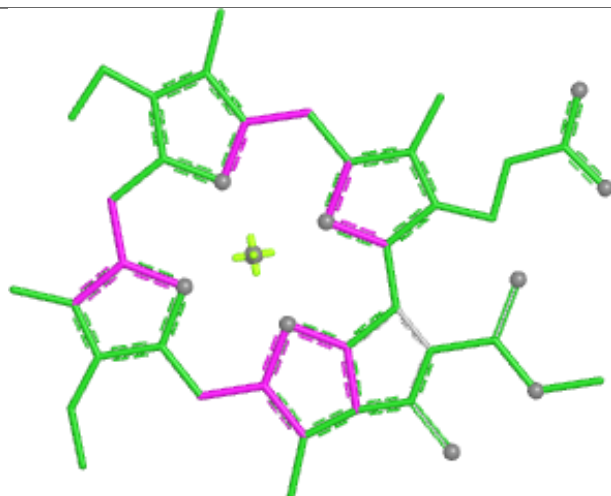




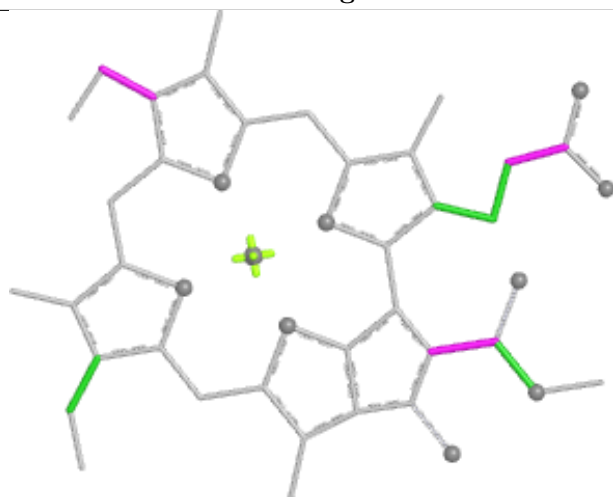
Ligand CLA H 307



Bond lengths



Bond angles

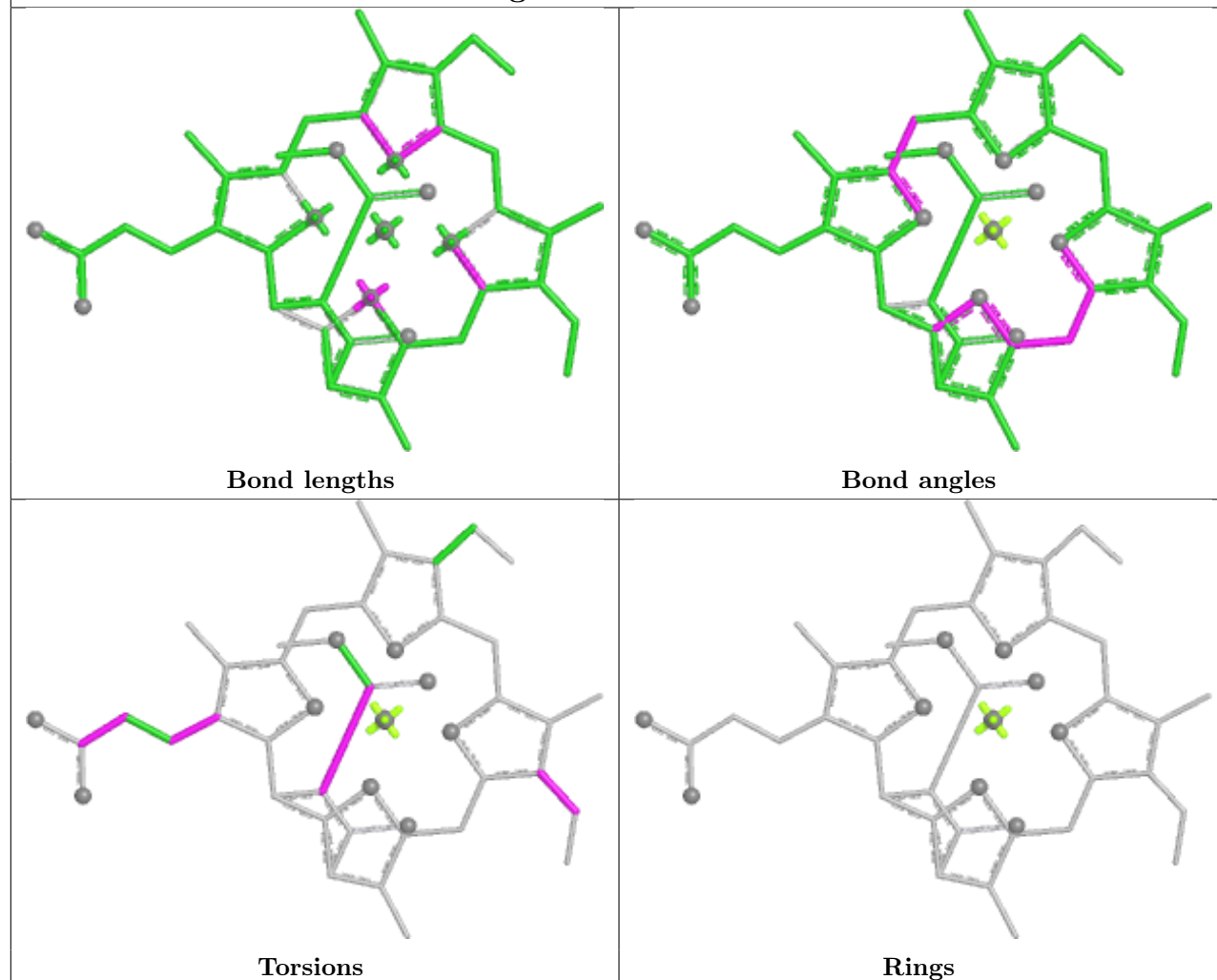


Torsions

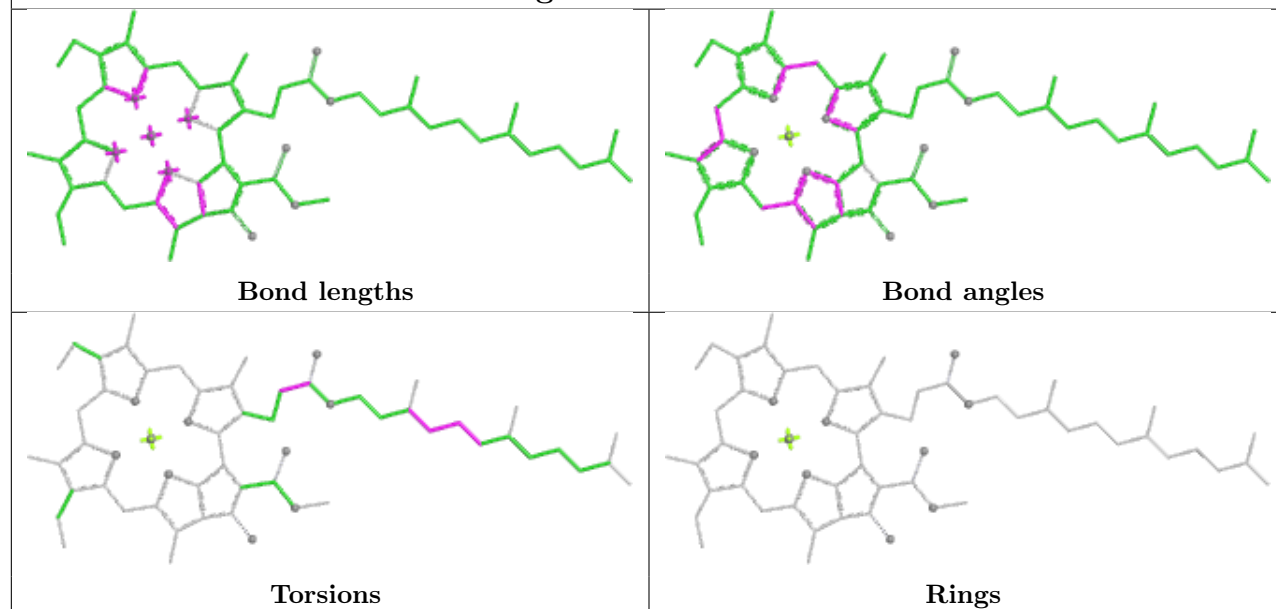


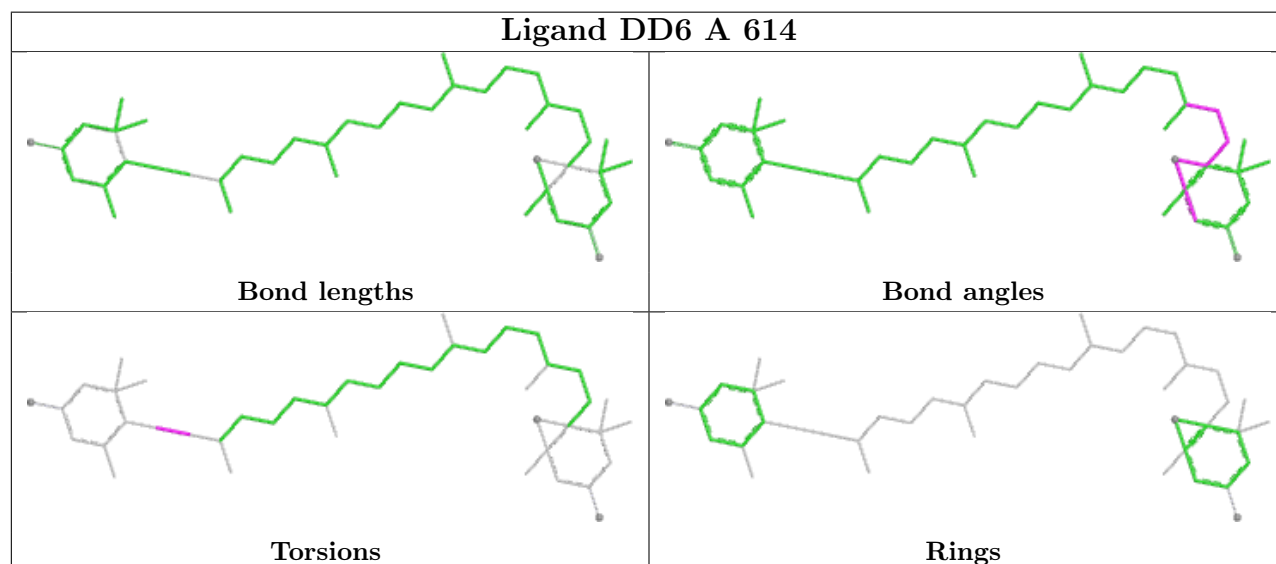
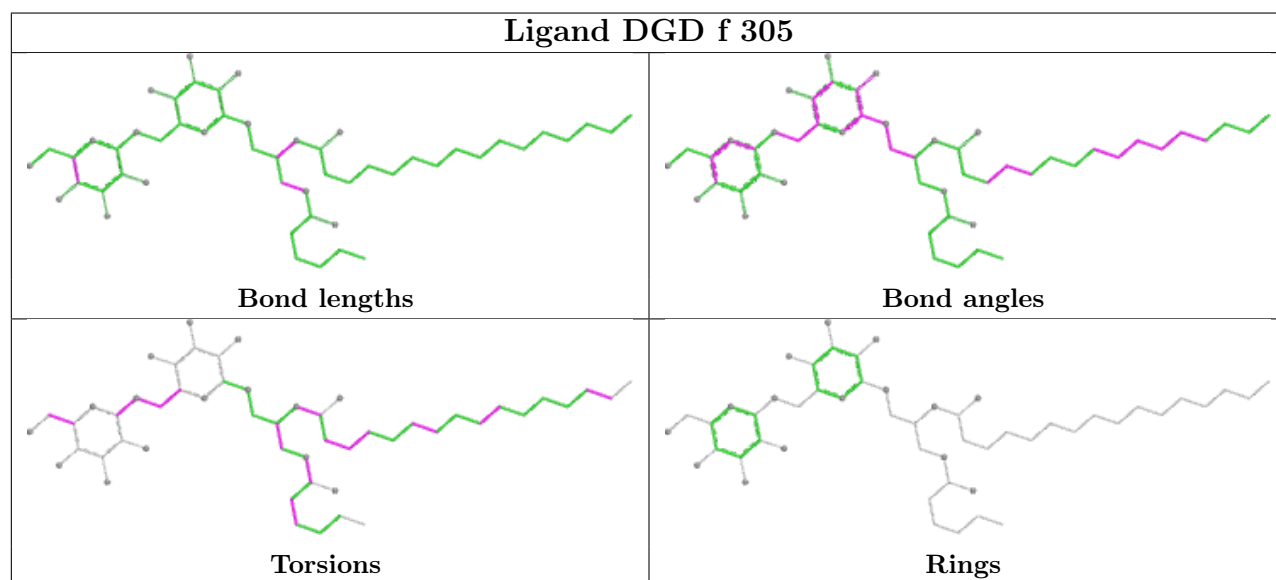
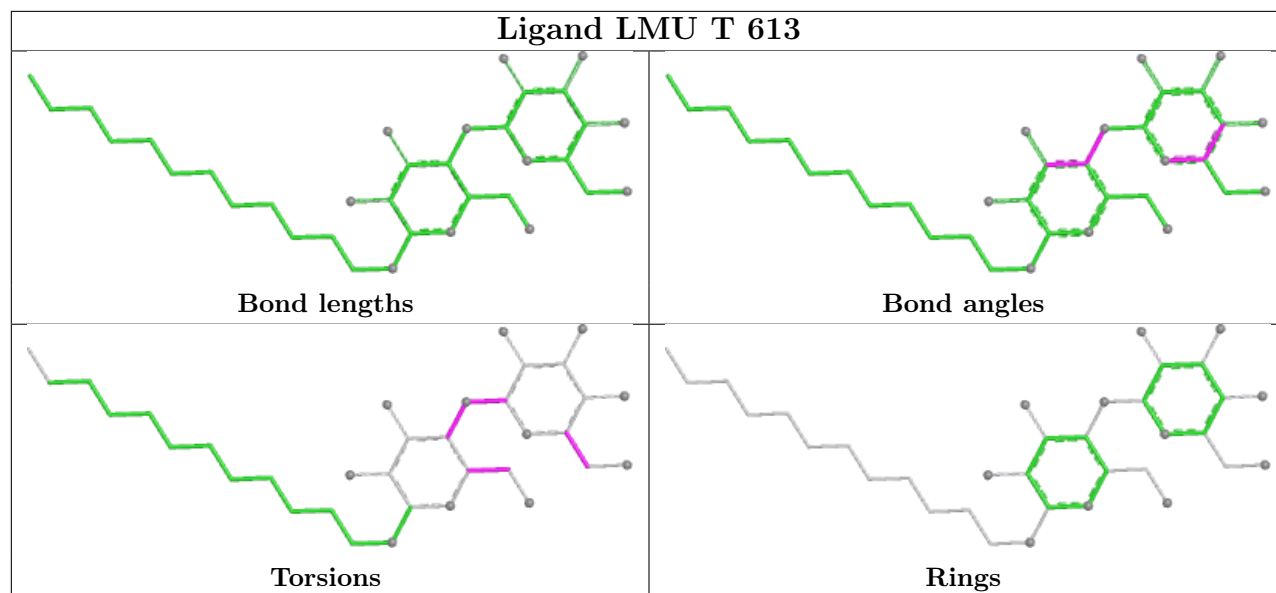
Rings

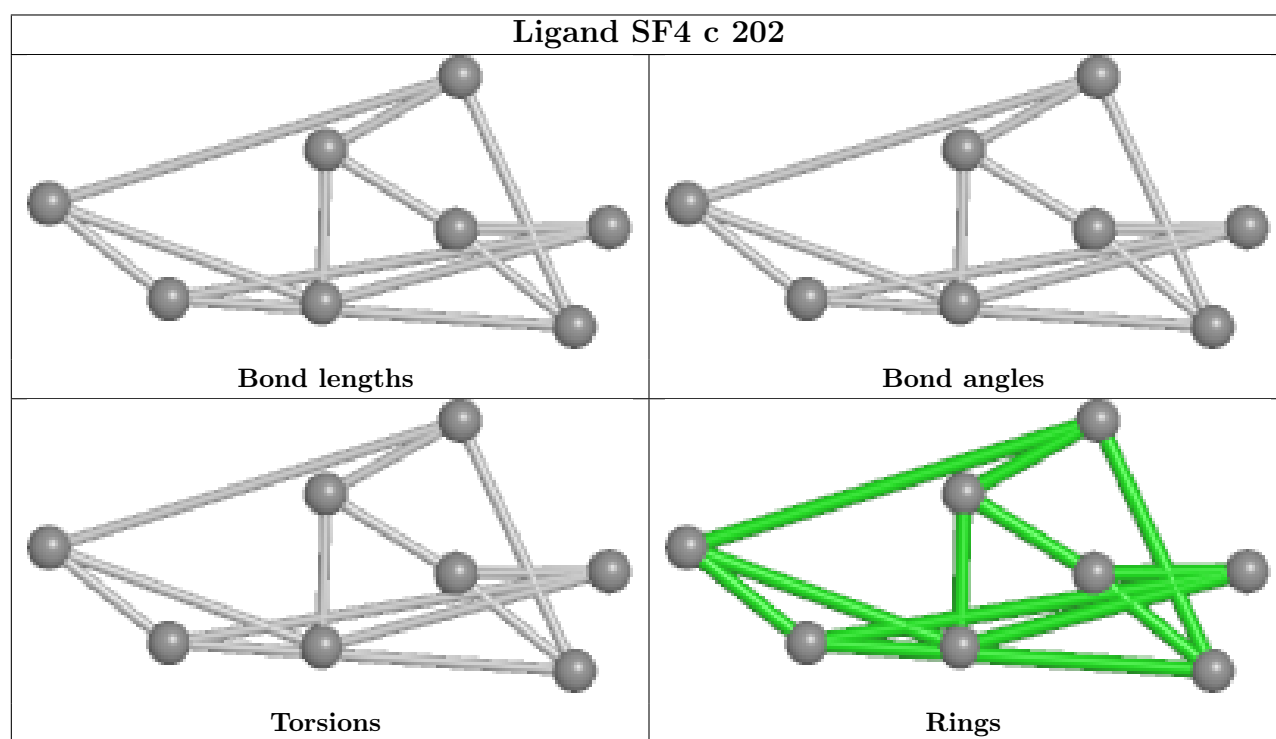
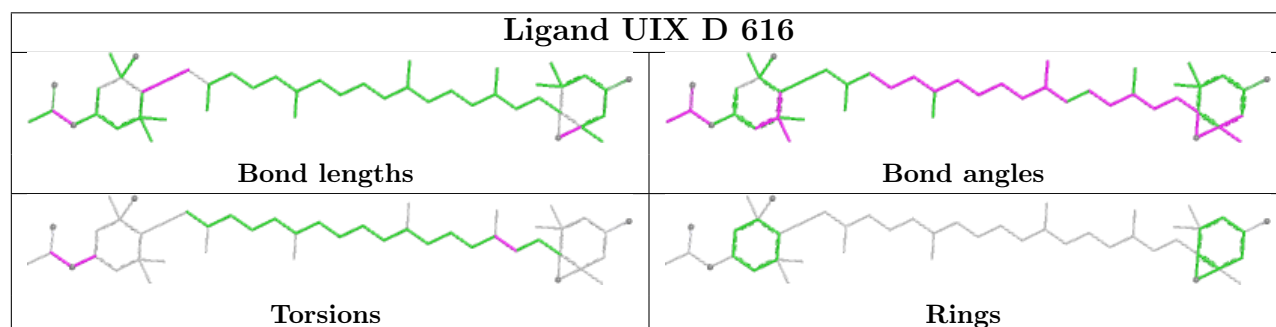
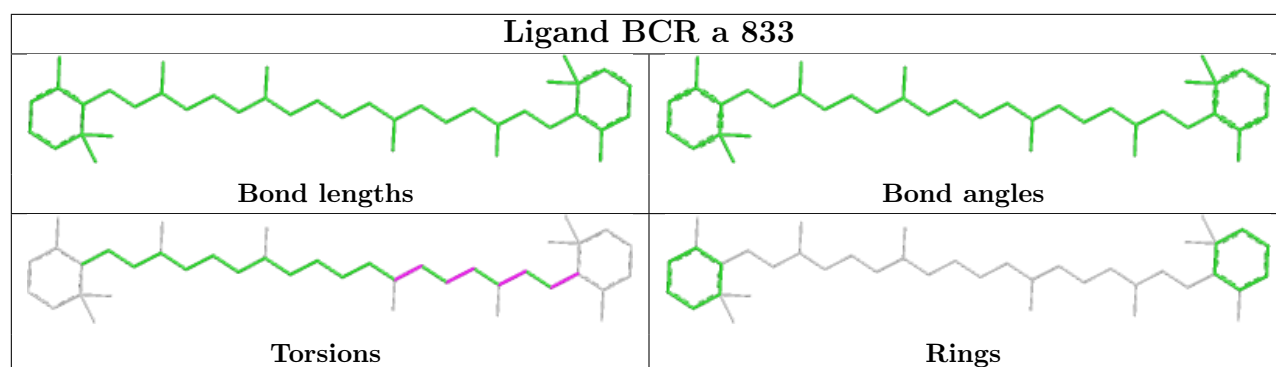
Ligand KC2 C 210

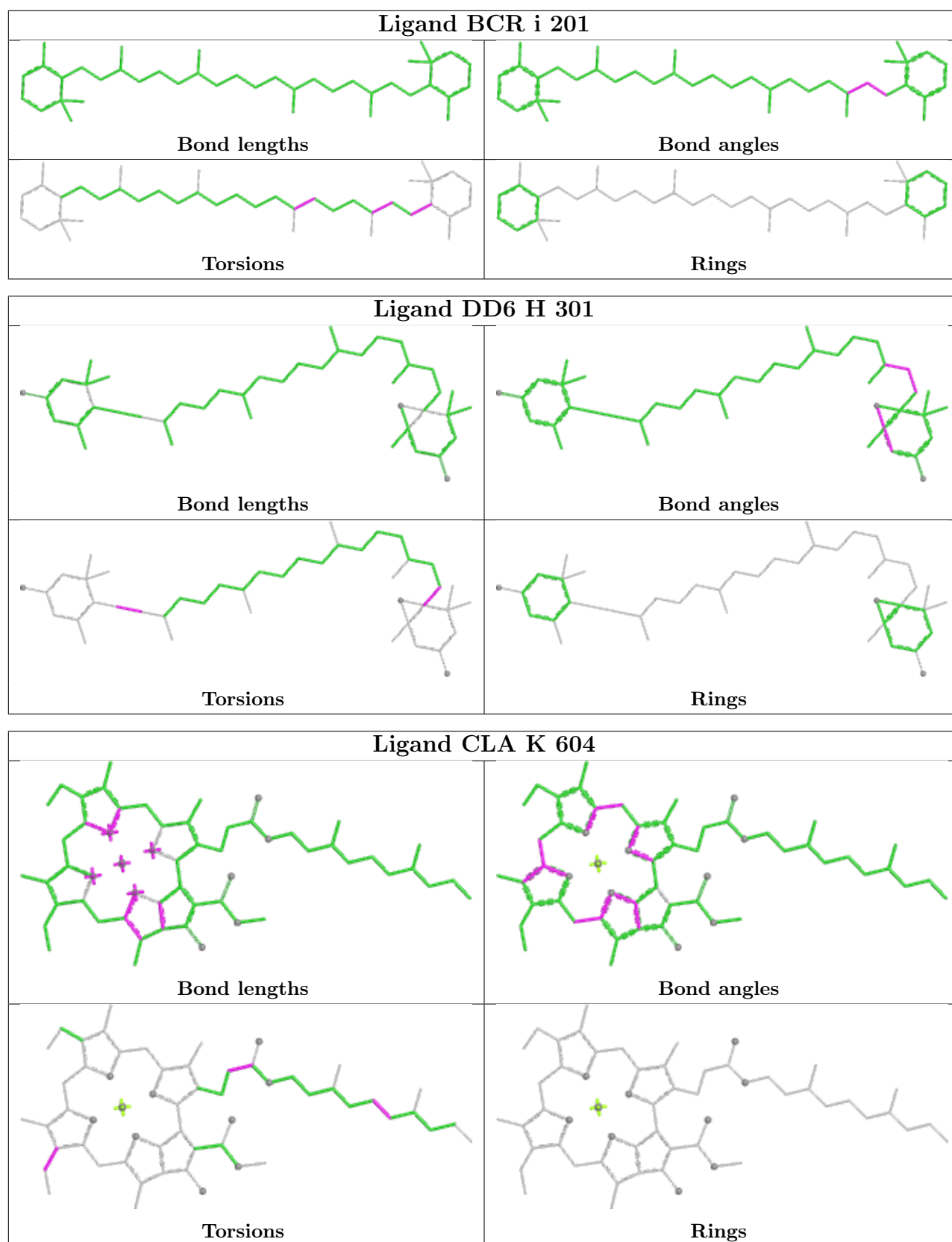


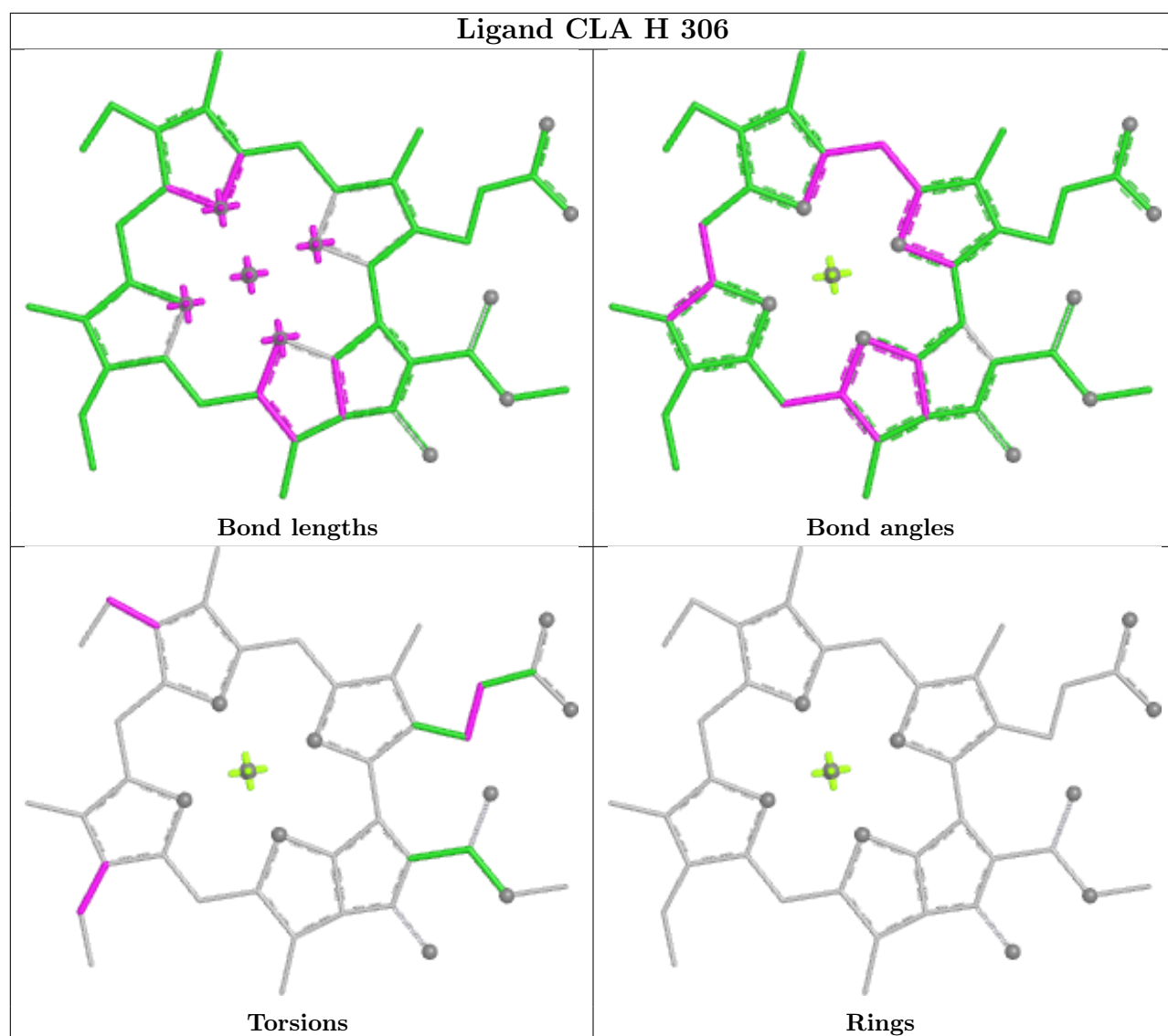
Ligand CLA J 605



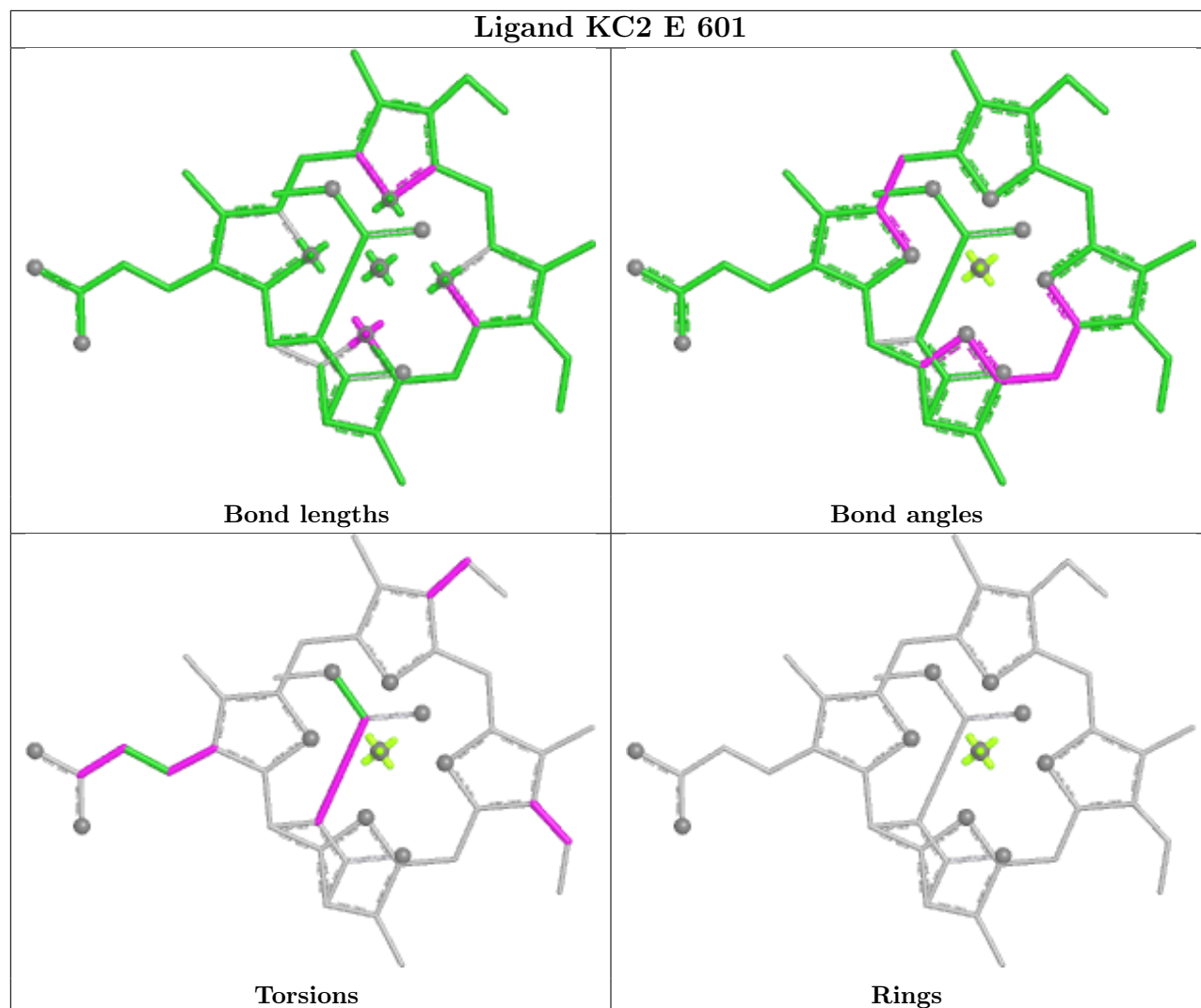




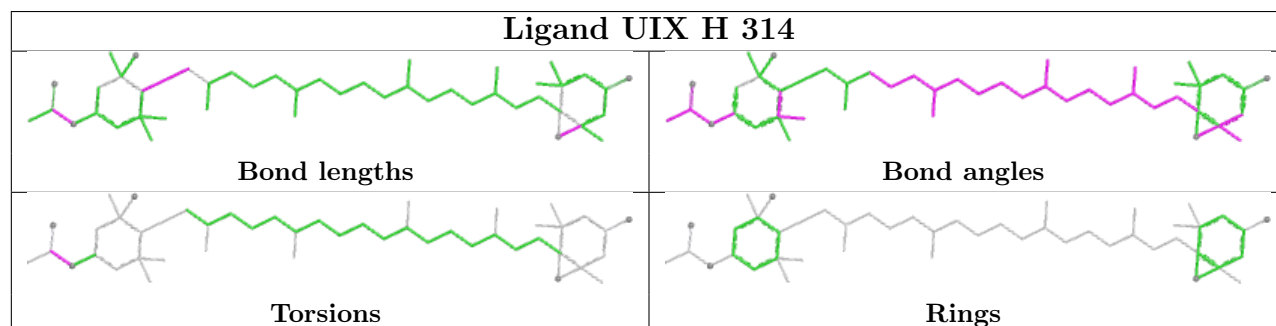


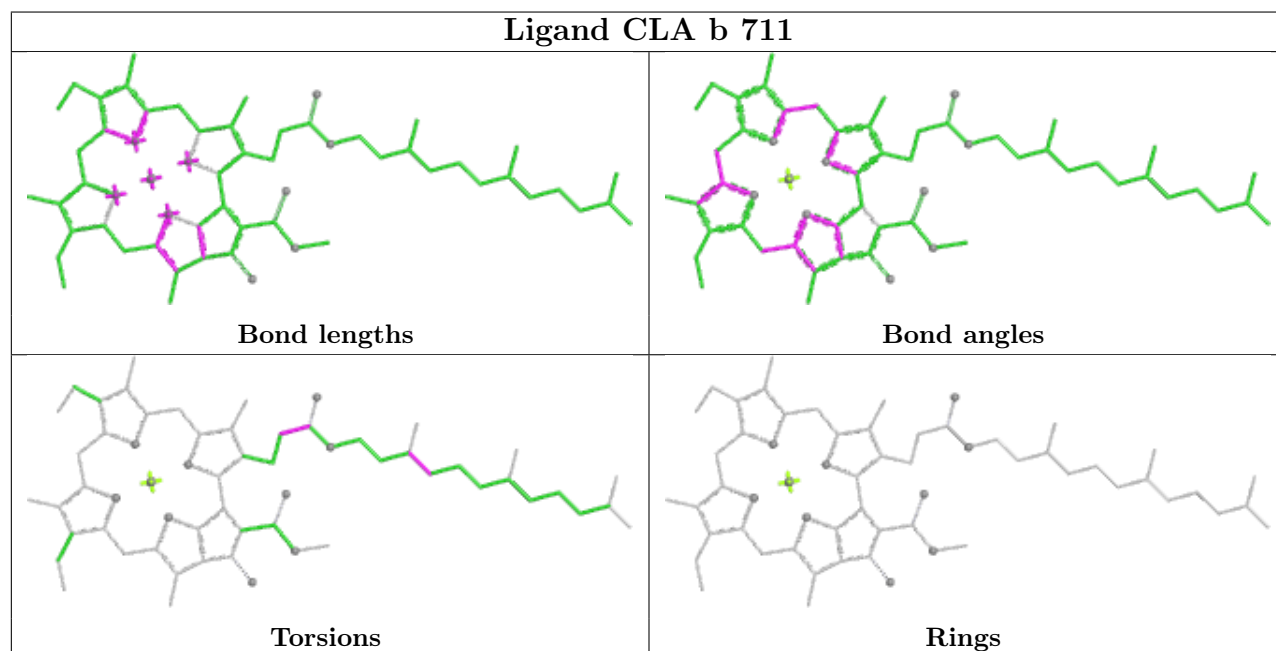
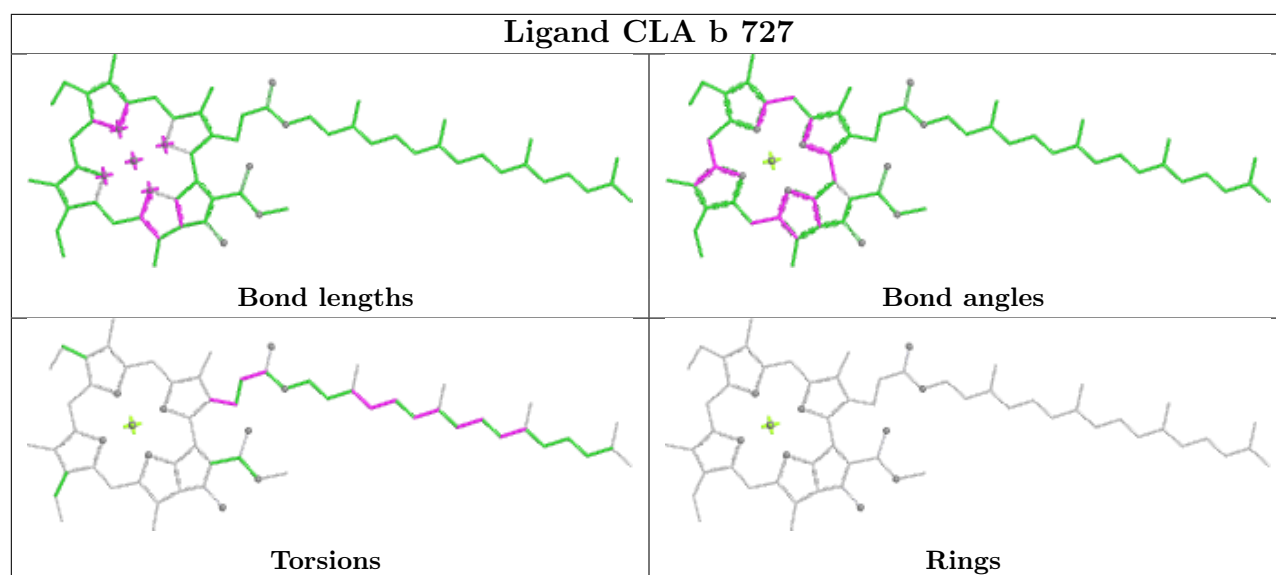


Ligand KC2 E 601

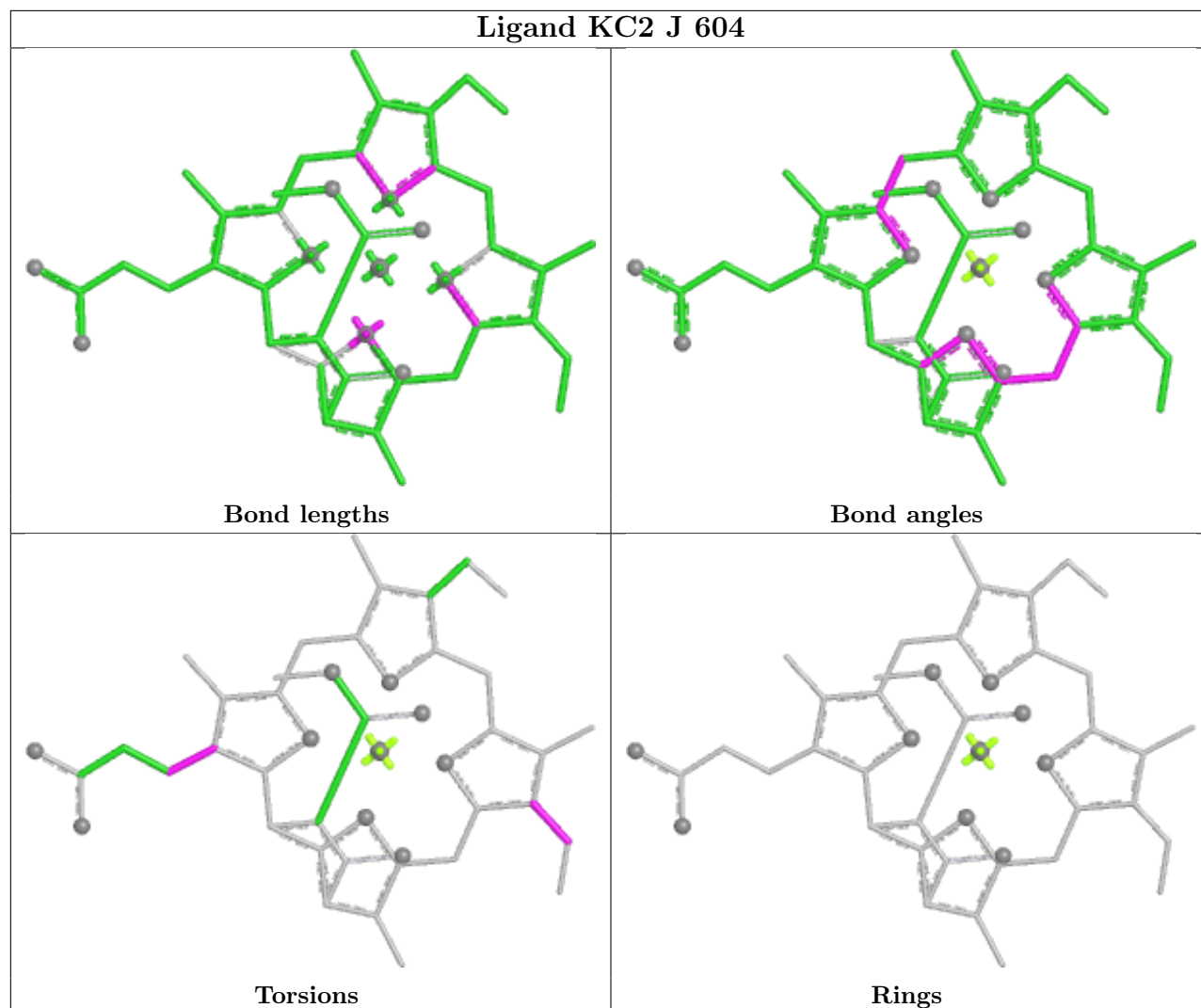


Ligand UIX H 314

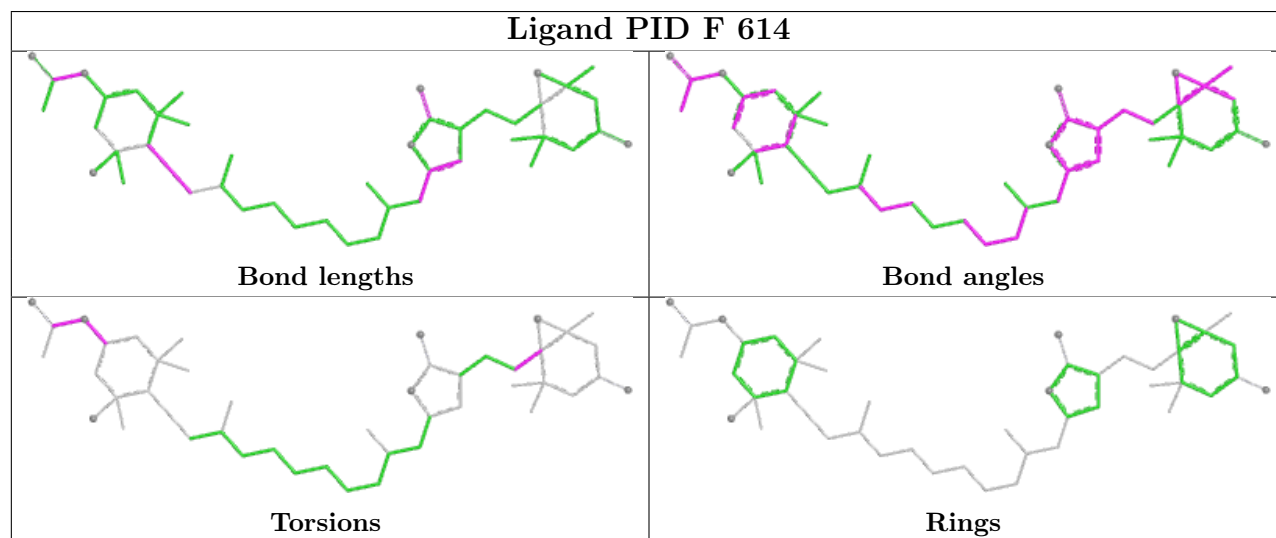




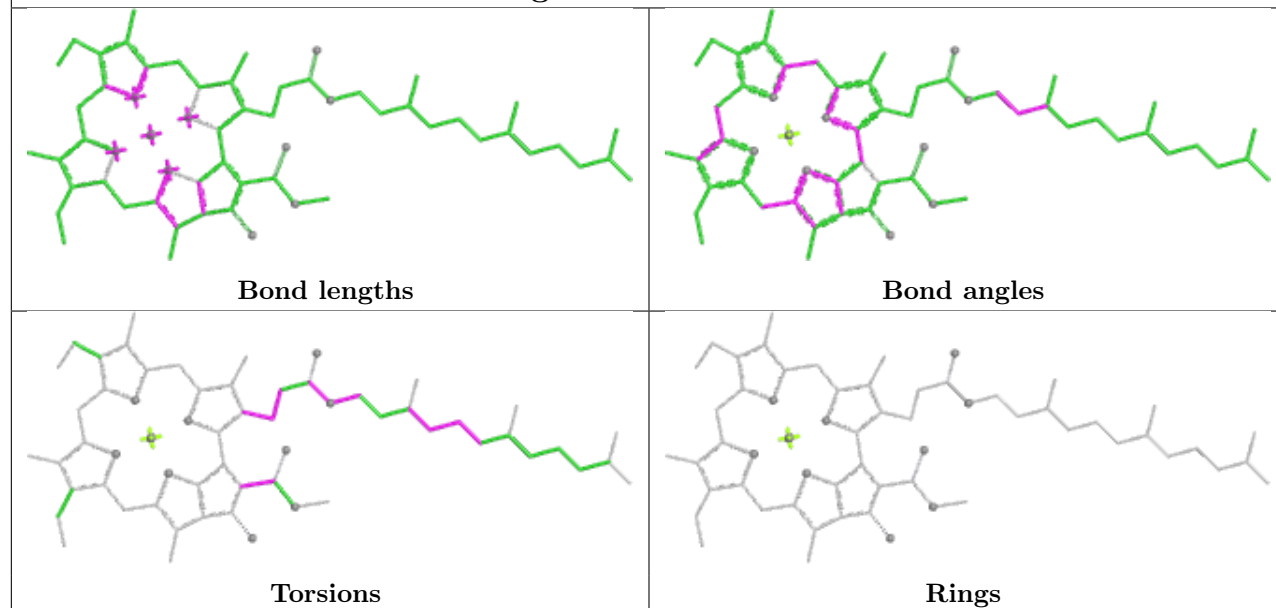
Ligand KC2 J 604



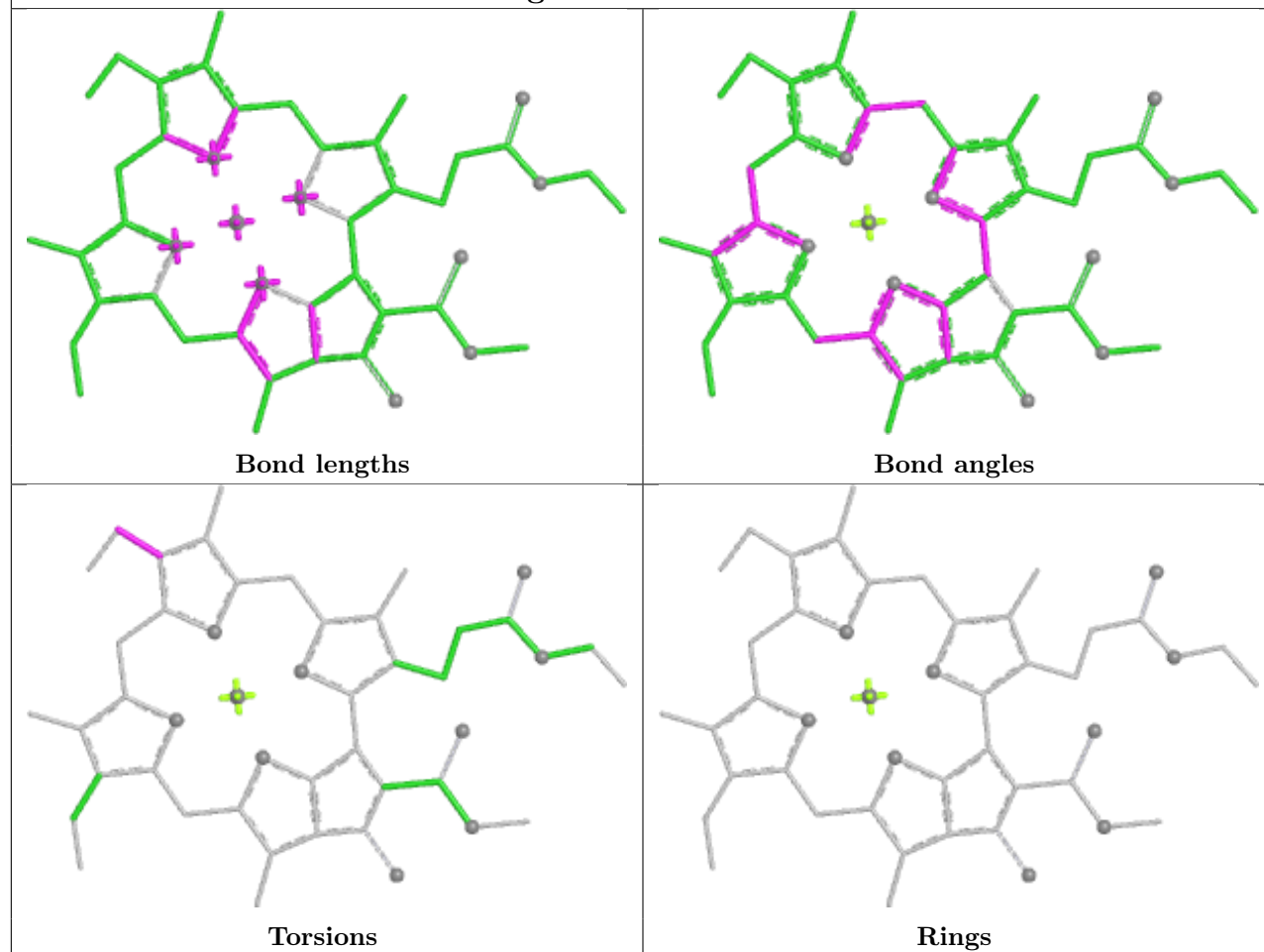
Ligand PID F 614



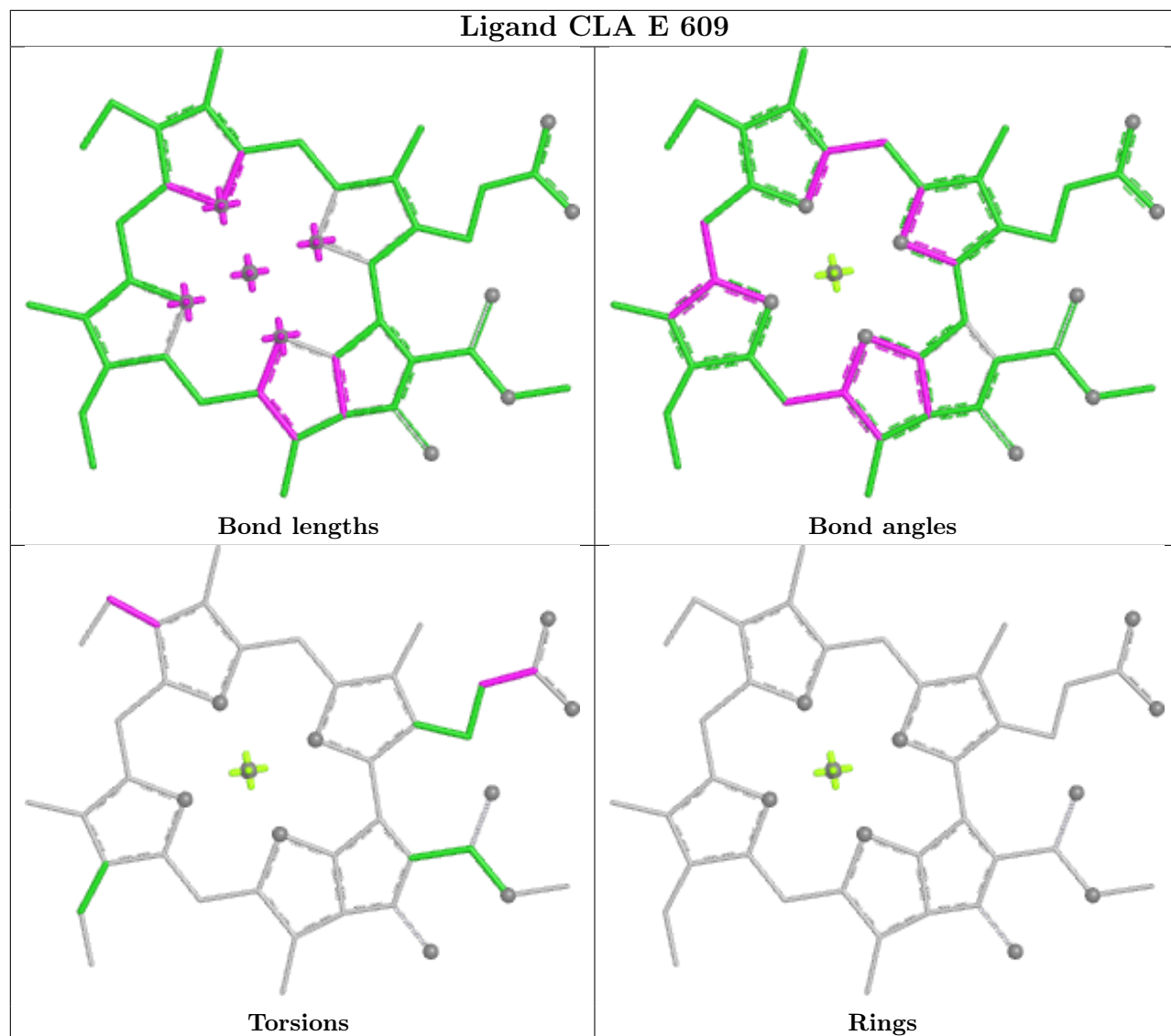
Ligand CLA H 305

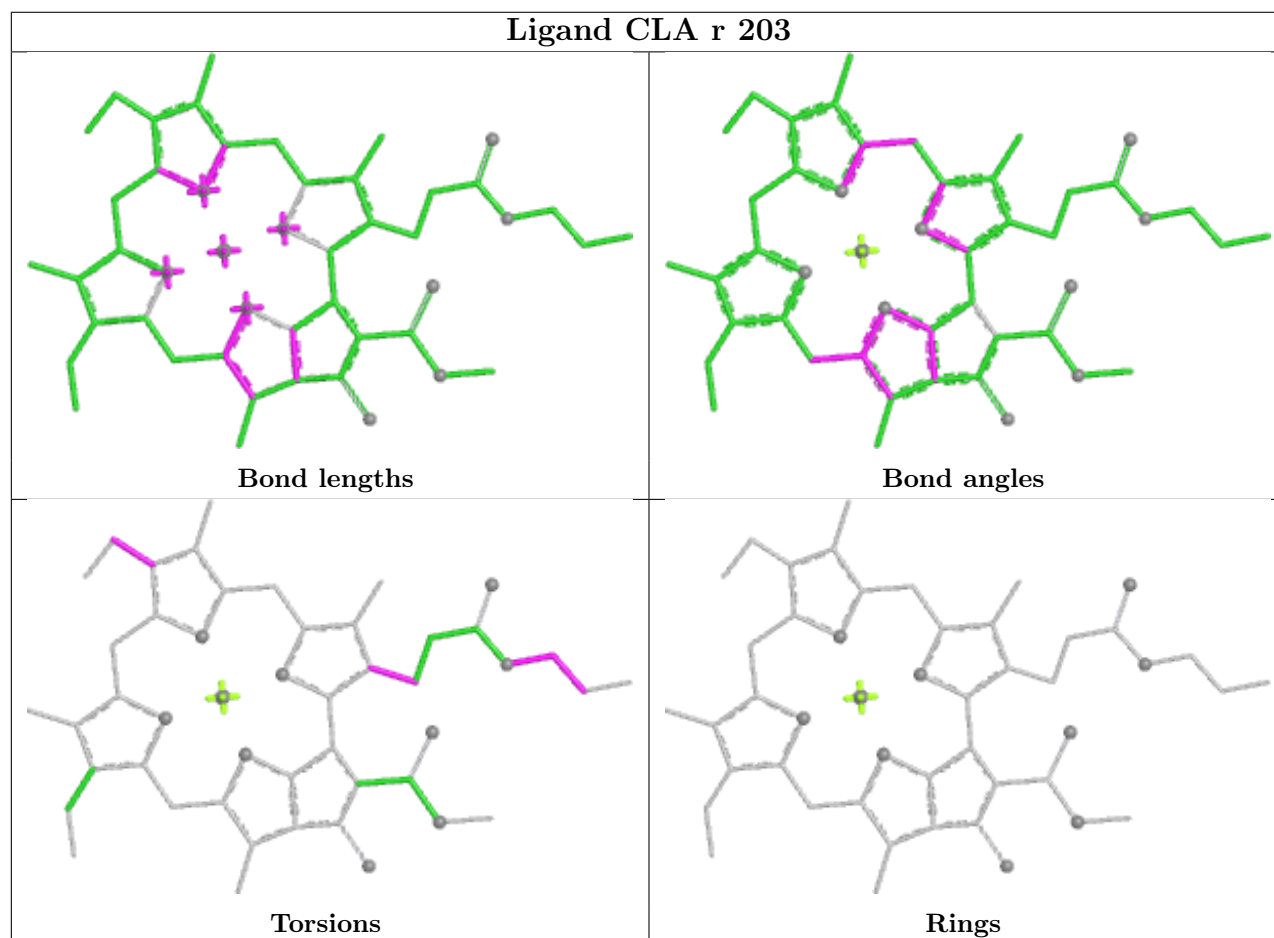
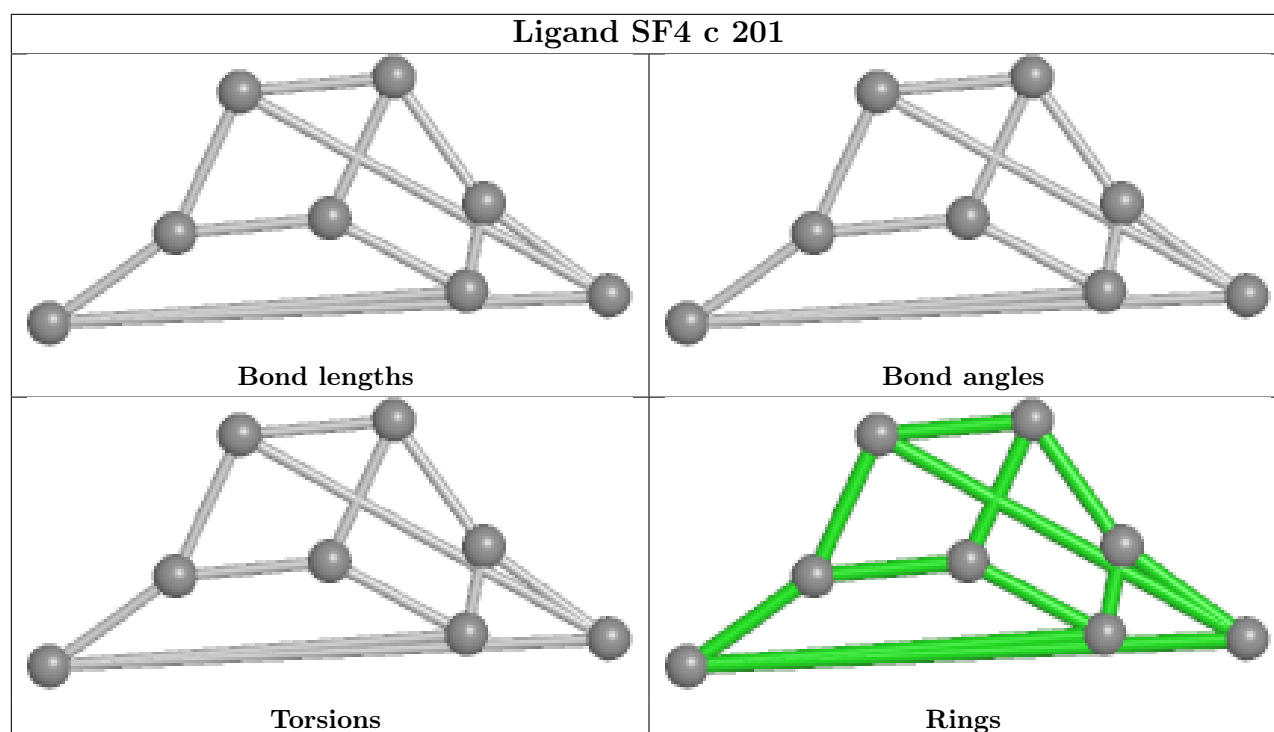


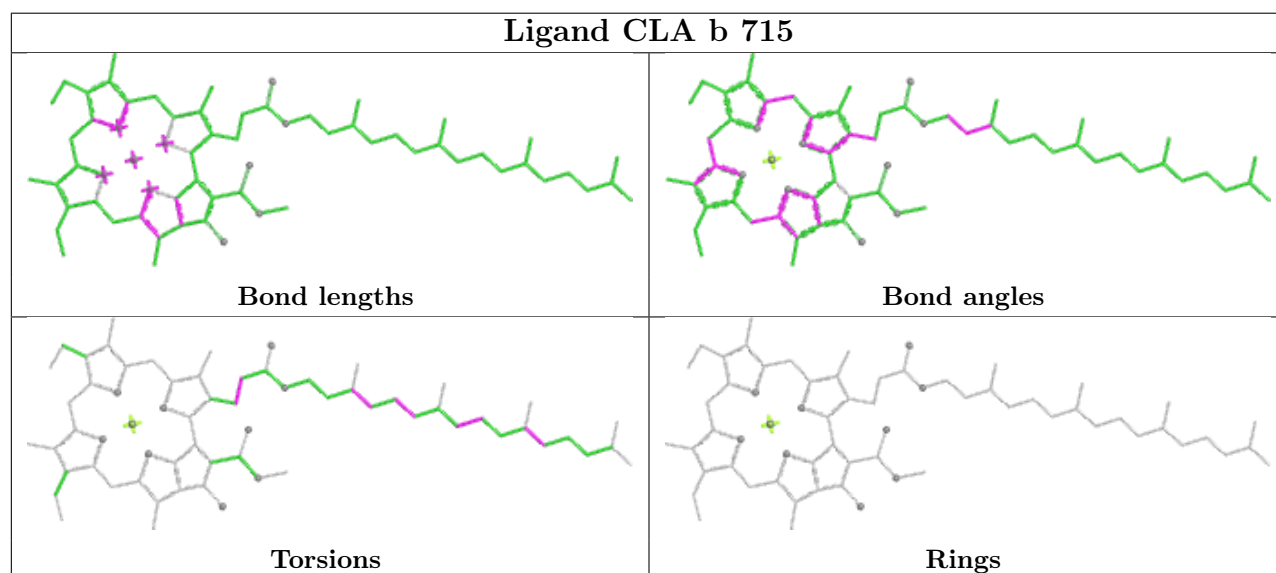
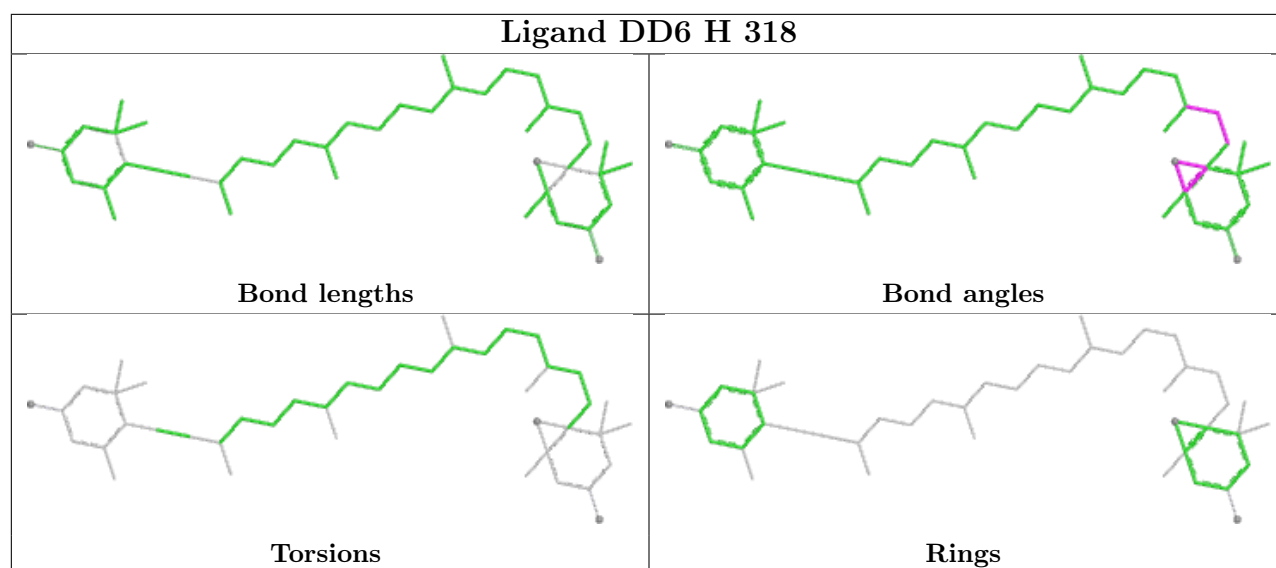
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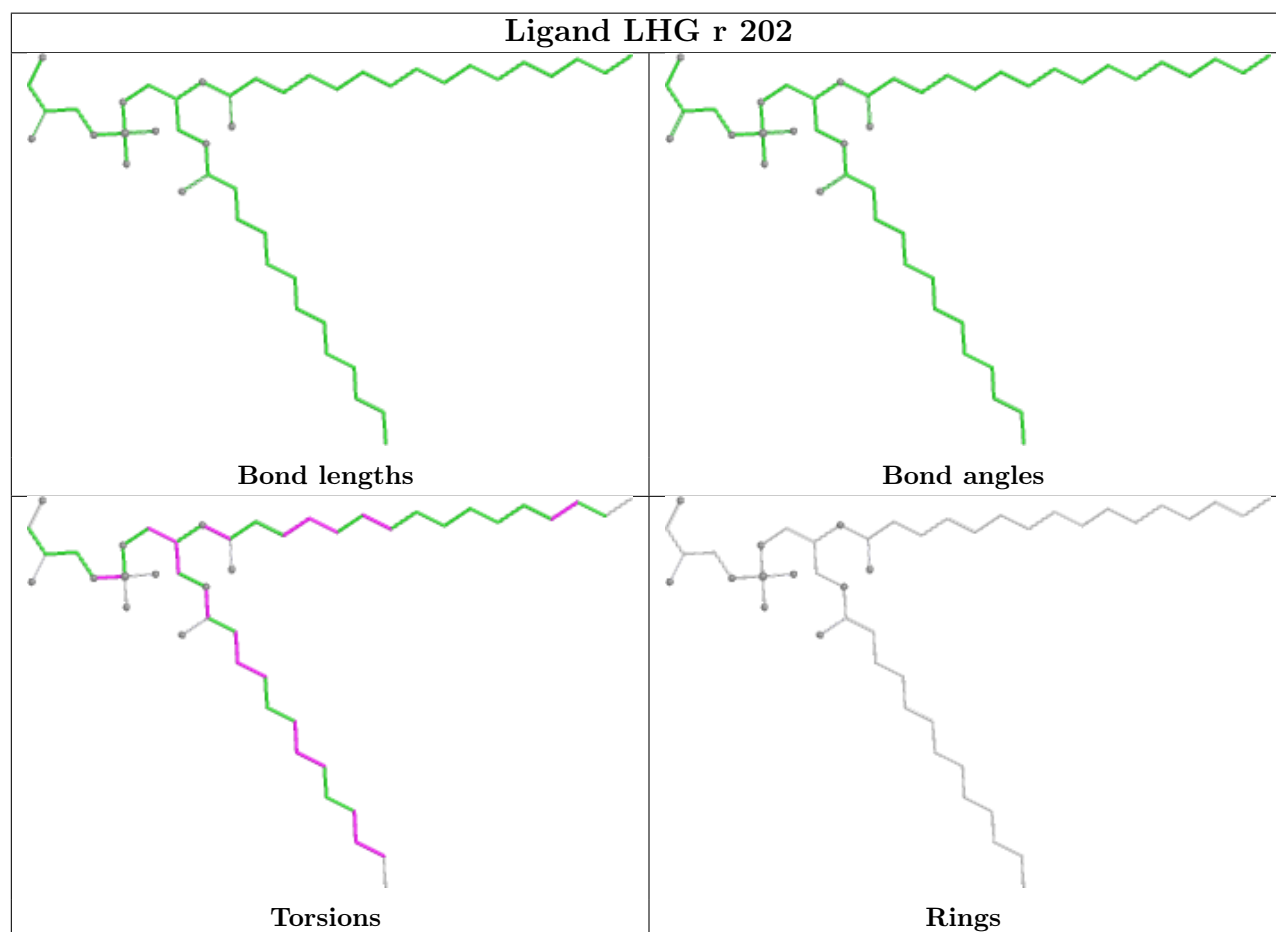
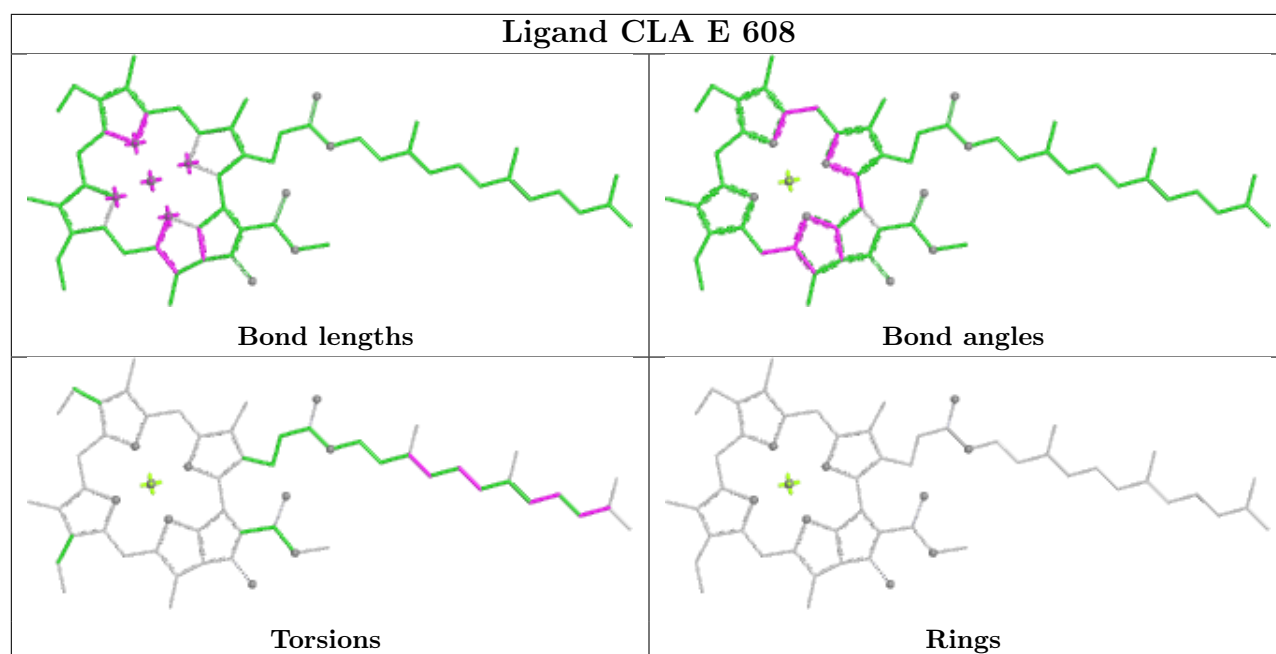


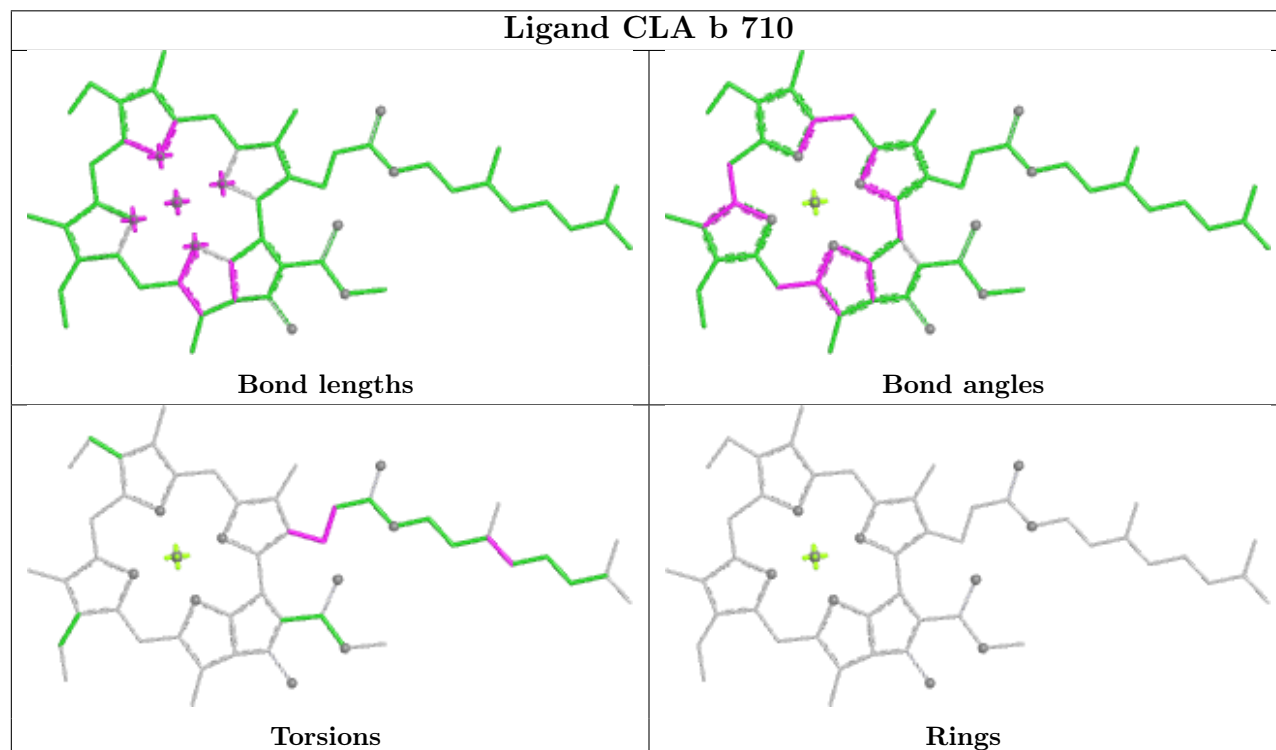
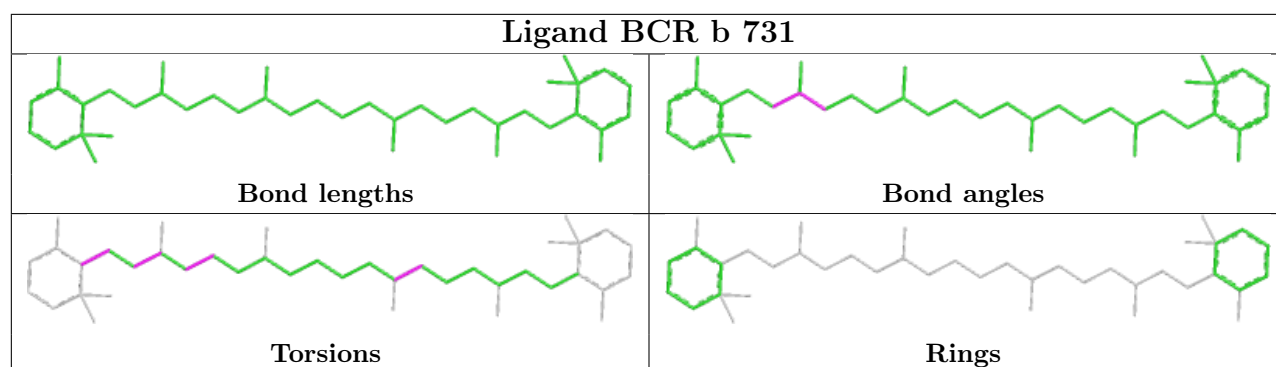
Ligand CLA E 609



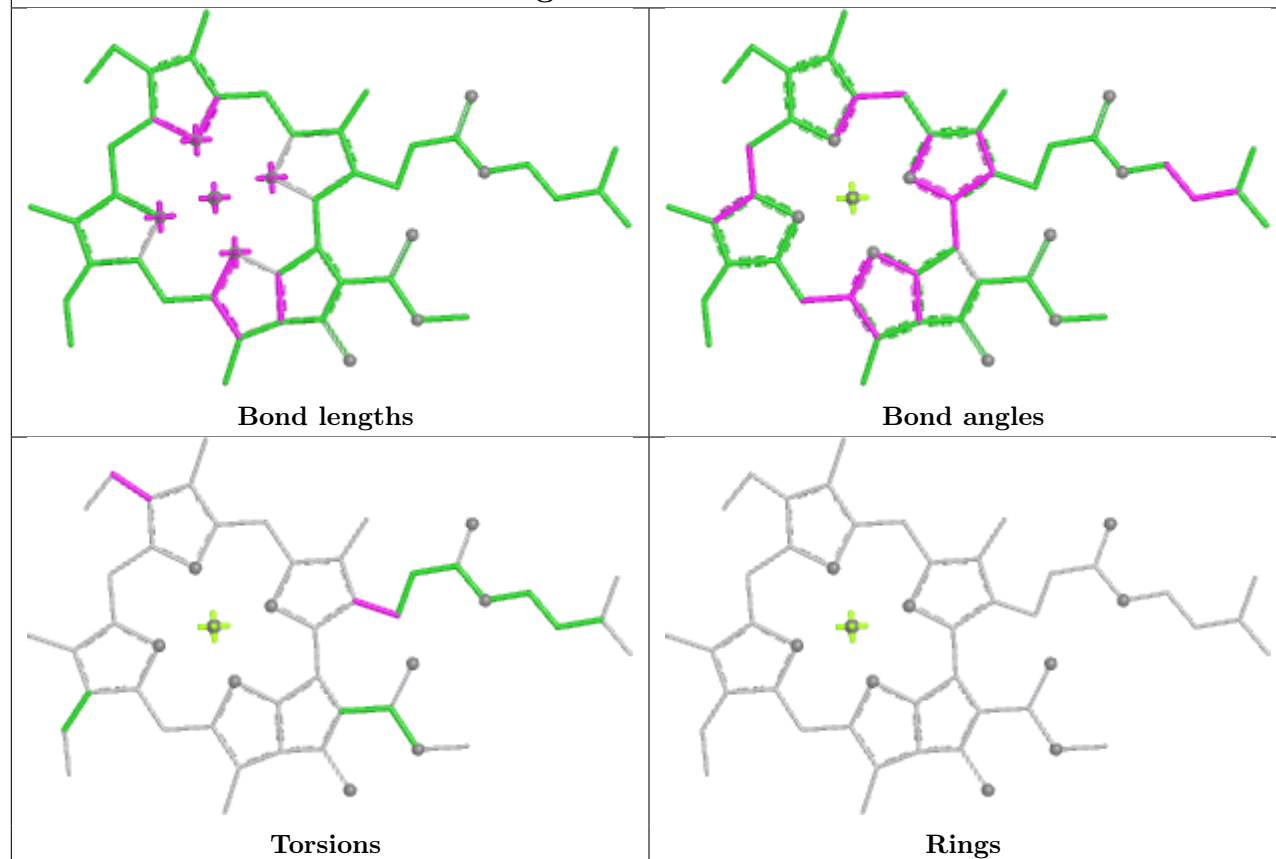




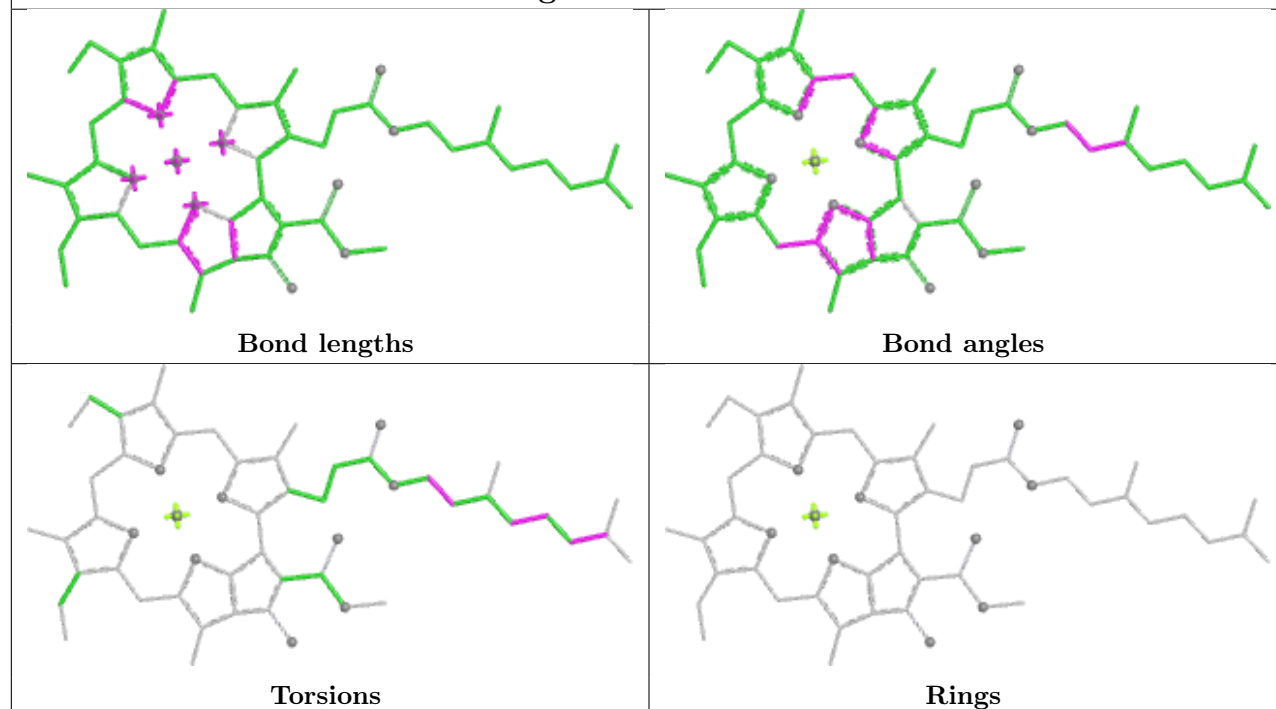




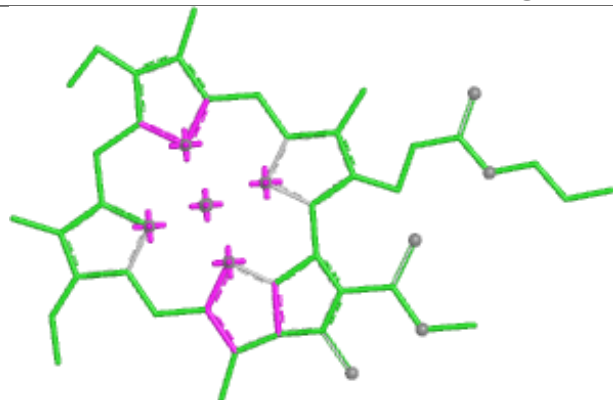
Ligand CLA a 812



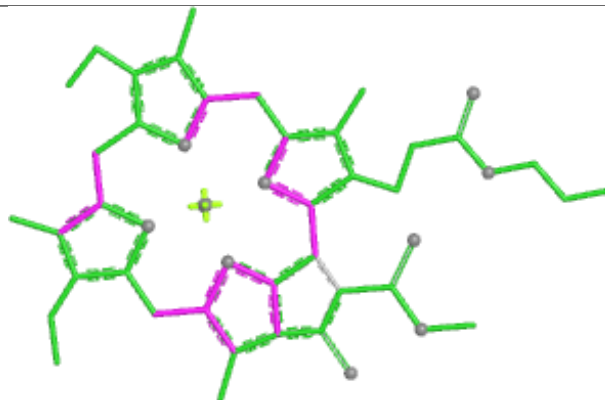
Ligand CLA I 610



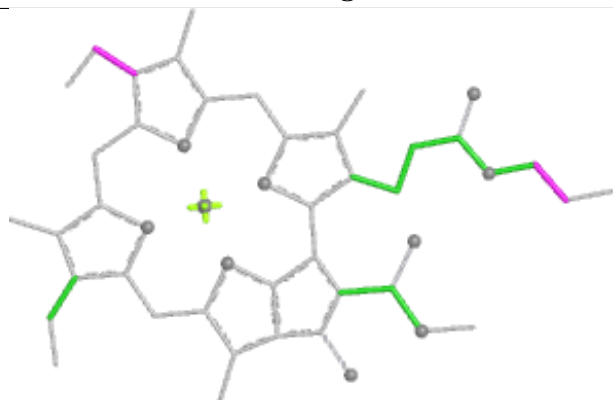
Ligand CLA a 811



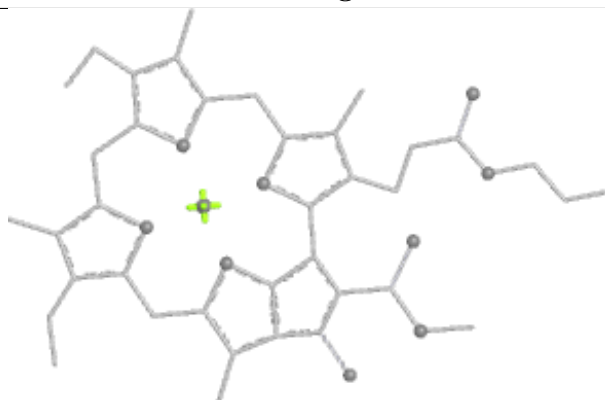
Bond lengths



Bond angles

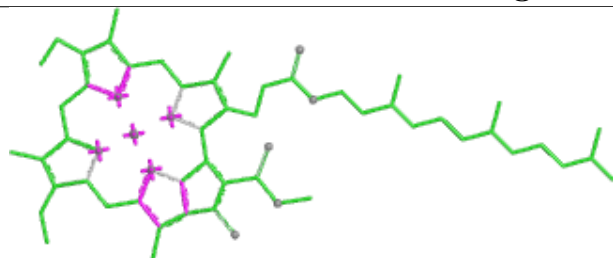


Torsions

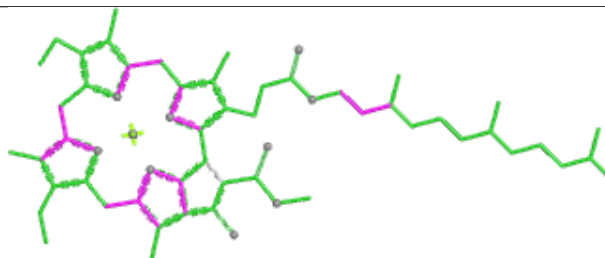


Rings

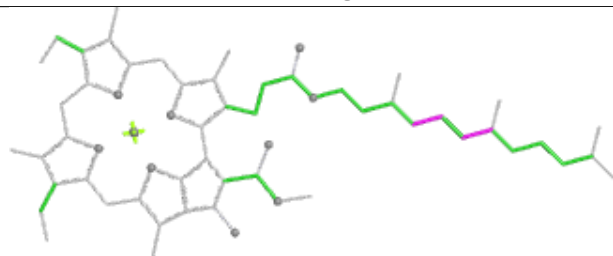
Ligand CLA H 313



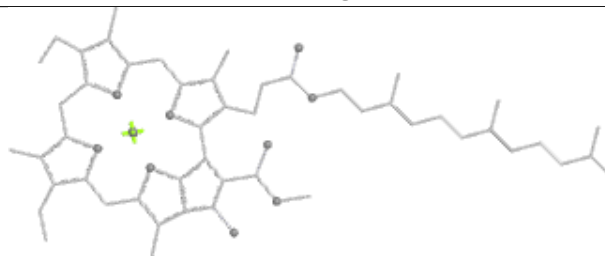
Bond lengths



Bond angles

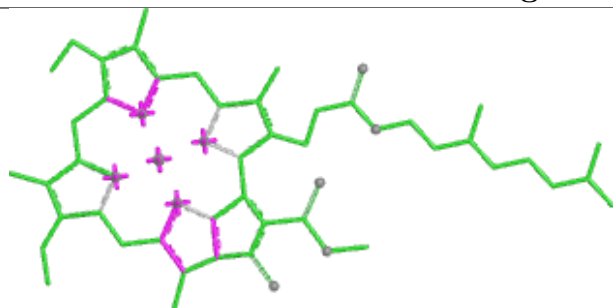


Torsions

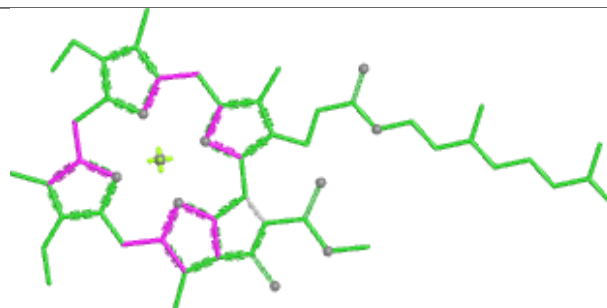


Rings

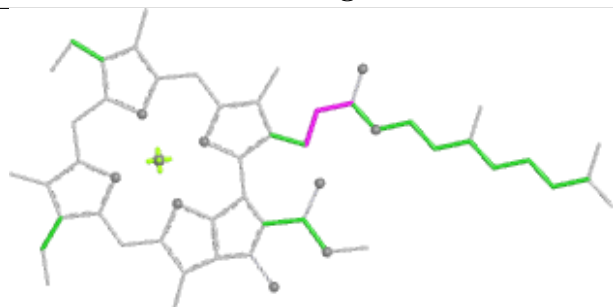
Ligand CLA I 606



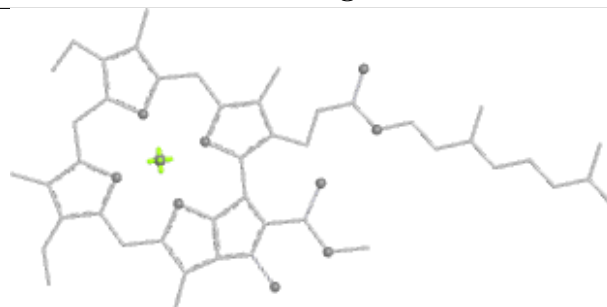
Bond lengths



Bond angles

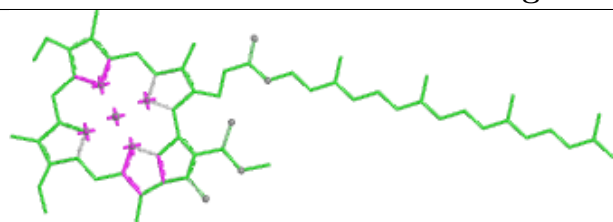


Torsions

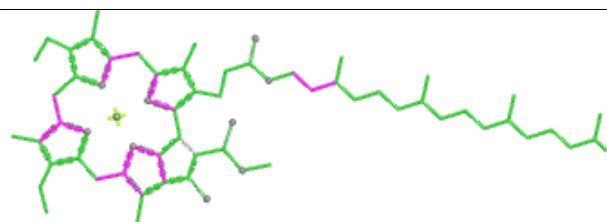


Rings

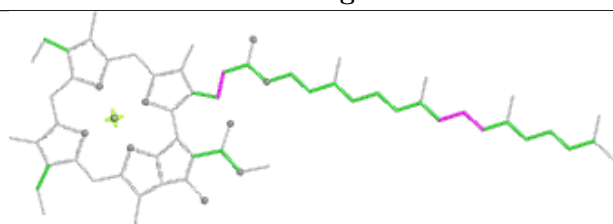
Ligand CLA I 406



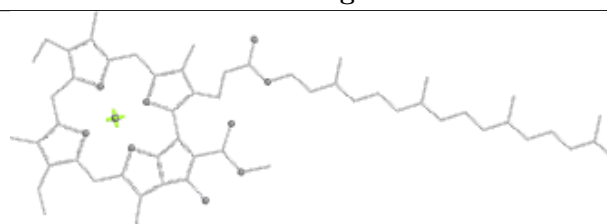
Bond lengths



Bond angles

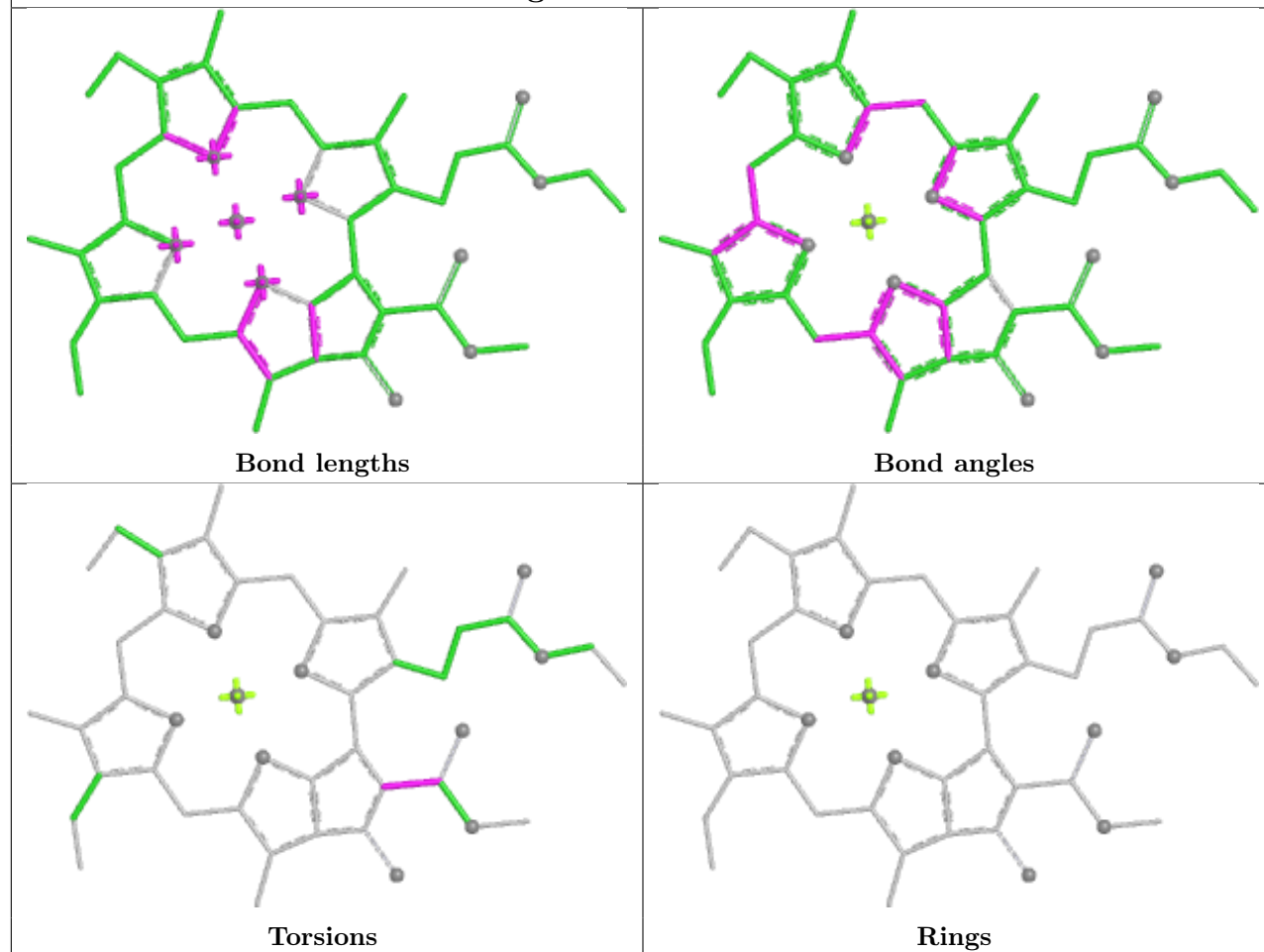


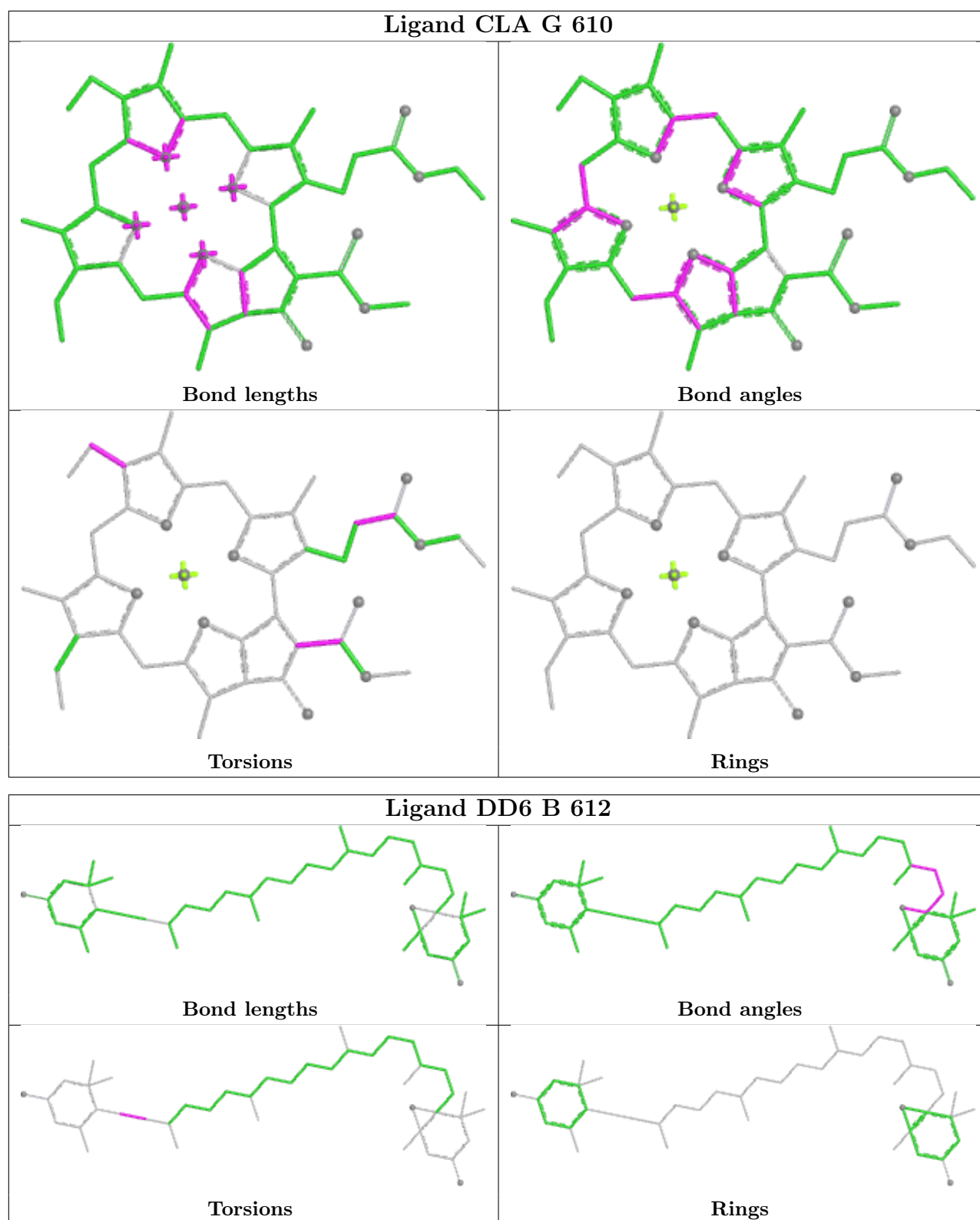
Torsions



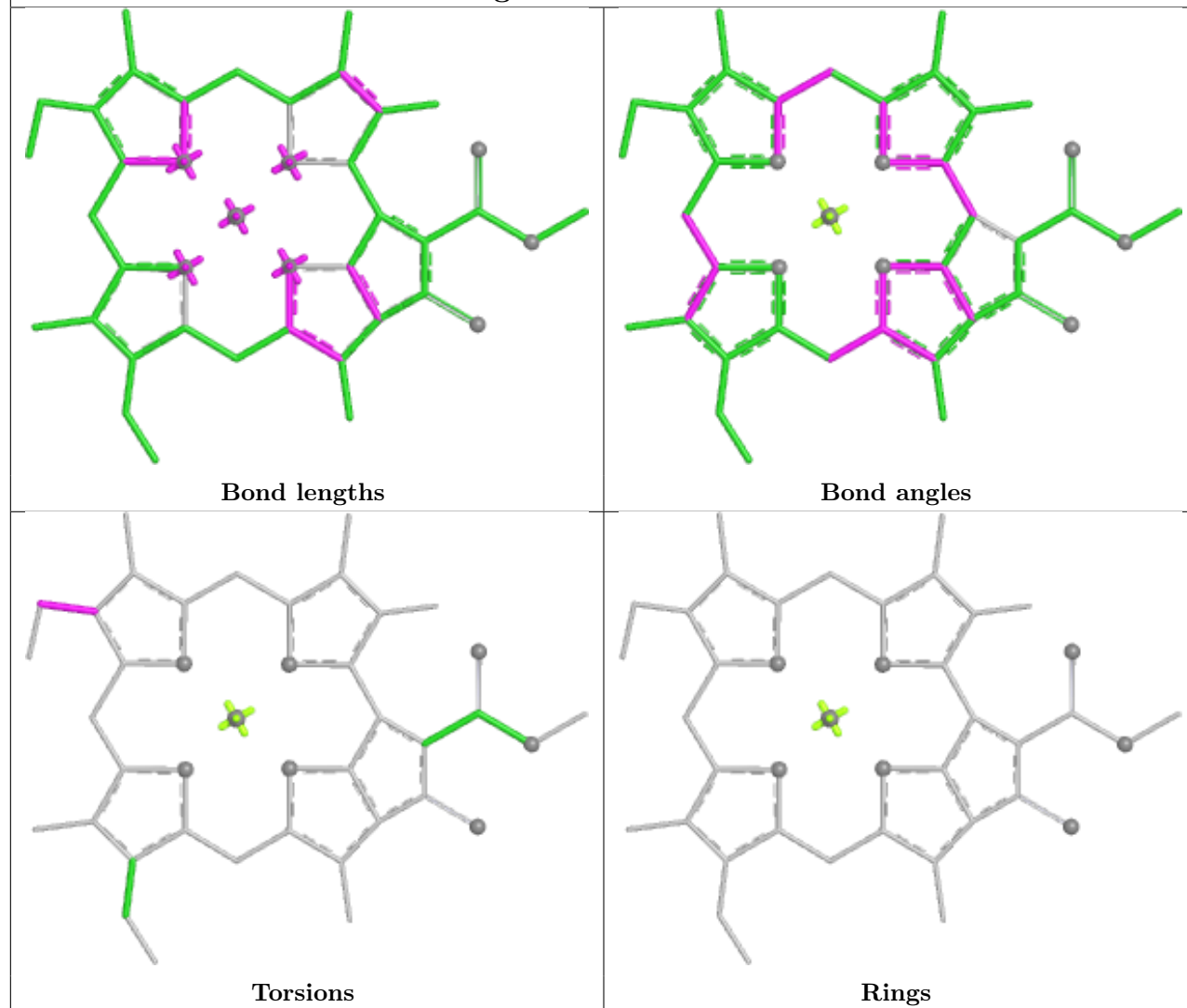
Rings

Ligand CLA C 206

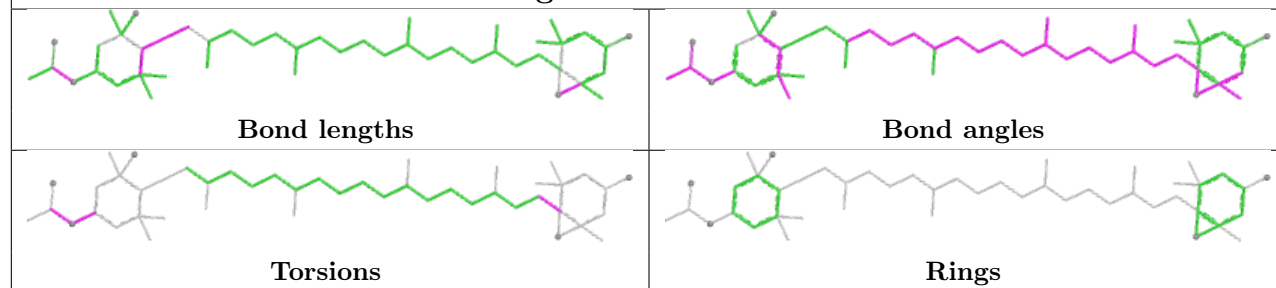




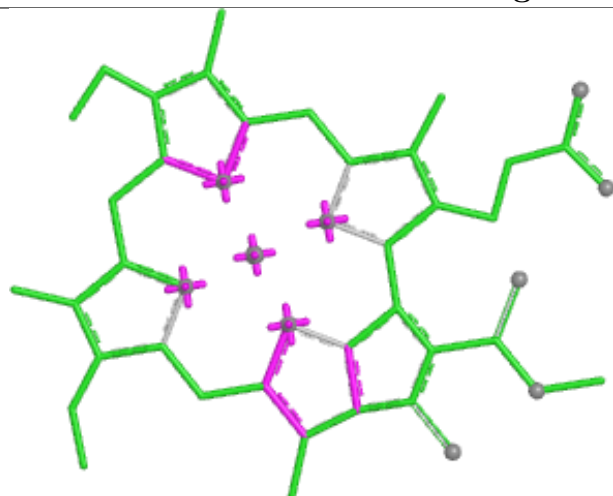
Ligand CLA K 606



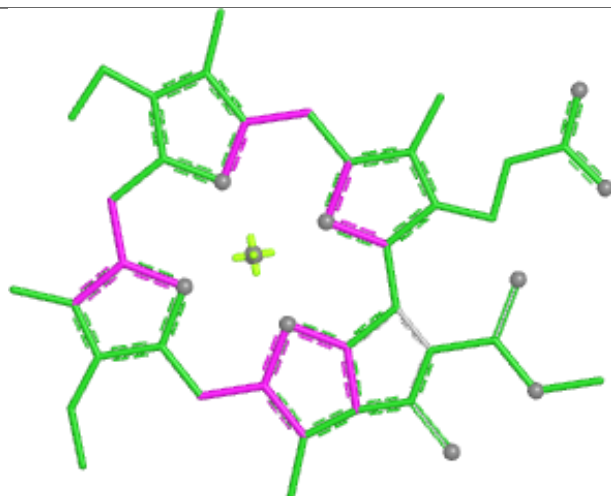
Ligand UIX T 612



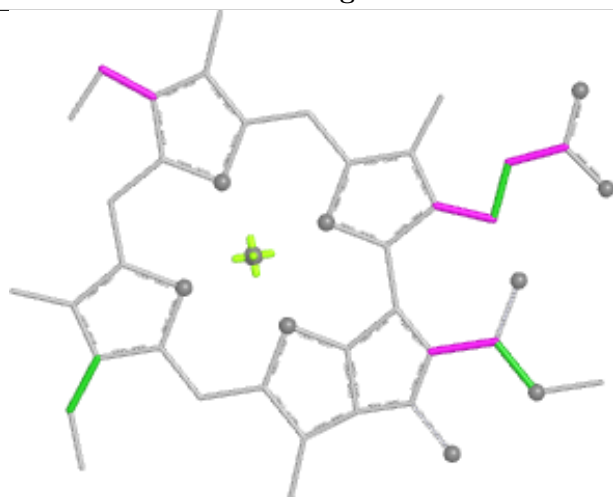
Ligand CLA U 606



Bond lengths



Bond angles

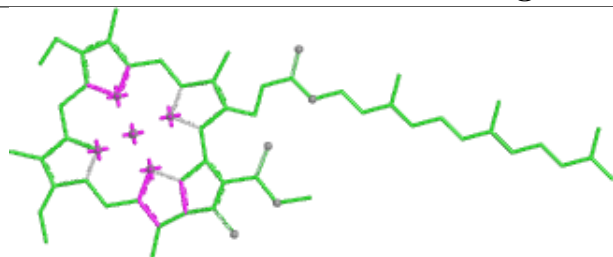


Torsions

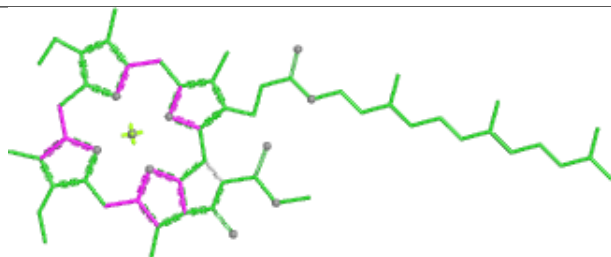


Rings

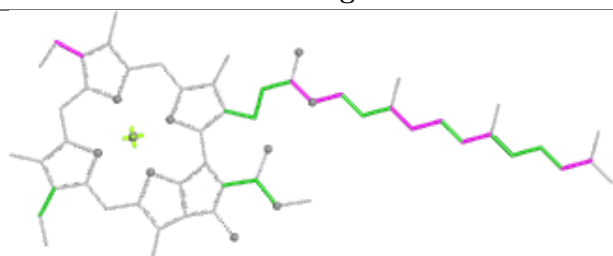
Ligand CLA F 617



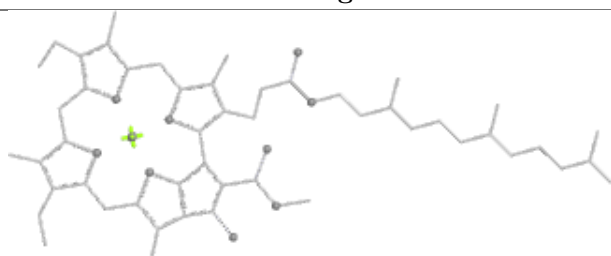
Bond lengths



Bond angles

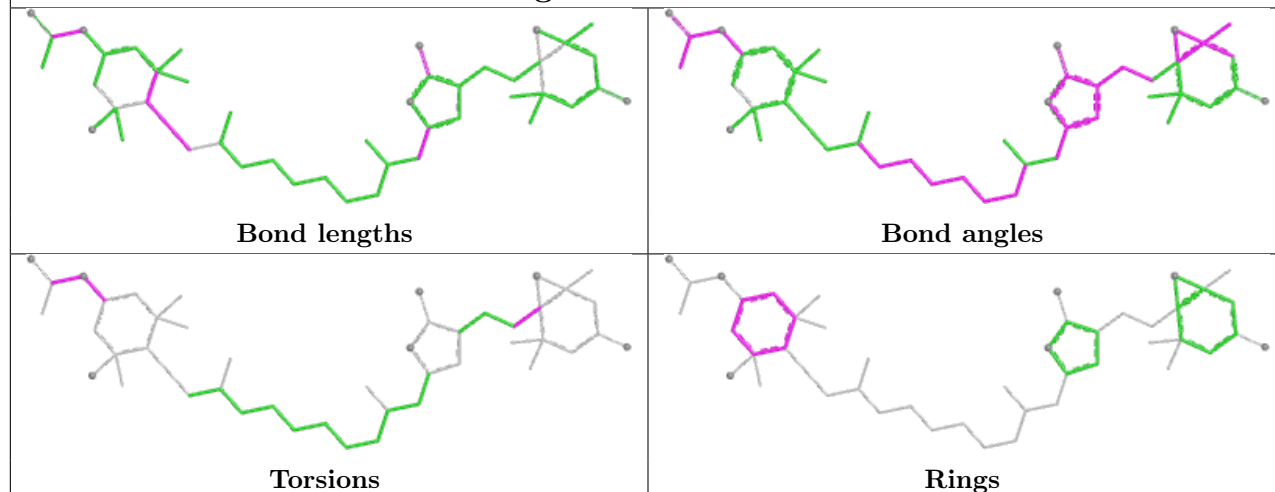


Torsions

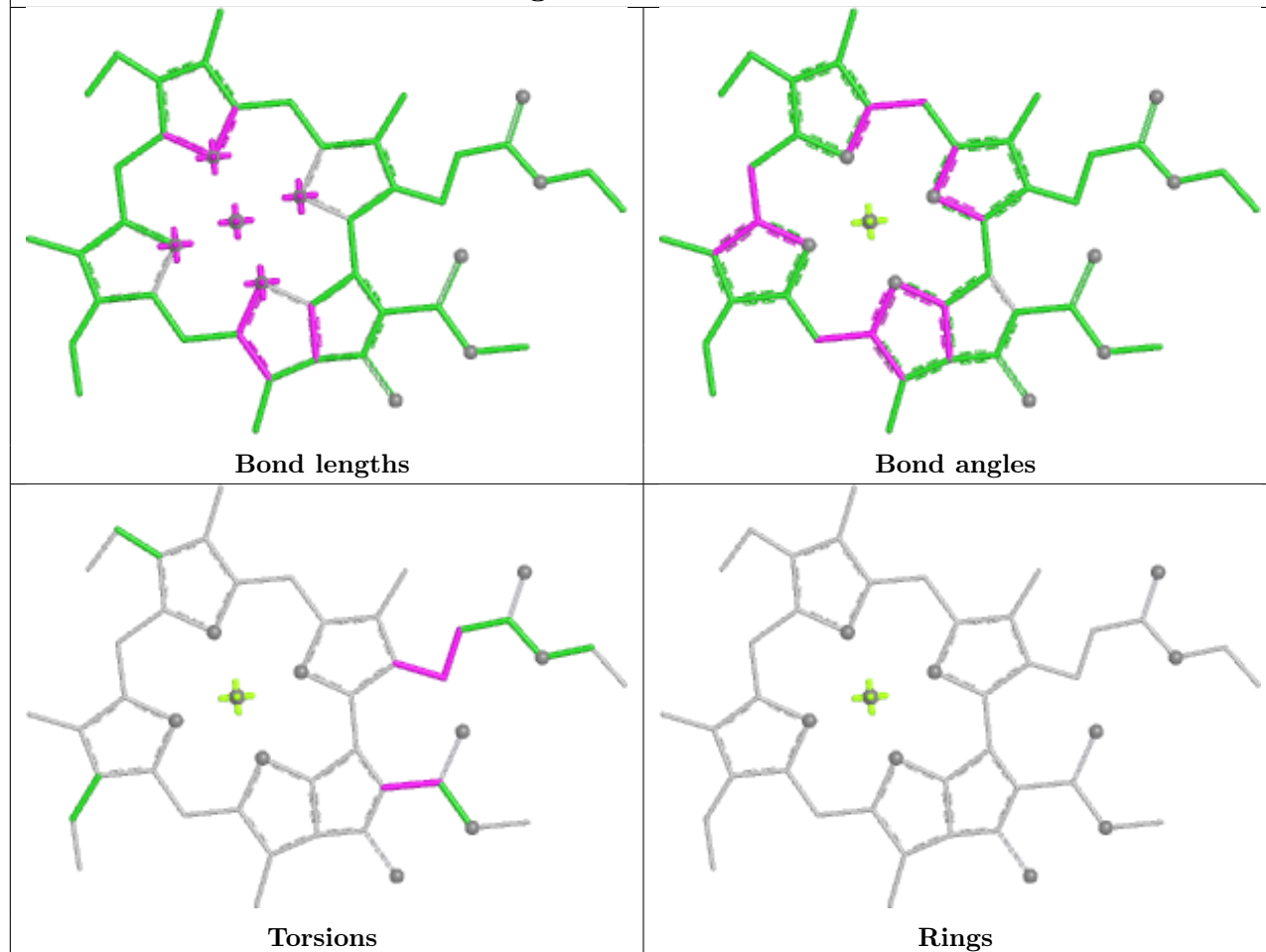


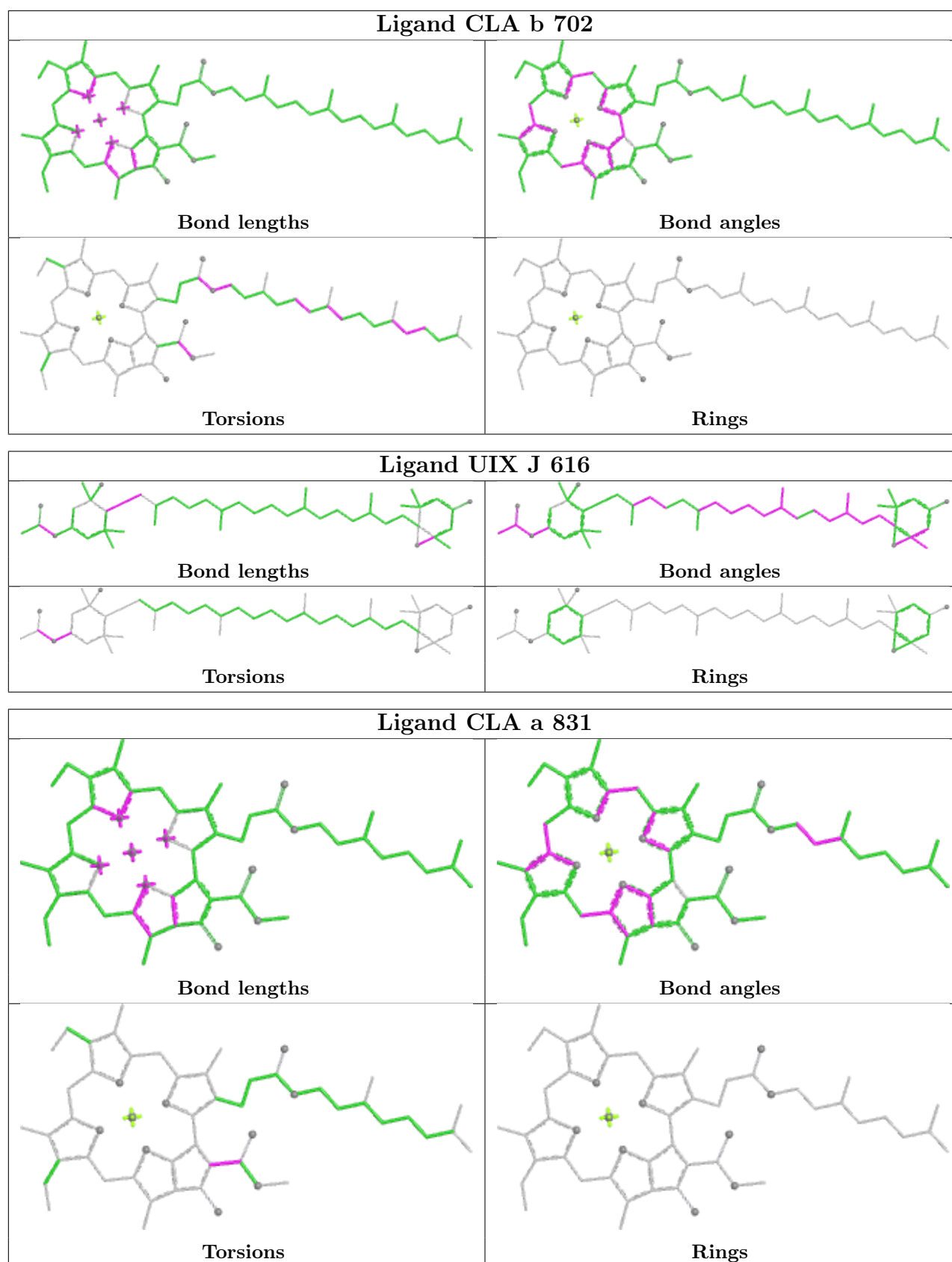
Rings

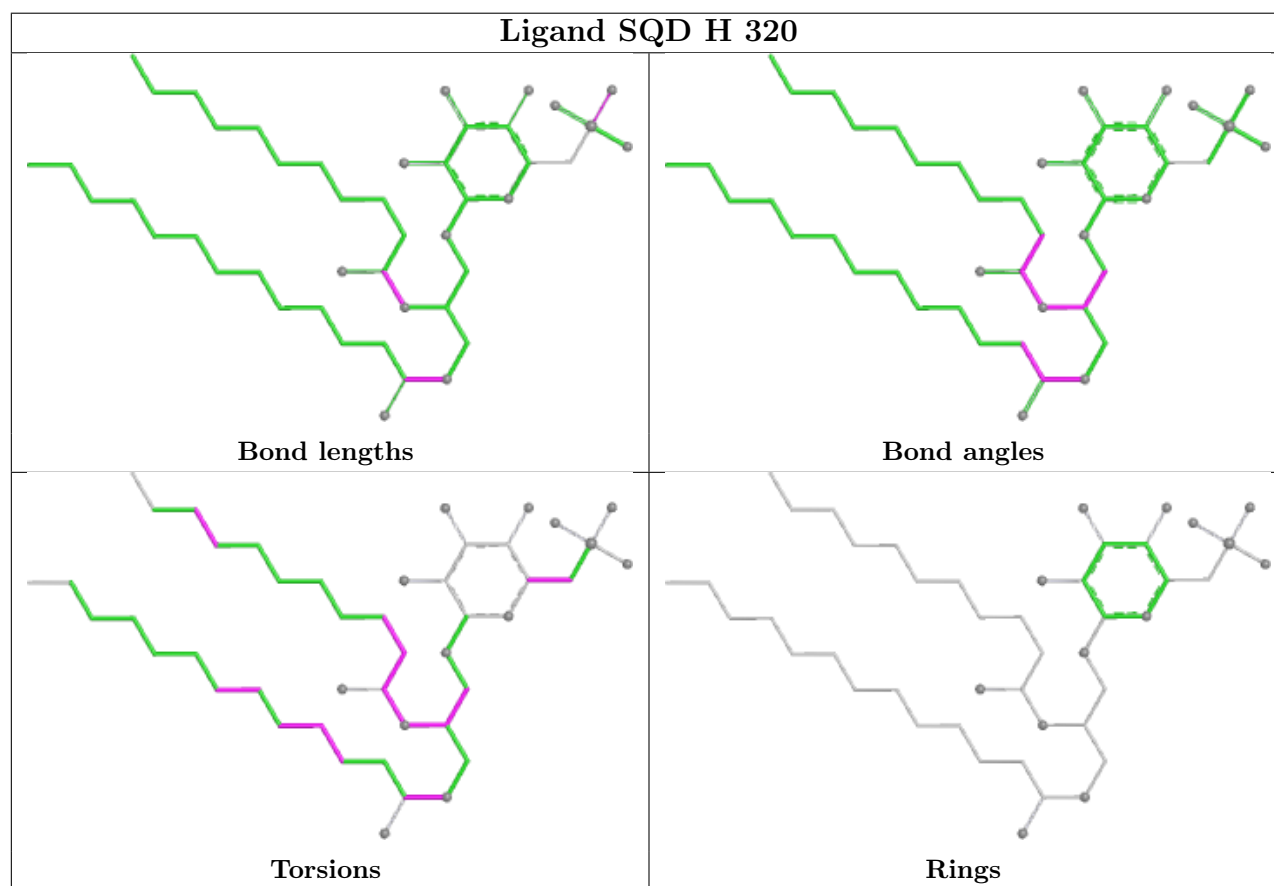
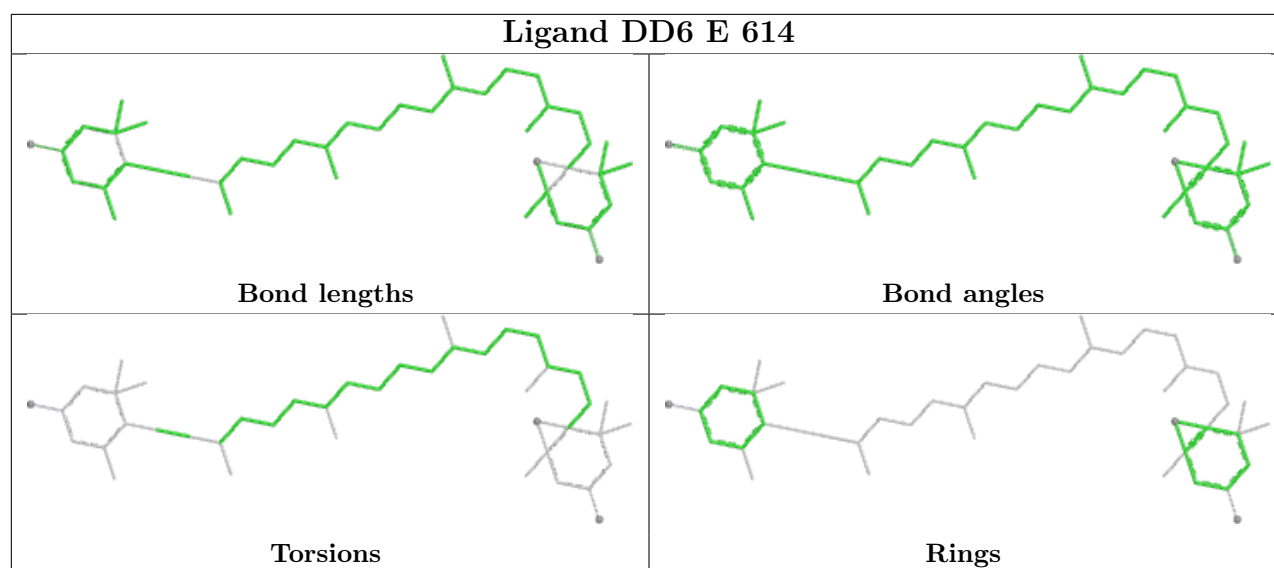
Ligand PID K 611

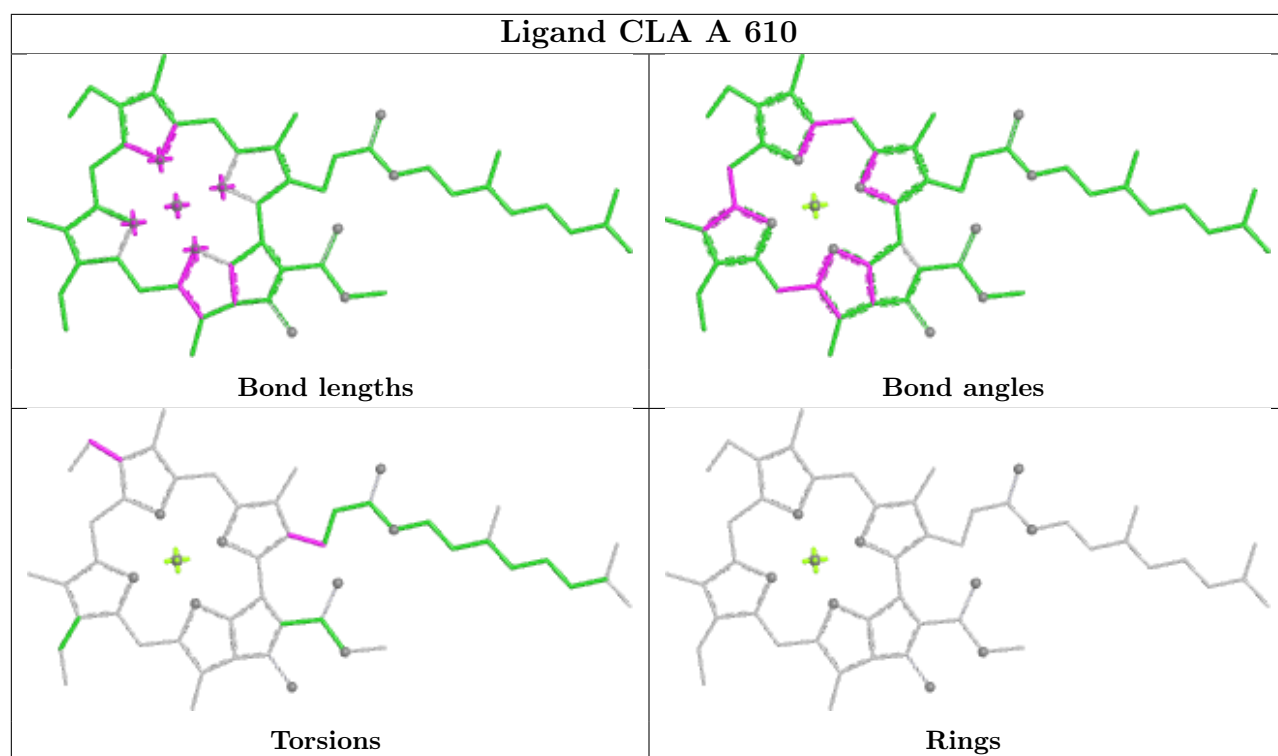


Ligand CLA F 610

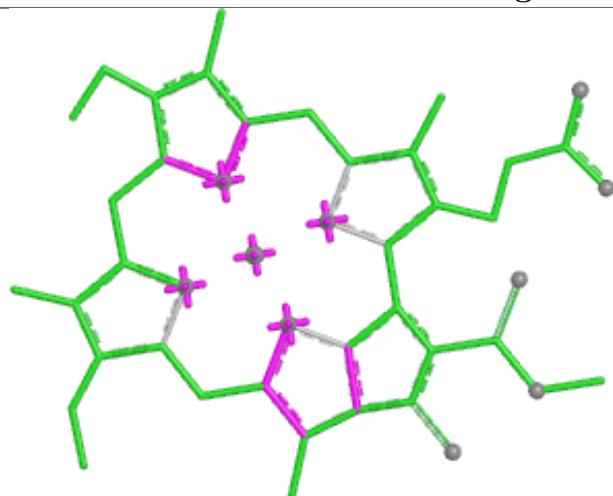




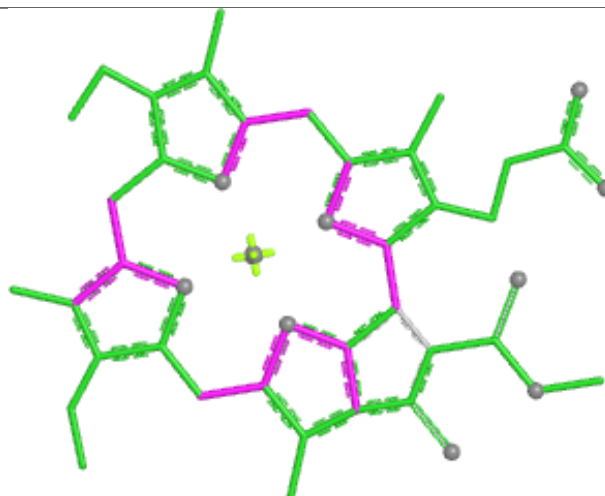




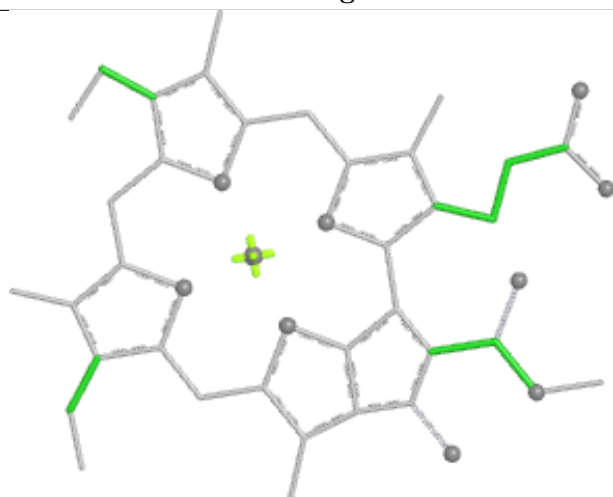
Ligand CLA T 605



Bond lengths



Bond angles

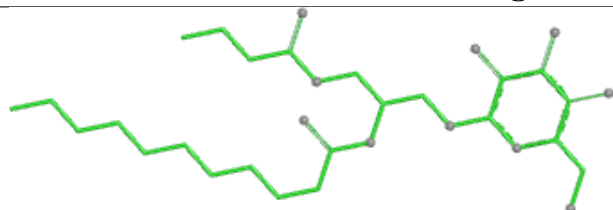


Torsions

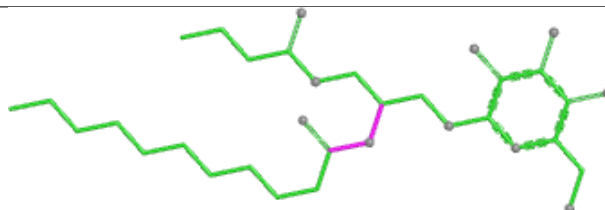


Rings

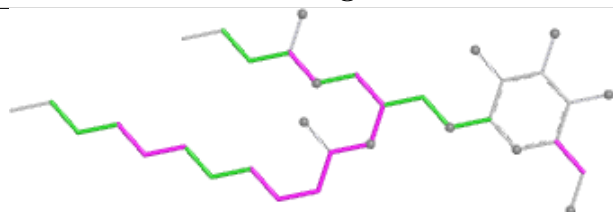
Ligand LMG C 217



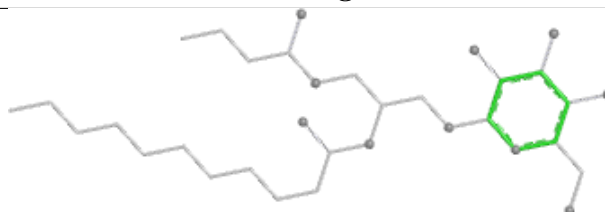
Bond lengths



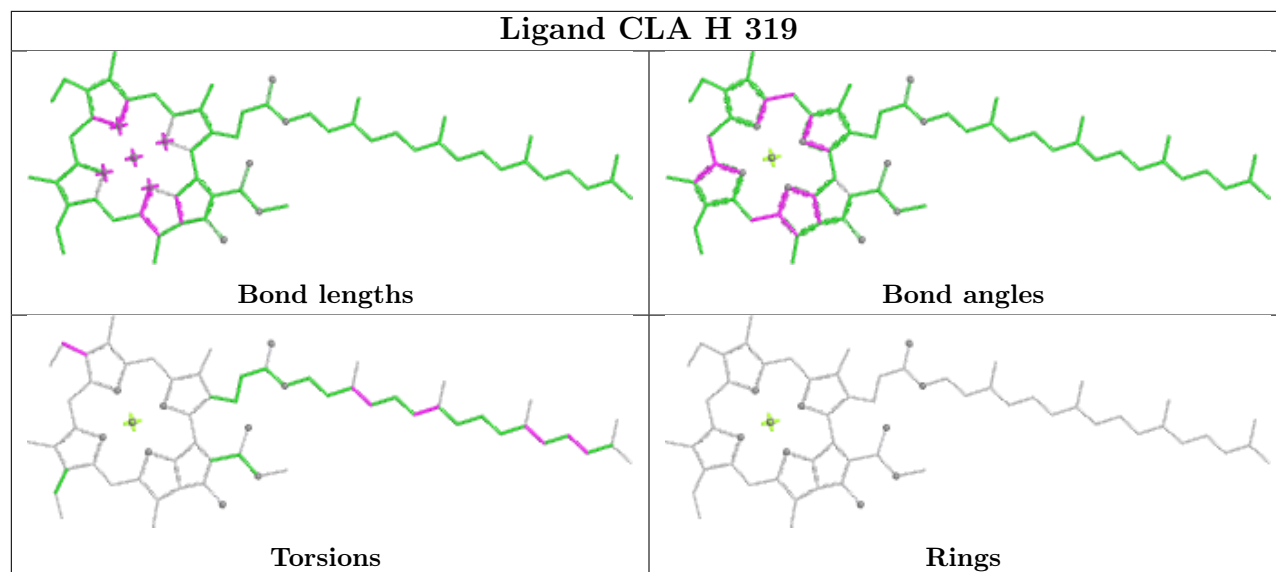
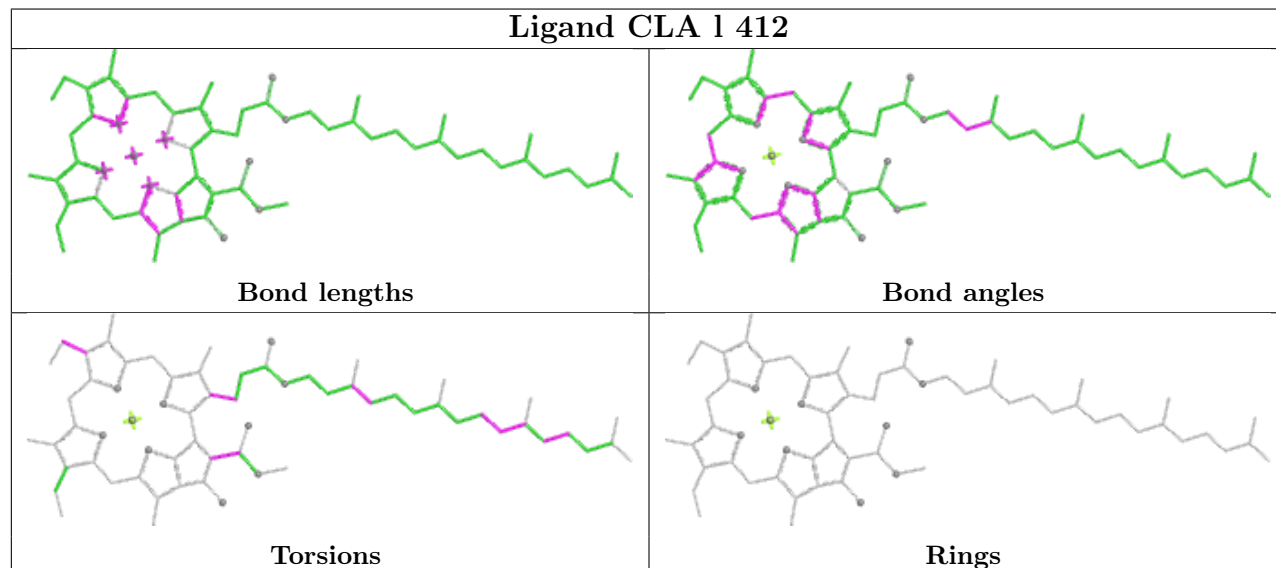
Bond angles

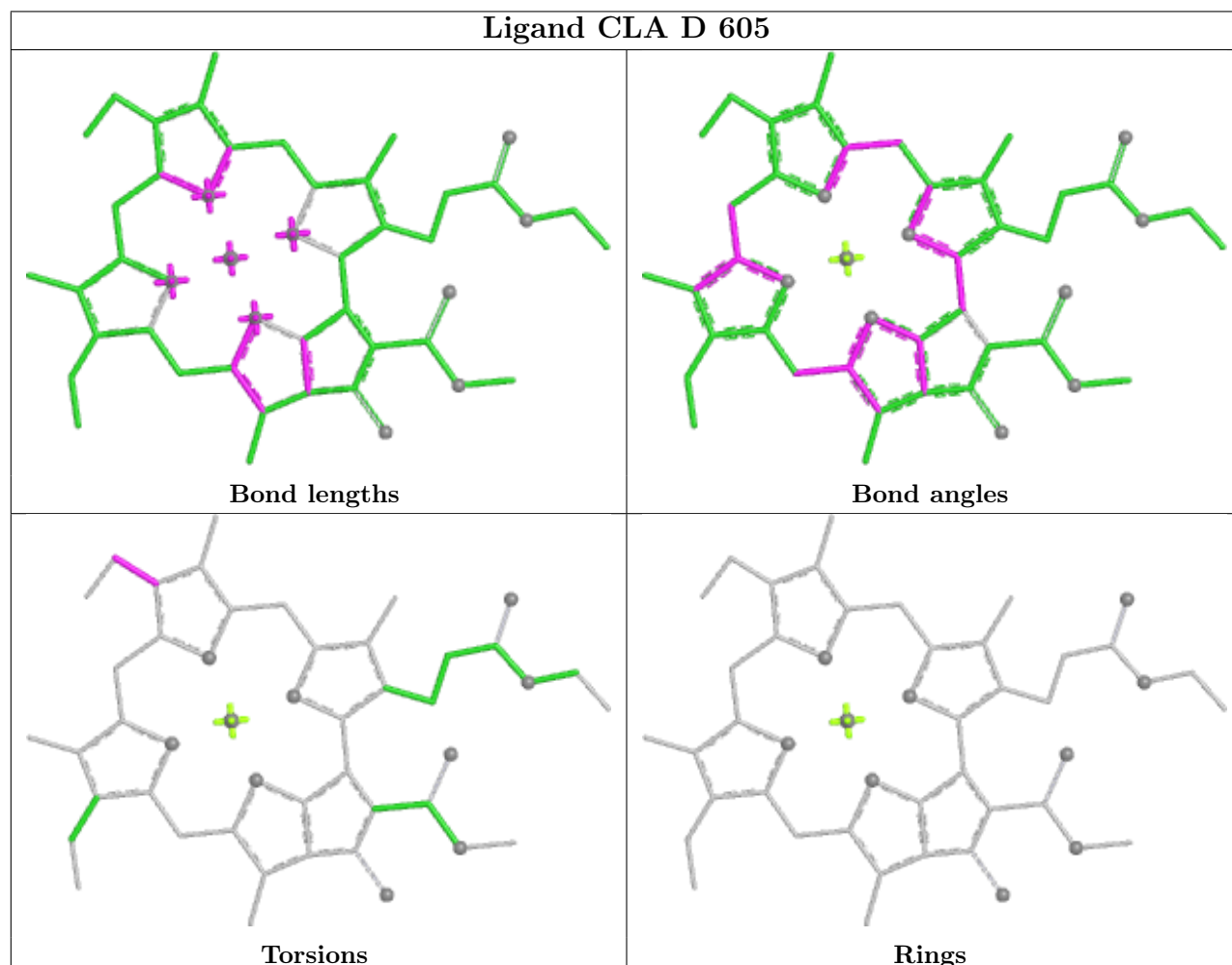
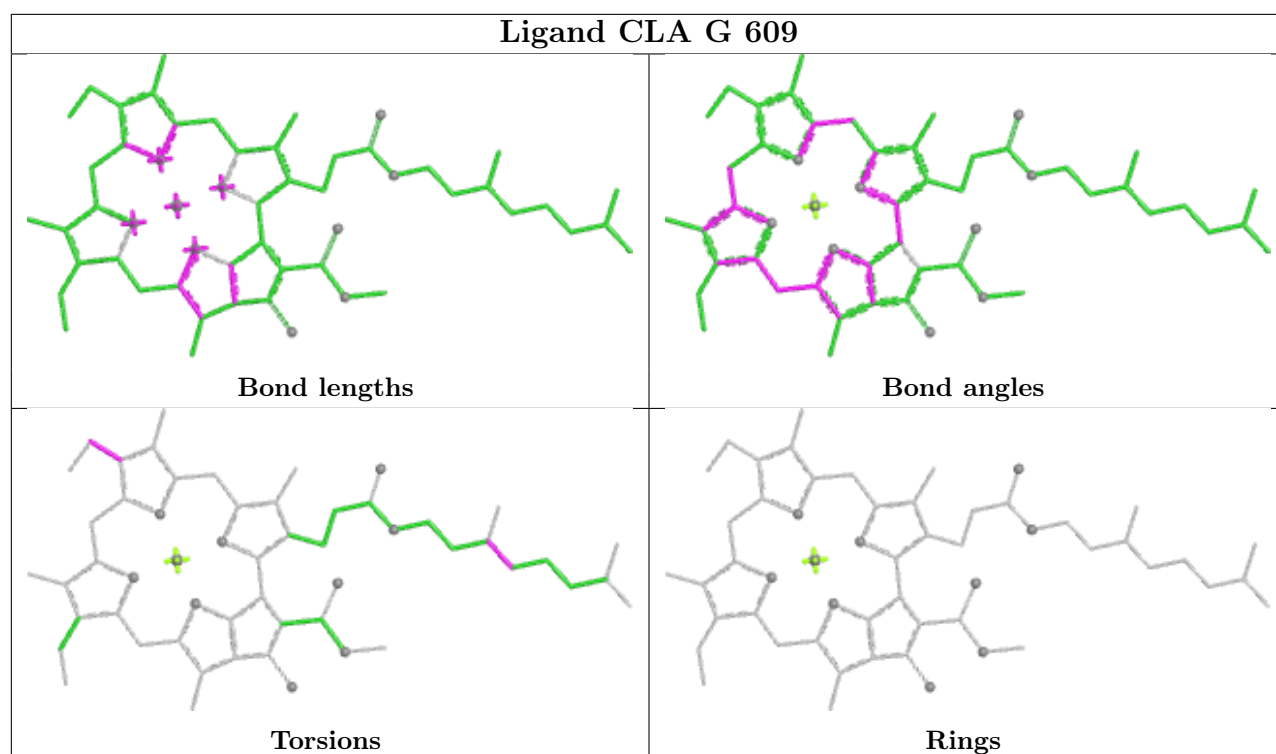


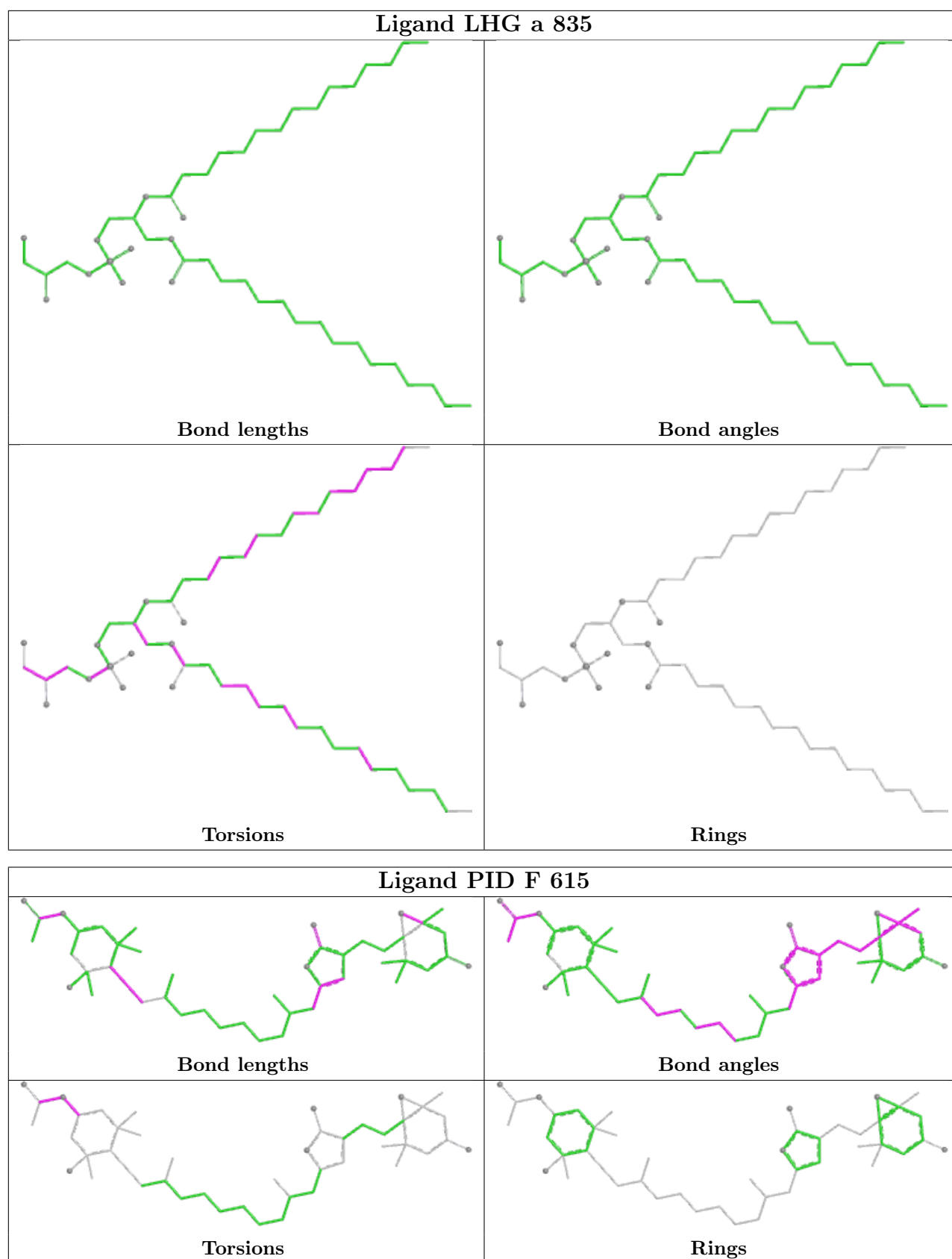
Torsions



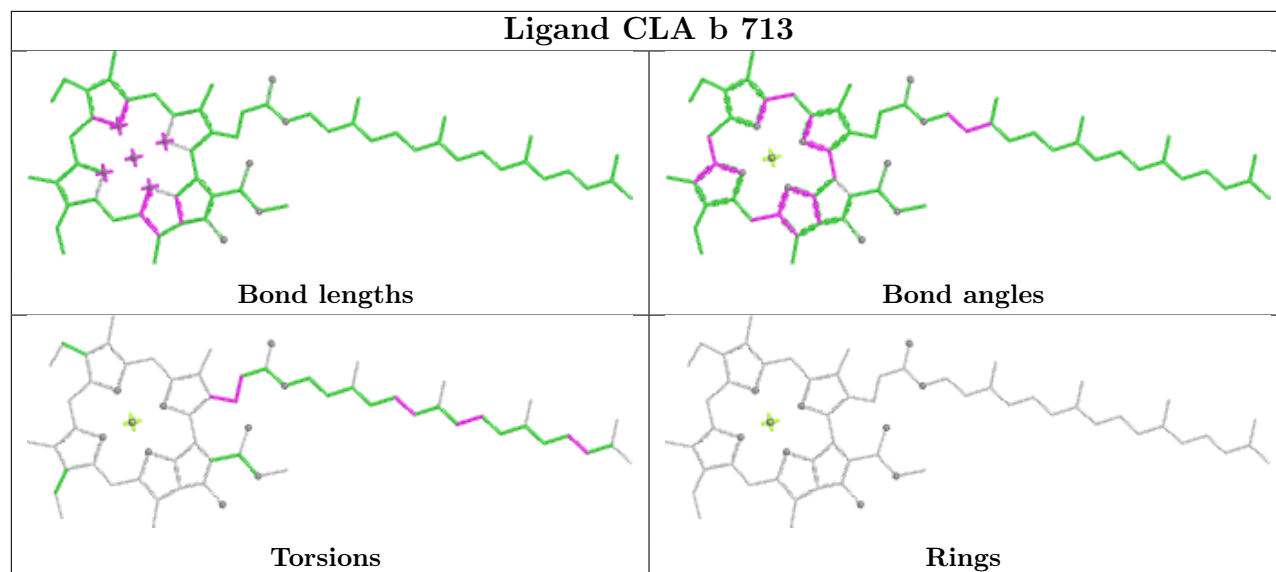
Rings

Ligand CLA H 319**Ligand CLA I 412**

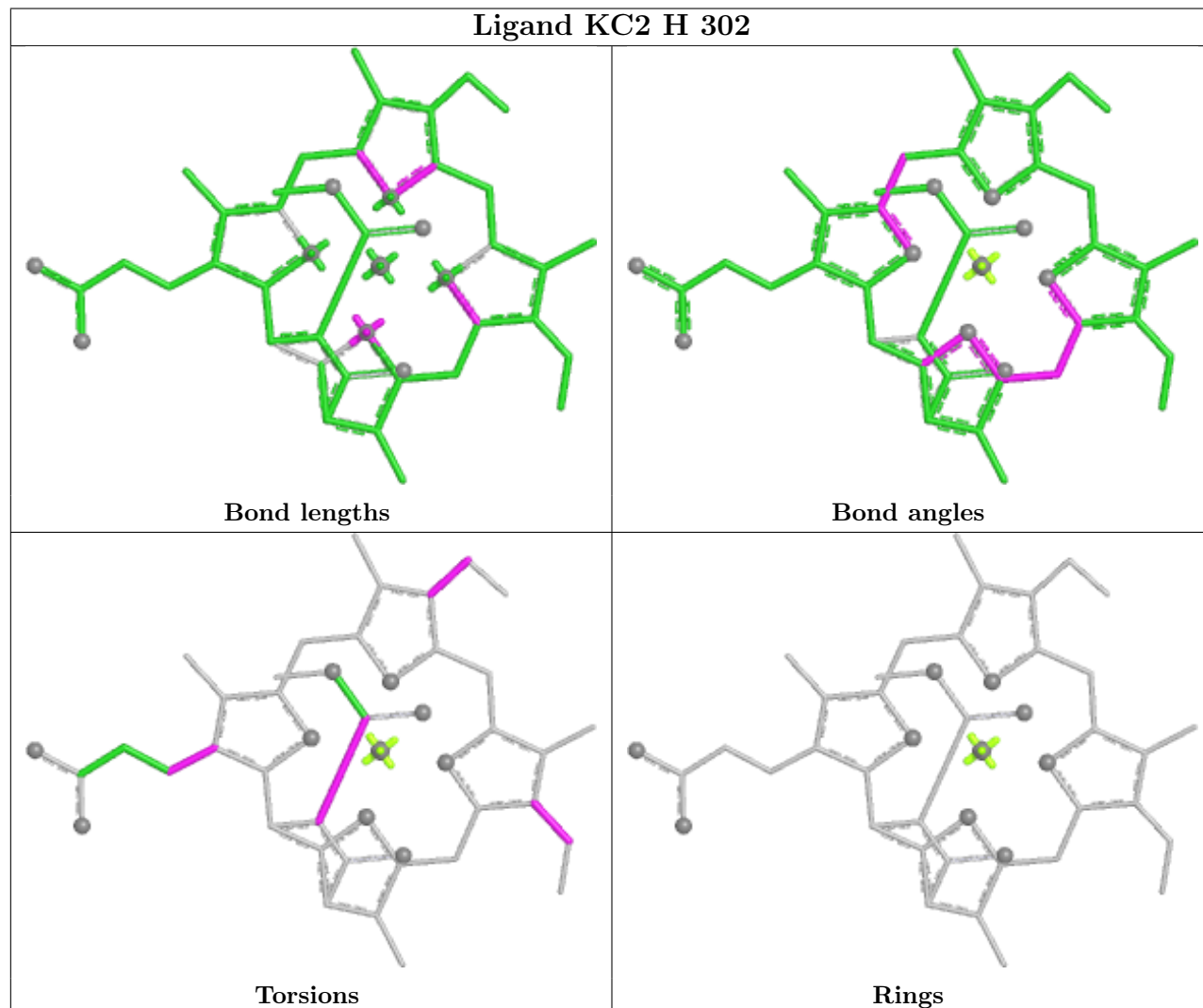




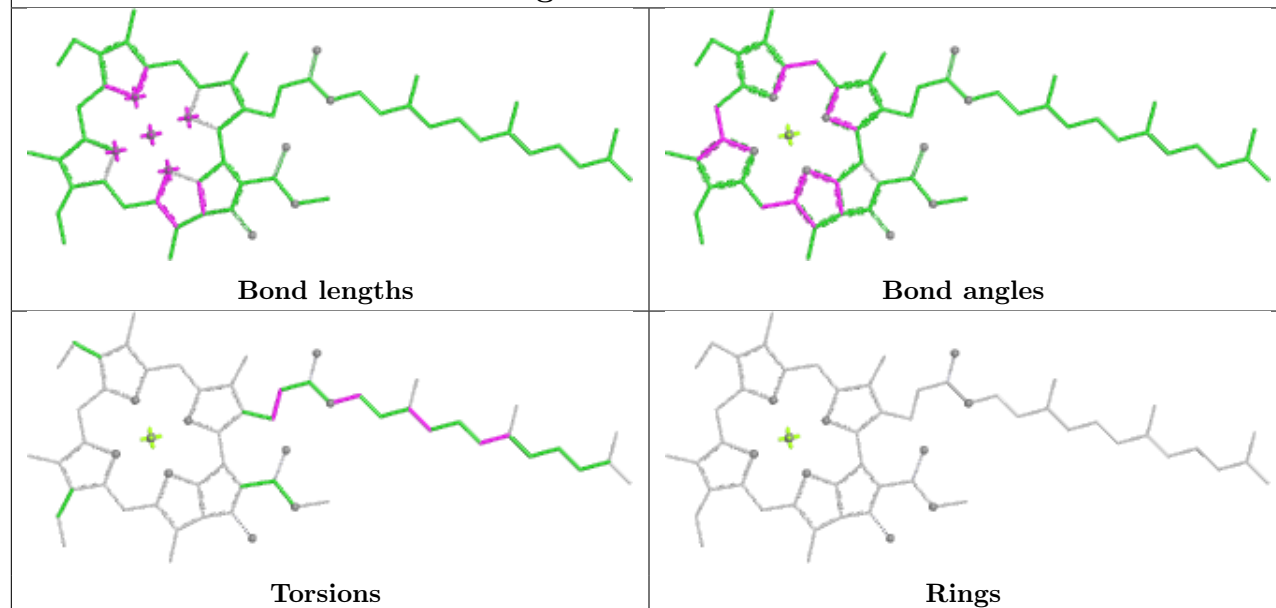
Ligand CLA b 713



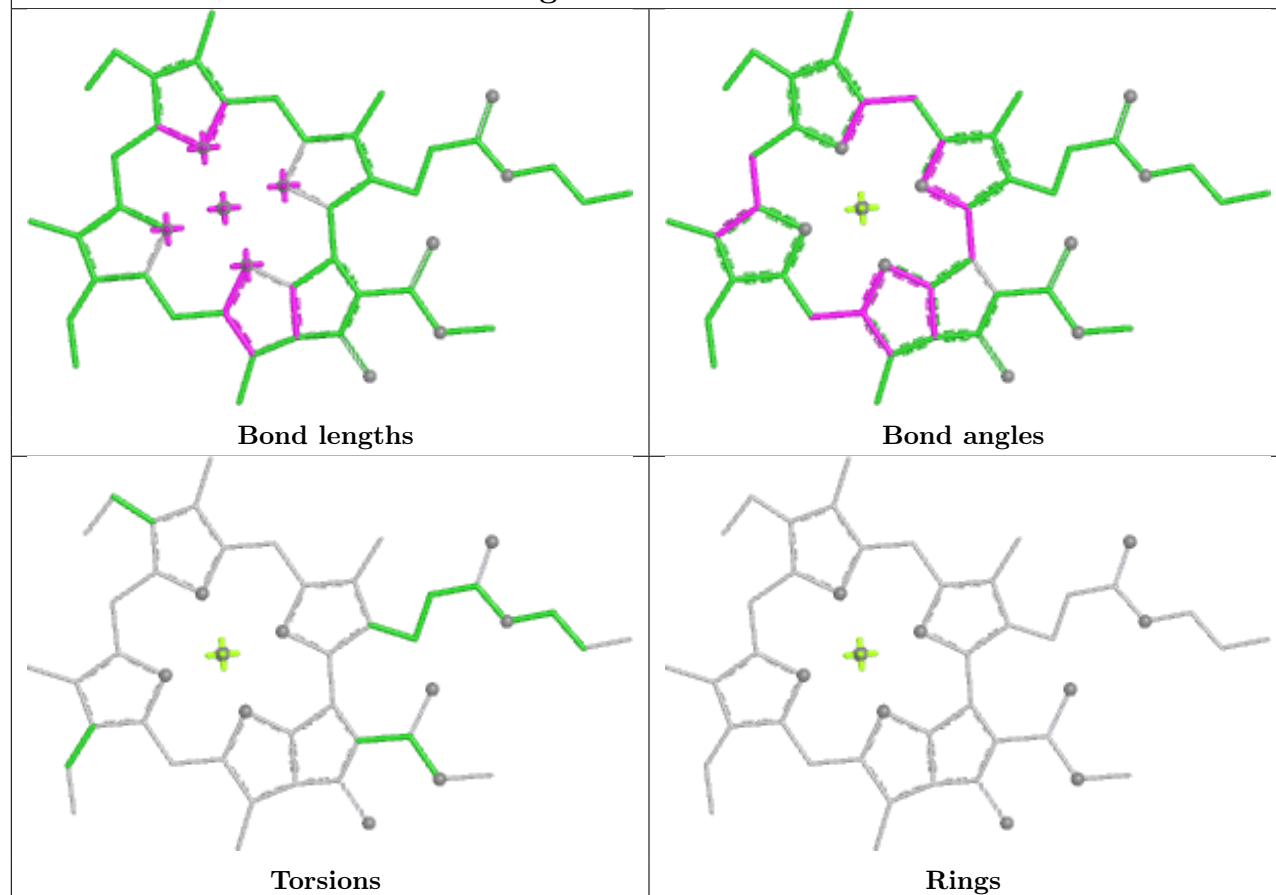
Ligand KC2 H 302



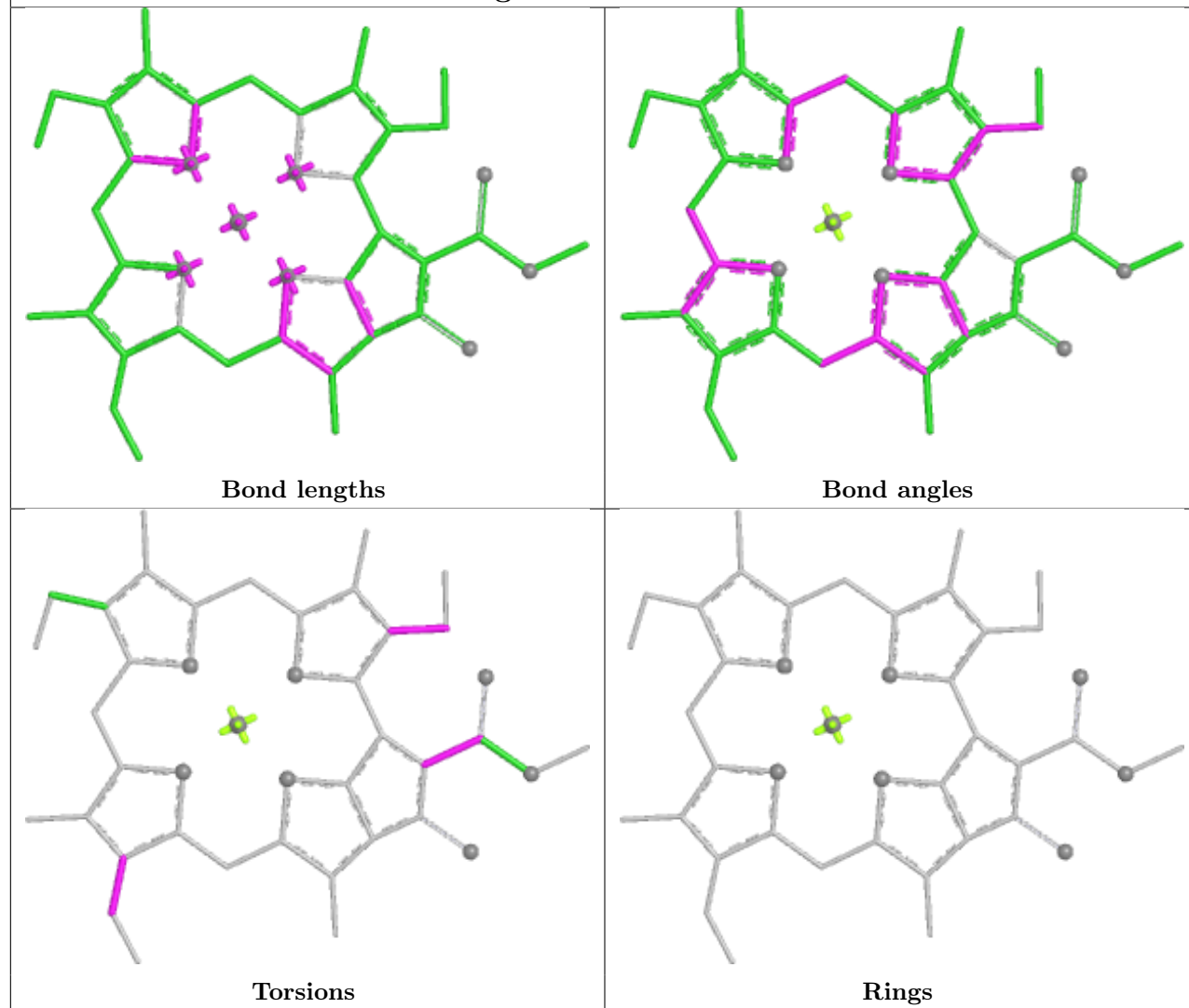
Ligand CLA a 815



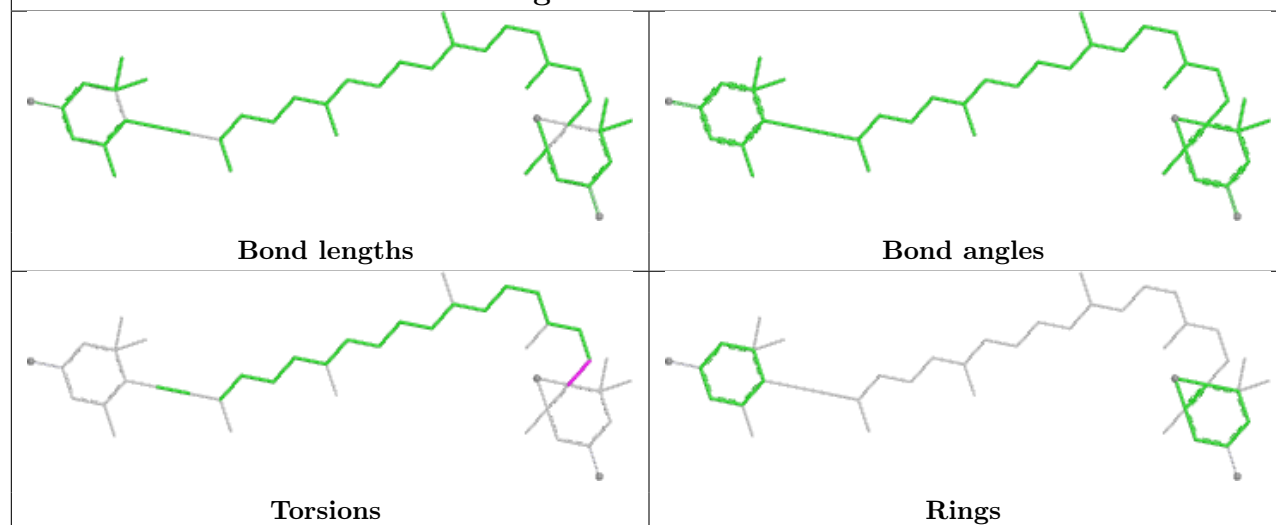
Ligand CLA f 303



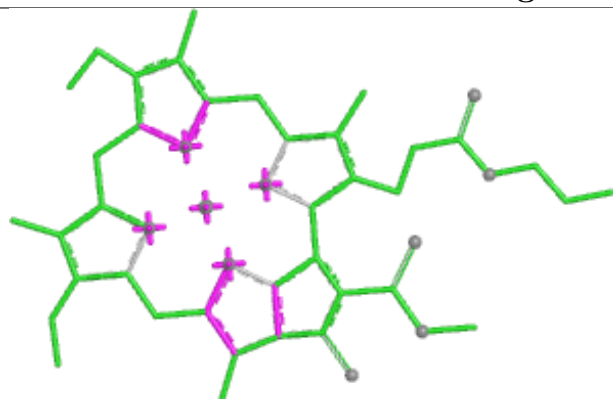
Ligand CLA H 312



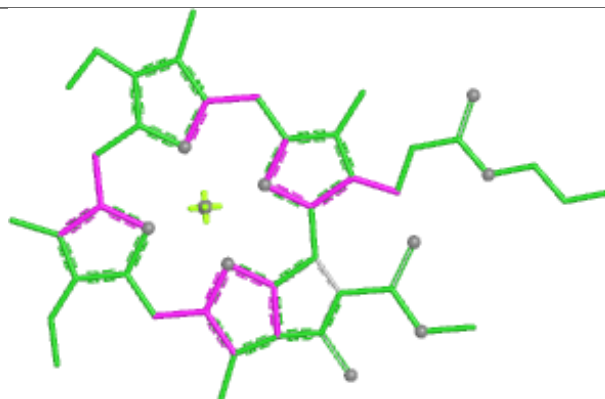
Ligand DD6 B 616



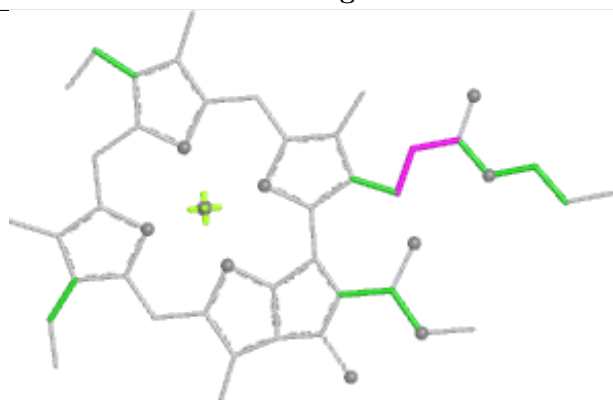
Ligand CLA b 712



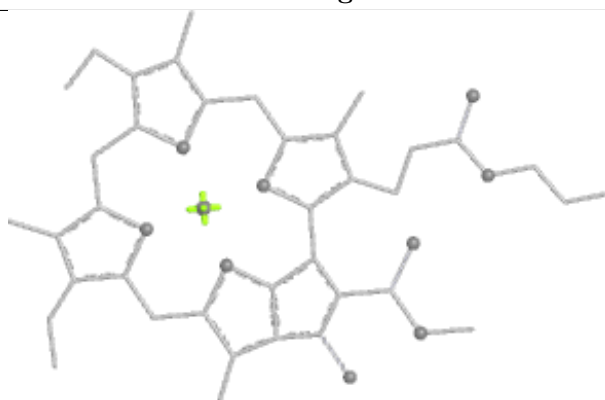
Bond lengths



Bond angles

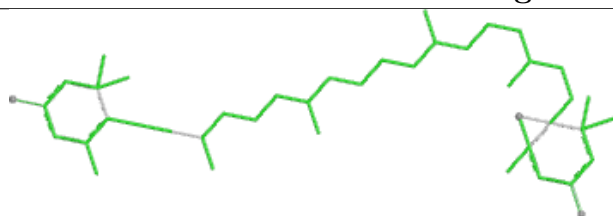


Torsions

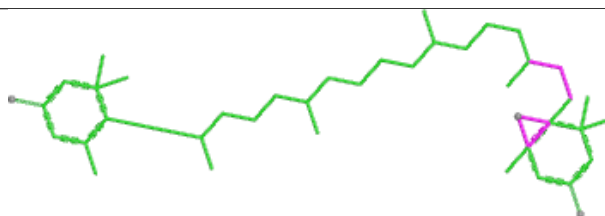


Rings

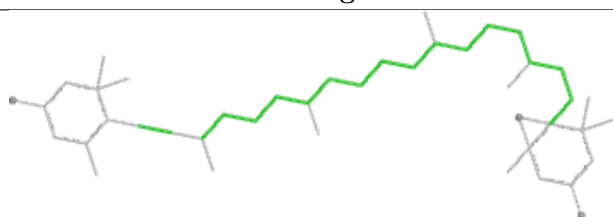
Ligand DD6 D 617



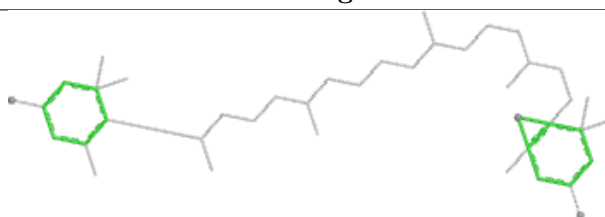
Bond lengths



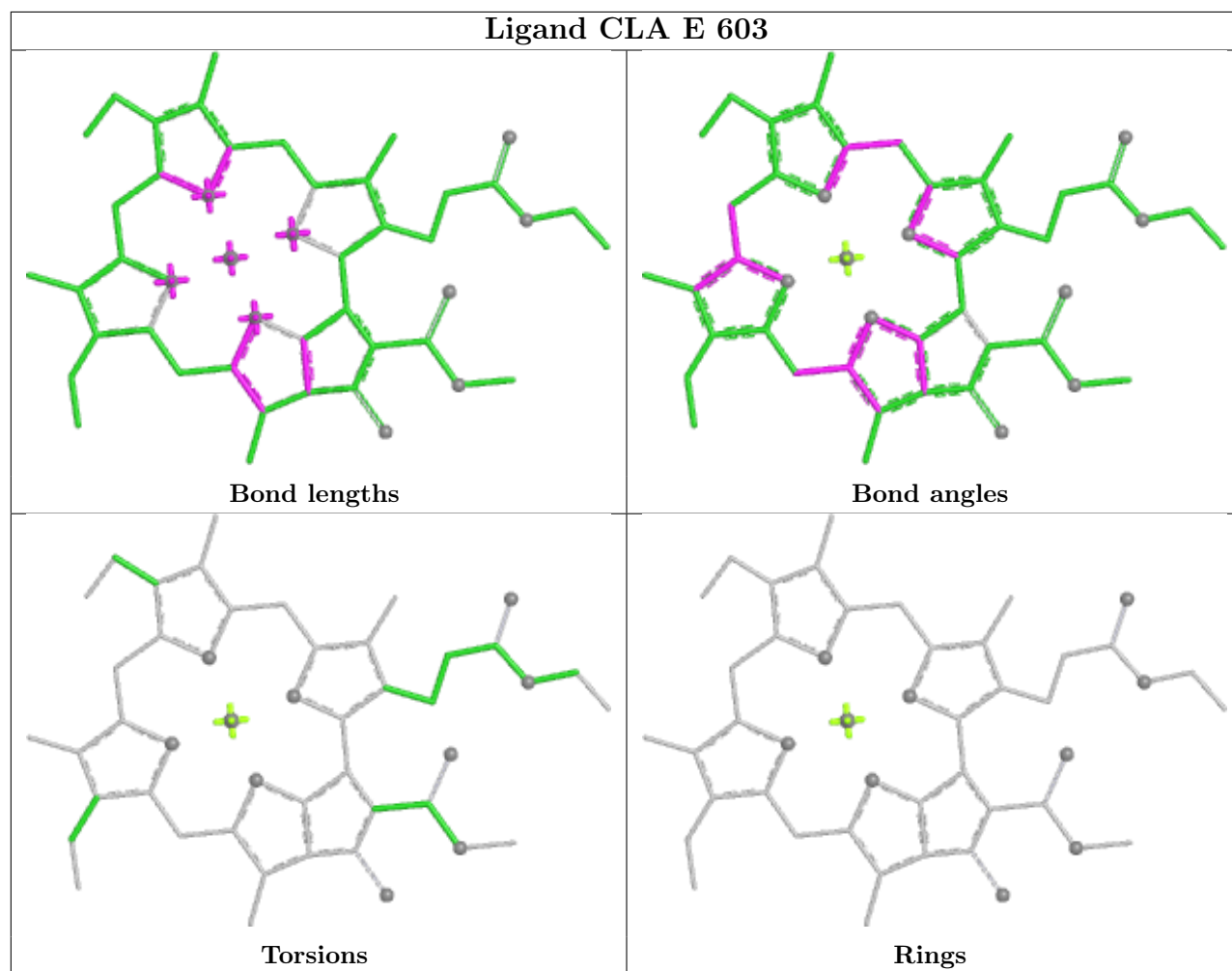
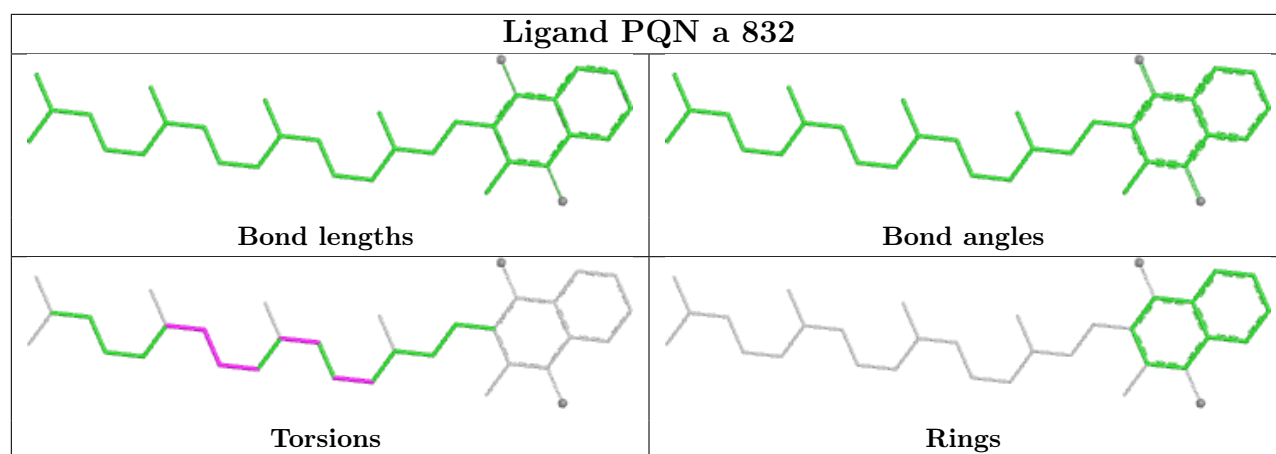
Bond angles



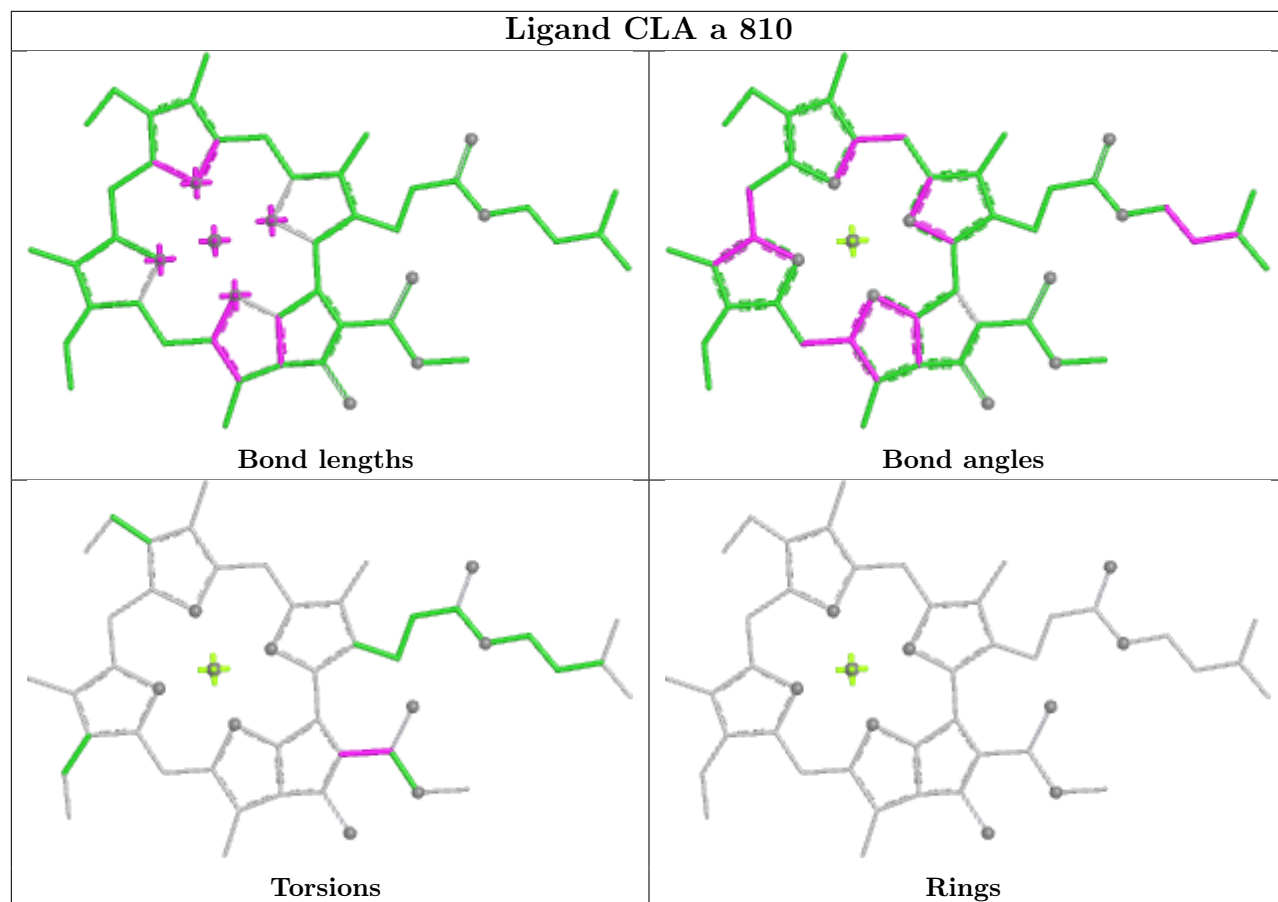
Torsions



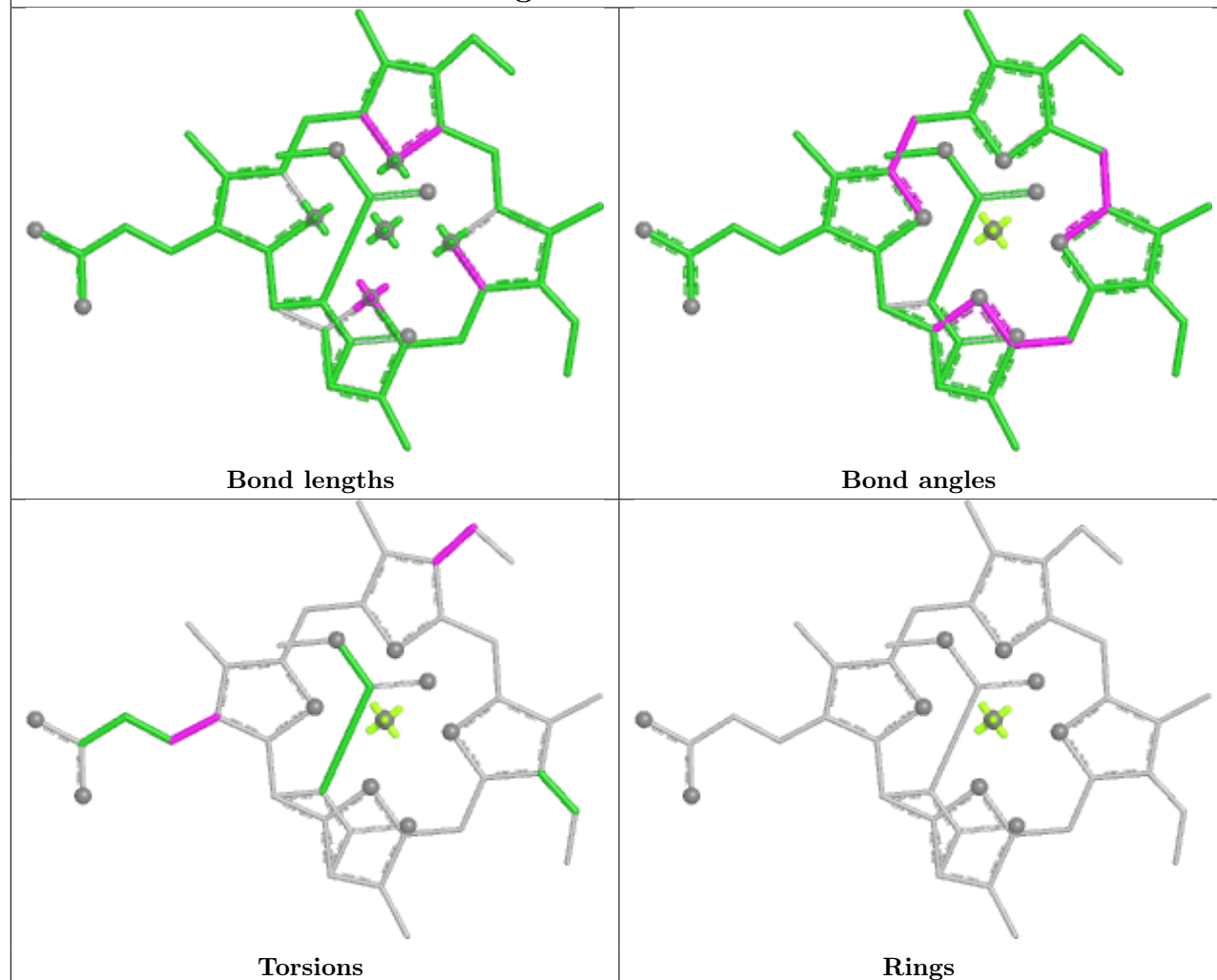
Rings



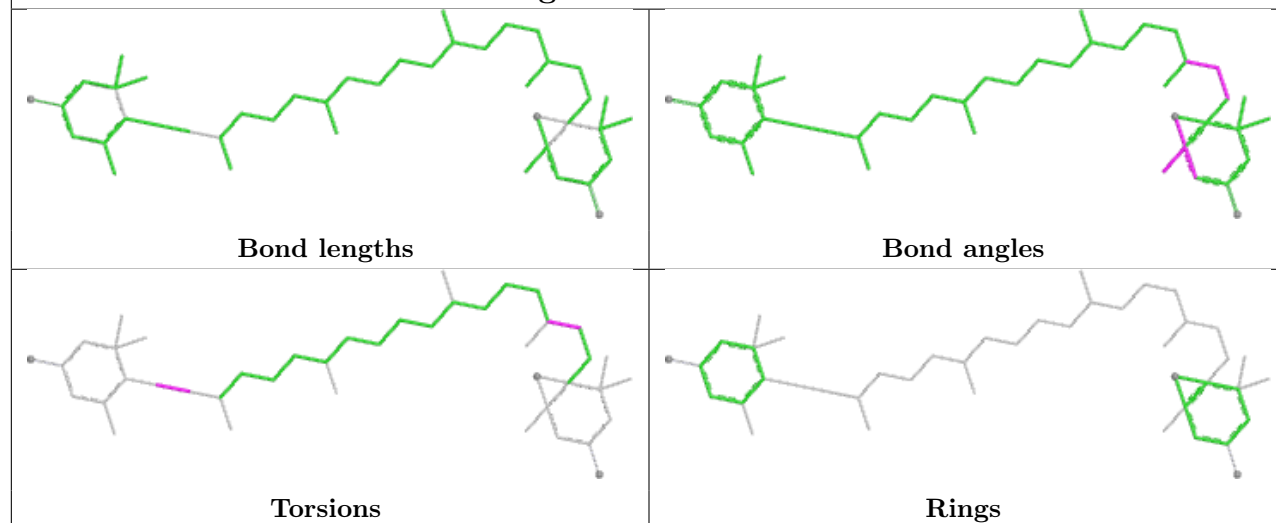
Ligand CLA a 810

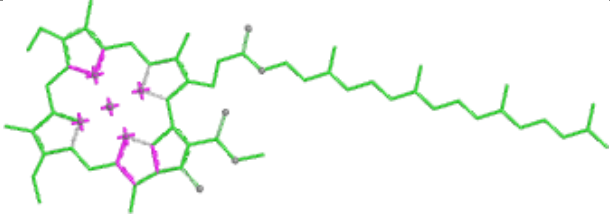
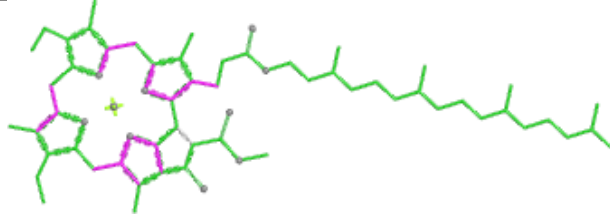
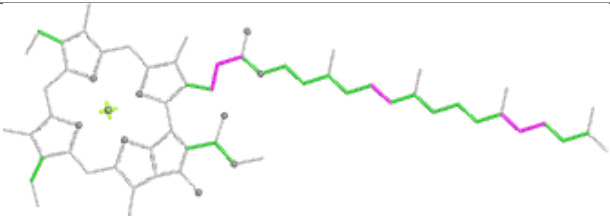
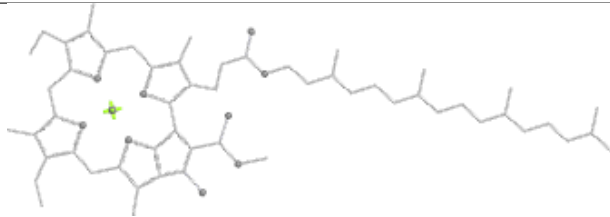
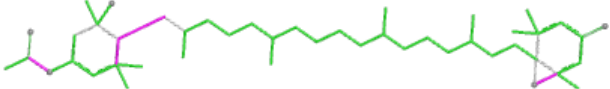
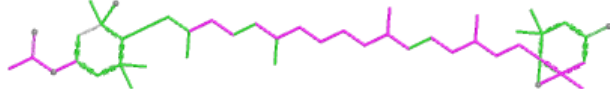
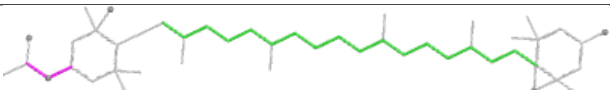
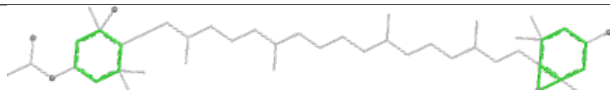
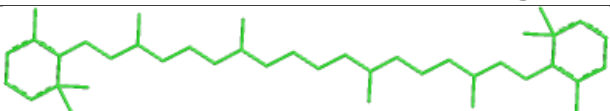
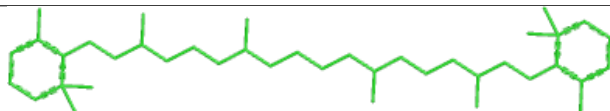
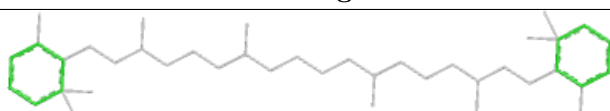


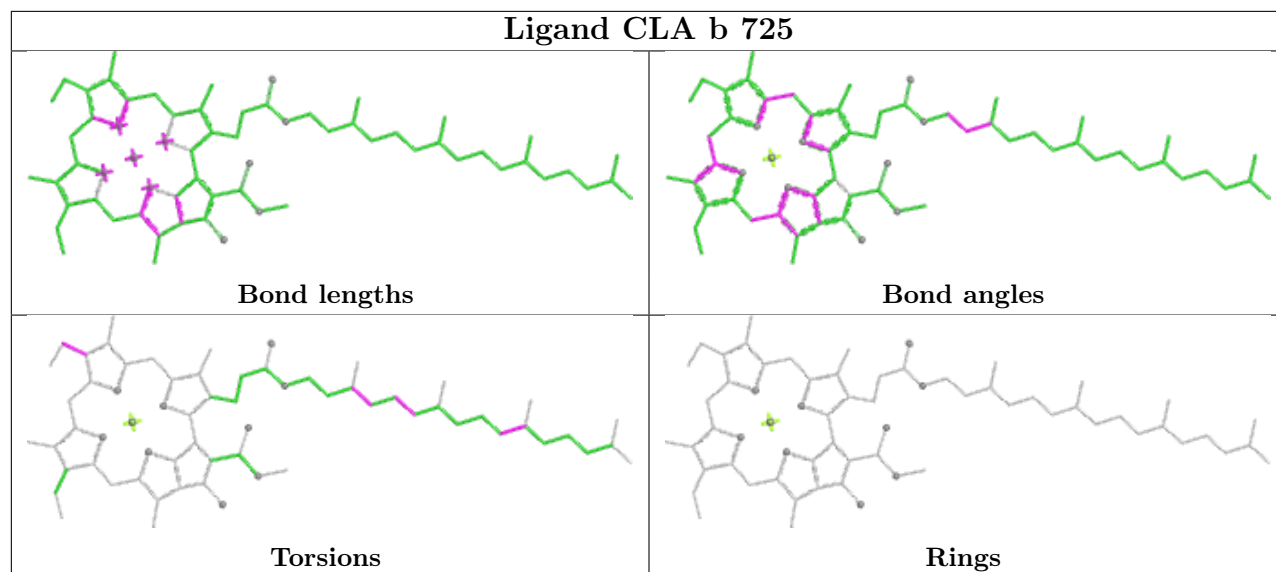
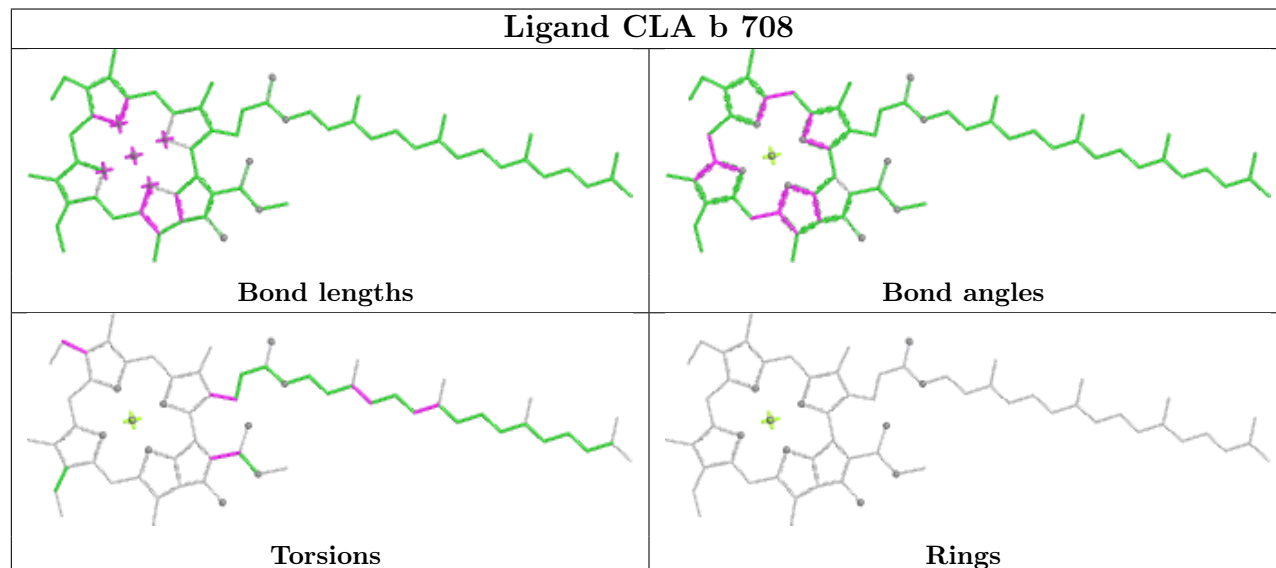
Ligand KC2 I 604

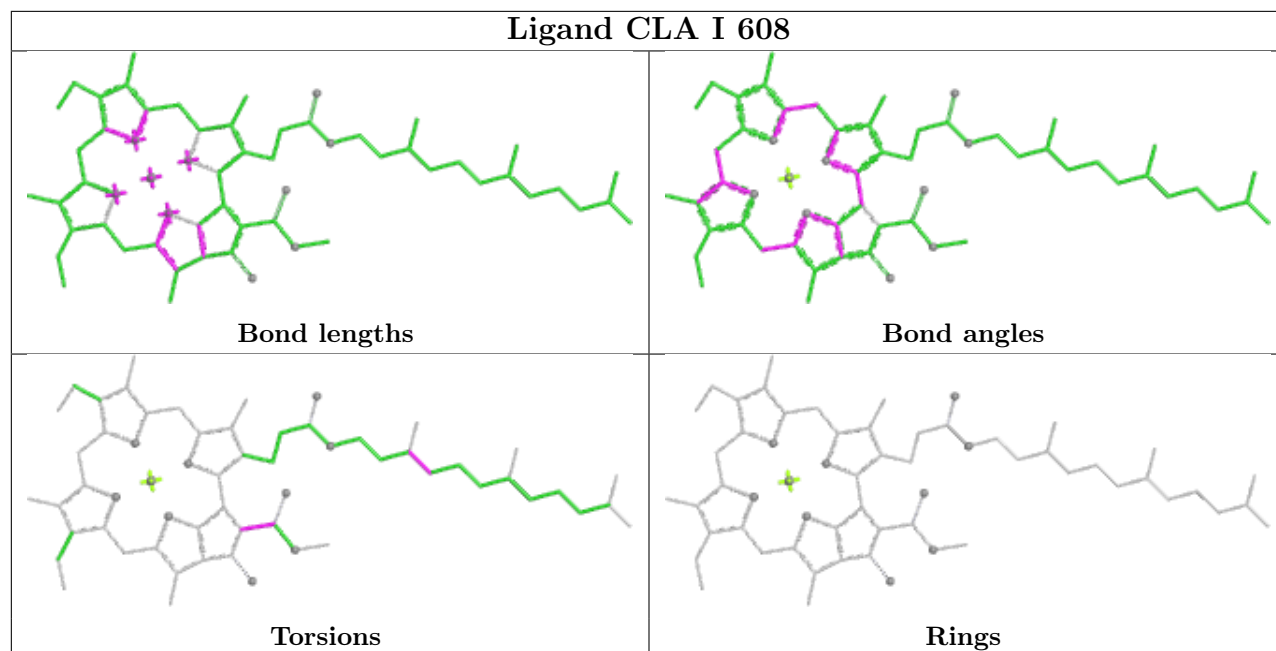
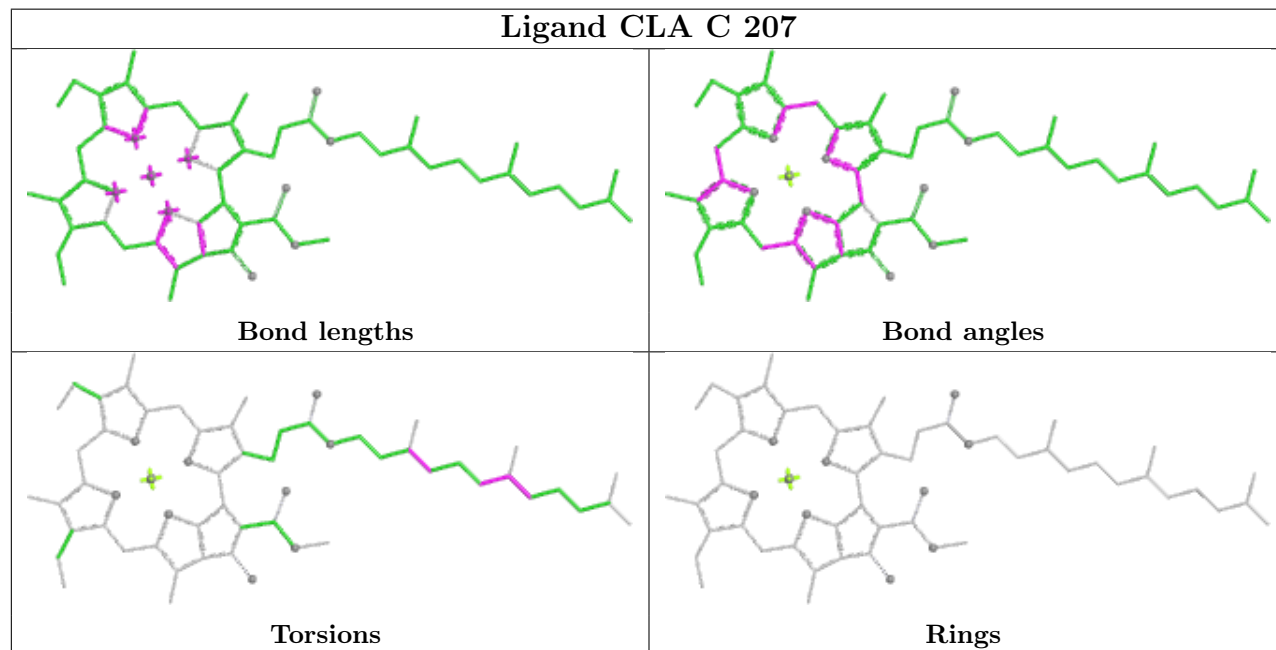


Ligand DD6 r 206

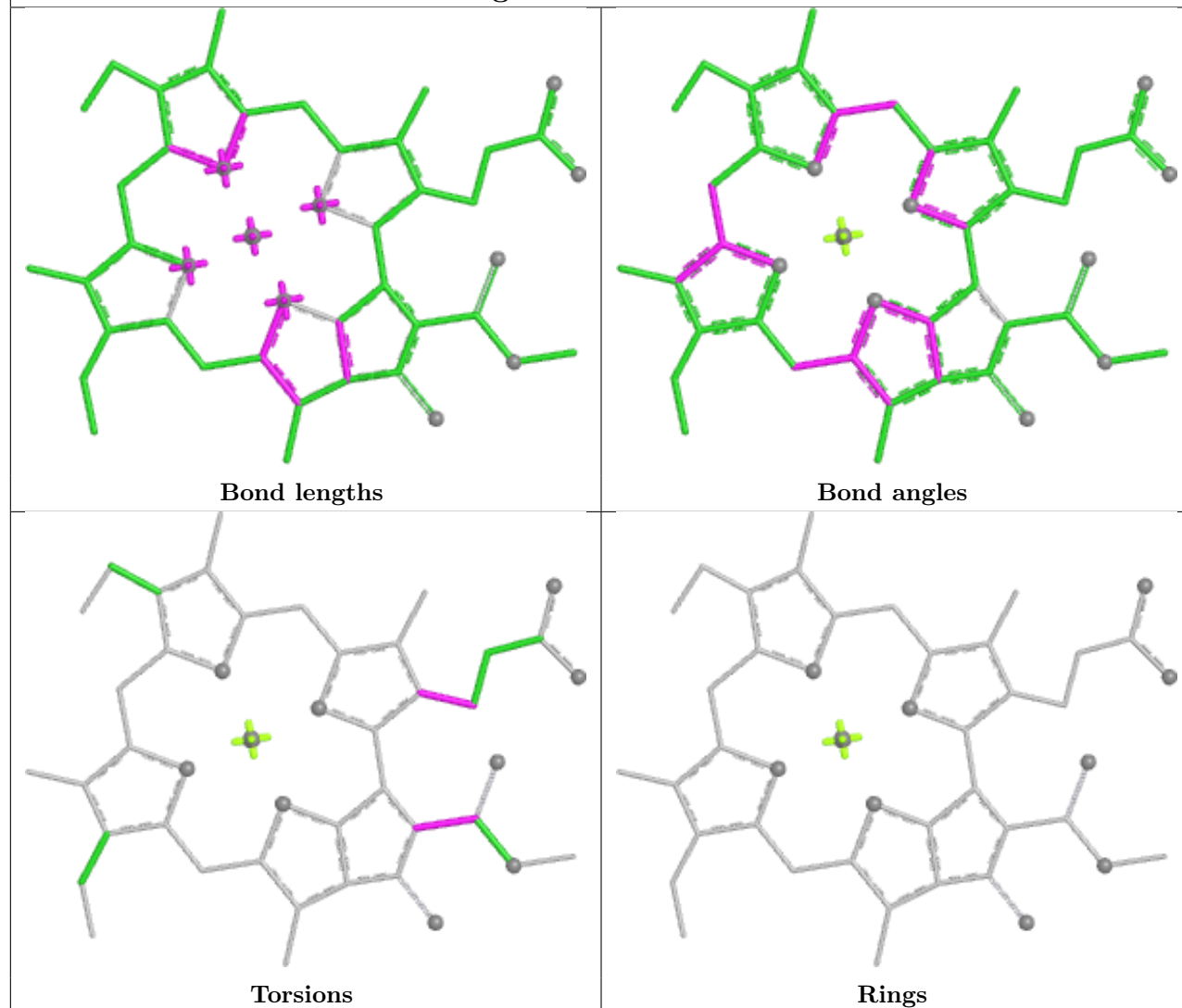


Ligand CLA B 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand UIX H 317	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 1 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

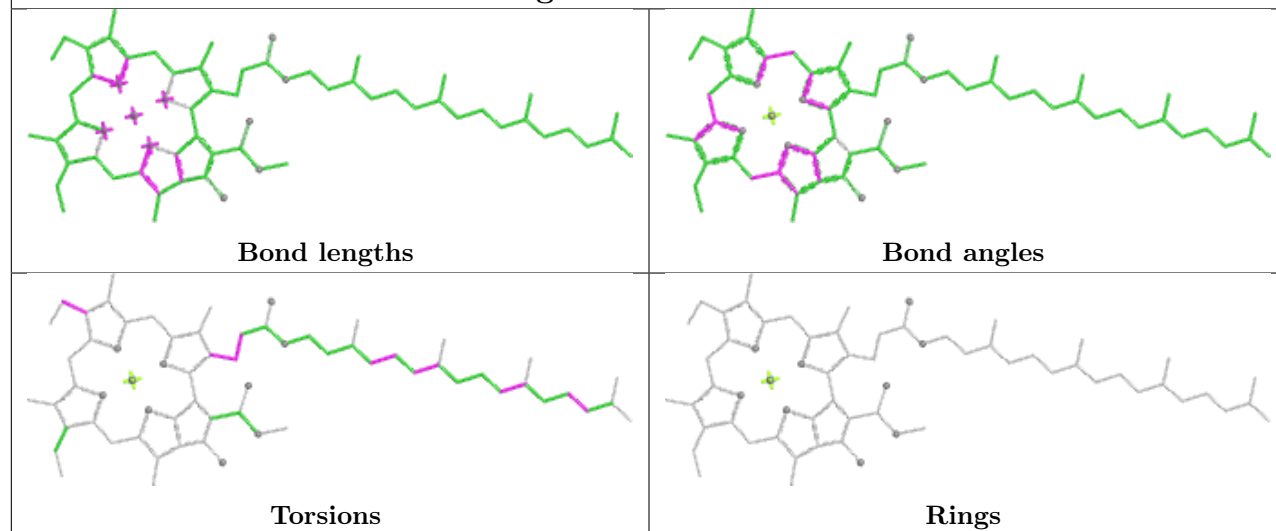
Ligand CLA b 725**Ligand CLA b 708**

Ligand CLA I 608**Ligand CLA C 207**

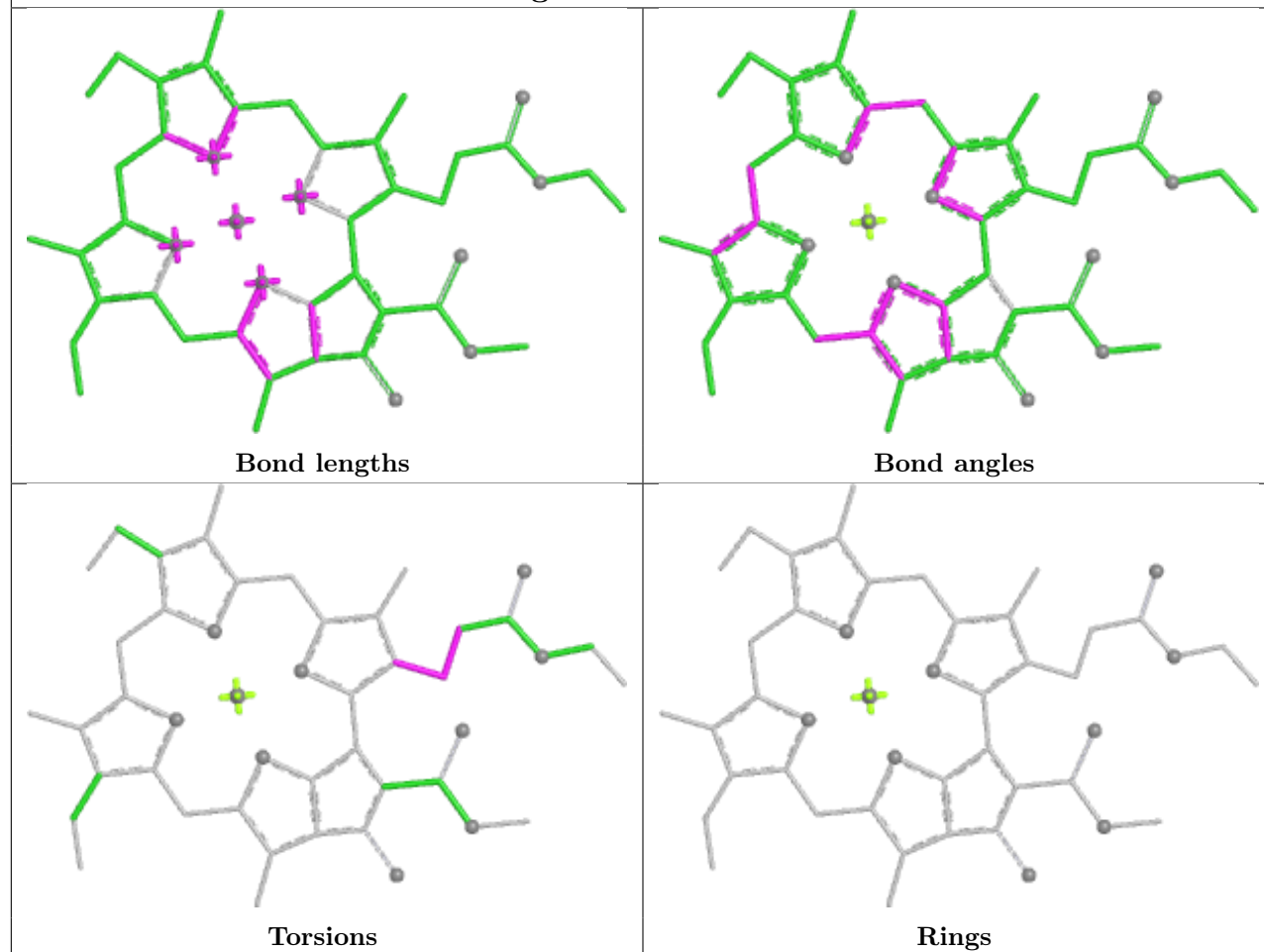
Ligand CLA A 611



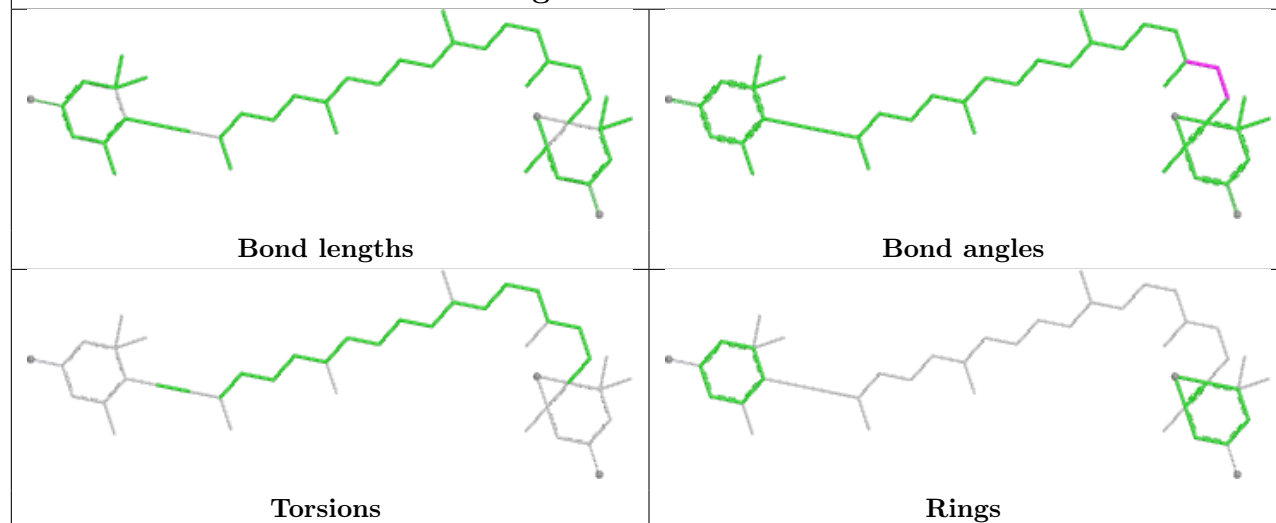
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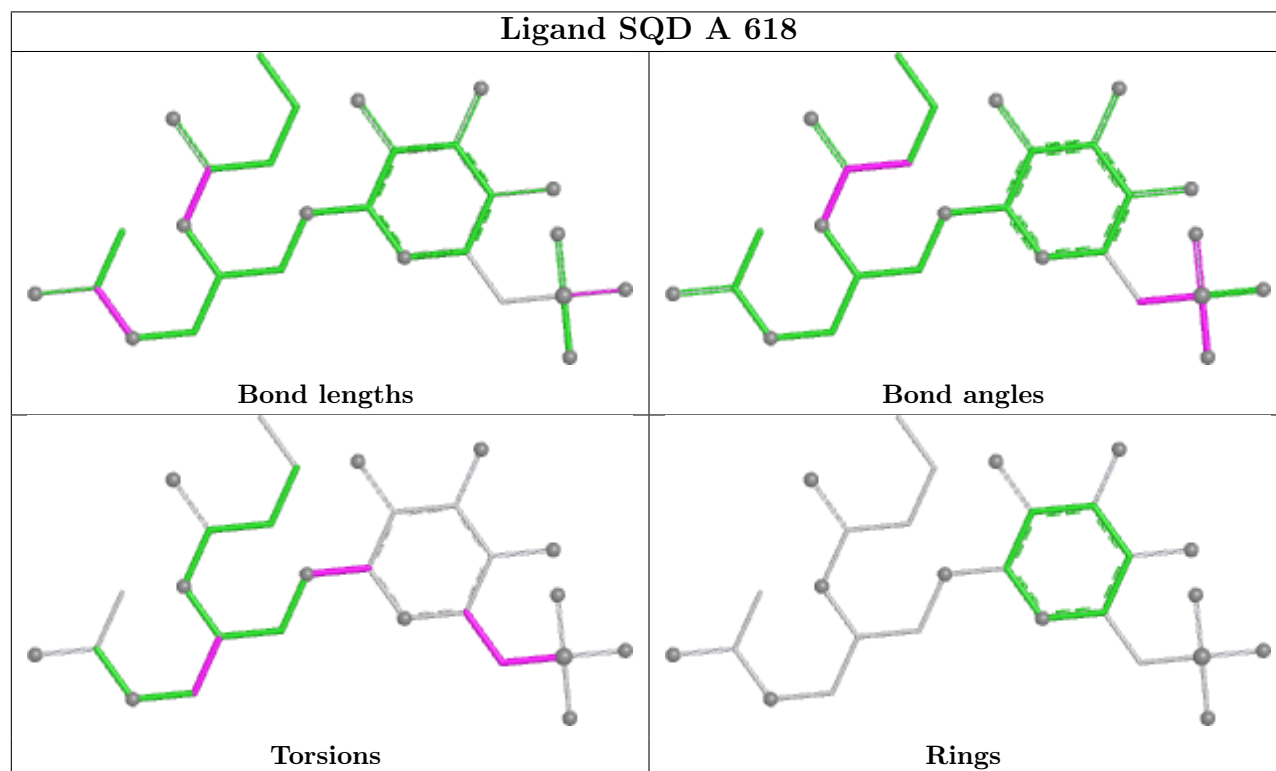
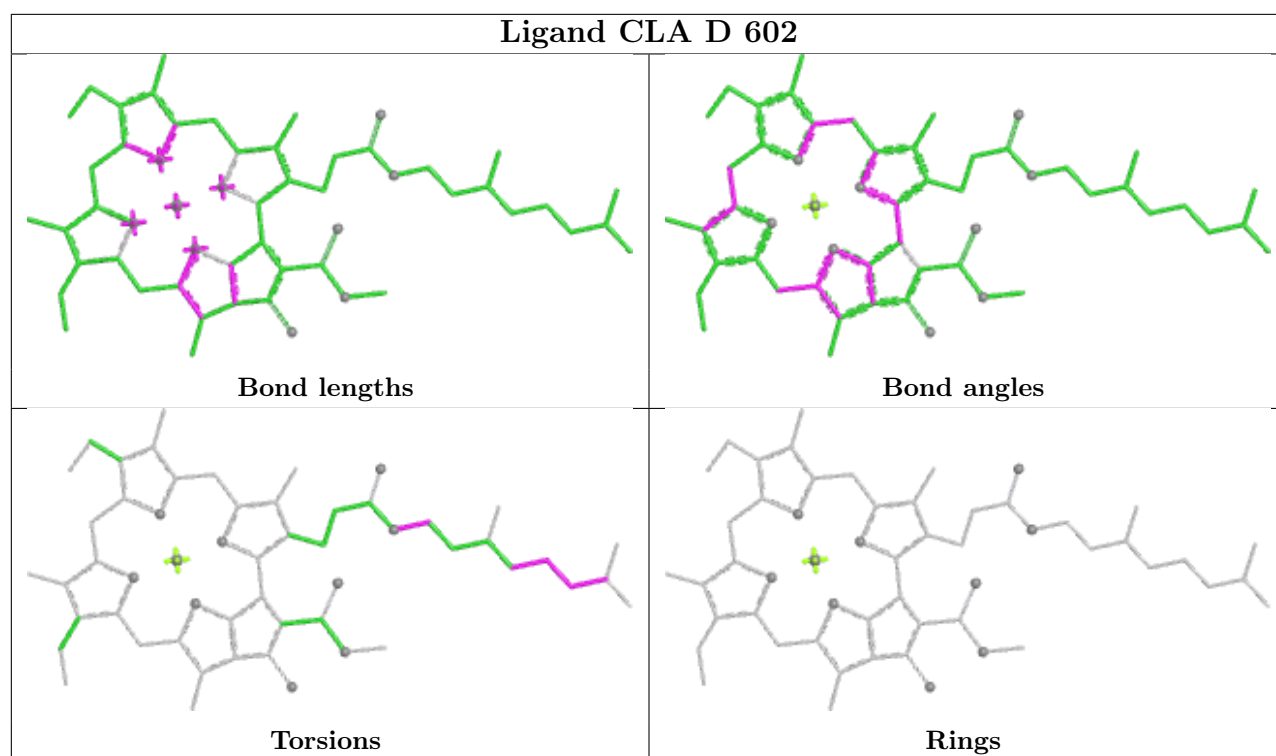


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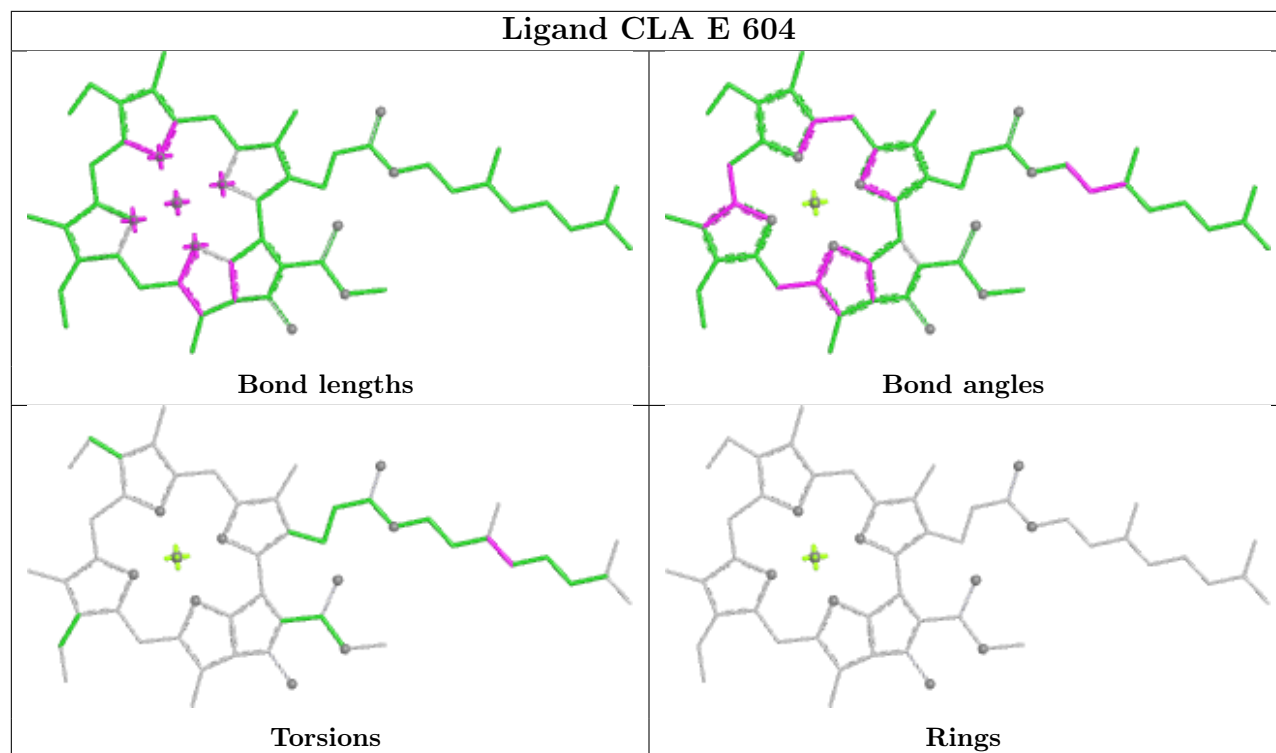


Ligand DD6 U 607

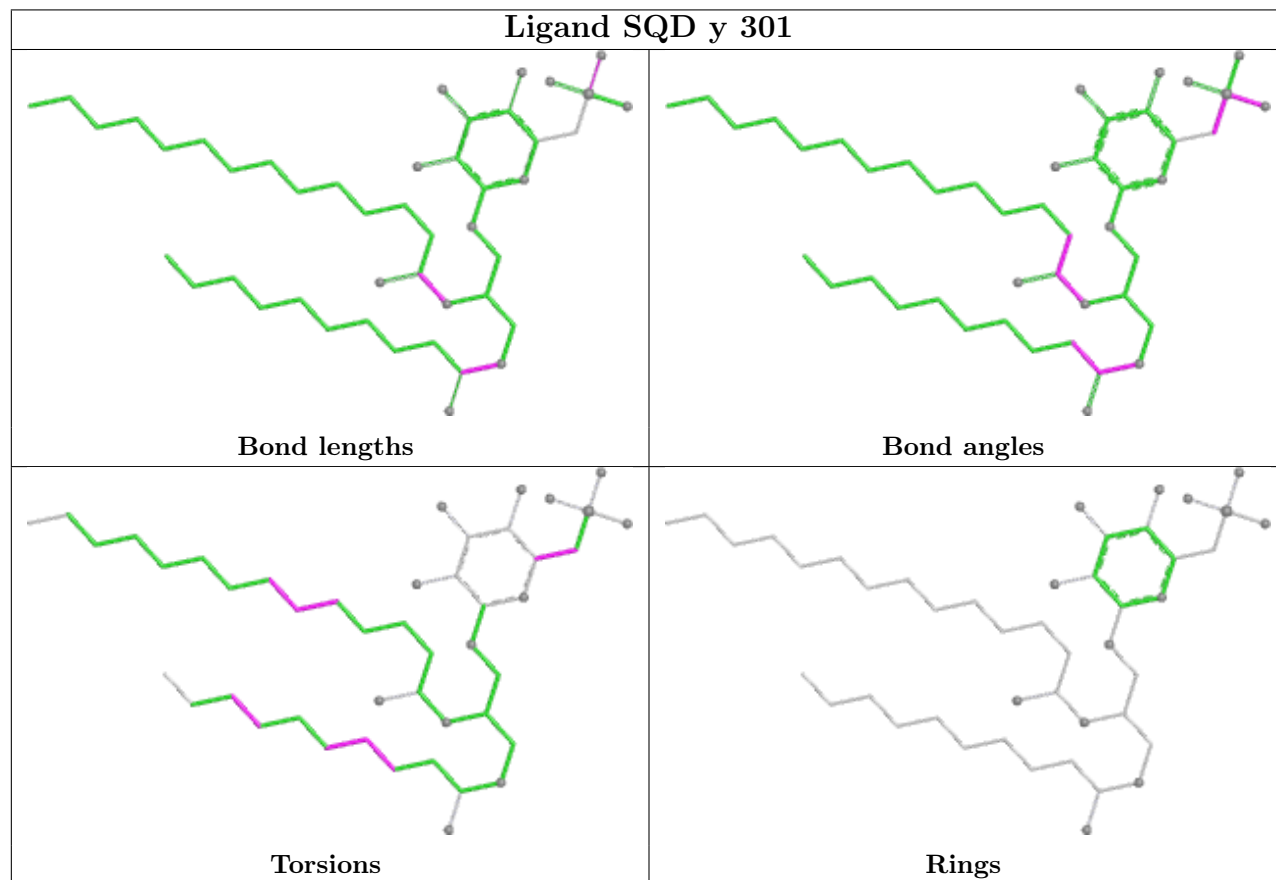


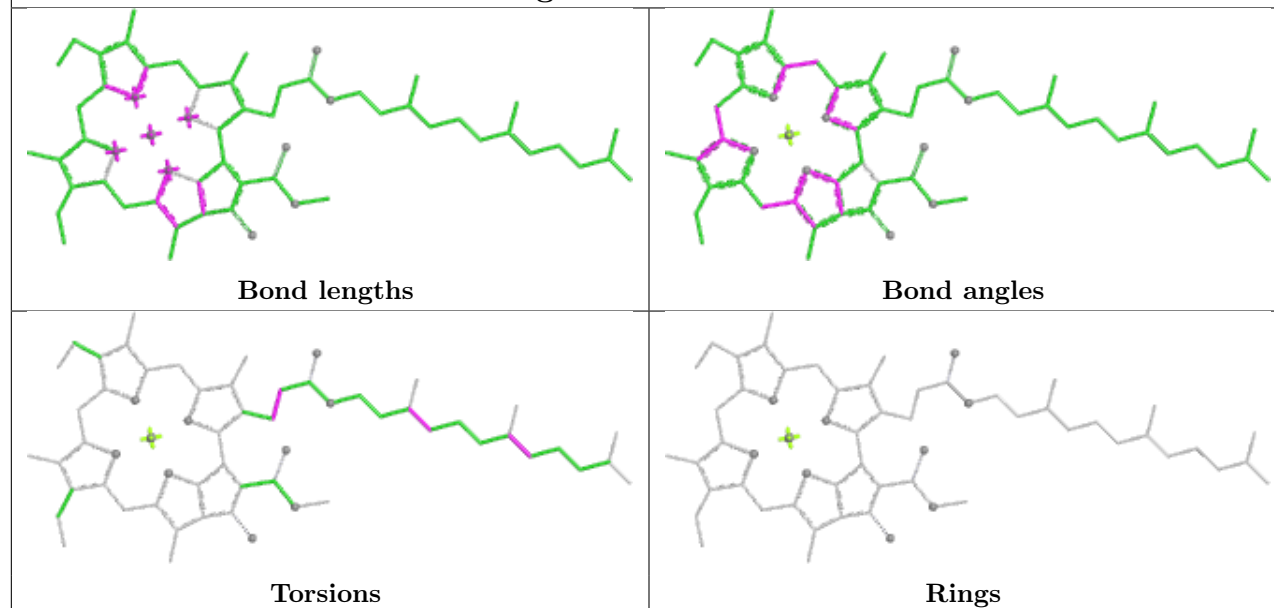
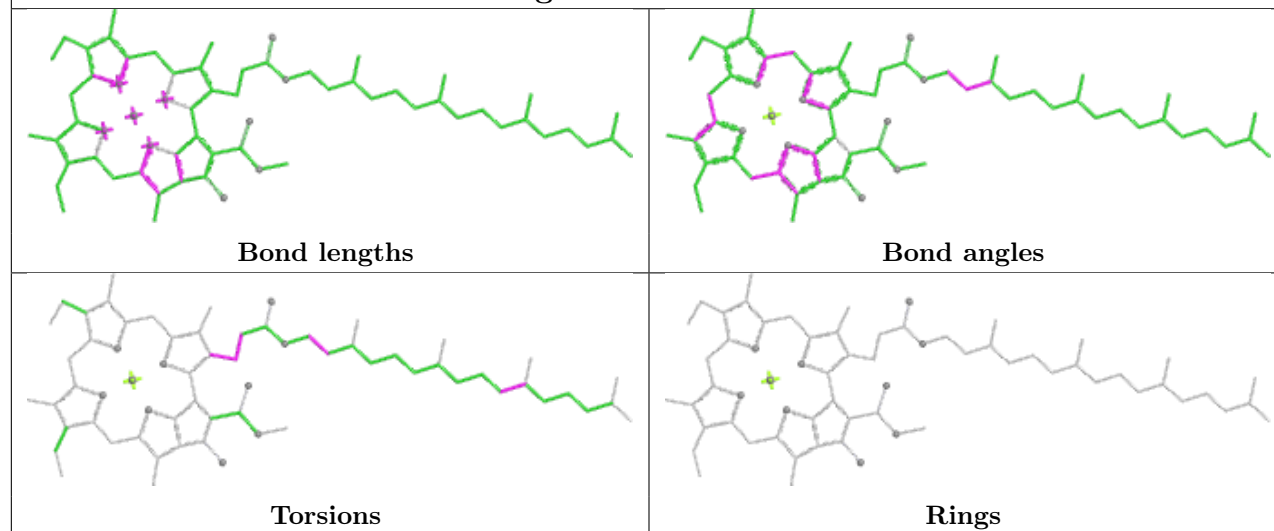


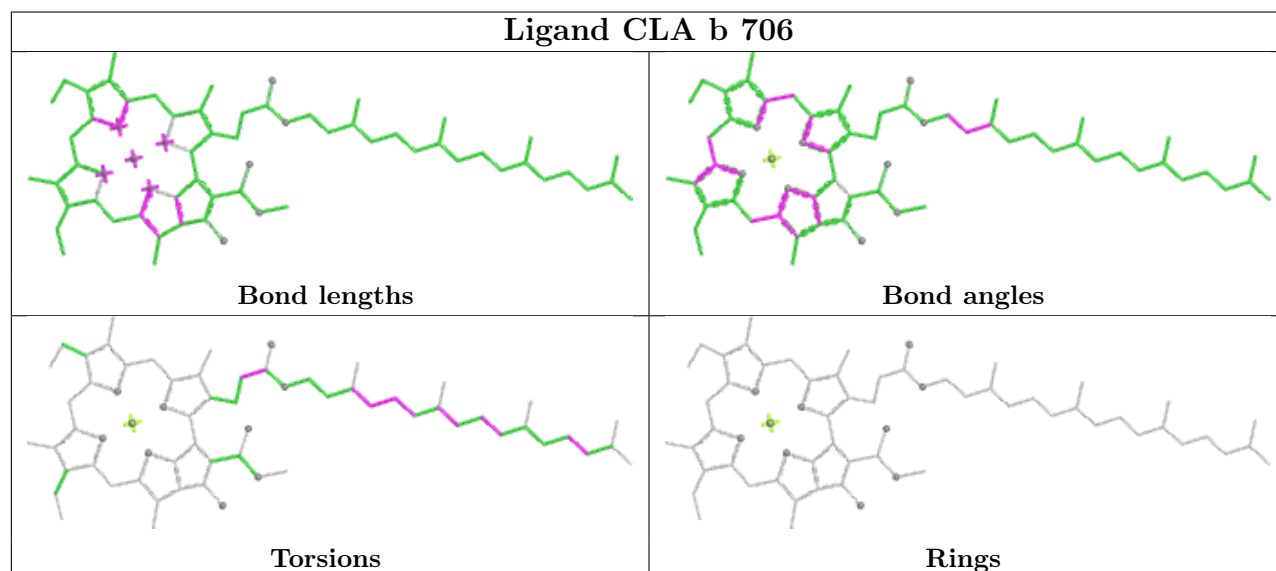
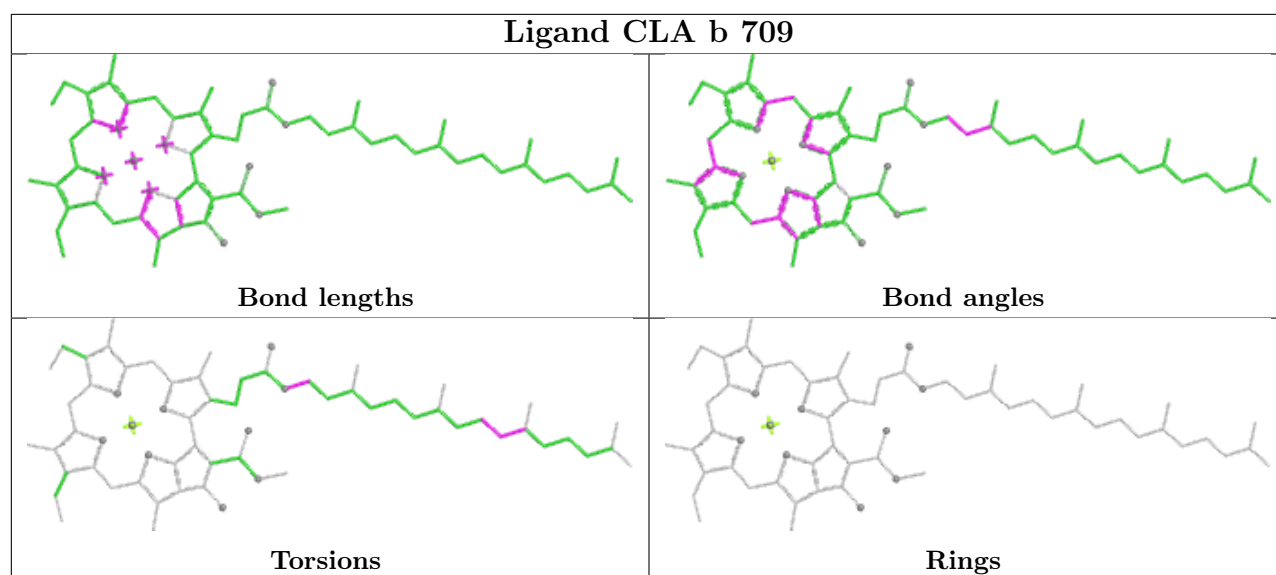
Ligand CLA E 604

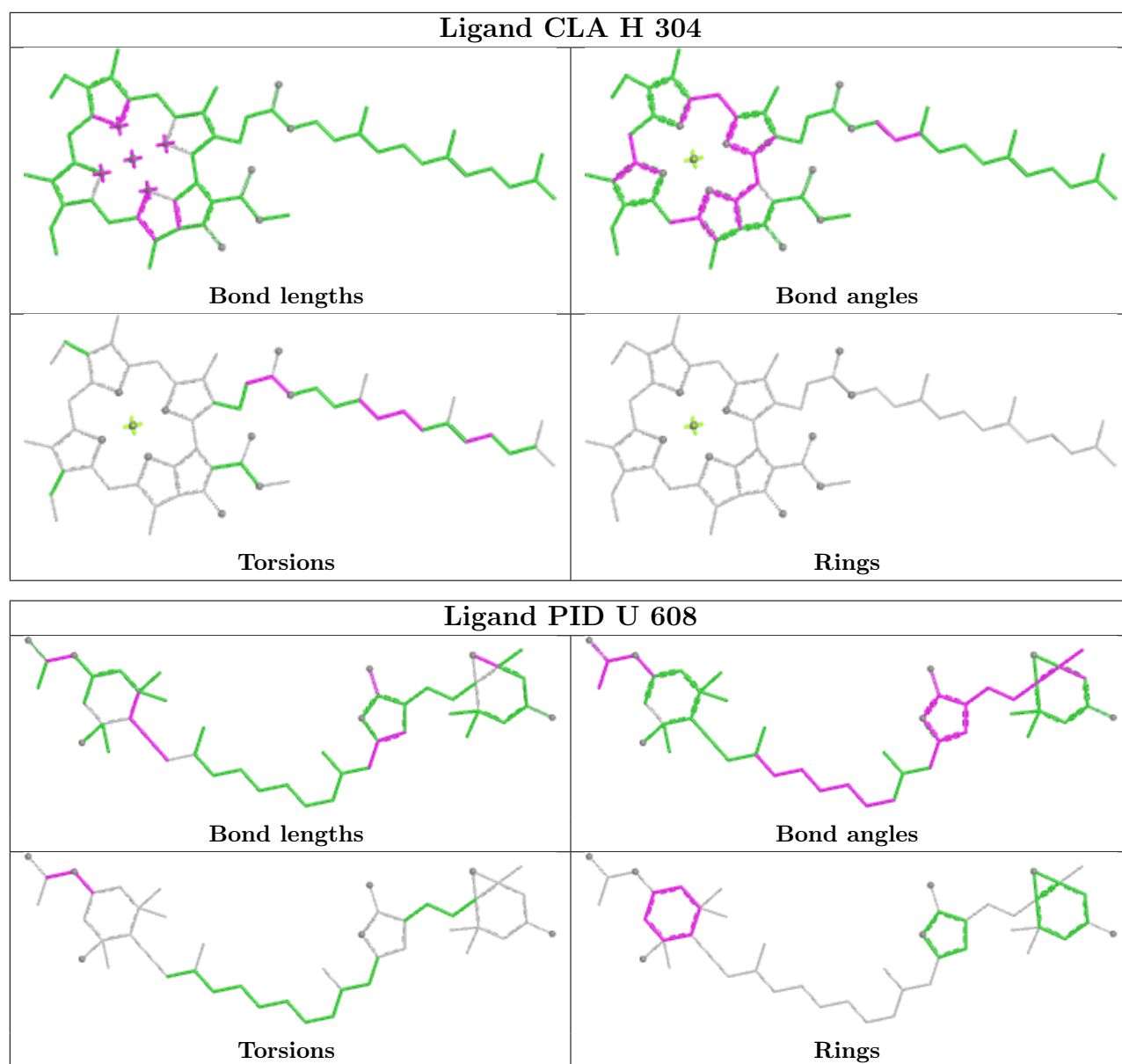


Ligand SQD y 301

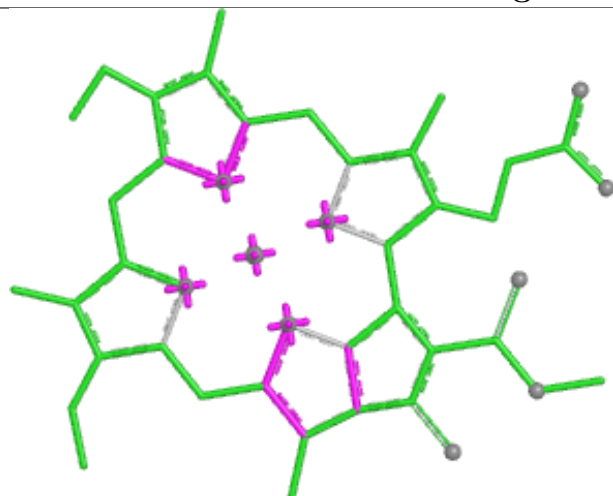


Ligand CLA a 819**Ligand CLA b 724**

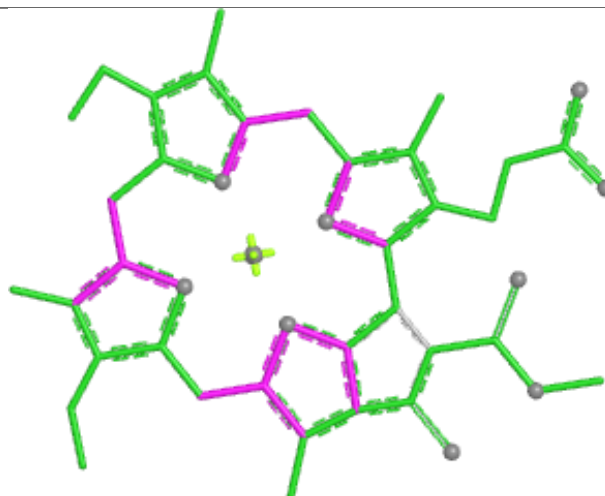




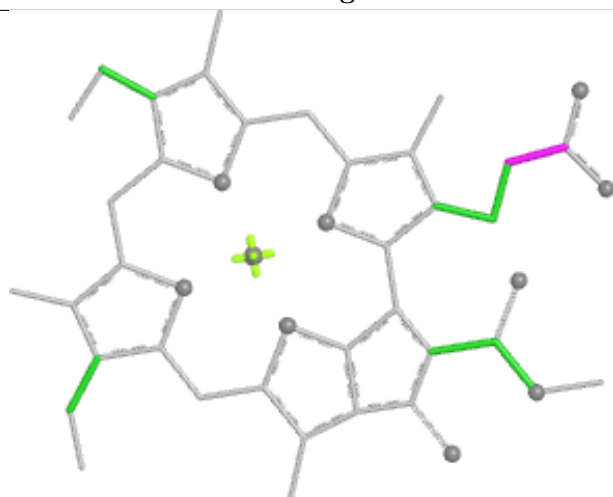
Ligand CLA D 609



Bond lengths



Bond angles

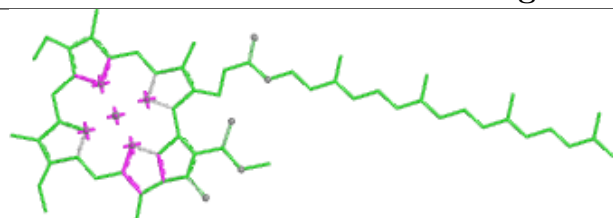


Torsions

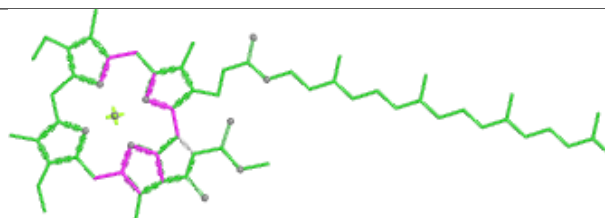


Rings

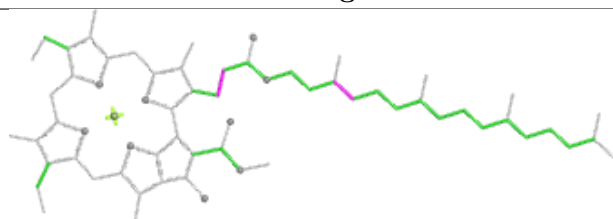
Ligand CLA a 837



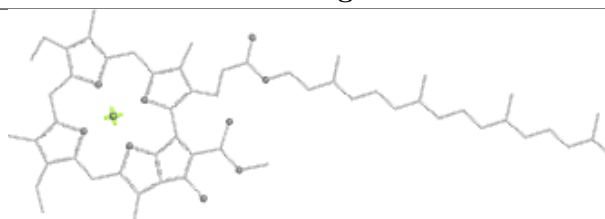
Bond lengths



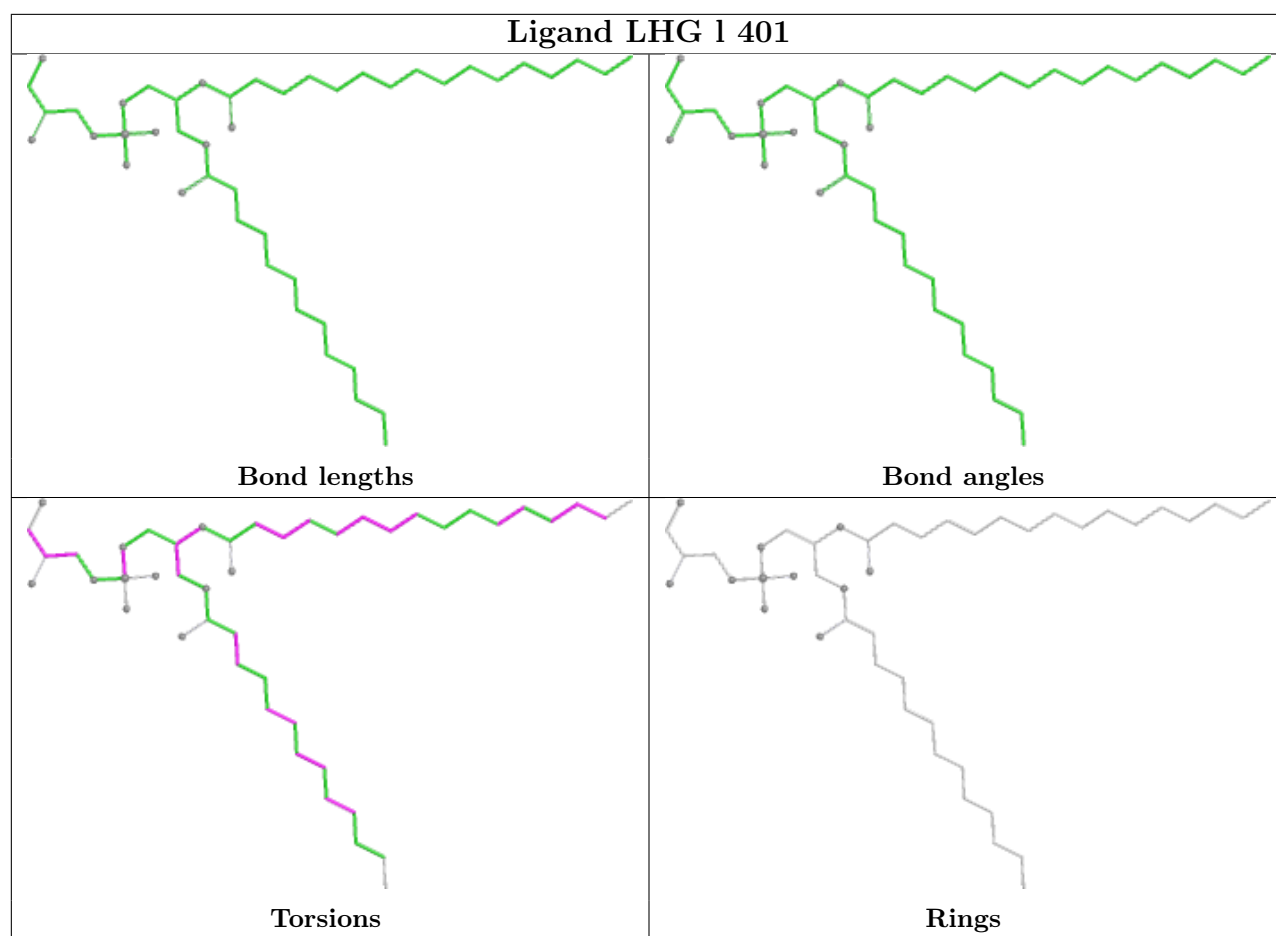
Bond angles

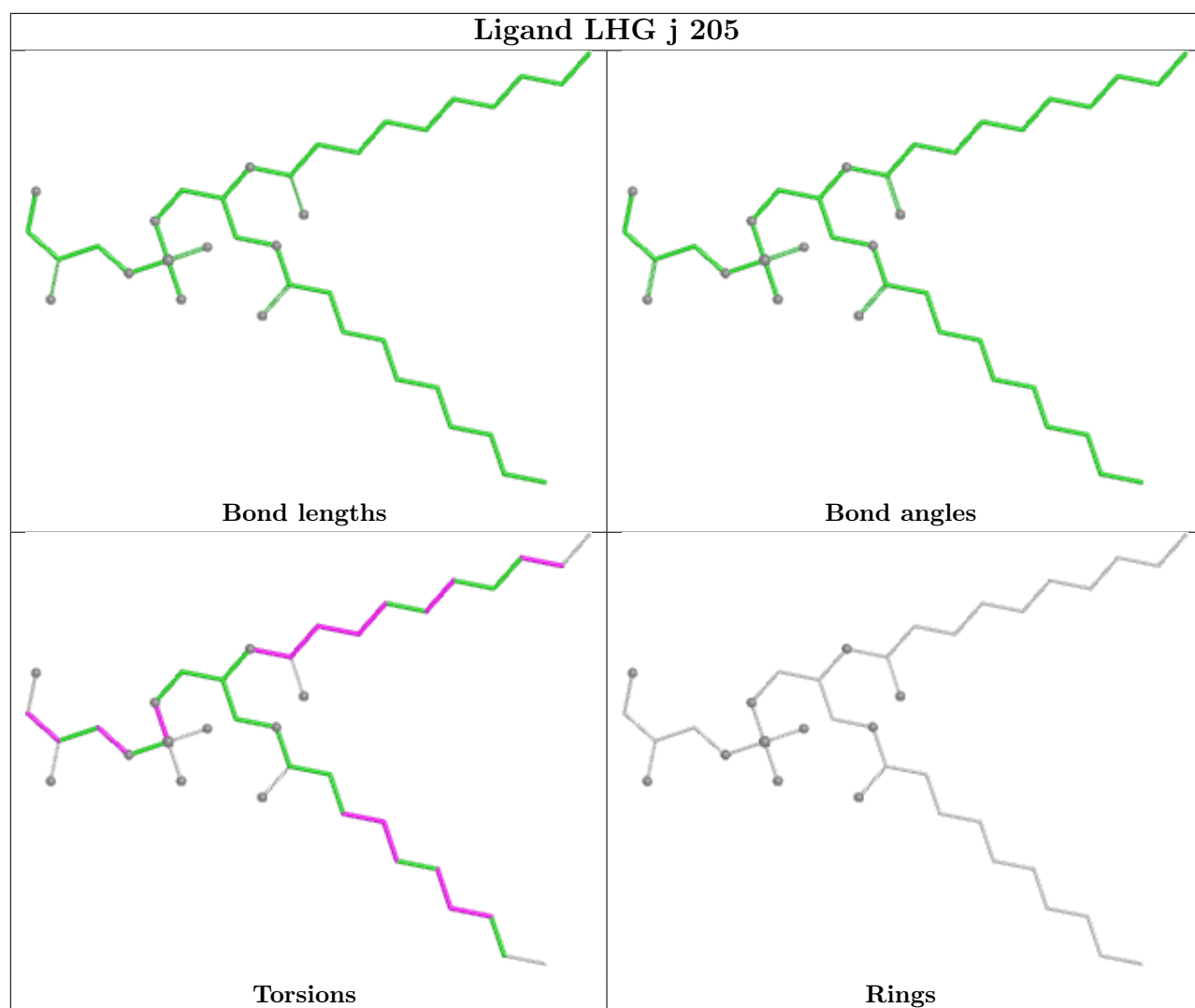


Torsions

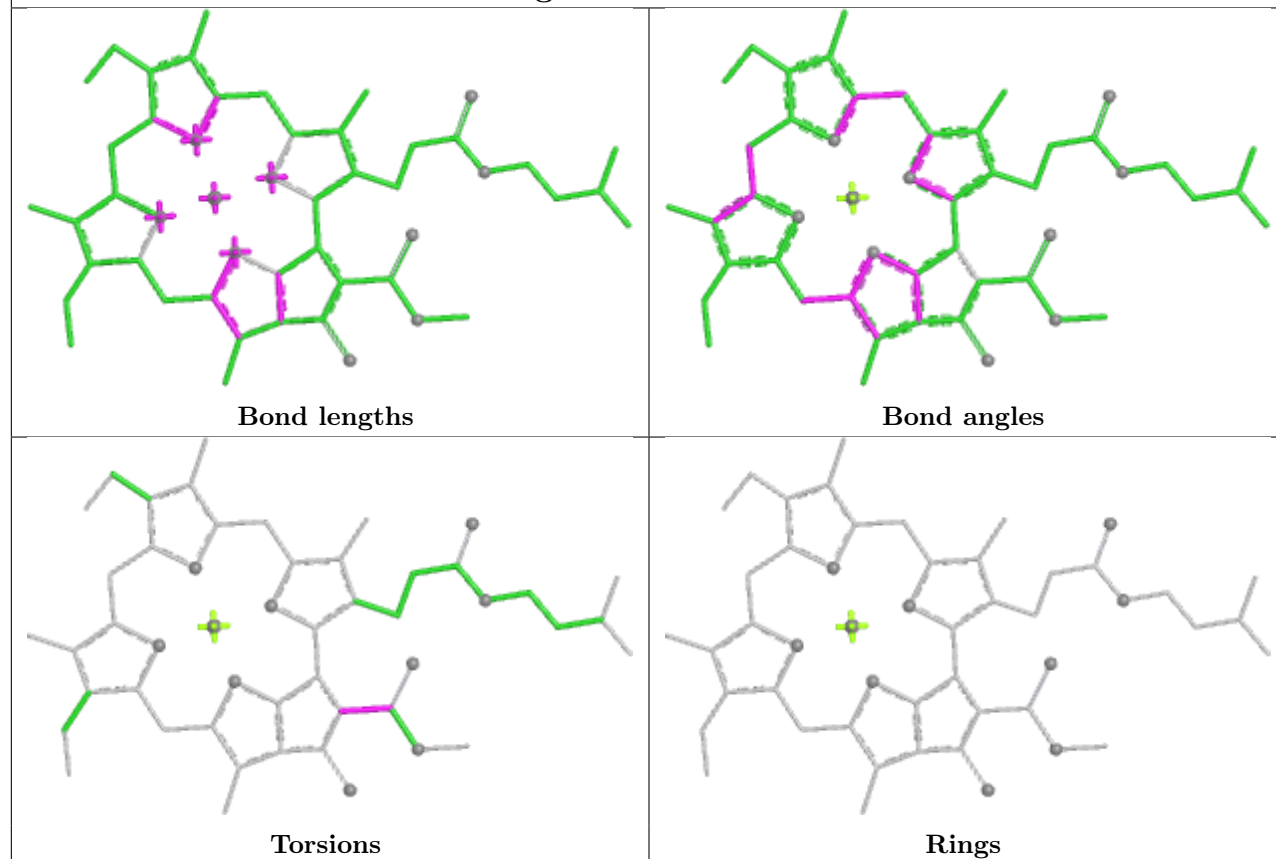


Rings



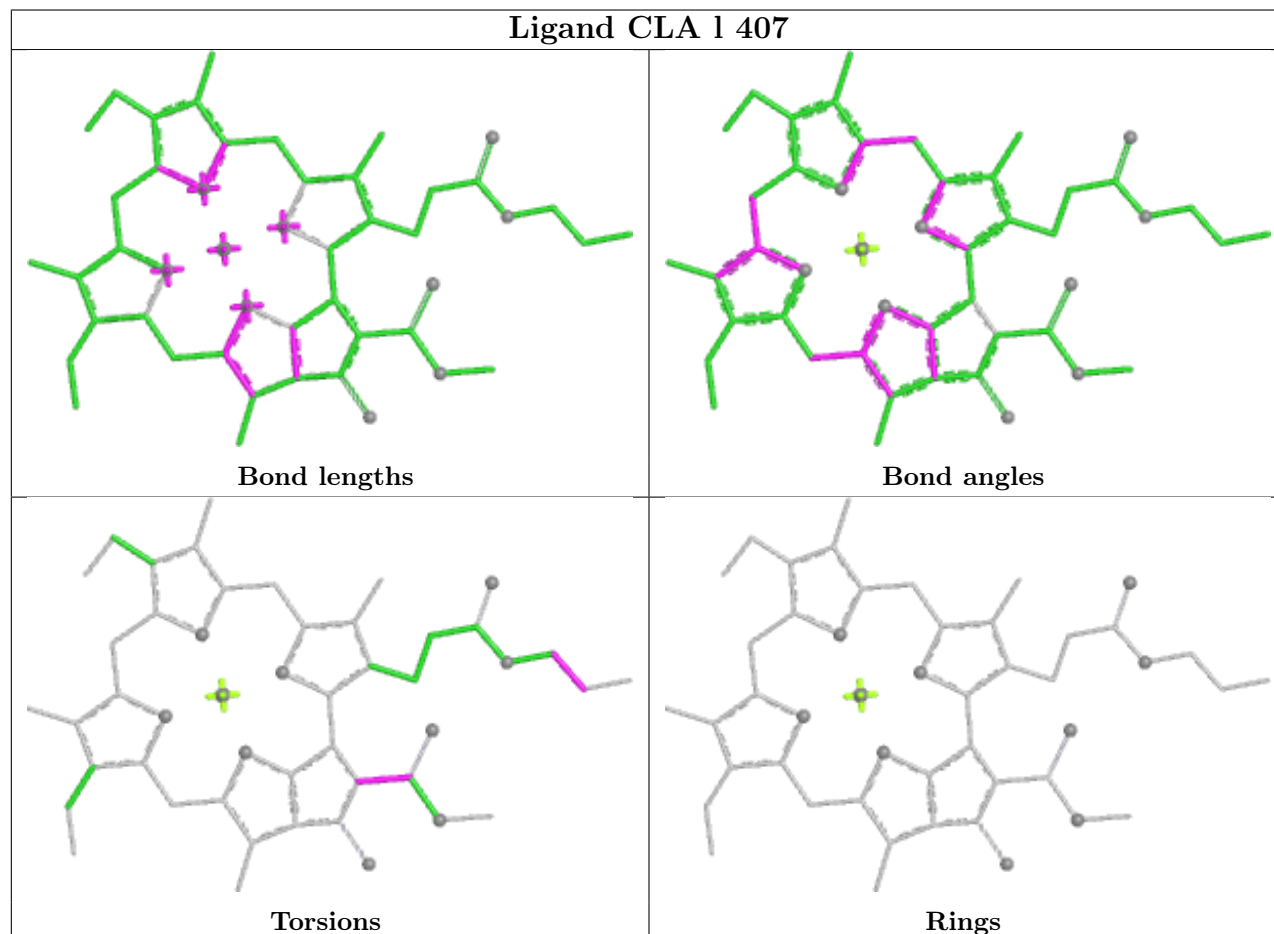
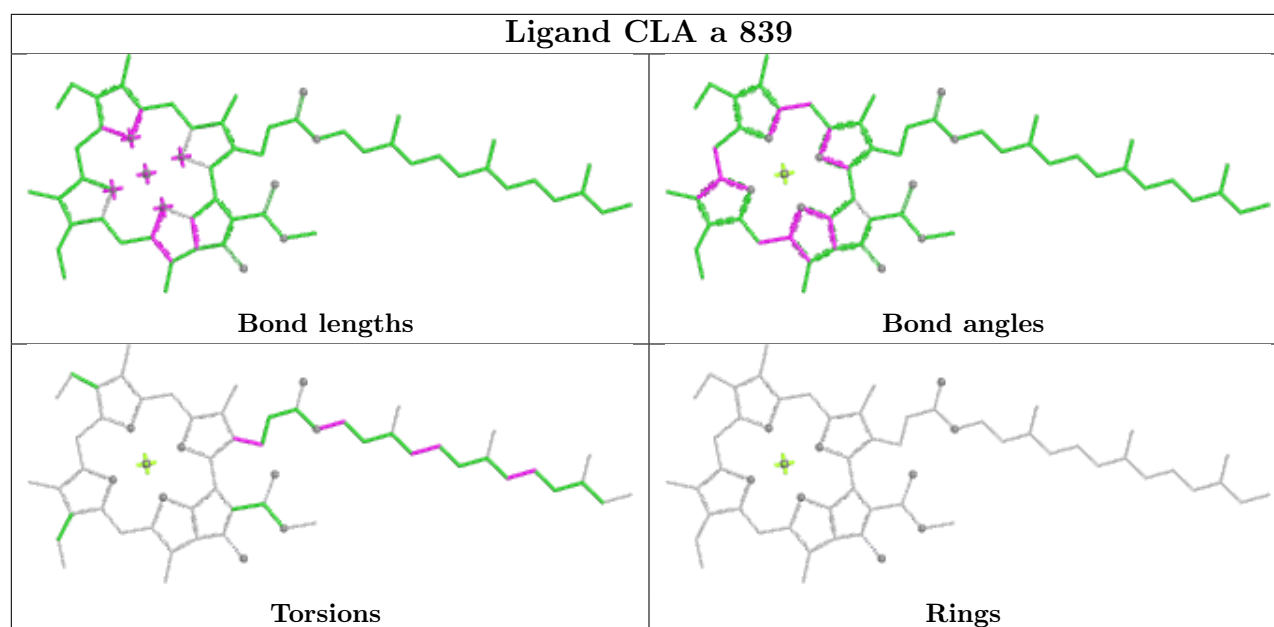


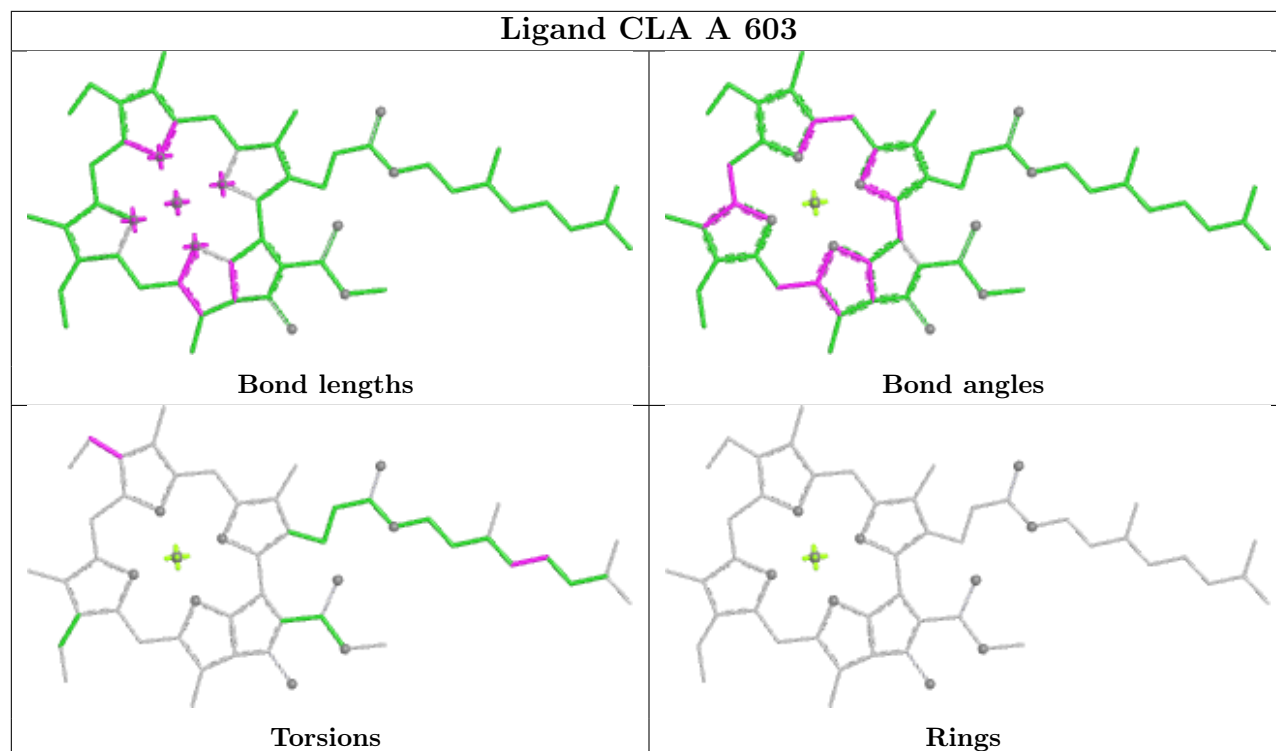
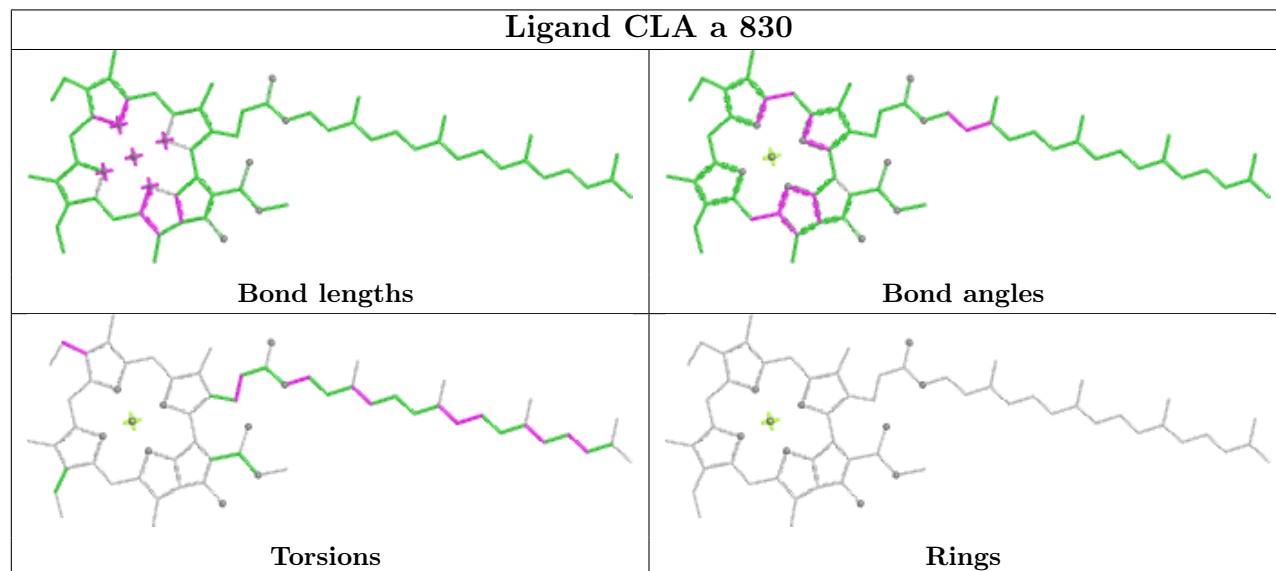
Ligand CLA b 721

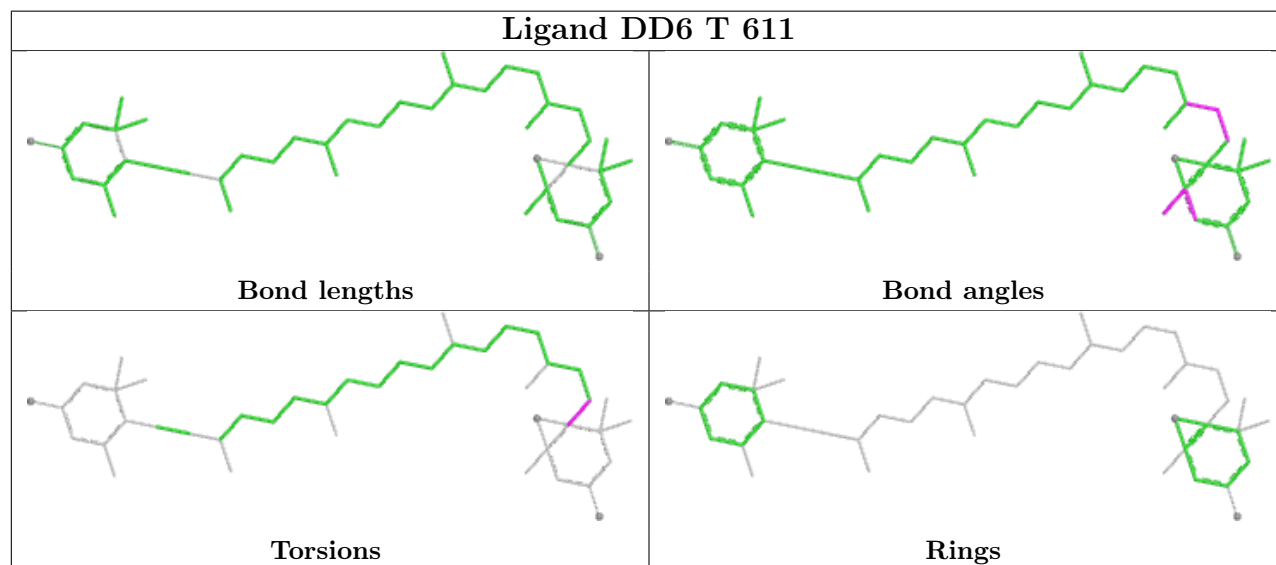
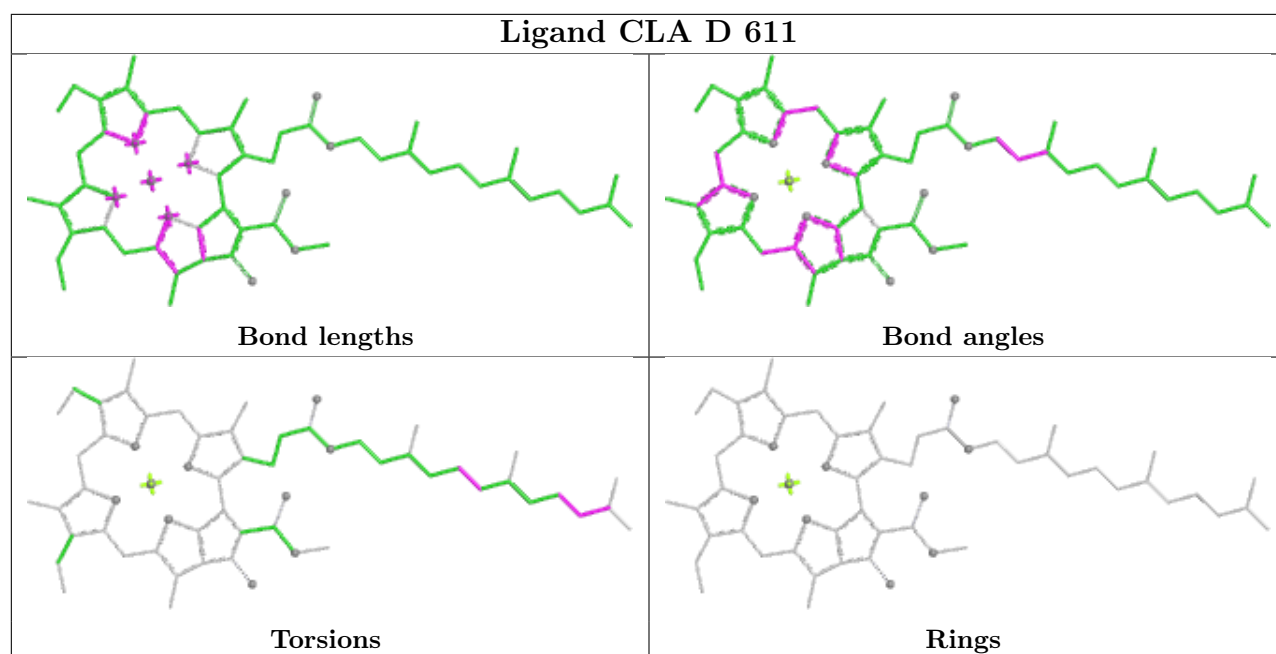


Ligand LMG 1 417

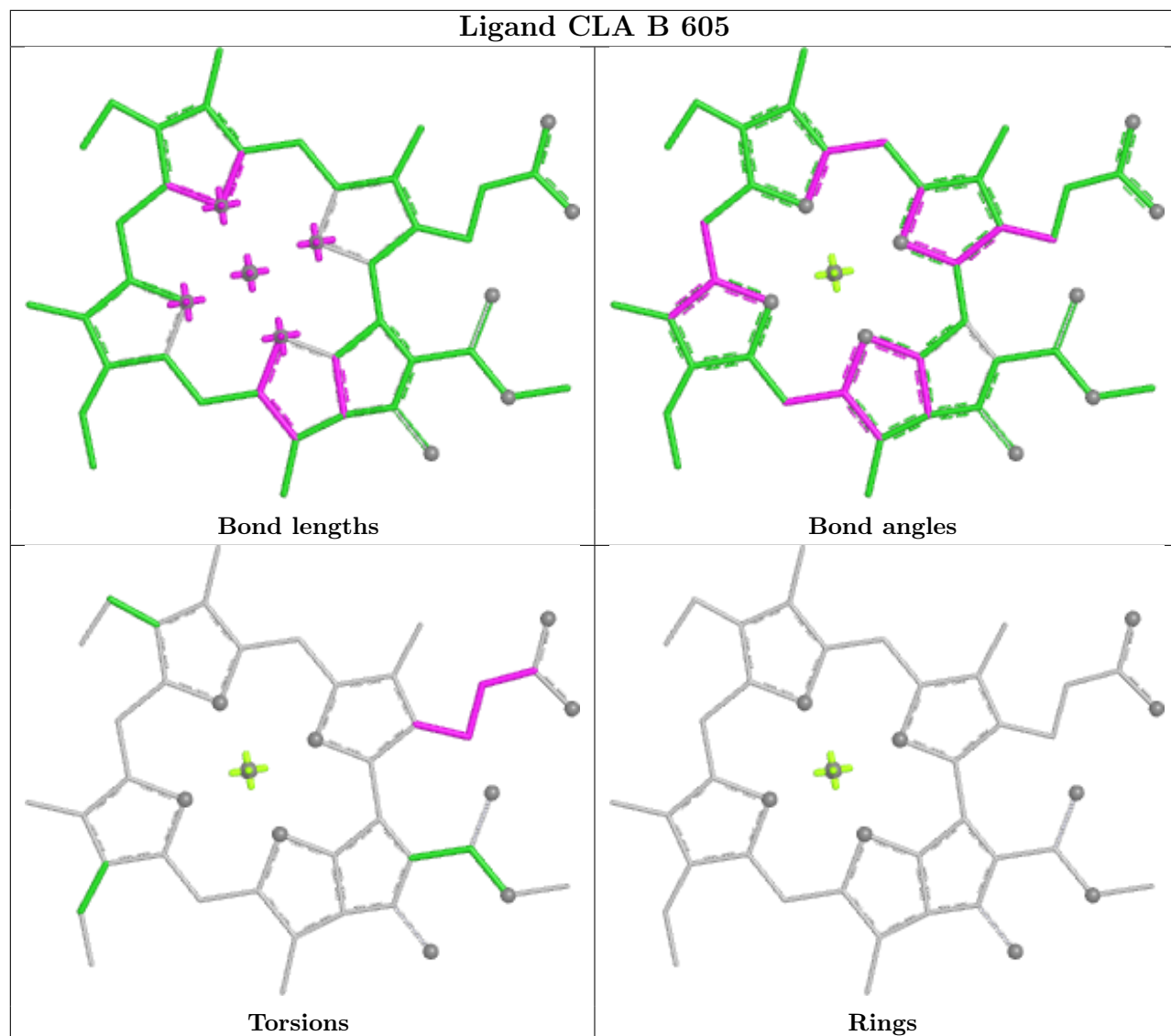




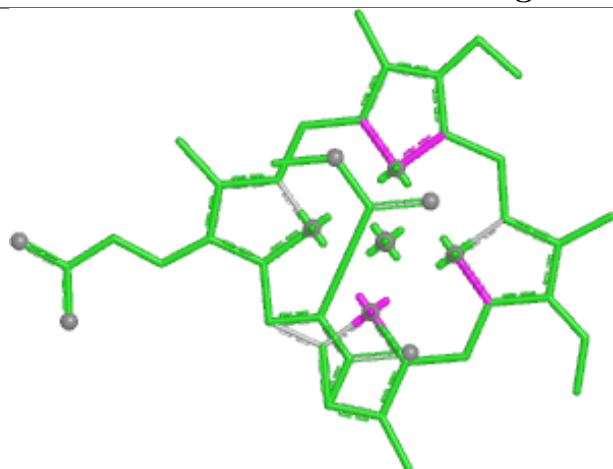
Ligand CLA A 603**Ligand CLA a 830**



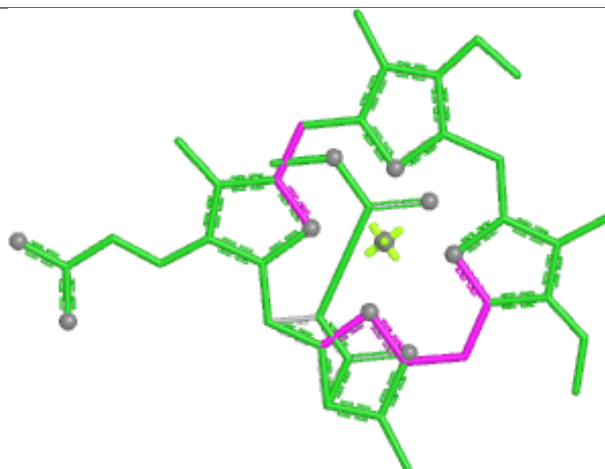
Ligand CLA B 605



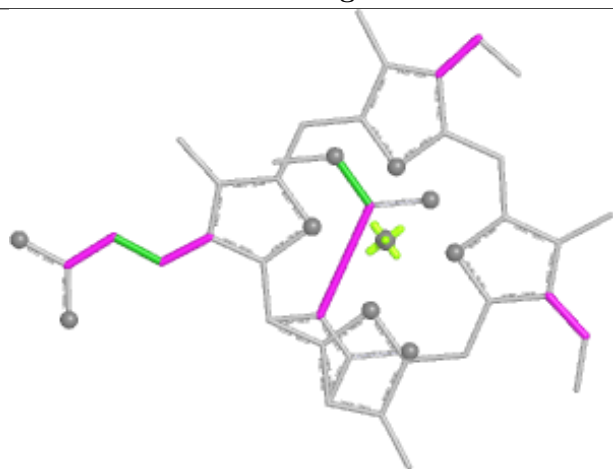
Ligand KC2 H 311



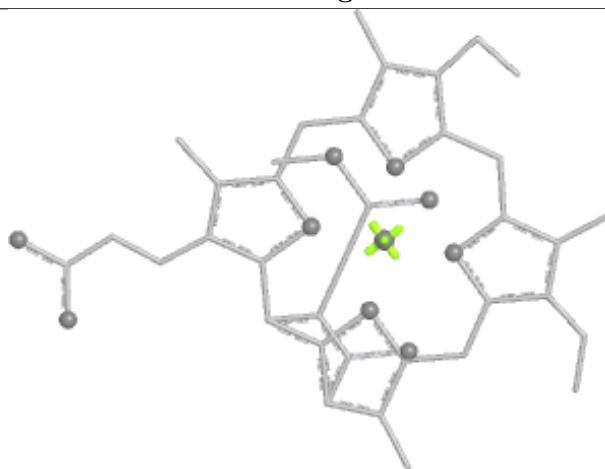
Bond lengths



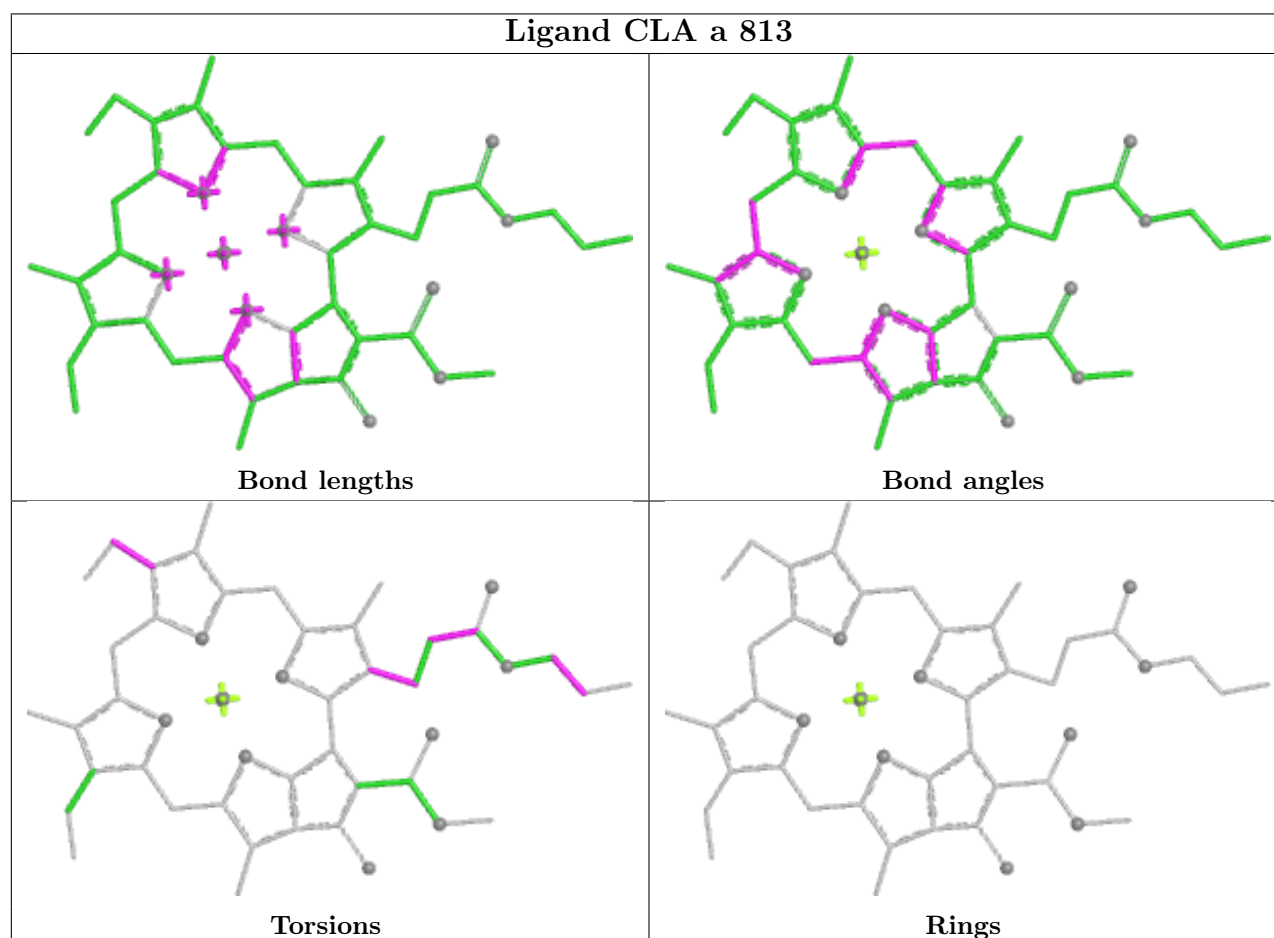
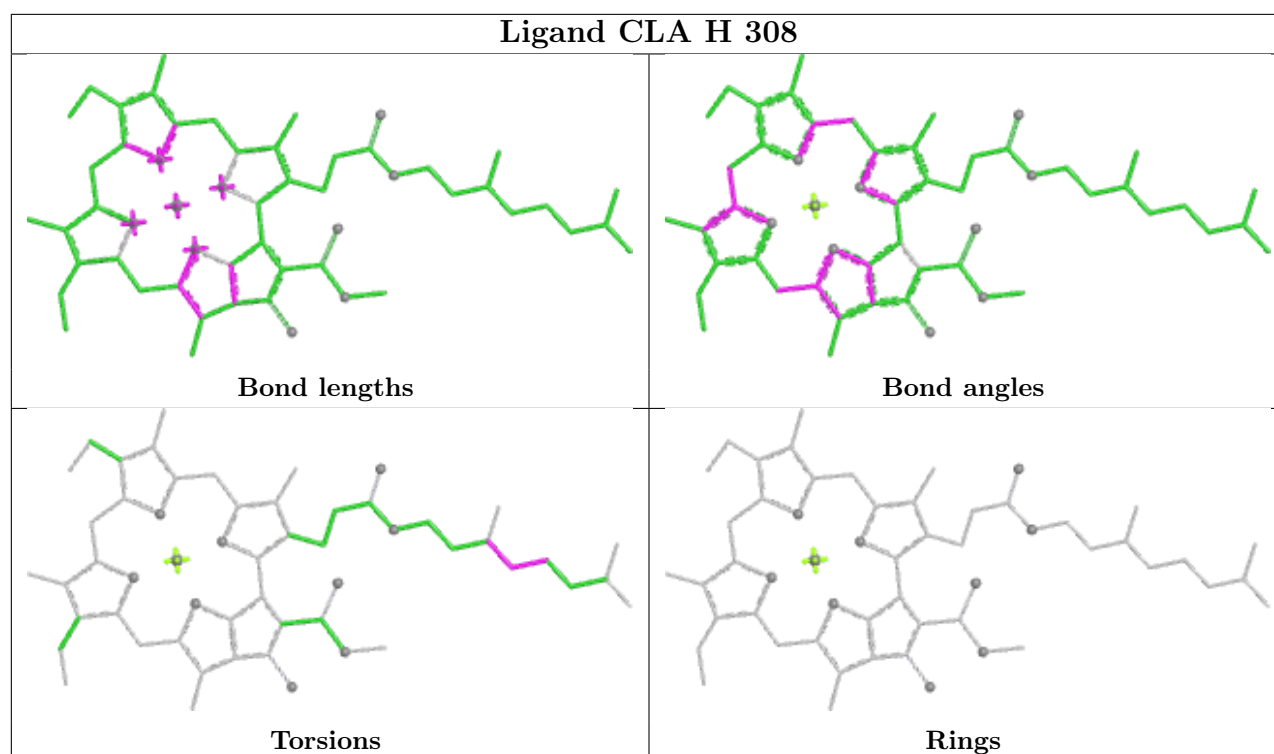
Bond angles

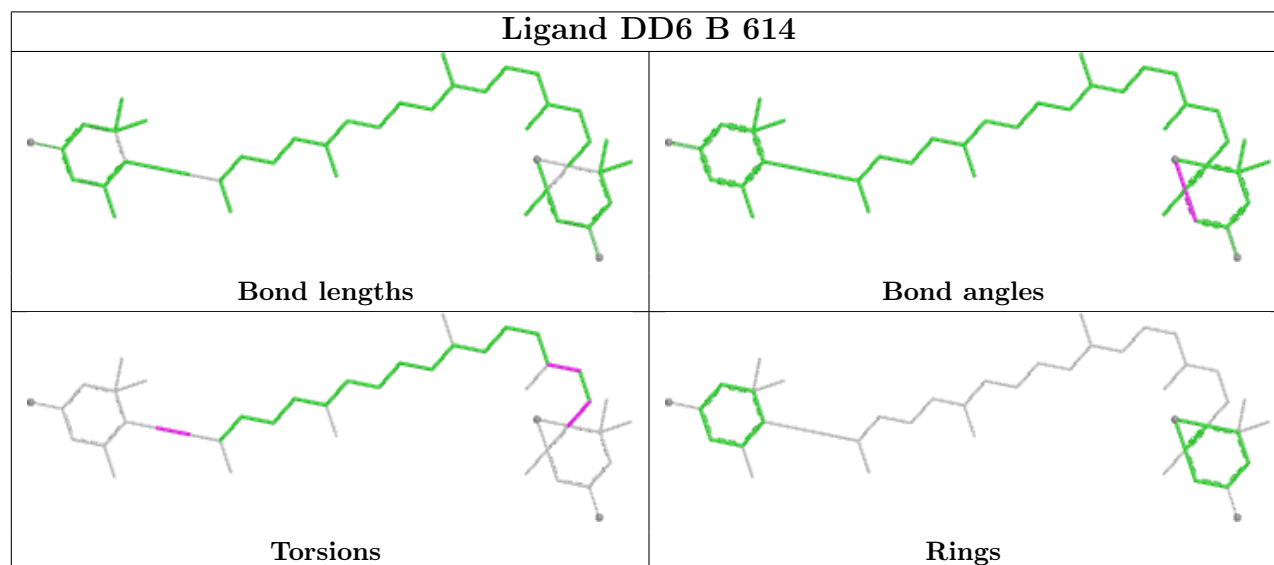
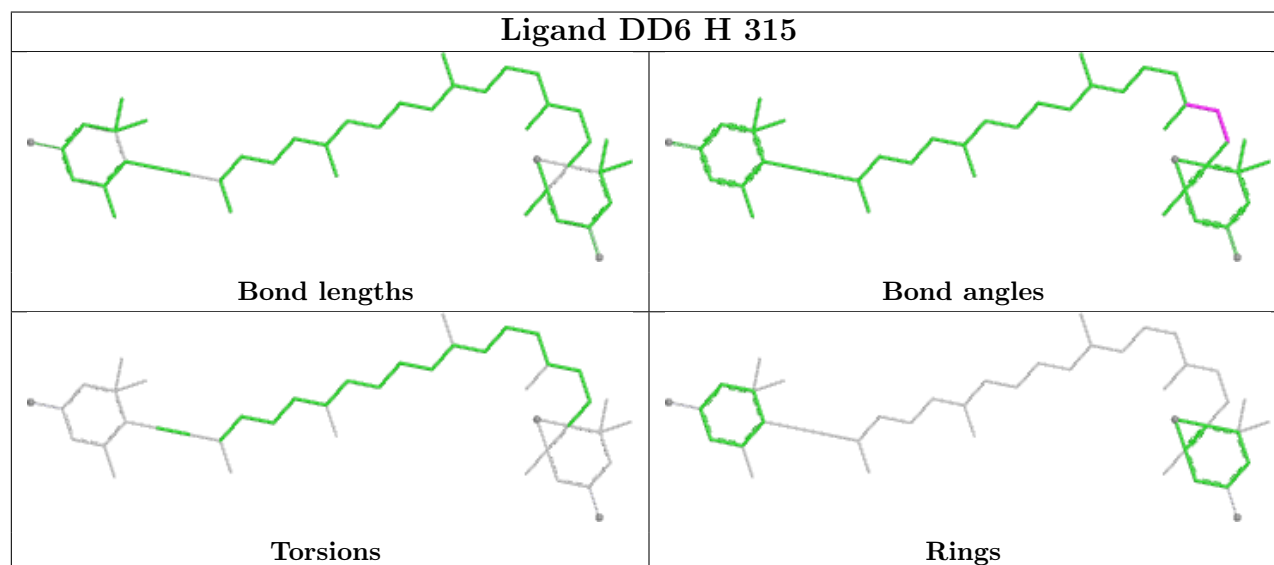
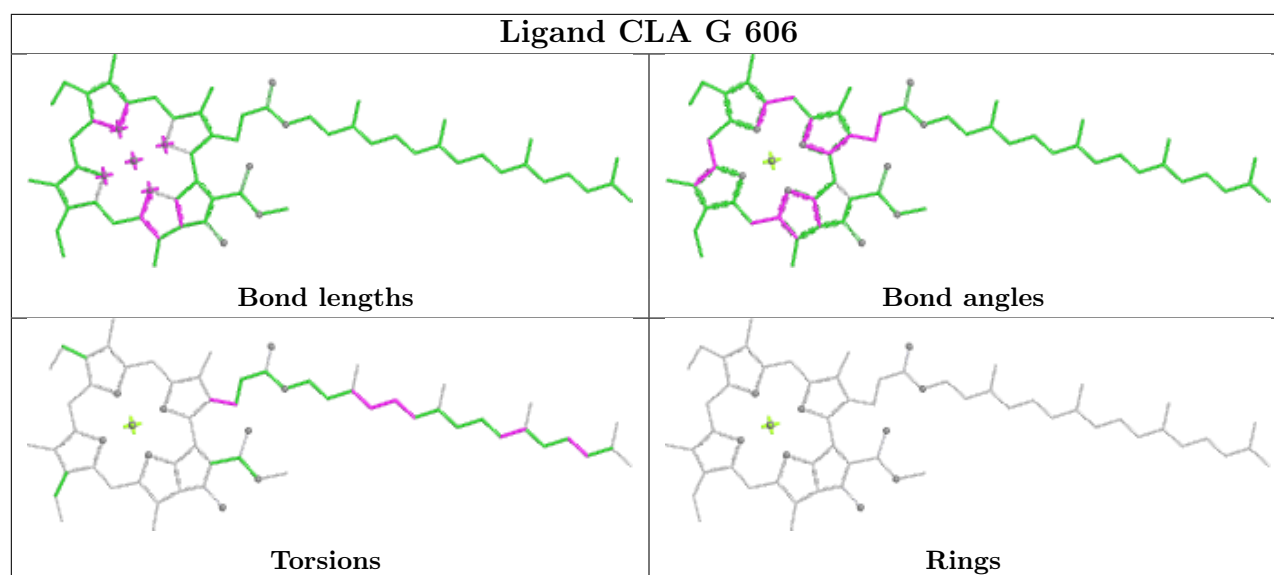


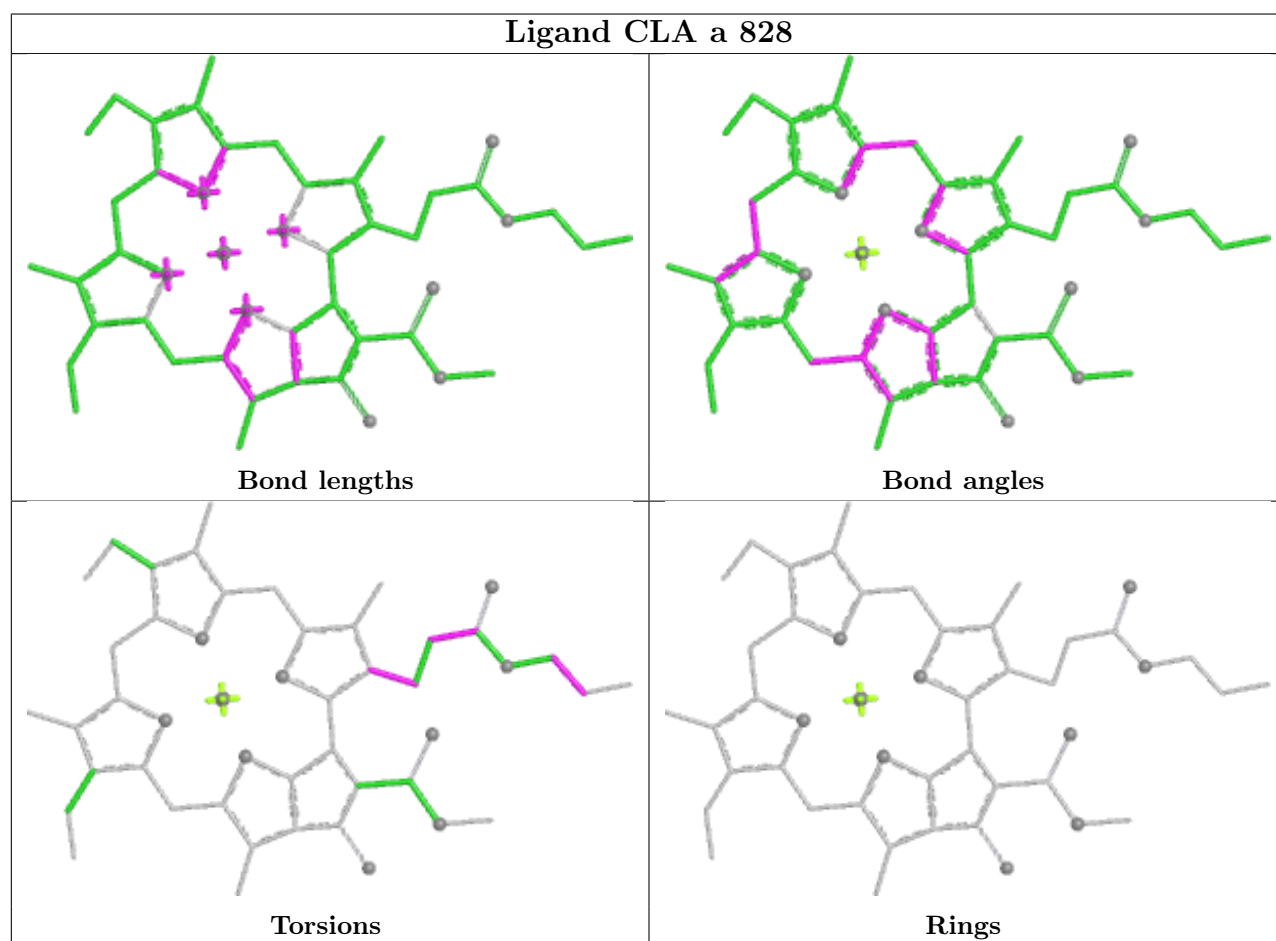
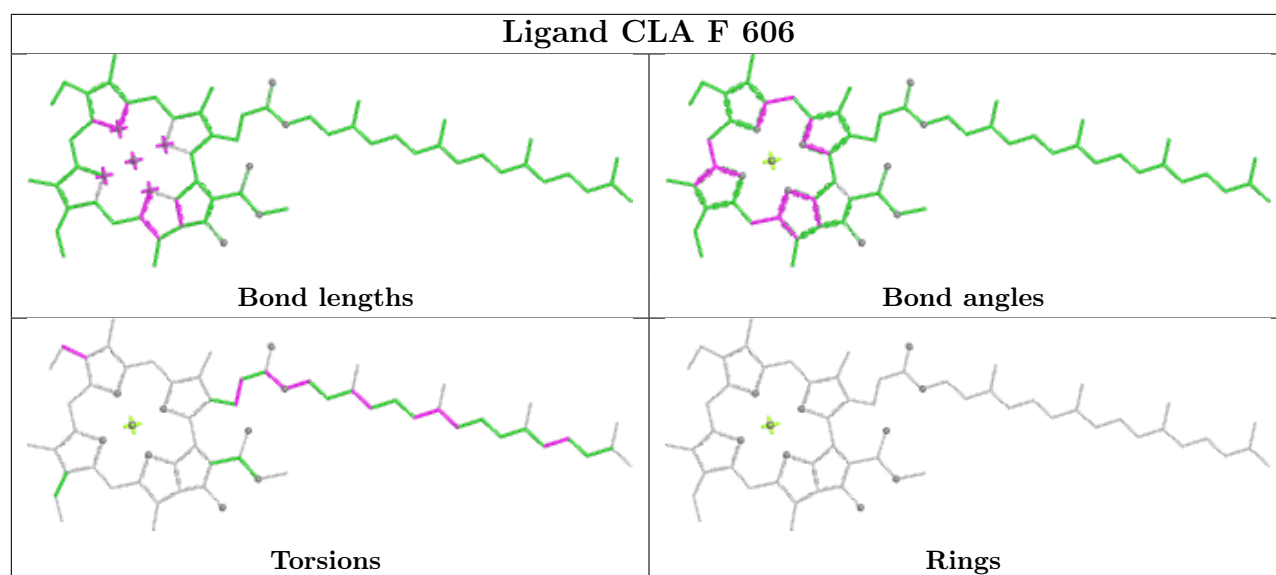
Torsions



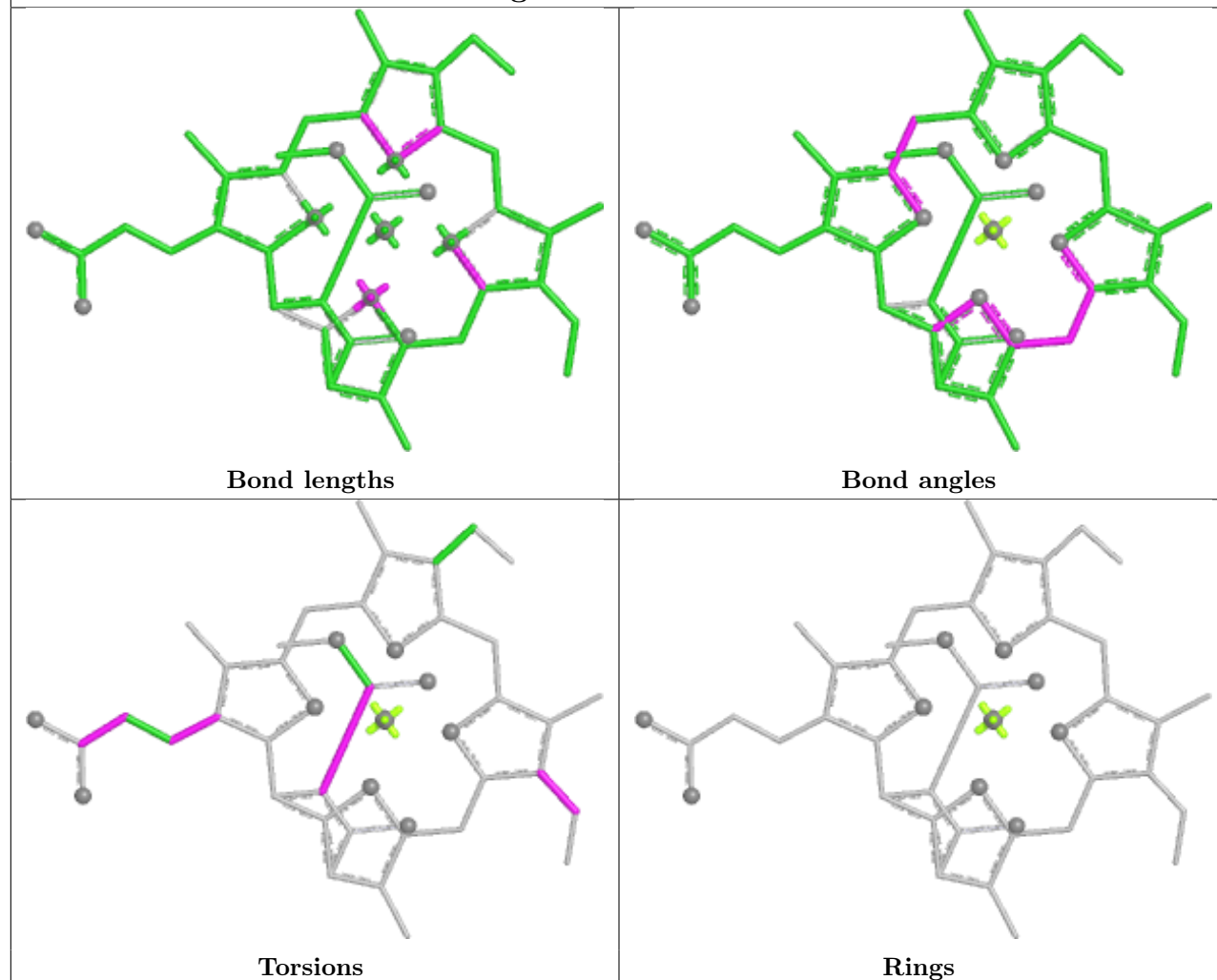
Rings



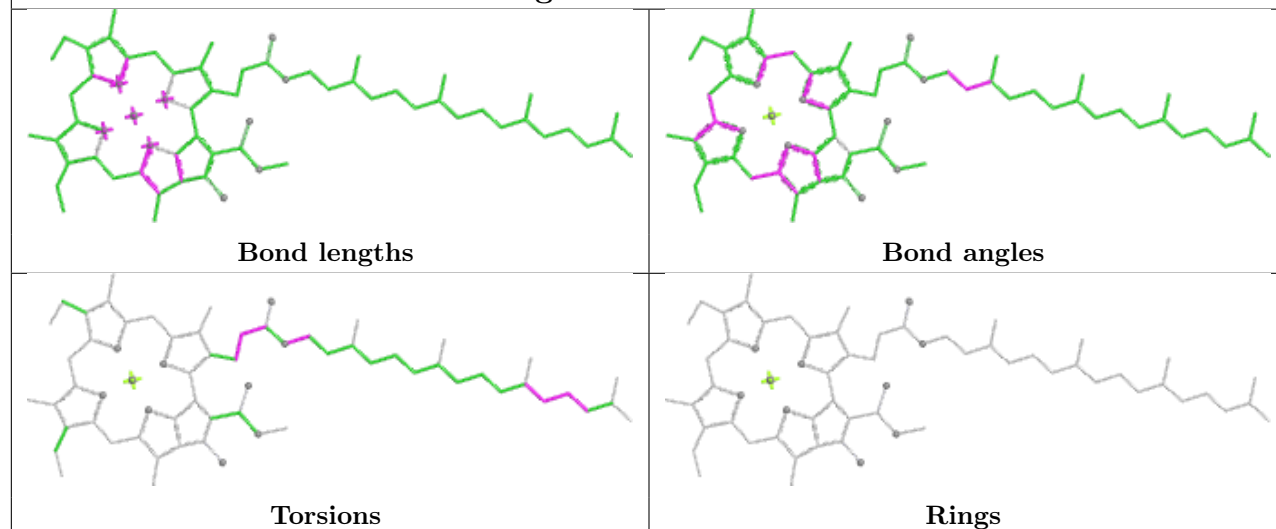


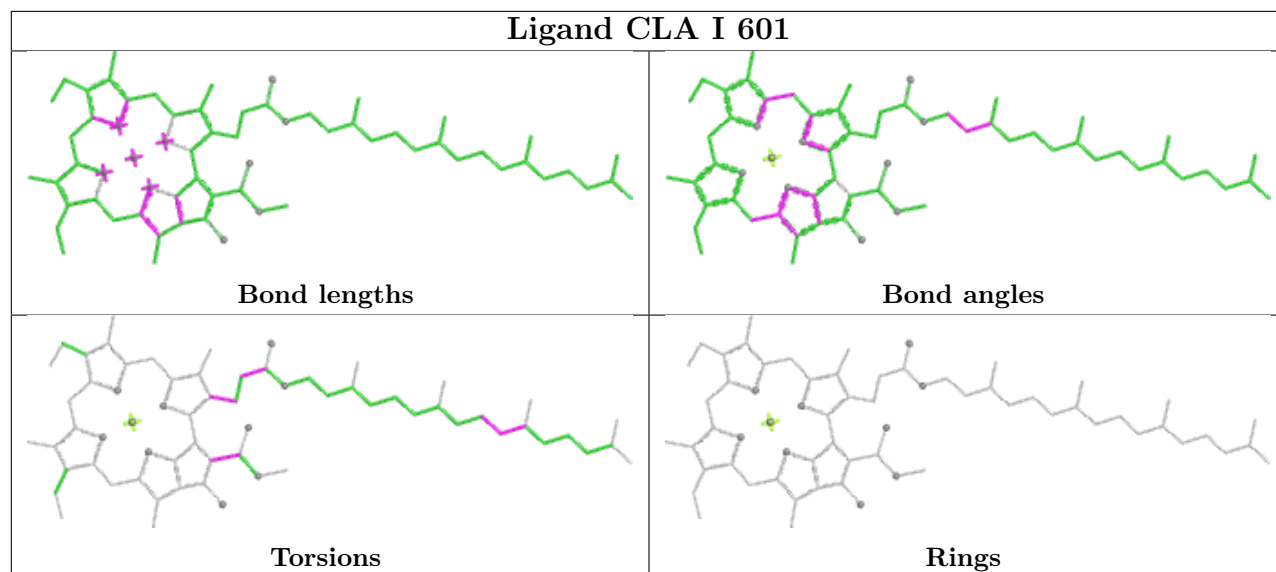
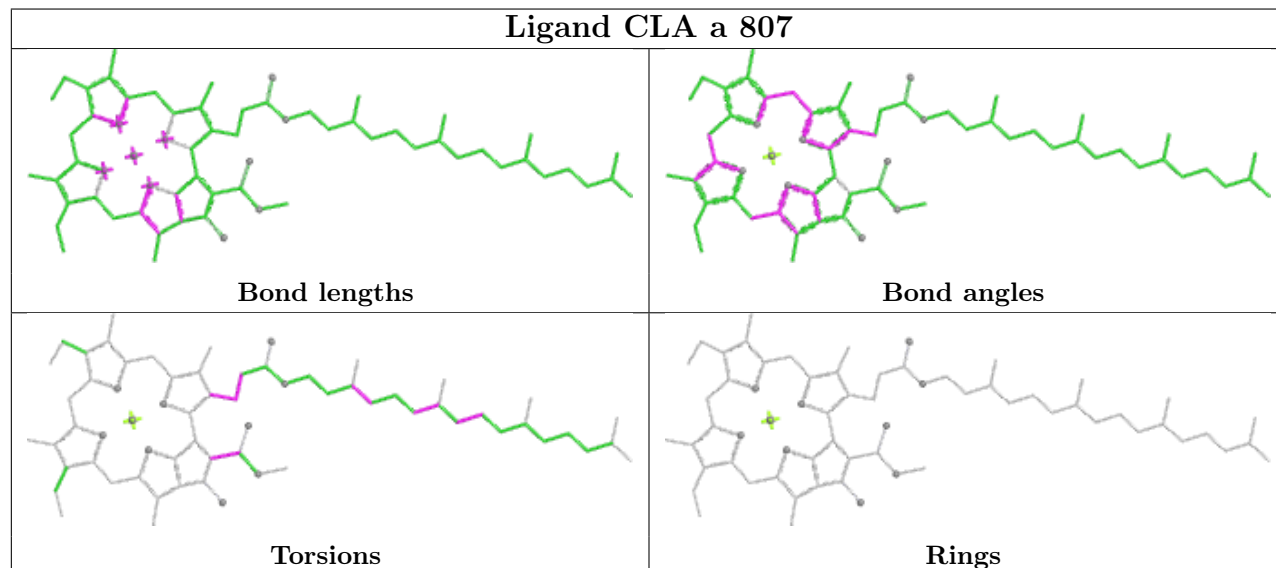


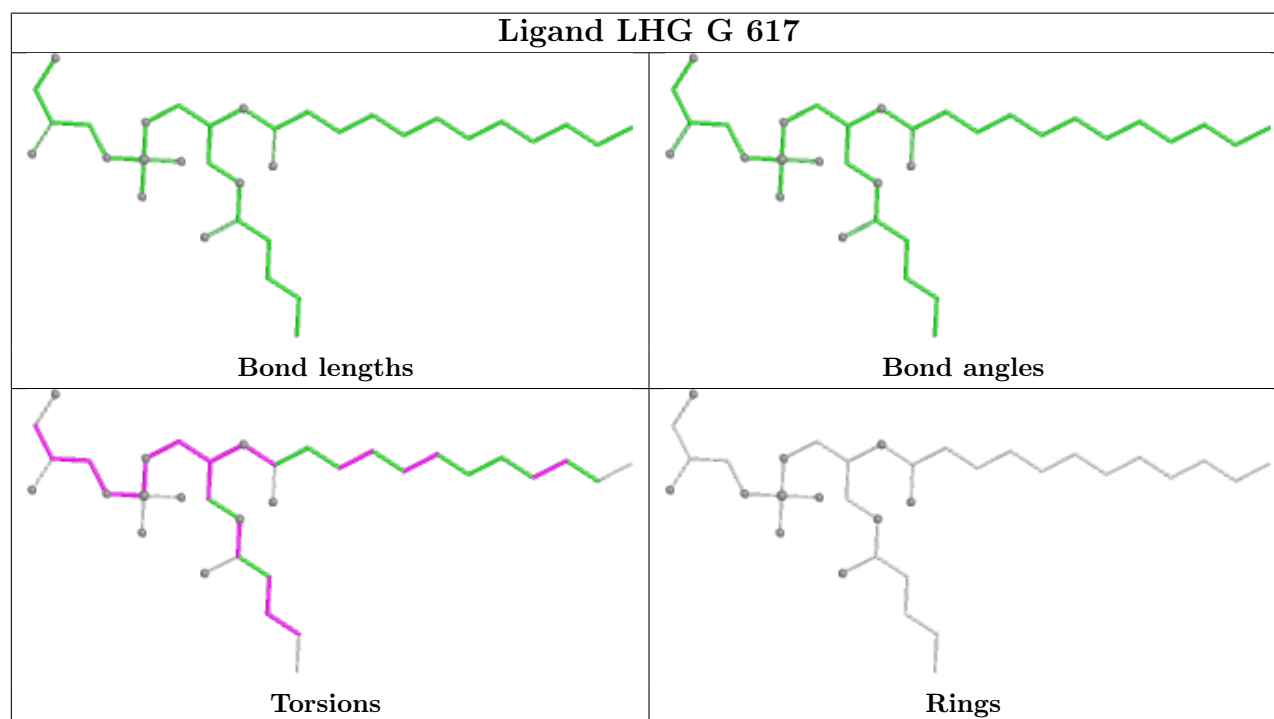
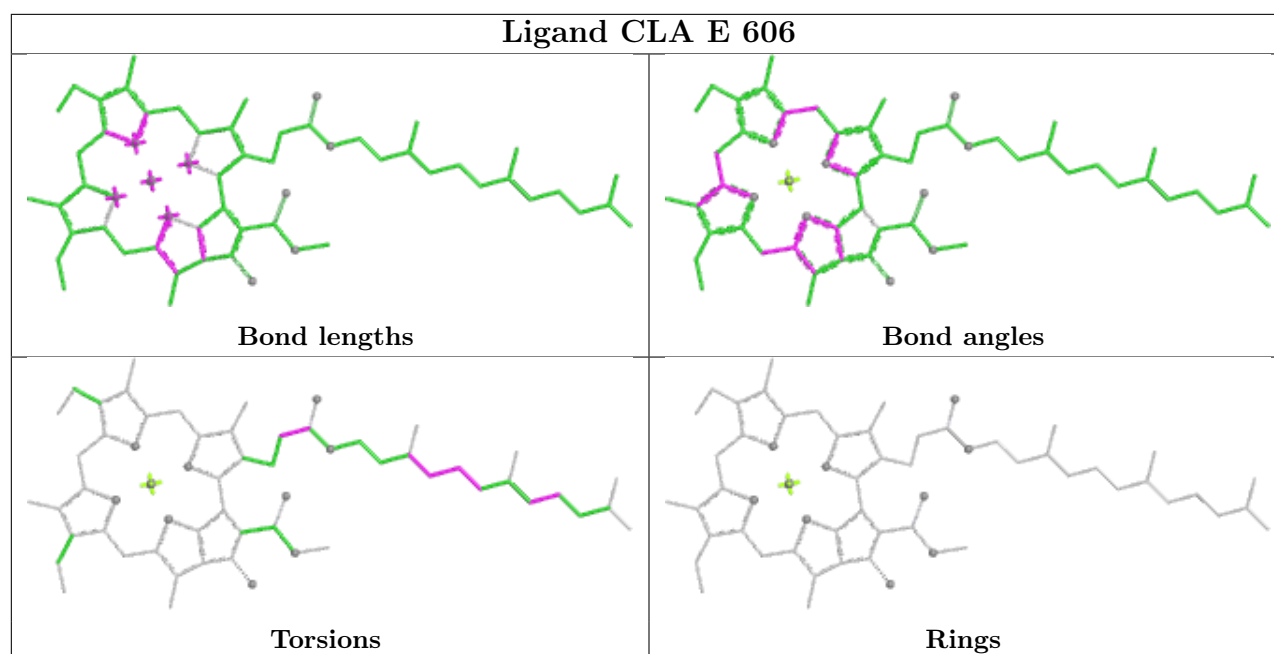
Ligand KC2 E 610

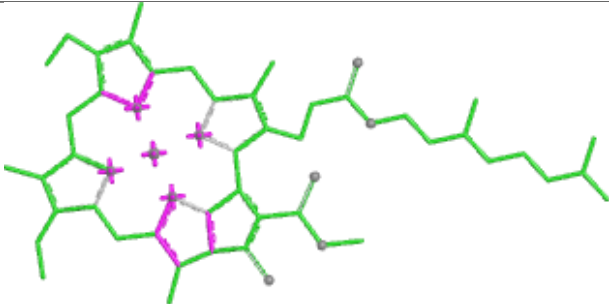
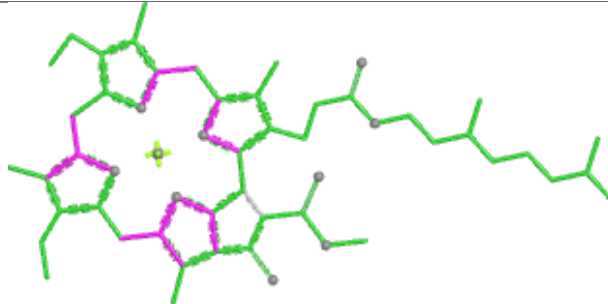
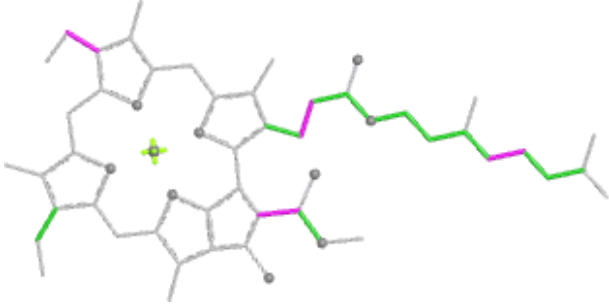
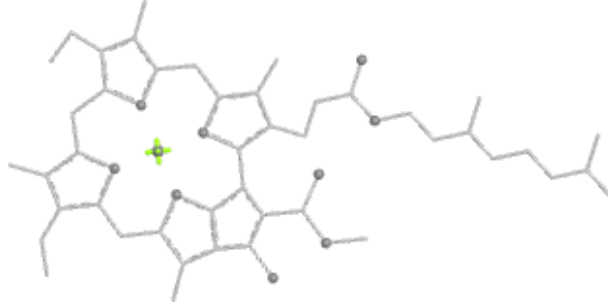


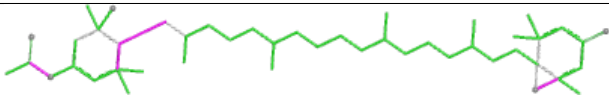
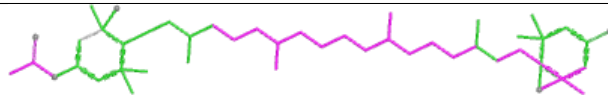
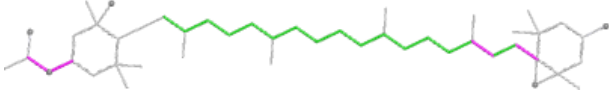
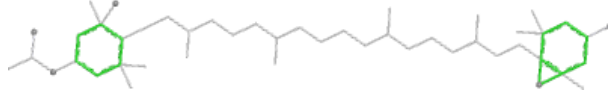
Ligand CLA b 728

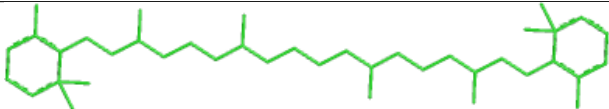
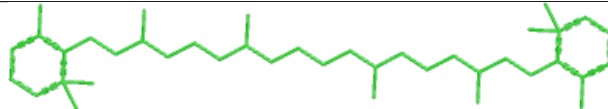
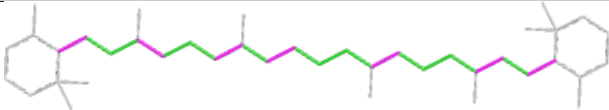
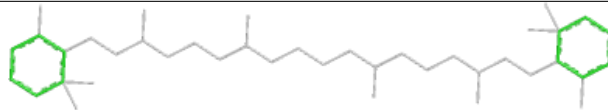


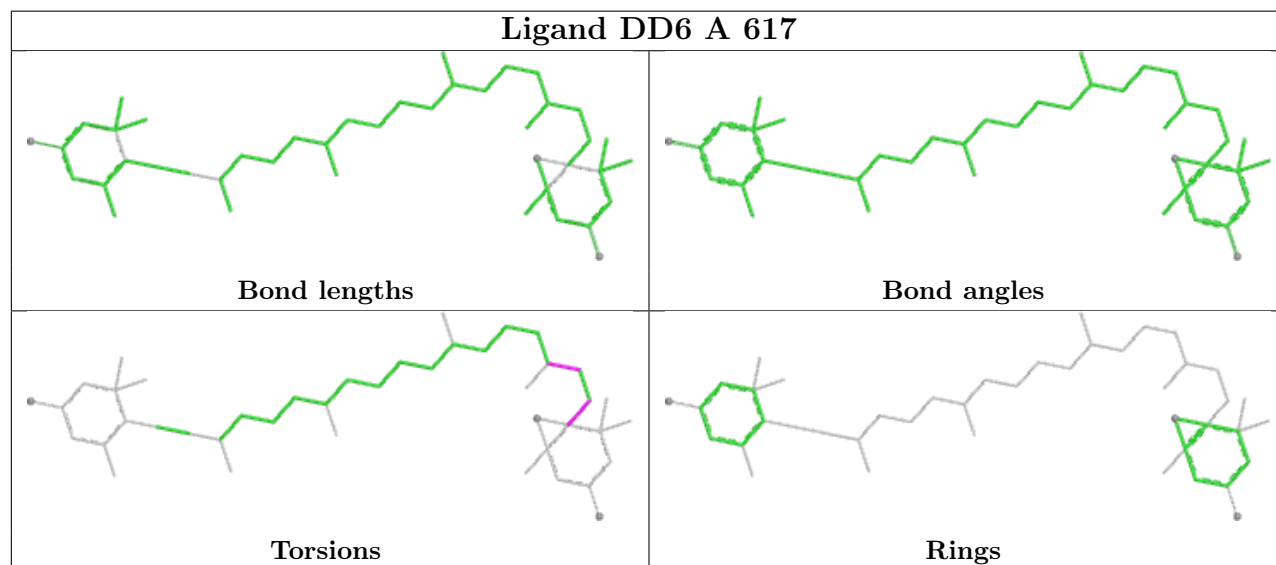
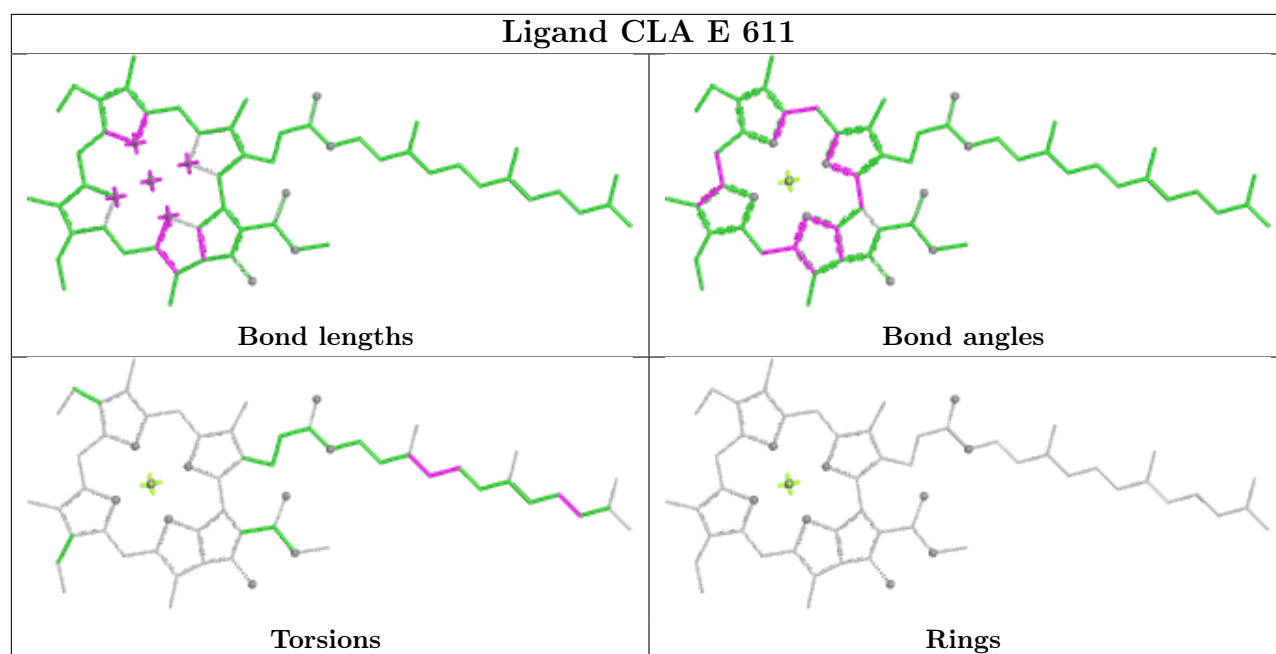
Ligand CLA I 601**Ligand CLA a 807**



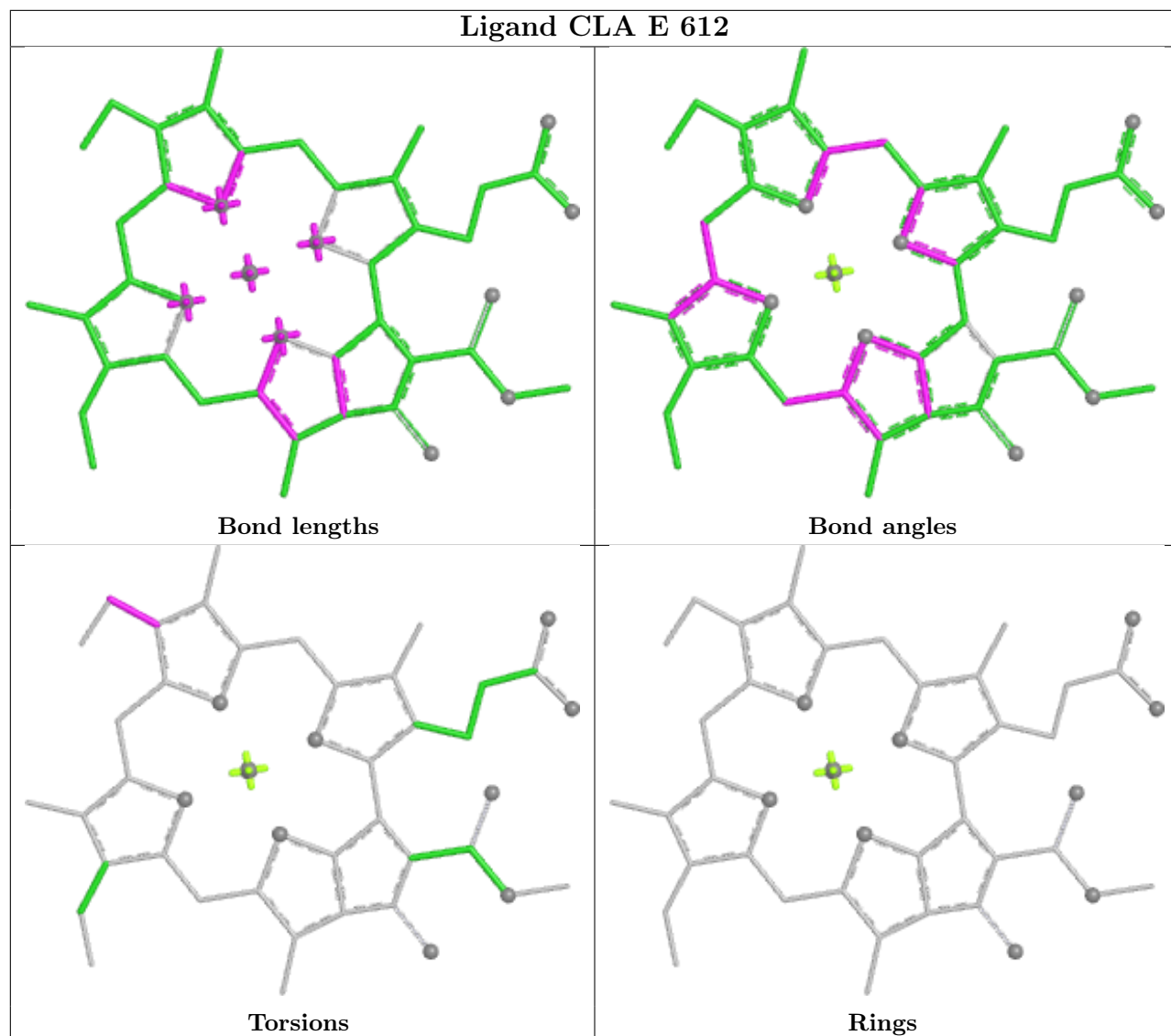
Ligand CLA I 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UIX j 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

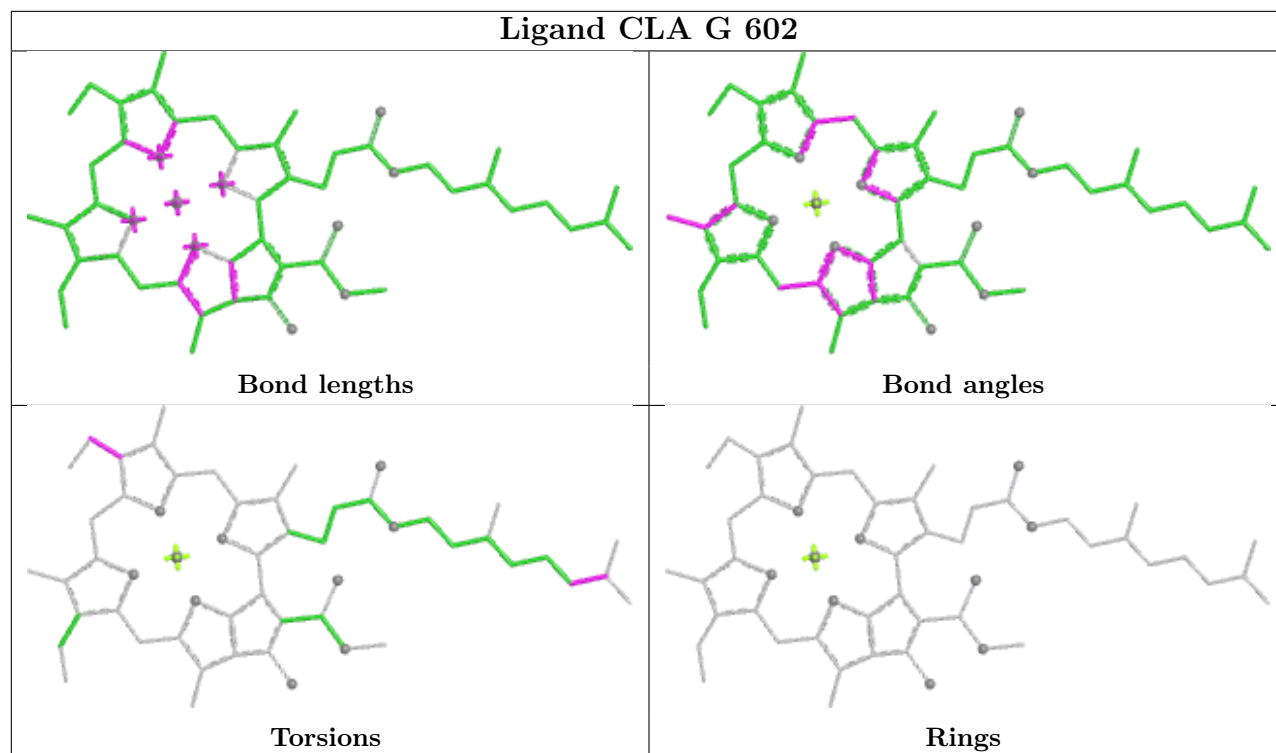
Ligand BCR 1 415	
	
Bond lengths	Bond angles
	
Torsions	Rings



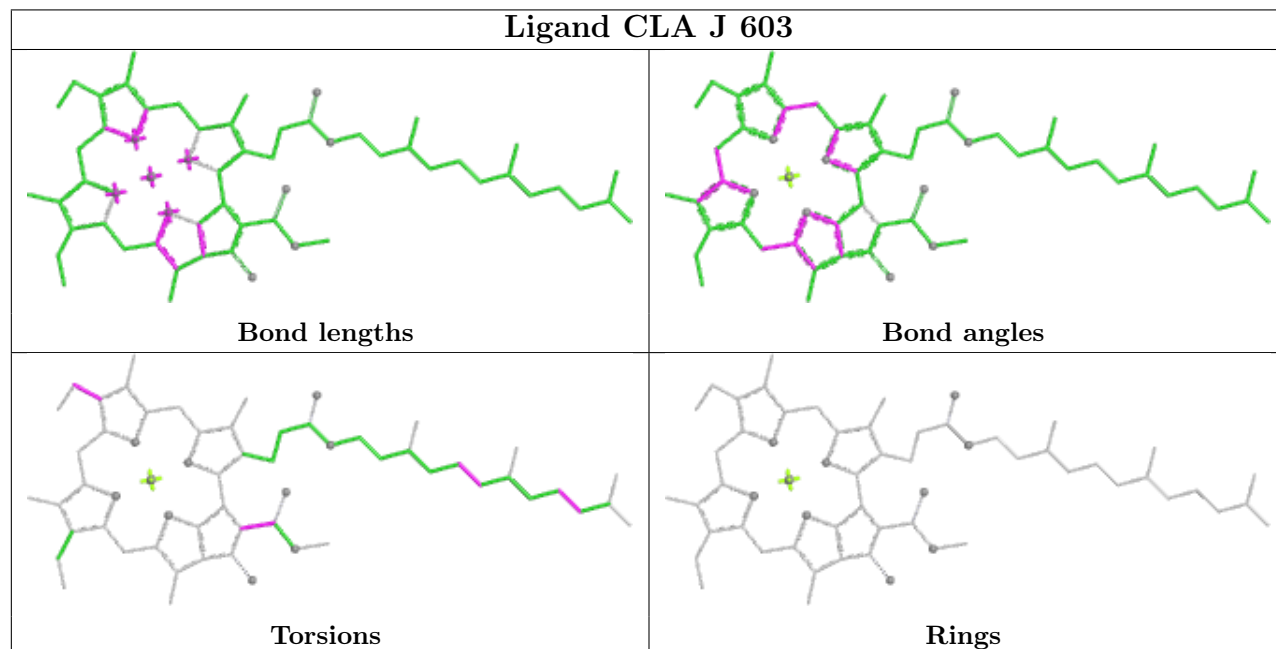
Ligand CLA E 612

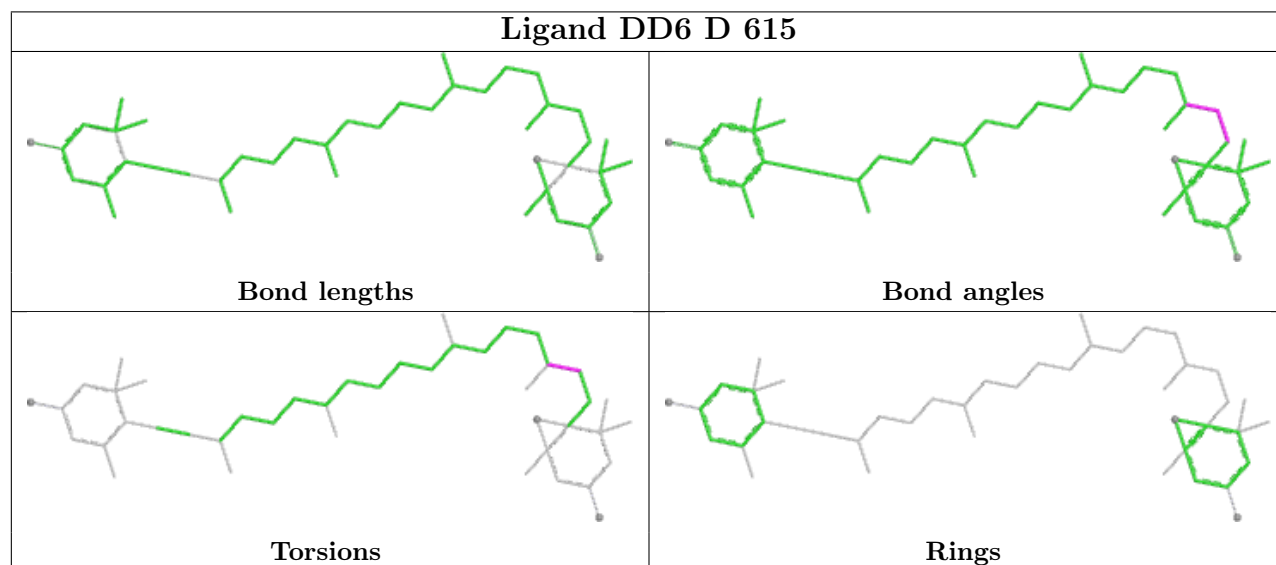
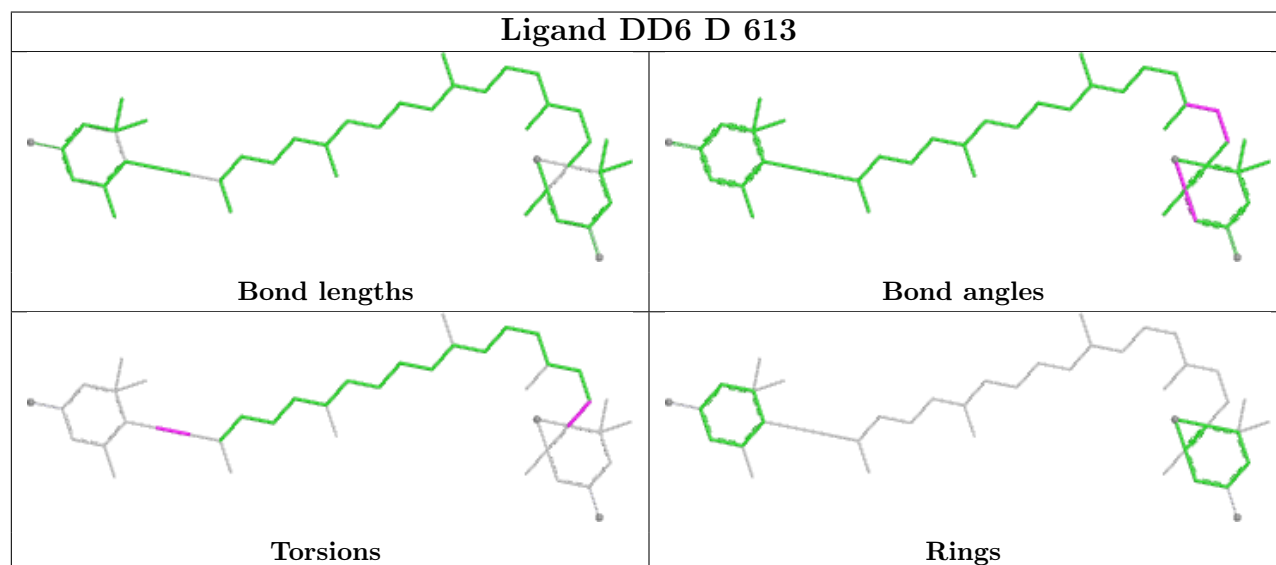
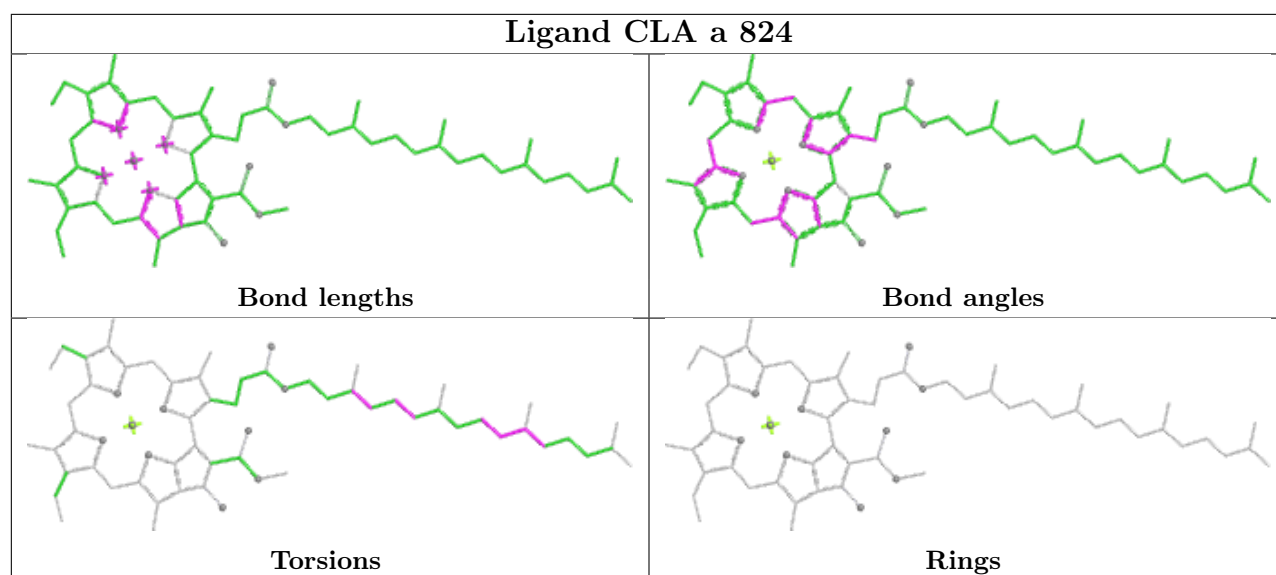


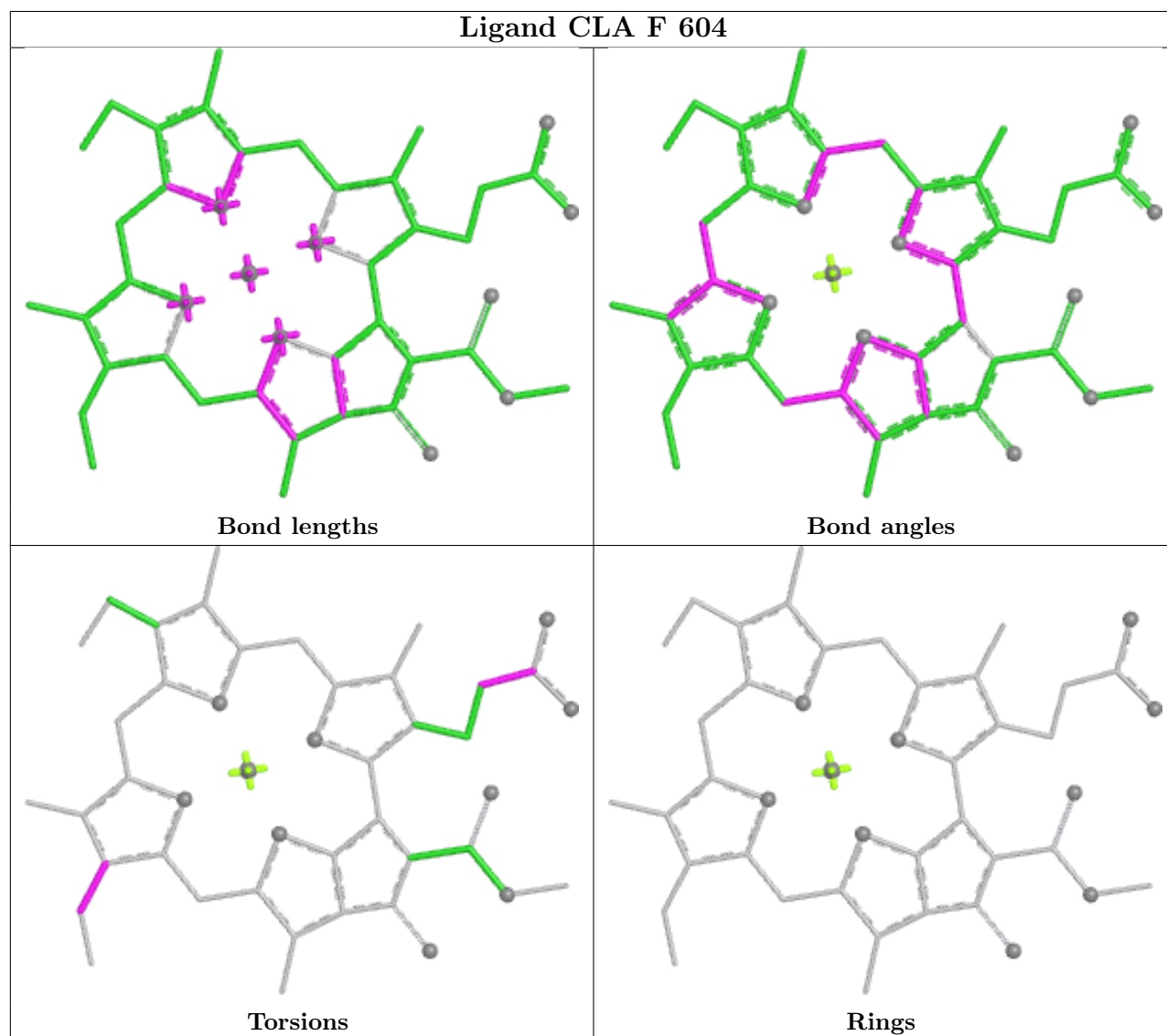
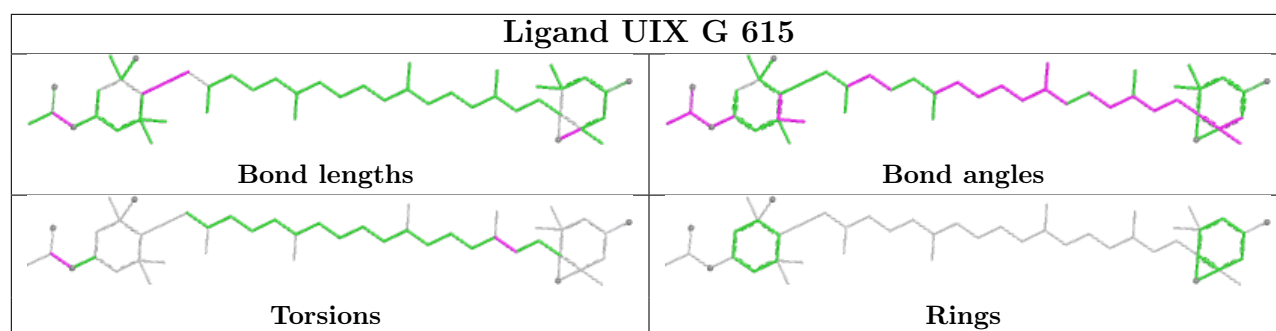
Ligand CLA G 602

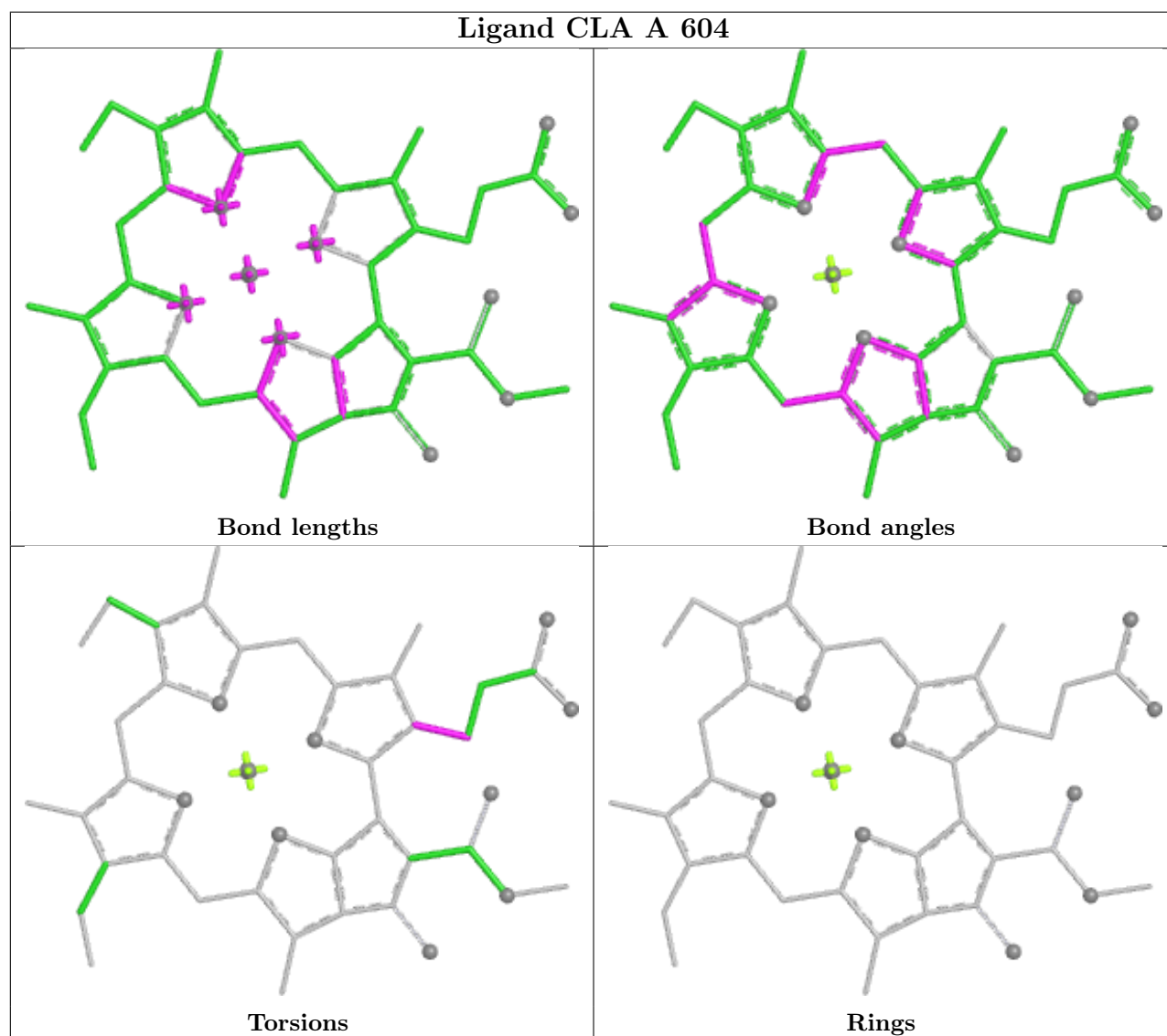
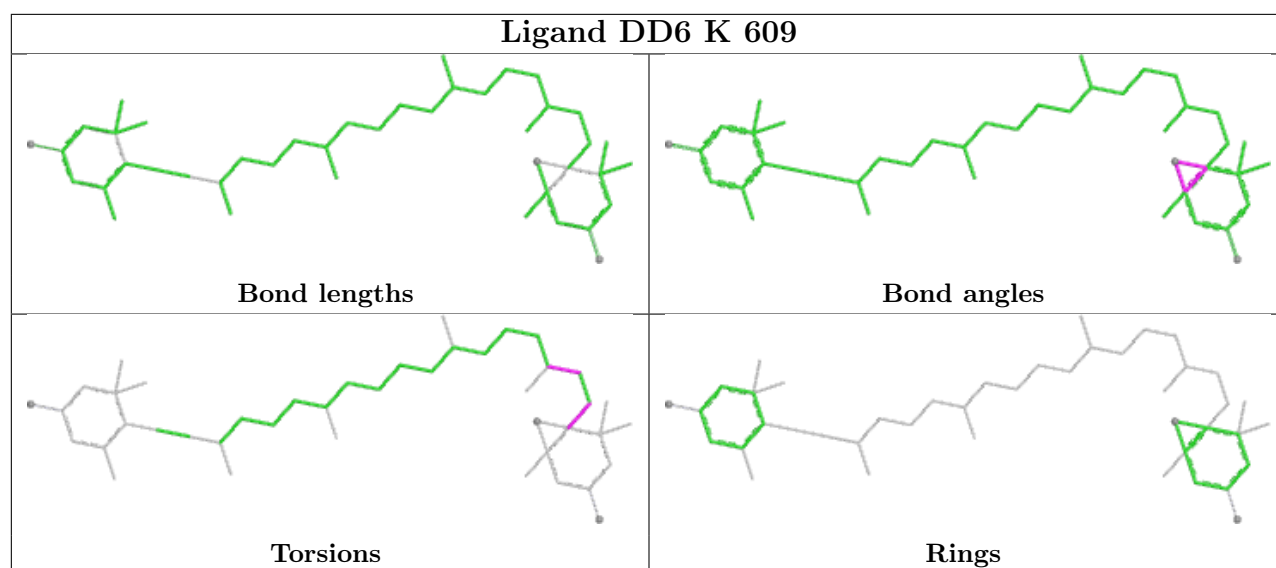


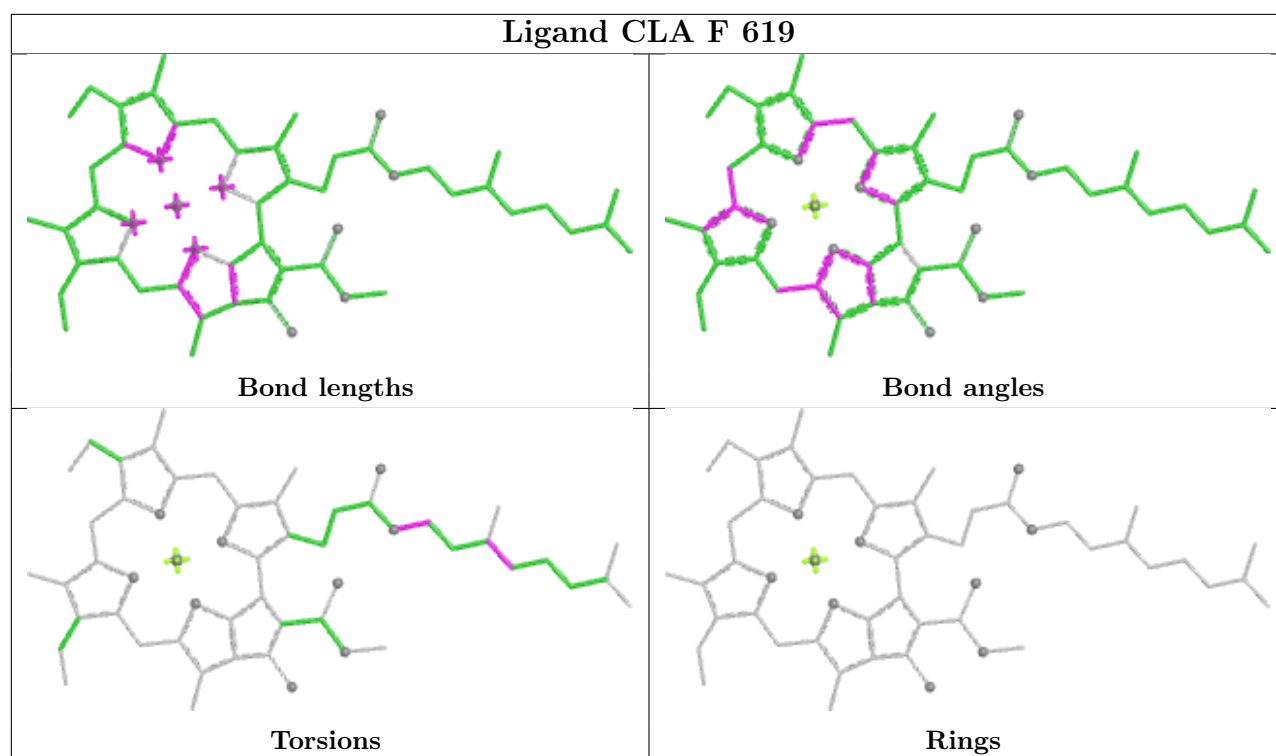
Ligand CLA J 603



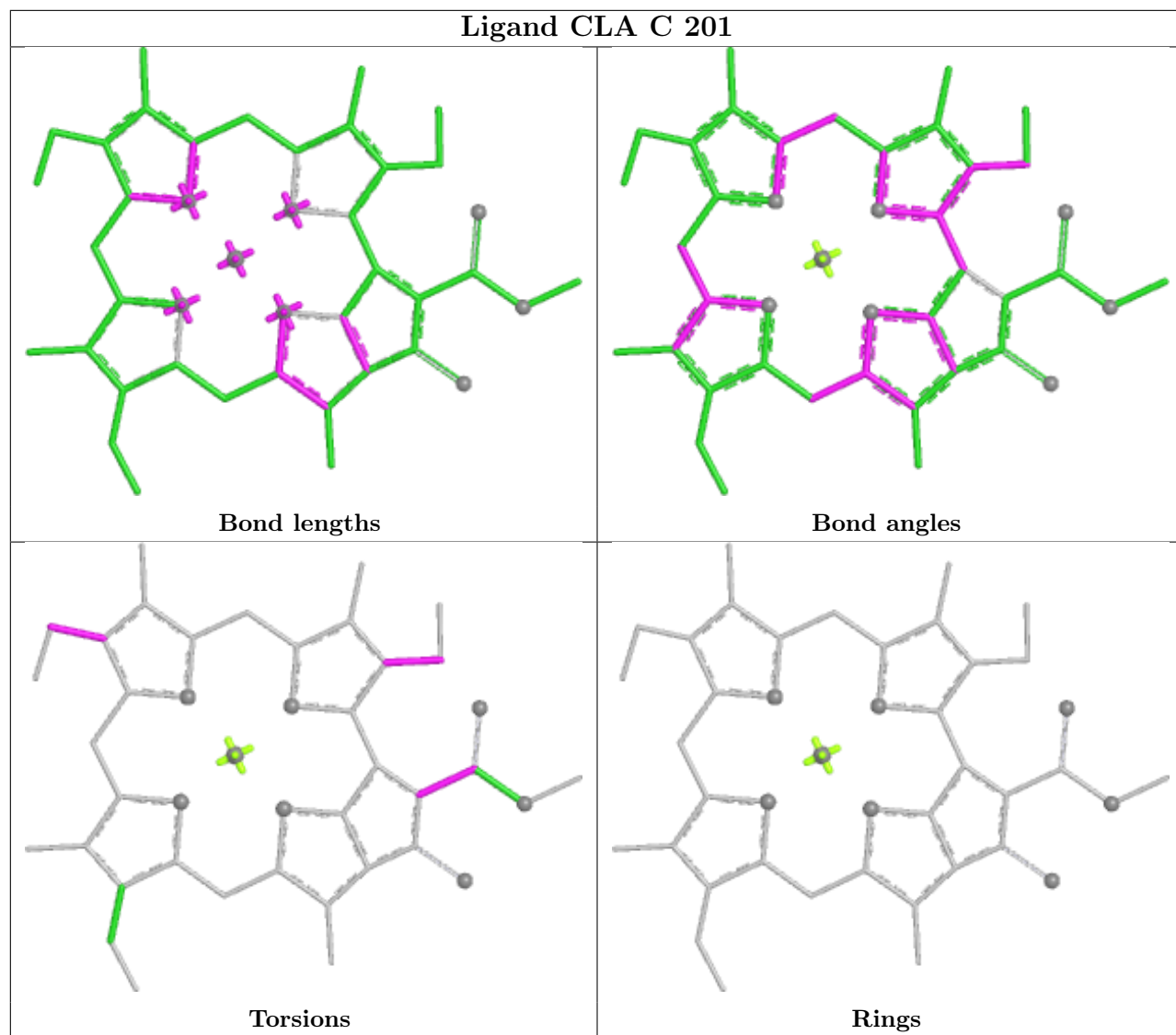




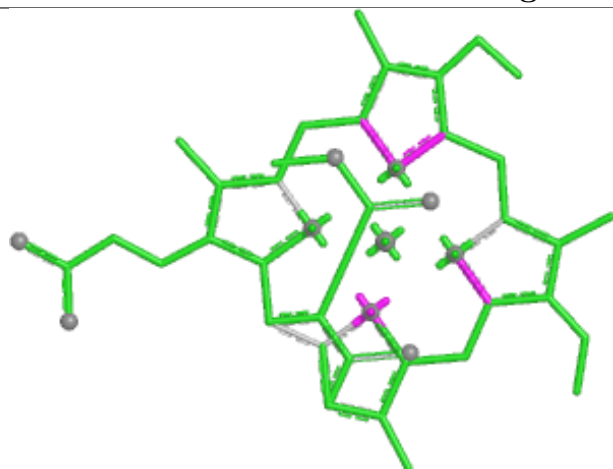




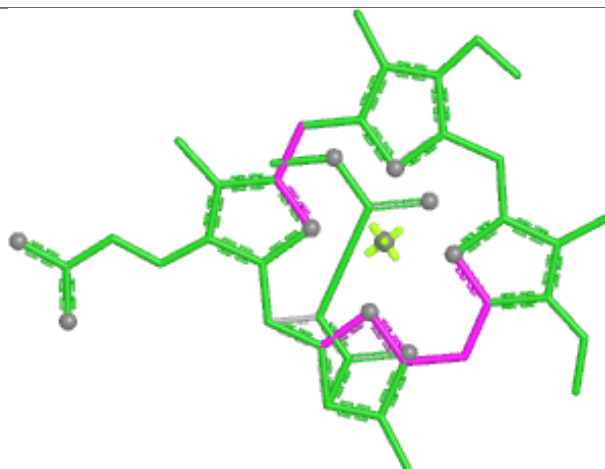
Ligand CLA C 201



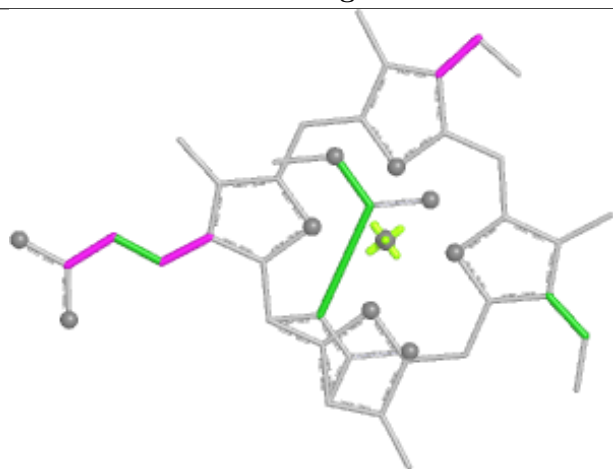
Ligand KC2 J 602



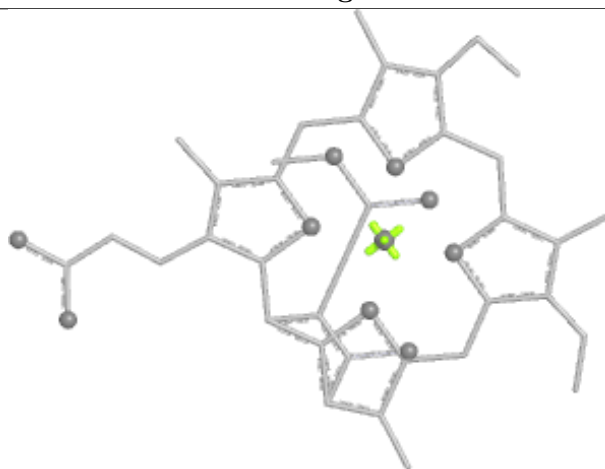
Bond lengths



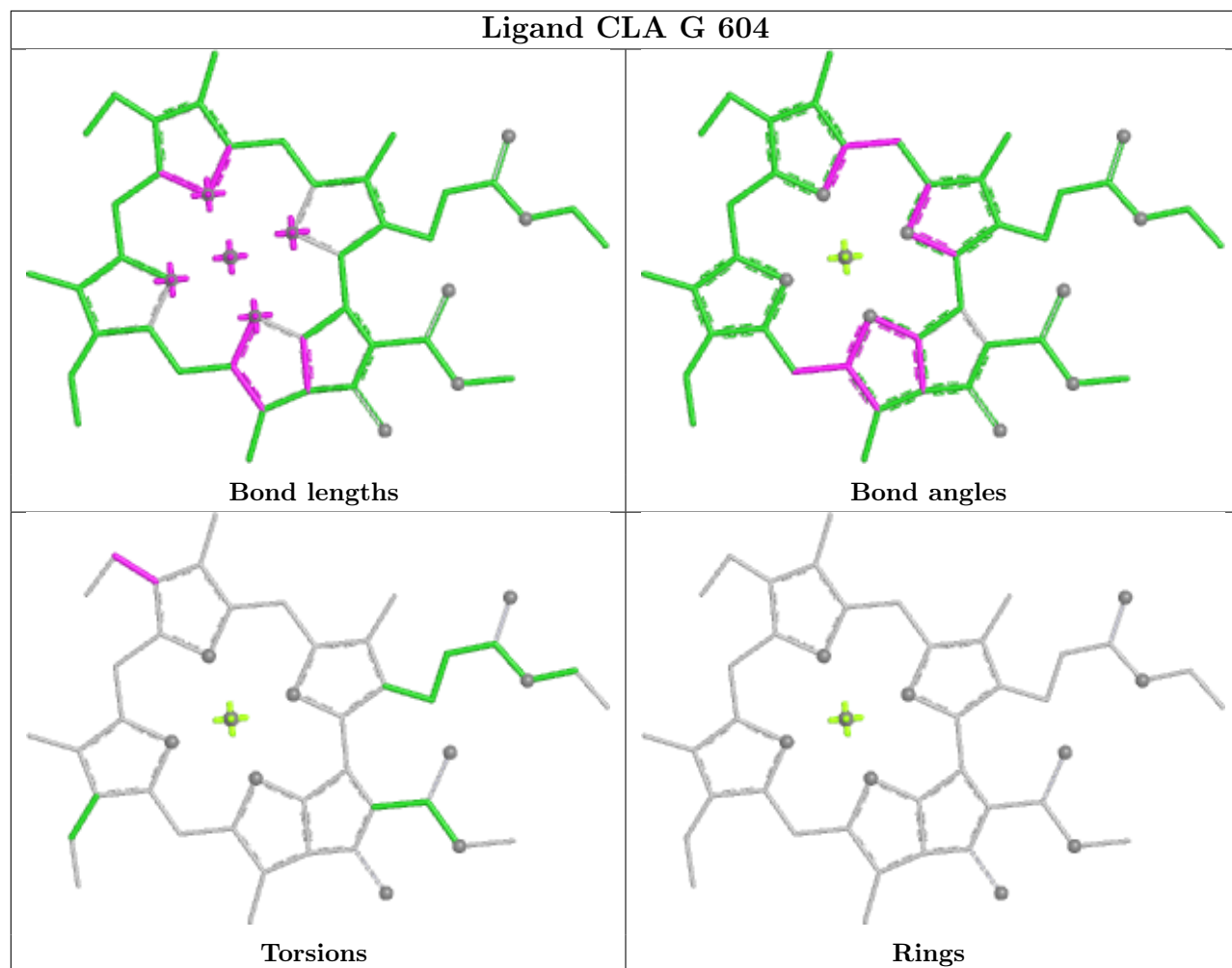
Bond angles



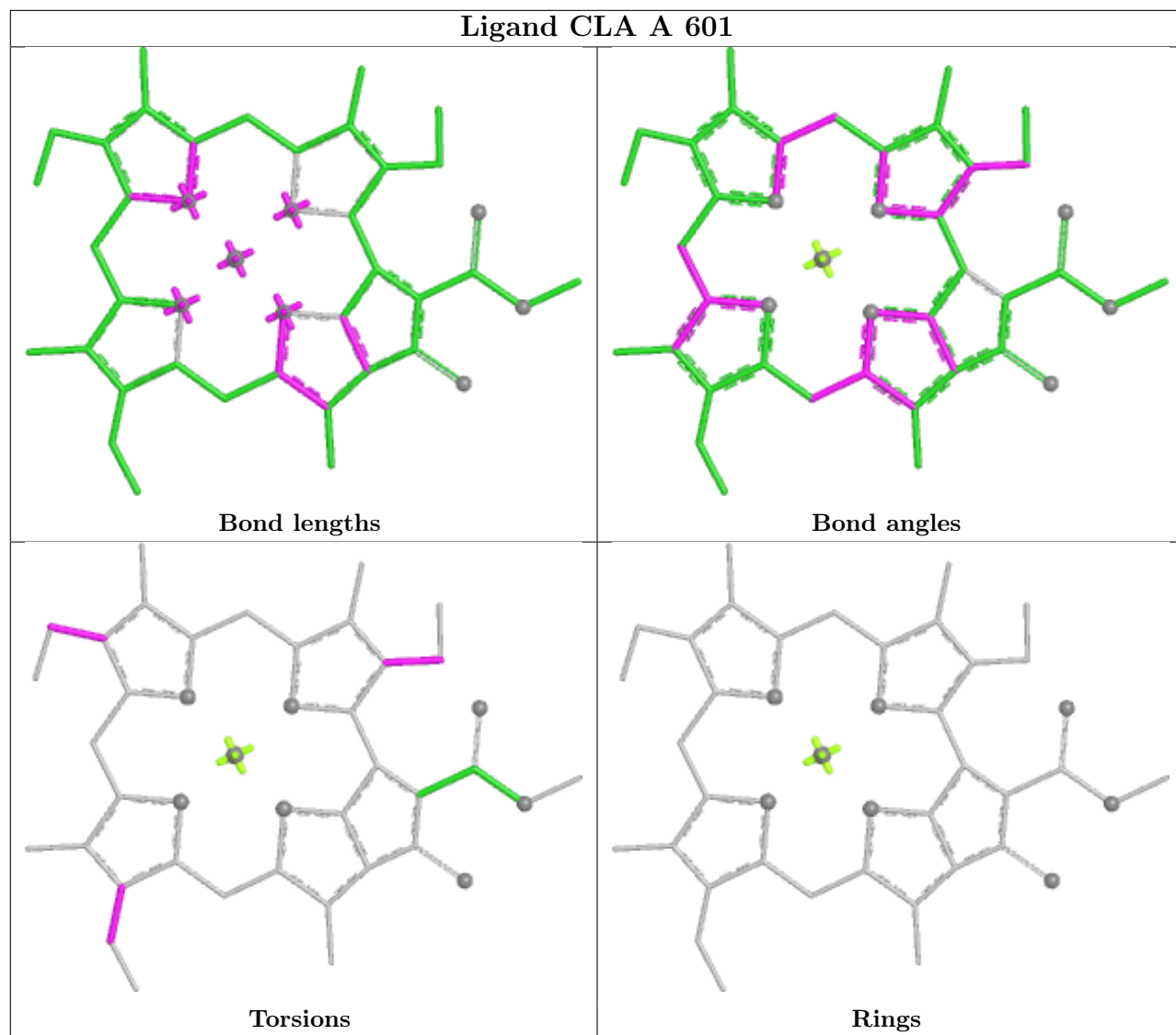
Torsions



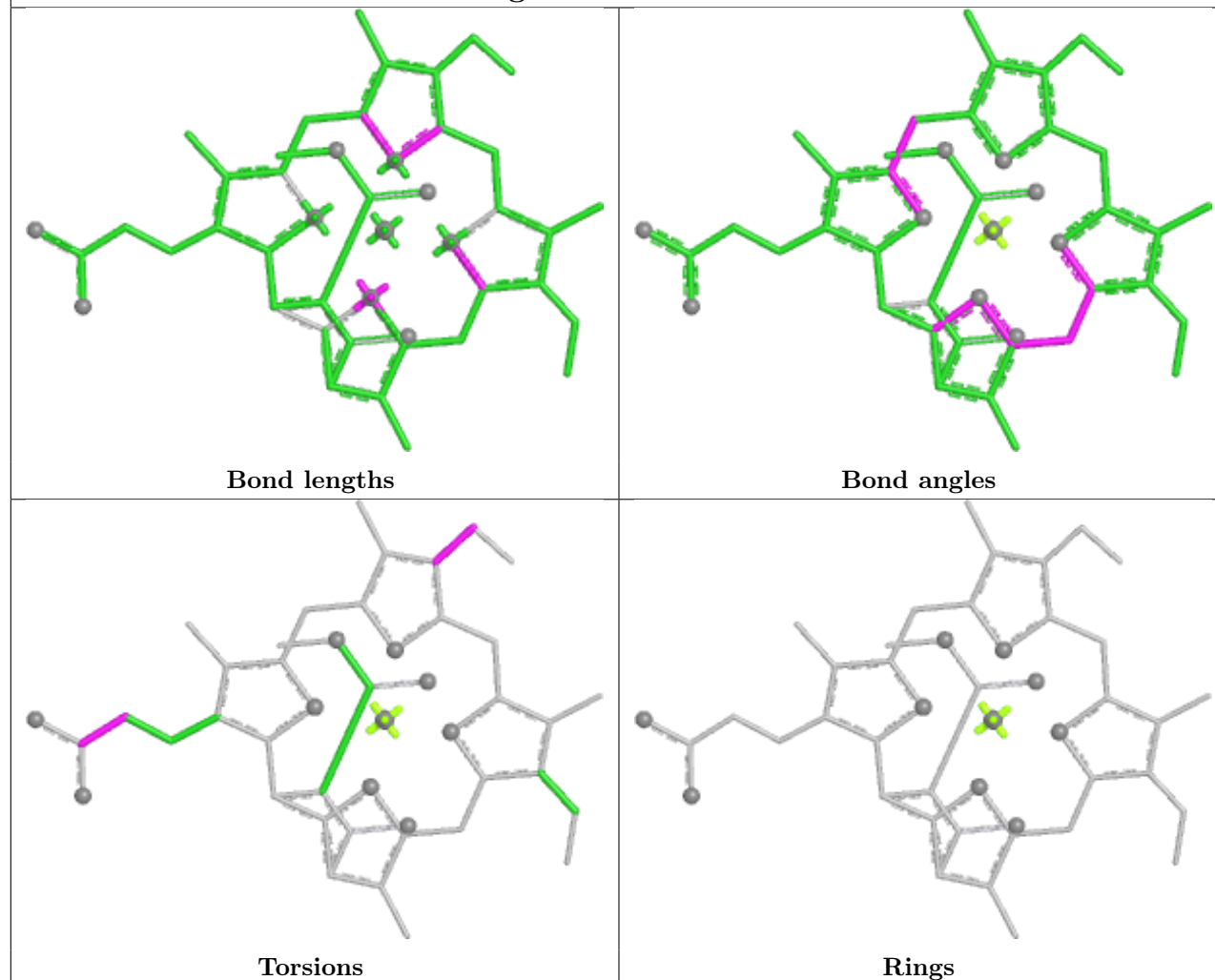
Rings



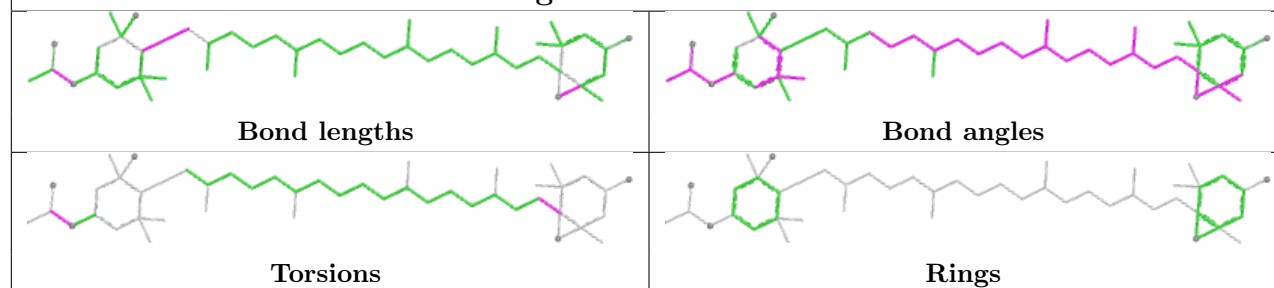
Ligand CLA A 601



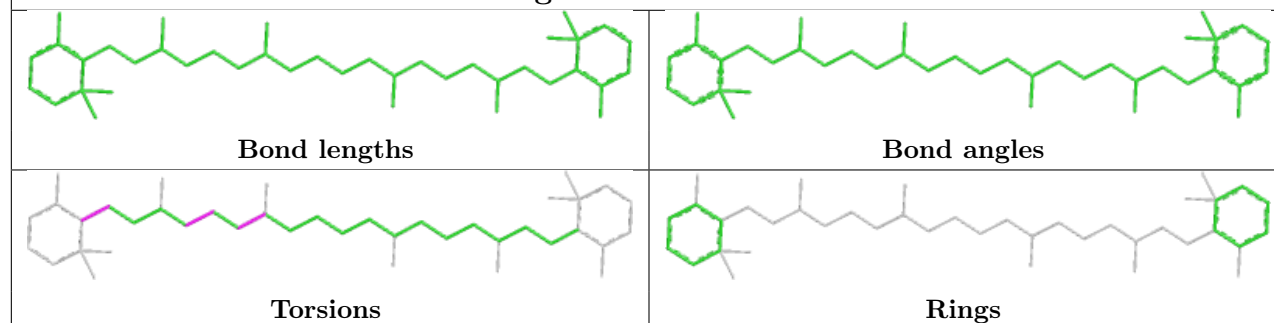
Ligand KC2 U 602

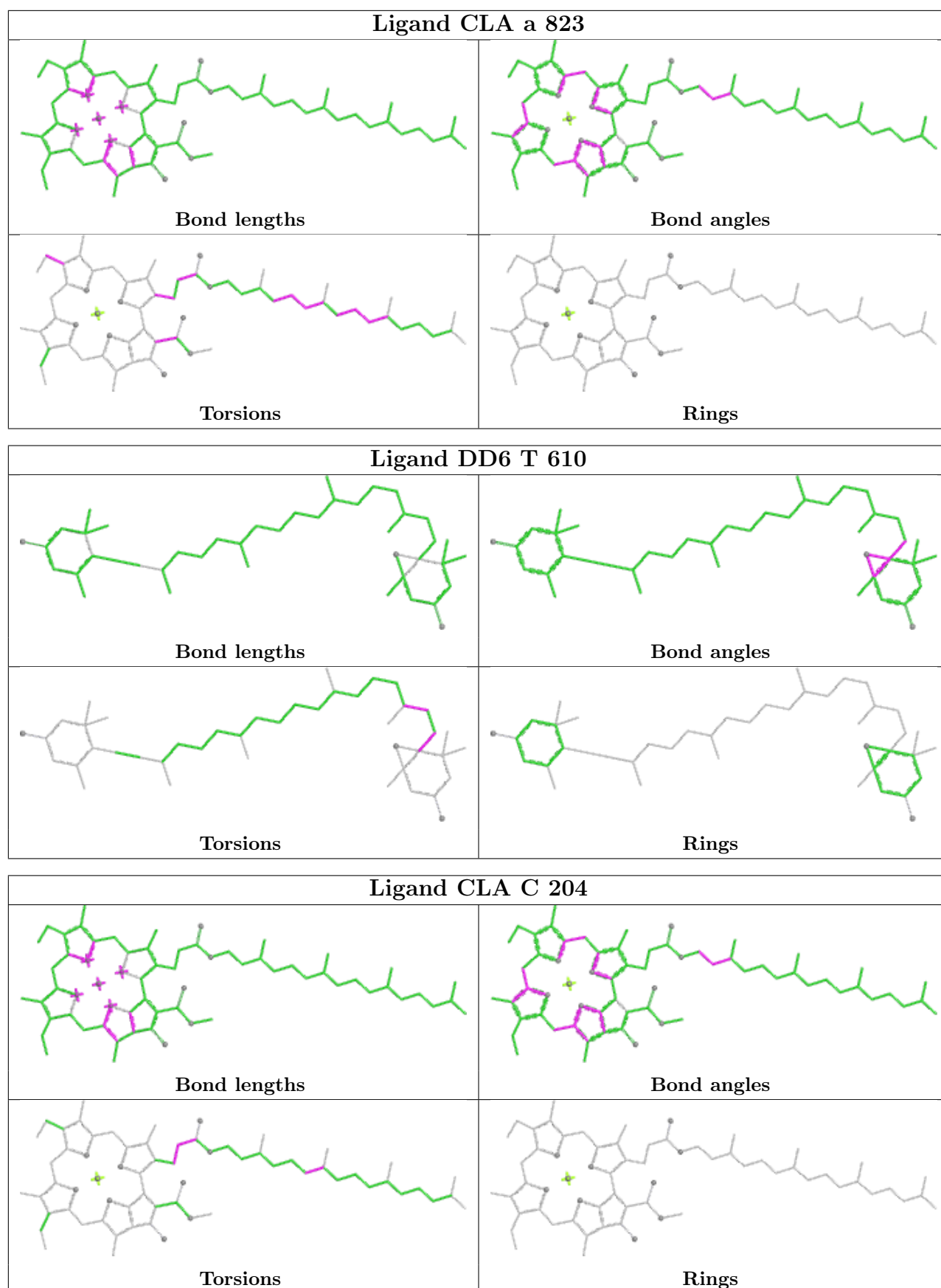


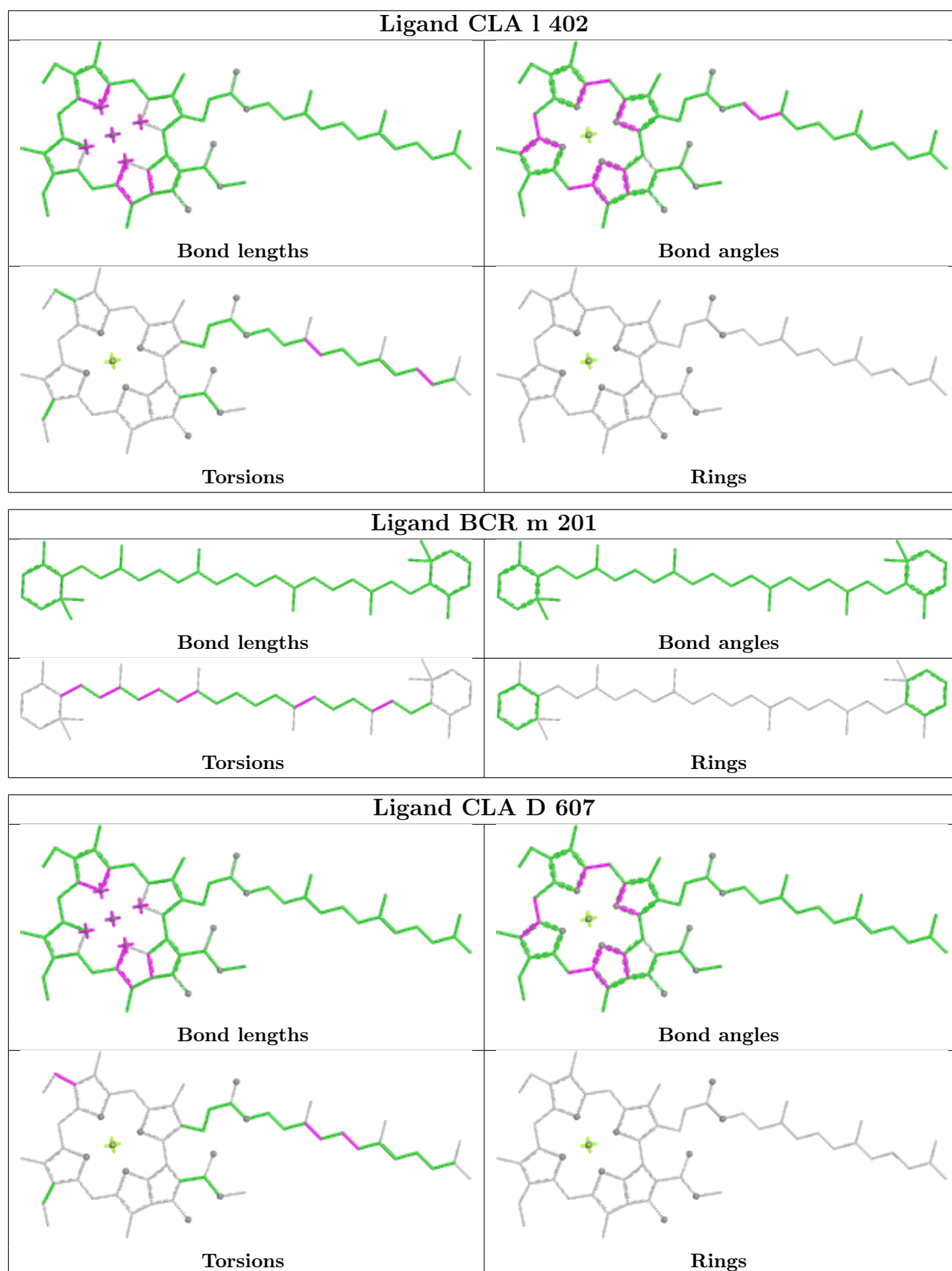
Ligand UIX C 215



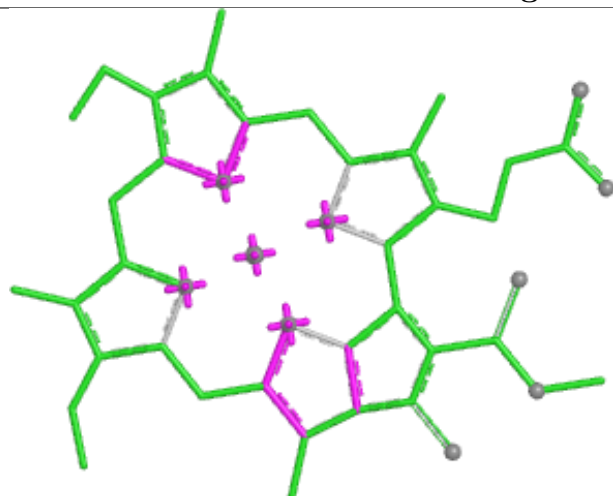
Ligand BCR a 834



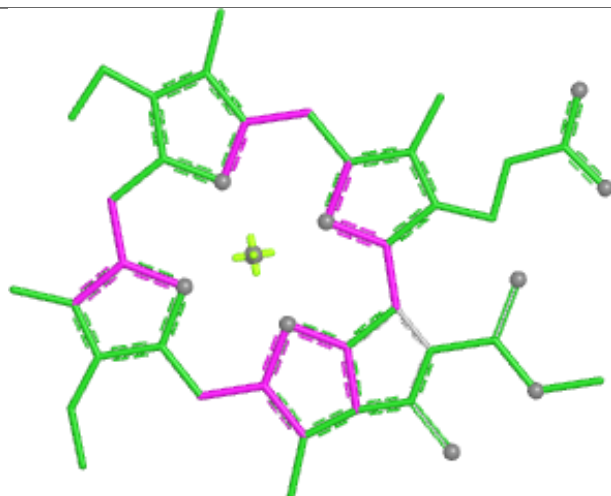




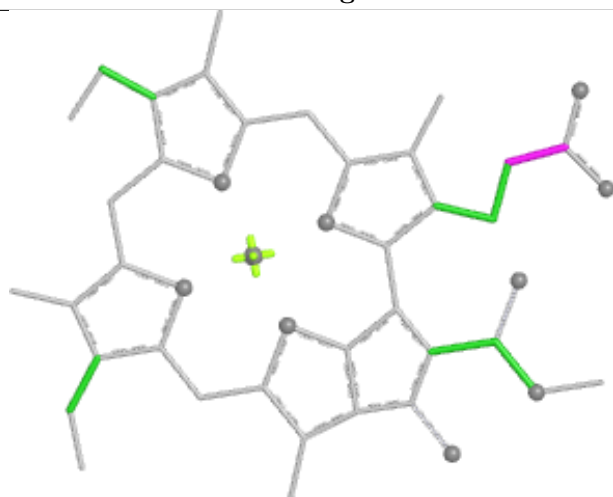
Ligand CLA I 609



Bond lengths



Bond angles

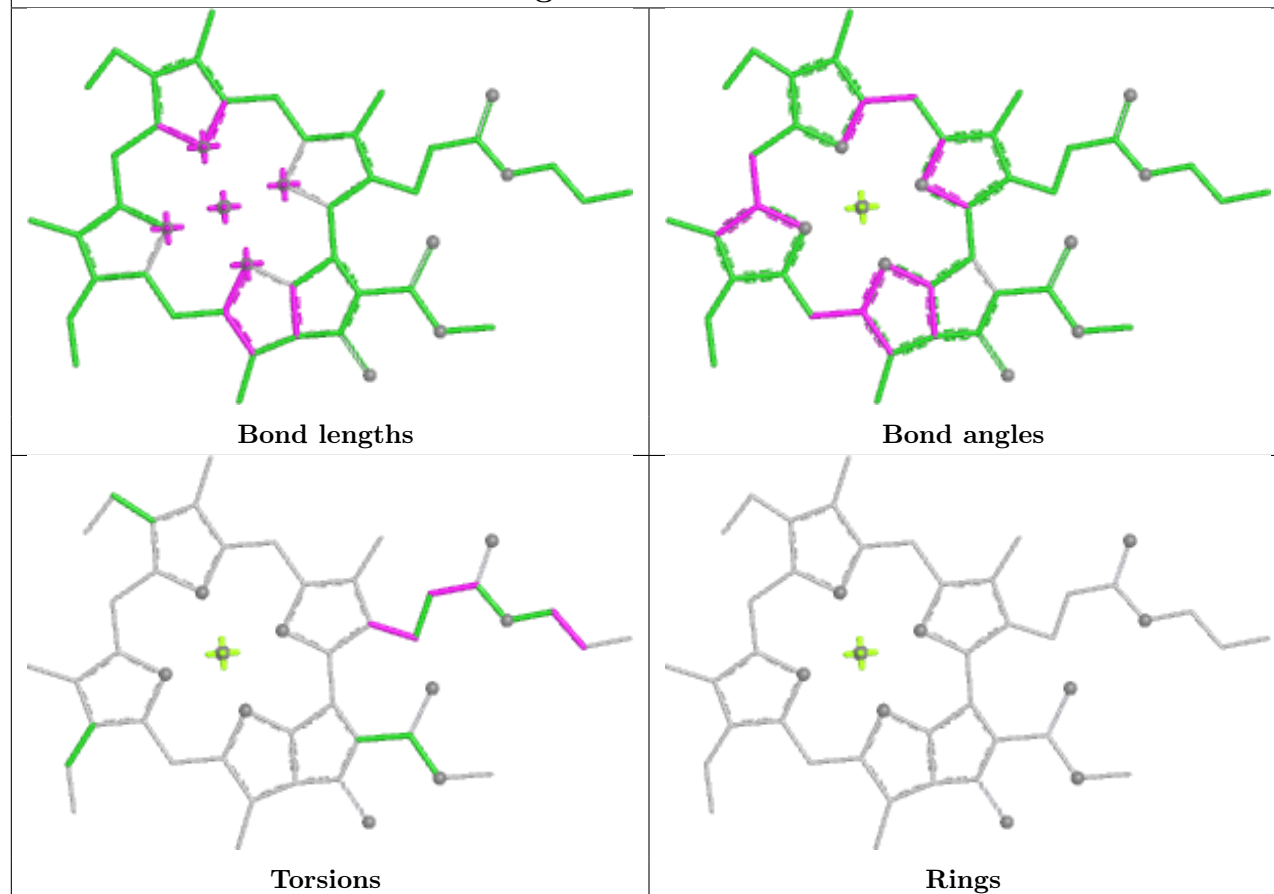


Torsions

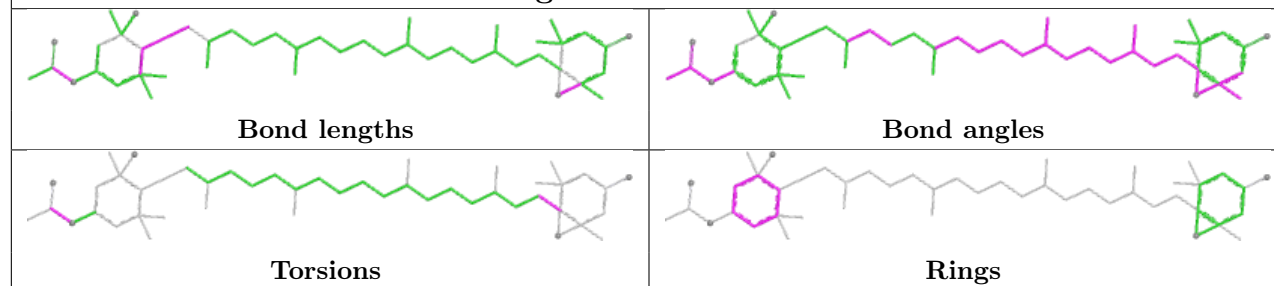


Rings

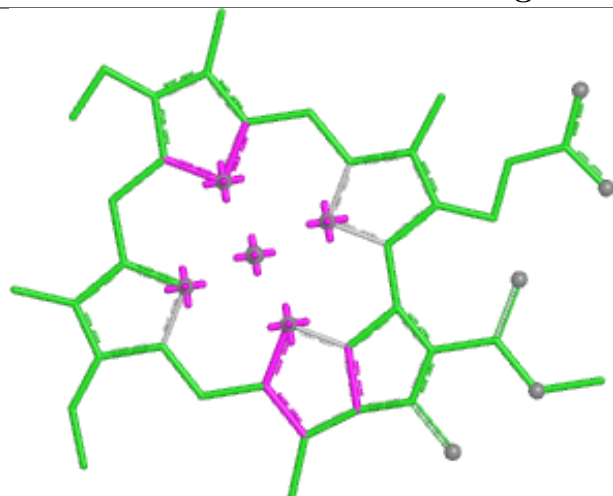
Ligand CLA b 722



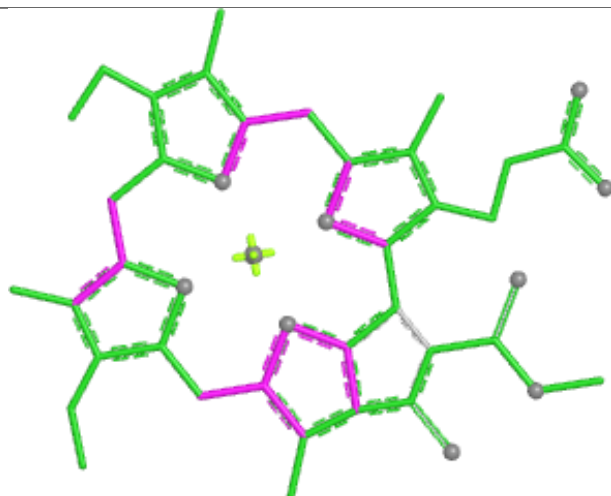
Ligand UIX B 615



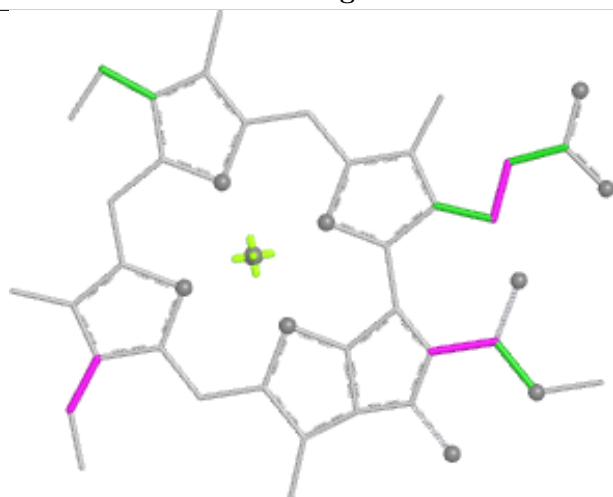
Ligand CLA T 603



Bond lengths



Bond angles

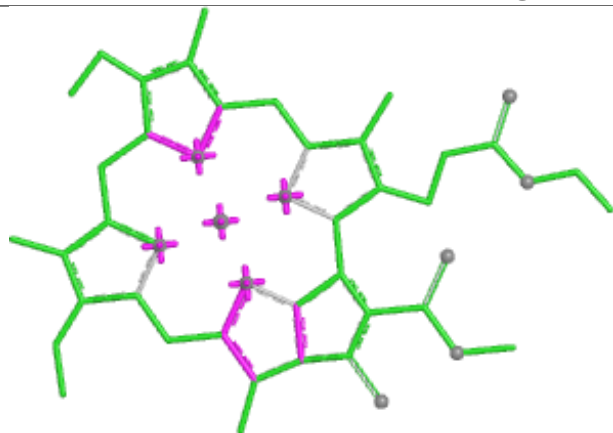


Torsions

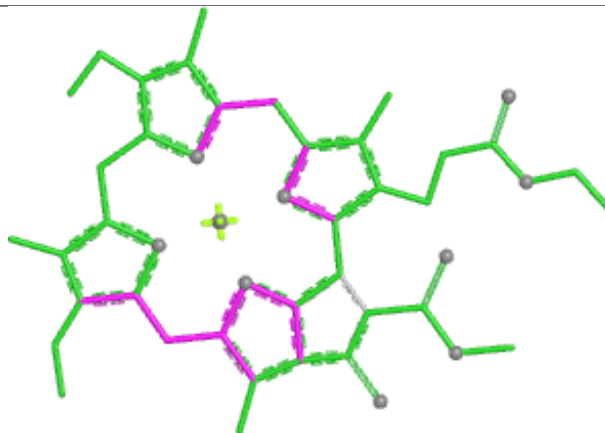


Rings

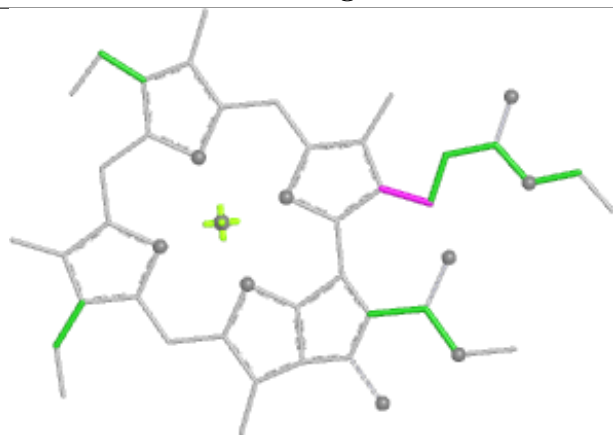
Ligand CLA A 606



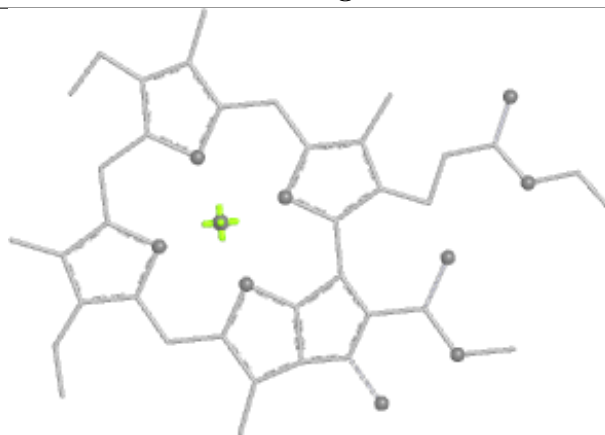
Bond lengths



Bond angles

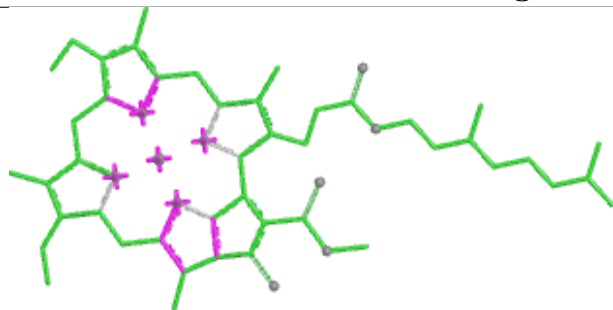


Torsions

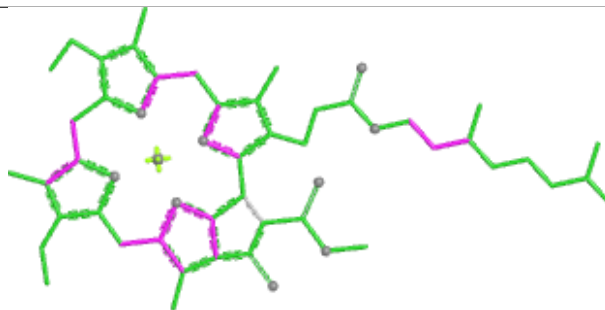


Rings

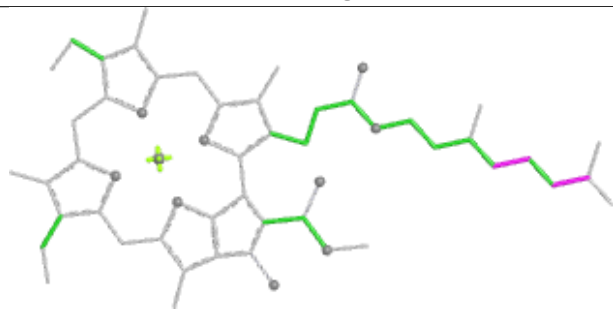
Ligand CLA D 603



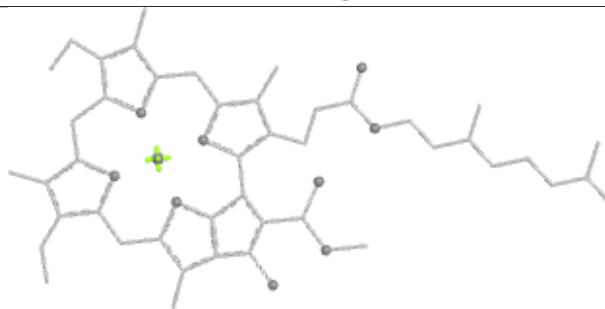
Bond lengths



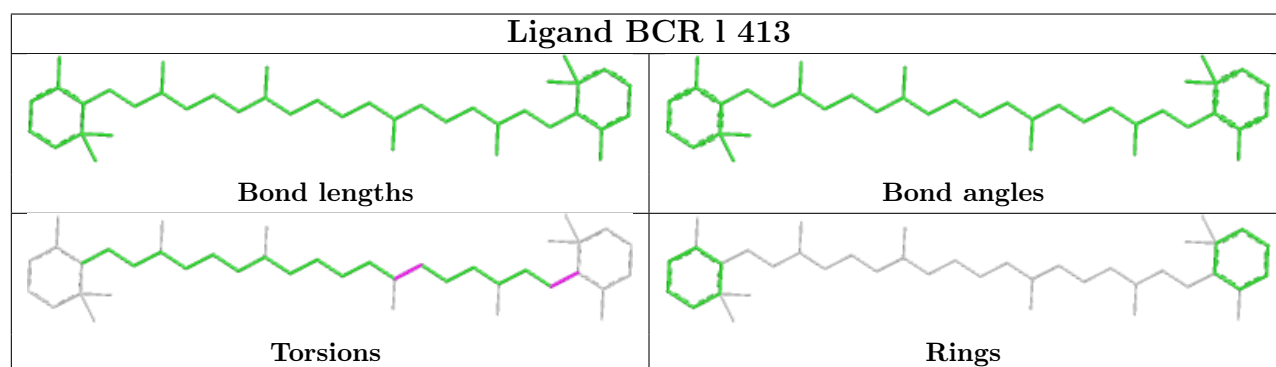
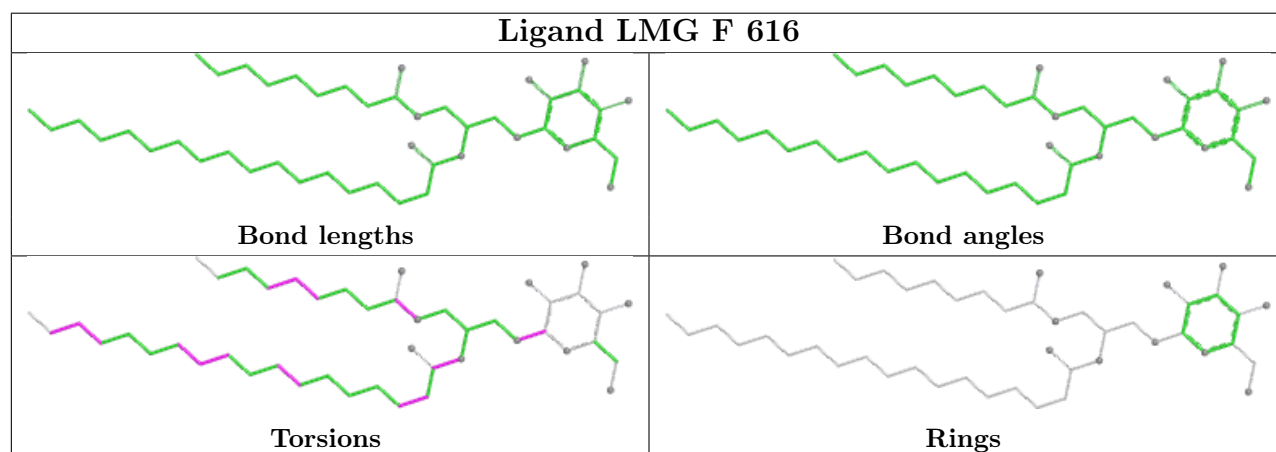
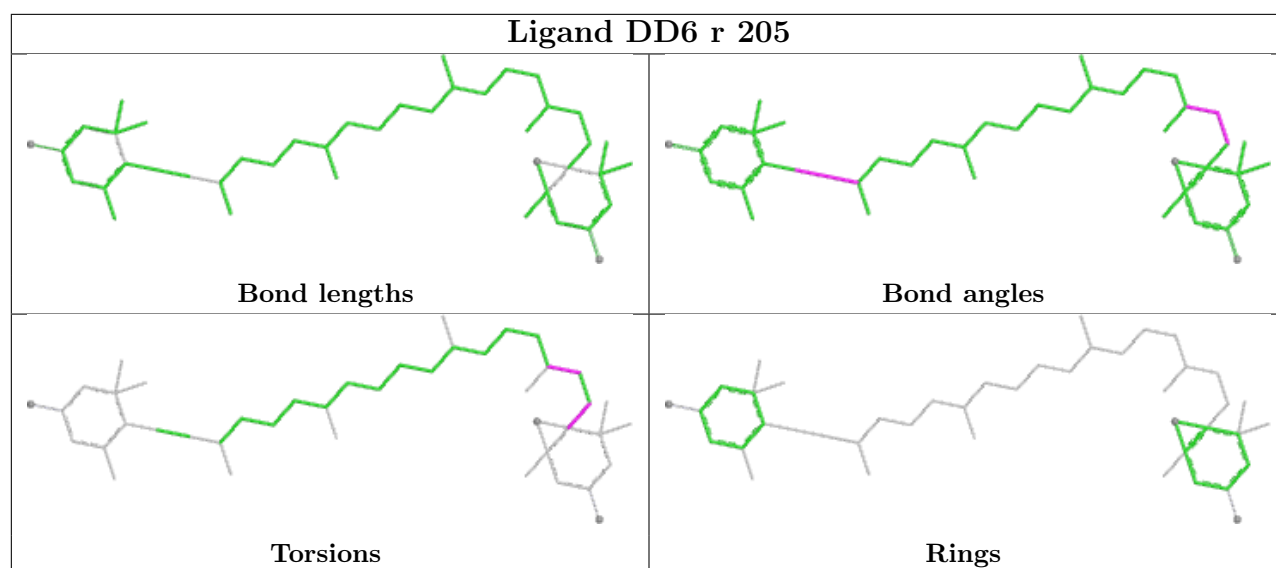
Bond angles

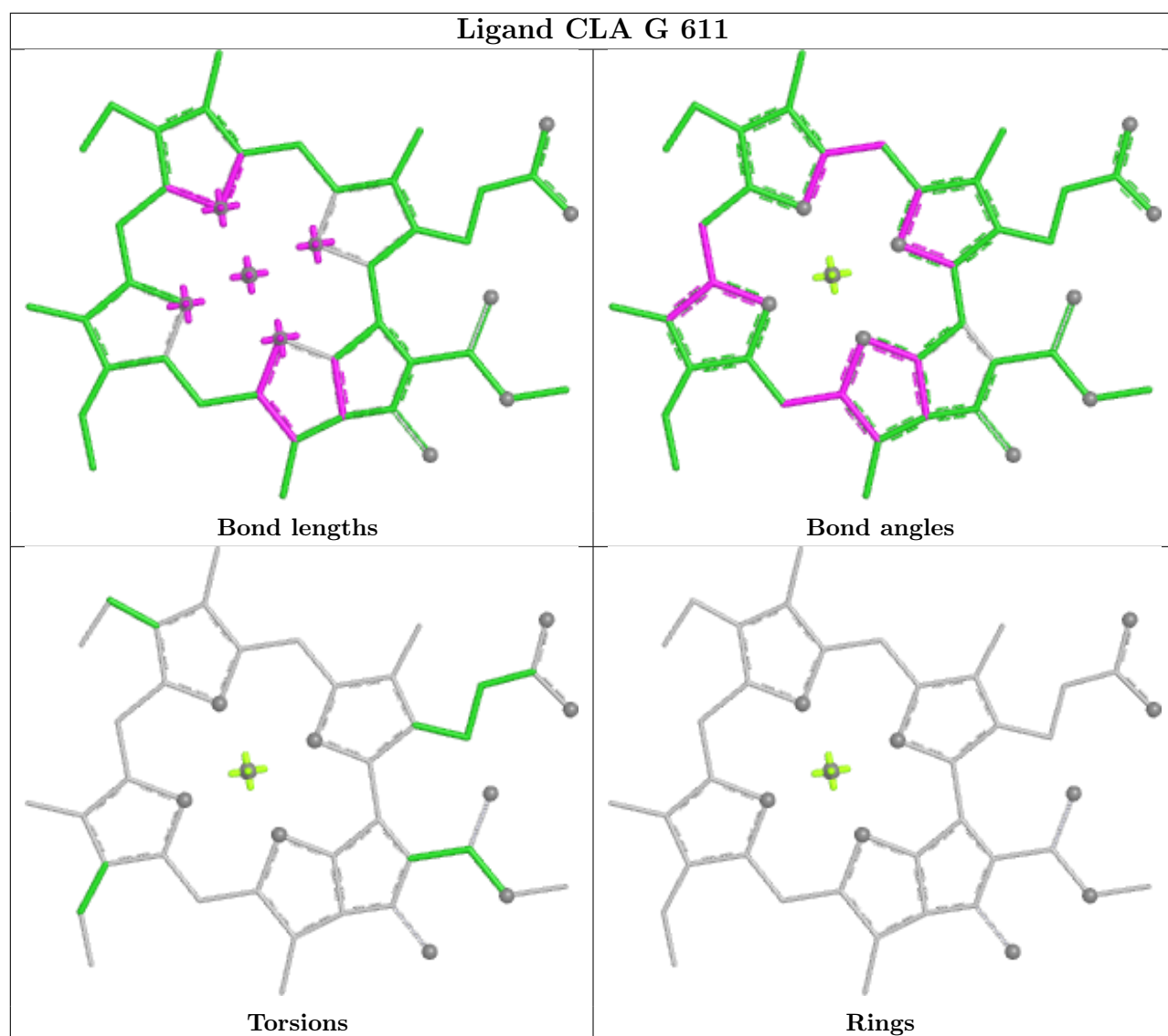


Torsions

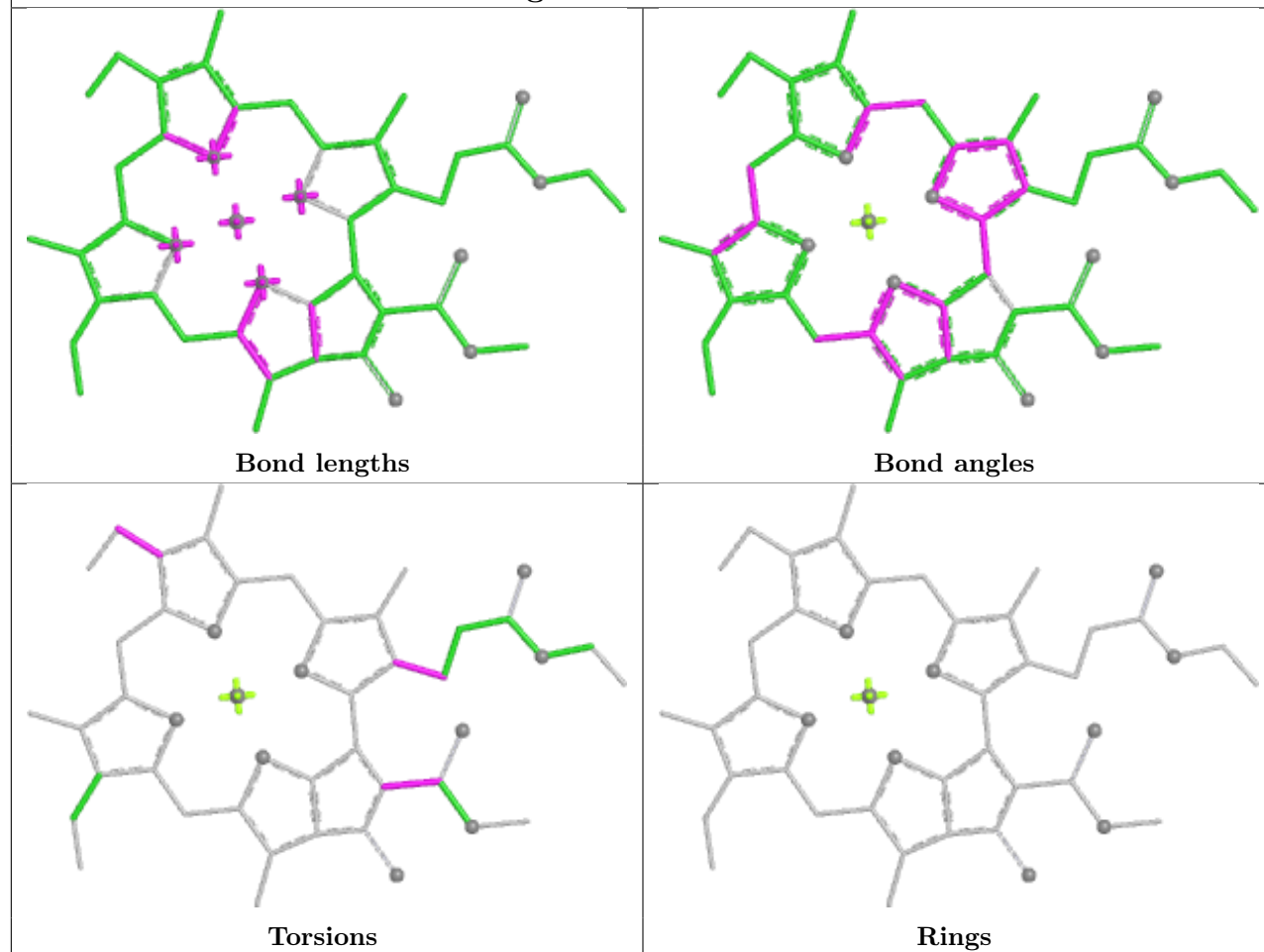


Rings

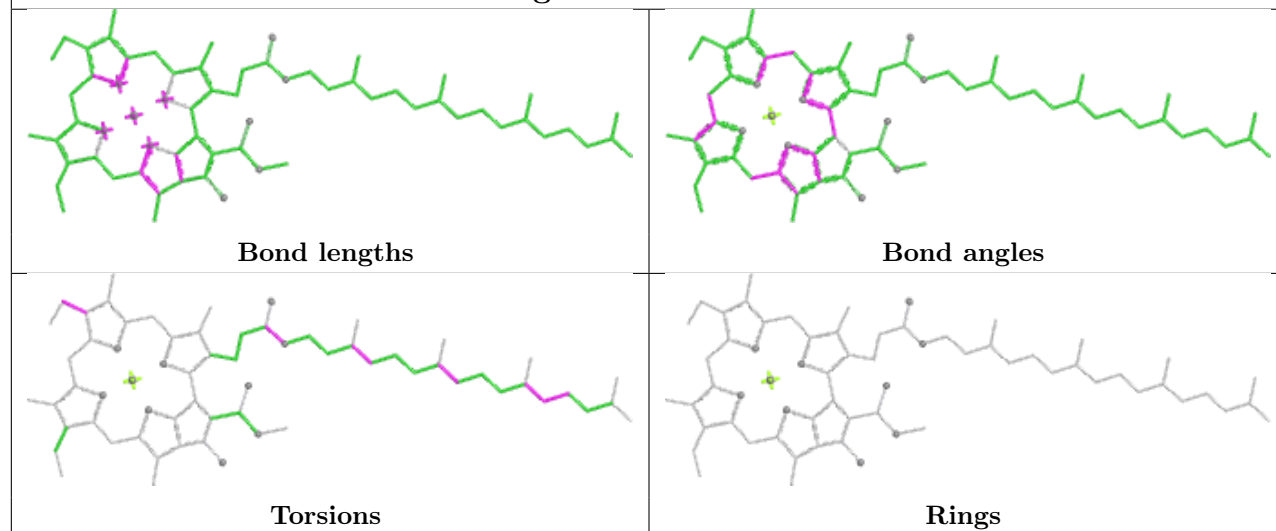


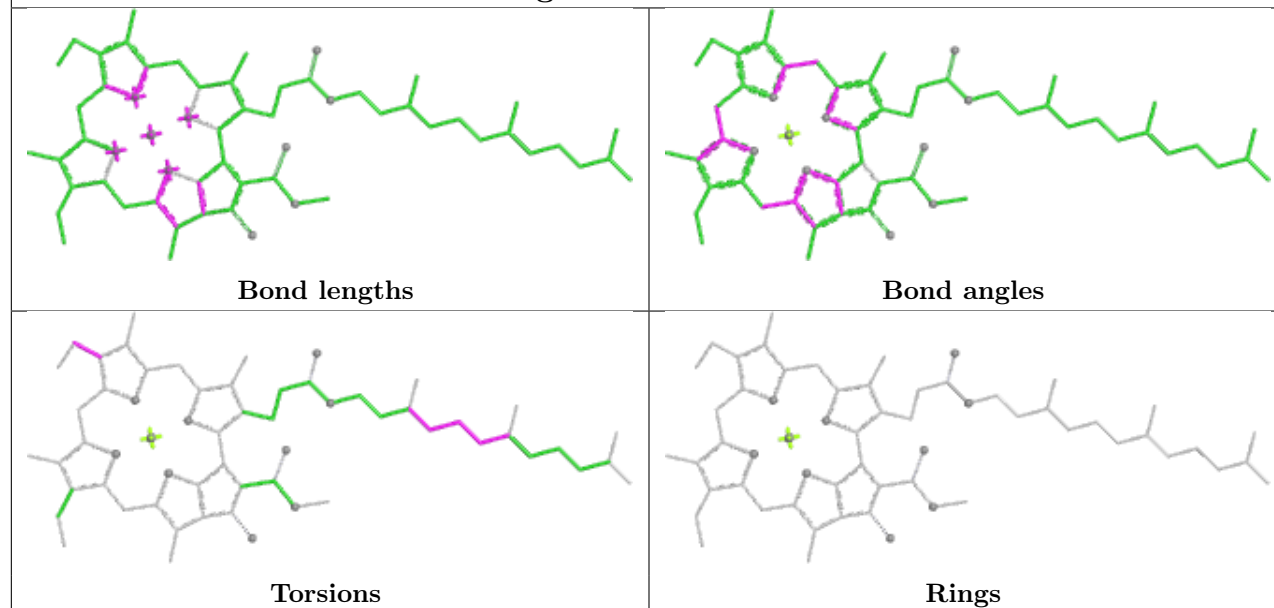
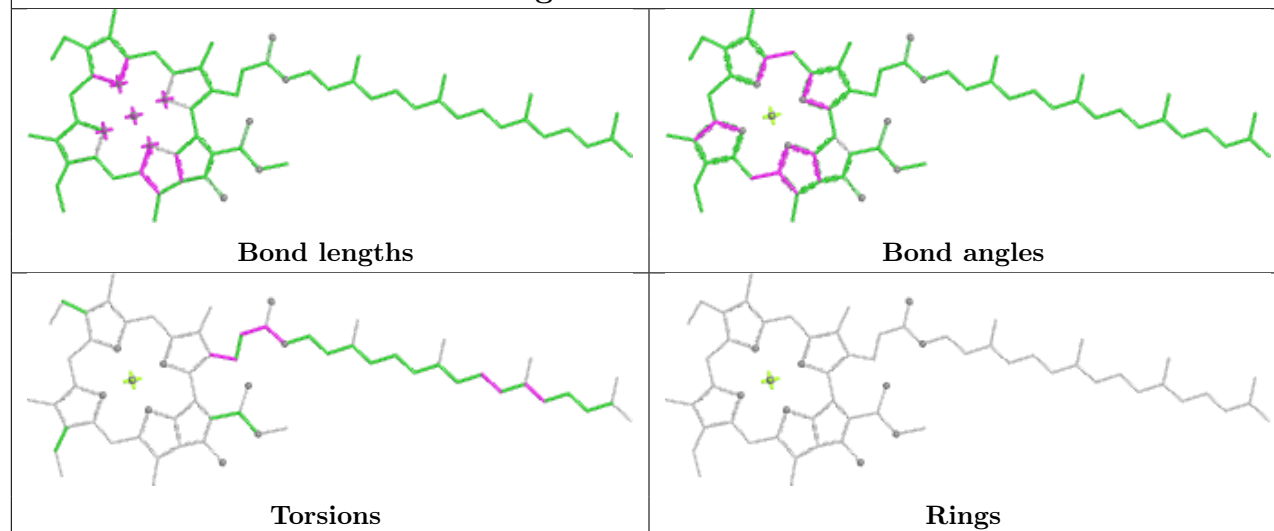


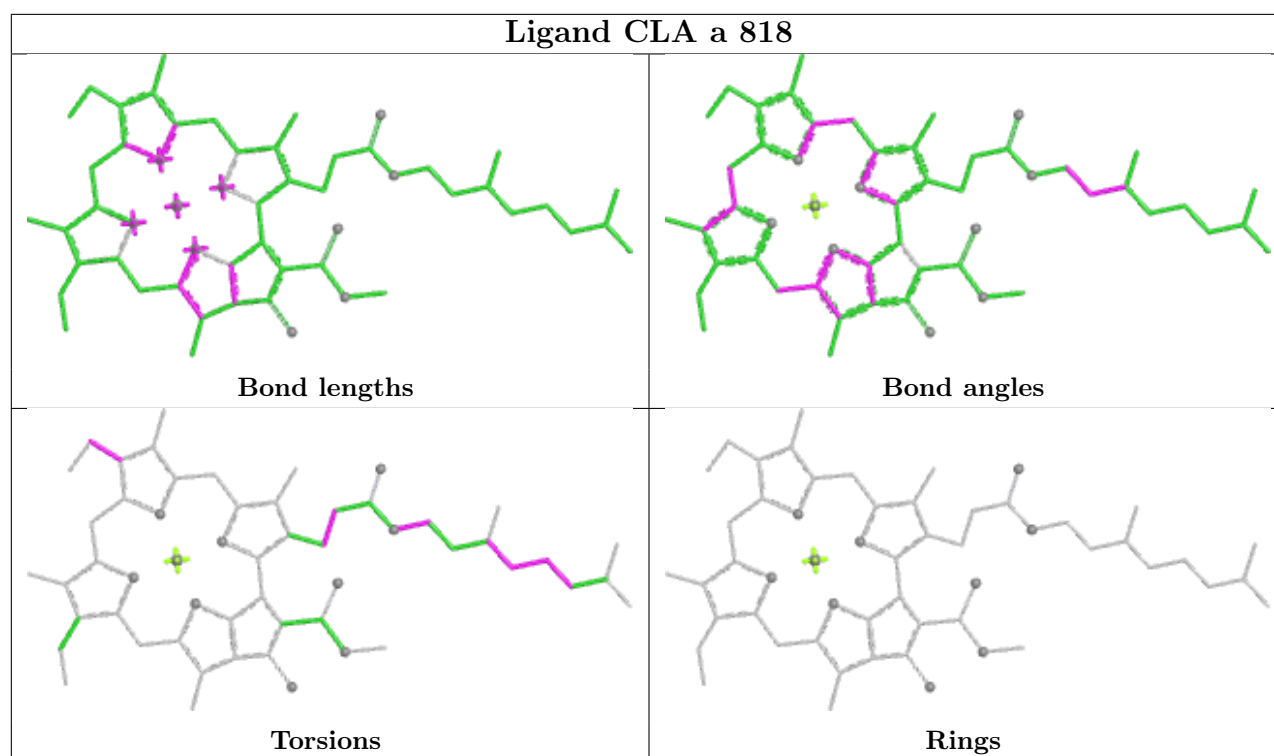
Ligand CLA A 612



Ligand CLA E 607



Ligand CLA a 816**Ligand CLA b 717**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

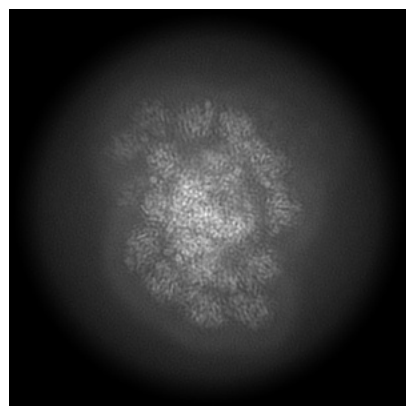
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36366. These allow visual inspection of the internal detail of the map and identification of artifacts.

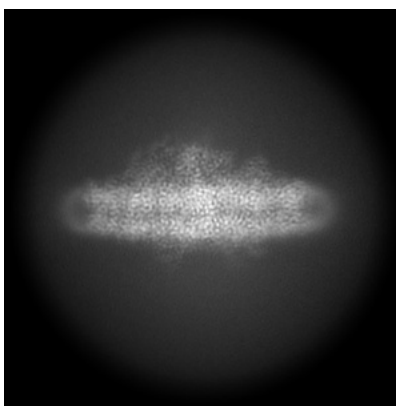
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

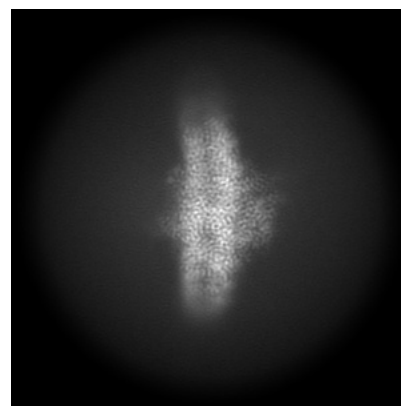
6.1.1 Primary map



X

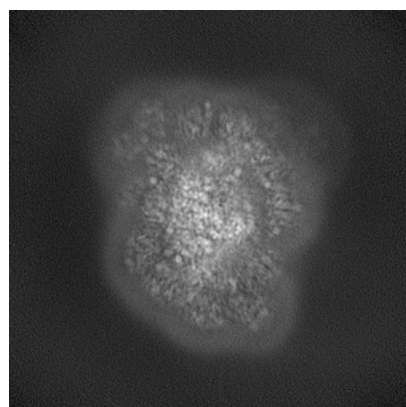


Y

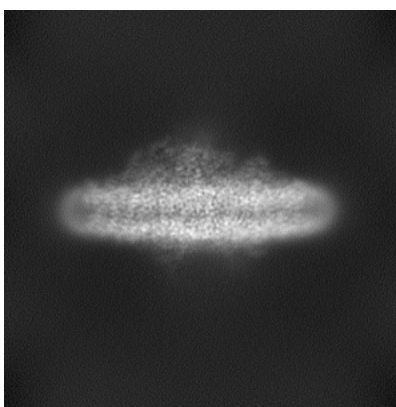


Z

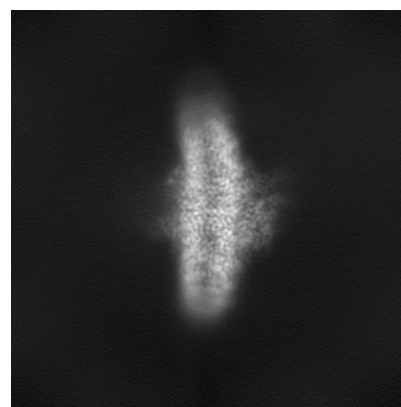
6.1.2 Raw map



X



Y

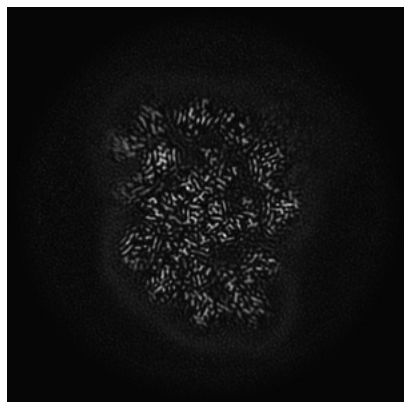


Z

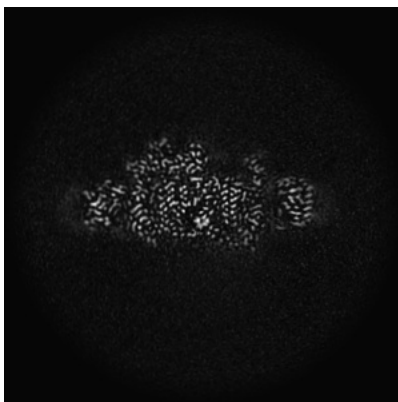
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

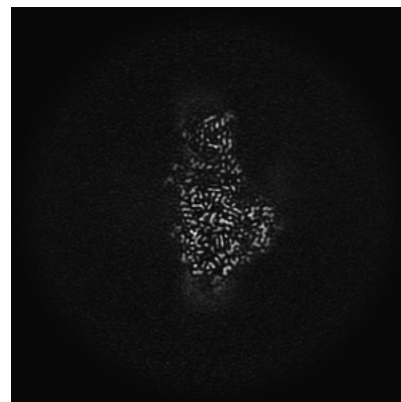
6.2.1 Primary map



X Index: 160

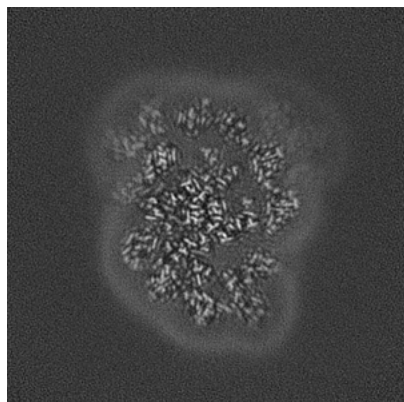


Y Index: 160

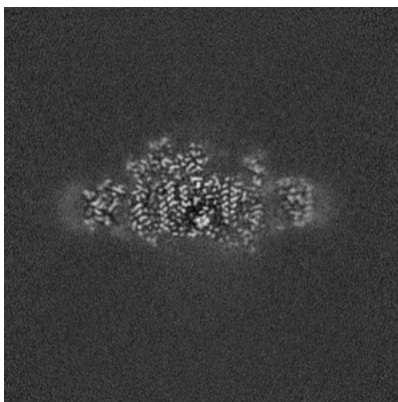


Z Index: 160

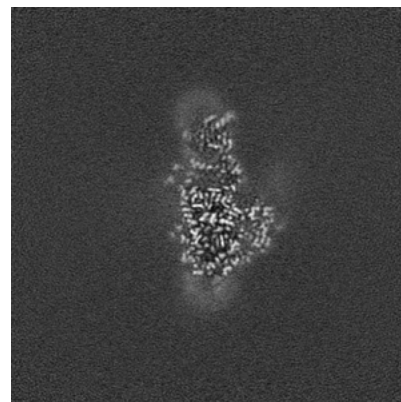
6.2.2 Raw map



X Index: 160



Y Index: 160

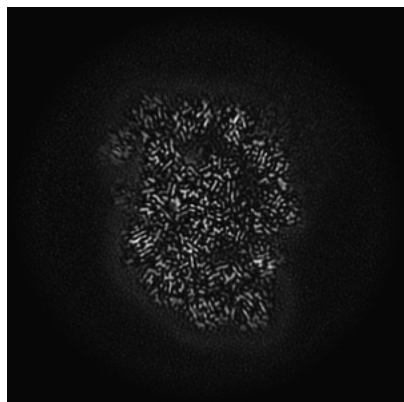


Z Index: 160

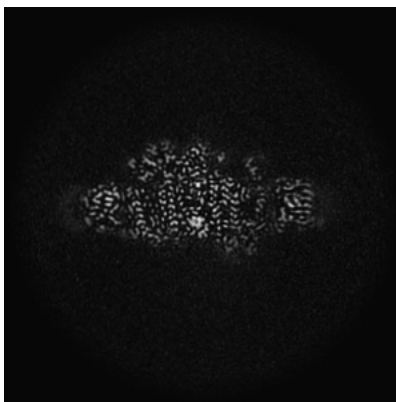
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

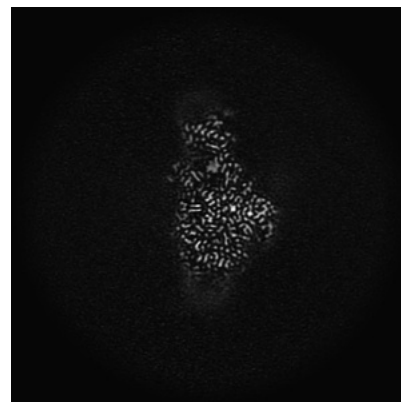
6.3.1 Primary map



X Index: 167

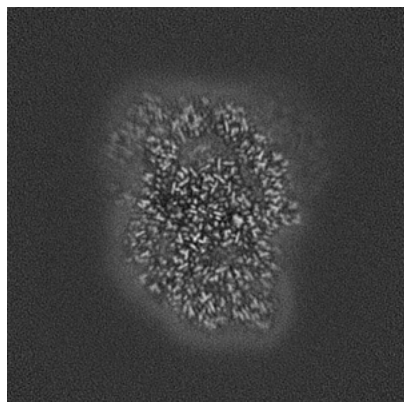


Y Index: 157

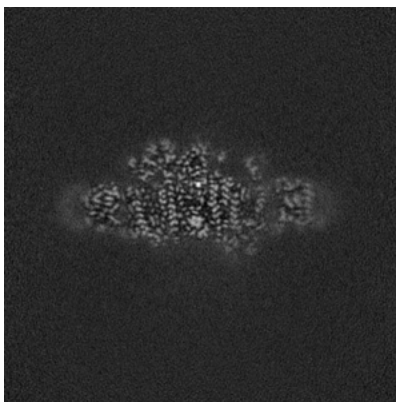


Z Index: 155

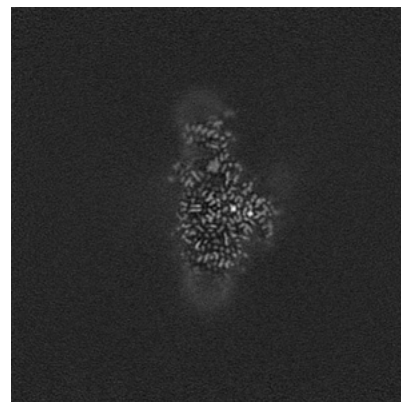
6.3.2 Raw map



X Index: 170



Y Index: 157

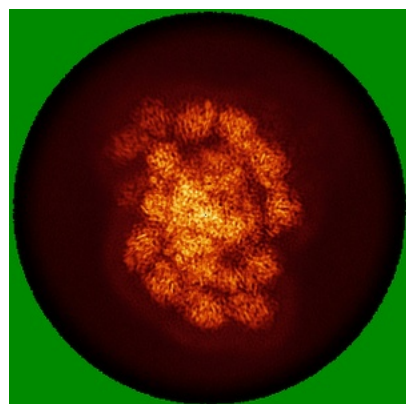


Z Index: 155

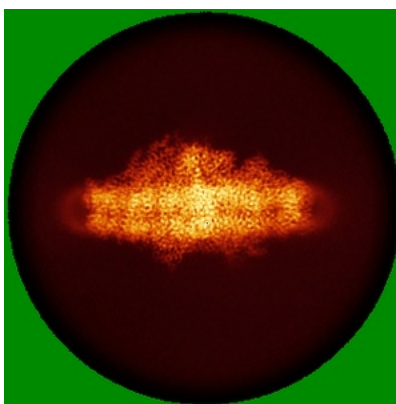
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

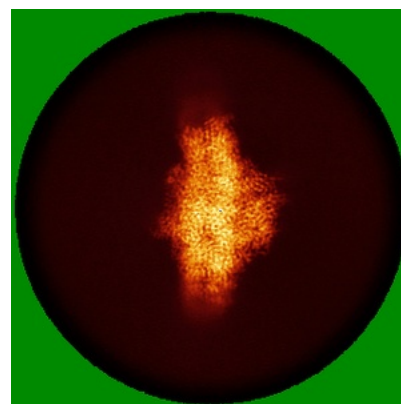
6.4.1 Primary map



X

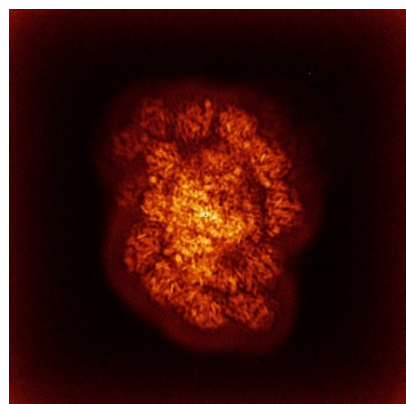


Y

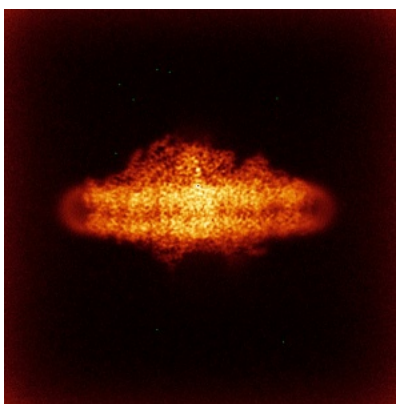


Z

6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

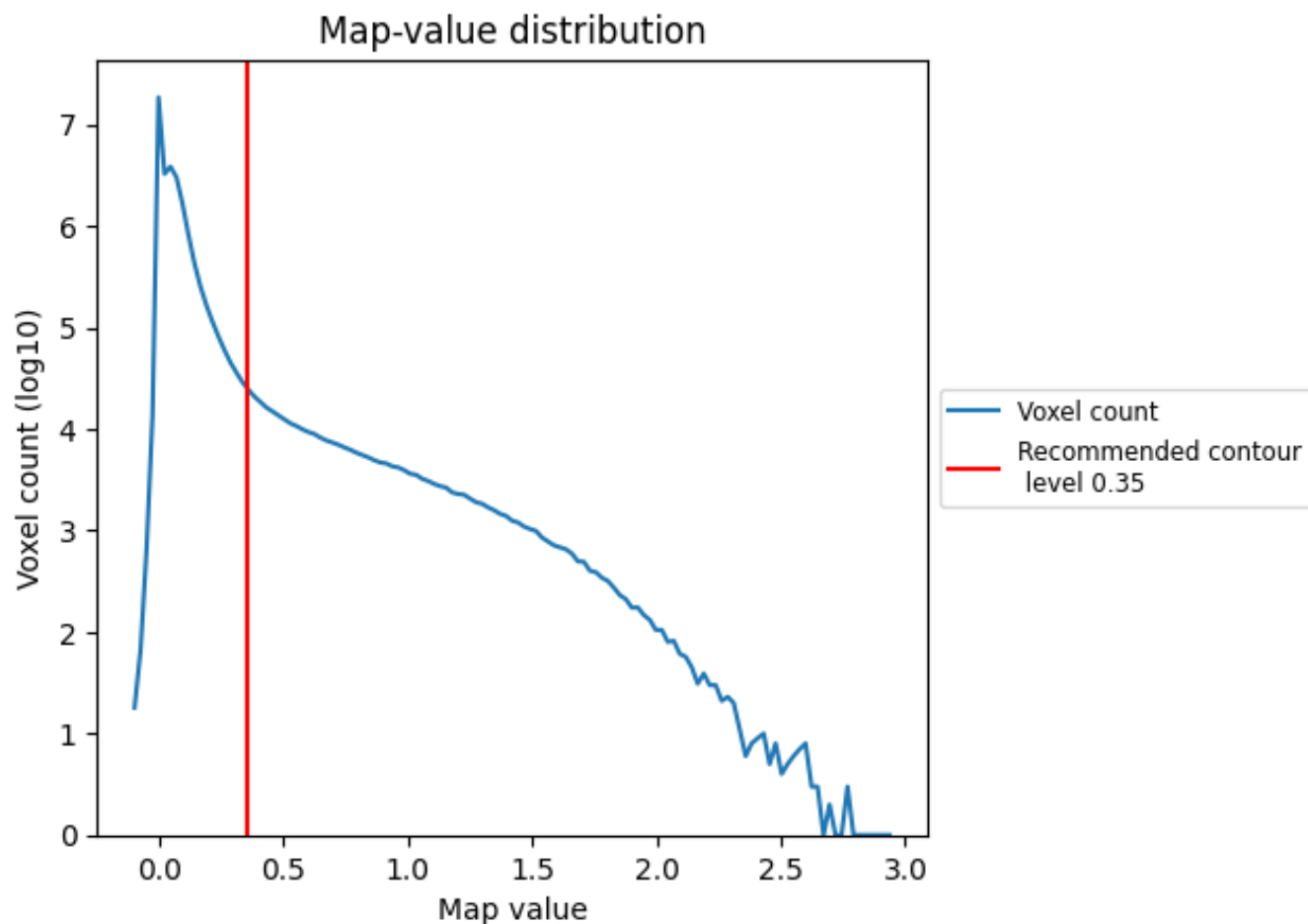
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

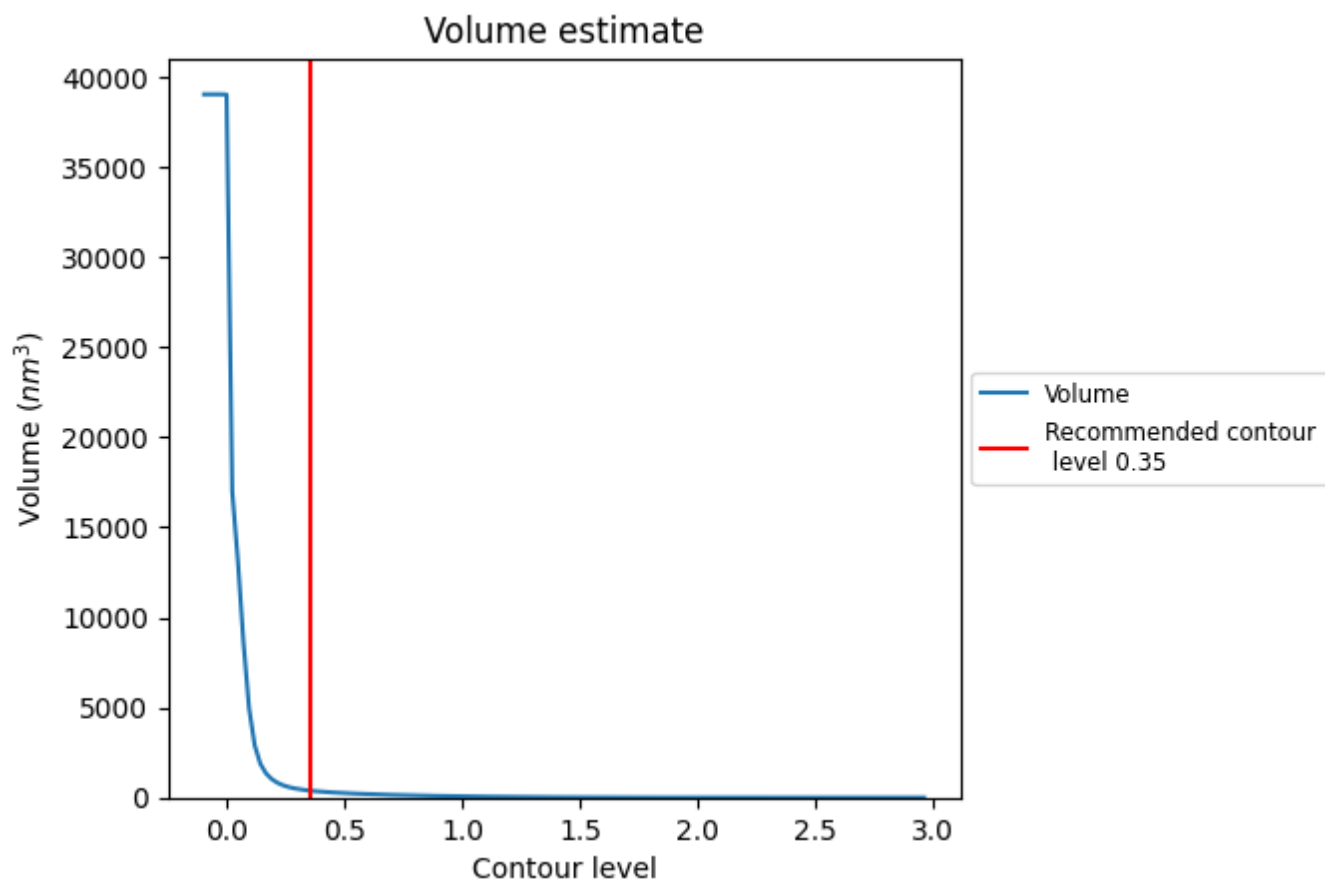
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

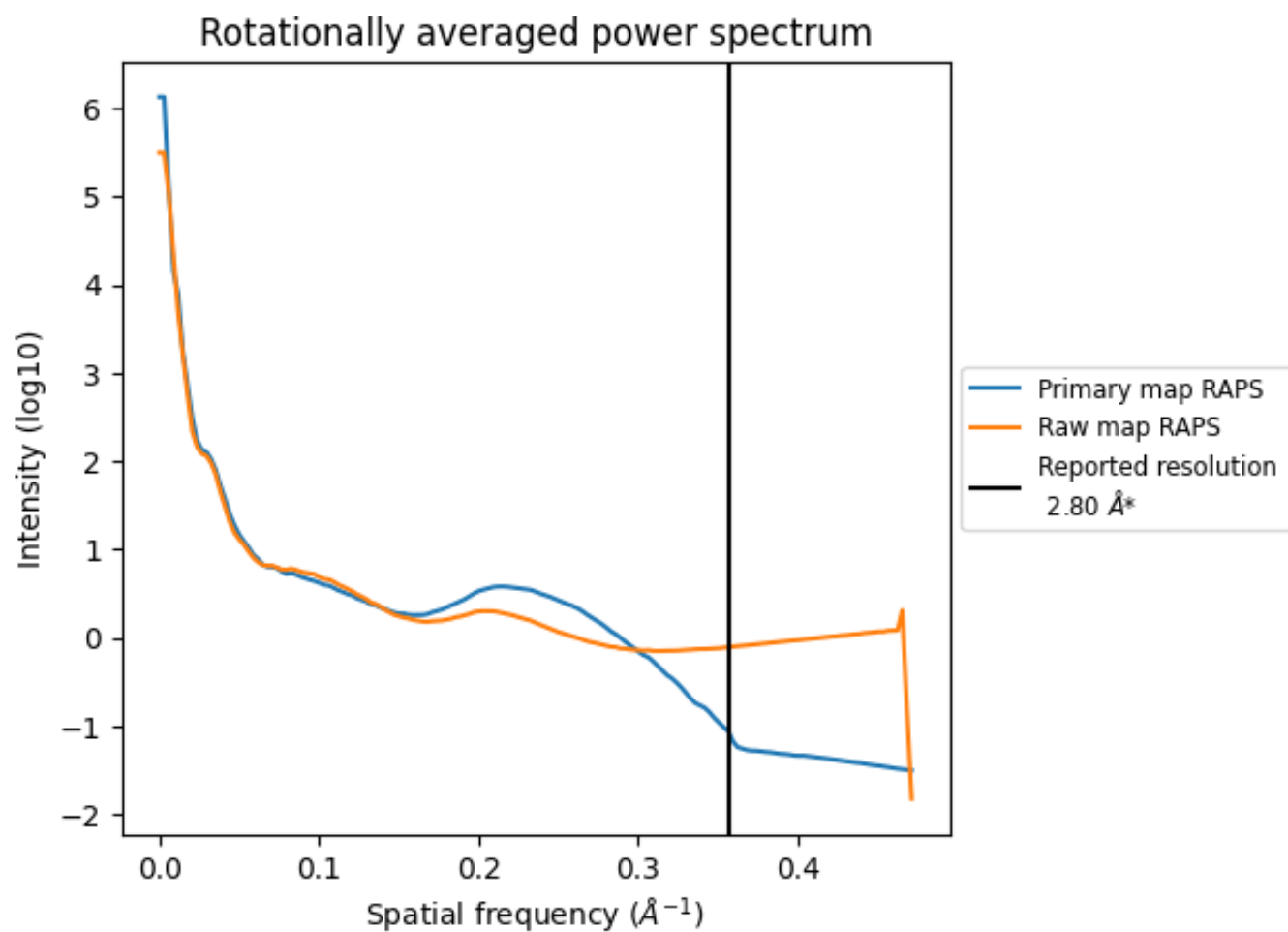
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm³; this corresponds to an approximate mass of 349 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

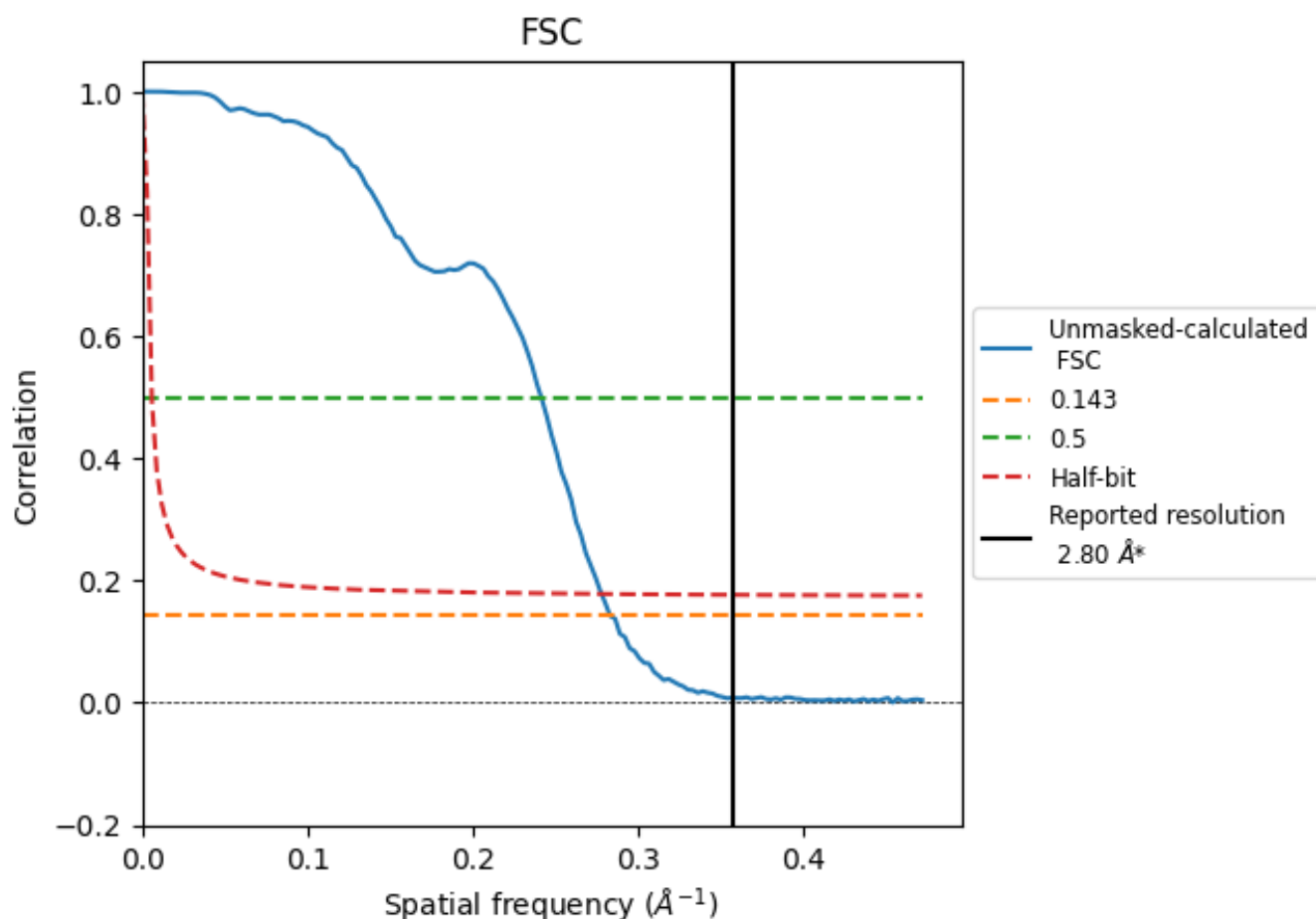


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

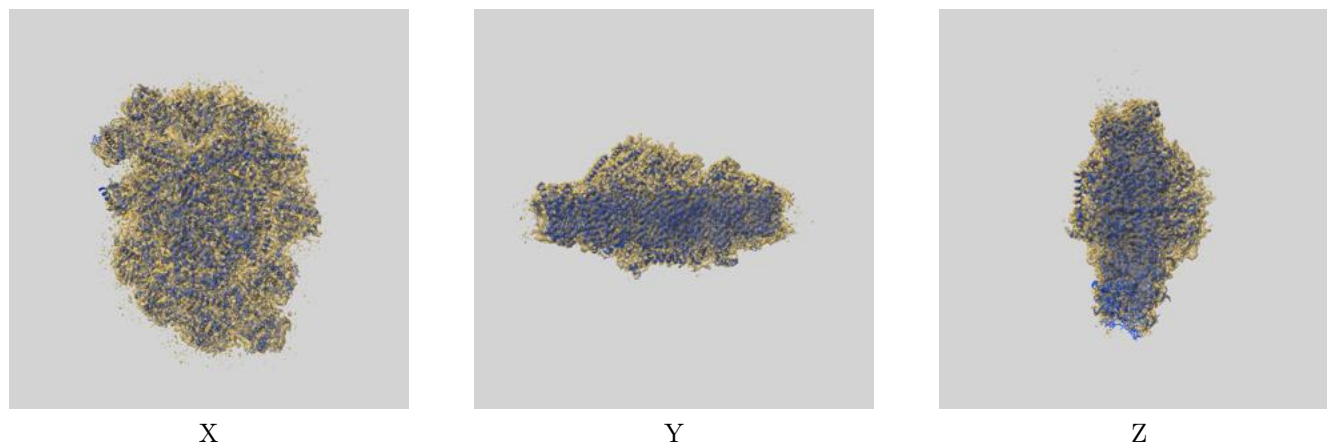
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.14	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

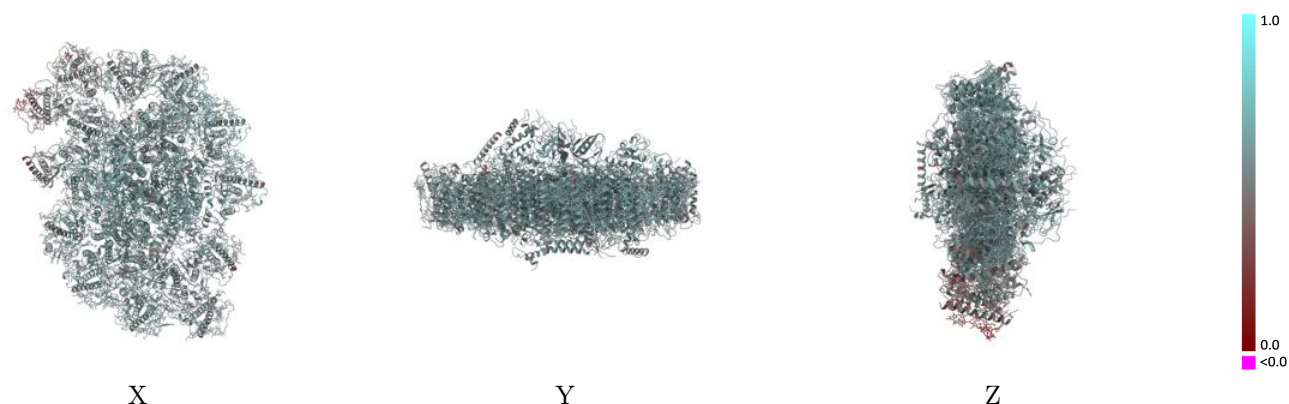
This section contains information regarding the fit between EMDB map EMD-36366 and PDB model 8JJR. Per-residue inclusion information can be found in [section 3](#) on [page 36](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

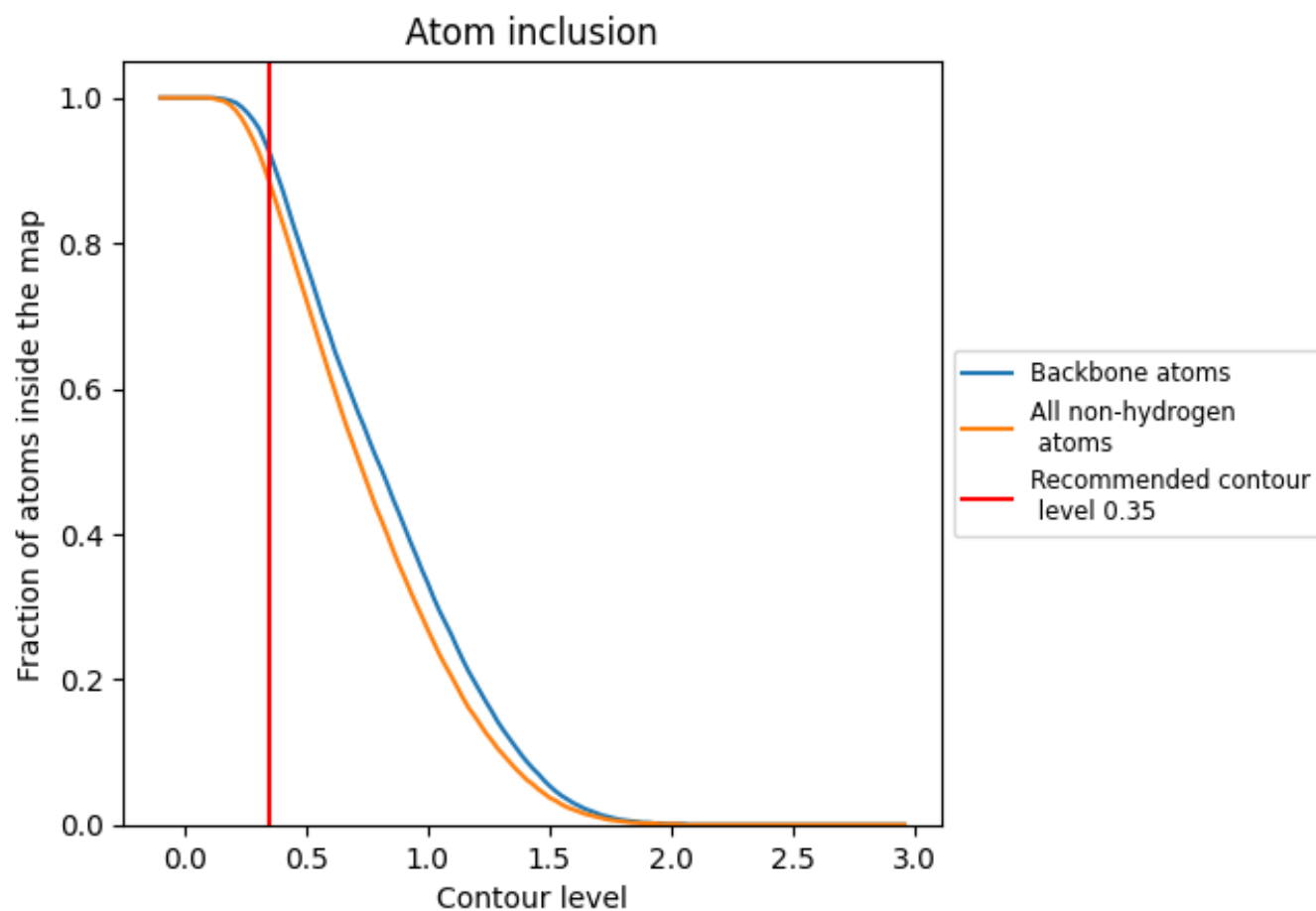


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5750
A	 0.8810	 0.5710
B	 0.9160	 0.5810
C	 0.8970	 0.5880
D	 0.9220	 0.6000
E	 0.9190	 0.5760
F	 0.8660	 0.5680
G	 0.8660	 0.5410
H	 0.9040	 0.5730
I	 0.8900	 0.5700
J	 0.8410	 0.5450
K	 0.6670	 0.4810
T	 0.6320	 0.4260
U	 0.6680	 0.4840
a	 0.9250	 0.6020
b	 0.9490	 0.6130
c	 0.9760	 0.6000
d	 0.9020	 0.5800
e	 0.9500	 0.6090
f	 0.8320	 0.5850
i	 0.8890	 0.5790
j	 0.8380	 0.5740
l	 0.9350	 0.6010
m	 0.9130	 0.6000
r	 0.9290	 0.5780
x	 0.9140	 0.5860
y	 0.7230	 0.5400

