



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 11:07 AM UTC

PDB ID : 9UEN / pdb_00009uen
EMDB ID : EMD-64087
Title : Cryo-EM structure of coccolithophore photosystem I
Authors : Zhao, L.S.; Sun, X.M.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2025-04-08
Resolution : 3.10 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:

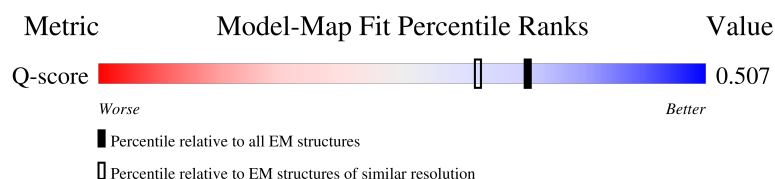
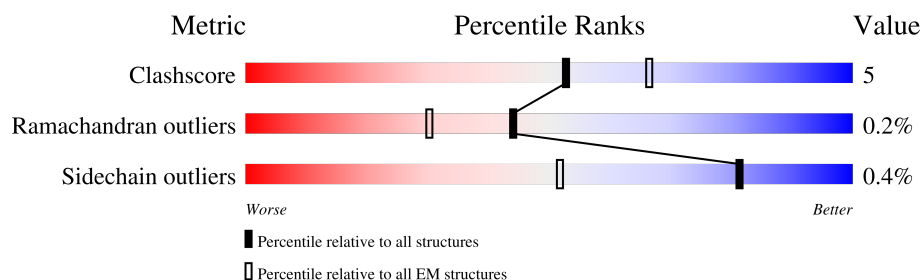
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	201	
2	B	219	
3	C	208	
4	D	255	

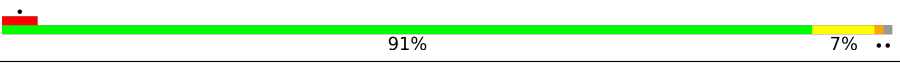
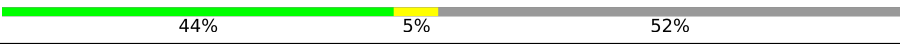
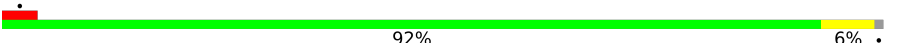
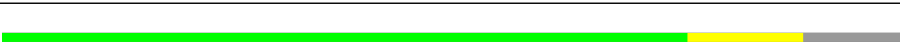
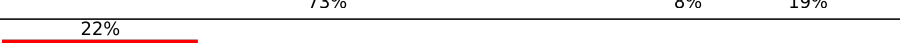
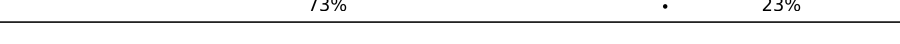
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Mol	Chain	Length	Quality of chain
5	E	217	
6	F	239	
7	G	198	
8	H	199	
9	I	196	
10	J	208	
11	K	204	
12	L	228	
13	M	224	
13	P	224	
13	W	224	
14	N	225	
15	O	210	
15	R	210	
15	T	210	
16	Q	187	
17	S	245	
18	U	198	
19	V	123	
20	X	253	
21	Y	244	
22	Z	254	
23	a	752	
24	b	734	
25	c	81	

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Mol	Chain	Length	Quality of chain
26	d	142	
27	e	131	
28	f	184	
29	i	36	
30	j	40	
31	k	112	
32	l	145	
33	m	30	
34	o	273	
35	p	255	
35	u	255	
35	x	255	
36	q	268	
36	v	268	
37	r	133	
38	t	260	
38	w	260	
38	y	260	
39	z	257	

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
40	CLA	A	301	X	-	-	-
40	CLA	A	302	X	-	-	-
40	CLA	A	303	X	-	-	-
40	CLA	A	304	X	-	-	-
40	CLA	A	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	A	306	X	-	-	-
40	CLA	A	307	X	-	-	-
40	CLA	A	308	X	-	-	-
40	CLA	A	309	X	-	-	-
40	CLA	A	311	X	-	-	-
40	CLA	B	301	X	-	-	-
40	CLA	B	302	X	-	-	-
40	CLA	B	303	X	-	-	-
40	CLA	B	304	X	-	-	-
40	CLA	B	306	X	-	-	-
40	CLA	B	307	X	-	-	-
40	CLA	C	301	X	-	-	-
40	CLA	C	302	X	-	-	-
40	CLA	C	304	X	-	-	-
40	CLA	C	305	X	-	-	-
40	CLA	C	306	X	-	-	-
40	CLA	C	307	X	-	-	-
40	CLA	C	308	X	-	-	-
40	CLA	C	309	X	-	-	-
40	CLA	D	301	X	-	-	-
40	CLA	D	302	X	-	-	-
40	CLA	D	303	X	-	-	-
40	CLA	D	304	X	-	-	-
40	CLA	D	305	X	-	-	-
40	CLA	D	306	X	-	-	-
40	CLA	D	307	X	-	-	-
40	CLA	D	308	X	-	-	-
40	CLA	D	309	X	-	-	-
40	CLA	D	310	X	-	-	-
40	CLA	D	311	X	-	-	-
40	CLA	D	312	X	-	-	-
40	CLA	E	302	X	-	-	-
40	CLA	E	303	X	-	-	-
40	CLA	E	304	X	-	-	-
40	CLA	E	305	X	-	-	-
40	CLA	E	306	X	-	-	-
40	CLA	E	307	X	-	-	-
40	CLA	E	308	X	-	-	-
40	CLA	E	309	X	-	-	-
40	CLA	E	310	X	-	-	-
40	CLA	E	311	X	-	-	-
40	CLA	E	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	E	313	X	-	-	-
40	CLA	E	314	X	-	-	-
40	CLA	F	301	X	-	-	-
40	CLA	F	303	X	-	-	-
40	CLA	F	304	X	-	-	-
40	CLA	F	305	X	-	-	-
40	CLA	F	306	X	-	-	-
40	CLA	F	307	X	-	-	-
40	CLA	F	308	X	-	-	-
40	CLA	F	310	X	-	-	-
40	CLA	F	311	X	-	-	-
40	CLA	F	321	X	-	-	-
40	CLA	G	201	X	-	-	-
40	CLA	G	203	X	-	-	-
40	CLA	G	204	X	-	-	-
40	CLA	G	205	X	-	-	-
40	CLA	G	206	X	-	-	-
40	CLA	G	207	X	-	-	-
40	CLA	G	213	X	-	-	-
40	CLA	H	301	X	-	-	-
40	CLA	H	302	X	-	-	-
40	CLA	H	304	X	-	-	-
40	CLA	H	305	X	-	-	-
40	CLA	H	306	X	-	-	-
40	CLA	H	307	X	-	-	-
40	CLA	H	308	X	-	-	-
40	CLA	H	309	X	-	-	-
40	CLA	H	310	X	-	-	-
40	CLA	H	311	X	-	-	-
40	CLA	I	201	X	-	-	-
40	CLA	I	202	X	-	-	-
40	CLA	I	203	X	-	-	-
40	CLA	I	204	X	-	-	-
40	CLA	I	205	X	-	-	-
40	CLA	I	206	X	-	-	-
40	CLA	I	207	X	-	-	-
40	CLA	I	208	X	-	-	-
40	CLA	J	302	X	-	-	-
40	CLA	J	303	X	-	-	-
40	CLA	J	305	X	-	-	-
40	CLA	J	306	X	-	-	-
40	CLA	J	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	J	308	X	-	-	-
40	CLA	J	309	X	-	-	-
40	CLA	J	310	X	-	-	-
40	CLA	J	311	X	-	-	-
40	CLA	J	312	X	-	-	-
40	CLA	J	318	X	-	-	-
40	CLA	K	301	X	-	-	-
40	CLA	K	304	X	-	-	-
40	CLA	K	306	X	-	-	-
40	CLA	K	307	X	-	-	-
40	CLA	K	308	X	-	-	-
40	CLA	K	312	X	-	-	-
40	CLA	L	301	X	-	-	-
40	CLA	L	304	X	-	-	-
40	CLA	L	305	X	-	-	-
40	CLA	L	306	X	-	-	-
40	CLA	L	307	X	-	-	-
40	CLA	L	310	X	-	-	-
40	CLA	L	311	X	-	-	-
40	CLA	L	312	X	-	-	-
40	CLA	M	304	X	-	-	-
40	CLA	M	305	X	-	-	-
40	CLA	M	306	X	-	-	-
40	CLA	M	307	X	-	-	-
40	CLA	M	310	X	-	-	-
40	CLA	M	311	X	-	-	-
40	CLA	M	312	X	-	-	-
40	CLA	N	304	X	-	-	-
40	CLA	N	305	X	-	-	-
40	CLA	N	306	X	-	-	-
40	CLA	N	307	X	-	-	-
40	CLA	N	310	X	-	-	-
40	CLA	N	311	X	-	-	-
40	CLA	O	304	X	-	-	-
40	CLA	O	305	X	-	-	-
40	CLA	O	306	X	-	-	-
40	CLA	O	307	X	-	-	-
40	CLA	O	310	X	-	-	-
40	CLA	O	316	X	-	-	-
40	CLA	P	305	X	-	-	-
40	CLA	P	306	X	-	-	-
40	CLA	P	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	P	308	X	-	-	-
40	CLA	P	311	X	-	-	-
40	CLA	P	312	X	-	-	-
40	CLA	P	313	X	-	-	-
40	CLA	Q	202	X	-	-	-
40	CLA	Q	203	X	-	-	-
40	CLA	Q	204	X	-	-	-
40	CLA	Q	205	X	-	-	-
40	CLA	Q	206	X	-	-	-
40	CLA	Q	207	X	-	-	-
40	CLA	Q	208	X	-	-	-
40	CLA	Q	209	X	-	-	-
40	CLA	R	304	X	-	-	-
40	CLA	R	305	X	-	-	-
40	CLA	R	306	X	-	-	-
40	CLA	R	307	X	-	-	-
40	CLA	R	310	X	-	-	-
40	CLA	R	316	X	-	-	-
40	CLA	S	301	X	-	-	-
40	CLA	S	302	X	-	-	-
40	CLA	S	305	X	-	-	-
40	CLA	S	306	X	-	-	-
40	CLA	S	307	X	-	-	-
40	CLA	S	308	X	-	-	-
40	CLA	S	311	X	-	-	-
40	CLA	S	312	X	-	-	-
40	CLA	S	313	X	-	-	-
40	CLA	S	314	X	-	-	-
40	CLA	S	319	X	-	-	-
40	CLA	T	304	X	-	-	-
40	CLA	T	305	X	-	-	-
40	CLA	T	306	X	-	-	-
40	CLA	T	307	X	-	-	-
40	CLA	T	310	X	-	-	-
40	CLA	T	317	X	-	-	-
40	CLA	U	202	X	-	-	-
40	CLA	U	203	X	-	-	-
40	CLA	U	204	X	-	-	-
40	CLA	U	205	X	-	-	-
40	CLA	U	206	X	-	-	-
40	CLA	U	207	X	-	-	-
40	CLA	U	208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	V	201	X	-	-	-
40	CLA	V	202	X	-	-	-
40	CLA	W	305	X	-	-	-
40	CLA	W	306	X	-	-	-
40	CLA	W	307	X	-	-	-
40	CLA	W	308	X	-	-	-
40	CLA	W	311	X	-	-	-
40	CLA	W	312	X	-	-	-
40	CLA	W	313	X	-	-	-
40	CLA	X	301	X	-	-	-
40	CLA	X	304	X	-	-	-
40	CLA	X	305	X	-	-	-
40	CLA	X	306	X	-	-	-
40	CLA	X	307	X	-	-	-
40	CLA	X	310	X	-	-	-
40	CLA	X	311	X	-	-	-
40	CLA	X	312	X	-	-	-
40	CLA	X	313	X	-	-	-
40	CLA	Y	301	X	-	-	-
40	CLA	Y	304	X	-	-	-
40	CLA	Y	305	X	-	-	-
40	CLA	Y	306	X	-	-	-
40	CLA	Y	307	X	-	-	-
40	CLA	Y	310	X	-	-	-
40	CLA	Y	311	X	-	-	-
40	CLA	Y	312	X	-	-	-
40	CLA	Y	313	X	-	-	-
40	CLA	Z	301	X	-	-	-
40	CLA	Z	304	X	-	-	-
40	CLA	Z	305	X	-	-	-
40	CLA	Z	306	X	-	-	-
40	CLA	Z	307	X	-	-	-
40	CLA	Z	310	X	-	-	-
40	CLA	Z	311	X	-	-	-
40	CLA	Z	312	X	-	-	-
40	CLA	Z	313	X	-	-	-
40	CLA	a	803	X	-	-	-
40	CLA	a	804	X	-	-	-
40	CLA	a	805	X	-	-	-
40	CLA	a	806	X	-	-	-
40	CLA	a	807	X	-	-	-
40	CLA	a	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	a	809	X	-	-	-
40	CLA	a	810	X	-	-	-
40	CLA	a	811	X	-	-	-
40	CLA	a	812	X	-	-	-
40	CLA	a	813	X	-	-	-
40	CLA	a	814	X	-	-	-
40	CLA	a	815	X	-	-	-
40	CLA	a	816	X	-	-	-
40	CLA	a	817	X	-	-	-
40	CLA	a	818	X	-	-	-
40	CLA	a	819	X	-	X	-
40	CLA	a	820	X	-	-	-
40	CLA	a	821	X	-	-	-
40	CLA	a	822	X	-	-	-
40	CLA	a	823	X	-	-	-
40	CLA	a	824	X	-	-	-
40	CLA	a	825	X	-	-	-
40	CLA	a	826	X	-	-	-
40	CLA	a	827	X	-	-	-
40	CLA	a	828	X	-	-	-
40	CLA	a	829	X	-	-	-
40	CLA	a	830	X	-	-	-
40	CLA	a	831	X	-	-	-
40	CLA	a	832	X	-	-	-
40	CLA	a	833	X	-	-	-
40	CLA	a	834	X	-	-	-
40	CLA	a	835	X	-	-	-
40	CLA	a	836	X	-	-	-
40	CLA	a	837	X	-	-	-
40	CLA	a	838	X	-	-	-
40	CLA	a	839	X	-	-	-
40	CLA	a	840	X	-	-	-
40	CLA	a	841	X	-	-	-
40	CLA	a	842	X	-	-	-
40	CLA	a	850	X	-	-	-
40	CLA	a	851	X	-	-	-
40	CLA	a	852	X	-	-	-
40	CLA	b	801	X	-	-	-
40	CLA	b	802	X	-	-	-
40	CLA	b	803	X	-	-	-
40	CLA	b	805	X	-	-	-
40	CLA	b	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	b	807	X	-	-	-
40	CLA	b	808	X	-	-	-
40	CLA	b	809	X	-	-	-
40	CLA	b	810	X	-	-	-
40	CLA	b	811	X	-	-	-
40	CLA	b	812	X	-	-	-
40	CLA	b	813	X	-	-	-
40	CLA	b	814	X	-	-	-
40	CLA	b	815	X	-	-	-
40	CLA	b	816	X	-	-	-
40	CLA	b	817	X	-	-	-
40	CLA	b	818	X	-	-	-
40	CLA	b	819	X	-	-	-
40	CLA	b	820	X	-	-	-
40	CLA	b	821	X	-	-	-
40	CLA	b	822	X	-	-	-
40	CLA	b	823	X	-	-	-
40	CLA	b	824	X	-	-	-
40	CLA	b	825	X	-	-	-
40	CLA	b	826	X	-	-	-
40	CLA	b	827	X	-	-	-
40	CLA	b	828	X	-	-	-
40	CLA	b	829	X	-	-	-
40	CLA	b	830	X	-	-	-
40	CLA	b	831	X	-	-	-
40	CLA	b	832	X	-	-	-
40	CLA	b	833	X	-	-	-
40	CLA	b	834	X	-	-	-
40	CLA	b	835	X	-	-	-
40	CLA	b	836	X	-	-	-
40	CLA	b	837	X	-	-	-
40	CLA	b	838	X	-	-	-
40	CLA	b	839	X	-	-	-
40	CLA	b	840	X	-	-	-
40	CLA	b	841	X	-	-	-
40	CLA	b	842	X	-	-	-
40	CLA	f	201	X	-	-	-
40	CLA	f	202	X	-	-	-
40	CLA	f	204	X	-	-	-
40	CLA	f	205	X	-	-	-
40	CLA	i	101	X	-	-	-
40	CLA	j	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	k	201	X	-	-	-
40	CLA	k	202	X	-	-	-
40	CLA	l	202	X	-	-	-
40	CLA	l	203	X	-	-	-
40	CLA	l	204	X	-	-	-
40	CLA	l	205	X	-	-	-
40	CLA	o	301	X	-	-	-
40	CLA	o	304	X	-	-	-
40	CLA	o	305	X	-	-	-
40	CLA	o	306	X	-	-	-
40	CLA	o	307	X	-	-	-
40	CLA	o	310	X	-	-	-
40	CLA	o	311	X	-	-	-
40	CLA	o	312	X	-	-	-
40	CLA	o	313	X	-	-	-
40	CLA	p	302	X	-	-	-
40	CLA	p	305	X	-	-	-
40	CLA	p	306	X	-	-	-
40	CLA	p	307	X	-	-	-
40	CLA	p	308	X	-	-	-
40	CLA	p	311	X	-	-	-
40	CLA	p	312	X	-	-	-
40	CLA	p	313	X	-	-	-
40	CLA	p	314	X	-	-	-
40	CLA	q	301	X	-	-	-
40	CLA	q	304	X	-	-	-
40	CLA	q	305	X	-	-	-
40	CLA	q	306	X	-	-	-
40	CLA	q	307	X	-	-	-
40	CLA	q	310	X	-	-	-
40	CLA	q	311	X	-	-	-
40	CLA	q	312	X	-	-	-
40	CLA	q	313	X	-	-	-
40	CLA	t	302	X	-	-	-
40	CLA	t	303	X	-	-	-
40	CLA	t	304	X	-	-	-
40	CLA	t	305	X	-	-	-
40	CLA	t	307	X	-	-	-
40	CLA	t	309	X	-	-	-
40	CLA	u	302	X	-	-	-
40	CLA	u	305	X	-	-	-
40	CLA	u	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	u	307	X	-	-	-
40	CLA	u	308	X	-	-	-
40	CLA	u	311	X	-	-	-
40	CLA	u	312	X	-	-	-
40	CLA	u	313	X	-	-	-
40	CLA	u	314	X	-	-	-
40	CLA	v	301	X	-	-	-
40	CLA	v	304	X	-	-	-
40	CLA	v	305	X	-	-	-
40	CLA	v	306	X	-	-	-
40	CLA	v	307	X	-	-	-
40	CLA	v	310	X	-	-	-
40	CLA	v	311	X	-	-	-
40	CLA	v	312	X	-	-	-
40	CLA	v	313	X	-	-	-
40	CLA	w	302	X	-	-	-
40	CLA	w	303	X	-	-	-
40	CLA	w	304	X	-	-	-
40	CLA	w	305	X	-	-	-
40	CLA	w	308	X	-	-	-
40	CLA	w	309	X	-	-	-
40	CLA	x	302	X	-	-	-
40	CLA	x	305	X	-	-	-
40	CLA	x	306	X	-	-	-
40	CLA	x	307	X	-	-	-
40	CLA	x	308	X	-	-	-
40	CLA	x	311	X	-	-	-
40	CLA	x	312	X	-	-	-
40	CLA	x	313	X	-	-	-
40	CLA	x	314	X	-	-	-
40	CLA	y	302	X	-	-	-
40	CLA	y	303	X	-	-	-
40	CLA	y	304	X	-	-	-
40	CLA	y	305	X	-	-	-
40	CLA	y	308	X	-	-	-
40	CLA	y	309	X	-	-	-
40	CLA	z	302	X	-	-	-
40	CLA	z	305	X	-	-	-
40	CLA	z	306	X	-	-	-
40	CLA	z	307	X	-	-	-
40	CLA	z	308	X	-	-	-
40	CLA	z	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	z	312	X	-	-	-
40	CLA	z	313	X	-	-	-
40	CLA	z	314	X	-	-	-
40	CLA	z	324	X	-	-	-
42	DD6	P	315	X	-	-	-
42	DD6	t	312	-	-	X	-
42	DD6	w	312	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 110086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	183	Total	C	N	O	S	0	0
			1419	916	229	264	10		

- Molecule 2 is a protein called EFCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	148	Total	C	N	O	S	0	0
			1108	711	186	205	6		

- Molecule 3 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1352	874	225	244	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	103	ALA	VAL	conflict	UNP A0A6V2SE28
C	104	GLU	ASP	conflict	UNP A0A6V2SE28

- Molecule 4 is a protein called EFCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	188	Total	C	N	O	S	1	0
			1446	943	232	265	6		

- Molecule 5 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	187	Total	C	N	O	S	0	0
			1383	896	222	257	8		

- Molecule 6 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	188	Total	C	N	O	S	0	0
			1414	909	244	252	9		

- Molecule 7 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	168	Total	C	N	O	S	0	0
			1248	803	206	231	8		

- Molecule 8 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	S	0	0
			1251	802	205	232	12		

- Molecule 9 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	155	Total	C	N	O	S	0	0
			1195	773	199	214	9		

- Molecule 10 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	166	Total	C	N	O	S	0	0
			1231	783	216	225	7		

- Molecule 11 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	171	Total	C	N	O	S	0	0
			1333	868	226	232	7		

- Molecule 12 is a protein called EFCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	189	Total	C	N	O	S	0	0
			1419	927	236	250	6		

- Molecule 13 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
13	P	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
13	W	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		

- Molecule 14 is a protein called EFCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	194	Total	C	N	O	S	0	0
			1454	943	245	257	9		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		
15	R	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		
15	T	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		

- Molecule 16 is a protein called EFCPI-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	156	Total	C	N	O	S	0	0
			1192	763	202	219	8		

- Molecule 17 is a protein called EFCPI-22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	210	Total	C	N	O	S	0	0
			1640	1082	264	288	6		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	144	Total	C	N	O	S	0	0
			1130	728	190	206	6		

- Molecule 19 is a protein called LEFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	47	Total	C	N	O	S	0	0
			351	225	59	65	2		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	211	Total	C	N	O	S	0	0
			1643	1069	273	294	7		

- Molecule 21 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	213	Total	C	N	O	S	0	0
			1660	1090	278	284	8		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	219	Total	C	N	O	S	0	0
			1714	1121	279	309	5		

- Molecule 23 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	741	Total	C	N	O	S	0	0
			5832	3815	993	994	30		

- Molecule 24 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	731	Total	C	N	O	S	0	0
			5807	3822	980	984	21		

- Molecule 25 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	80	Total	C	N	O	S	0	0
			597	365	105	116	11		

- Molecule 26 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	140	Total	C	N	O	S	0	0
			1103	710	184	206	3		

- Molecule 27 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	63	Total	C	N	O	S	0	0
			493	313	86	93	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	81	ALA	PRO	conflict	UNP R1EZZ6
e	85	THR	PRO	conflict	UNP R1EZZ6

- Molecule 28 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	161	Total	C	N	O	S	0	0
			1238	800	210	224	4		

- Molecule 29 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	31	Total	C	N	O	S	0	0
			243	170	32	40	1		

- Molecule 30 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	40	Total	C	N	O	S	0	0
			317	211	47	56	3		

- Molecule 31 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	70	Total	C	N	O	S	0	0
			510	331	83	90	6		

- Molecule 32 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	143	Total	C	N	O	S	0	0
			1084	716	172	195	1		

- Molecule 33 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	30	Total	C	N	O	S	0	0
			224	149	35	38	2		

- Molecule 34 is a protein called EFCPI-30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	236	Total	C	N	O	S	0	0
			1760	1142	290	318	10		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
35	u	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
35	x	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	238	Total	C	N	O	S	0	0
			1790	1163	296	323	8		
36	v	238	Total	C	N	O	S	0	0
			1790	1163	296	323	8		

- Molecule 37 is a protein called Psar.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	91	Total	C	N	O	S	0	0
			681	443	111	126	1		

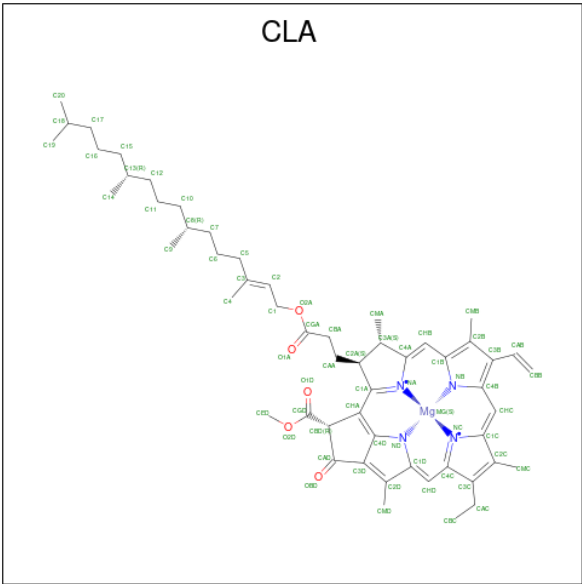
- Molecule 38 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	211	Total	C	N	O	S	0	0
			1631	1057	272	295	7		
38	w	211	Total	C	N	O	S	0	0
			1631	1057	272	295	7		
38	y	201	Total	C	N	O	S	0	0
			1546	1001	261	277	7		

- Molecule 39 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	z	222	Total	C	N	O	S	0	0
			1718	1126	280	307	5		

- Molecule 40 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
40	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	D	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	D	1	Total 44	C 35	Mg 1	N 4	O 4	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	D	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	E	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 53	C 43	Mg 1	N 4	O 5	0
40	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	F	1	Total 59	C 49	Mg 1	N 4	O 5	0
40	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	I	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	I	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	I	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	J	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	K	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	K	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	K	1	Total 59	C 49	Mg 1	N 4	O 5	0
40	K	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	M	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	M	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	M	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	P	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Q	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	Q	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	R	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	S	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	T	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	T	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	U	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	U	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	U	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	U	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	U	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	V	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	X	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	Z	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	Z	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Z	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	b	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
40	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	j	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	l	1	Total 64	C 54	Mg 1	N 4	O 5	0
40	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	o	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	p	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	q	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	q	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	t	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	t	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	t	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	t	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	u	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	u	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	u	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	v	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	v	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	w	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	w	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 55	C 45	Mg 1	N 4	O 5	0

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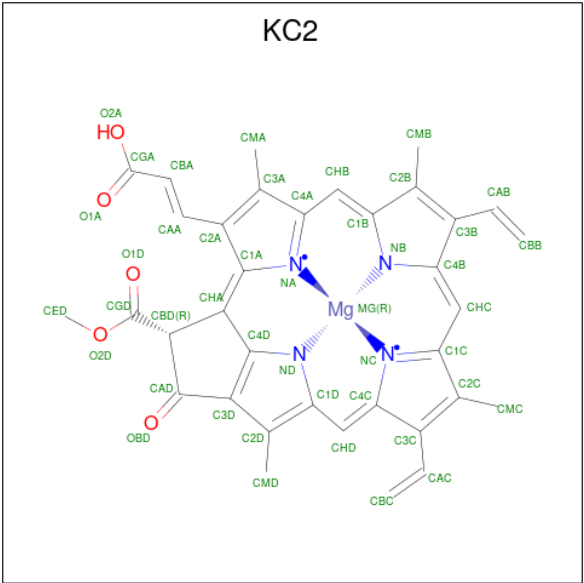
Mol	Chain	Residues	Atoms					AltConf
40	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	x	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	x	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	y	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 41 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0

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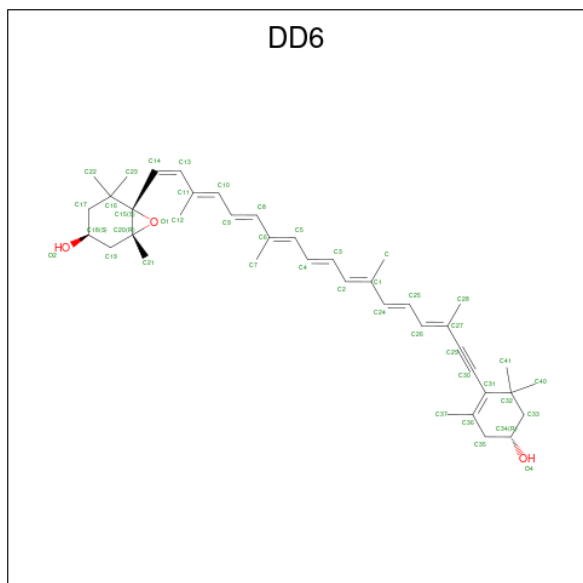
Mol	Chain	Residues	Atoms					AltConf
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	x	1	Total 45	C 35	Mg 1	N 4	O 5	0

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

- Molecule 42 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: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	C	O	0
			43	40	3	

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

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Mol	Chain	Residues	Atoms			AltConf
42	H	1	Total 43	C 40	O 3	0
42	H	1	Total 43	C 40	O 3	0
42	H	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	K	1	Total 43	C 40	O 3	0
42	K	1	Total 43	C 40	O 3	0
42	L	1	Total 43	C 40	O 3	0
42	L	1	Total 43	C 40	O 3	0
42	M	1	Total 43	C 40	O 3	0
42	N	1	Total 43	C 40	O 3	0
42	N	1	Total 43	C 40	O 3	0
42	N	1	Total 43	C 40	O 3	0

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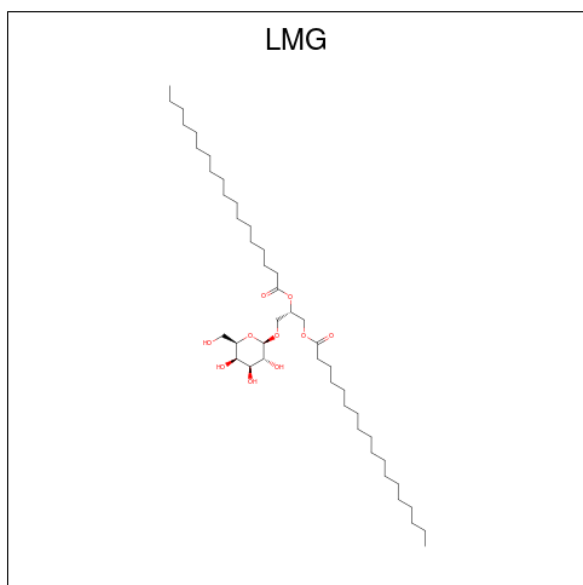
Mol	Chain	Residues	Atoms			AltConf
42	O	1	Total 43	C 40	O 3	0
42	P	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	R	1	Total 43	C 40	O 3	0
42	T	1	Total 43	C 40	O 3	0
42	U	1	Total 43	C 40	O 3	0
42	U	1	Total 43	C 40	O 3	0
42	W	1	Total 43	C 40	O 3	0
42	X	1	Total 43	C 40	O 3	0
42	Y	1	Total 43	C 40	O 3	0
42	Z	1	Total 43	C 40	O 3	0
42	j	1	Total 43	C 40	O 3	0
42	k	1	Total 43	C 40	O 3	0
42	o	1	Total 43	C 40	O 3	0
42	o	1	Total 43	C 40	O 3	0
42	p	1	Total 43	C 40	O 3	0
42	q	1	Total 43	C 40	O 3	0
42	q	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
42	t	1	Total	C	O	0
			43	40	3	
42	u	1	Total	C	O	0
			43	40	3	
42	v	1	Total	C	O	0
			43	40	3	
42	v	1	Total	C	O	0
			43	40	3	
42	w	1	Total	C	O	0
			43	40	3	
42	x	1	Total	C	O	0
			43	40	3	
42	y	1	Total	C	O	0
			43	40	3	
42	z	1	Total	C	O	0
			43	40	3	
42	z	1	Total	C	O	0
			43	40	3	

- Molecule 43 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



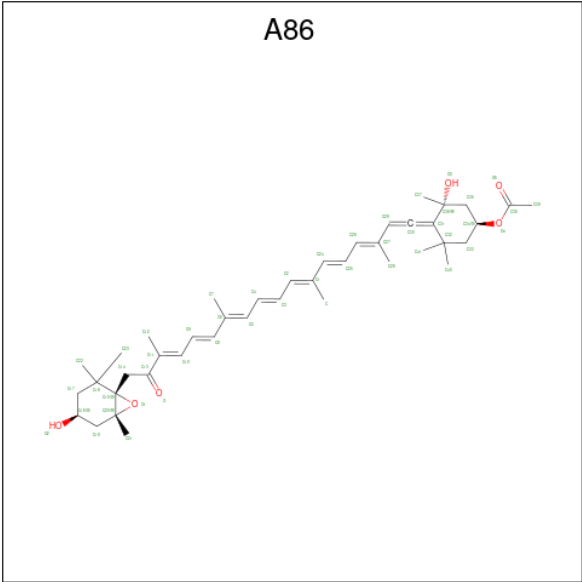
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			40	30	10	
43	D	1	Total	C	O	0
			40	30	10	

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Mol	Chain	Residues	Atoms			AltConf
43	E	1	Total	C	O	0
			31	21	10	
43	E	1	Total	C	O	0
			31	21	10	
43	E	1	Total	C	O	0
			40	30	10	
43	F	1	Total	C	O	0
			39	29	10	
43	L	1	Total	C	O	0
			37	27	10	
43	M	1	Total	C	O	0
			39	29	10	
43	P	1	Total	C	O	0
			39	29	10	
43	S	1	Total	C	O	0
			39	29	10	
43	T	1	Total	C	O	0
			40	30	10	
43	W	1	Total	C	O	0
			39	29	10	
43	a	1	Total	C	O	0
			35	25	10	
43	a	1	Total	C	O	0
			35	25	10	
43	j	1	Total	C	O	0
			30	20	10	
43	l	1	Total	C	O	0
			39	29	10	
43	p	1	Total	C	O	0
			39	29	10	
43	u	1	Total	C	O	0
			39	29	10	
43	x	1	Total	C	O	0
			39	29	10	

- Molecule 44 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
44	C	1	Total	C	O	0
			48	42	6	
44	D	1	Total	C	O	0
			48	42	6	
44	D	1	Total	C	O	0
			48	42	6	
44	F	1	Total	C	O	0
			48	42	6	
44	F	1	Total	C	O	0
			48	42	6	
44	F	1	Total	C	O	0
			48	42	6	
44	G	1	Total	C	O	0
			48	42	6	
44	G	1	Total	C	O	0
			48	42	6	
44	H	1	Total	C	O	0
			48	42	6	
44	K	1	Total	C	O	0
			48	42	6	
44	L	1	Total	C	O	0
			48	42	6	
44	M	1	Total	C	O	0
			48	42	6	
44	M	1	Total	C	O	0
			48	42	6	
44	M	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
44	M	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	O	1	Total	C	O	0
			48	42	6	
44	O	1	Total	C	O	0
			48	42	6	
44	O	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	Q	1	Total	C	O	0
			48	42	6	
44	Q	1	Total	C	O	0
			48	42	6	
44	R	1	Total	C	O	0
			48	42	6	
44	R	1	Total	C	O	0
			48	42	6	
44	R	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
44	T	1	Total	C	O	0
			48	42	6	
44	T	1	Total	C	O	0
			48	42	6	
44	T	1	Total	C	O	0
			48	42	6	
44	T	1	Total	C	O	0
			48	42	6	
44	U	1	Total	C	O	0
			48	42	6	
44	W	1	Total	C	O	0
			48	42	6	
44	W	1	Total	C	O	0
			48	42	6	
44	W	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	

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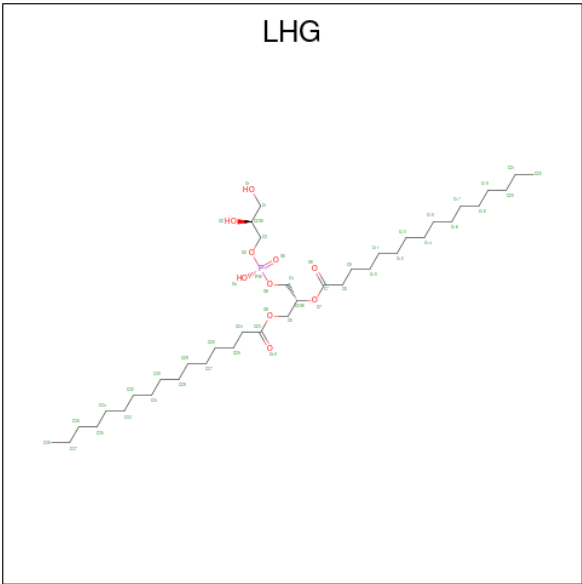
Mol	Chain	Residues	Atoms			AltConf
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	

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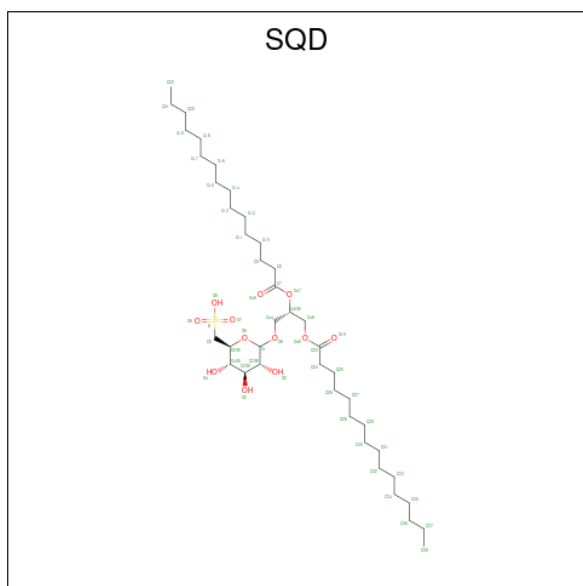
Mol	Chain	Residues	Atoms			AltConf
44	x	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	
44	y	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	

- Molecule 45 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
45	F	1	Total	C	O	P	0
			40	29	10	1	
45	S	1	Total	C	O	P	0
			40	29	10	1	
45	a	1	Total	C	O	P	0
			48	37	10	1	
45	a	1	Total	C	O	P	0
			30	19	10	1	

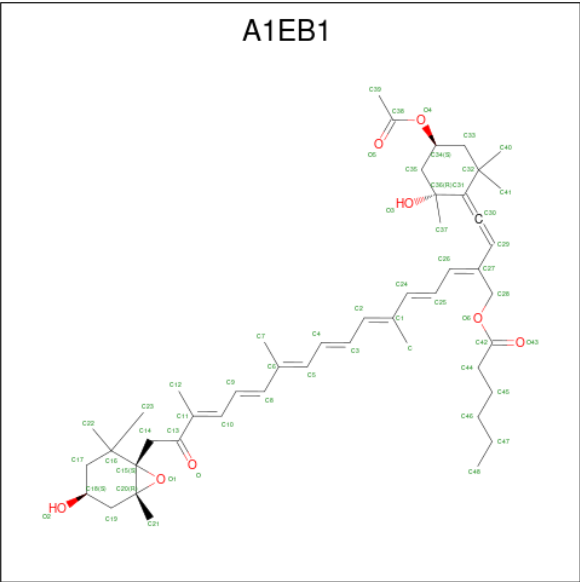
- Molecule 46 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
46	F	1	Total	C	O	S	0
			36	23	12	1	
46	I	1	Total	C	O	S	0
			54	41	12	1	
46	M	1	Total	C	O	S	0
			32	19	12	1	
46	P	1	Total	C	O	S	0
			32	19	12	1	
46	W	1	Total	C	O	S	0
			32	19	12	1	
46	k	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 47 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acety

loxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]ethenyl]-6,11,15-trimethyl-16-oxidanylidene-17-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]heptadeca-2,4,6,8,10,12,14-heptaenyl] hexanoate (CCD ID: A1EB1) (formula: C₄₈H₆₈O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
47	F	1	Total	C	O	0
			56	48	8	
47	G	1	Total	C	O	0
			56	48	8	
47	K	1	Total	C	O	0
			56	48	8	
47	K	1	Total	C	O	0
			56	48	8	
47	L	1	Total	C	O	0
			56	48	8	
47	L	1	Total	C	O	0
			56	48	8	
47	N	1	Total	C	O	0
			56	48	8	
47	O	1	Total	C	O	0
			56	48	8	
47	P	1	Total	C	O	0
			56	48	8	
47	R	1	Total	C	O	0
			56	48	8	
47	S	1	Total	C	O	0
			56	48	8	

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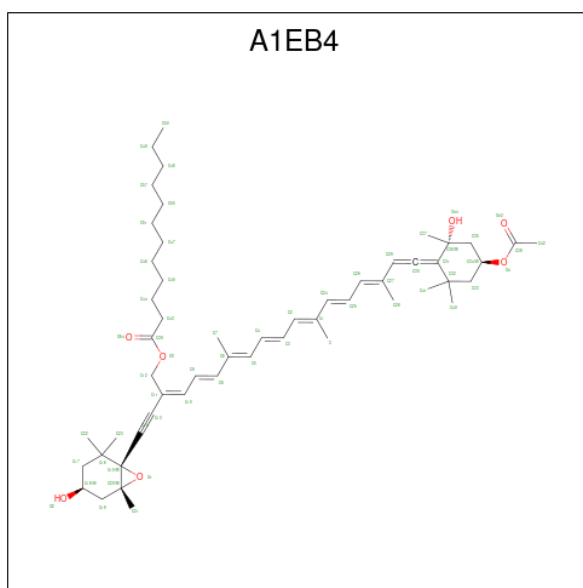
Mol	Chain	Residues	Atoms			AltConf
47	S	1	Total	C	O	0
			56	48	8	
47	T	1	Total	C	O	0
			56	48	8	
47	T	1	Total	C	O	0
			56	48	8	
47	Y	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	o	1	Total	C	O	0
			56	48	8	
47	o	1	Total	C	O	0
			56	48	8	
47	p	1	Total	C	O	0
			56	48	8	
47	p	1	Total	C	O	0
			56	48	8	
47	q	1	Total	C	O	0
			56	48	8	
47	q	1	Total	C	O	0
			56	48	8	
47	q	1	Total	C	O	0
			56	48	8	
47	t	1	Total	C	O	0
			56	48	8	
47	t	1	Total	C	O	0
			56	48	8	
47	t	1	Total	C	O	0
			56	48	8	
47	u	1	Total	C	O	0
			56	48	8	
47	u	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	

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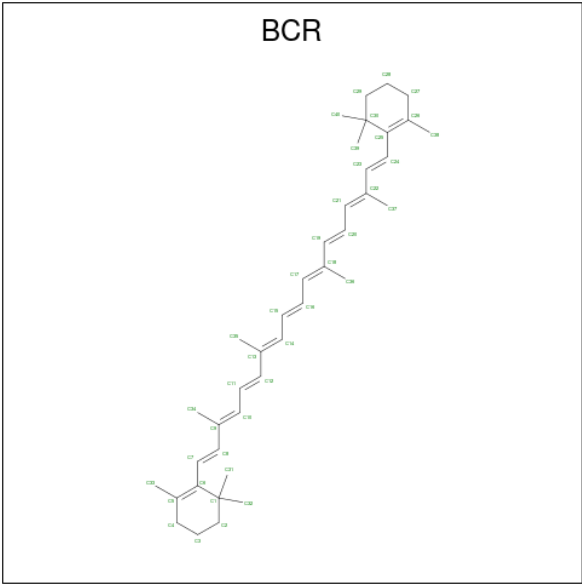
Mol	Chain	Residues	Atoms			AltConf
47	v	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	
47	w	1	Total	C	O	0
			56	48	8	
47	w	1	Total	C	O	0
			56	48	8	
47	x	1	Total	C	O	0
			56	48	8	
47	x	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	z	1	Total	C	O	0
			56	48	8	

- Molecule 48 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[2-[(1 {R},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethynyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] dodecanoate (CCD ID: A1EB4) (formula: C₅₄H₇₈O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
48	M	1	Total	C	O	0
			56	49	7	
48	P	1	Total	C	O	0
			56	49	7	
48	W	1	Total	C	O	0
			56	49	7	

- Molecule 49 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



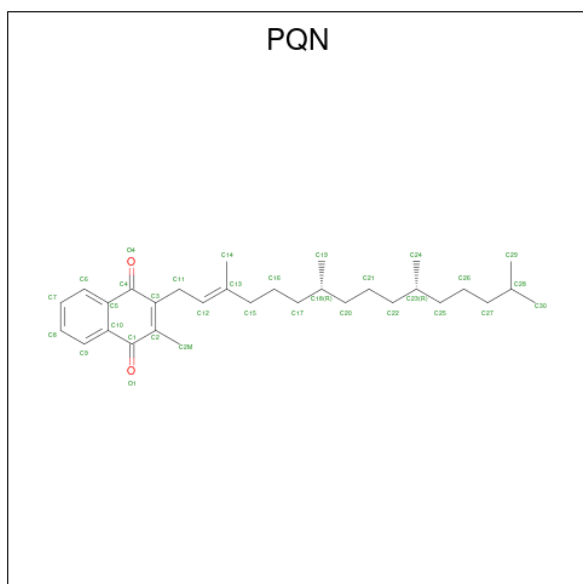
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	

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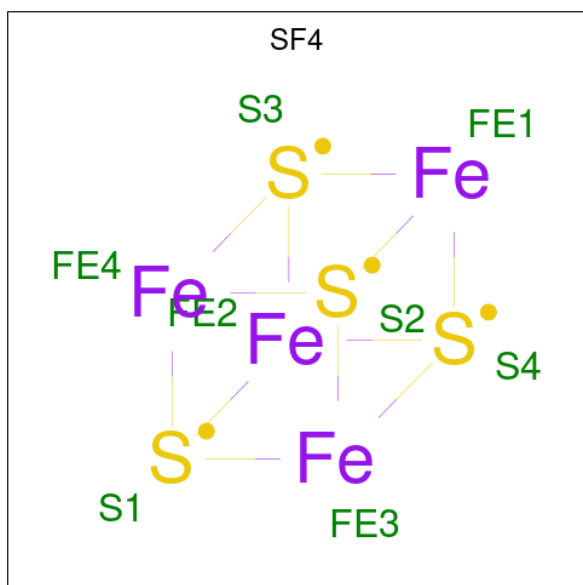
Mol	Chain	Residues	Atoms	AltConf
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	i	1	Total C 40 40	0
49	j	1	Total C 40 40	0
49	k	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	m	1	Total C 40 40	0
49	r	1	Total C 40 40	0

- Molecule 50 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



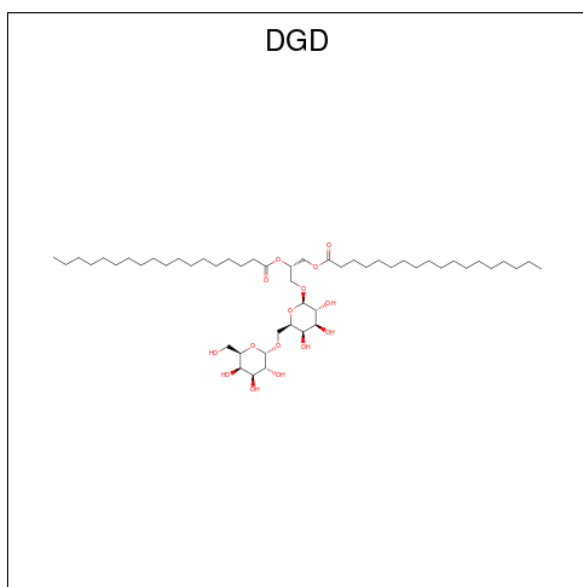
Mol	Chain	Residues	Atoms			AltConf
50	a	1	Total	C	O	0
			28	26	2	
50	b	1	Total	C	O	0
			28	26	2	

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
51	b	1	Total	Fe	S	0
			8	4	4	
51	c	1	Total	Fe	S	0
			8	4	4	
51	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	b	1	56	41	15	0

3 Residue-property plots

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

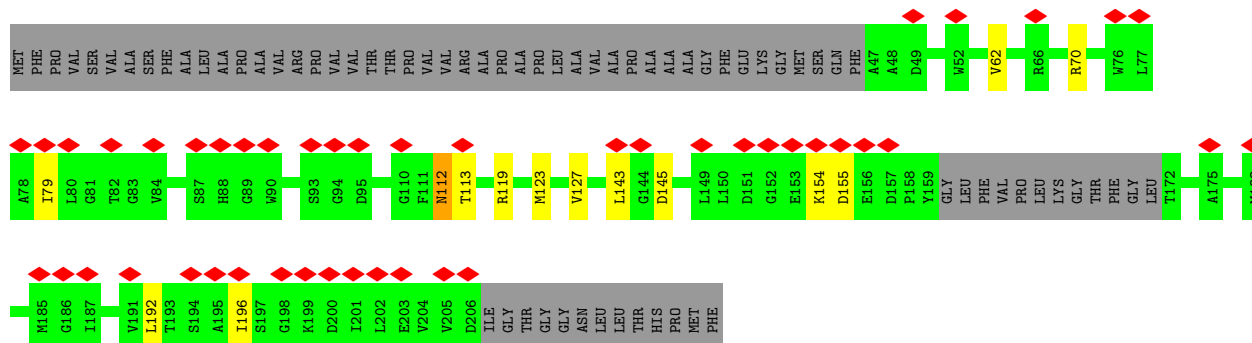
- Molecule 1: Light harvesting protein

Chain A: 



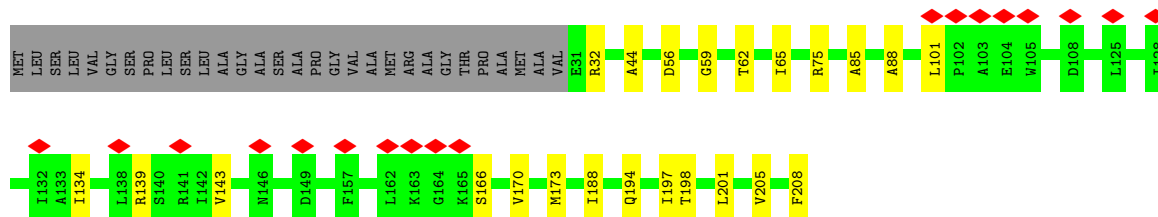
- Molecule 2: EFCPI-1

Chain B: 



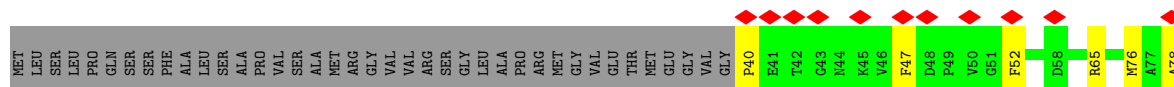
- Molecule 3: Light harvesting protein

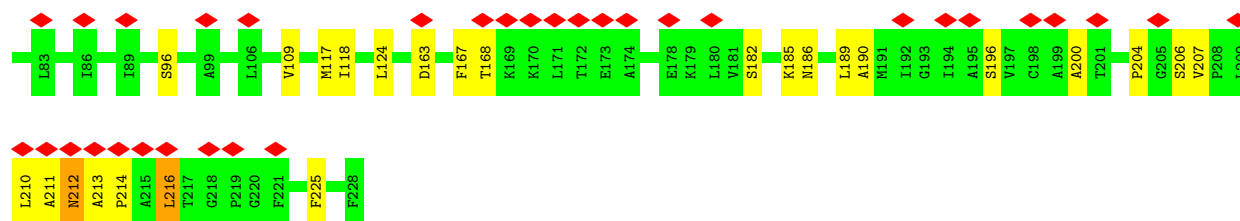
Chain C: 



- Molecule 4: EFCPI-6

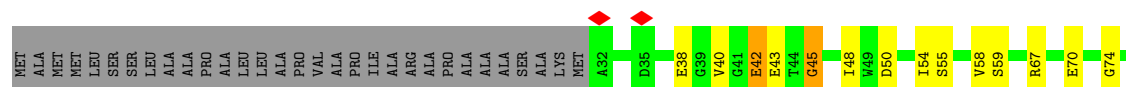
Chain D: 





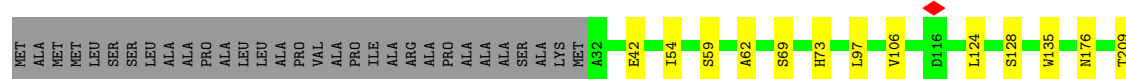
- Molecule 13: Light harvesting protein

Chain M: 74% 12% 14%



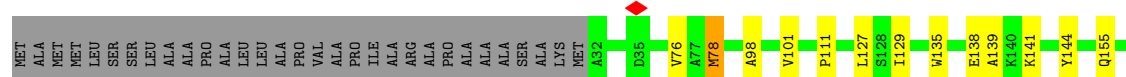
- Molecule 13: Light harvesting protein

Chain P: 79% 7% 14%



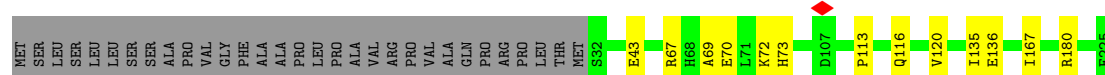
- Molecule 13: Light harvesting protein

Chain W: 76% 9% 14%



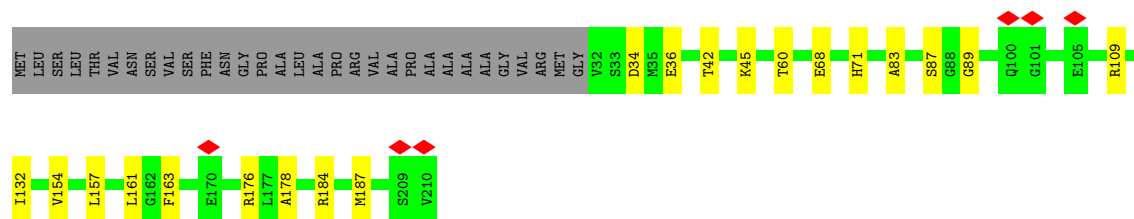
- Molecule 14: EFCPI-17

Chain N: 80% 6% 14%



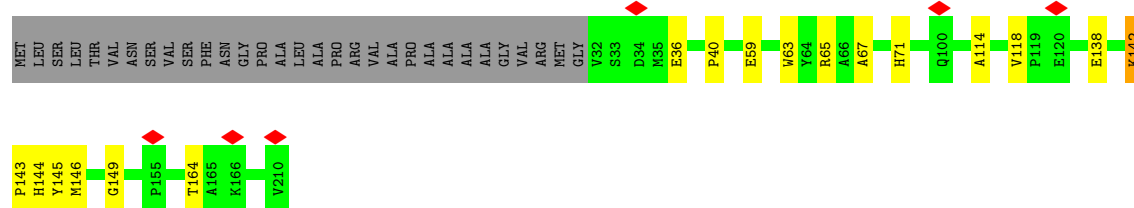
- Molecule 15: Light harvesting protein

Chain O: 76% 10% 15%



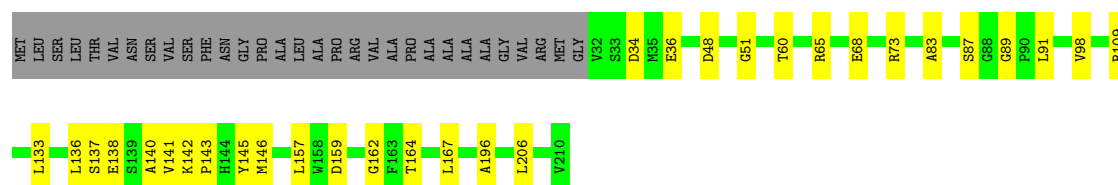
- Molecule 15: Light harvesting protein

Chain R: 77% 8% 15%



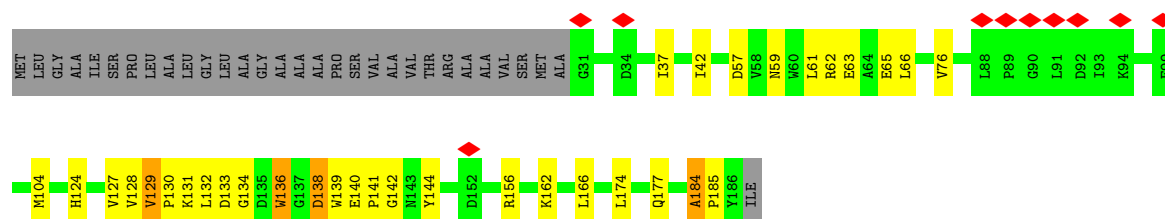
- Molecule 15: Light harvesting protein

Chain T: 70% 15% 15%



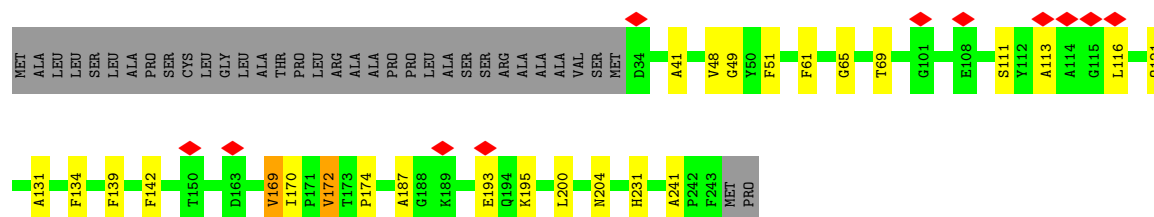
- Molecule 16: EFCPI-18

Chain Q: 5% 65% 16% 17%

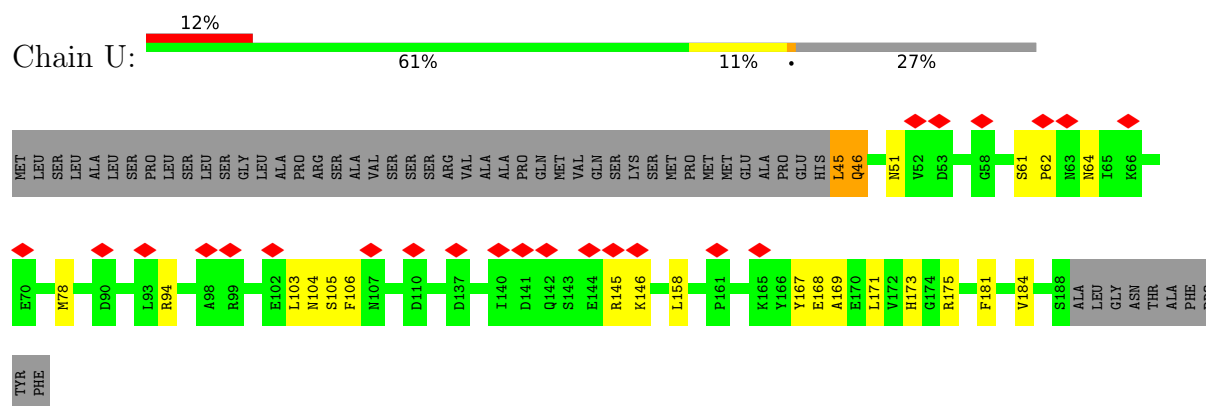


- Molecule 17: EFCPI-22

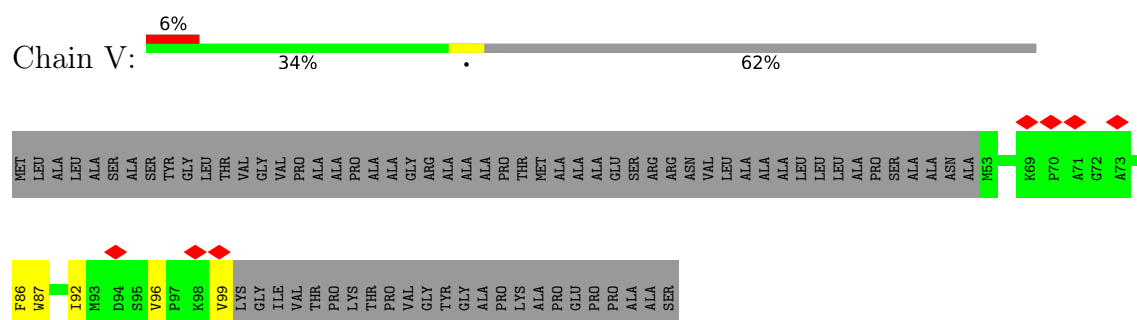
Chain S: 75% 10% 14%



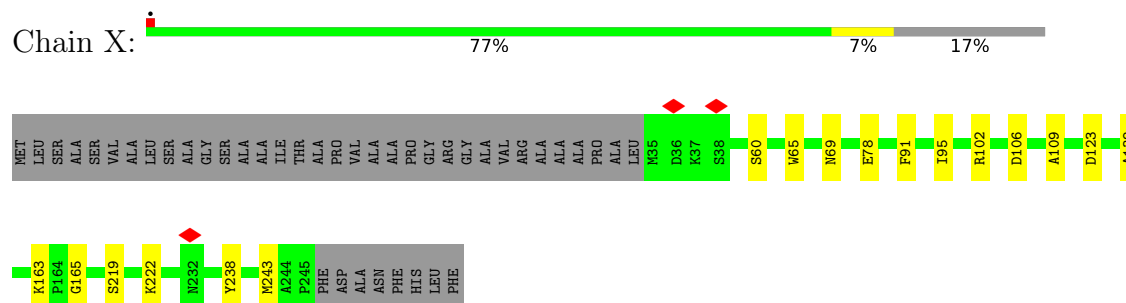
- Molecule 18: Light harvesting protein



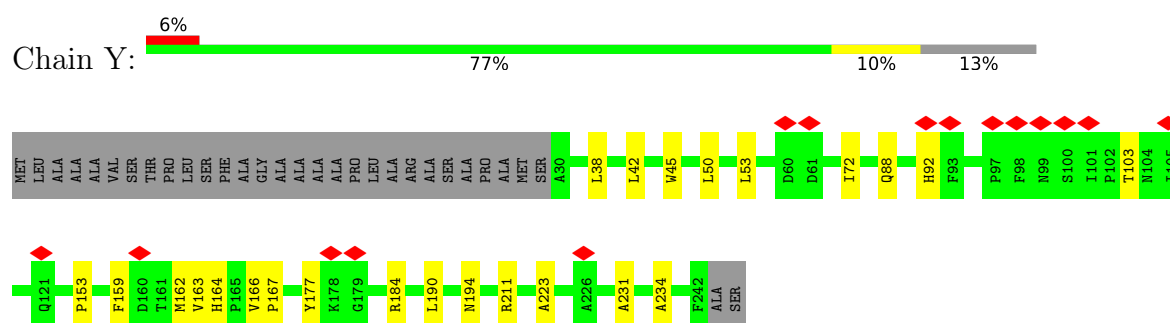
- Molecule 19: LEFP



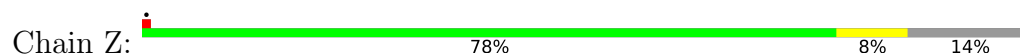
- Molecule 20: Light harvesting protein

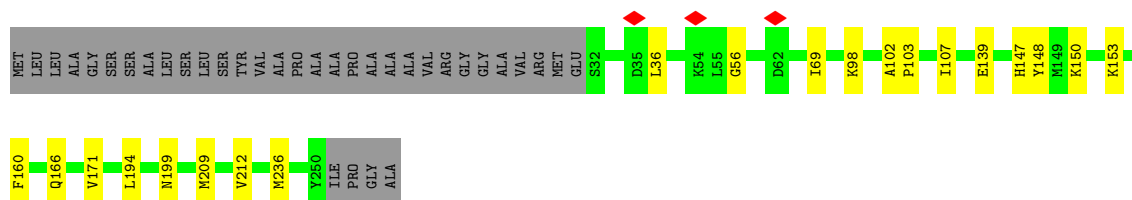


- Molecule 21: Light harvesting protein



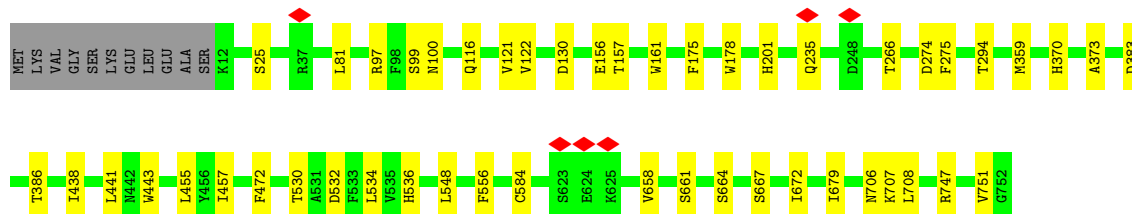
- Molecule 22: Light harvesting protein





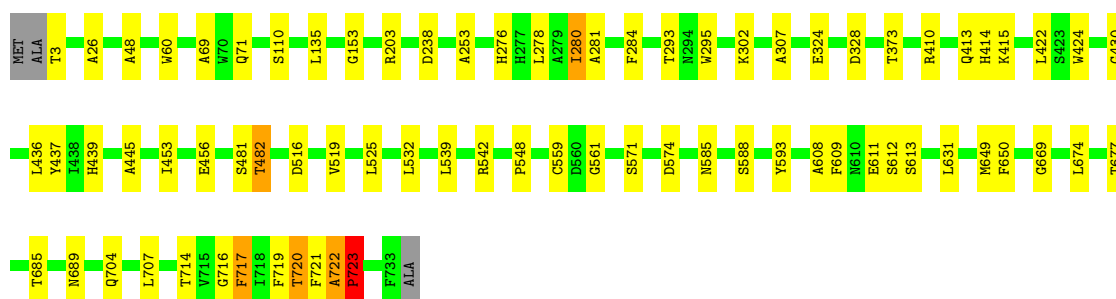
- Molecule 23: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 92% 7% .



- Molecule 24: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 89% 10% .



- Molecule 25: Photosystem I iron-sulfur center

Chain c: 88% 11% .



- Molecule 26: Photosystem I reaction center subunit II

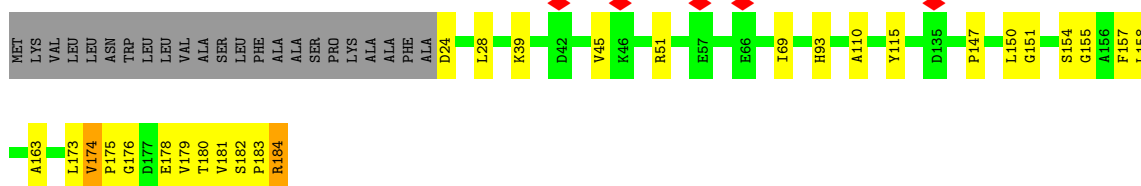
Chain d: 91% 7% ..



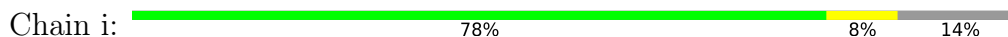
- Molecule 27: Photosystem I reaction center subunit IV

Chain e: 44% 5% 52%

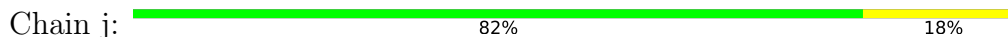
- Molecule 28: Photosystem I reaction center subunit III



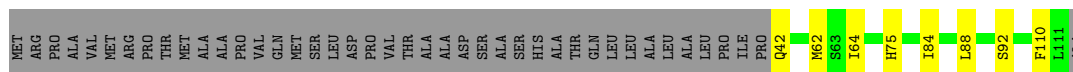
- Molecule 29: Photosystem I reaction center subunit VIII



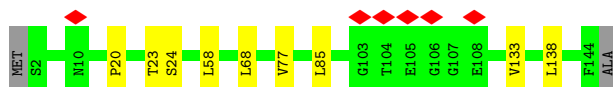
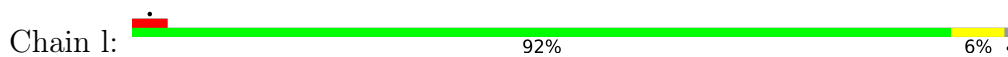
- Molecule 30: Photosystem I reaction center subunit IX



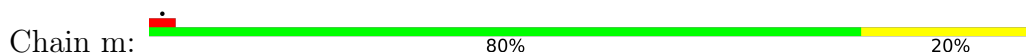
- Molecule 31: PSI-K

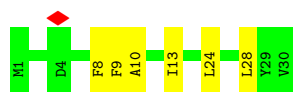


- Molecule 32: Photosystem I reaction center subunit XI

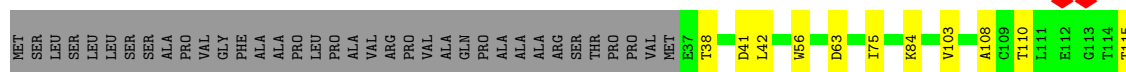
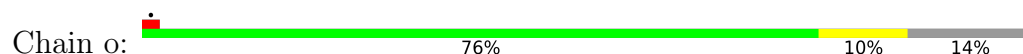


- Molecule 33: Photosystem I reaction center subunit XII

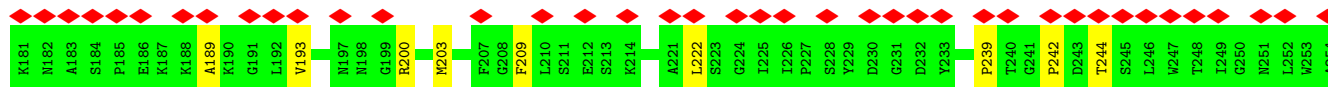
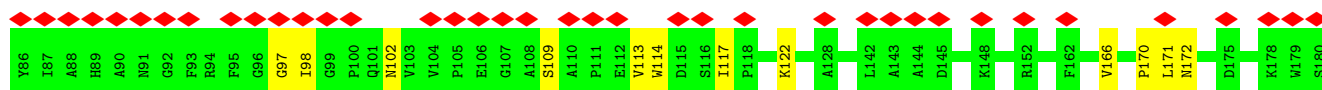
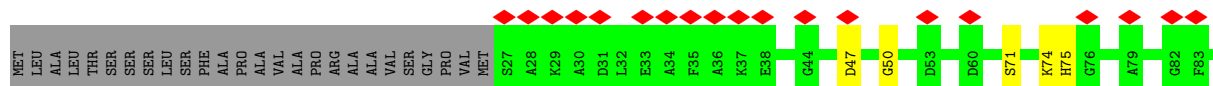
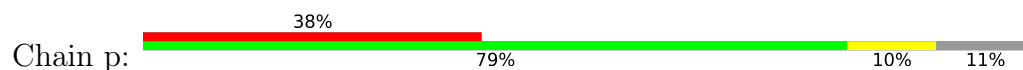




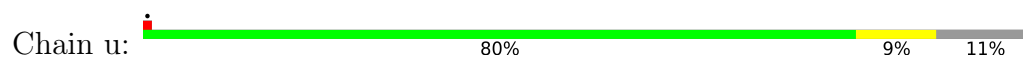
- Molecule 34: EFCPI-30



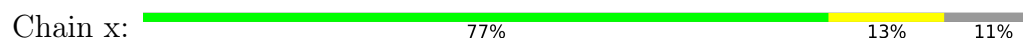
- Molecule 35: Light harvesting protein



- Molecule 35: Light harvesting protein

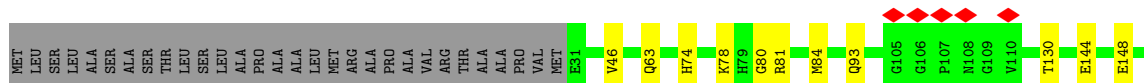
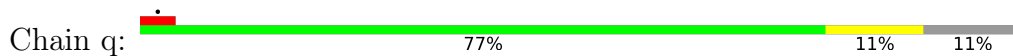


- Molecule 35: Light harvesting protein

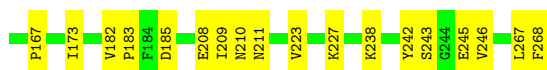
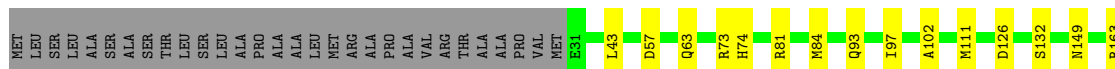
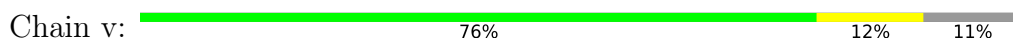




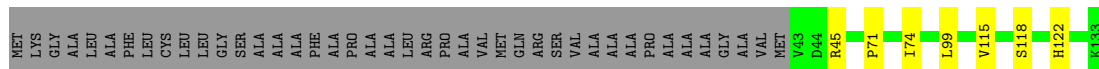
- Molecule 36: Light harvesting protein



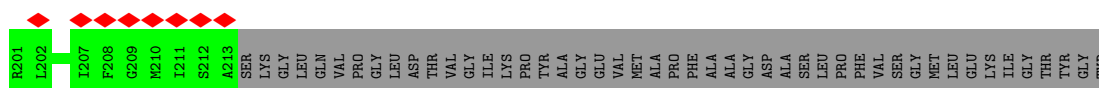
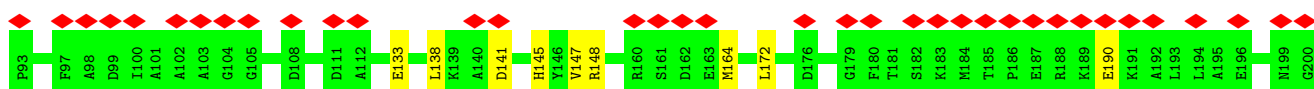
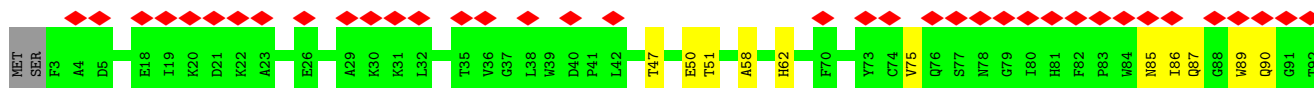
- Molecule 36: Light harvesting protein



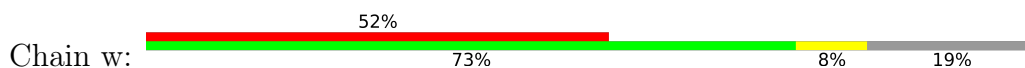
- Molecule 37: PsaR

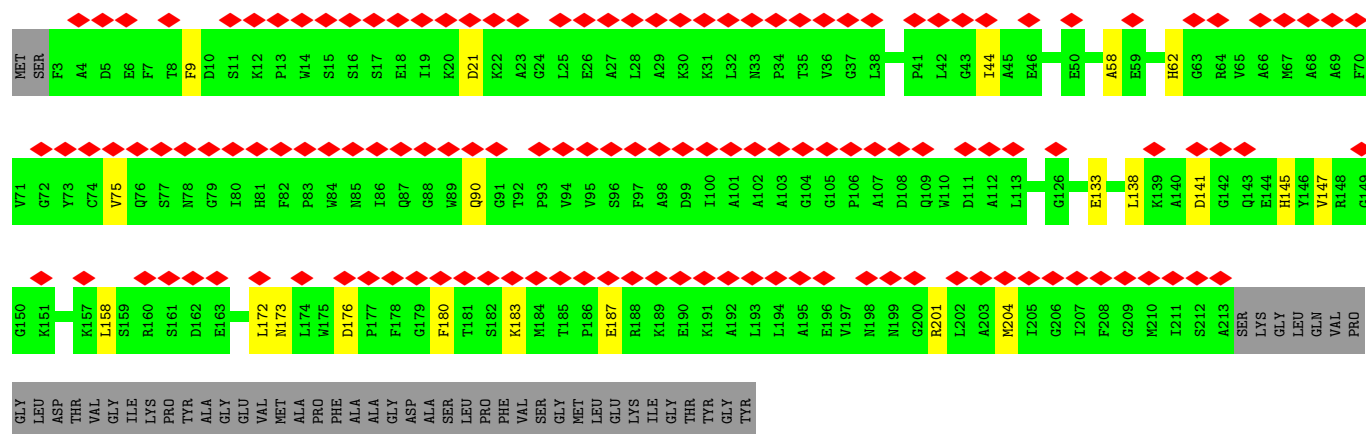


- Molecule 38: Light harvesting protein

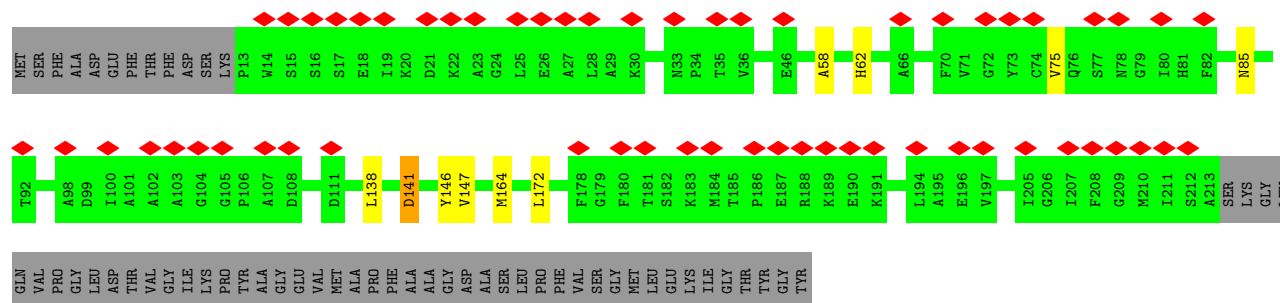
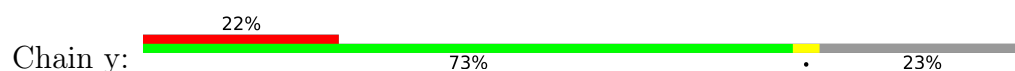


- Molecule 38: Light harvesting protein

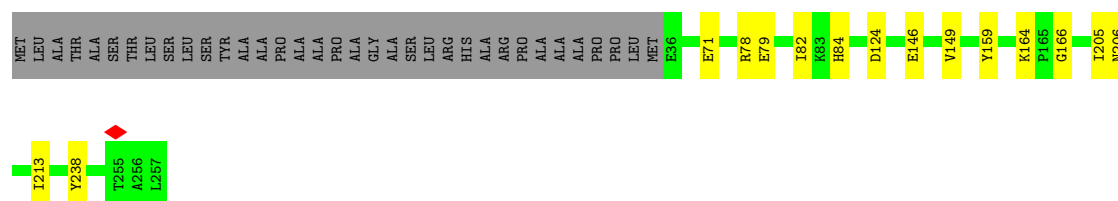
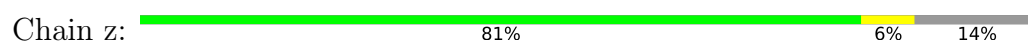




• Molecule 38: Light harvesting protein



• Molecule 39: Light harvesting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	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	1.457	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	530.0, 530.0, 530.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, DD6, CLA, SF4, LMG, A1EB4, A86, SQD, LHG, BCR, KC2, DGD, A1EB1

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	0.20	0/1458	0.41	0/1979
2	B	0.30	0/1135	0.60	1/1545 (0.1%)
3	C	0.23	0/1381	0.46	0/1865
4	D	0.45	0/1486	0.52	1/2020 (0.0%)
5	E	0.21	0/1416	0.43	0/1933
6	F	0.30	0/1452	0.51	3/1970 (0.2%)
7	G	0.19	0/1277	0.37	0/1739
8	H	0.23	0/1283	0.49	0/1739
9	I	0.20	0/1225	0.40	0/1656
10	J	0.23	0/1254	0.52	0/1692
11	K	0.20	0/1378	0.41	0/1874
12	L	0.28	0/1462	0.55	1/1989 (0.1%)
13	M	0.41	0/1491	0.52	2/2020 (0.1%)
13	P	0.20	0/1491	0.43	0/2020
13	W	0.21	0/1491	0.47	0/2020
14	N	0.19	0/1494	0.43	0/2027
15	O	0.22	0/1360	0.48	0/1850
15	R	0.38	0/1360	0.53	0/1850
15	T	0.23	0/1360	0.51	0/1850
16	Q	0.47	1/1223 (0.1%)	0.64	4/1659 (0.2%)
17	S	0.21	0/1700	0.49	2/2315 (0.1%)
18	U	0.25	0/1158	0.55	1/1567 (0.1%)
19	V	0.22	0/362	0.49	0/492
20	X	0.23	0/1695	0.48	0/2300
21	Y	0.26	0/1719	0.53	0/2342
22	Z	0.24	0/1773	0.50	0/2423
23	a	0.20	0/6024	0.39	0/8200
24	b	0.38	6/6017 (0.1%)	0.46	4/8208 (0.0%)
25	c	0.22	0/607	0.45	0/824
26	d	0.20	0/1128	0.42	0/1525
27	e	0.20	0/503	0.44	0/681
28	f	0.28	0/1269	0.45	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	i	0.23	0/250	0.45	0/342
30	j	0.23	0/324	0.49	0/438
31	k	0.20	0/520	0.40	0/701
32	l	0.19	0/1113	0.37	0/1513
33	m	0.22	0/226	0.35	0/306
34	o	0.26	0/1809	0.54	0/2460
35	p	0.25	0/1801	0.49	0/2451
35	u	0.28	0/1801	0.49	0/2451
35	x	0.24	0/1801	0.48	0/2451
36	q	0.26	0/1843	0.48	0/2503
36	v	0.26	0/1843	0.49	0/2503
37	r	0.23	0/700	0.42	0/958
38	t	0.26	0/1682	0.49	0/2286
38	w	0.24	0/1682	0.51	0/2286
38	y	0.22	0/1594	0.47	0/2167
39	z	0.25	0/1772	0.46	0/2414
All	All	0.27	7/72193 (0.0%)	0.47	19/98125 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	T	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	281	ALA	CA-C	-6.35	1.44	1.52
24	b	284	PHE	C-O	-6.20	1.16	1.24
24	b	281	ALA	C-O	-5.83	1.17	1.24
16	Q	136	TRP	CA-C	-5.79	1.45	1.52
24	b	722	ALA	C-O	-5.38	1.19	1.24

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	722	ALA	CA-C-N	-7.89	109.97	119.84
24	b	722	ALA	C-N-CA	-7.89	109.97	119.84
4	D	93	VAL	N-CA-C	-7.55	103.92	111.77
6	F	152	ALA	N-CA-C	-7.37	103.18	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	129	VAL	O-C-N	6.28	124.44	120.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	T	142	LYS	Peptide
15	T	162	GLY	Peptide

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	1419	0	1408	15	0
2	B	1108	0	1082	10	0
3	C	1352	0	1383	15	0
4	D	1446	0	1404	35	0
5	E	1383	0	1399	48	0
6	F	1414	0	1411	21	0
7	G	1248	0	1251	10	0
8	H	1251	0	1225	9	0
9	I	1195	0	1197	8	0
10	J	1231	0	1245	25	0
11	K	1333	0	1297	16	0
12	L	1419	0	1413	37	0
13	M	1455	0	1468	22	0
13	P	1455	0	1468	25	0
13	W	1455	0	1468	24	0
14	N	1454	0	1469	9	0
15	O	1325	0	1344	13	0
15	R	1325	0	1344	16	0
15	T	1325	0	1344	19	0
16	Q	1192	0	1163	39	0
17	S	1640	0	1586	22	0
18	U	1130	0	1116	12	0
19	V	351	0	350	13	0
20	X	1643	0	1607	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Y	1660	0	1617	16	0
22	Z	1714	0	1670	14	0
23	a	5832	0	5730	59	0
24	b	5807	0	5630	63	0
25	c	597	0	581	7	0
26	d	1103	0	1113	8	0
27	e	493	0	482	4	0
28	f	1238	0	1242	40	0
29	i	243	0	255	5	0
30	j	317	0	333	15	0
31	k	510	0	520	9	0
32	l	1084	0	1090	8	0
33	m	224	0	243	5	0
34	o	1760	0	1757	18	0
35	p	1744	0	1703	16	0
35	u	1744	0	1703	16	0
35	x	1744	0	1703	24	0
36	q	1790	0	1776	27	0
36	v	1790	0	1776	26	0
37	r	681	0	667	4	0
38	t	1631	0	1593	29	0
38	w	1631	0	1593	19	0
38	y	1546	0	1523	9	0
39	z	1718	0	1701	13	0
40	A	581	0	562	24	0
40	B	287	0	218	3	0
40	C	429	0	381	4	0
40	D	668	0	613	7	0
40	E	711	0	640	35	0
40	F	544	0	482	12	0
40	G	363	0	303	4	0
40	H	521	0	442	2	0
40	I	445	0	412	0	0
40	J	549	0	441	14	0
40	K	327	0	294	6	0
40	L	394	0	312	10	0
40	M	420	0	413	3	0
40	N	345	0	324	3	0
40	O	328	0	299	0	0
40	P	393	0	364	11	0
40	Q	432	0	375	11	0
40	R	320	0	278	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	S	580	0	496	21	0
40	T	330	0	296	1	0
40	U	345	0	273	1	0
40	V	113	0	104	6	0
40	W	425	0	429	5	0
40	X	484	0	425	2	0
40	Y	478	0	415	0	0
40	Z	507	0	469	2	0
40	a	2596	0	2627	48	0
40	b	2503	0	2570	31	0
40	f	219	0	201	7	0
40	i	55	0	49	4	0
40	j	47	0	35	2	0
40	k	110	0	98	17	0
40	l	259	0	284	4	0
40	o	507	0	469	5	0
40	p	478	0	418	2	0
40	q	508	0	469	2	0
40	t	305	0	249	1	0
40	u	491	0	442	0	0
40	v	508	0	469	4	0
40	w	305	0	249	6	0
40	x	508	0	472	3	0
40	y	305	0	249	7	0
40	z	551	0	498	5	0
41	A	45	0	0	0	0
41	C	45	0	0	1	0
41	E	45	0	0	0	0
41	F	90	0	0	0	0
41	G	90	0	0	0	0
41	H	90	0	0	0	0
41	I	90	0	0	0	0
41	J	45	0	0	0	0
41	K	180	0	0	0	0
41	L	225	0	0	1	0
41	M	225	0	0	2	0
41	N	315	0	0	1	0
41	O	270	0	0	1	0
41	P	225	0	0	1	0
41	Q	90	0	0	10	0
41	R	270	0	0	0	0
41	S	180	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	T	270	0	0	3	0
41	U	45	0	0	0	0
41	W	225	0	0	1	0
41	X	180	0	0	1	0
41	Y	225	0	0	9	0
41	Z	180	0	0	2	0
41	o	180	0	0	1	0
41	p	225	0	0	0	0
41	q	180	0	0	0	0
41	t	135	0	0	15	0
41	u	225	0	0	0	0
41	v	180	0	0	1	0
41	w	135	0	0	13	0
41	x	225	0	0	0	0
41	y	135	0	0	8	0
41	z	180	0	0	1	0
42	A	215	0	0	10	0
42	B	43	0	0	1	0
42	C	129	0	0	1	0
42	D	215	0	0	1	0
42	E	172	0	0	0	0
42	F	129	0	0	1	0
42	G	43	0	0	0	0
42	H	129	0	0	1	0
42	I	172	0	0	2	0
42	J	258	0	0	16	0
42	K	86	0	0	0	0
42	L	86	0	0	32	0
42	M	43	0	0	1	0
42	N	129	0	0	1	0
42	O	43	0	0	1	0
42	P	43	0	0	5	0
42	Q	172	0	0	1	0
42	R	43	0	0	0	0
42	T	43	0	0	0	0
42	U	86	0	0	0	0
42	W	43	0	0	1	0
42	X	43	0	0	0	0
42	Y	43	0	0	9	0
42	Z	43	0	0	0	0
42	j	43	0	0	0	0
42	k	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	o	86	0	0	2	0
42	p	43	0	0	1	0
42	q	86	0	0	7	0
42	t	43	0	0	29	0
42	u	43	0	0	1	0
42	v	86	0	0	5	0
42	w	43	0	0	26	0
42	x	43	0	0	2	0
42	y	43	0	0	17	0
42	z	86	0	0	0	0
43	A	40	0	50	0	0
43	D	40	0	50	1	0
43	E	102	0	114	6	0
43	F	39	0	48	0	0
43	L	37	0	44	0	0
43	M	39	0	48	0	0
43	P	39	0	48	0	0
43	S	39	0	48	0	0
43	T	40	0	50	0	0
43	W	39	0	48	0	0
43	a	70	0	80	3	0
43	j	30	0	30	13	0
43	l	39	0	48	0	0
43	p	39	0	48	0	0
43	u	39	0	48	1	0
43	x	39	0	48	5	0
44	C	48	0	0	0	0
44	D	96	0	0	1	0
44	F	144	0	0	0	0
44	G	96	0	0	3	0
44	H	48	0	0	0	0
44	K	48	0	0	0	0
44	L	48	0	0	1	0
44	M	192	0	0	1	0
44	N	192	0	0	7	0
44	O	144	0	0	0	0
44	P	192	0	0	1	0
44	Q	96	0	0	1	0
44	R	144	0	0	0	0
44	S	192	0	0	0	0
44	T	192	0	0	0	0
44	U	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	W	144	0	0	2	0
44	X	384	0	0	3	0
44	Y	336	0	0	3	0
44	Z	192	0	0	1	0
44	o	240	0	0	1	0
44	p	288	0	0	1	0
44	q	288	0	0	0	0
44	t	144	0	0	1	0
44	u	240	0	0	0	0
44	v	288	0	0	0	0
44	w	192	0	0	1	0
44	x	192	0	0	0	0
44	y	48	0	0	1	0
44	z	336	0	0	1	0
45	F	40	0	50	0	0
45	S	40	0	50	2	0
45	a	78	0	99	0	0
46	F	36	0	36	2	0
46	I	54	0	78	2	0
46	M	32	0	28	1	0
46	P	32	0	28	5	0
46	W	32	0	28	4	0
46	k	36	0	36	3	0
47	F	56	0	0	0	0
47	G	56	0	0	0	0
47	K	112	0	0	1	0
47	L	112	0	0	0	0
47	N	56	0	0	0	0
47	O	56	0	0	0	0
47	P	56	0	0	9	0
47	R	56	0	0	0	0
47	S	112	0	0	0	0
47	T	112	0	0	1	0
47	Y	56	0	0	0	0
47	Z	168	0	0	1	0
47	o	112	0	0	0	0
47	p	112	0	0	2	0
47	q	168	0	0	1	0
47	t	168	0	0	2	0
47	u	112	0	0	2	0
47	v	224	0	0	5	0
47	w	112	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	x	112	0	0	2	0
47	y	168	0	0	4	0
47	z	56	0	0	0	0
48	M	56	0	0	0	0
48	P	56	0	0	4	0
48	W	56	0	0	7	0
49	a	160	0	224	7	0
49	b	240	0	336	2	0
49	f	80	0	112	4	0
49	i	40	0	56	3	0
49	j	40	0	56	0	0
49	k	40	0	56	0	0
49	l	120	0	168	4	0
49	m	40	0	56	4	0
49	r	40	0	56	1	0
50	a	28	0	33	1	0
50	b	28	0	33	2	0
51	b	8	0	0	0	0
51	c	16	0	0	0	0
52	b	56	0	70	7	0
All	All	110086	0	91890	1072	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 5.

The worst 5 of 1072 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)
13:P:54:ILE:CG2	47:P:301:A1EB1:O43	1.73	1.36
30:j:1:MET:CE	43:j:101:LMG:H292	1.56	1.34
16:Q:162:LYS:NZ	41:Q:216:KC2:O2A	1.65	1.27
16:Q:42:ILE:HD12	41:Q:216:KC2:CED	1.67	1.23
4:D:103:ILE:CG2	23:a:175:PHE:CZ	2.23	1.20

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/201 (90%)	177 (98%)	4 (2%)	0	100	100
2	B	144/219 (66%)	136 (94%)	7 (5%)	1 (1%)	18	49
3	C	176/208 (85%)	166 (94%)	9 (5%)	1 (1%)	21	52
4	D	187/255 (73%)	178 (95%)	8 (4%)	1 (0%)	24	57
5	E	185/217 (85%)	176 (95%)	8 (4%)	1 (0%)	24	57
6	F	186/239 (78%)	175 (94%)	10 (5%)	1 (0%)	24	57
7	G	166/198 (84%)	161 (97%)	5 (3%)	0	100	100
8	H	165/199 (83%)	157 (95%)	8 (5%)	0	100	100
9	I	153/196 (78%)	147 (96%)	6 (4%)	0	100	100
10	J	164/208 (79%)	157 (96%)	6 (4%)	1 (1%)	21	52
11	K	169/204 (83%)	158 (94%)	10 (6%)	1 (1%)	21	52
12	L	187/228 (82%)	173 (92%)	12 (6%)	2 (1%)	11	39
13	M	191/224 (85%)	184 (96%)	7 (4%)	0	100	100
13	P	191/224 (85%)	183 (96%)	8 (4%)	0	100	100
13	W	191/224 (85%)	182 (95%)	9 (5%)	0	100	100
14	N	192/225 (85%)	182 (95%)	10 (5%)	0	100	100
15	O	177/210 (84%)	164 (93%)	13 (7%)	0	100	100
15	R	177/210 (84%)	171 (97%)	6 (3%)	0	100	100
15	T	177/210 (84%)	164 (93%)	12 (7%)	1 (1%)	21	52
16	Q	154/187 (82%)	141 (92%)	10 (6%)	3 (2%)	6	27
17	S	208/245 (85%)	189 (91%)	18 (9%)	1 (0%)	24	57
18	U	142/198 (72%)	128 (90%)	11 (8%)	3 (2%)	5	25
19	V	45/123 (37%)	43 (96%)	2 (4%)	0	100	100
20	X	209/253 (83%)	201 (96%)	8 (4%)	0	100	100
21	Y	211/244 (86%)	199 (94%)	11 (5%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Z	217/254 (85%)	210 (97%)	7 (3%)	0	100	100
23	a	739/752 (98%)	711 (96%)	28 (4%)	0	100	100
24	b	729/734 (99%)	706 (97%)	22 (3%)	1 (0%)	48	78
25	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
26	d	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
27	e	61/131 (47%)	59 (97%)	2 (3%)	0	100	100
28	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
29	i	29/36 (81%)	27 (93%)	2 (7%)	0	100	100
30	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
31	k	68/112 (61%)	65 (96%)	2 (3%)	1 (2%)	8	32
32	l	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
33	m	28/30 (93%)	28 (100%)	0	0	100	100
34	o	234/273 (86%)	225 (96%)	8 (3%)	1 (0%)	30	61
35	p	226/255 (89%)	223 (99%)	3 (1%)	0	100	100
35	u	226/255 (89%)	221 (98%)	5 (2%)	0	100	100
35	x	226/255 (89%)	220 (97%)	6 (3%)	0	100	100
36	q	236/268 (88%)	229 (97%)	7 (3%)	0	100	100
36	v	236/268 (88%)	224 (95%)	12 (5%)	0	100	100
37	r	89/133 (67%)	88 (99%)	1 (1%)	0	100	100
38	t	209/260 (80%)	200 (96%)	9 (4%)	0	100	100
38	w	209/260 (80%)	202 (97%)	7 (3%)	0	100	100
38	y	199/260 (76%)	194 (98%)	5 (2%)	0	100	100
39	z	220/257 (86%)	215 (98%)	5 (2%)	0	100	100
All	All	9063/10734 (84%)	8676 (96%)	366 (4%)	21 (0%)	44	73

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	81	GLU
5	E	210	VAL
10	J	71	ILE
11	K	139	PRO
12	L	204	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/170 (91%)	155 (100%)	0	100	100
2	B	108/160 (68%)	108 (100%)	0	100	100
3	C	142/161 (88%)	141 (99%)	1 (1%)	76	82
4	D	146/193 (76%)	145 (99%)	1 (1%)	76	82
5	E	146/163 (90%)	146 (100%)	0	100	100
6	F	140/180 (78%)	138 (99%)	2 (1%)	59	76
7	G	127/149 (85%)	127 (100%)	0	100	100
8	H	130/154 (84%)	130 (100%)	0	100	100
9	I	125/153 (82%)	125 (100%)	0	100	100
10	J	123/150 (82%)	123 (100%)	0	100	100
11	K	131/153 (86%)	131 (100%)	0	100	100
12	L	144/174 (83%)	143 (99%)	1 (1%)	76	82
13	M	146/165 (88%)	146 (100%)	0	100	100
13	P	146/165 (88%)	146 (100%)	0	100	100
13	W	146/165 (88%)	144 (99%)	2 (1%)	59	76
14	N	149/174 (86%)	148 (99%)	1 (1%)	76	82
15	O	136/157 (87%)	136 (100%)	0	100	100
15	R	136/157 (87%)	135 (99%)	1 (1%)	76	82
15	T	136/157 (87%)	135 (99%)	1 (1%)	76	82
16	Q	123/141 (87%)	122 (99%)	1 (1%)	73	81
17	S	163/188 (87%)	163 (100%)	0	100	100
18	U	118/162 (73%)	116 (98%)	2 (2%)	53	74
19	V	39/85 (46%)	39 (100%)	0	100	100
20	X	169/194 (87%)	169 (100%)	0	100	100
21	Y	166/183 (91%)	166 (100%)	0	100	100
22	Z	177/198 (89%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	a	607/616 (98%)	607 (100%)	0	100	100
24	b	591/592 (100%)	587 (99%)	4 (1%)	76	82
25	c	68/69 (99%)	68 (100%)	0	100	100
26	d	120/122 (98%)	119 (99%)	1 (1%)	73	81
27	e	51/90 (57%)	51 (100%)	0	100	100
28	f	127/144 (88%)	123 (97%)	4 (3%)	35	64
29	i	28/32 (88%)	28 (100%)	0	100	100
30	j	36/36 (100%)	36 (100%)	0	100	100
31	k	52/85 (61%)	52 (100%)	0	100	100
32	l	114/115 (99%)	114 (100%)	0	100	100
33	m	23/23 (100%)	23 (100%)	0	100	100
34	o	180/208 (86%)	178 (99%)	2 (1%)	65	78
35	p	179/199 (90%)	179 (100%)	0	100	100
35	u	179/199 (90%)	178 (99%)	1 (1%)	78	83
35	x	179/199 (90%)	179 (100%)	0	100	100
36	q	183/204 (90%)	182 (100%)	1 (0%)	81	85
36	v	183/204 (90%)	182 (100%)	1 (0%)	81	85
37	r	71/94 (76%)	70 (99%)	1 (1%)	59	76
38	t	168/204 (82%)	168 (100%)	0	100	100
38	w	168/204 (82%)	167 (99%)	1 (1%)	78	83
38	y	159/204 (78%)	158 (99%)	1 (1%)	78	83
39	z	177/199 (89%)	177 (100%)	0	100	100
All	All	7210/8293 (87%)	7180 (100%)	30 (0%)	81	86

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	b	717	PHE
36	v	84	MET
26	d	38	SER
38	y	141	ASP
36	q	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
36	q	44	ASN
36	q	195	ASN
35	u	140	ASN
16	Q	59	ASN
14	N	110	GLN

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](#)

790 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	$\# Z > 2$
40	CLA	K	301	-	51,55,73	1.96	9 (17%)	60,91,113	1.43	7 (11%)
40	CLA	Y	310	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	6 (8%)
40	CLA	Q	206	-	62,68,73	1.72	9 (14%)	74,105,113	1.76	10 (13%)
41	KC2	I	209	9	49,53,53	1.83	4 (8%)	60,89,89	1.12	6 (10%)
40	CLA	H	307	-	64,68,73	1.80	9 (14%)	76,107,113	1.47	9 (11%)
40	CLA	W	305	13	69,73,73	1.70	9 (13%)	82,113,113	1.28	8 (9%)
41	KC2	R	311	15	49,53,53	1.84	4 (8%)	60,89,89	1.07	4 (6%)
49	BCR	f	203	-	41,41,41	0.22	0	56,56,56	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	a	828	23	69,73,73	1.66	9 (13%)	82,113,113	1.27	6 (7%)
44	A86	D	319	-	47,50,50	0.45	1 (2%)	51,76,76	1.02	2 (3%)
40	CLA	E	304	5	59,63,73	1.84	10 (16%)	70,101,113	1.39	6 (8%)
40	CLA	b	821	-	69,73,73	1.67	9 (13%)	82,113,113	1.22	7 (8%)
40	CLA	o	307	34	64,68,73	1.78	9 (14%)	76,107,113	1.51	11 (14%)
44	A86	T	313	-	47,50,50	0.40	1 (2%)	51,76,76	0.90	3 (5%)
40	CLA	U	203	-	59,63,73	1.93	9 (15%)	70,101,113	1.49	10 (14%)
40	CLA	w	308	-	51,55,73	1.97	9 (17%)	60,91,113	1.44	5 (8%)
40	CLA	U	206	-	51,55,73	2.01	9 (17%)	60,91,113	1.39	7 (11%)
41	KC2	N	302	14	49,53,53	1.85	4 (8%)	60,89,89	1.07	5 (8%)
44	A86	N	318	-	47,50,50	0.66	1 (2%)	51,76,76	0.49	0
40	CLA	F	306	6	64,68,73	1.77	9 (14%)	76,107,113	1.33	7 (9%)
41	KC2	M	309	-	49,53,53	1.88	4 (8%)	60,89,89	1.03	3 (5%)
41	KC2	p	310	-	49,53,53	1.86	4 (8%)	60,89,89	1.05	3 (5%)
40	CLA	I	204	9	51,55,73	1.97	9 (17%)	60,91,113	1.43	6 (10%)
40	CLA	N	311	14	64,68,73	1.78	9 (14%)	76,107,113	1.45	7 (9%)
40	CLA	a	851	-	69,73,73	1.70	9 (13%)	82,113,113	1.32	7 (8%)
41	KC2	U	201	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
42	DD6	A	315	-	40,45,45	0.16	0	51,67,67	0.70	1 (1%)
42	DD6	x	320	-	40,45,45	0.19	0	51,67,67	0.67	2 (3%)
44	A86	P	317	-	47,50,50	0.44	1 (2%)	51,76,76	0.79	2 (3%)
41	KC2	K	303	11	49,53,53	1.85	4 (8%)	60,89,89	1.07	5 (8%)
47	A1EB1	v	323	-	54,58,58	0.51	1 (1%)	60,85,85	0.62	1 (1%)
47	A1EB1	w	313	-	54,58,58	0.43	1 (1%)	60,85,85	0.66	1 (1%)
40	CLA	T	317	47	51,55,73	1.96	8 (15%)	60,91,113	1.38	8 (13%)
40	CLA	a	840	23	59,63,73	1.83	9 (15%)	70,101,113	1.39	7 (10%)
41	KC2	x	315	-	49,53,53	1.85	4 (8%)	60,89,89	1.14	4 (6%)
42	DD6	U	211	-	40,45,45	0.20	0	51,67,67	0.71	1 (1%)
44	A86	R	312	-	47,50,50	0.76	1 (2%)	51,76,76	1.30	3 (5%)
41	KC2	R	303	-	49,53,53	1.84	4 (8%)	60,89,89	1.18	5 (8%)
40	CLA	J	318	10	51,55,73	1.99	9 (17%)	60,91,113	1.49	8 (13%)
40	CLA	B	302	2	51,55,73	1.99	9 (17%)	60,91,113	1.38	6 (10%)
40	CLA	b	815	-	61,65,73	1.82	9 (14%)	72,103,113	1.38	6 (8%)
42	DD6	O	314	-	40,45,45	0.20	0	51,67,67	0.69	1 (1%)
40	CLA	O	304	15	69,73,73	1.69	9 (13%)	82,113,113	1.33	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	V	201	-	62,66,73	1.80	9 (14%)	73,104,113	1.34	5 (6%)
40	CLA	u	306	35	51,55,73	1.98	9 (17%)	60,91,113	1.49	7 (11%)
40	CLA	S	307	17	64,68,73	1.76	10 (15%)	76,107,113	1.41	6 (7%)
47	A1EB1	K	313	-	54,58,58	0.55	1 (1%)	60,85,85	1.24	2 (3%)
40	CLA	B	306	-	56,60,73	1.99	9 (16%)	65,97,113	1.50	9 (13%)
40	CLA	J	310	-	51,55,73	2.08	9 (17%)	60,91,113	1.66	9 (15%)
40	CLA	b	837	24	64,68,73	1.74	9 (14%)	76,107,113	1.40	6 (7%)
40	CLA	u	305	35	51,55,73	1.99	9 (17%)	60,91,113	1.66	8 (13%)
47	A1EB1	w	314	-	54,58,58	0.51	1 (1%)	60,85,85	0.68	1 (1%)
41	KC2	Y	314	-	49,53,53	1.86	4 (8%)	60,89,89	1.13	5 (8%)
44	A86	q	315	-	47,50,50	0.49	1 (2%)	51,76,76	0.92	2 (3%)
44	A86	v	315	-	47,50,50	0.56	1 (2%)	51,76,76	0.85	1 (1%)
44	A86	z	316	-	47,50,50	0.52	1 (2%)	51,76,76	1.49	3 (5%)
40	CLA	a	824	-	66,70,73	1.74	9 (13%)	78,109,113	1.30	6 (7%)
40	CLA	w	302	38	51,55,73	1.97	9 (17%)	60,91,113	1.53	6 (10%)
42	DD6	z	322	-	40,45,45	0.23	0	51,67,67	1.00	4 (7%)
40	CLA	S	308	-	53,57,73	2.00	9 (16%)	65,94,113	1.56	10 (15%)
42	DD6	H	312	-	40,45,45	0.22	0	51,67,67	0.98	3 (5%)
41	KC2	O	308	15	49,53,53	1.83	4 (8%)	60,89,89	1.12	4 (6%)
42	DD6	k	204	-	40,45,45	0.20	0	51,67,67	0.82	4 (7%)
44	A86	u	320	-	47,50,50	0.38	1 (2%)	51,76,76	1.01	2 (3%)
40	CLA	M	307	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	8 (10%)
47	A1EB1	x	322	-	54,58,58	0.56	1 (1%)	60,85,85	0.60	1 (1%)
40	CLA	a	809	-	54,58,73	1.98	9 (16%)	64,95,113	1.44	8 (12%)
40	CLA	l	204	-	69,73,73	1.71	9 (13%)	82,113,113	1.20	6 (7%)
40	CLA	Q	208	-	64,68,73	1.77	8 (12%)	76,107,113	1.31	8 (10%)
49	BCR	f	206	-	41,41,41	0.20	0	56,56,56	0.53	0
42	DD6	u	321	-	40,45,45	0.21	0	51,67,67	0.67	1 (1%)
40	CLA	M	310	-	60,64,73	1.78	9 (15%)	71,102,113	1.31	8 (11%)
44	A86	X	317	-	47,50,50	0.50	1 (2%)	51,76,76	0.97	3 (5%)
44	A86	v	325	-	47,50,50	0.35	0	51,76,76	1.05	2 (3%)
40	CLA	A	305	1	65,69,73	1.76	9 (13%)	77,108,113	1.38	7 (9%)
42	DD6	J	315	-	40,45,45	0.22	0	51,67,67	0.76	3 (5%)
40	CLA	b	820	-	69,73,73	1.73	9 (13%)	82,113,113	1.33	8 (9%)
40	CLA	C	305	3	64,68,73	1.78	9 (14%)	76,107,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	a	827	23	69,73,73	1.70	9 (13%)	82,113,113	1.27	5 (6%)
42	DD6	H	313	-	40,45,45	0.25	0	51,67,67	0.86	2 (3%)
42	DD6	I	210	-	40,45,45	0.17	0	51,67,67	0.97	3 (5%)
40	CLA	L	305	12	51,55,73	2.04	9 (17%)	60,91,113	1.50	6 (10%)
40	CLA	X	312	-	51,55,73	2.06	9 (17%)	60,91,113	1.56	8 (13%)
49	BCR	b	846	-	41,41,41	0.12	0	56,56,56	0.67	1 (1%)
40	CLA	b	805	-	65,69,73	1.77	9 (13%)	77,108,113	1.34	6 (7%)
41	KC2	w	307	-	49,53,53	1.84	4 (8%)	60,89,89	1.09	4 (6%)
40	CLA	u	311	-	59,63,73	1.94	9 (15%)	70,101,113	1.71	12 (17%)
47	A1EB1	P	301	-	54,58,58	0.52	1 (1%)	60,85,85	0.59	0
40	CLA	J	312	-	62,66,73	1.79	9 (14%)	73,104,113	1.32	6 (8%)
49	BCR	b	844	-	41,41,41	0.25	0	56,56,56	0.60	1 (1%)
40	CLA	D	310	4	64,68,73	1.73	9 (14%)	76,107,113	1.31	9 (11%)
40	CLA	b	817	24	69,73,73	1.66	9 (13%)	82,113,113	1.28	7 (8%)
47	A1EB1	t	315	-	54,58,58	0.45	1 (1%)	60,85,85	0.80	2 (3%)
40	CLA	H	310	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	6 (7%)
40	CLA	Q	204	16	54,58,73	1.96	9 (16%)	62,94,113	1.88	12 (19%)
44	A86	R	313	-	47,50,50	0.60	1 (2%)	51,76,76	0.66	0
41	KC2	O	302	15	49,53,53	1.86	5 (10%)	60,89,89	1.15	4 (6%)
40	CLA	x	307	-	59,63,73	1.90	9 (15%)	70,101,113	1.64	8 (11%)
40	CLA	U	207	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	8 (13%)
44	A86	M	316	-	47,50,50	0.48	1 (2%)	51,76,76	0.84	3 (5%)
40	CLA	N	304	14	64,68,73	1.76	9 (14%)	76,107,113	1.37	6 (7%)
41	KC2	Y	303	21	49,53,53	1.79	4 (8%)	60,89,89	1.01	4 (6%)
40	CLA	Y	307	21	64,68,73	1.80	9 (14%)	76,107,113	1.45	8 (10%)
40	CLA	D	304	4	60,64,73	1.84	10 (16%)	71,102,113	1.49	8 (11%)
40	CLA	a	819	23	65,69,73	1.76	9 (13%)	77,108,113	1.43	8 (10%)
42	DD6	I	213	-	40,45,45	0.26	0	51,67,67	0.80	2 (3%)
40	CLA	p	314	35	51,55,73	2.04	9 (17%)	60,91,113	1.61	7 (11%)
41	KC2	y	301	38	49,53,53	1.85	4 (8%)	60,89,89	1.07	3 (5%)
41	KC2	Y	302	-	49,53,53	1.87	4 (8%)	60,89,89	1.03	5 (8%)
41	KC2	W	303	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	5 (8%)
40	CLA	q	306	36	64,68,73	1.78	9 (14%)	76,107,113	1.39	7 (9%)
40	CLA	b	810	24	69,73,73	1.68	9 (13%)	82,113,113	1.26	8 (9%)
40	CLA	A	309	1	69,73,73	1.73	9 (13%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	F	311	-	51,55,73	2.00	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	z	305	39	64,68,73	1.74	9 (14%)	76,107,113	1.42	8 (10%)
40	CLA	z	312	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	7 (9%)
41	KC2	q	309	-	49,53,53	1.83	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	T	310	-	62,66,73	1.80	9 (14%)	73,104,113	1.40	7 (9%)
40	CLA	A	311	1	51,55,73	1.97	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	A	304	1	69,73,73	1.74	9 (13%)	82,113,113	1.44	10 (12%)
40	CLA	H	301	-	51,55,73	2.00	9 (17%)	60,91,113	1.48	8 (13%)
40	CLA	f	202	24	69,73,73	1.65	9 (13%)	82,113,113	1.23	6 (7%)
40	CLA	R	316	47	51,55,73	1.95	8 (15%)	60,91,113	1.34	7 (11%)
41	KC2	T	309	15	49,53,53	1.84	4 (8%)	60,89,89	1.05	3 (5%)
40	CLA	I	201	-	69,73,73	1.71	9 (13%)	82,113,113	1.30	6 (7%)
41	KC2	T	311	15	49,53,53	1.85	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	C	307	3	64,68,73	1.83	9 (14%)	76,107,113	1.52	8 (10%)
40	CLA	b	823	24	59,63,73	1.82	9 (15%)	70,101,113	1.46	7 (10%)
41	KC2	X	303	20	49,53,53	1.84	4 (8%)	60,89,89	1.04	5 (8%)
47	A1EB1	K	315	-	54,58,58	0.55	1 (1%)	60,85,85	0.50	0
40	CLA	a	815	23	69,73,73	1.73	9 (13%)	82,113,113	1.36	8 (9%)
40	CLA	t	307	-	59,63,73	1.90	9 (15%)	70,101,113	1.57	8 (11%)
41	KC2	p	309	-	49,53,53	1.84	4 (8%)	60,89,89	1.13	4 (6%)
40	CLA	Q	207	-	51,55,73	2.12	9 (17%)	60,91,113	1.73	11 (18%)
40	CLA	q	313	36	51,55,73	2.00	9 (17%)	60,91,113	1.52	7 (11%)
40	CLA	Z	310	-	59,63,73	1.94	9 (15%)	70,101,113	1.70	12 (17%)
42	DD6	p	322	-	40,45,45	0.18	0	51,67,67	0.68	0
43	LMG	D	318	-	40,40,55	0.80	0	48,48,63	1.23	5 (10%)
41	KC2	P	304	13	49,53,53	1.87	4 (8%)	60,89,89	1.08	5 (8%)
41	KC2	T	308	15	49,53,53	1.85	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	T	307	-	59,63,73	1.85	9 (15%)	70,101,113	1.46	7 (10%)
44	A86	W	301	-	47,50,50	0.43	1 (2%)	51,76,76	0.63	1 (1%)
44	A86	p	320	-	47,50,50	0.34	0	51,76,76	1.09	3 (5%)
47	A1EB1	Y	323	-	54,58,58	0.38	1 (1%)	60,85,85	0.87	3 (5%)
40	CLA	b	826	24	68,72,73	1.72	9 (13%)	80,111,113	1.30	5 (6%)
44	A86	G	211	-	47,50,50	0.53	1 (2%)	51,76,76	0.78	1 (1%)
40	CLA	b	841	24	69,73,73	1.67	9 (13%)	82,113,113	1.26	7 (8%)
44	A86	p	321	-	47,50,50	0.35	0	51,76,76	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	z	304	39	49,53,53	1.82	5 (10%)	60,89,89	1.11	5 (8%)
43	LMG	u	301	-	39,39,55	0.83	1 (2%)	47,47,63	1.29	5 (10%)
40	CLA	b	834	-	69,73,73	1.72	9 (13%)	82,113,113	1.30	5 (6%)
47	A1EB1	Z	320	-	54,58,58	0.29	0	60,85,85	0.62	0
42	DD6	J	313	-	40,45,45	0.19	0	51,67,67	0.69	1 (1%)
41	KC2	w	301	38	49,53,53	1.84	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	b	839	24	69,73,73	1.72	9 (13%)	82,113,113	1.40	6 (7%)
40	CLA	M	306	13	66,70,73	1.71	9 (13%)	78,109,113	1.30	5 (6%)
40	CLA	S	319	-	51,55,73	1.97	9 (17%)	60,91,113	1.39	6 (10%)
44	A86	X	318	-	47,50,50	0.62	1 (2%)	51,76,76	1.77	4 (7%)
47	A1EB1	v	324	-	54,58,58	0.62	1 (1%)	60,85,85	1.16	4 (6%)
41	KC2	p	303	-	49,53,53	1.87	4 (8%)	60,89,89	1.03	5 (8%)
40	CLA	L	306	12	51,55,73	2.09	9 (17%)	60,91,113	1.74	10 (16%)
40	CLA	J	308	10	59,63,73	1.84	10 (16%)	70,101,113	1.40	8 (11%)
40	CLA	a	825	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	6 (7%)
40	CLA	i	101	-	59,63,73	1.93	9 (15%)	70,101,113	1.58	8 (11%)
44	A86	S	315	-	47,50,50	0.36	1 (2%)	51,76,76	1.08	2 (3%)
47	A1EB1	q	322	-	54,58,58	0.35	0	60,85,85	0.80	1 (1%)
40	CLA	D	307	4	69,73,73	1.70	9 (13%)	82,113,113	1.37	10 (12%)
41	KC2	t	308	-	49,53,53	1.86	4 (8%)	60,89,89	1.10	5 (8%)
42	DD6	N	316	-	40,45,45	0.22	0	51,67,67	0.96	2 (3%)
40	CLA	J	311	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	7 (11%)
40	CLA	X	301	-	64,68,73	1.76	9 (14%)	76,107,113	1.32	6 (7%)
40	CLA	a	822	-	69,73,73	1.69	9 (13%)	82,113,113	1.34	8 (9%)
44	A86	T	312	-	47,50,50	0.46	1 (2%)	51,76,76	1.10	3 (5%)
40	CLA	E	305	5	64,68,73	1.81	9 (14%)	76,107,113	1.36	8 (10%)
42	DD6	Y	322	-	40,45,45	0.17	0	51,67,67	0.69	2 (3%)
40	CLA	D	302	43	62,66,73	1.82	9 (14%)	73,104,113	1.41	6 (8%)
40	CLA	v	311	-	67,71,73	1.78	9 (13%)	79,110,113	1.37	8 (10%)
40	CLA	B	303	-	51,55,73	1.98	9 (17%)	60,91,113	1.47	6 (10%)
44	A86	y	310	-	47,50,50	0.52	1 (2%)	51,76,76	1.09	4 (7%)
41	KC2	P	309	13	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
49	BCR	b	843	-	41,41,41	0.13	0	56,56,56	0.44	0
40	CLA	S	312	-	51,55,73	2.05	9 (17%)	60,91,113	1.64	9 (15%)
46	SQD	P	319	-	30,32,54	1.46	3 (10%)	40,43,65	1.36	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	z	306	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	7 (10%)
44	A86	o	316	-	47,50,50	0.55	1 (2%)	51,76,76	1.05	3 (5%)
49	BCR	b	847	-	41,41,41	0.19	0	56,56,56	0.58	0
40	CLA	b	824	24	69,73,73	1.66	9 (13%)	82,113,113	1.31	9 (10%)
40	CLA	A	302	-	64,68,73	1.78	9 (14%)	76,107,113	1.30	6 (7%)
42	DD6	v	320	-	40,45,45	0.20	0	51,67,67	0.70	0
41	KC2	S	303	17	49,53,53	1.86	4 (8%)	60,89,89	1.10	5 (8%)
40	CLA	Z	307	22	64,68,73	1.80	9 (14%)	76,107,113	1.40	9 (11%)
40	CLA	J	303	-	51,55,73	2.07	8 (15%)	60,91,113	1.56	8 (13%)
44	A86	T	315	-	47,50,50	0.66	1 (2%)	51,76,76	0.99	1 (1%)
40	CLA	H	306	8	54,58,73	1.94	9 (16%)	64,95,113	1.43	6 (9%)
40	CLA	C	302	-	51,55,73	2.03	9 (17%)	60,91,113	1.65	7 (11%)
44	A86	z	317	-	47,50,50	0.56	1 (2%)	51,76,76	1.48	2 (3%)
40	CLA	G	213	-	51,55,73	2.04	9 (17%)	60,91,113	1.63	9 (15%)
40	CLA	a	833	23	64,68,73	1.77	9 (14%)	76,107,113	1.38	7 (9%)
40	CLA	o	311	-	67,71,73	1.76	9 (13%)	79,110,113	1.37	6 (7%)
44	A86	R	315	-	47,50,50	0.49	1 (2%)	51,76,76	1.28	3 (5%)
42	DD6	F	315	-	40,45,45	0.21	0	51,67,67	0.92	1 (1%)
41	KC2	W	310	13	49,53,53	1.88	4 (8%)	60,89,89	1.06	4 (6%)
41	KC2	L	302	-	49,53,53	1.86	4 (8%)	60,89,89	1.07	5 (8%)
44	A86	p	317	-	47,50,50	0.56	1 (2%)	51,76,76	1.11	2 (3%)
44	A86	Y	315	-	47,50,50	0.58	1 (2%)	51,76,76	1.18	2 (3%)
48	A1EB4	M	319	-	53,58,63	0.60	1 (1%)	59,84,89	0.60	1 (1%)
40	CLA	O	306	15	64,68,73	1.78	10 (15%)	76,107,113	1.45	8 (10%)
44	A86	Q	210	-	47,50,50	0.42	1 (2%)	51,76,76	0.92	1 (1%)
44	A86	z	318	-	47,50,50	0.55	1 (2%)	51,76,76	0.91	2 (3%)
49	BCR	b	848	-	41,41,41	0.14	0	56,56,56	0.34	0
44	A86	v	317	-	47,50,50	0.45	1 (2%)	51,76,76	0.73	1 (1%)
41	KC2	x	303	-	49,53,53	1.88	4 (8%)	60,89,89	1.01	4 (6%)
41	KC2	K	309	11	49,53,53	1.84	4 (8%)	60,89,89	1.11	5 (8%)
40	CLA	E	310	-	64,68,73	1.77	9 (14%)	76,107,113	1.40	6 (7%)
41	KC2	z	310	39	49,53,53	1.83	4 (8%)	60,89,89	1.05	4 (6%)
41	KC2	R	309	15	49,53,53	1.88	4 (8%)	60,89,89	1.11	5 (8%)
40	CLA	a	850	-	69,73,73	1.67	9 (13%)	82,113,113	1.39	8 (9%)
41	KC2	N	312	14	49,53,53	1.83	4 (8%)	60,89,89	1.07	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	y	303	-	51,55,73	2.06	9 (17%)	60,91,113	1.66	8 (13%)
41	KC2	v	303	36	49,53,53	1.85	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	P	311	-	51,55,73	2.02	9 (17%)	60,91,113	1.59	10 (16%)
41	KC2	x	309	-	49,53,53	1.82	4 (8%)	60,89,89	1.16	5 (8%)
44	A86	q	316	-	47,50,50	0.54	1 (2%)	51,76,76	1.29	1 (1%)
40	CLA	Y	312	-	51,55,73	2.11	9 (17%)	60,91,113	1.76	11 (18%)
42	DD6	E	318	-	40,45,45	0.20	0	51,67,67	0.76	3 (5%)
40	CLA	b	828	24	59,63,73	1.87	9 (15%)	70,101,113	1.46	8 (11%)
43	LMG	x	301	-	39,39,55	0.87	1 (2%)	47,47,63	1.23	5 (10%)
40	CLA	N	306	-	64,68,73	1.77	9 (14%)	76,107,113	1.29	7 (9%)
41	KC2	p	304	35	49,53,53	1.84	4 (8%)	60,89,89	1.06	3 (5%)
41	KC2	N	308	14	49,53,53	1.86	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	v	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	5 (6%)
40	CLA	E	311	-	54,58,73	1.99	9 (16%)	64,95,113	1.50	7 (10%)
40	CLA	O	305	15	51,55,73	2.02	9 (17%)	60,91,113	1.52	7 (11%)
41	KC2	v	309	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	4 (6%)
44	A86	U	210	-	47,50,50	0.43	1 (2%)	51,76,76	1.06	3 (5%)
43	LMG	E	321	-	40,40,55	0.86	1 (2%)	48,48,63	1.28	7 (14%)
40	CLA	E	307	-	69,73,73	1.68	9 (13%)	82,113,113	1.20	5 (6%)
40	CLA	f	204	28	51,55,73	1.94	9 (17%)	60,91,113	1.49	7 (11%)
40	CLA	H	311	-	51,55,73	2.03	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	Z	301	-	64,68,73	1.78	9 (14%)	76,107,113	1.30	5 (6%)
40	CLA	a	814	-	54,58,73	1.94	9 (16%)	64,95,113	1.46	6 (9%)
40	CLA	a	823	23	59,63,73	1.84	9 (15%)	70,101,113	1.37	6 (8%)
42	DD6	Q	213	-	40,45,45	0.21	0	51,67,67	0.76	3 (5%)
40	CLA	w	305	-	53,57,73	1.97	9 (16%)	65,94,113	1.50	5 (7%)
42	DD6	o	319	-	40,45,45	0.21	0	51,67,67	0.78	3 (5%)
47	A1EB1	y	312	-	54,58,58	0.43	1 (1%)	60,85,85	0.70	1 (1%)
49	BCR	k	203	-	41,41,41	0.17	0	56,56,56	0.47	1 (1%)
40	CLA	S	302	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	7 (9%)
41	KC2	y	306	-	49,53,53	1.84	4 (8%)	60,89,89	1.02	3 (5%)
40	CLA	x	314	35	51,55,73	1.99	9 (17%)	60,91,113	1.53	7 (11%)
44	A86	M	320	-	47,50,50	0.37	1 (2%)	51,76,76	0.64	0
40	CLA	J	302	10	51,55,73	2.00	9 (17%)	60,91,113	1.43	6 (10%)
40	CLA	G	204	7	59,63,73	1.85	9 (15%)	70,101,113	1.43	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	x	317	-	47,50,50	0.55	1 (2%)	51,76,76	0.89	2 (3%)
41	KC2	M	303	13	49,53,53	1.85	4 (8%)	60,89,89	1.08	5 (8%)
40	CLA	o	301	-	64,68,73	1.80	9 (14%)	76,107,113	1.31	5 (6%)
42	DD6	D	315	-	40,45,45	0.18	0	51,67,67	0.94	2 (3%)
41	KC2	T	301	-	49,53,53	1.83	4 (8%)	60,89,89	1.05	4 (6%)
43	LMG	E	320	-	31,31,55	0.98	1 (3%)	39,39,63	1.18	2 (5%)
42	DD6	N	319	-	40,45,45	0.16	0	51,67,67	1.07	4 (7%)
41	KC2	M	302	13	49,53,53	1.86	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	l	202	-	69,73,73	1.70	9 (13%)	82,113,113	1.31	8 (9%)
40	CLA	y	302	38	51,55,73	2.09	9 (17%)	60,91,113	1.59	8 (13%)
41	KC2	u	309	-	49,53,53	1.83	4 (8%)	60,89,89	1.11	4 (6%)
44	A86	L	314	-	47,50,50	0.71	1 (2%)	51,76,76	1.06	2 (3%)
40	CLA	H	302	-	51,55,73	2.04	9 (17%)	60,91,113	1.51	8 (13%)
40	CLA	C	304	3	60,64,73	1.84	10 (16%)	71,102,113	1.43	11 (15%)
42	DD6	C	313	-	40,45,45	0.19	0	51,67,67	0.59	1 (1%)
40	CLA	z	302	-	64,68,73	1.75	9 (14%)	76,107,113	1.29	5 (6%)
46	SQD	W	318	-	30,32,54	1.48	4 (13%)	40,43,65	1.30	4 (10%)
47	A1EB1	y	314	-	54,58,58	0.55	1 (1%)	60,85,85	0.44	0
42	DD6	A	313	-	40,45,45	0.17	0	51,67,67	0.67	2 (3%)
40	CLA	a	804	23	65,69,73	1.79	10 (15%)	76,107,113	1.75	10 (13%)
40	CLA	b	825	-	69,73,73	1.65	9 (13%)	82,113,113	1.30	6 (7%)
40	CLA	I	206	9	69,73,73	1.70	9 (13%)	82,113,113	1.32	8 (9%)
44	A86	t	310	-	47,50,50	0.51	1 (2%)	51,76,76	0.96	3 (5%)
40	CLA	B	304	-	51,55,73	2.04	9 (17%)	60,91,113	1.53	7 (11%)
41	KC2	O	301	15	49,53,53	1.84	4 (8%)	60,89,89	1.10	5 (8%)
44	A86	X	321	-	47,50,50	0.79	1 (2%)	51,76,76	1.16	3 (5%)
40	CLA	a	839	45	69,73,73	1.68	9 (13%)	82,113,113	1.32	6 (7%)
40	CLA	x	302	-	69,73,73	1.78	9 (13%)	82,113,113	1.43	7 (8%)
44	A86	p	316	-	47,50,50	0.44	0	51,76,76	1.16	3 (5%)
40	CLA	S	311	-	51,55,73	2.11	9 (17%)	60,91,113	1.76	10 (16%)
44	A86	u	319	-	47,50,50	0.38	1 (2%)	51,76,76	1.27	4 (7%)
40	CLA	b	830	24	65,69,73	1.77	9 (13%)	77,108,113	1.51	9 (11%)
40	CLA	H	309	-	60,64,73	1.89	9 (15%)	71,102,113	1.64	9 (12%)
40	CLA	u	314	35	51,55,73	2.06	9 (17%)	60,91,113	1.69	8 (13%)
40	CLA	K	312	-	51,55,73	1.94	9 (17%)	60,91,113	1.47	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	G	210	-	40,45,45	0.22	0	51,67,67	0.73	2 (3%)
40	CLA	I	207	9	51,55,73	2.03	9 (17%)	60,91,113	1.61	7 (11%)
40	CLA	M	304	13	64,68,73	1.74	9 (14%)	76,107,113	1.34	5 (6%)
41	KC2	Y	308	-	49,53,53	1.83	4 (8%)	60,89,89	1.09	5 (8%)
41	KC2	q	308	36	49,53,53	1.83	4 (8%)	60,89,89	1.12	4 (6%)
40	CLA	q	307	36	64,68,73	1.80	9 (14%)	76,107,113	1.50	10 (13%)
40	CLA	p	312	-	51,55,73	2.02	9 (17%)	60,91,113	1.52	7 (11%)
40	CLA	b	838	-	69,73,73	1.71	9 (13%)	82,113,113	1.38	7 (8%)
40	CLA	a	832	23	69,73,73	1.70	9 (13%)	82,113,113	1.28	7 (8%)
40	CLA	P	306	13	51,55,73	1.97	9 (17%)	60,91,113	1.43	7 (11%)
40	CLA	W	308	-	64,68,73	1.86	9 (14%)	76,107,113	1.51	9 (11%)
44	A86	u	317	-	47,50,50	0.55	1 (2%)	51,76,76	1.19	2 (3%)
42	DD6	Q	214	-	40,45,45	0.24	0	51,67,67	0.85	1 (1%)
44	A86	o	315	-	47,50,50	0.54	1 (2%)	51,76,76	1.02	3 (5%)
47	A1EB1	L	316	-	54,58,58	0.54	1 (1%)	60,85,85	0.77	1 (1%)
42	DD6	L	315	-	40,45,45	0.15	0	51,67,67	0.53	1 (1%)
40	CLA	b	816	24	51,55,73	2.00	9 (17%)	60,91,113	1.63	9 (15%)
42	DD6	z	321	-	40,45,45	0.22	0	51,67,67	0.76	1 (1%)
43	LMG	j	101	-	30,30,55	0.91	1 (3%)	38,38,63	1.30	3 (7%)
47	A1EB1	t	314	-	54,58,58	0.61	1 (1%)	60,85,85	0.91	3 (5%)
40	CLA	U	205	-	51,55,73	2.03	9 (17%)	60,91,113	1.56	8 (13%)
44	A86	x	318	-	47,50,50	0.48	1 (2%)	51,76,76	1.19	2 (3%)
41	KC2	X	309	-	49,53,53	1.88	4 (8%)	60,89,89	1.09	2 (3%)
40	CLA	x	311	-	59,63,73	1.94	9 (15%)	70,101,113	1.74	12 (17%)
40	CLA	v	301	-	59,63,73	1.87	9 (15%)	70,101,113	1.42	6 (8%)
40	CLA	z	308	39	64,68,73	1.73	9 (14%)	76,107,113	1.44	10 (13%)
40	CLA	q	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.27	5 (6%)
44	A86	W	314	-	47,50,50	0.65	1 (2%)	51,76,76	0.90	2 (3%)
44	A86	Y	318	-	47,50,50	0.65	1 (2%)	51,76,76	0.94	3 (5%)
44	A86	q	319	-	47,50,50	0.35	0	51,76,76	1.34	4 (7%)
42	DD6	R	314	-	40,45,45	0.18	0	51,67,67	0.94	1 (1%)
47	A1EB1	u	322	-	54,58,58	0.35	0	60,85,85	1.32	6 (10%)
47	A1EB1	x	321	-	54,58,58	0.52	1 (1%)	60,85,85	0.58	1 (1%)
40	CLA	F	310	-	51,55,73	1.99	10 (19%)	60,91,113	1.53	10 (16%)
40	CLA	U	202	18	59,63,73	1.91	9 (15%)	70,101,113	1.55	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	Y	311	-	51,55,73	2.02	9 (17%)	60,91,113	1.46	7 (11%)
40	CLA	p	305	35	51,55,73	1.92	9 (17%)	60,91,113	1.57	7 (11%)
40	CLA	T	304	15	64,68,73	1.78	9 (14%)	76,107,113	1.36	6 (7%)
40	CLA	Z	312	-	51,55,73	2.09	9 (17%)	60,91,113	1.67	14 (23%)
40	CLA	S	301	-	64,68,73	1.82	9 (14%)	76,107,113	1.39	6 (7%)
44	A86	x	316	-	47,50,50	0.46	1 (2%)	51,76,76	1.25	3 (5%)
41	KC2	F	302	6	49,53,53	1.85	4 (8%)	60,89,89	1.07	4 (6%)
41	KC2	Z	309	-	49,53,53	1.89	4 (8%)	60,89,89	1.00	2 (3%)
44	A86	F	317	-	47,50,50	0.42	1 (2%)	51,76,76	0.83	2 (3%)
42	DD6	E	315	-	40,45,45	0.20	0	51,67,67	0.89	3 (5%)
42	DD6	P	315	-	40,45,45	0.39	0	51,67,67	0.94	2 (3%)
47	A1EB1	G	212	-	54,58,58	0.58	1 (1%)	60,85,85	0.75	1 (1%)
40	CLA	w	303	38	51,55,73	2.02	9 (17%)	60,91,113	1.52	6 (10%)
40	CLA	B	301	2	51,55,73	2.07	9 (17%)	60,91,113	1.77	9 (15%)
40	CLA	a	842	-	69,73,73	1.66	9 (13%)	82,113,113	1.26	7 (8%)
40	CLA	D	312	4	59,63,73	1.89	9 (15%)	70,101,113	1.43	6 (8%)
40	CLA	b	807	-	69,73,73	1.66	9 (13%)	82,113,113	1.23	8 (9%)
41	KC2	R	308	15	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
44	A86	u	318	-	47,50,50	0.44	1 (2%)	51,76,76	1.37	3 (5%)
47	A1EB1	z	323	-	54,58,58	0.52	1 (1%)	60,85,85	1.00	2 (3%)
47	A1EB1	t	313	-	54,58,58	0.41	1 (1%)	60,85,85	0.85	4 (6%)
40	CLA	b	811	24	51,55,73	1.93	9 (17%)	60,91,113	1.53	8 (13%)
41	KC2	T	302	-	49,53,53	1.86	5 (10%)	60,89,89	1.07	4 (6%)
41	KC2	C	303	-	49,53,53	1.86	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	Y	301	-	64,68,73	1.80	9 (14%)	76,107,113	1.31	6 (7%)
40	CLA	D	303	4	64,68,73	1.74	10 (15%)	76,107,113	1.36	7 (9%)
40	CLA	l	203	-	68,72,73	1.70	10 (14%)	80,111,113	1.51	9 (11%)
42	DD6	M	314	-	40,45,45	0.21	0	51,67,67	0.74	1 (1%)
40	CLA	a	817	23	54,58,73	1.90	9 (16%)	64,95,113	1.43	6 (9%)
40	CLA	O	316	47	51,55,73	1.97	9 (17%)	60,91,113	1.37	6 (10%)
44	A86	M	315	-	47,50,50	0.56	1 (2%)	51,76,76	1.15	3 (5%)
44	A86	F	313	-	47,50,50	0.42	1 (2%)	51,76,76	0.80	2 (3%)
44	A86	o	317	-	47,50,50	0.47	1 (2%)	51,76,76	0.99	3 (5%)
40	CLA	Q	203	-	53,57,73	1.98	9 (16%)	62,93,113	1.89	9 (14%)
40	CLA	D	308	4	59,63,73	1.85	9 (15%)	70,101,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	z	324	-	51,55,73	2.04	9 (17%)	60,91,113	1.56	9 (15%)
40	CLA	b	803	-	69,73,73	1.70	9 (13%)	82,113,113	1.36	8 (9%)
44	A86	Z	317	-	47,50,50	0.58	1 (2%)	51,76,76	0.82	1 (1%)
40	CLA	u	302	-	69,73,73	1.72	9 (13%)	82,113,113	1.35	8 (9%)
44	A86	G	209	-	47,50,50	0.54	1 (2%)	51,76,76	1.14	3 (5%)
40	CLA	R	305	15	64,68,73	1.78	9 (14%)	76,107,113	1.38	5 (6%)
40	CLA	A	303	1	65,69,73	1.73	9 (13%)	77,108,113	1.32	7 (9%)
51	SF4	c	102	-	0,12,12	-	-	-		
47	A1EB1	Z	321	-	54,58,58	0.51	1 (1%)	60,85,85	0.40	0
42	DD6	w	312	-	40,45,45	0.17	0	51,67,67	0.97	3 (5%)
40	CLA	M	305	13	64,68,73	1.75	9 (14%)	76,107,113	1.35	7 (9%)
41	KC2	Z	303	22	49,53,53	1.81	4 (8%)	60,89,89	1.01	4 (6%)
49	BCR	r	201	-	41,41,41	0.19	0	56,56,56	0.40	0
40	CLA	k	202	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	7 (10%)
40	CLA	C	308	-	51,55,73	2.11	9 (17%)	60,91,113	1.69	10 (16%)
40	CLA	b	833	24	64,68,73	1.73	9 (14%)	76,107,113	1.37	9 (11%)
44	A86	p	318	-	47,50,50	0.47	1 (2%)	51,76,76	1.14	3 (5%)
40	CLA	o	312	-	51,55,73	2.06	9 (17%)	60,91,113	1.61	7 (11%)
41	KC2	O	309	15	49,53,53	1.83	4 (8%)	60,89,89	1.12	5 (8%)
41	KC2	t	306	-	49,53,53	1.83	4 (8%)	60,89,89	1.03	3 (5%)
49	BCR	m	101	-	41,41,41	0.17	0	56,56,56	0.34	0
51	SF4	b	804	-	0,12,12	-	-	-		
40	CLA	a	829	-	69,73,73	1.72	9 (13%)	82,113,113	1.41	9 (10%)
41	KC2	o	309	34	49,53,53	1.85	4 (8%)	60,89,89	1.04	4 (6%)
41	KC2	Q	201	16	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	v	305	-	64,68,73	1.79	9 (14%)	76,107,113	1.42	9 (11%)
47	A1EB1	Z	319	-	54,58,58	0.50	1 (1%)	60,85,85	0.71	1 (1%)
40	CLA	X	304	-	51,55,73	1.97	9 (17%)	60,91,113	1.46	6 (10%)
41	KC2	L	308	12	49,53,53	1.86	4 (8%)	60,89,89	0.99	3 (5%)
40	CLA	P	305	13	64,68,73	1.73	9 (14%)	76,107,113	1.35	7 (9%)
43	LMG	S	322	-	39,39,55	0.94	2 (5%)	47,47,63	1.22	4 (8%)
40	CLA	a	816	23	69,73,73	1.68	9 (13%)	82,113,113	1.46	9 (10%)
40	CLA	p	306	35	51,55,73	2.00	9 (17%)	60,91,113	1.50	7 (11%)
41	KC2	x	304	35	49,53,53	1.83	4 (8%)	60,89,89	1.03	3 (5%)
42	DD6	C	310	-	40,45,45	0.19	0	51,67,67	0.87	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	B	305	-	40,45,45	0.19	0	51,67,67	0.80	2 (3%)
47	A1EB1	v	322	-	54,58,58	0.35	0	60,85,85	0.82	1 (1%)
40	CLA	X	306	20	59,63,73	1.87	9 (15%)	70,101,113	1.53	10 (14%)
40	CLA	a	830	-	62,66,73	1.77	9 (14%)	73,104,113	1.41	9 (12%)
40	CLA	F	307	6	61,67,73	1.72	9 (14%)	74,105,113	1.49	8 (10%)
44	A86	H	315	-	47,50,50	0.48	1 (2%)	51,76,76	1.25	4 (7%)
47	A1EB1	p	324	-	54,58,58	0.49	1 (1%)	60,85,85	0.44	1 (1%)
41	KC2	A	310	1	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
40	CLA	B	307	-	51,55,73	2.04	9 (17%)	60,91,113	1.69	9 (15%)
40	CLA	P	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.32	7 (9%)
42	DD6	Z	318	-	40,45,45	0.22	0	51,67,67	0.91	2 (3%)
45	LHG	a	849	40	29,29,48	0.78	0	32,35,54	1.23	2 (6%)
42	DD6	J	314	-	40,45,45	0.19	0	51,67,67	0.72	3 (5%)
40	CLA	W	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.31	9 (11%)
40	CLA	J	306	10	56,60,73	1.93	9 (16%)	65,97,113	1.51	8 (12%)
40	CLA	t	302	38	51,55,73	2.01	9 (17%)	60,91,113	1.50	6 (10%)
40	CLA	p	313	-	59,63,73	1.88	9 (15%)	70,101,113	1.32	6 (8%)
41	KC2	Z	302	-	49,53,53	1.87	4 (8%)	60,89,89	1.03	4 (6%)
42	DD6	J	317	-	40,45,45	0.20	0	51,67,67	0.77	1 (1%)
40	CLA	a	838	23	59,63,73	1.90	9 (15%)	70,101,113	1.55	7 (10%)
40	CLA	Z	311	22	67,71,73	1.77	9 (13%)	79,110,113	1.40	8 (10%)
40	CLA	X	311	20	67,71,73	1.78	9 (13%)	79,110,113	1.39	7 (8%)
41	KC2	H	303	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	H	305	8	64,68,73	1.76	9 (14%)	76,107,113	1.34	10 (13%)
41	KC2	t	301	38	49,53,53	1.84	5 (10%)	60,89,89	1.05	4 (6%)
40	CLA	D	301	4	59,63,73	1.82	9 (15%)	70,101,113	1.37	6 (8%)
40	CLA	q	304	-	56,60,73	1.86	9 (16%)	65,97,113	1.39	8 (12%)
40	CLA	t	309	-	51,55,73	2.01	9 (17%)	60,91,113	1.51	6 (10%)
42	DD6	F	314	-	40,45,45	0.29	0	51,67,67	0.85	3 (5%)
47	A1EB1	o	321	-	54,58,58	0.51	1 (1%)	60,85,85	0.65	0
41	KC2	O	303	15	49,53,53	1.85	4 (8%)	60,89,89	1.06	5 (8%)
40	CLA	D	311	-	51,55,73	2.01	9 (17%)	60,91,113	1.64	7 (11%)
44	A86	X	320	-	47,50,50	0.50	1 (2%)	51,76,76	0.92	2 (3%)
40	CLA	b	809	24	64,68,73	1.83	9 (14%)	76,107,113	1.54	9 (11%)
42	DD6	K	310	-	40,45,45	0.22	0	51,67,67	0.62	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	F	304	6	59,63,73	1.93	9 (15%)	70,101,113	1.49	10 (14%)
43	LMG	W	317	-	39,39,55	0.84	0	47,47,63	1.29	6 (12%)
40	CLA	v	313	36	51,55,73	2.03	9 (17%)	60,91,113	1.61	8 (13%)
40	CLA	C	301	3	51,55,73	2.03	9 (17%)	60,91,113	1.55	7 (11%)
42	DD6	D	316	-	40,45,45	0.21	0	51,67,67	0.63	0
40	CLA	I	205	9	60,64,73	1.82	9 (15%)	71,102,113	1.36	8 (11%)
40	CLA	P	313	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	6 (7%)
40	CLA	E	314	5	51,55,73	2.08	9 (17%)	60,91,113	1.95	12 (20%)
40	CLA	a	806	23	69,73,73	1.72	10 (14%)	82,113,113	1.45	7 (8%)
40	CLA	o	306	34	64,68,73	1.80	10 (15%)	76,107,113	1.40	9 (11%)
41	KC2	M	308	13	49,53,53	1.84	4 (8%)	60,89,89	1.11	5 (8%)
41	KC2	u	304	35	49,53,53	1.83	4 (8%)	60,89,89	1.07	3 (5%)
40	CLA	a	821	23	69,73,73	1.69	9 (13%)	82,113,113	1.26	7 (8%)
47	A1EB1	o	322	-	54,58,58	0.54	1 (1%)	60,85,85	0.71	1 (1%)
40	CLA	H	308	8	51,55,73	1.98	9 (17%)	60,91,113	1.46	5 (8%)
41	KC2	v	302	-	49,53,53	1.87	4 (8%)	60,89,89	1.06	4 (6%)
41	KC2	W	304	13	49,53,53	1.83	4 (8%)	60,89,89	1.07	6 (10%)
40	CLA	y	309	-	59,63,73	1.92	9 (15%)	70,101,113	1.59	8 (11%)
46	SQD	k	205	-	34,36,54	1.39	4 (11%)	44,47,65	1.25	3 (6%)
40	CLA	b	827	24	64,68,73	1.80	9 (14%)	76,107,113	1.46	7 (9%)
42	DD6	K	311	-	40,45,45	0.17	0	51,67,67	0.72	2 (3%)
45	LHG	F	319	-	39,39,48	0.68	1 (2%)	42,45,54	1.19	2 (4%)
41	KC2	Q	216	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	4 (6%)
42	DD6	E	317	-	40,45,45	0.18	0	51,67,67	0.69	2 (3%)
47	A1EB1	v	321	-	54,58,58	0.52	1 (1%)	60,85,85	0.94	3 (5%)
42	DD6	A	312	-	40,45,45	0.20	0	51,67,67	0.88	1 (1%)
41	KC2	u	310	-	49,53,53	1.82	4 (8%)	60,89,89	1.04	3 (5%)
40	CLA	p	302	-	69,73,73	1.72	9 (13%)	82,113,113	1.37	8 (9%)
40	CLA	E	306	5	59,63,73	1.84	9 (15%)	70,101,113	1.40	6 (8%)
42	DD6	y	311	-	40,45,45	0.18	0	51,67,67	0.99	3 (5%)
40	CLA	a	807	-	60,64,73	1.82	9 (15%)	71,102,113	1.45	7 (9%)
40	CLA	a	820	23	64,68,73	1.81	9 (14%)	76,107,113	1.49	8 (10%)
44	A86	X	316	-	47,50,50	0.51	1 (2%)	51,76,76	1.14	2 (3%)
44	A86	t	316	-	47,50,50	0.56	1 (2%)	51,76,76	0.52	0
40	CLA	T	306	15	64,68,73	1.76	10 (15%)	76,107,113	1.36	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	o	318	-	47,50,50	0.58	1 (2%)	51,76,76	0.53	0
40	CLA	S	306	17	60,64,73	1.82	9 (15%)	71,102,113	1.37	8 (11%)
42	DD6	o	320	-	40,45,45	0.18	0	51,67,67	0.59	1 (1%)
41	KC2	N	301	14	49,53,53	1.84	4 (8%)	60,89,89	1.07	2 (3%)
44	A86	z	320	-	47,50,50	0.57	1 (2%)	51,76,76	0.66	1 (1%)
41	KC2	S	304	17	49,53,53	1.83	4 (8%)	60,89,89	1.09	5 (8%)
41	KC2	K	305	11	49,53,53	1.82	4 (8%)	60,89,89	1.09	4 (6%)
40	CLA	L	310	-	51,55,73	2.04	9 (17%)	60,91,113	1.63	9 (15%)
42	DD6	C	312	-	40,45,45	0.16	0	51,67,67	1.03	2 (3%)
40	CLA	R	304	15	55,59,73	1.90	9 (16%)	64,96,113	1.58	10 (15%)
40	CLA	Z	305	22	59,63,73	1.83	9 (15%)	70,101,113	1.30	6 (8%)
42	DD6	D	313	-	40,45,45	0.18	0	51,67,67	0.85	2 (3%)
40	CLA	a	837	23	59,63,73	1.86	9 (15%)	70,101,113	1.38	6 (8%)
40	CLA	E	313	5	51,55,73	1.97	9 (17%)	60,91,113	1.50	6 (10%)
42	DD6	D	314	-	40,45,45	0.20	0	51,67,67	0.86	1 (1%)
44	A86	Y	317	41	47,50,50	0.56	1 (2%)	51,76,76	0.99	3 (5%)
49	BCR	l	208	-	41,41,41	0.20	0	56,56,56	0.67	2 (3%)
41	KC2	L	303	12	49,53,53	1.84	4 (8%)	60,89,89	1.05	5 (8%)
41	KC2	o	302	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	K	304	11	64,68,73	1.73	9 (14%)	76,107,113	1.38	6 (7%)
41	KC2	z	309	39	49,53,53	1.81	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	S	313	-	51,55,73	1.95	9 (17%)	60,91,113	1.43	7 (11%)
40	CLA	a	810	-	64,68,73	1.76	9 (14%)	76,107,113	1.40	8 (10%)
44	A86	W	316	-	47,50,50	0.42	1 (2%)	51,76,76	0.71	1 (1%)
44	A86	Z	316	-	47,50,50	0.59	1 (2%)	51,76,76	1.18	3 (5%)
40	CLA	a	852	-	59,63,73	1.84	9 (15%)	70,101,113	1.37	5 (7%)
45	LHG	S	323	-	39,39,48	0.69	2 (5%)	42,45,54	1.28	4 (9%)
40	CLA	b	818	24	66,70,73	1.71	9 (13%)	78,109,113	1.35	7 (8%)
44	A86	S	317	-	47,50,50	0.45	1 (2%)	51,76,76	0.95	2 (3%)
44	A86	Q	215	-	47,50,50	0.42	1 (2%)	51,76,76	1.20	2 (3%)
40	CLA	W	311	-	59,63,73	1.88	9 (15%)	70,101,113	1.49	7 (10%)
40	CLA	A	308	-	59,63,73	1.85	9 (15%)	70,101,113	1.34	5 (7%)
41	KC2	q	303	36	49,53,53	1.83	4 (8%)	60,89,89	1.02	3 (5%)
40	CLA	G	201	7	51,55,73	1.98	9 (17%)	60,91,113	1.43	6 (10%)
40	CLA	L	312	-	51,55,73	2.04	9 (17%)	60,91,113	1.48	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	P	310	-	49,53,53	1.84	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	u	313	-	59,63,73	1.85	9 (15%)	70,101,113	1.31	6 (8%)
42	DD6	t	312	-	40,45,45	0.15	0	51,67,67	1.04	4 (7%)
44	A86	O	315	-	47,50,50	0.39	1 (2%)	51,76,76	0.73	1 (1%)
44	A86	T	319	-	47,50,50	0.61	1 (2%)	51,76,76	0.78	2 (3%)
49	BCR	a	845	-	41,41,41	0.13	0	56,56,56	0.47	0
41	KC2	q	302	36	49,53,53	1.88	4 (8%)	60,89,89	1.09	6 (10%)
42	DD6	T	314	-	40,45,45	0.20	0	51,67,67	0.66	1 (1%)
40	CLA	R	306	15	64,68,73	1.78	9 (14%)	76,107,113	1.37	7 (9%)
40	CLA	S	314	17	59,63,73	1.88	9 (15%)	70,101,113	1.54	7 (10%)
40	CLA	q	311	-	67,71,73	1.80	9 (13%)	79,110,113	1.39	8 (10%)
44	A86	Z	315	-	47,50,50	0.48	1 (2%)	51,76,76	1.08	3 (5%)
40	CLA	k	201	31	59,63,73	1.84	9 (15%)	70,101,113	1.44	7 (10%)
42	DD6	J	301	-	40,45,45	0.22	0	51,67,67	0.69	1 (1%)
47	A1EB1	q	321	-	54,58,58	0.53	1 (1%)	60,85,85	0.97	3 (5%)
40	CLA	N	305	14	59,63,73	1.83	9 (15%)	70,101,113	1.41	6 (8%)
44	A86	O	313	-	47,50,50	0.30	0	51,76,76	0.82	2 (3%)
44	A86	Y	321	-	47,50,50	0.63	1 (2%)	51,76,76	0.75	1 (1%)
40	CLA	W	307	13	69,73,73	1.69	9 (13%)	82,113,113	1.27	8 (9%)
40	CLA	b	840	-	69,73,73	1.75	9 (13%)	82,113,113	1.39	8 (9%)
41	KC2	P	303	13	49,53,53	1.88	4 (8%)	60,89,89	1.07	3 (5%)
40	CLA	O	310	-	51,55,73	2.06	9 (17%)	60,91,113	1.70	11 (18%)
41	KC2	u	303	-	49,53,53	1.88	4 (8%)	60,89,89	1.01	4 (6%)
40	CLA	b	832	24	69,73,73	1.72	9 (13%)	82,113,113	1.45	8 (9%)
40	CLA	f	205	-	51,55,73	1.97	9 (17%)	60,91,113	1.43	7 (11%)
43	LMG	P	318	-	39,39,55	0.99	3 (7%)	47,47,63	1.32	7 (14%)
44	A86	v	316	-	47,50,50	0.56	1 (2%)	51,76,76	1.30	1 (1%)
40	CLA	Y	305	21	59,63,73	1.85	9 (15%)	70,101,113	1.41	7 (10%)
41	KC2	P	302	-	49,53,53	1.83	4 (8%)	60,89,89	1.08	5 (8%)
44	A86	u	316	-	47,50,50	0.43	1 (2%)	51,76,76	1.25	3 (5%)
40	CLA	E	302	5	51,55,73	2.02	9 (17%)	60,91,113	1.72	8 (13%)
40	CLA	u	312	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	5 (6%)
42	DD6	X	322	-	40,45,45	0.18	0	51,67,67	0.65	1 (1%)
40	CLA	o	305	34	59,63,73	1.86	9 (15%)	70,101,113	1.38	8 (11%)
41	KC2	z	303	39	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	A	307	1	64,68,73	1.80	10 (15%)	76,107,113	1.44	8 (10%)
40	CLA	l	205	32	69,73,73	1.75	9 (13%)	82,113,113	1.38	8 (9%)
40	CLA	z	307	-	64,68,73	1.80	9 (14%)	76,107,113	1.47	10 (13%)
40	CLA	F	308	-	59,63,73	1.88	9 (15%)	70,101,113	1.43	6 (8%)
40	CLA	a	805	23,40	58,62,73	1.82	9 (15%)	68,99,113	1.41	6 (8%)
47	A1EB1	q	323	-	54,58,58	0.54	1 (1%)	60,85,85	0.54	0
40	CLA	U	208	-	51,55,73	1.94	9 (17%)	60,91,113	1.43	9 (15%)
41	KC2	X	308	20	49,53,53	1.84	4 (8%)	60,89,89	1.02	3 (5%)
40	CLA	O	307	-	66,70,73	1.76	9 (13%)	78,109,113	1.33	6 (7%)
47	A1EB1	y	313	-	54,58,58	0.44	1 (1%)	60,85,85	0.82	2 (3%)
40	CLA	K	306	-	64,68,73	1.73	9 (14%)	76,107,113	1.39	10 (13%)
49	BCR	a	844	-	41,41,41	0.17	0	56,56,56	0.47	0
44	A86	X	315	-	47,50,50	0.50	0	51,76,76	1.66	6 (11%)
44	A86	O	312	-	47,50,50	0.46	1 (2%)	51,76,76	0.97	2 (3%)
40	CLA	E	309	-	64,68,73	1.77	9 (14%)	76,107,113	1.34	7 (9%)
44	A86	q	317	-	47,50,50	0.48	1 (2%)	51,76,76	0.87	1 (1%)
47	A1EB1	R	317	40	54,58,58	0.58	1 (1%)	60,85,85	1.15	2 (3%)
41	KC2	S	310	-	49,53,53	1.84	4 (8%)	60,89,89	1.04	3 (5%)
40	CLA	u	308	35	64,68,73	1.78	9 (14%)	76,107,113	1.42	7 (9%)
40	CLA	a	834	-	64,68,73	1.80	9 (14%)	76,107,113	1.44	8 (10%)
40	CLA	x	306	35	64,68,73	1.73	9 (14%)	76,107,113	1.32	9 (11%)
40	CLA	a	835	-	69,73,73	1.67	9 (13%)	82,113,113	1.30	7 (8%)
42	DD6	U	209	-	40,45,45	0.27	0	51,67,67	0.81	2 (3%)
40	CLA	L	307	-	59,63,73	1.84	9 (15%)	70,101,113	1.40	6 (8%)
44	A86	N	314	-	47,50,50	0.53	1 (2%)	51,76,76	1.10	4 (7%)
41	KC2	K	302	11	49,53,53	1.85	4 (8%)	60,89,89	1.07	3 (5%)
44	A86	v	319	-	47,50,50	0.36	0	51,76,76	1.32	4 (7%)
40	CLA	T	305	15	54,58,73	1.92	9 (16%)	64,95,113	1.42	6 (9%)
40	CLA	Y	306	21	64,68,73	1.79	10 (15%)	76,107,113	1.44	9 (11%)
40	CLA	S	305	-	56,60,73	1.95	9 (16%)	65,97,113	1.64	11 (16%)
40	CLA	z	313	-	51,55,73	2.06	9 (17%)	60,91,113	1.64	8 (13%)
41	KC2	R	302	15	49,53,53	1.88	5 (10%)	60,89,89	1.07	5 (8%)
44	A86	z	319	-	47,50,50	0.53	1 (2%)	51,76,76	0.96	1 (1%)
47	A1EB1	O	317	40	54,58,58	0.54	1 (1%)	60,85,85	0.80	1 (1%)
40	CLA	b	822	-	68,72,73	1.75	9 (13%)	80,111,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	v	306	36	64,68,73	1.77	9 (14%)	76,107,113	1.35	7 (9%)
43	LMG	a	802	-	35,35,55	0.89	1 (2%)	43,43,63	1.31	7 (16%)
40	CLA	y	304	-	64,68,73	1.79	10 (15%)	76,107,113	1.36	10 (13%)
50	PQN	b	849	-	29,29,34	0.45	0	37,39,45	0.79	1 (2%)
40	CLA	H	304	-	51,55,73	2.02	10 (19%)	60,91,113	1.53	9 (15%)
40	CLA	b	808	-	69,73,73	1.73	9 (13%)	82,113,113	1.21	9 (10%)
44	A86	o	314	-	47,50,50	0.47	1 (2%)	51,76,76	1.41	5 (9%)
40	CLA	x	313	-	59,63,73	1.85	9 (15%)	70,101,113	1.31	7 (10%)
40	CLA	b	812	24	64,68,73	1.74	9 (14%)	76,107,113	1.26	7 (9%)
44	A86	t	311	-	47,50,50	0.62	1 (2%)	51,76,76	1.22	3 (5%)
47	A1EB1	F	322	-	54,58,58	0.52	1 (1%)	60,85,85	0.42	0
41	KC2	x	310	-	49,53,53	1.84	4 (8%)	60,89,89	1.05	4 (6%)
41	KC2	S	309	17	49,53,53	1.82	4 (8%)	60,89,89	1.12	5 (8%)
44	A86	Z	314	-	47,50,50	0.50	1 (2%)	51,76,76	1.34	3 (5%)
41	KC2	O	311	-	49,53,53	1.84	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	Y	313	21	51,55,73	2.09	9 (17%)	60,91,113	1.72	9 (15%)
42	DD6	E	316	-	40,45,45	0.21	0	51,67,67	0.86	3 (5%)
47	A1EB1	L	318	-	54,58,58	0.57	1 (1%)	60,85,85	0.73	1 (1%)
40	CLA	D	309	-	62,66,73	1.81	9 (14%)	73,104,113	1.35	6 (8%)
40	CLA	Q	205	16	65,69,73	1.80	9 (13%)	76,107,113	1.74	12 (15%)
49	BCR	l	207	-	41,41,41	0.25	0	56,56,56	0.92	3 (5%)
43	LMG	M	317	-	39,39,55	0.88	2 (5%)	47,47,63	1.34	4 (8%)
41	KC2	w	306	38	49,53,53	1.84	4 (8%)	60,89,89	1.05	5 (8%)
45	LHG	a	848	-	47,47,48	0.62	0	50,53,54	1.14	3 (6%)
42	DD6	A	314	-	40,45,45	0.16	0	51,67,67	0.77	1 (1%)
40	CLA	G	203	7	56,62,73	1.75	8 (14%)	68,99,113	1.56	11 (16%)
43	LMG	F	318	-	39,39,55	0.78	0	47,47,63	1.34	6 (12%)
40	CLA	b	801	-	67,71,73	1.75	10 (14%)	79,110,113	1.42	12 (15%)
44	A86	Y	320	-	47,50,50	0.62	1 (2%)	51,76,76	1.41	3 (5%)
40	CLA	b	802	-	69,73,73	1.67	9 (13%)	82,113,113	1.29	8 (9%)
40	CLA	C	309	-	51,55,73	2.06	9 (17%)	60,91,113	1.55	7 (11%)
44	A86	N	321	-	47,50,50	0.46	1 (2%)	51,76,76	0.87	2 (3%)
40	CLA	t	305	-	53,57,73	1.99	9 (16%)	65,94,113	1.51	6 (9%)
47	A1EB1	p	323	-	54,58,58	0.38	0	60,85,85	1.27	5 (8%)
44	A86	Y	316	-	47,50,50	0.44	1 (2%)	51,76,76	0.63	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	N	313	14	49,53,53	1.84	4 (8%)	60,89,89	1.03	4 (6%)
41	KC2	J	304	-	49,53,53	1.85	4 (8%)	60,89,89	1.09	4 (6%)
40	CLA	b	829	-	51,55,73	2.02	9 (17%)	60,91,113	1.44	8 (13%)
44	A86	q	314	-	47,50,50	0.59	1 (2%)	51,76,76	1.43	5 (9%)
44	A86	v	314	-	47,50,50	0.54	1 (2%)	51,76,76	1.54	5 (9%)
42	DD6	D	317	-	40,45,45	0.19	0	51,67,67	0.79	2 (3%)
40	CLA	b	813	24	54,58,73	1.89	9 (16%)	64,95,113	1.48	8 (12%)
48	A1EB4	W	319	-	53,58,63	0.67	1 (1%)	59,84,89	0.68	1 (1%)
44	A86	C	311	-	47,50,50	0.69	1 (2%)	51,76,76	1.02	3 (5%)
41	KC2	u	315	-	49,53,53	1.84	4 (8%)	60,89,89	1.11	4 (6%)
46	SQD	I	215	-	52,54,54	1.13	3 (5%)	62,65,65	1.10	3 (4%)
41	KC2	Y	309	21,44	49,53,53	1.84	4 (8%)	60,89,89	1.01	3 (5%)
44	A86	S	316	-	47,50,50	0.53	1 (2%)	51,76,76	1.09	4 (7%)
42	DD6	I	211	-	40,45,45	0.22	0	51,67,67	1.02	3 (5%)
43	LMG	a	801	-	35,35,55	0.95	1 (2%)	43,43,63	1.18	4 (9%)
40	CLA	X	305	-	54,58,73	1.97	9 (16%)	64,95,113	1.44	8 (12%)
40	CLA	b	819	24	68,72,73	1.71	9 (13%)	80,111,113	1.31	6 (7%)
44	A86	q	324	-	47,50,50	0.34	0	51,76,76	1.06	3 (5%)
40	CLA	X	310	-	59,63,73	1.94	8 (13%)	70,101,113	1.71	11 (15%)
40	CLA	N	307	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	6 (7%)
40	CLA	a	808	-	69,73,73	1.76	9 (13%)	82,113,113	1.55	10 (12%)
43	LMG	L	319	-	37,37,55	0.84	0	45,45,63	1.24	4 (8%)
44	A86	P	314	-	47,50,50	0.40	0	51,76,76	0.97	3 (5%)
40	CLA	y	305	-	53,57,73	1.99	9 (16%)	65,94,113	1.50	7 (10%)
40	CLA	K	308	11	63,67,73	1.77	9 (14%)	74,105,113	1.47	9 (12%)
47	A1EB1	S	320	-	54,58,58	0.49	1 (1%)	60,85,85	0.85	2 (3%)
41	KC2	M	301	13	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
40	CLA	J	305	10	59,63,73	1.89	10 (16%)	70,101,113	1.42	6 (8%)
40	CLA	F	321	-	64,68,73	1.78	9 (14%)	76,107,113	1.39	8 (10%)
41	KC2	y	307	-	49,53,53	1.85	4 (8%)	60,89,89	1.09	5 (8%)
40	CLA	F	301	-	57,61,73	1.90	9 (15%)	67,98,113	1.42	6 (8%)
40	CLA	a	803	-	69,73,73	1.67	9 (13%)	82,113,113	1.25	8 (9%)
42	DD6	J	316	-	40,45,45	0.14	0	51,67,67	0.67	3 (5%)
46	SQD	F	320	-	34,36,54	1.36	3 (8%)	44,47,65	1.36	6 (13%)
40	CLA	o	313	-	51,55,73	2.08	10 (19%)	60,91,113	1.81	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	p	308	-	64,68,73	1.77	9 (14%)	76,107,113	1.45	7 (9%)
40	CLA	x	305	-	55,59,73	1.86	9 (16%)	64,96,113	1.48	7 (10%)
42	DD6	I	212	-	40,45,45	0.18	0	51,67,67	0.63	1 (1%)
43	LMG	T	318	-	40,40,55	0.93	3 (7%)	48,48,63	1.24	5 (10%)
40	CLA	X	307	20	64,68,73	1.77	9 (14%)	76,107,113	1.37	7 (9%)
52	DGD	b	850	-	57,57,67	0.96	2 (3%)	71,71,81	1.47	9 (12%)
40	CLA	G	206	7	60,64,73	1.79	9 (15%)	71,102,113	1.37	8 (11%)
40	CLA	I	203	9	59,63,73	1.91	9 (15%)	70,101,113	1.48	7 (10%)
44	A86	P	321	-	47,50,50	0.51	1 (2%)	51,76,76	1.15	2 (3%)
40	CLA	Z	306	22	64,68,73	1.81	9 (14%)	76,107,113	1.44	8 (10%)
40	CLA	q	305	-	64,68,73	1.77	9 (14%)	76,107,113	1.40	8 (10%)
41	KC2	Z	308	22	49,53,53	1.82	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	t	304	-	64,68,73	1.77	9 (14%)	76,107,113	1.35	8 (10%)
42	DD6	F	316	-	40,45,45	0.20	0	51,67,67	0.89	2 (3%)
43	LMG	l	201	-	39,39,55	0.84	2 (5%)	47,47,63	1.25	4 (8%)
42	DD6	L	317	-	40,45,45	0.15	0	51,67,67	0.71	1 (1%)
41	KC2	o	303	34	49,53,53	1.87	5 (10%)	60,89,89	1.07	4 (6%)
44	A86	p	319	-	47,50,50	0.40	1 (2%)	51,76,76	1.45	4 (7%)
46	SQD	M	318	-	30,32,54	1.44	3 (10%)	40,43,65	1.18	6 (15%)
40	CLA	V	202	19	59,63,73	1.87	9 (15%)	70,101,113	1.43	9 (12%)
40	CLA	b	806	24	69,73,73	1.68	9 (13%)	82,113,113	1.26	5 (6%)
40	CLA	U	204	18	51,55,73	2.03	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	D	306	4	59,63,73	1.86	9 (15%)	70,101,113	1.40	7 (10%)
44	A86	w	316	-	47,50,50	0.59	1 (2%)	51,76,76	1.09	3 (5%)
40	CLA	b	835	24	66,72,73	1.62	8 (12%)	80,111,113	1.46	10 (12%)
40	CLA	M	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.39	7 (9%)
40	CLA	a	811	23,40	65,69,73	1.81	9 (13%)	76,107,113	1.66	9 (11%)
40	CLA	f	201	-	64,68,73	1.76	9 (14%)	76,107,113	1.27	6 (7%)
44	A86	F	312	-	47,50,50	0.51	1 (2%)	51,76,76	0.88	2 (3%)
40	CLA	A	306	1	64,68,73	1.76	9 (14%)	76,107,113	1.29	6 (7%)
41	KC2	v	308	36	49,53,53	1.84	4 (8%)	60,89,89	1.13	4 (6%)
49	BCR	j	103	-	41,41,41	0.23	0	56,56,56	0.55	0
40	CLA	L	304	12	61,65,73	1.85	9 (14%)	72,103,113	1.44	7 (9%)
40	CLA	t	303	38	51,55,73	2.00	9 (17%)	60,91,113	1.50	7 (11%)
41	KC2	G	202	-	49,53,53	1.83	4 (8%)	60,89,89	1.12	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	C	306	3	69,73,73	1.71	9 (13%)	82,113,113	1.26	8 (9%)
41	KC2	T	303	-	49,53,53	1.86	4 (8%)	60,89,89	1.17	6 (10%)
42	DD6	Q	212	-	40,45,45	0.19	0	51,67,67	0.69	2 (3%)
47	A1EB1	u	323	-	54,58,58	0.49	1 (1%)	60,85,85	0.49	0
49	BCR	b	845	-	41,41,41	0.18	0	56,56,56	0.40	0
40	CLA	E	312	-	51,55,73	2.00	9 (17%)	60,91,113	1.63	6 (10%)
40	CLA	Y	304	-	51,55,73	2.05	9 (17%)	60,91,113	1.50	7 (11%)
40	CLA	Q	202	16	62,66,73	1.83	9 (14%)	73,104,113	1.47	7 (9%)
44	A86	Y	319	-	47,50,50	0.44	1 (2%)	51,76,76	1.07	3 (5%)
40	CLA	G	205	7	54,58,73	1.91	9 (16%)	64,95,113	1.43	6 (9%)
40	CLA	b	836	24	64,68,73	1.81	9 (14%)	76,107,113	1.36	7 (9%)
43	LMG	E	301	40	31,31,55	0.91	0	39,39,63	1.24	5 (12%)
40	CLA	o	304	34	64,68,73	1.75	9 (14%)	76,107,113	1.34	6 (7%)
47	A1EB1	N	320	-	54,58,58	0.42	0	60,85,85	1.12	3 (5%)
40	CLA	I	202	9	59,63,73	1.81	9 (15%)	70,101,113	1.37	5 (7%)
40	CLA	b	831	24	55,59,73	1.89	9 (16%)	64,96,113	1.43	6 (9%)
40	CLA	Z	304	-	64,68,73	1.79	9 (14%)	76,107,113	1.32	7 (9%)
44	A86	D	320	-	47,50,50	0.46	1 (2%)	51,76,76	0.89	2 (3%)
40	CLA	E	303	-	64,68,73	1.82	9 (14%)	76,107,113	1.45	7 (9%)
40	CLA	o	310	-	59,63,73	1.94	9 (15%)	70,101,113	1.57	11 (15%)
51	SF4	c	101	-	0,12,12	-	-	-	-	-
49	BCR	a	843	-	41,41,41	0.20	0	56,56,56	0.45	0
42	DD6	A	316	-	40,45,45	0.16	0	51,67,67	0.60	2 (3%)
42	DD6	v	318	-	40,45,45	0.22	0	51,67,67	0.86	4 (7%)
41	KC2	p	315	-	49,53,53	1.84	4 (8%)	60,89,89	1.12	4 (6%)
40	CLA	u	307	35	59,63,73	1.88	9 (15%)	70,101,113	1.62	8 (11%)
40	CLA	E	308	5	62,66,73	1.79	9 (14%)	73,104,113	1.43	7 (9%)
40	CLA	P	308	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	7 (9%)
40	CLA	F	305	-	51,55,73	2.00	9 (17%)	60,91,113	1.57	7 (11%)
40	CLA	L	311	12	51,55,73	2.06	9 (17%)	60,91,113	1.57	7 (11%)
40	CLA	v	304	-	56,60,73	1.86	9 (16%)	65,97,113	1.38	8 (12%)
44	A86	K	314	-	47,50,50	0.46	1 (2%)	51,76,76	0.94	3 (5%)
41	KC2	G	208	-	49,53,53	1.83	4 (8%)	60,89,89	1.01	3 (5%)
43	LMG	A	317	-	40,40,55	0.83	0	48,48,63	1.23	4 (8%)
44	A86	N	315	-	47,50,50	0.64	1 (2%)	51,76,76	1.13	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	p	311	-	59,63,73	1.98	9 (15%)	70,101,113	1.69	11 (15%)
41	KC2	o	308	34	49,53,53	1.82	4 (8%)	60,89,89	1.05	4 (6%)
40	CLA	Z	313	22	51,55,73	2.04	9 (17%)	60,91,113	1.71	9 (15%)
40	CLA	b	842	-	65,69,73	1.77	9 (13%)	77,108,113	1.34	7 (9%)
40	CLA	X	313	20	51,55,73	2.02	9 (17%)	60,91,113	1.66	9 (15%)
42	DD6	q	320	-	40,45,45	0.20	0	51,67,67	0.69	0
44	A86	w	315	-	47,50,50	0.61	1 (2%)	51,76,76	0.67	2 (3%)
44	A86	z	301	-	47,50,50	0.48	1 (2%)	51,76,76	0.99	2 (3%)
40	CLA	z	314	-	51,55,73	2.02	9 (17%)	60,91,113	1.70	9 (15%)
40	CLA	w	309	-	59,63,73	1.91	9 (15%)	70,101,113	1.57	7 (10%)
40	CLA	N	310	-	54,58,73	1.96	9 (16%)	64,95,113	1.58	10 (15%)
40	CLA	W	306	13	64,68,73	1.78	10 (15%)	76,107,113	1.40	8 (10%)
40	CLA	a	812	23	59,63,73	1.82	9 (15%)	70,101,113	1.35	8 (11%)
42	DD6	j	104	-	40,45,45	0.19	0	51,67,67	0.69	1 (1%)
41	KC2	L	313	12	49,53,53	1.86	4 (8%)	60,89,89	1.06	4 (6%)
42	DD6	H	314	-	40,45,45	0.23	0	51,67,67	0.95	4 (7%)
44	A86	w	311	-	47,50,50	0.56	2 (4%)	51,76,76	1.13	3 (5%)
40	CLA	W	313	13	64,68,73	1.78	9 (14%)	76,107,113	1.34	6 (7%)
40	CLA	I	208	-	59,63,73	1.90	9 (15%)	70,101,113	1.50	7 (10%)
40	CLA	J	307	10	51,55,73	2.02	9 (17%)	60,91,113	1.60	11 (18%)
49	BCR	a	846	-	41,41,41	0.15	0	56,56,56	0.41	0
49	BCR	i	102	-	41,41,41	0.36	0	56,56,56	0.70	0
41	KC2	X	302	-	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)
40	CLA	a	831	-	64,68,73	1.79	9 (14%)	76,107,113	1.32	5 (6%)
42	DD6	Q	211	-	40,45,45	0.20	0	51,67,67	0.72	2 (3%)
40	CLA	a	826	-	65,69,73	1.71	9 (13%)	77,108,113	1.39	8 (10%)
40	CLA	D	305	4	47,51,73	1.93	10 (21%)	60,82,113	2.60	10 (16%)
40	CLA	a	813	23	64,68,73	1.81	9 (14%)	76,107,113	1.38	7 (9%)
41	KC2	N	309	-	49,53,53	1.83	4 (8%)	60,89,89	1.03	5 (8%)
43	LMG	p	301	-	39,39,55	0.80	0	47,47,63	1.19	3 (6%)
44	A86	S	318	-	47,50,50	0.41	1 (2%)	51,76,76	1.00	1 (1%)
41	KC2	I	214	-	49,53,53	1.85	4 (8%)	60,89,89	1.05	3 (5%)
44	A86	x	319	-	47,50,50	0.29	0	51,76,76	1.27	2 (3%)
50	PQN	a	847	-	29,29,34	0.44	0	37,39,45	0.78	2 (5%)
41	KC2	E	319	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	q	318	-	40,45,45	0.20	0	51,67,67	0.91	3 (5%)
44	A86	w	310	-	47,50,50	0.44	1 (2%)	51,76,76	1.13	2 (3%)
42	DD6	W	315	-	40,45,45	0.19	0	51,67,67	0.71	2 (3%)
40	CLA	y	308	-	51,55,73	1.97	9 (17%)	60,91,113	1.44	5 (8%)
40	CLA	R	310	-	51,55,73	2.01	9 (17%)	60,91,113	1.56	7 (11%)
41	KC2	L	309	12	49,53,53	1.87	4 (8%)	60,89,89	1.00	3 (5%)
40	CLA	a	818	-	51,55,73	1.95	9 (17%)	60,91,113	1.56	8 (13%)
40	CLA	x	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.37	8 (10%)
42	DD6	N	317	-	40,45,45	0.22	0	51,67,67	1.17	5 (9%)
41	KC2	W	302	-	49,53,53	1.84	4 (8%)	60,89,89	1.04	3 (5%)
40	CLA	j	102	30	51,55,73	2.07	9 (17%)	60,91,113	1.63	10 (16%)
49	BCR	l	206	-	41,41,41	0.14	0	56,56,56	0.42	0
40	CLA	x	308	35	64,68,73	1.77	9 (14%)	76,107,113	1.41	7 (9%)
40	CLA	J	309	-	51,55,73	2.01	9 (17%)	60,91,113	1.44	6 (10%)
47	A1EB1	T	316	40	54,58,58	0.48	1 (1%)	60,85,85	0.77	1 (1%)
48	A1EB4	P	320	-	53,58,63	0.79	1 (1%)	59,84,89	1.23	2 (3%)
40	CLA	K	307	11	58,62,73	1.85	9 (15%)	68,99,113	1.30	6 (8%)
40	CLA	q	310	-	55,59,73	1.92	9 (16%)	64,96,113	1.56	8 (12%)
40	CLA	v	310	-	55,59,73	1.92	9 (16%)	64,96,113	1.57	9 (14%)
44	A86	X	319	-	47,50,50	0.43	1 (2%)	51,76,76	1.32	4 (7%)
44	A86	z	315	-	47,50,50	0.40	0	51,76,76	1.44	4 (7%)
40	CLA	R	307	-	59,63,73	1.85	9 (15%)	70,101,113	1.44	6 (8%)
40	CLA	A	301	1	51,55,73	2.01	9 (17%)	60,91,113	1.52	9 (15%)
40	CLA	b	814	24	69,73,73	1.66	9 (13%)	82,113,113	1.30	5 (6%)
41	KC2	W	309	-	49,53,53	1.86	4 (8%)	60,89,89	1.12	5 (8%)
40	CLA	F	303	6	65,69,73	1.78	9 (13%)	76,107,113	1.73	10 (13%)
44	A86	M	313	-	47,50,50	0.41	1 (2%)	51,76,76	1.85	3 (5%)
40	CLA	G	207	-	58,62,73	1.88	9 (15%)	68,99,113	1.41	7 (10%)
40	CLA	z	311	-	59,63,73	1.94	9 (15%)	70,101,113	1.77	11 (15%)
44	A86	P	316	-	47,50,50	0.39	1 (2%)	51,76,76	0.99	3 (5%)
47	A1EB1	S	321	-	54,58,58	0.45	1 (1%)	60,85,85	0.75	1 (1%)
40	CLA	p	307	35	59,63,73	1.92	9 (15%)	70,101,113	1.62	8 (11%)
41	KC2	F	309	6	49,53,53	1.83	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	a	841	23	69,73,73	1.71	9 (13%)	82,113,113	1.34	7 (8%)
41	KC2	N	303	14	49,53,53	1.80	4 (8%)	60,89,89	1.12	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	L	301	-	51,55,73	2.04	8 (15%)	60,91,113	1.50	7 (11%)
40	CLA	v	307	36	64,68,73	1.80	9 (14%)	76,107,113	1.51	10 (13%)
40	CLA	M	311	13	66,70,73	1.77	9 (13%)	78,109,113	1.33	9 (11%)
44	A86	X	314	-	47,50,50	0.59	1 (2%)	51,76,76	1.11	4 (7%)
40	CLA	P	307	13	63,67,73	1.78	9 (14%)	74,105,113	1.41	7 (9%)
40	CLA	Q	209	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	8 (13%)
40	CLA	w	304	-	64,68,73	1.77	9 (14%)	76,107,113	1.33	7 (9%)
41	KC2	H	316	-	49,53,53	1.81	4 (8%)	60,89,89	1.16	6 (10%)
40	CLA	a	836	23	69,73,73	1.68	9 (13%)	82,113,113	1.27	8 (9%)
47	A1EB1	T	320	-	54,58,58	0.42	1 (1%)	60,85,85	0.71	1 (1%)
40	CLA	q	301	-	59,63,73	1.87	9 (15%)	70,101,113	1.46	6 (8%)
41	KC2	R	301	15	49,53,53	1.80	4 (8%)	60,89,89	1.09	5 (8%)

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
40	CLA	K	301	-	1/1/11/20	4/18/94/115	-
40	CLA	Y	310	-	1/1/13/20	9/27/103/115	-
40	CLA	Q	206	-	1/1/14/20	7/35/112/115	-
41	KC2	I	209	9	-	8/15/71/71	-
40	CLA	H	307	-	1/1/14/20	16/33/109/115	-
40	CLA	W	305	13	1/1/15/20	6/39/115/115	-
41	KC2	R	311	15	-	8/15/71/71	-
49	BCR	f	203	-	-	0/29/63/63	0/2/2/2
40	CLA	a	828	23	1/1/15/20	13/39/115/115	-
44	A86	D	319	-	-	4/34/90/90	0/3/3/3
40	CLA	E	304	5	1/1/13/20	0/27/103/115	-
40	CLA	b	821	-	1/1/15/20	4/39/115/115	-
40	CLA	o	307	34	1/1/14/20	13/33/109/115	-
44	A86	T	313	-	-	2/34/90/90	0/3/3/3
40	CLA	U	203	-	1/1/13/20	8/27/103/115	-
40	CLA	w	308	-	1/1/11/20	6/18/94/115	-
40	CLA	U	206	-	1/1/11/20	1/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	N	302	14	-	5/15/71/71	-
44	A86	N	318	-	-	2/34/90/90	0/3/3/3
40	CLA	F	306	6	1/1/14/20	7/33/109/115	-
41	KC2	M	309	-	-	4/15/71/71	-
41	KC2	p	310	-	-	5/15/71/71	-
40	CLA	I	204	9	1/1/11/20	2/18/94/115	-
40	CLA	N	311	14	1/1/14/20	11/33/109/115	-
40	CLA	a	851	-	1/1/15/20	11/39/115/115	-
41	KC2	U	201	-	-	6/15/71/71	-
42	DD6	A	315	-	-	0/26/80/80	0/3/3/3
42	DD6	x	320	-	-	0/26/80/80	0/3/3/3
44	A86	P	317	-	-	3/34/90/90	0/3/3/3
41	KC2	K	303	11	-	10/15/71/71	-
47	A1EB1	v	323	-	-	16/43/100/100	1/3/3/3
47	A1EB1	w	313	-	-	12/43/100/100	0/3/3/3
40	CLA	T	317	47	1/1/11/20	4/18/94/115	-
40	CLA	a	840	23	1/1/13/20	8/27/103/115	-
41	KC2	x	315	-	-	6/15/71/71	-
42	DD6	U	211	-	-	0/26/80/80	0/3/3/3
44	A86	R	312	-	-	4/34/90/90	0/3/3/3
41	KC2	R	303	-	-	10/15/71/71	-
40	CLA	J	318	10	1/1/11/20	1/18/94/115	-
40	CLA	B	302	2	1/1/11/20	4/18/94/115	-
40	CLA	b	815	-	1/1/13/20	4/30/106/115	-
42	DD6	O	314	-	-	1/26/80/80	0/3/3/3
40	CLA	O	304	15	1/1/15/20	7/39/115/115	-
40	CLA	V	201	-	1/1/13/20	8/31/107/115	-
40	CLA	u	306	35	1/1/11/20	7/18/94/115	-
40	CLA	S	307	17	1/1/14/20	9/33/109/115	-
47	A1EB1	K	313	-	-	3/43/100/100	0/3/3/3
40	CLA	B	306	-	1/1/12/20	9/24/100/115	-
40	CLA	J	310	-	1/1/11/20	2/18/94/115	-
40	CLA	b	837	24	1/1/14/20	6/33/109/115	-
40	CLA	u	305	35	1/1/11/20	1/18/94/115	-
47	A1EB1	w	314	-	-	11/43/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	Y	314	-	-	10/15/71/71	-
44	A86	q	315	-	-	5/34/90/90	0/3/3/3
44	A86	v	315	-	-	5/34/90/90	0/3/3/3
44	A86	z	316	-	-	7/34/90/90	1/3/3/3
40	CLA	a	824	-	1/1/14/20	12/36/112/115	-
40	CLA	w	302	38	1/1/11/20	0/18/94/115	-
42	DD6	z	322	-	-	2/26/80/80	0/3/3/3
40	CLA	S	308	-	1/1/12/20	3/19/95/115	-
42	DD6	H	312	-	-	0/26/80/80	0/3/3/3
41	KC2	O	308	15	-	8/15/71/71	-
42	DD6	k	204	-	-	1/26/80/80	0/3/3/3
44	A86	u	320	-	-	5/34/90/90	0/3/3/3
40	CLA	M	307	-	1/1/14/20	7/33/109/115	-
47	A1EB1	x	322	-	-	5/43/100/100	0/3/3/3
40	CLA	a	809	-	1/1/12/20	4/21/97/115	-
40	CLA	l	204	-	1/1/15/20	11/39/115/115	-
40	CLA	Q	208	-	1/1/14/20	7/33/109/115	-
49	BCR	f	206	-	-	4/29/63/63	0/2/2/2
42	DD6	u	321	-	-	1/26/80/80	0/3/3/3
40	CLA	M	310	-	1/1/13/20	7/29/105/115	-
44	A86	X	317	-	-	6/34/90/90	0/3/3/3
44	A86	v	325	-	-	7/34/90/90	0/3/3/3
40	CLA	A	305	1	1/1/14/20	7/35/111/115	-
42	DD6	J	315	-	-	1/26/80/80	0/3/3/3
40	CLA	b	820	-	1/1/15/20	9/39/115/115	-
40	CLA	C	305	3	1/1/14/20	5/33/109/115	-
40	CLA	a	827	23	1/1/15/20	1/39/115/115	-
42	DD6	H	313	-	-	5/26/80/80	0/3/3/3
42	DD6	I	210	-	-	0/26/80/80	0/3/3/3
40	CLA	L	305	12	1/1/11/20	4/18/94/115	-
40	CLA	X	312	-	1/1/11/20	5/18/94/115	-
49	BCR	b	846	-	-	3/29/63/63	0/2/2/2
40	CLA	b	805	-	1/1/14/20	6/35/111/115	-
41	KC2	w	307	-	-	4/15/71/71	-
40	CLA	u	311	-	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	A1EB1	P	301	-	-	14/43/100/100	0/3/3/3
40	CLA	J	312	-	1/1/13/20	9/31/107/115	-
49	BCR	b	844	-	-	6/29/63/63	0/2/2/2
40	CLA	D	310	4	1/1/14/20	11/33/109/115	-
40	CLA	b	817	24	1/1/15/20	6/39/115/115	-
47	A1EB1	t	315	-	-	13/43/100/100	0/3/3/3
40	CLA	H	310	-	1/1/14/20	4/33/109/115	-
40	CLA	Q	204	16	1/1/12/20	2/23/99/115	-
44	A86	R	313	-	-	6/34/90/90	0/3/3/3
41	KC2	O	302	15	-	10/15/71/71	-
40	CLA	x	307	-	1/1/13/20	9/27/103/115	-
40	CLA	U	207	-	1/1/11/20	3/18/94/115	-
44	A86	M	316	-	-	2/34/90/90	0/3/3/3
40	CLA	N	304	14	1/1/14/20	10/33/109/115	-
41	KC2	Y	303	21	-	6/15/71/71	-
40	CLA	Y	307	21	1/1/14/20	9/33/109/115	-
40	CLA	D	304	4	1/1/13/20	7/29/105/115	-
40	CLA	a	819	23	1/1/14/20	9/35/111/115	-
42	DD6	I	213	-	-	1/26/80/80	0/3/3/3
40	CLA	p	314	35	1/1/11/20	8/18/94/115	-
41	KC2	y	301	38	-	10/15/71/71	-
41	KC2	Y	302	-	-	5/15/71/71	-
41	KC2	W	303	-	-	7/15/71/71	-
40	CLA	q	306	36	1/1/14/20	7/33/109/115	-
40	CLA	b	810	24	1/1/15/20	11/39/115/115	-
40	CLA	A	309	1	1/1/15/20	12/39/115/115	-
40	CLA	F	311	-	1/1/11/20	4/18/94/115	-
40	CLA	z	305	39	1/1/14/20	14/33/109/115	-
40	CLA	z	312	-	1/1/14/20	10/33/109/115	-
41	KC2	q	309	-	-	6/15/71/71	-
40	CLA	T	310	-	1/1/13/20	9/31/107/115	-
40	CLA	A	311	1	1/1/11/20	4/18/94/115	-
40	CLA	A	304	1	1/1/15/20	15/39/115/115	-
40	CLA	H	301	-	1/1/11/20	4/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	f	202	24	1/1/15/20	7/39/115/115	-
40	CLA	R	316	47	1/1/11/20	2/18/94/115	-
41	KC2	T	309	15	-	4/15/71/71	-
40	CLA	I	201	-	1/1/15/20	7/39/115/115	-
41	KC2	T	311	15	-	10/15/71/71	-
40	CLA	C	307	3	1/1/14/20	9/33/109/115	-
40	CLA	b	823	24	1/1/13/20	3/27/103/115	-
41	KC2	X	303	20	-	1/15/71/71	-
47	A1EB1	K	315	-	-	15/43/100/100	1/3/3/3
40	CLA	a	815	23	1/1/15/20	5/39/115/115	-
40	CLA	t	307	-	1/1/13/20	11/27/103/115	-
41	KC2	p	309	-	-	6/15/71/71	-
40	CLA	Q	207	-	1/1/11/20	2/18/94/115	-
40	CLA	q	313	36	1/1/11/20	7/18/94/115	-
40	CLA	Z	310	-	1/1/13/20	9/27/103/115	-
42	DD6	p	322	-	-	1/26/80/80	0/3/3/3
43	LMG	D	318	-	-	15/35/55/70	0/1/1/1
41	KC2	P	304	13	-	5/15/71/71	-
41	KC2	T	308	15	-	8/15/71/71	-
40	CLA	T	307	-	1/1/13/20	0/27/103/115	-
44	A86	W	301	-	-	1/34/90/90	0/3/3/3
44	A86	p	320	-	-	8/34/90/90	0/3/3/3
47	A1EB1	Y	323	-	-	3/43/100/100	0/3/3/3
40	CLA	b	826	24	1/1/14/20	7/38/114/115	-
44	A86	G	211	-	-	7/34/90/90	0/3/3/3
40	CLA	b	841	24	1/1/15/20	5/39/115/115	-
44	A86	p	321	-	-	7/34/90/90	0/3/3/3
41	KC2	z	304	39	-	5/15/71/71	-
43	LMG	u	301	-	-	14/34/54/70	0/1/1/1
40	CLA	b	834	-	1/1/15/20	8/39/115/115	-
47	A1EB1	Z	320	-	-	7/43/100/100	0/3/3/3
42	DD6	J	313	-	-	1/26/80/80	0/3/3/3
41	KC2	w	301	38	-	9/15/71/71	-
40	CLA	b	839	24	1/1/15/20	12/39/115/115	-
40	CLA	M	306	13	1/1/14/20	5/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	S	319	-	1/1/11/20	7/18/94/115	-
44	A86	X	318	-	-	5/34/90/90	0/3/3/3
47	A1EB1	v	324	-	-	13/43/100/100	0/3/3/3
41	KC2	p	303	-	-	6/15/71/71	-
40	CLA	L	306	12	1/1/11/20	6/18/94/115	-
40	CLA	J	308	10	1/1/13/20	8/27/103/115	-
40	CLA	a	825	-	1/1/15/20	5/39/115/115	-
40	CLA	i	101	-	1/1/13/20	12/27/103/115	-
44	A86	S	315	-	-	7/34/90/90	0/3/3/3
47	A1EB1	q	322	-	-	7/43/100/100	0/3/3/3
40	CLA	D	307	4	1/1/15/20	8/39/115/115	-
41	KC2	t	308	-	-	6/15/71/71	-
42	DD6	N	316	-	-	2/26/80/80	0/3/3/3
40	CLA	J	311	-	1/1/11/20	4/18/94/115	-
40	CLA	X	301	-	1/1/14/20	4/33/109/115	-
40	CLA	a	822	-	1/1/15/20	10/39/115/115	-
44	A86	T	312	-	-	4/34/90/90	0/3/3/3
40	CLA	E	305	5	1/1/14/20	6/33/109/115	-
42	DD6	Y	322	-	-	3/26/80/80	0/3/3/3
40	CLA	D	302	43	1/1/13/20	7/31/107/115	-
40	CLA	v	311	-	1/1/14/20	9/37/113/115	-
40	CLA	B	303	-	1/1/11/20	3/18/94/115	-
44	A86	y	310	-	-	7/34/90/90	0/3/3/3
41	KC2	P	309	13	-	5/15/71/71	-
49	BCR	b	843	-	-	0/29/63/63	0/2/2/2
40	CLA	S	312	-	1/1/11/20	4/18/94/115	-
46	SQD	P	319	-	-	7/27/47/69	0/1/1/1
40	CLA	z	306	-	1/1/13/20	5/27/103/115	-
44	A86	o	316	-	-	11/34/90/90	0/3/3/3
49	BCR	b	847	-	-	4/29/63/63	0/2/2/2
40	CLA	b	824	24	1/1/15/20	15/39/115/115	-
40	CLA	A	302	-	1/1/14/20	7/33/109/115	-
42	DD6	v	320	-	-	6/26/80/80	0/3/3/3
41	KC2	S	303	17	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	Z	307	22	1/1/14/20	8/33/109/115	-
40	CLA	J	303	-	1/1/11/20	4/18/94/115	-
44	A86	T	315	-	-	11/34/90/90	1/3/3/3
40	CLA	H	306	8	1/1/12/20	0/21/97/115	-
40	CLA	C	302	-	1/1/11/20	5/18/94/115	-
44	A86	z	317	-	-	6/34/90/90	0/3/3/3
40	CLA	G	213	-	1/1/11/20	8/18/94/115	-
40	CLA	a	833	23	1/1/14/20	9/33/109/115	-
40	CLA	o	311	-	1/1/14/20	8/37/113/115	-
44	A86	R	315	-	-	7/34/90/90	0/3/3/3
42	DD6	F	315	-	-	3/26/80/80	0/3/3/3
41	KC2	W	310	13	-	6/15/71/71	-
41	KC2	L	302	-	-	7/15/71/71	-
44	A86	p	317	-	-	1/34/90/90	0/3/3/3
44	A86	Y	315	-	-	8/34/90/90	0/3/3/3
48	A1EB4	M	319	-	-	6/38/98/103	0/3/3/3
40	CLA	O	306	15	1/1/14/20	7/33/109/115	-
44	A86	Q	210	-	-	5/34/90/90	0/3/3/3
44	A86	z	318	-	-	4/34/90/90	1/3/3/3
49	BCR	b	848	-	-	3/29/63/63	0/2/2/2
44	A86	v	317	-	-	1/34/90/90	0/3/3/3
41	KC2	x	303	-	-	7/15/71/71	-
41	KC2	K	309	11	-	8/15/71/71	-
40	CLA	E	310	-	1/1/14/20	6/33/109/115	-
41	KC2	z	310	39	-	8/15/71/71	-
41	KC2	R	309	15	-	7/15/71/71	-
40	CLA	a	850	-	1/1/15/20	4/39/115/115	-
41	KC2	N	312	14	-	8/15/71/71	-
40	CLA	y	303	-	1/1/11/20	4/18/94/115	-
41	KC2	v	303	36	-	6/15/71/71	-
40	CLA	P	311	-	1/1/11/20	4/18/94/115	-
41	KC2	x	309	-	-	4/15/71/71	-
44	A86	q	316	-	-	3/34/90/90	1/3/3/3
40	CLA	Y	312	-	1/1/11/20	2/18/94/115	-
42	DD6	E	318	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	b	828	24	1/1/13/20	1/27/103/115	-
43	LMG	x	301	-	-	15/34/54/70	0/1/1/1
40	CLA	N	306	-	1/1/14/20	2/33/109/115	-
41	KC2	p	304	35	-	8/15/71/71	-
41	KC2	N	308	14	-	8/15/71/71	-
40	CLA	v	312	-	1/1/14/20	7/33/109/115	-
40	CLA	E	311	-	1/1/12/20	5/21/97/115	-
40	CLA	O	305	15	1/1/11/20	2/18/94/115	-
41	KC2	v	309	-	-	6/15/71/71	-
44	A86	U	210	-	-	2/34/90/90	0/3/3/3
43	LMG	E	321	-	-	12/35/55/70	0/1/1/1
40	CLA	E	307	-	1/1/15/20	10/39/115/115	-
40	CLA	f	204	28	1/1/11/20	2/18/94/115	-
40	CLA	H	311	-	1/1/11/20	3/18/94/115	-
40	CLA	Z	301	-	1/1/14/20	6/33/109/115	-
40	CLA	a	814	-	1/1/12/20	2/21/97/115	-
40	CLA	a	823	23	1/1/13/20	5/27/103/115	-
42	DD6	Q	213	-	-	0/26/80/80	0/3/3/3
40	CLA	w	305	-	1/1/12/20	3/19/95/115	-
42	DD6	o	319	-	-	1/26/80/80	0/3/3/3
47	A1EB1	y	312	-	-	11/43/100/100	0/3/3/3
49	BCR	k	203	-	-	4/29/63/63	0/2/2/2
40	CLA	S	302	-	1/1/14/20	13/33/109/115	-
41	KC2	y	306	-	-	8/15/71/71	-
40	CLA	x	314	35	1/1/11/20	4/18/94/115	-
44	A86	M	320	-	-	5/34/90/90	0/3/3/3
40	CLA	J	302	10	1/1/11/20	8/18/94/115	-
40	CLA	G	204	7	1/1/13/20	2/27/103/115	-
44	A86	x	317	-	-	6/34/90/90	0/3/3/3
41	KC2	M	303	13	-	4/15/71/71	-
40	CLA	o	301	-	1/1/14/20	6/33/109/115	-
42	DD6	D	315	-	-	0/26/80/80	0/3/3/3
41	KC2	T	301	-	-	4/15/71/71	-
43	LMG	E	320	-	-	15/26/46/70	0/1/1/1
42	DD6	N	319	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	M	302	13	-	3/15/71/71	-
40	CLA	l	202	-	1/1/15/20	14/39/115/115	-
40	CLA	y	302	38	1/1/11/20	4/18/94/115	-
41	KC2	u	309	-	-	5/15/71/71	-
44	A86	L	314	-	-	4/34/90/90	0/3/3/3
40	CLA	H	302	-	1/1/11/20	8/18/94/115	-
40	CLA	C	304	3	1/1/13/20	3/29/105/115	-
42	DD6	C	313	-	-	2/26/80/80	0/3/3/3
40	CLA	z	302	-	1/1/14/20	6/33/109/115	-
46	SQD	W	318	-	-	7/27/47/69	0/1/1/1
47	A1EB1	y	314	-	-	8/43/100/100	0/3/3/3
42	DD6	A	313	-	-	1/26/80/80	0/3/3/3
40	CLA	a	804	23	1/1/14/20	8/36/112/115	-
40	CLA	b	825	-	1/1/15/20	9/39/115/115	-
40	CLA	I	206	9	1/1/15/20	7/39/115/115	-
44	A86	t	310	-	-	7/34/90/90	0/3/3/3
40	CLA	B	304	-	1/1/11/20	6/18/94/115	-
41	KC2	O	301	15	-	6/15/71/71	-
44	A86	X	321	-	-	5/34/90/90	0/3/3/3
40	CLA	a	839	45	1/1/15/20	10/39/115/115	-
40	CLA	x	302	-	1/1/15/20	8/39/115/115	-
44	A86	p	316	-	-	5/34/90/90	0/3/3/3
40	CLA	S	311	-	1/1/11/20	6/18/94/115	-
44	A86	u	319	-	-	11/34/90/90	0/3/3/3
40	CLA	b	830	24	1/1/14/20	5/35/111/115	-
40	CLA	H	309	-	1/1/13/20	6/29/105/115	-
40	CLA	u	314	35	1/1/11/20	5/18/94/115	-
40	CLA	K	312	-	1/1/11/20	2/18/94/115	-
42	DD6	G	210	-	-	1/26/80/80	0/3/3/3
40	CLA	I	207	9	1/1/11/20	4/18/94/115	-
40	CLA	M	304	13	1/1/14/20	7/33/109/115	-
41	KC2	Y	308	-	-	7/15/71/71	-
41	KC2	q	308	36	-	10/15/71/71	-
40	CLA	q	307	36	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	p	312	-	1/1/11/20	3/18/94/115	-
40	CLA	b	838	-	1/1/15/20	9/39/115/115	-
40	CLA	a	832	23	1/1/15/20	12/39/115/115	-
40	CLA	P	306	13	1/1/11/20	1/18/94/115	-
40	CLA	W	308	-	1/1/14/20	8/33/109/115	-
44	A86	u	317	-	-	1/34/90/90	0/3/3/3
42	DD6	Q	214	-	-	1/26/80/80	0/3/3/3
44	A86	o	315	-	-	7/34/90/90	0/3/3/3
47	A1EB1	L	316	-	-	8/43/100/100	0/3/3/3
42	DD6	L	315	-	-	0/26/80/80	0/3/3/3
40	CLA	b	816	24	1/1/11/20	5/18/94/115	-
42	DD6	z	321	-	-	1/26/80/80	0/3/3/3
43	LMG	j	101	-	-	10/25/45/70	0/1/1/1
47	A1EB1	t	314	-	-	18/43/100/100	1/3/3/3
40	CLA	U	205	-	1/1/11/20	4/18/94/115	-
44	A86	x	318	-	-	8/34/90/90	0/3/3/3
41	KC2	X	309	-	-	6/15/71/71	-
40	CLA	x	311	-	1/1/13/20	9/27/103/115	-
40	CLA	v	301	-	1/1/13/20	4/27/103/115	-
40	CLA	z	308	39	1/1/14/20	12/33/109/115	-
40	CLA	q	312	-	1/1/14/20	8/33/109/115	-
44	A86	W	314	-	-	5/34/90/90	0/3/3/3
44	A86	Y	318	-	-	9/34/90/90	0/3/3/3
44	A86	q	319	-	-	12/34/90/90	0/3/3/3
42	DD6	R	314	-	-	0/26/80/80	0/3/3/3
47	A1EB1	u	322	-	-	8/43/100/100	0/3/3/3
47	A1EB1	x	321	-	-	2/43/100/100	0/3/3/3
40	CLA	F	310	-	1/1/11/20	6/18/94/115	-
40	CLA	U	202	18	1/1/13/20	9/27/103/115	-
40	CLA	Y	311	-	1/1/11/20	5/18/94/115	-
40	CLA	p	305	35	1/1/11/20	6/18/94/115	-
40	CLA	T	304	15	1/1/14/20	4/33/109/115	-
40	CLA	Z	312	-	1/1/11/20	6/18/94/115	-
40	CLA	S	301	-	1/1/14/20	5/33/109/115	-
44	A86	x	316	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	F	302	6	-	8/15/71/71	-
41	KC2	Z	309	-	-	6/15/71/71	-
44	A86	F	317	-	-	8/34/90/90	0/3/3/3
42	DD6	P	315	-	1/1/12/24	1/26/80/80	0/3/3/3
42	DD6	E	315	-	-	1/26/80/80	0/3/3/3
47	A1EB1	G	212	-	-	14/43/100/100	0/3/3/3
40	CLA	w	303	38	1/1/11/20	4/18/94/115	-
40	CLA	B	301	2	1/1/11/20	9/18/94/115	-
40	CLA	a	842	-	1/1/15/20	14/39/115/115	-
40	CLA	D	312	4	1/1/13/20	9/27/103/115	-
40	CLA	b	807	-	1/1/15/20	9/39/115/115	-
41	KC2	R	308	15	-	8/15/71/71	-
44	A86	u	318	-	-	11/34/90/90	0/3/3/3
47	A1EB1	z	323	-	-	8/43/100/100	0/3/3/3
47	A1EB1	t	313	-	-	15/43/100/100	0/3/3/3
40	CLA	b	811	24	1/1/11/20	4/18/94/115	-
41	KC2	T	302	-	-	2/15/71/71	-
41	KC2	C	303	-	-	7/15/71/71	-
40	CLA	Y	301	-	1/1/14/20	7/33/109/115	-
40	CLA	D	303	4	1/1/14/20	12/33/109/115	-
40	CLA	l	203	-	1/1/14/20	12/38/114/115	-
42	DD6	M	314	-	-	1/26/80/80	0/3/3/3
40	CLA	a	817	23	1/1/12/20	0/21/97/115	-
40	CLA	O	316	47	1/1/11/20	2/18/94/115	-
44	A86	M	315	-	-	5/34/90/90	1/3/3/3
44	A86	F	313	-	-	6/34/90/90	0/3/3/3
44	A86	o	317	-	-	7/34/90/90	0/3/3/3
40	CLA	Q	203	-	1/1/12/20	4/21/97/115	-
40	CLA	D	308	4	1/1/13/20	2/27/103/115	-
40	CLA	z	324	-	1/1/11/20	5/18/94/115	-
40	CLA	b	803	-	1/1/15/20	13/39/115/115	-
44	A86	Z	317	-	-	2/34/90/90	1/3/3/3
40	CLA	u	302	-	1/1/15/20	8/39/115/115	-
44	A86	G	209	-	-	9/34/90/90	0/3/3/3
40	CLA	R	305	15	1/1/14/20	6/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	A	303	1	1/1/14/20	10/35/111/115	-
51	SF4	c	102	-	-	-	0/6/5/5
47	A1EB1	Z	321	-	-	10/43/100/100	0/3/3/3
42	DD6	w	312	-	-	1/26/80/80	0/3/3/3
40	CLA	M	305	13	1/1/14/20	10/33/109/115	-
41	KC2	Z	303	22	-	4/15/71/71	-
49	BCR	r	201	-	-	2/29/63/63	0/2/2/2
40	CLA	k	202	-	1/1/13/20	5/27/103/115	-
40	CLA	C	308	-	1/1/11/20	5/18/94/115	-
40	CLA	b	833	24	1/1/14/20	10/33/109/115	-
44	A86	p	318	-	-	10/34/90/90	0/3/3/3
40	CLA	o	312	-	1/1/11/20	5/18/94/115	-
41	KC2	O	309	15	-	9/15/71/71	-
41	KC2	t	306	-	-	8/15/71/71	-
49	BCR	m	101	-	-	0/29/63/63	0/2/2/2
51	SF4	b	804	-	-	-	0/6/5/5
40	CLA	a	829	-	1/1/15/20	15/39/115/115	-
41	KC2	o	309	34	-	10/15/71/71	-
41	KC2	Q	201	16	-	6/15/71/71	-
40	CLA	v	305	-	1/1/14/20	3/33/109/115	-
47	A1EB1	Z	319	-	-	6/43/100/100	0/3/3/3
40	CLA	X	304	-	1/1/11/20	6/18/94/115	-
41	KC2	L	308	12	-	4/15/71/71	-
40	CLA	P	305	13	1/1/14/20	9/33/109/115	-
43	LMG	S	322	-	-	9/34/54/70	0/1/1/1
40	CLA	a	816	23	1/1/15/20	6/39/115/115	-
40	CLA	p	306	35	1/1/11/20	5/18/94/115	-
41	KC2	x	304	35	-	8/15/71/71	-
42	DD6	C	310	-	-	1/26/80/80	0/3/3/3
42	DD6	B	305	-	-	3/26/80/80	0/3/3/3
47	A1EB1	v	322	-	-	7/43/100/100	0/3/3/3
40	CLA	X	306	20	1/1/13/20	7/27/103/115	-
40	CLA	a	830	-	1/1/13/20	6/31/107/115	-
40	CLA	F	307	6	1/1/14/20	6/32/109/115	-
44	A86	H	315	-	-	4/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	A1EB1	p	324	-	-	4/43/100/100	0/3/3/3
41	KC2	A	310	1	-	6/15/71/71	-
40	CLA	B	307	-	1/1/11/20	7/18/94/115	-
40	CLA	P	312	13	1/1/14/20	13/33/109/115	-
42	DD6	Z	318	-	-	1/26/80/80	0/3/3/3
45	LHG	a	849	40	-	17/34/34/53	-
42	DD6	J	314	-	-	0/26/80/80	0/3/3/3
40	CLA	W	312	13	1/1/14/20	9/33/109/115	-
40	CLA	J	306	10	1/1/12/20	1/24/100/115	-
40	CLA	t	302	38	1/1/11/20	0/18/94/115	-
40	CLA	p	313	-	1/1/13/20	2/27/103/115	-
41	KC2	Z	302	-	-	8/15/71/71	-
42	DD6	J	317	-	-	1/26/80/80	0/3/3/3
40	CLA	a	838	23	1/1/13/20	8/27/103/115	-
40	CLA	Z	311	22	1/1/14/20	5/37/113/115	-
40	CLA	X	311	20	1/1/14/20	11/37/113/115	-
41	KC2	H	303	-	-	4/15/71/71	-
40	CLA	H	305	8	1/1/14/20	12/33/109/115	-
41	KC2	t	301	38	-	8/15/71/71	-
40	CLA	D	301	4	1/1/13/20	6/27/103/115	-
40	CLA	q	304	-	1/1/12/20	4/24/100/115	-
40	CLA	t	309	-	1/1/11/20	4/18/94/115	-
42	DD6	F	314	-	-	1/26/80/80	0/3/3/3
47	A1EB1	o	321	-	-	9/43/100/100	1/3/3/3
41	KC2	O	303	15	-	6/15/71/71	-
40	CLA	D	311	-	1/1/11/20	4/18/94/115	-
44	A86	X	320	-	-	6/34/90/90	0/3/3/3
40	CLA	b	809	24	1/1/14/20	8/33/109/115	-
42	DD6	K	310	-	-	0/26/80/80	0/3/3/3
40	CLA	F	304	6	1/1/13/20	3/27/103/115	-
43	LMG	W	317	-	-	7/34/54/70	0/1/1/1
40	CLA	v	313	36	1/1/11/20	3/18/94/115	-
40	CLA	C	301	3	1/1/11/20	6/18/94/115	-
42	DD6	D	316	-	-	1/26/80/80	0/3/3/3
40	CLA	I	205	9	1/1/13/20	8/29/105/115	-
40	CLA	P	313	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	E	314	5	1/1/11/20	11/18/94/115	-
40	CLA	a	806	23	1/1/15/20	12/39/115/115	-
40	CLA	o	306	34	1/1/14/20	7/33/109/115	-
41	KC2	M	308	13	-	7/15/71/71	-
41	KC2	u	304	35	-	8/15/71/71	-
40	CLA	a	821	23	1/1/15/20	11/39/115/115	-
47	A1EB1	o	322	-	-	12/43/100/100	0/3/3/3
40	CLA	H	308	8	1/1/11/20	3/18/94/115	-
41	KC2	v	302	-	-	6/15/71/71	-
41	KC2	W	304	13	-	7/15/71/71	-
40	CLA	y	309	-	1/1/13/20	9/27/103/115	-
46	SQD	k	205	-	-	3/31/51/69	0/1/1/1
40	CLA	b	827	24	1/1/14/20	6/33/109/115	-
42	DD6	K	311	-	-	2/26/80/80	0/3/3/3
45	LHG	F	319	-	-	18/44/44/53	-
41	KC2	Q	216	-	-	7/15/71/71	-
42	DD6	E	317	-	-	1/26/80/80	0/3/3/3
47	A1EB1	v	321	-	-	16/43/100/100	1/3/3/3
42	DD6	A	312	-	-	0/26/80/80	0/3/3/3
41	KC2	u	310	-	-	5/15/71/71	-
40	CLA	p	302	-	1/1/15/20	7/39/115/115	-
40	CLA	E	306	5	1/1/13/20	9/27/103/115	-
42	DD6	y	311	-	-	0/26/80/80	0/3/3/3
40	CLA	a	807	-	1/1/13/20	7/29/105/115	-
40	CLA	a	820	23	1/1/14/20	13/33/109/115	-
44	A86	X	316	-	-	4/34/90/90	0/3/3/3
44	A86	t	316	-	-	7/34/90/90	0/3/3/3
40	CLA	T	306	15	1/1/14/20	3/33/109/115	-
44	A86	o	318	-	-	3/34/90/90	0/3/3/3
40	CLA	S	306	17	1/1/13/20	7/29/105/115	-
42	DD6	o	320	-	-	0/26/80/80	0/3/3/3
41	KC2	N	301	14	-	4/15/71/71	-
44	A86	z	320	-	-	2/34/90/90	0/3/3/3
41	KC2	S	304	17	-	6/15/71/71	-
41	KC2	K	305	11	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	L	310	-	1/1/11/20	6/18/94/115	-
42	DD6	C	312	-	-	2/26/80/80	0/3/3/3
40	CLA	R	304	15	1/1/12/20	6/23/99/115	-
40	CLA	Z	305	22	1/1/13/20	6/27/103/115	-
42	DD6	D	313	-	-	0/26/80/80	0/3/3/3
40	CLA	a	837	23	1/1/13/20	8/27/103/115	-
40	CLA	E	313	5	1/1/11/20	1/18/94/115	-
42	DD6	D	314	-	-	3/26/80/80	0/3/3/3
44	A86	Y	317	41	-	6/34/90/90	0/3/3/3
49	BCR	l	208	-	-	5/29/63/63	0/2/2/2
41	KC2	L	303	12	-	6/15/71/71	-
41	KC2	o	302	-	-	6/15/71/71	-
40	CLA	K	304	11	1/1/14/20	6/33/109/115	-
41	KC2	z	309	39	-	7/15/71/71	-
40	CLA	S	313	-	1/1/11/20	3/18/94/115	-
40	CLA	a	810	-	1/1/14/20	5/33/109/115	-
44	A86	W	316	-	-	4/34/90/90	0/3/3/3
44	A86	Z	316	-	-	5/34/90/90	1/3/3/3
40	CLA	a	852	-	1/1/13/20	7/27/103/115	-
45	LHG	S	323	-	-	19/44/44/53	-
40	CLA	b	818	24	1/1/14/20	13/36/112/115	-
44	A86	S	317	-	-	5/34/90/90	0/3/3/3
44	A86	Q	215	-	-	3/34/90/90	0/3/3/3
40	CLA	W	311	-	1/1/13/20	8/27/103/115	-
40	CLA	A	308	-	1/1/13/20	2/27/103/115	-
41	KC2	q	303	36	-	7/15/71/71	-
40	CLA	G	201	7	1/1/11/20	4/18/94/115	-
40	CLA	L	312	-	1/1/11/20	2/18/94/115	-
41	KC2	P	310	-	-	7/15/71/71	-
40	CLA	u	313	-	1/1/13/20	1/27/103/115	-
42	DD6	t	312	-	-	0/26/80/80	0/3/3/3
44	A86	O	315	-	-	5/34/90/90	0/3/3/3
44	A86	T	319	-	-	3/34/90/90	0/3/3/3
49	BCR	a	845	-	-	2/29/63/63	0/2/2/2
41	KC2	q	302	36	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	T	314	-	-	1/26/80/80	0/3/3/3
40	CLA	R	306	15	1/1/14/20	5/33/109/115	-
40	CLA	S	314	17	1/1/13/20	11/27/103/115	-
40	CLA	q	311	-	1/1/14/20	11/37/113/115	-
44	A86	Z	315	-	-	12/34/90/90	0/3/3/3
40	CLA	k	201	31	1/1/13/20	6/27/103/115	-
42	DD6	J	301	-	-	2/26/80/80	0/3/3/3
47	A1EB1	q	321	-	-	17/43/100/100	1/3/3/3
40	CLA	N	305	14	1/1/13/20	5/27/103/115	-
44	A86	O	313	-	-	4/34/90/90	0/3/3/3
44	A86	Y	321	-	-	4/34/90/90	0/3/3/3
40	CLA	W	307	13	1/1/15/20	10/39/115/115	-
40	CLA	b	840	-	1/1/15/20	12/39/115/115	-
41	KC2	P	303	13	-	2/15/71/71	-
40	CLA	O	310	-	1/1/11/20	6/18/94/115	-
41	KC2	u	303	-	-	6/15/71/71	-
40	CLA	b	832	24	1/1/15/20	6/39/115/115	-
40	CLA	f	205	-	1/1/11/20	1/18/94/115	-
43	LMG	P	318	-	-	11/34/54/70	0/1/1/1
44	A86	v	316	-	-	3/34/90/90	1/3/3/3
40	CLA	Y	305	21	1/1/13/20	7/27/103/115	-
41	KC2	P	302	-	-	4/15/71/71	-
44	A86	u	316	-	-	5/34/90/90	0/3/3/3
40	CLA	E	302	5	1/1/11/20	8/18/94/115	-
40	CLA	u	312	-	1/1/14/20	8/33/109/115	-
42	DD6	X	322	-	-	0/26/80/80	0/3/3/3
40	CLA	o	305	34	1/1/13/20	8/27/103/115	-
41	KC2	z	303	39	-	6/15/71/71	-
40	CLA	A	307	1	1/1/14/20	7/33/109/115	-
40	CLA	l	205	32	1/1/15/20	12/39/115/115	-
40	CLA	z	307	-	1/1/14/20	7/33/109/115	-
40	CLA	F	308	-	1/1/13/20	3/27/103/115	-
40	CLA	a	805	23,40	1/1/12/20	4/26/102/115	-
47	A1EB1	q	323	-	-	14/43/100/100	0/3/3/3
40	CLA	U	208	-	1/1/11/20	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	X	308	20	-	5/15/71/71	-
40	CLA	O	307	-	1/1/14/20	9/36/112/115	-
47	A1EB1	y	313	-	-	12/43/100/100	0/3/3/3
40	CLA	K	306	-	1/1/14/20	6/33/109/115	-
49	BCR	a	844	-	-	2/29/63/63	0/2/2/2
44	A86	X	315	-	-	5/34/90/90	0/3/3/3
44	A86	O	312	-	-	5/34/90/90	0/3/3/3
40	CLA	E	309	-	1/1/14/20	11/33/109/115	-
44	A86	q	317	-	-	1/34/90/90	0/3/3/3
47	A1EB1	R	317	40	-	9/43/100/100	0/3/3/3
41	KC2	S	310	-	-	6/15/71/71	-
40	CLA	u	308	35	1/1/14/20	7/33/109/115	-
40	CLA	a	834	-	1/1/14/20	6/33/109/115	-
40	CLA	x	306	35	1/1/14/20	14/33/109/115	-
40	CLA	a	835	-	1/1/15/20	1/39/115/115	-
42	DD6	U	209	-	-	0/26/80/80	0/3/3/3
40	CLA	L	307	-	1/1/13/20	2/27/103/115	-
44	A86	N	314	-	-	2/34/90/90	0/3/3/3
41	KC2	K	302	11	-	6/15/71/71	-
44	A86	v	319	-	-	13/34/90/90	0/3/3/3
40	CLA	T	305	15	1/1/12/20	4/21/97/115	-
40	CLA	Y	306	21	1/1/14/20	7/33/109/115	-
40	CLA	S	305	-	1/1/12/20	7/24/100/115	-
40	CLA	z	313	-	1/1/11/20	4/18/94/115	-
41	KC2	R	302	15	-	4/15/71/71	-
44	A86	z	319	-	-	5/34/90/90	0/3/3/3
47	A1EB1	O	317	40	-	9/43/100/100	1/3/3/3
40	CLA	b	822	-	1/1/14/20	9/38/114/115	-
40	CLA	v	306	36	1/1/14/20	9/33/109/115	-
43	LMG	a	802	-	-	11/30/50/70	0/1/1/1
40	CLA	y	304	-	1/1/14/20	8/33/109/115	-
50	PQN	b	849	-	-	3/17/37/43	0/2/2/2
40	CLA	H	304	-	1/1/11/20	3/18/94/115	-
40	CLA	b	808	-	1/1/15/20	8/39/115/115	-
44	A86	o	314	-	-	12/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	x	313	-	1/1/13/20	4/27/103/115	-
40	CLA	b	812	24	1/1/14/20	8/33/109/115	-
44	A86	t	311	-	-	12/34/90/90	1/3/3/3
47	A1EB1	F	322	-	-	7/43/100/100	0/3/3/3
41	KC2	x	310	-	-	6/15/71/71	-
41	KC2	S	309	17	-	9/15/71/71	-
44	A86	Z	314	-	-	3/34/90/90	0/3/3/3
41	KC2	O	311	-	-	6/15/71/71	-
40	CLA	Y	313	21	1/1/11/20	8/18/94/115	-
42	DD6	E	316	-	-	0/26/80/80	0/3/3/3
47	A1EB1	L	318	-	-	15/43/100/100	0/3/3/3
40	CLA	D	309	-	1/1/13/20	6/31/107/115	-
40	CLA	Q	205	16	1/1/14/20	12/36/112/115	-
49	BCR	l	207	-	-	6/29/63/63	0/2/2/2
43	LMG	M	317	-	-	9/34/54/70	0/1/1/1
41	KC2	w	306	38	-	9/15/71/71	-
45	LHG	a	848	-	-	22/52/52/53	-
42	DD6	A	314	-	-	1/26/80/80	0/3/3/3
40	CLA	G	203	7	1/1/13/20	5/26/103/115	-
43	LMG	F	318	-	-	10/34/54/70	0/1/1/1
40	CLA	b	801	-	1/1/14/20	6/37/113/115	-
44	A86	Y	320	-	-	9/34/90/90	0/3/3/3
40	CLA	b	802	-	1/1/15/20	8/39/115/115	-
40	CLA	C	309	-	1/1/11/20	1/18/94/115	-
44	A86	N	321	-	-	8/34/90/90	0/3/3/3
40	CLA	t	305	-	1/1/12/20	2/19/95/115	-
47	A1EB1	p	323	-	-	8/43/100/100	0/3/3/3
44	A86	Y	316	-	-	3/34/90/90	0/3/3/3
41	KC2	N	313	14	-	4/15/71/71	-
41	KC2	J	304	-	-	9/15/71/71	-
40	CLA	b	829	-	1/1/11/20	2/18/94/115	-
44	A86	q	314	-	-	3/34/90/90	0/3/3/3
44	A86	v	314	-	-	3/34/90/90	0/3/3/3
42	DD6	D	317	-	-	1/26/80/80	0/3/3/3
40	CLA	b	813	24	1/1/12/20	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A1EB4	W	319	-	-	11/38/98/103	0/3/3/3
44	A86	C	311	-	-	8/34/90/90	1/3/3/3
41	KC2	u	315	-	-	8/15/71/71	-
46	SQD	I	215	-	-	17/49/69/69	0/1/1/1
41	KC2	Y	309	21,44	-	8/15/71/71	-
44	A86	S	316	-	-	8/34/90/90	0/3/3/3
42	DD6	I	211	-	-	6/26/80/80	0/3/3/3
43	LMG	a	801	-	-	13/30/50/70	0/1/1/1
40	CLA	X	305	-	1/1/12/20	8/21/97/115	-
40	CLA	b	819	24	1/1/14/20	15/38/114/115	-
44	A86	q	324	-	-	7/34/90/90	0/3/3/3
40	CLA	X	310	-	1/1/13/20	9/27/103/115	-
40	CLA	N	307	-	1/1/14/20	6/33/109/115	-
40	CLA	a	808	-	1/1/15/20	6/39/115/115	-
43	LMG	L	319	-	-	15/32/52/70	0/1/1/1
44	A86	P	314	-	-	6/34/90/90	0/3/3/3
40	CLA	y	305	-	1/1/12/20	3/19/95/115	-
40	CLA	K	308	11	1/1/13/20	9/32/108/115	-
47	A1EB1	S	320	-	-	6/43/100/100	1/3/3/3
41	KC2	M	301	13	-	6/15/71/71	-
40	CLA	J	305	10	1/1/13/20	7/27/103/115	-
40	CLA	F	321	-	1/1/14/20	12/33/109/115	-
41	KC2	y	307	-	-	6/15/71/71	-
40	CLA	F	301	-	1/1/12/20	10/25/101/115	-
40	CLA	a	803	-	1/1/15/20	4/39/115/115	-
42	DD6	J	316	-	-	0/26/80/80	0/3/3/3
46	SQD	F	320	-	-	10/31/51/69	0/1/1/1
40	CLA	o	313	-	1/1/11/20	5/18/94/115	-
40	CLA	p	308	-	1/1/14/20	7/33/109/115	-
40	CLA	x	305	-	1/1/12/20	2/23/99/115	-
42	DD6	I	212	-	-	0/26/80/80	0/3/3/3
43	LMG	T	318	-	-	15/35/55/70	0/1/1/1
40	CLA	X	307	20	1/1/14/20	5/33/109/115	-
52	DGD	b	850	-	-	19/45/85/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	G	206	7	1/1/13/20	9/29/105/115	-
40	CLA	I	203	9	1/1/13/20	6/27/103/115	-
44	A86	P	321	-	-	6/34/90/90	0/3/3/3
40	CLA	Z	306	22	1/1/14/20	14/33/109/115	-
40	CLA	q	305	-	1/1/14/20	3/33/109/115	-
41	KC2	Z	308	22	-	5/15/71/71	-
40	CLA	t	304	-	1/1/14/20	8/33/109/115	-
42	DD6	F	316	-	-	2/26/80/80	0/3/3/3
43	LMG	l	201	-	-	19/34/54/70	0/1/1/1
42	DD6	L	317	-	-	0/26/80/80	0/3/3/3
41	KC2	o	303	34	-	4/15/71/71	-
44	A86	p	319	-	-	11/34/90/90	0/3/3/3
46	SQD	M	318	-	-	8/27/47/69	0/1/1/1
40	CLA	V	202	19	1/1/13/20	8/27/103/115	-
40	CLA	b	806	24	1/1/15/20	14/39/115/115	-
40	CLA	U	204	18	1/1/11/20	8/18/94/115	-
40	CLA	D	306	4	1/1/13/20	6/27/103/115	-
44	A86	w	316	-	-	12/34/90/90	0/3/3/3
40	CLA	b	835	24	1/1/15/20	13/38/115/115	-
40	CLA	M	312	13	1/1/14/20	14/33/109/115	-
40	CLA	a	811	23,40	1/1/14/20	12/36/112/115	-
40	CLA	f	201	-	1/1/14/20	5/33/109/115	-
44	A86	F	312	-	-	4/34/90/90	0/3/3/3
40	CLA	A	306	1	1/1/14/20	9/33/109/115	-
41	KC2	v	308	36	-	10/15/71/71	-
49	BCR	j	103	-	-	4/29/63/63	0/2/2/2
40	CLA	L	304	12	1/1/13/20	2/30/106/115	-
40	CLA	t	303	38	1/1/11/20	3/18/94/115	-
41	KC2	G	202	-	-	10/15/71/71	-
40	CLA	C	306	3	1/1/15/20	17/39/115/115	-
41	KC2	T	303	-	-	4/15/71/71	-
42	DD6	Q	212	-	-	1/26/80/80	0/3/3/3
47	A1EB1	u	323	-	-	3/43/100/100	0/3/3/3
49	BCR	b	845	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	E	312	-	1/1/11/20	4/18/94/115	-
40	CLA	Y	304	-	1/1/11/20	1/18/94/115	-
40	CLA	Q	202	16	1/1/13/20	5/31/107/115	-
44	A86	Y	319	-	-	6/34/90/90	0/3/3/3
40	CLA	G	205	7	1/1/12/20	0/21/97/115	-
40	CLA	b	836	24	1/1/14/20	6/33/109/115	-
43	LMG	E	301	40	-	14/26/46/70	0/1/1/1
40	CLA	o	304	34	1/1/14/20	6/33/109/115	-
47	A1EB1	N	320	-	-	8/43/100/100	0/3/3/3
40	CLA	I	202	9	1/1/13/20	8/27/103/115	-
40	CLA	b	831	24	1/1/12/20	5/23/99/115	-
40	CLA	Z	304	-	1/1/14/20	4/33/109/115	-
44	A86	D	320	-	-	5/34/90/90	0/3/3/3
40	CLA	E	303	-	1/1/14/20	5/33/109/115	-
40	CLA	o	310	-	1/1/13/20	9/27/103/115	-
51	SF4	c	101	-	-	-	0/6/5/5
49	BCR	a	843	-	-	4/29/63/63	0/2/2/2
42	DD6	A	316	-	-	1/26/80/80	0/3/3/3
42	DD6	v	318	-	-	0/26/80/80	0/3/3/3
41	KC2	p	315	-	-	8/15/71/71	-
40	CLA	u	307	35	1/1/13/20	8/27/103/115	-
40	CLA	E	308	5	1/1/13/20	6/31/107/115	-
40	CLA	P	308	-	1/1/14/20	12/33/109/115	-
40	CLA	F	305	-	1/1/11/20	4/18/94/115	-
40	CLA	L	311	12	1/1/11/20	6/18/94/115	-
40	CLA	v	304	-	1/1/12/20	4/24/100/115	-
44	A86	K	314	-	-	4/34/90/90	0/3/3/3
41	KC2	G	208	-	-	4/15/71/71	-
43	LMG	A	317	-	-	22/35/55/70	0/1/1/1
44	A86	N	315	-	-	6/34/90/90	0/3/3/3
40	CLA	p	311	-	1/1/13/20	10/27/103/115	-
41	KC2	o	308	34	-	8/15/71/71	-
40	CLA	Z	313	22	1/1/11/20	5/18/94/115	-
40	CLA	b	842	-	1/1/14/20	8/35/111/115	-
40	CLA	X	313	20	1/1/11/20	1/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	q	320	-	-	6/26/80/80	0/3/3/3
44	A86	w	315	-	-	8/34/90/90	1/3/3/3
44	A86	z	301	-	-	6/34/90/90	0/3/3/3
40	CLA	z	314	-	1/1/11/20	4/18/94/115	-
40	CLA	w	309	-	1/1/13/20	9/27/103/115	-
40	CLA	N	310	-	1/1/12/20	5/21/97/115	-
40	CLA	W	306	13	1/1/14/20	12/33/109/115	-
40	CLA	a	812	23	1/1/13/20	0/27/103/115	-
42	DD6	j	104	-	-	1/26/80/80	0/3/3/3
41	KC2	L	313	12	-	8/15/71/71	-
42	DD6	H	314	-	-	2/26/80/80	0/3/3/3
44	A86	w	311	-	-	10/34/90/90	0/3/3/3
40	CLA	W	313	13	1/1/14/20	9/33/109/115	-
40	CLA	I	208	-	1/1/13/20	6/27/103/115	-
40	CLA	J	307	10	1/1/11/20	4/18/94/115	-
49	BCR	a	846	-	-	2/29/63/63	0/2/2/2
49	BCR	i	102	-	-	4/29/63/63	0/2/2/2
41	KC2	X	302	-	-	4/15/71/71	-
40	CLA	a	831	-	1/1/14/20	8/33/109/115	-
42	DD6	Q	211	-	-	1/26/80/80	0/3/3/3
40	CLA	a	826	-	1/1/14/20	11/35/111/115	-
40	CLA	D	305	4	1/1/9/20	2/18/82/115	-
40	CLA	a	813	23	1/1/14/20	6/33/109/115	-
41	KC2	N	309	-	-	4/15/71/71	-
43	LMG	p	301	-	-	9/34/54/70	0/1/1/1
44	A86	S	318	-	-	2/34/90/90	0/3/3/3
41	KC2	I	214	-	-	7/15/71/71	-
44	A86	x	319	-	-	12/34/90/90	0/3/3/3
50	PQN	a	847	-	-	3/17/37/43	0/2/2/2
41	KC2	E	319	-	-	10/15/71/71	-
42	DD6	q	318	-	-	0/26/80/80	0/3/3/3
44	A86	w	310	-	-	7/34/90/90	0/3/3/3
42	DD6	W	315	-	-	1/26/80/80	0/3/3/3
40	CLA	y	308	-	1/1/11/20	5/18/94/115	-
40	CLA	R	310	-	1/1/11/20	3/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	L	309	12	-	8/15/71/71	-
40	CLA	a	818	-	1/1/11/20	2/18/94/115	-
40	CLA	x	312	-	1/1/14/20	9/33/109/115	-
42	DD6	N	317	-	-	3/26/80/80	0/3/3/3
41	KC2	W	302	-	-	6/15/71/71	-
40	CLA	j	102	30	1/1/11/20	4/18/94/115	-
49	BCR	l	206	-	-	6/29/63/63	0/2/2/2
40	CLA	x	308	35	1/1/14/20	6/33/109/115	-
40	CLA	J	309	-	1/1/11/20	2/18/94/115	-
47	A1EB1	T	316	40	-	5/43/100/100	0/3/3/3
48	A1EB4	P	320	-	-	7/38/98/103	0/3/3/3
40	CLA	K	307	11	1/1/12/20	10/26/102/115	-
40	CLA	q	310	-	1/1/12/20	11/23/99/115	-
40	CLA	v	310	-	1/1/12/20	11/23/99/115	-
44	A86	X	319	-	-	7/34/90/90	0/3/3/3
44	A86	z	315	-	-	7/34/90/90	0/3/3/3
40	CLA	R	307	-	1/1/13/20	5/27/103/115	-
40	CLA	A	301	1	1/1/11/20	3/18/94/115	-
40	CLA	b	814	24	1/1/15/20	10/39/115/115	-
41	KC2	W	309	-	-	7/15/71/71	-
40	CLA	F	303	6	1/1/14/20	8/36/112/115	-
44	A86	M	313	-	-	3/34/90/90	0/3/3/3
40	CLA	G	207	-	1/1/12/20	5/26/102/115	-
40	CLA	z	311	-	1/1/13/20	9/27/103/115	-
44	A86	P	316	-	-	6/34/90/90	0/3/3/3
47	A1EB1	S	321	-	-	9/43/100/100	1/3/3/3
40	CLA	p	307	35	1/1/13/20	7/27/103/115	-
41	KC2	F	309	6	-	6/15/71/71	-
40	CLA	a	841	23	1/1/15/20	8/39/115/115	-
41	KC2	N	303	14	-	5/15/71/71	-
40	CLA	L	301	-	1/1/11/20	2/18/94/115	-
40	CLA	v	307	36	1/1/14/20	11/33/109/115	-
40	CLA	M	311	13	1/1/14/20	12/36/112/115	-
44	A86	X	314	-	-	4/34/90/90	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	P	307	13	1/1/13/20	6/32/108/115	-
40	CLA	Q	209	-	1/1/11/20	6/18/94/115	-
40	CLA	w	304	-	1/1/14/20	8/33/109/115	-
41	KC2	H	316	-	-	4/15/71/71	-
40	CLA	a	836	23	1/1/15/20	10/39/115/115	-
47	A1EB1	T	320	-	-	12/43/100/100	0/3/3/3
40	CLA	q	301	-	1/1/13/20	4/27/103/115	-
41	KC2	R	301	15	-	4/15/71/71	-

The worst 5 of 4168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	309	KC2	MG-ND	-10.40	1.85	2.05
41	Z	309	KC2	MG-ND	-10.36	1.85	2.05
41	v	303	KC2	MG-ND	-10.32	1.85	2.05
41	M	303	KC2	MG-ND	-10.26	1.85	2.05
41	P	304	KC2	MG-ND	-10.26	1.85	2.05

The worst 5 of 4057 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	M	313	A86	O1-C20-C19	-11.55	102.66	113.49
40	F	303	CLA	C1C-NC-C4C	-9.80	102.21	106.68
40	Q	206	CLA	C1C-NC-C4C	-9.59	102.31	106.68
44	X	318	A86	O1-C20-C19	9.46	122.36	113.49
40	D	305	CLA	CBD-CHA-C1A	9.36	131.24	118.85

5 of 388 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	A	301	CLA	ND
40	A	302	CLA	ND
40	A	303	CLA	ND
40	A	304	CLA	ND
40	A	305	CLA	ND

5 of 4962 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	A	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	A	303	CLA	C3A-C2A-CAA-CBA
40	A	304	CLA	C1A-C2A-CAA-CBA
40	A	304	CLA	C3A-C2A-CAA-CBA
40	A	305	CLA	C2B-C3B-CAB-CBB

5 of 21 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	t	311	A86	C31-C32-C33-C34-C35-C36
44	X	314	A86	C31-C32-C33-C34-C35-C36
44	C	311	A86	C31-C32-C33-C34-C35-C36
44	Z	317	A86	C31-C32-C33-C34-C35-C36
44	Z	316	A86	C31-C32-C33-C34-C35-C36

264 monomers are involved in 562 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	K	301	CLA	2	0
40	Q	206	CLA	9	0
40	H	307	CLA	1	0
40	W	305	CLA	1	0
44	D	319	A86	1	0
40	o	307	CLA	1	0
40	U	203	CLA	1	0
40	w	308	CLA	5	0
41	N	302	KC2	1	0
40	F	306	CLA	1	0
42	x	320	DD6	2	0
44	P	317	A86	1	0
40	J	318	CLA	2	0
42	O	314	DD6	1	0
40	V	201	CLA	2	0
40	a	824	CLA	1	0
40	S	308	CLA	3	0
42	H	312	DD6	1	0
40	M	307	CLA	1	0
47	x	322	A1EB1	1	0
40	a	809	CLA	1	0
49	f	206	BCR	4	0
42	u	321	DD6	1	0
44	X	317	A86	3	0
40	A	305	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	J	315	DD6	1	0
40	b	820	CLA	1	0
42	I	210	DD6	1	0
40	L	305	CLA	1	0
49	b	846	BCR	1	0
41	w	307	KC2	1	0
47	P	301	A1EB1	9	0
47	t	315	A1EB1	1	0
40	Q	204	CLA	1	0
40	N	304	CLA	1	0
40	D	304	CLA	1	0
40	a	819	CLA	21	0
40	b	810	CLA	2	0
40	z	305	CLA	3	0
40	A	311	CLA	3	0
40	H	301	CLA	1	0
40	f	202	CLA	3	0
40	C	307	CLA	2	0
41	X	303	KC2	1	0
47	K	315	A1EB1	1	0
40	a	815	CLA	12	0
40	Q	207	CLA	1	0
42	p	322	DD6	1	0
43	D	318	LMG	1	0
41	T	308	KC2	1	0
44	W	301	A86	1	0
40	b	826	CLA	1	0
41	z	304	KC2	1	0
43	u	301	LMG	1	0
40	b	834	CLA	2	0
40	b	839	CLA	1	0
40	S	319	CLA	1	0
47	v	324	A1EB1	4	0
40	L	306	CLA	7	0
40	i	101	CLA	4	0
47	q	322	A1EB1	1	0
40	D	307	CLA	1	0
41	t	308	KC2	1	0
42	N	316	DD6	1	0
42	Y	322	DD6	9	0
40	v	311	CLA	1	0
44	y	310	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	S	312	CLA	6	0
46	P	319	SQD	5	0
40	z	306	CLA	1	0
49	b	847	BCR	1	0
40	b	824	CLA	2	0
40	A	302	CLA	2	0
42	v	320	DD6	1	0
40	C	302	CLA	1	0
40	G	213	CLA	2	0
40	o	311	CLA	1	0
41	W	310	KC2	1	0
44	Y	315	A86	1	0
44	Q	210	A86	1	0
40	a	850	CLA	1	0
40	b	828	CLA	1	0
43	x	301	LMG	5	0
40	N	306	CLA	1	0
40	v	312	CLA	2	0
40	E	311	CLA	6	0
43	E	321	LMG	3	0
40	E	307	CLA	12	0
40	a	814	CLA	1	0
40	a	823	CLA	1	0
40	w	305	CLA	1	0
41	y	306	KC2	7	0
41	M	303	KC2	1	0
40	o	301	CLA	1	0
41	T	301	KC2	1	0
43	E	320	LMG	2	0
40	l	202	CLA	2	0
40	y	302	CLA	1	0
44	L	314	A86	1	0
40	z	302	CLA	1	0
46	W	318	SQD	4	0
44	t	310	A86	1	0
41	O	301	KC2	1	0
41	Y	308	KC2	9	0
40	a	832	CLA	2	0
40	P	306	CLA	1	0
42	Q	214	DD6	1	0
44	o	315	A86	1	0
42	L	315	DD6	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	j	101	LMG	13	0
47	t	314	A1EB1	1	0
40	v	301	CLA	1	0
44	W	314	A86	1	0
47	u	322	A1EB1	1	0
47	x	321	A1EB1	1	0
40	p	305	CLA	1	0
40	S	301	CLA	9	0
41	Z	309	KC2	1	0
42	P	315	DD6	5	0
40	a	842	CLA	1	0
40	b	807	CLA	1	0
41	C	303	KC2	1	0
40	D	303	CLA	1	0
40	l	203	CLA	1	0
42	M	314	DD6	1	0
40	a	817	CLA	1	0
44	M	315	A86	1	0
40	b	803	CLA	1	0
44	G	209	A86	3	0
40	R	305	CLA	1	0
47	Z	321	A1EB1	1	0
42	w	312	DD6	26	0
40	M	305	CLA	1	0
41	Z	303	KC2	1	0
49	r	201	BCR	1	0
40	k	202	CLA	16	0
40	b	833	CLA	1	0
44	p	318	A86	1	0
40	o	312	CLA	2	0
41	t	306	KC2	14	0
49	m	101	BCR	4	0
41	Q	201	KC2	2	0
40	X	304	CLA	2	0
40	P	305	CLA	3	0
40	a	816	CLA	1	0
40	p	306	CLA	1	0
42	C	310	DD6	1	0
42	B	305	DD6	1	0
47	v	322	A1EB1	1	0
40	a	830	CLA	1	0
40	F	307	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	p	324	A1EB1	1	0
40	B	307	CLA	3	0
40	W	312	CLA	2	0
42	F	314	DD6	1	0
40	D	311	CLA	2	0
40	b	809	CLA	3	0
40	P	313	CLA	1	0
46	k	205	SQD	3	0
40	b	827	CLA	1	0
41	Q	216	KC2	8	0
40	E	306	CLA	8	0
42	y	311	DD6	17	0
42	o	320	DD6	2	0
40	Z	305	CLA	1	0
49	l	208	BCR	1	0
41	L	303	KC2	1	0
40	S	313	CLA	1	0
44	Z	316	A86	1	0
45	S	323	LHG	2	0
40	W	311	CLA	1	0
40	A	308	CLA	4	0
40	G	201	CLA	1	0
40	L	312	CLA	1	0
42	t	312	DD6	29	0
49	a	845	BCR	1	0
40	R	306	CLA	1	0
40	S	314	CLA	1	0
40	q	311	CLA	2	0
40	k	201	CLA	1	0
40	N	305	CLA	1	0
41	P	303	KC2	1	0
40	b	832	CLA	2	0
40	f	205	CLA	4	0
40	E	302	CLA	1	0
40	l	205	CLA	1	0
47	y	313	A1EB1	4	0
40	K	306	CLA	1	0
40	x	306	CLA	1	0
40	a	835	CLA	1	0
40	L	307	CLA	1	0
40	T	305	CLA	1	0
40	S	305	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	z	319	A86	1	0
43	a	802	LMG	1	0
50	b	849	PQN	2	0
49	l	207	BCR	3	0
41	w	306	KC2	12	0
40	G	203	CLA	1	0
44	Y	320	A86	1	0
40	b	802	CLA	2	0
40	t	305	CLA	1	0
47	p	323	A1EB1	1	0
40	b	829	CLA	2	0
42	D	317	DD6	1	0
40	b	813	CLA	2	0
48	W	319	A1EB4	7	0
46	I	215	SQD	2	0
43	a	801	LMG	2	0
40	b	819	CLA	1	0
40	a	808	CLA	1	0
40	y	305	CLA	1	0
40	K	308	CLA	2	0
41	M	301	KC2	1	0
41	y	307	KC2	1	0
40	F	301	CLA	7	0
42	J	316	DD6	15	0
46	F	320	SQD	2	0
40	x	305	CLA	1	0
42	I	212	DD6	1	0
52	b	850	DGD	7	0
40	Z	306	CLA	1	0
42	L	317	DD6	17	0
46	M	318	SQD	1	0
40	V	202	CLA	4	0
40	b	806	CLA	3	0
40	D	306	CLA	1	0
44	w	316	A86	1	0
40	b	835	CLA	3	0
40	A	306	CLA	12	0
41	v	308	KC2	1	0
40	C	306	CLA	1	0
41	T	303	KC2	1	0
47	u	323	A1EB1	1	0
44	Y	319	A86	1	0

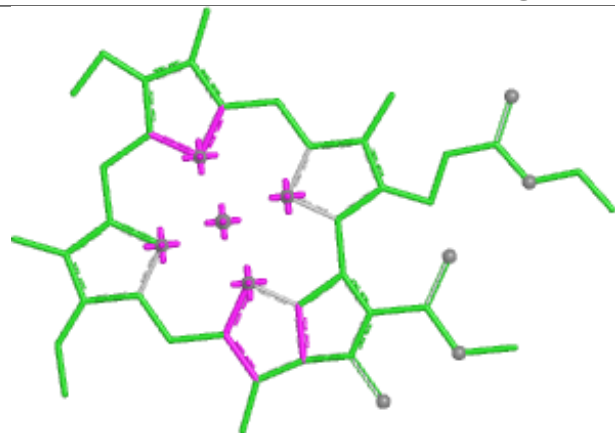
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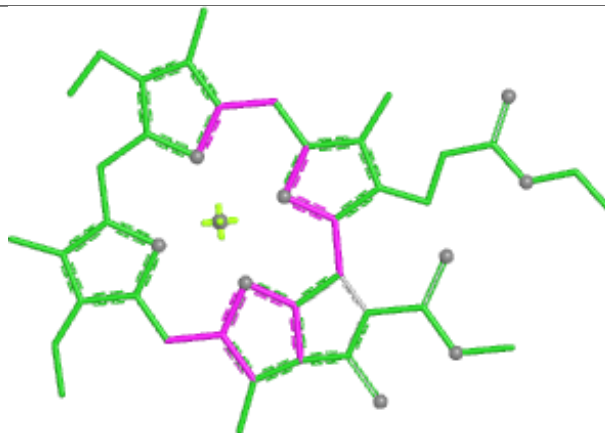
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40	E	303	CLA	4	0
49	a	843	BCR	5	0
42	A	316	DD6	10	0
42	v	318	DD6	4	0
40	E	308	CLA	4	0
40	P	308	CLA	6	0
40	F	305	CLA	1	0
44	N	315	A86	7	0
41	o	308	KC2	1	0
42	q	320	DD6	1	0
40	N	310	CLA	1	0
40	W	306	CLA	1	0
49	a	846	BCR	1	0
49	i	102	BCR	3	0
40	D	305	CLA	1	0
50	a	847	PQN	1	0
42	q	318	DD6	6	0
42	W	315	DD6	1	0
40	y	308	CLA	5	0
40	x	312	CLA	1	0
40	j	102	CLA	2	0
40	J	309	CLA	12	0
48	P	320	A1EB4	4	0
40	K	307	CLA	1	0
40	b	814	CLA	3	0
40	a	841	CLA	2	0
40	M	311	CLA	1	0
47	T	320	A1EB1	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.

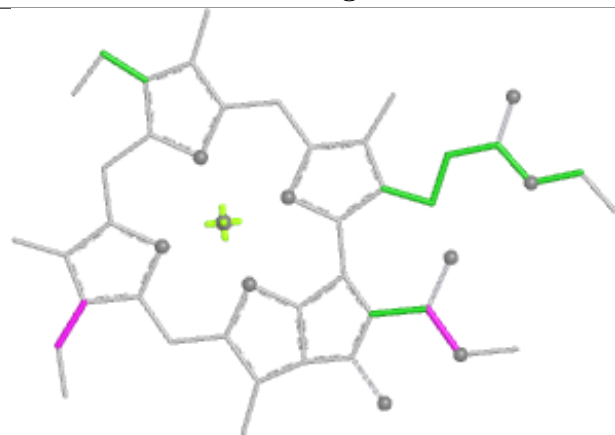
Ligand CLA K 301



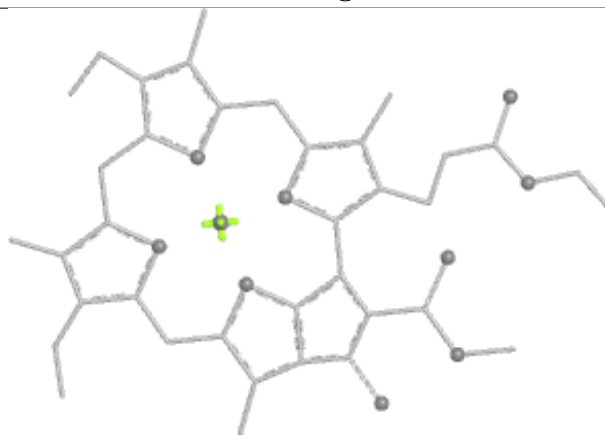
Bond lengths



Bond angles

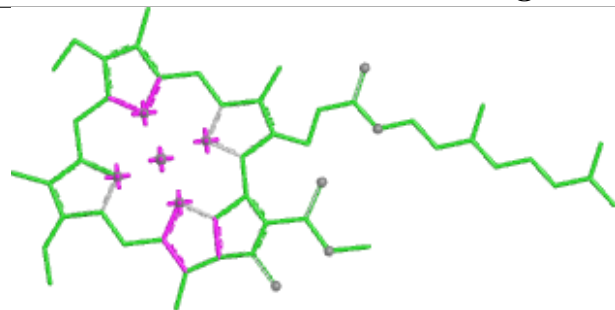


Torsions

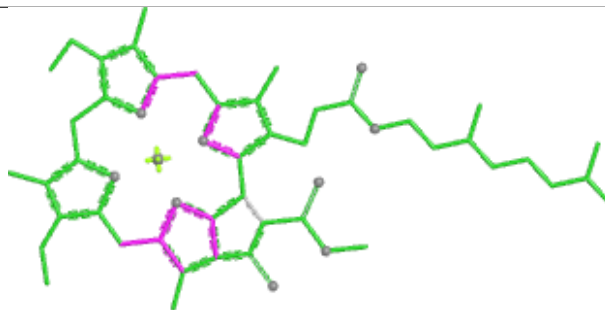


Rings

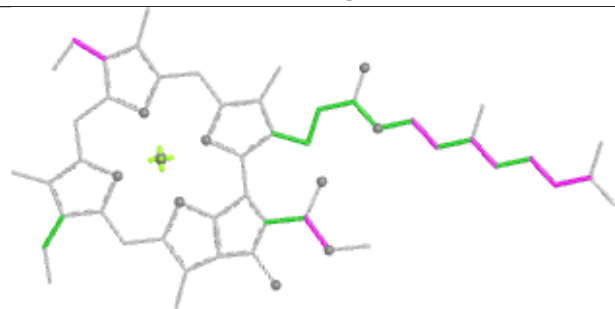
Ligand CLA Y 310



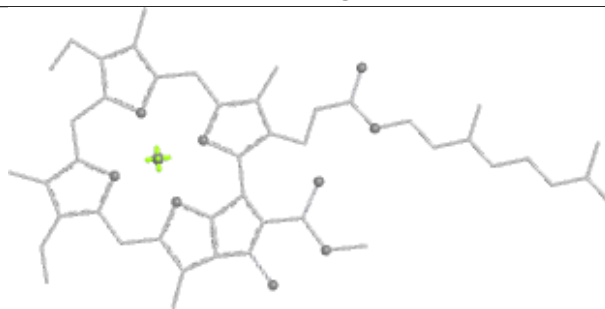
Bond lengths



Bond angles

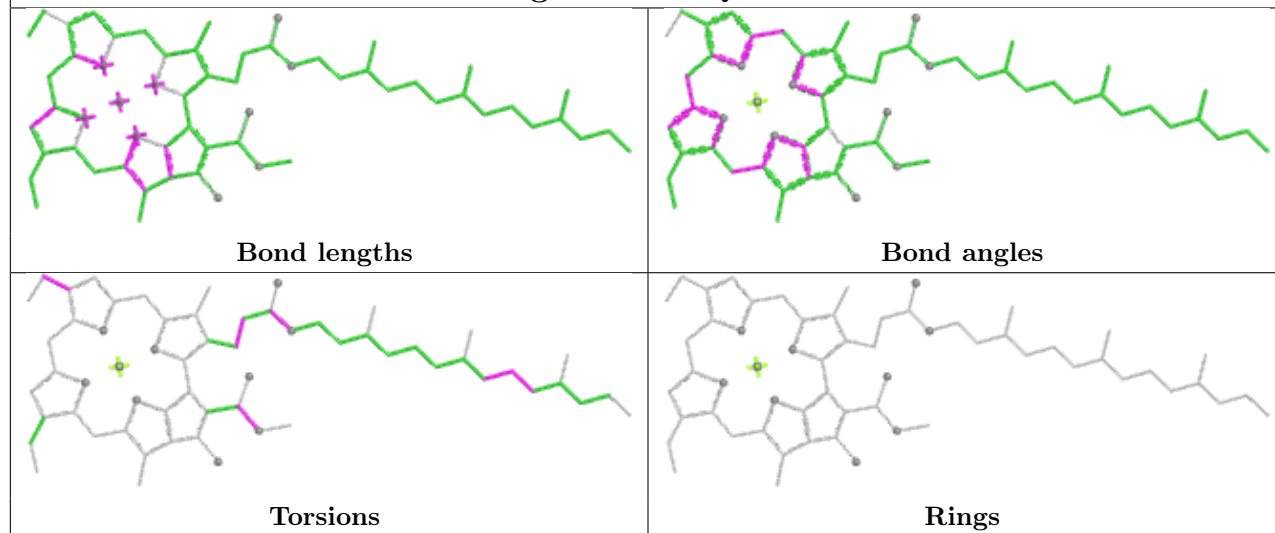


Torsions

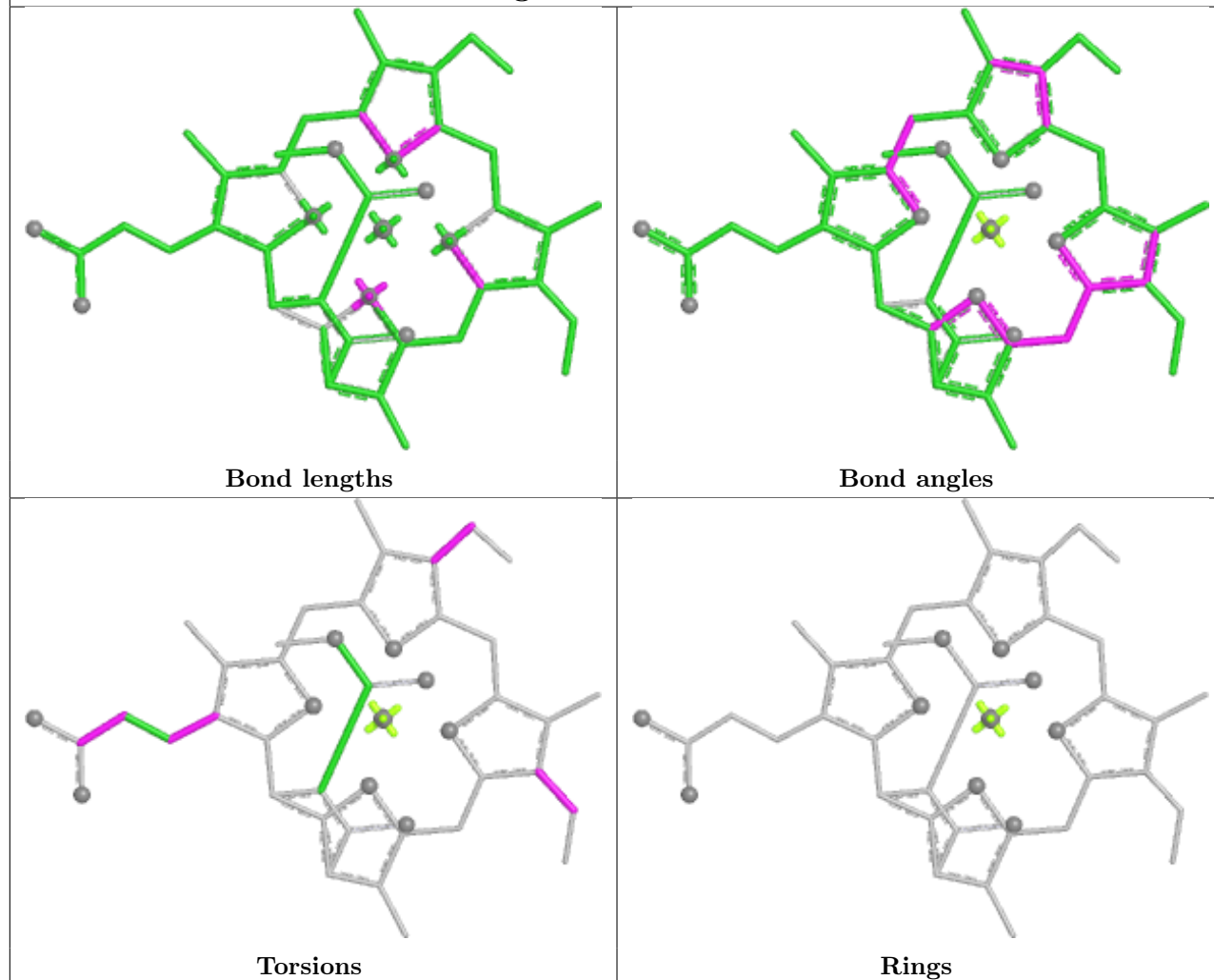


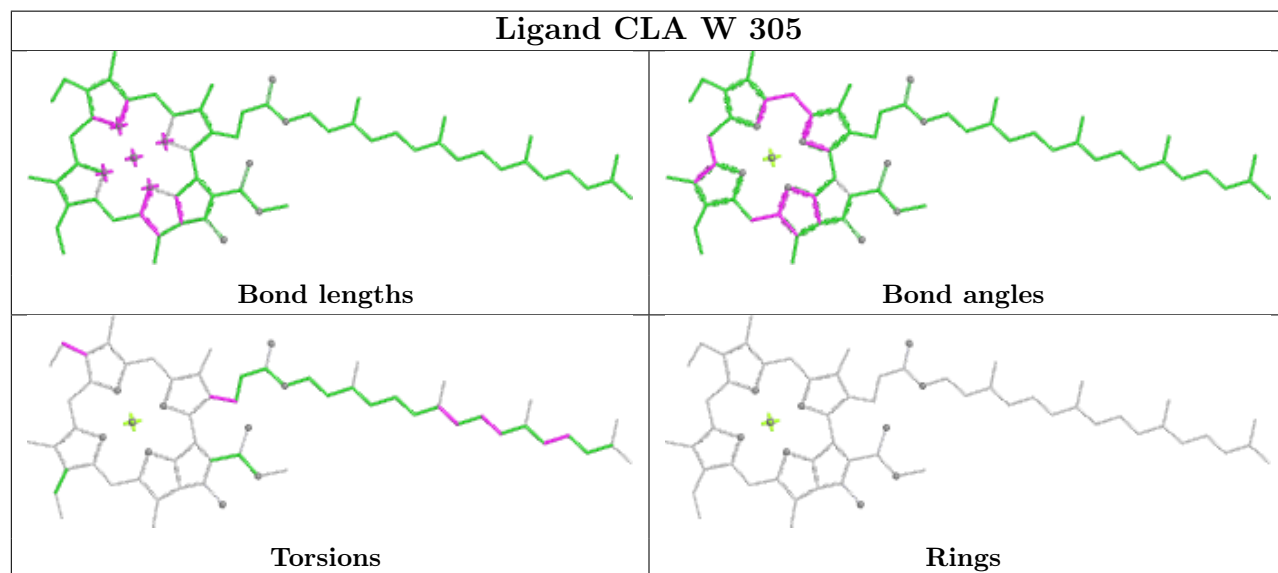
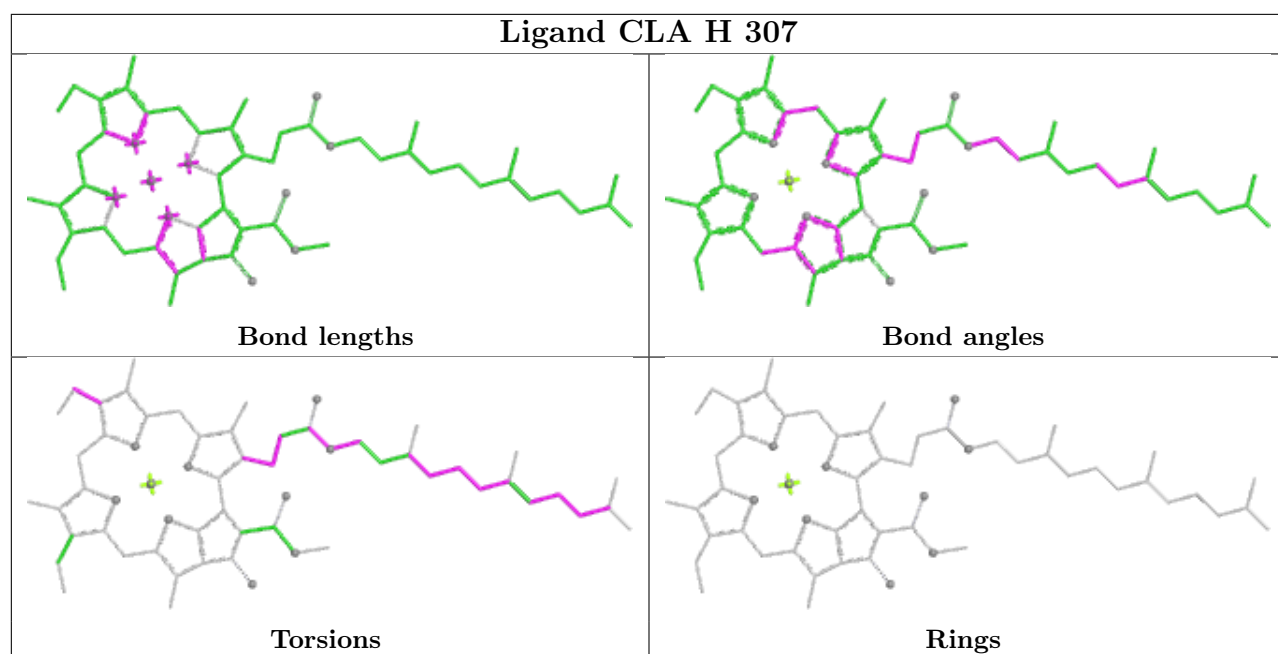
Rings

Ligand CLA Q 206

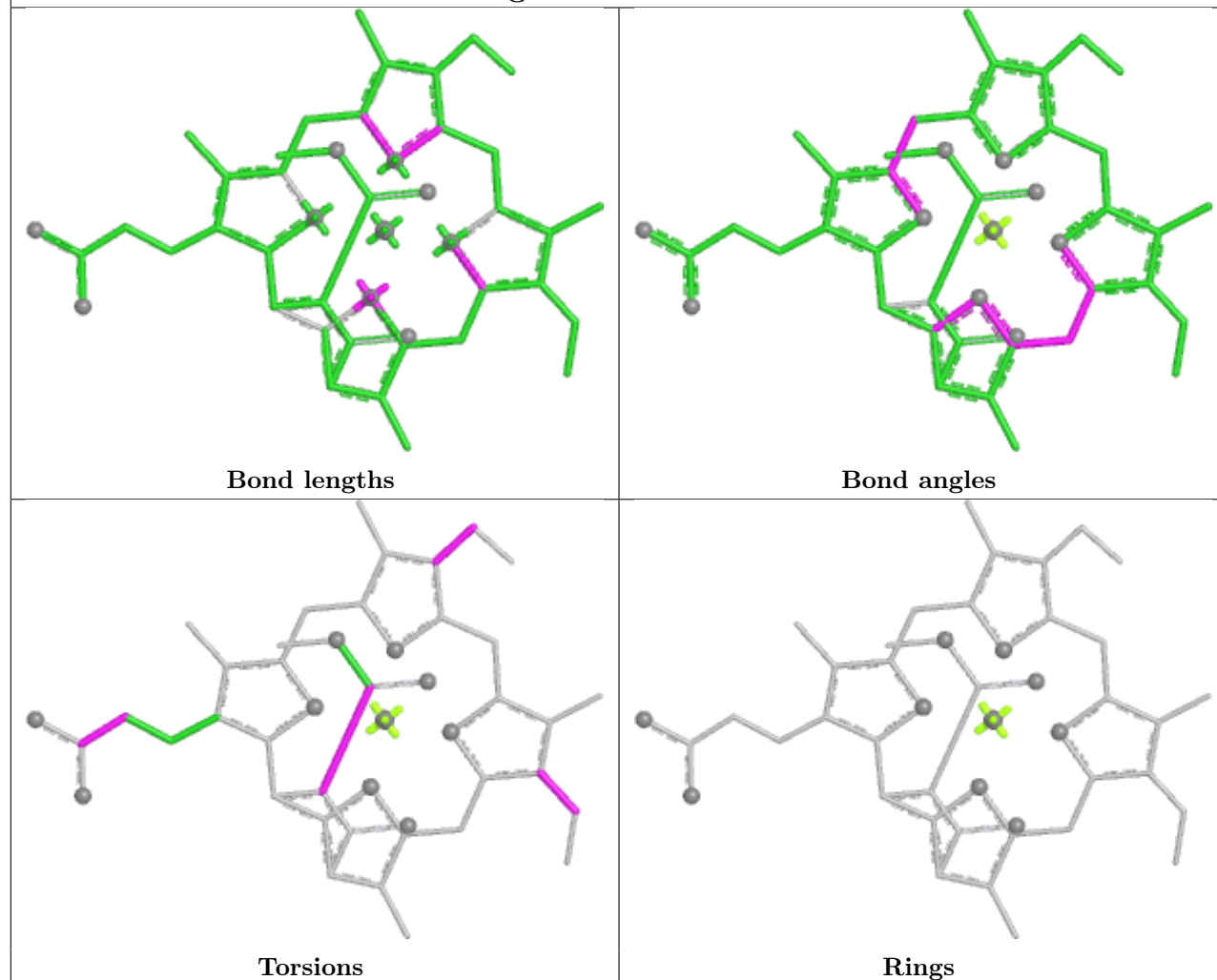


Ligand KC2 I 209

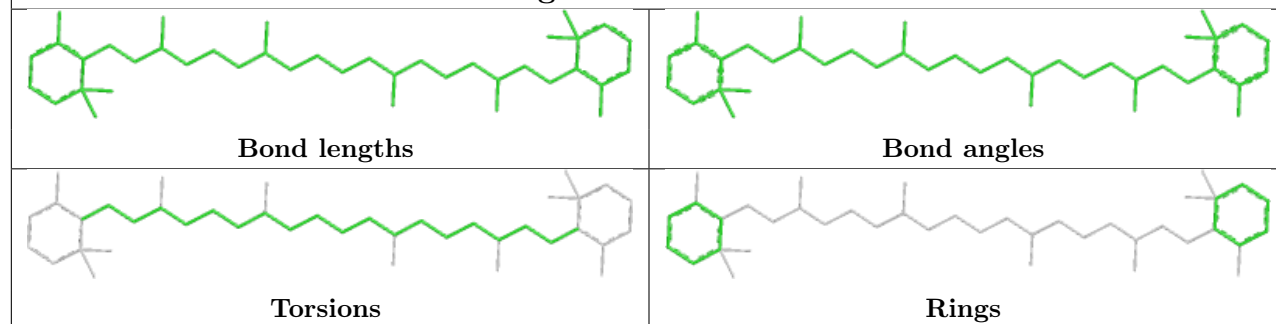


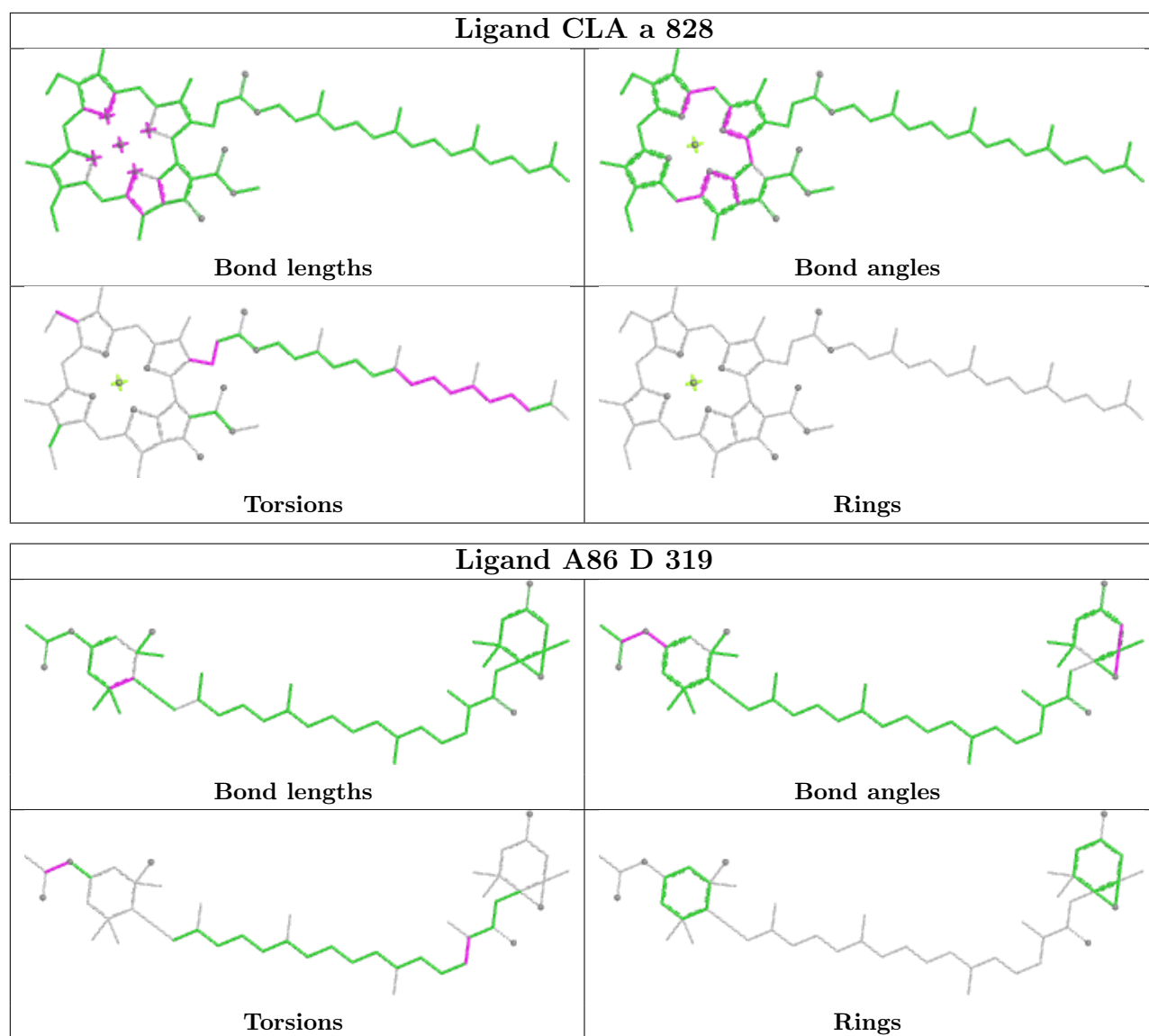


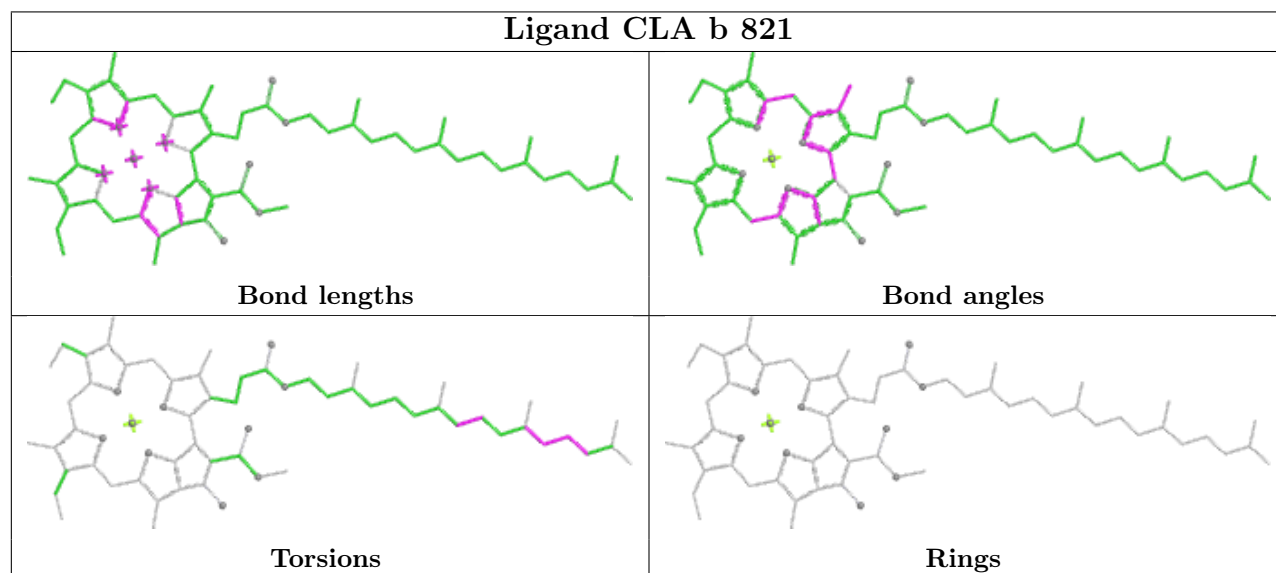
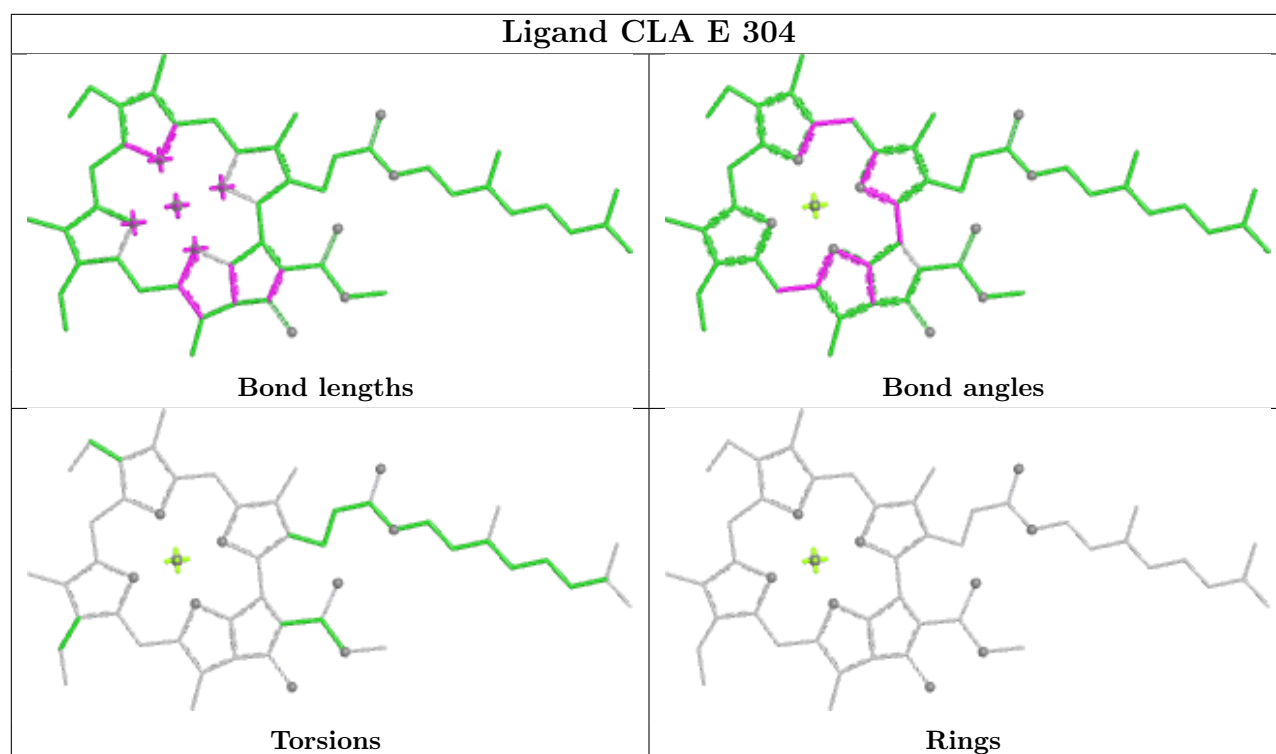
Ligand KC2 R 311

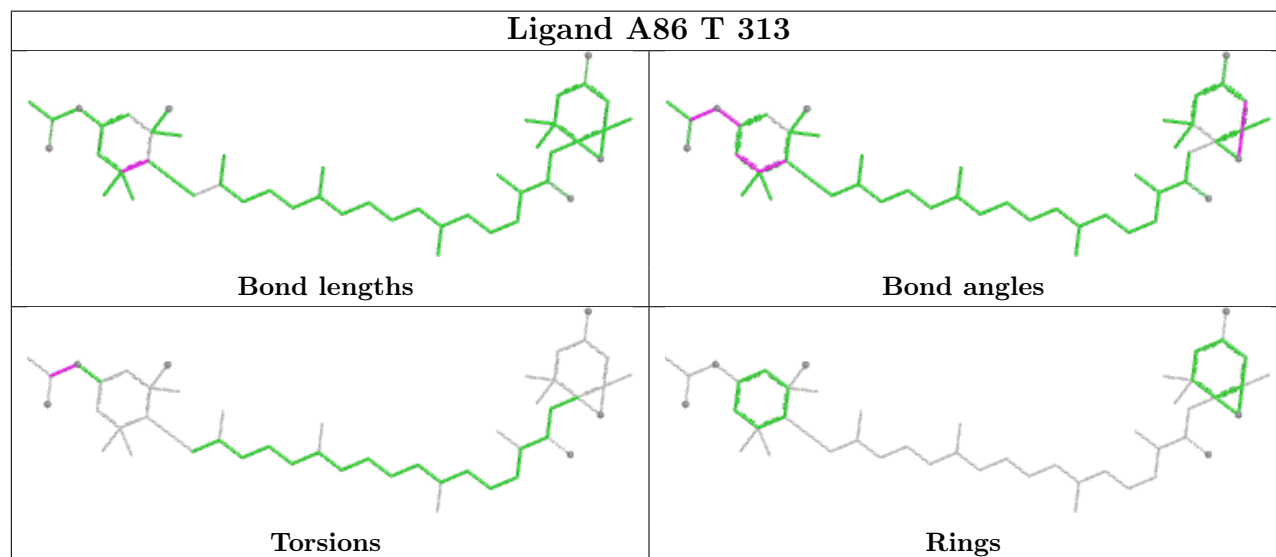
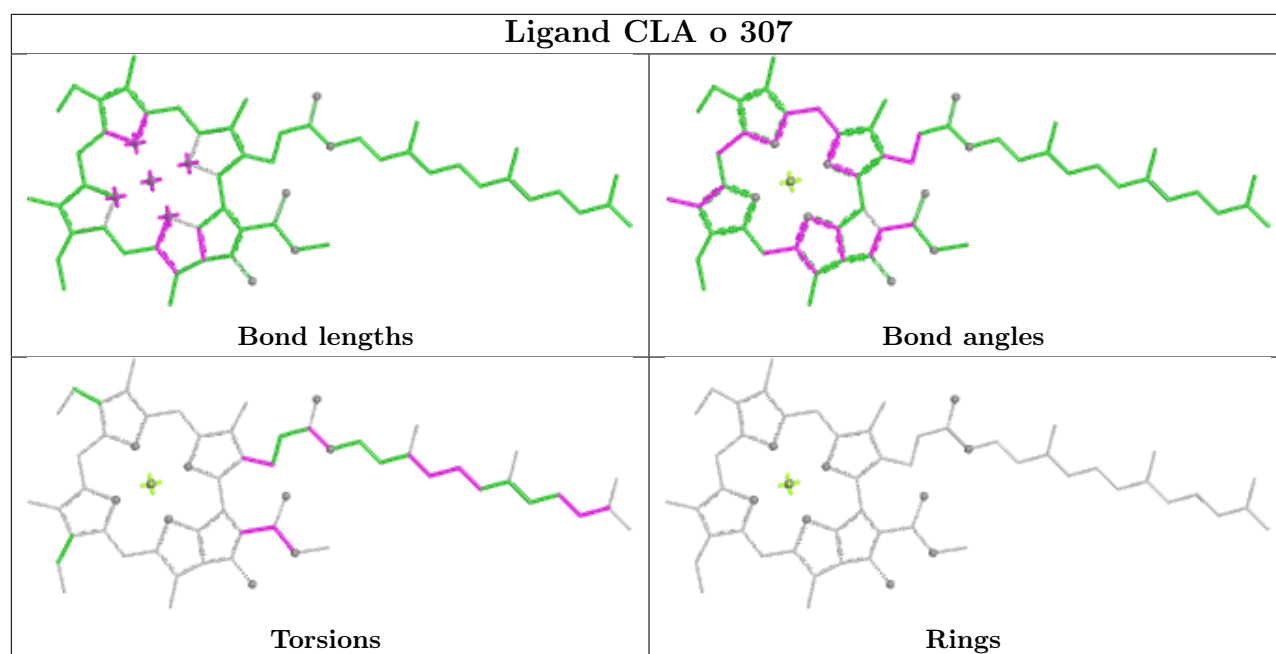


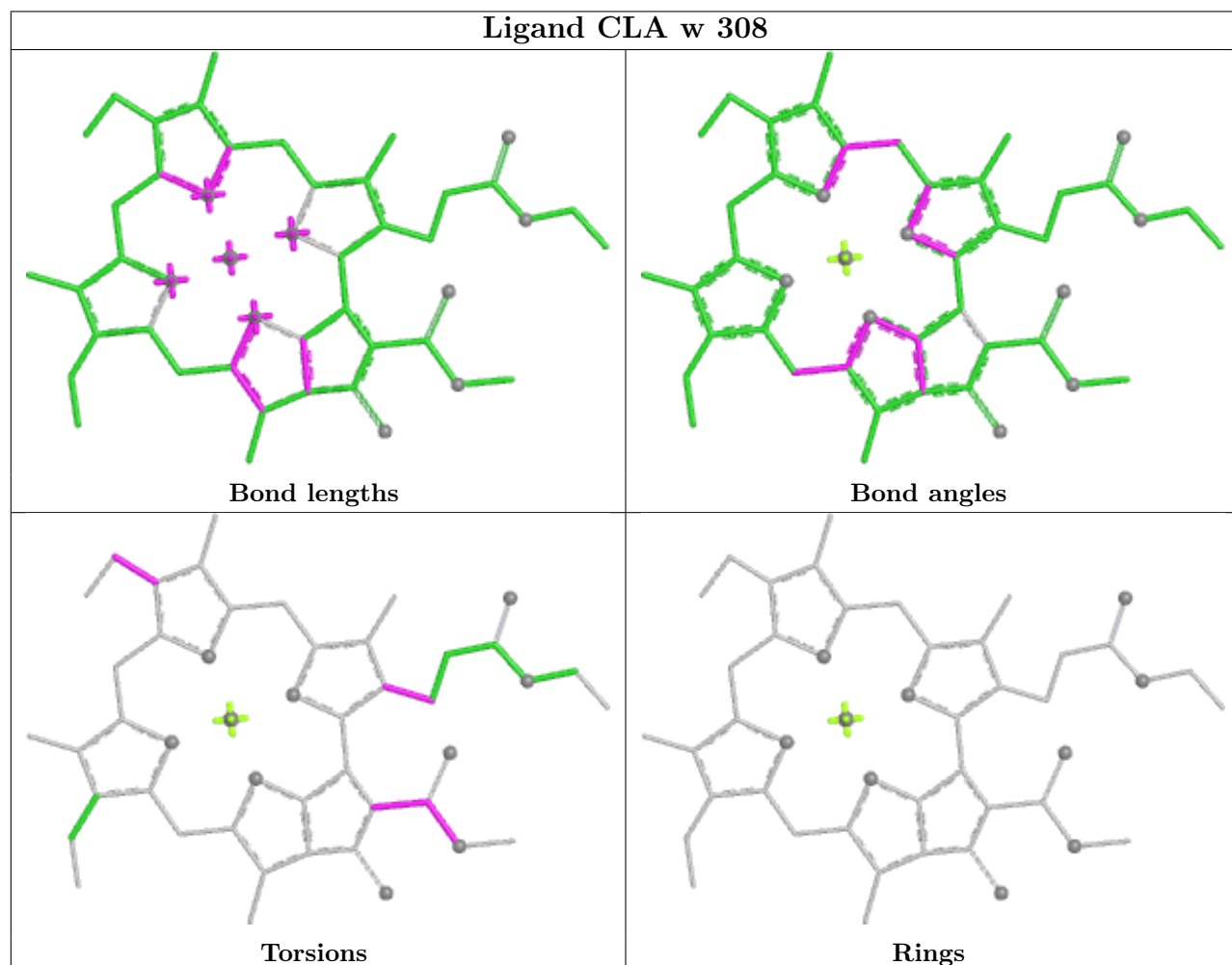
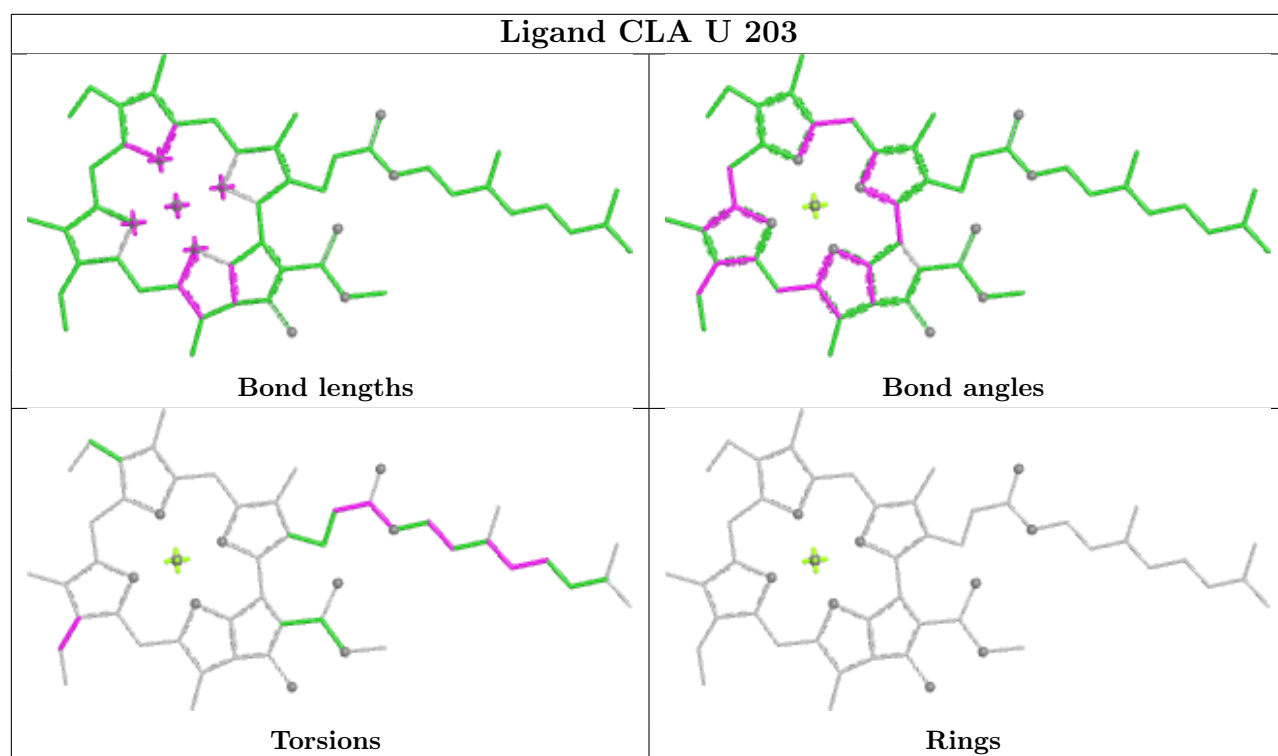
Ligand BCR f 203



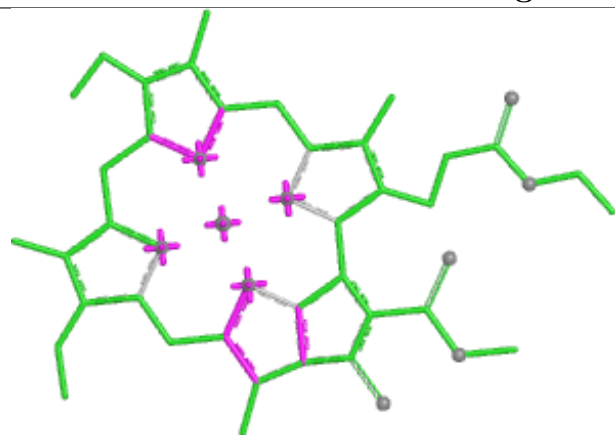




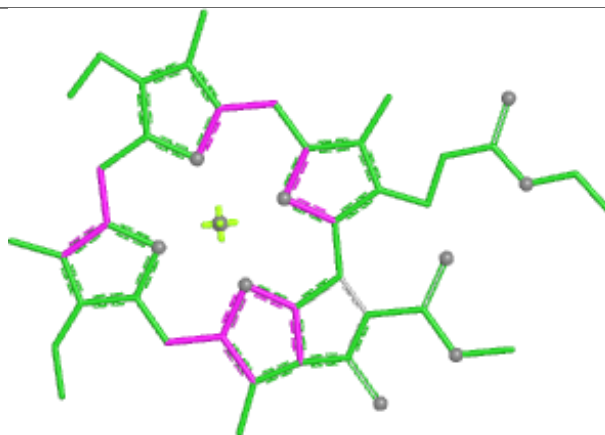




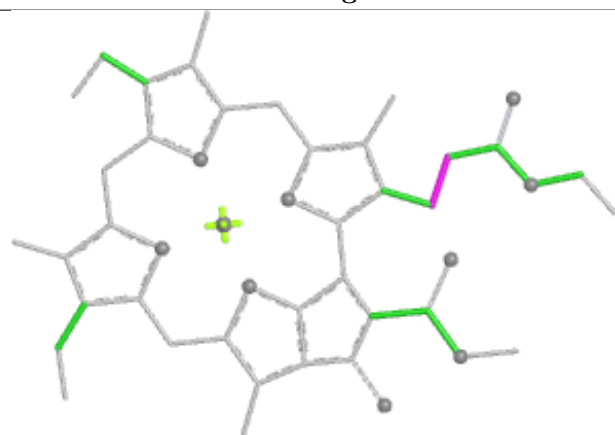
Ligand CLA U 206



Bond lengths



Bond angles

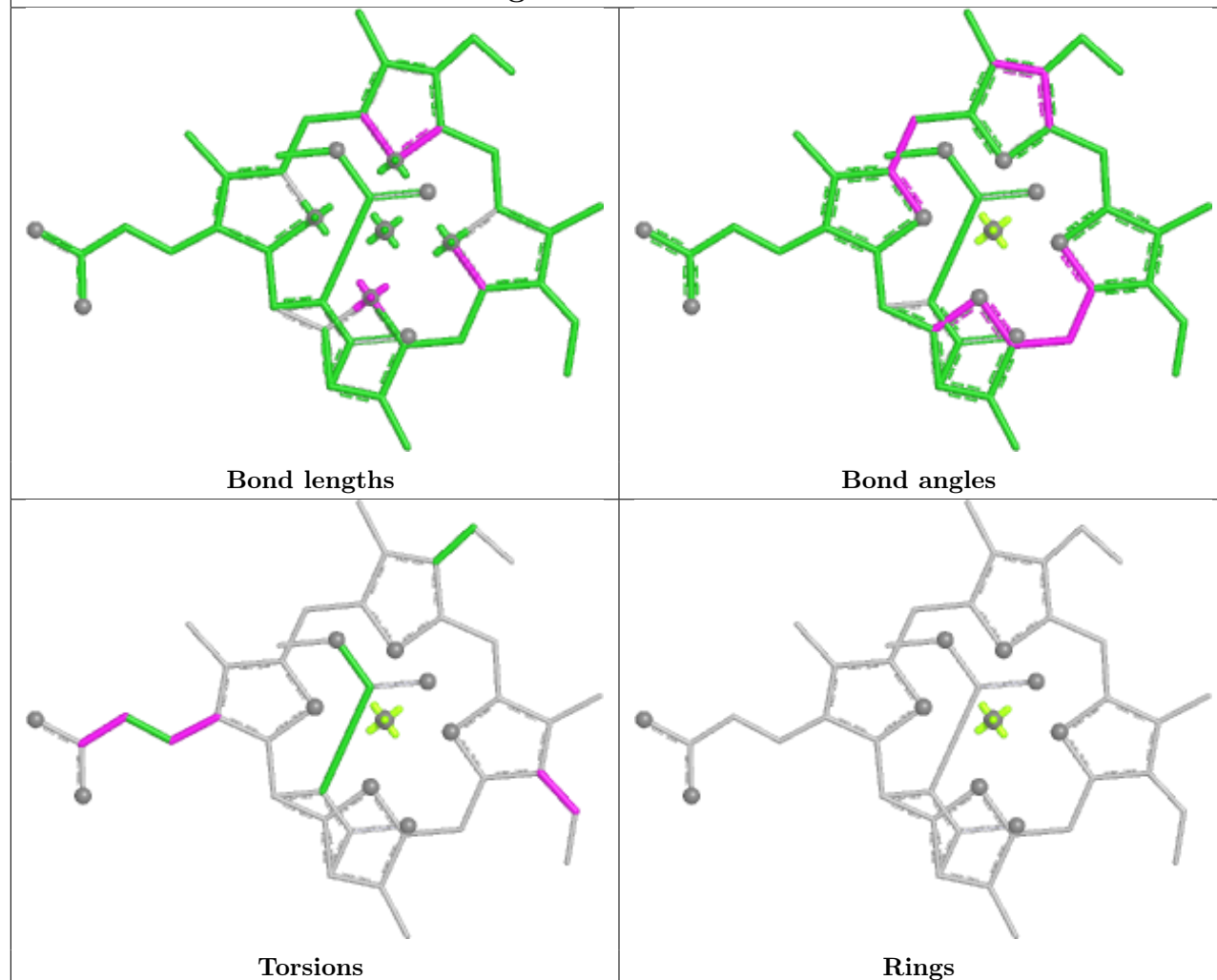


Torsions

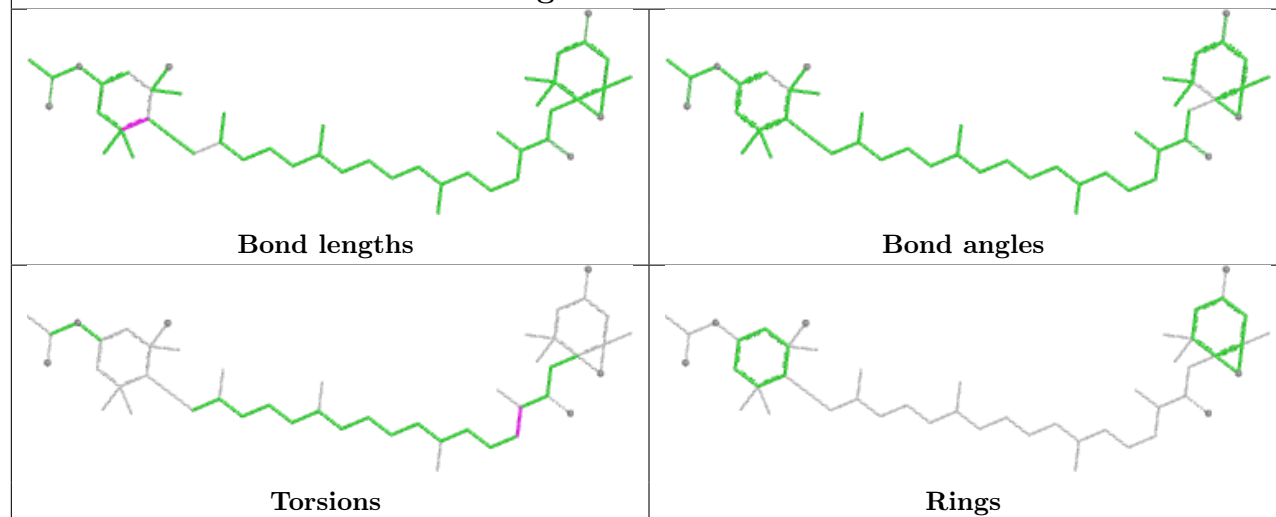


Rings

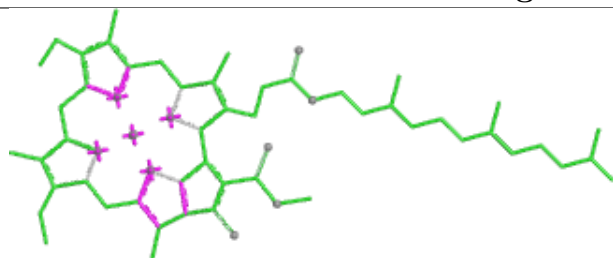
Ligand KC2 N 302



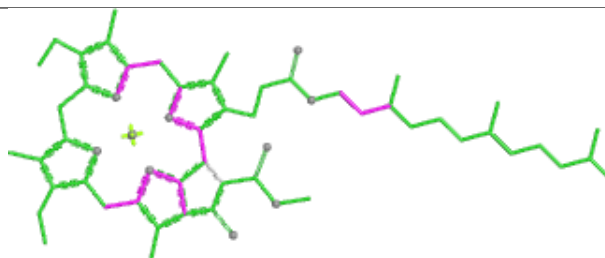
Ligand A86 N 318



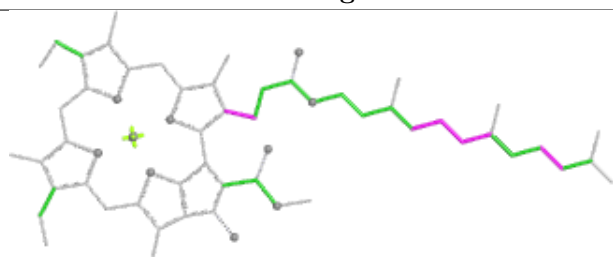
Ligand CLA F 306



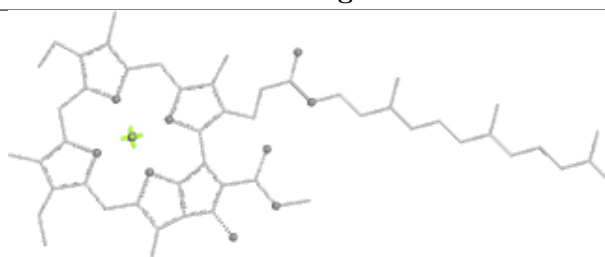
Bond lengths



Bond angles

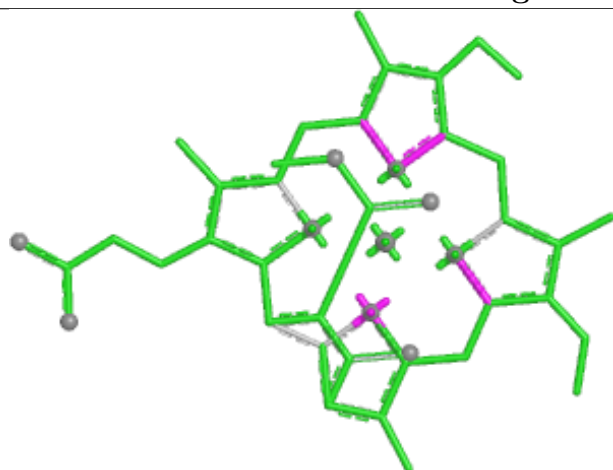


Torsions

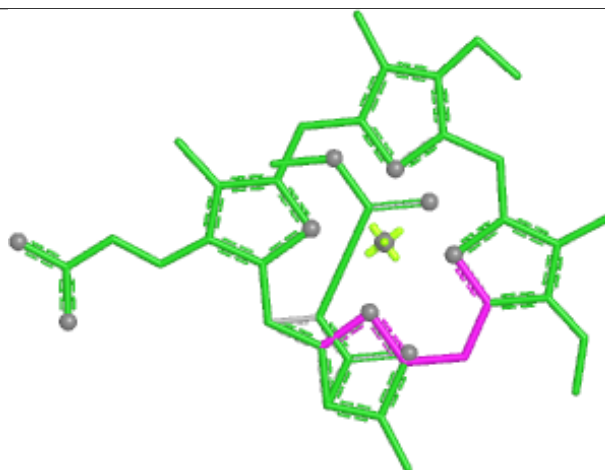


Rings

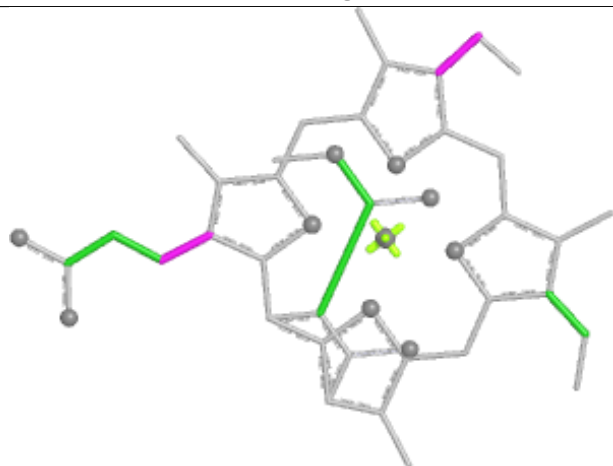
Ligand KC2 M 309



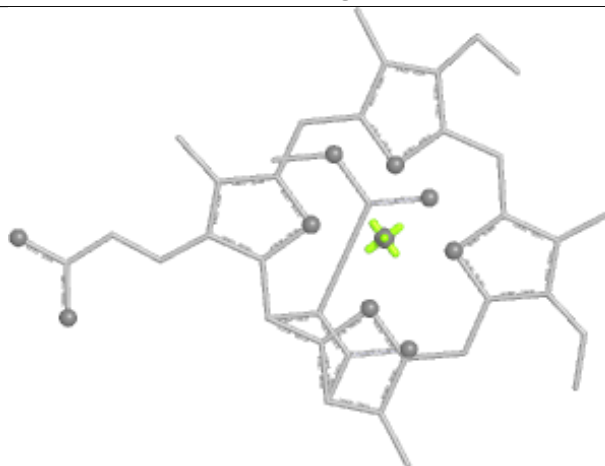
Bond lengths



Bond angles

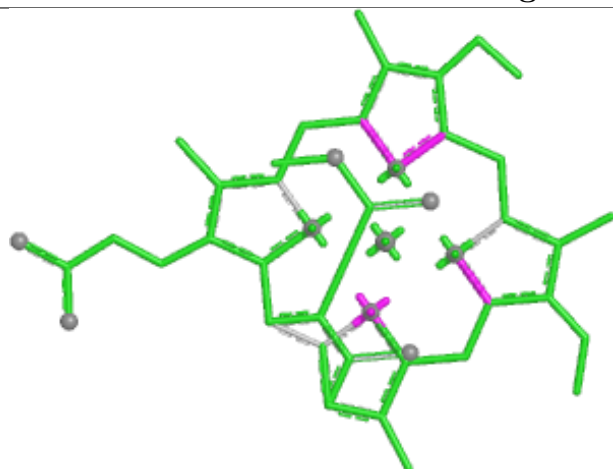


Torsions

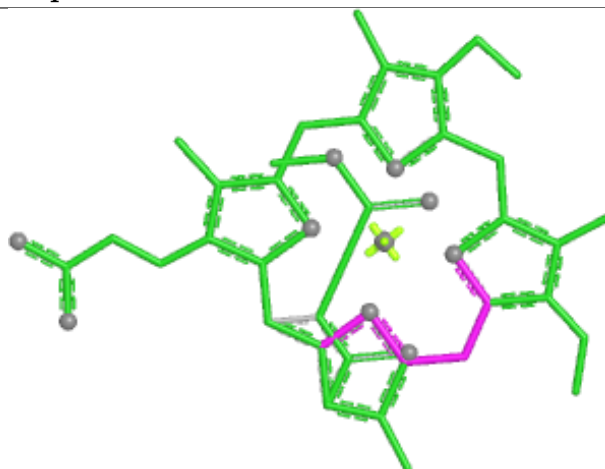


Rings

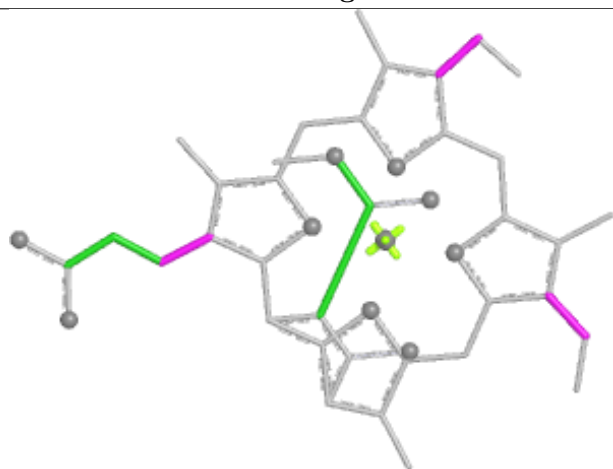
Ligand KC2 p 310



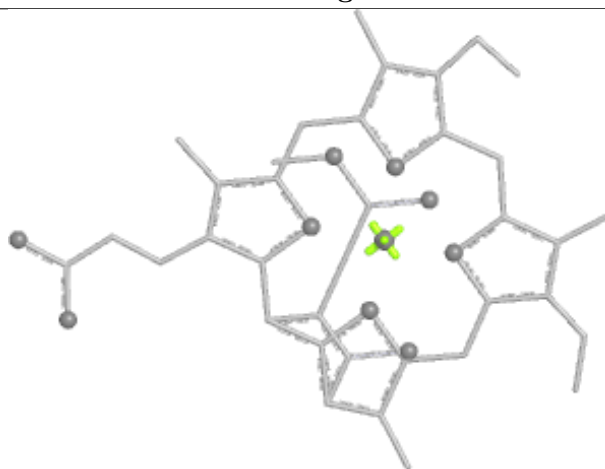
Bond lengths



Bond angles

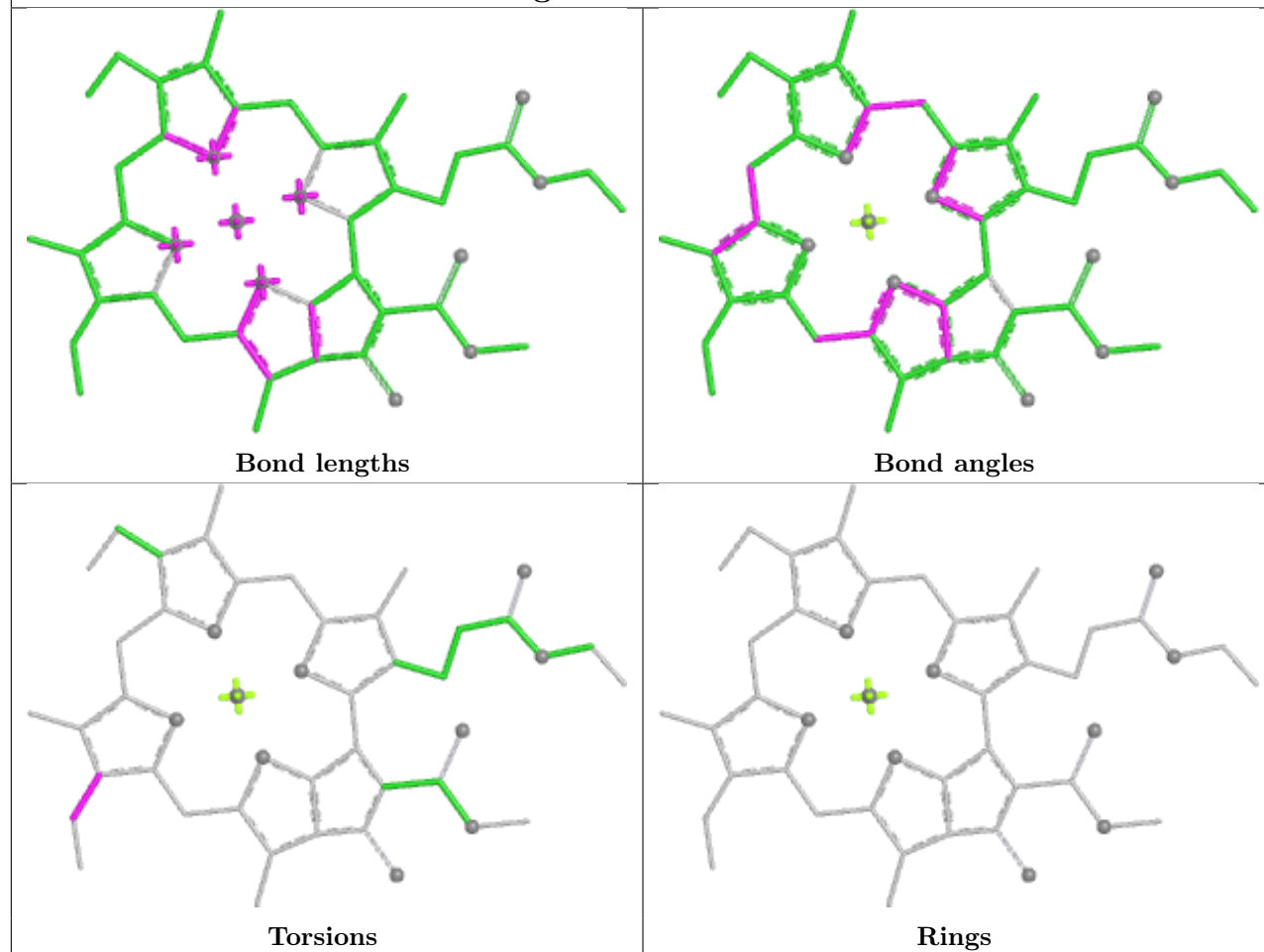


Torsions

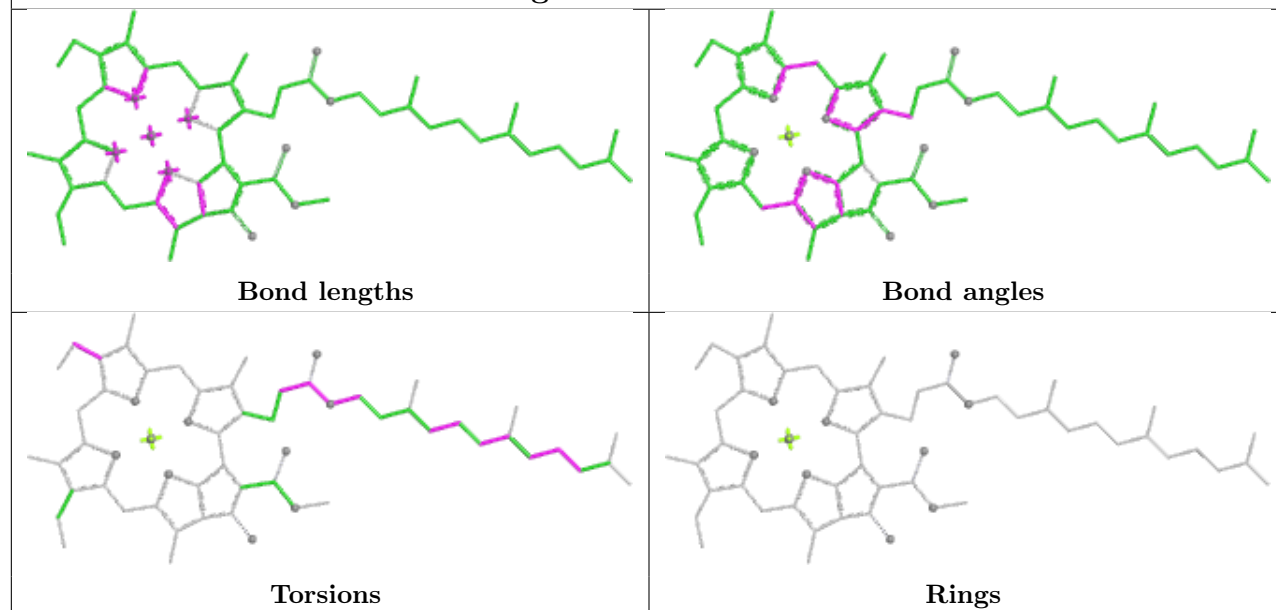


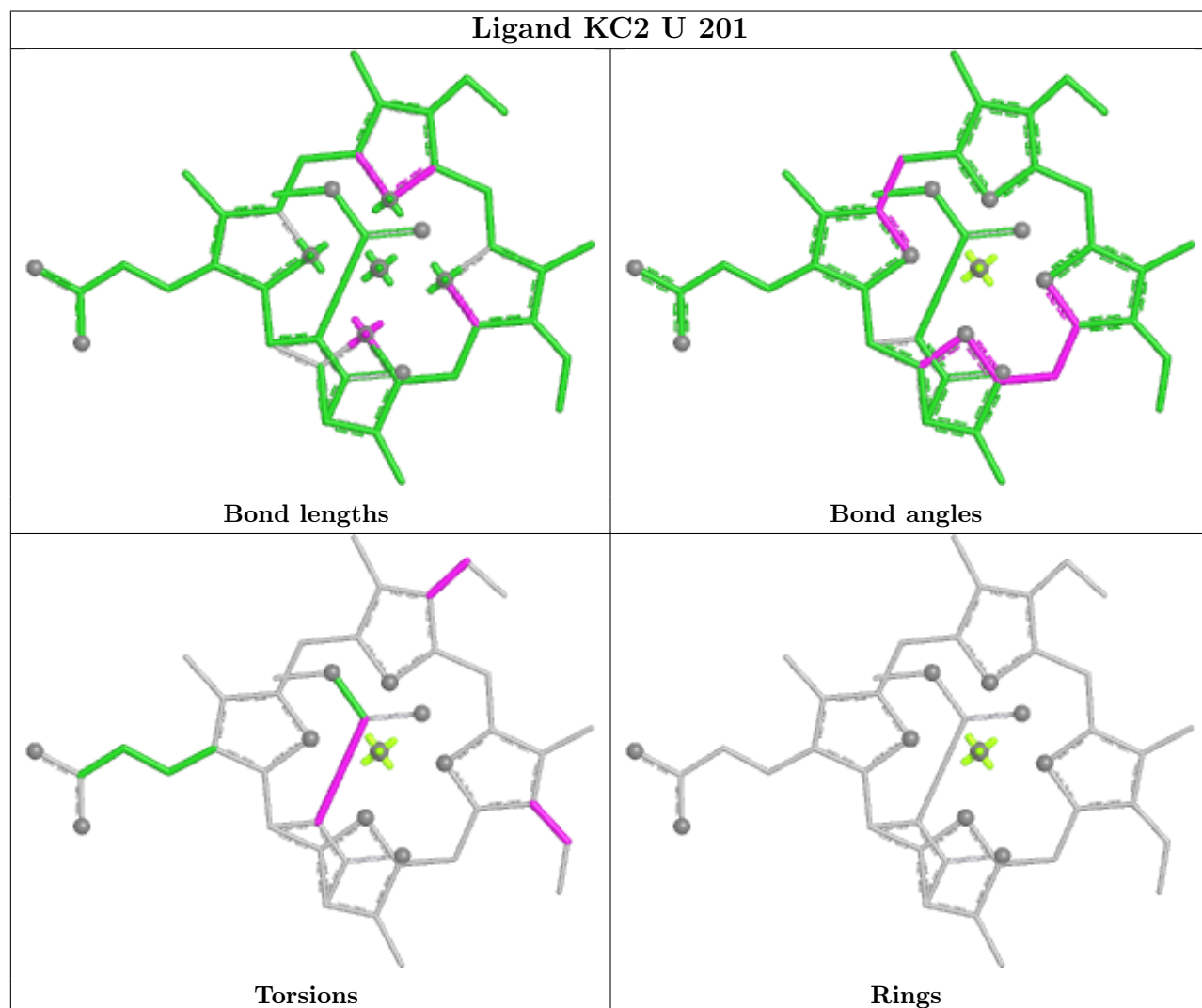
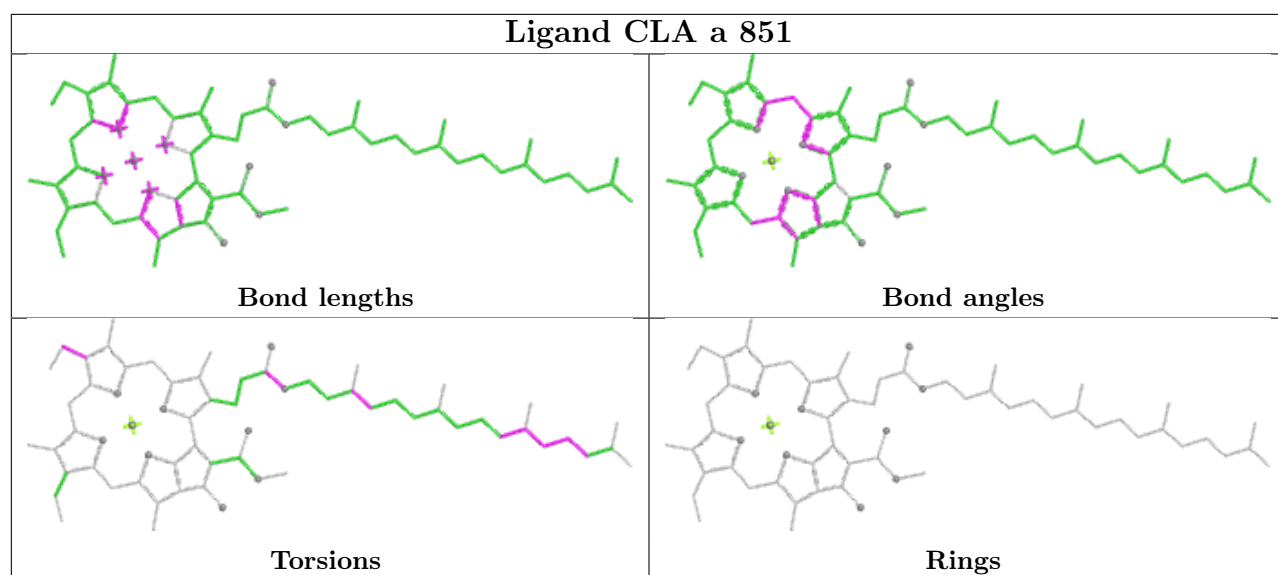
Rings

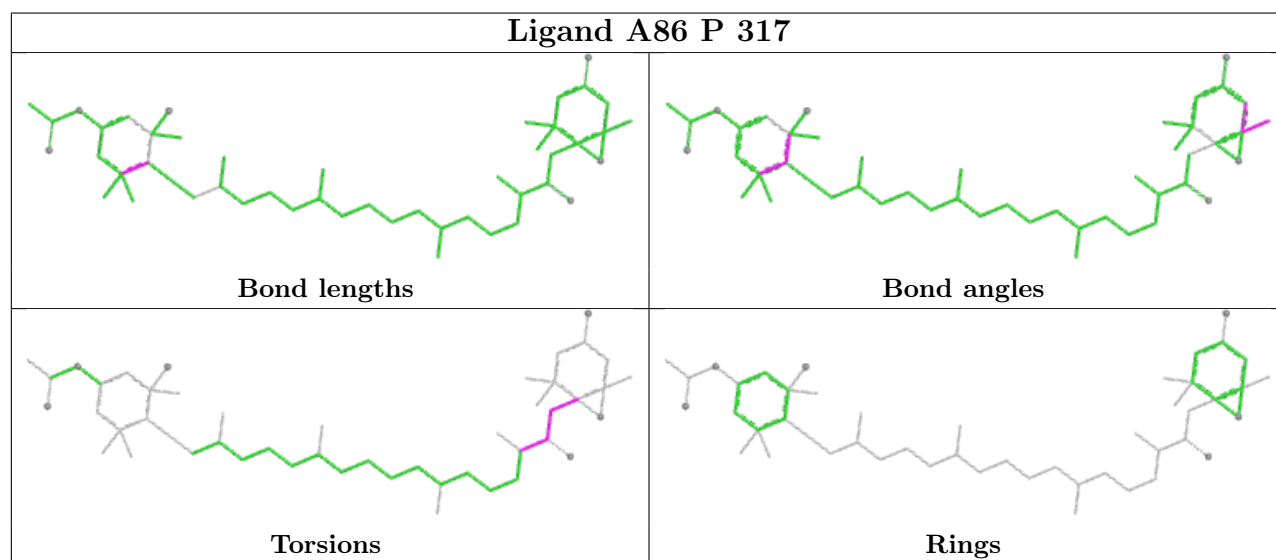
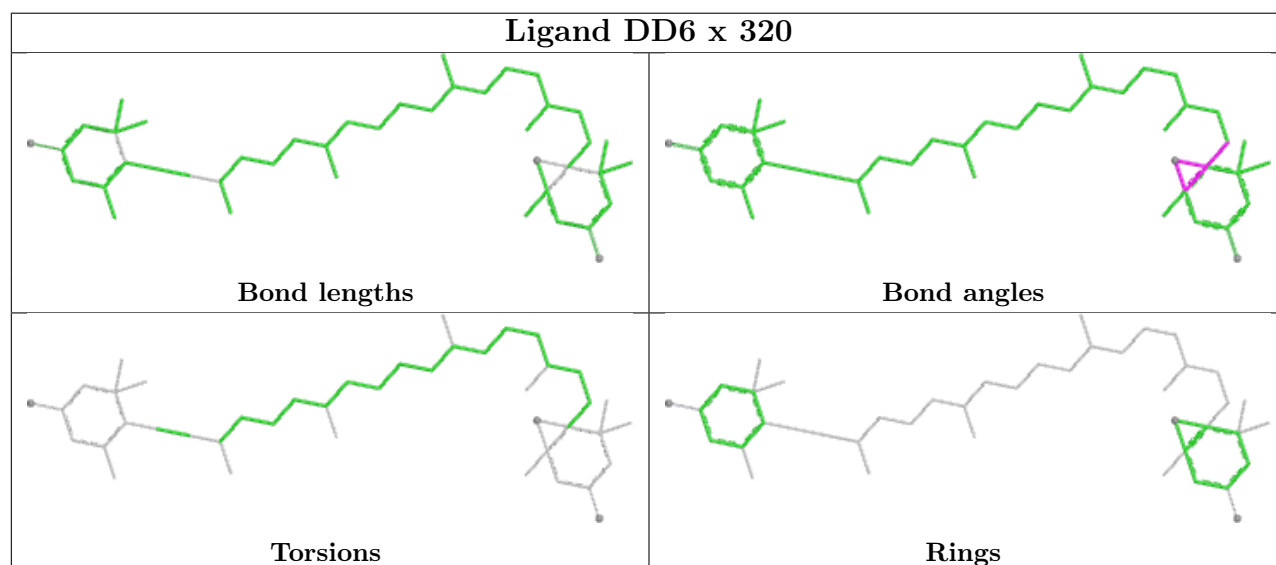
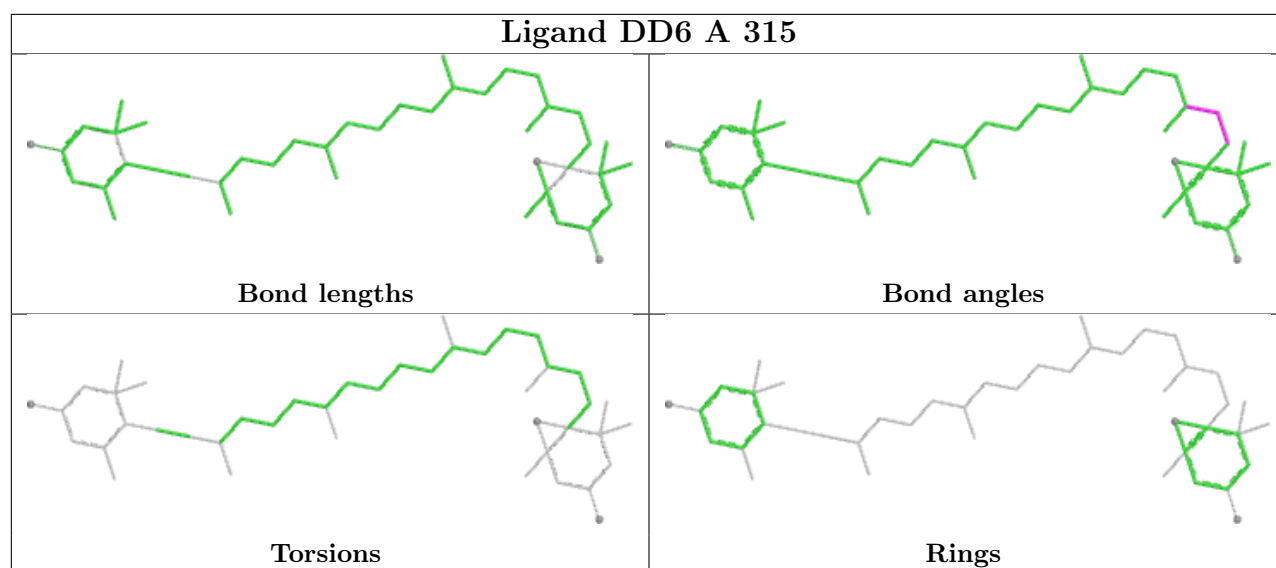
Ligand CLA I 204

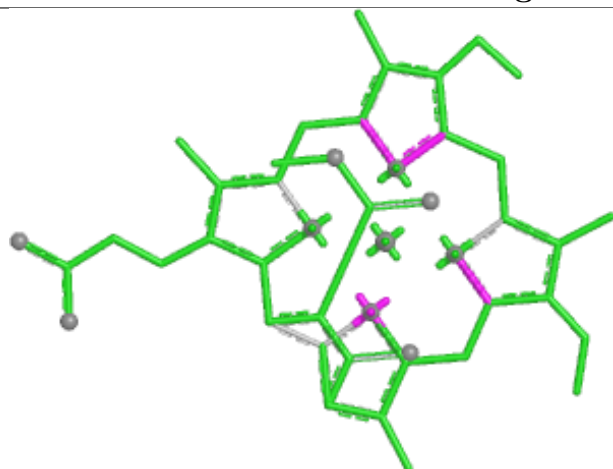


Ligand CLA N 311

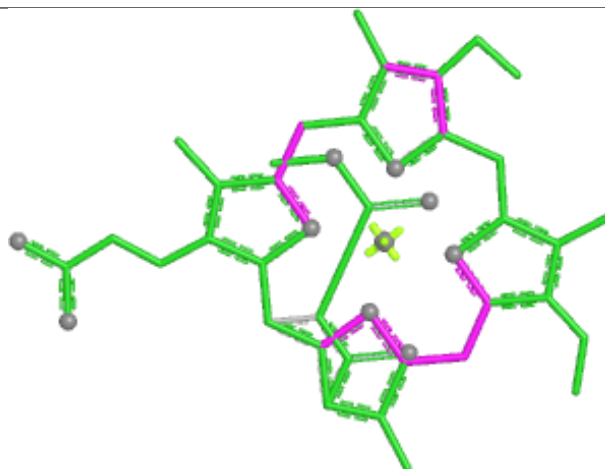




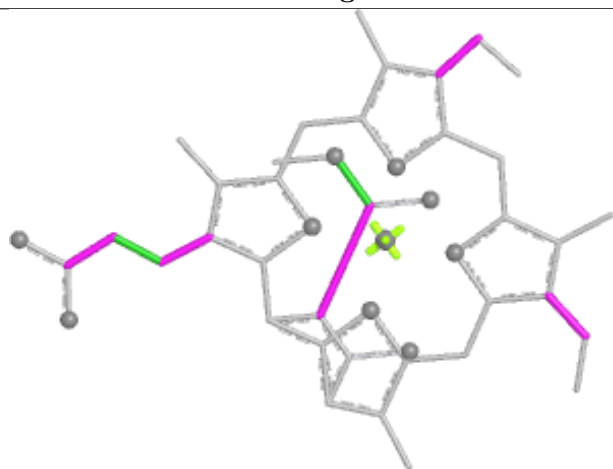


Ligand KC2 K 303

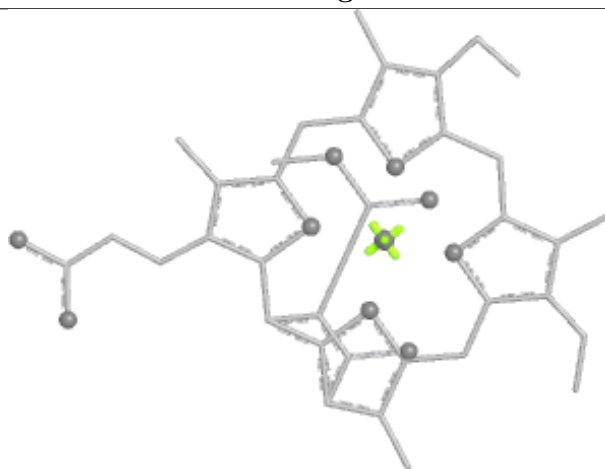
Bond lengths



Bond angles



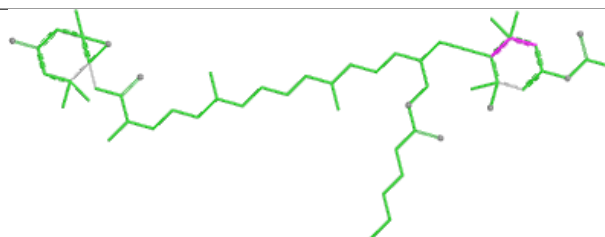
Torsions



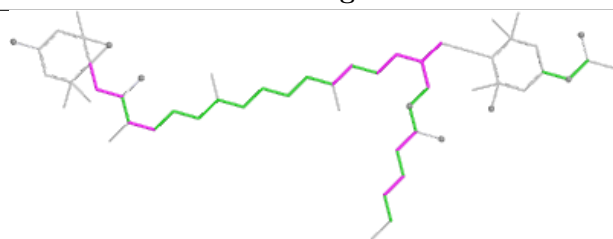
Rings

Ligand A1EB1 v 323

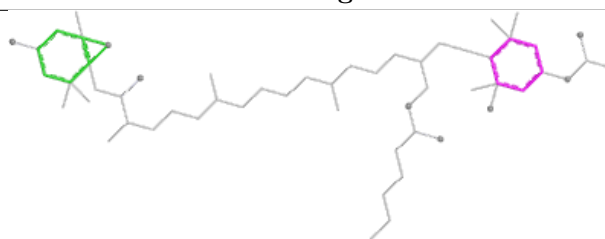
Bond lengths



Bond angles

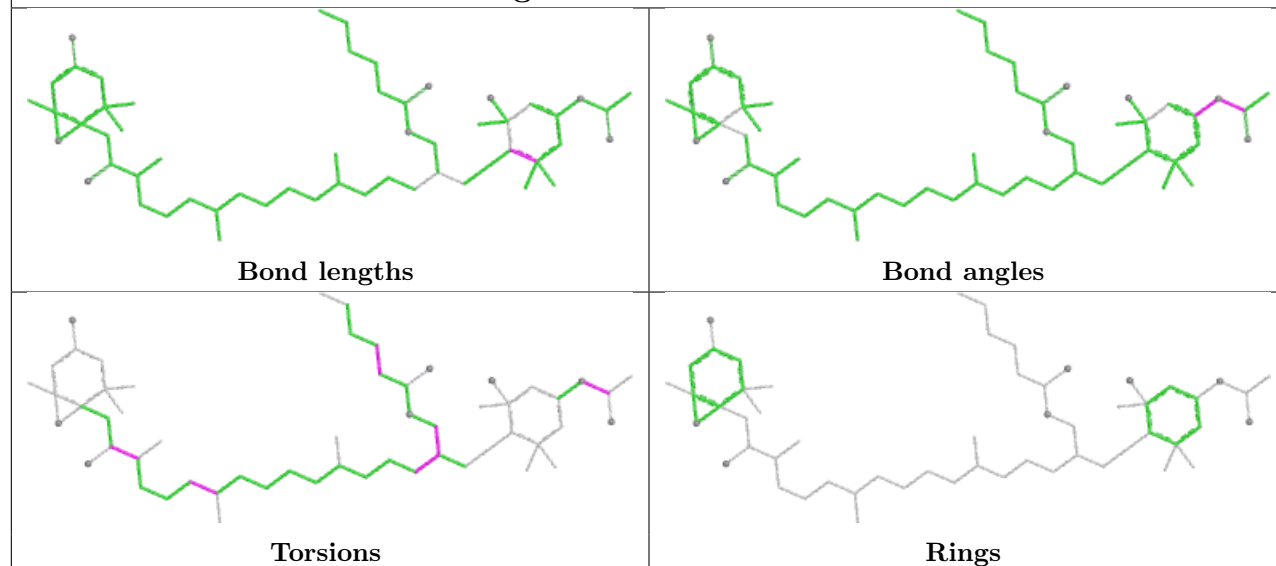


Torsions

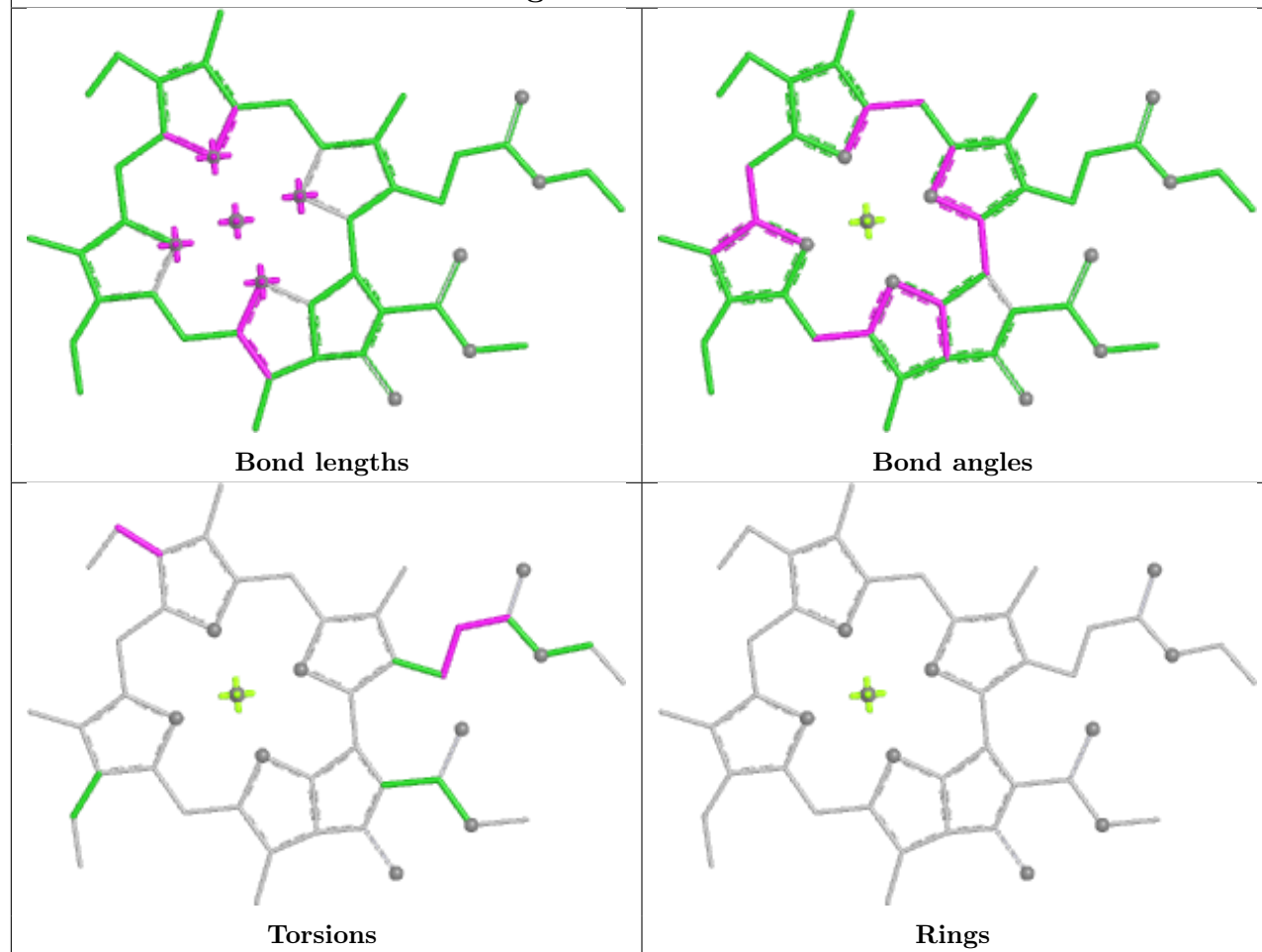


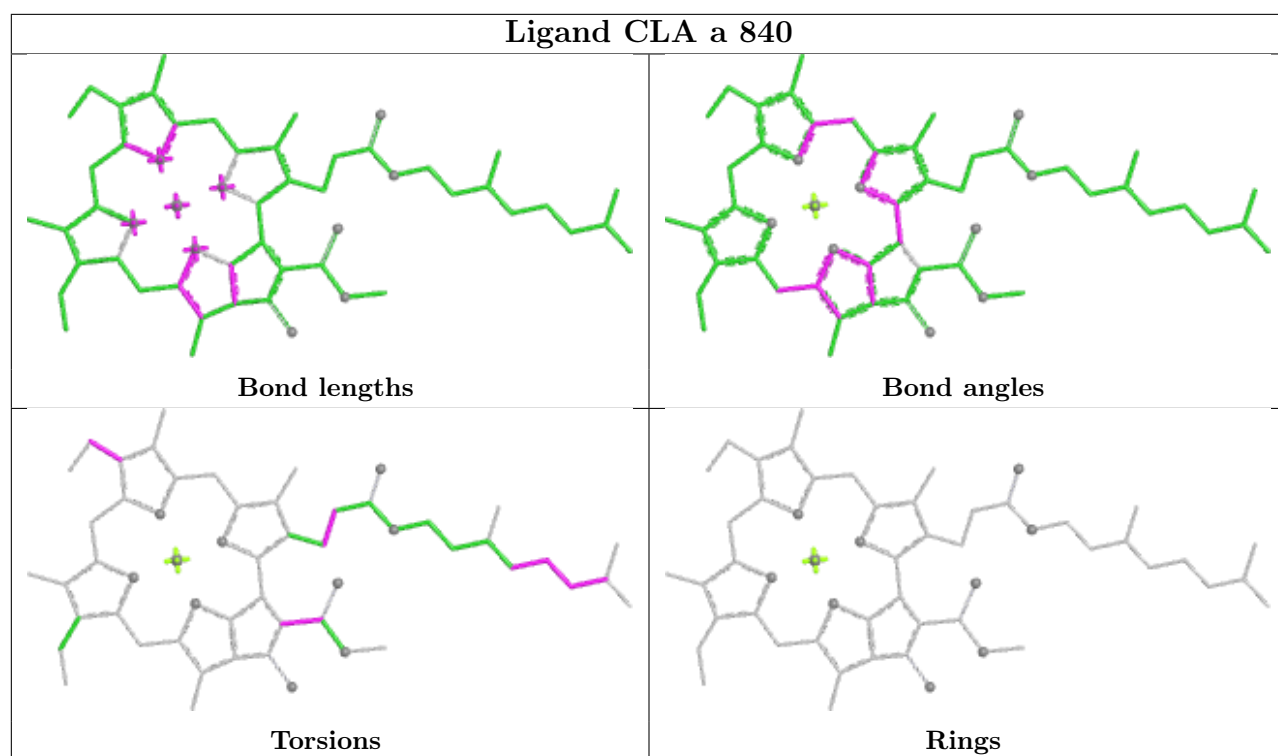
Rings

Ligand A1EB1 w 313

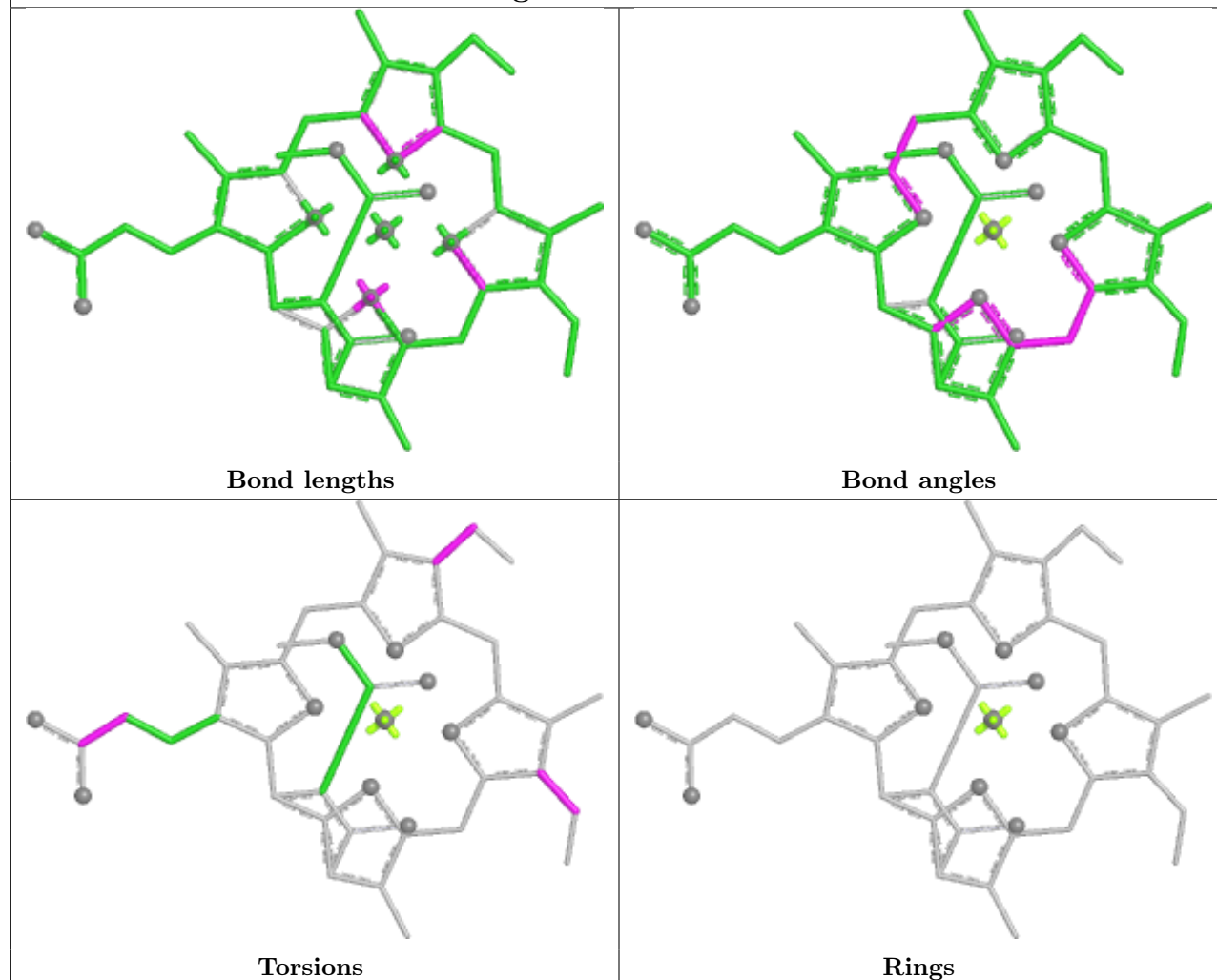


Ligand CLA T 317

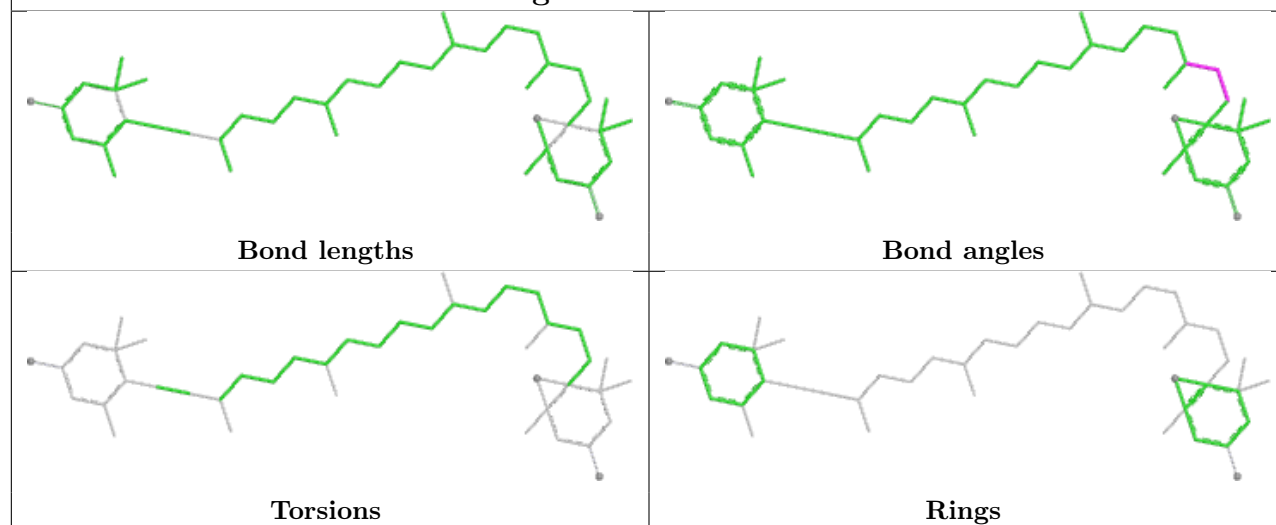


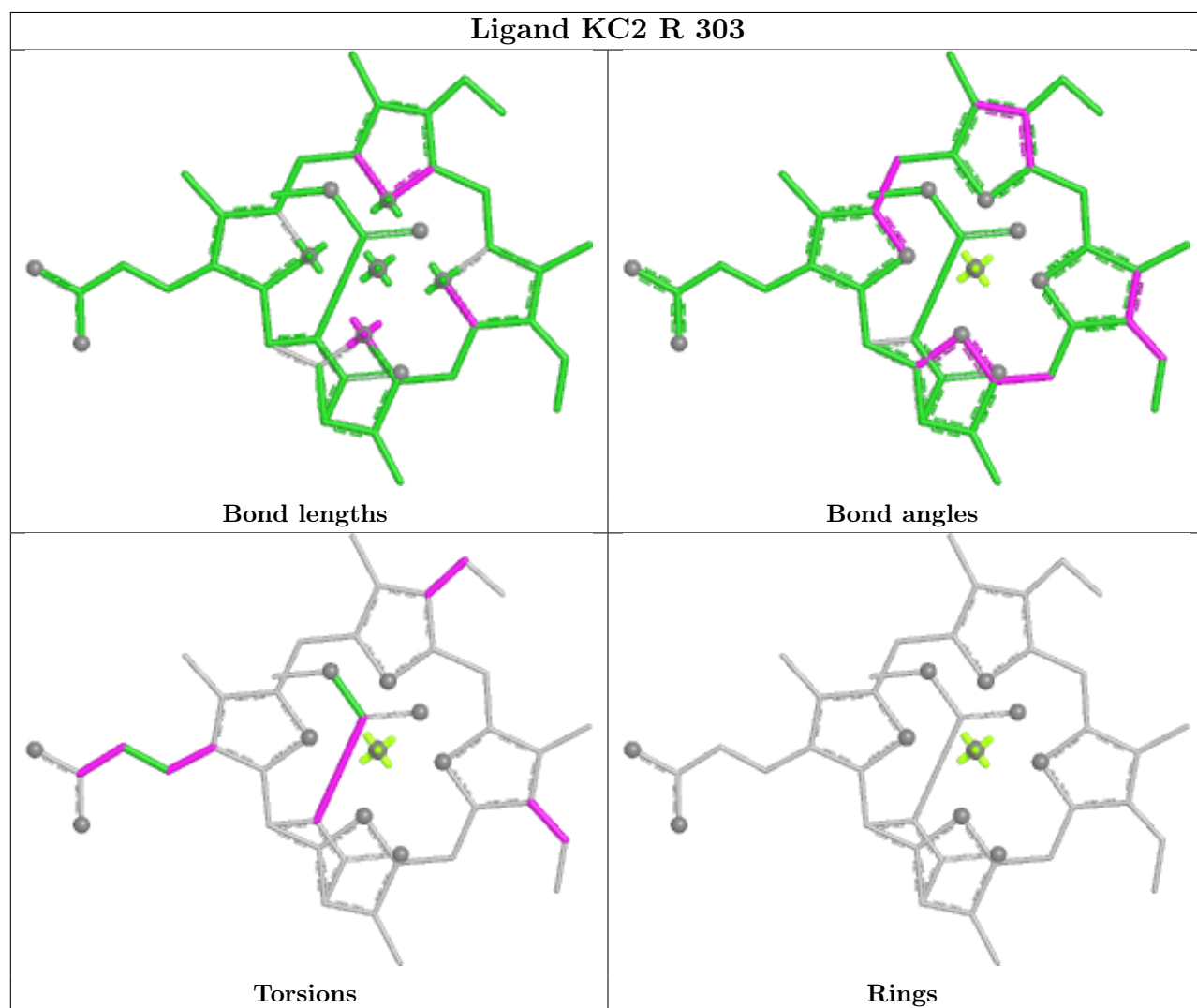
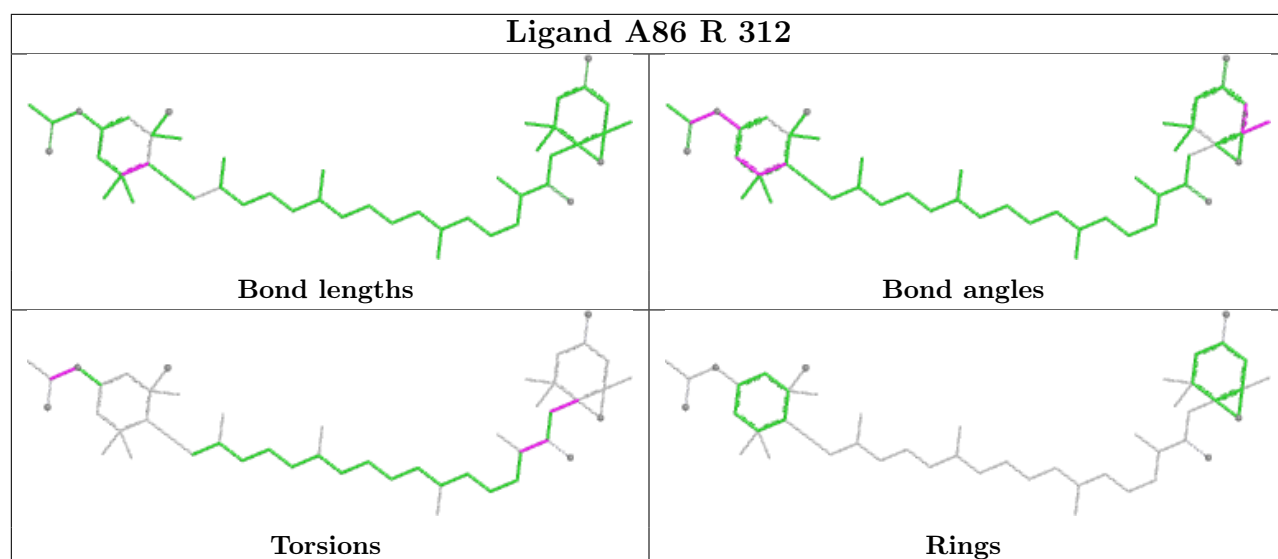


Ligand KC2 x 315

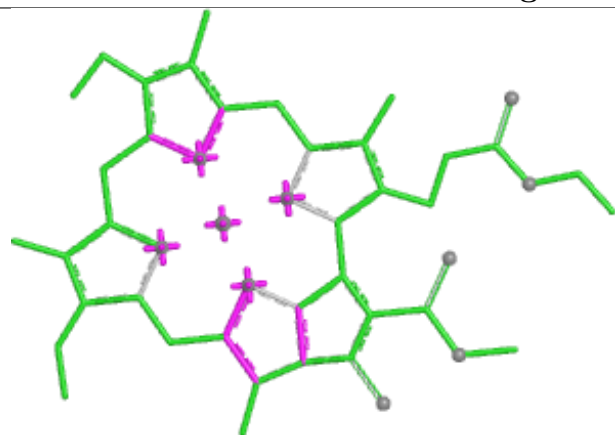


Ligand DD6 U 211

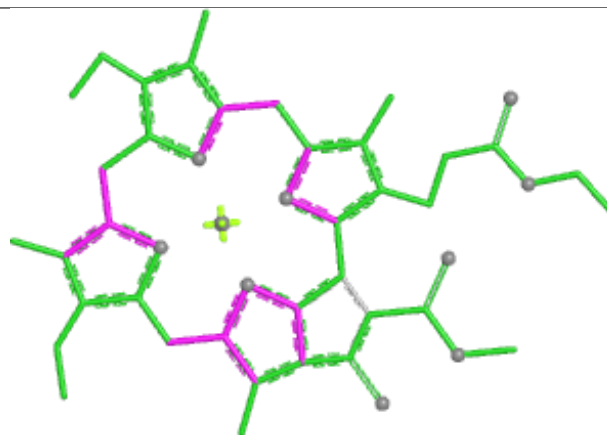




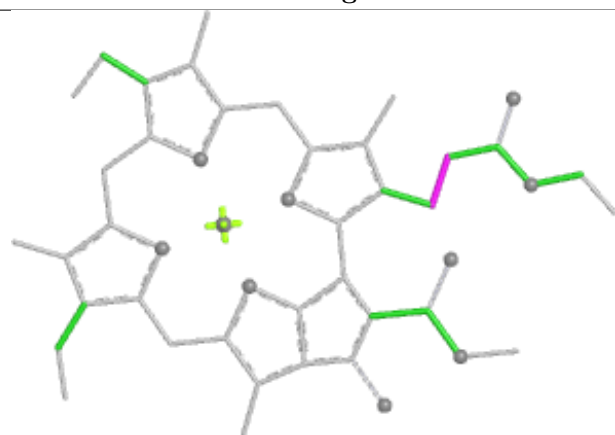
Ligand CLA J 318



Bond lengths



Bond angles

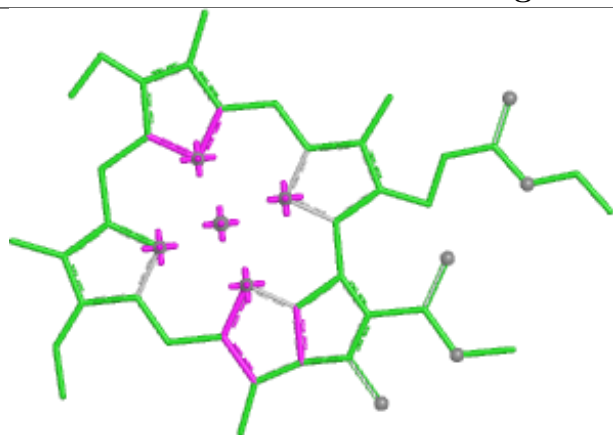


Torsions

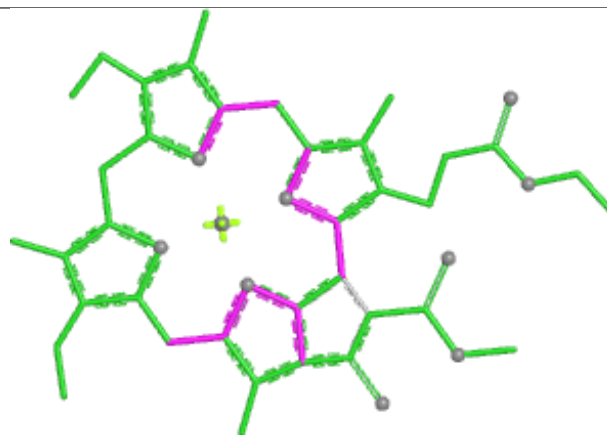


Rings

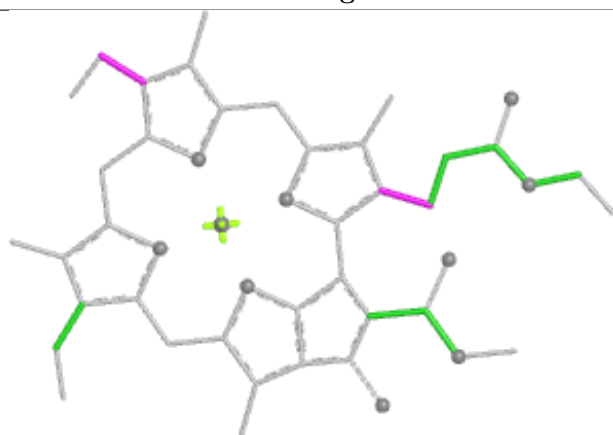
Ligand CLA B 302



Bond lengths



Bond angles

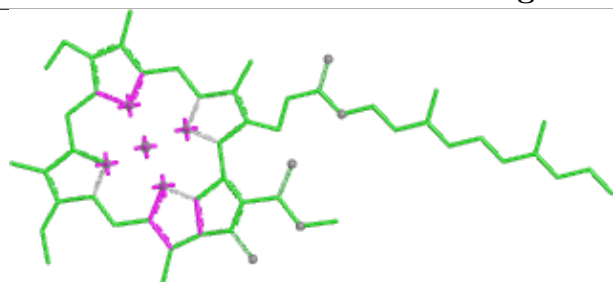


Torsions

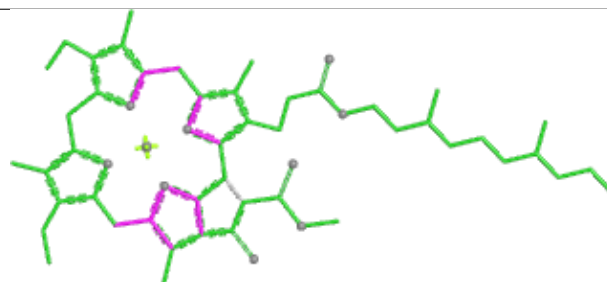


Rings

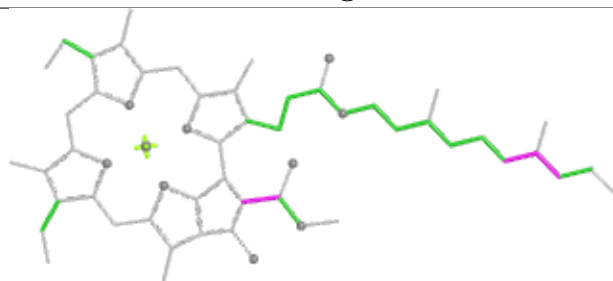
Ligand CLA b 815



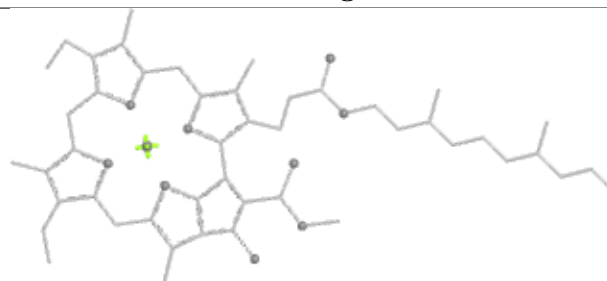
Bond lengths



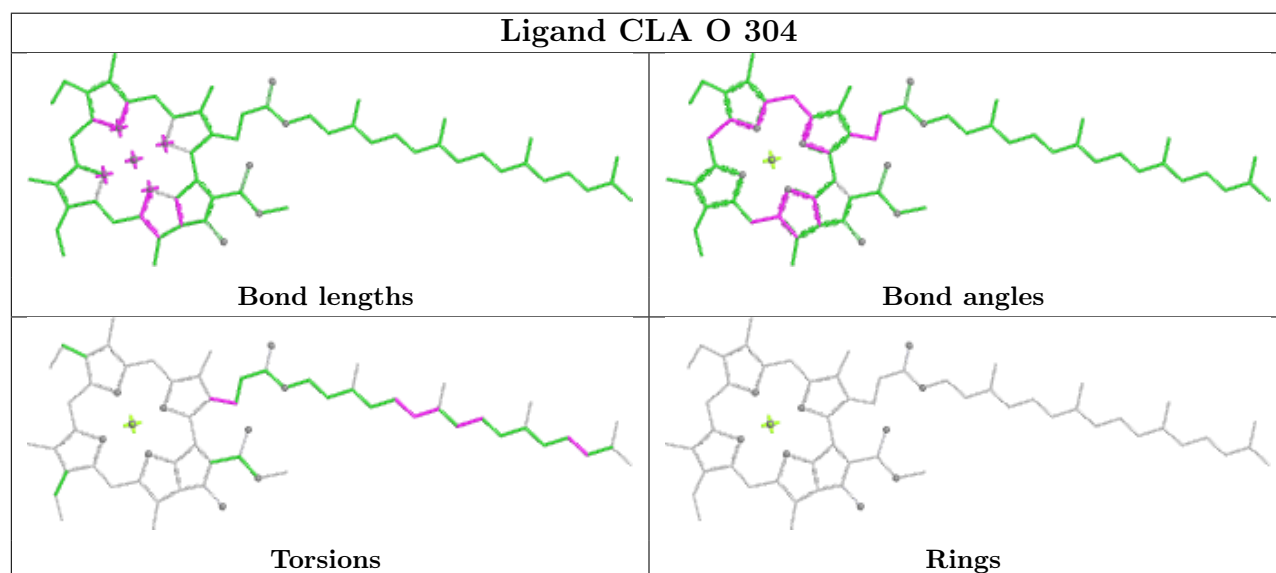
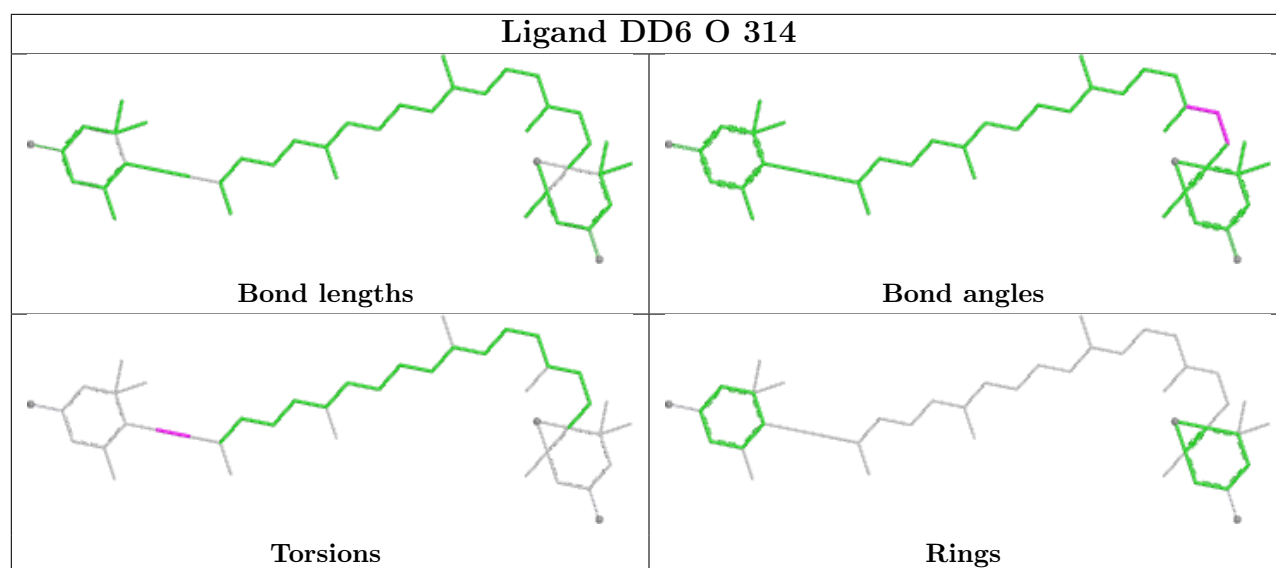
Bond angles



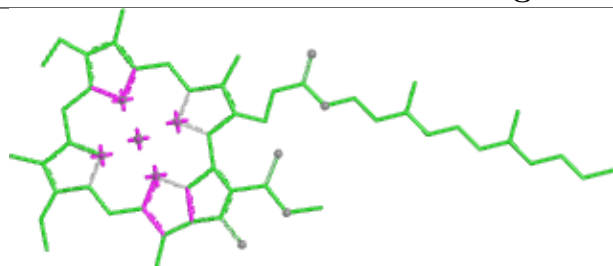
Torsions



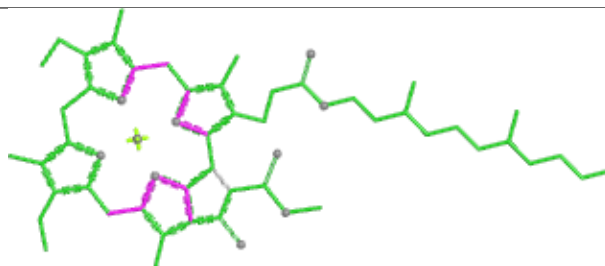
Rings



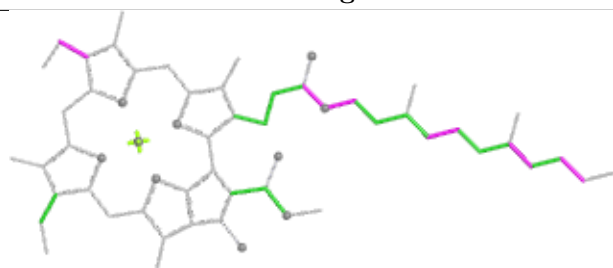
Ligand CLA V 201



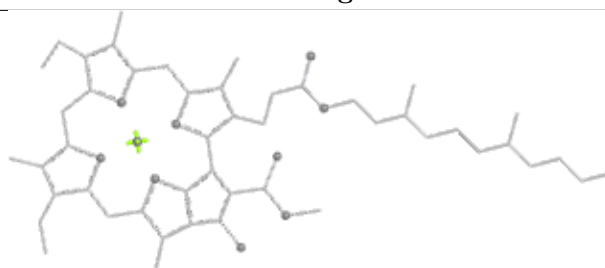
Bond lengths



Bond angles

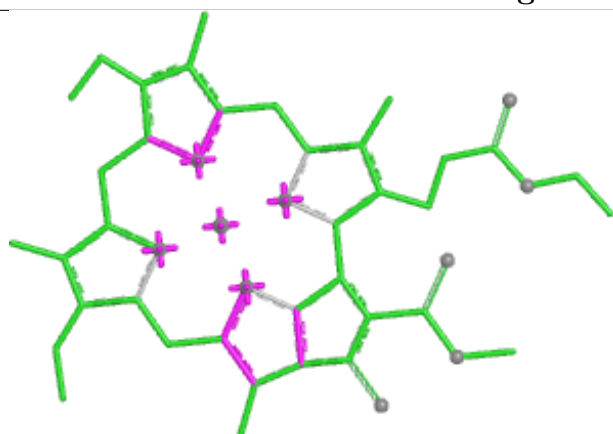


Torsions

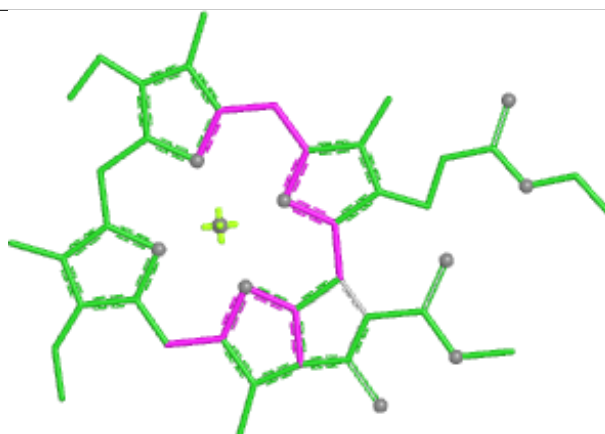


Rings

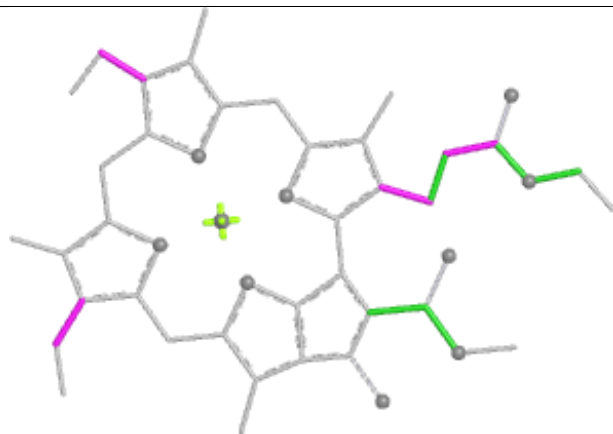
Ligand CLA u 306



Bond lengths



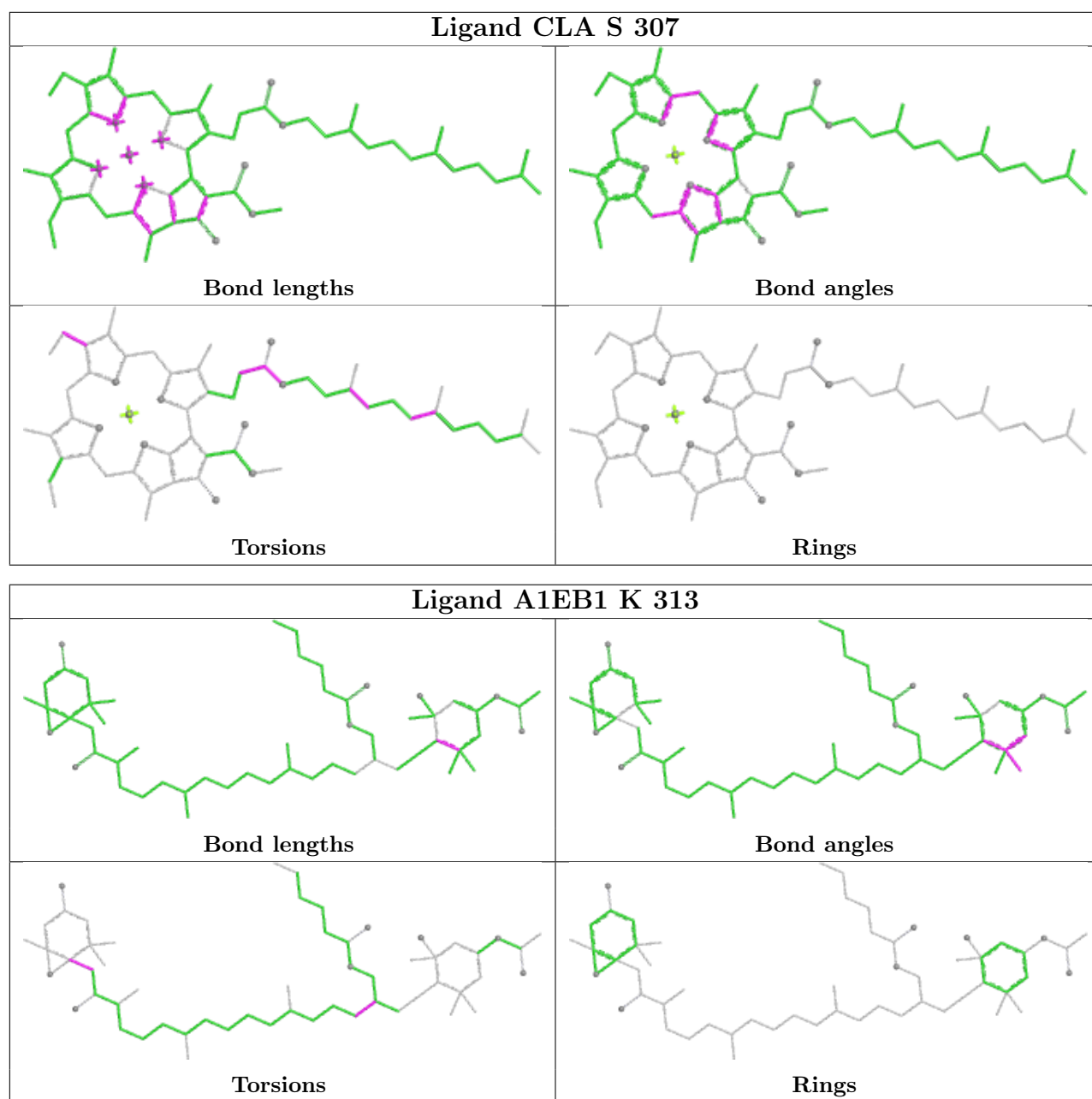
Bond angles

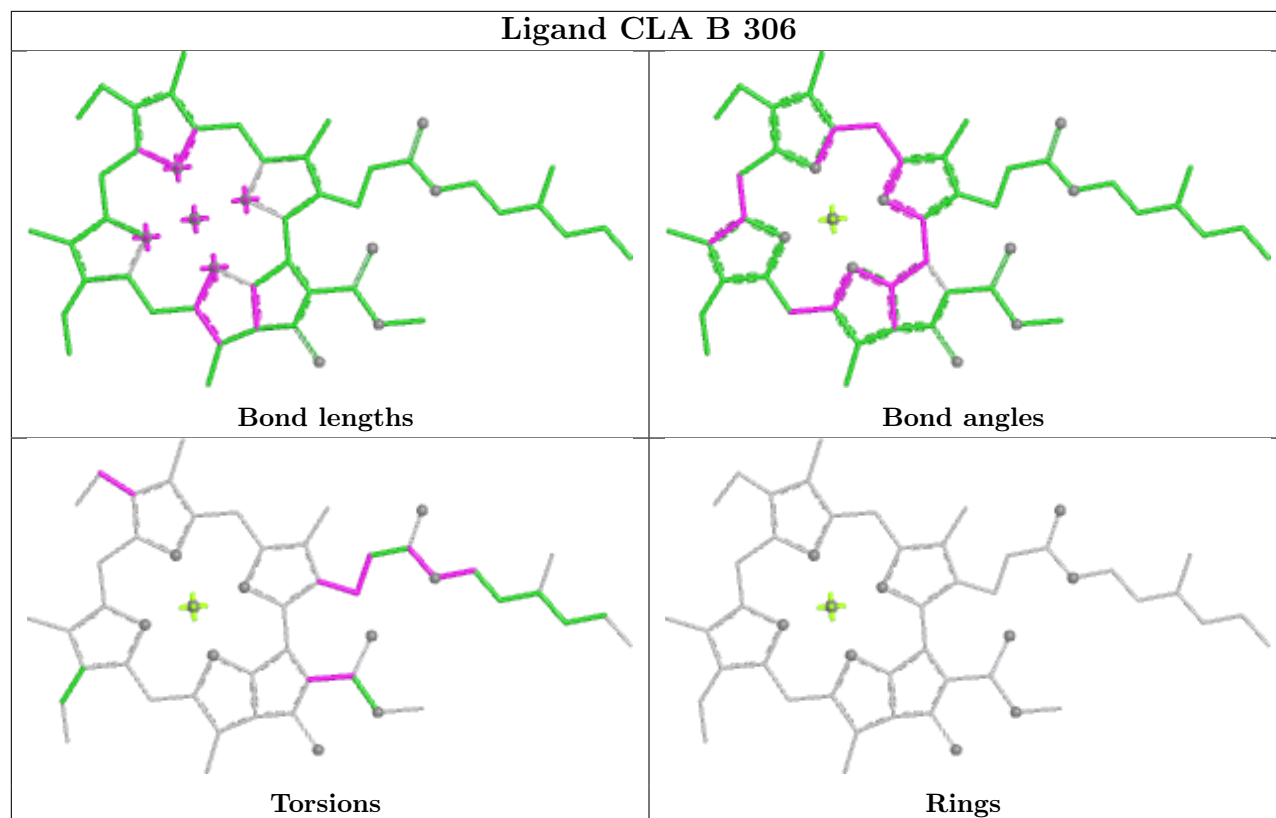


Torsions

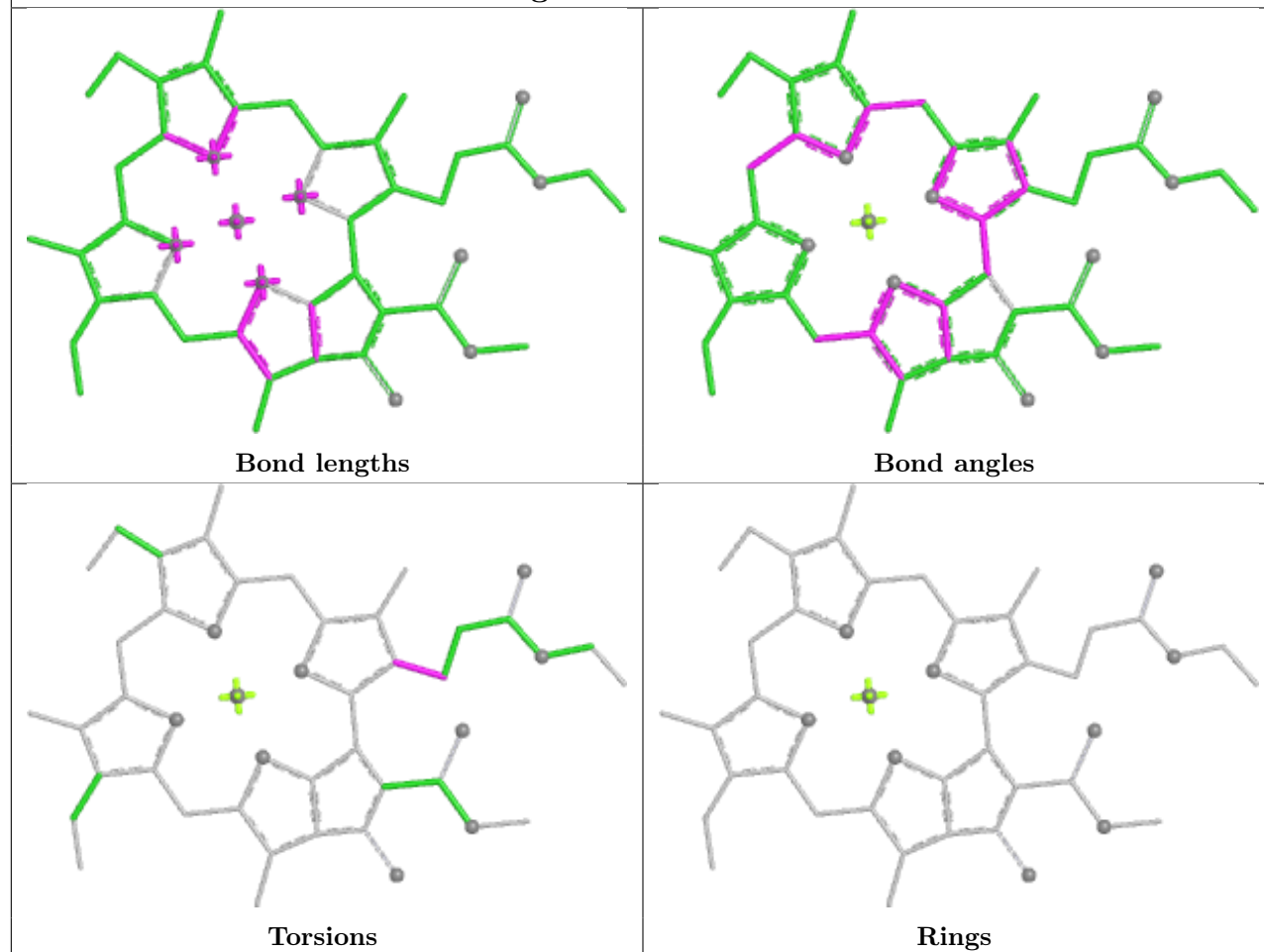


Rings

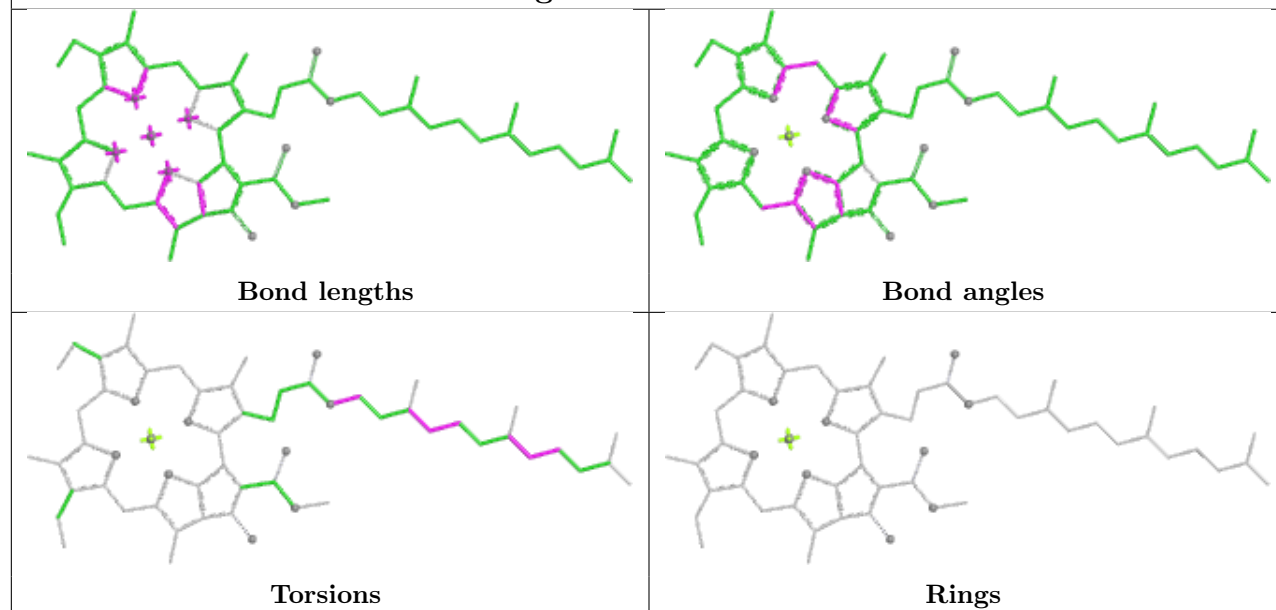




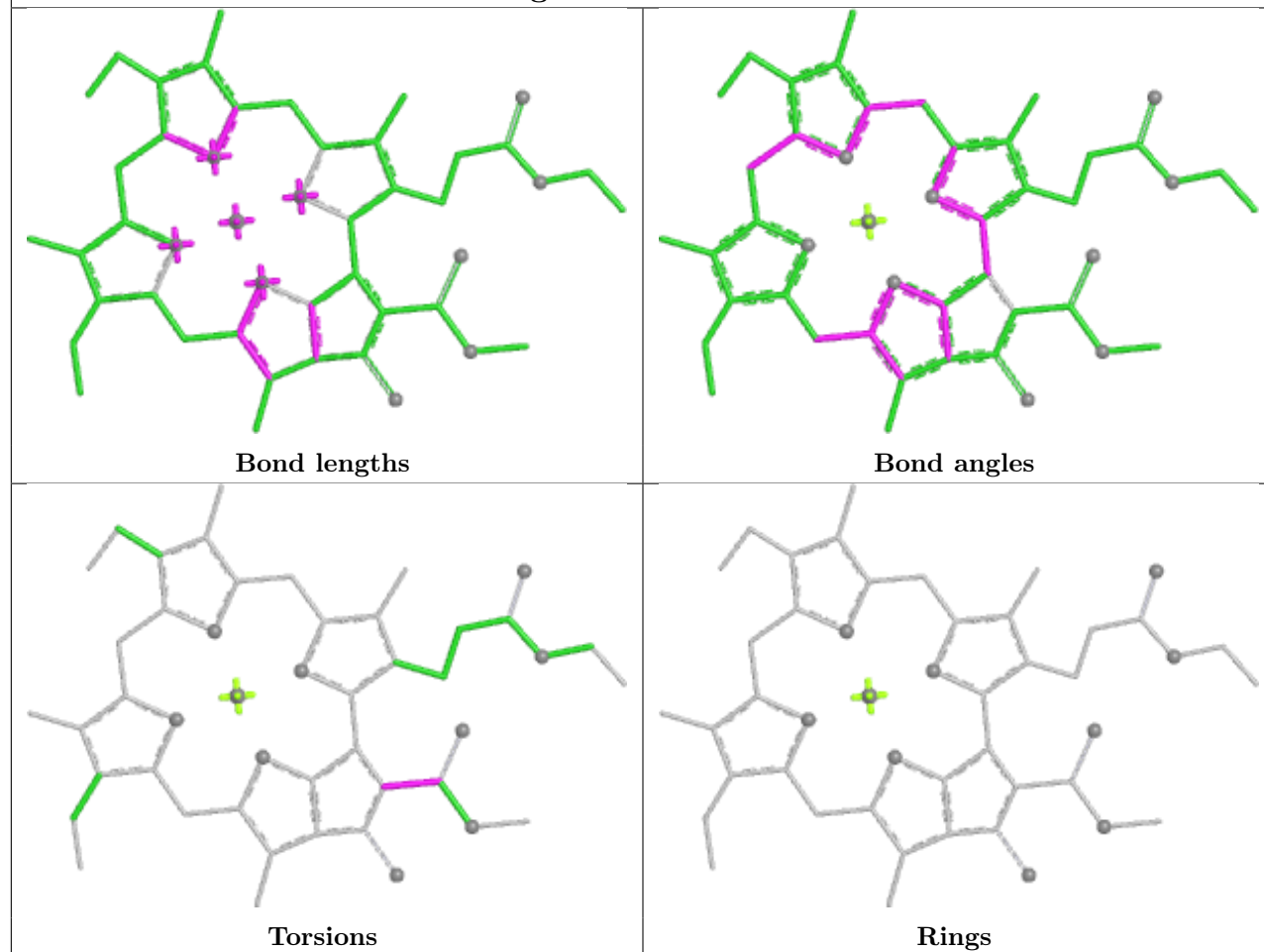
Ligand CLA J 310



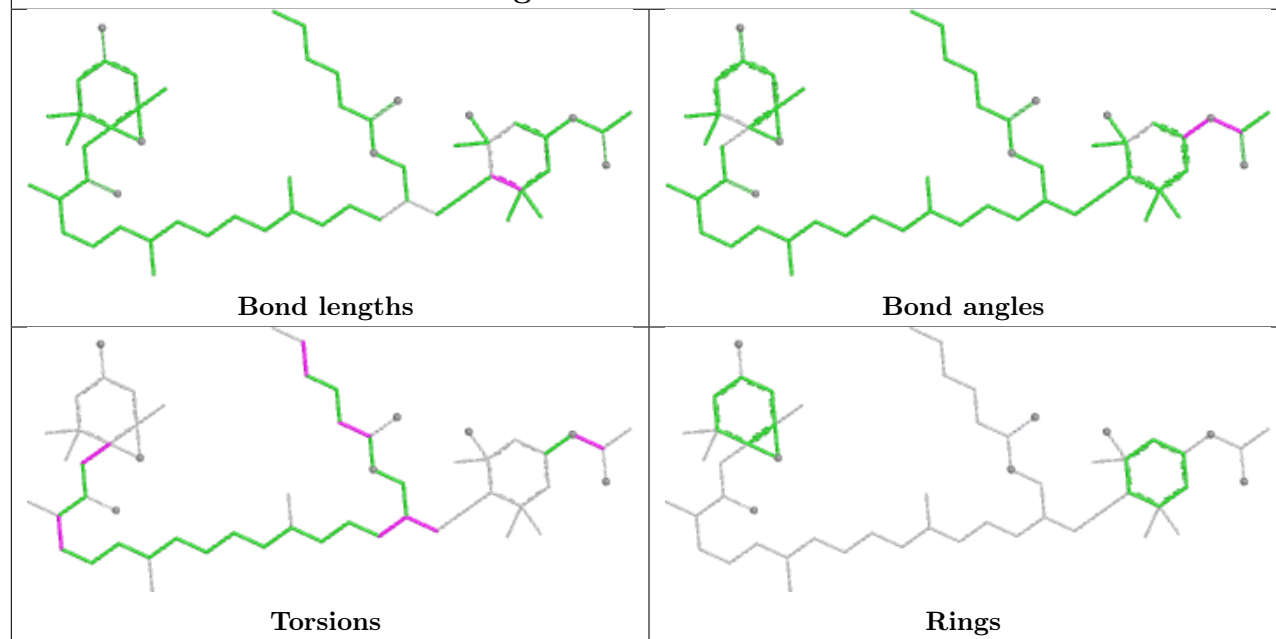
Ligand CLA b 837



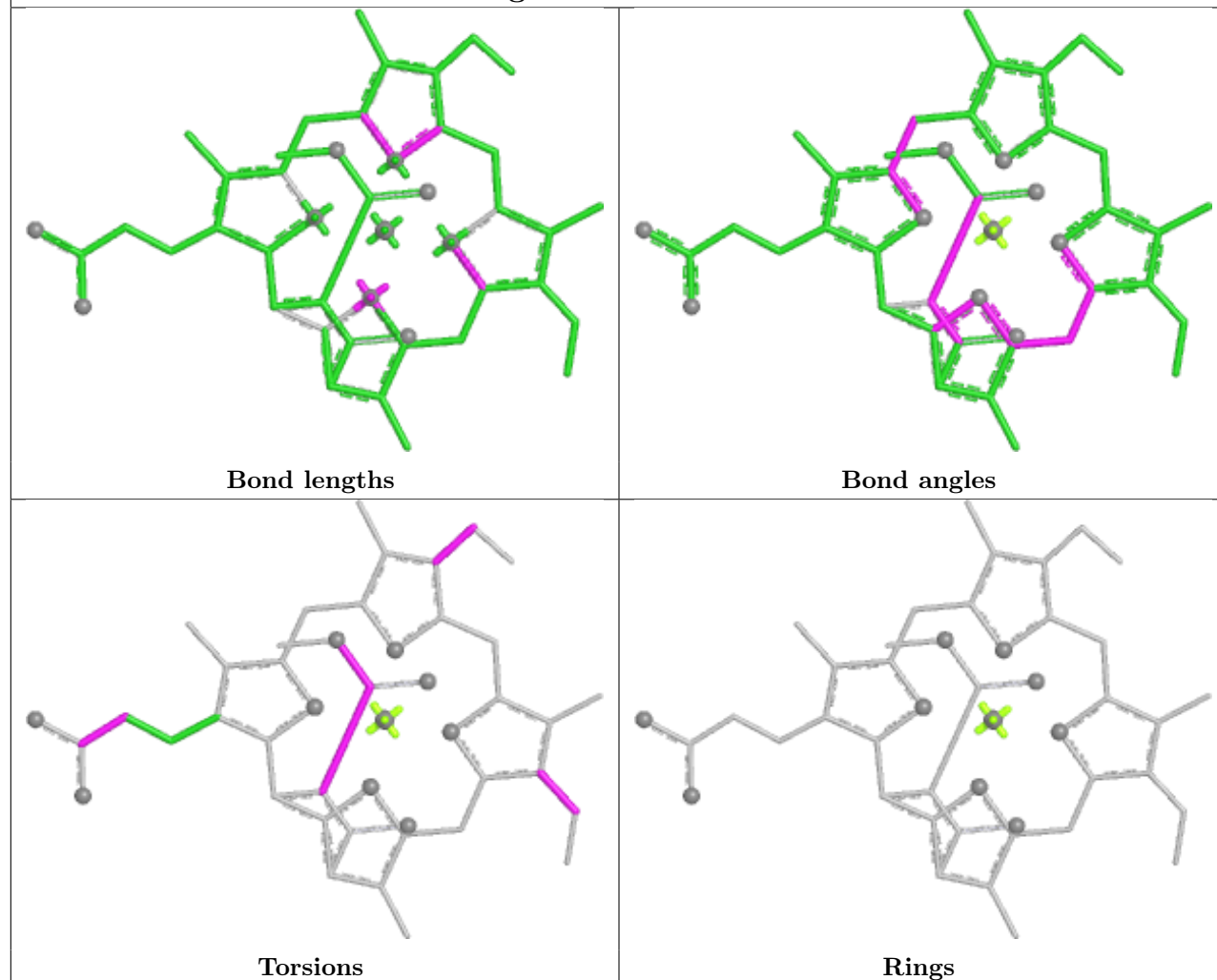
Ligand CLA u 305



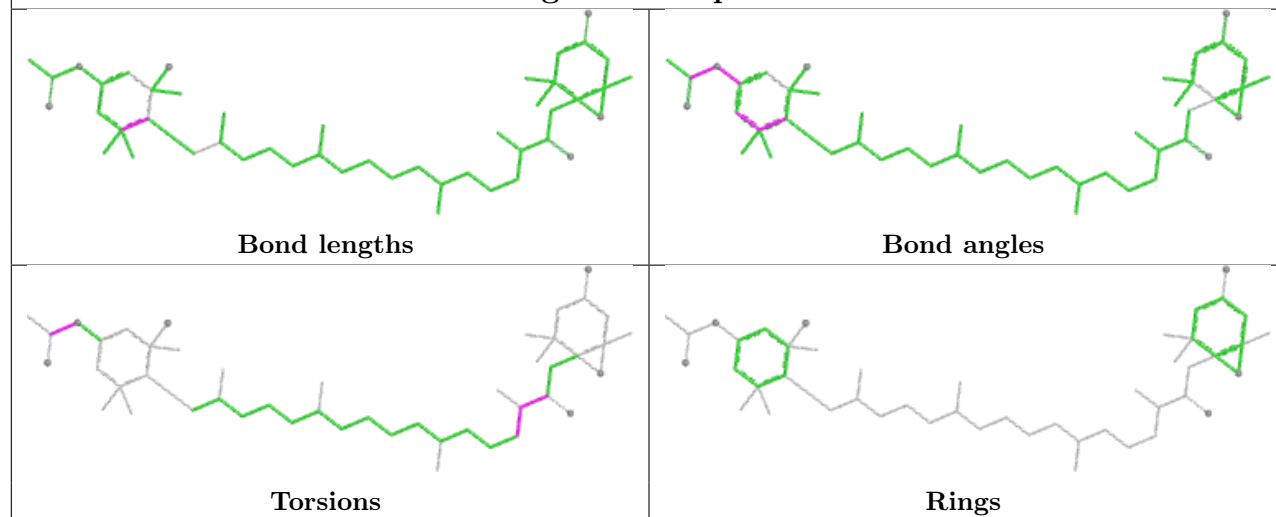
Ligand A1EB1 w 314

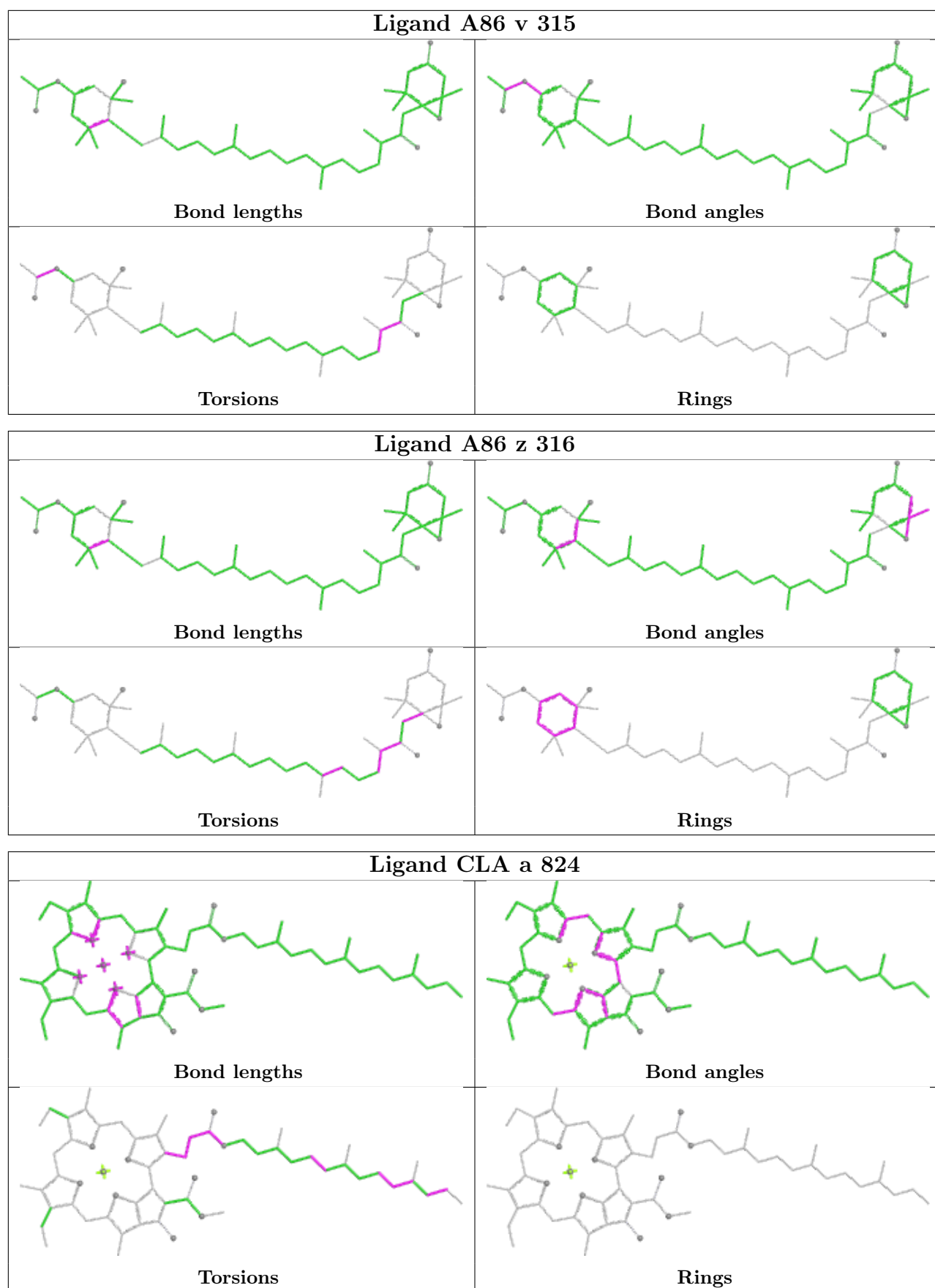


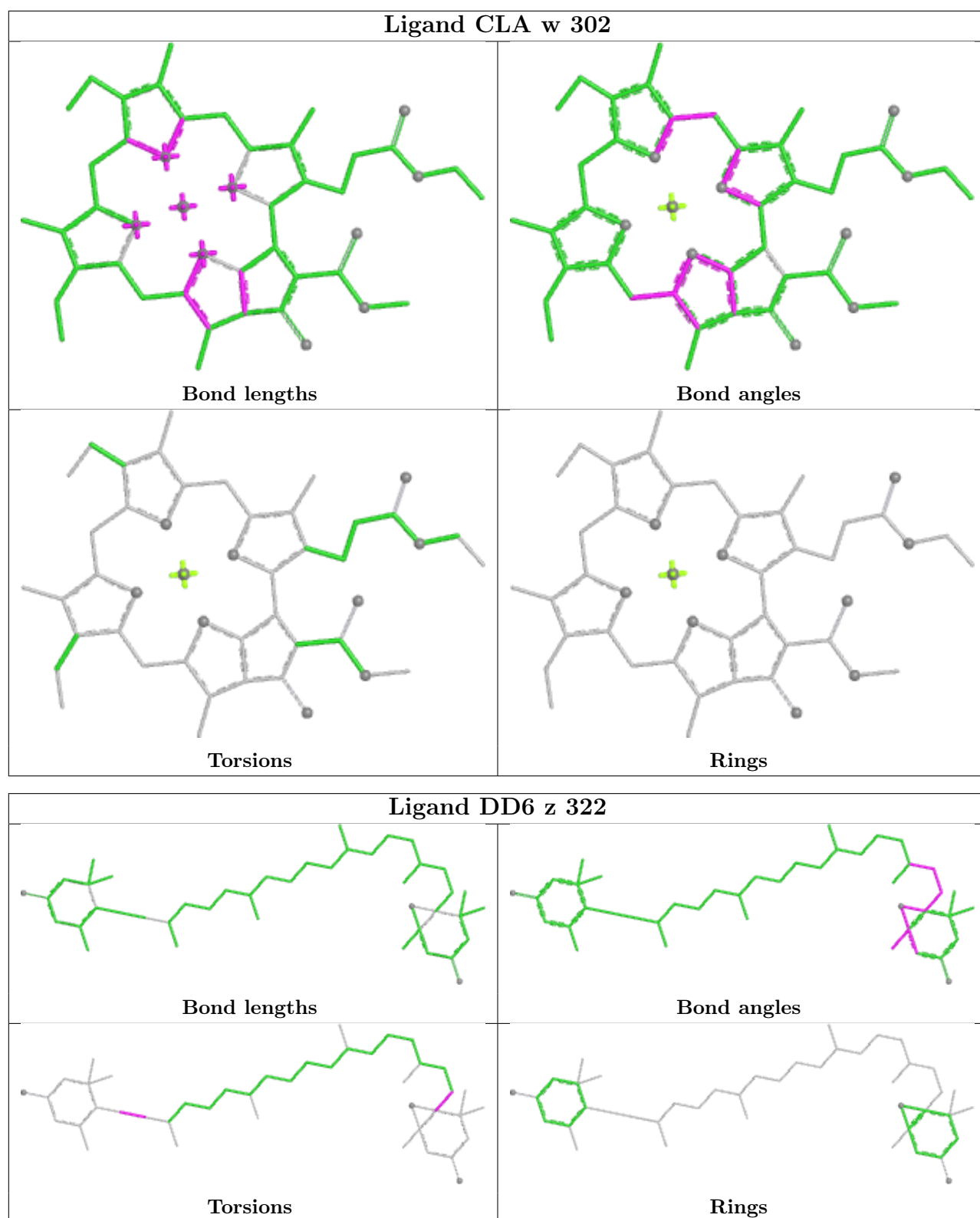
Ligand KC2 Y 314



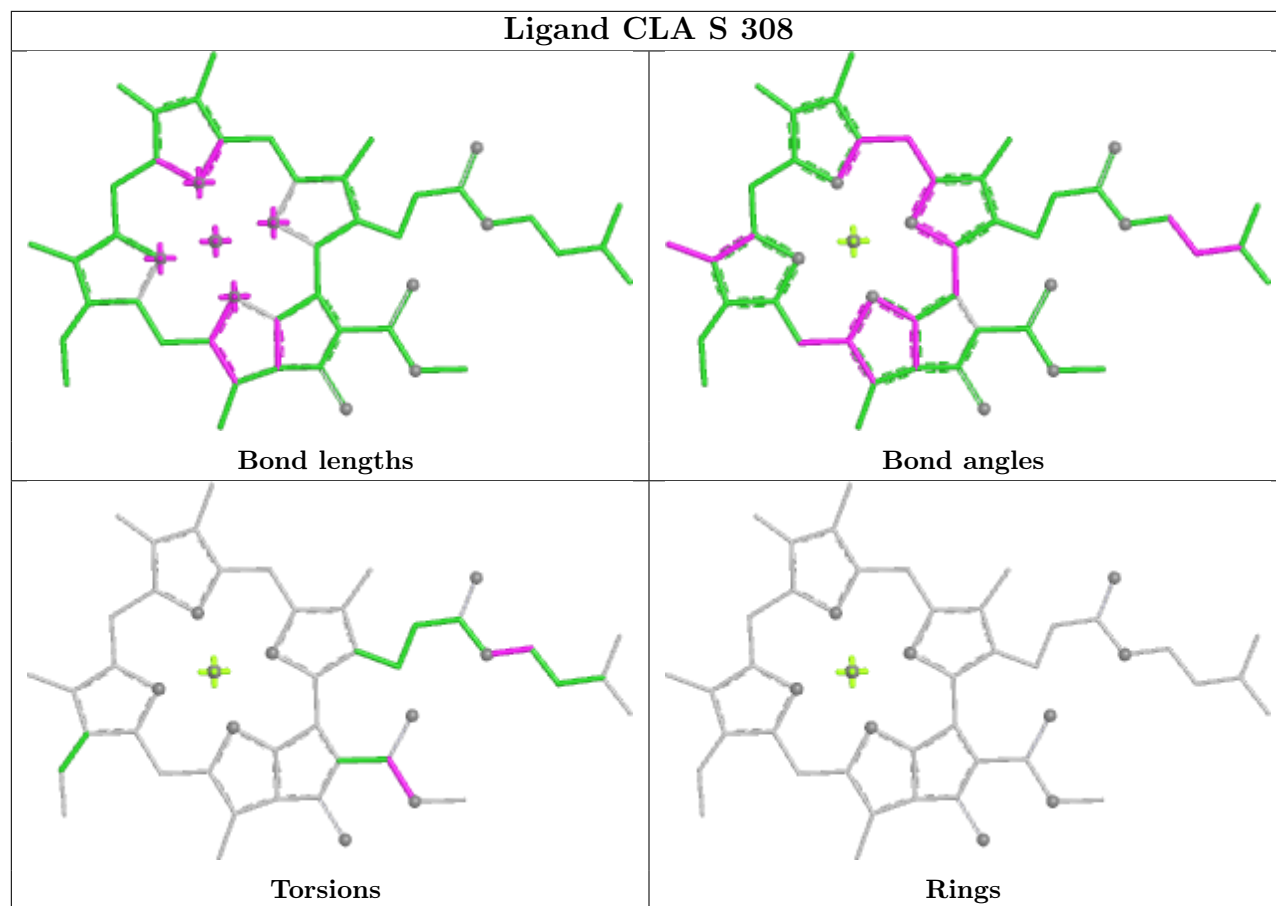
Ligand A86 q 315



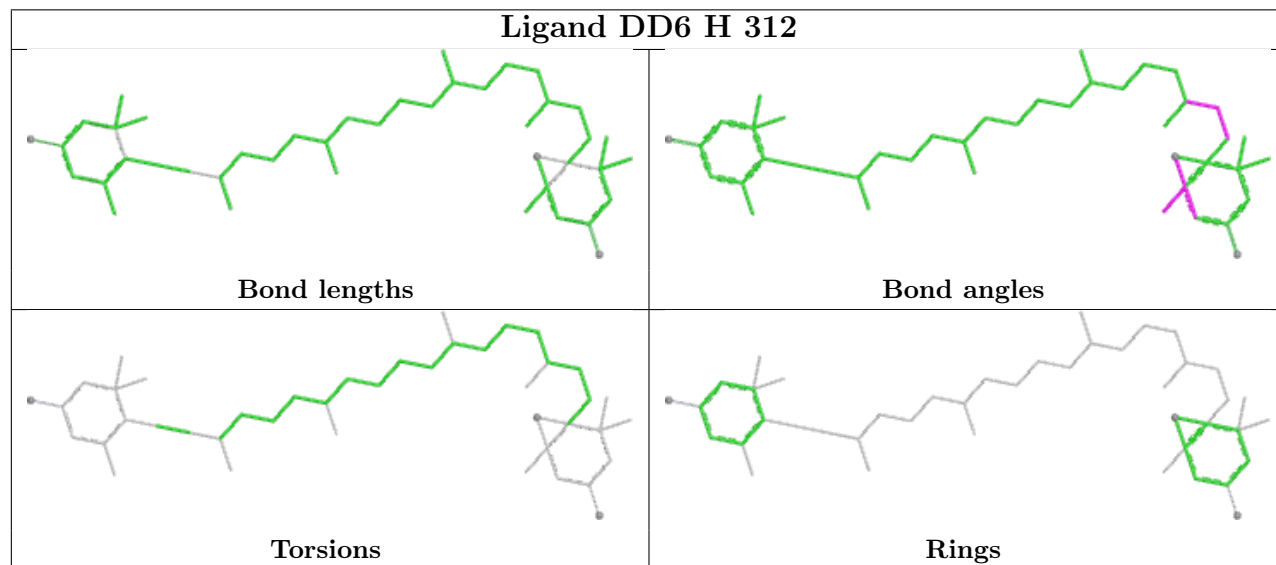




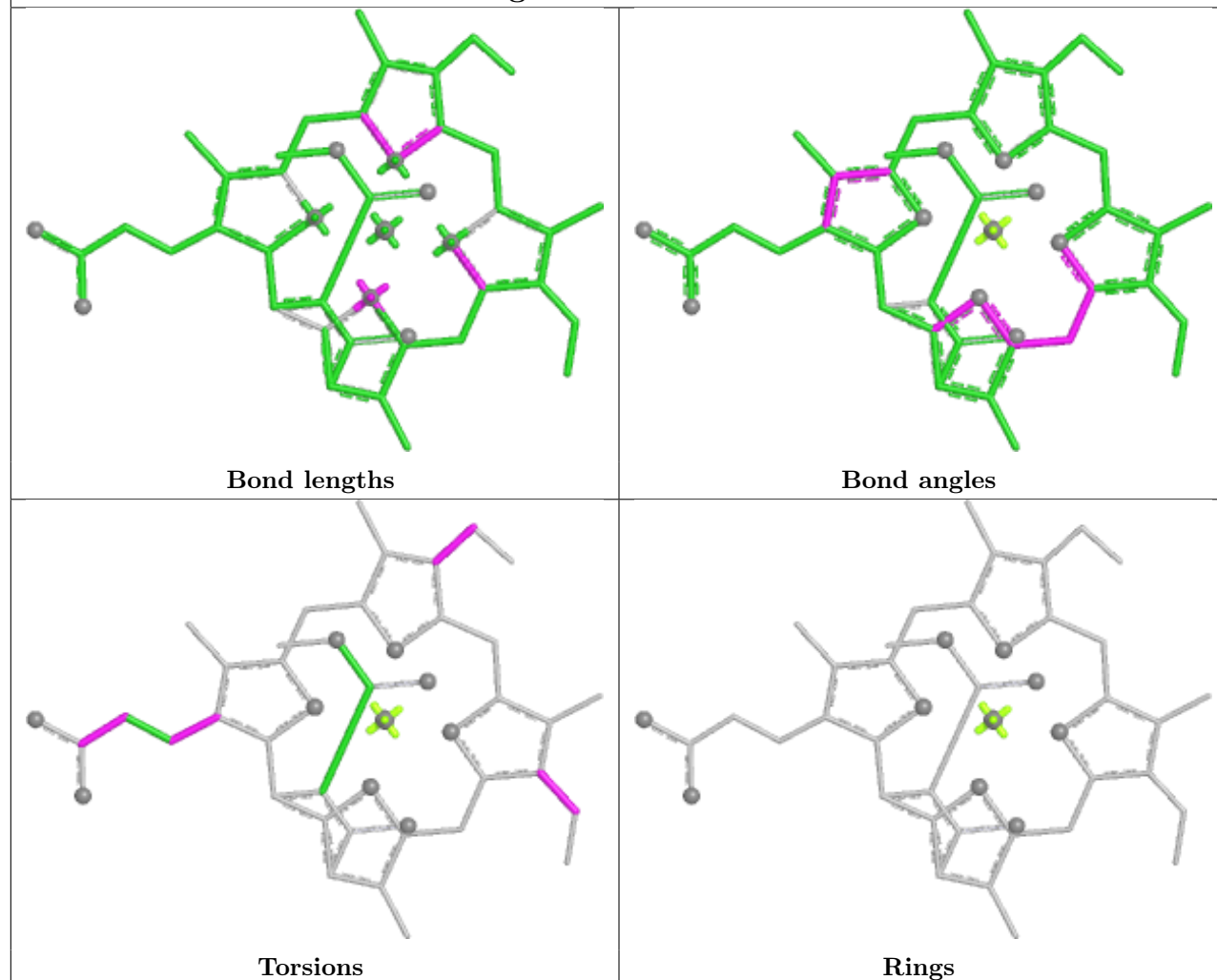
Ligand CLA S 308



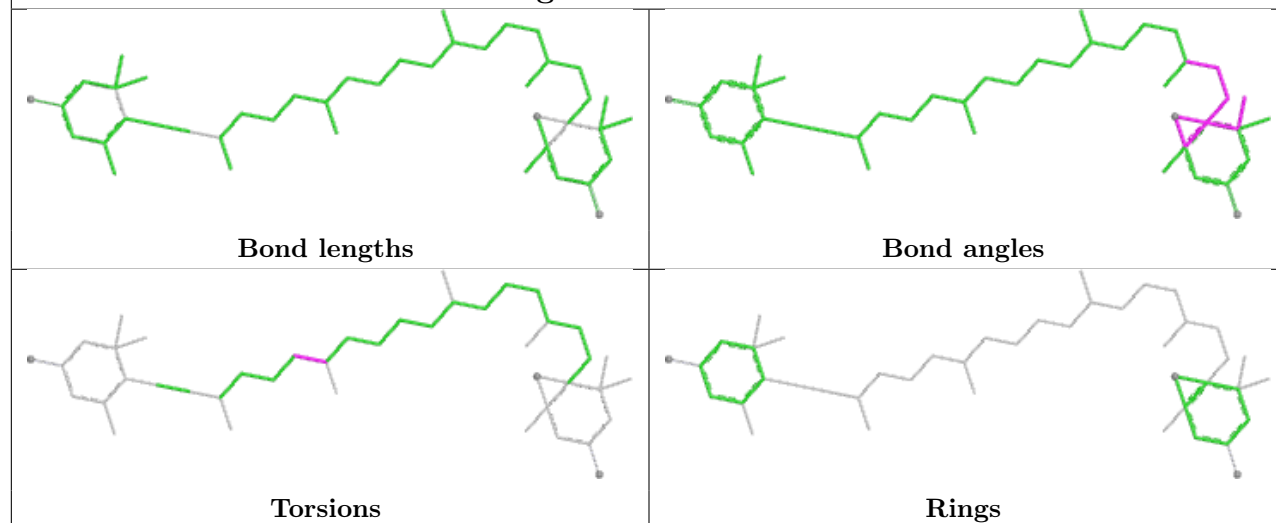
Ligand DD6 H 312

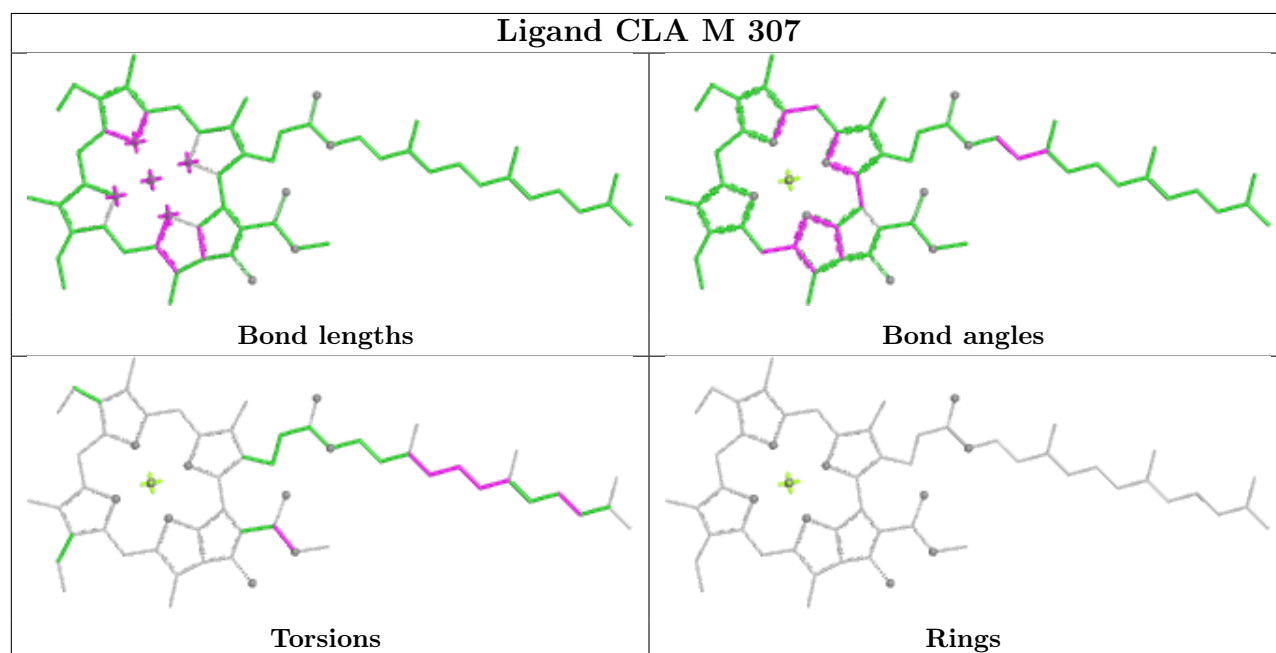
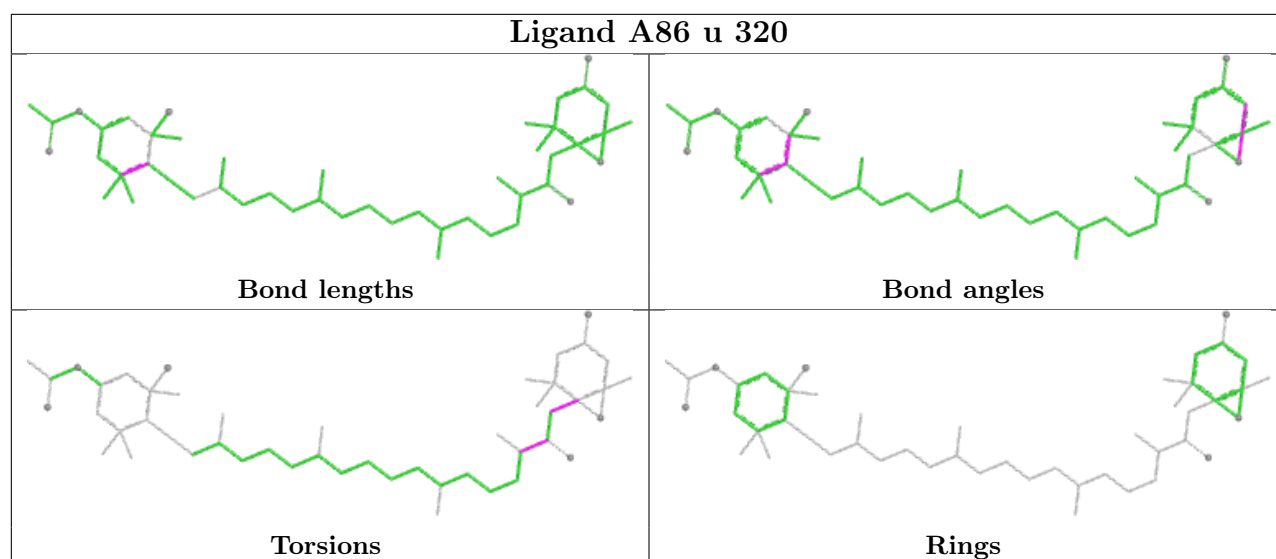


Ligand KC2 O 308

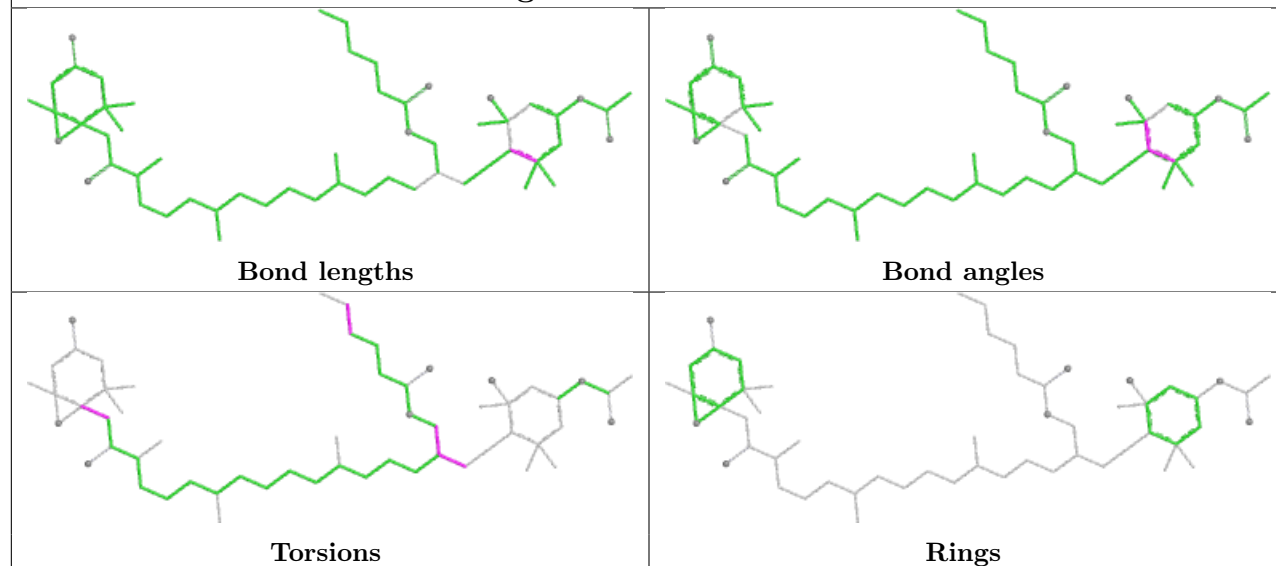


Ligand DD6 k 204

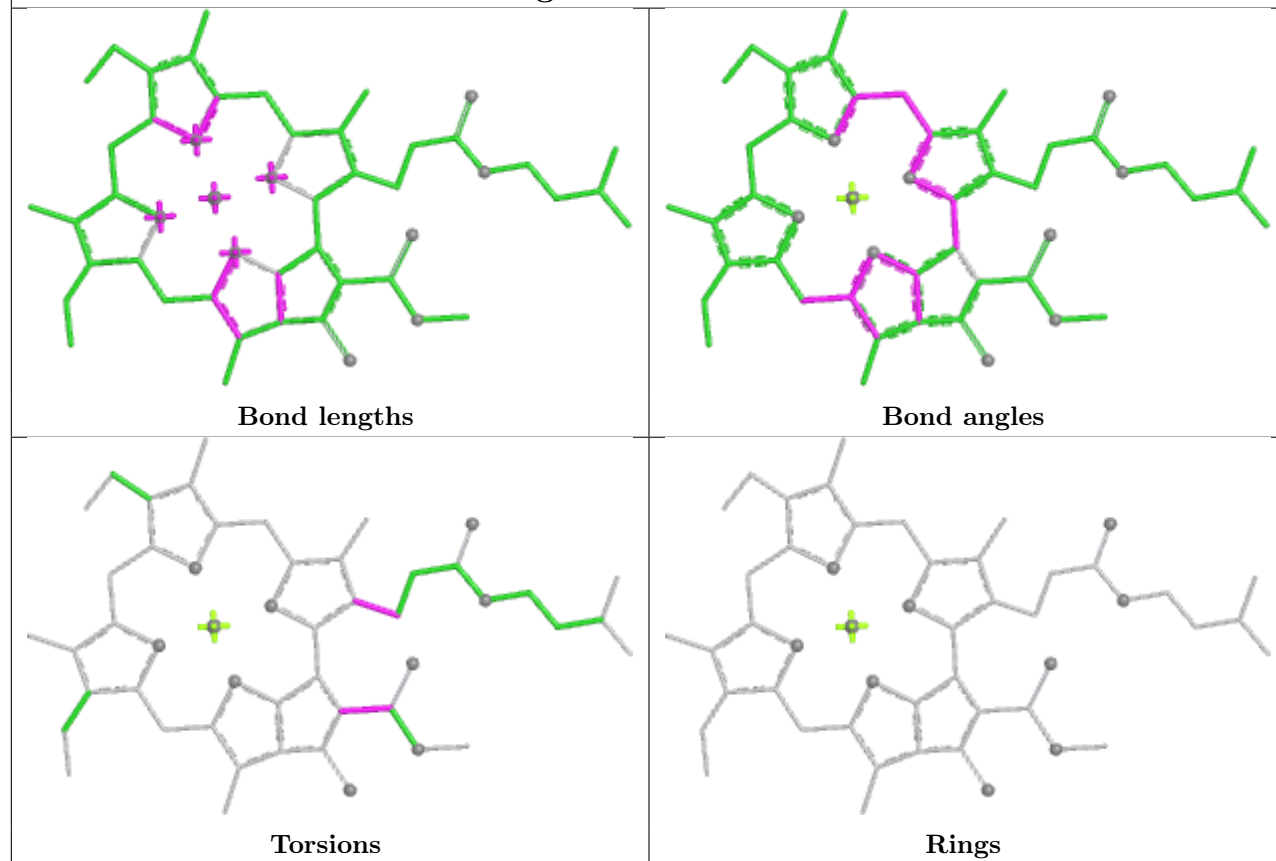


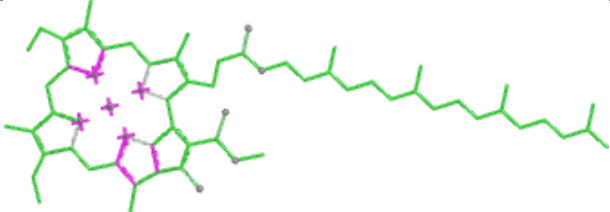
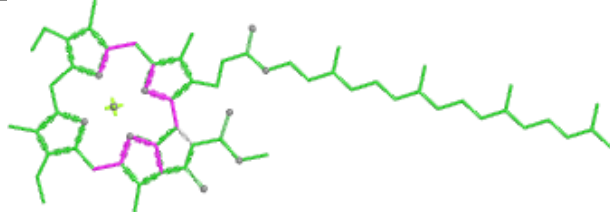
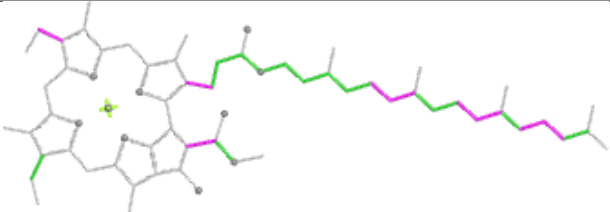
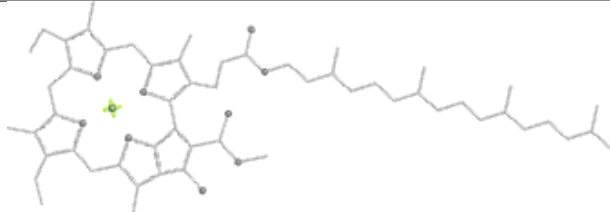
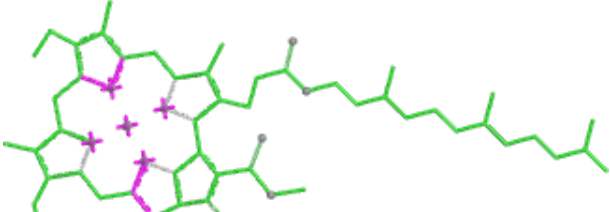
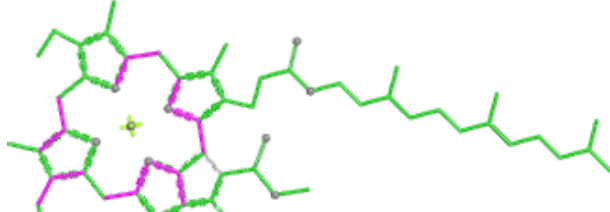
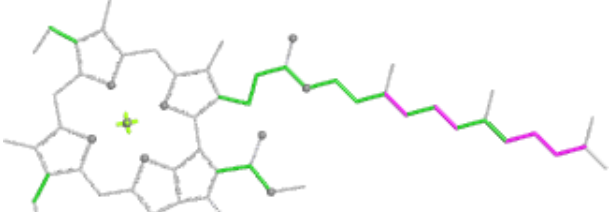
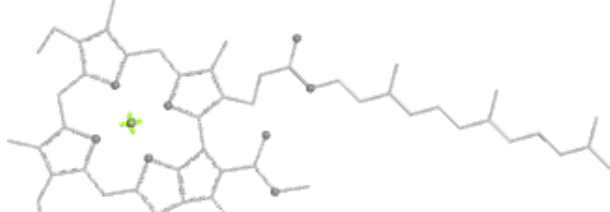
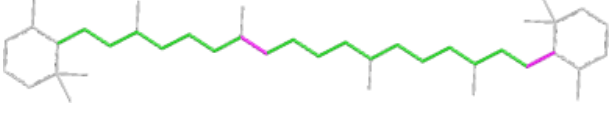
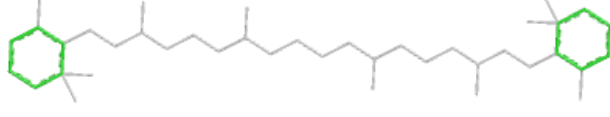


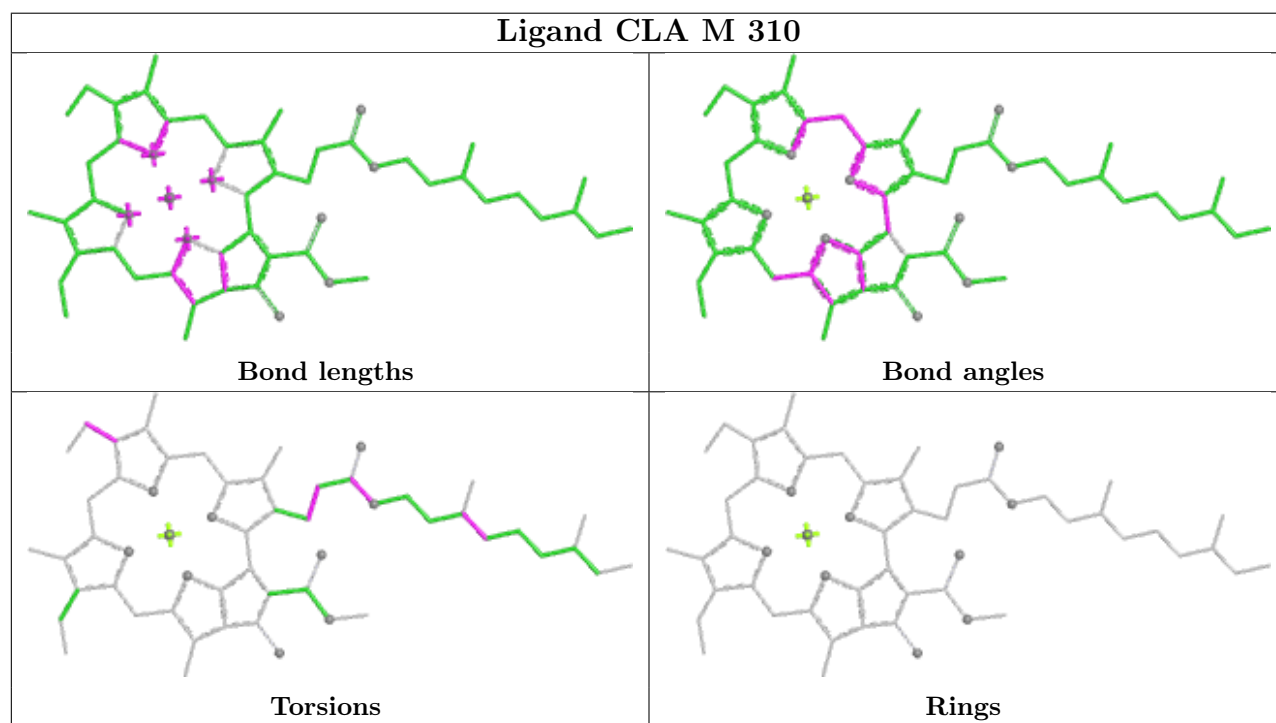
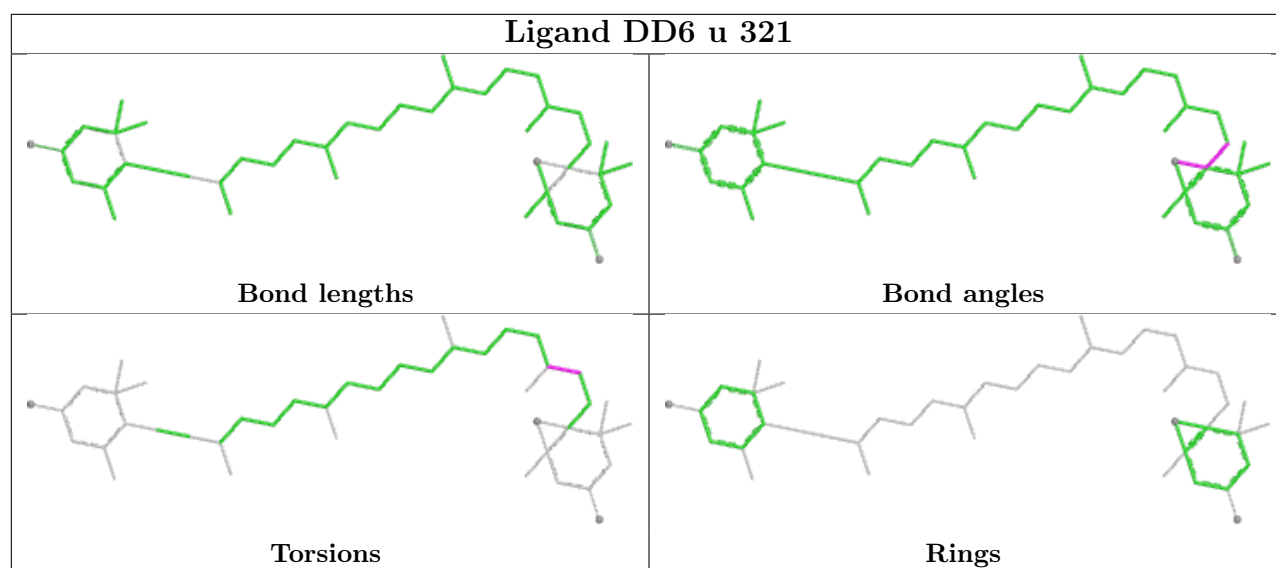
Ligand A1EB1 x 322

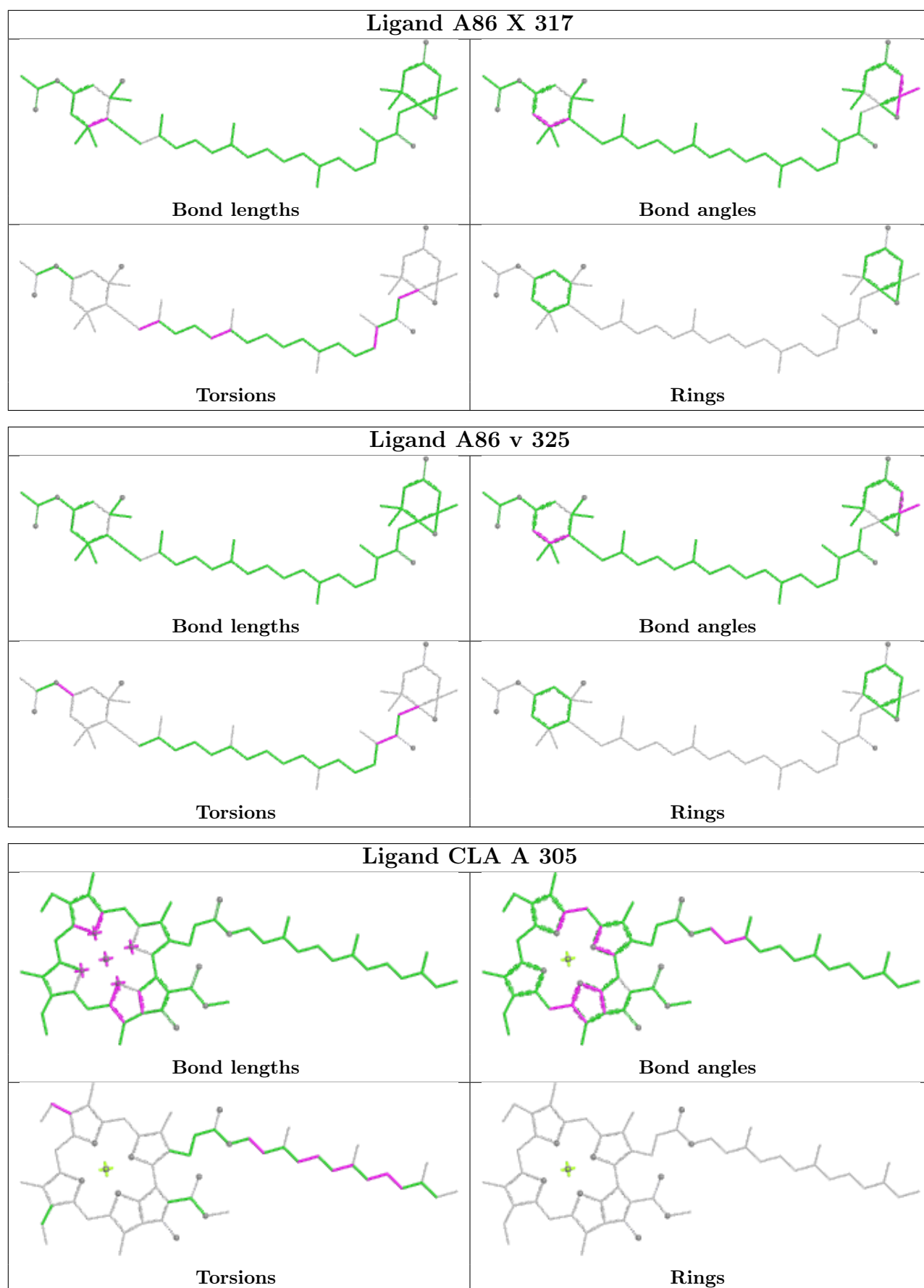


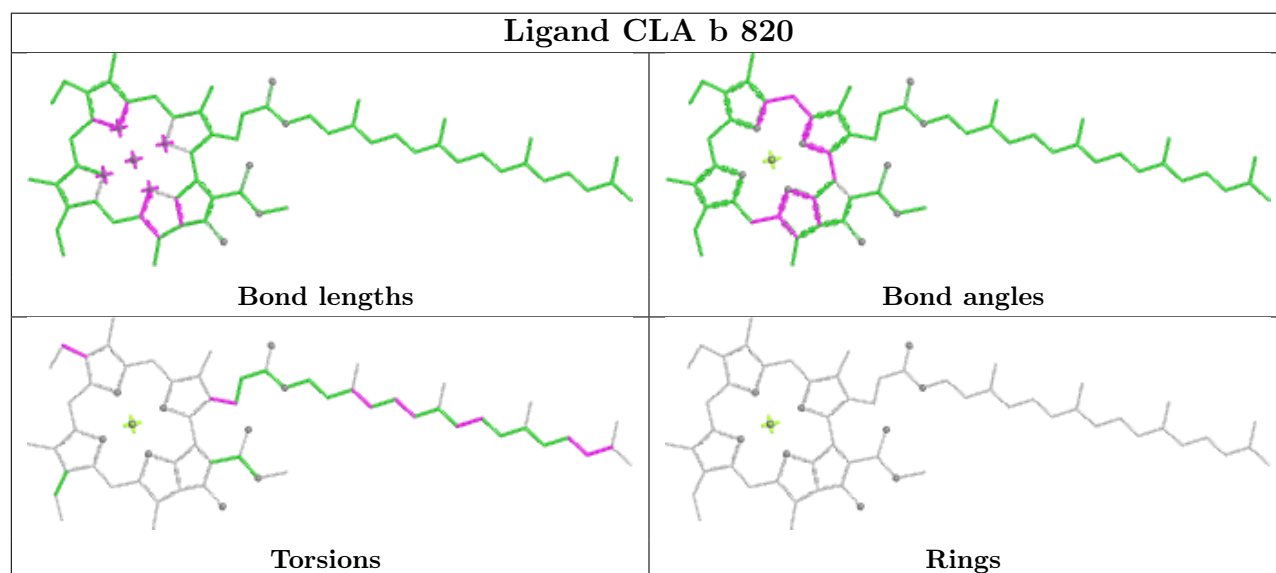
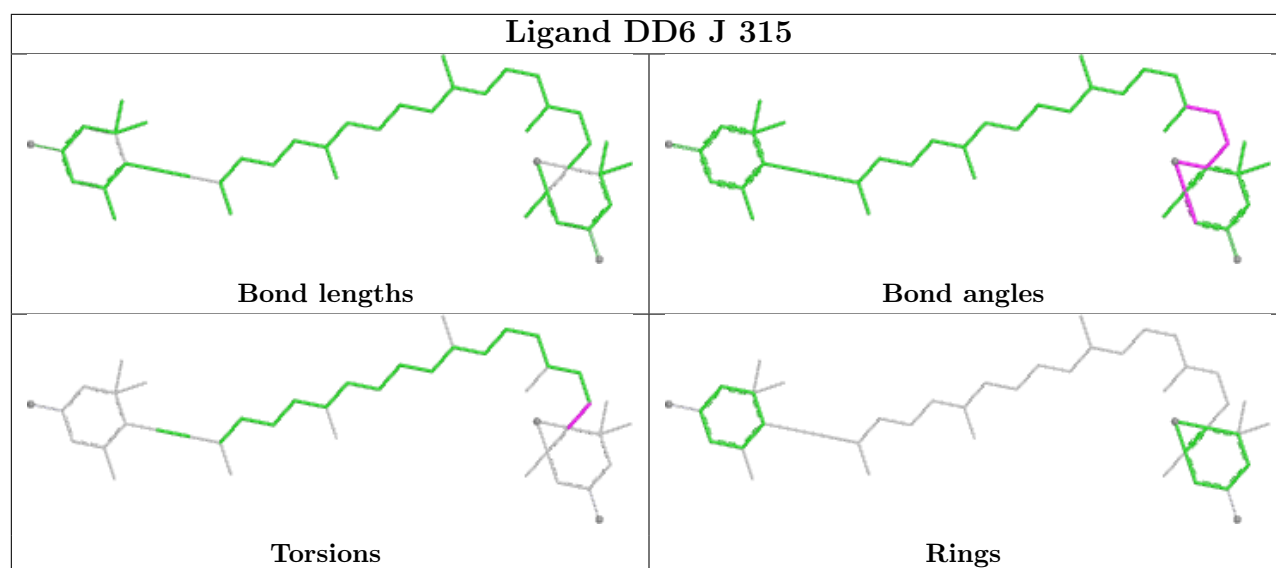
Ligand CLA a 809

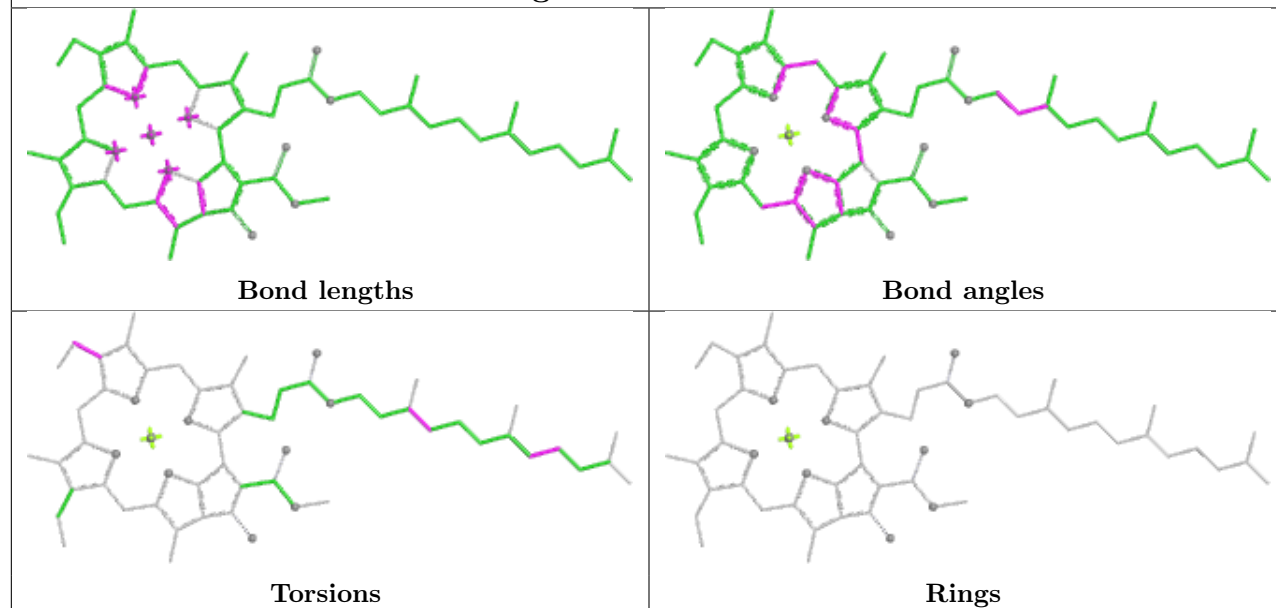
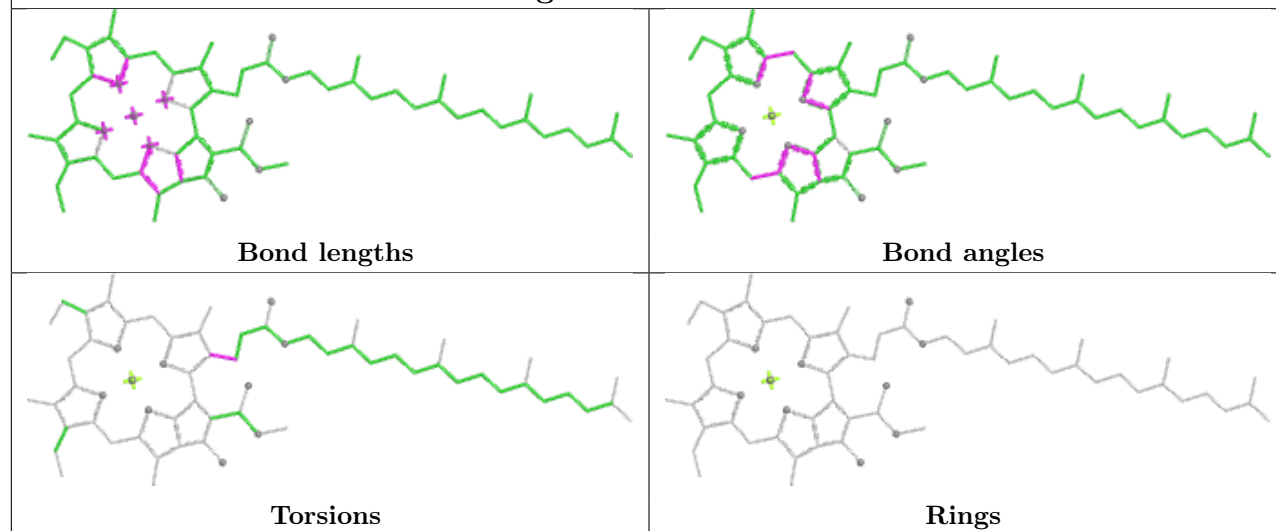


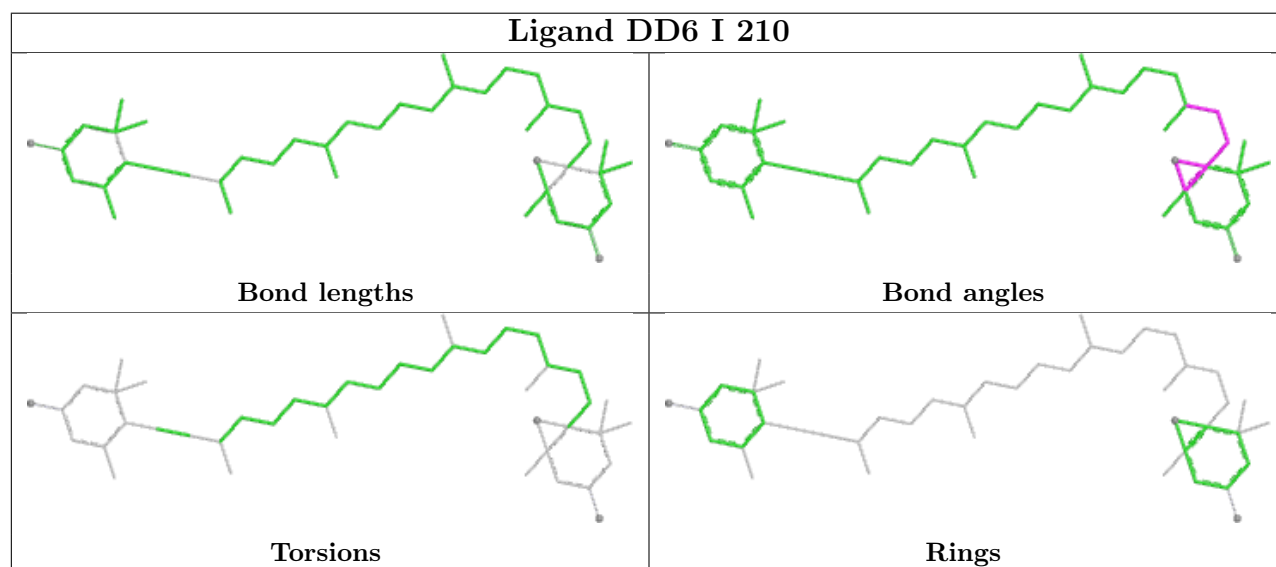
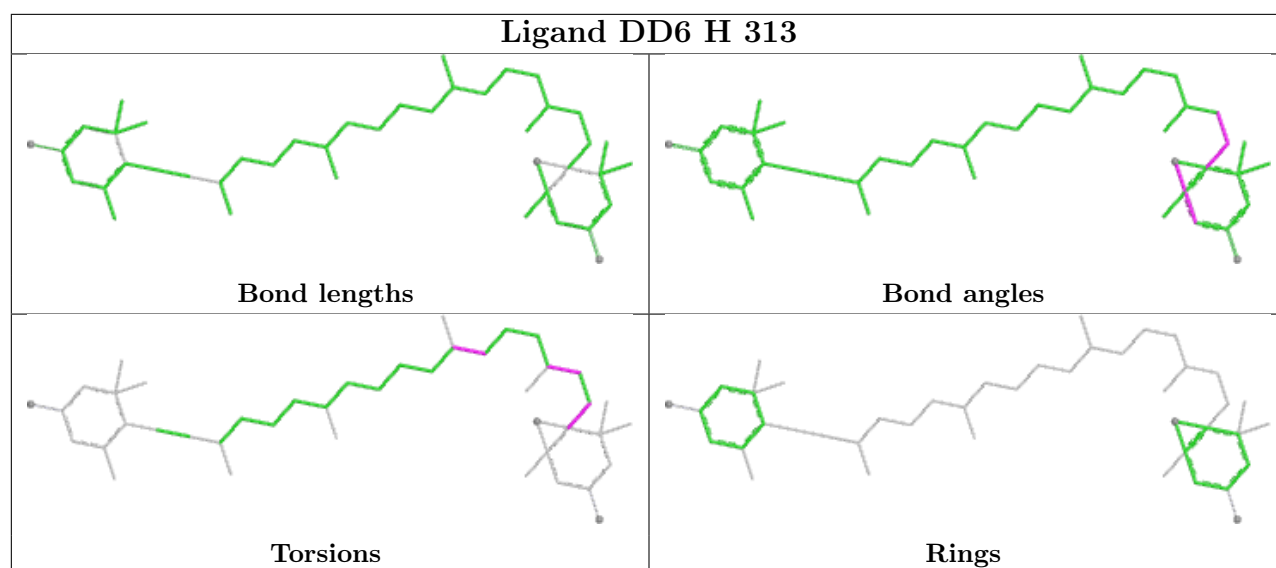
Ligand CLA I 204	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA Q 208	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR f 206	
 Bond lengths	 Bond angles
 Torsions	 Rings



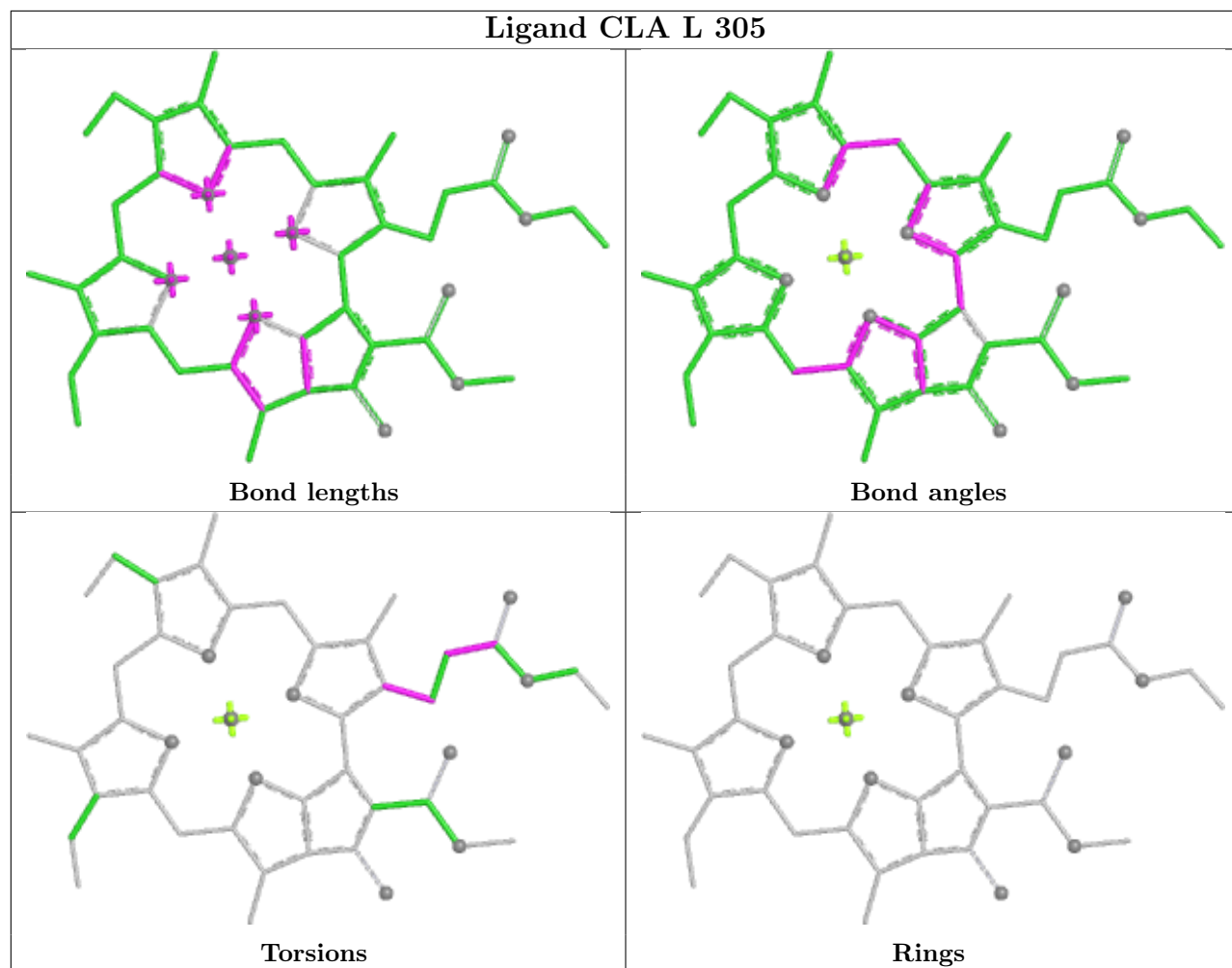




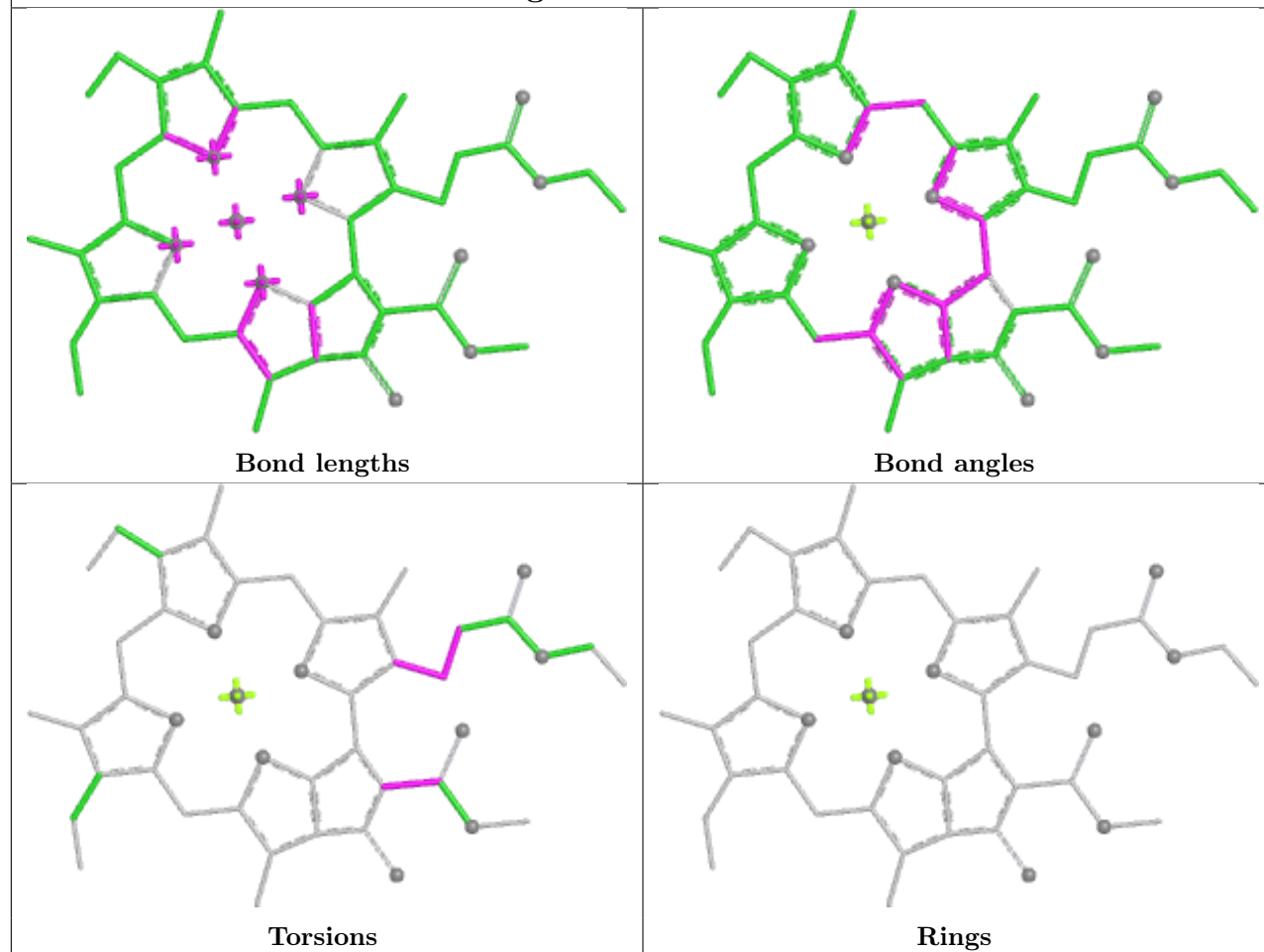
Ligand CLA C 305**Ligand CLA a 827**



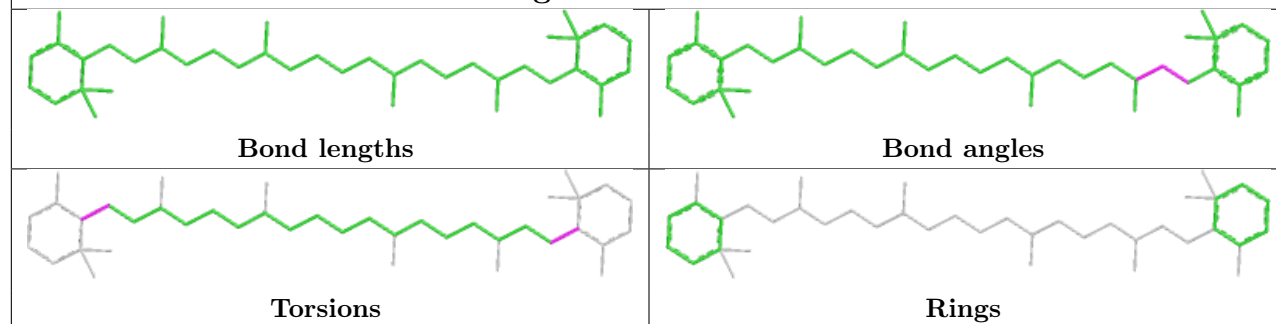
Ligand CLA L 305

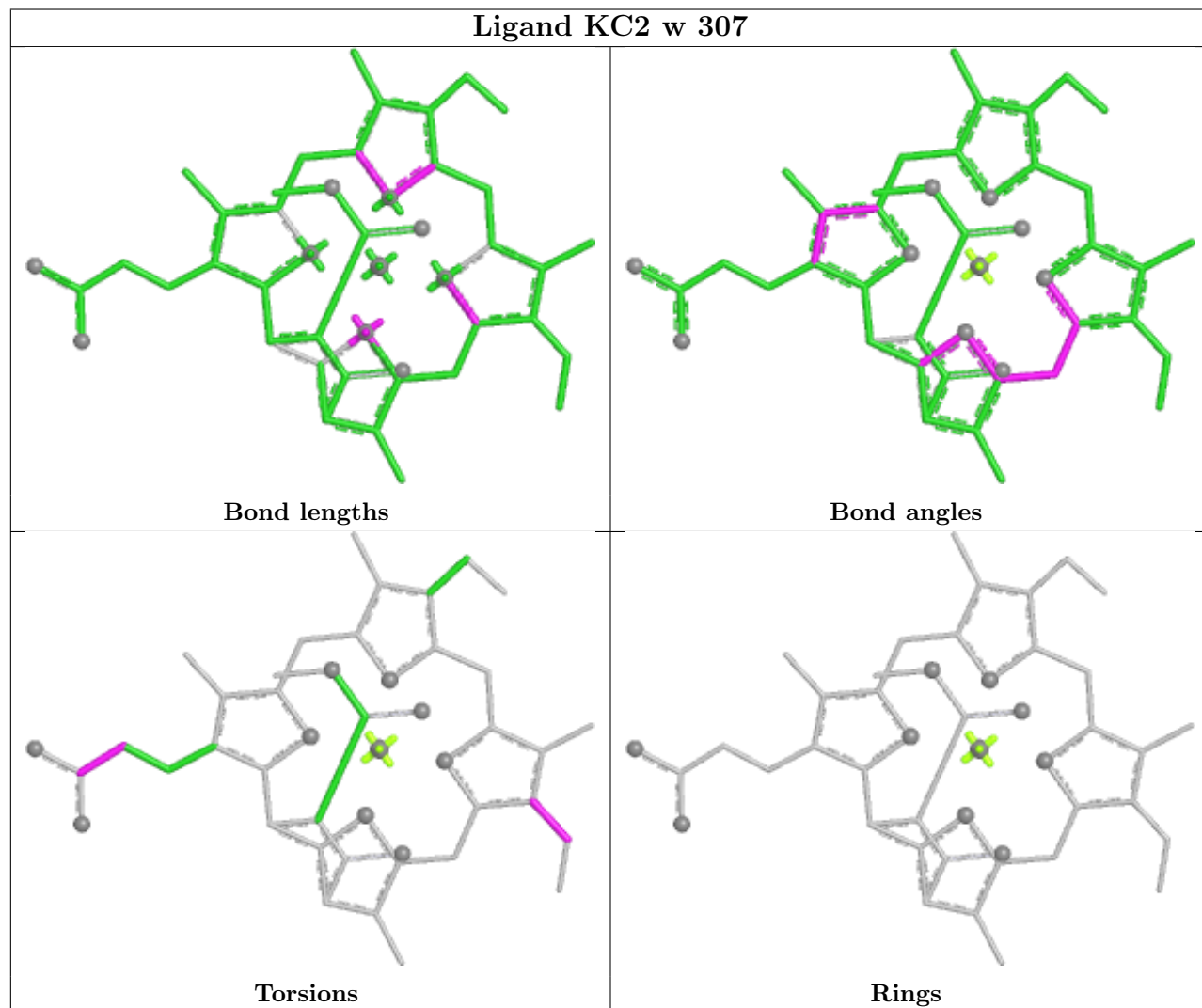
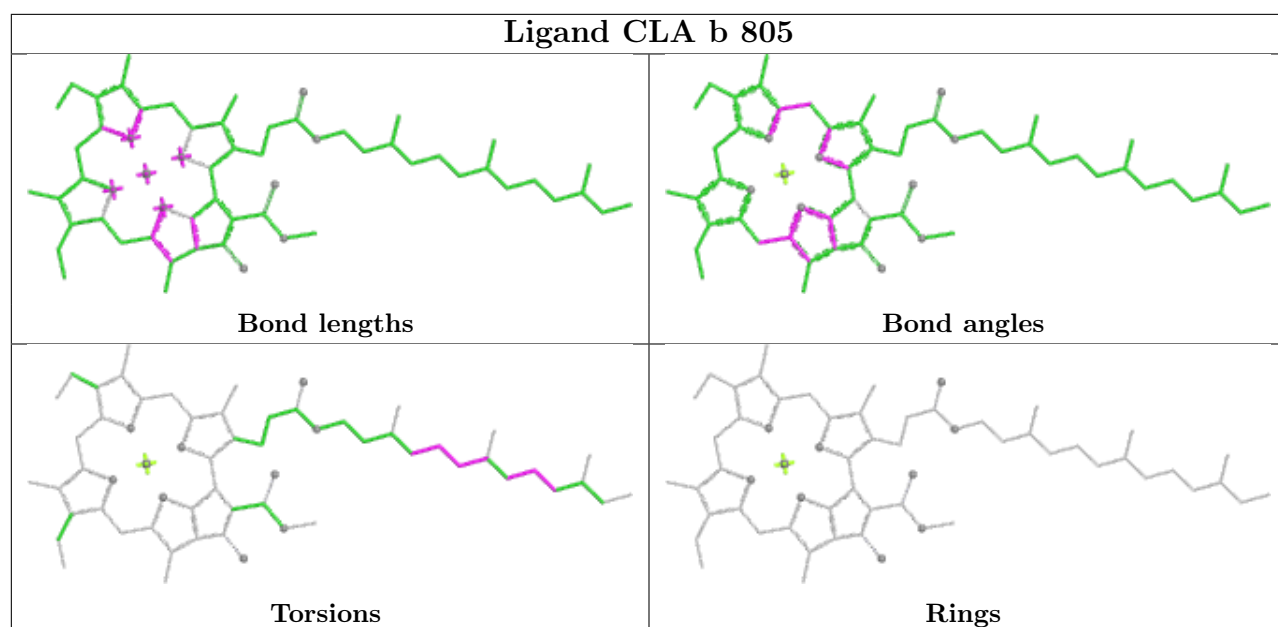


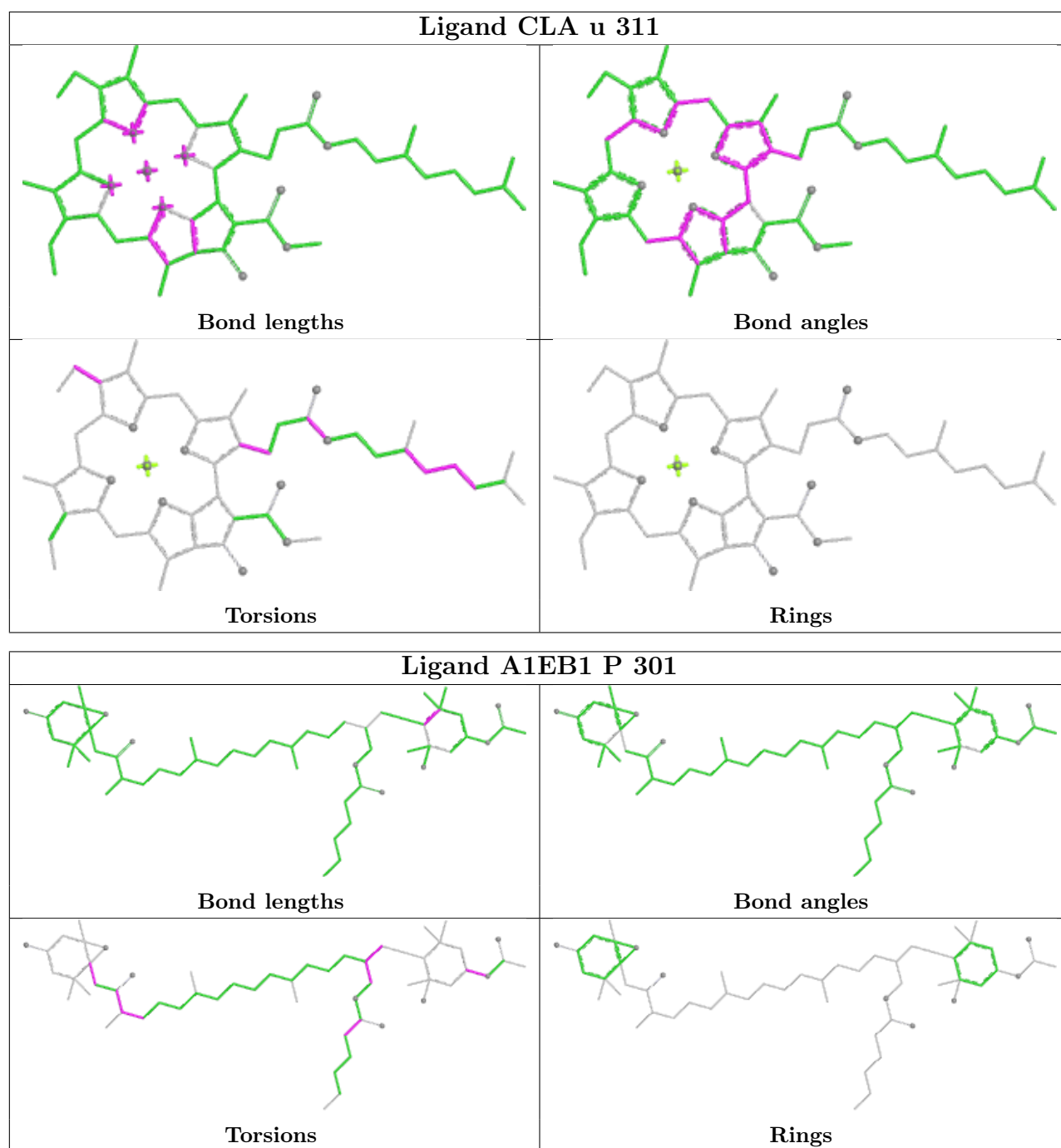
Ligand CLA X 312

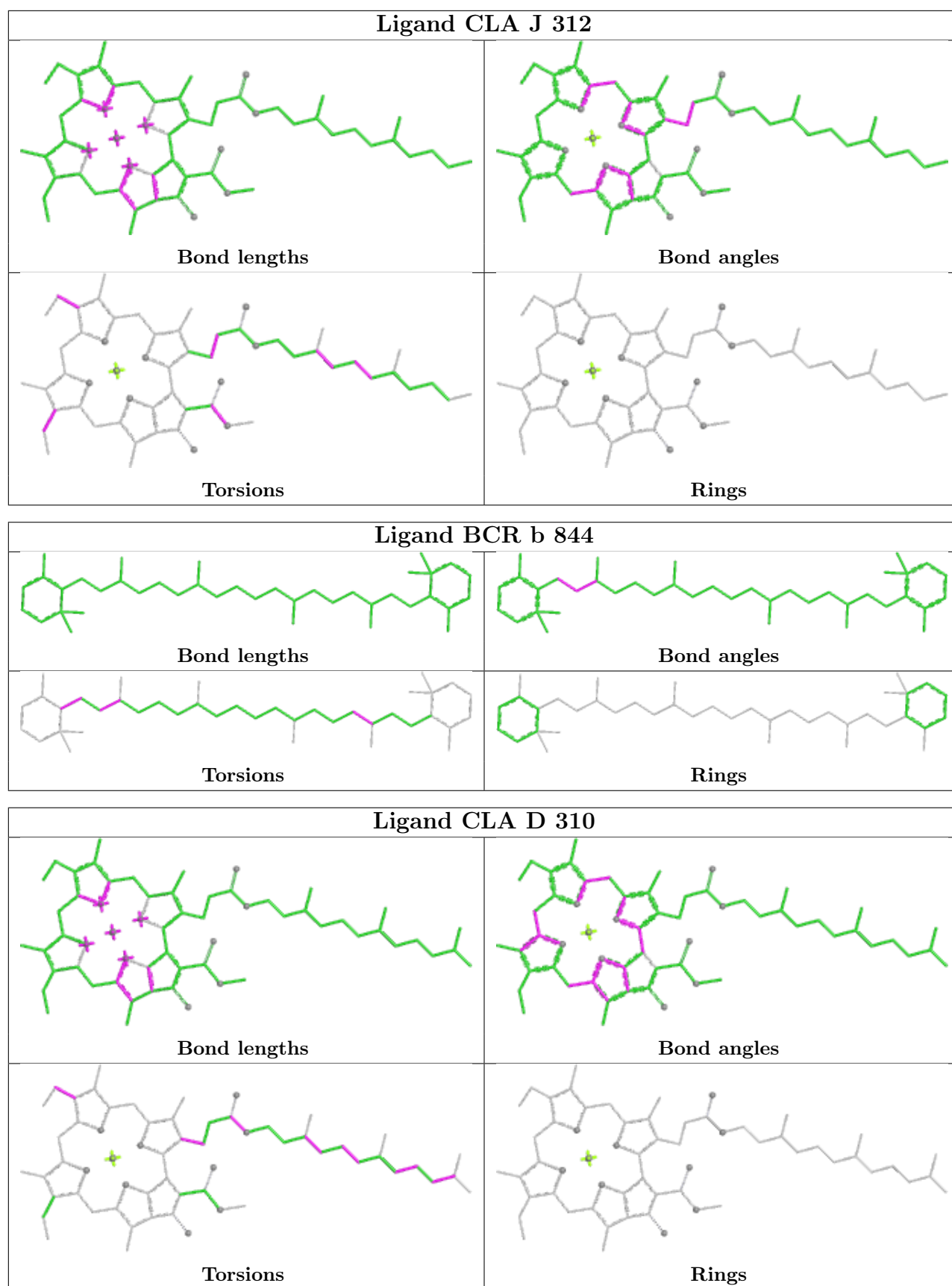


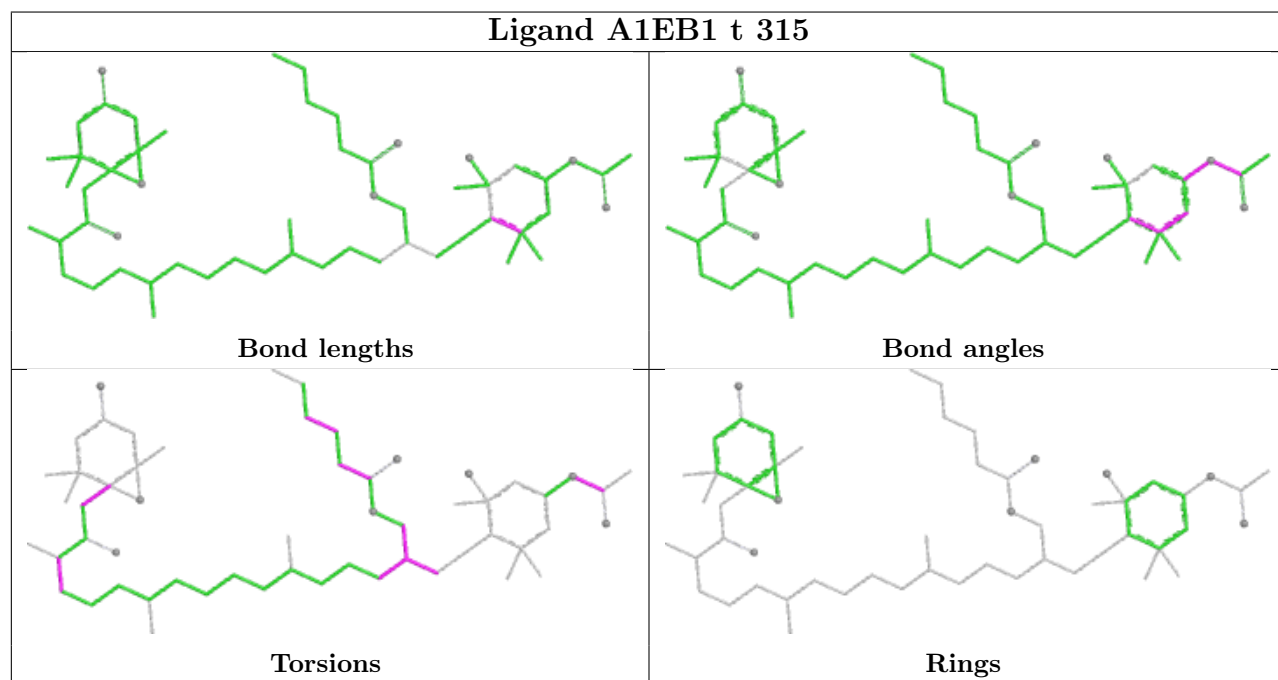
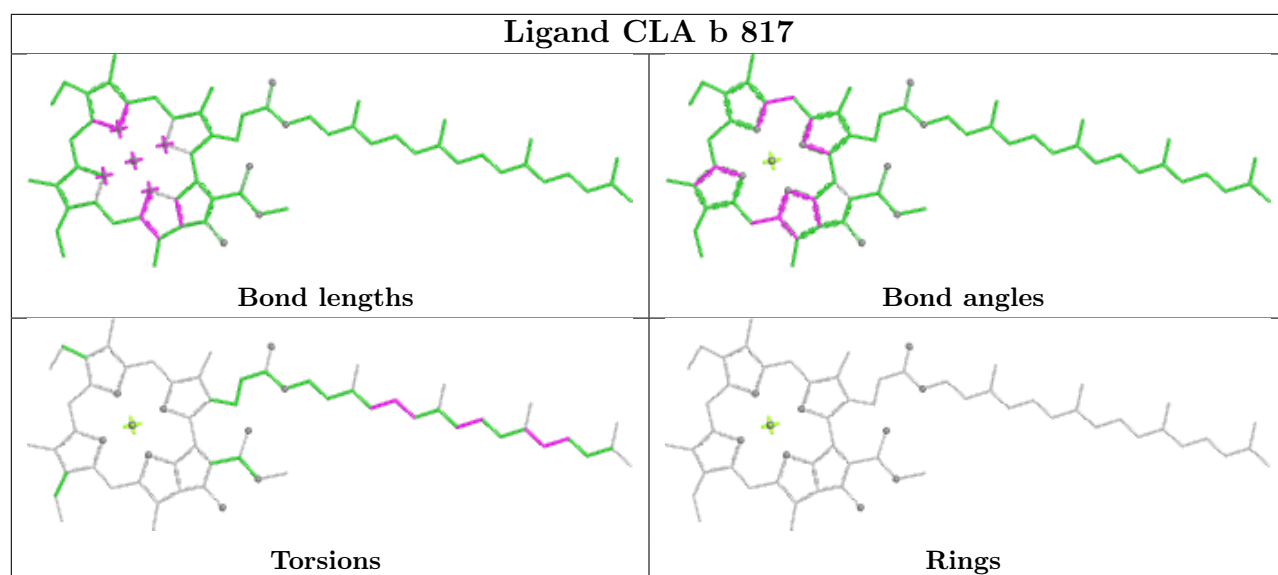
Ligand BCR b 846



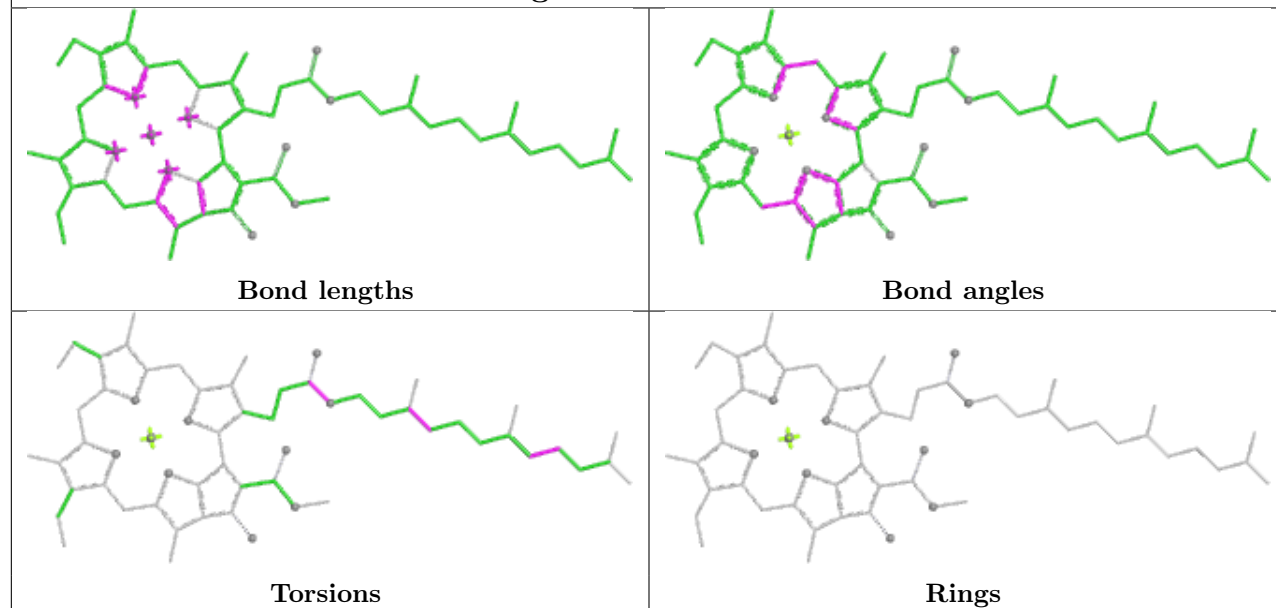




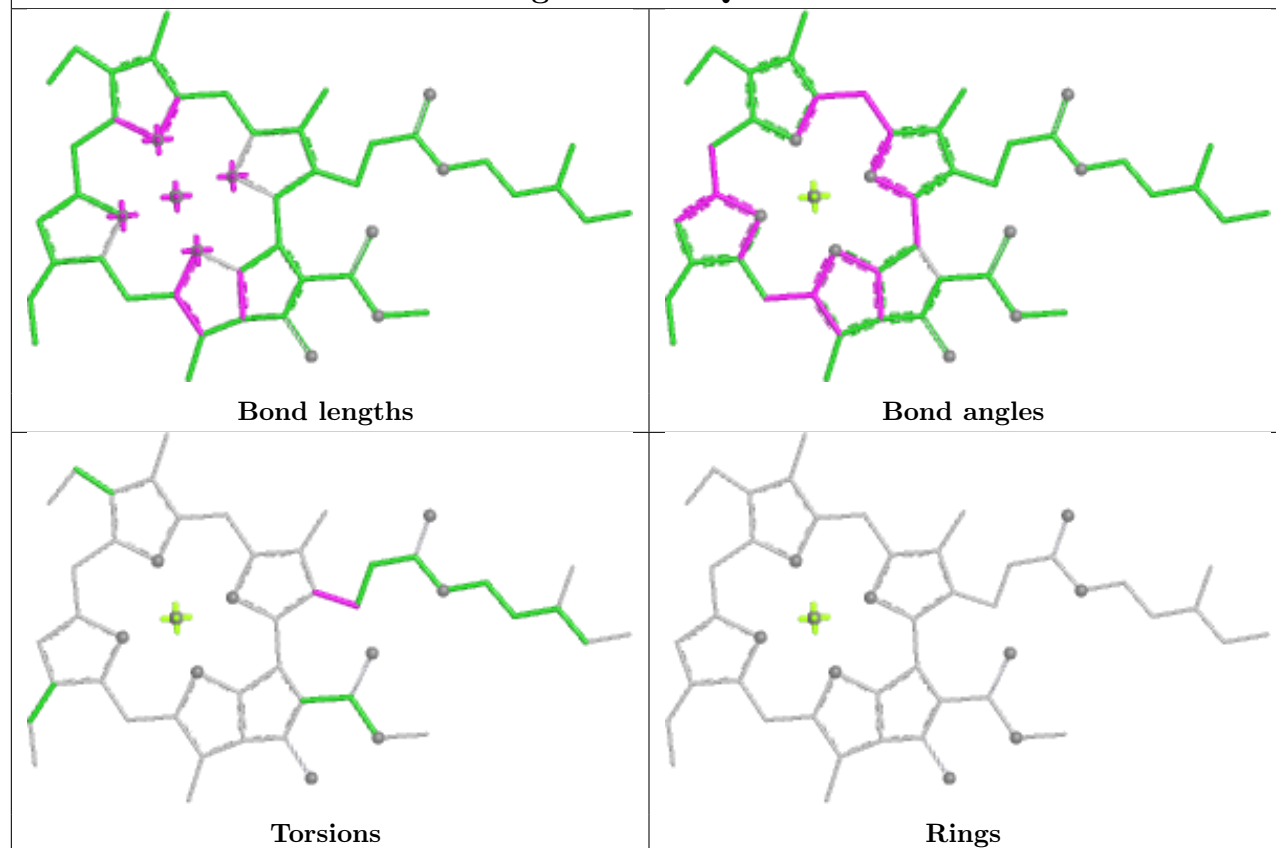


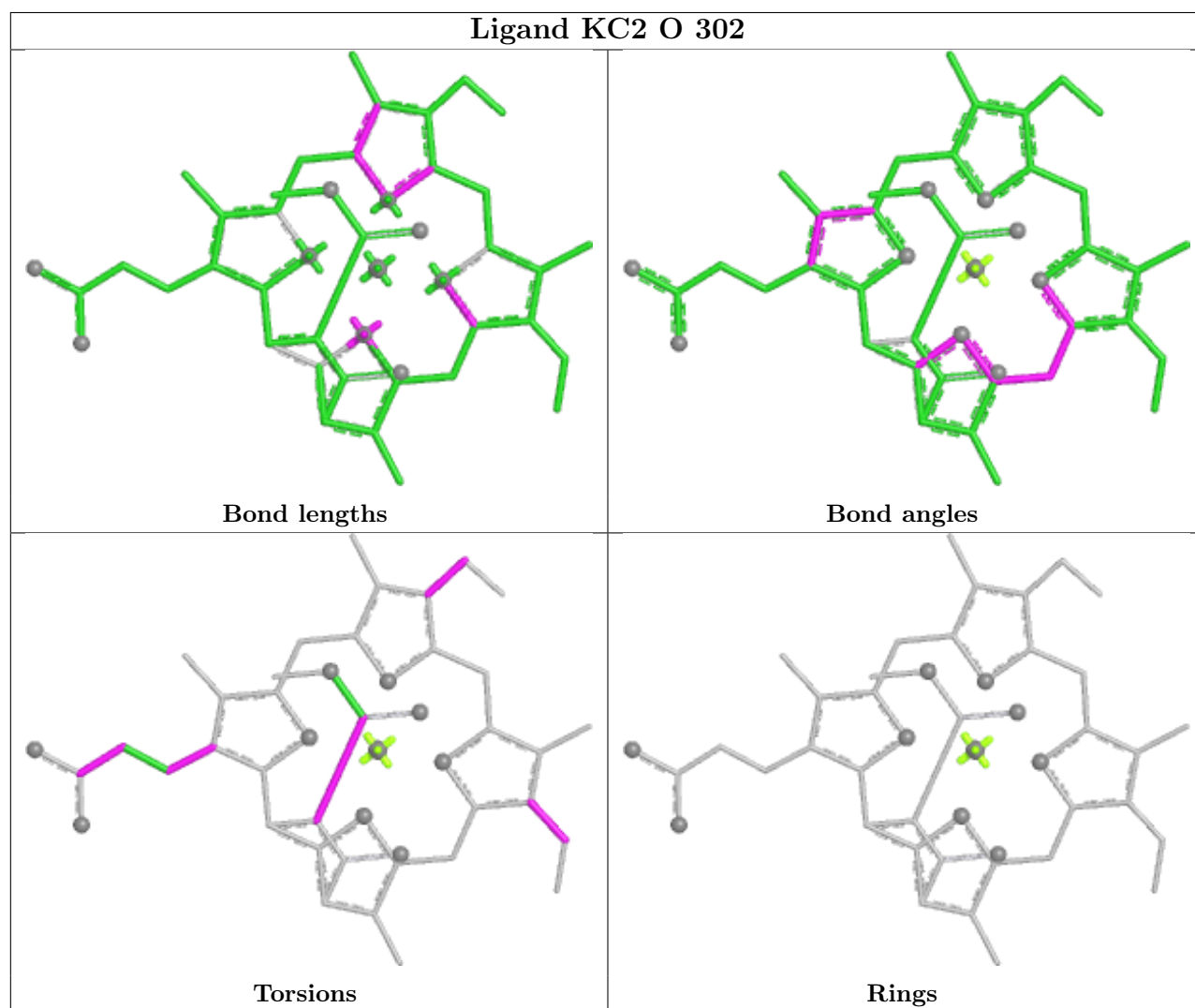
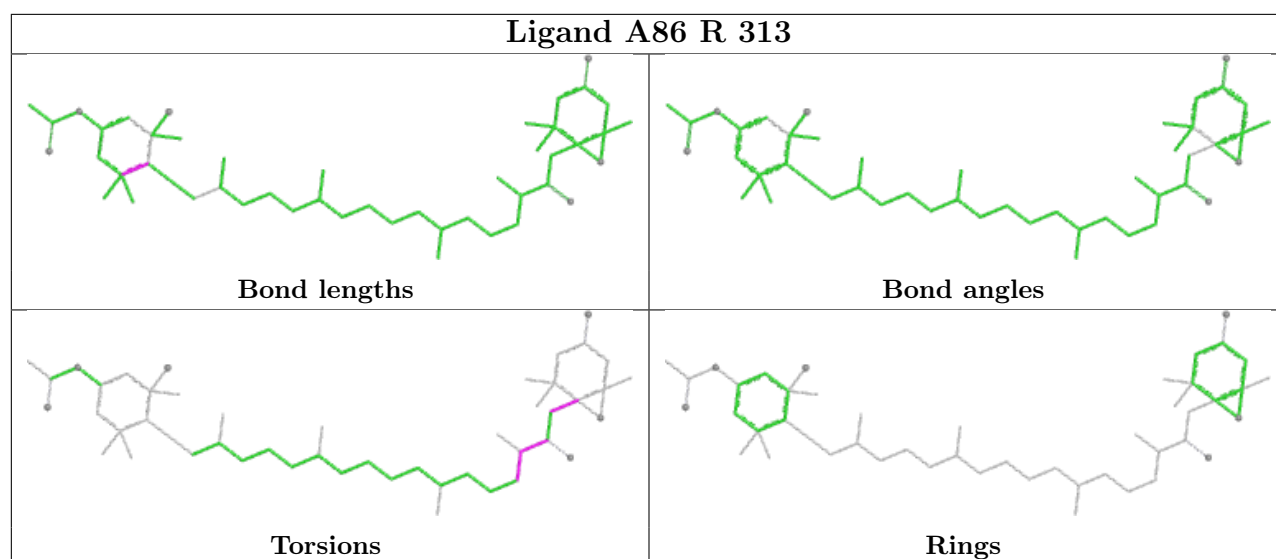


Ligand CLA H 310

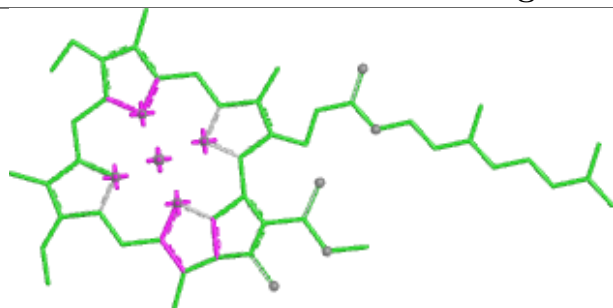


Ligand CLA Q 204

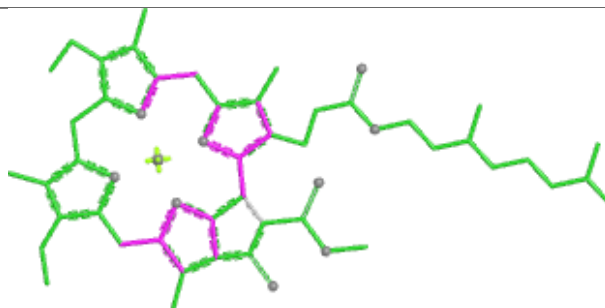




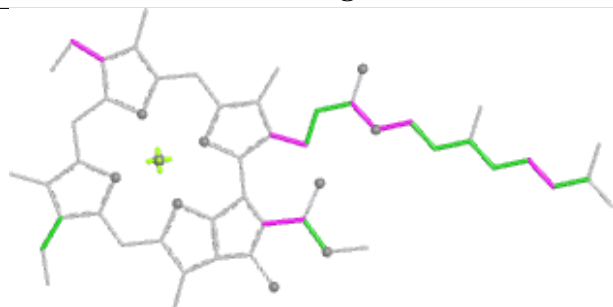
Ligand CLA x 307



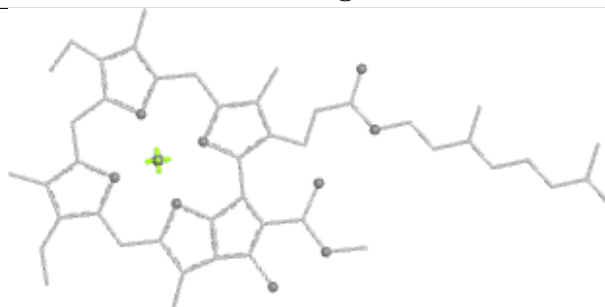
Bond lengths



Bond angles

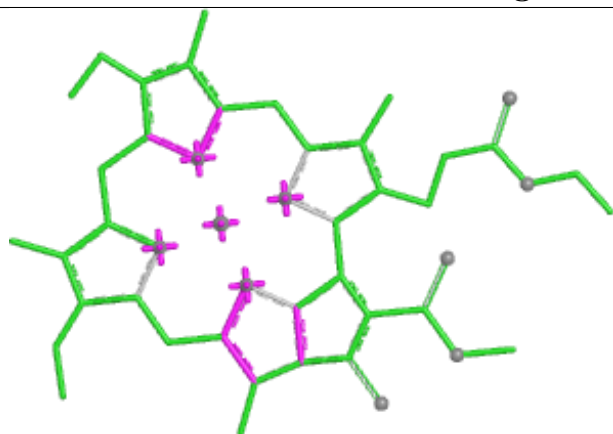


Torsions

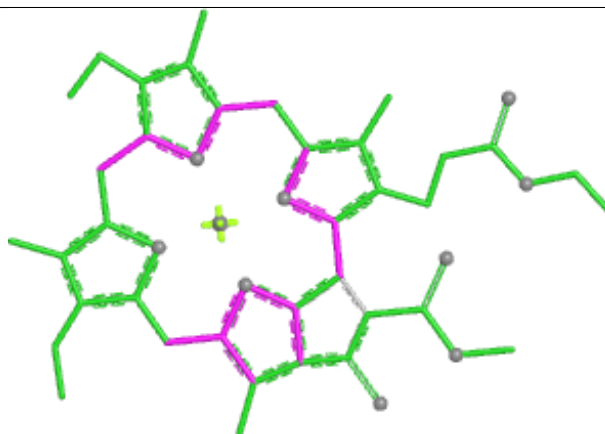


Rings

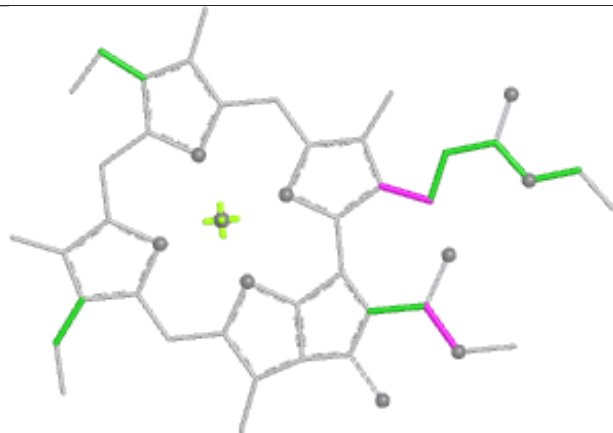
Ligand CLA U 207



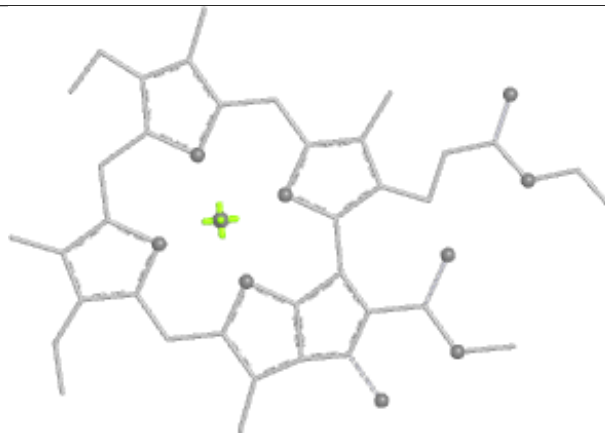
Bond lengths



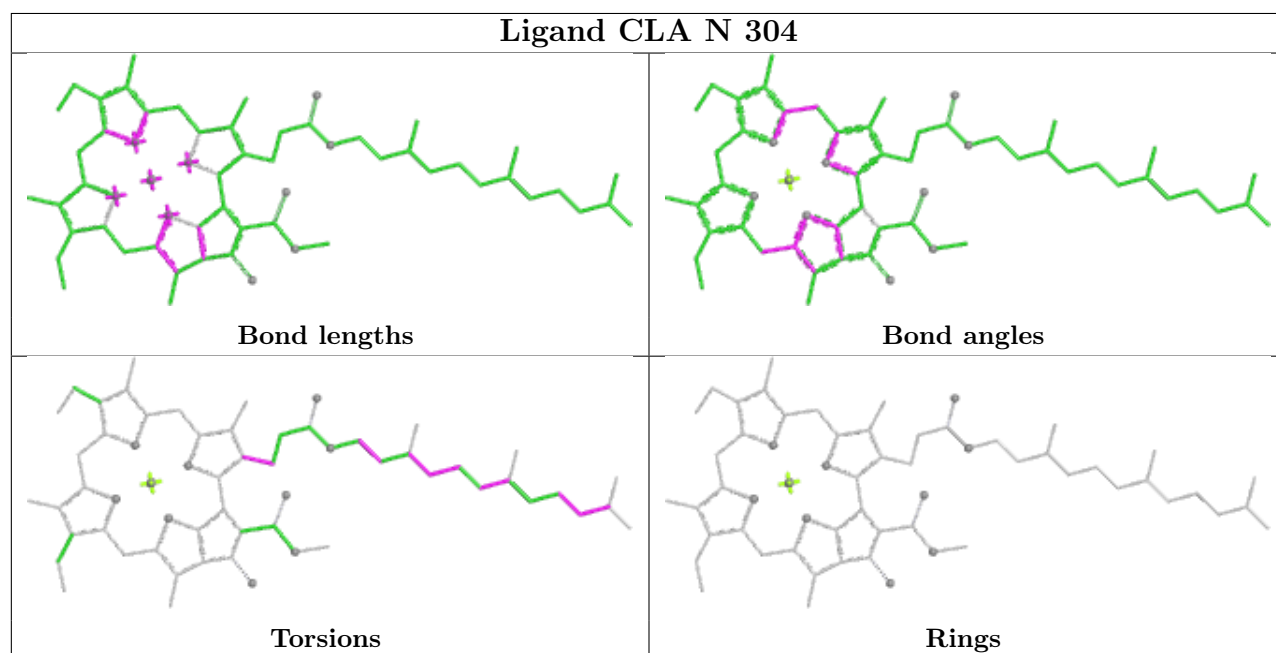
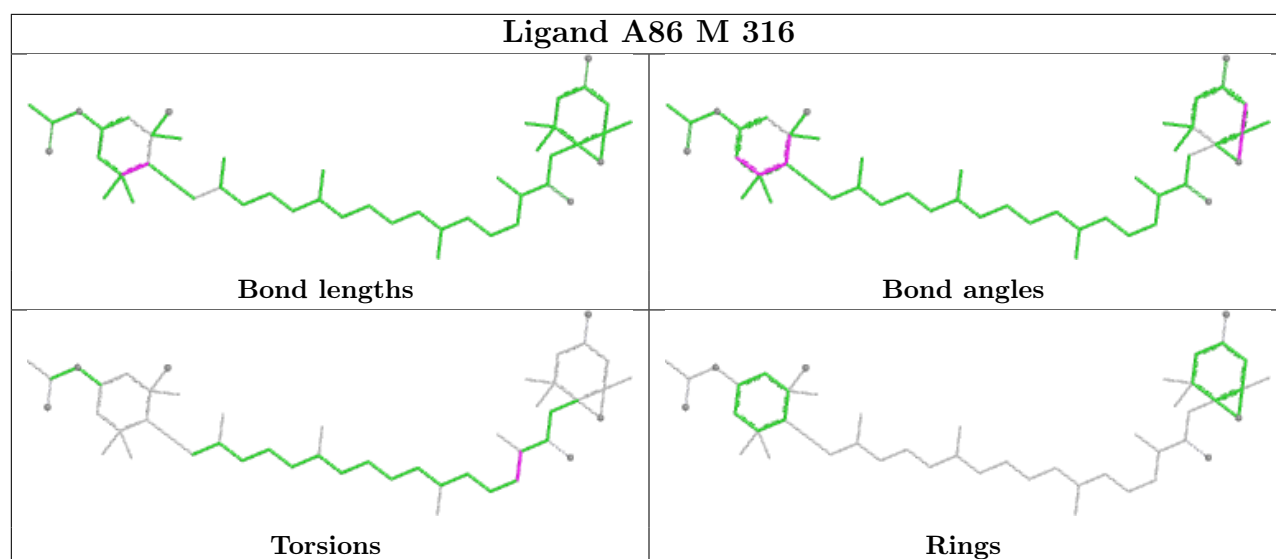
Bond angles



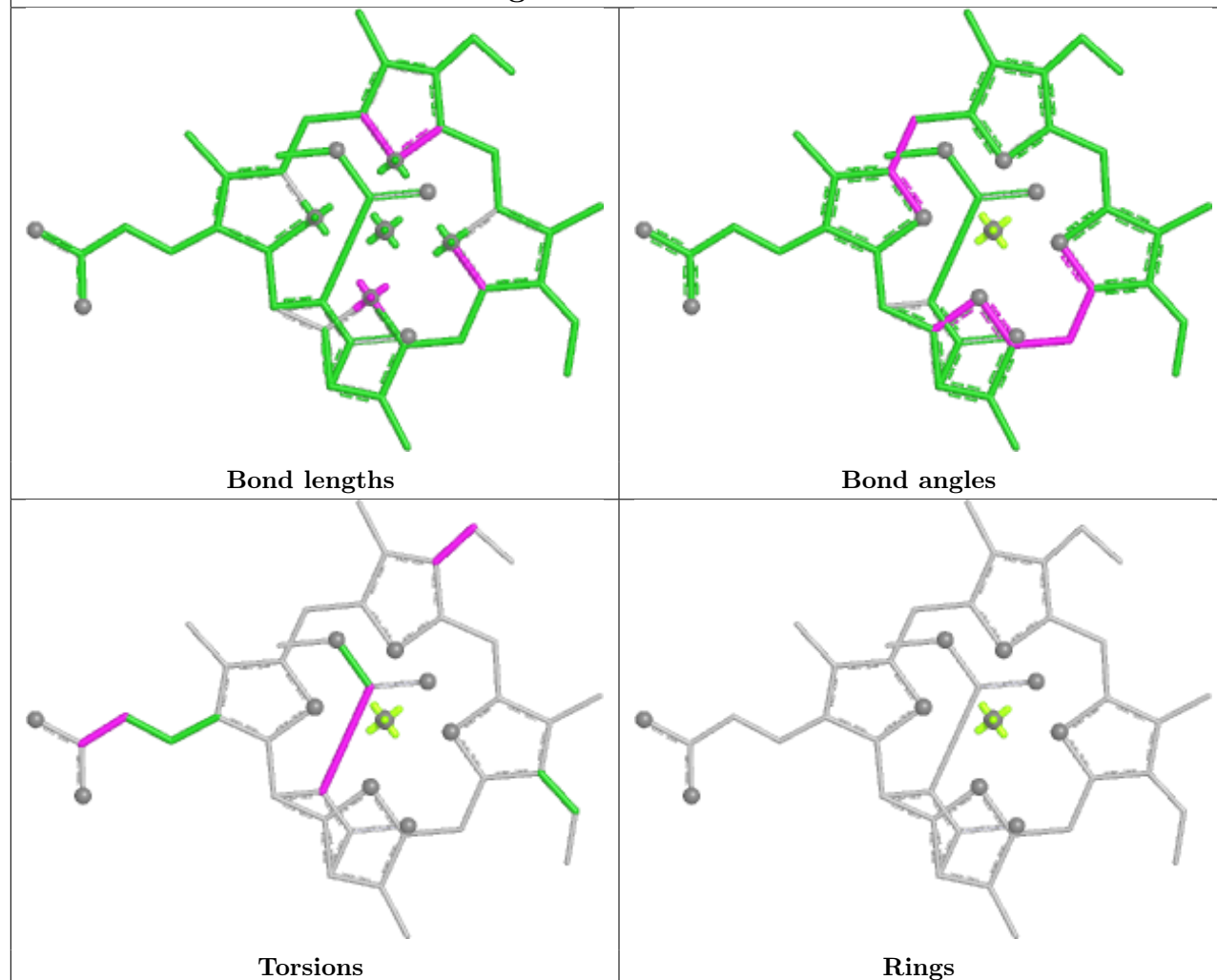
Torsions



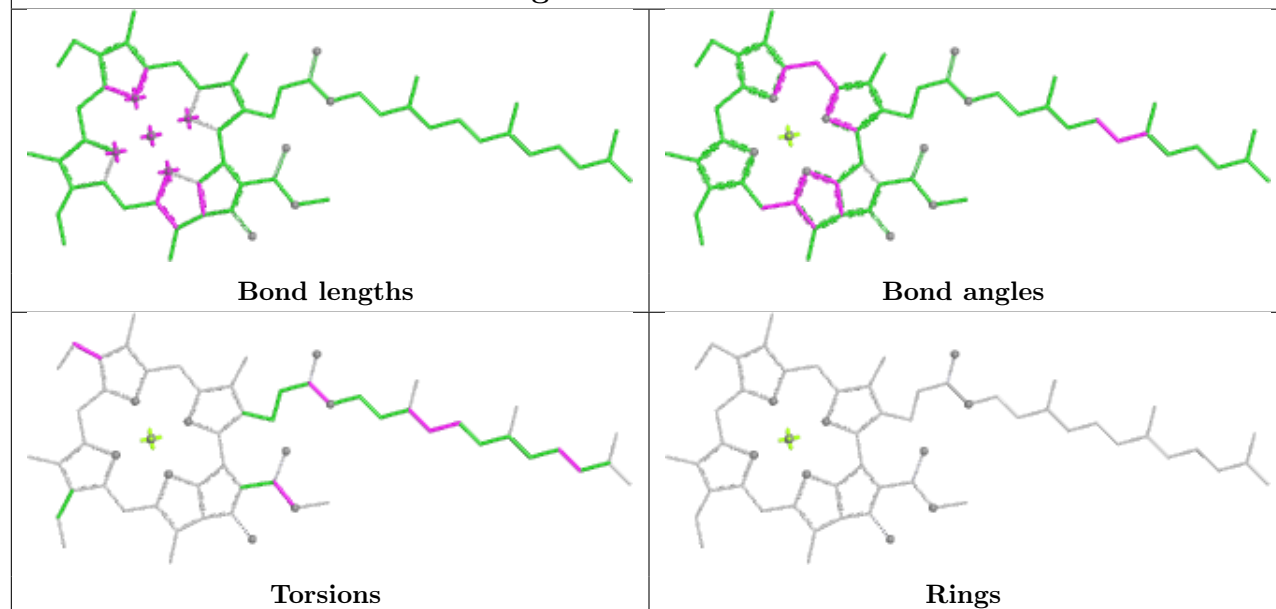
Rings

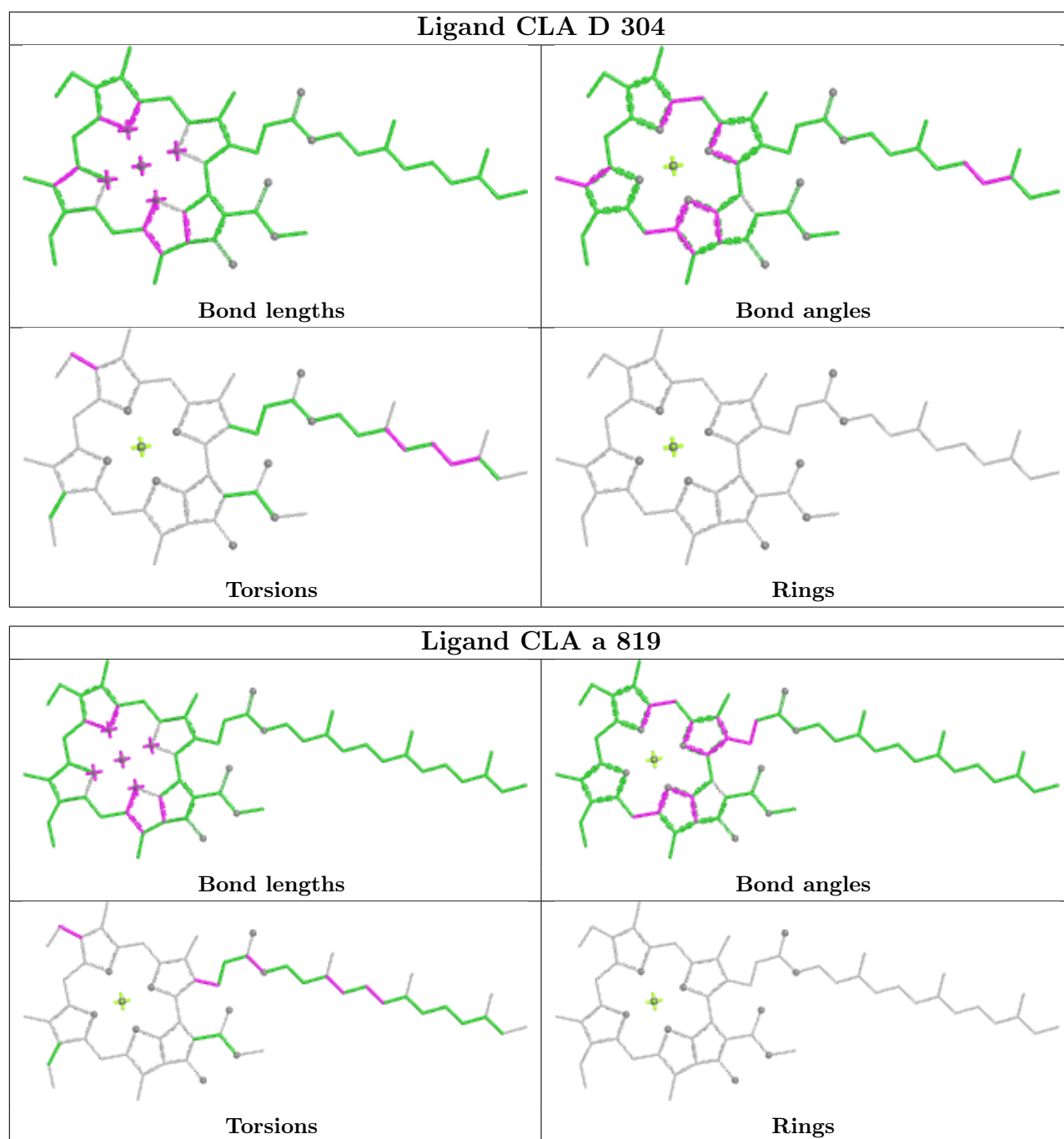


Ligand KC2 Y 303

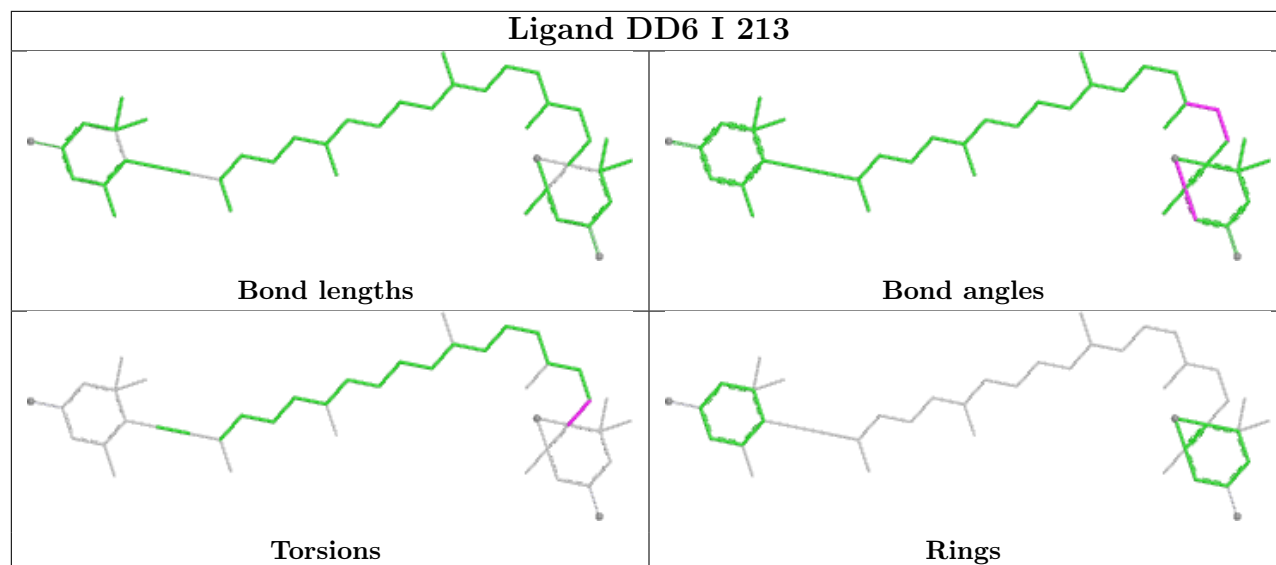


Ligand CLA Y 307

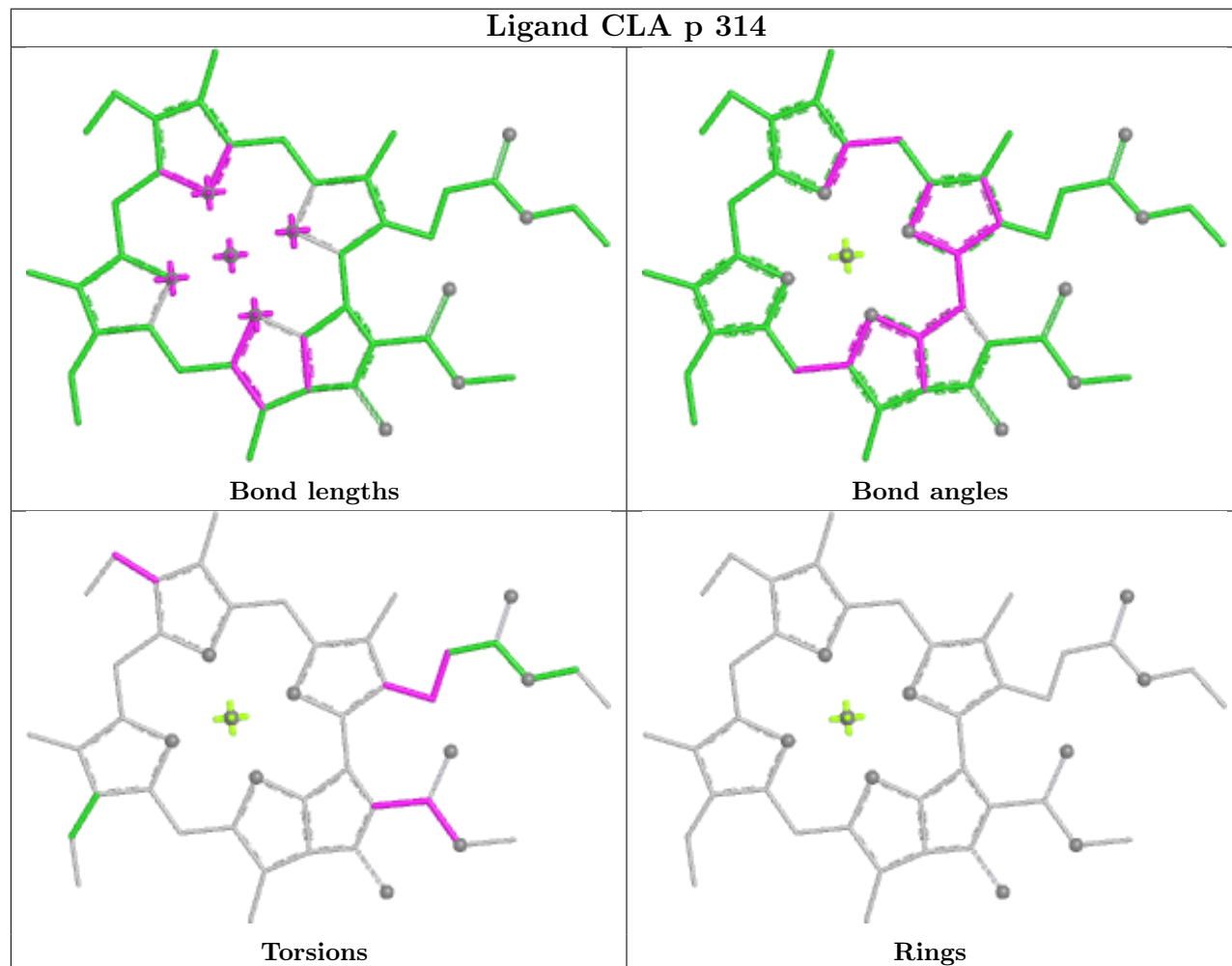




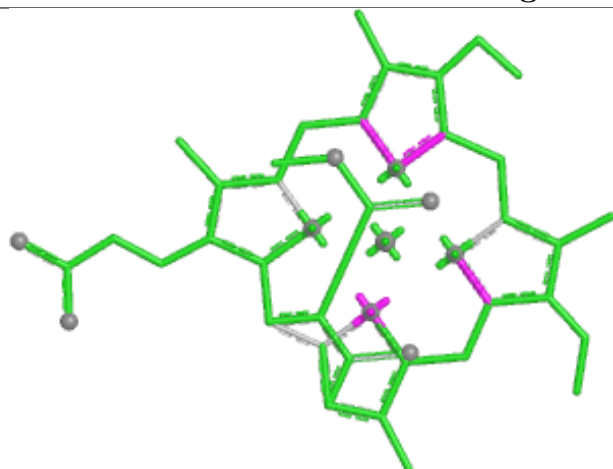
Ligand DD6 I 213



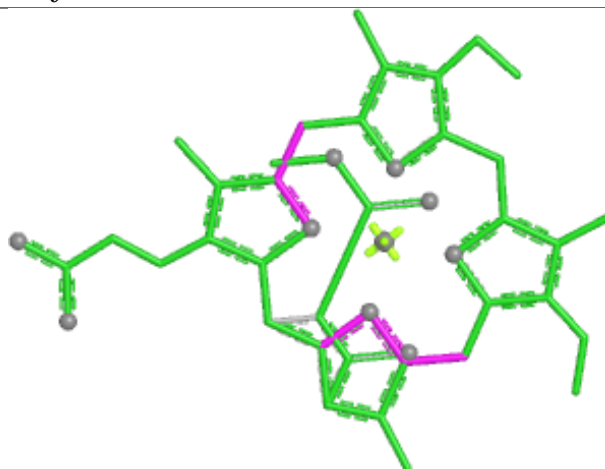
Ligand CLA p 314



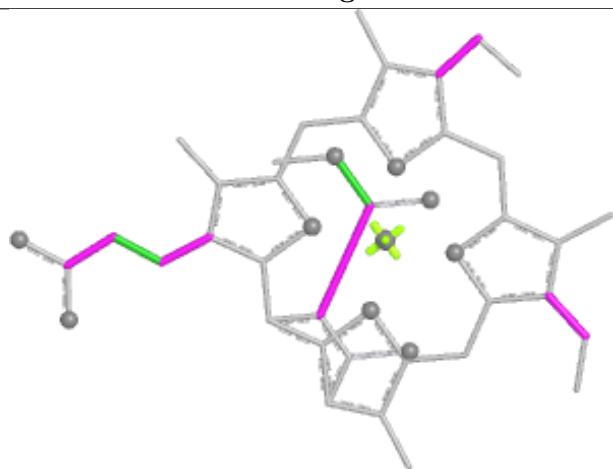
Ligand KC2 y 301



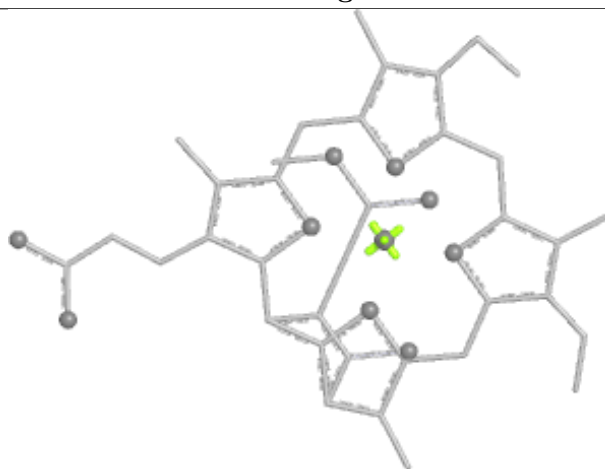
Bond lengths



Bond angles

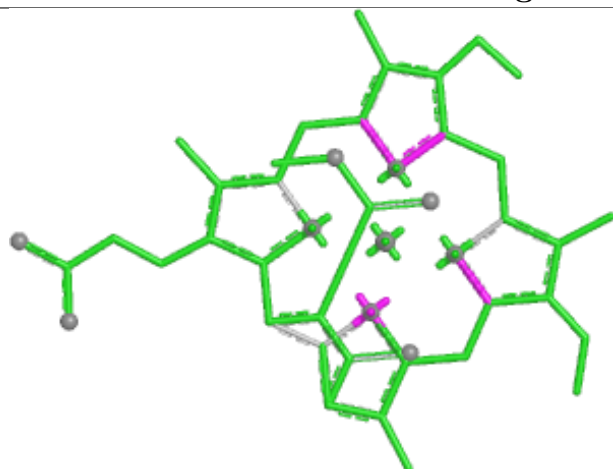


Torsions

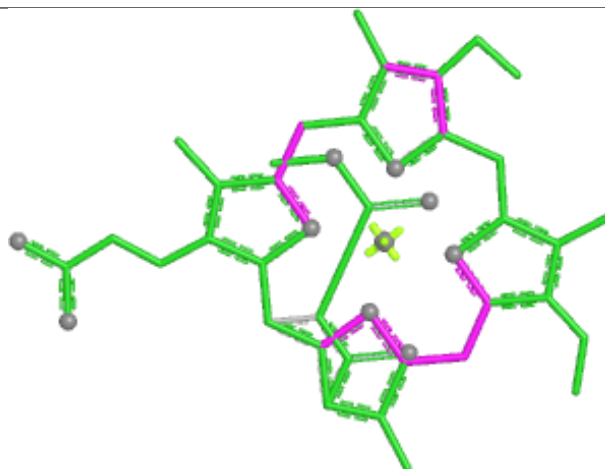


Rings

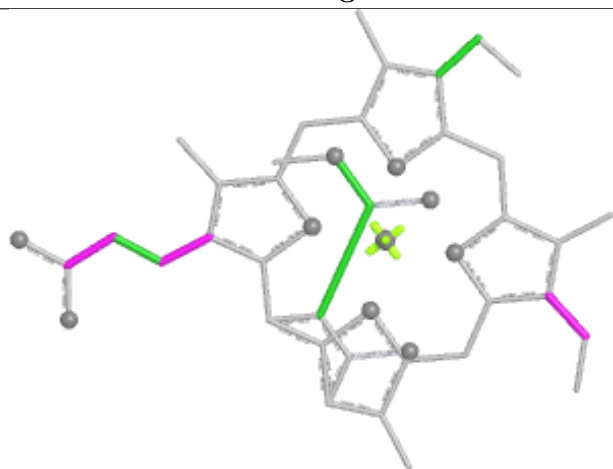
Ligand KC2 Y 302



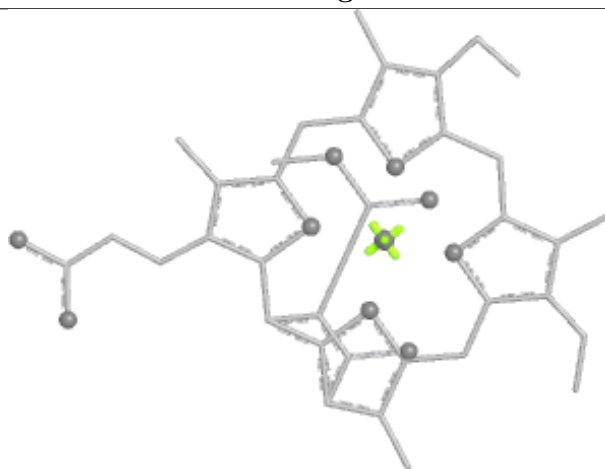
Bond lengths



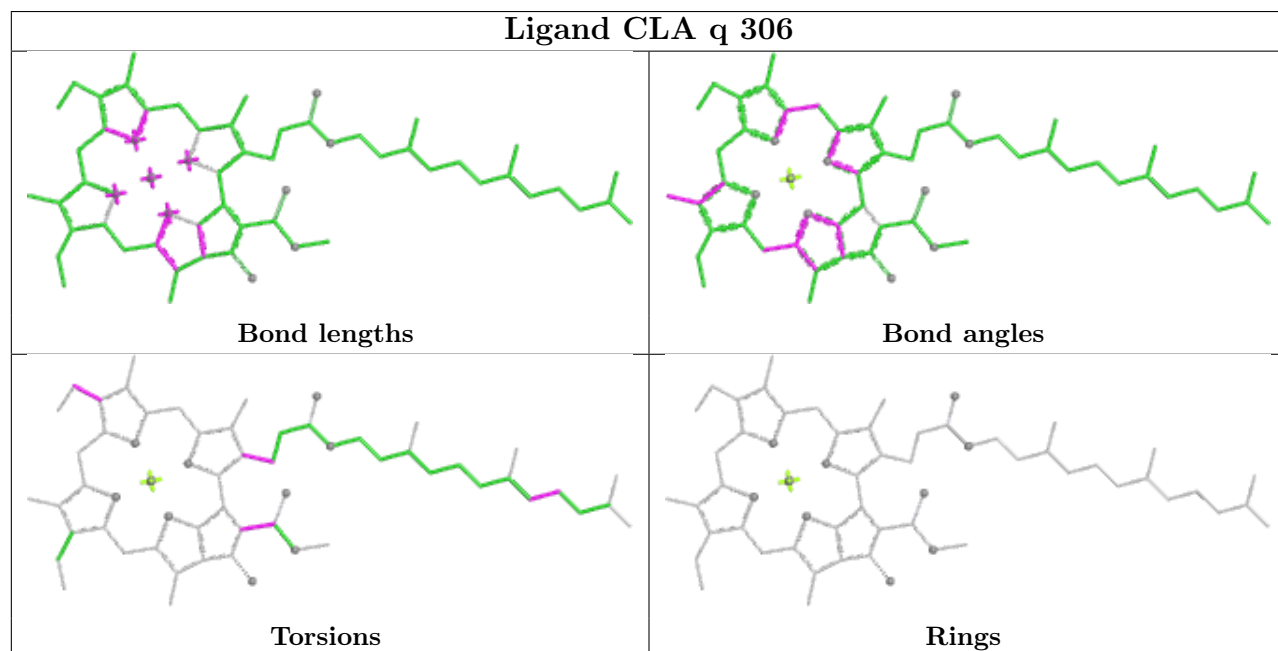
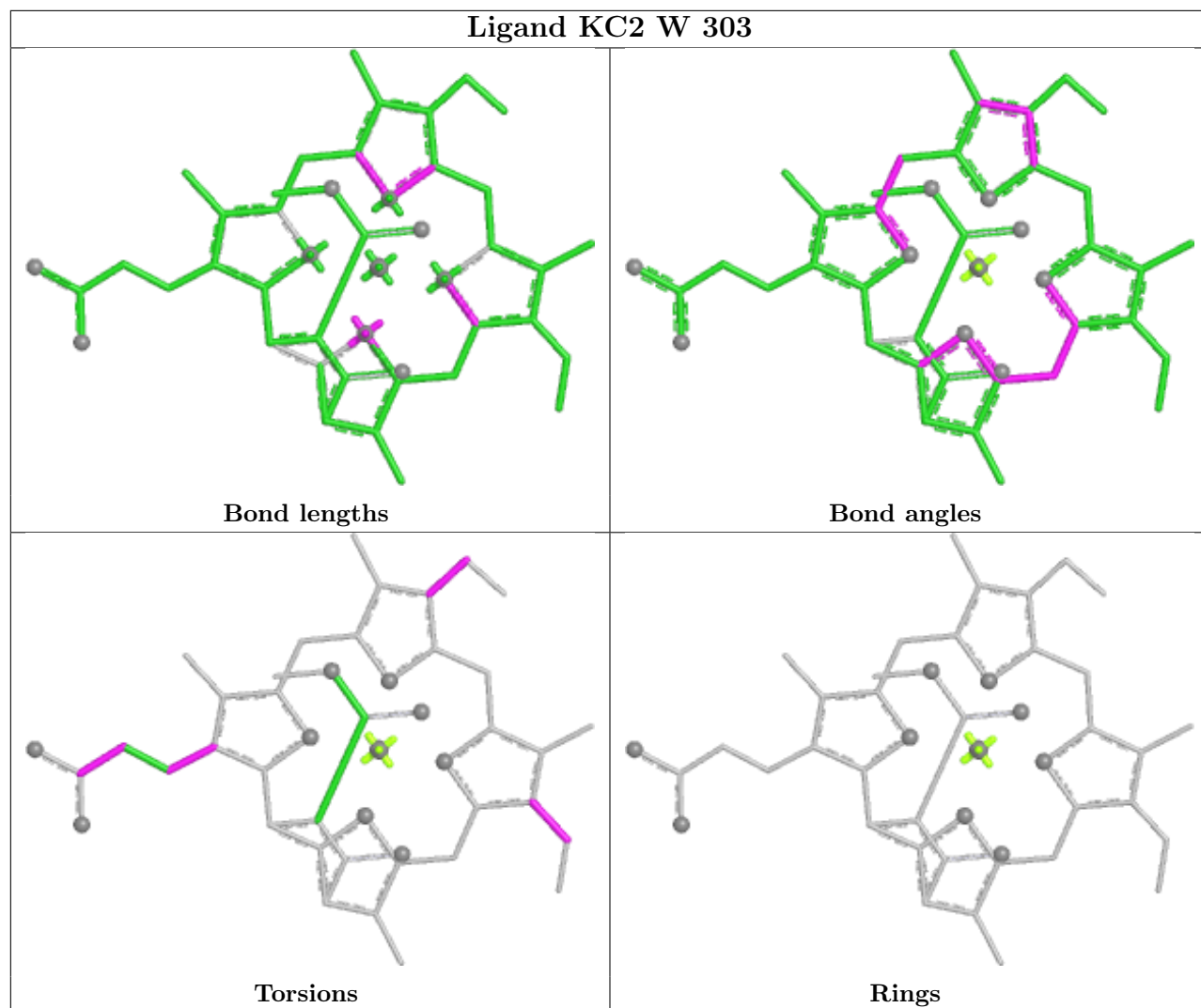
Bond angles

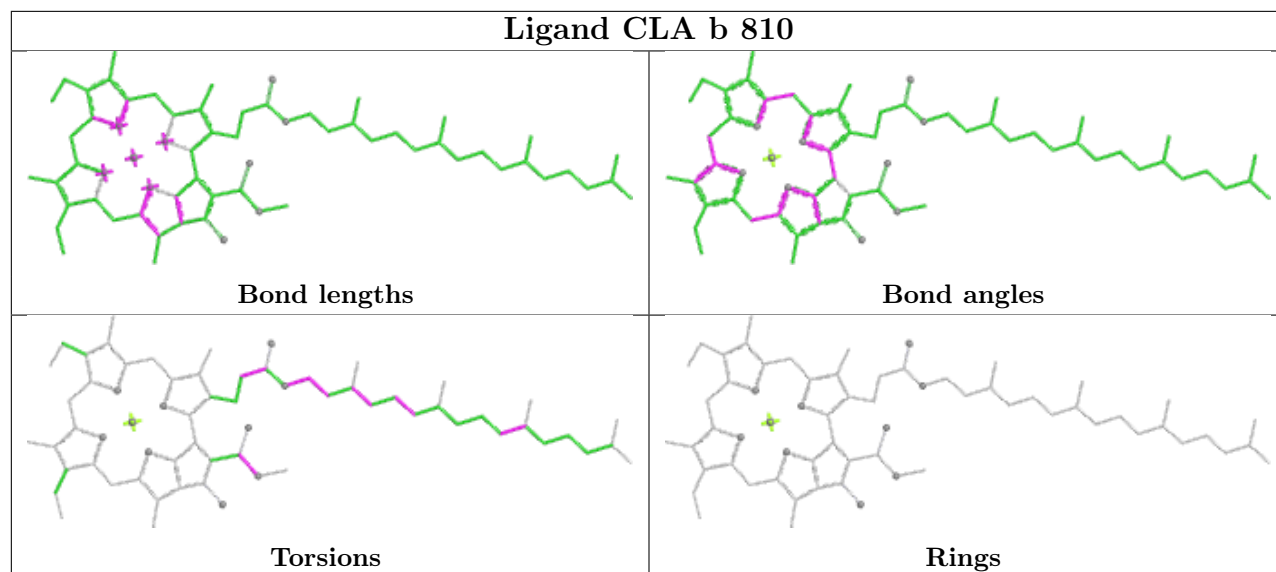
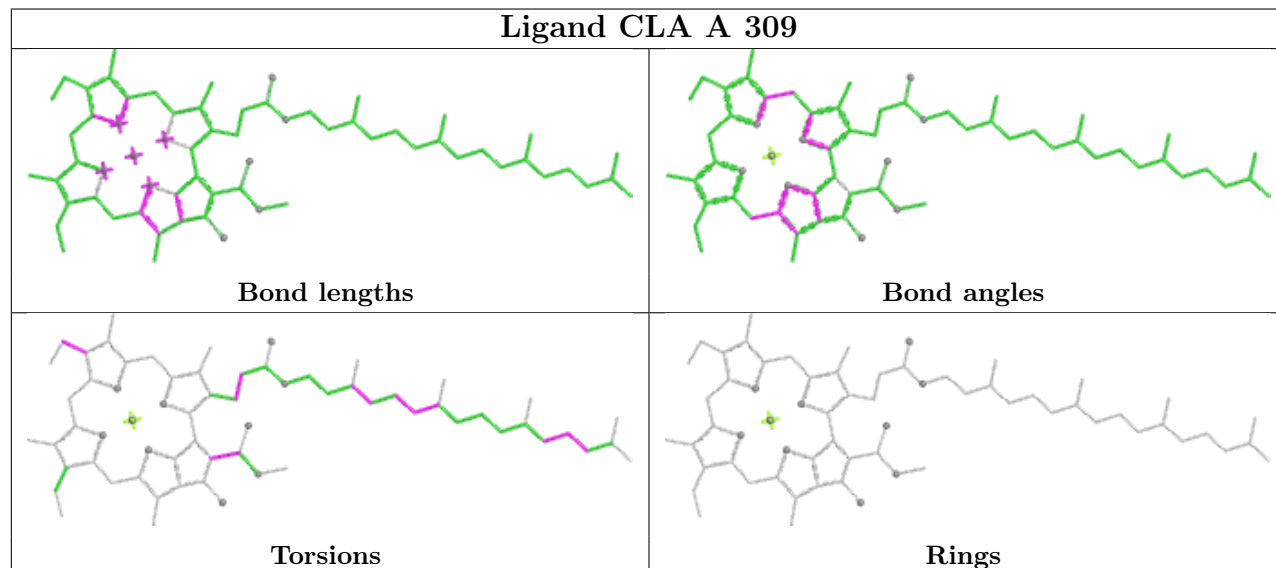


Torsions

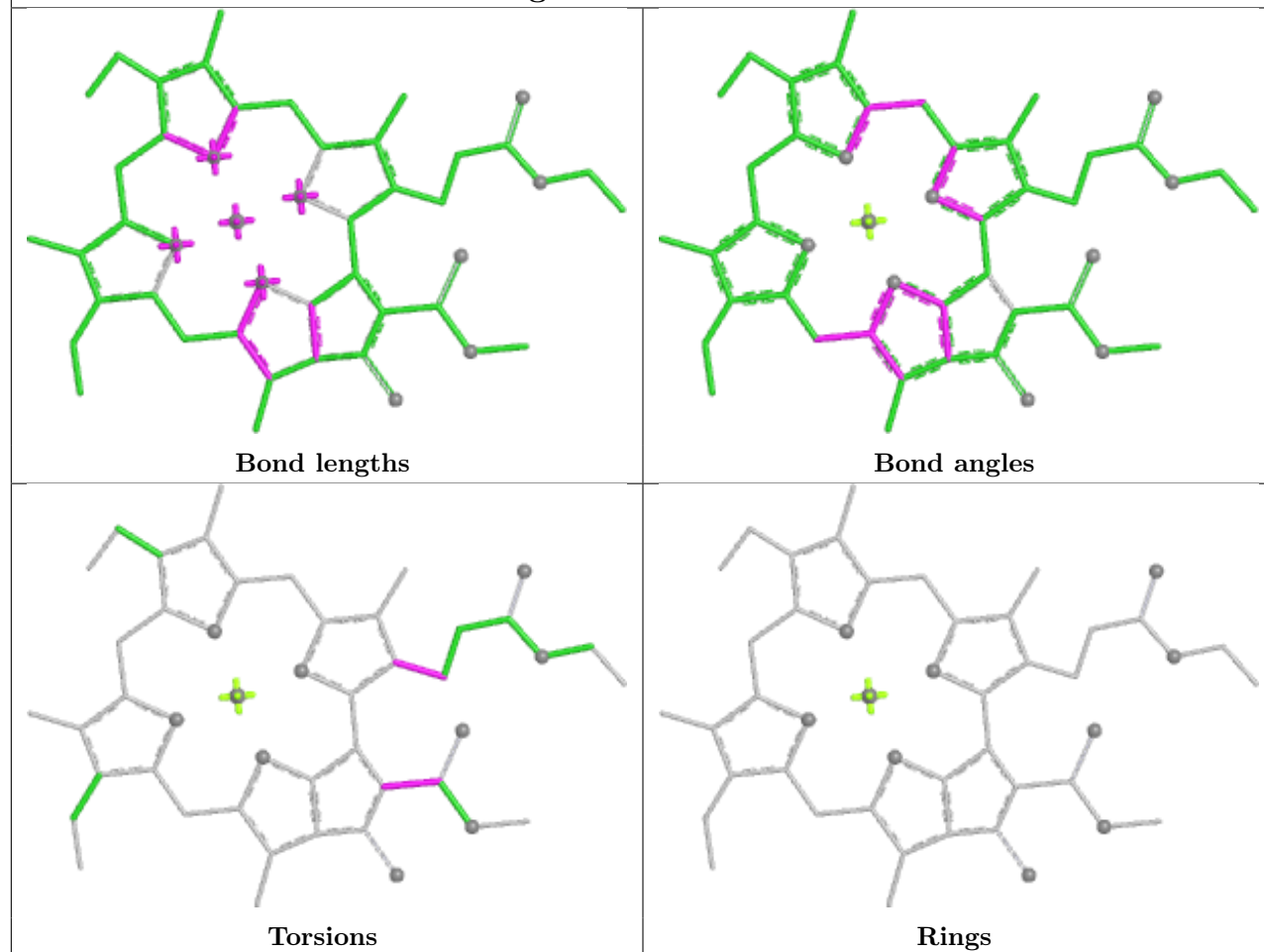


Rings

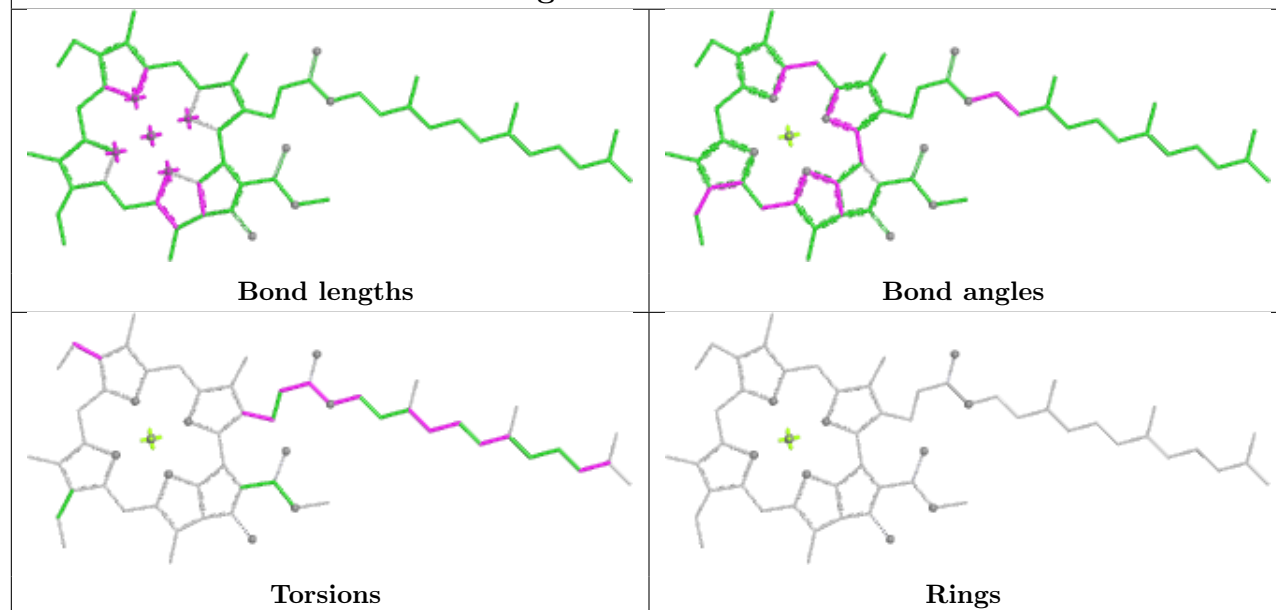


Ligand CLA b 810**Ligand CLA A 309**

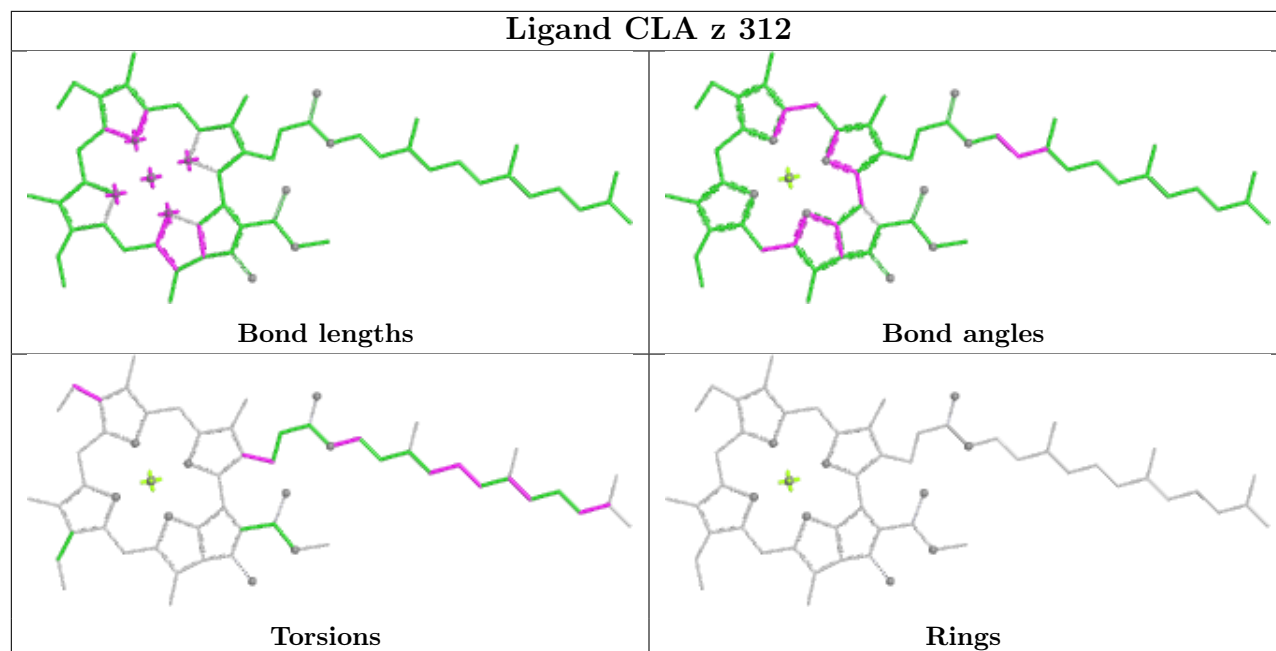
Ligand CLA F 311



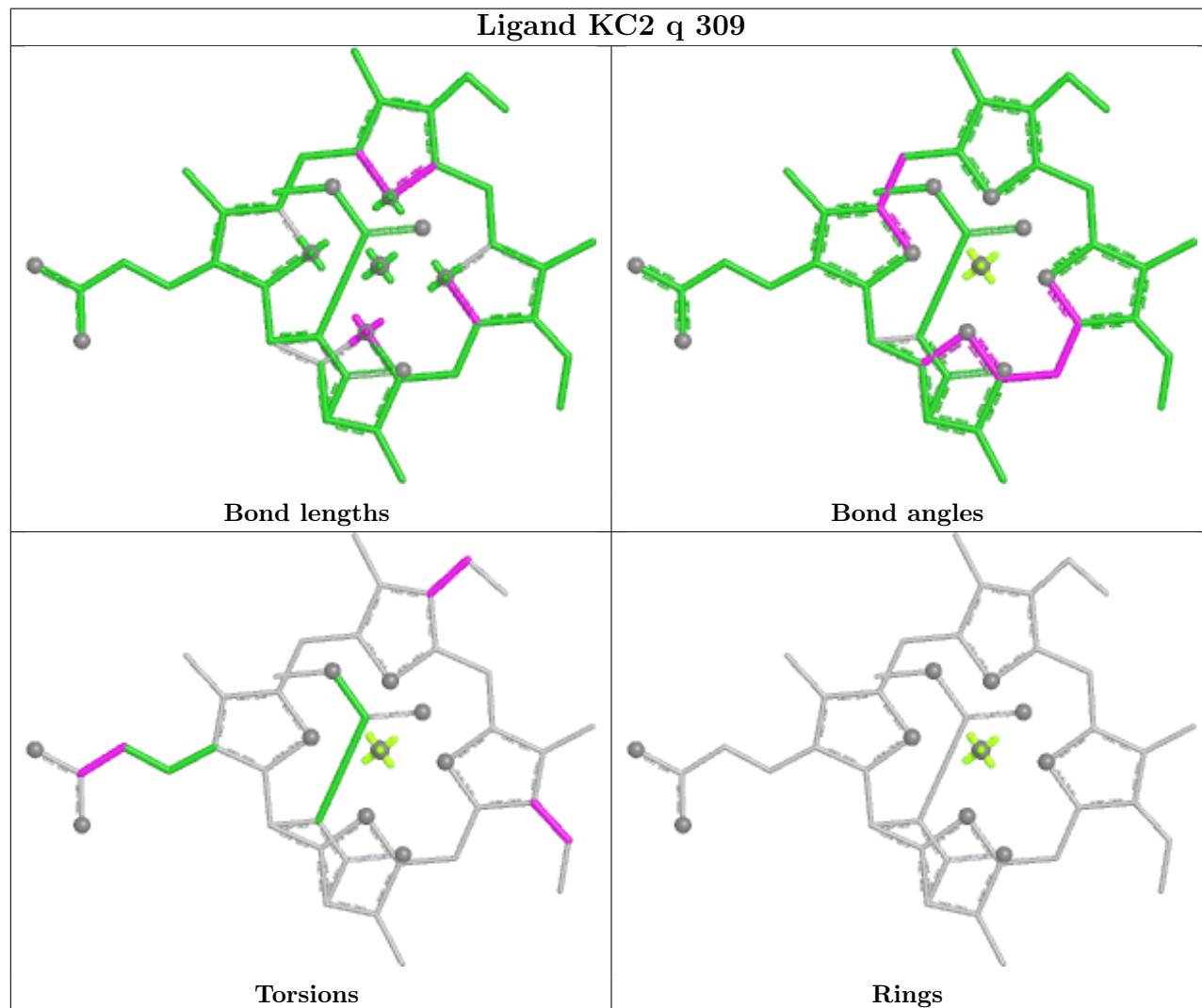
Ligand CLA z 305



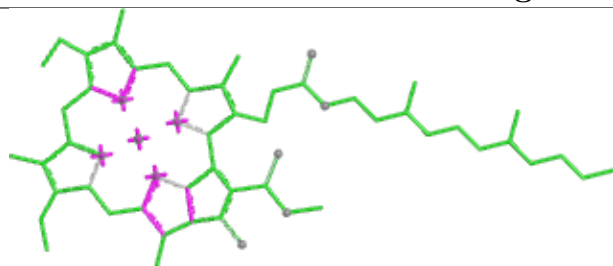
Ligand CLA z 312



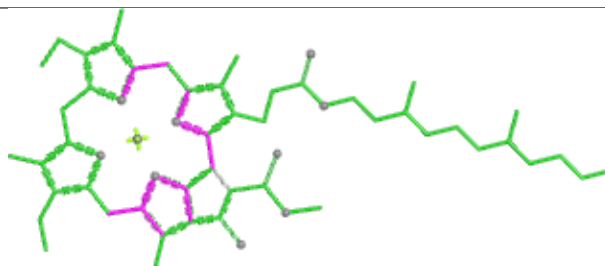
Ligand KC2 q 309



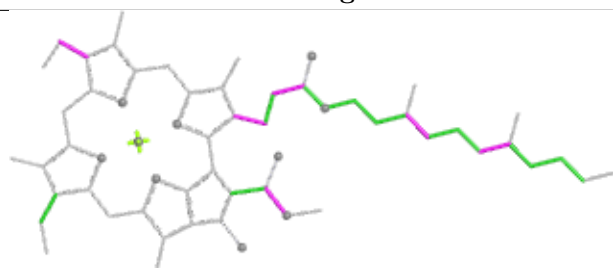
Ligand CLA T 310



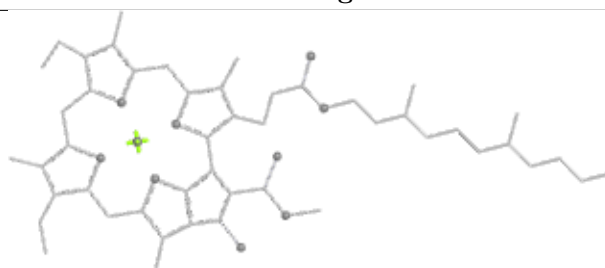
Bond lengths



Bond angles

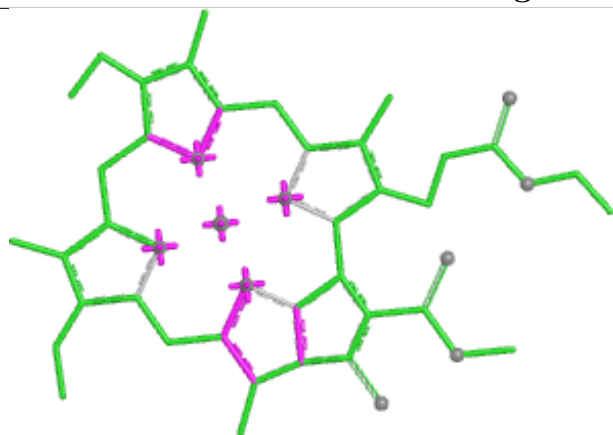


Torsions

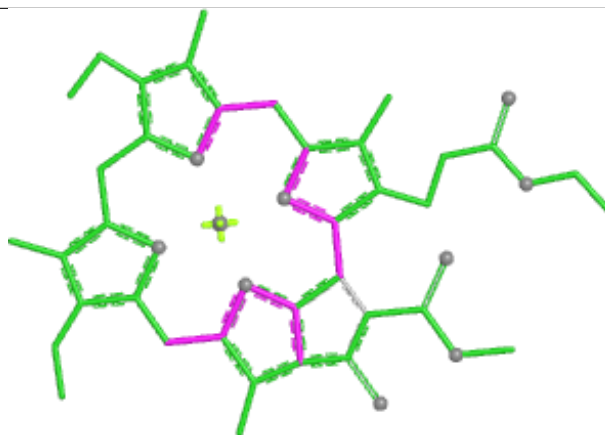


Rings

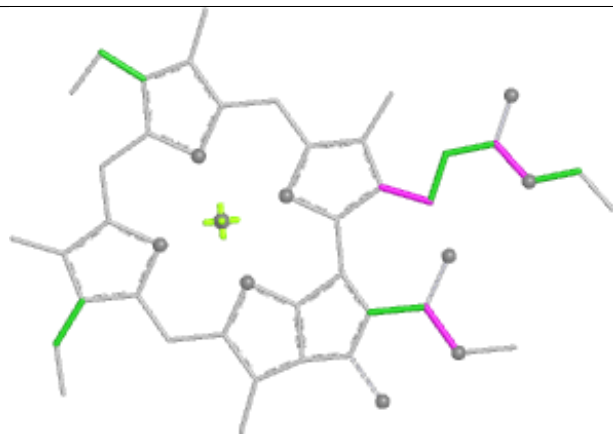
Ligand CLA A 311



Bond lengths



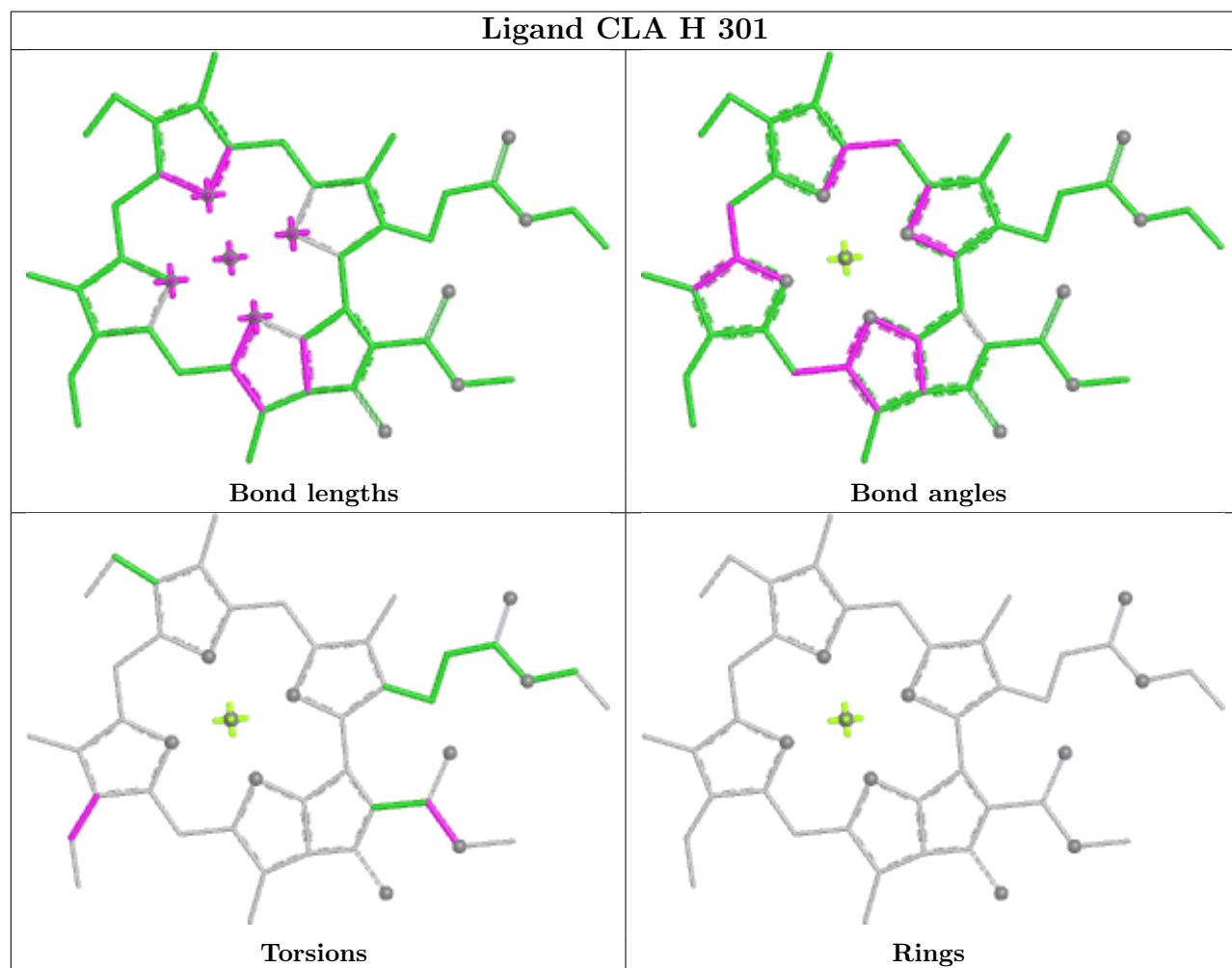
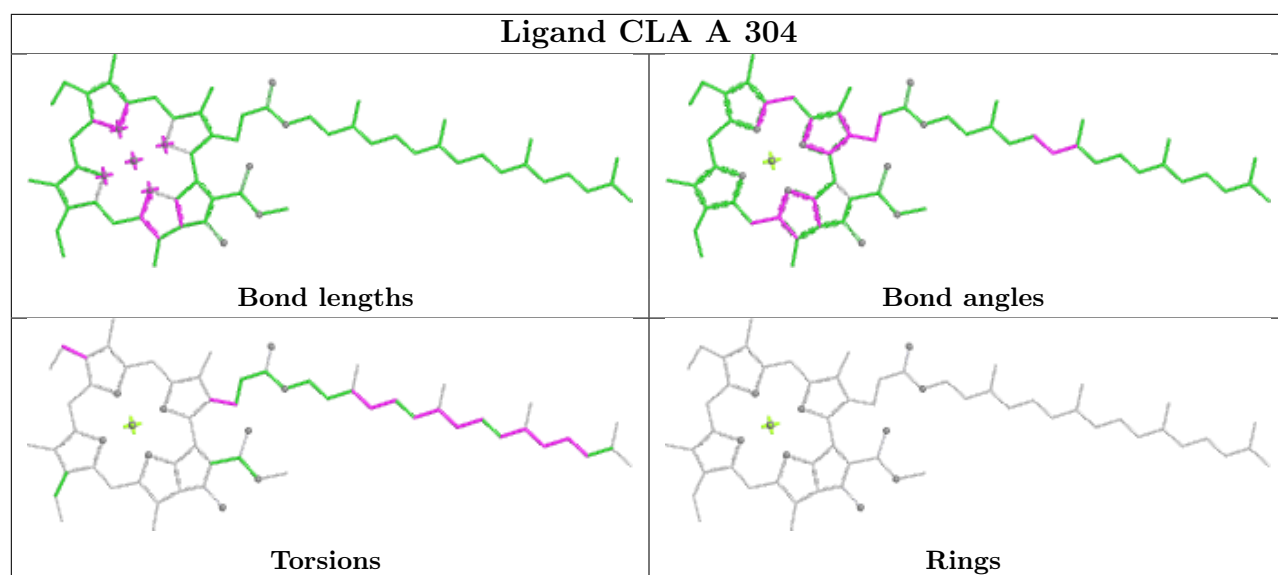
Bond angles



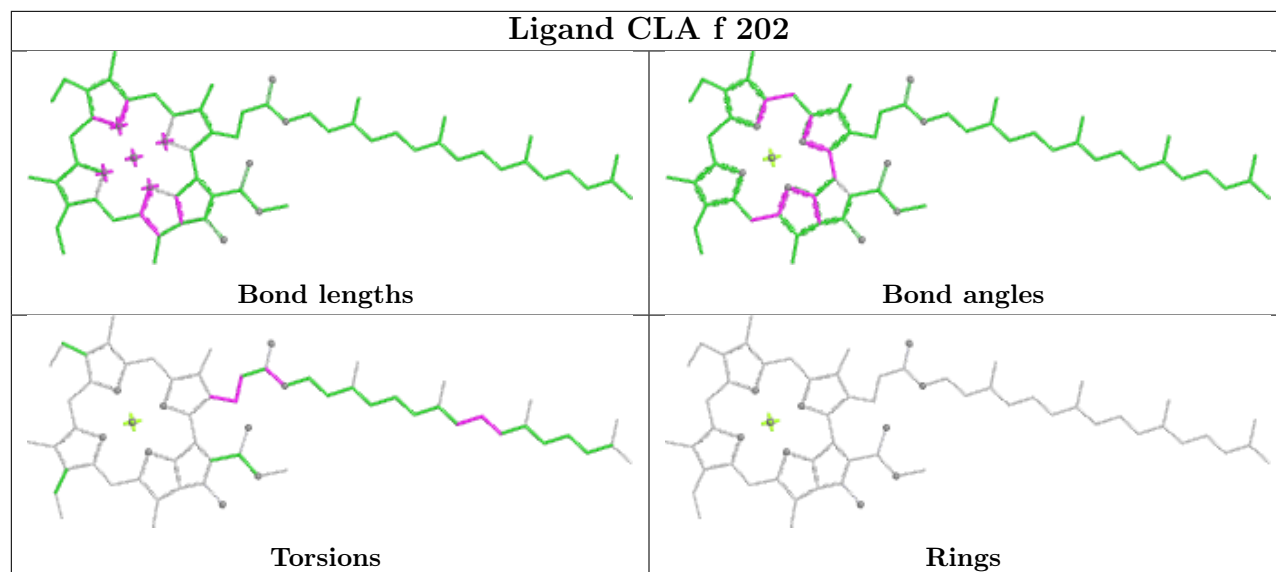
Torsions



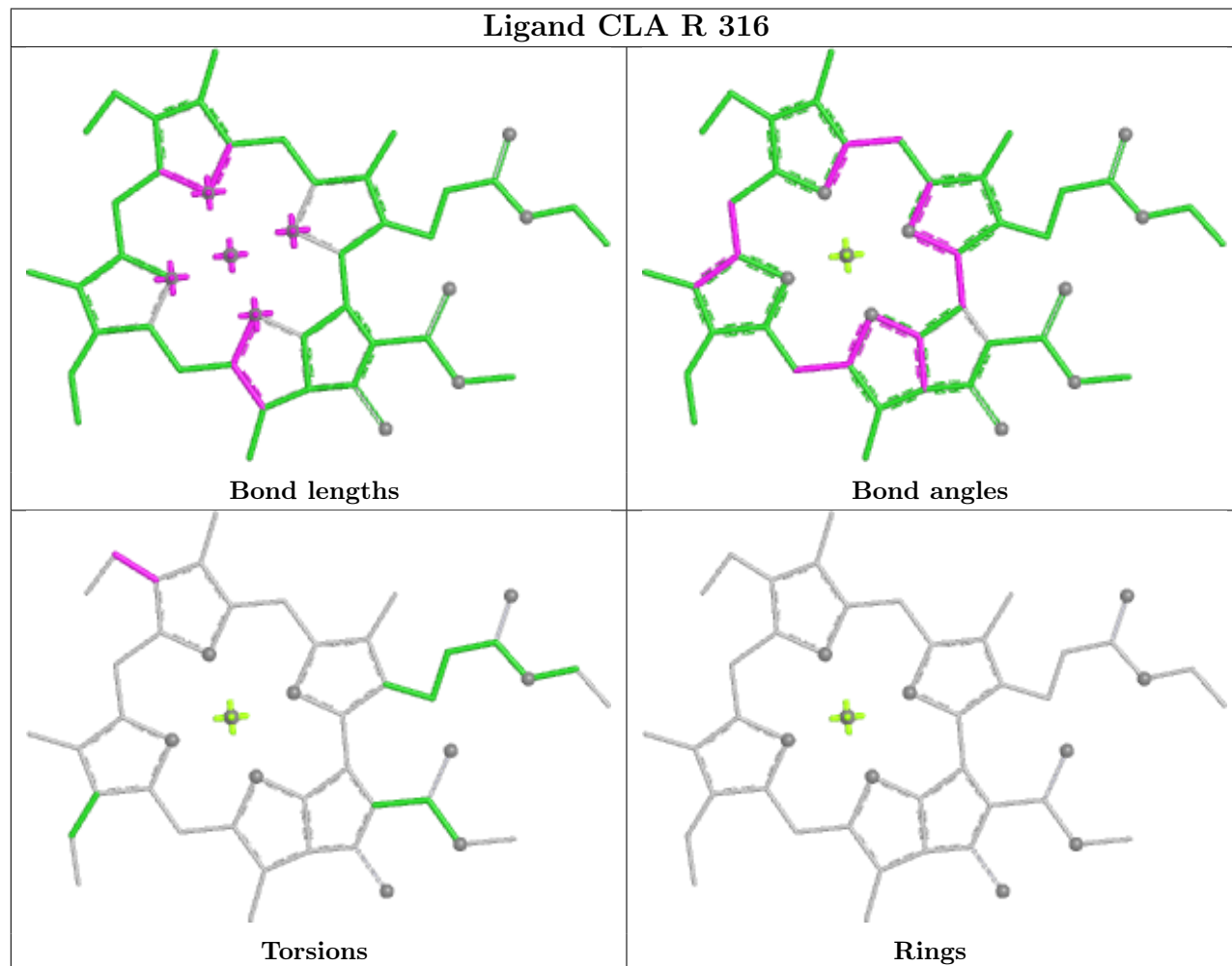
Rings



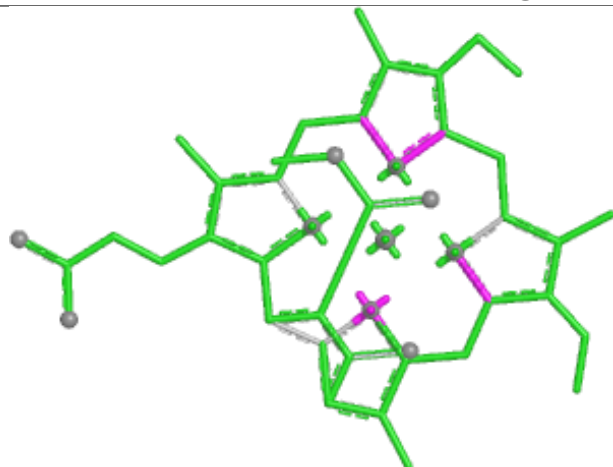
Ligand CLA f 202



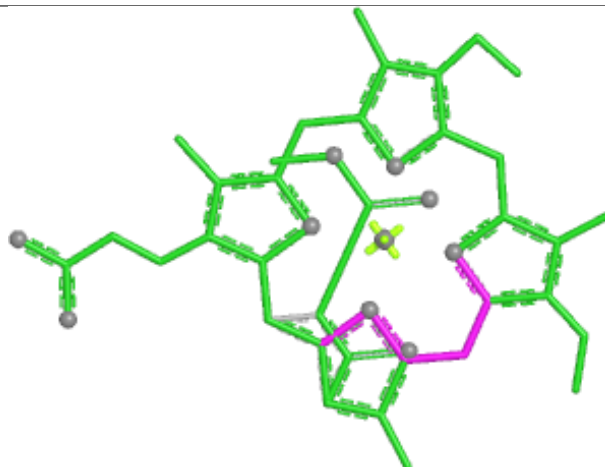
Ligand CLA R 316



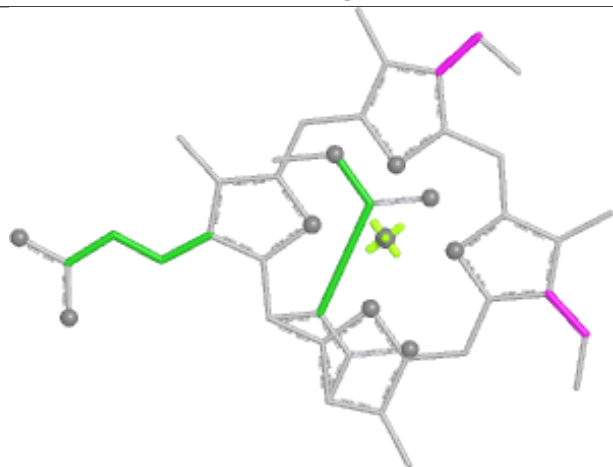
Ligand KC2 T 309



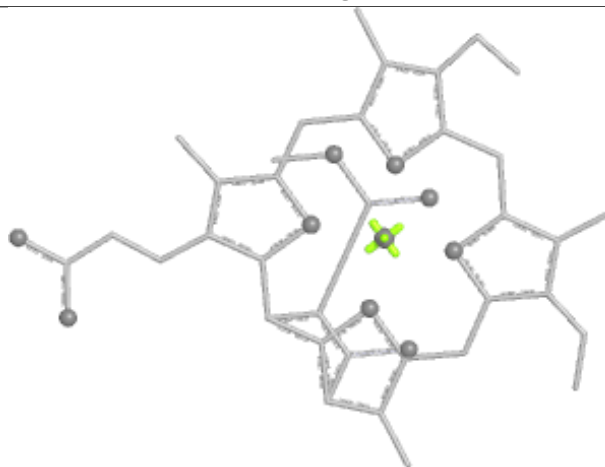
Bond lengths



Bond angles

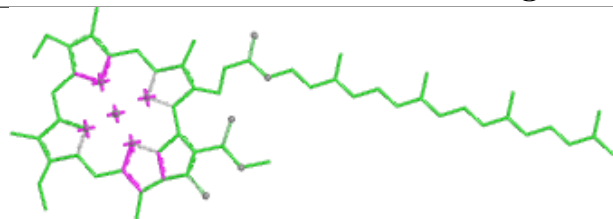


Torsions

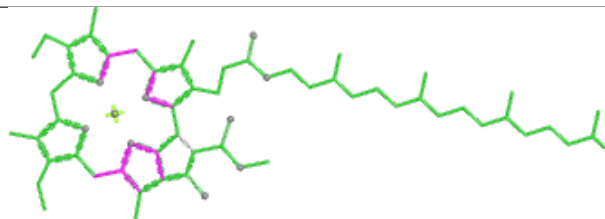


Rings

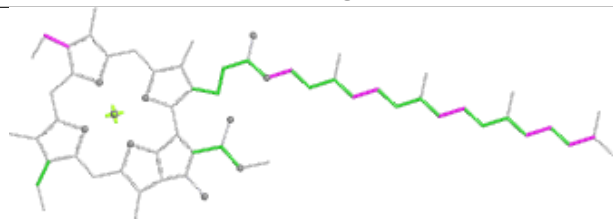
Ligand CLA I 201



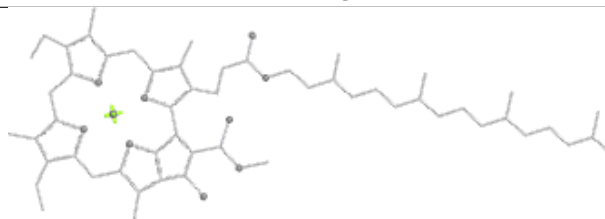
Bond lengths



Bond angles

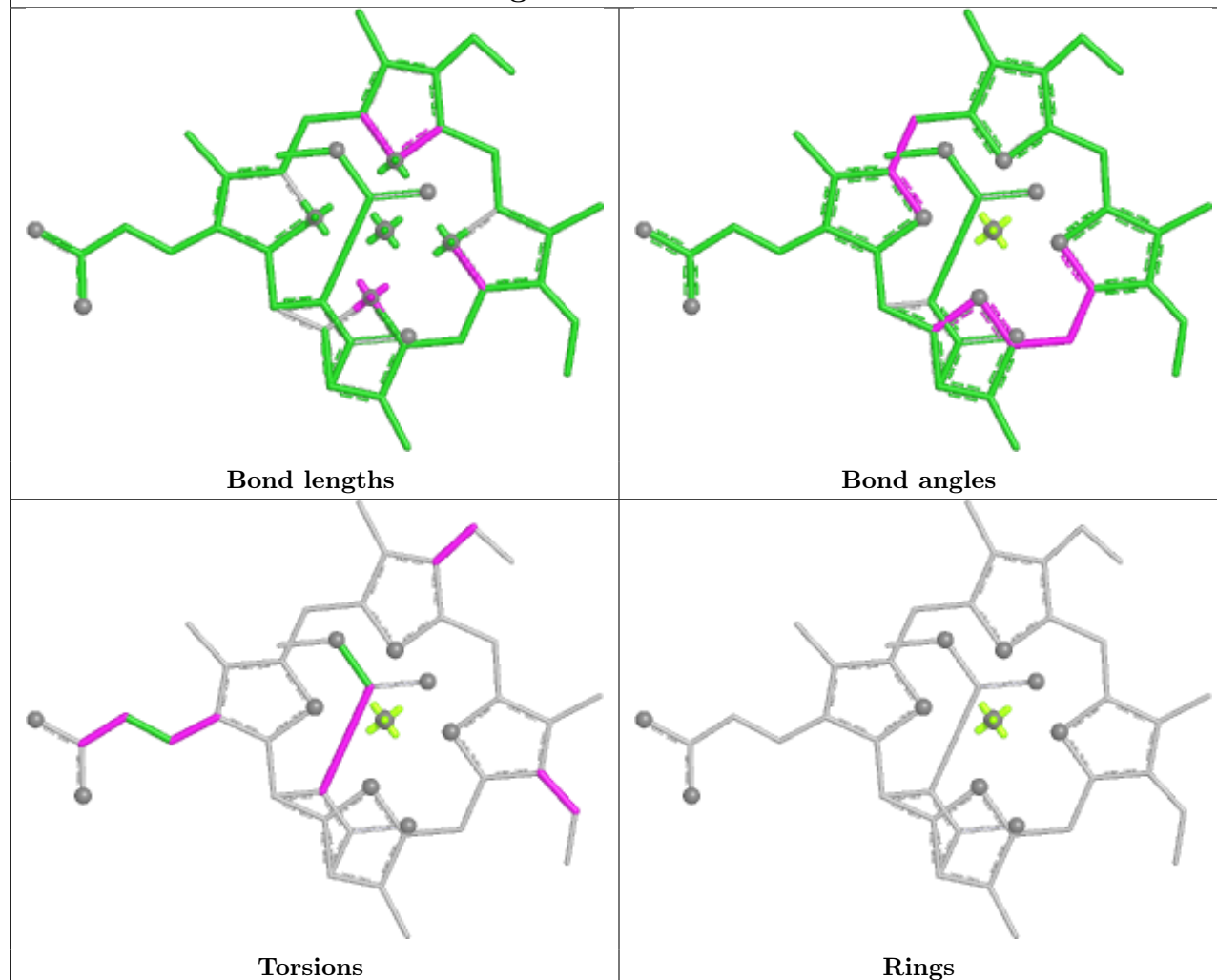


Torsions

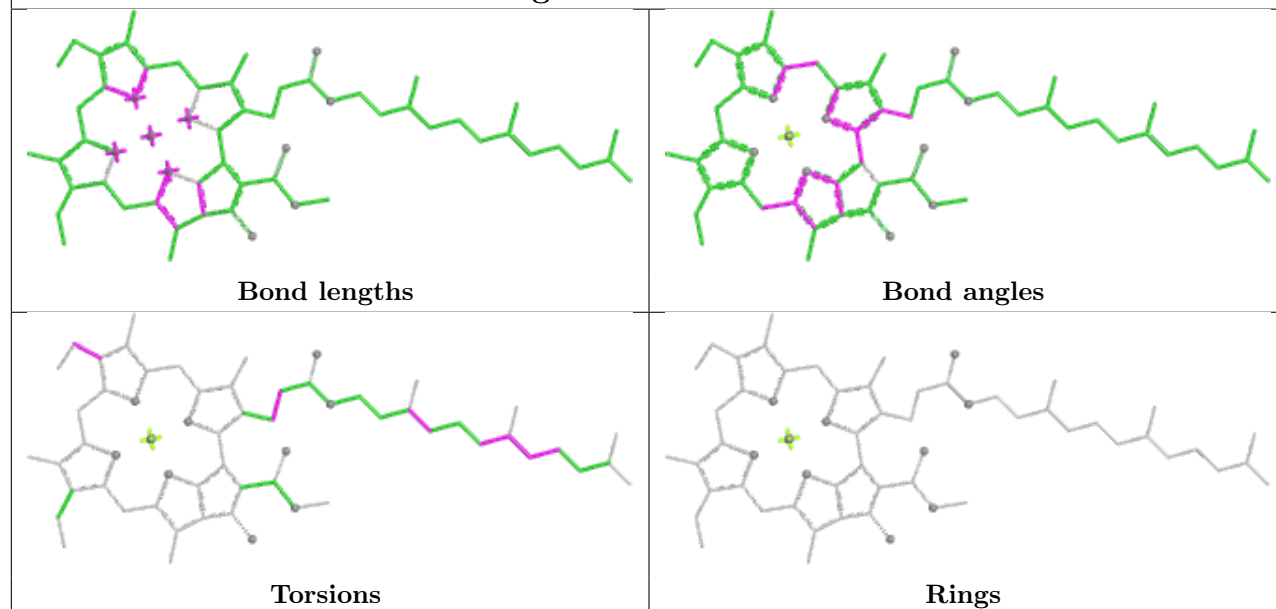


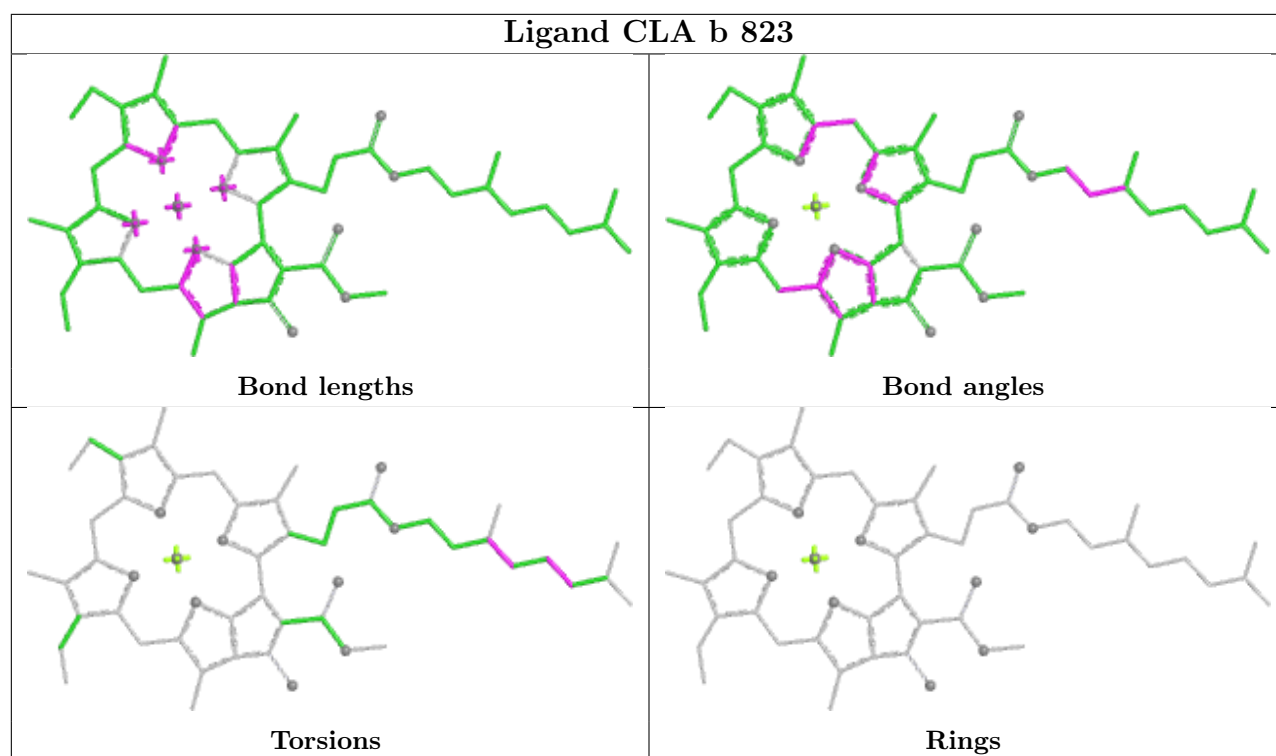
Rings

Ligand KC2 T 311

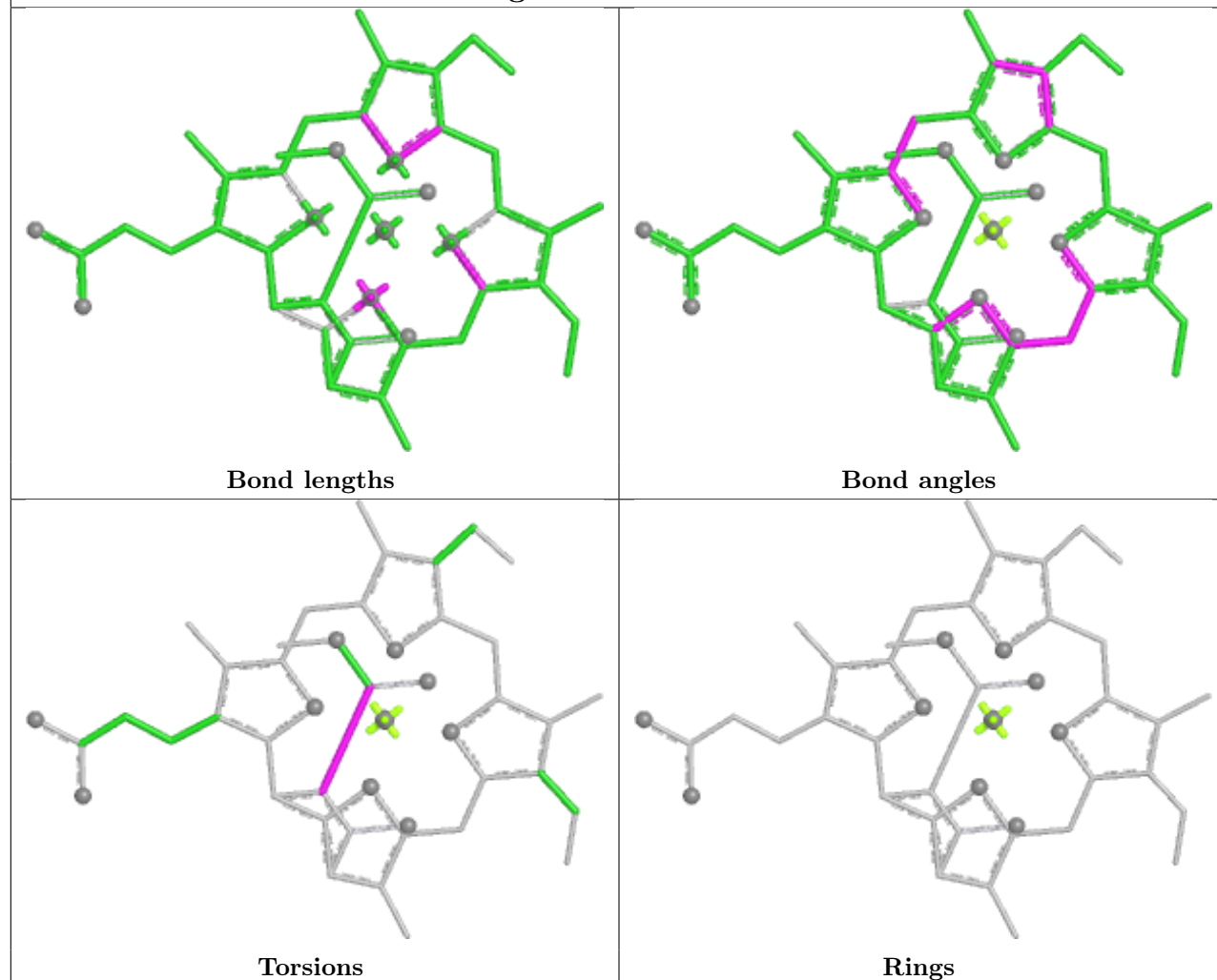


Ligand CLA C 307

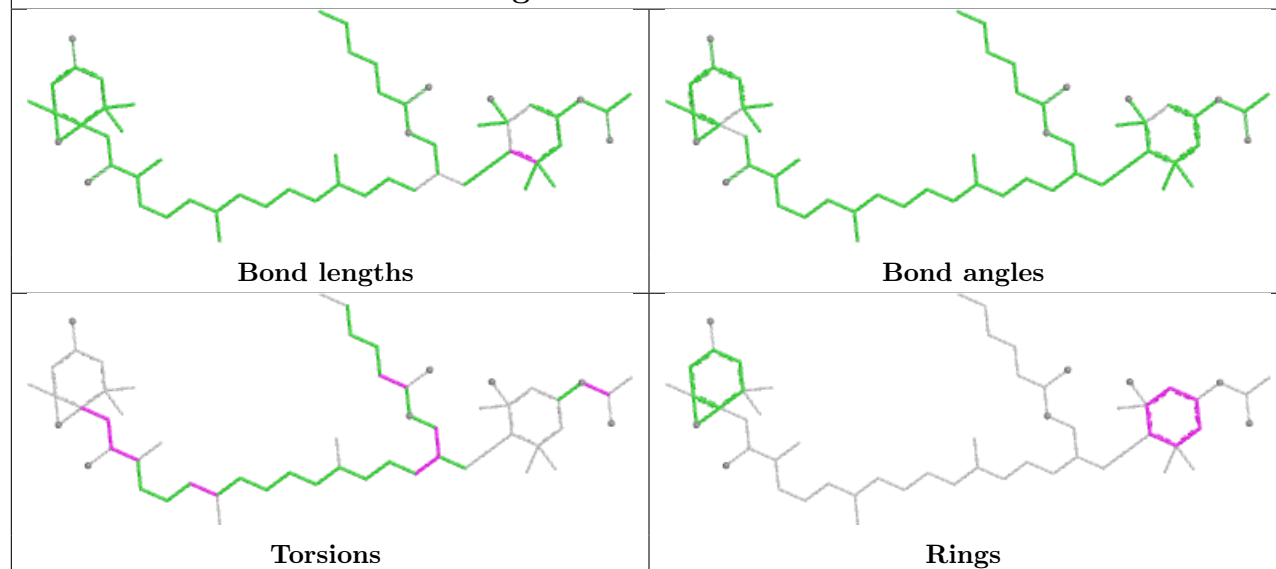


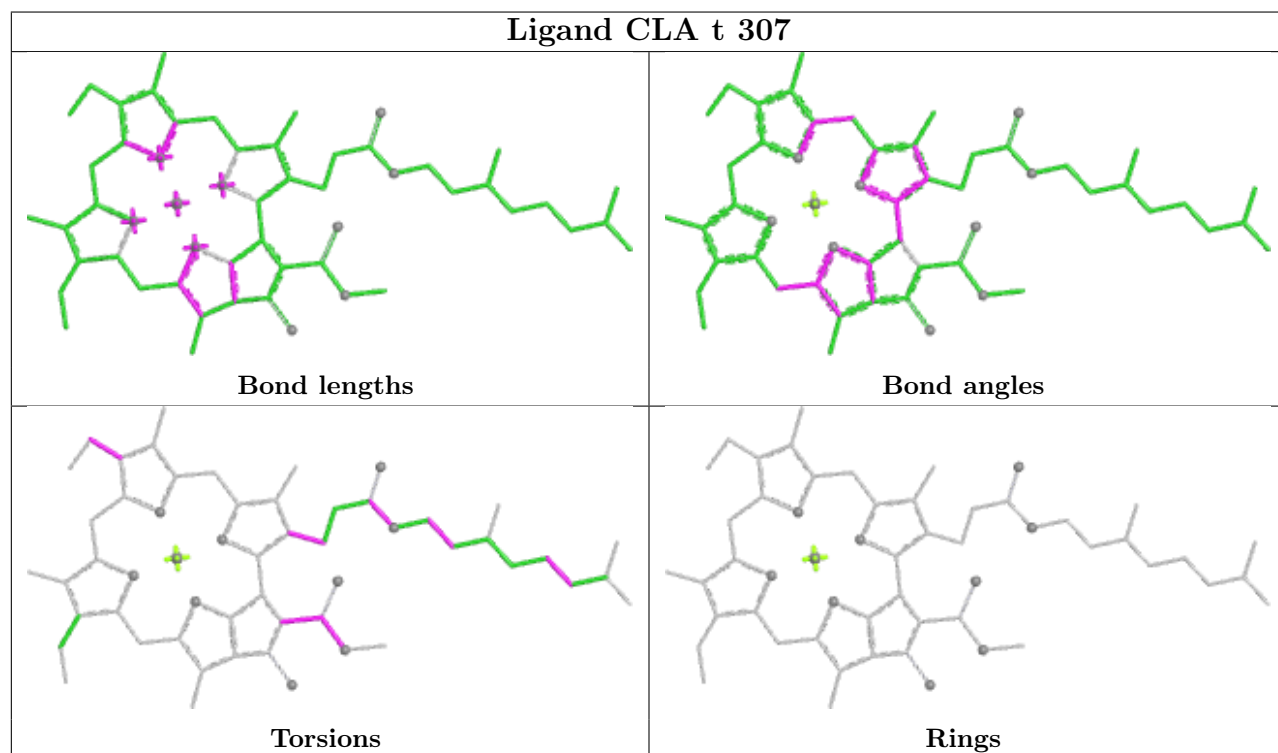
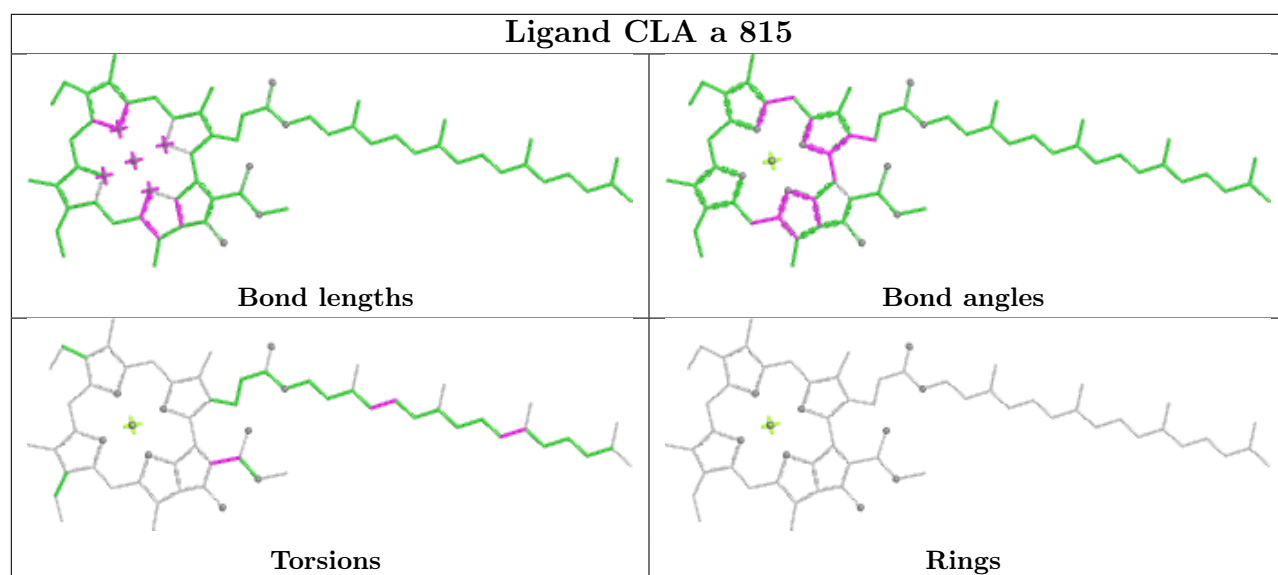


Ligand KC2 X 303

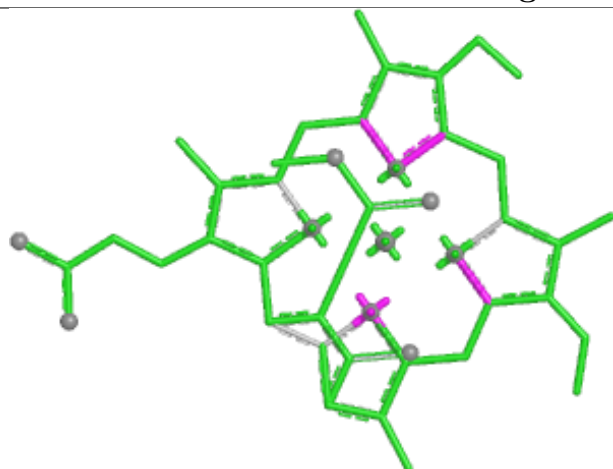


Ligand A1EB1 K 315

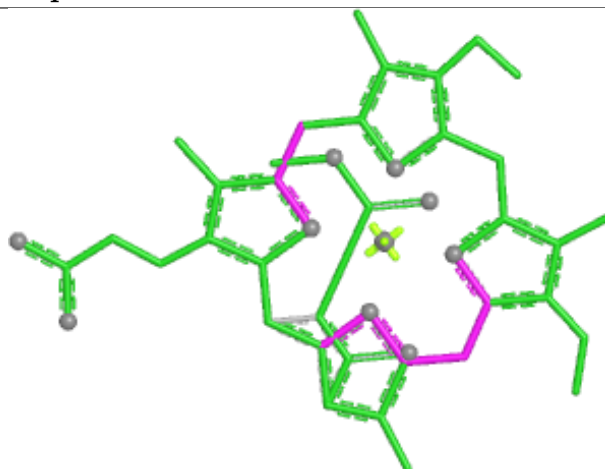




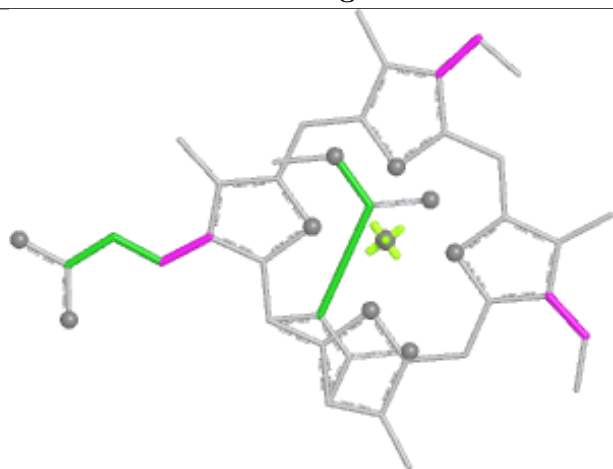
Ligand KC2 p 309



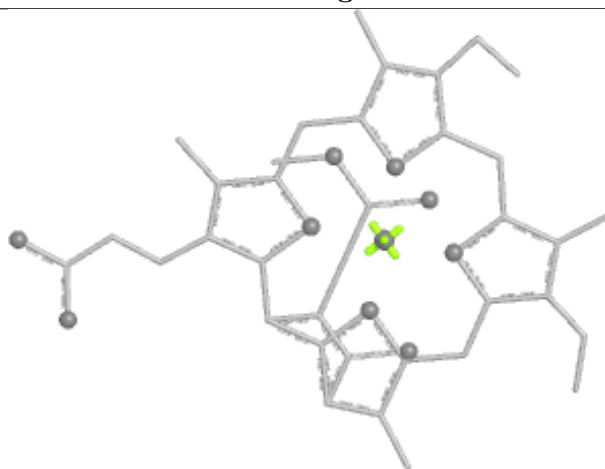
Bond lengths



Bond angles

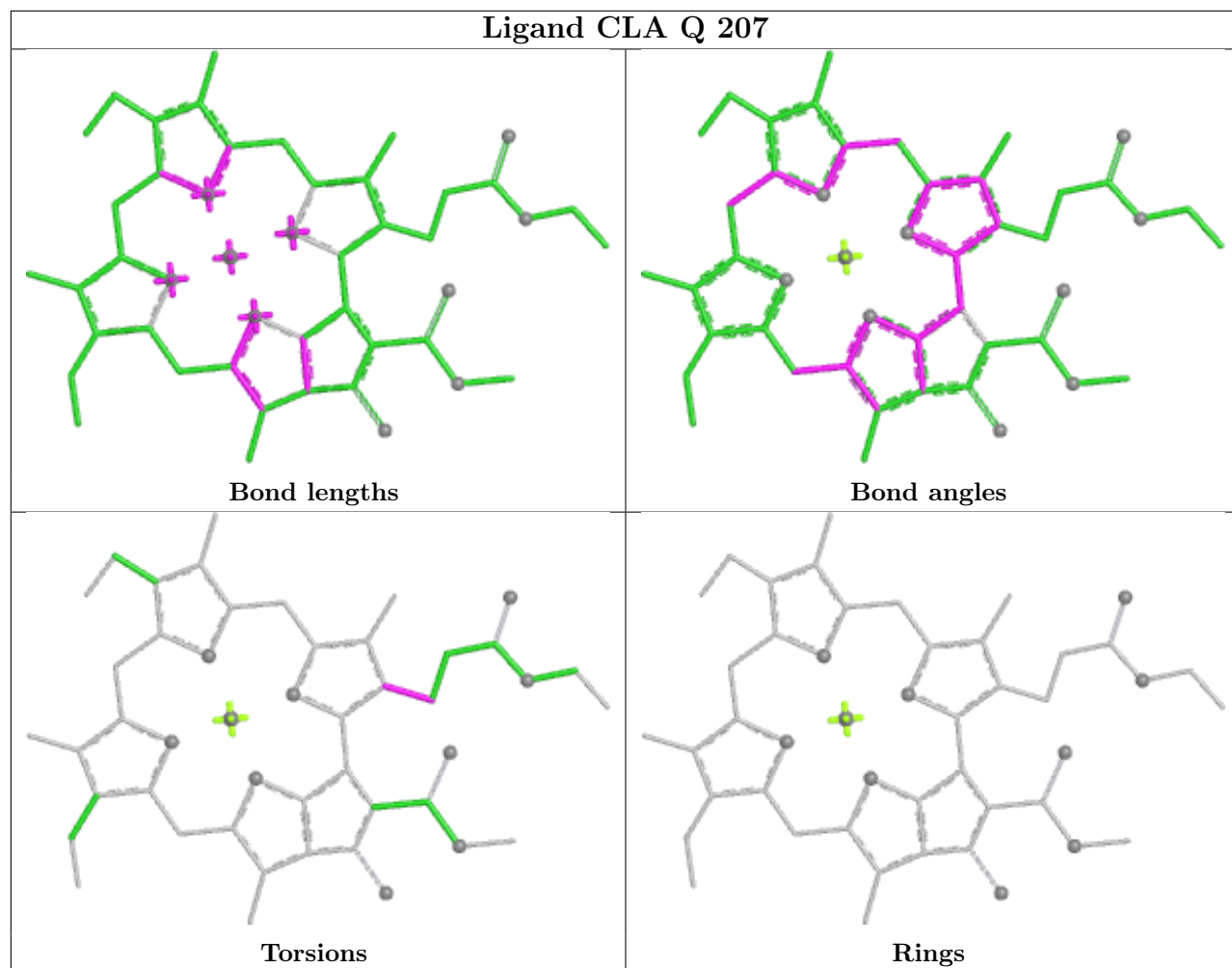


Torsions

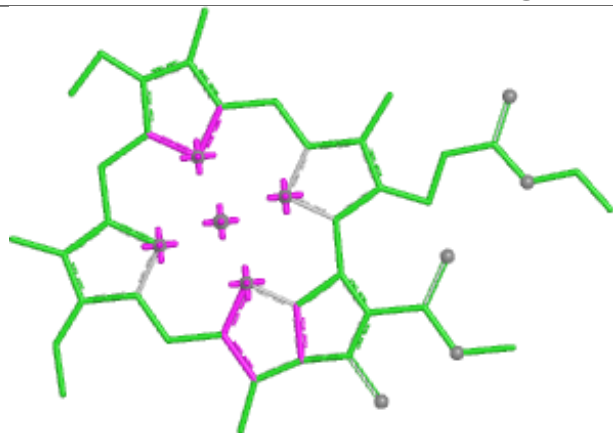


Rings

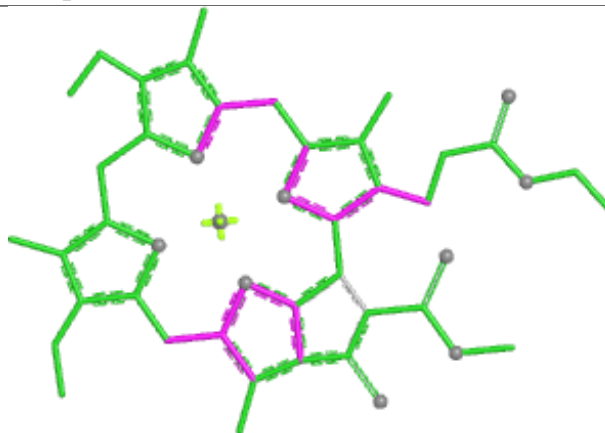
Ligand CLA Q 207



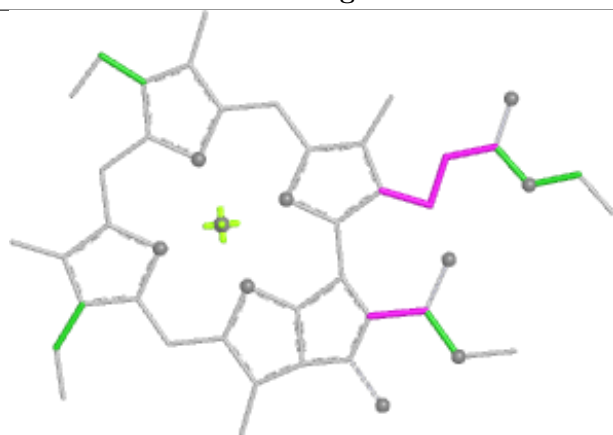
Ligand CLA q 313



Bond lengths



Bond angles

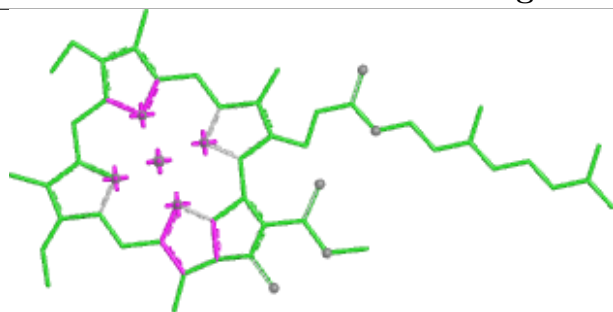


Torsions

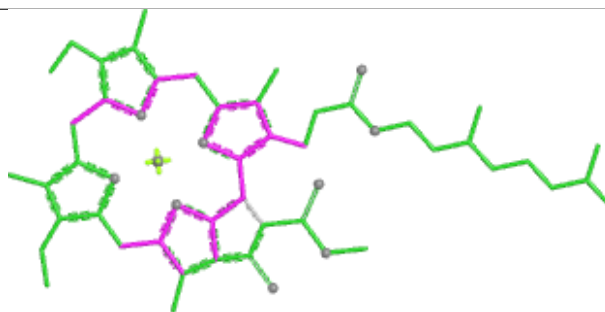


Rings

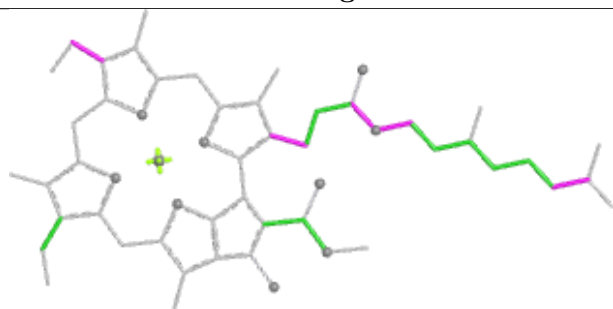
Ligand CLA Z 310



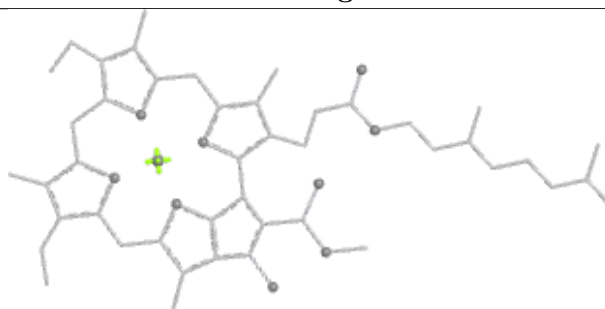
Bond lengths



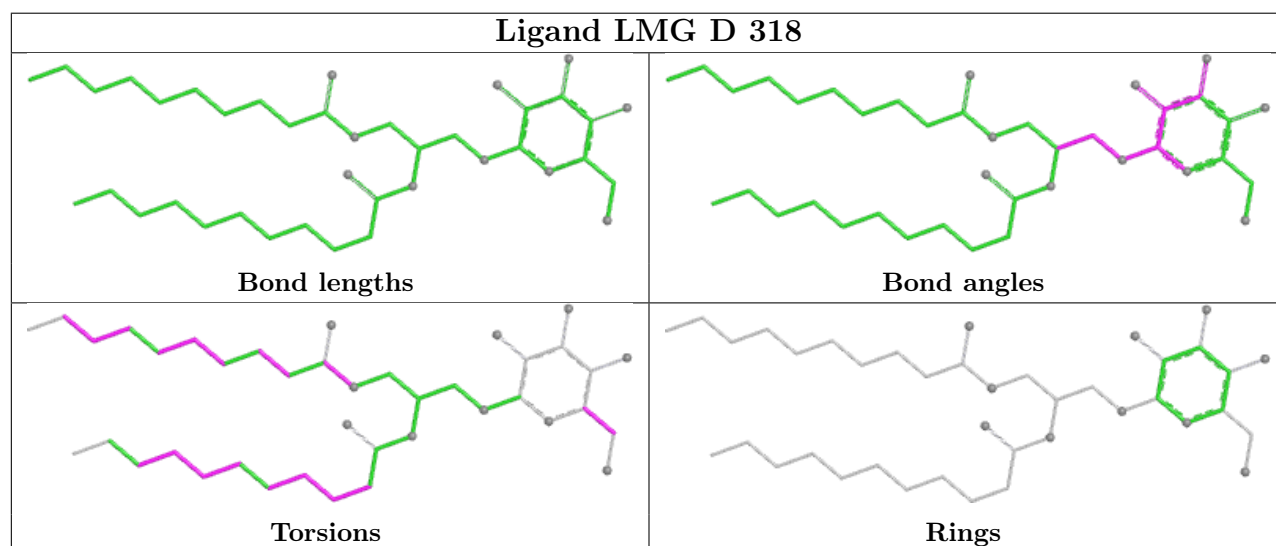
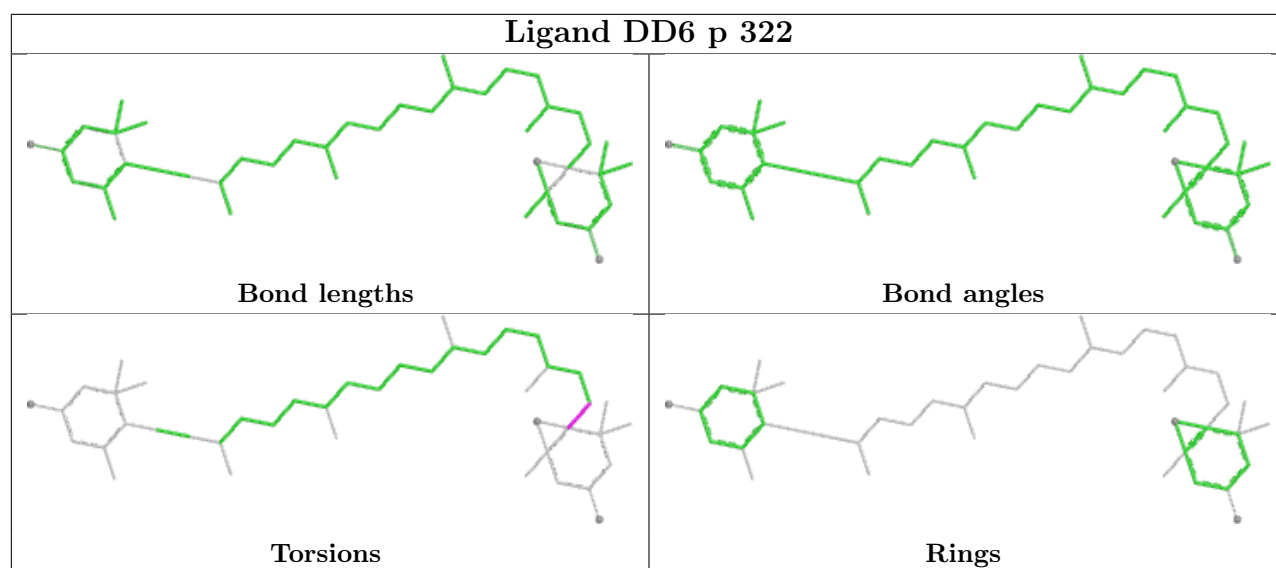
Bond angles



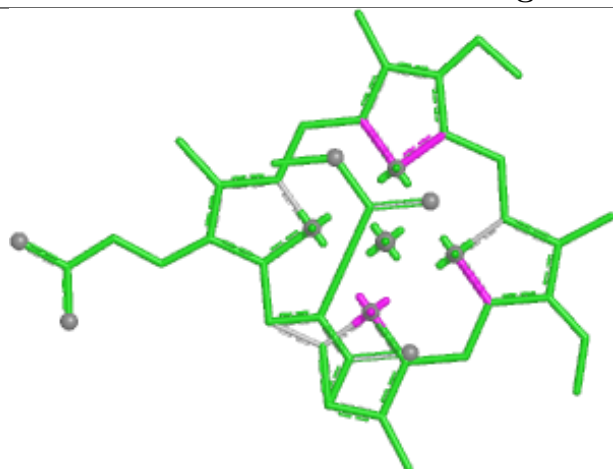
Torsions



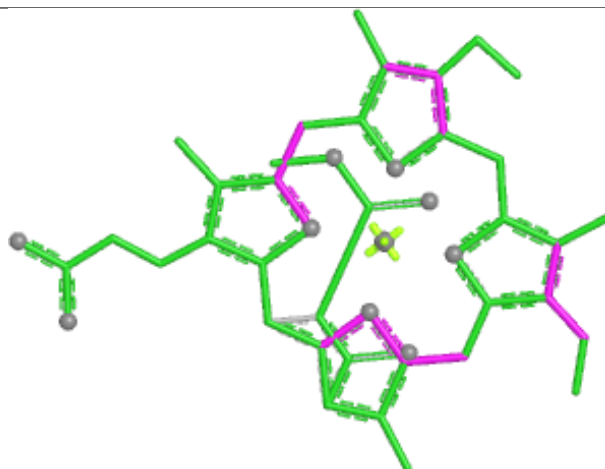
Rings



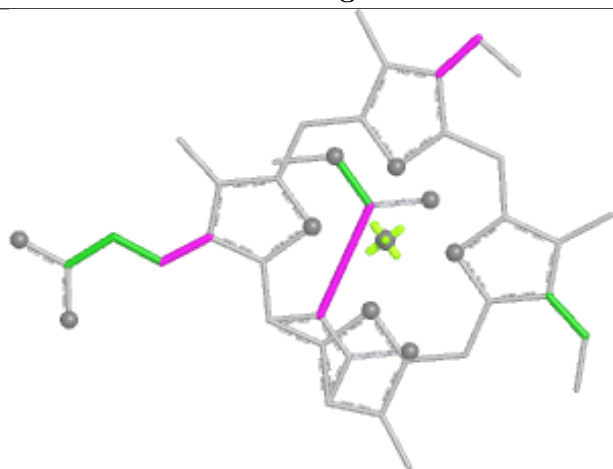
Ligand KC2 P 304



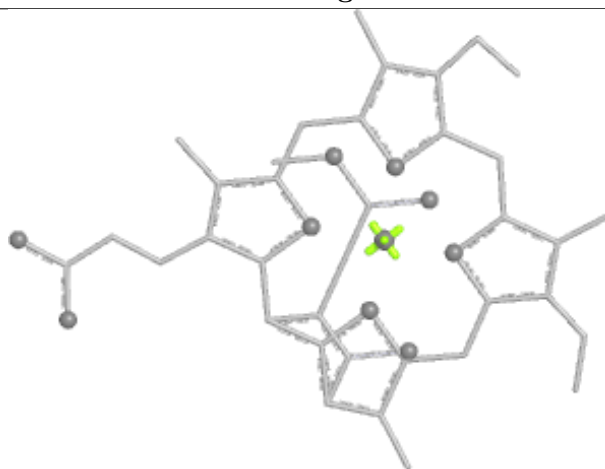
Bond lengths



Bond angles

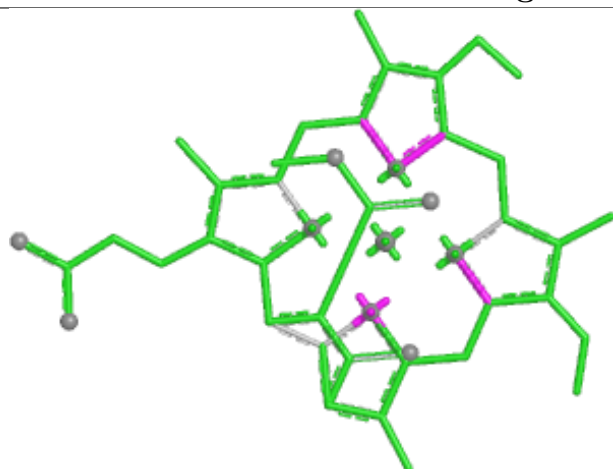


Torsions

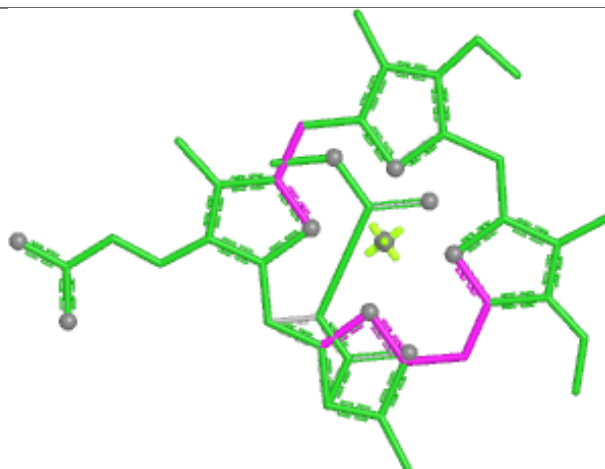


Rings

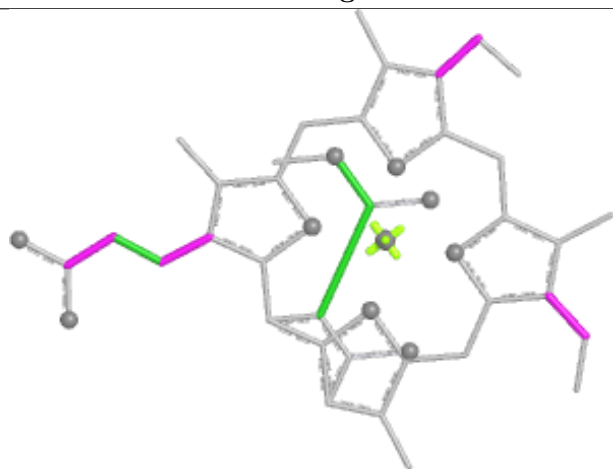
Ligand KC2 T 308



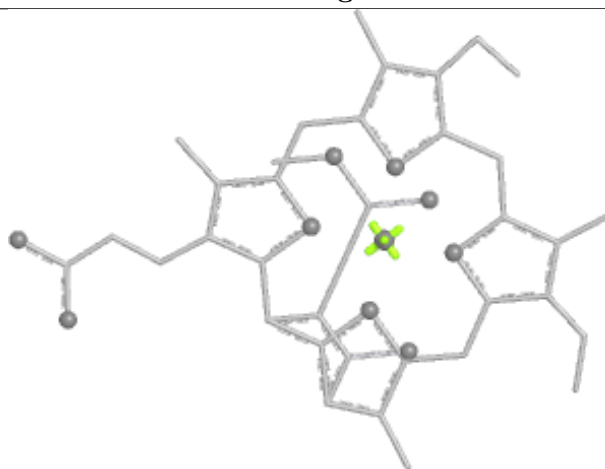
Bond lengths



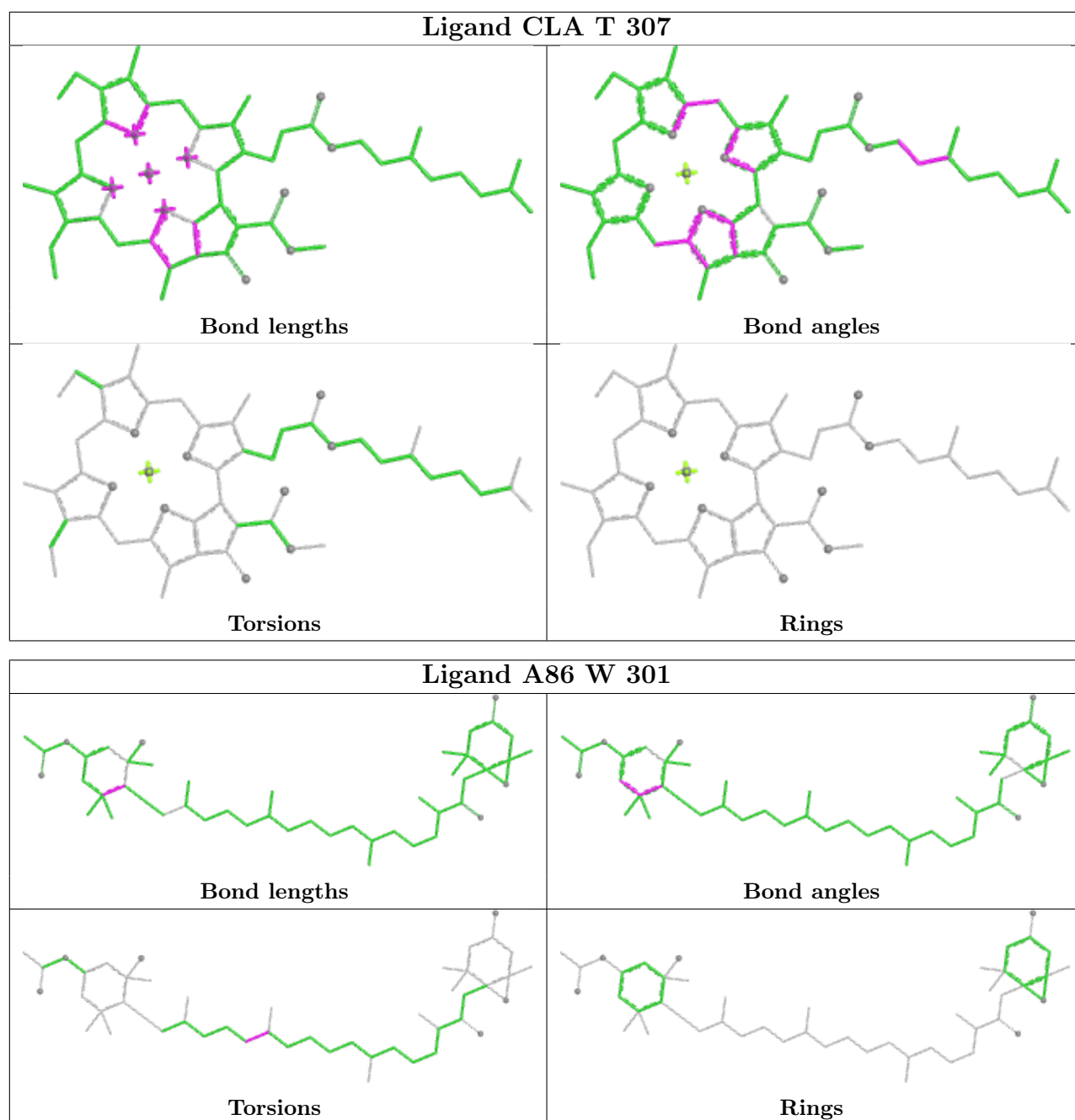
Bond angles

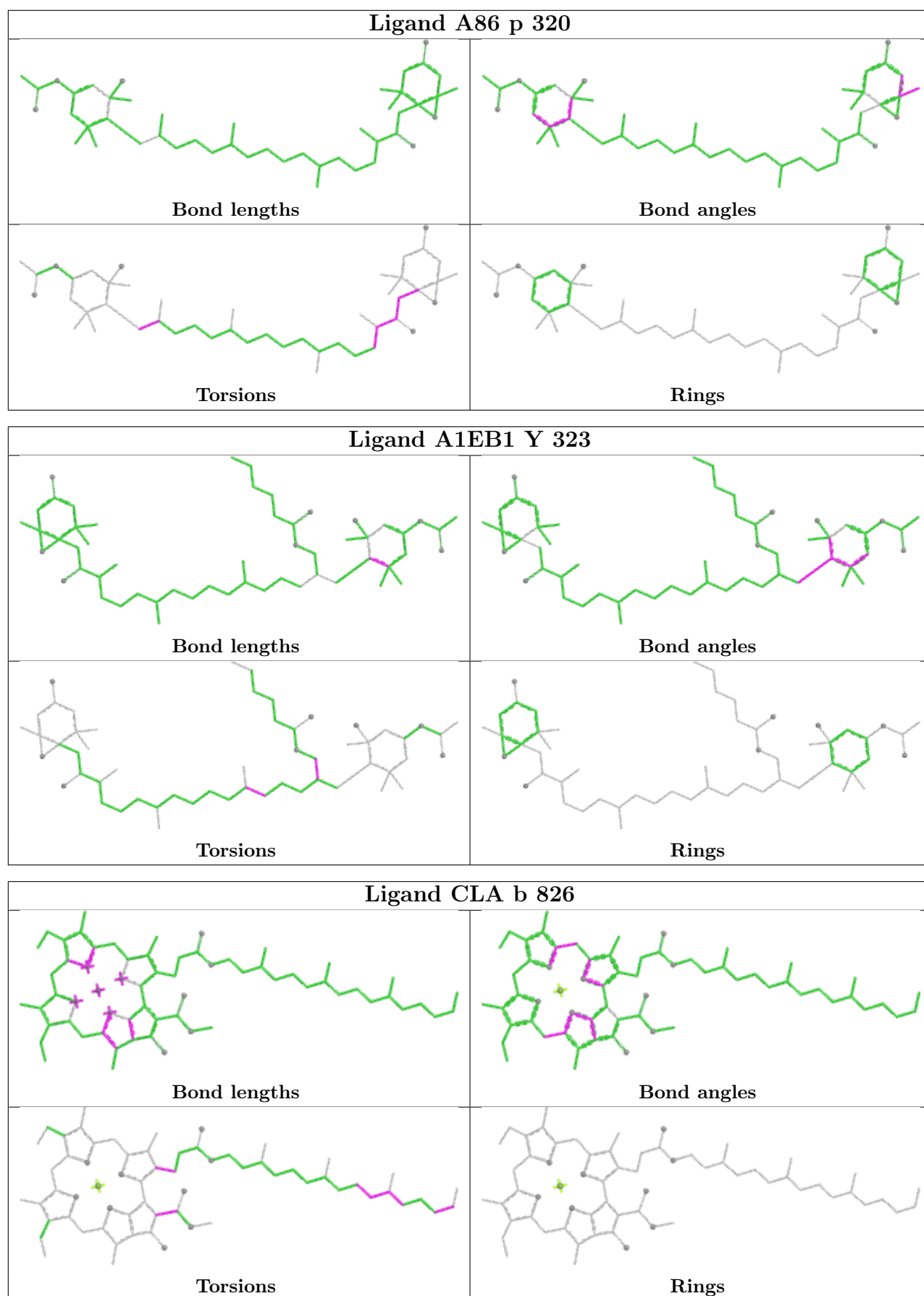


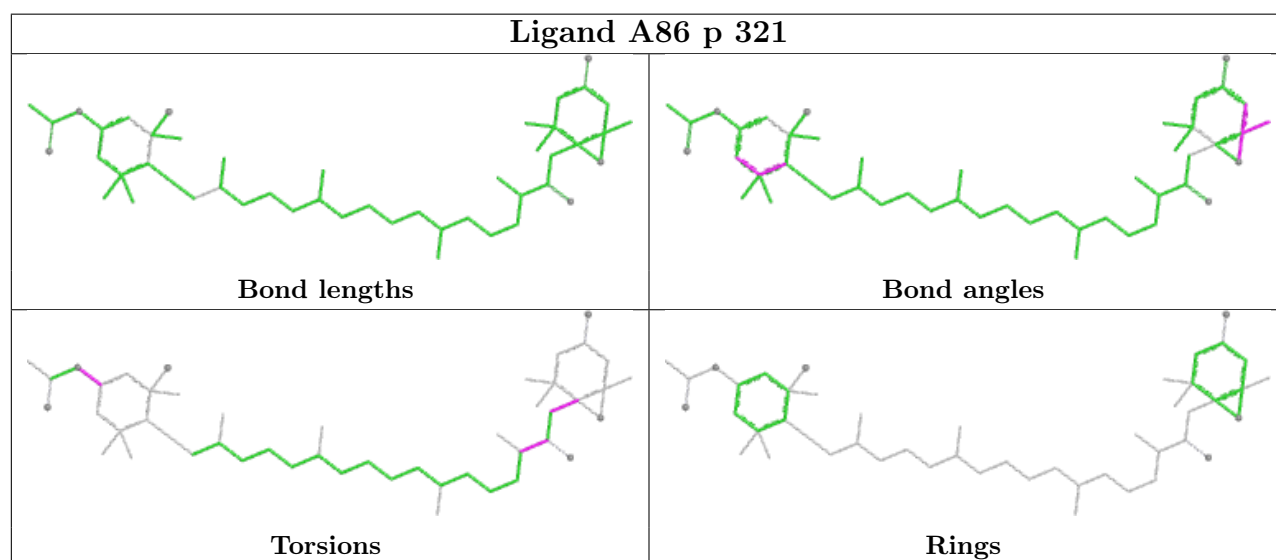
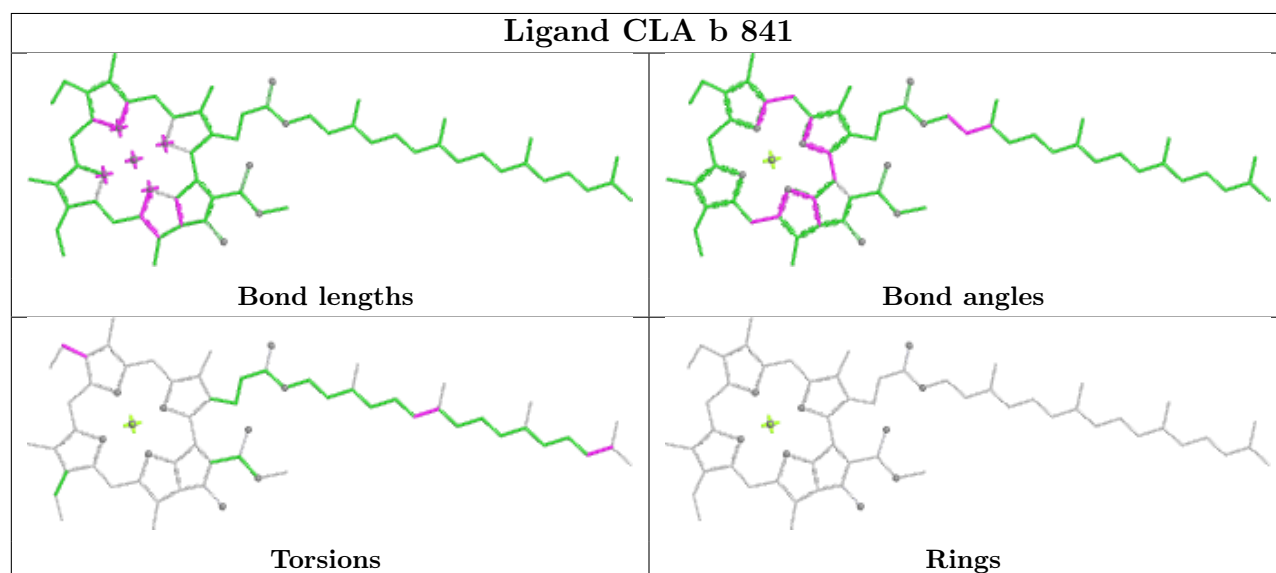
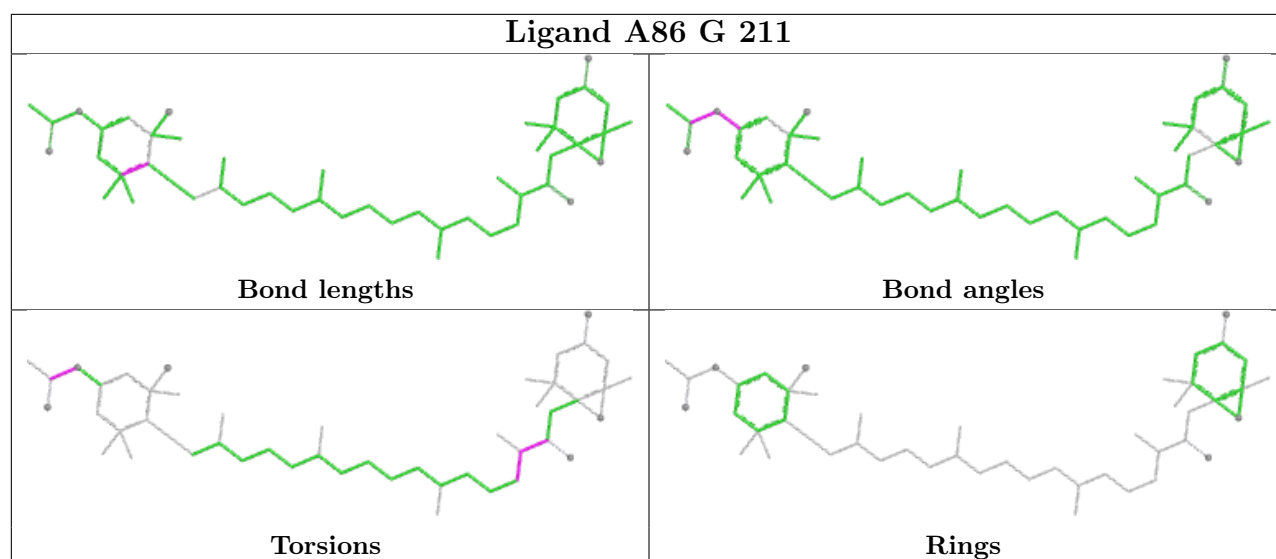
Torsions



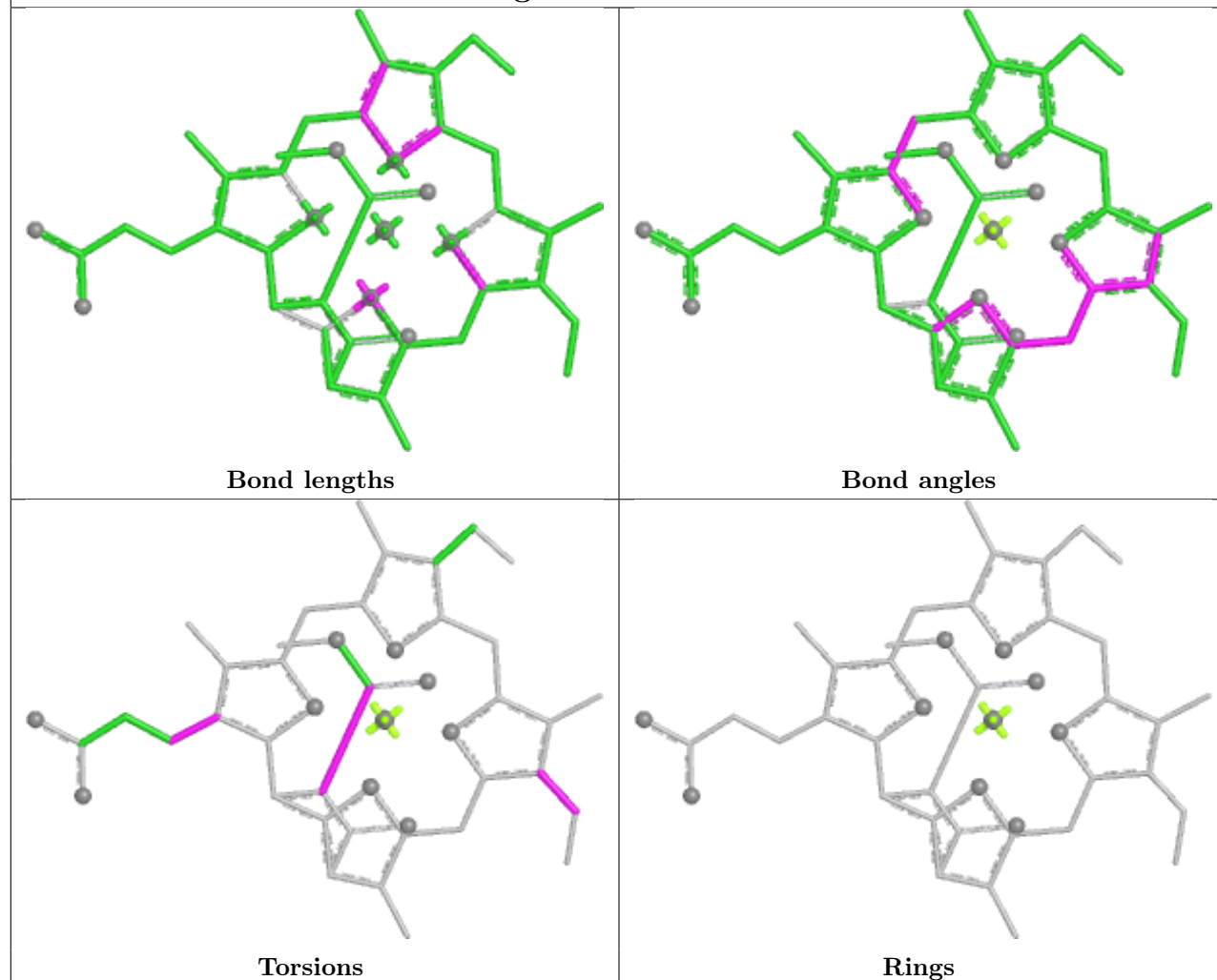
Rings



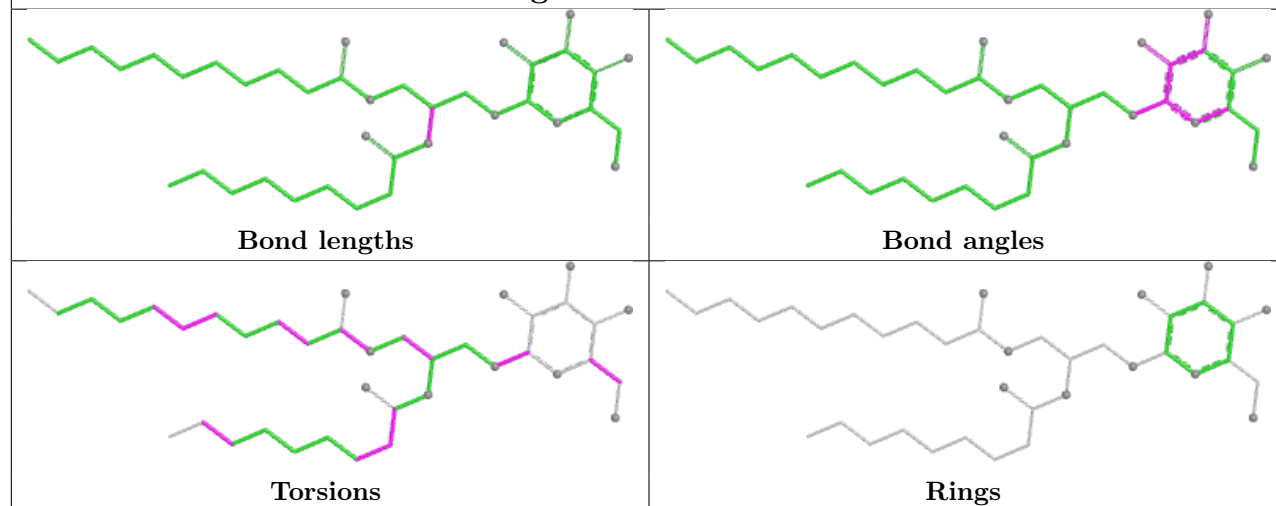


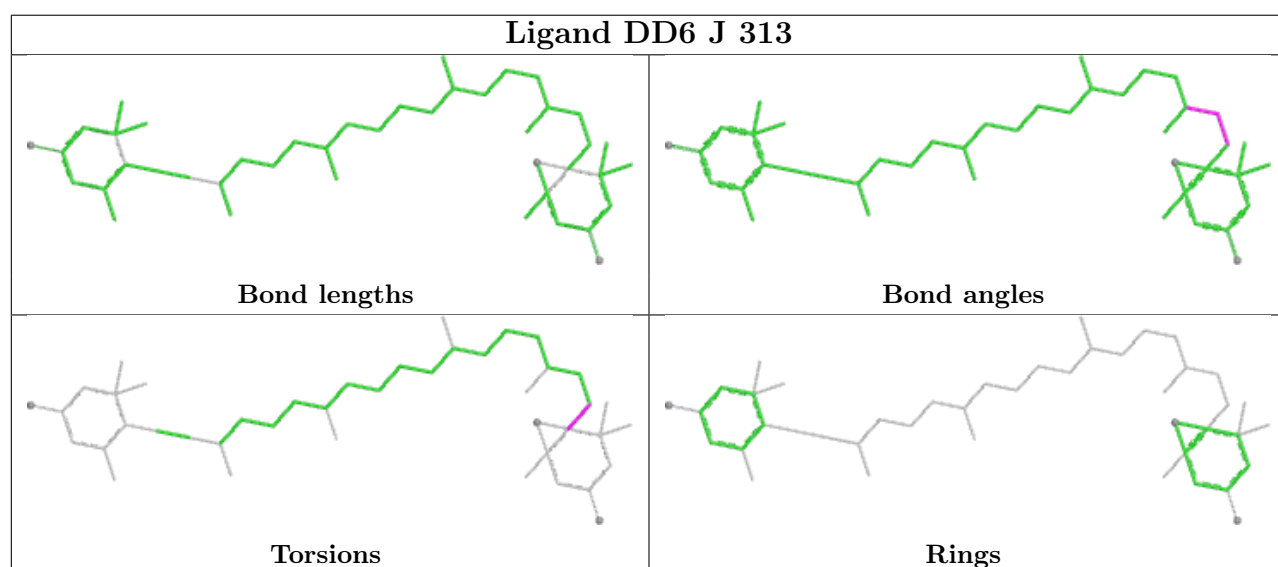
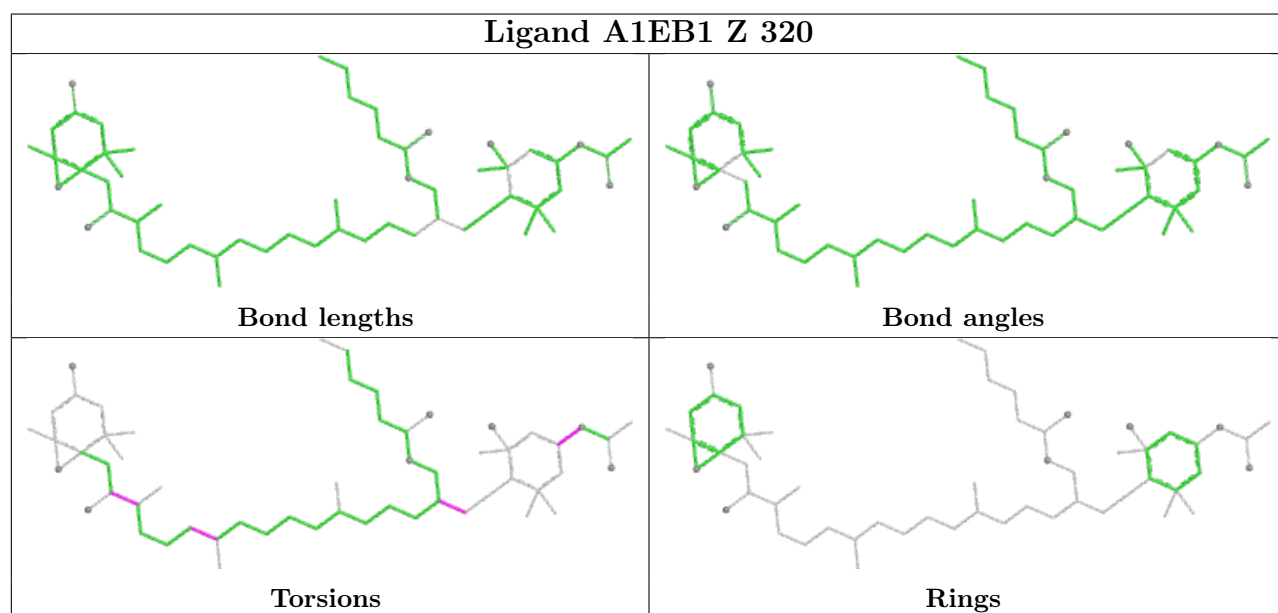
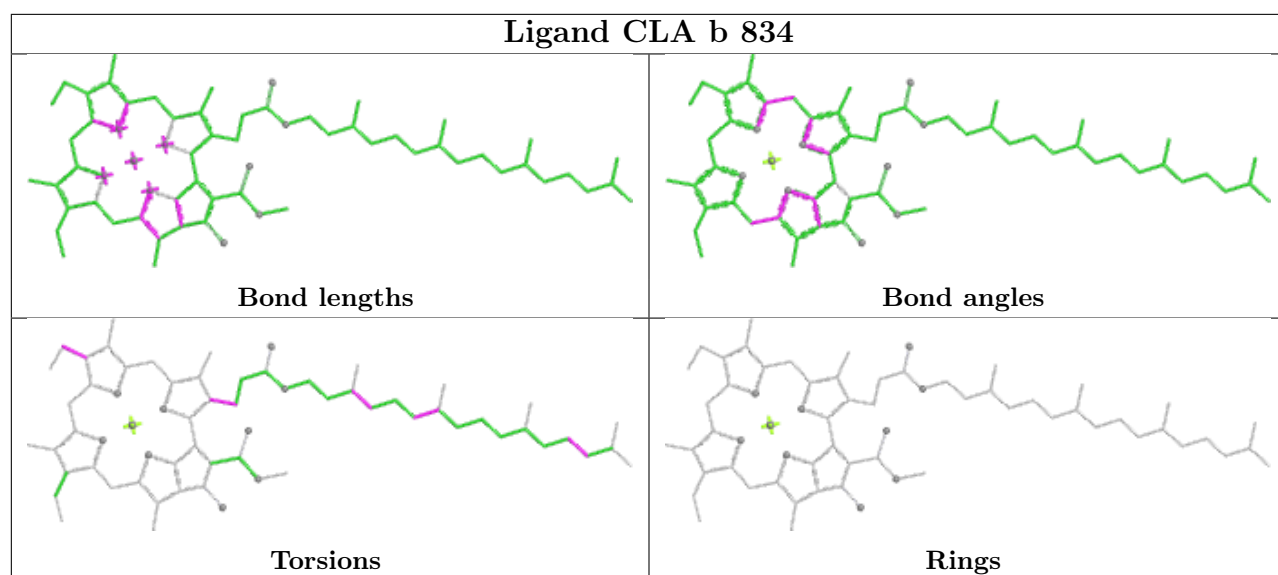


Ligand KC2 z 304

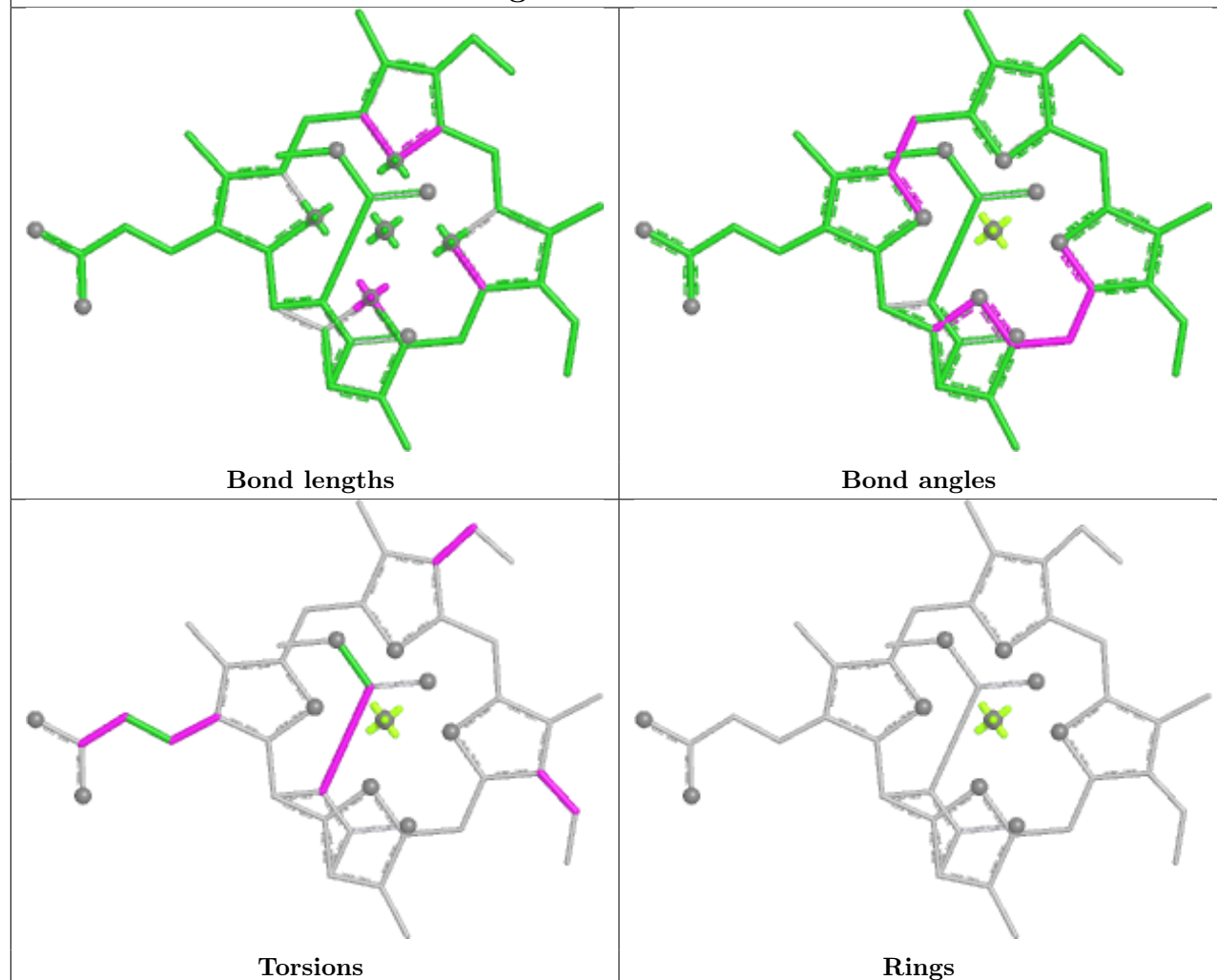


Ligand LMG u 301

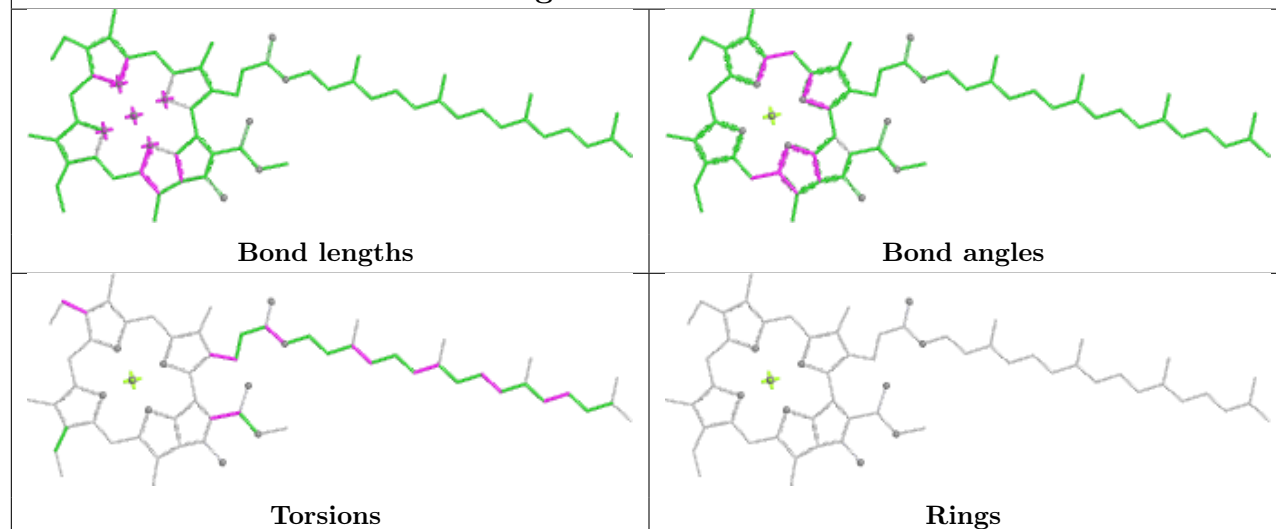


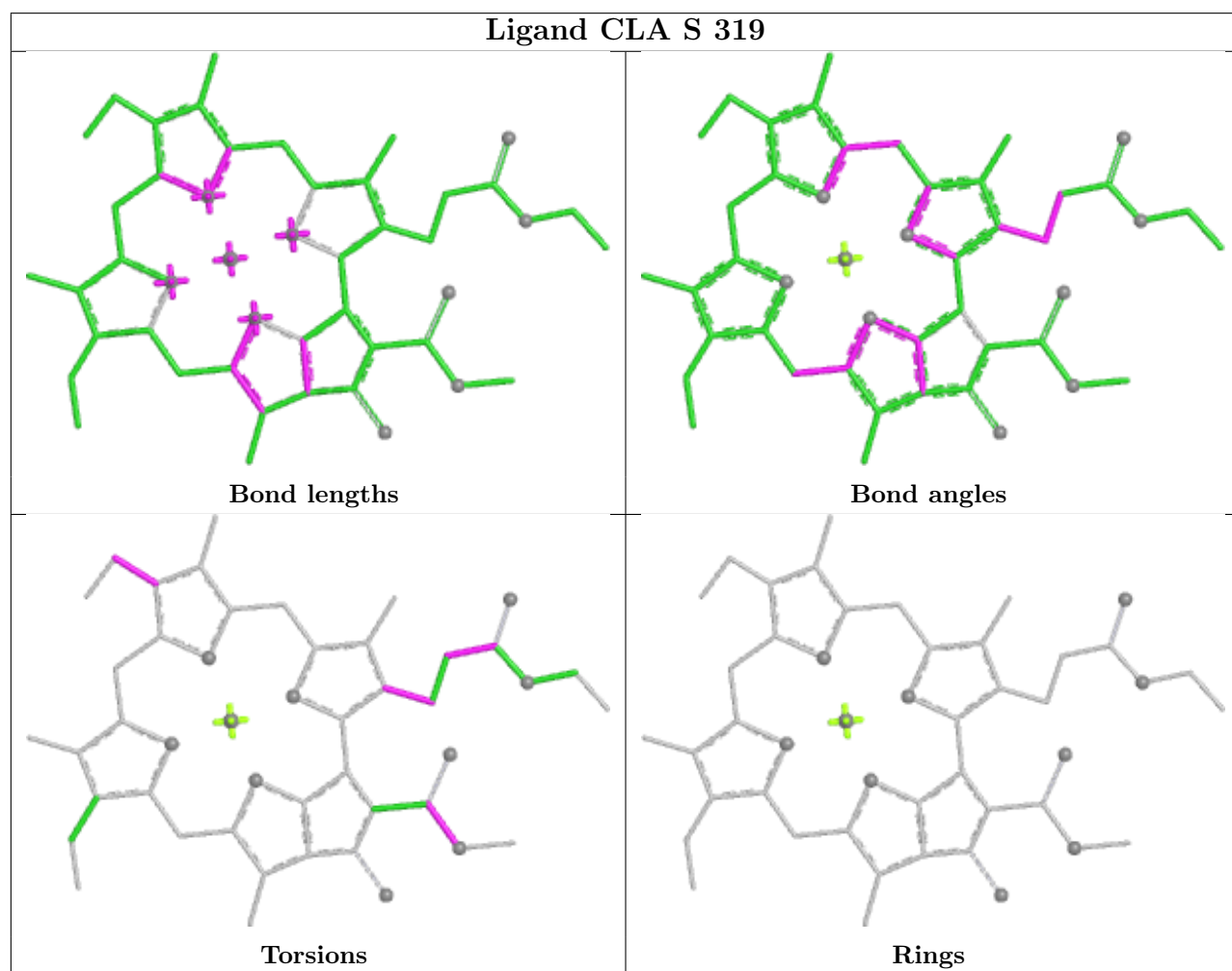
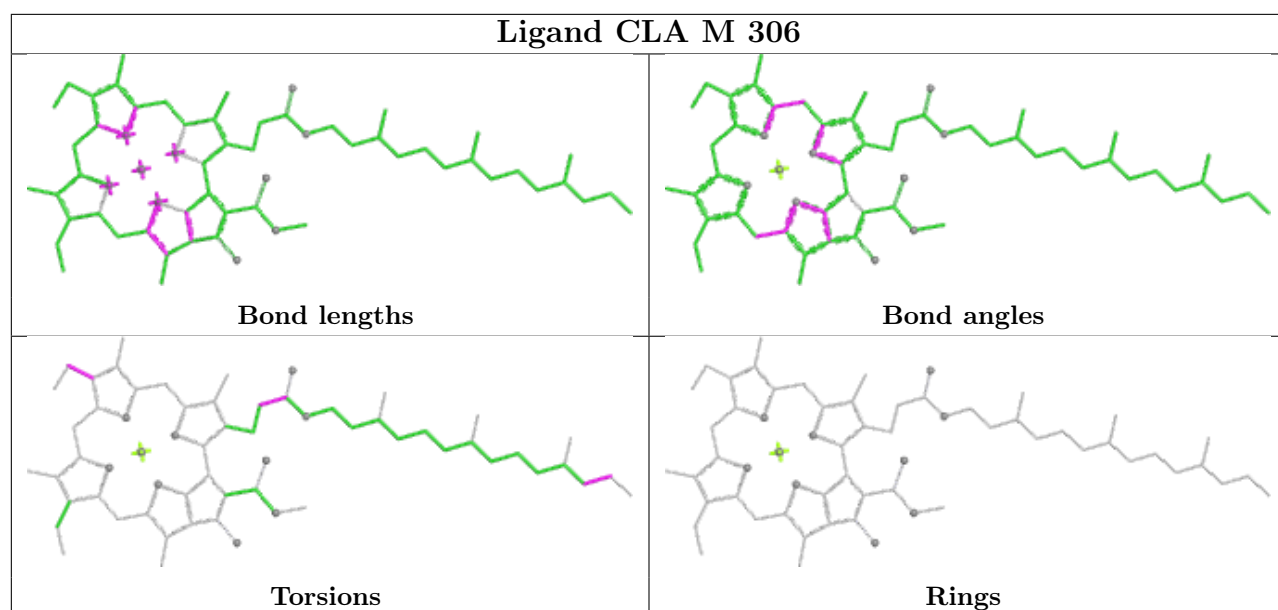


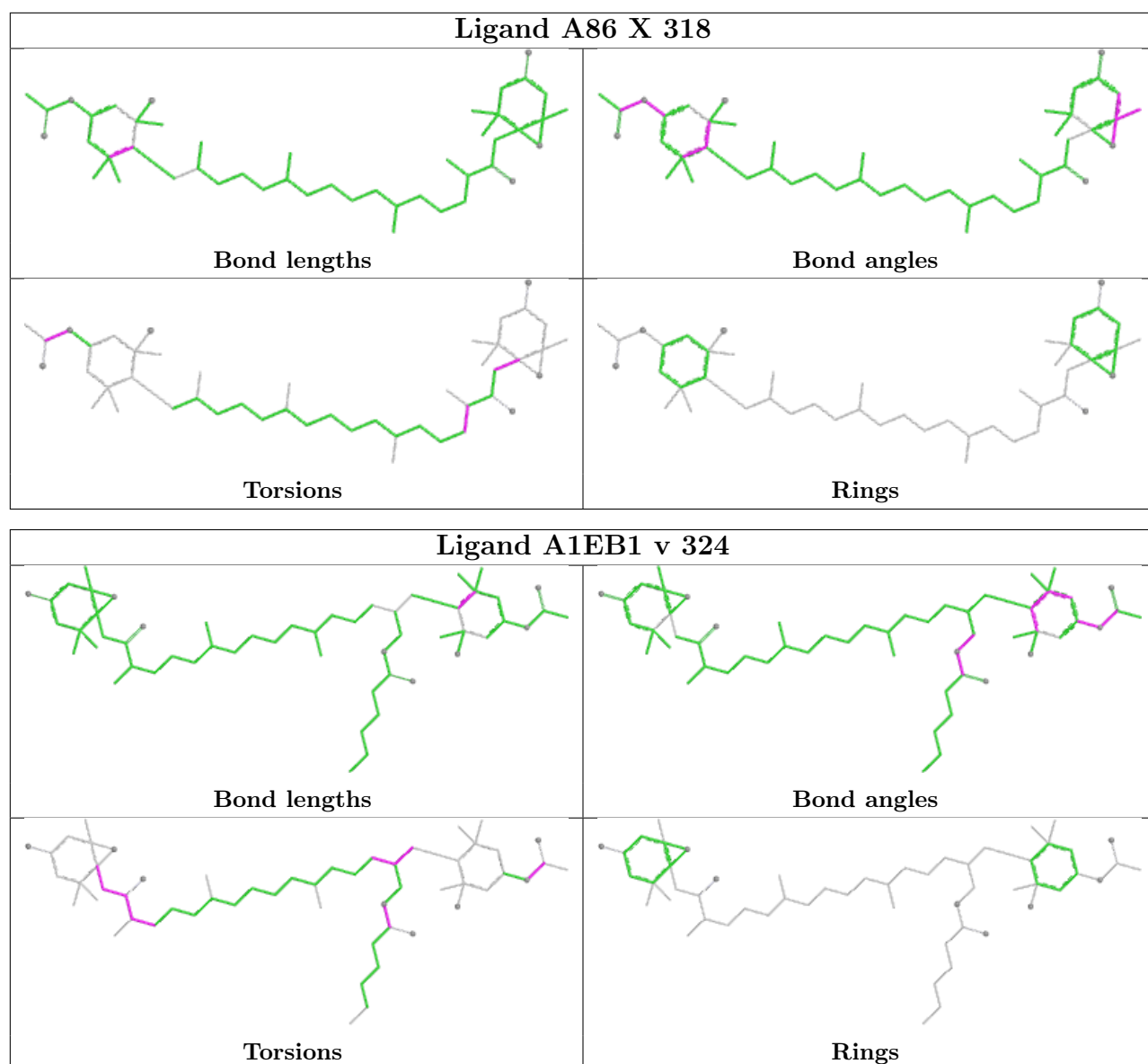
Ligand KC2 w 301



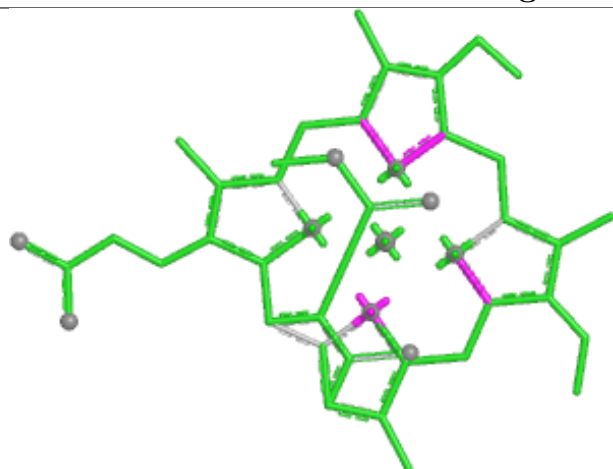
Ligand CLA b 839



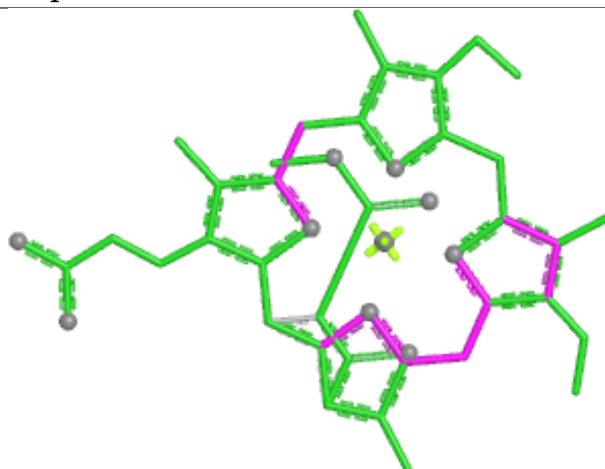




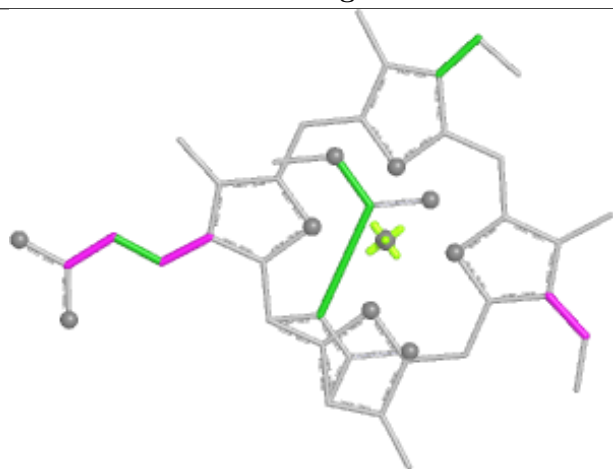
Ligand KC2 p 303



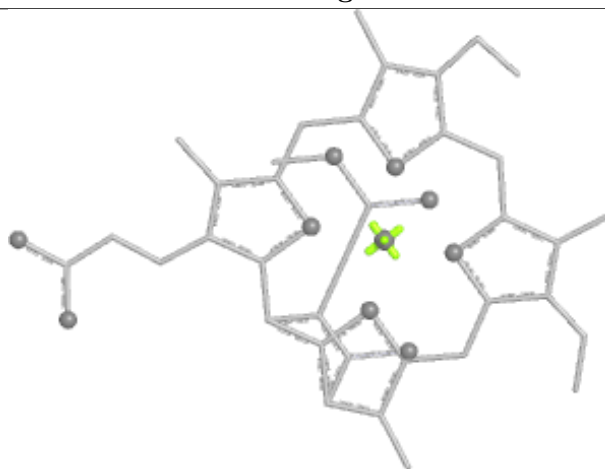
Bond lengths



Bond angles

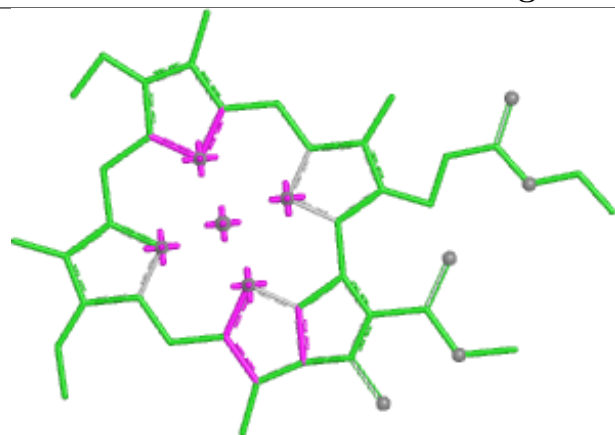


Torsions

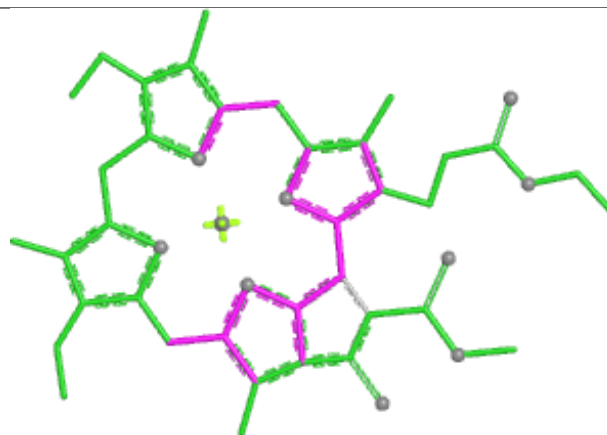


Rings

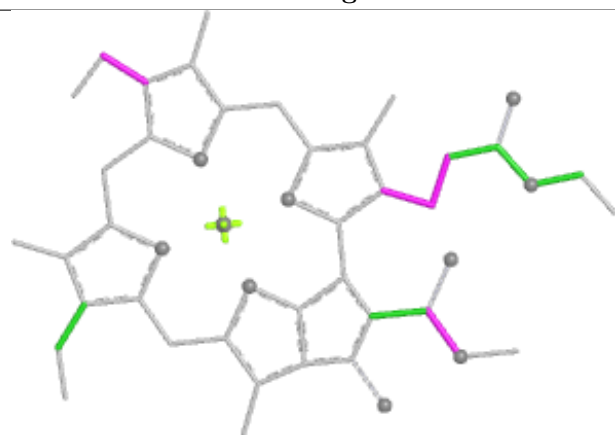
Ligand CLA L 306



Bond lengths



Bond angles

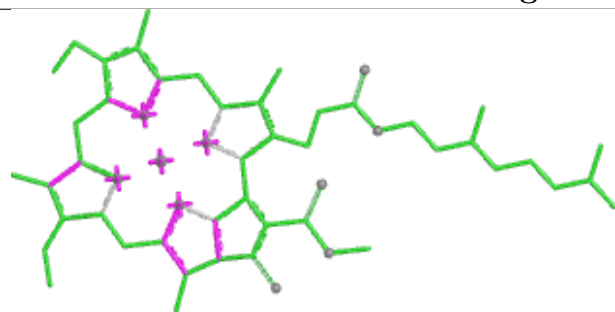


Torsions

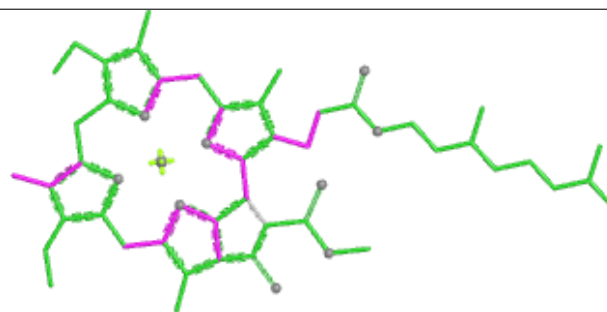


Rings

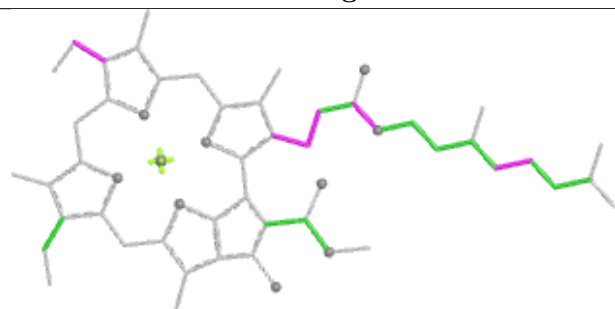
Ligand CLA J 308



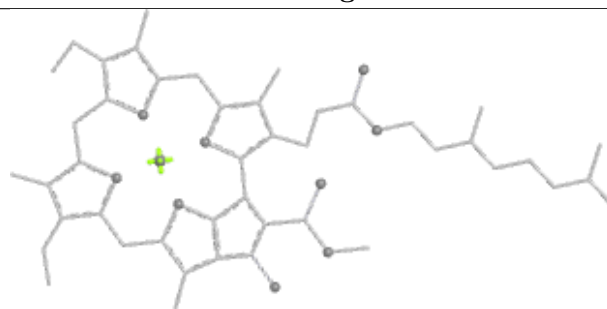
Bond lengths



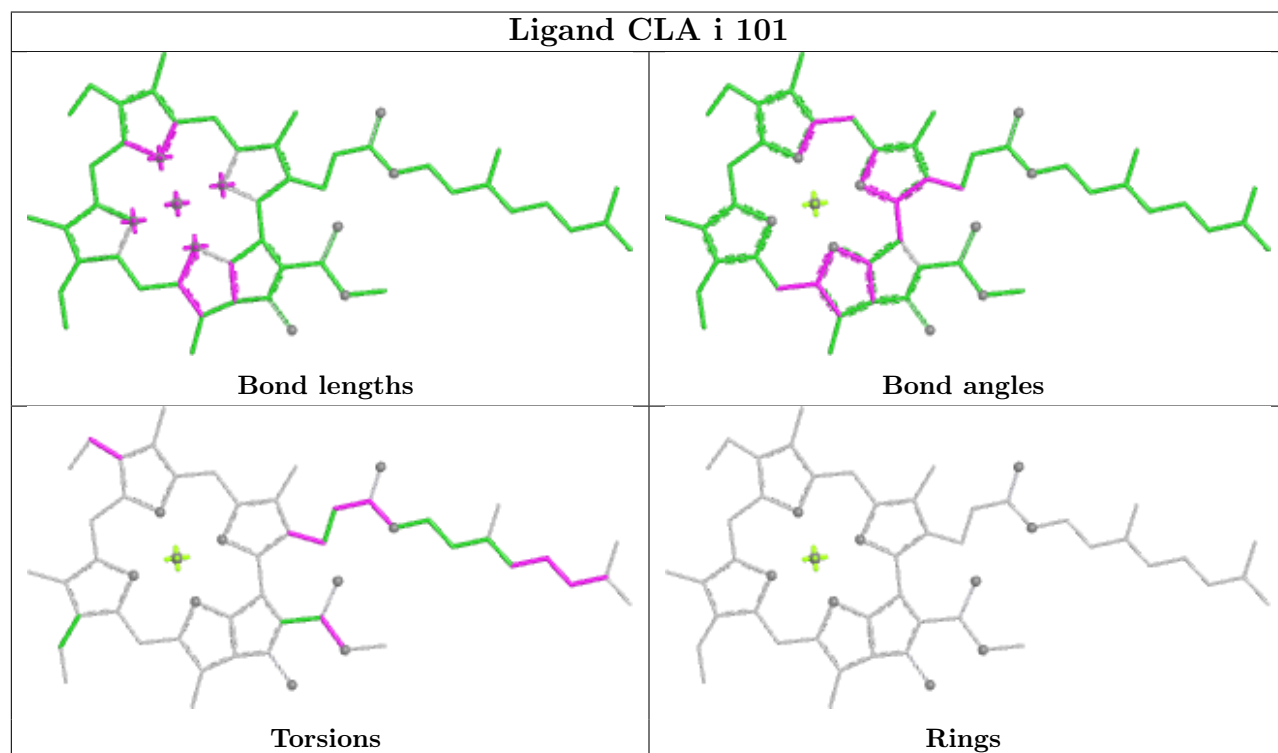
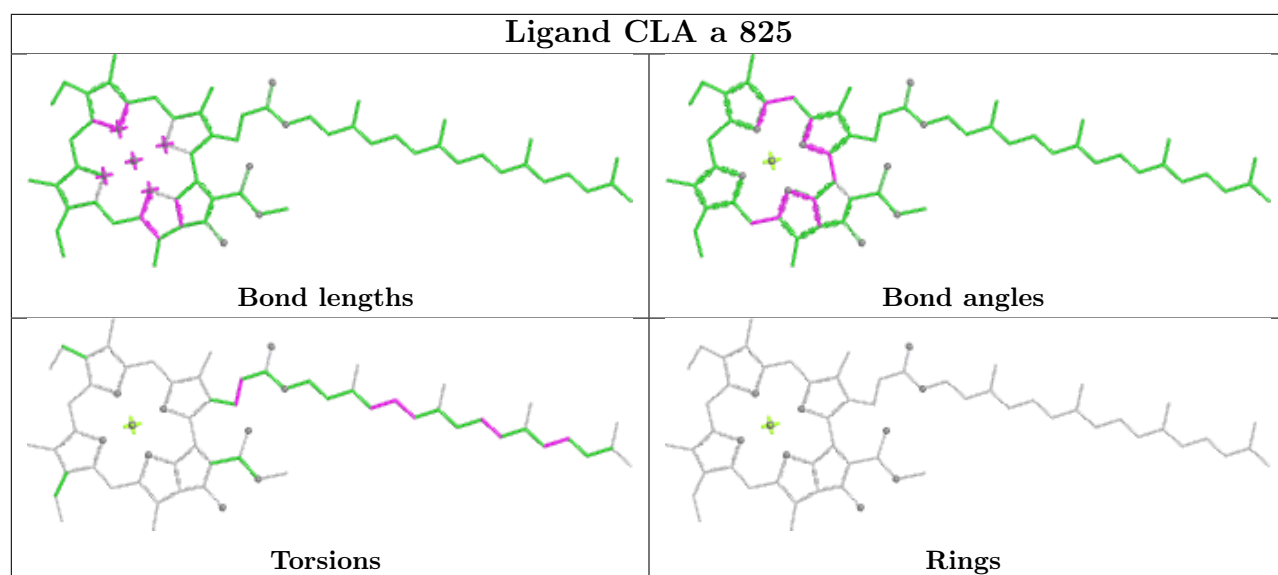
Bond angles

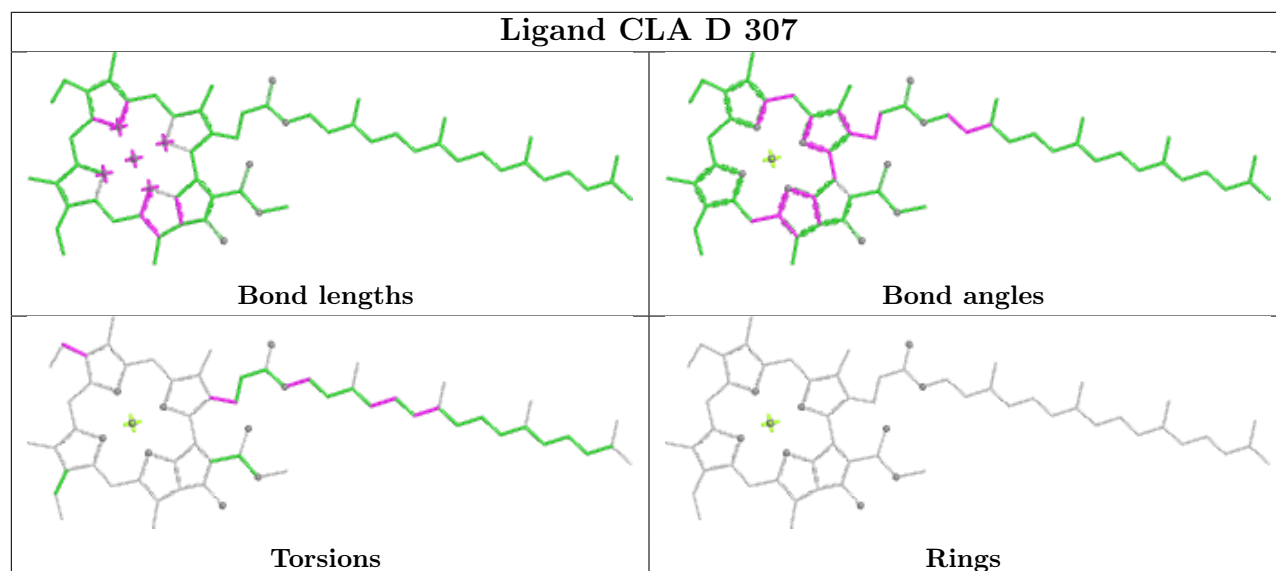
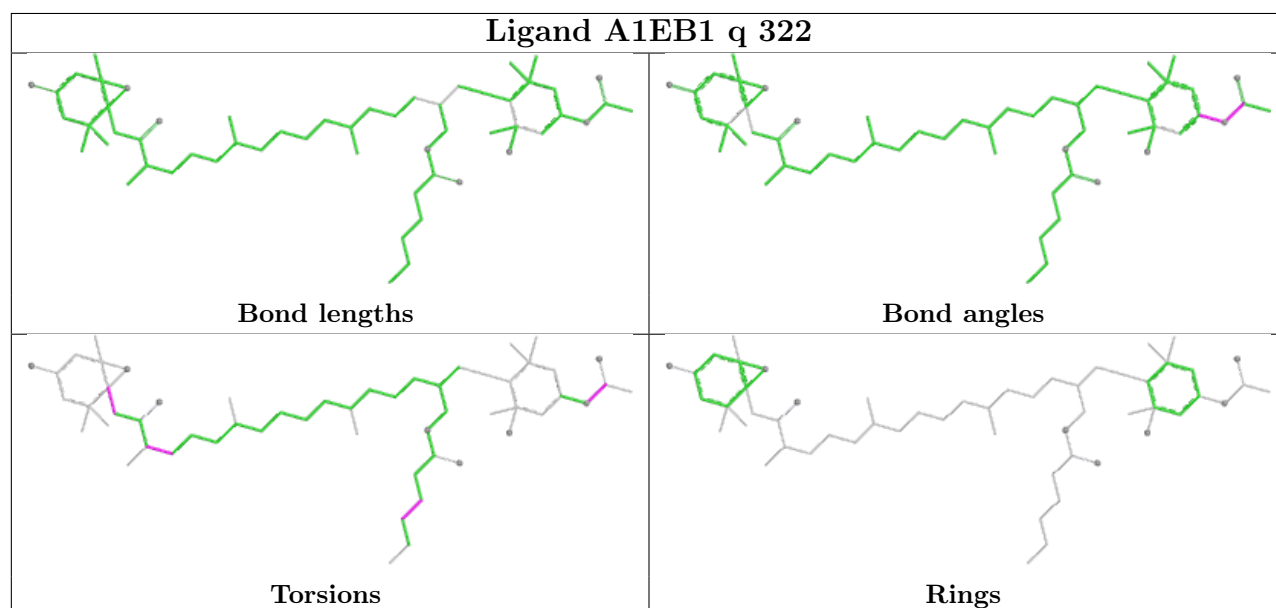
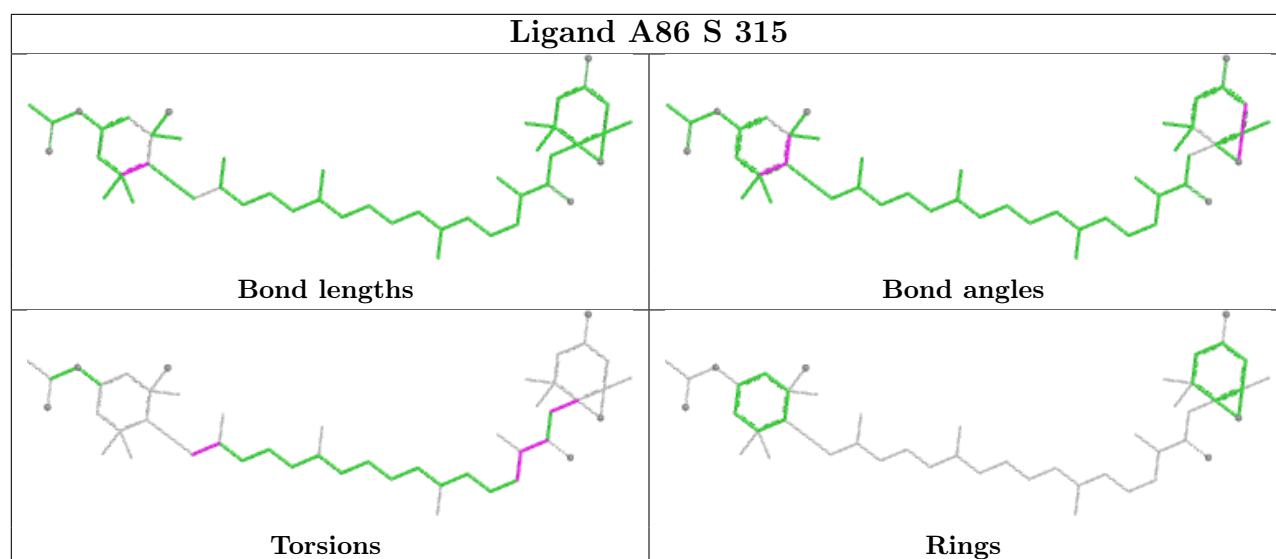


Torsions

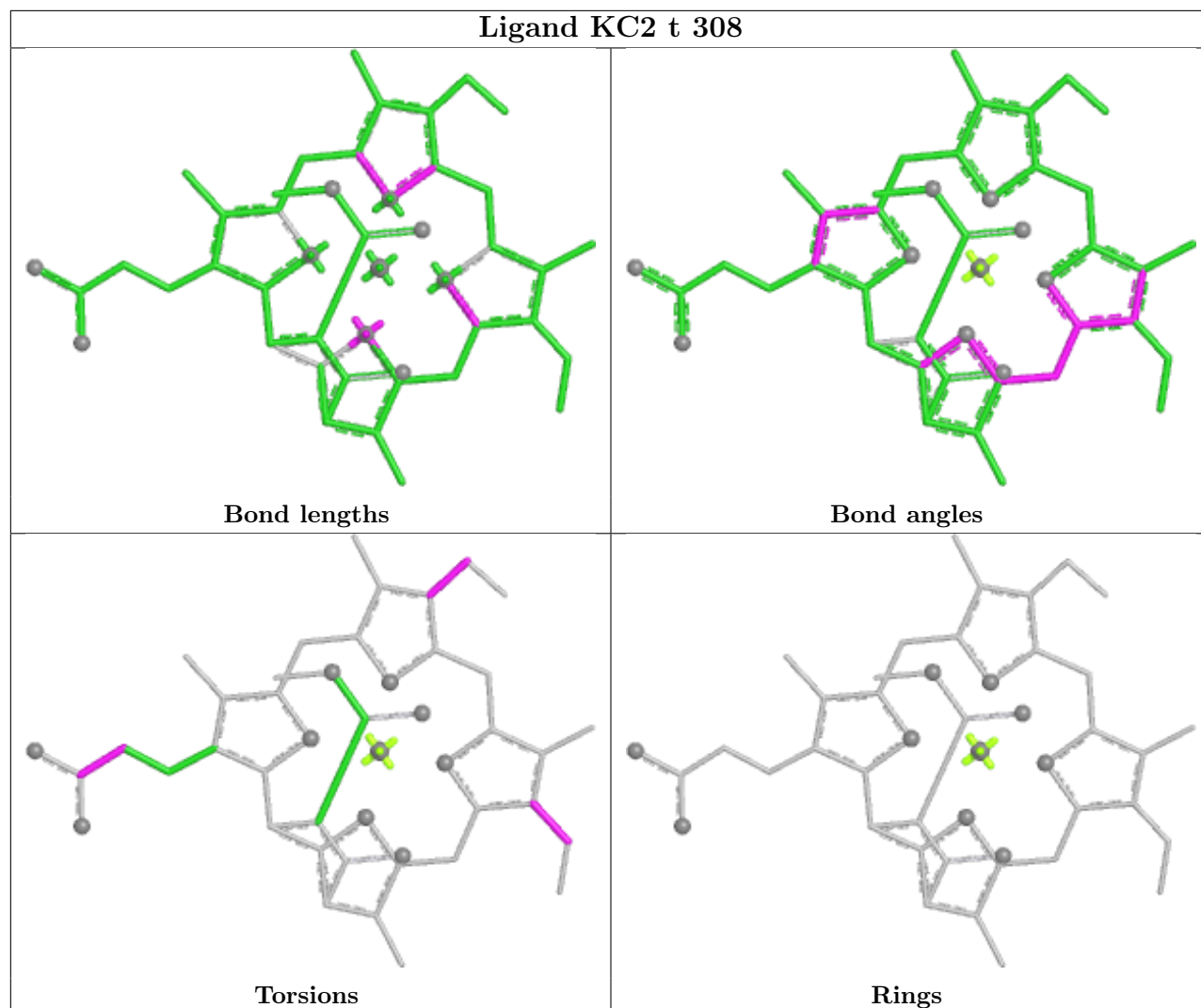


Rings

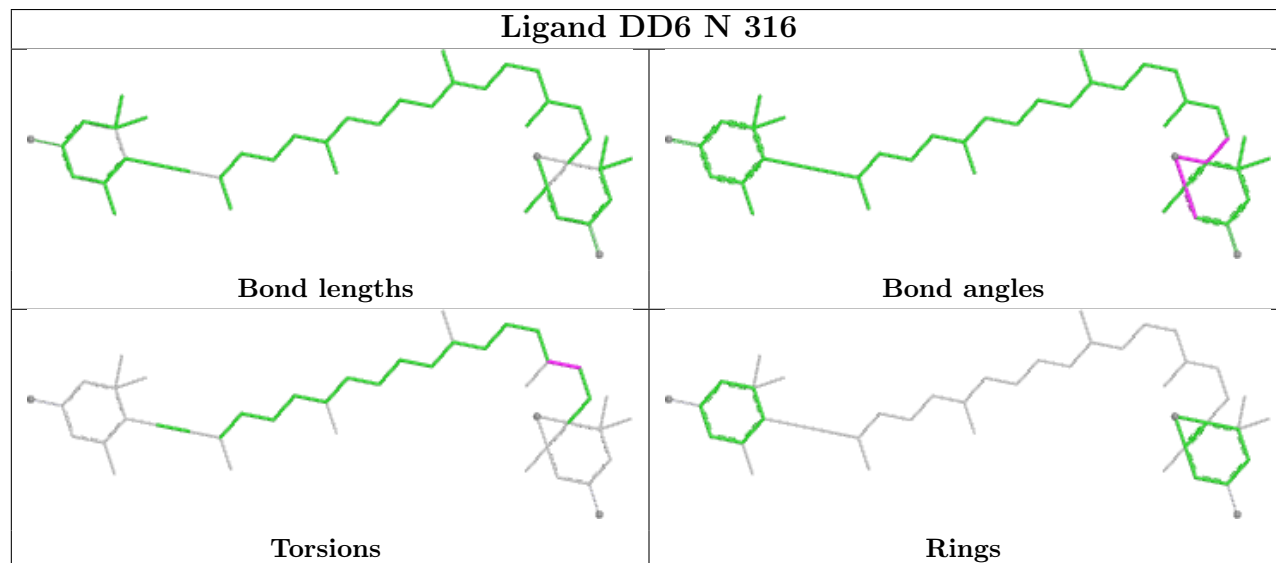




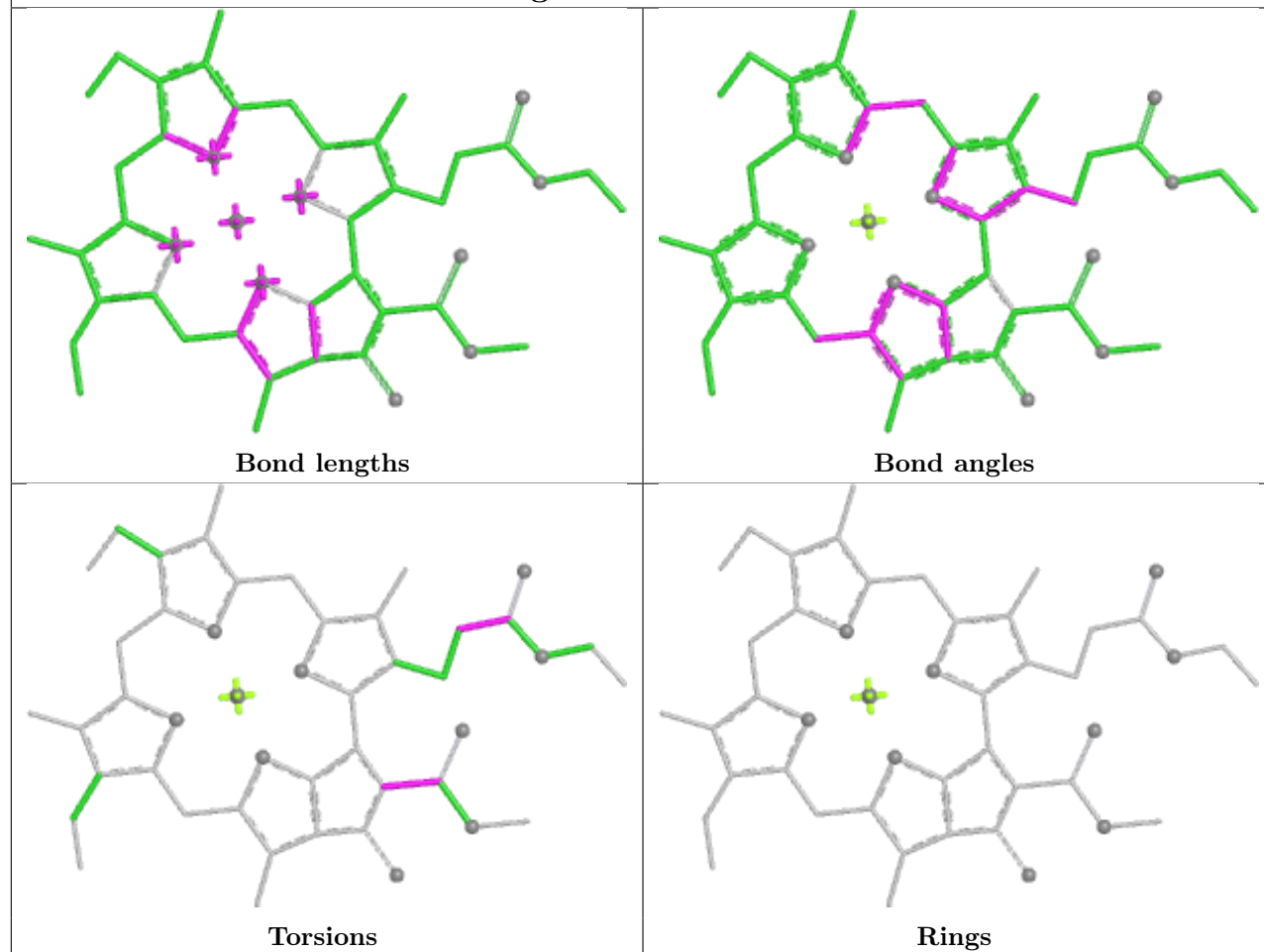
Ligand KC2 t 308



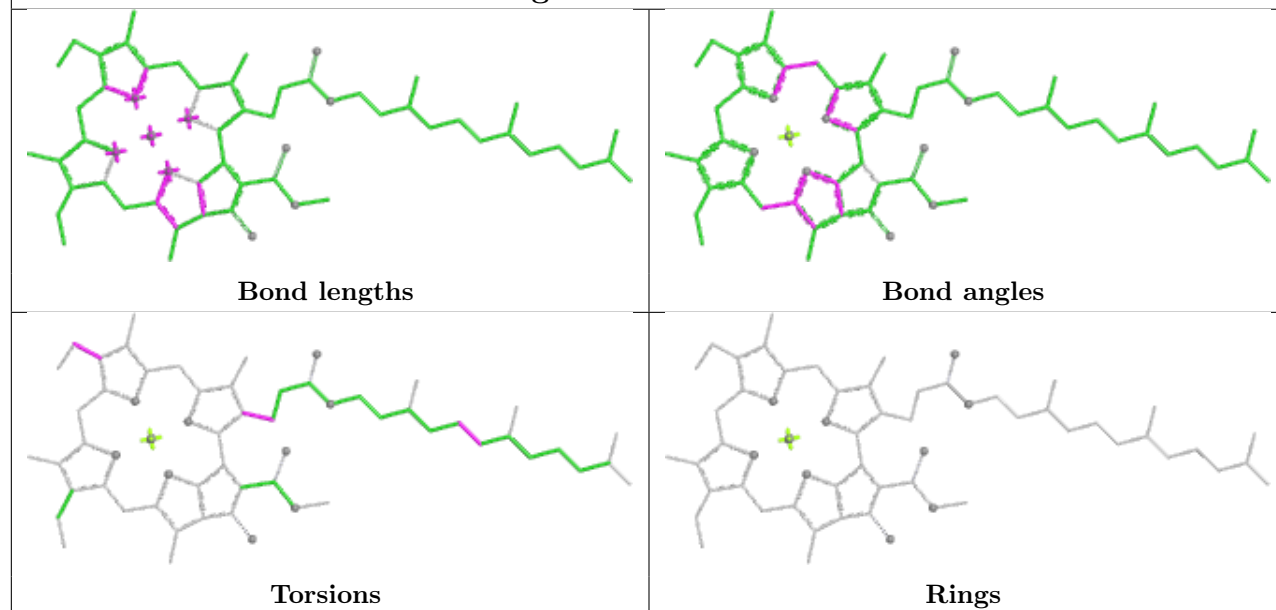
Ligand DD6 N 316

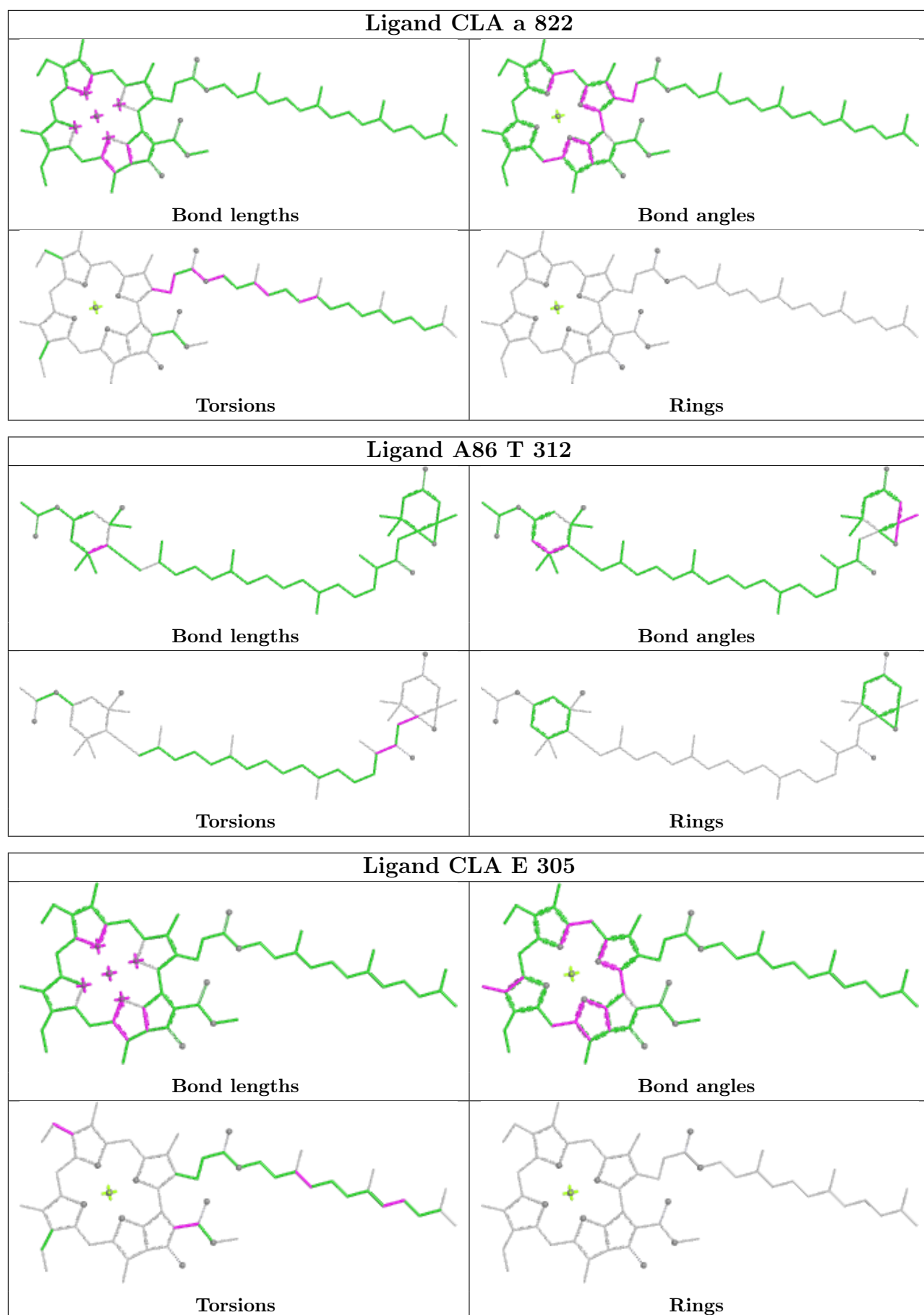


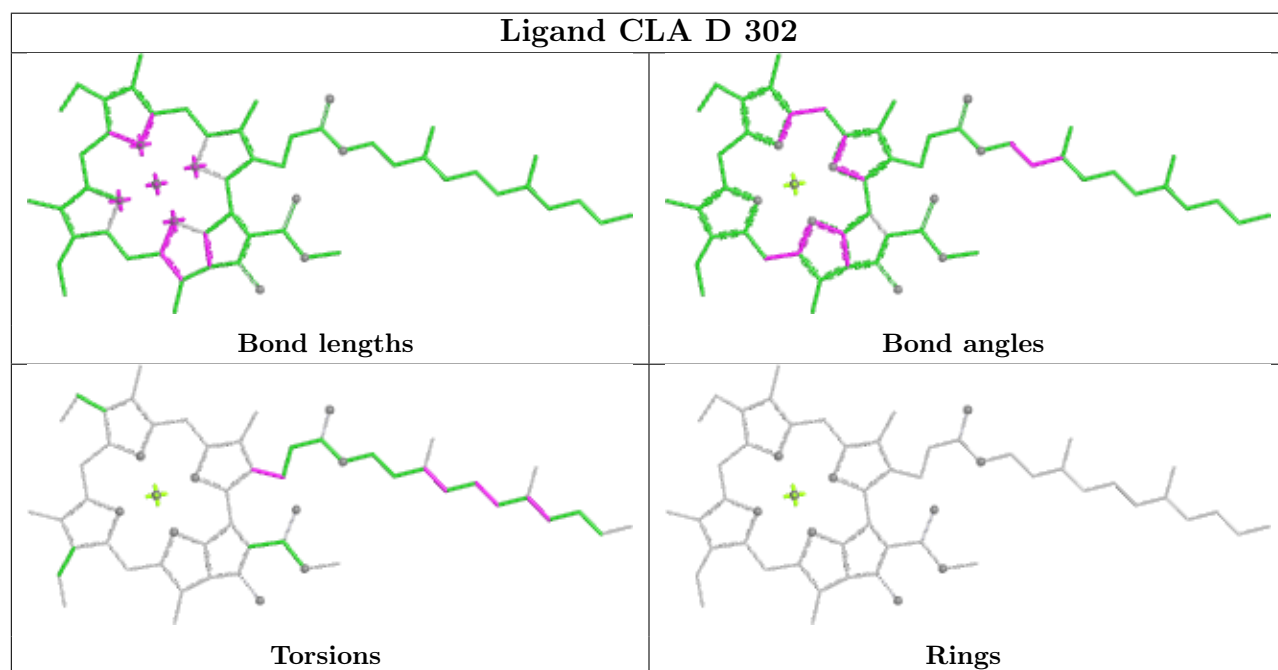
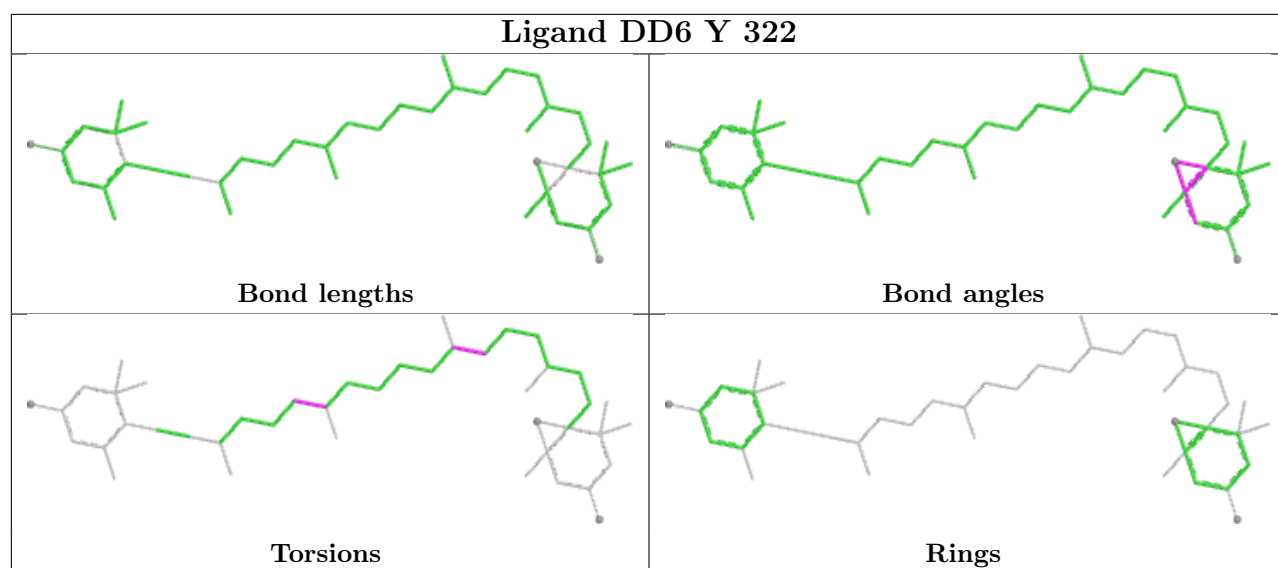
Ligand CLA J 311



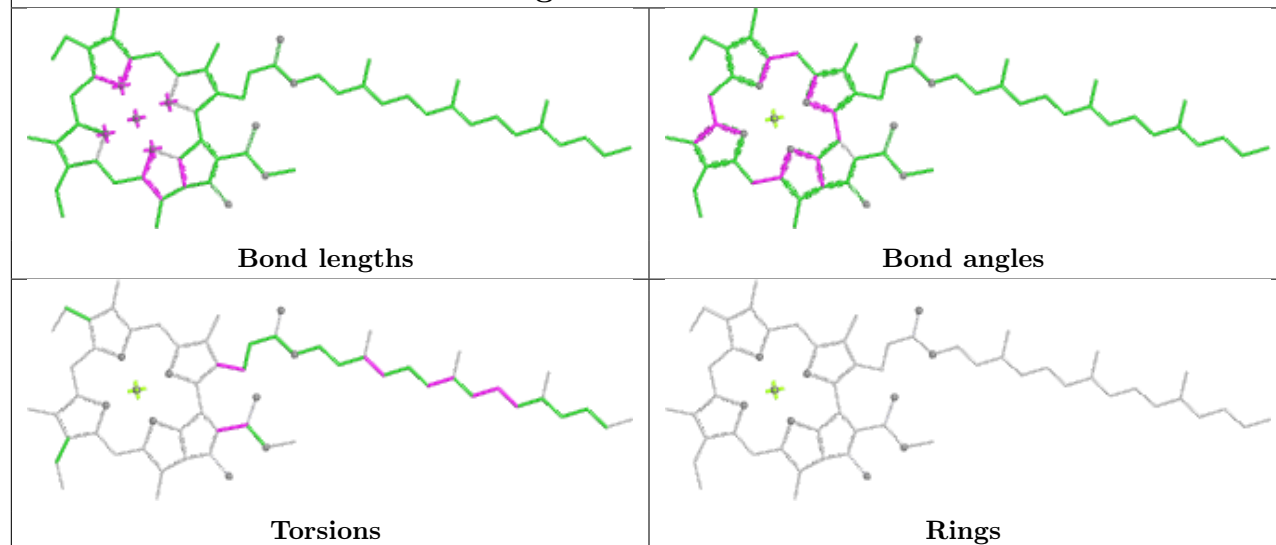
Ligand CLA X 301



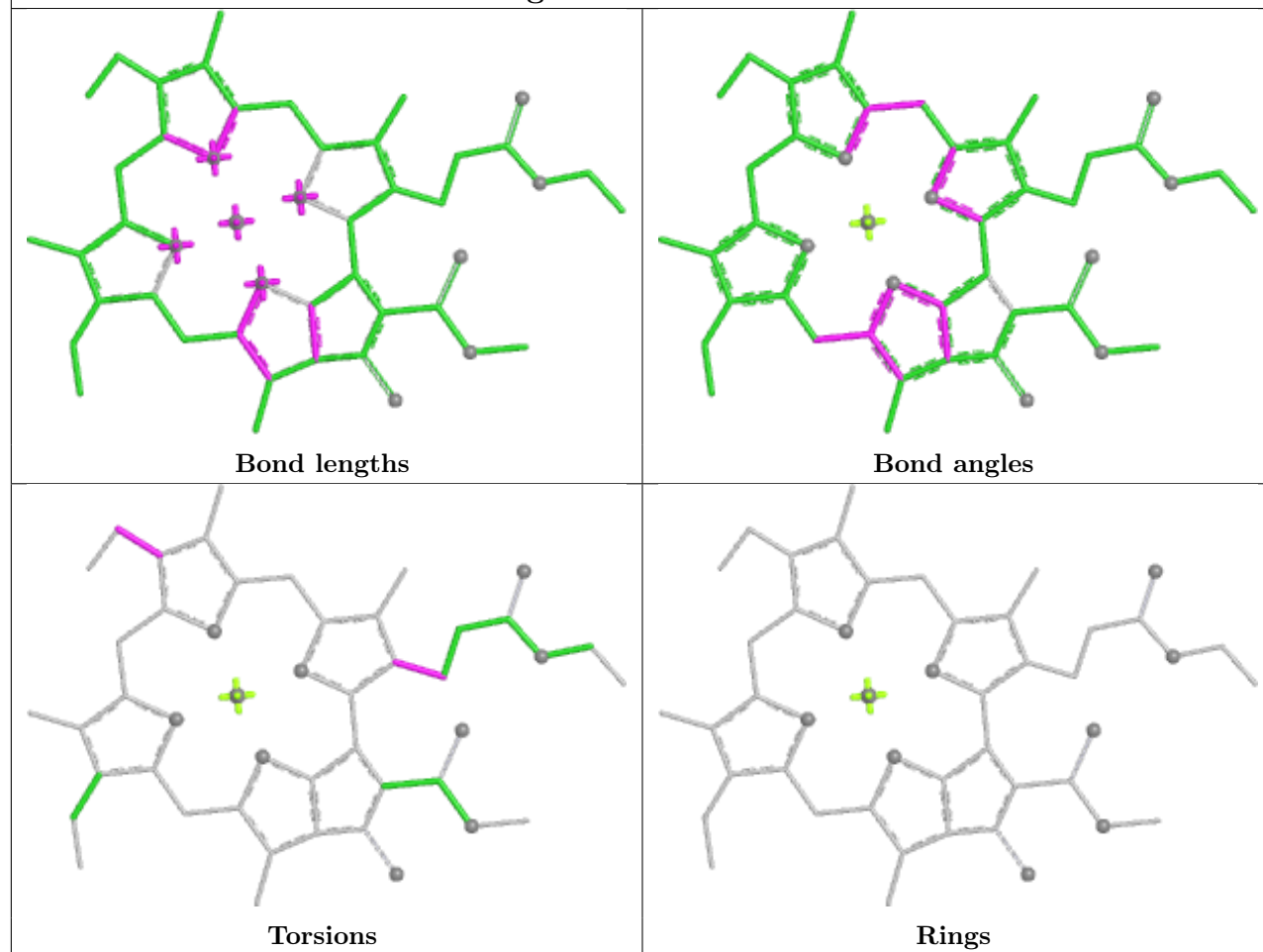


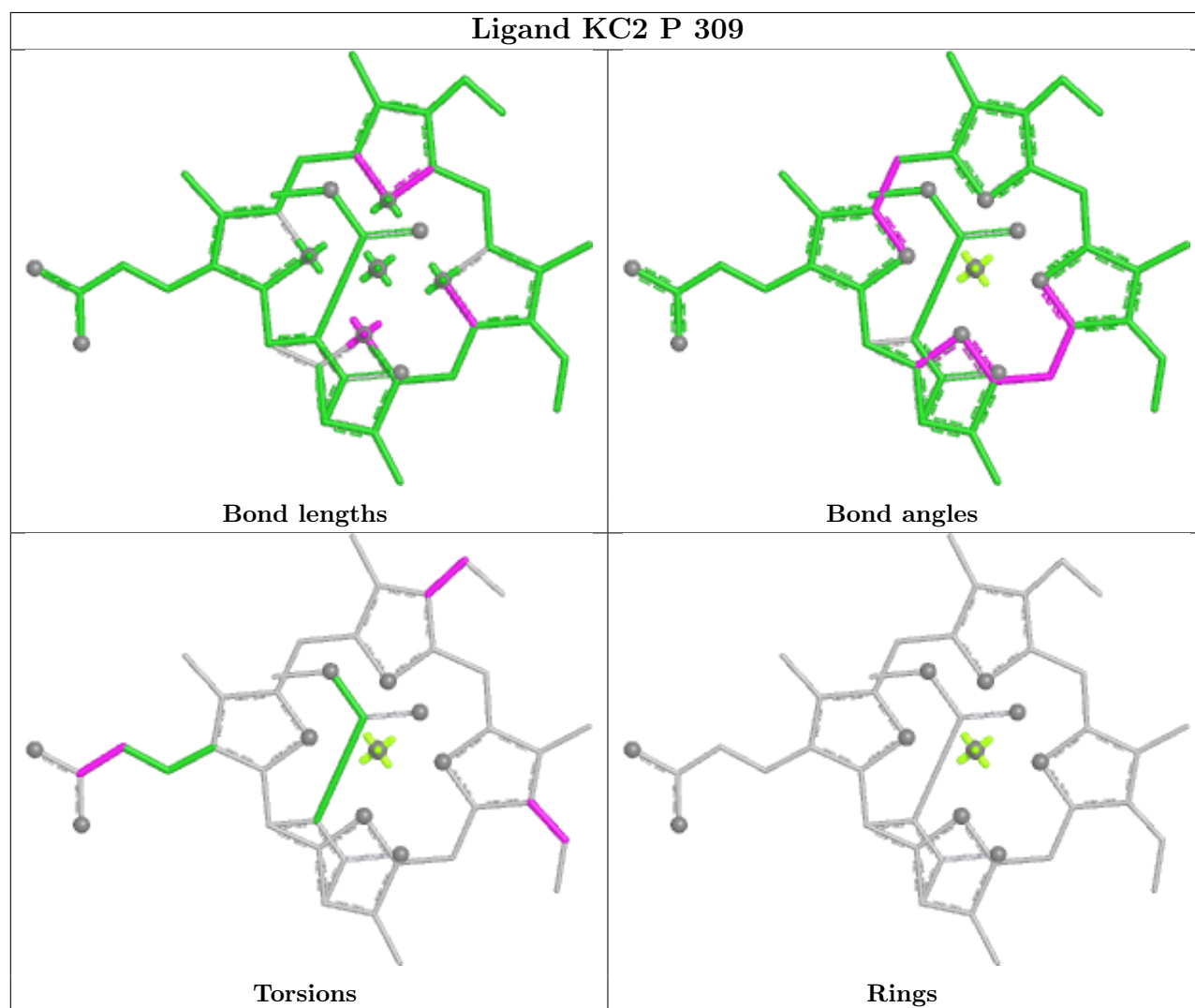
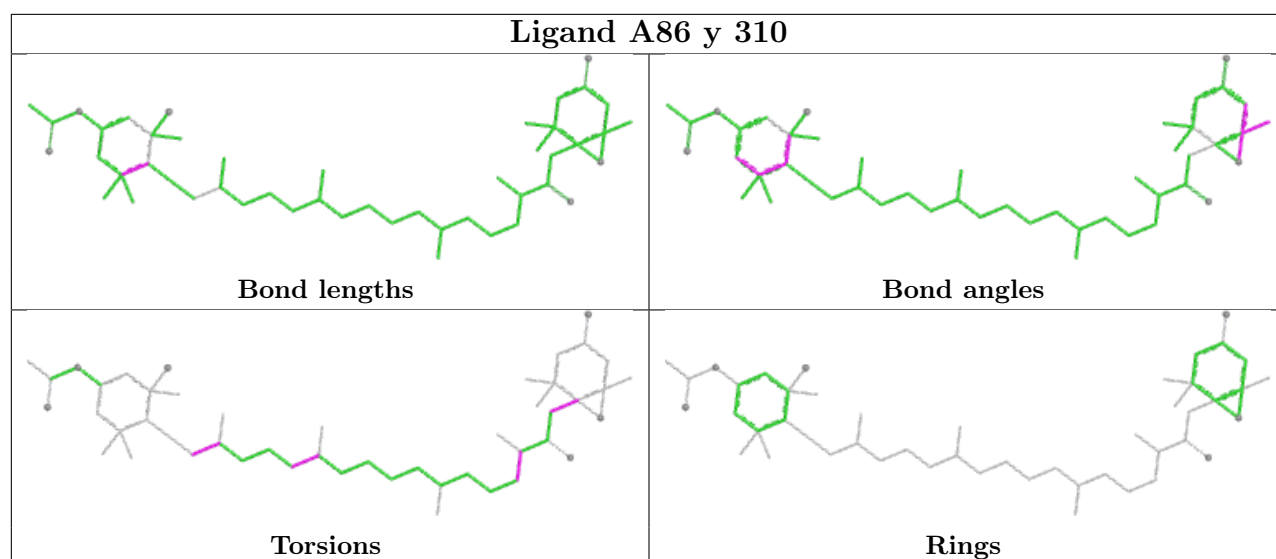


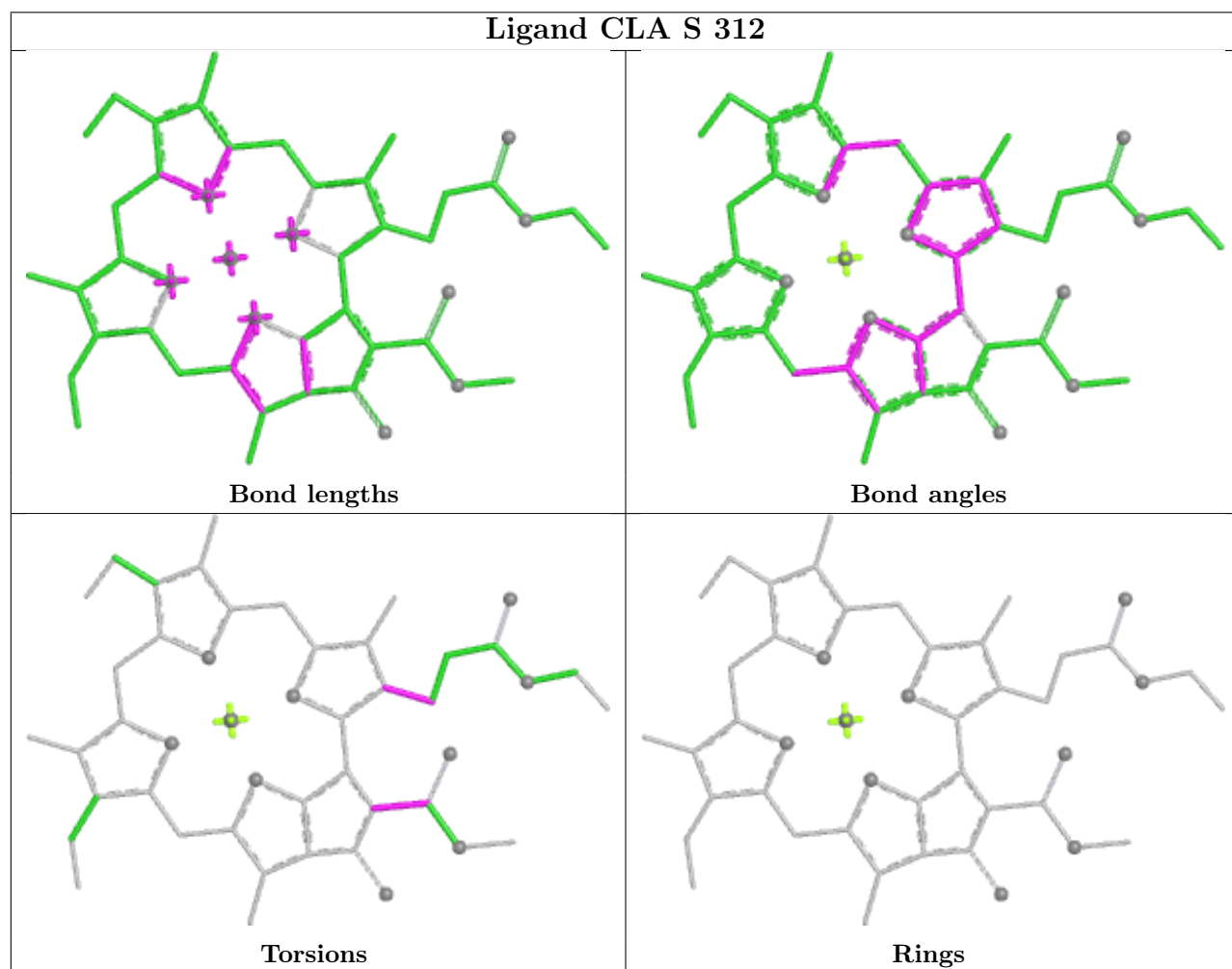
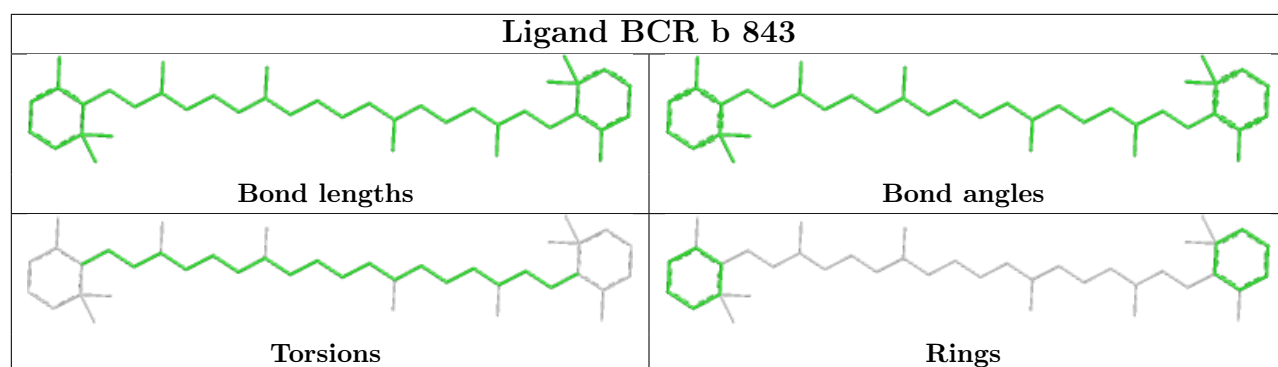
Ligand CLA v 311



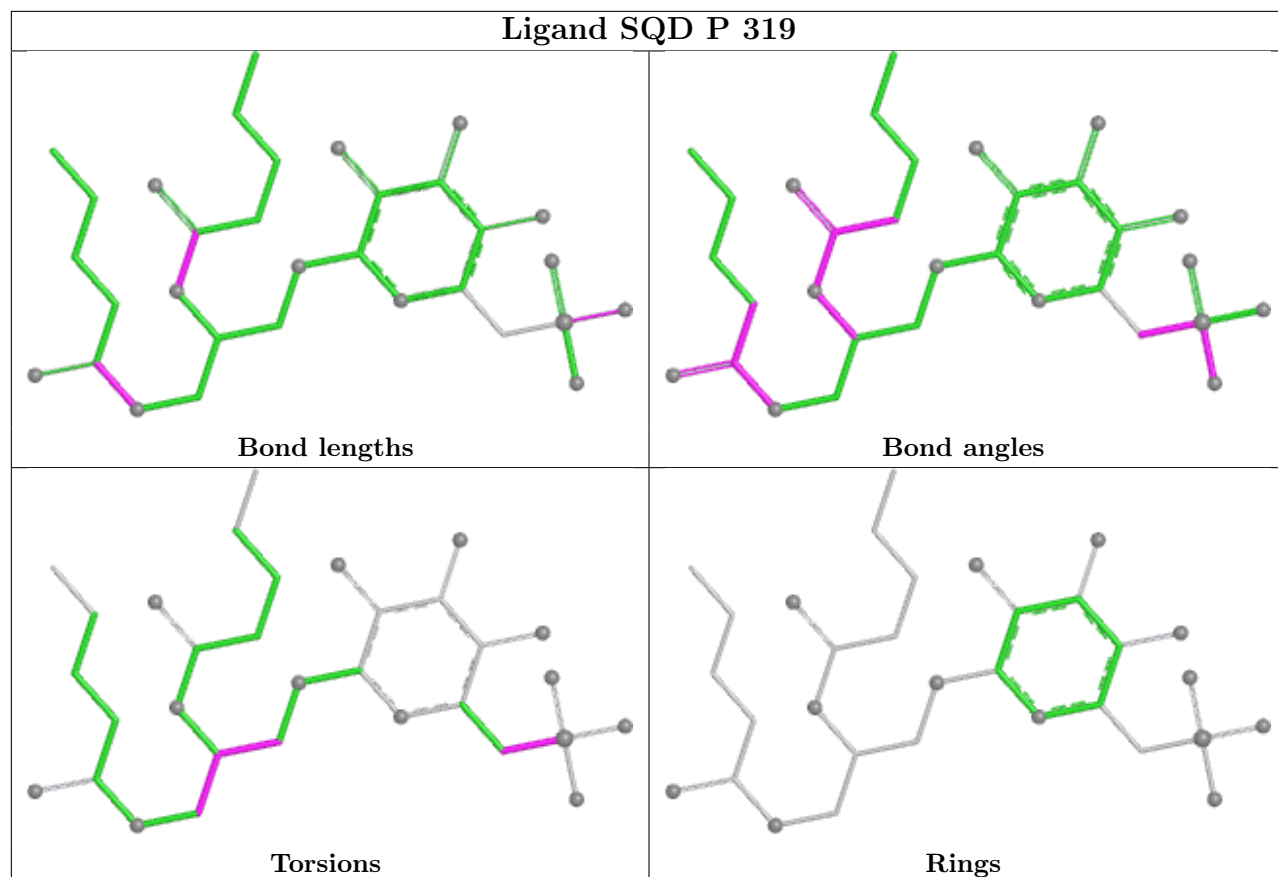
Ligand CLA B 303



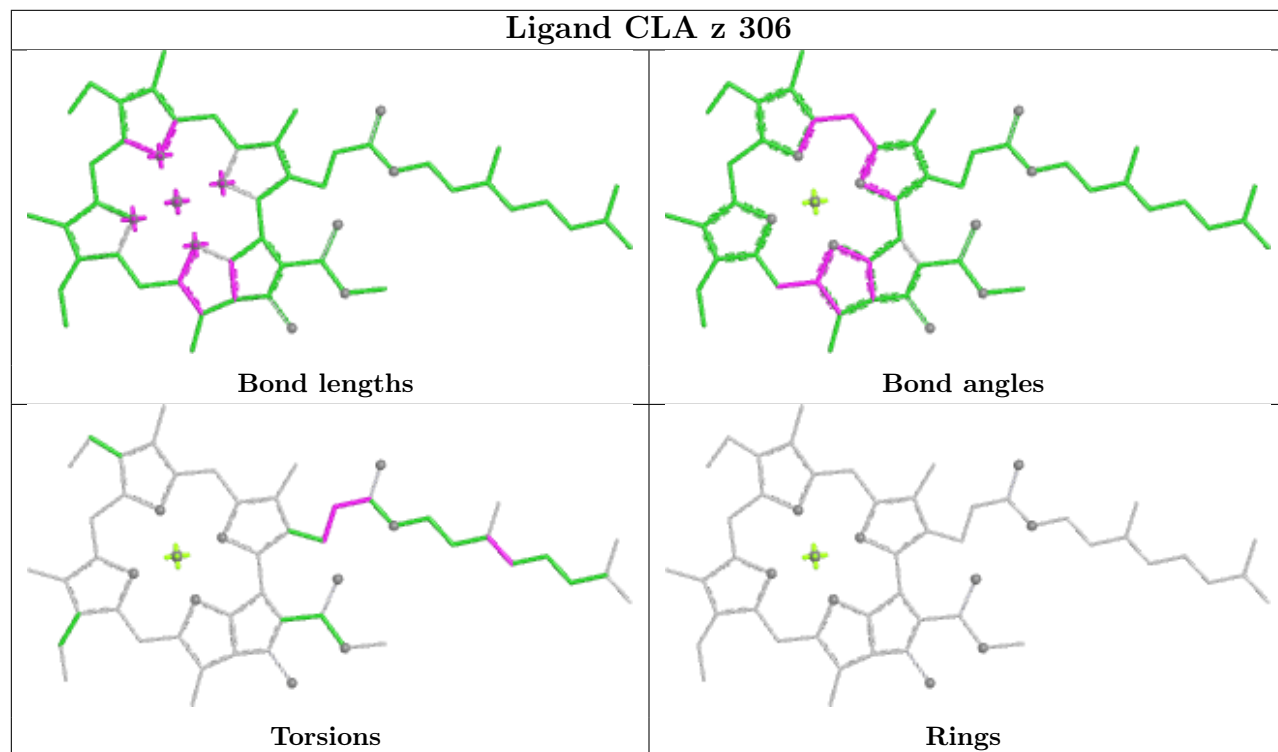


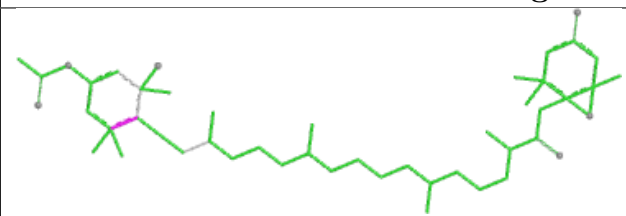
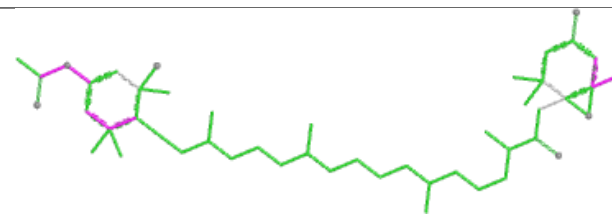
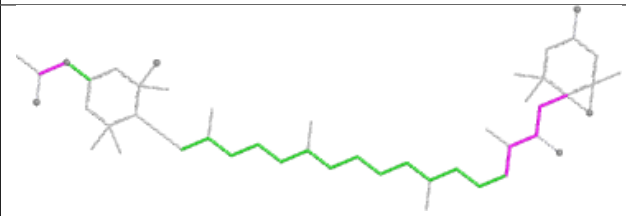
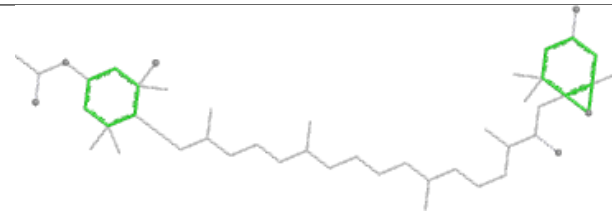


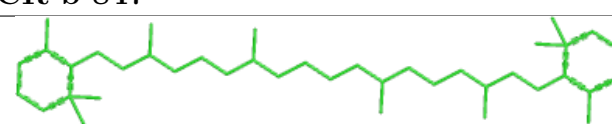
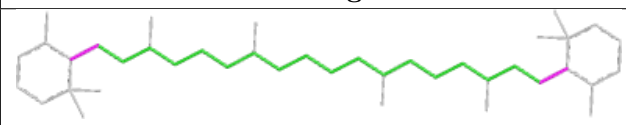
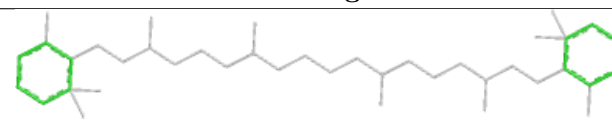
Ligand SQD P 319

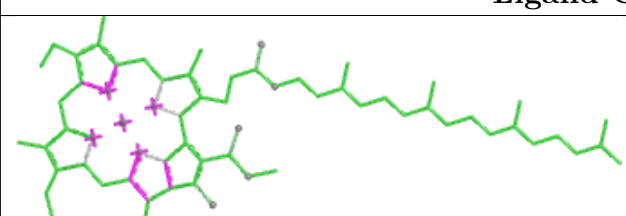
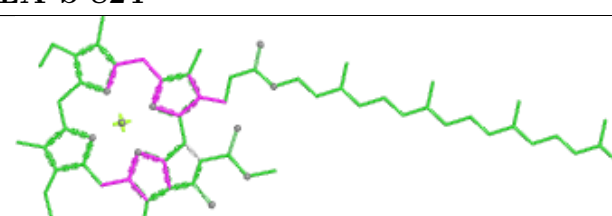
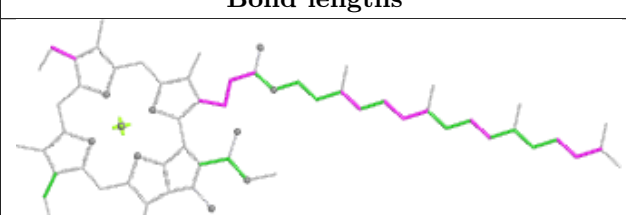
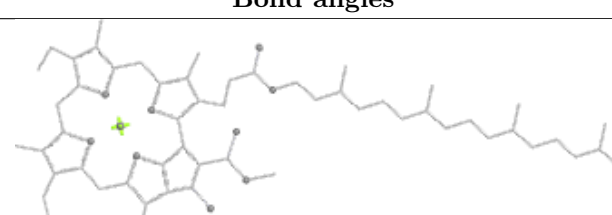


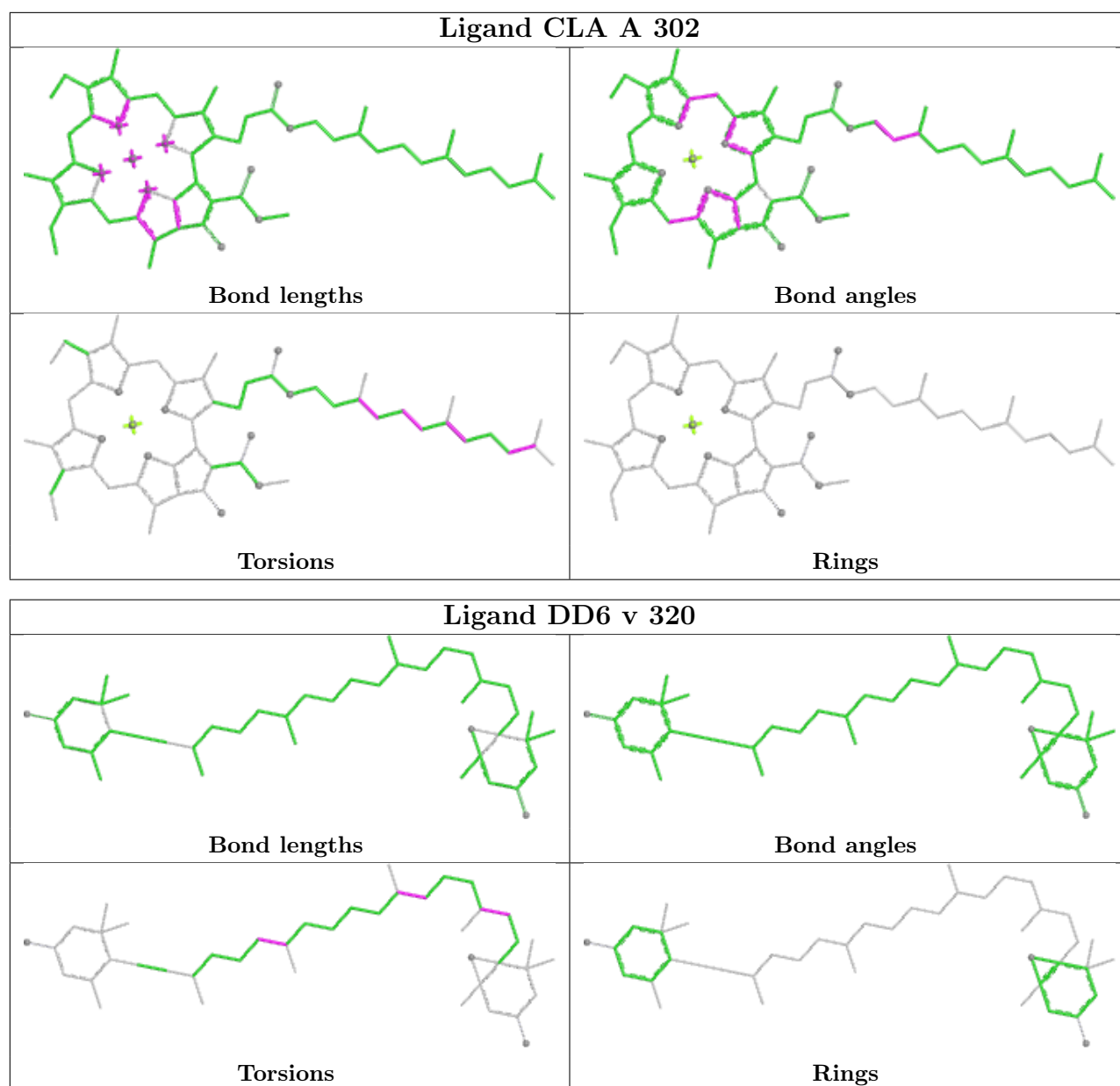
Ligand CLA z 306



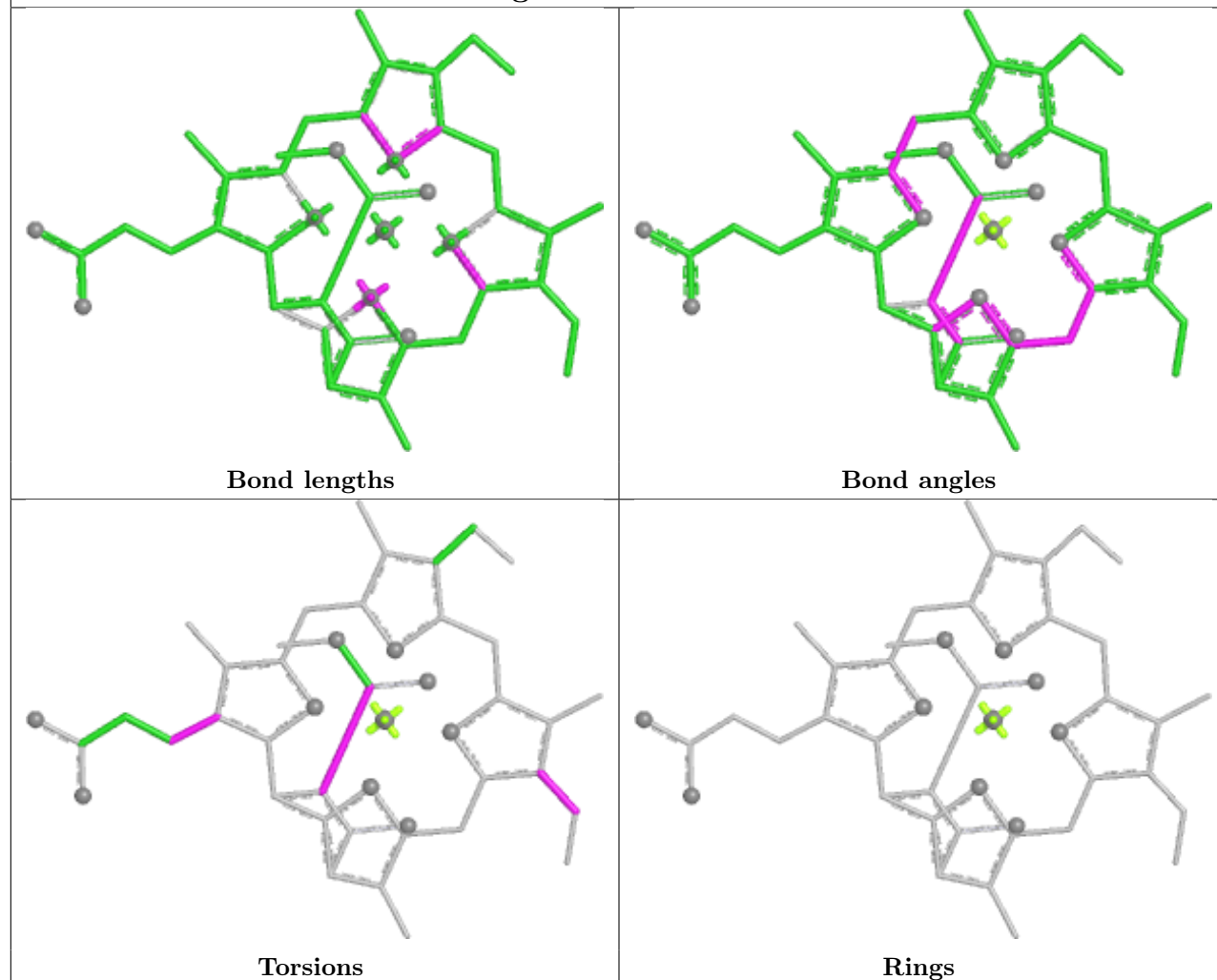
Ligand A86 o 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

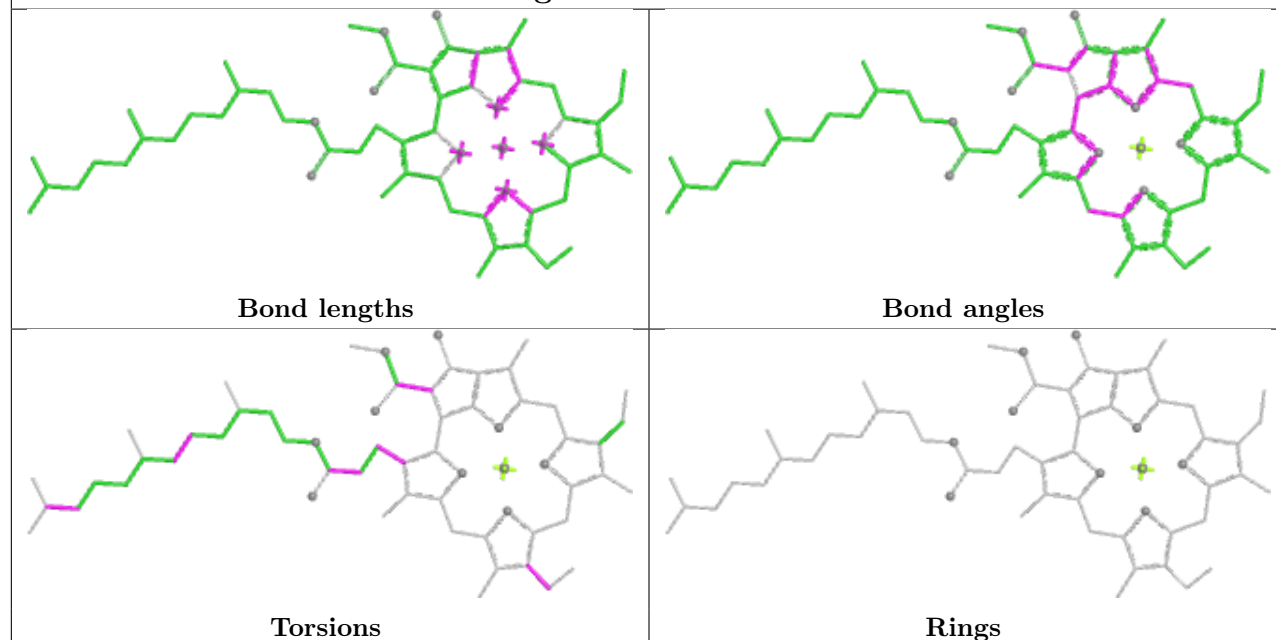
Ligand CLA b 824	
	
Bond lengths	Bond angles
	
Torsions	Rings



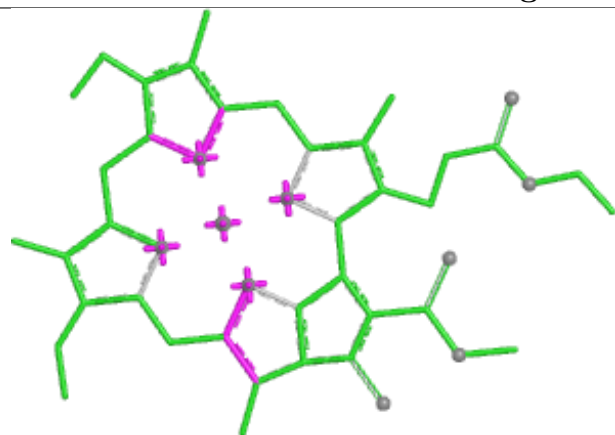
Ligand KC2 S 303



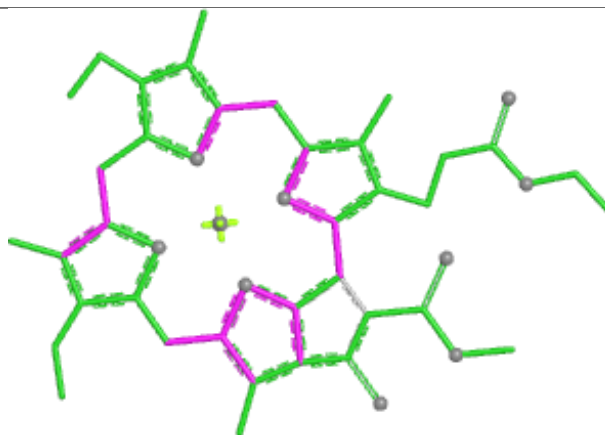
Ligand CLA Z 307



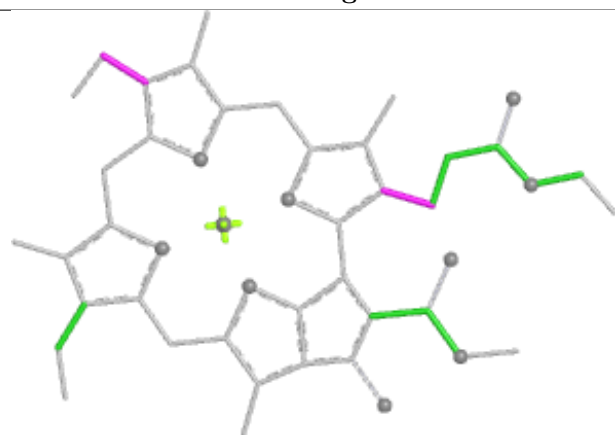
Ligand CLA J 303



Bond lengths



Bond angles

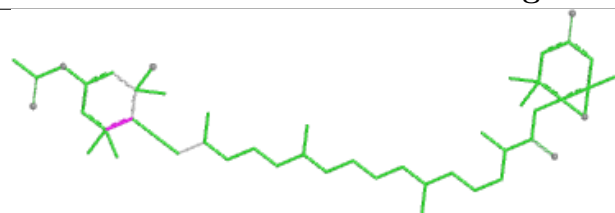


Torsions

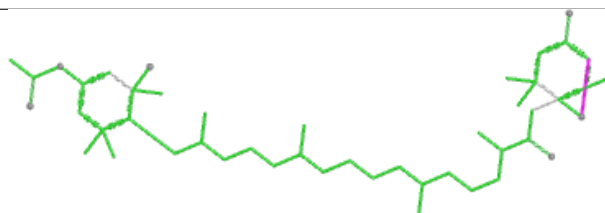


Rings

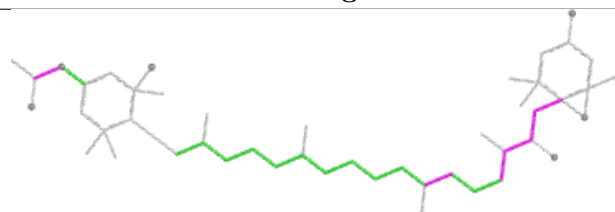
Ligand A86 T 315



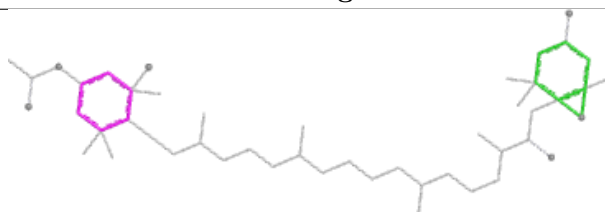
Bond lengths



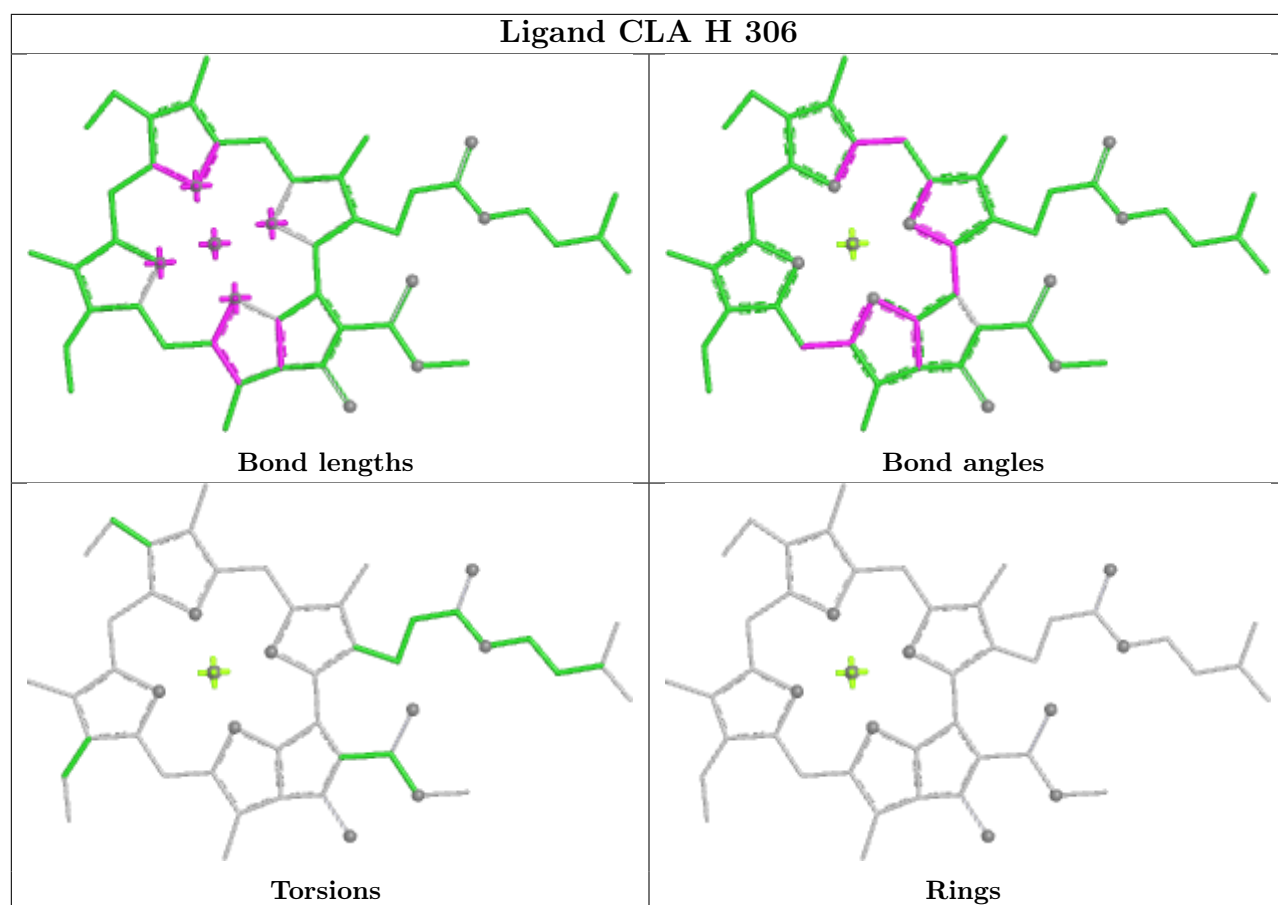
Bond angles



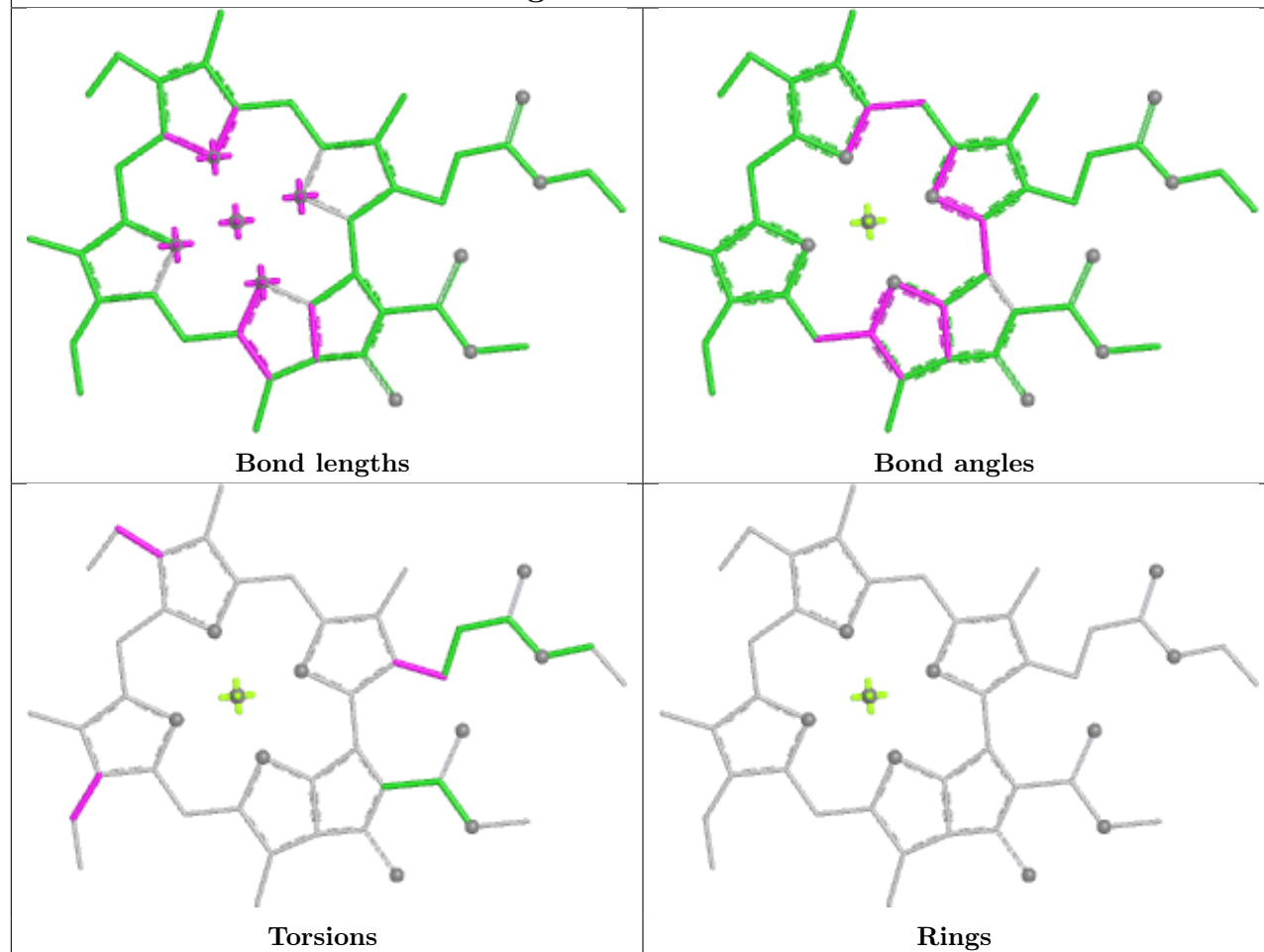
Torsions



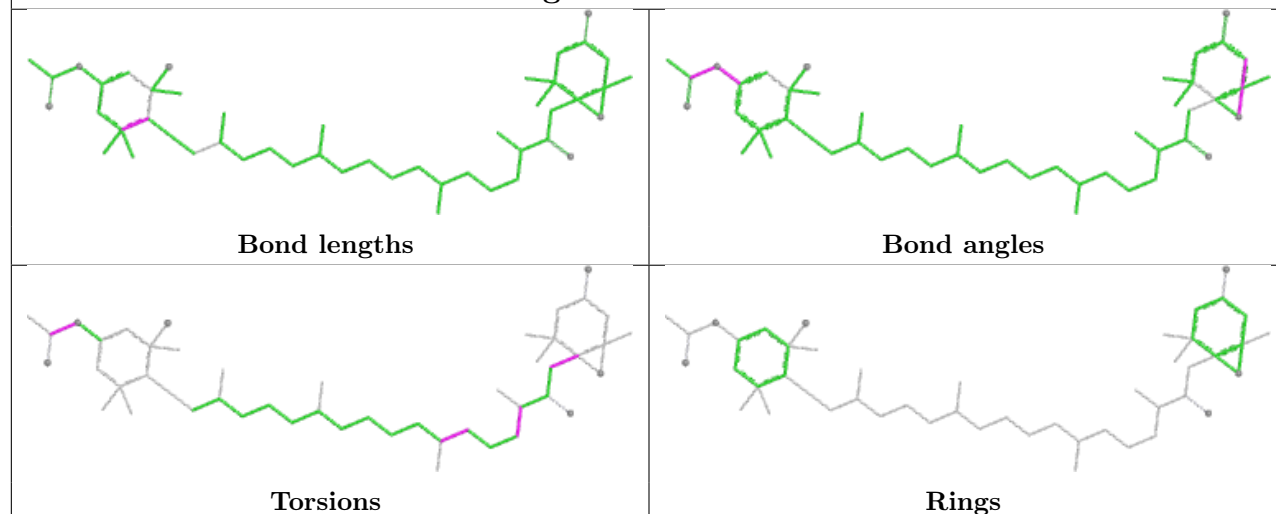
Rings



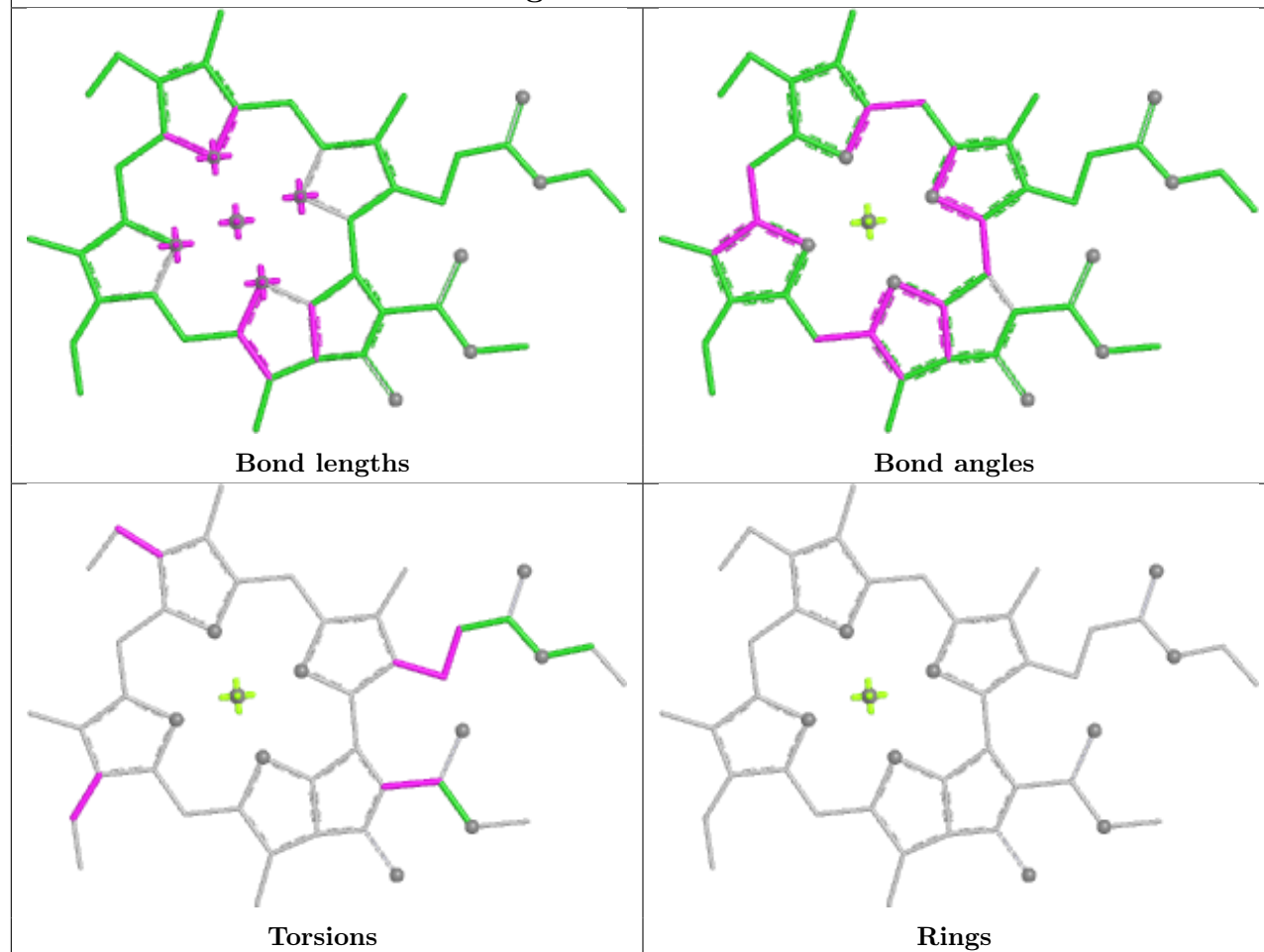
Ligand CLA C 302



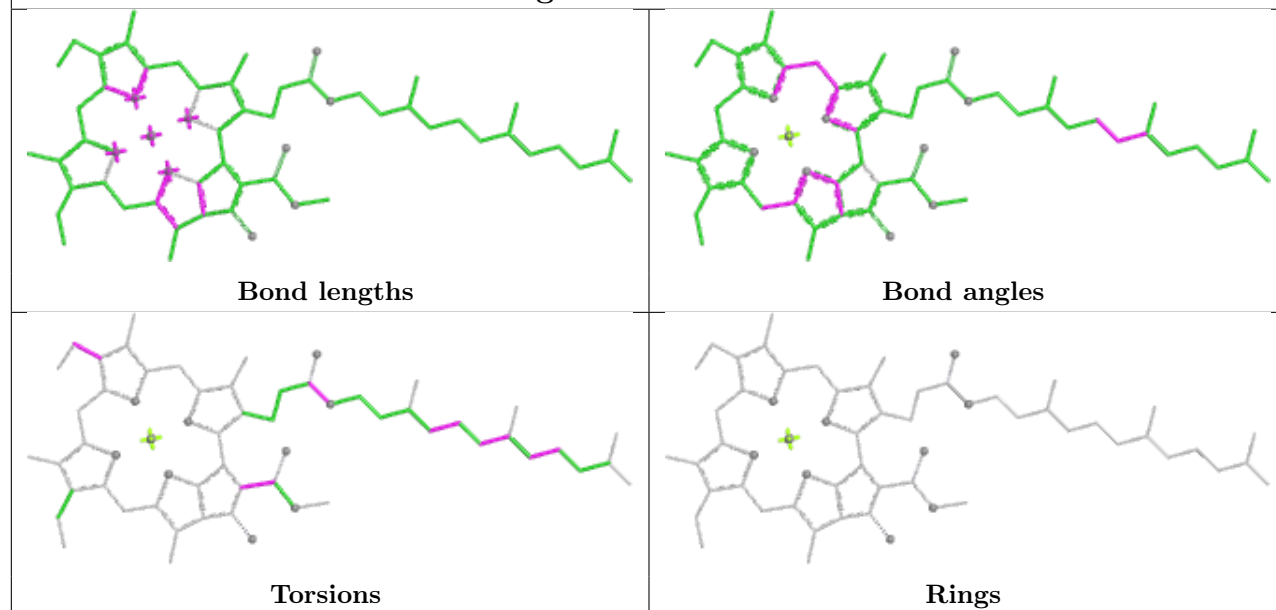
Ligand A86 z 317

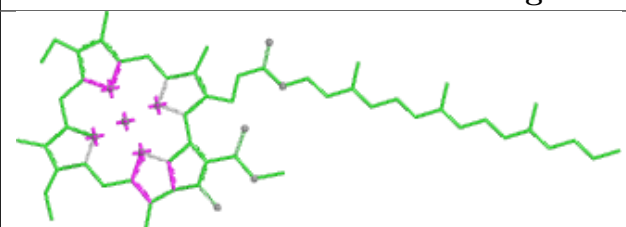
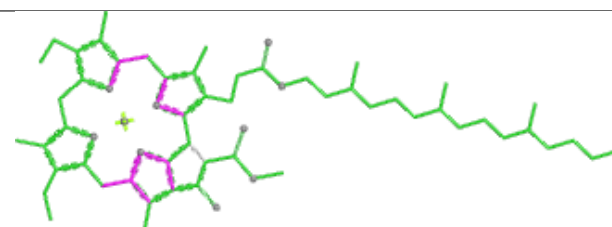
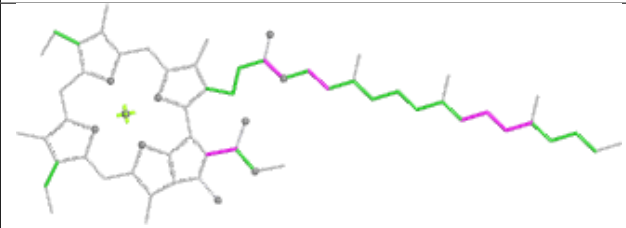
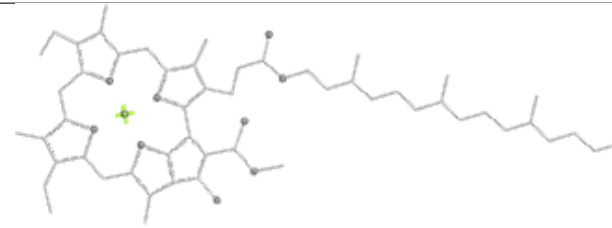
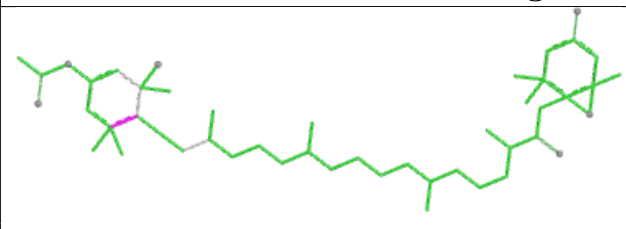
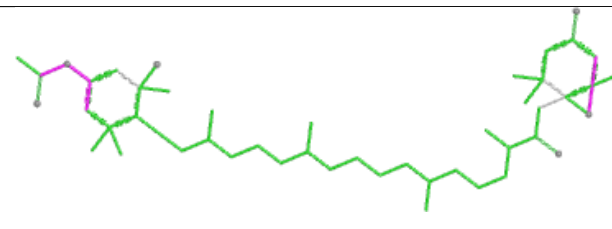
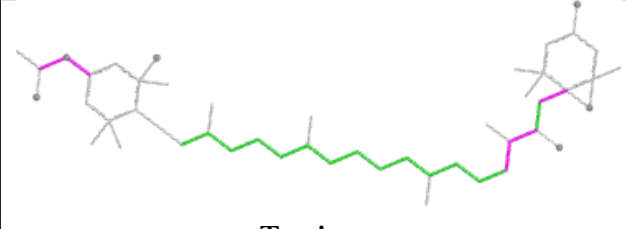
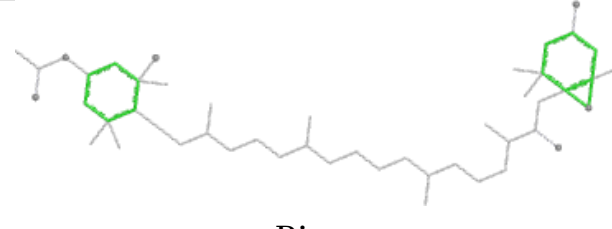
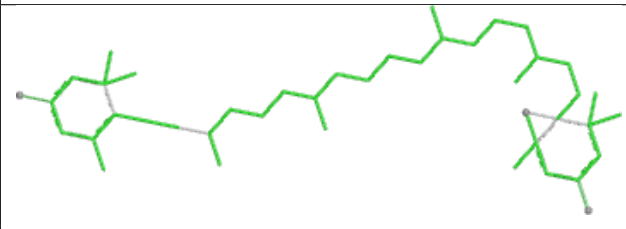
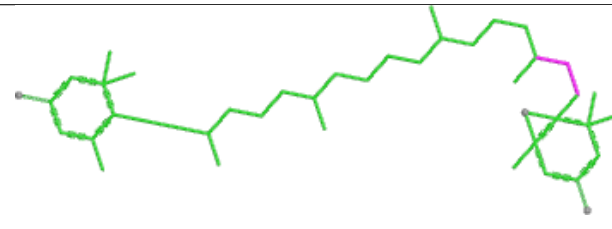
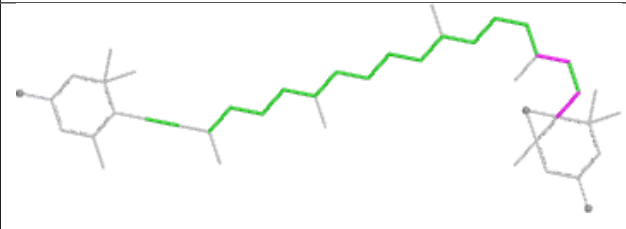
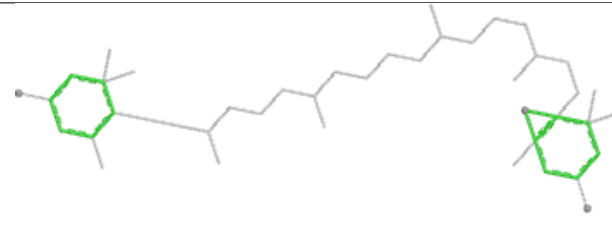


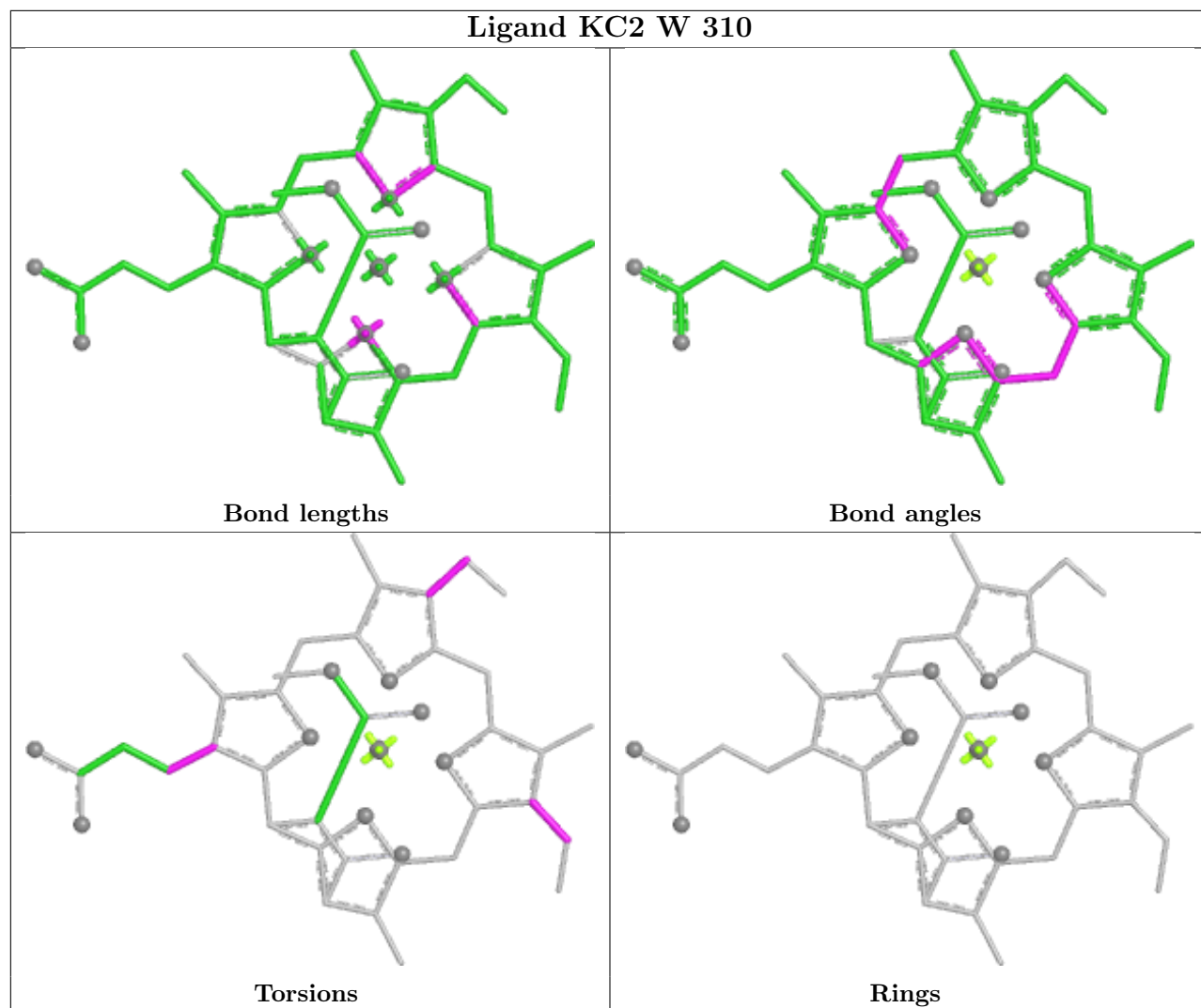
Ligand CLA G 213



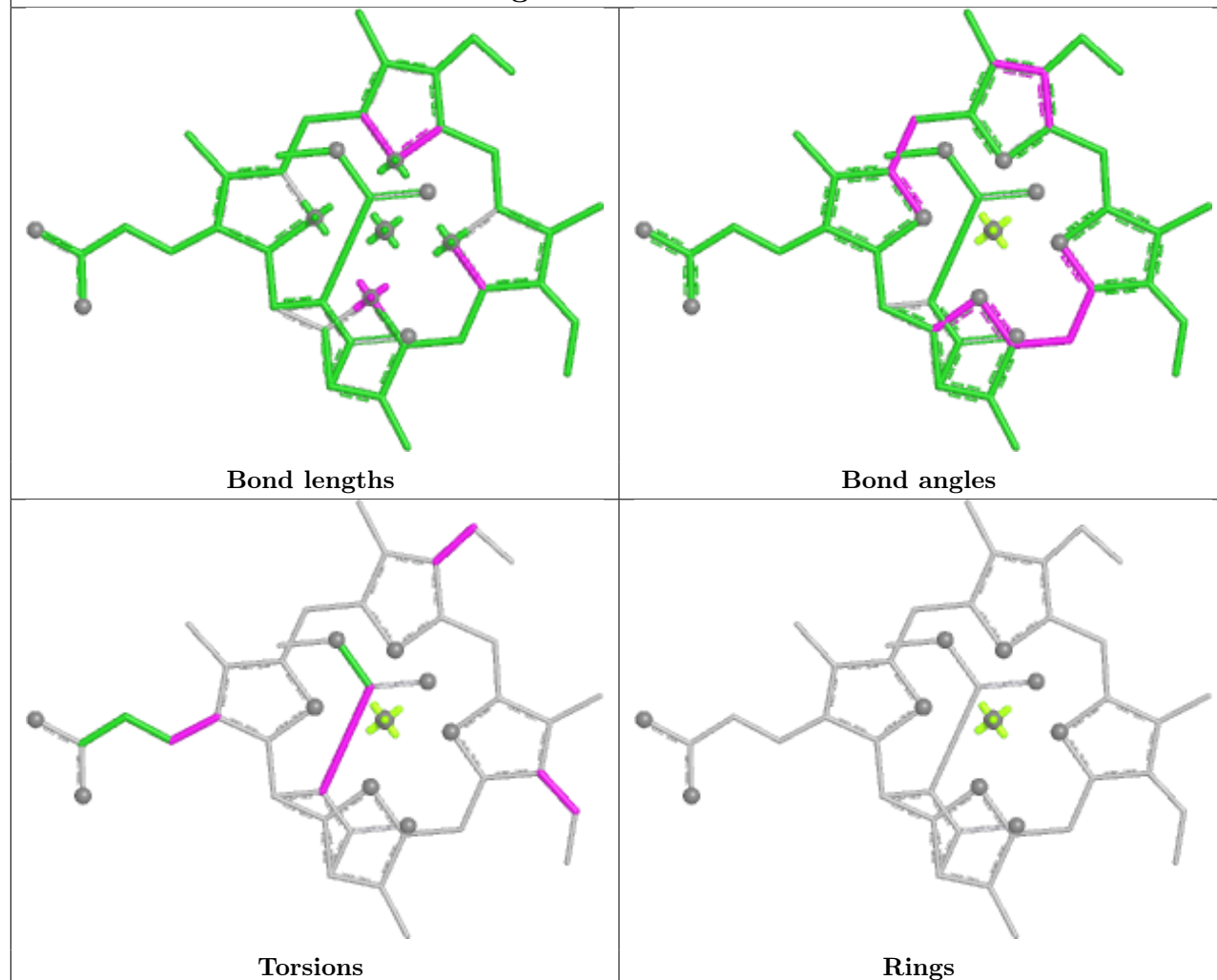
Ligand CLA a 833



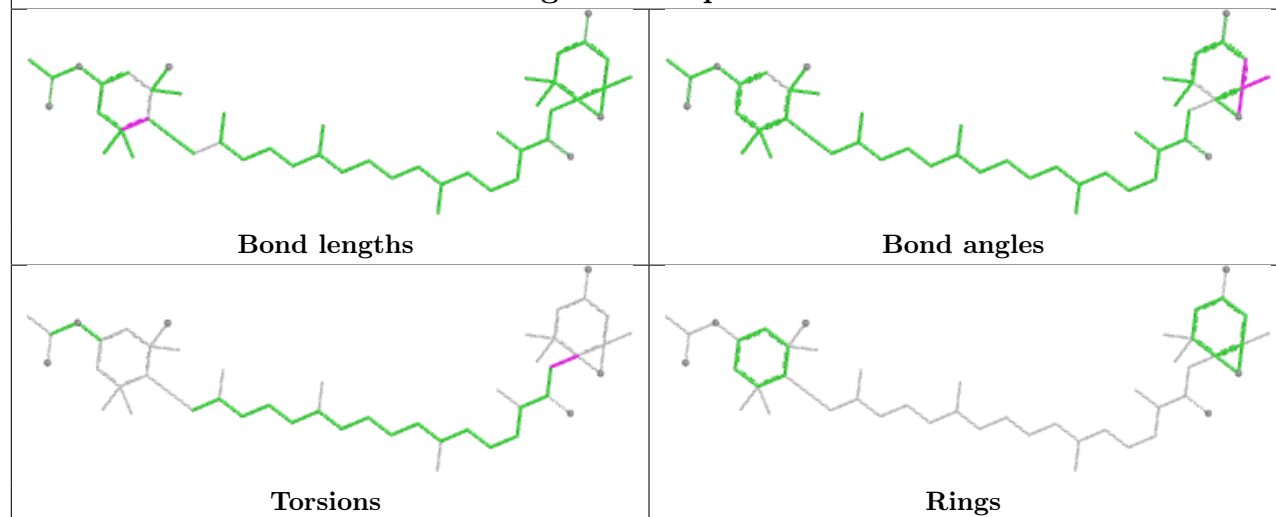
Ligand CLA o 311	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A86 R 315	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DD6 F 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

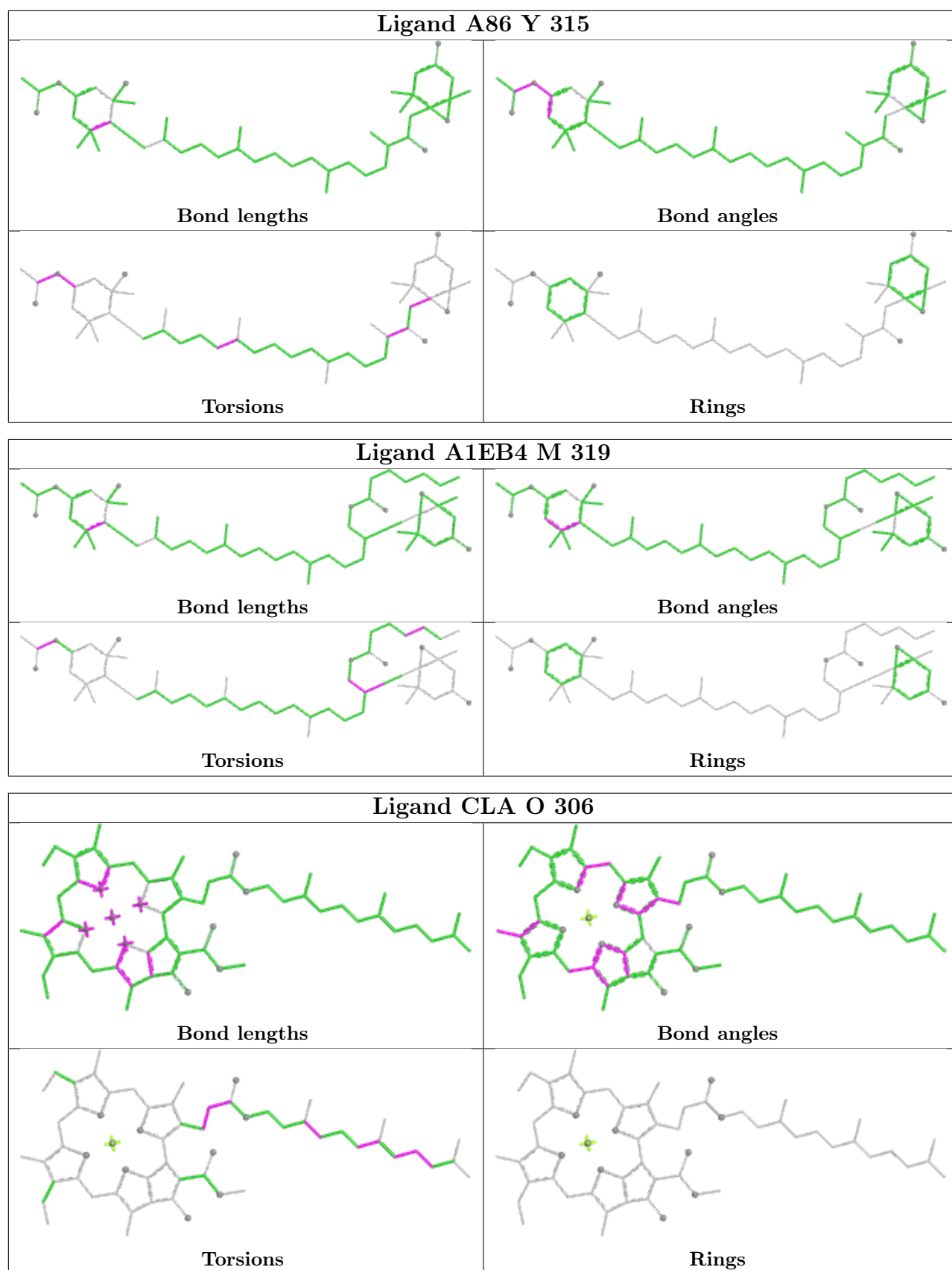


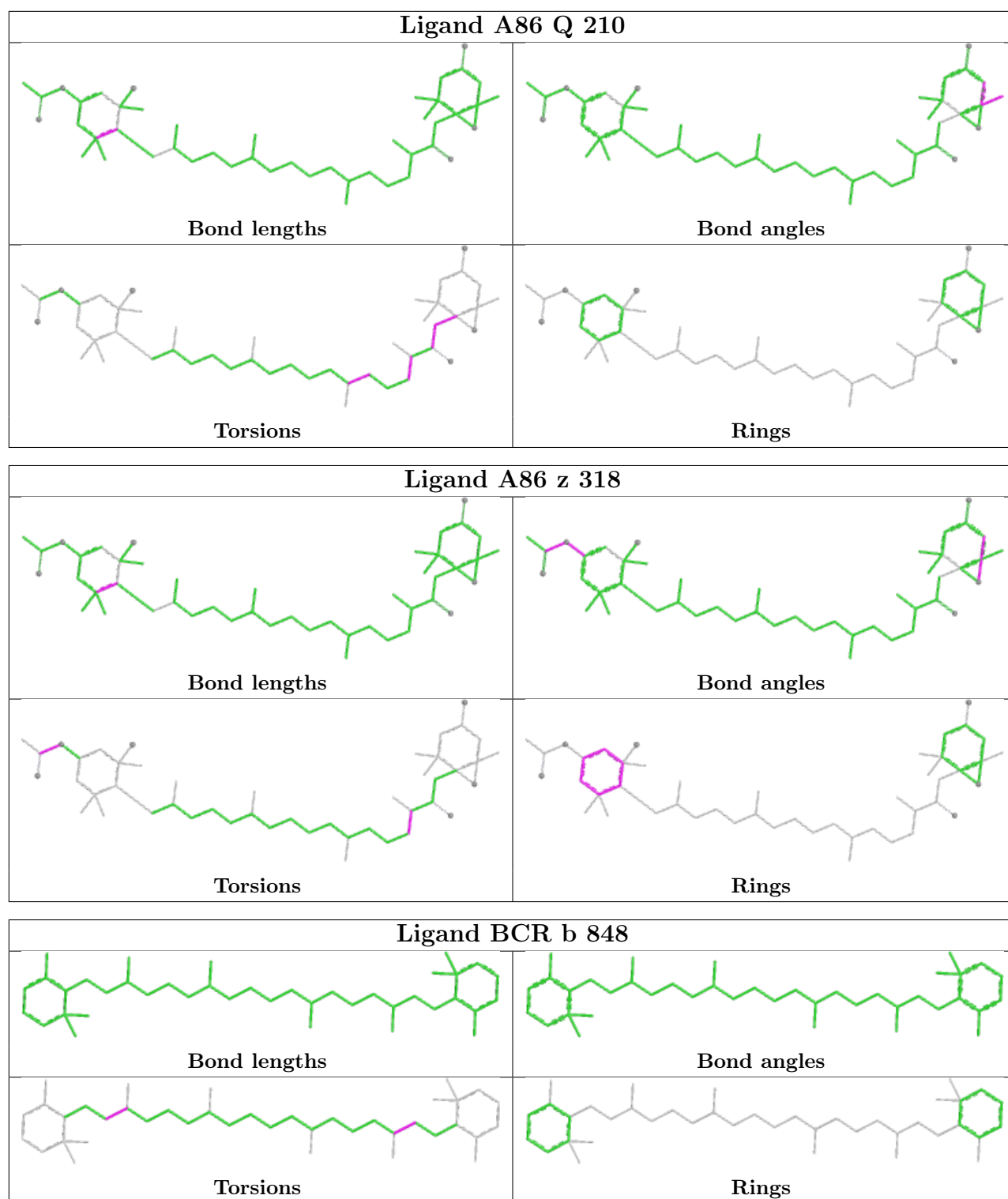
Ligand KC2 L 302

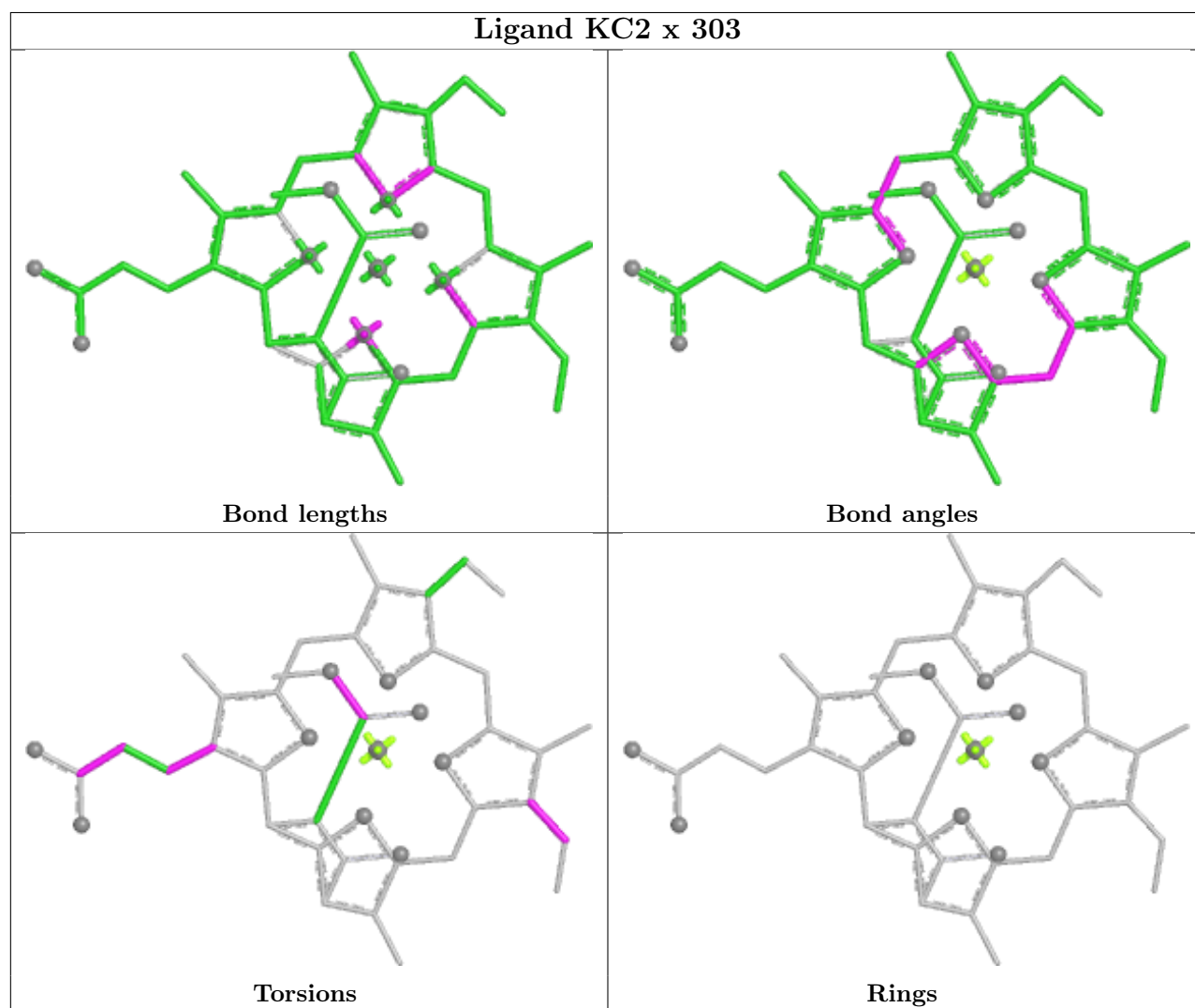
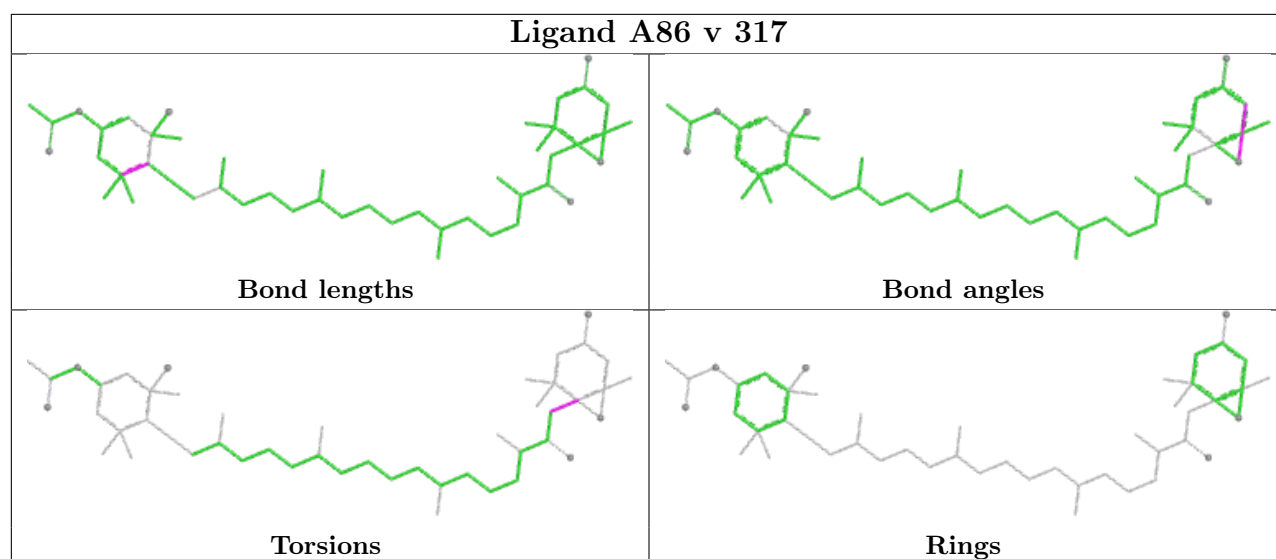


Ligand A86 p 317

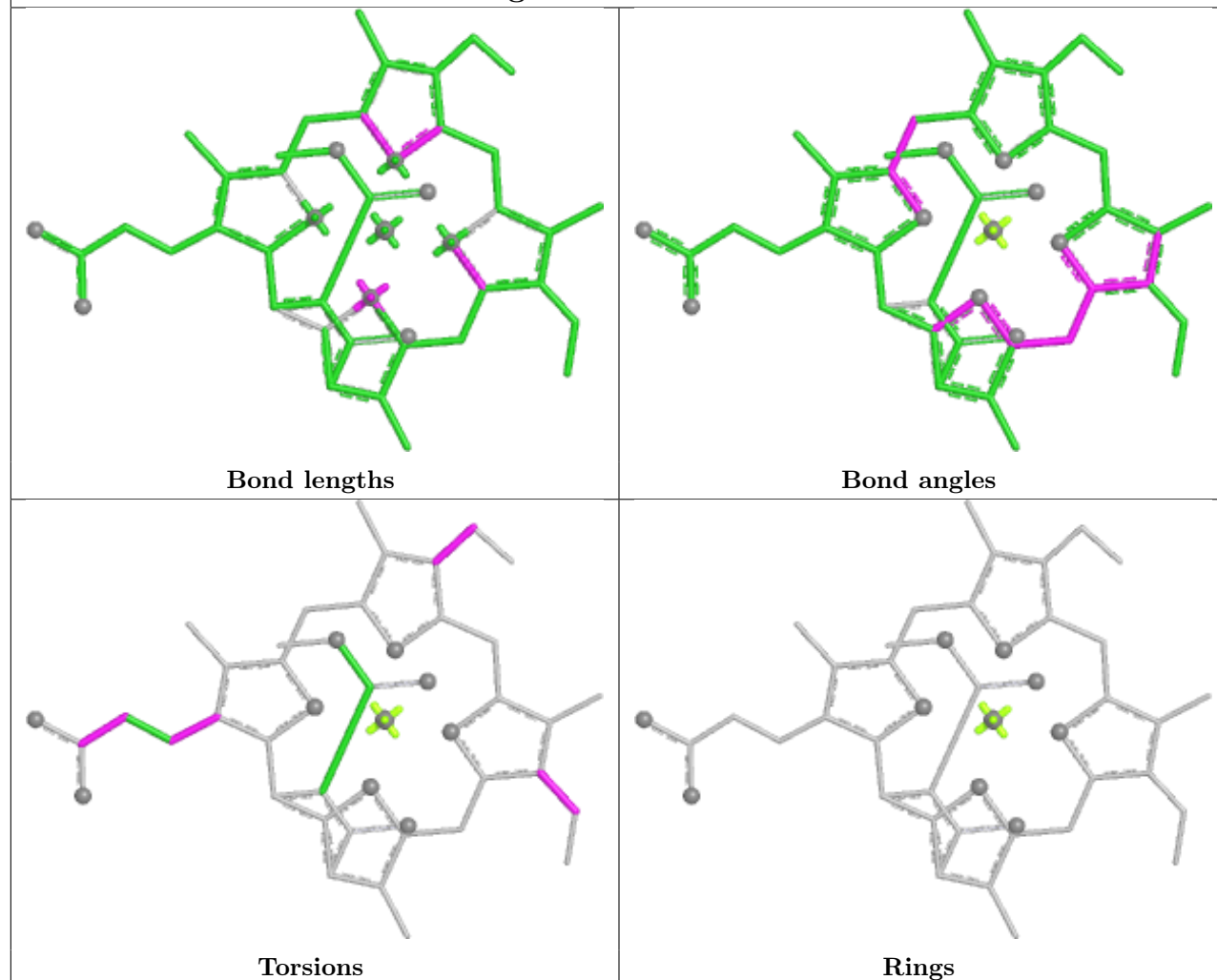




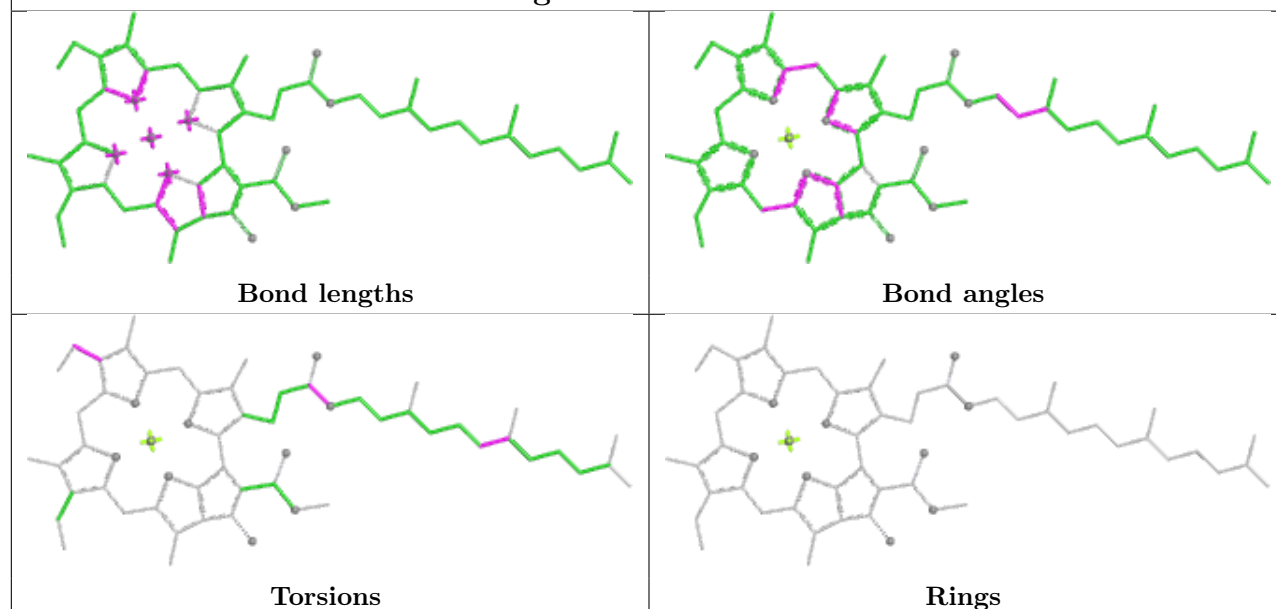




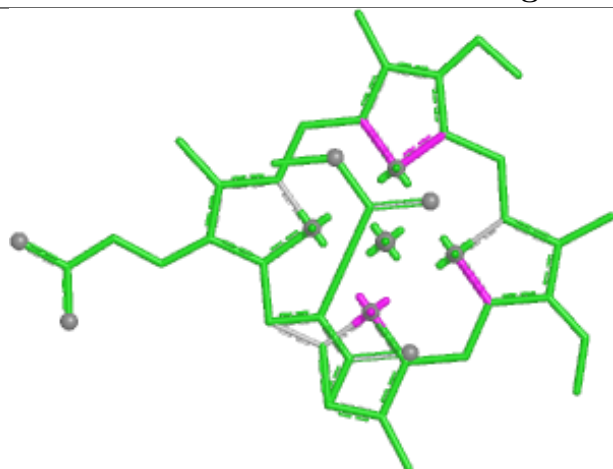
Ligand KC2 K 309



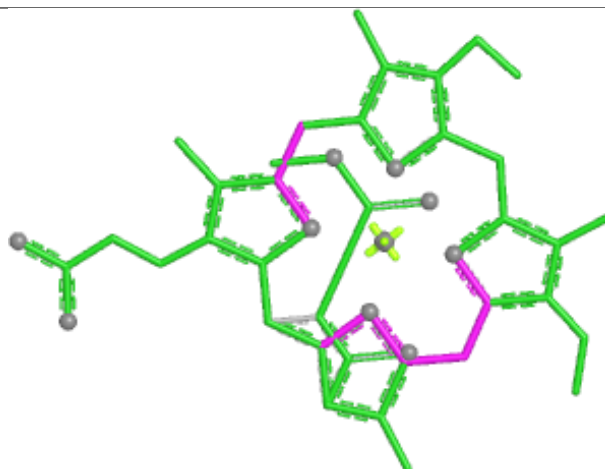
Ligand CLA E 310



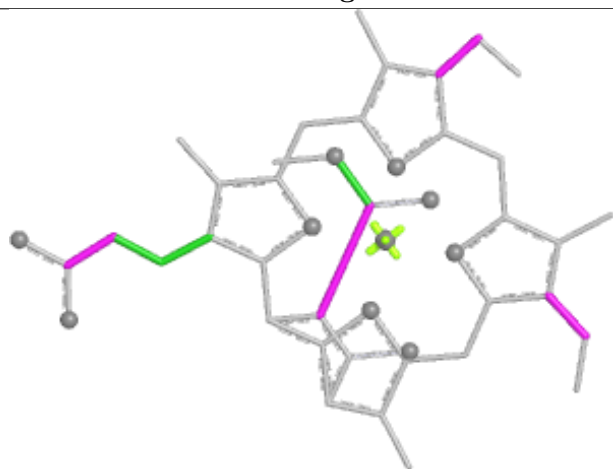
Ligand KC2 z 310



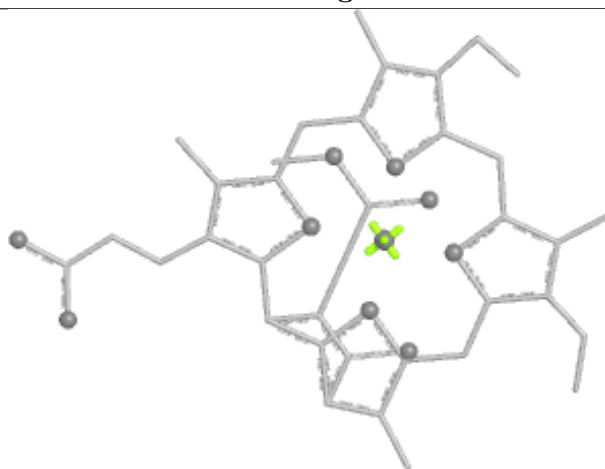
Bond lengths



Bond angles

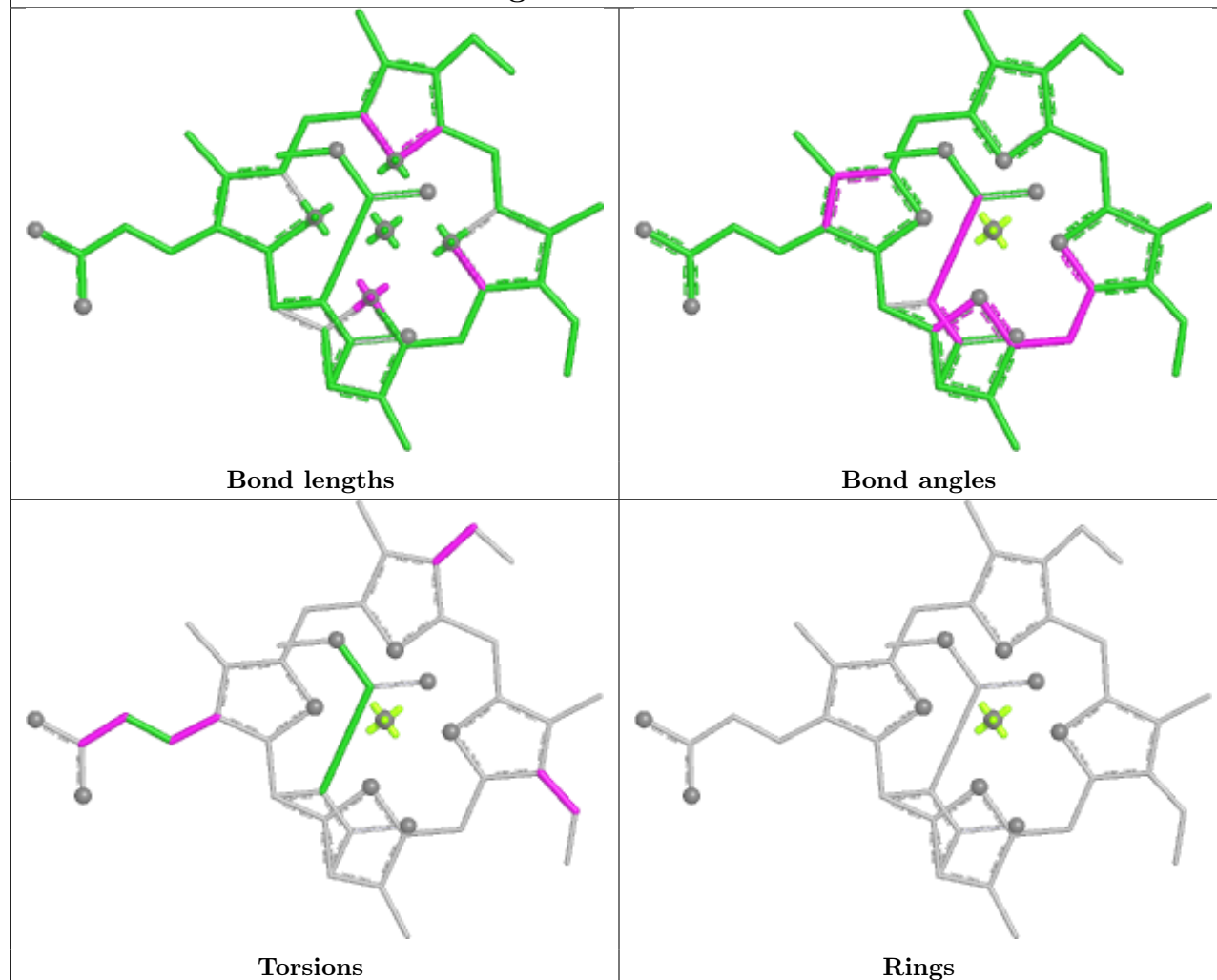


Torsions

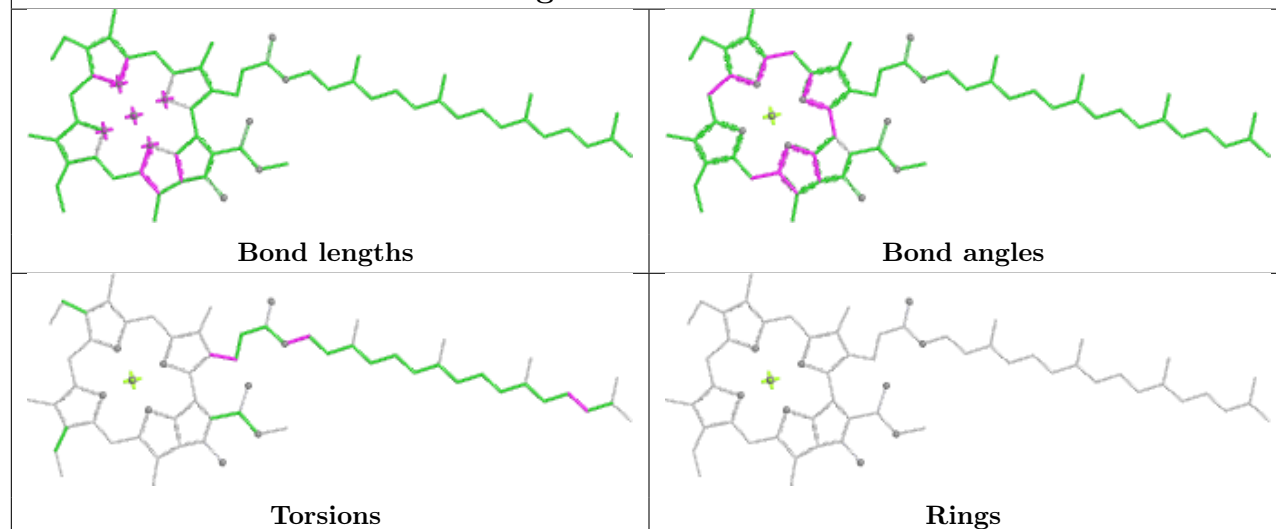


Rings

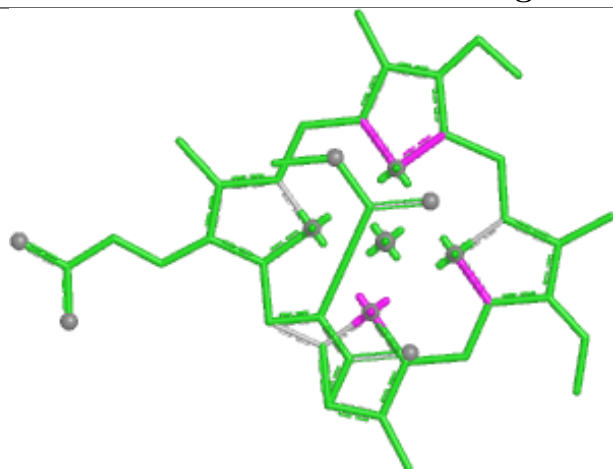
Ligand KC2 R 309



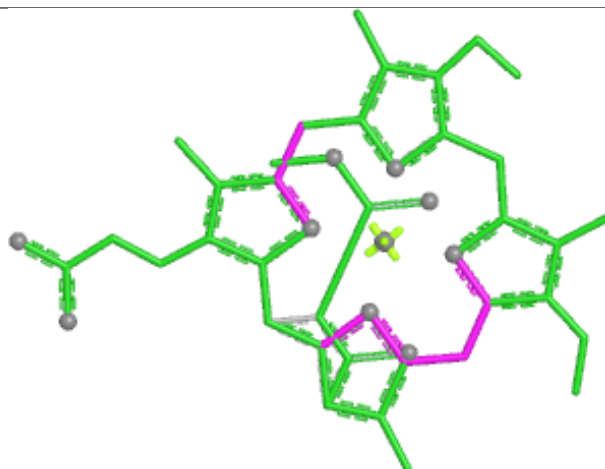
Ligand CLA a 850



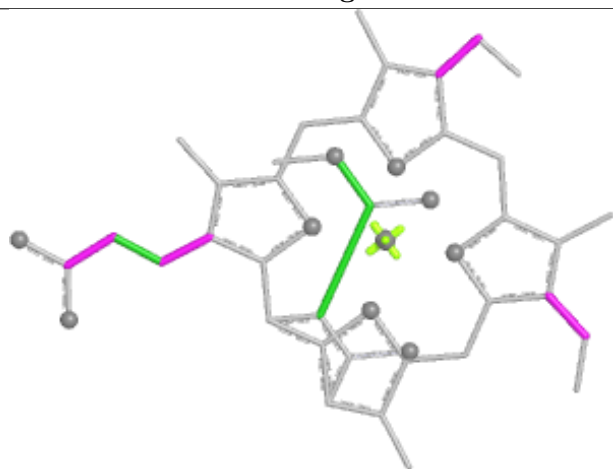
Ligand KC2 N 312



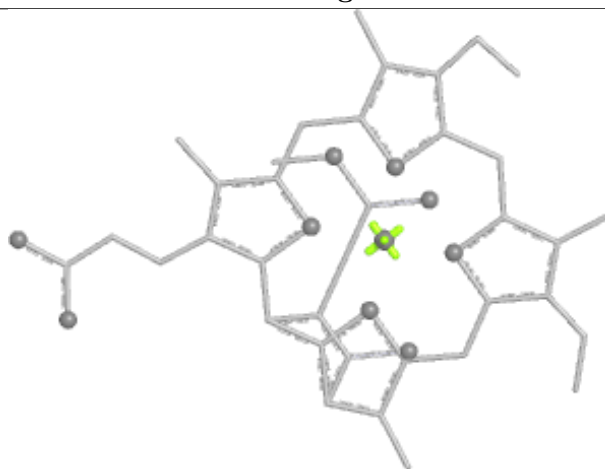
Bond lengths



Bond angles

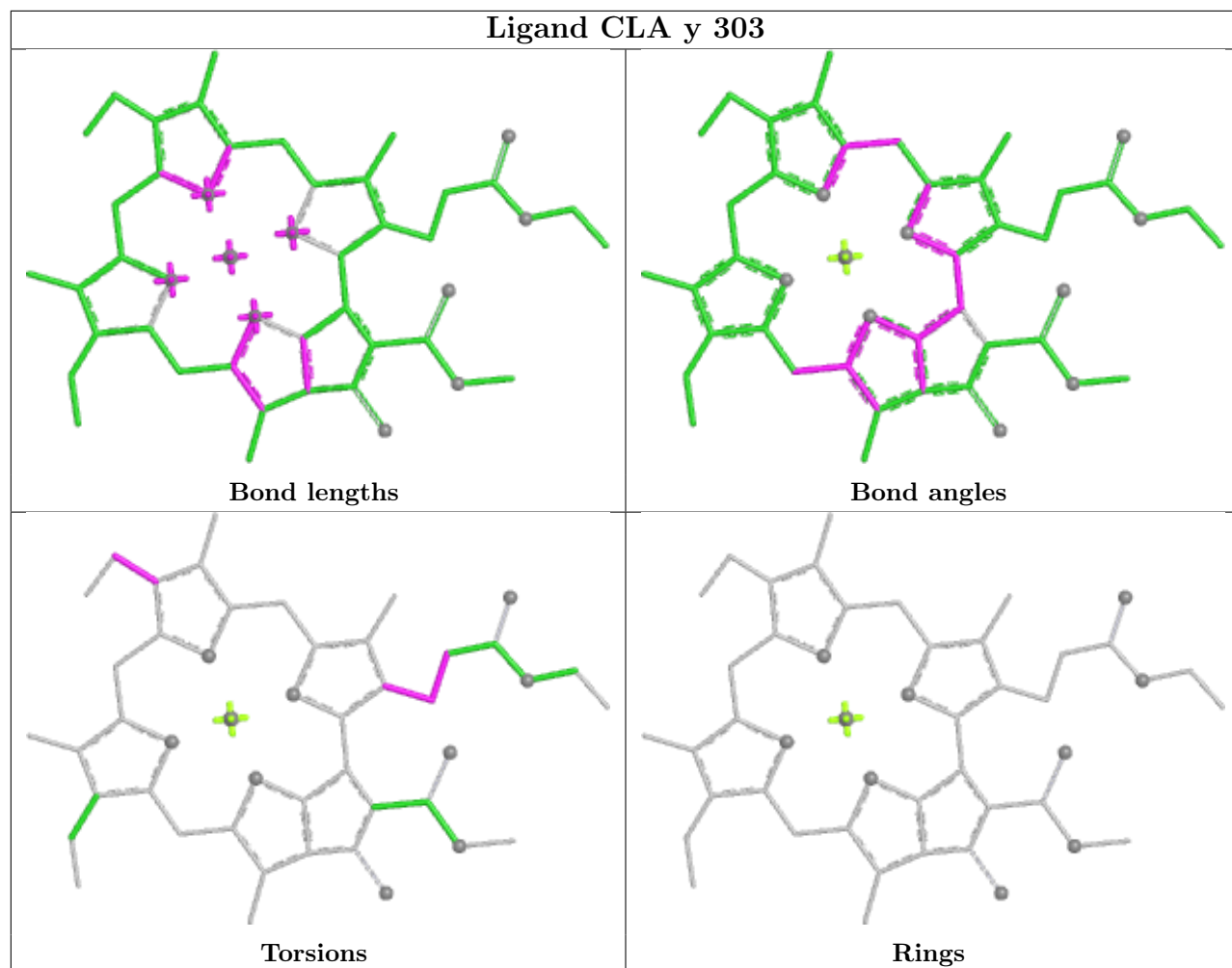


Torsions

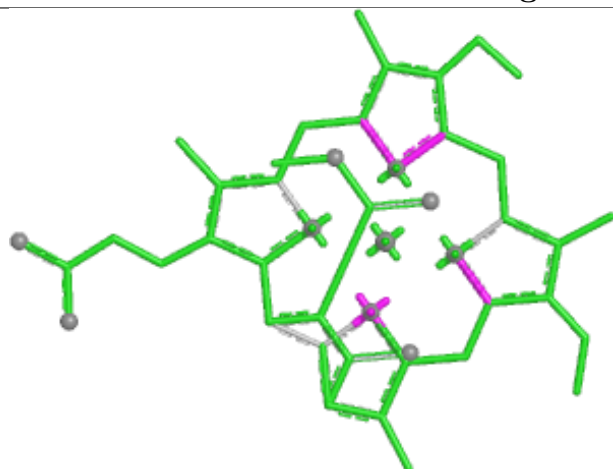


Rings

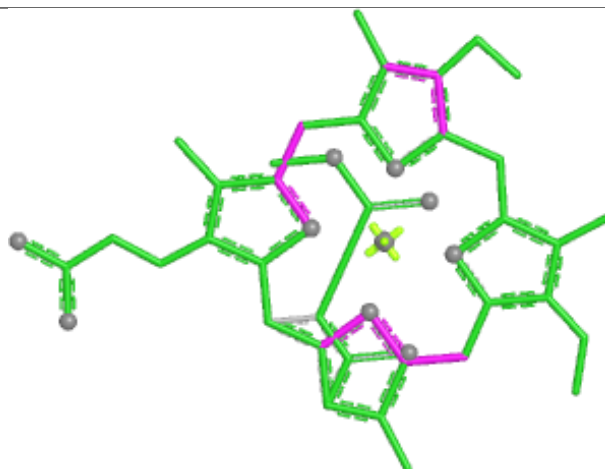
Ligand CLA y 303



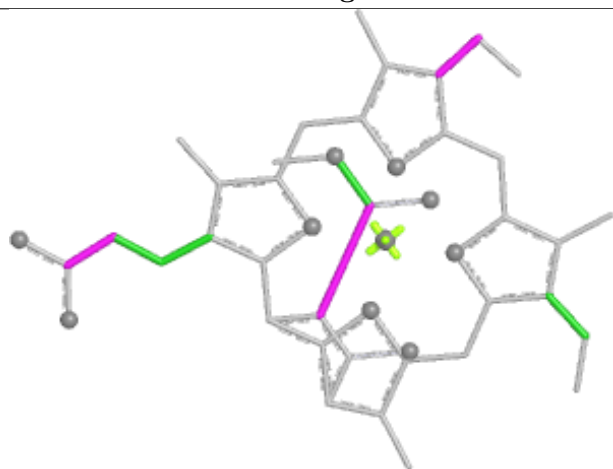
Ligand KC2 v 303



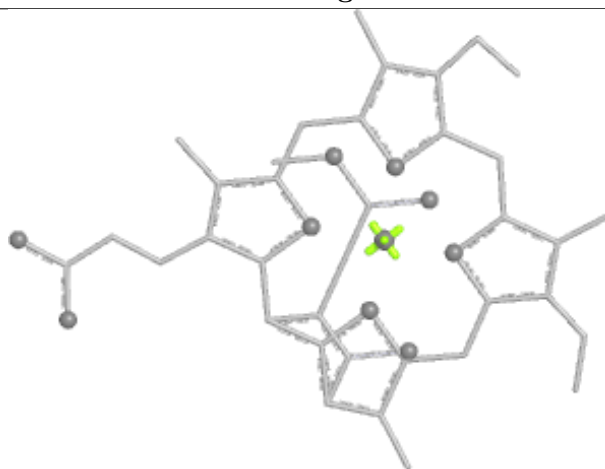
Bond lengths



Bond angles

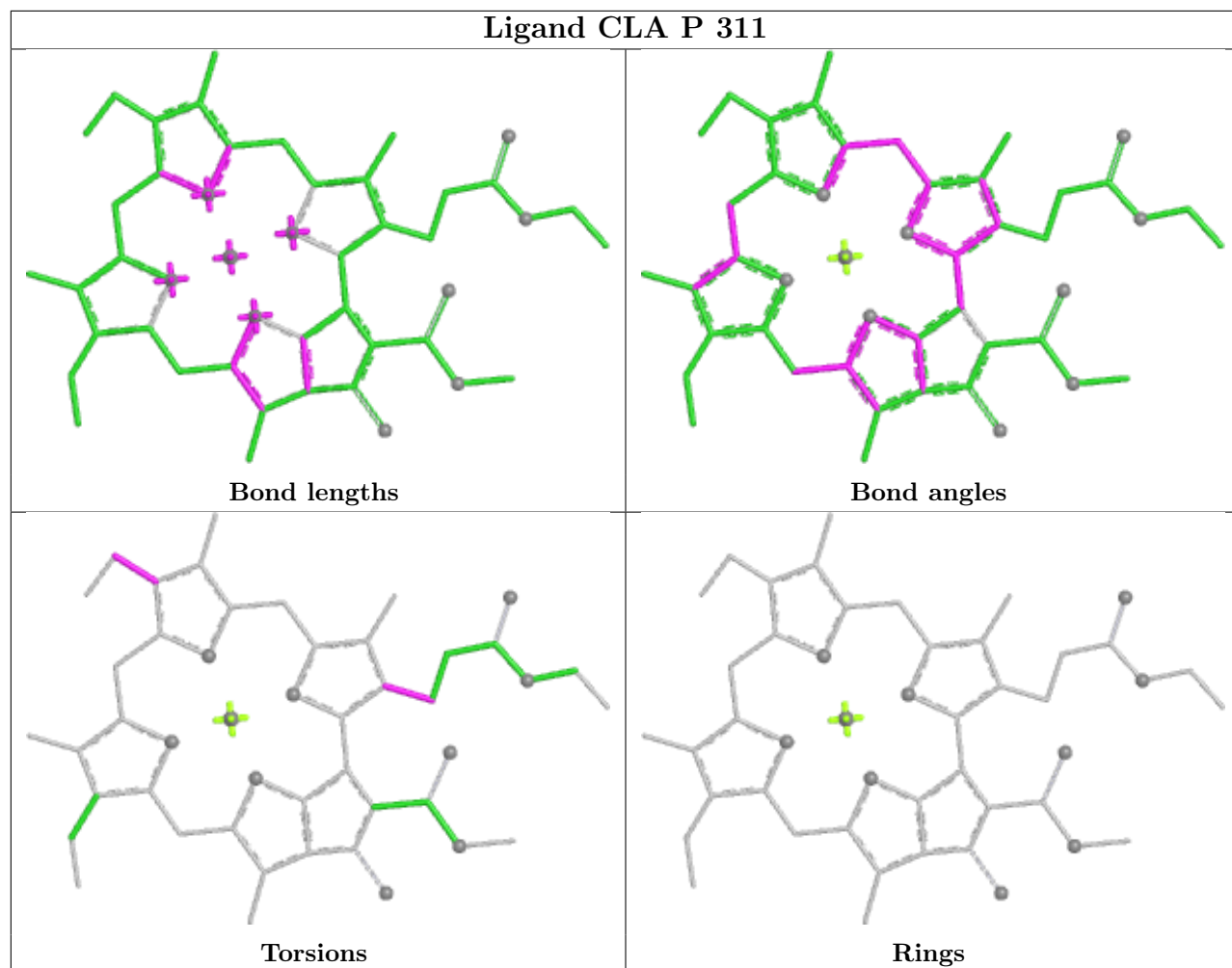


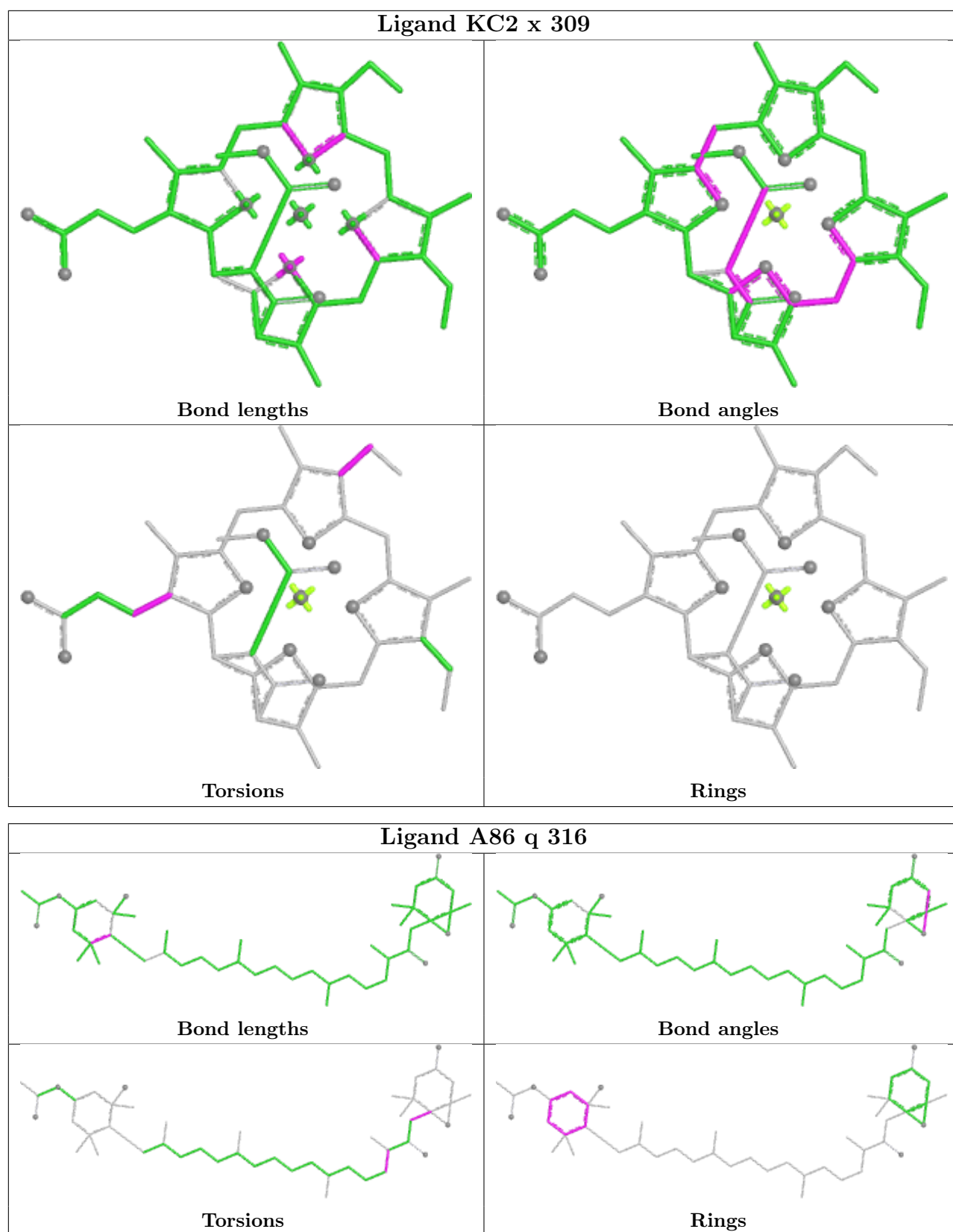
Torsions



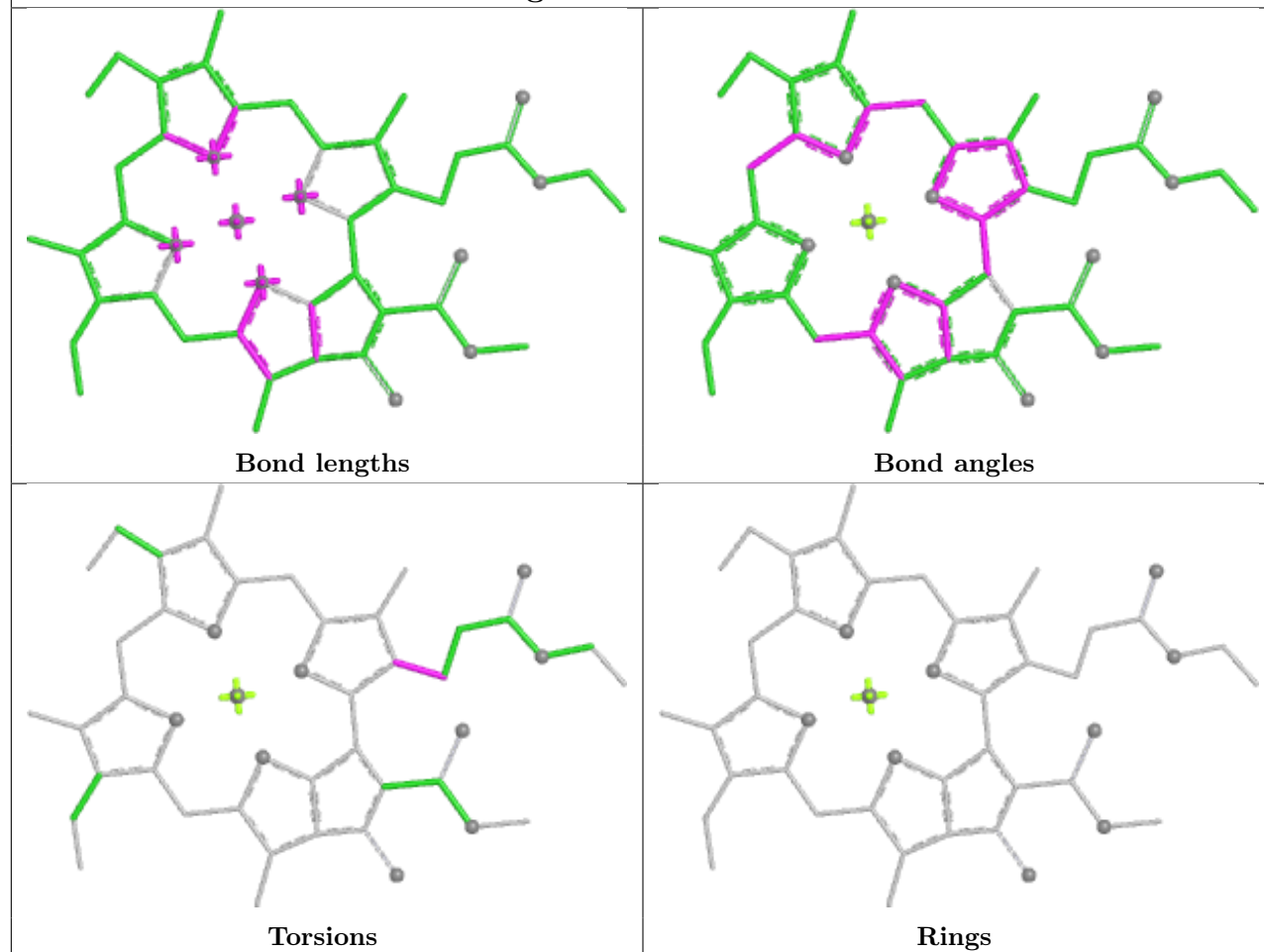
Rings

Ligand CLA P 311

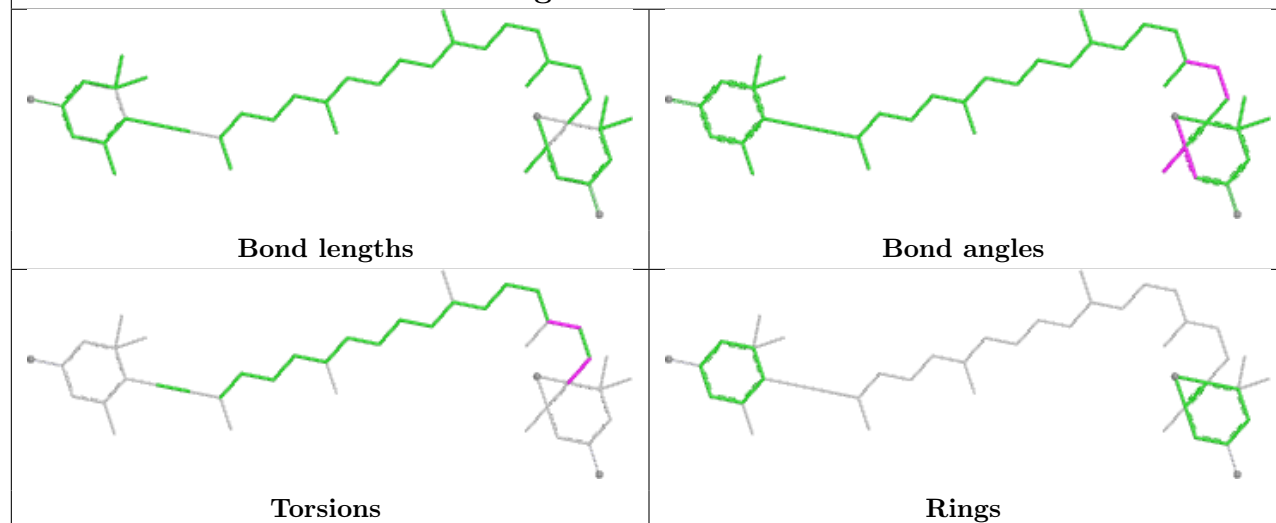


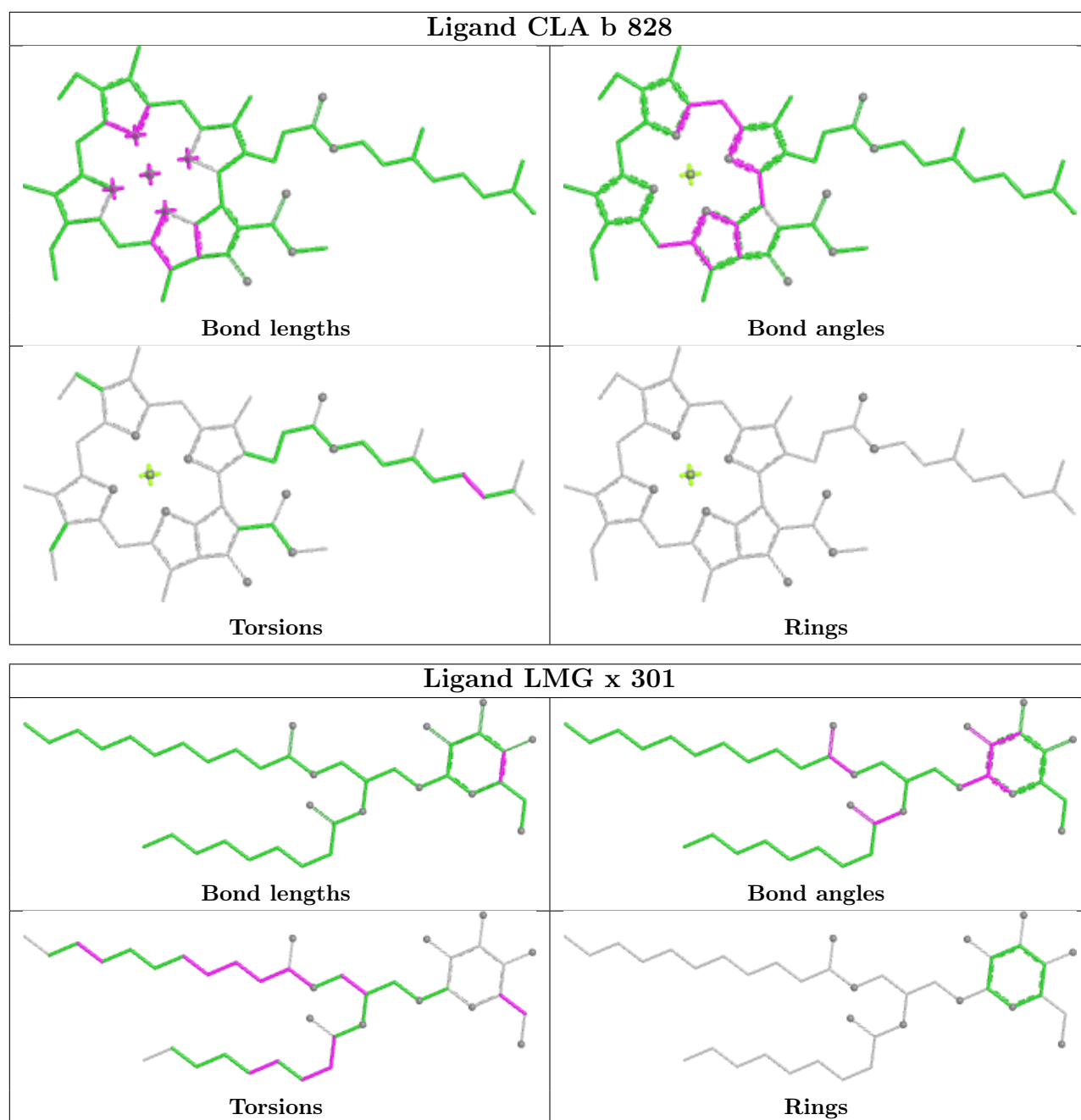


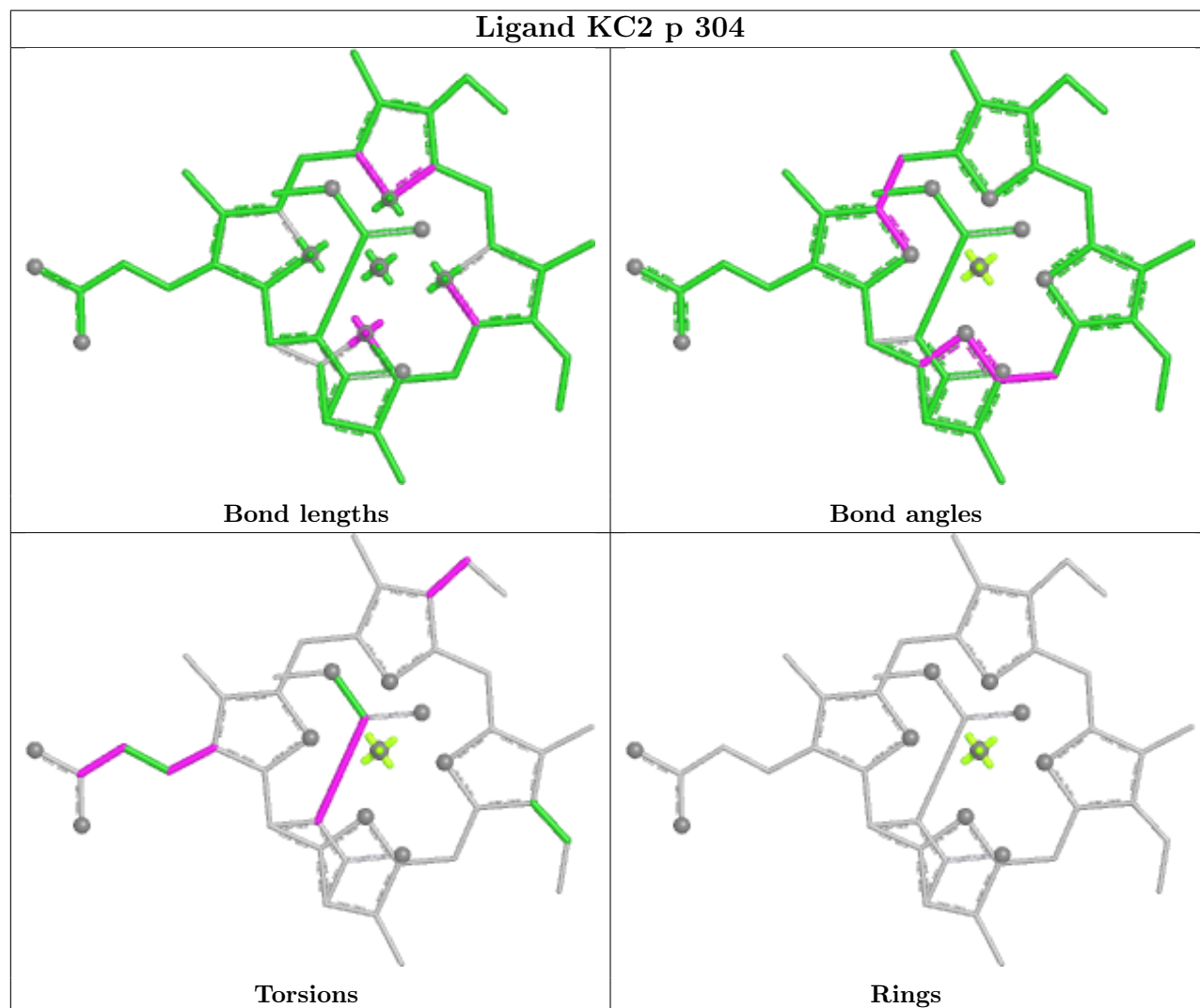
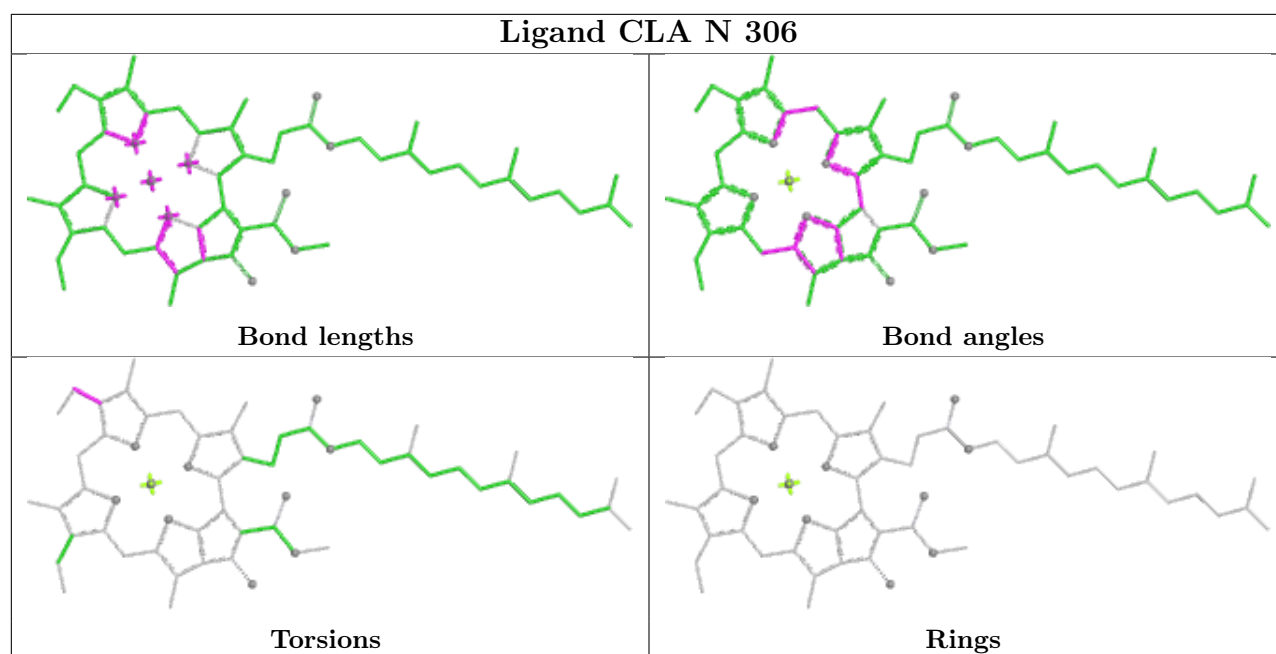
Ligand CLA Y 312



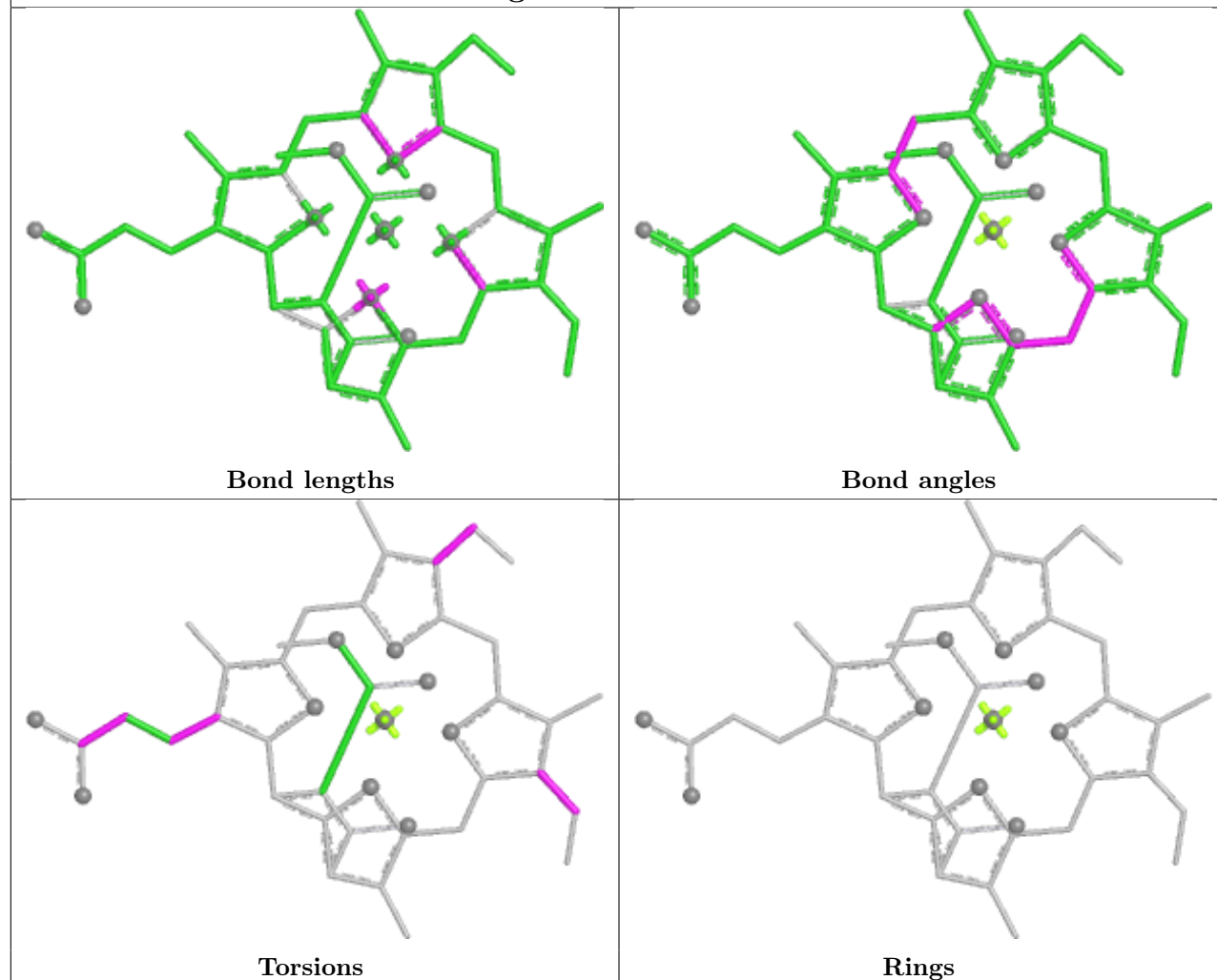
Ligand DD6 E 318



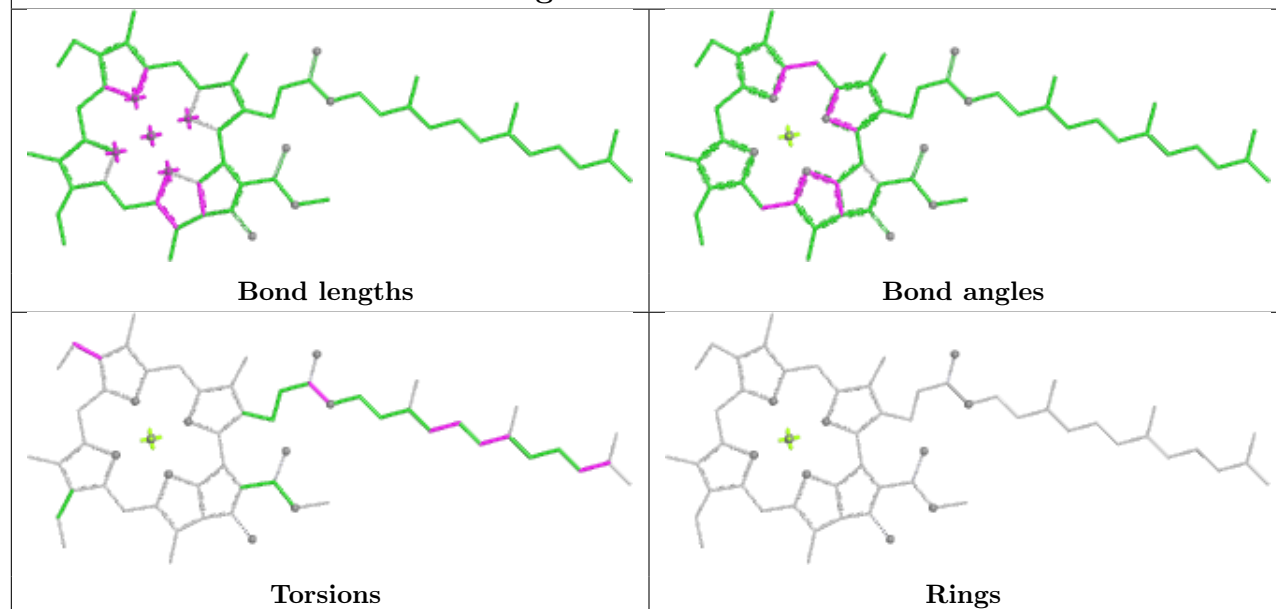


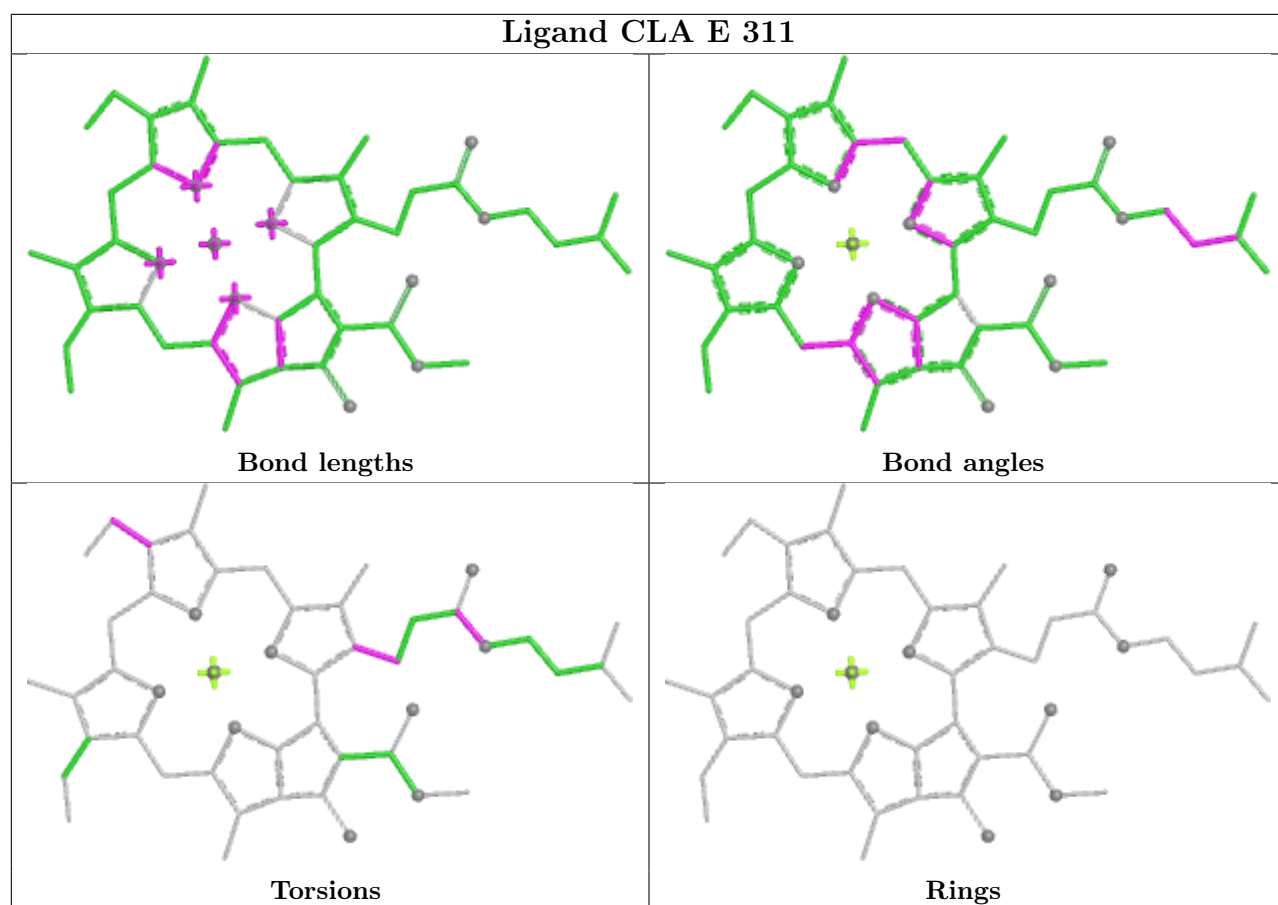


Ligand KC2 N 308

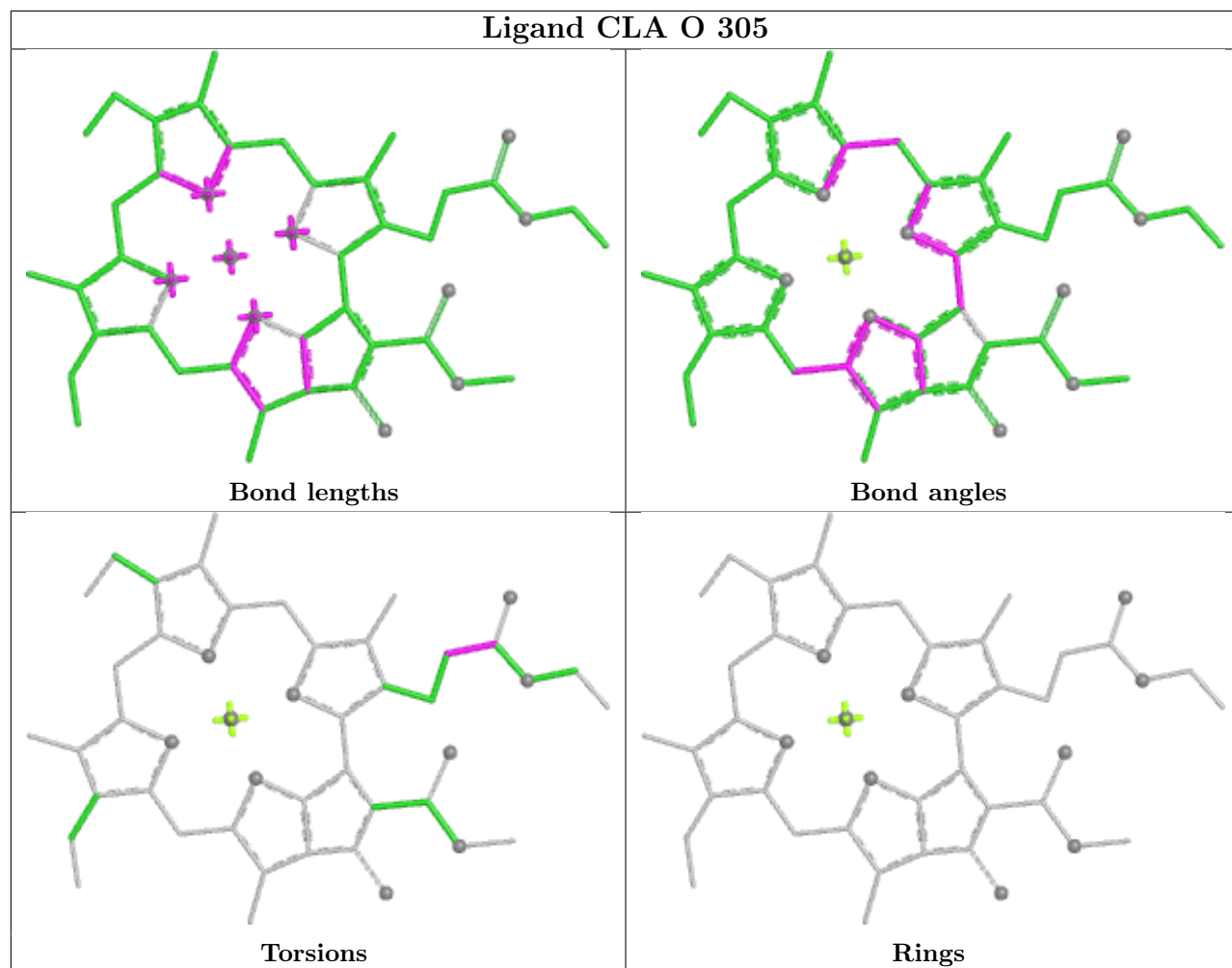


Ligand CLA v 312

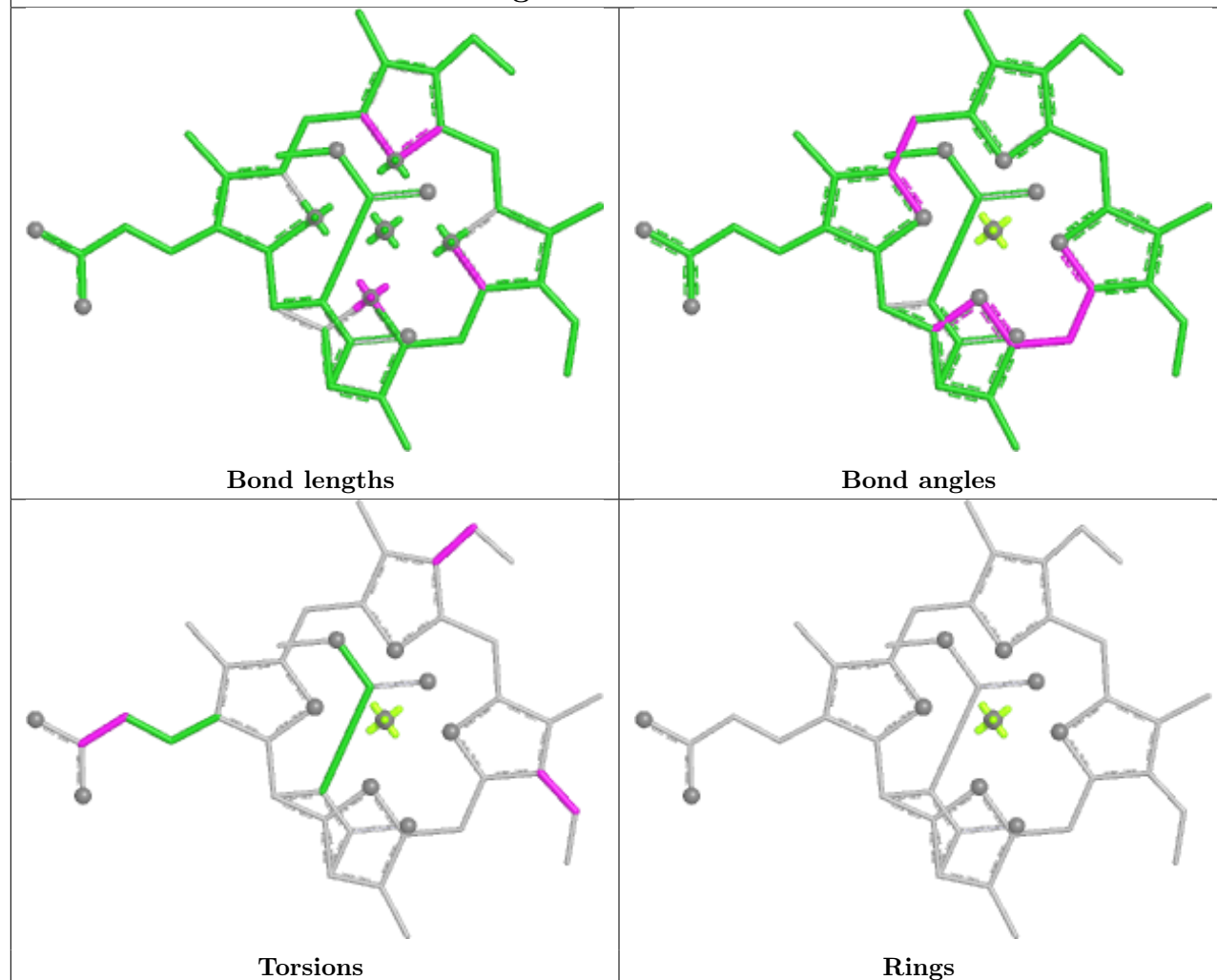




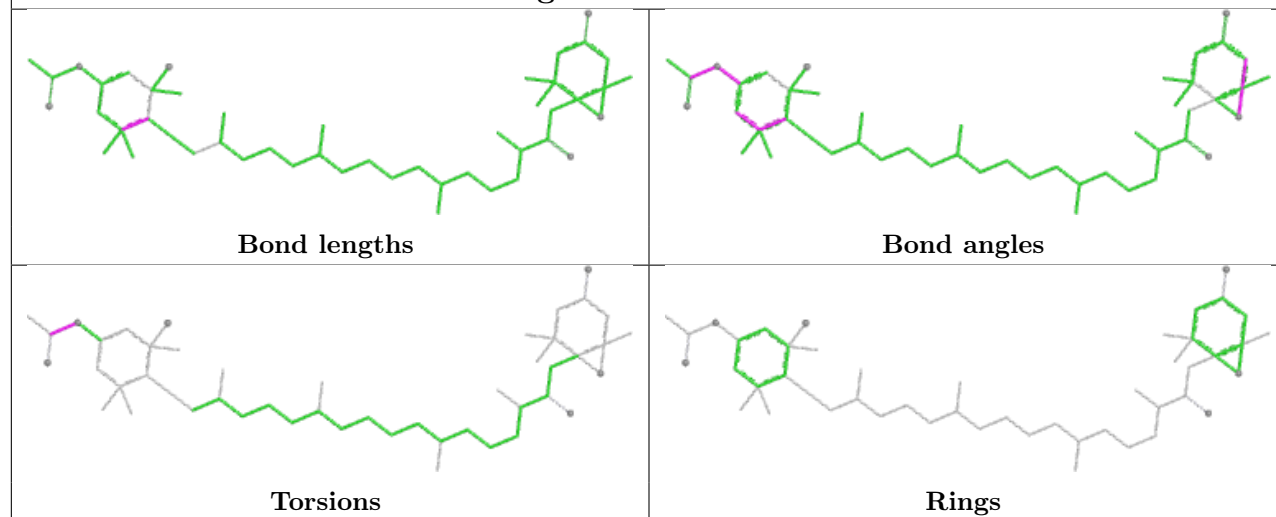
Ligand CLA O 305

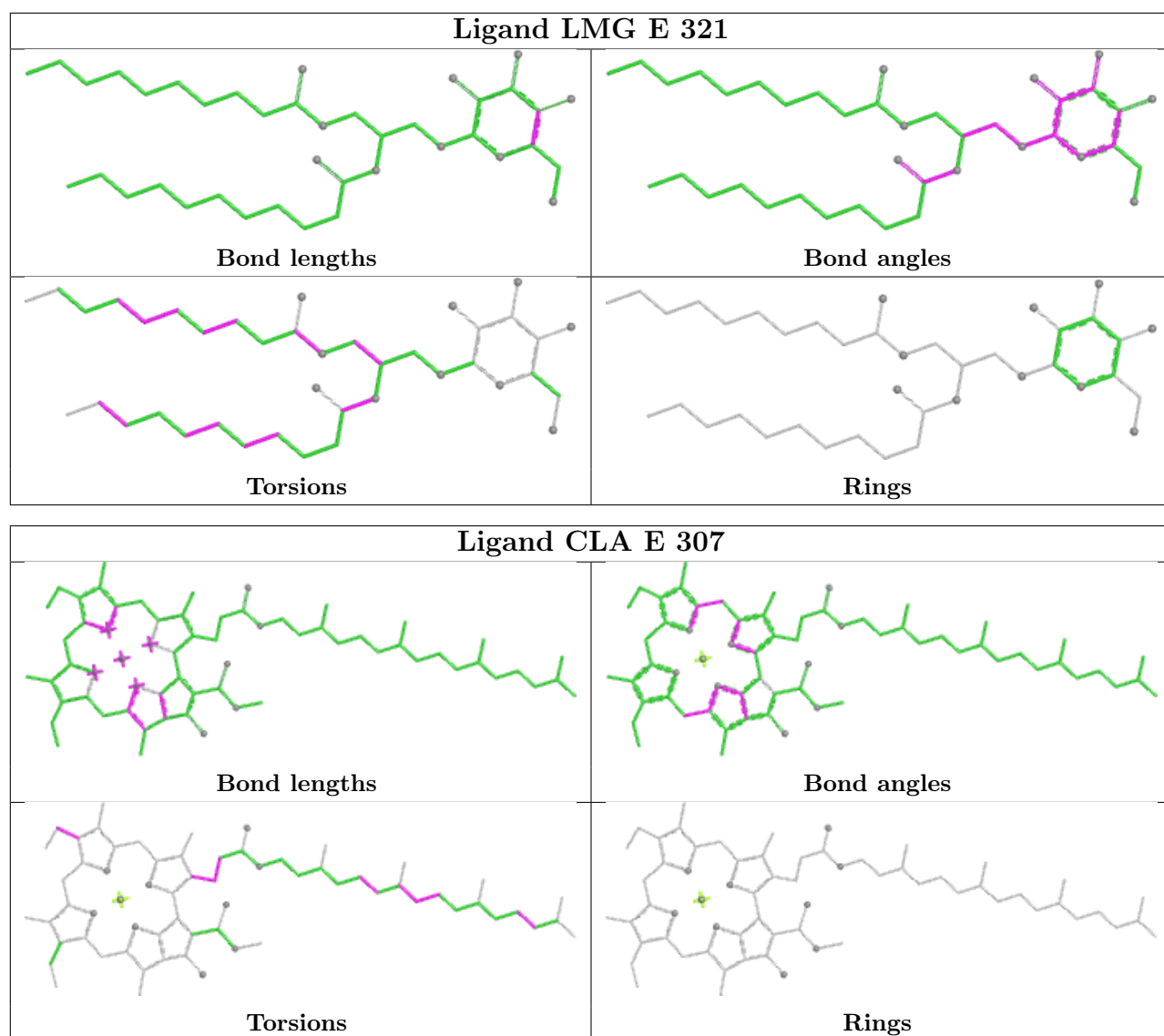


Ligand KC2 v 309

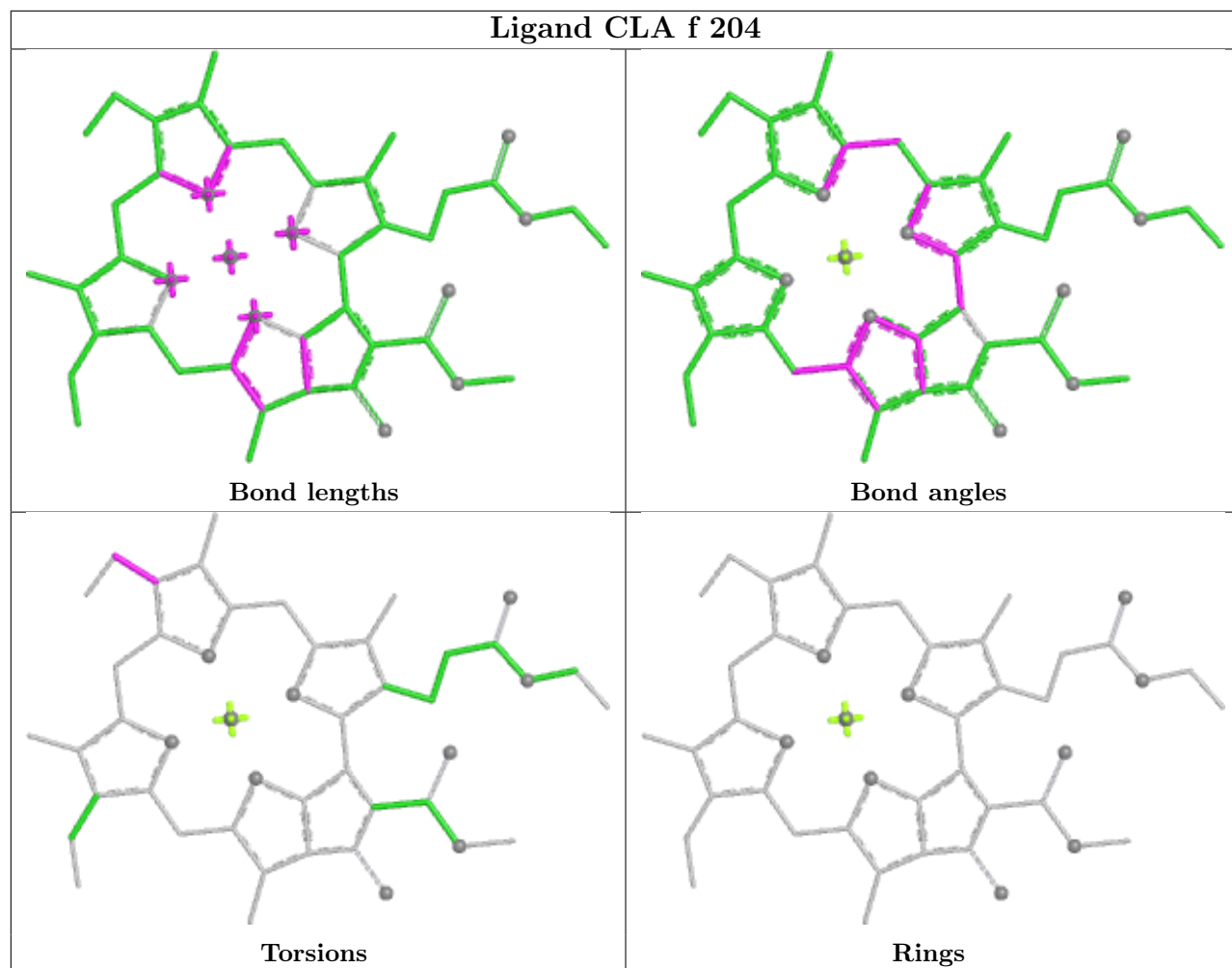


Ligand A86 U 210

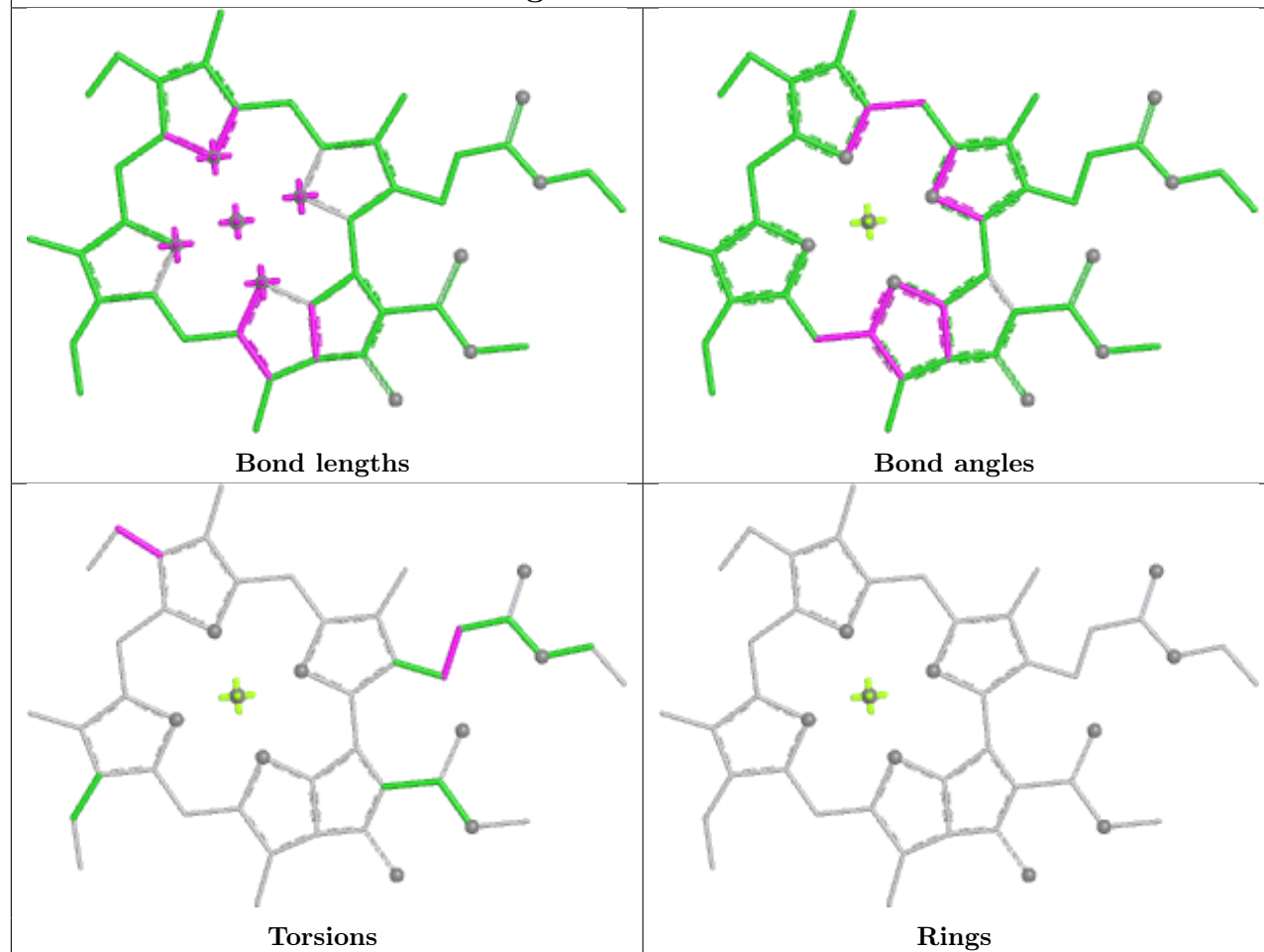




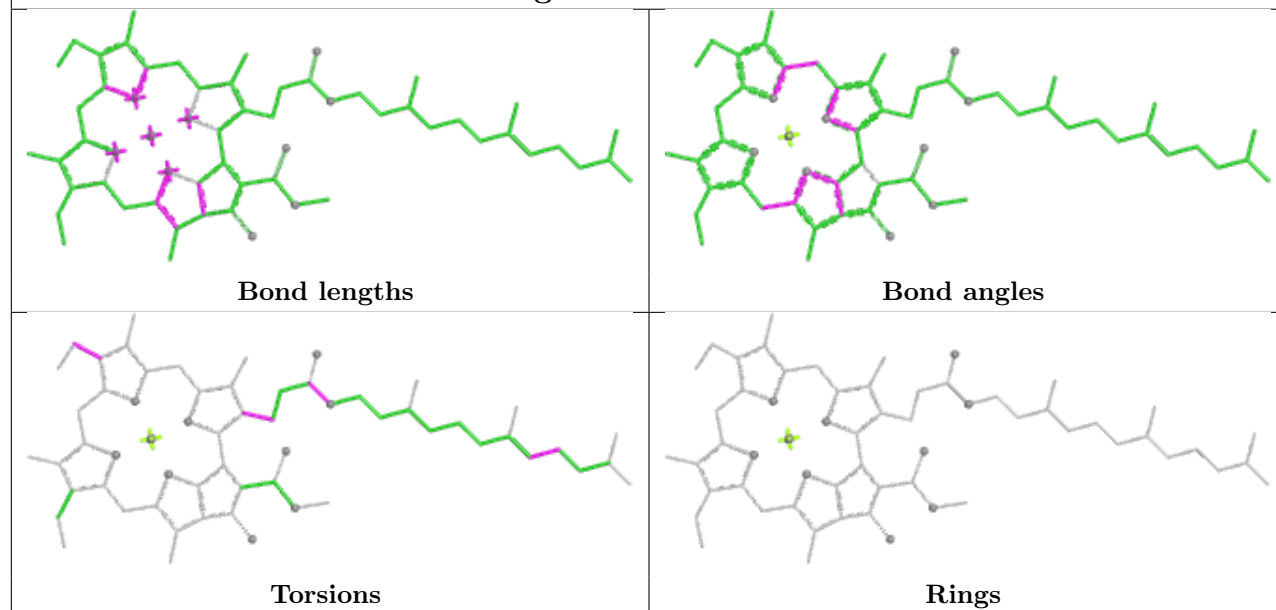
Ligand CLA f 204



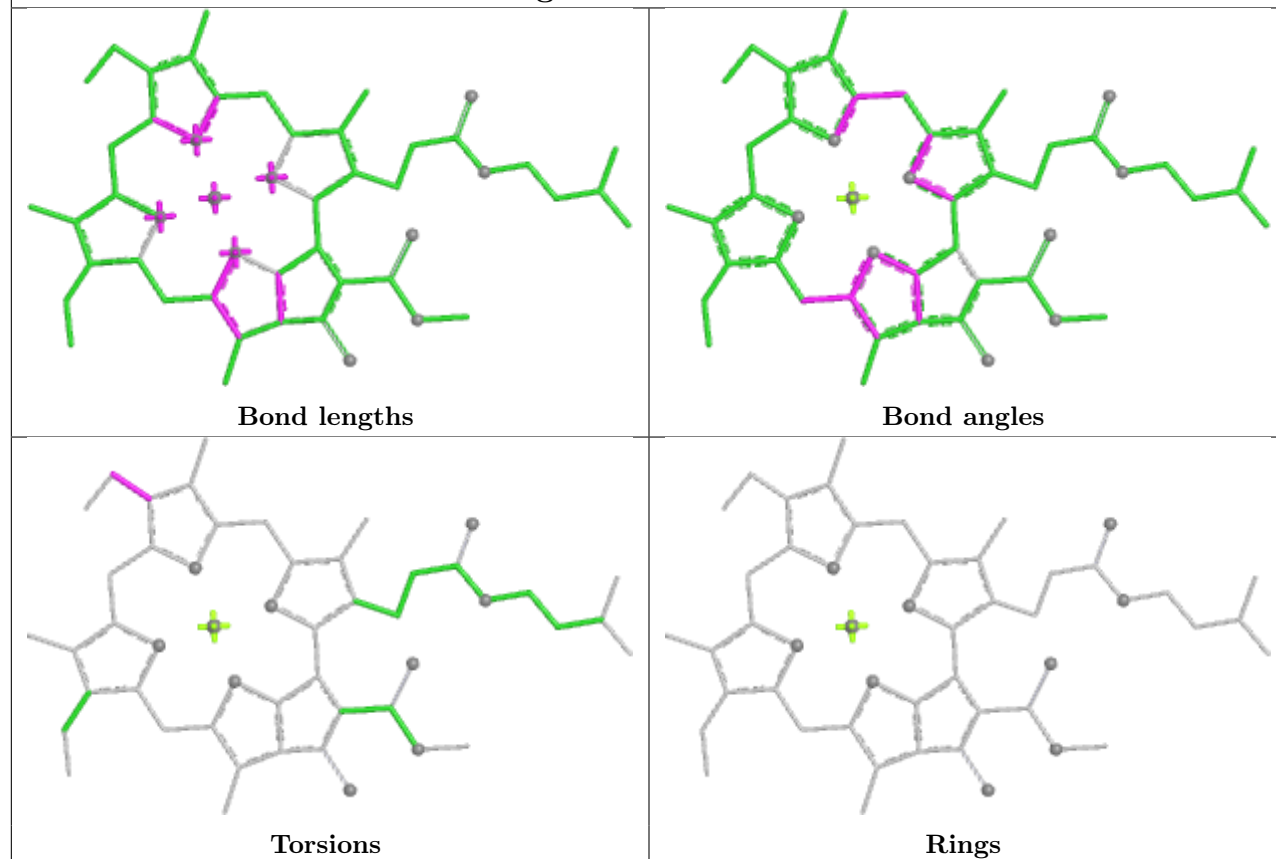
Ligand CLA H 311



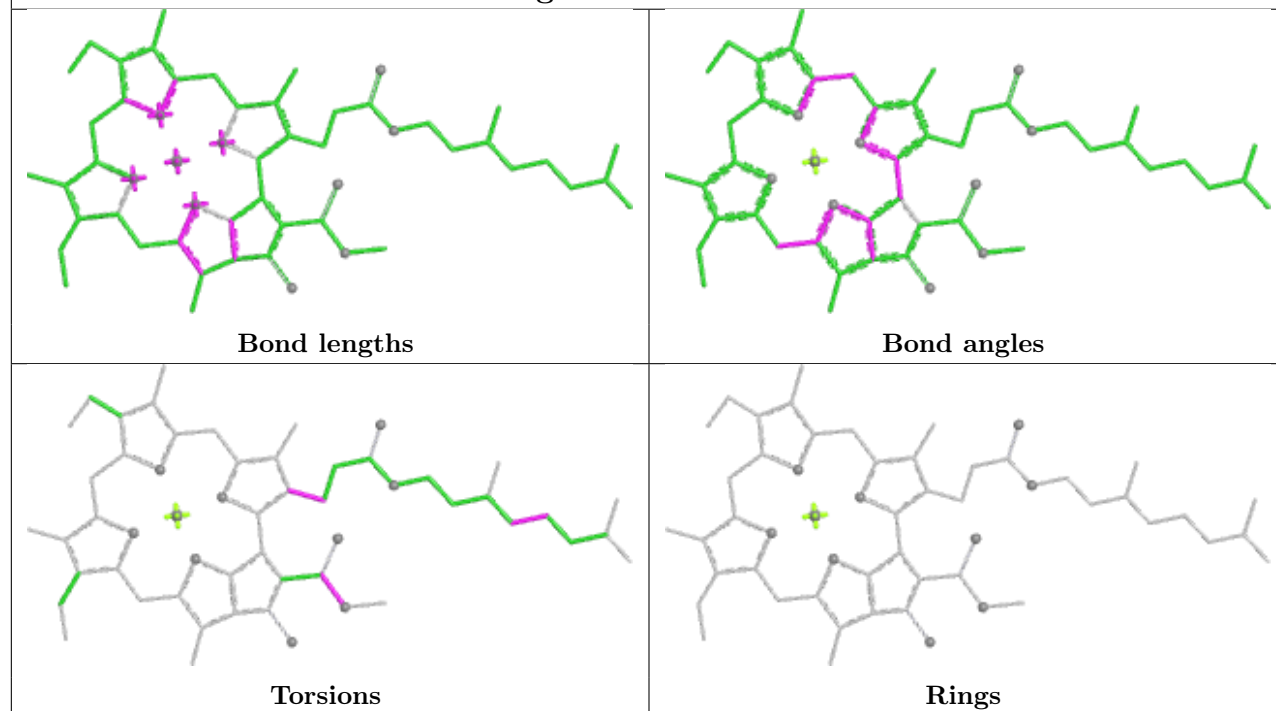
Ligand CLA Z 301

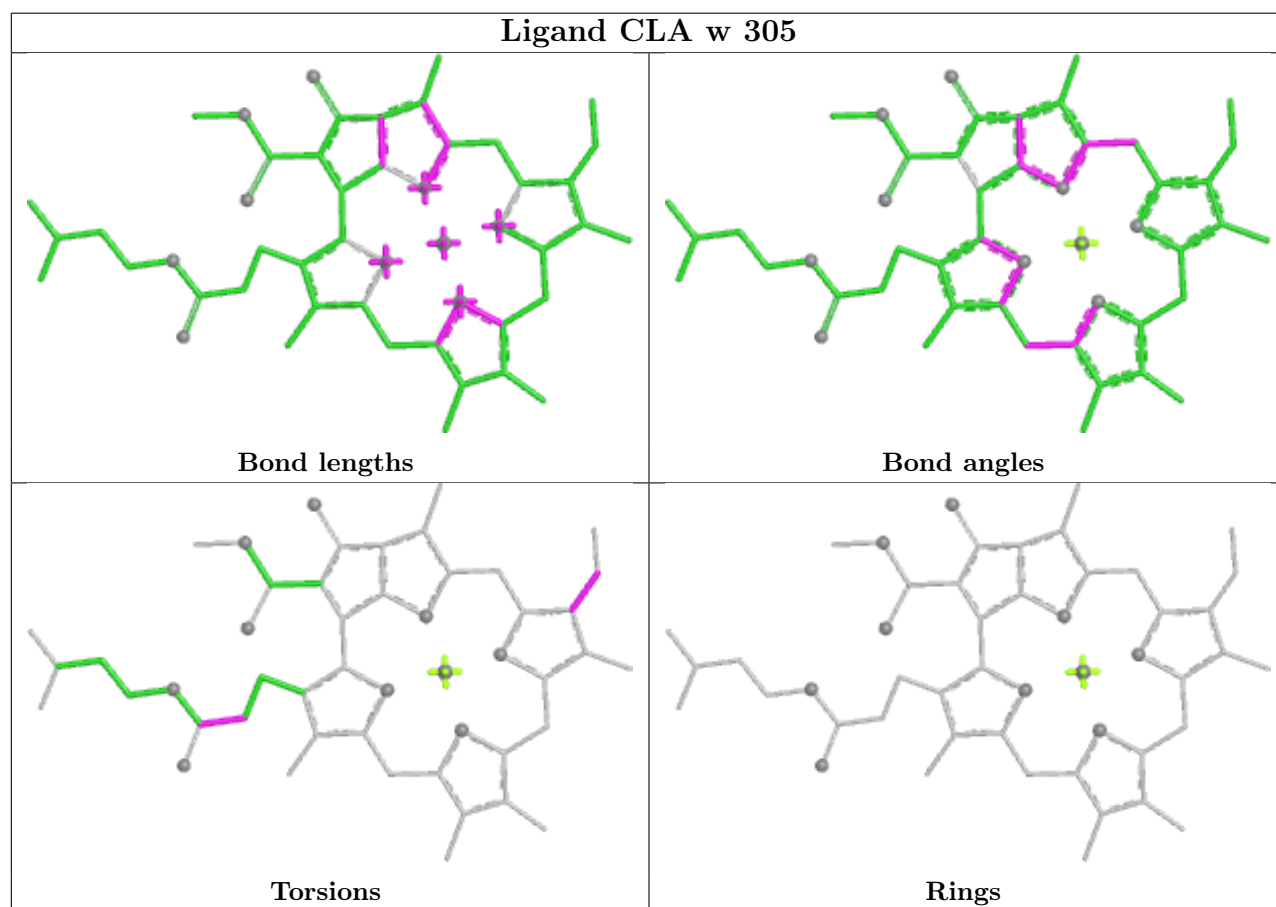
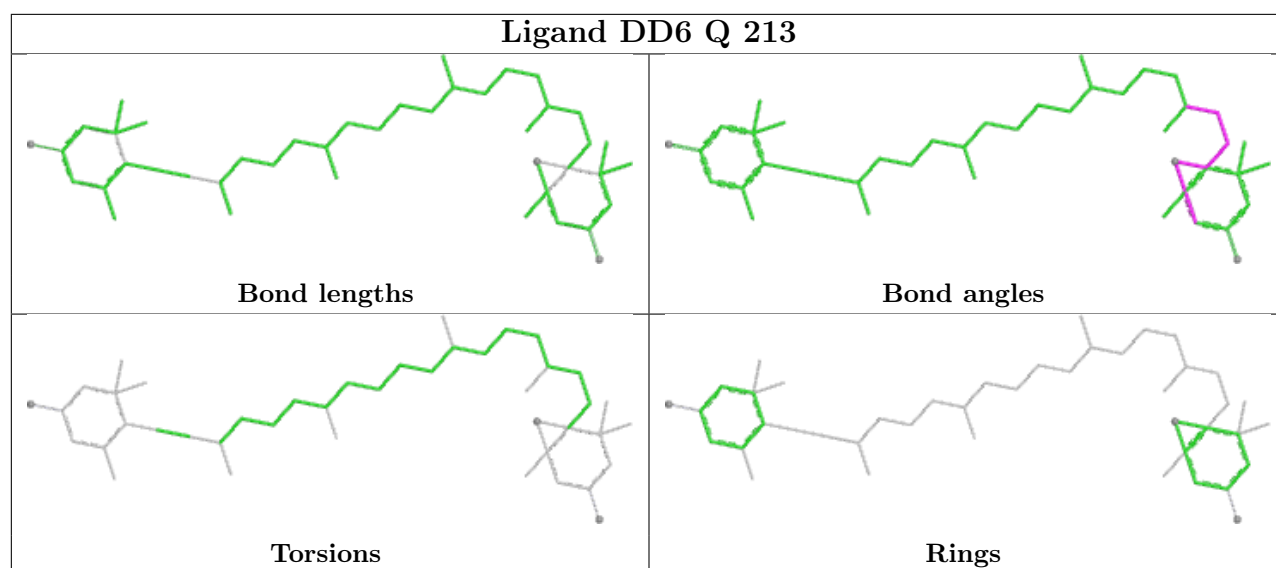


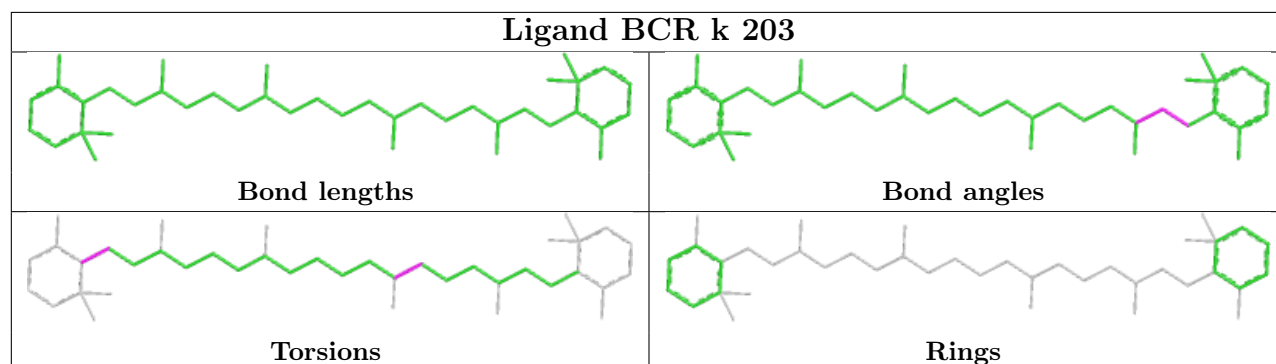
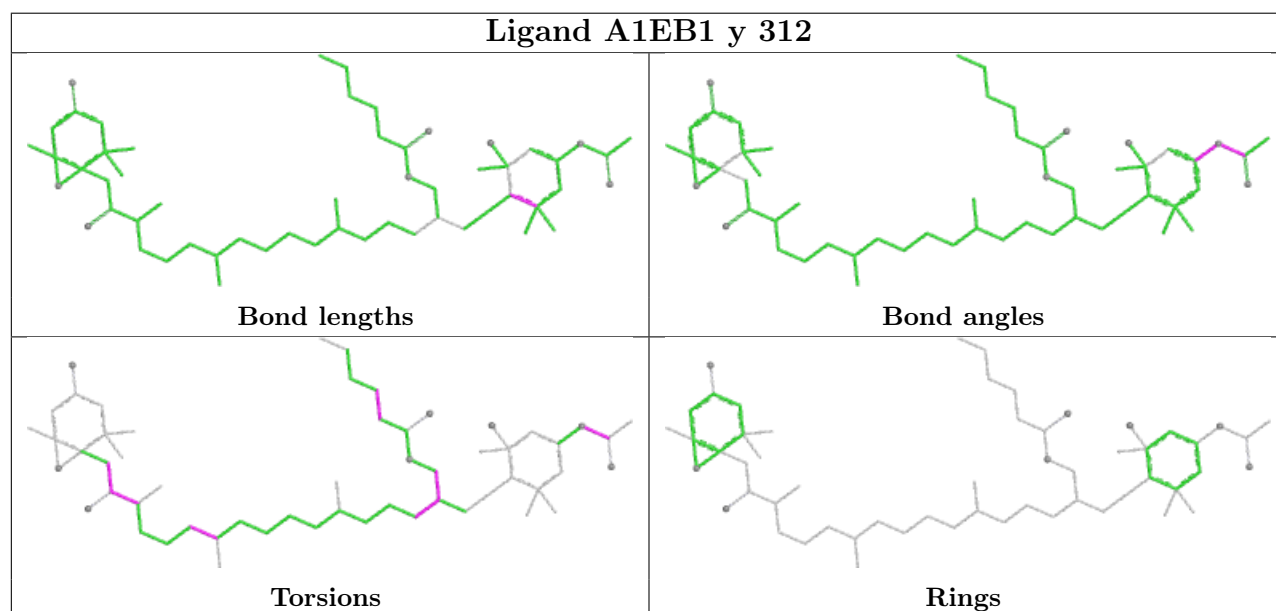
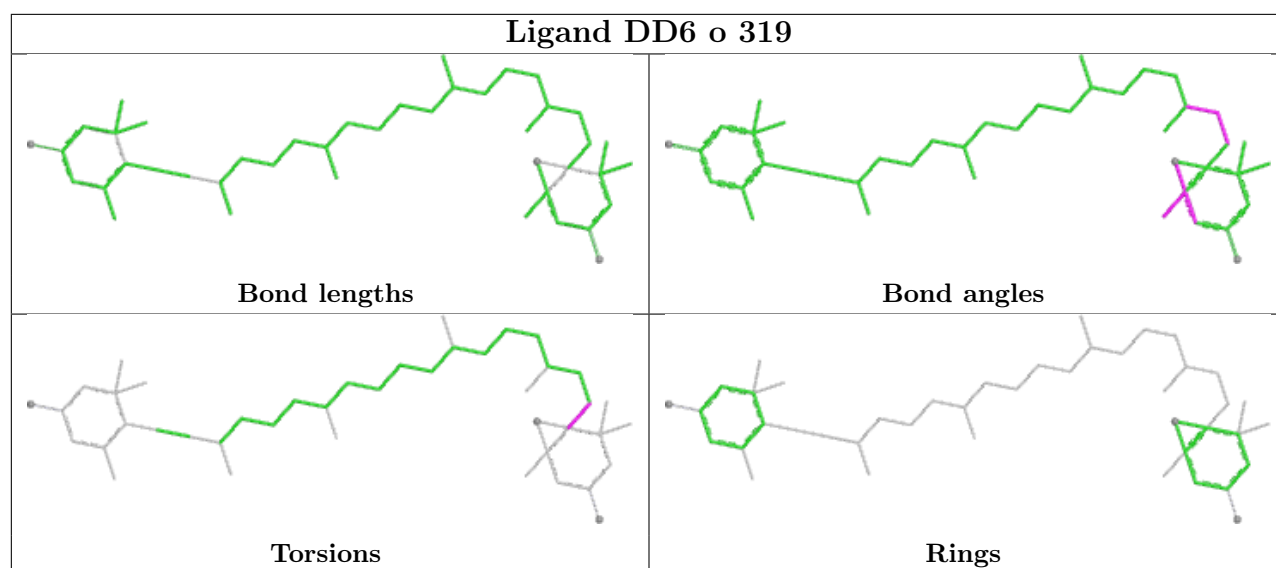
Ligand CLA a 814



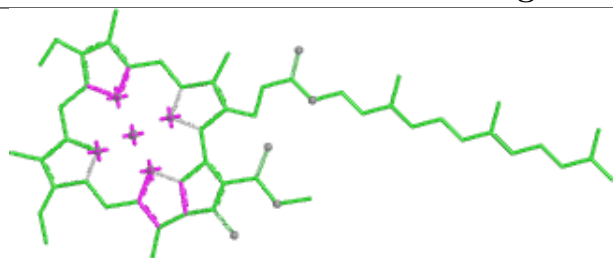
Ligand CLA a 823



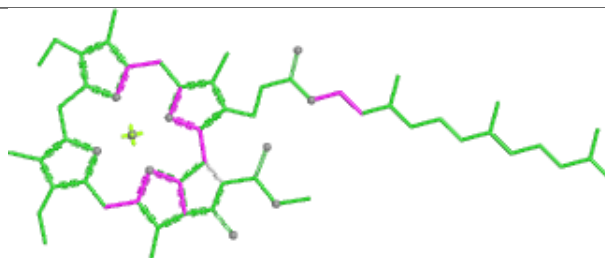




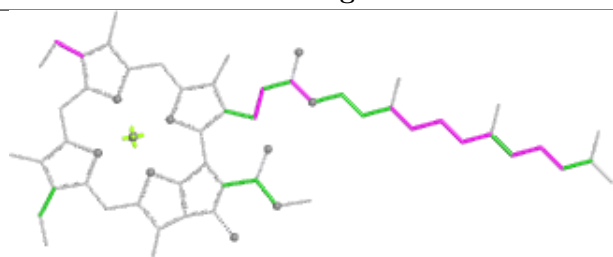
Ligand CLA S 302



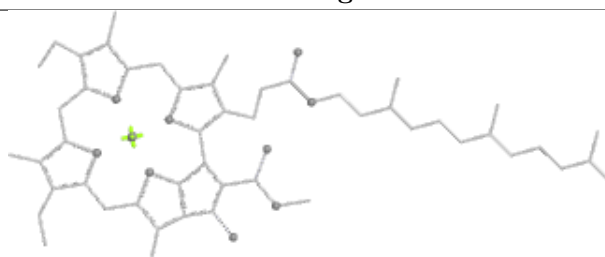
Bond lengths



Bond angles

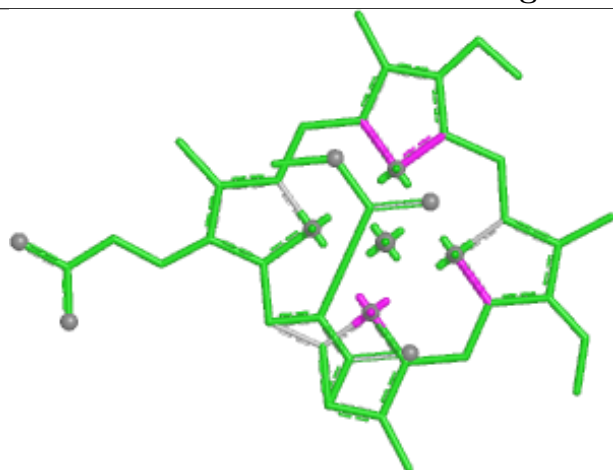


Torsions

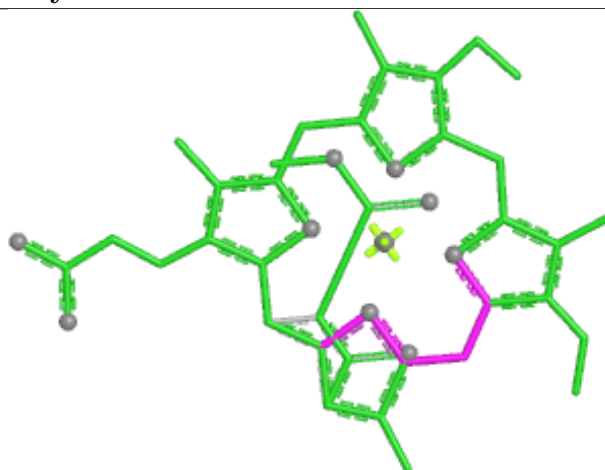


Rings

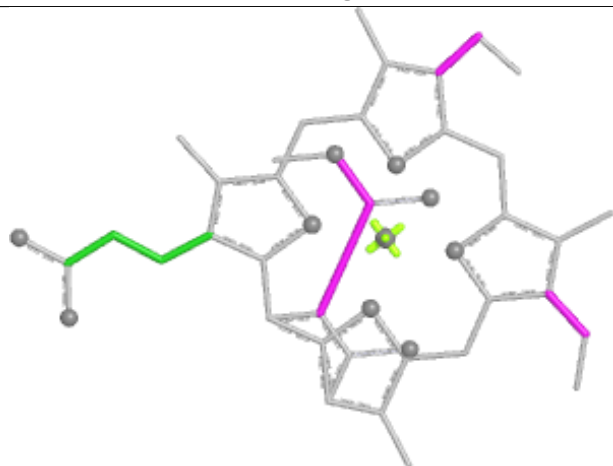
Ligand KC2 y 306



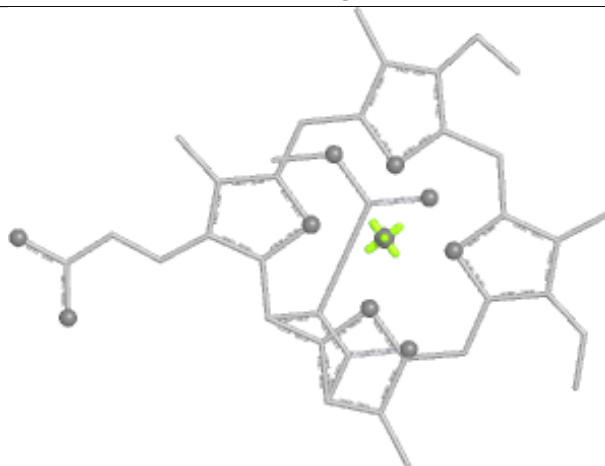
Bond lengths



Bond angles

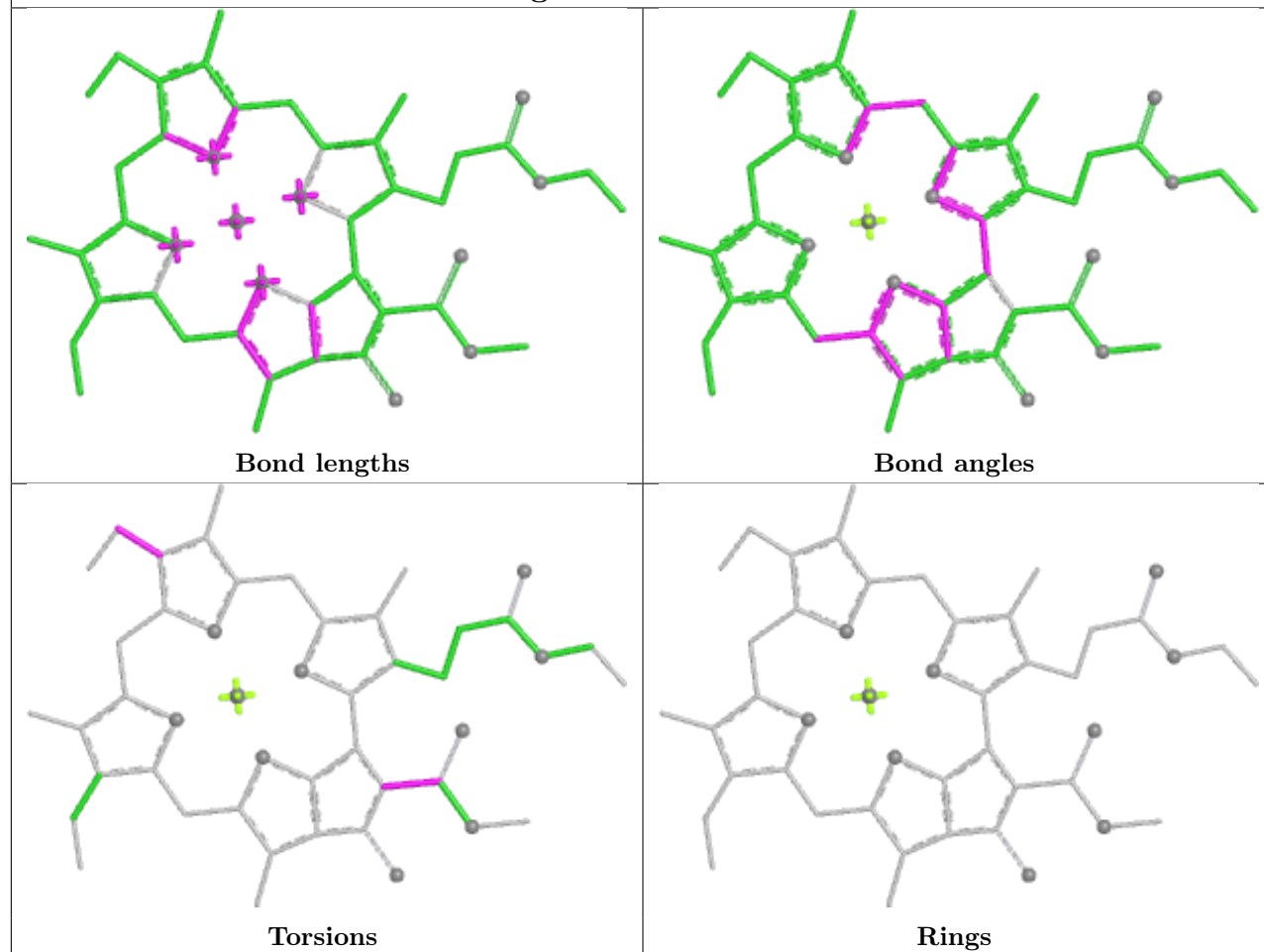


Torsions

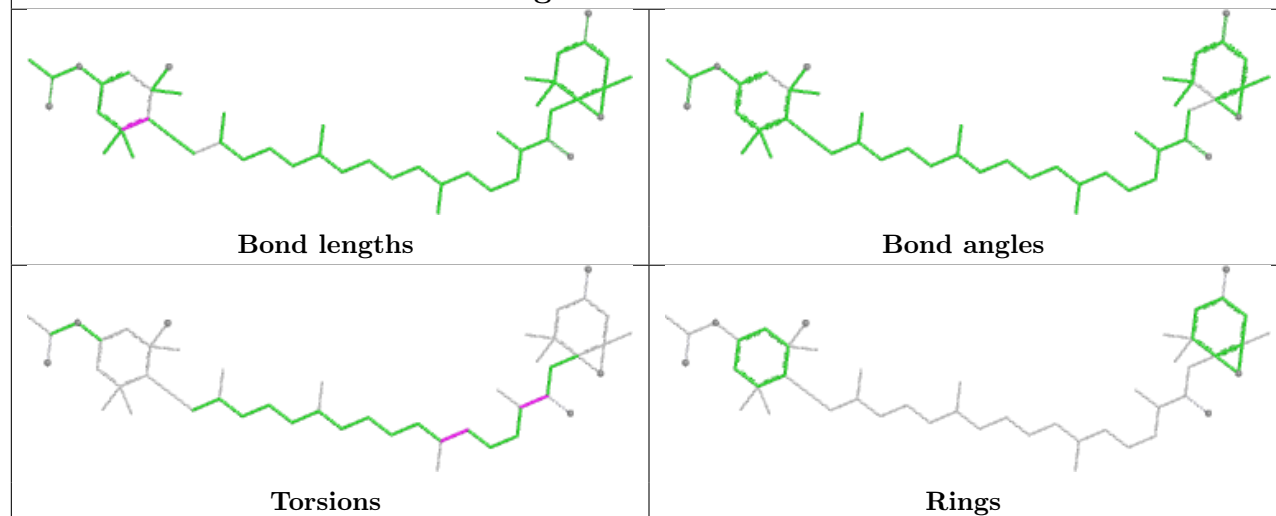


Rings

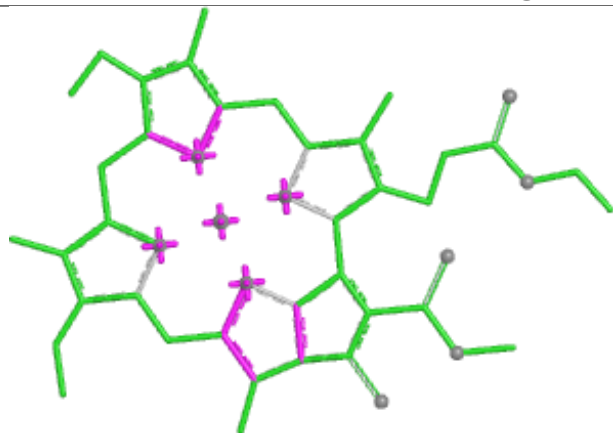
Ligand CLA x 314



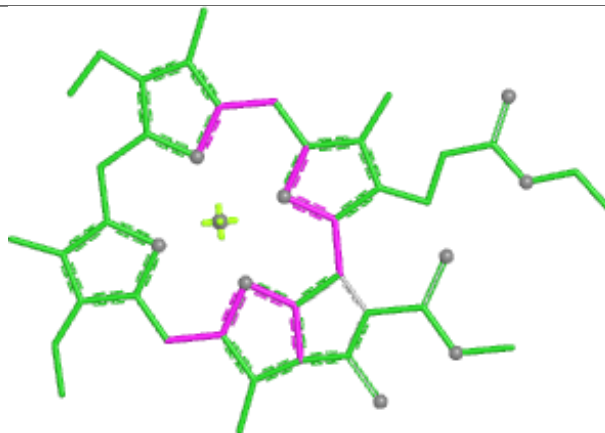
Ligand A86 M 320



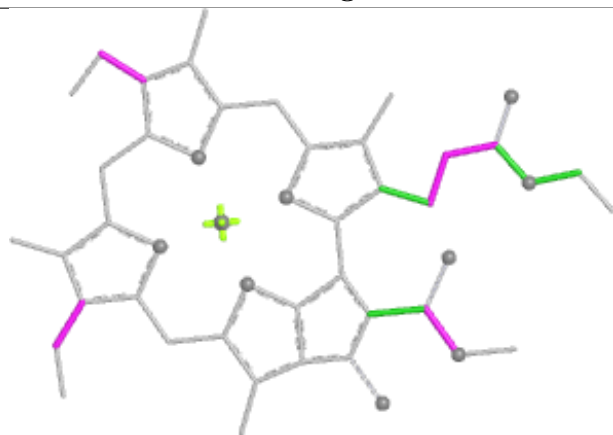
Ligand CLA J 302



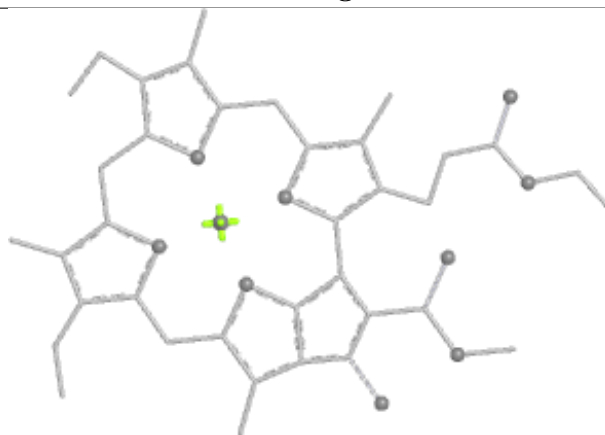
Bond lengths



Bond angles

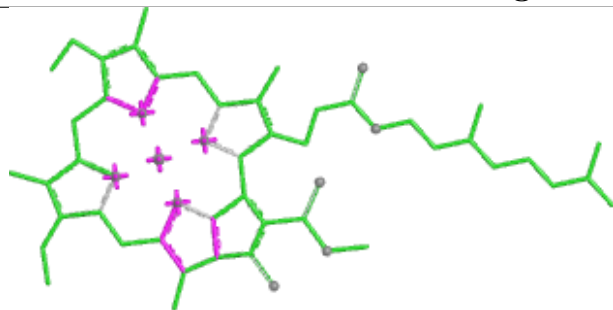


Torsions

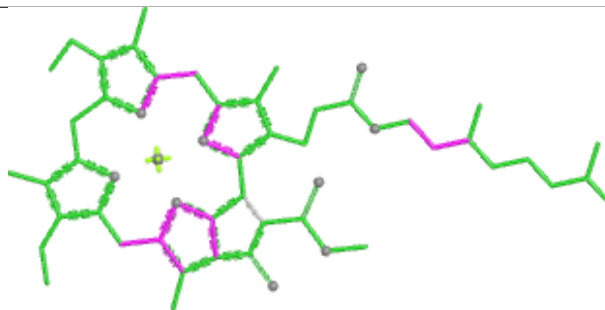


Rings

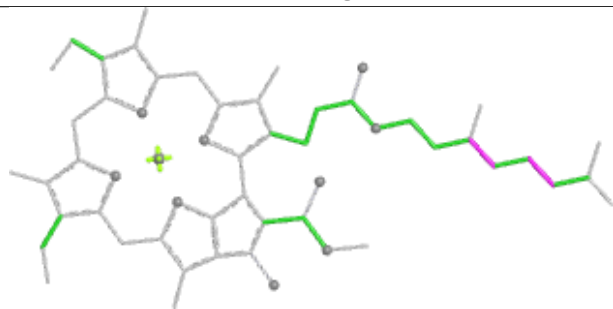
Ligand CLA G 204



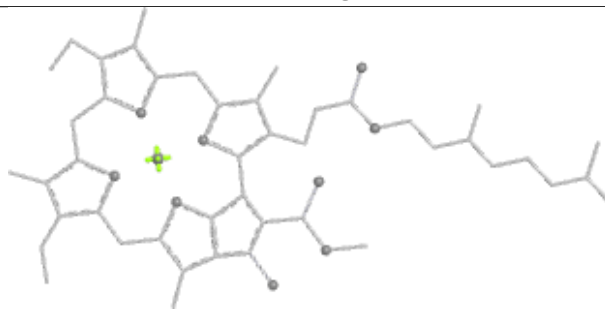
Bond lengths



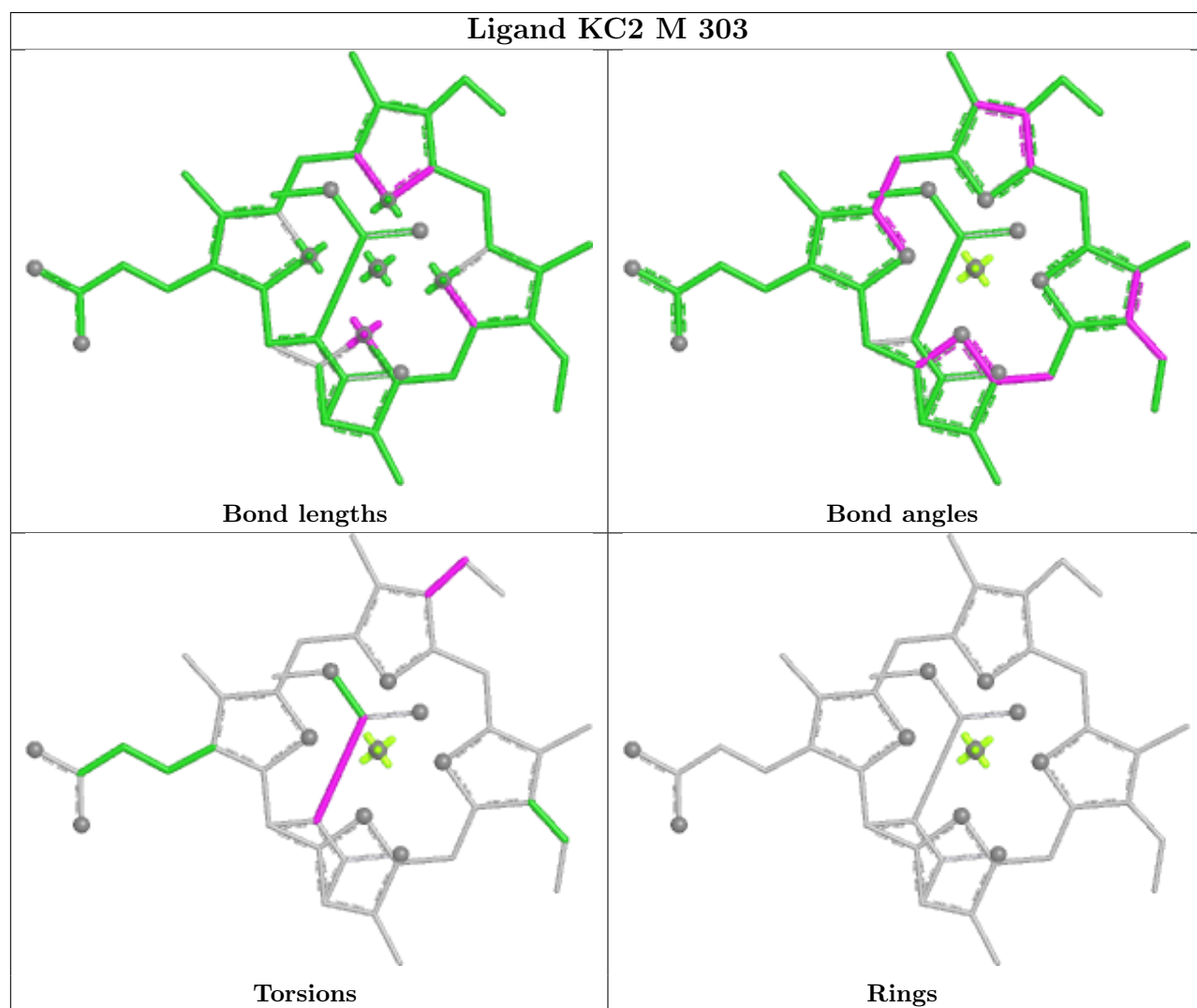
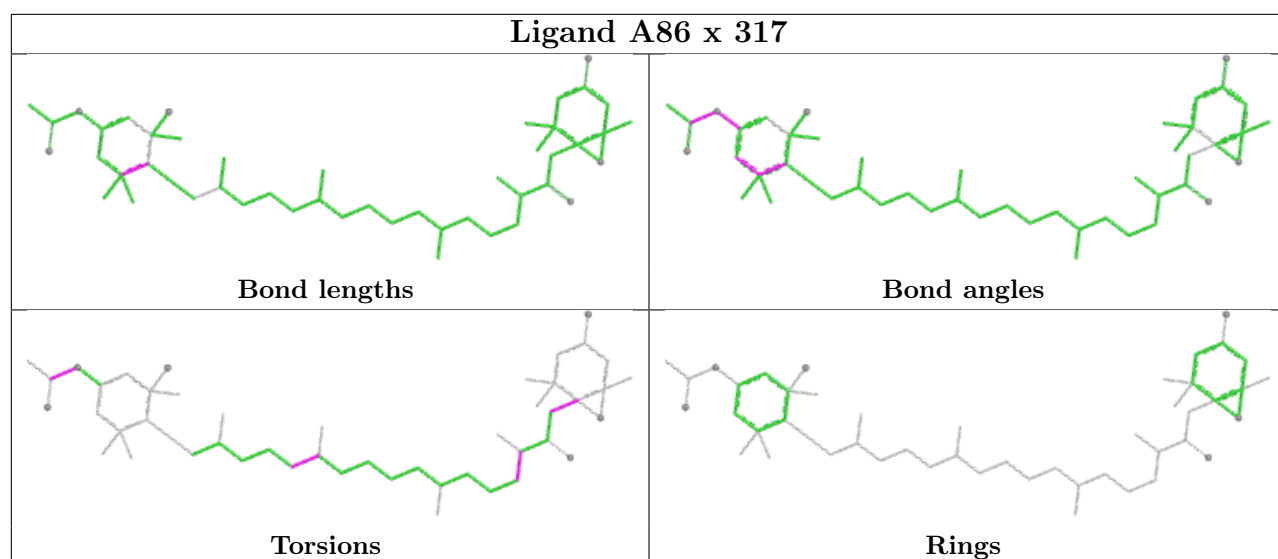
Bond angles

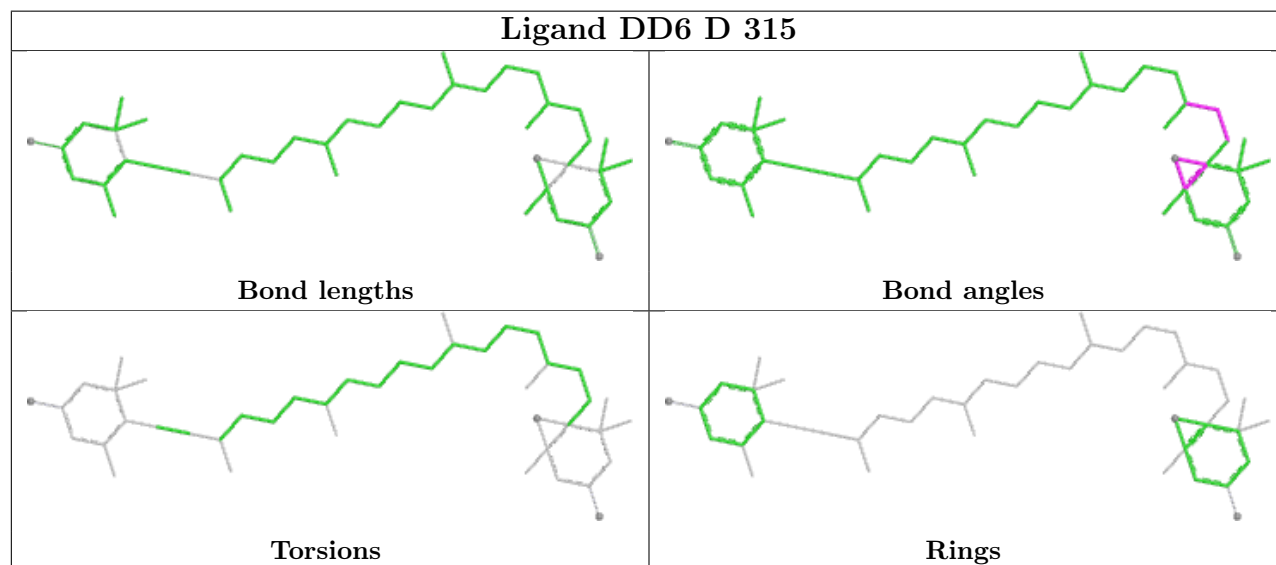
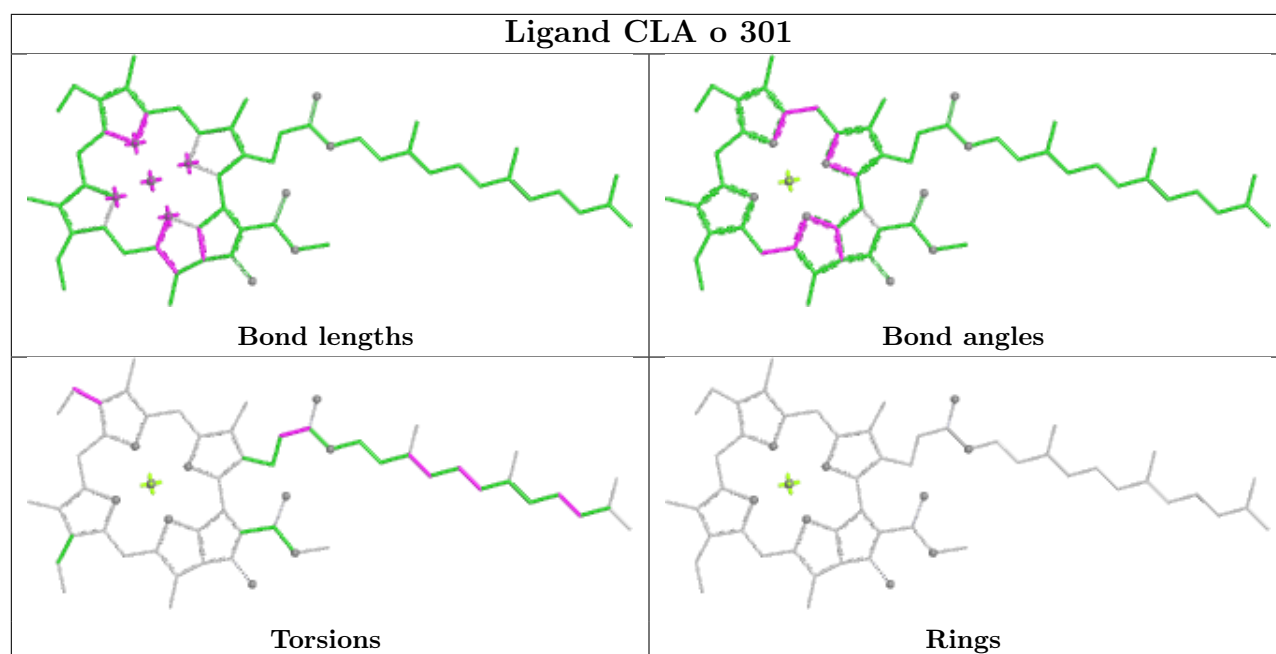


Torsions

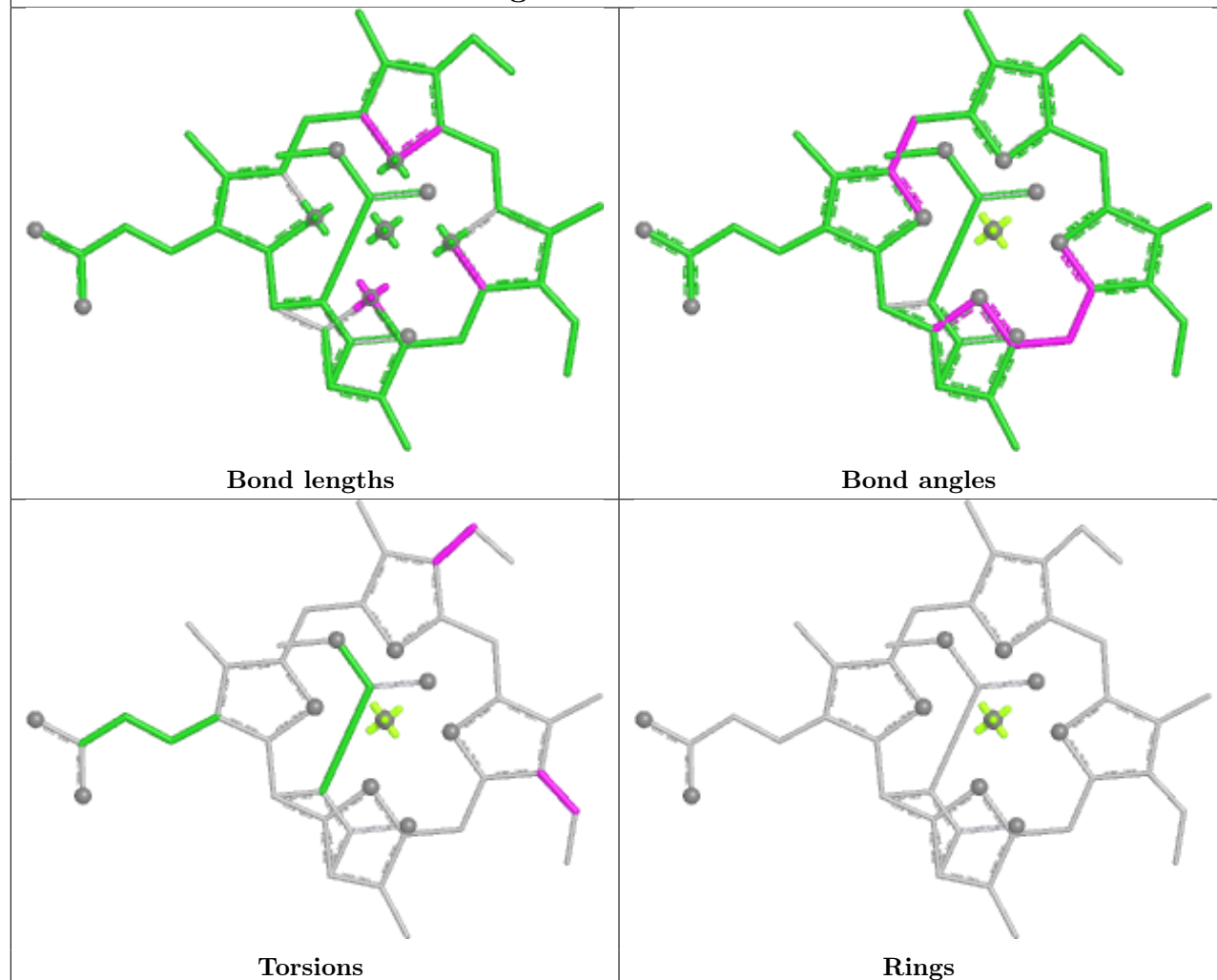


Rings

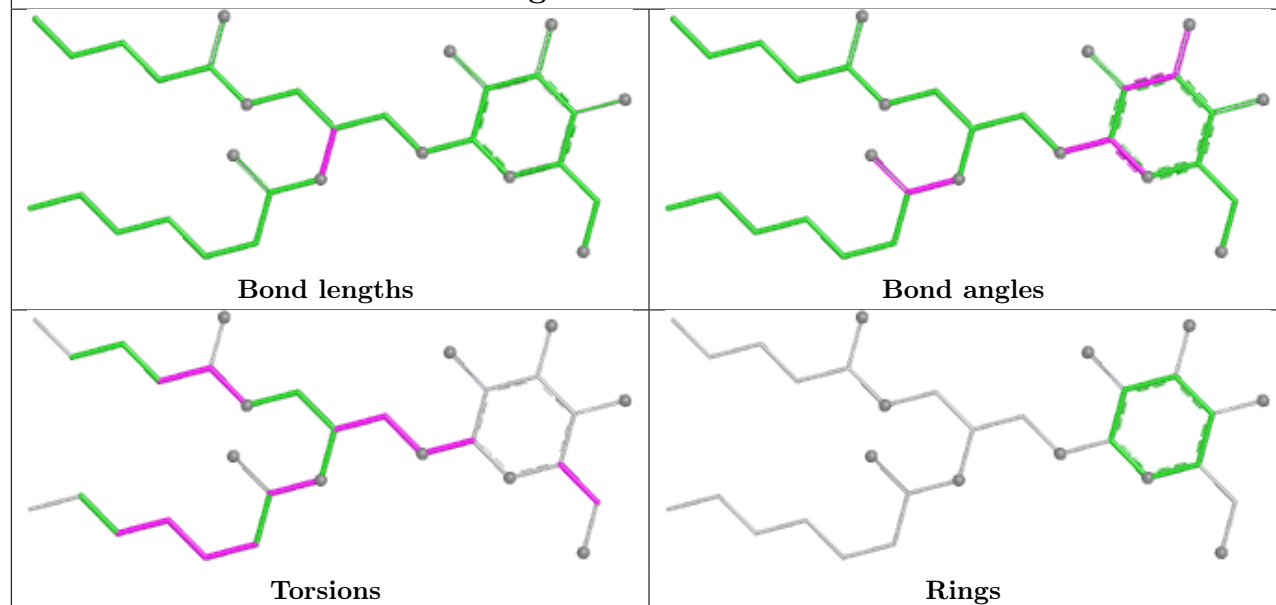


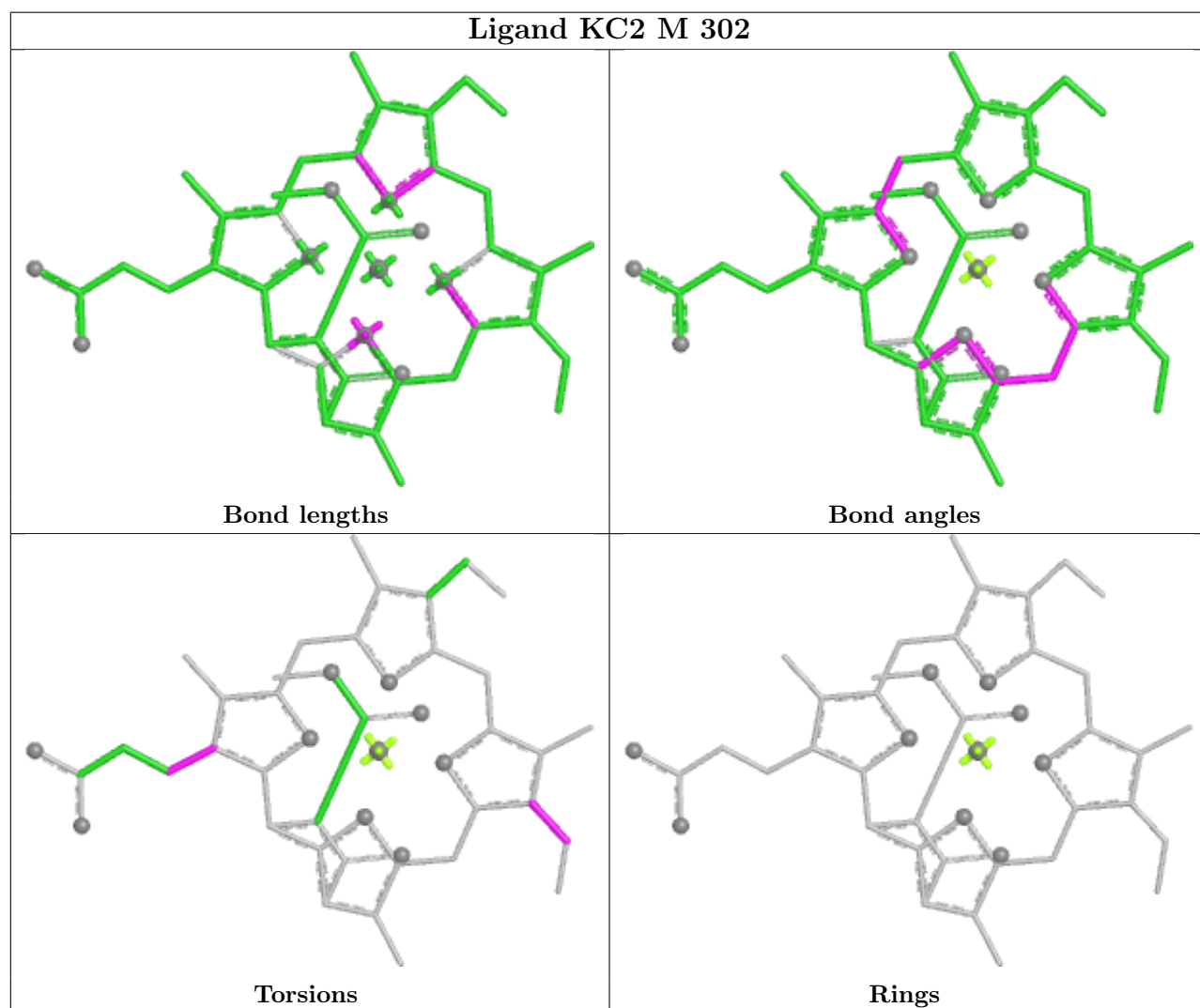
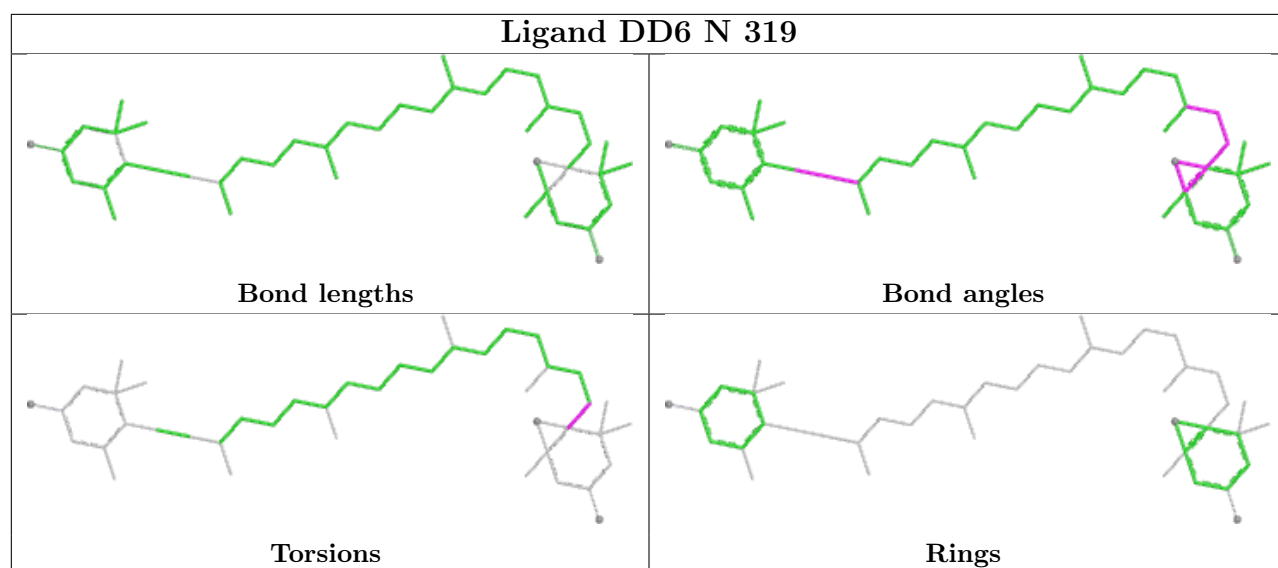


Ligand KC2 T 301

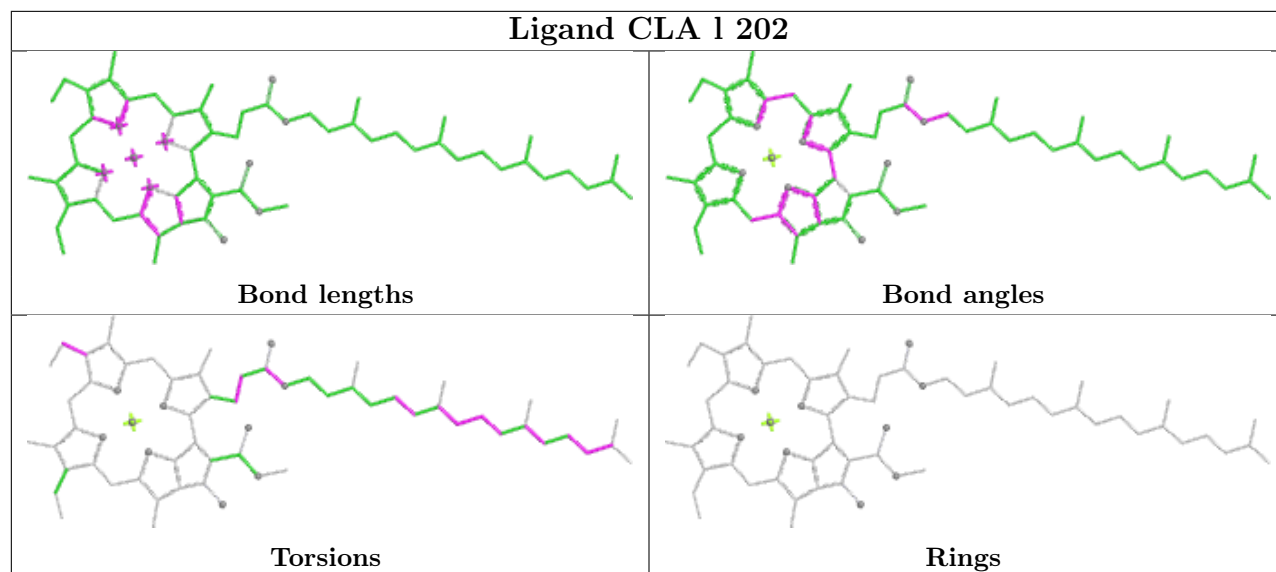


Ligand LMG E 320

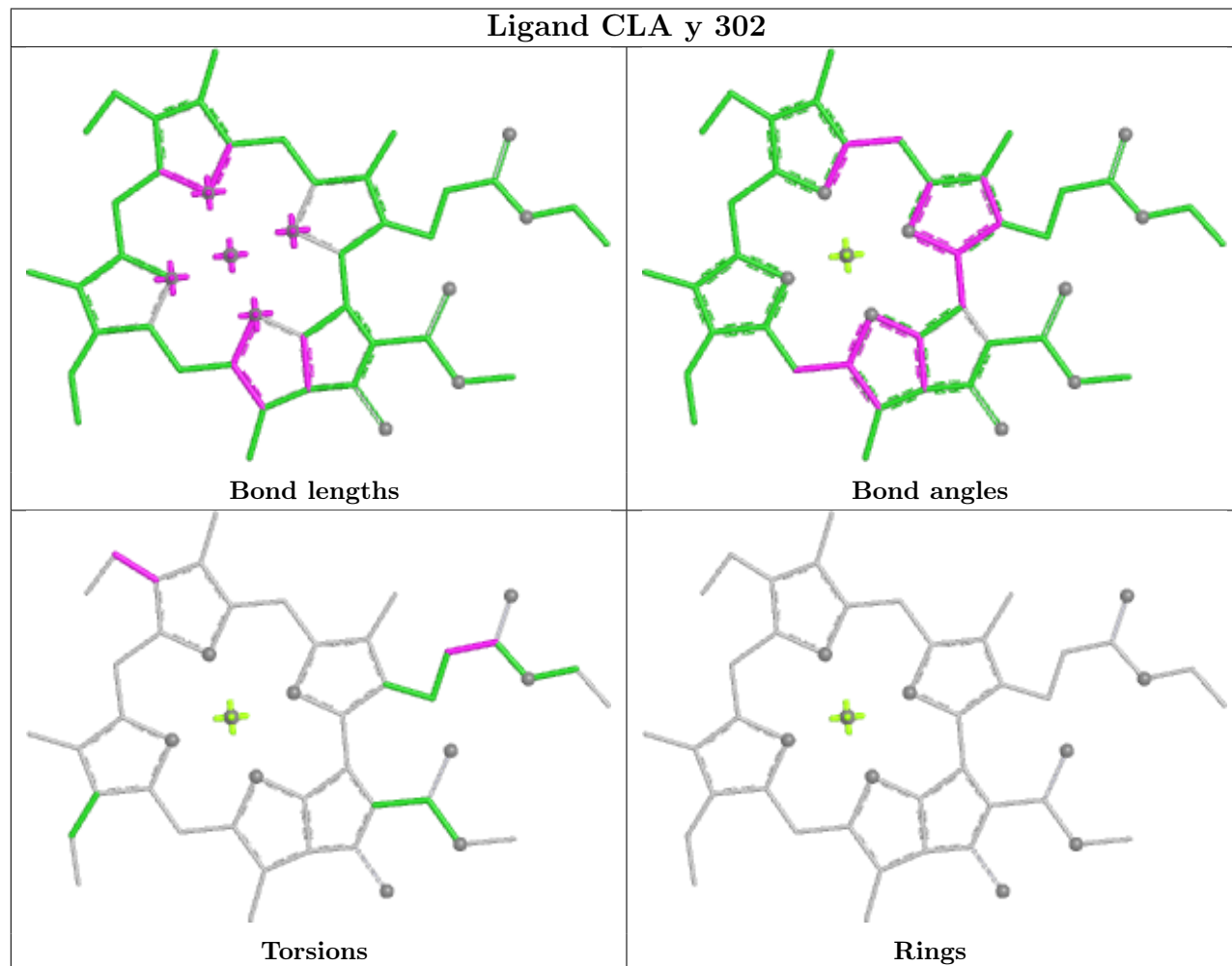




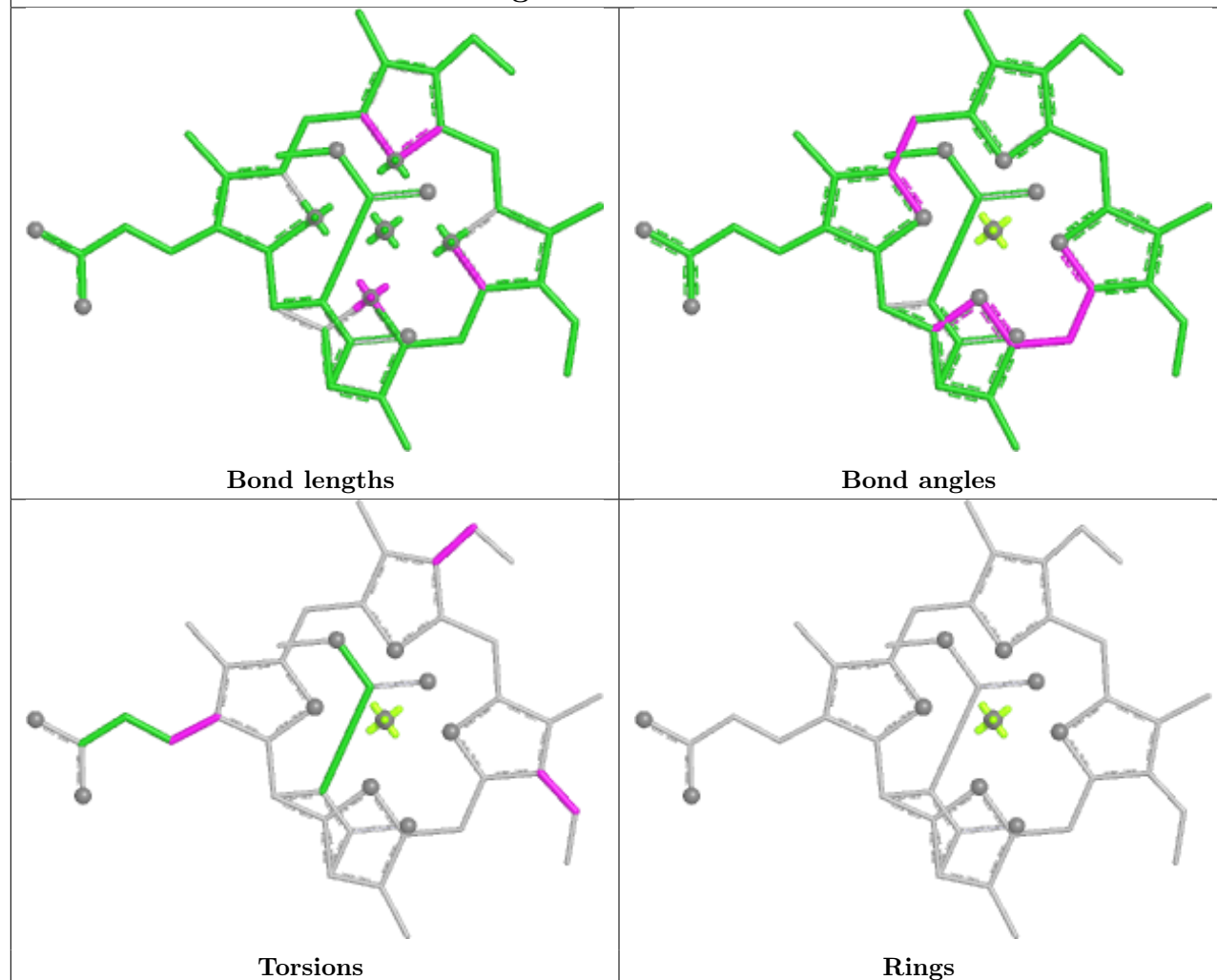
Ligand CLA 1 202



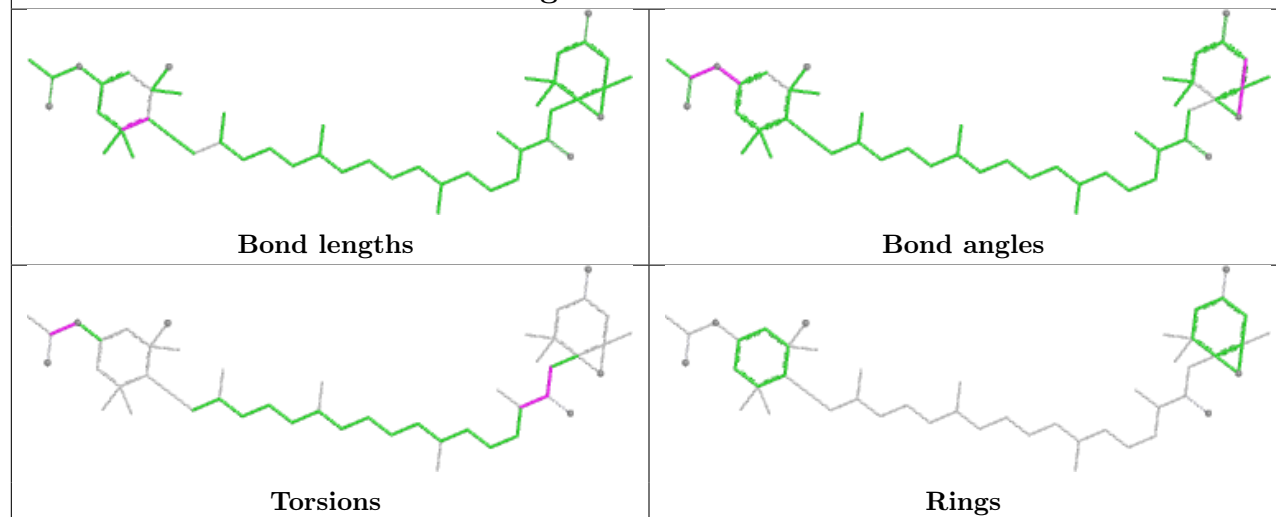
Ligand CLA y 302



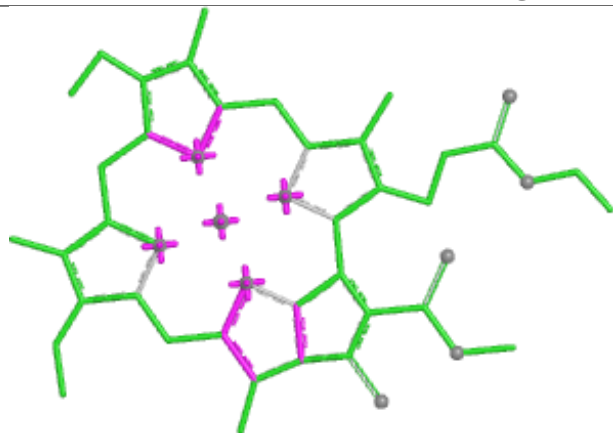
Ligand KC2 u 309



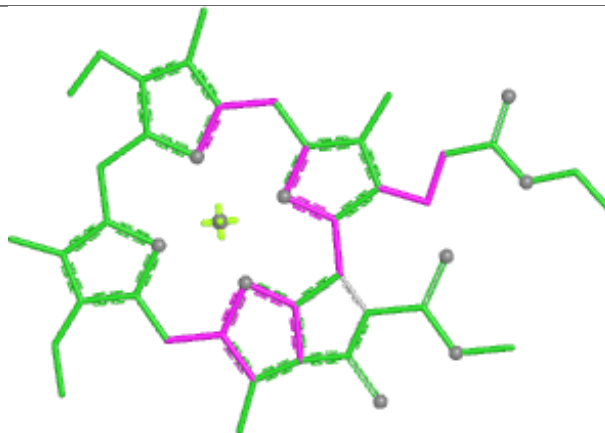
Ligand A86 L 314



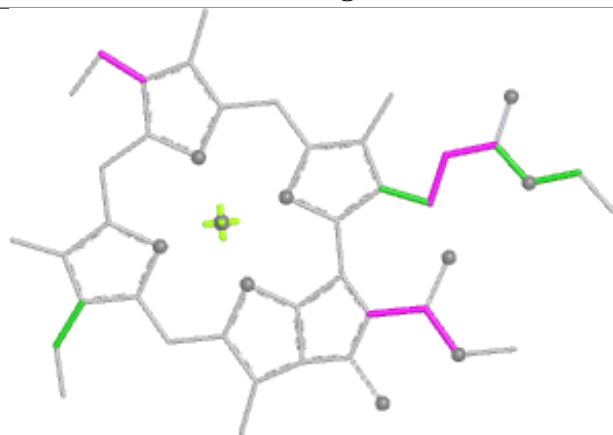
Ligand CLA H 302



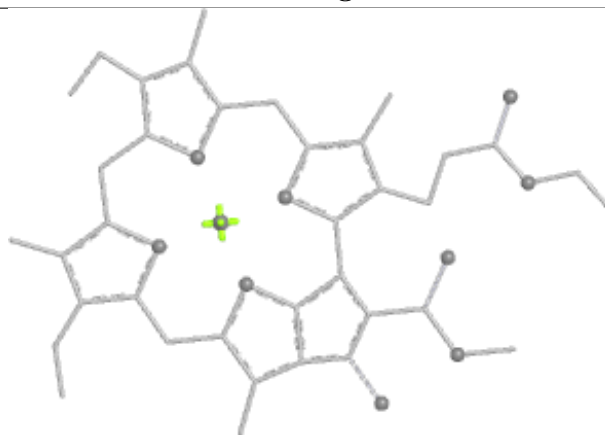
Bond lengths



Bond angles

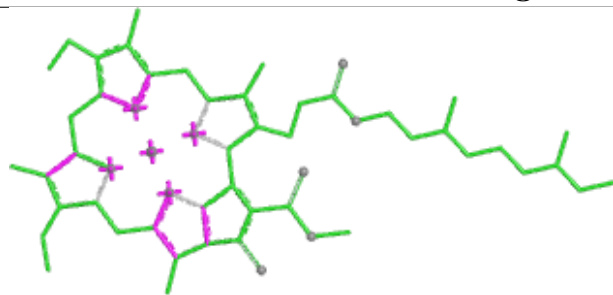


Torsions

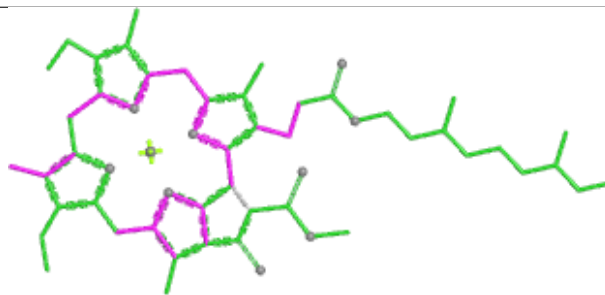


Rings

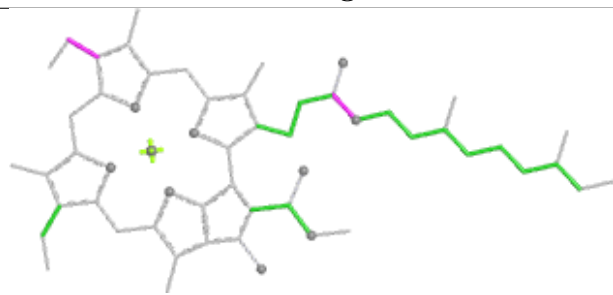
Ligand CLA C 304



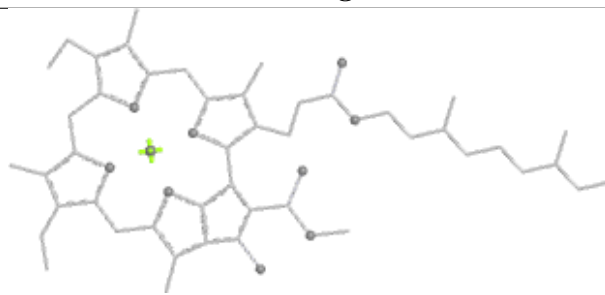
Bond lengths



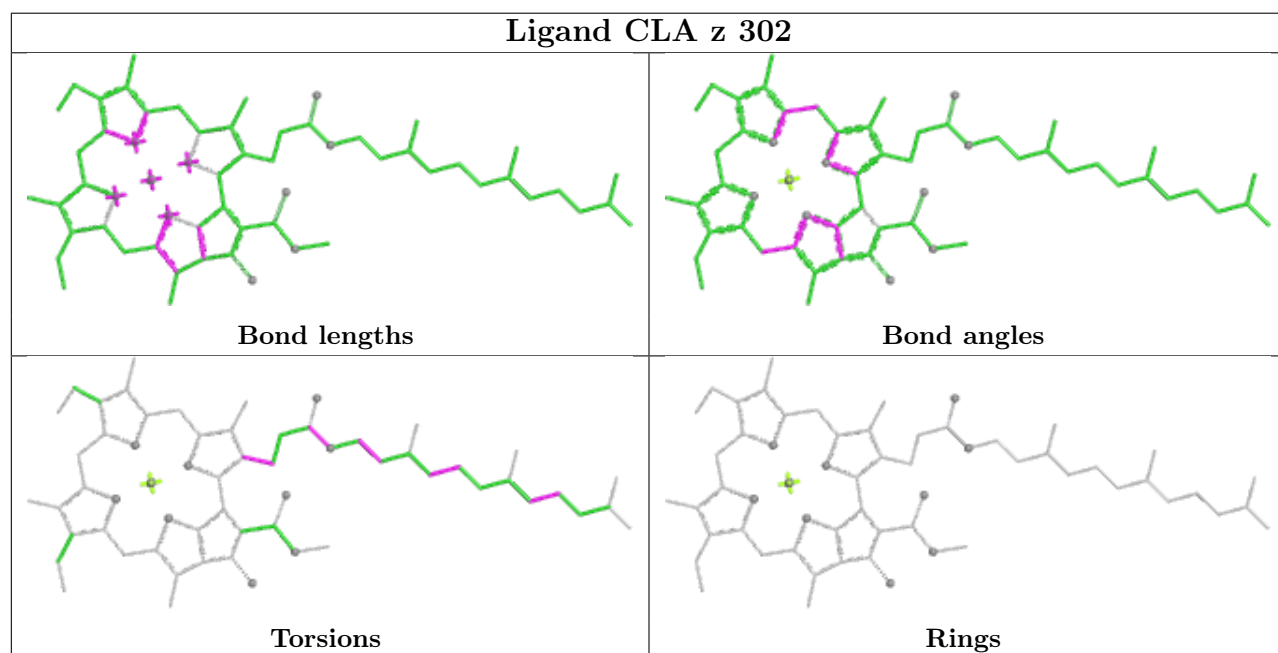
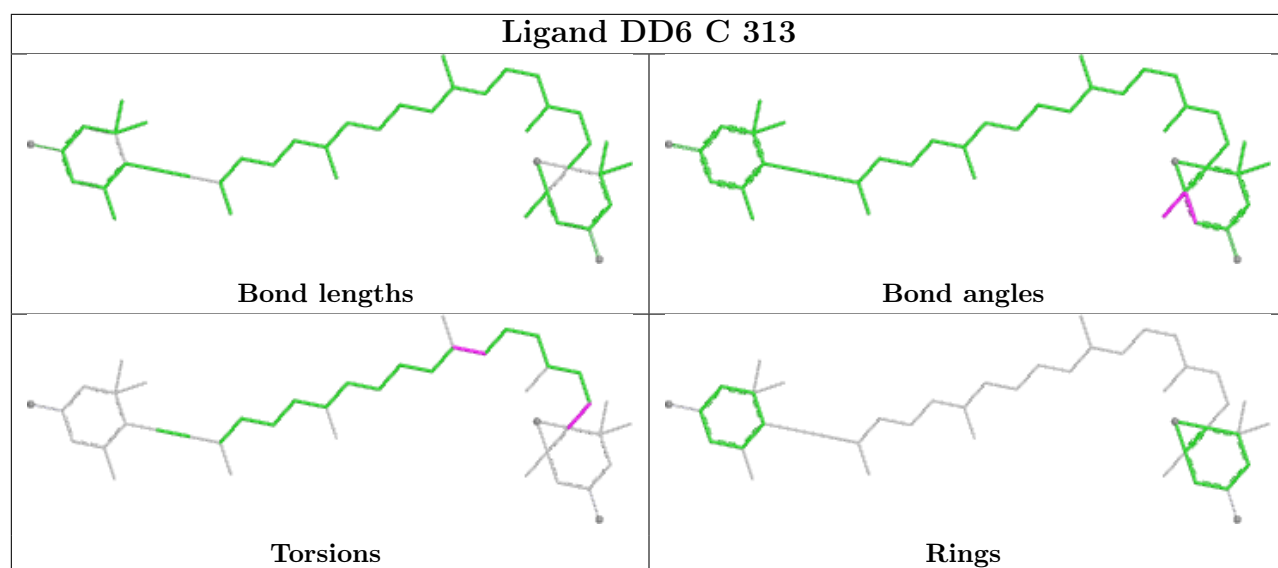
Bond angles

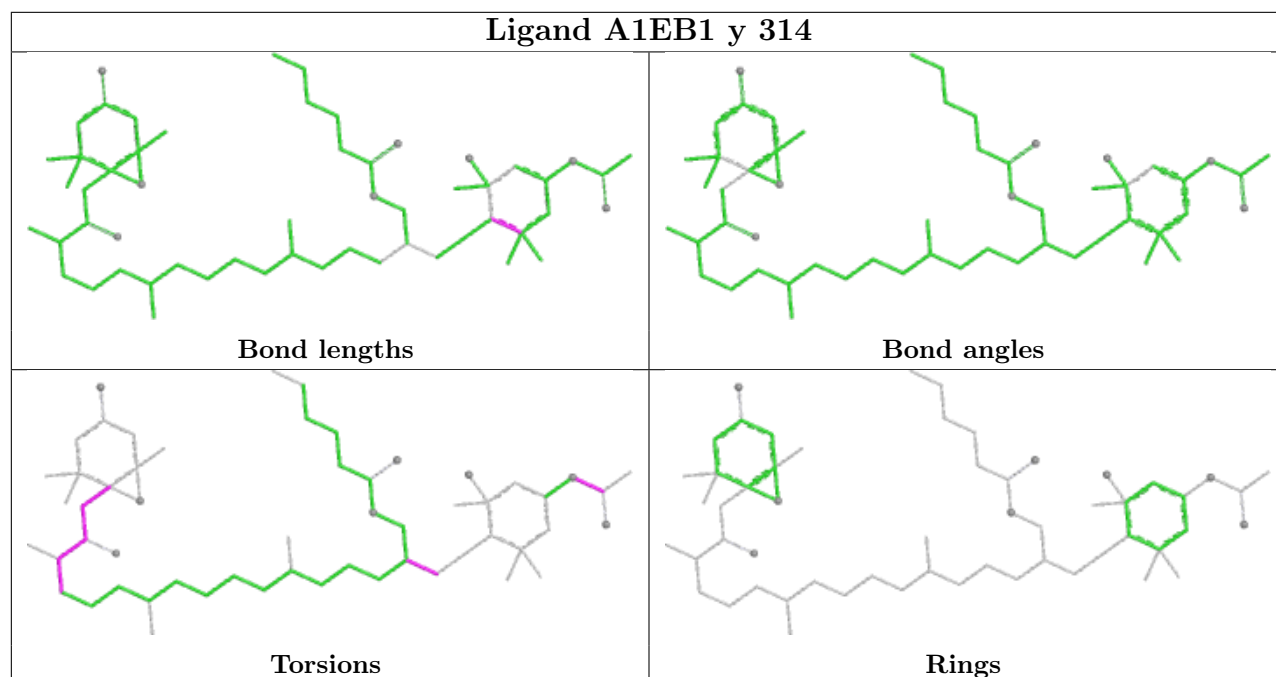
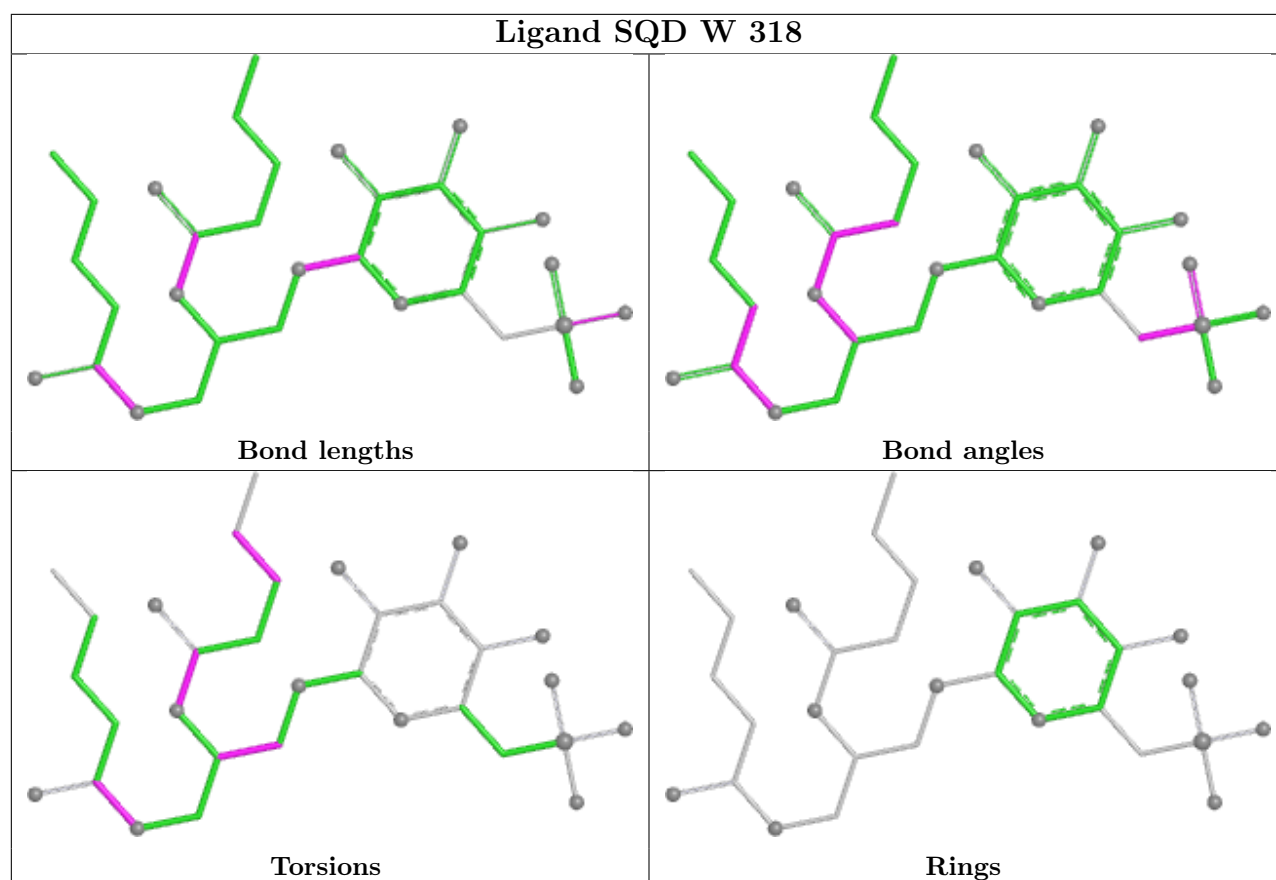


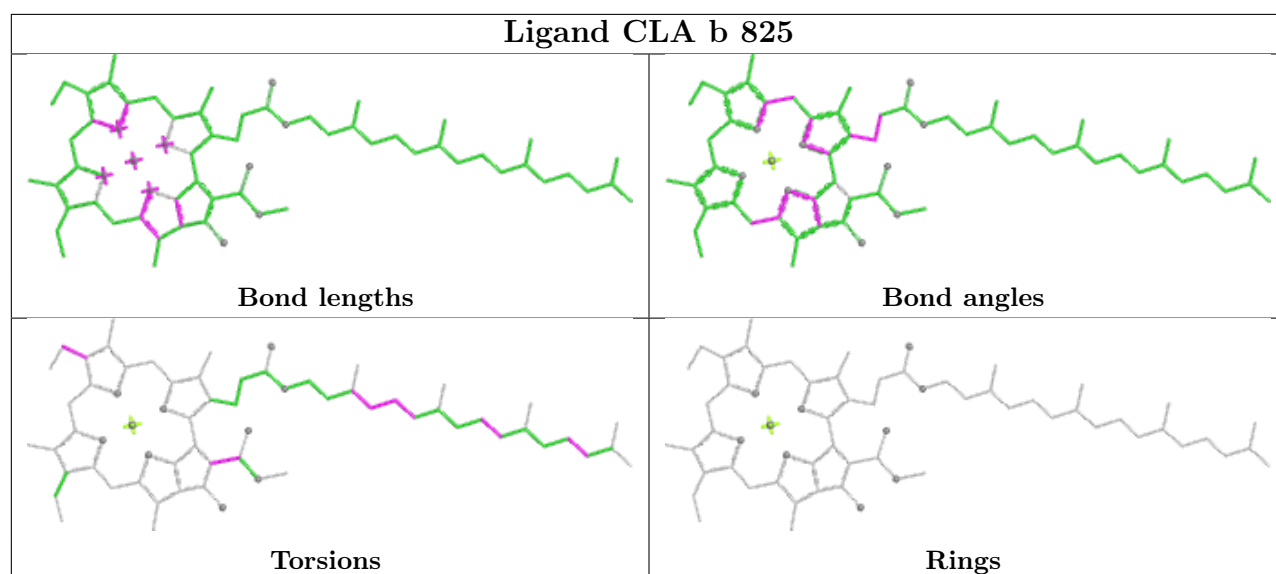
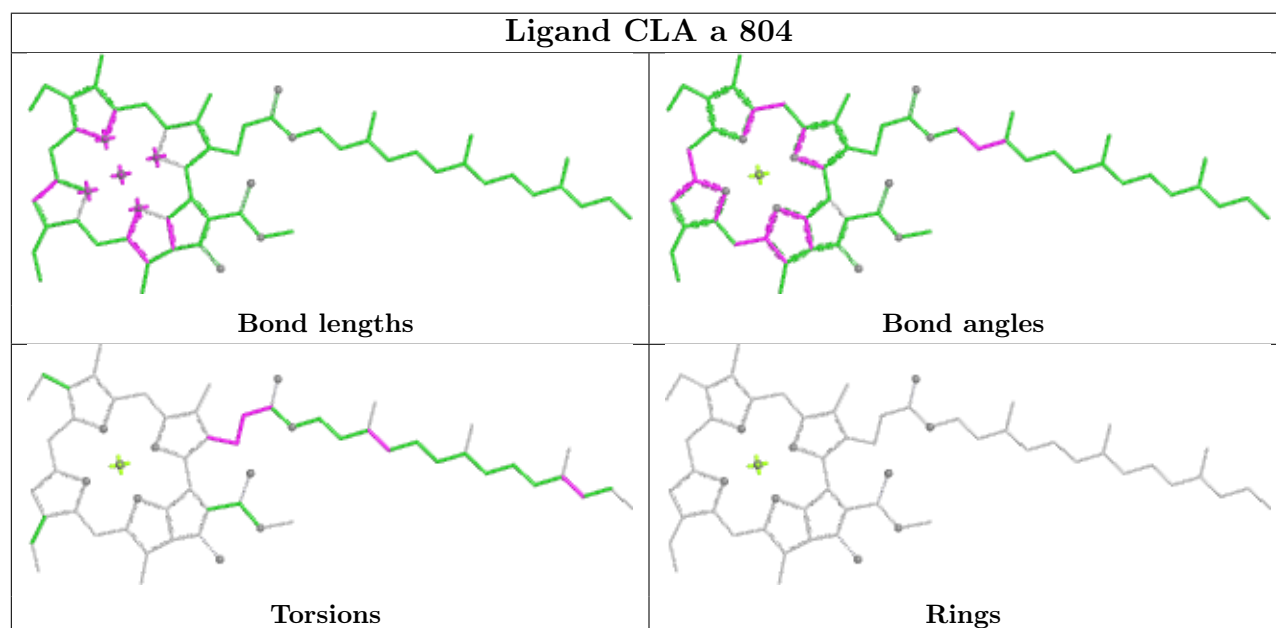
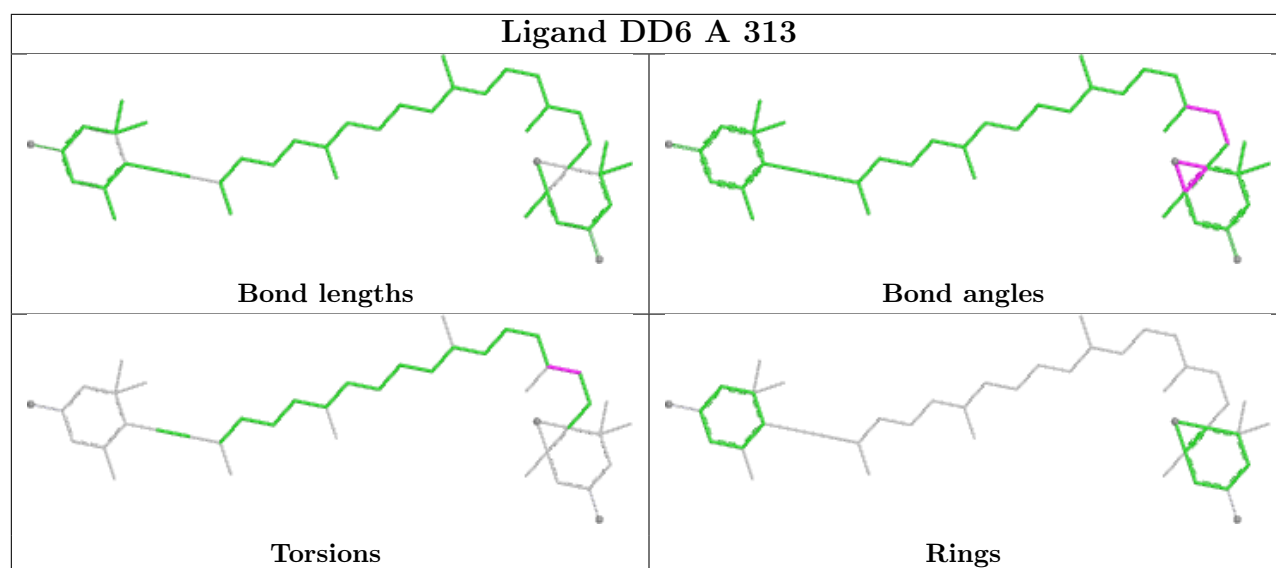
Torsions

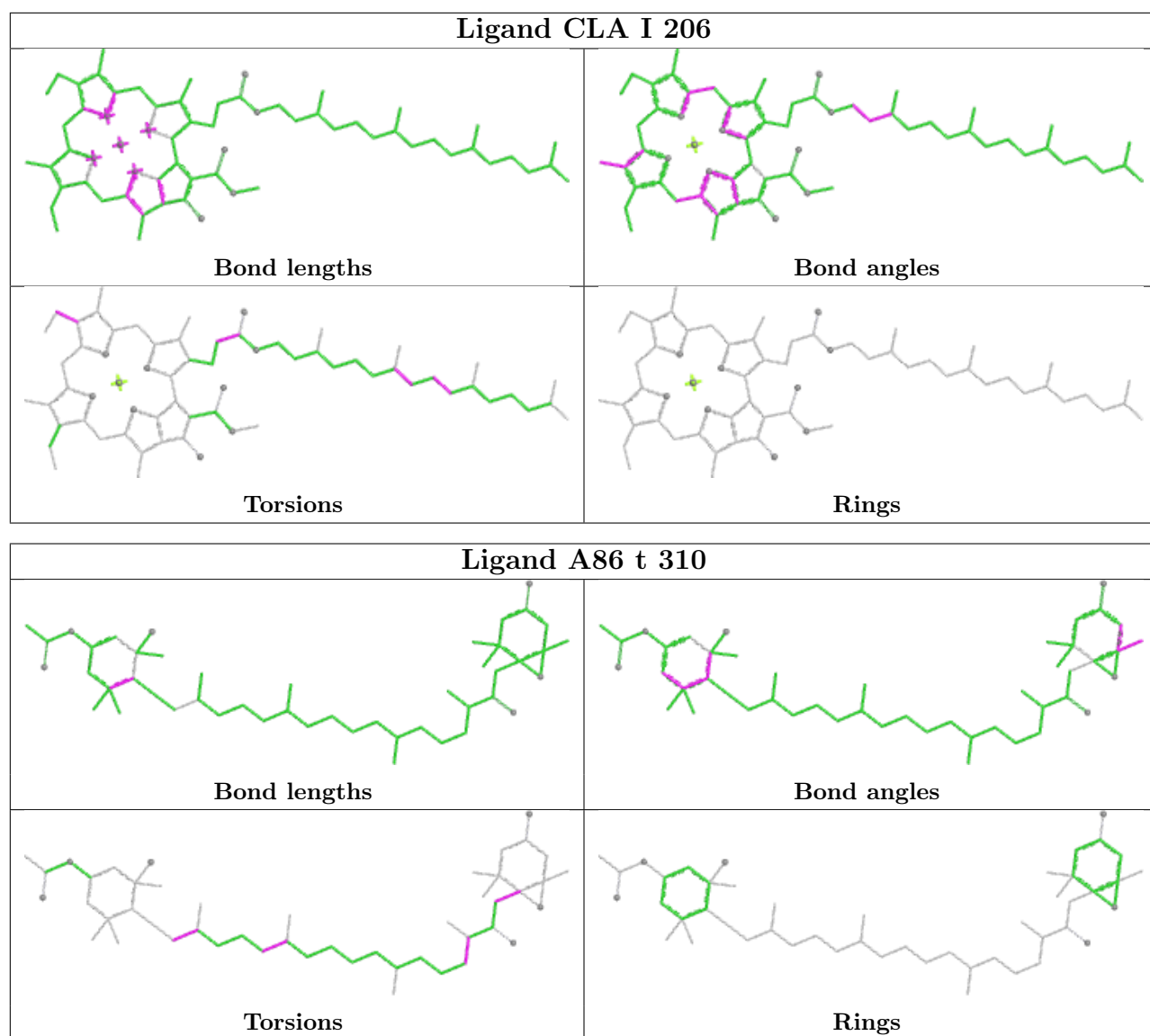


Rings

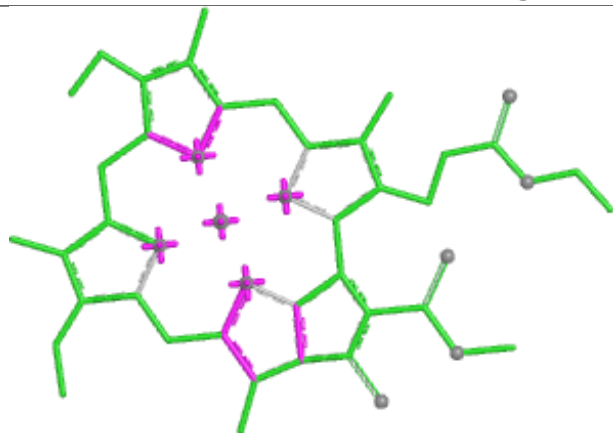




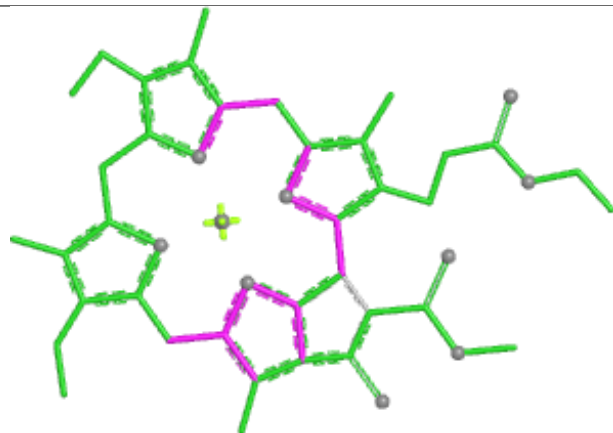




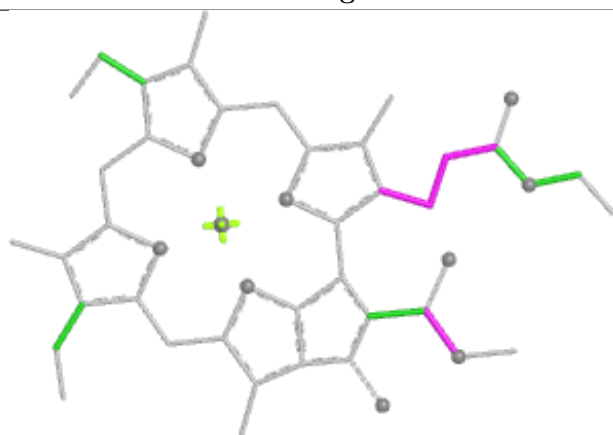
Ligand CLA B 304



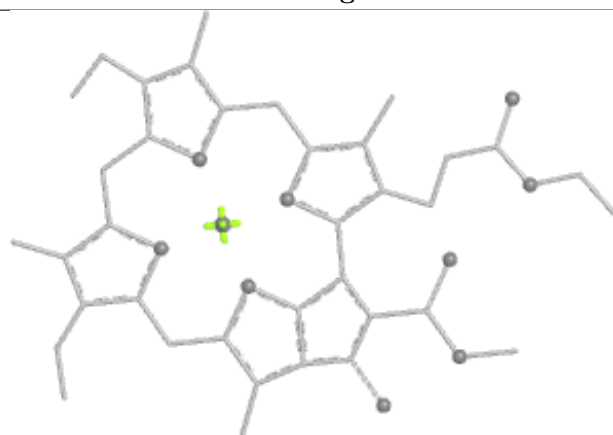
Bond lengths



Bond angles

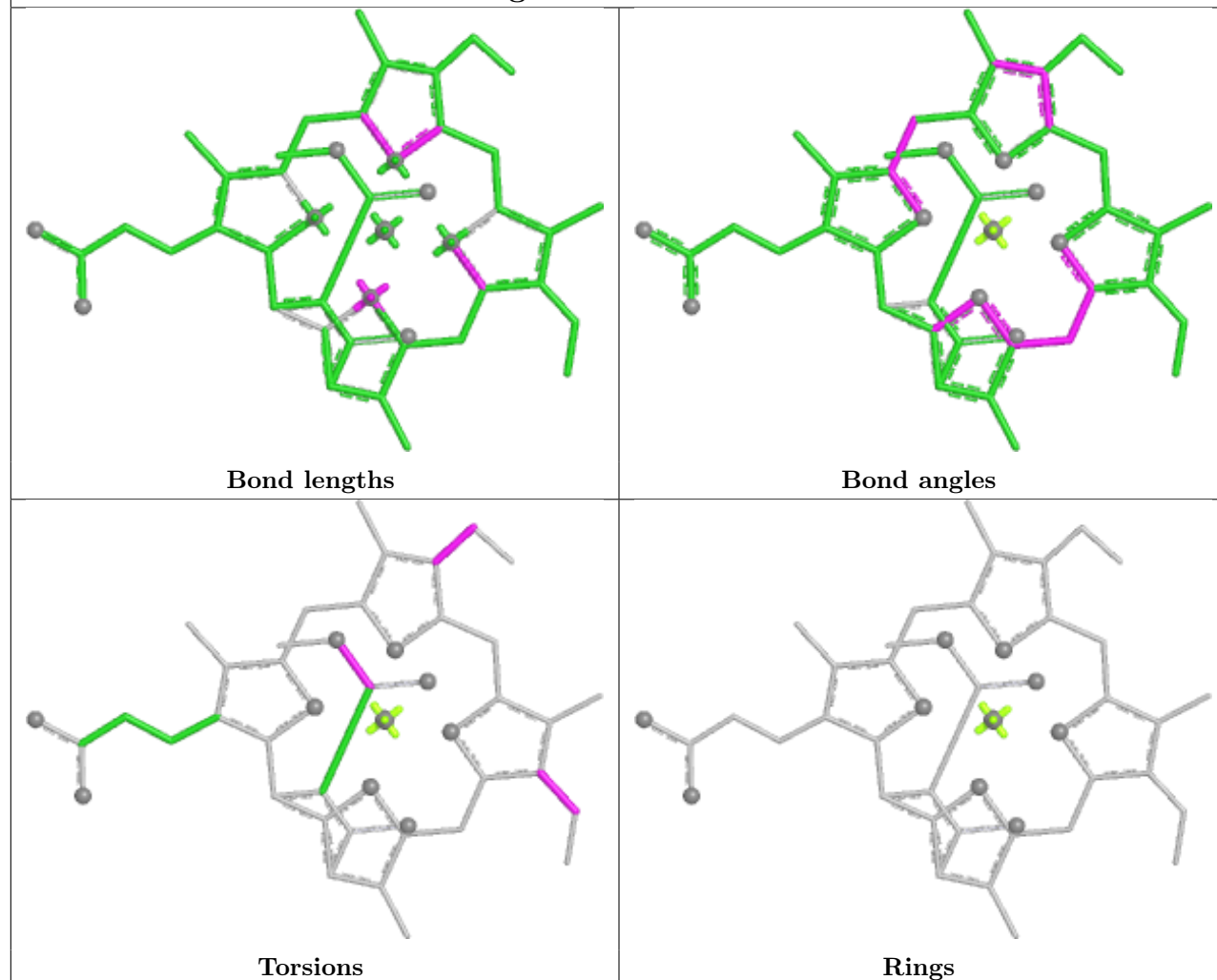


Torsions

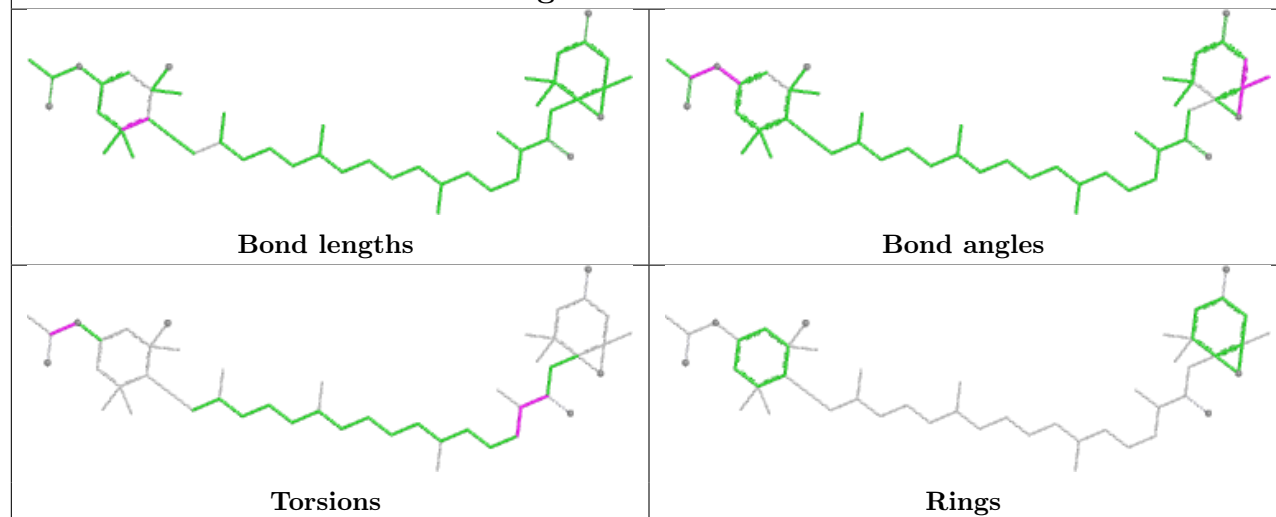


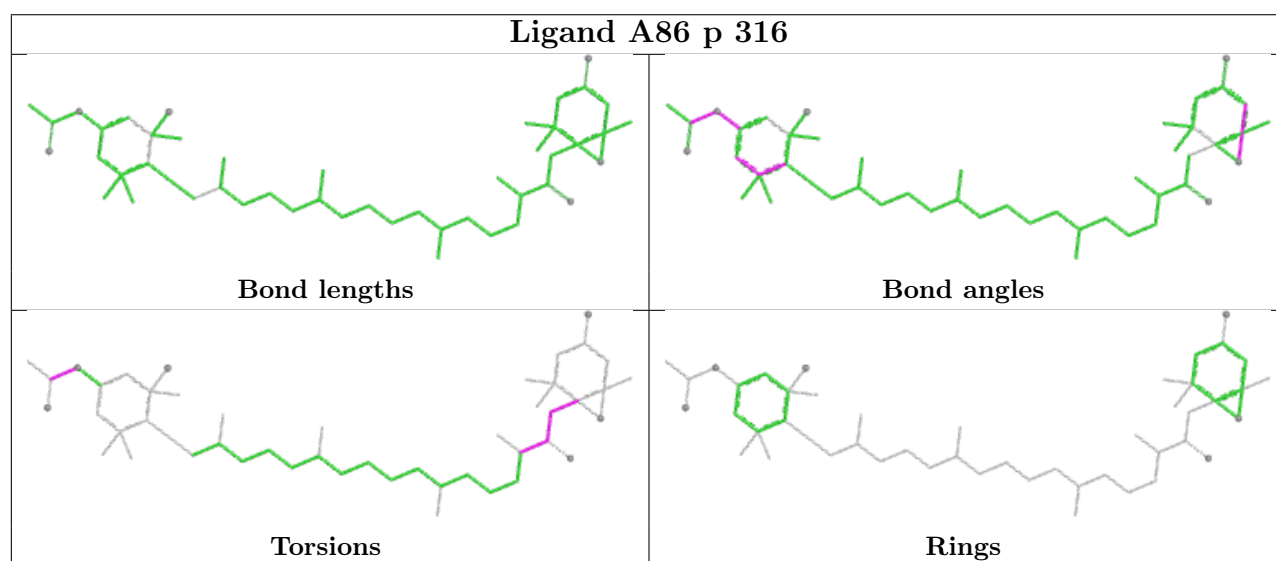
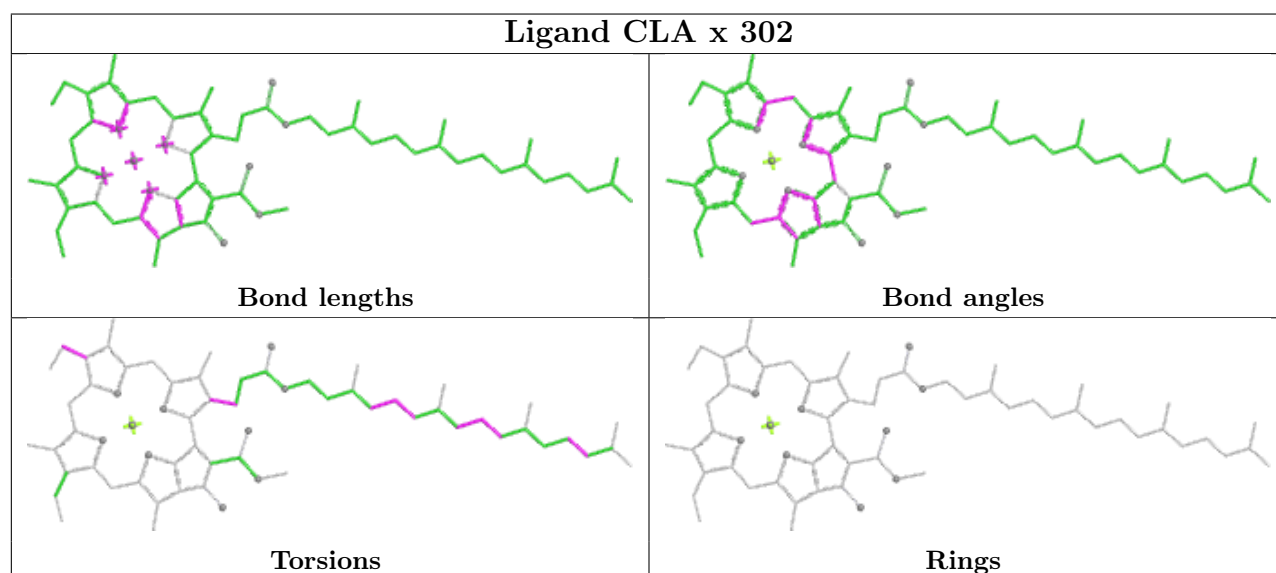
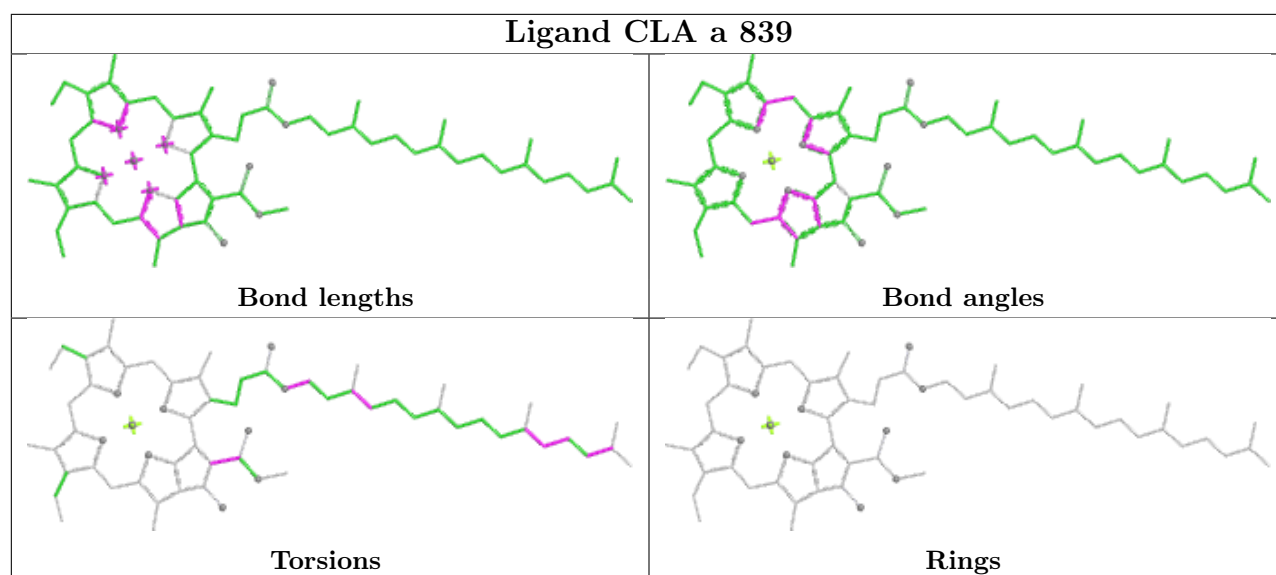
Rings

Ligand KC2 O 301

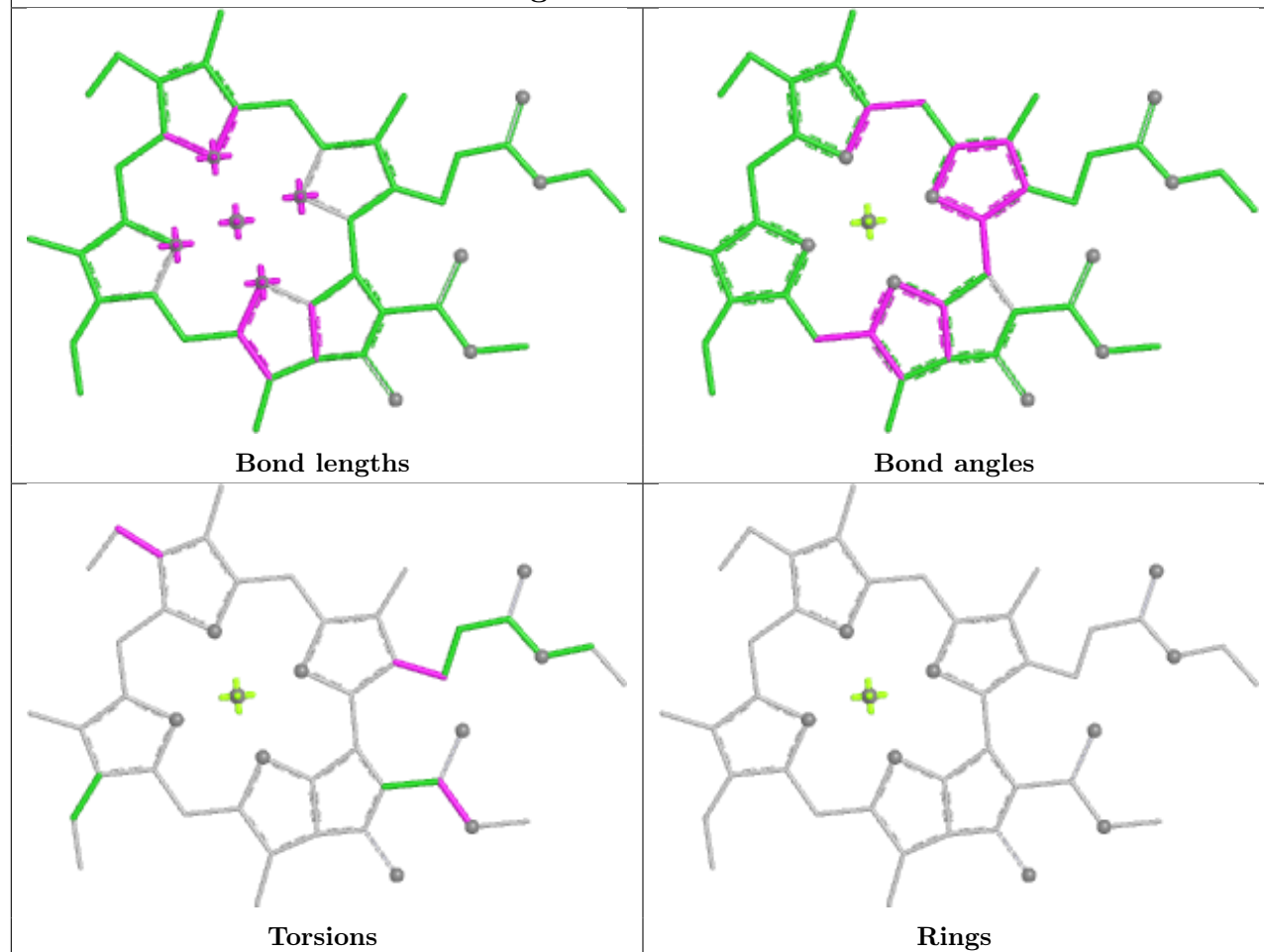


Ligand A86 X 321

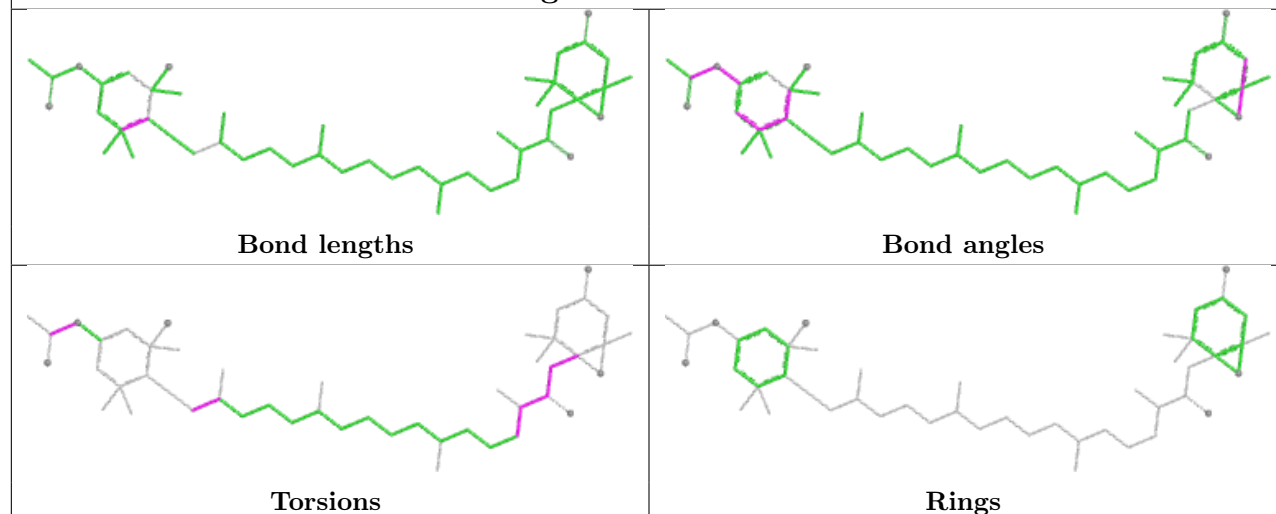




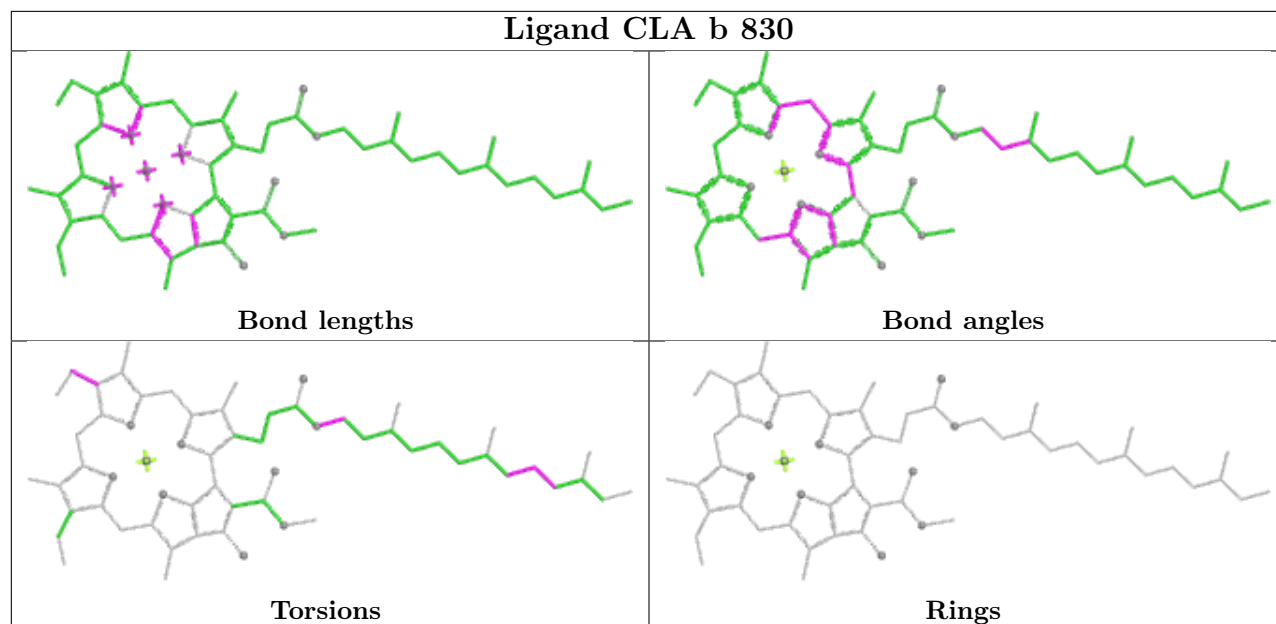
Ligand CLA S 311



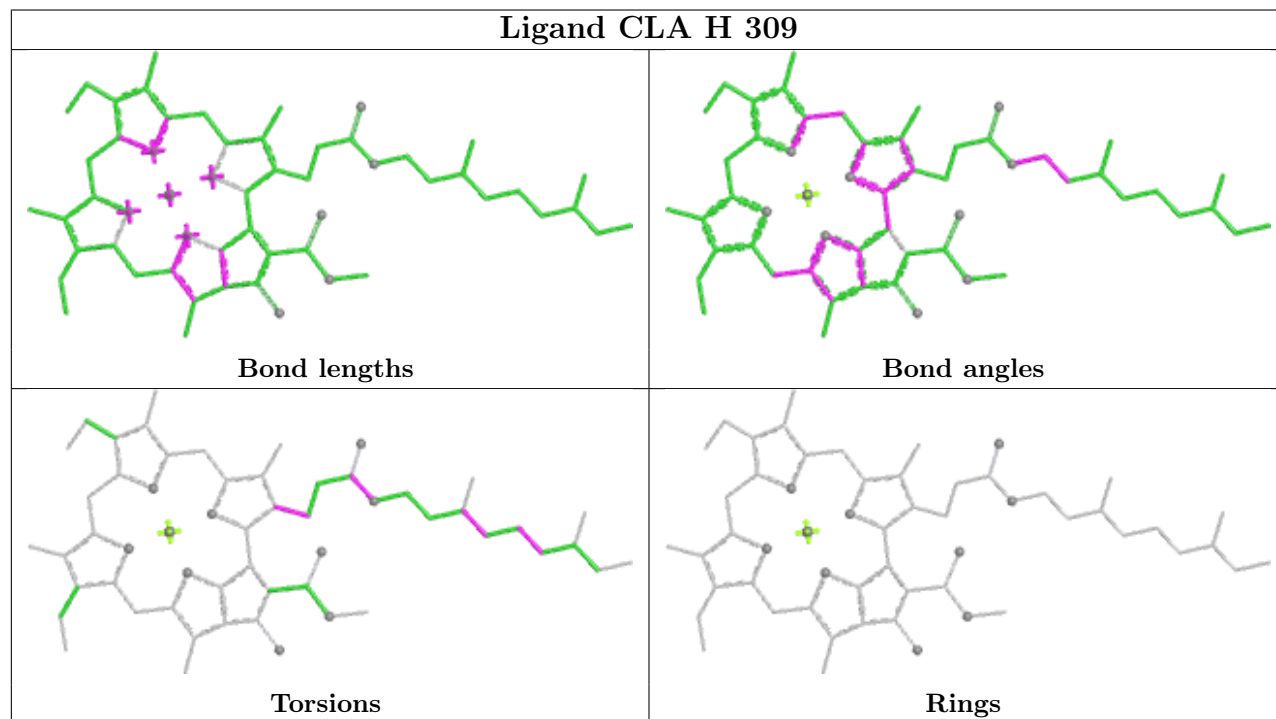
Ligand A86 u 319



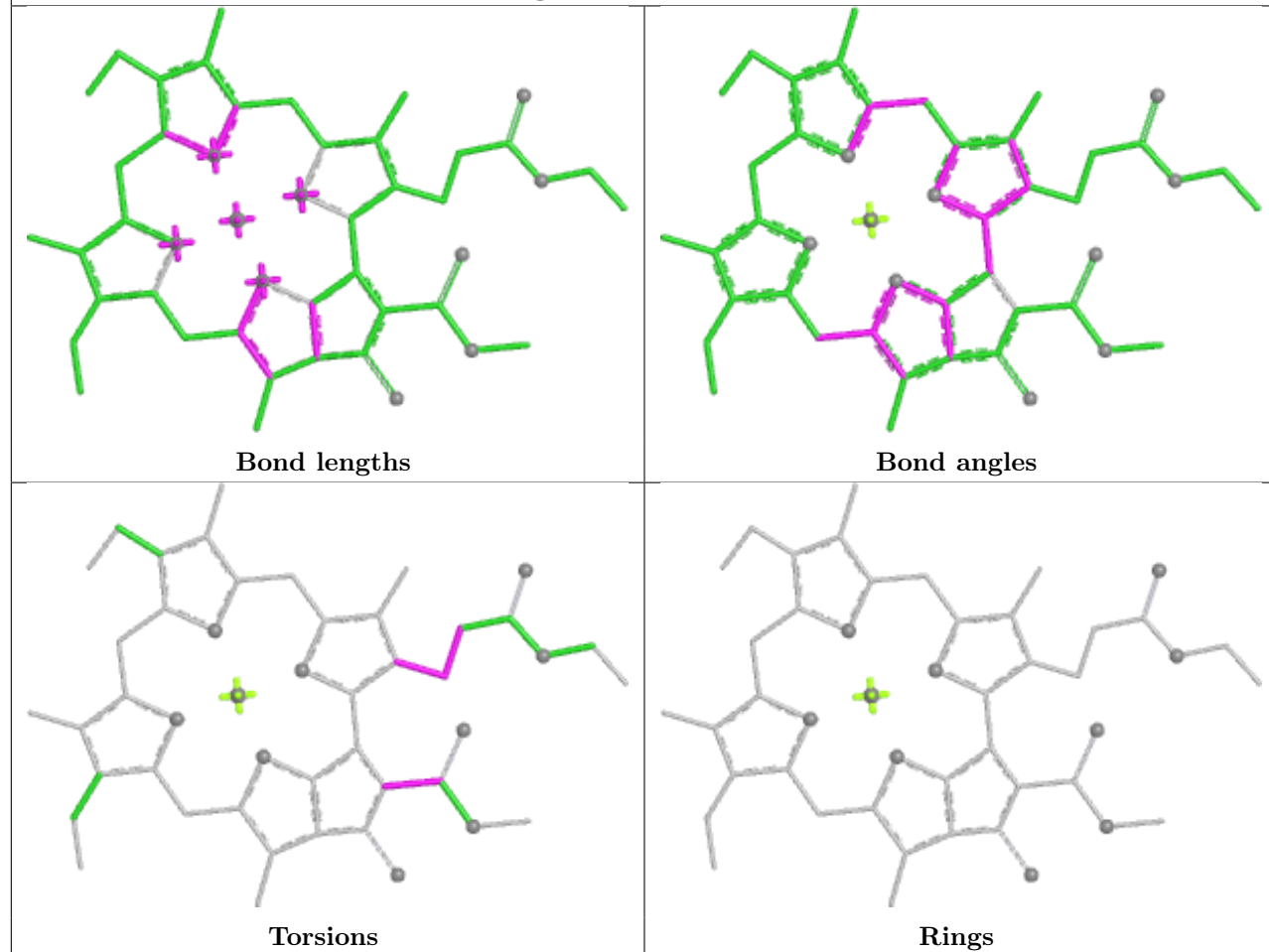
Ligand CLA b 830



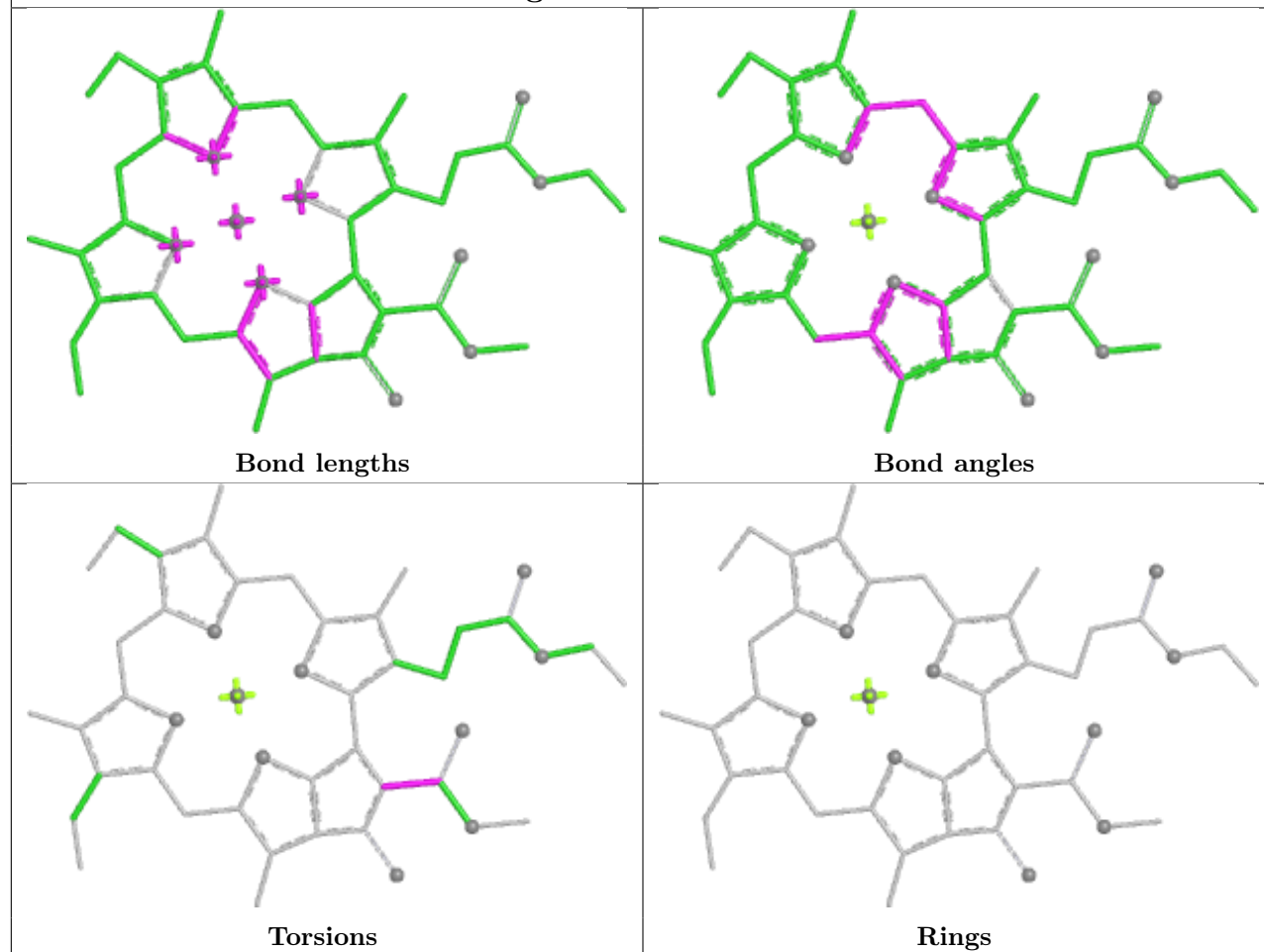
Ligand CLA H 309



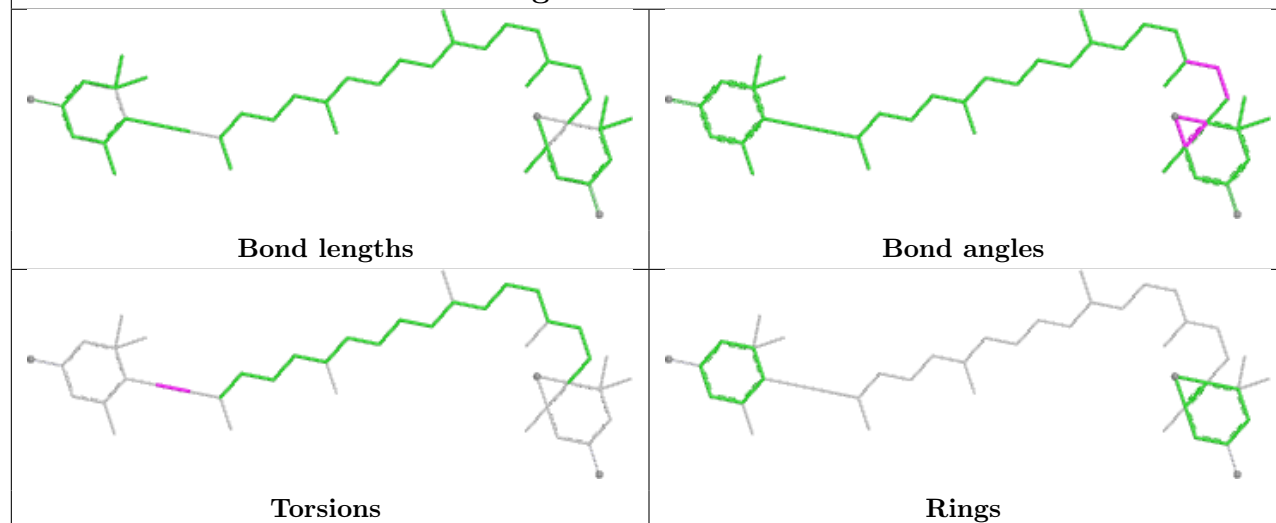
Ligand CLA u 314



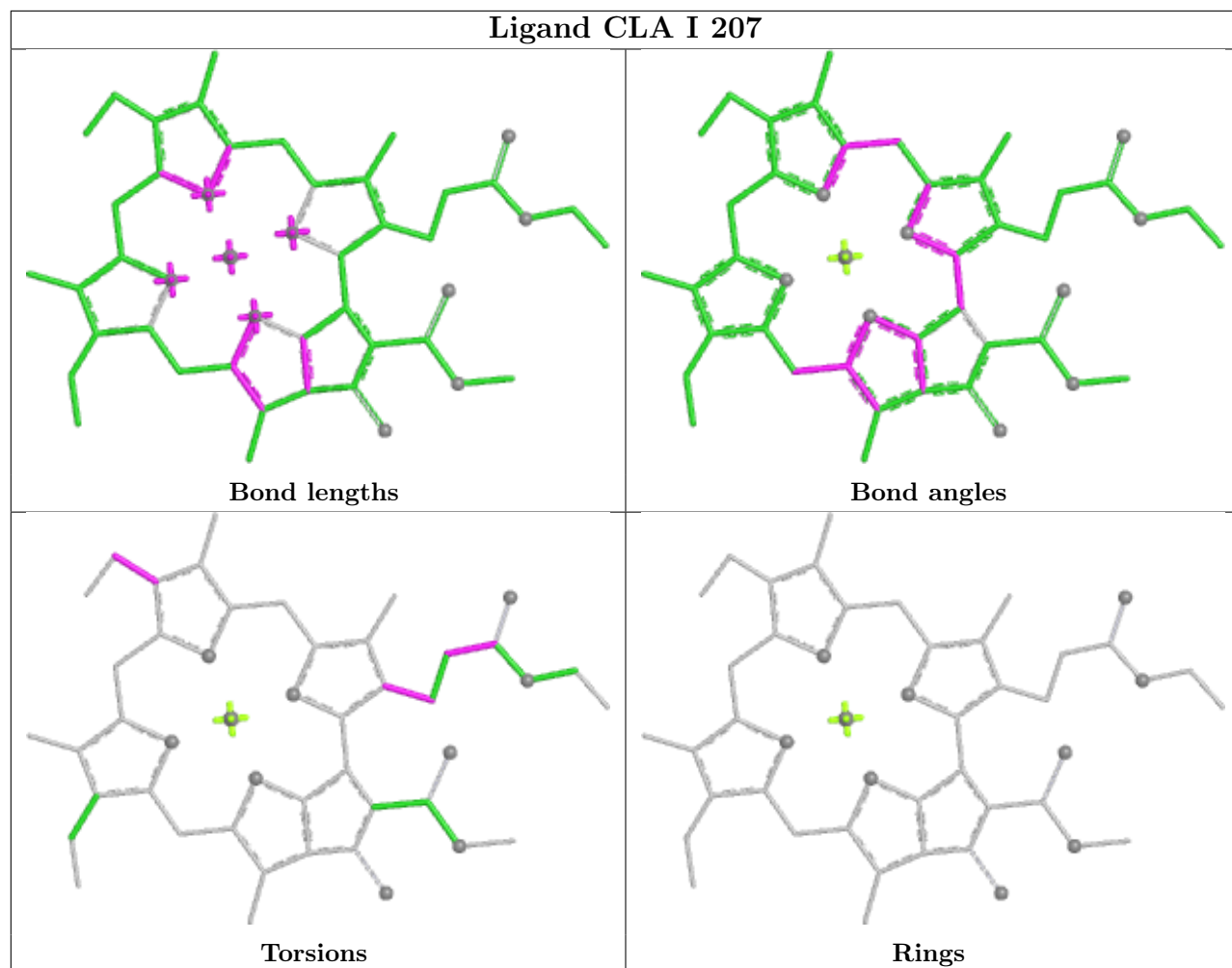
Ligand CLA K 312



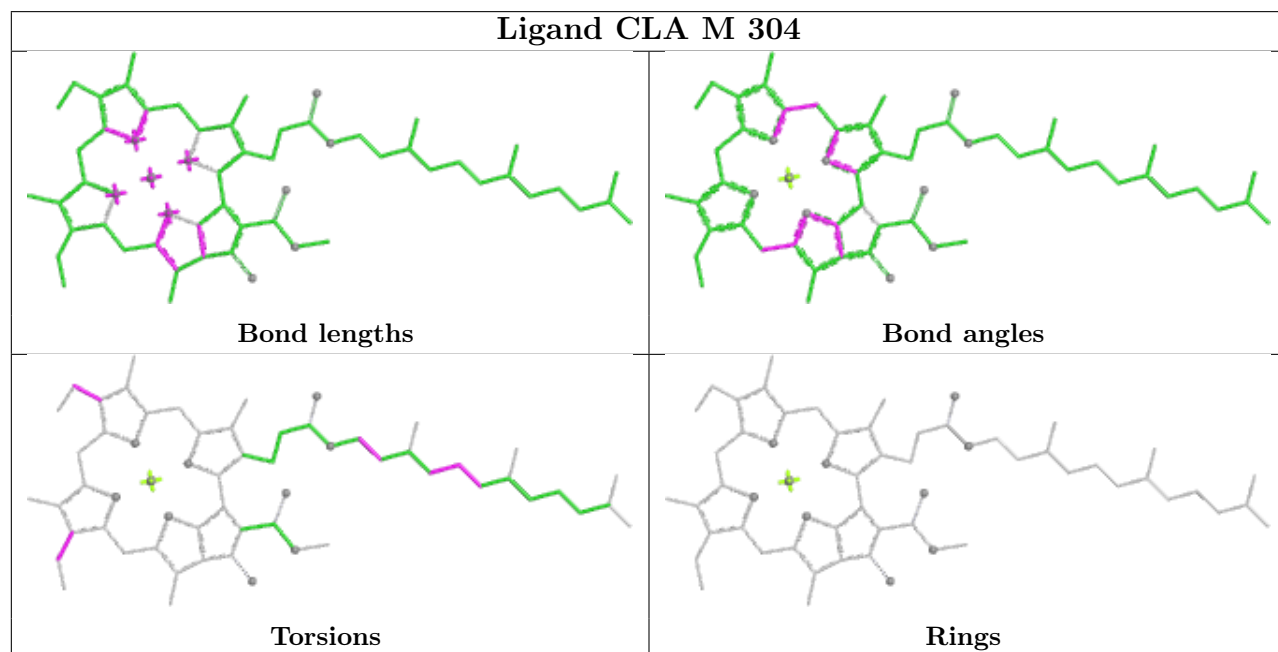
Ligand DD6 G 210



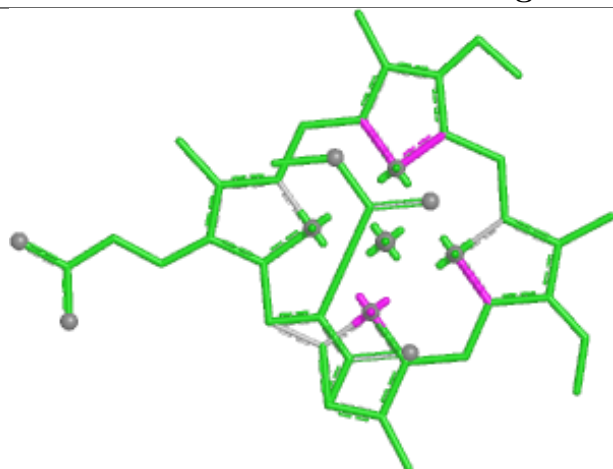
Ligand CLA I 207



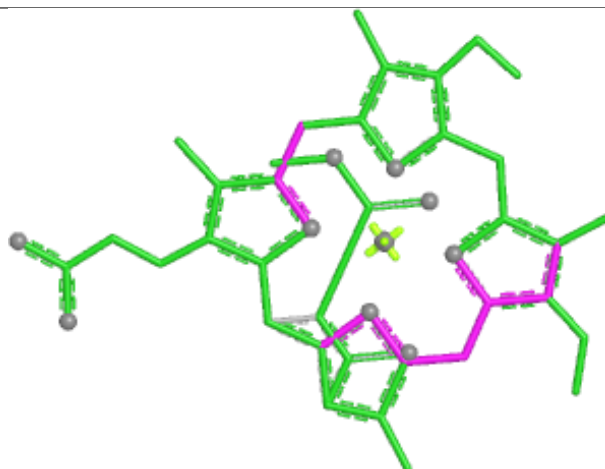
Ligand CLA M 304



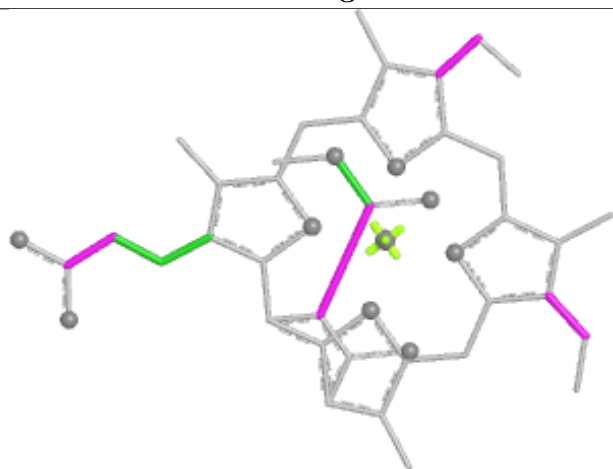
Ligand KC2 Y 308



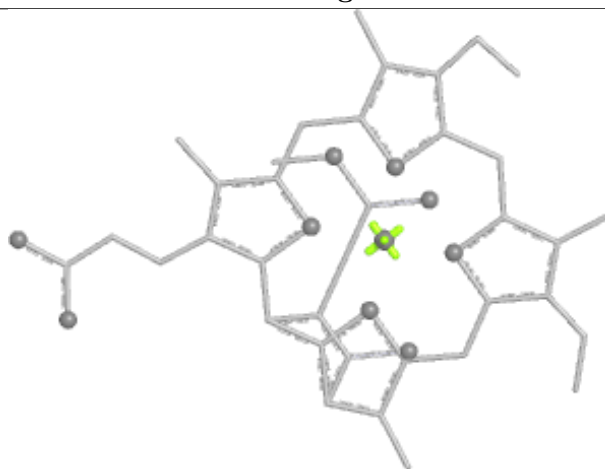
Bond lengths



Bond angles

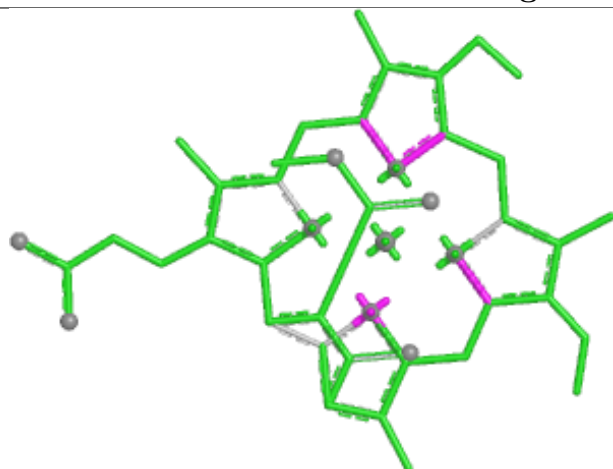


Torsions

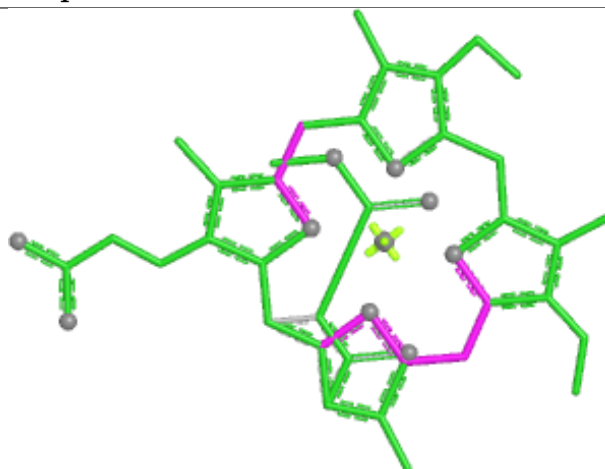


Rings

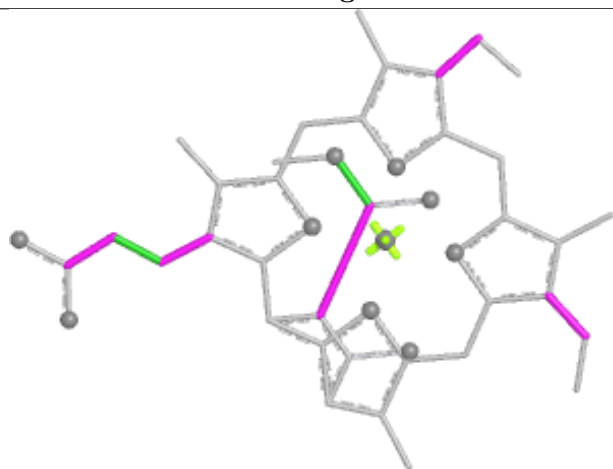
Ligand KC2 q 308



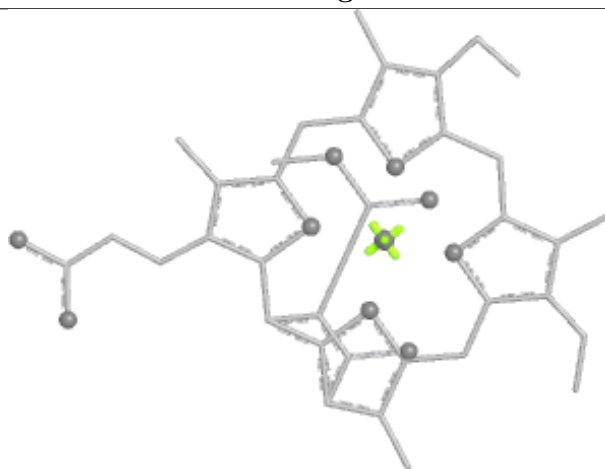
Bond lengths



Bond angles

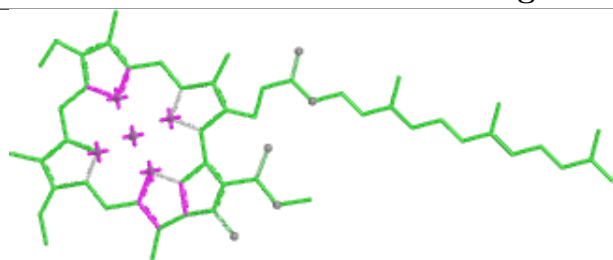


Torsions

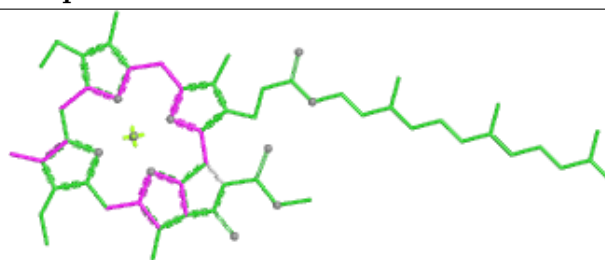


Rings

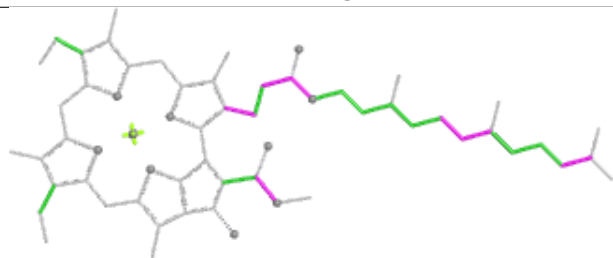
Ligand CLA q 307



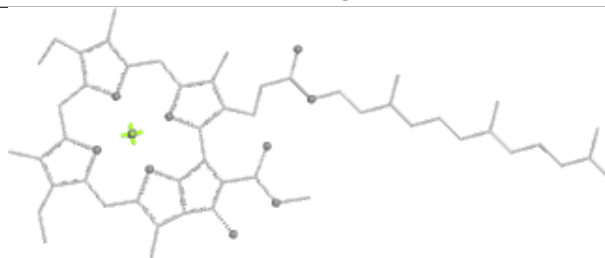
Bond lengths



Bond angles

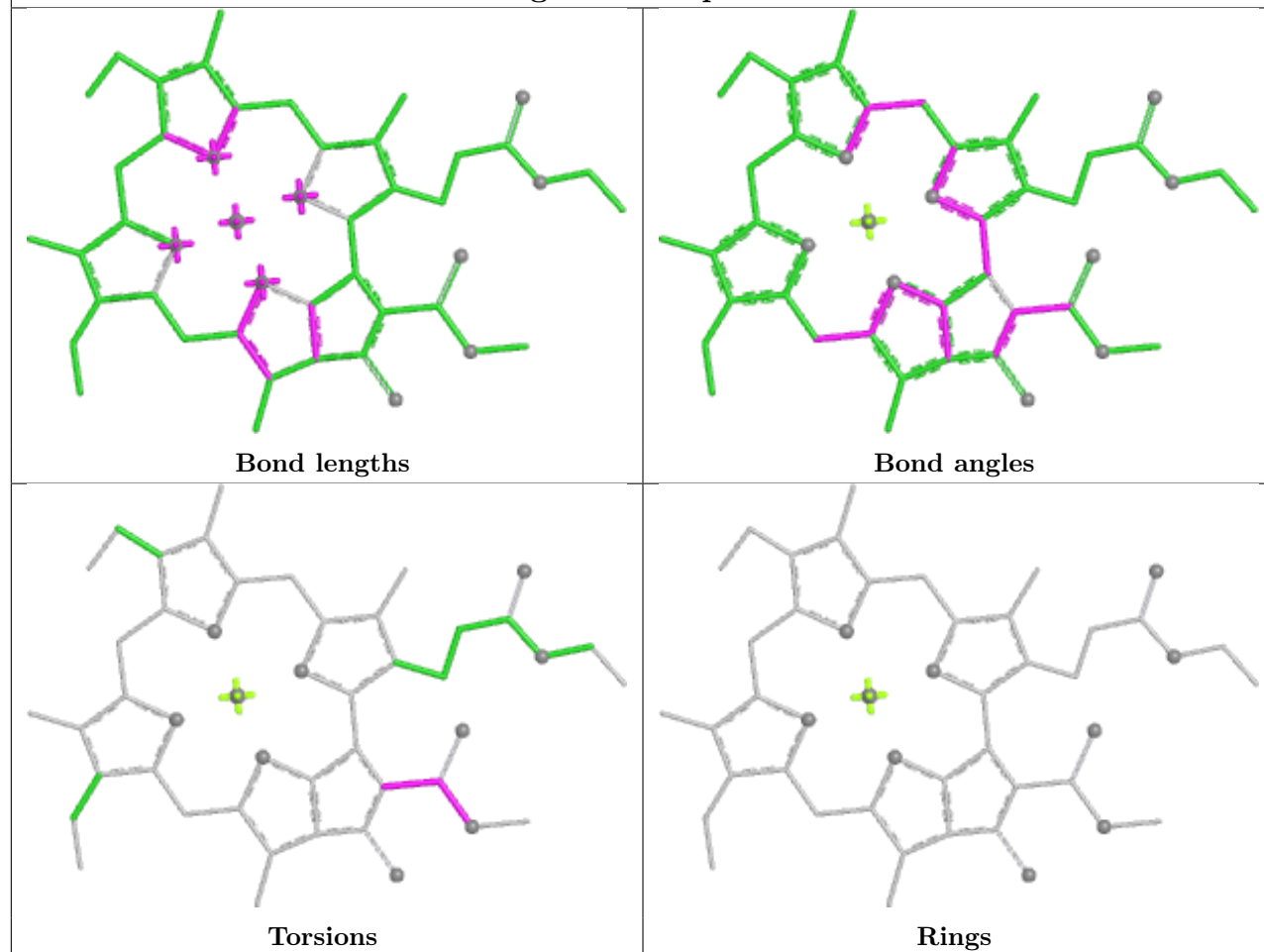


Torsions

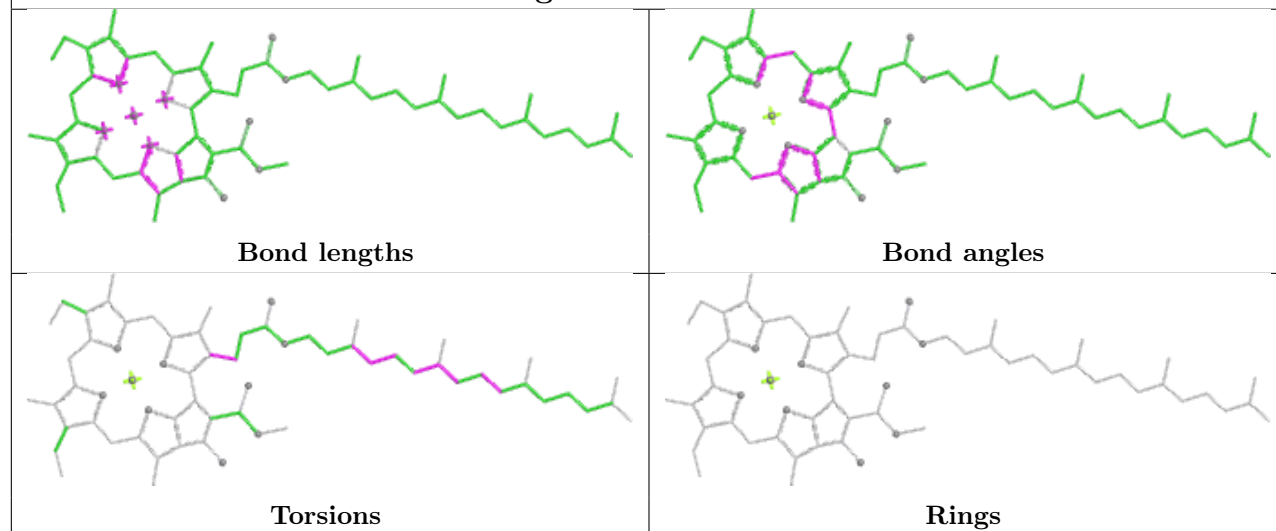


Rings

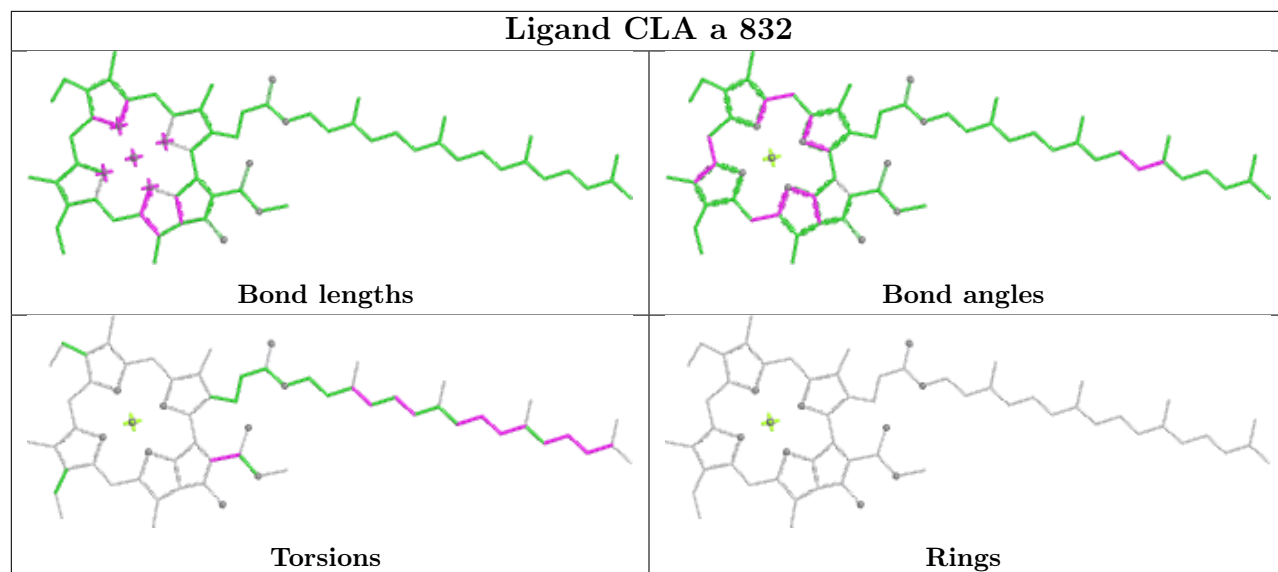
Ligand CLA p 312



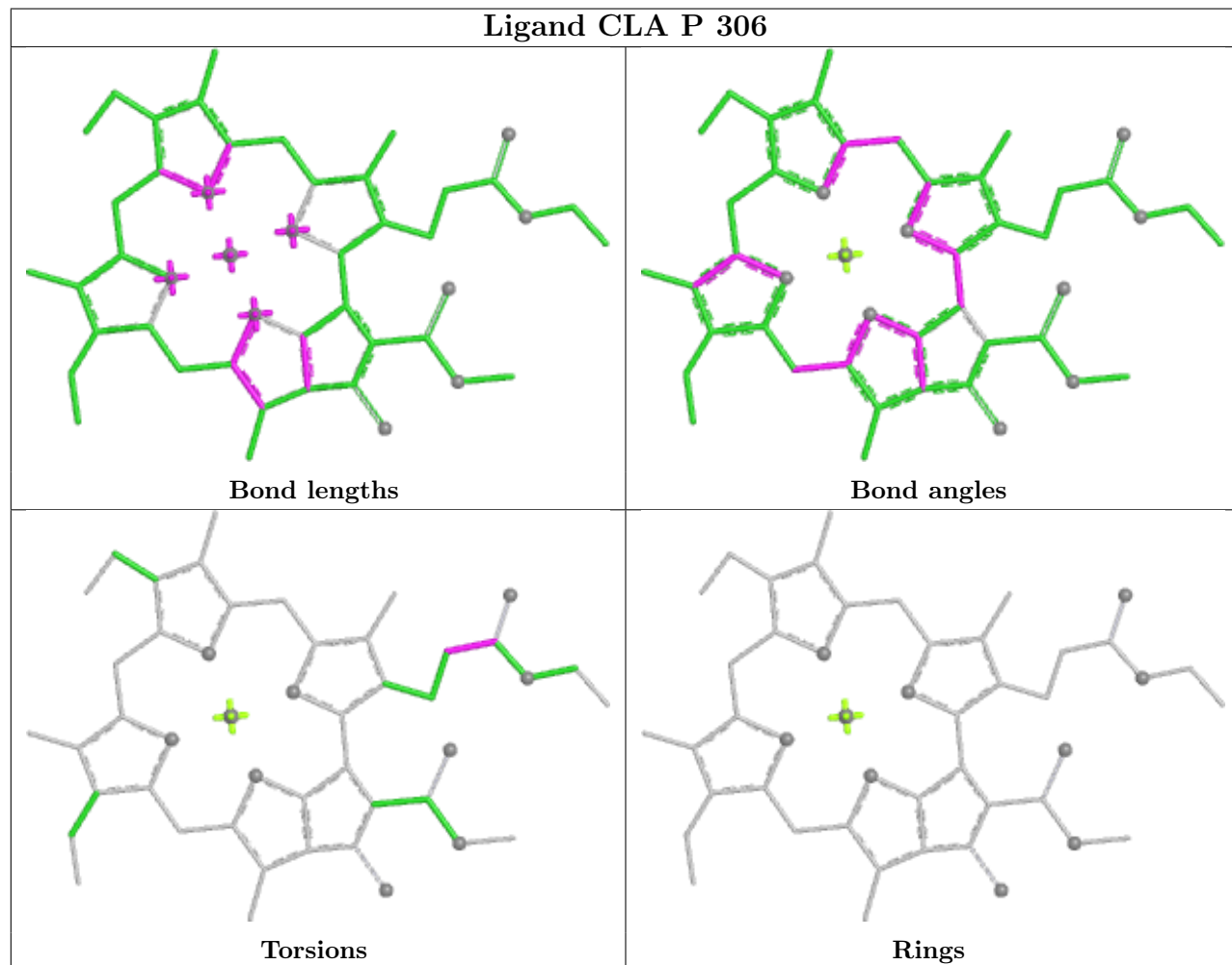
Ligand CLA b 838

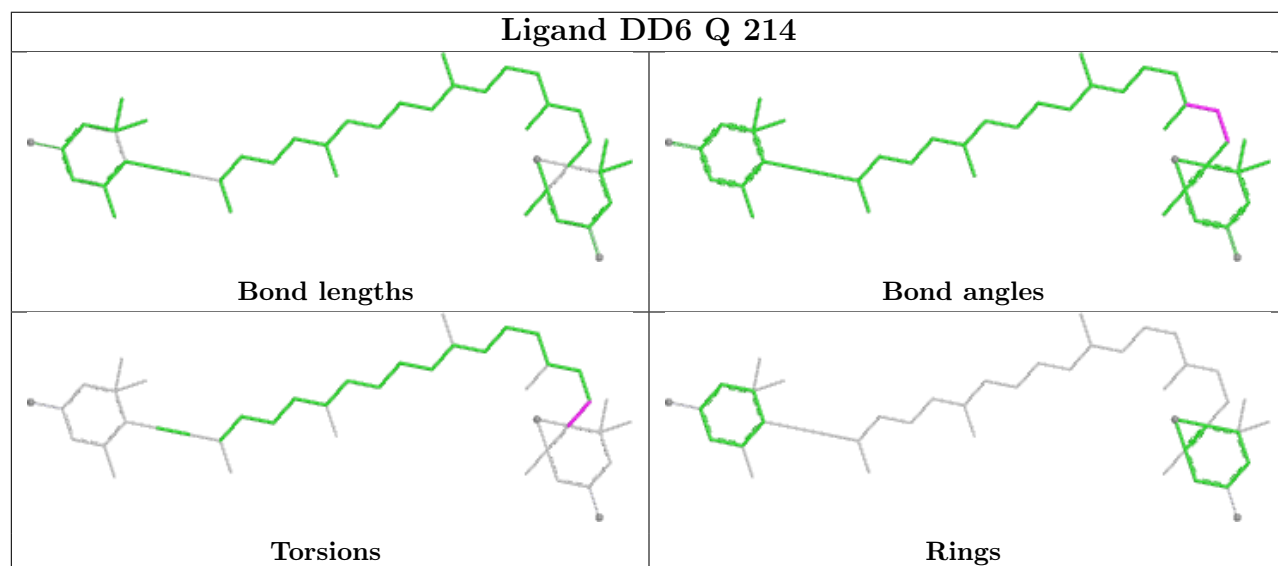
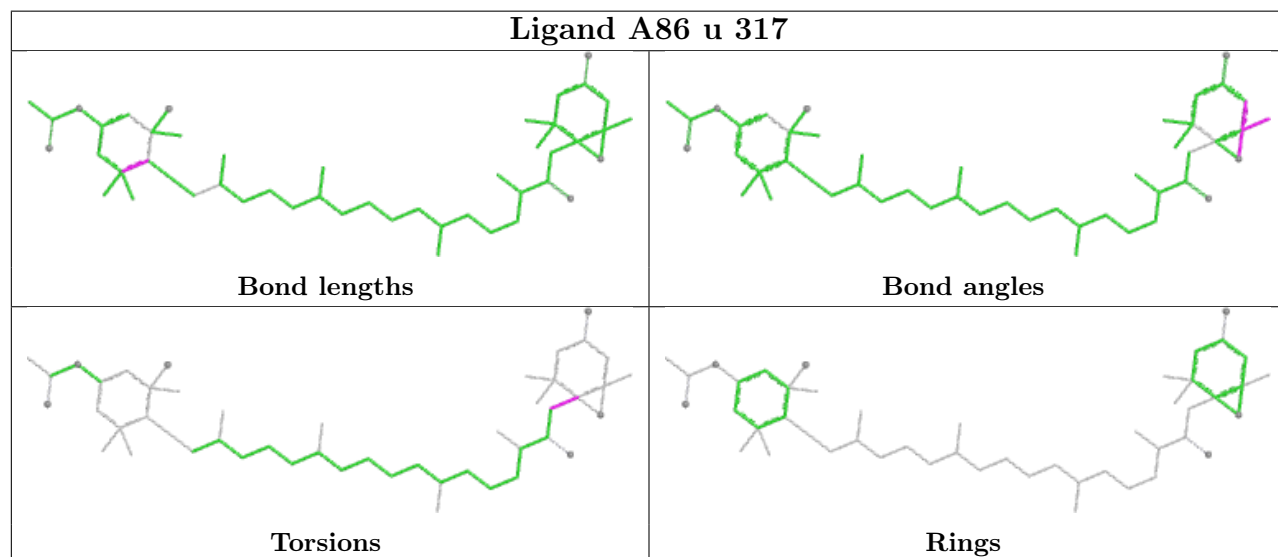
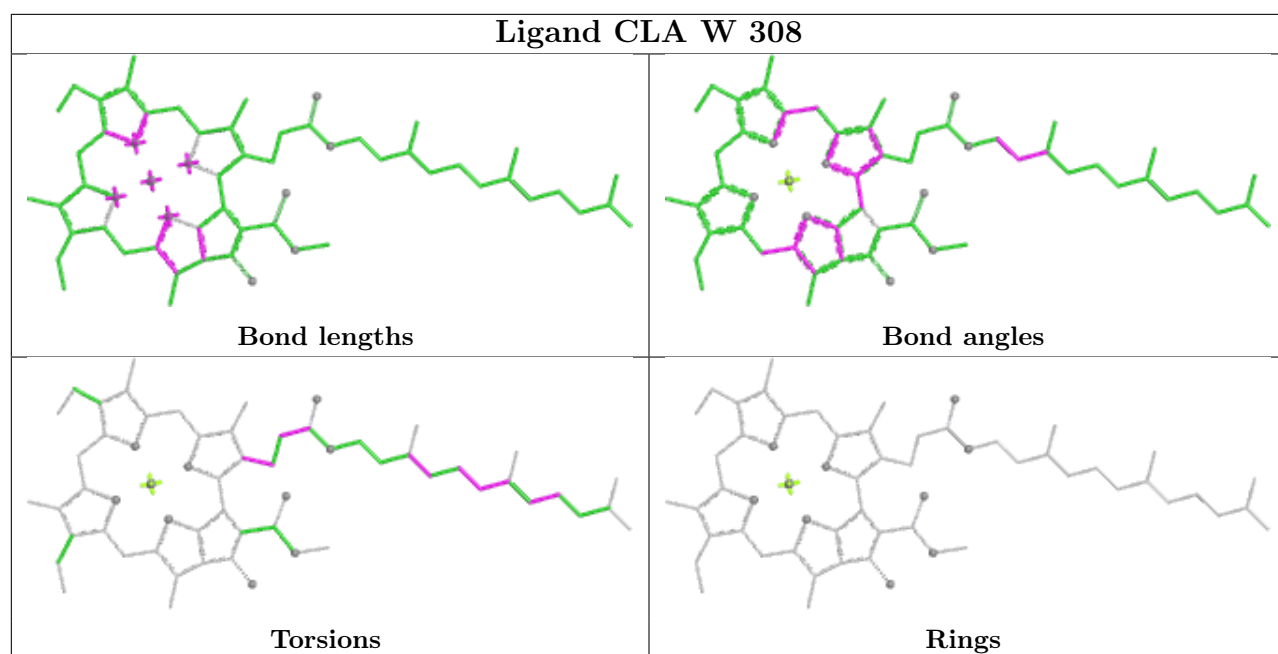


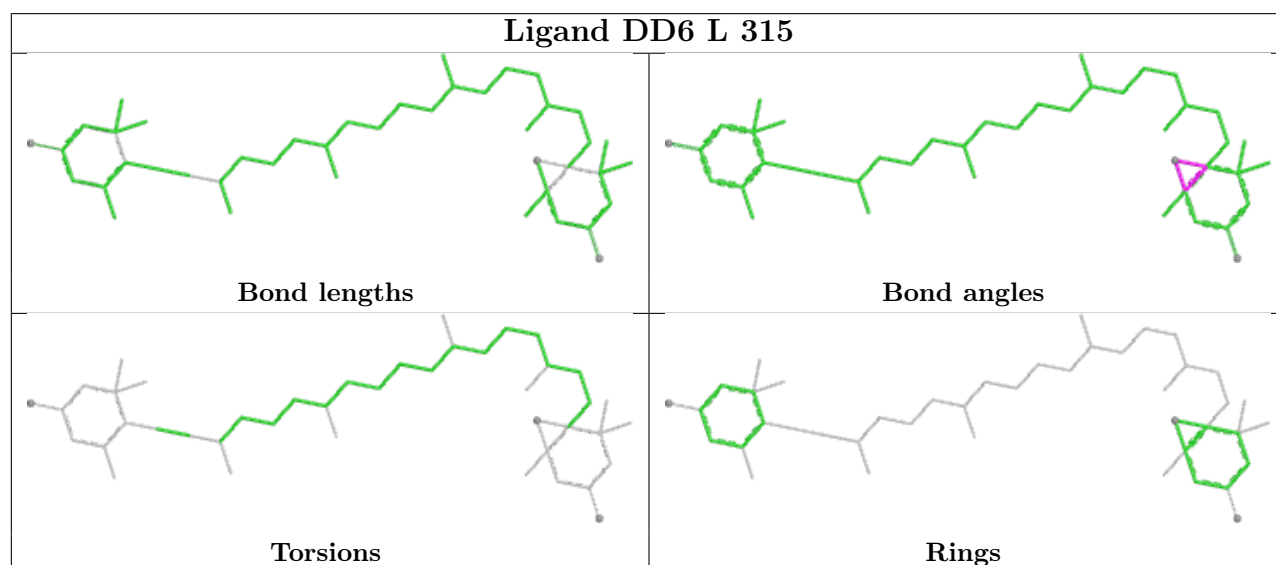
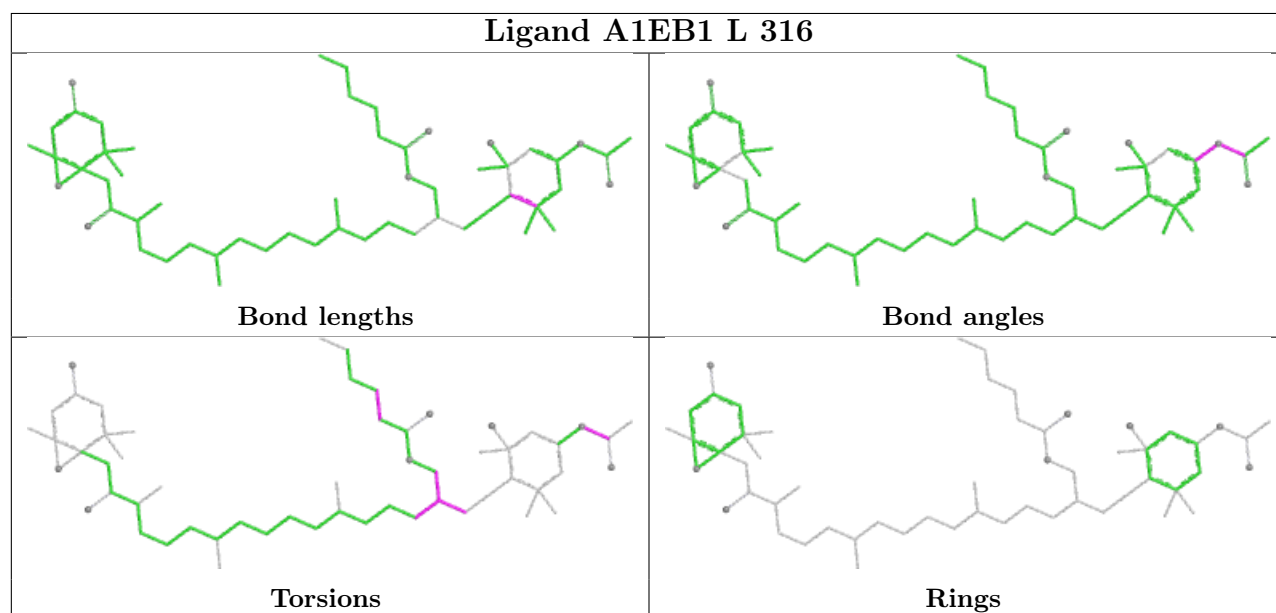
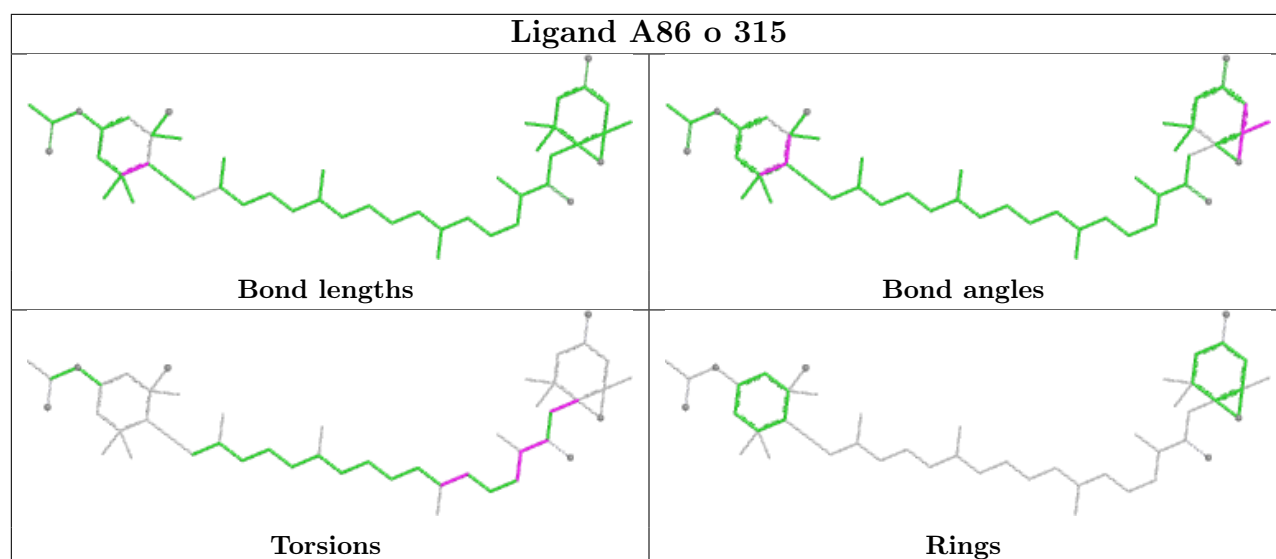
Ligand CLA a 832



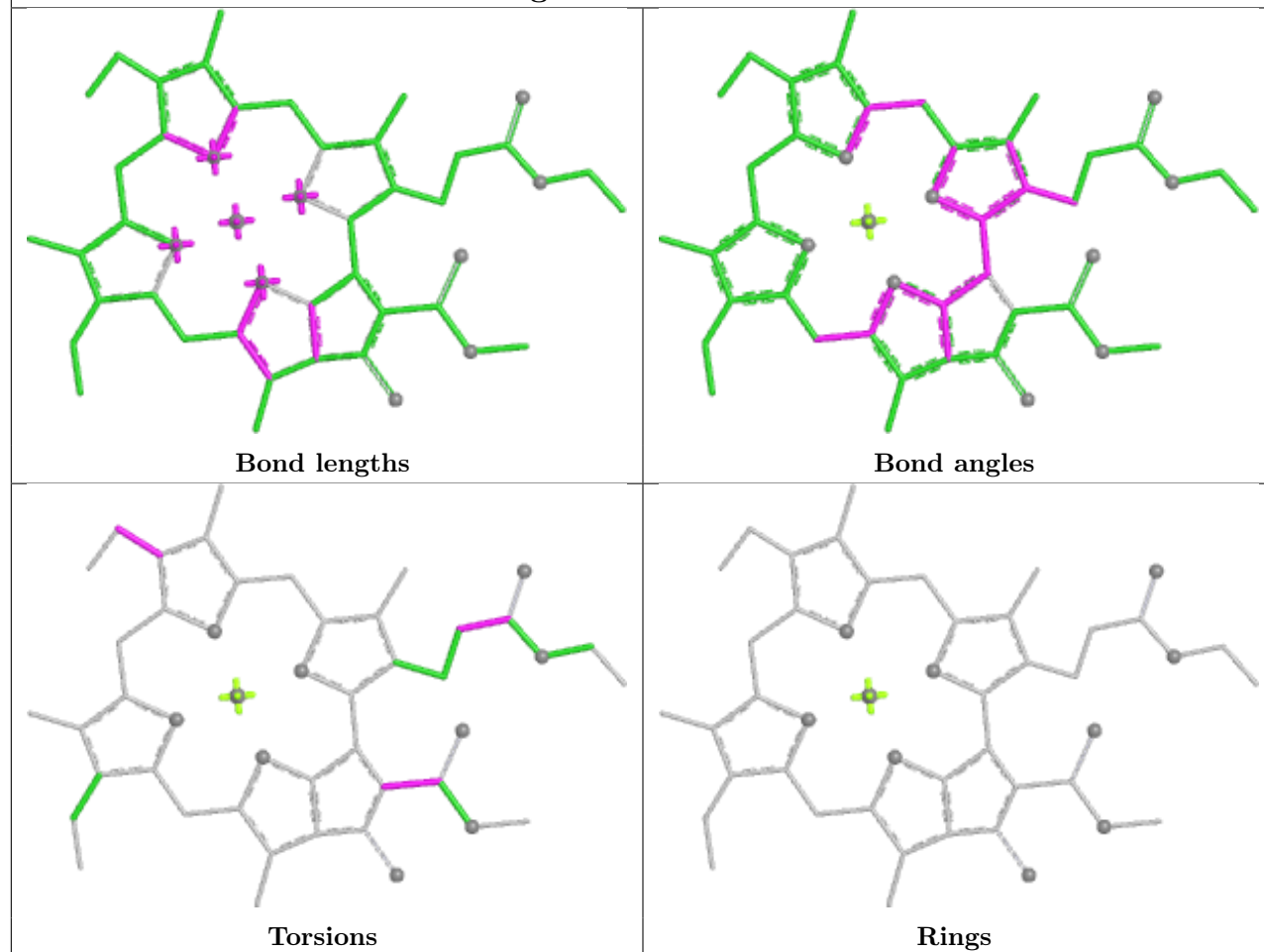
Ligand CLA P 306



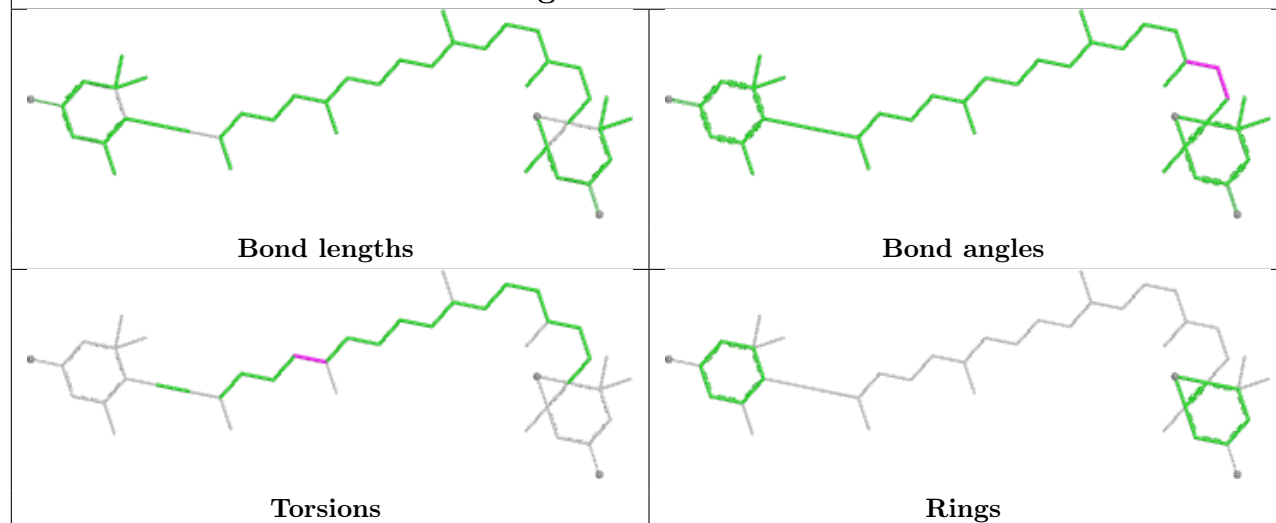


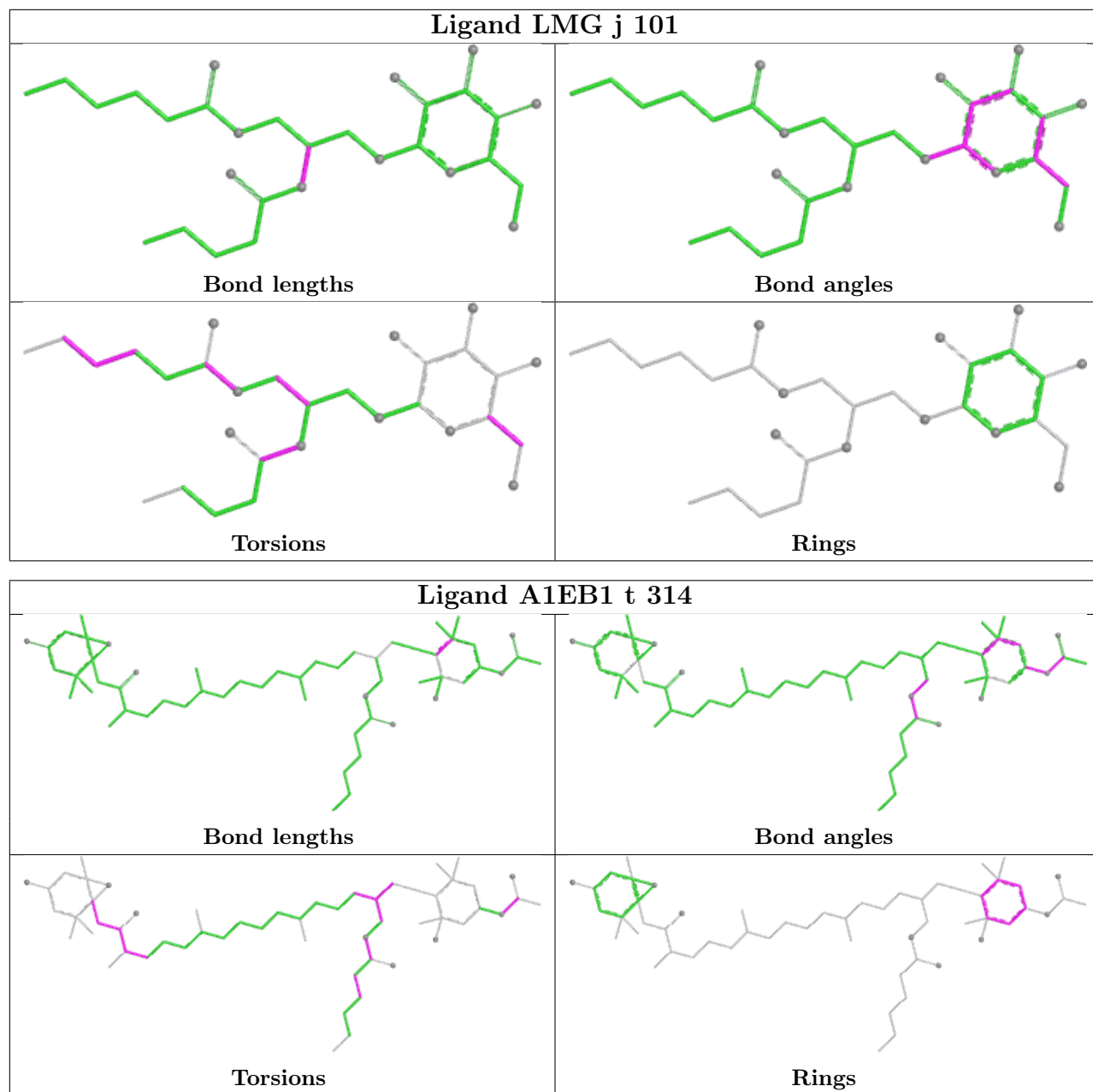


Ligand CLA b 816

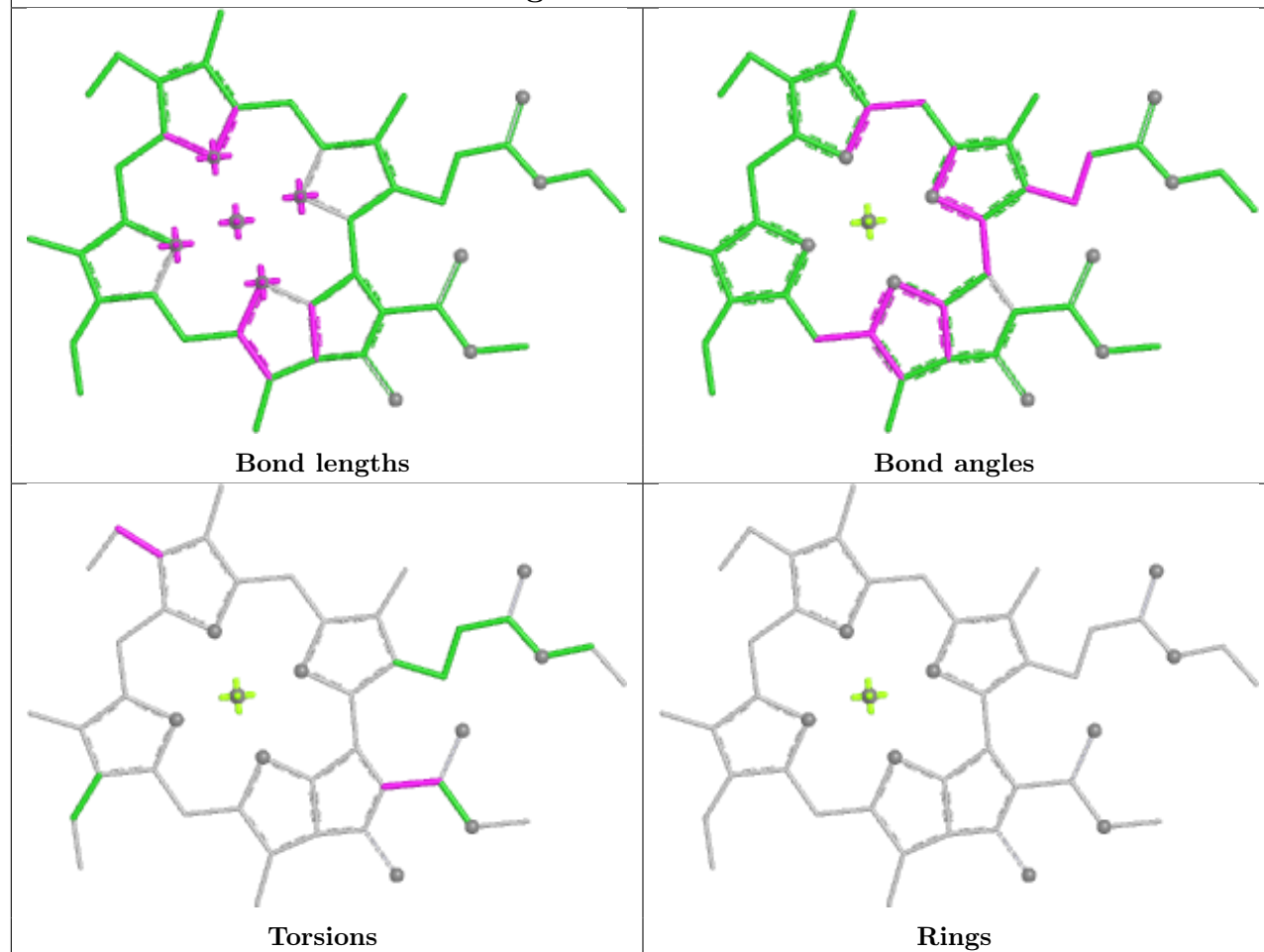


Ligand DD6 z 321

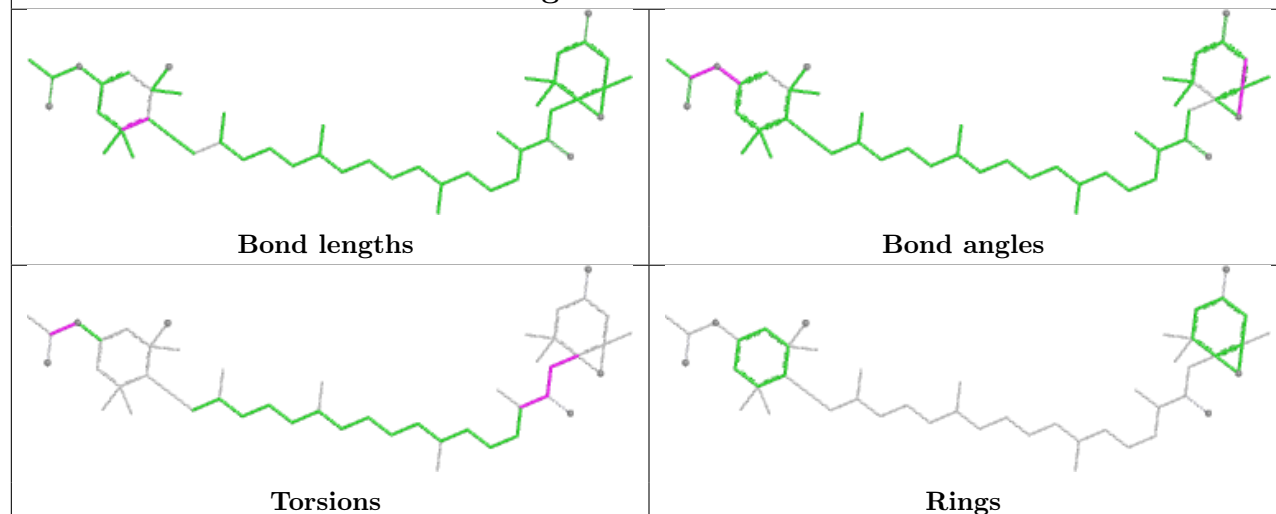




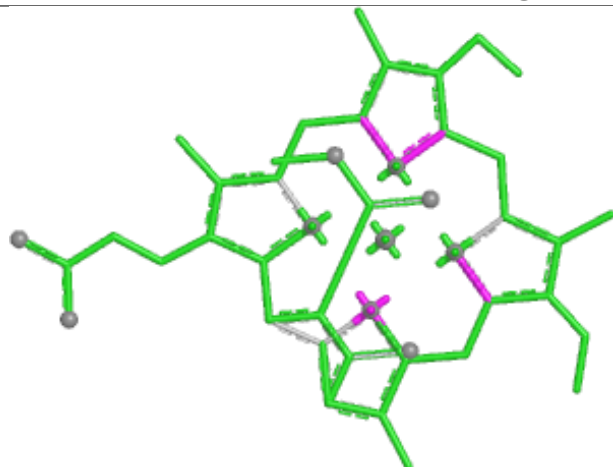
Ligand CLA U 205



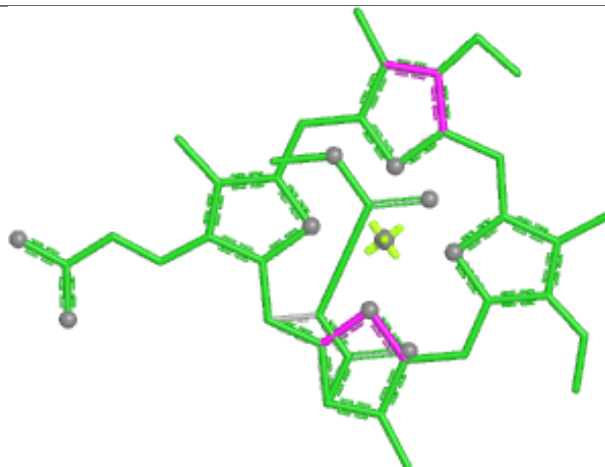
Ligand A86 x 318



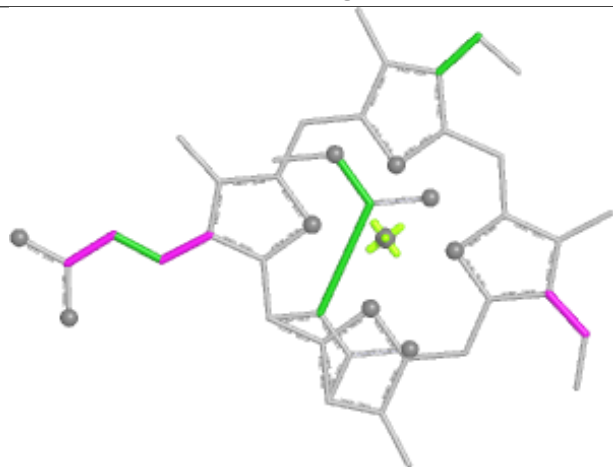
Ligand KC2 X 309



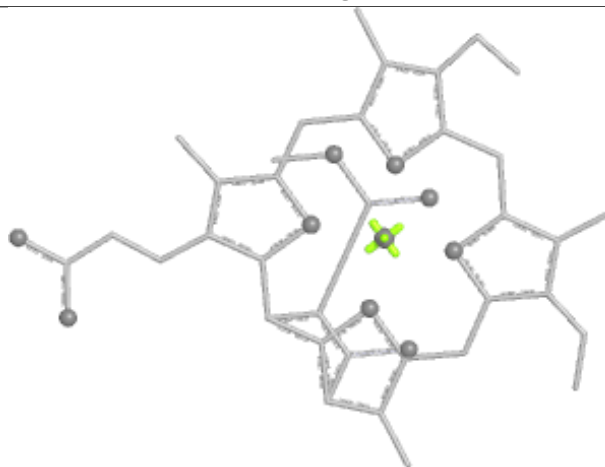
Bond lengths



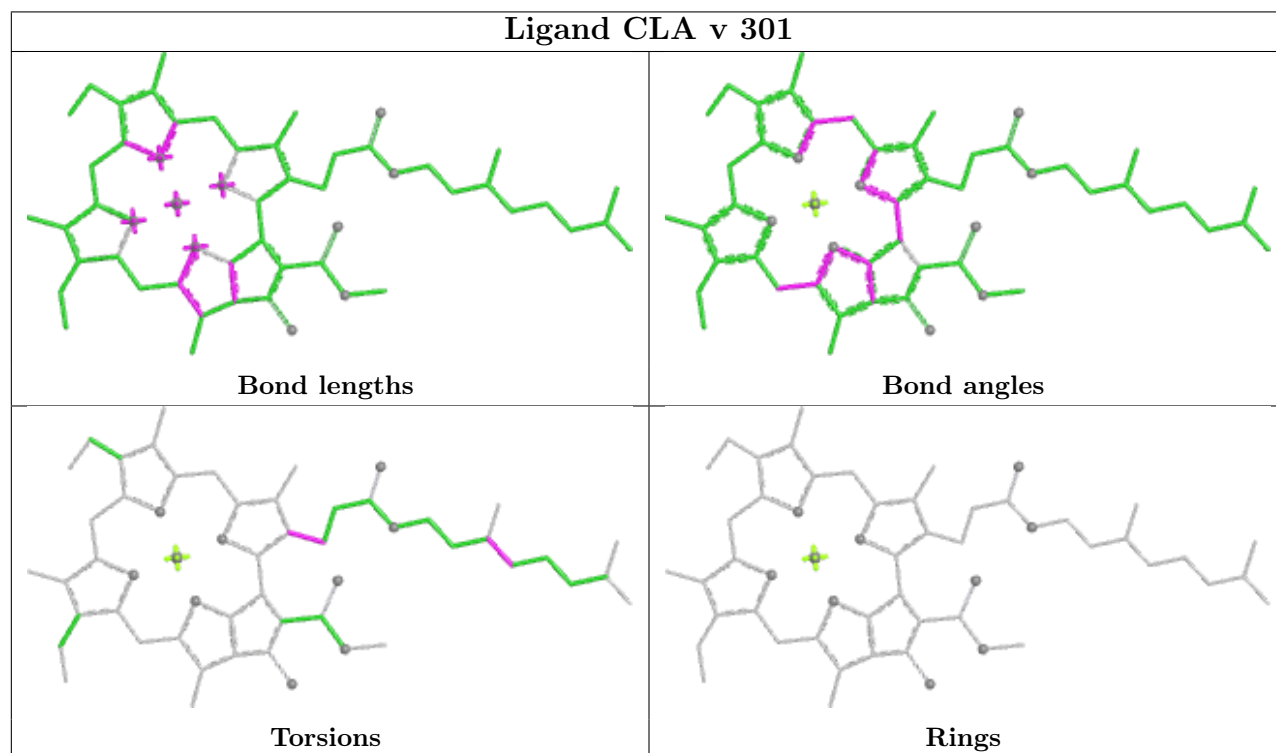
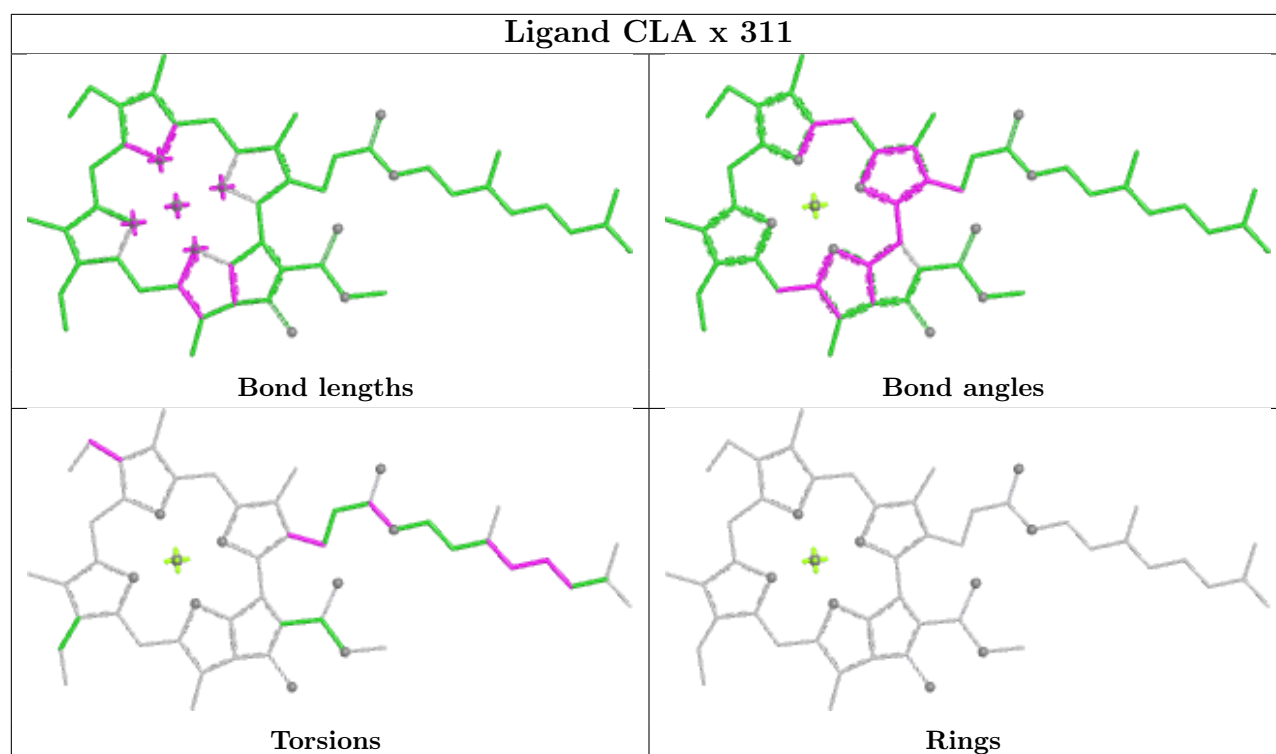
Bond angles

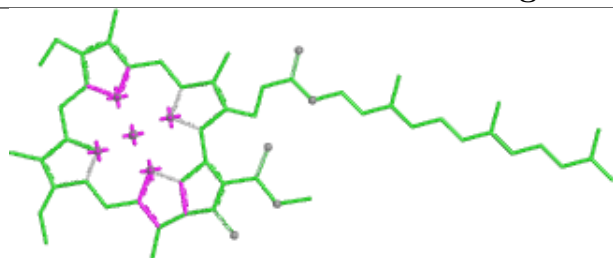
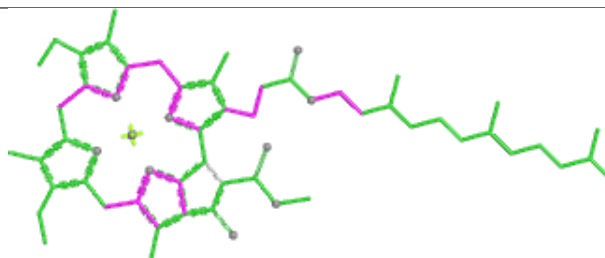
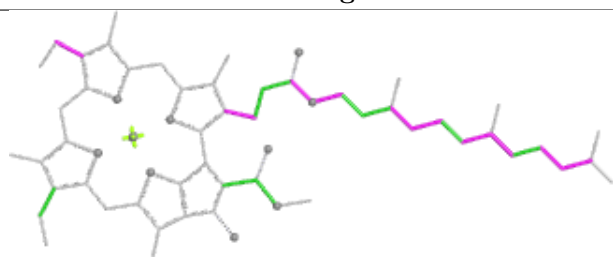
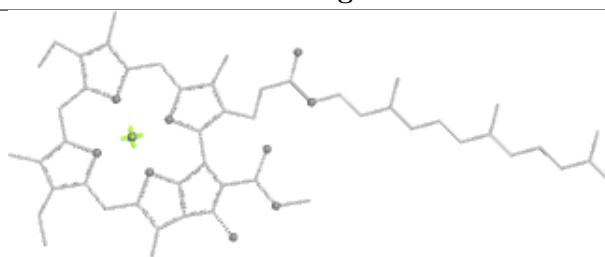
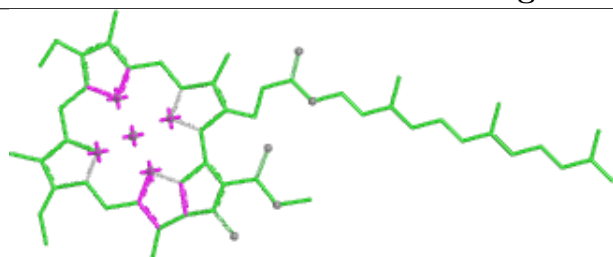
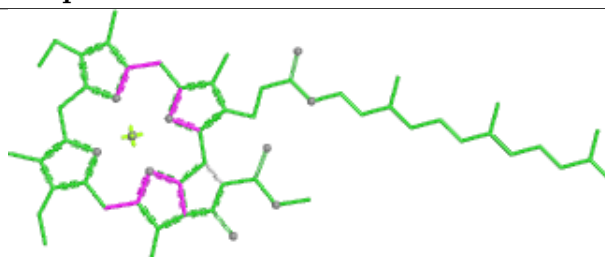
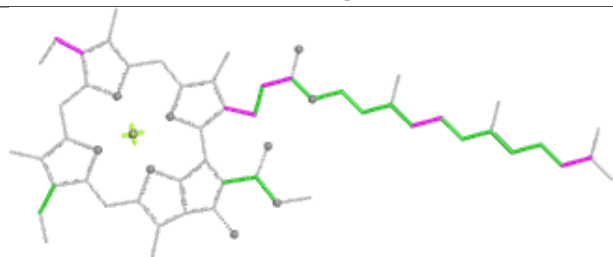
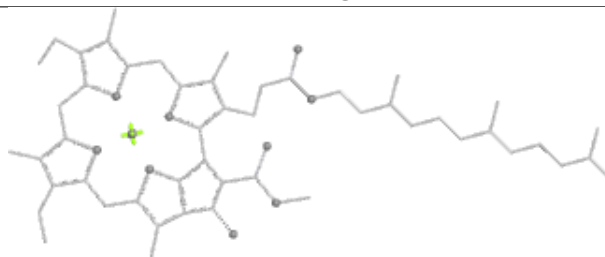


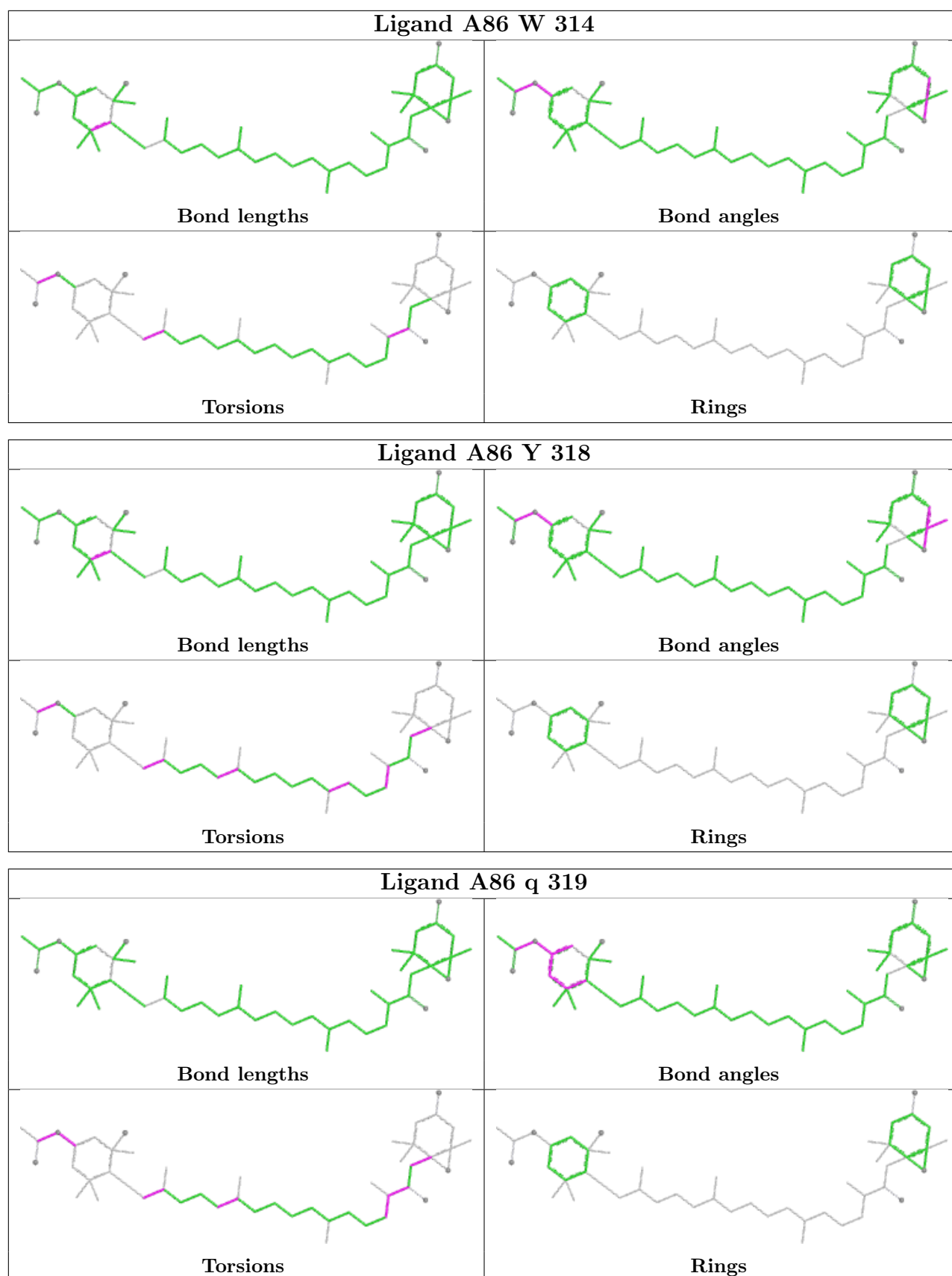
Torsions

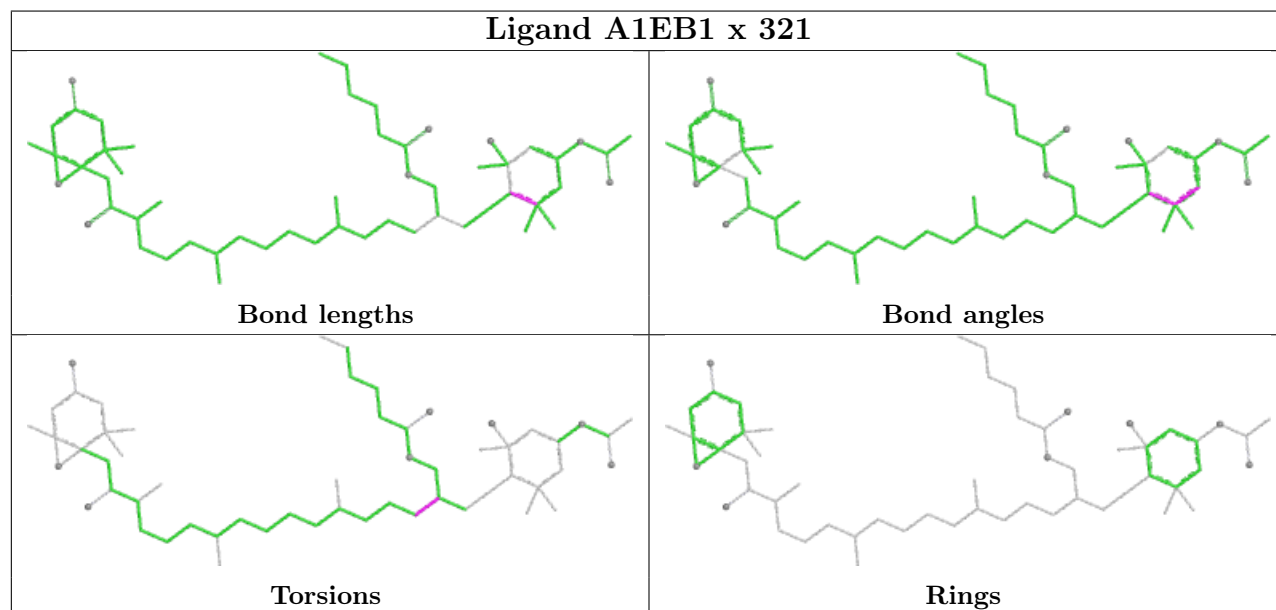
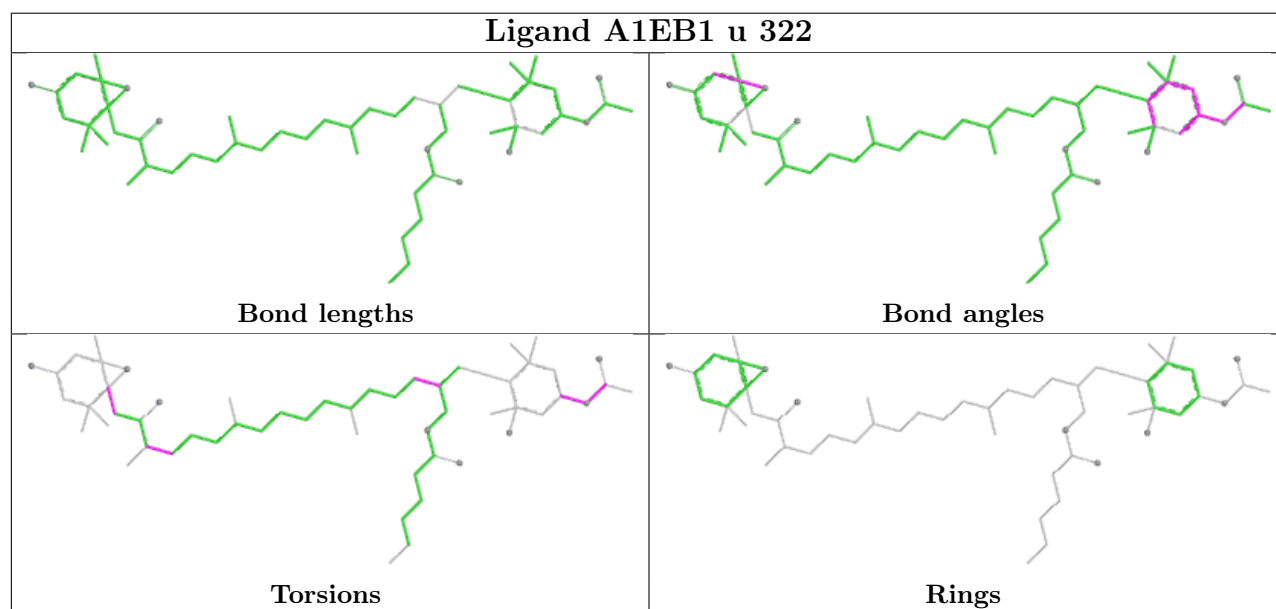
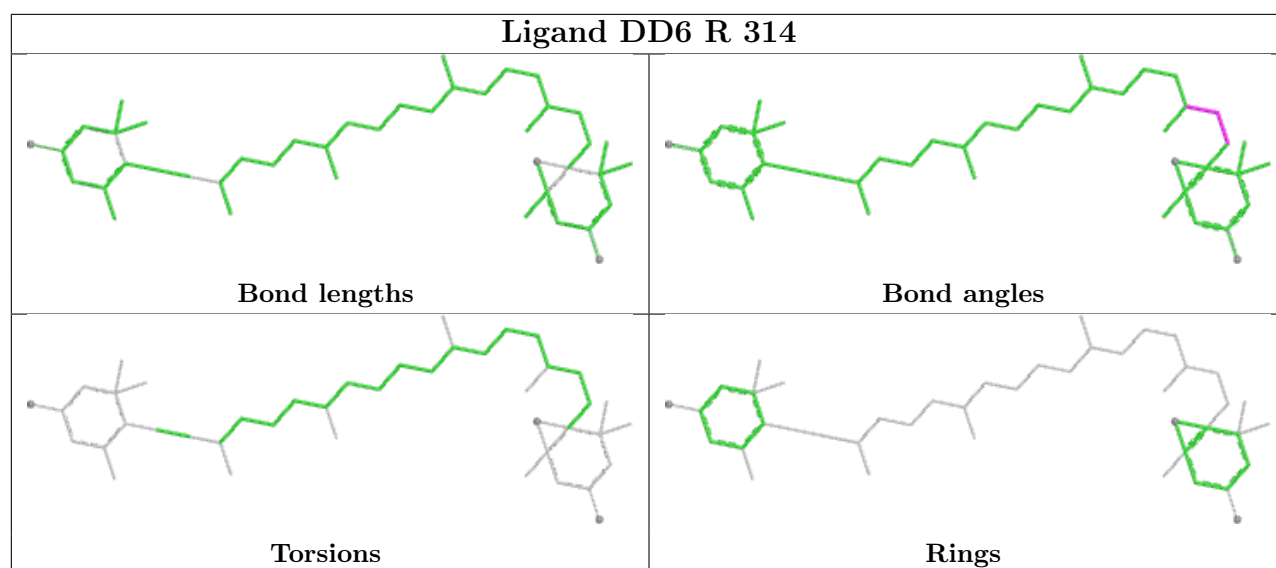


Rings

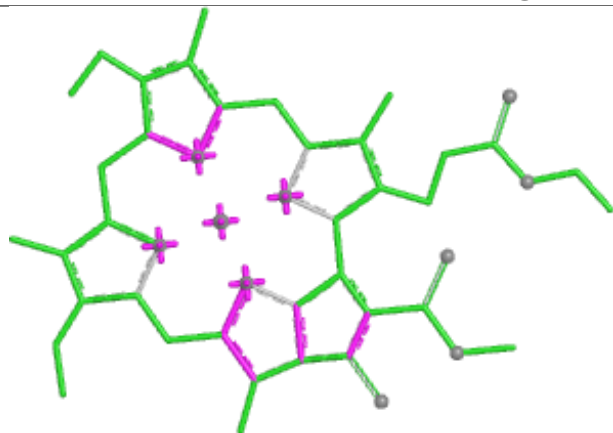


Ligand CLA z 308**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA q 312****Bond lengths****Bond angles****Torsions****Rings**

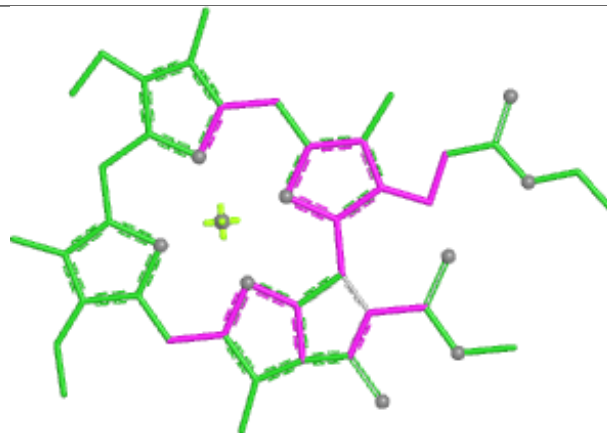




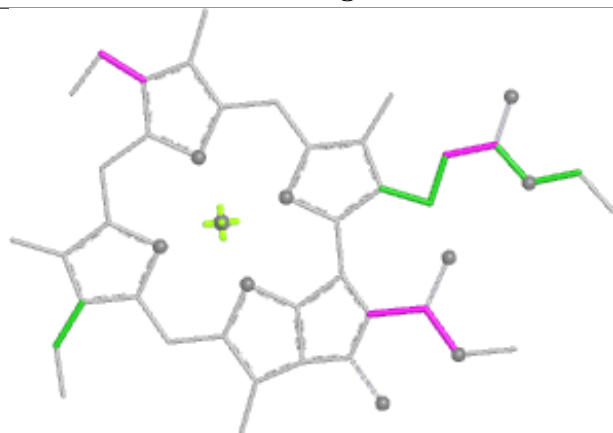
Ligand CLA F 310



Bond lengths



Bond angles

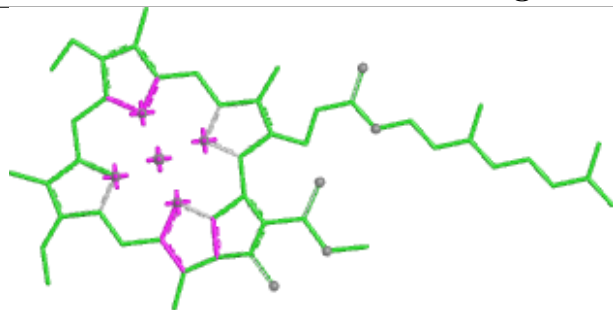


Torsions

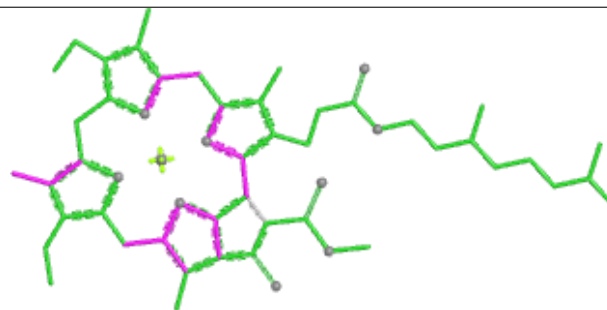


Rings

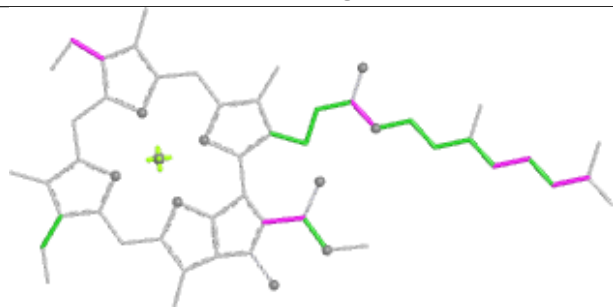
Ligand CLA U 202



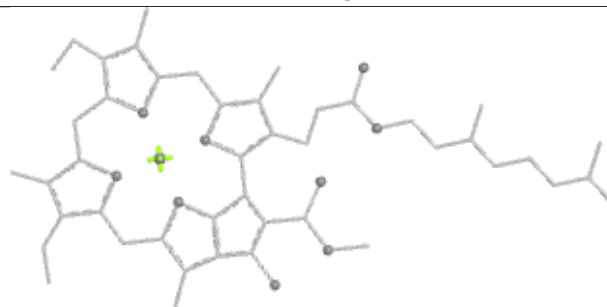
Bond lengths



Bond angles

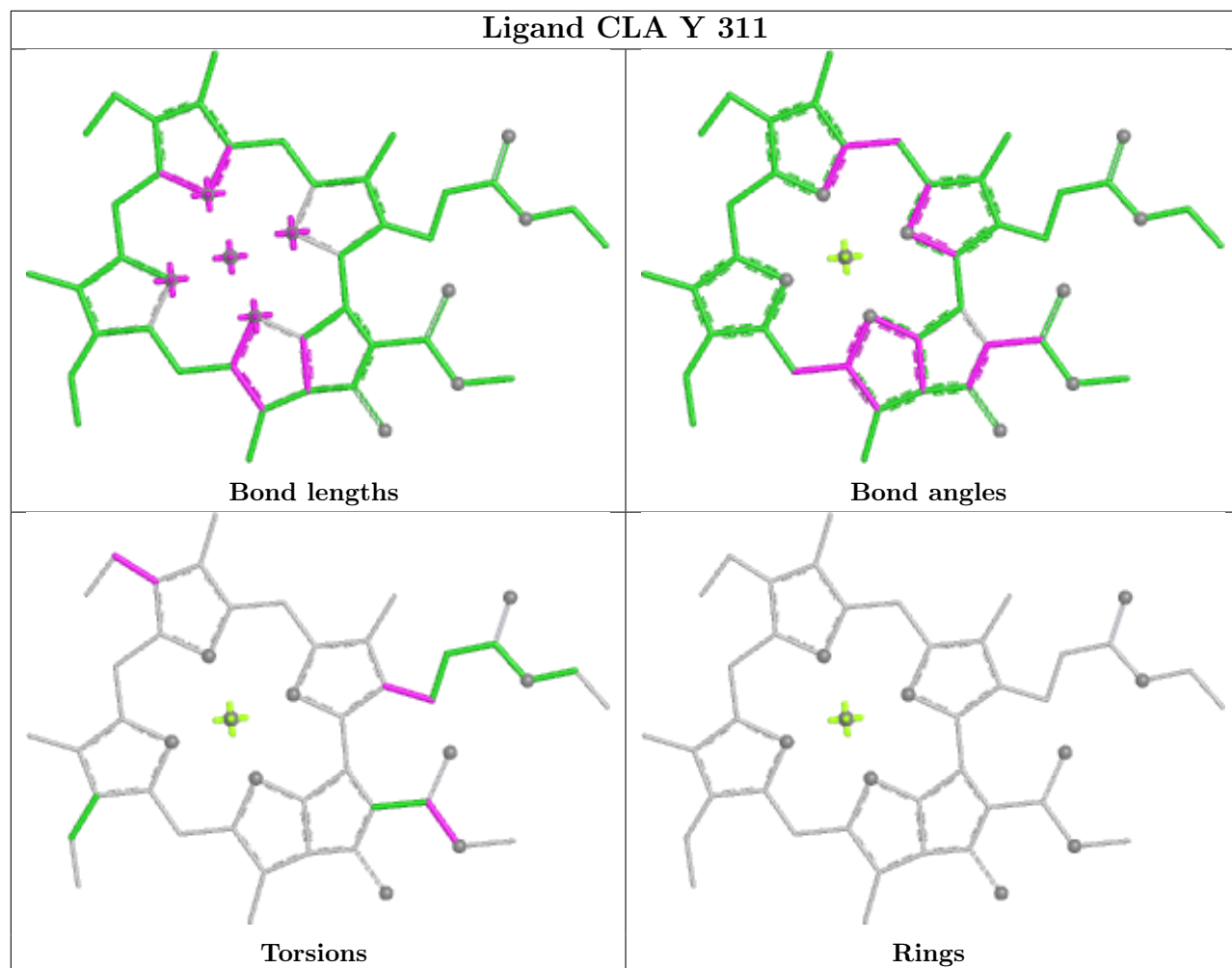


Torsions

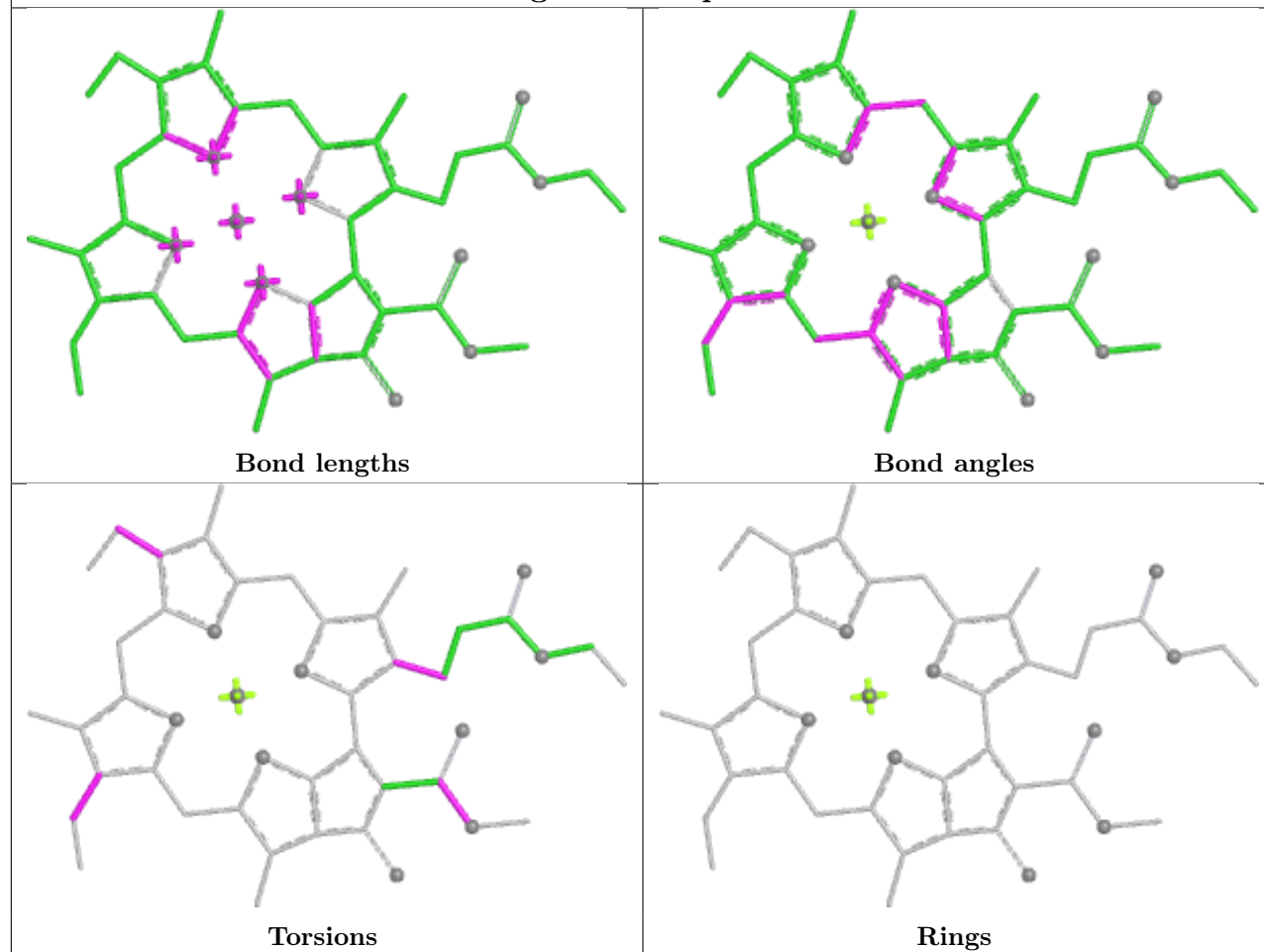


Rings

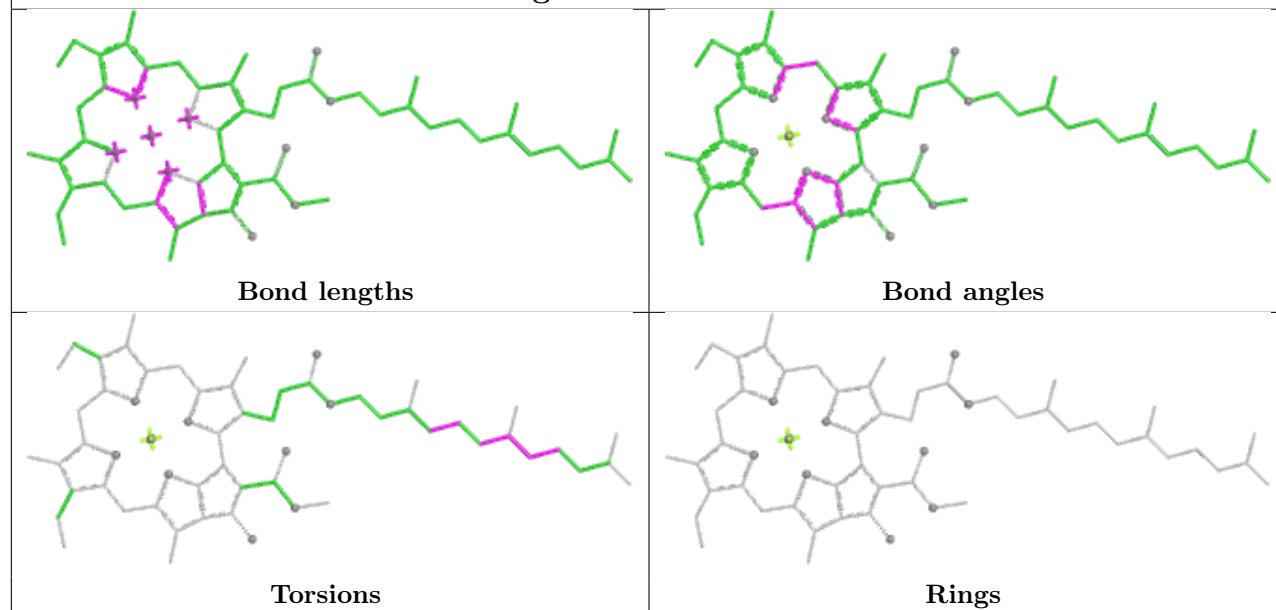
Ligand CLA Y 311



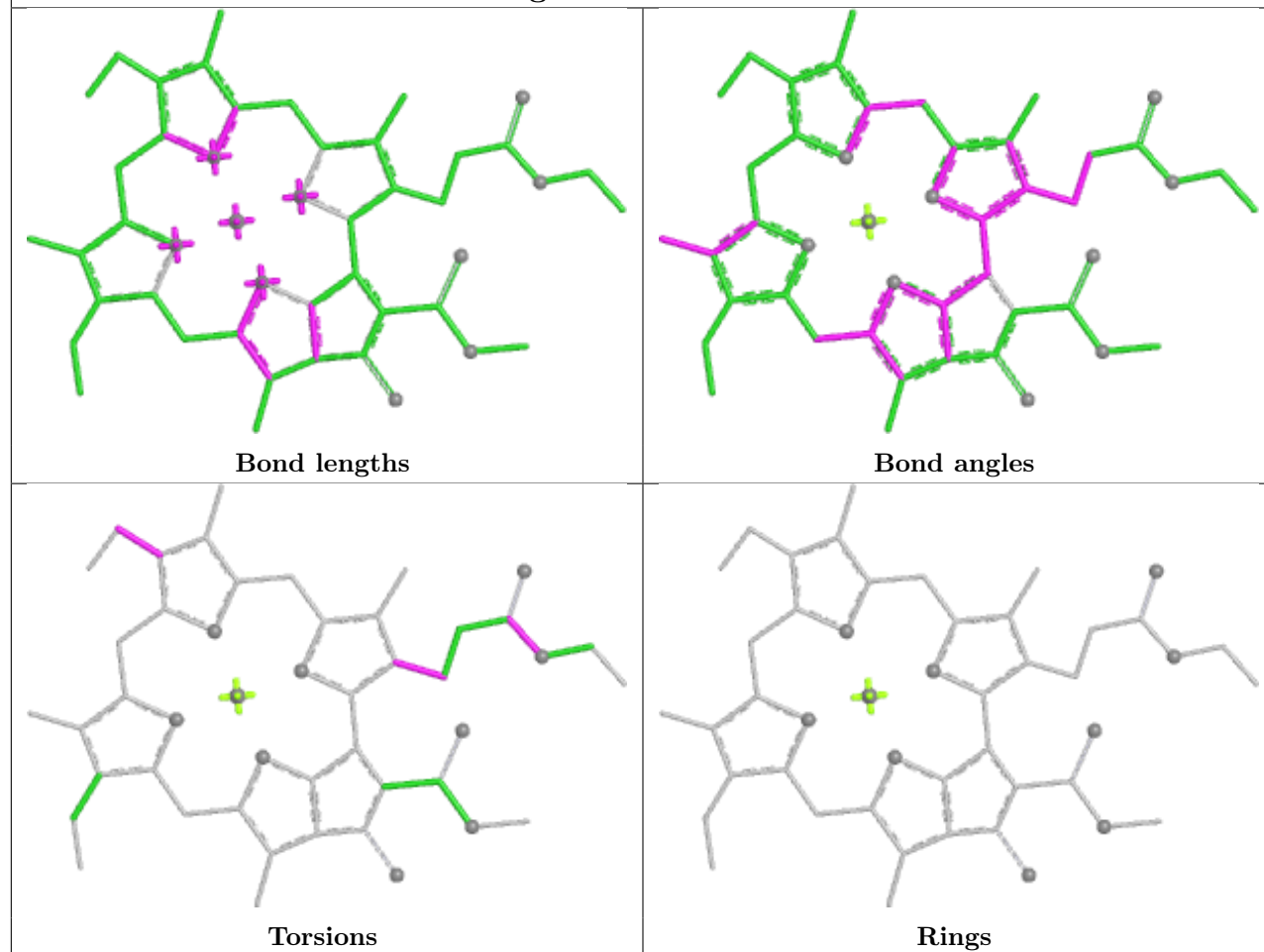
Ligand CLA p 305



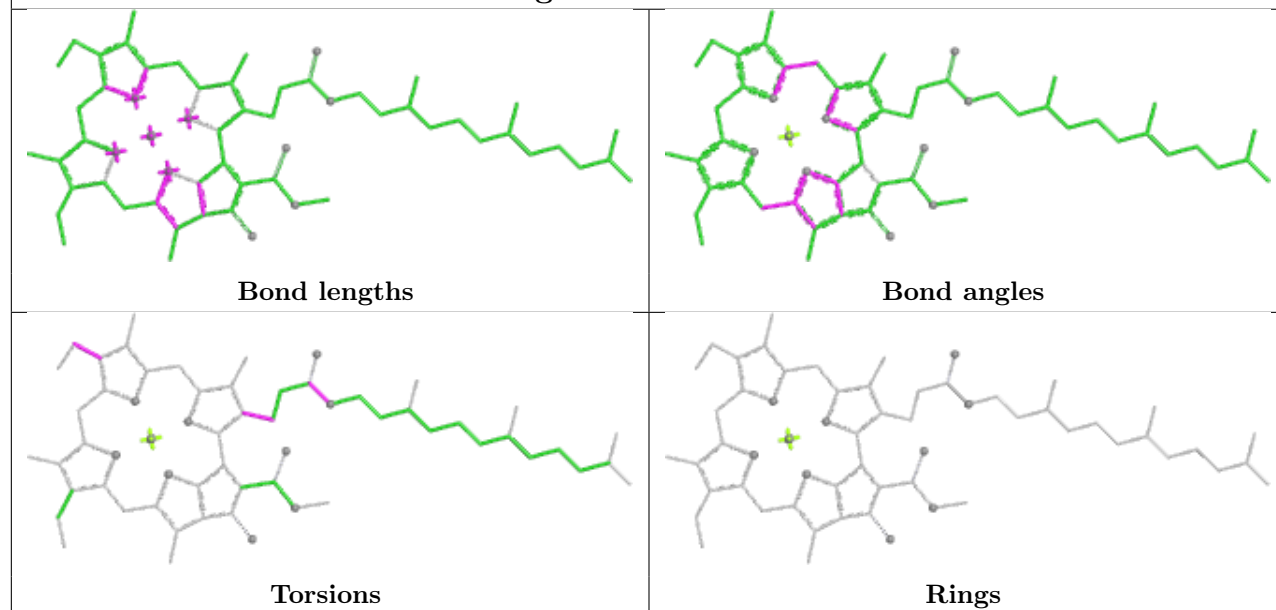
Ligand CLA T 304

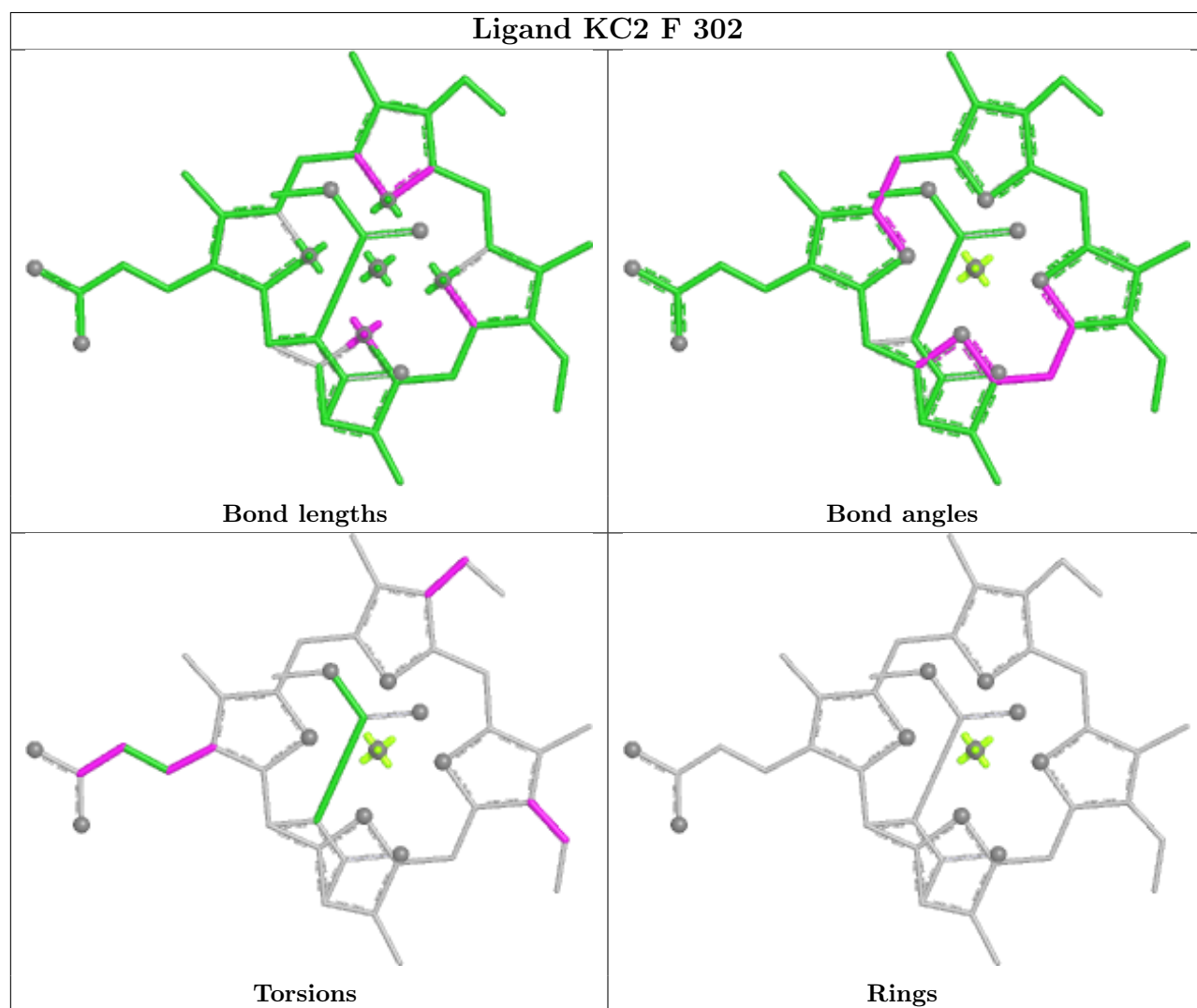
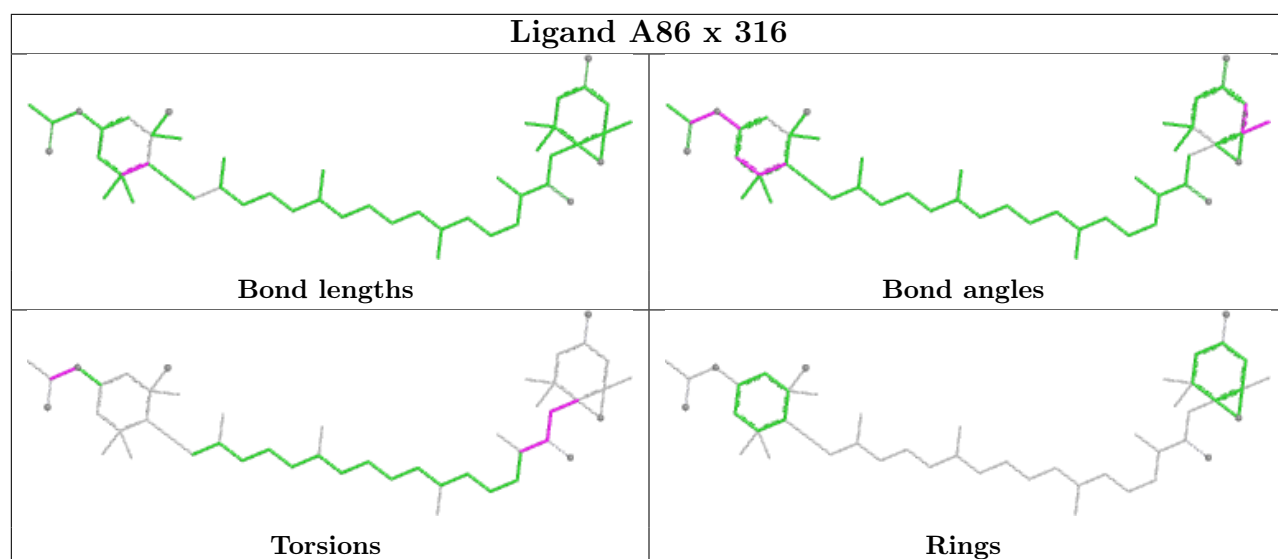


Ligand CLA Z 312

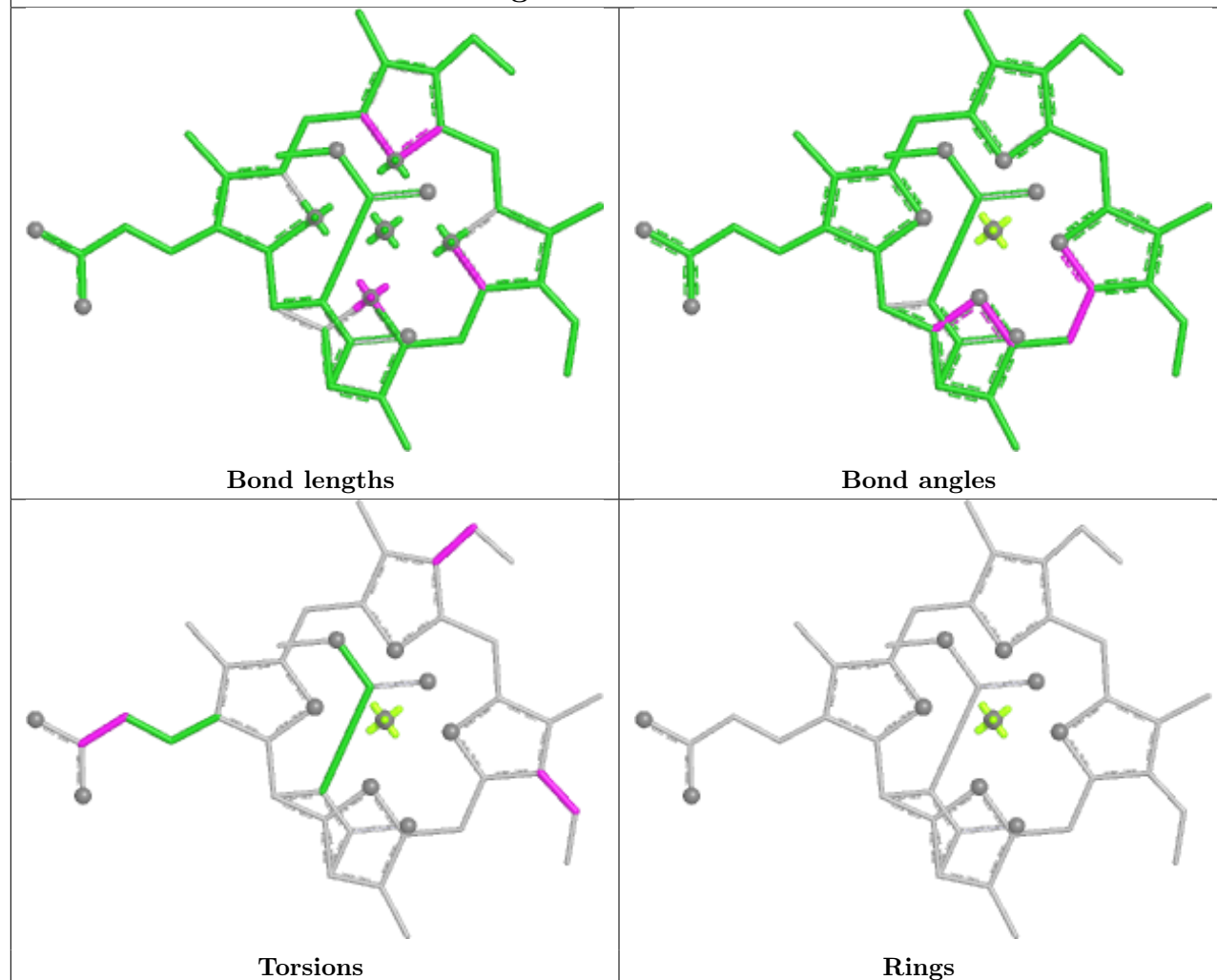


Ligand CLA S 301

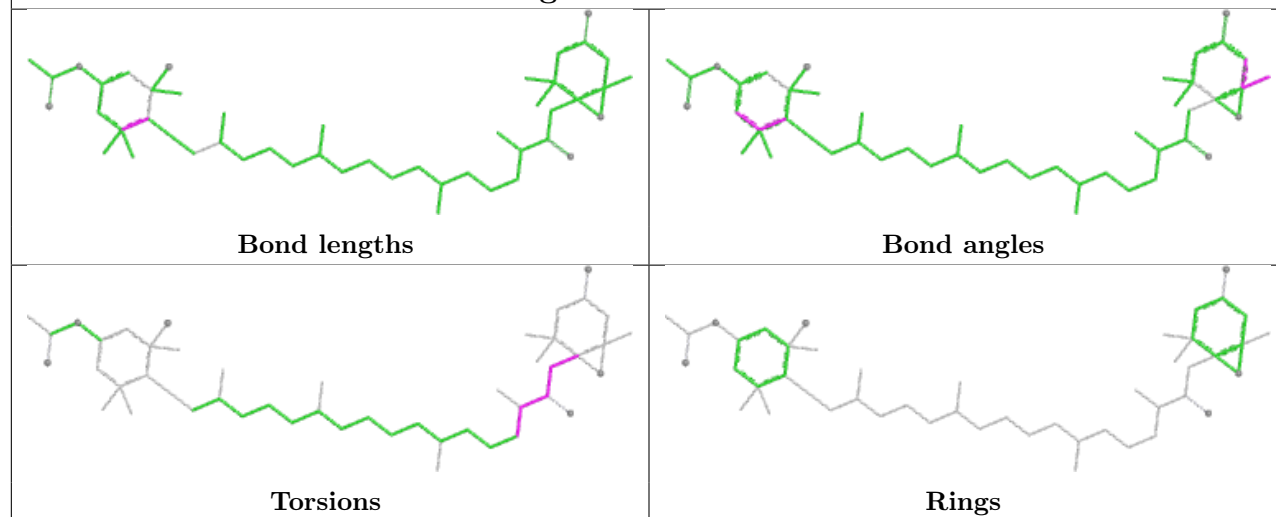


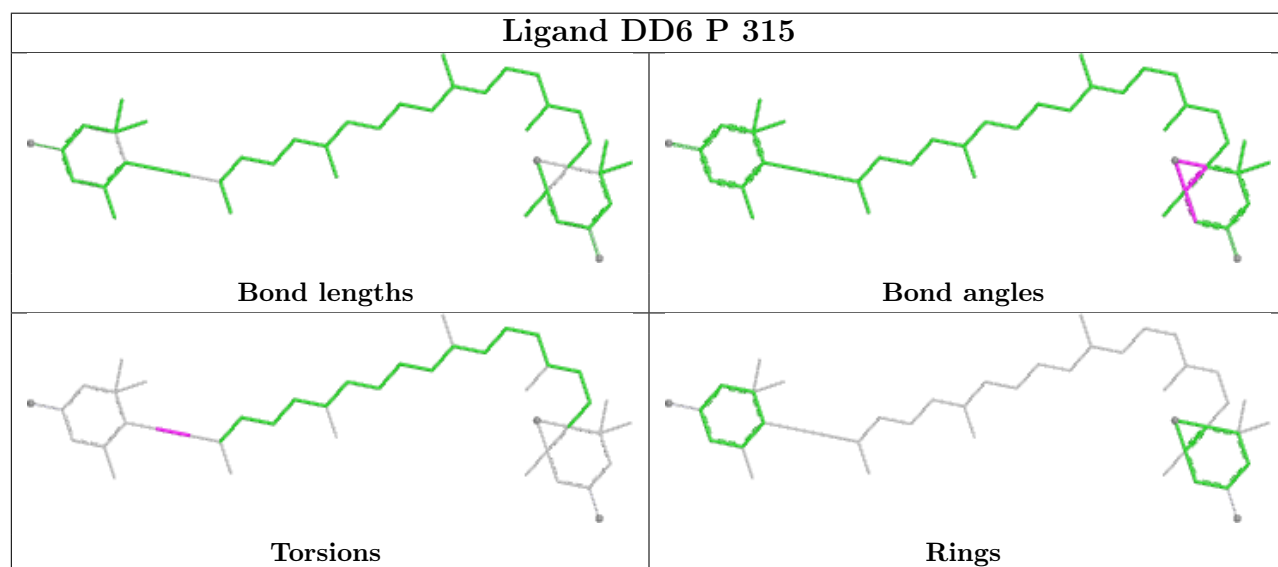
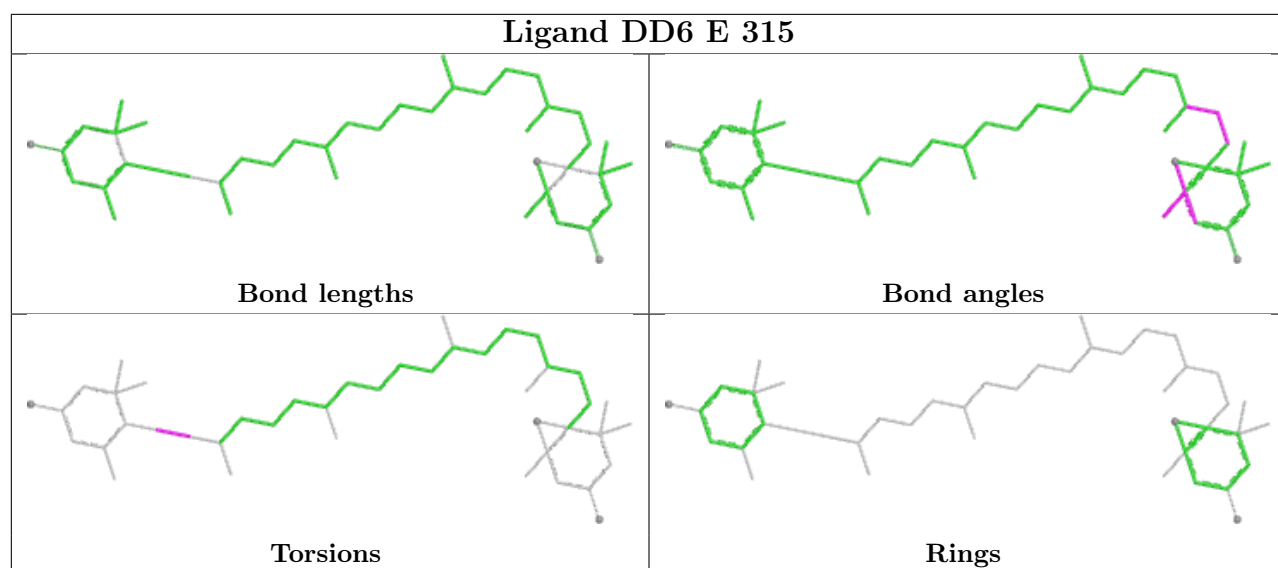


Ligand KC2 Z 309

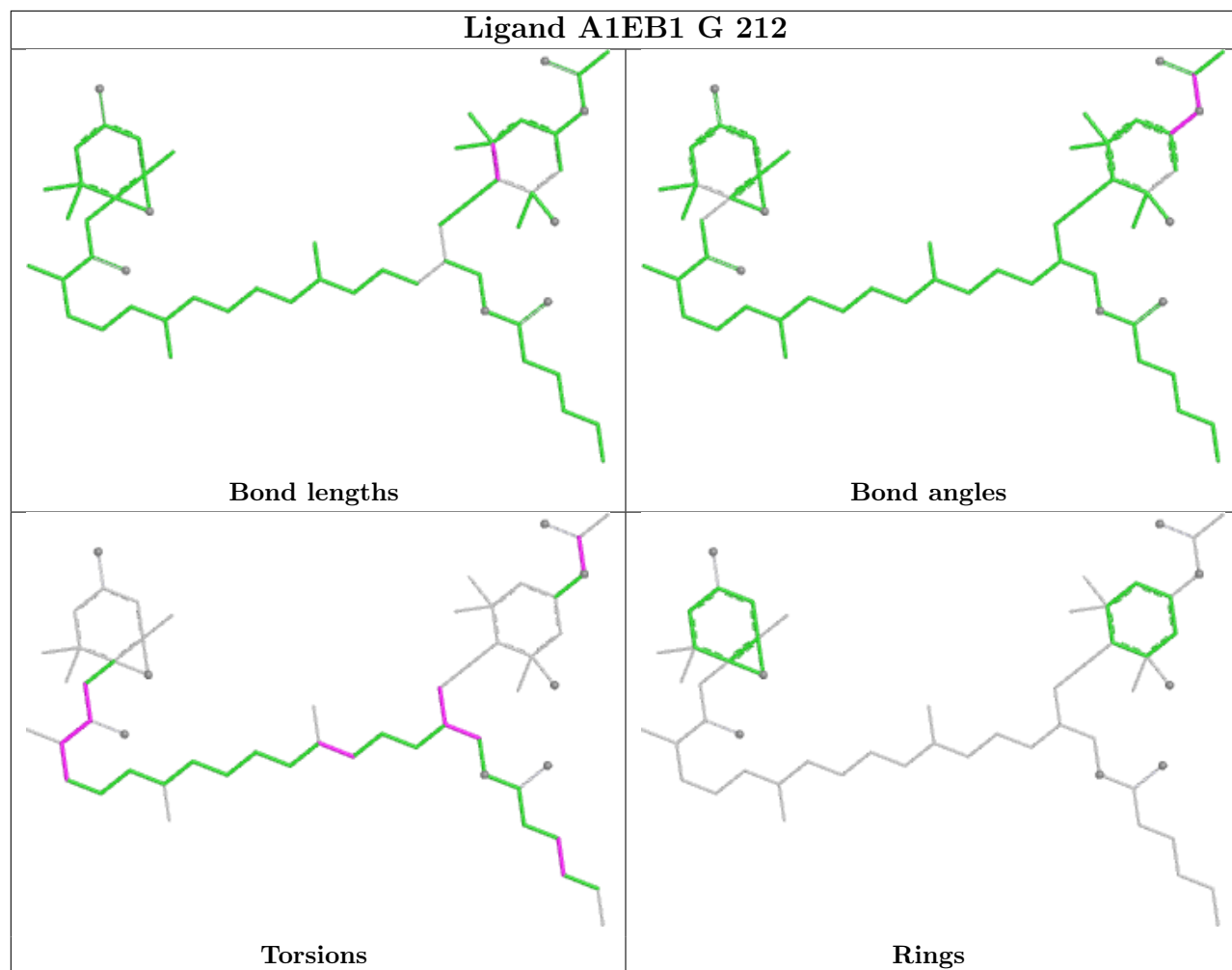


Ligand A86 F 317

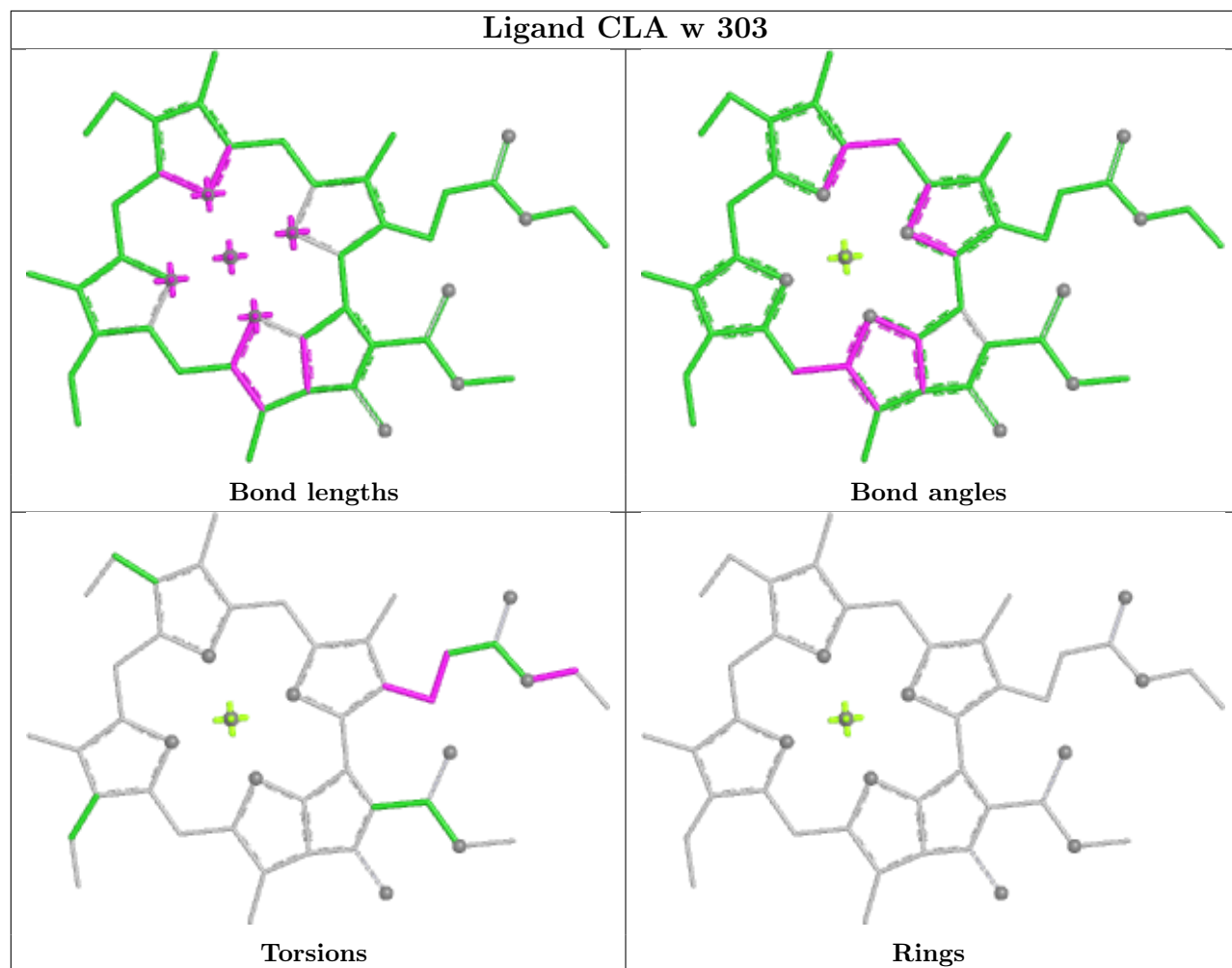




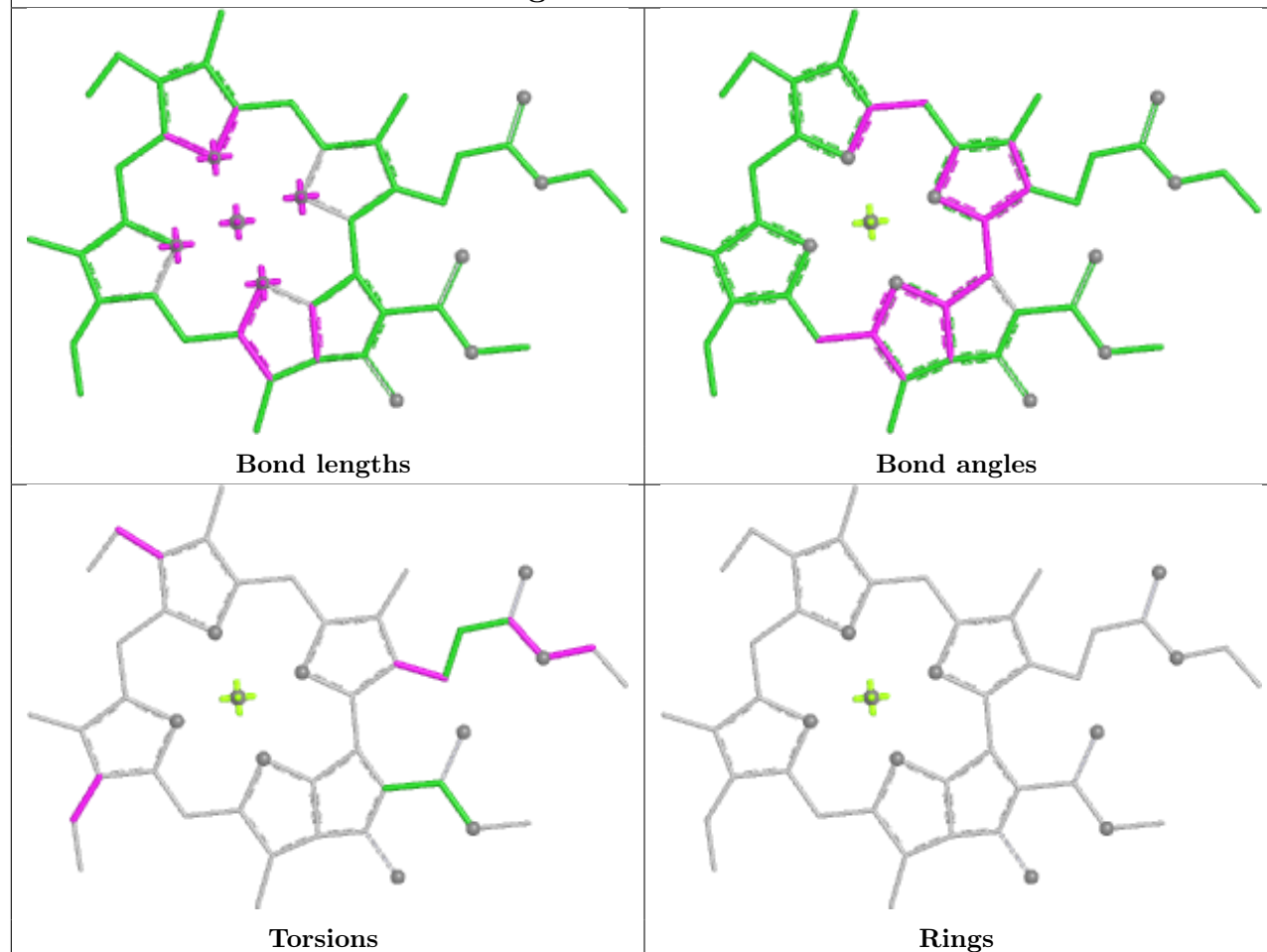
Ligand A1EB1 G 212



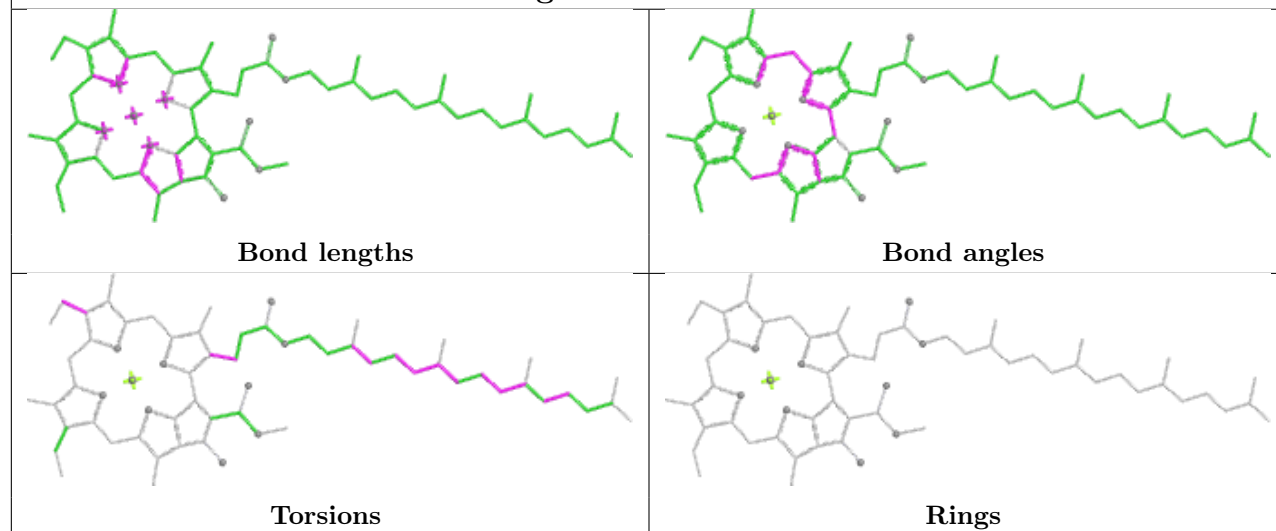
Ligand CLA w 303



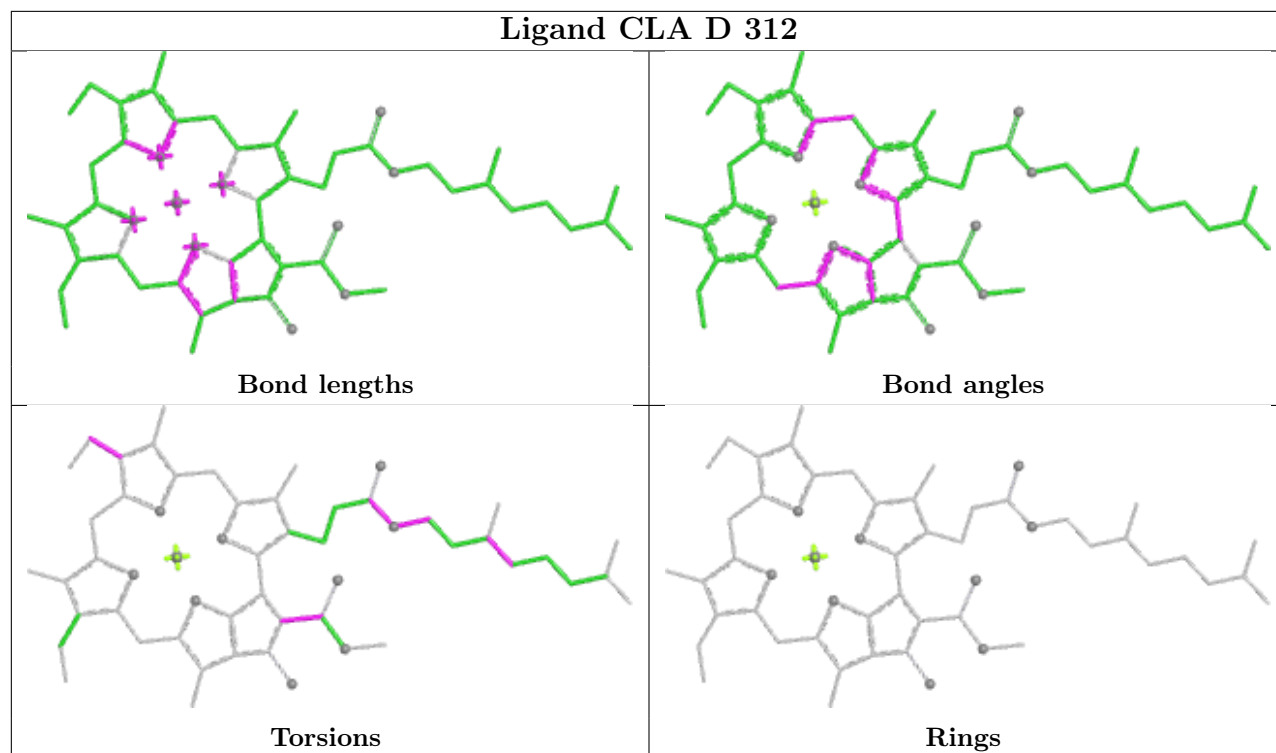
Ligand CLA B 301



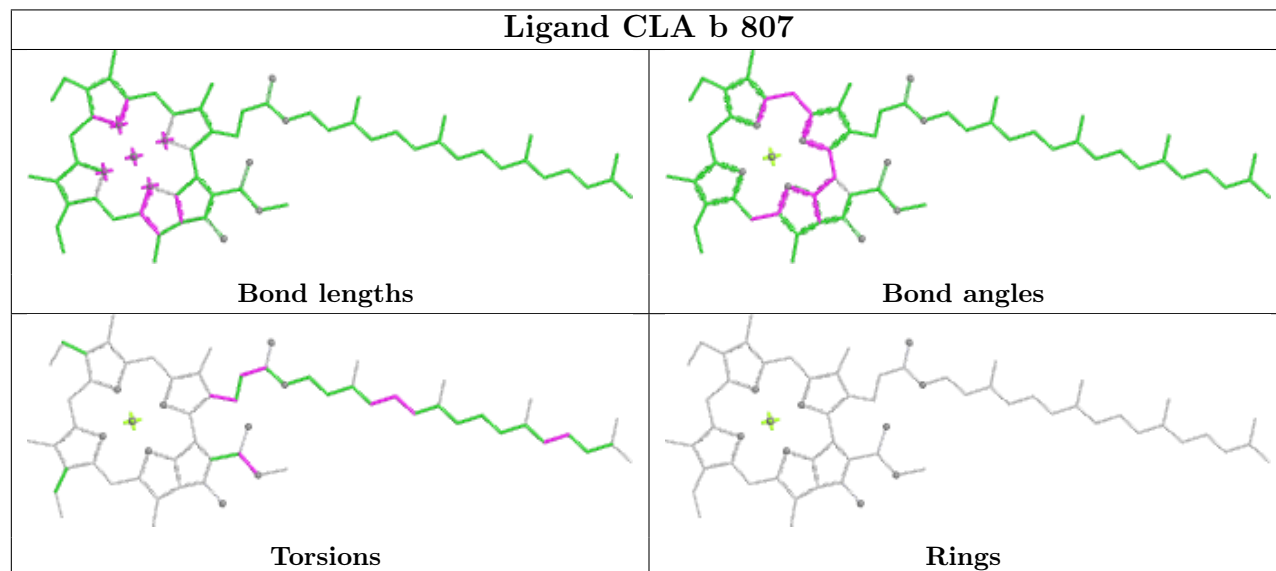
Ligand CLA a 842



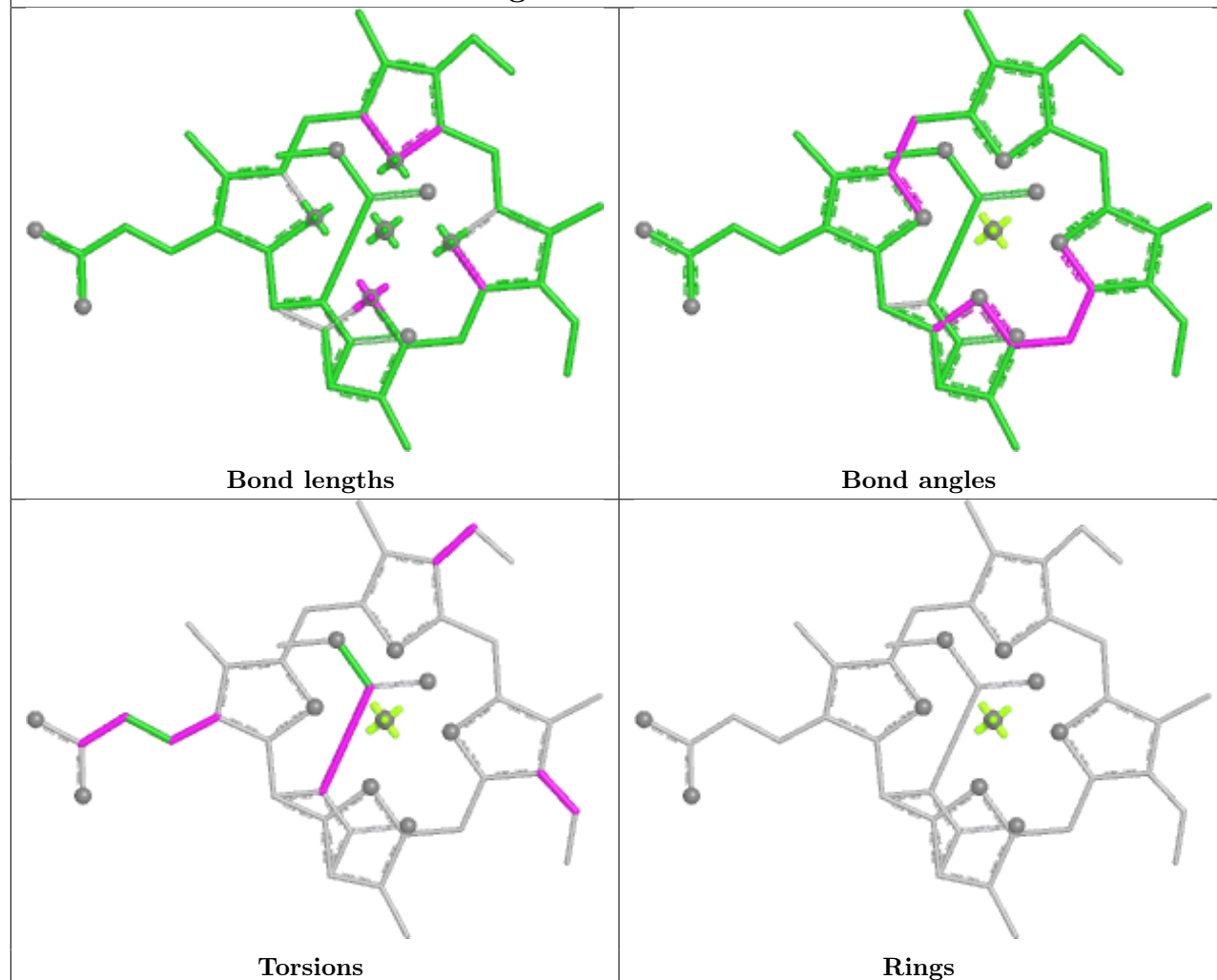
Ligand CLA D 312



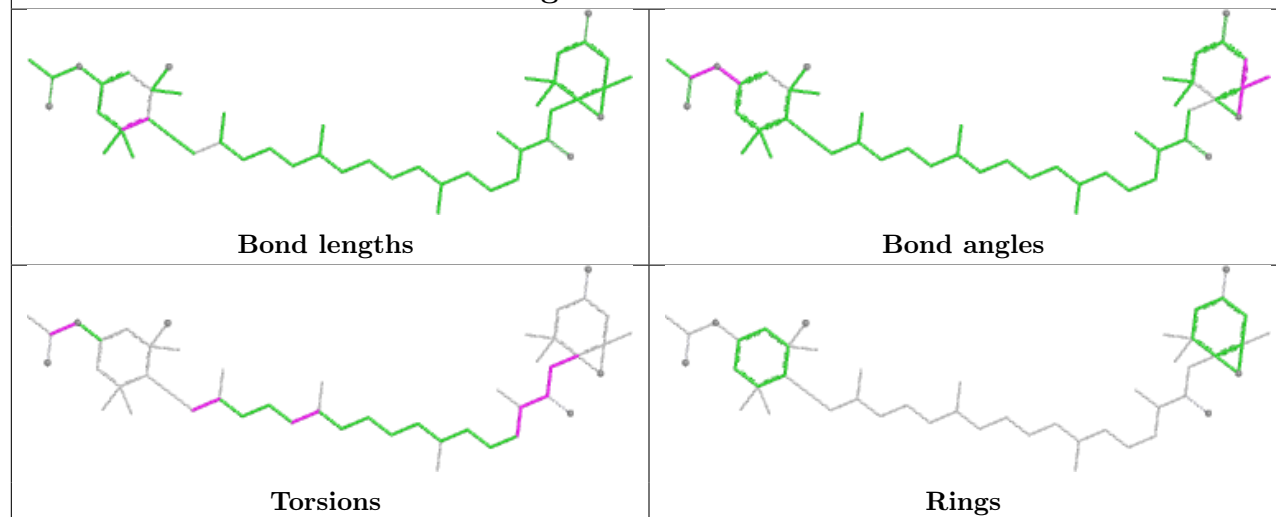
Ligand CLA b 807

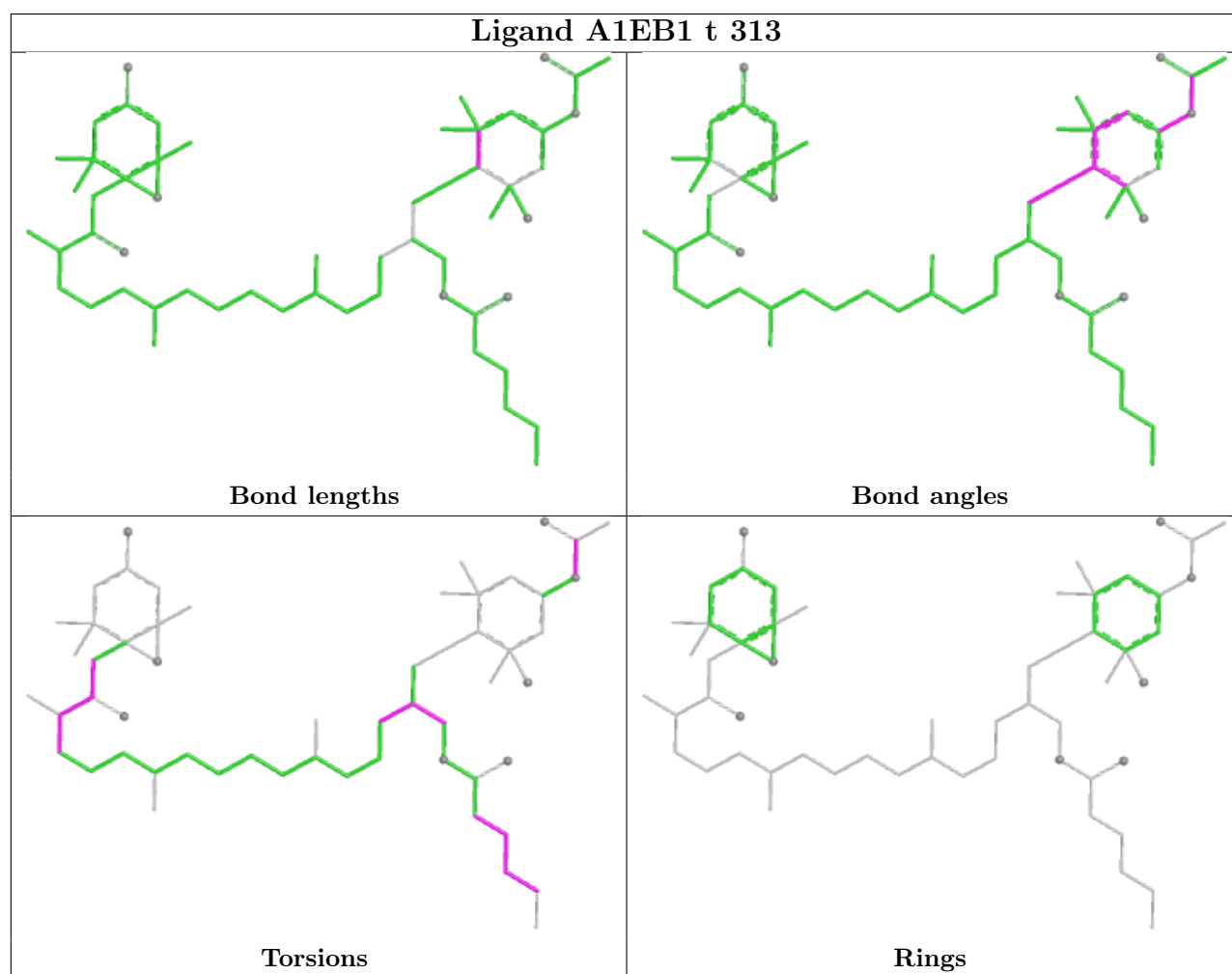
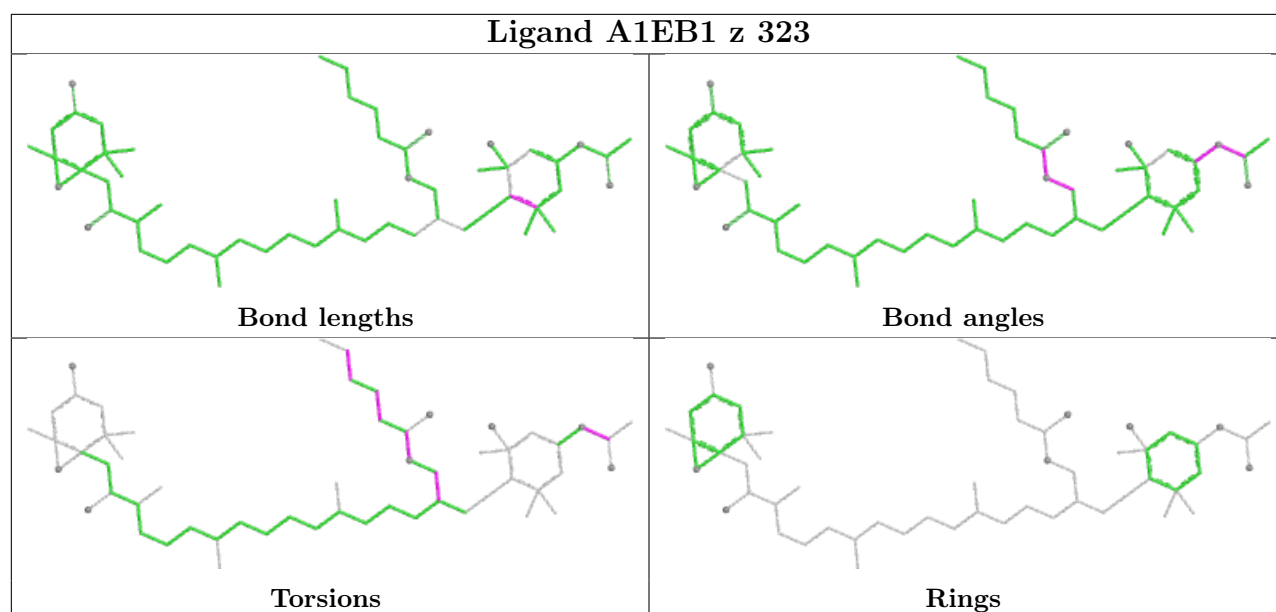


Ligand KC2 R 308

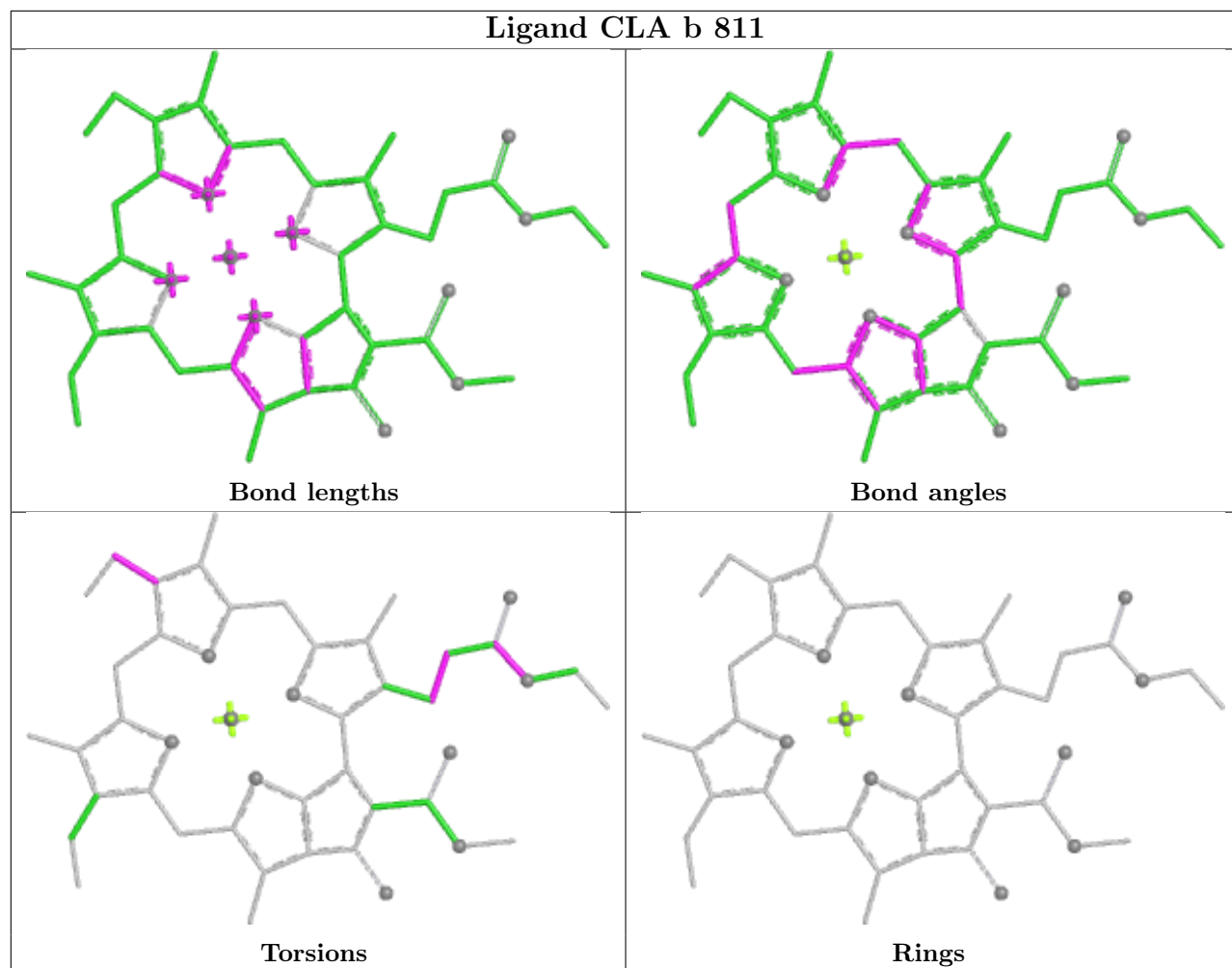


Ligand A86 u 318

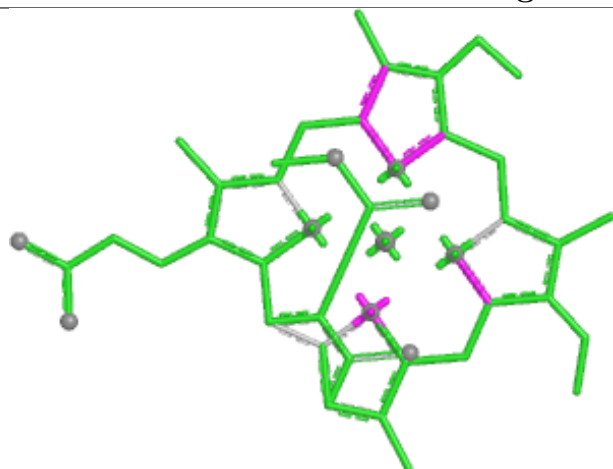




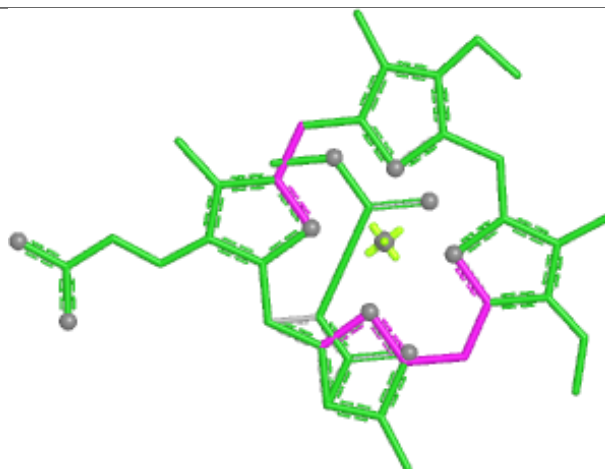
Ligand CLA b 811



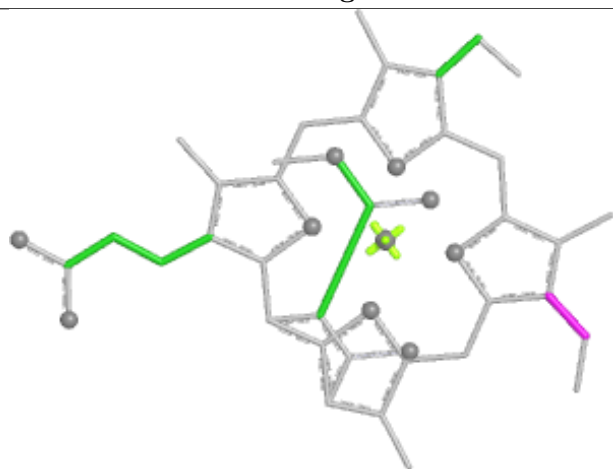
Ligand KC2 T 302



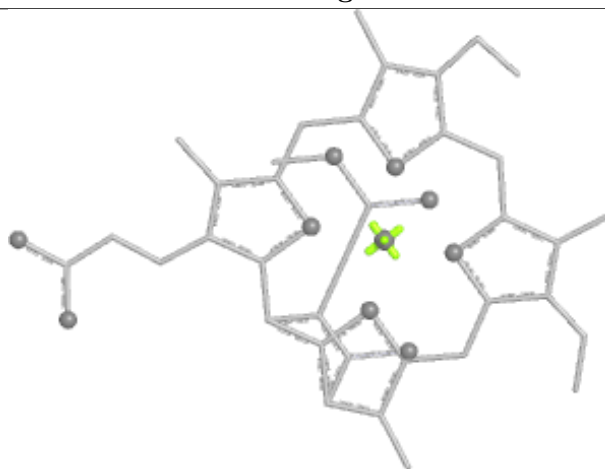
Bond lengths



Bond angles

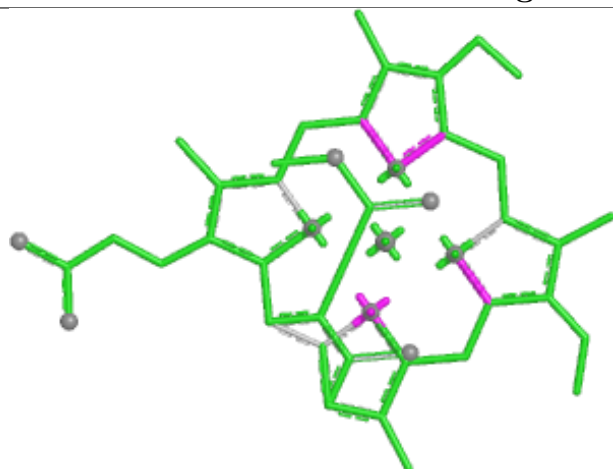


Torsions

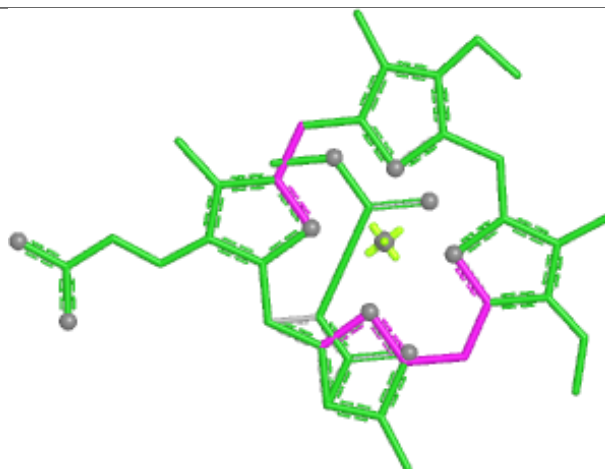


Rings

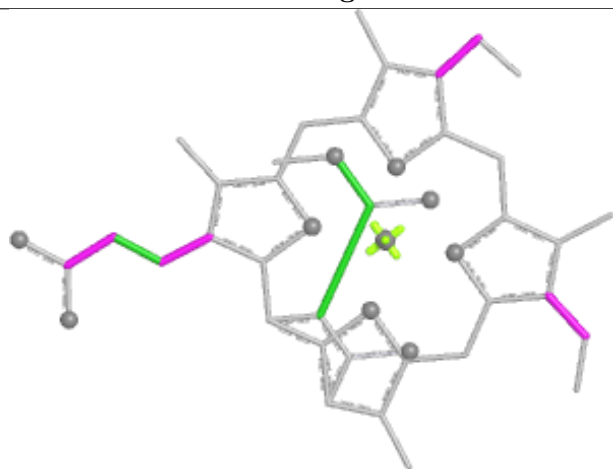
Ligand KC2 C 303



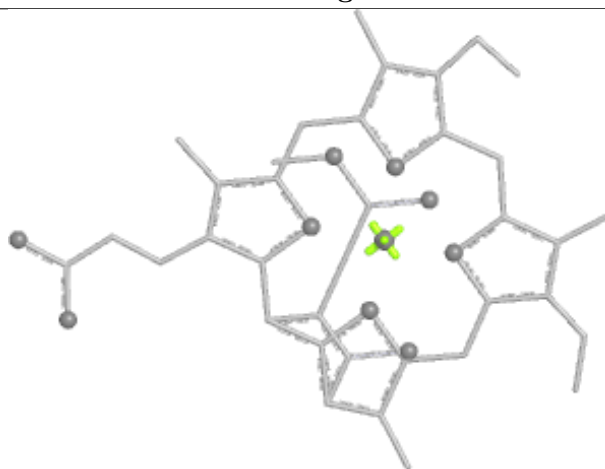
Bond lengths



Bond angles

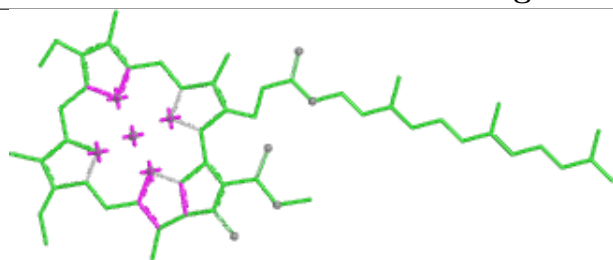


Torsions

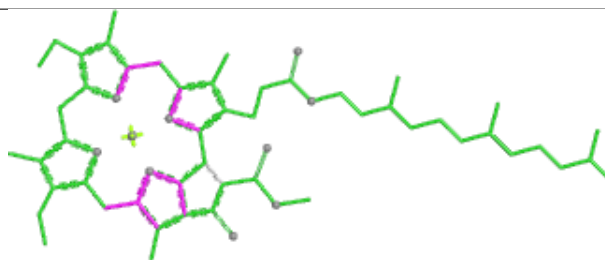


Rings

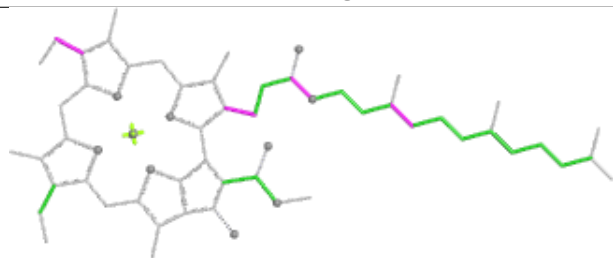
Ligand CLA Y 301



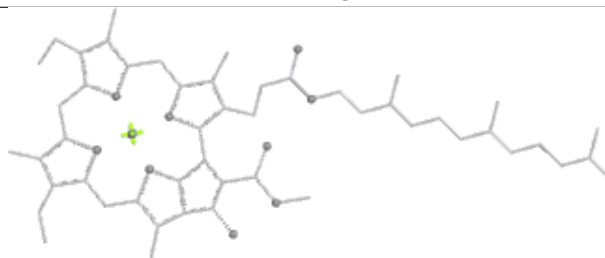
Bond lengths



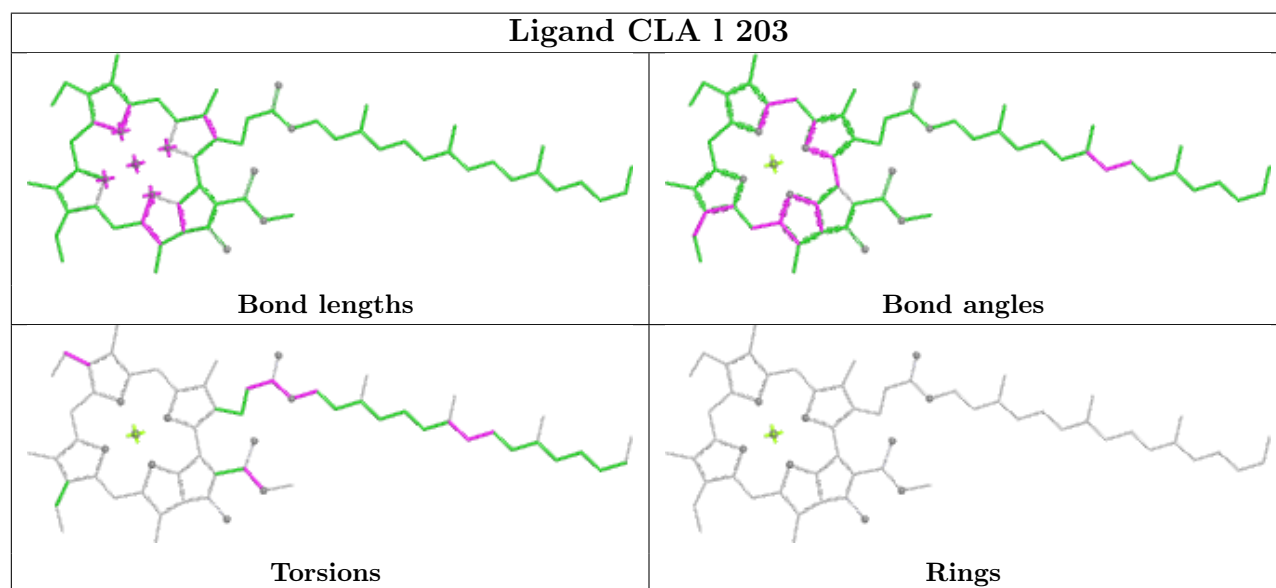
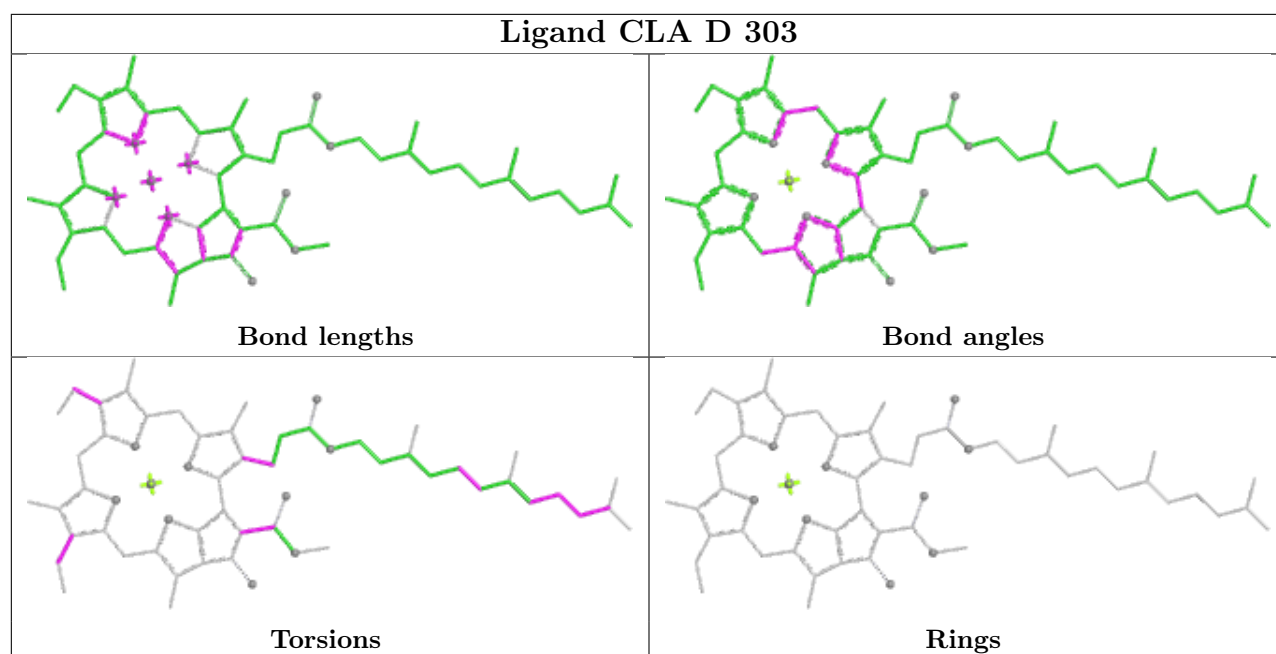
Bond angles

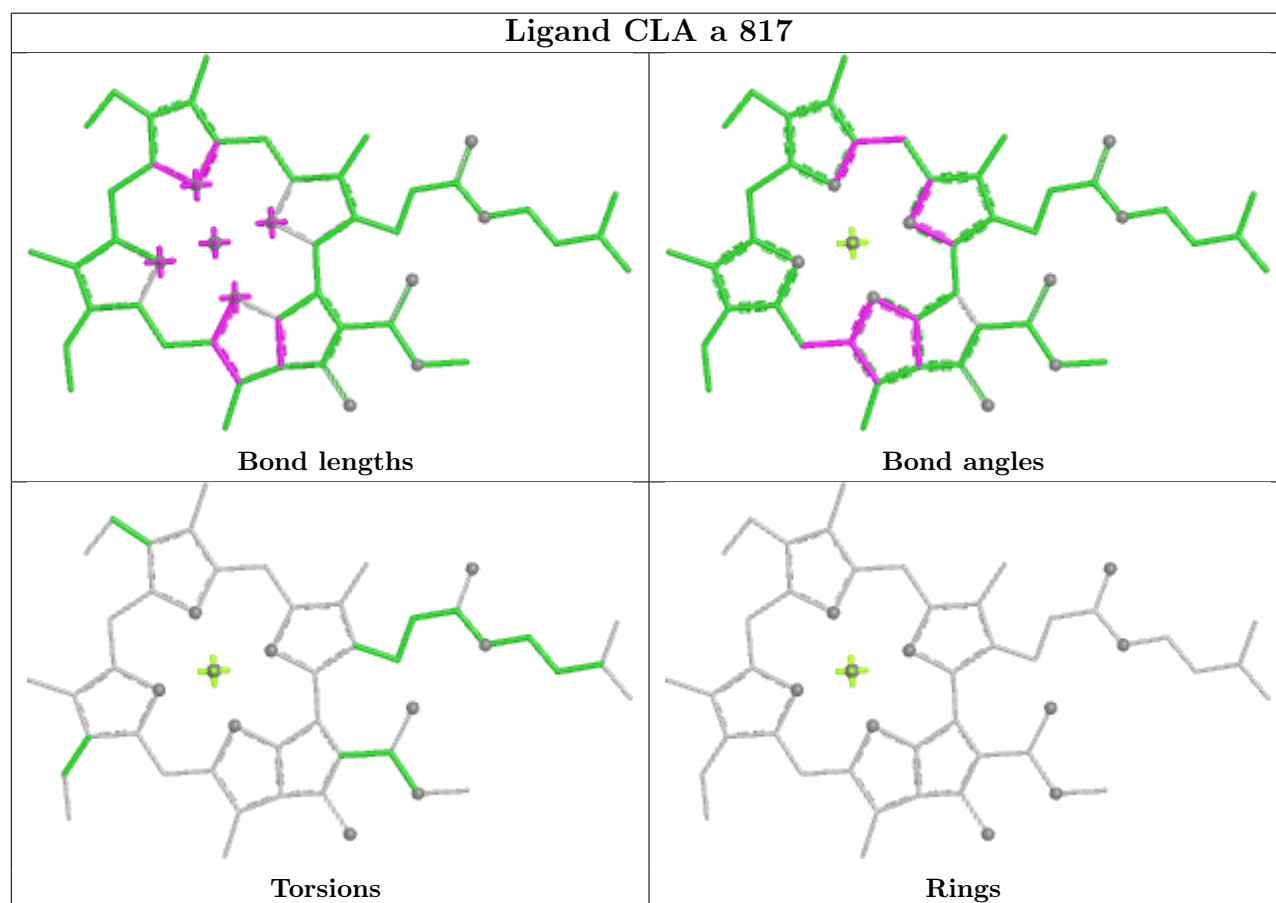
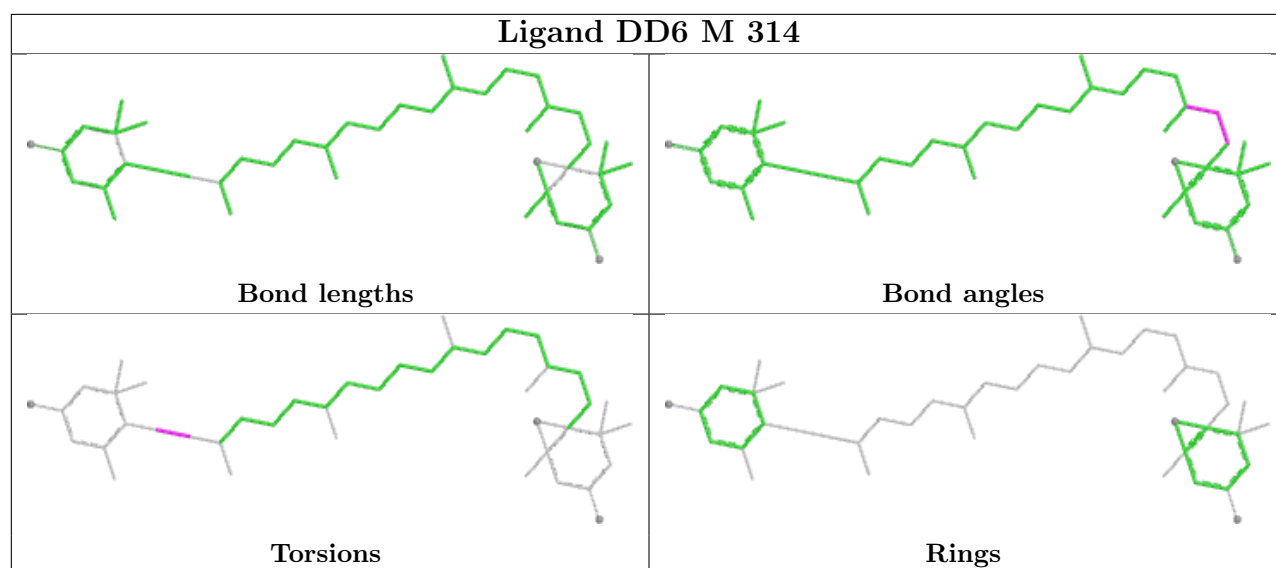


Torsions

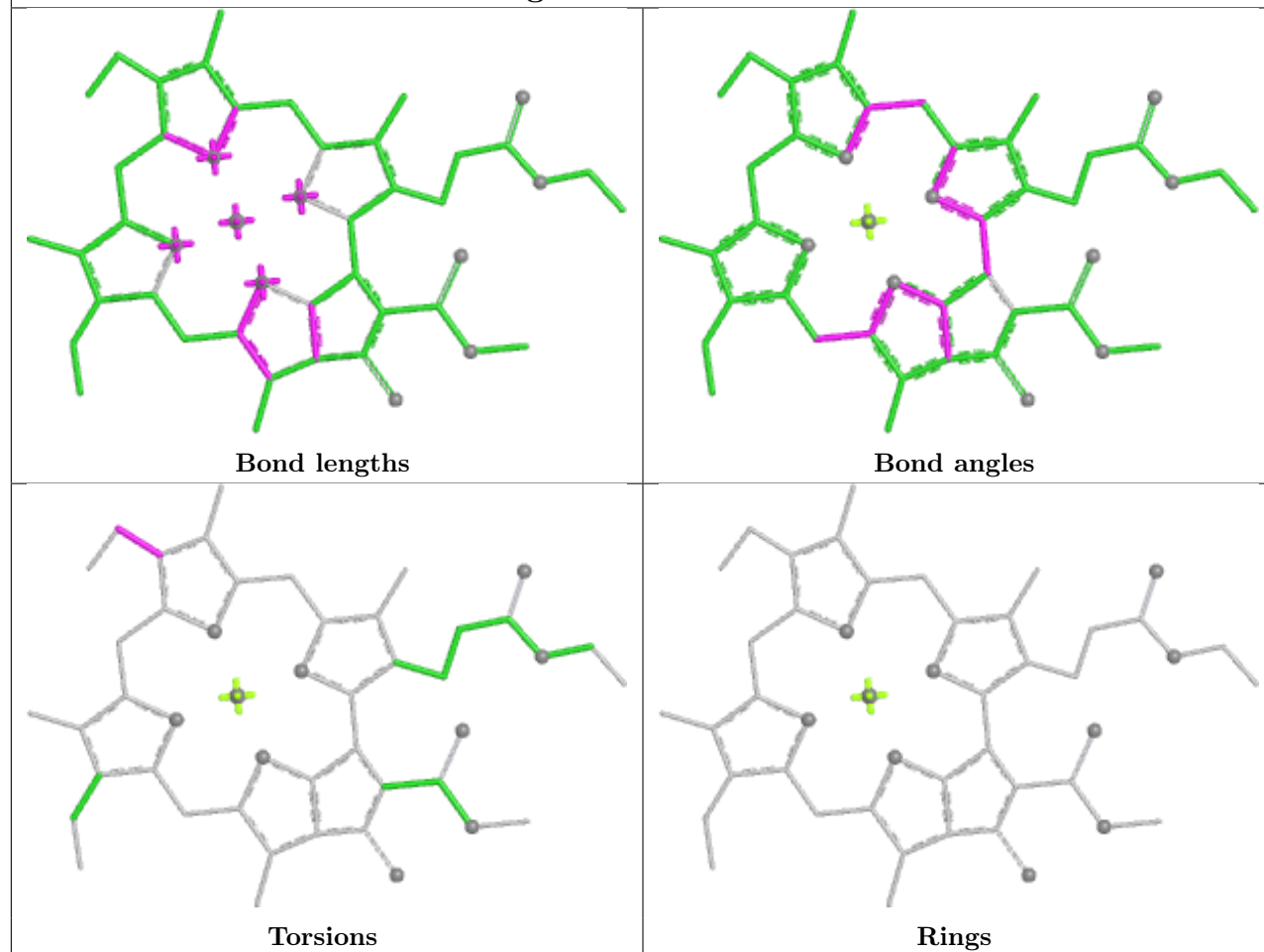


Rings

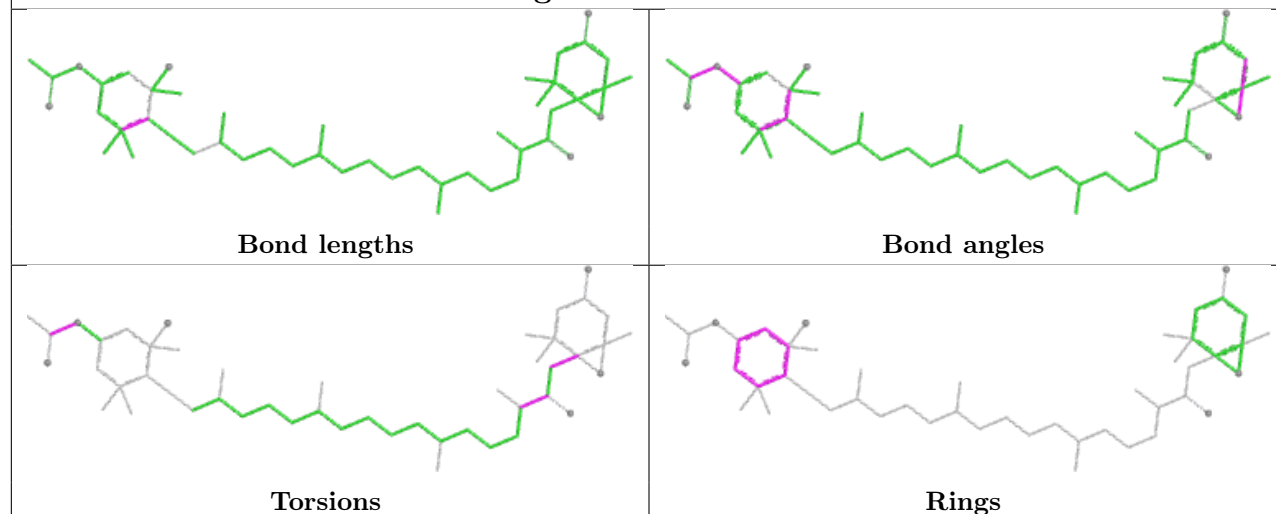


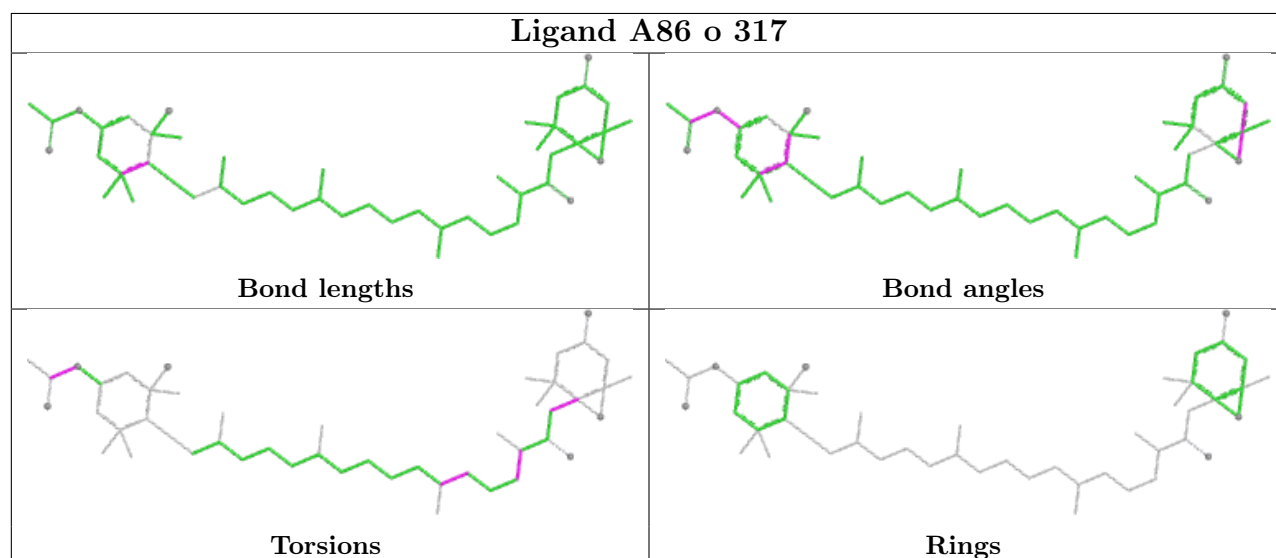
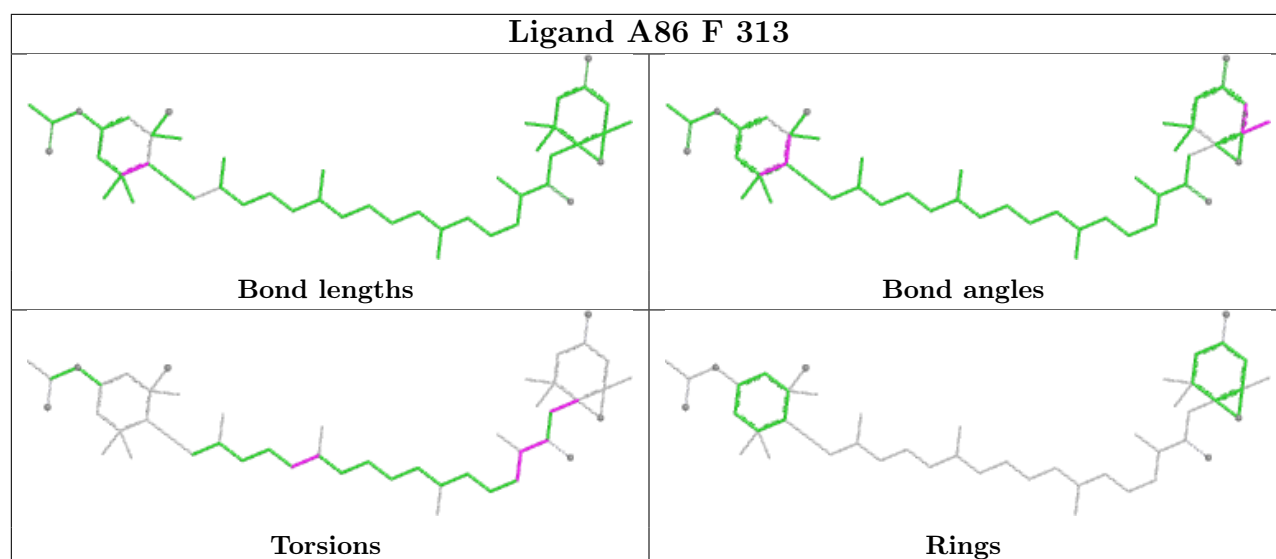


Ligand CLA O 316

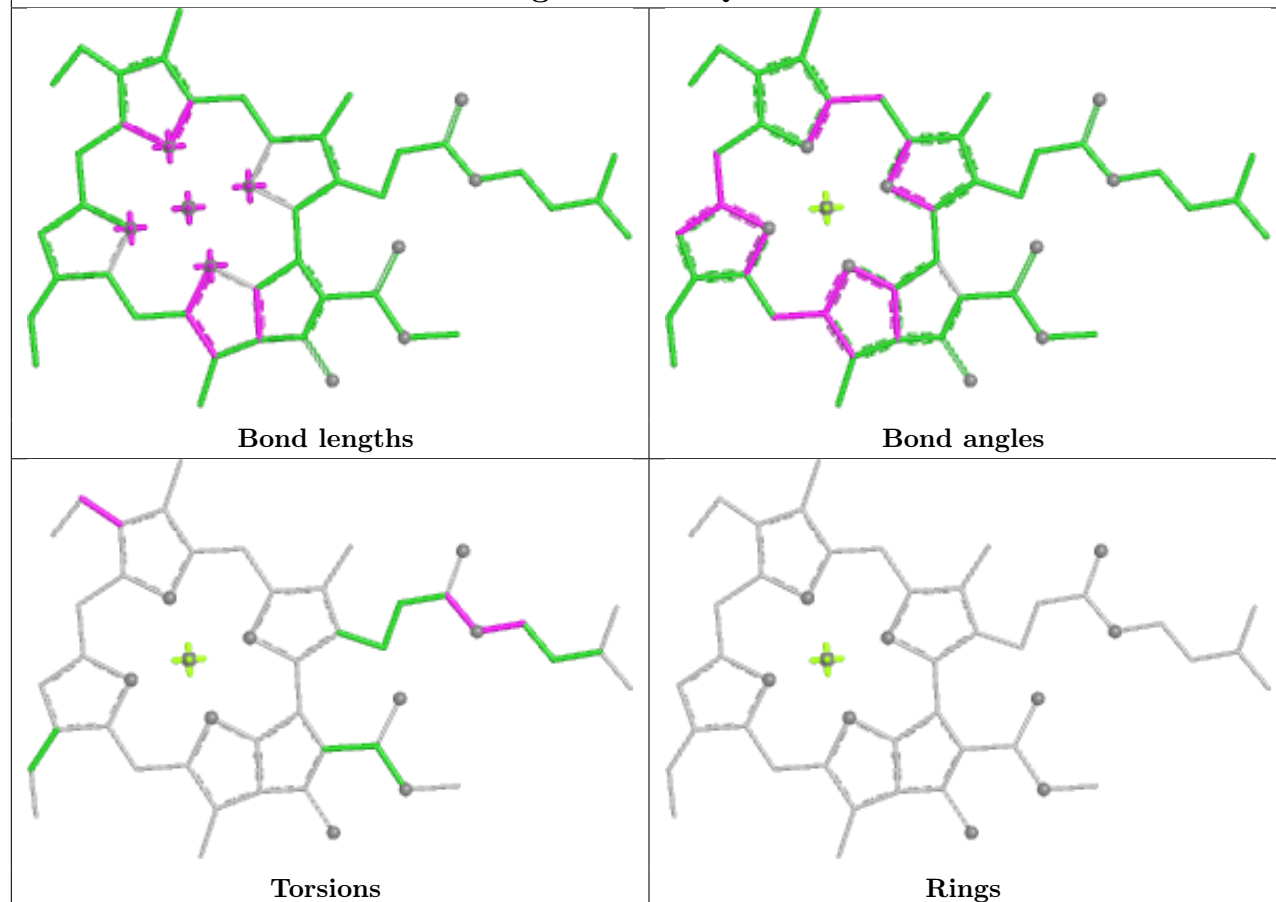


Ligand A86 M 315

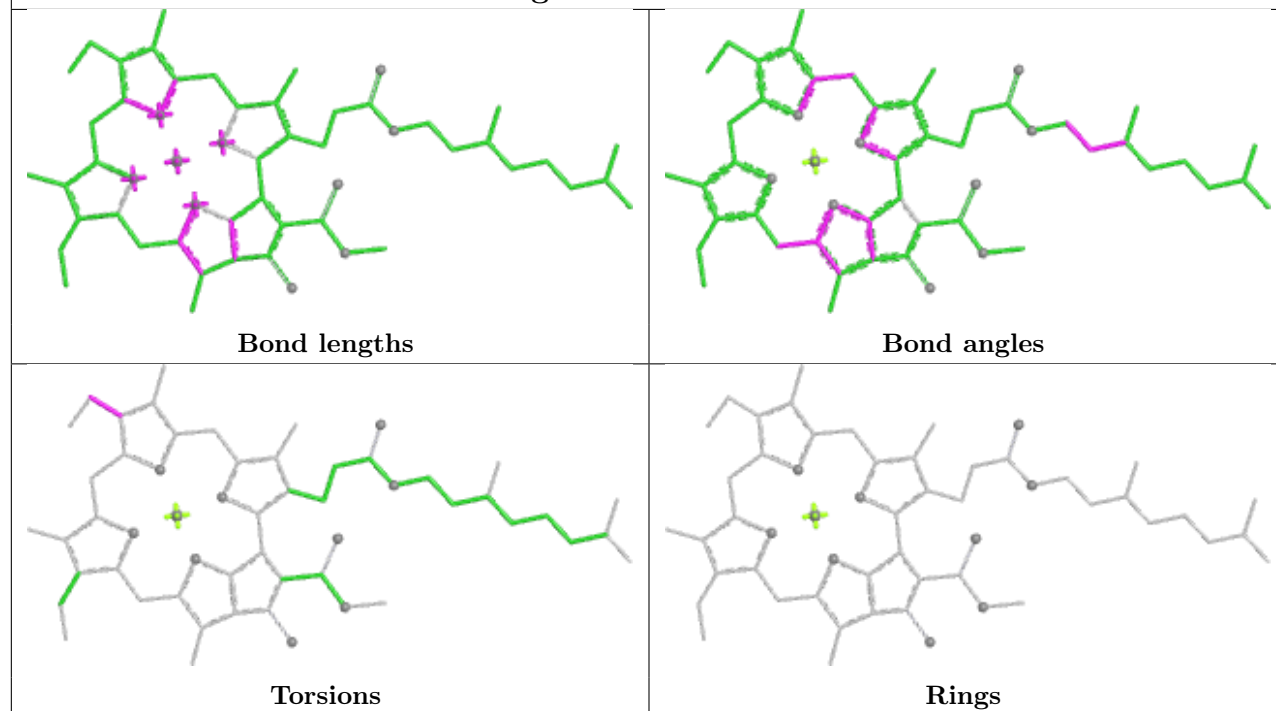




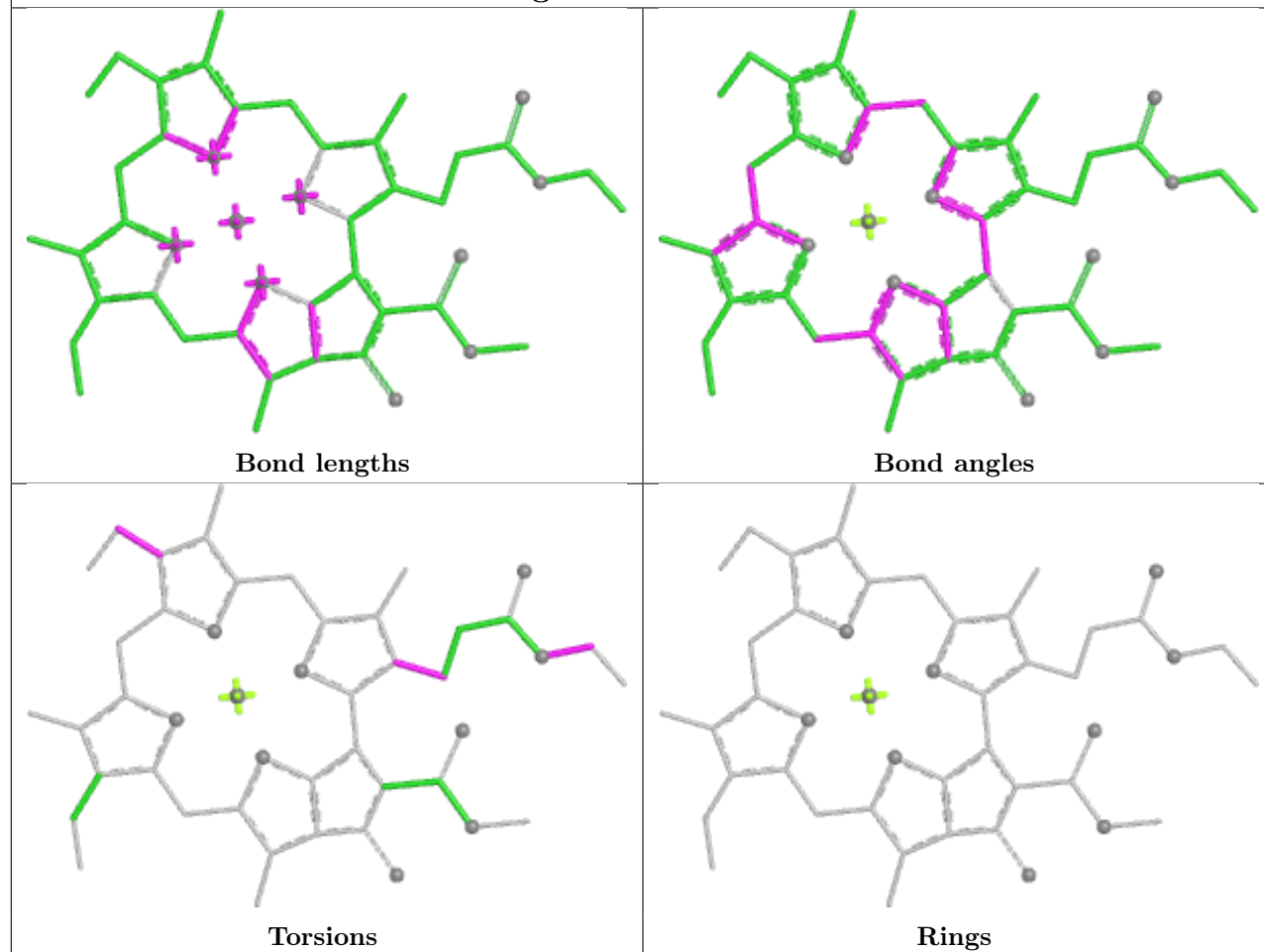
Ligand CLA Q 203



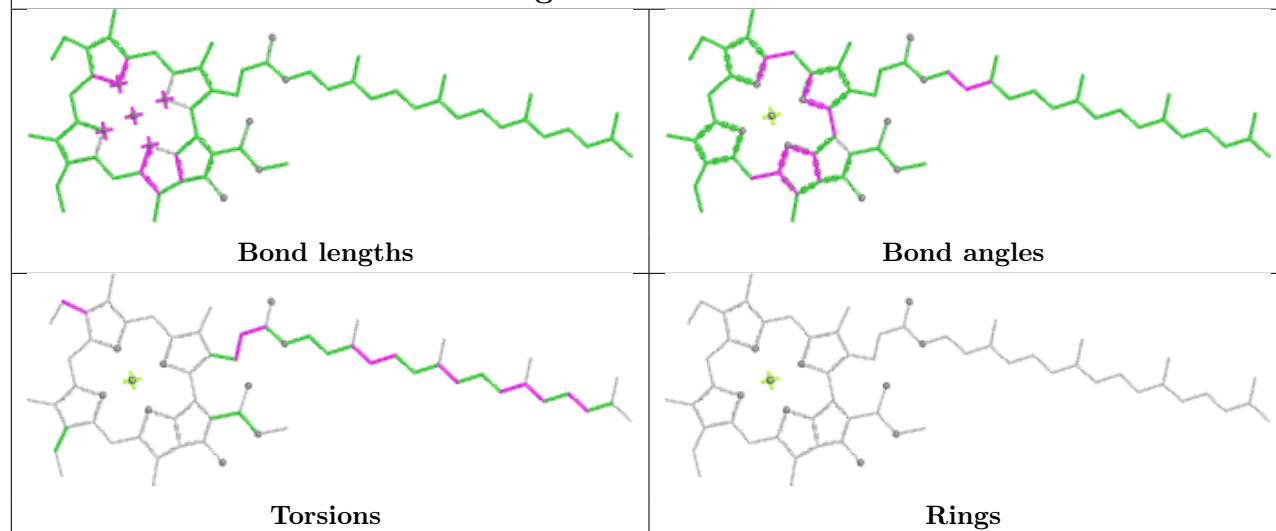
Ligand CLA D 308

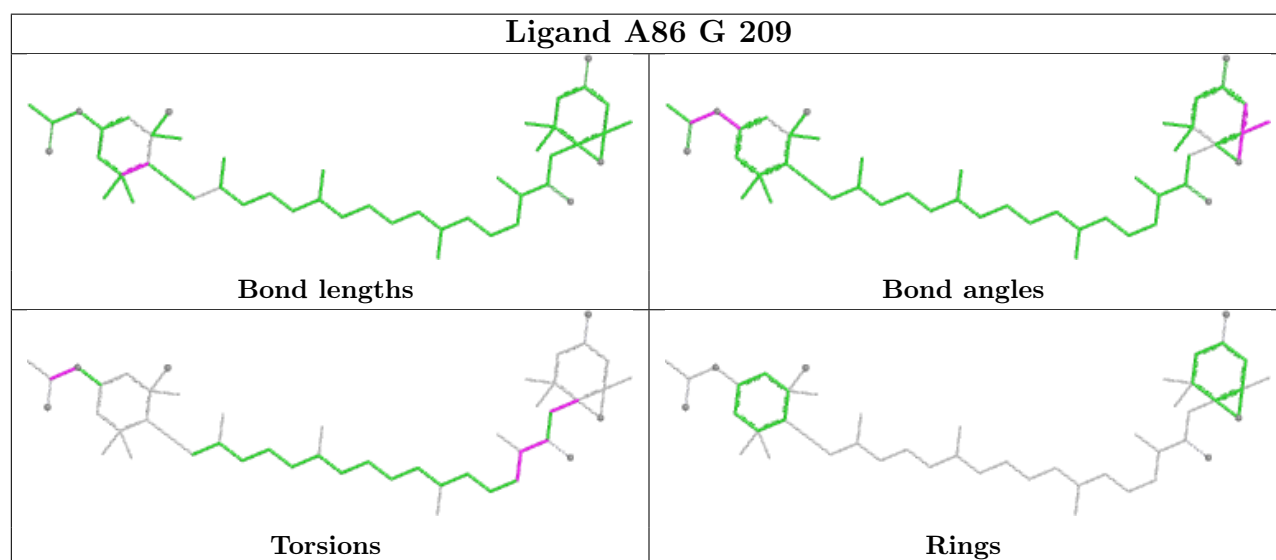
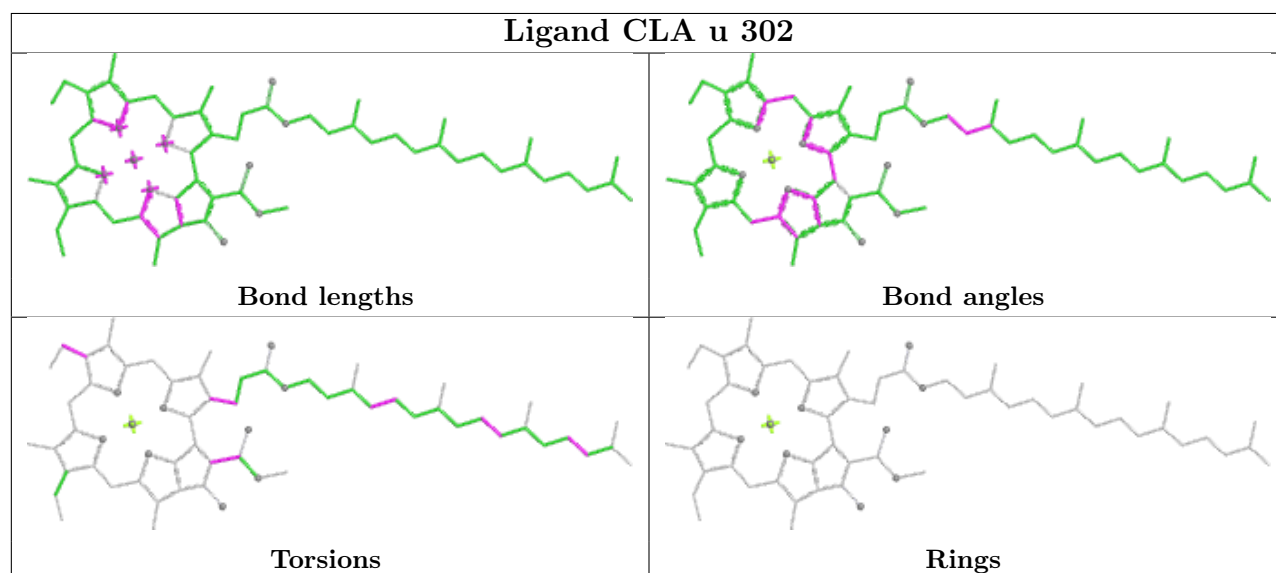
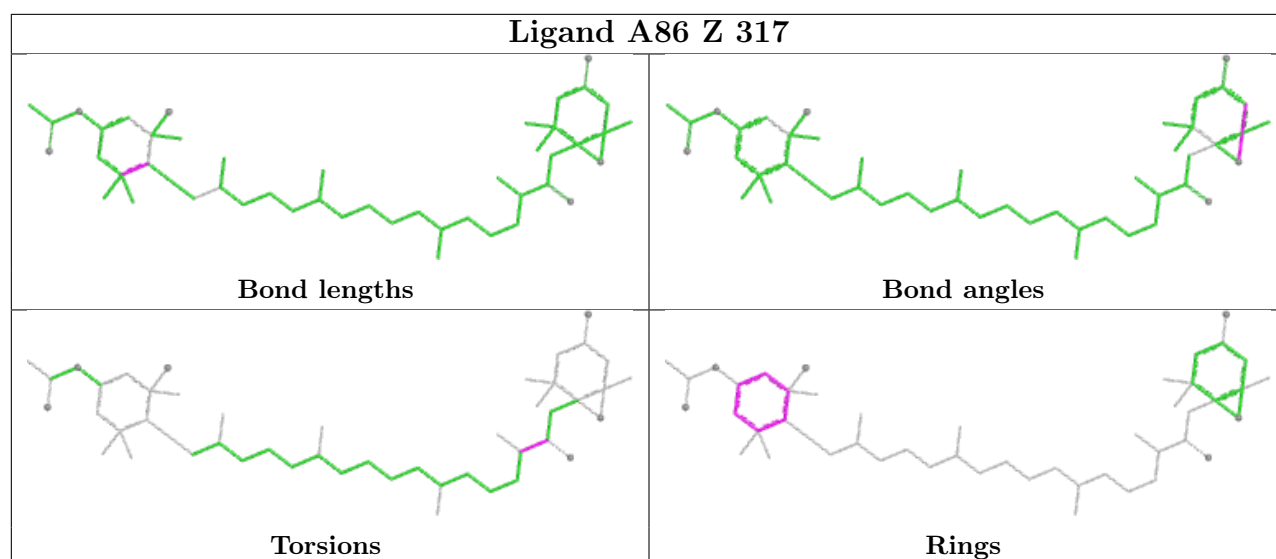


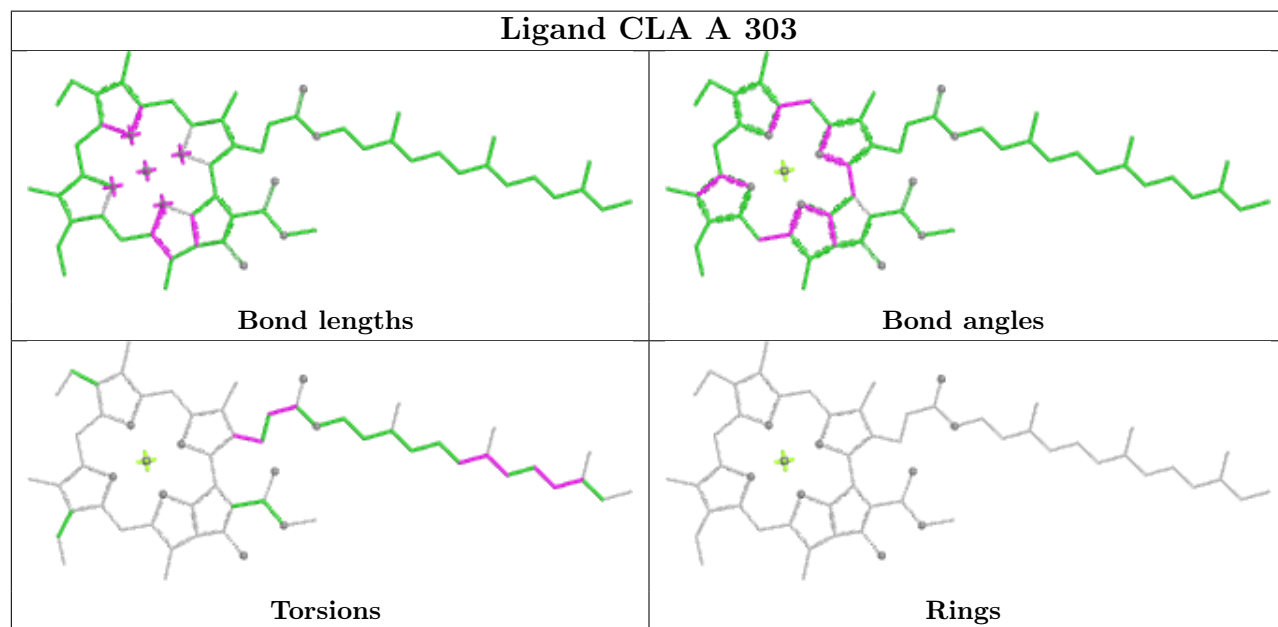
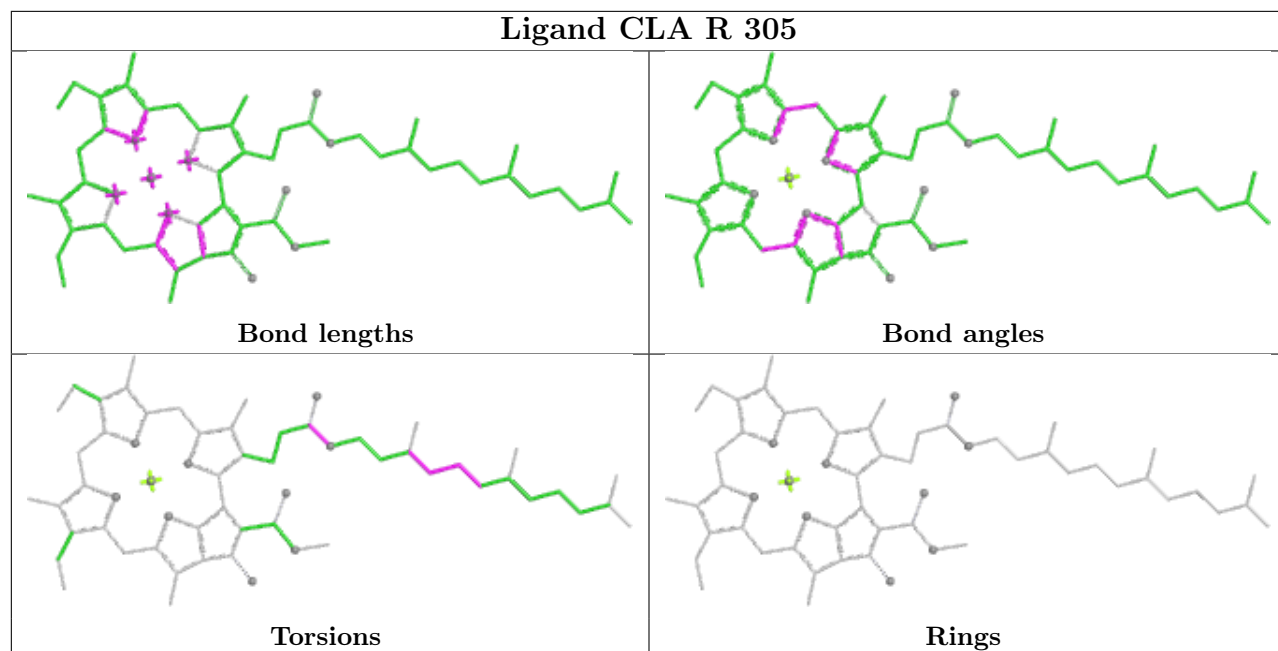
Ligand CLA z 324



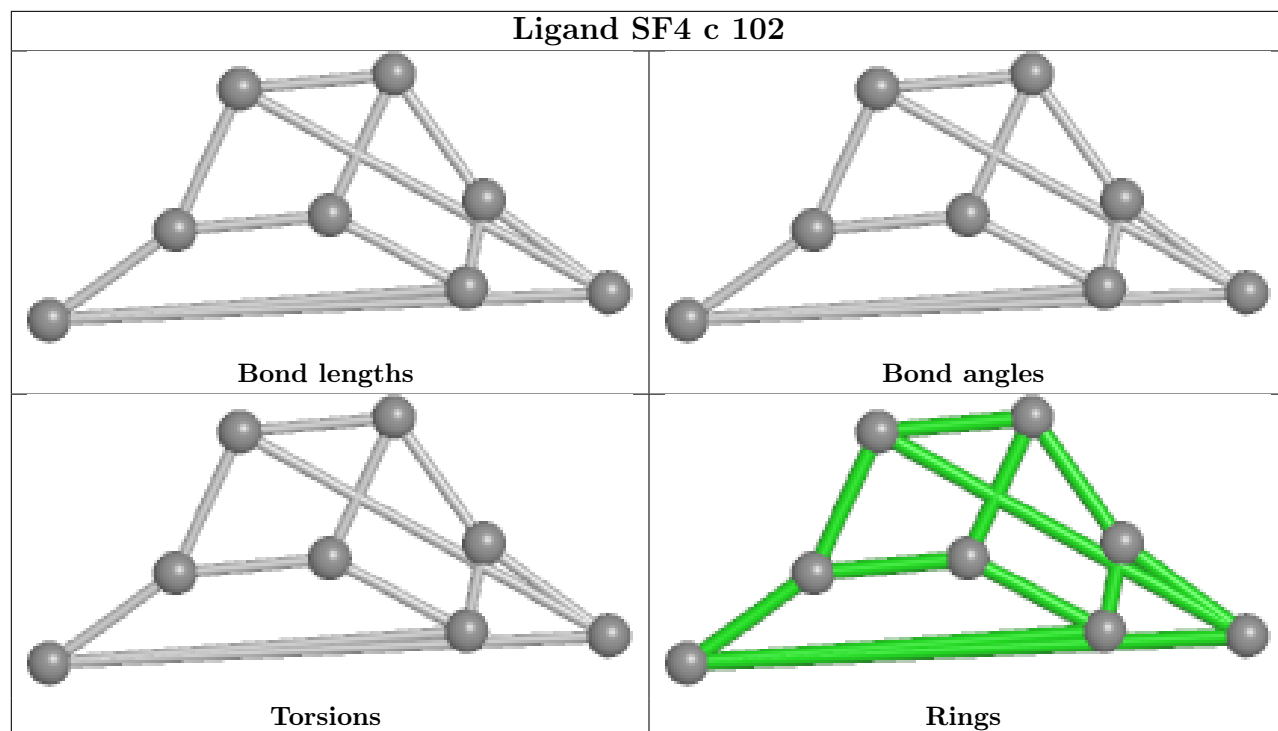
Ligand CLA b 803



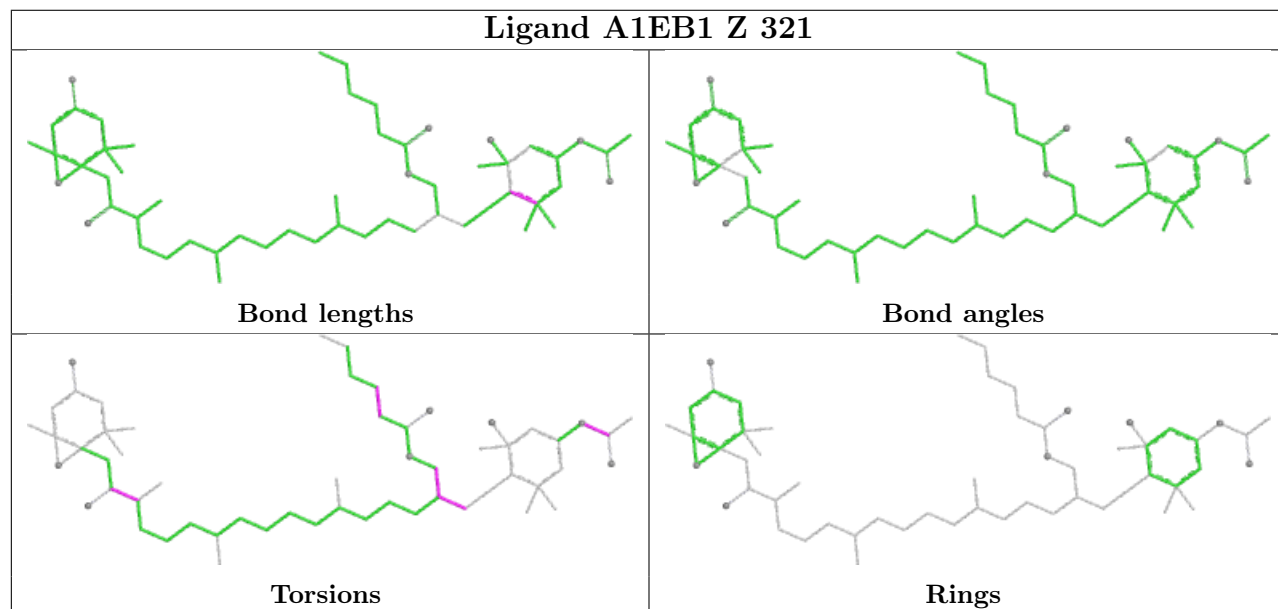


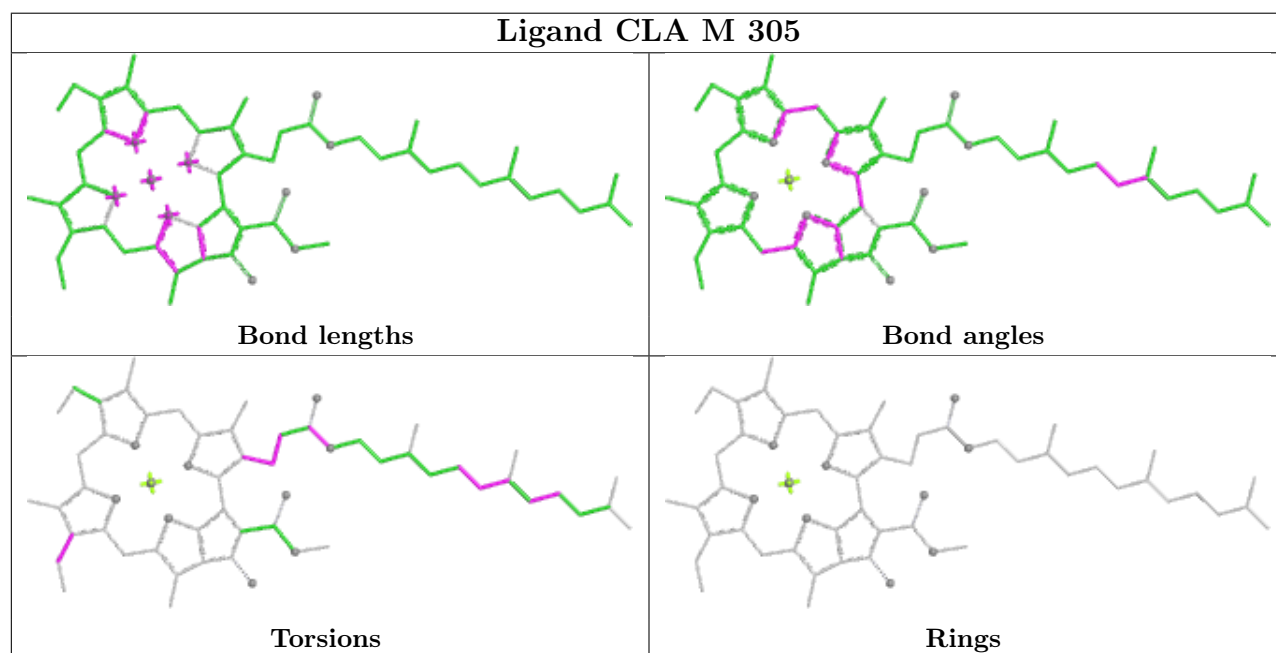
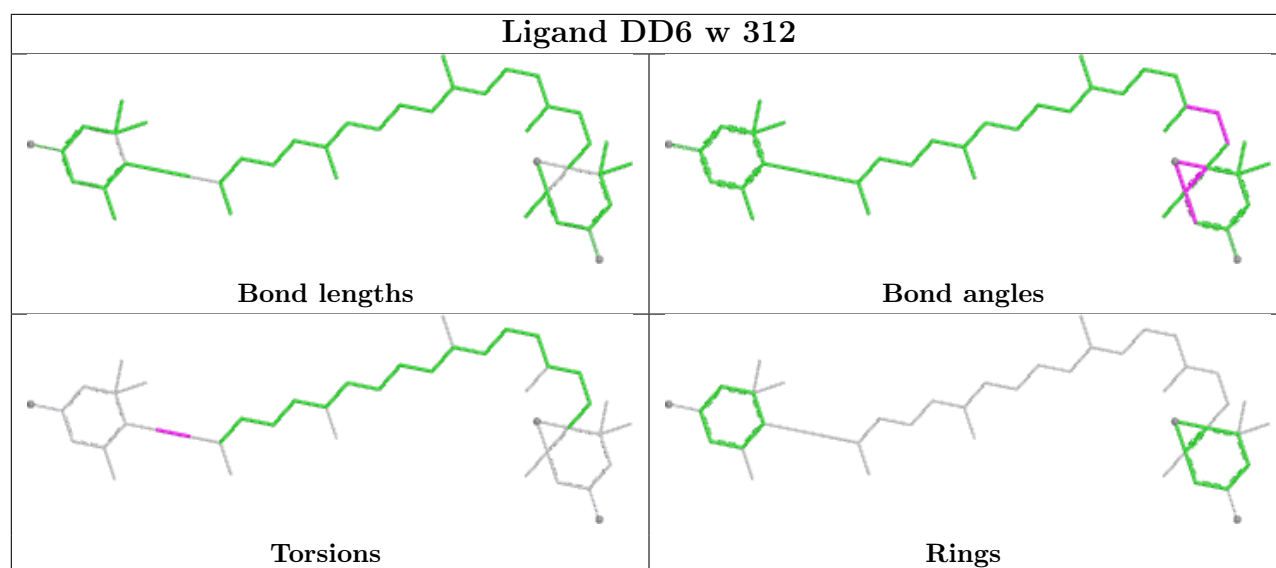


Ligand SF4 c 102

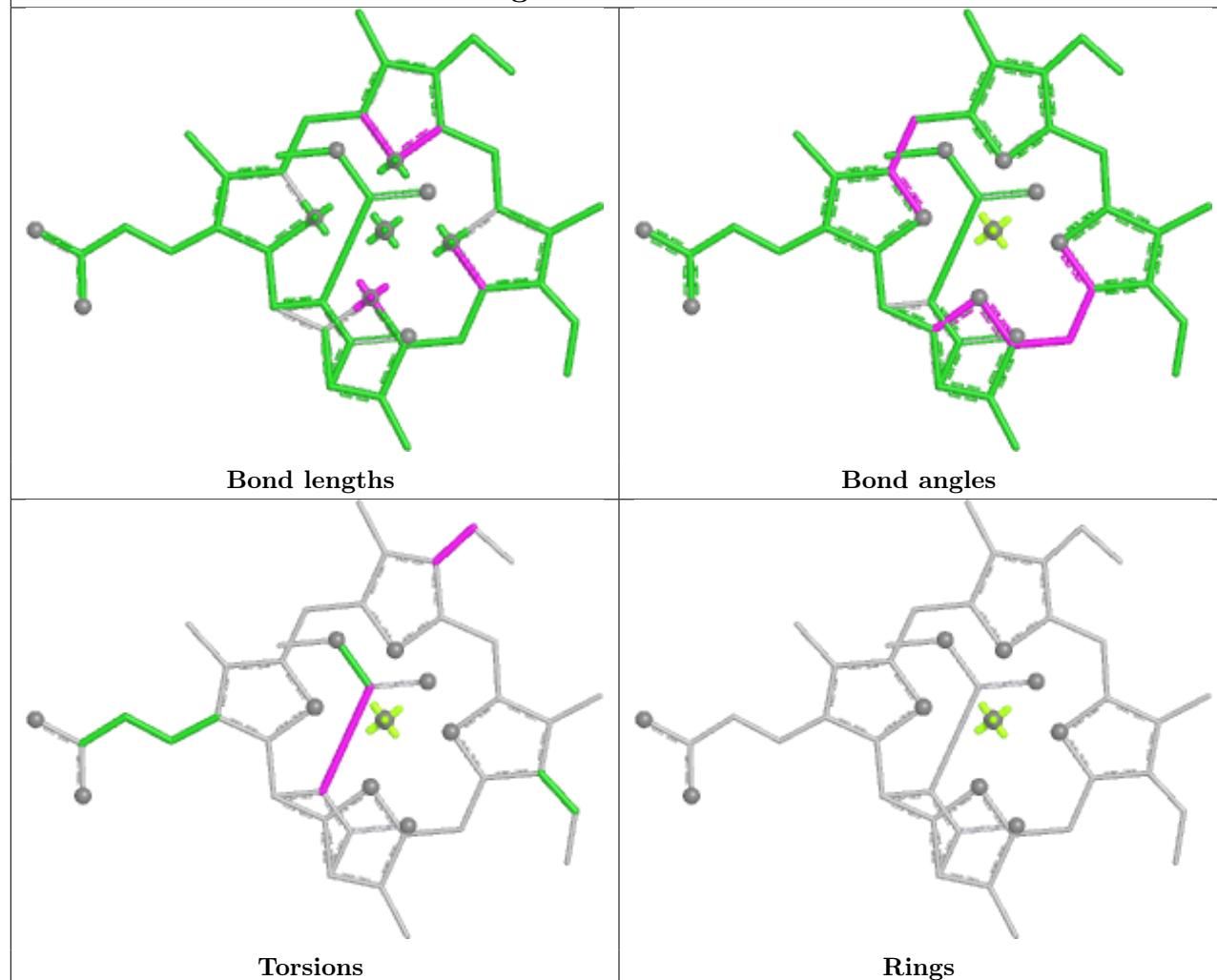


Ligand A1EB1 Z 321

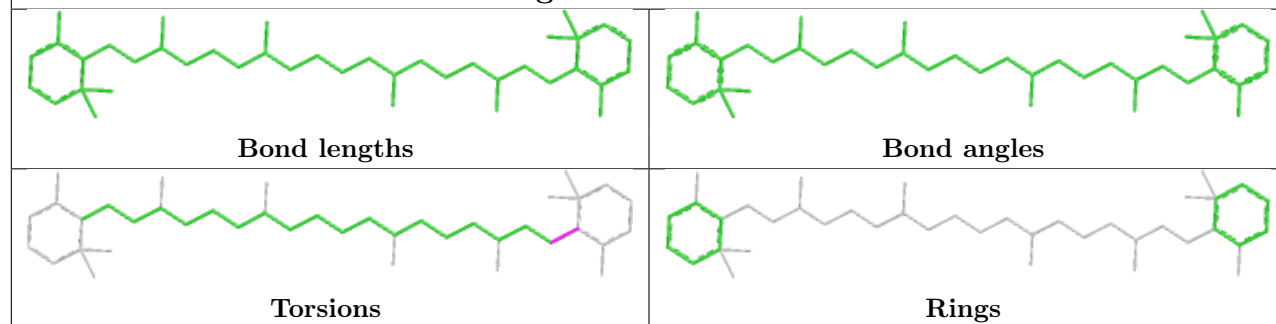




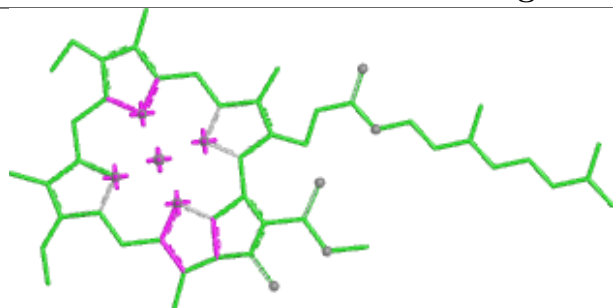
Ligand KC2 Z 303



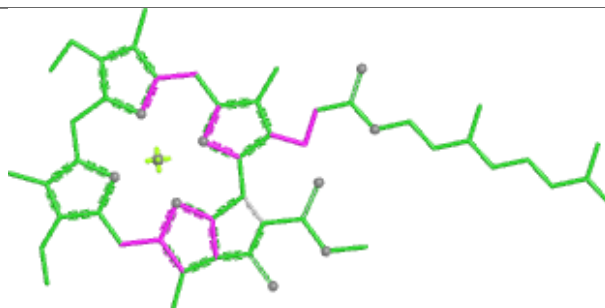
Ligand BCR r 201



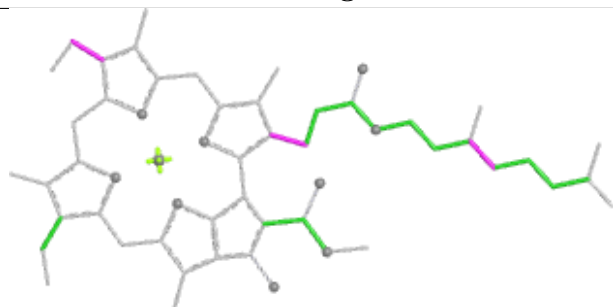
Ligand CLA k 202



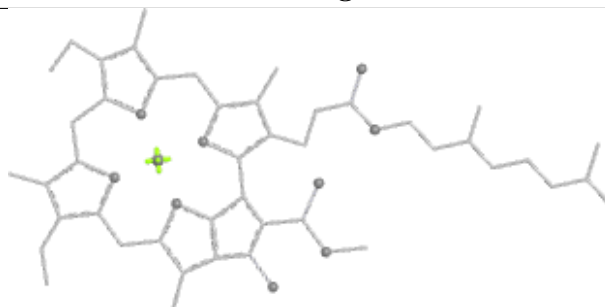
Bond lengths



Bond angles

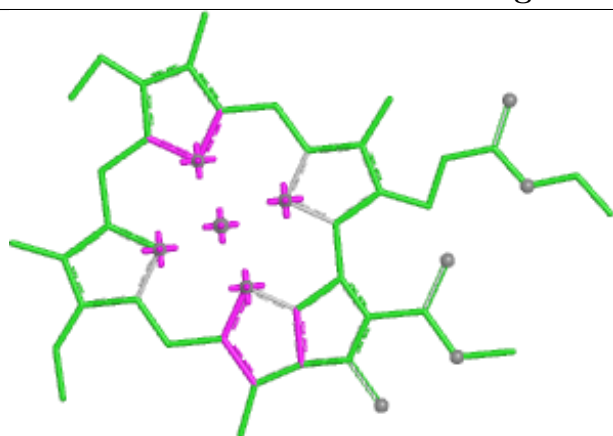


Torsions

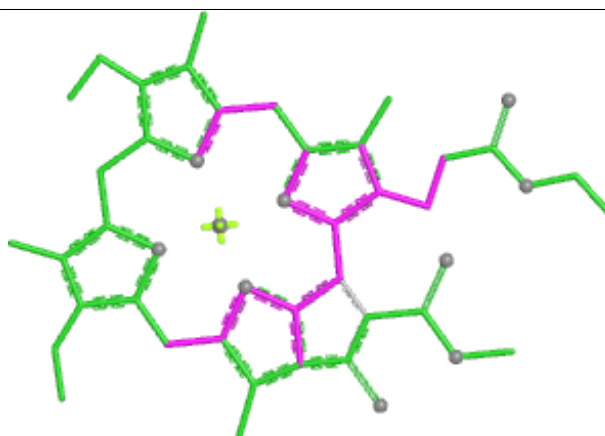


Rings

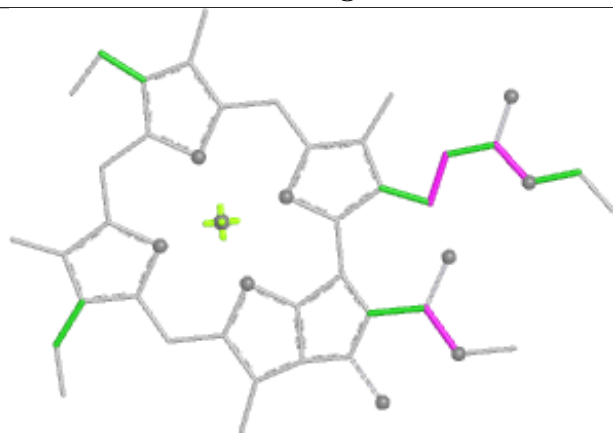
Ligand CLA C 308



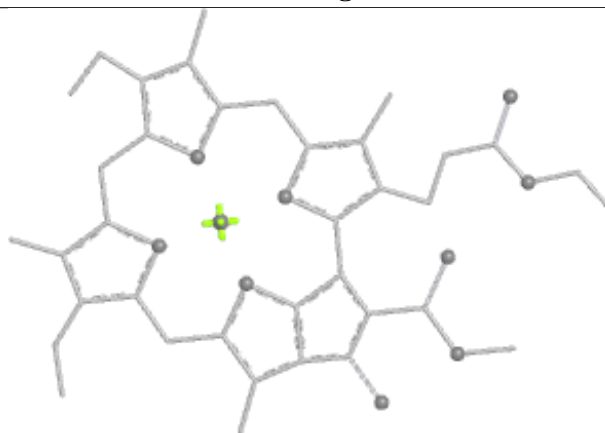
Bond lengths



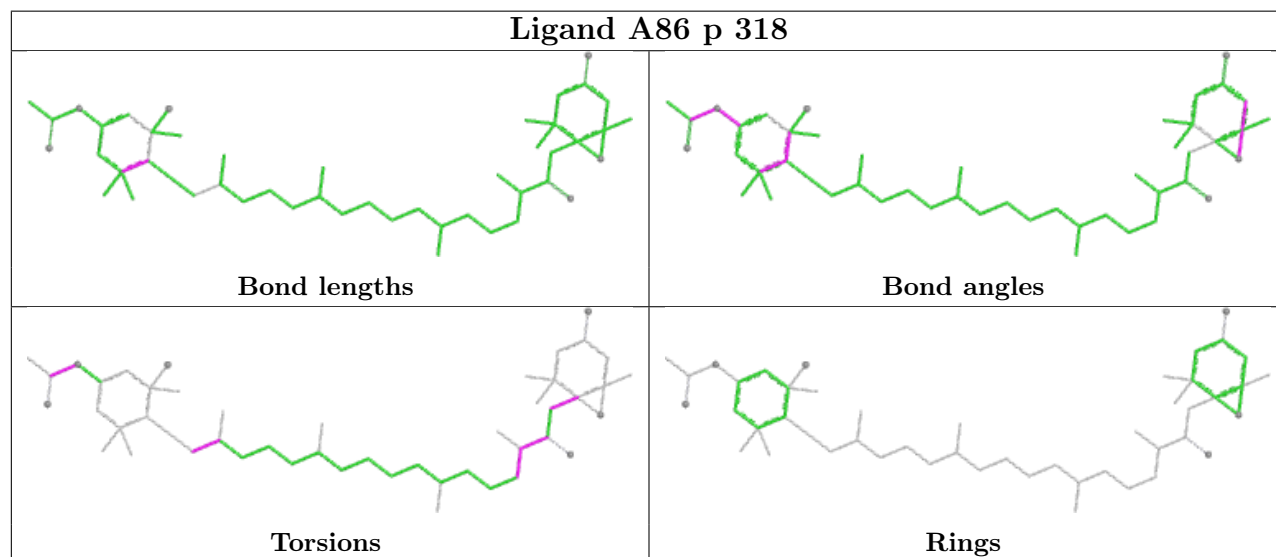
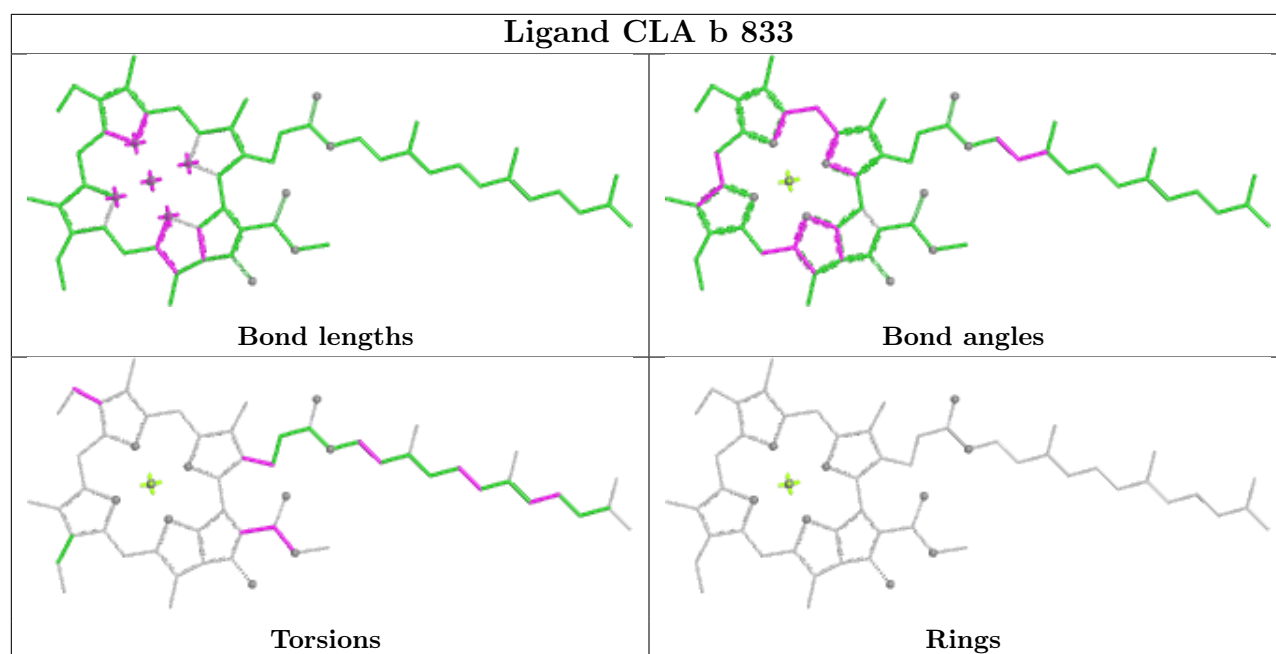
Bond angles



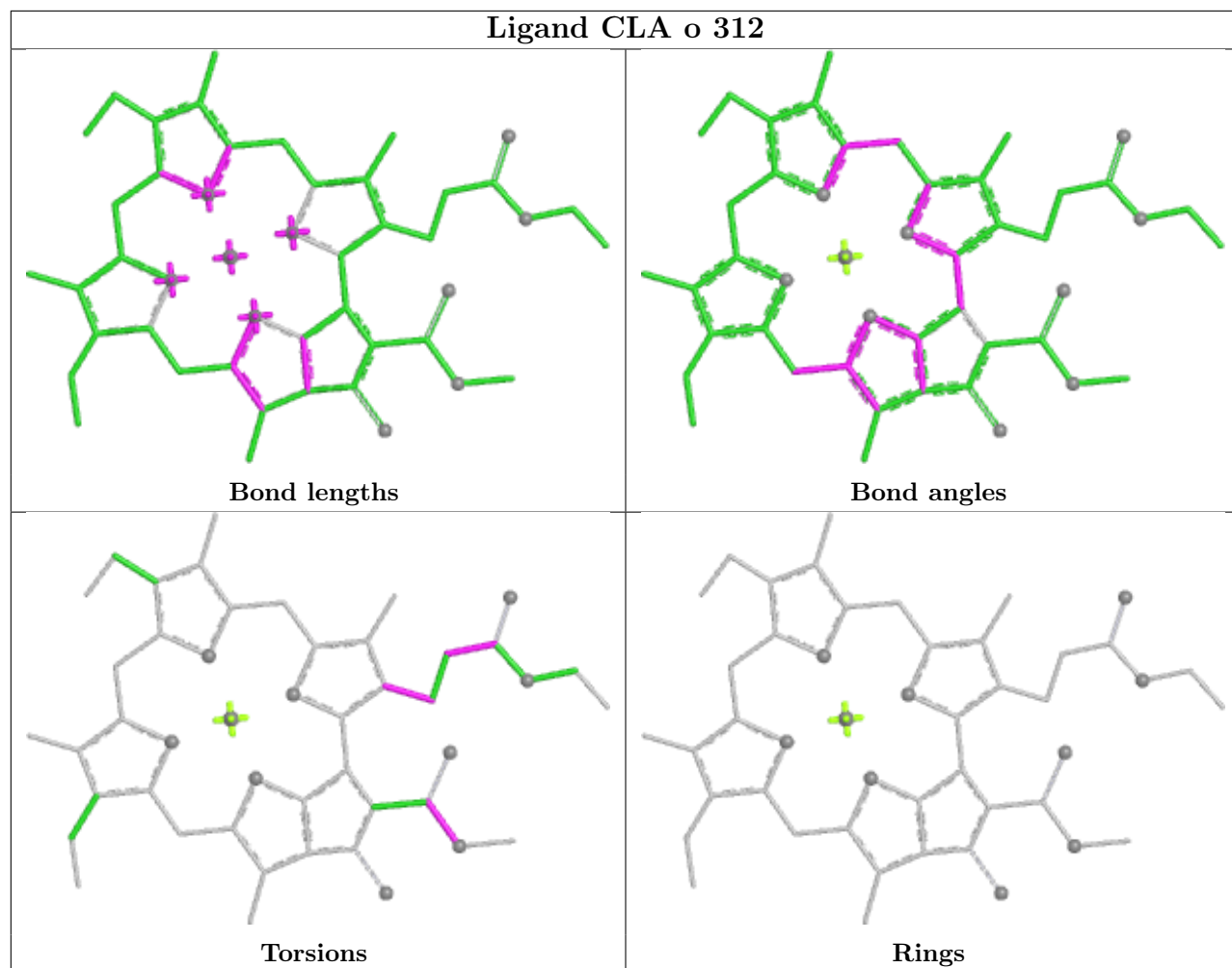
Torsions



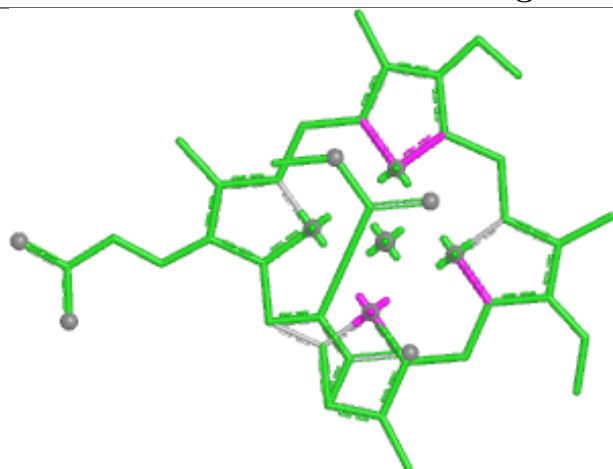
Rings



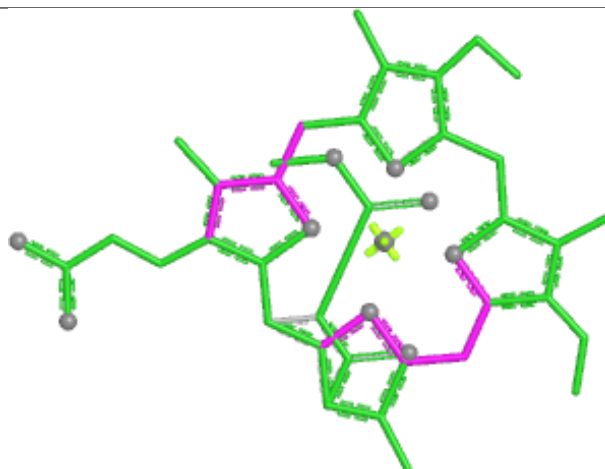
Ligand CLA o 312



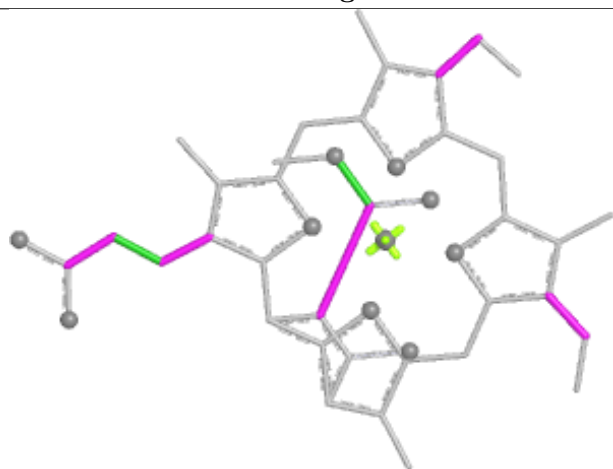
Ligand KC2 O 309



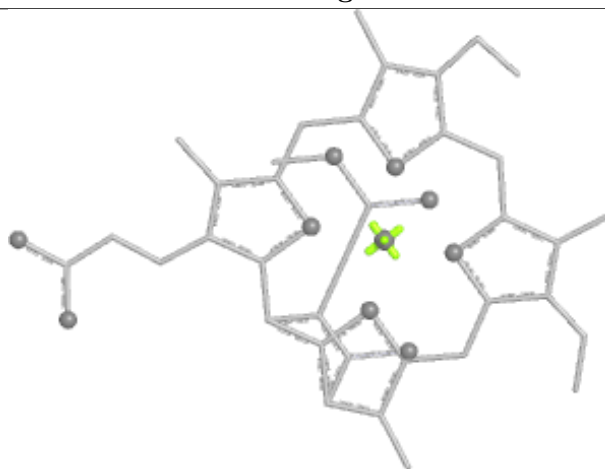
Bond lengths



Bond angles

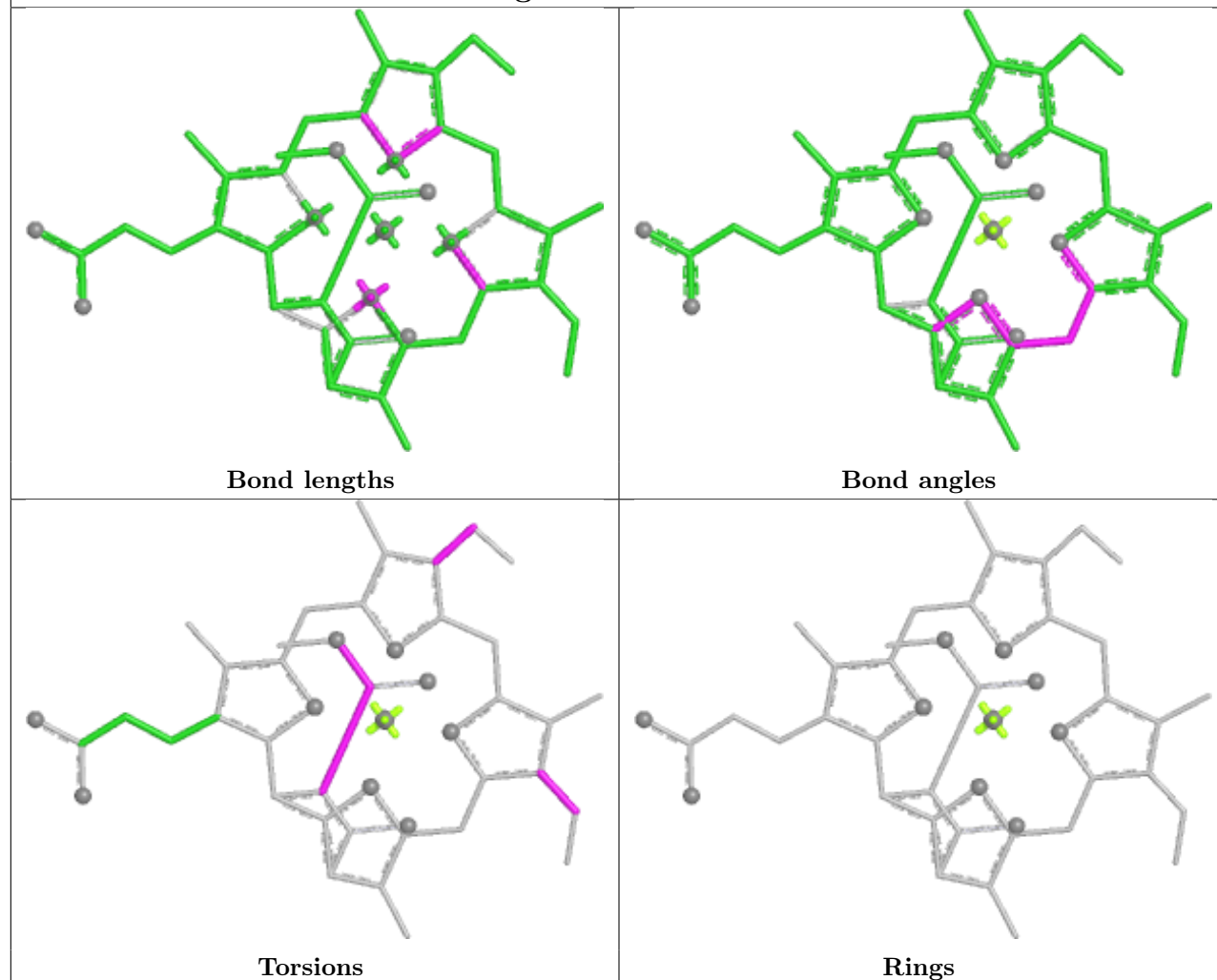


Torsions

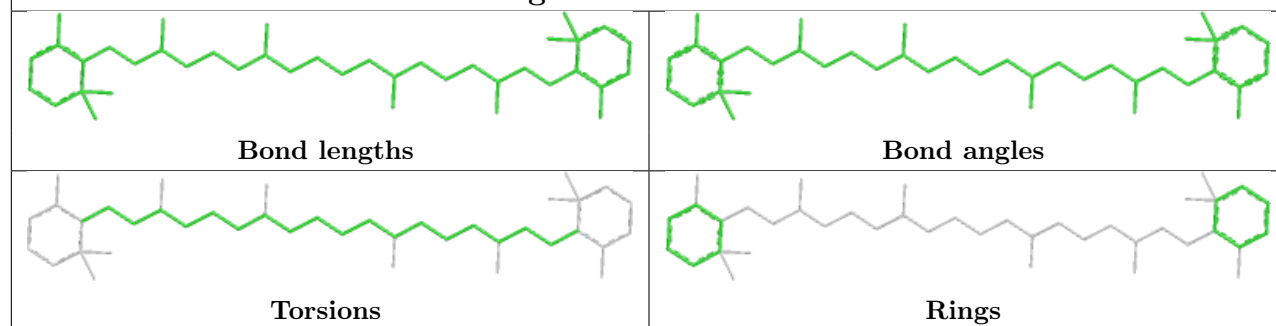


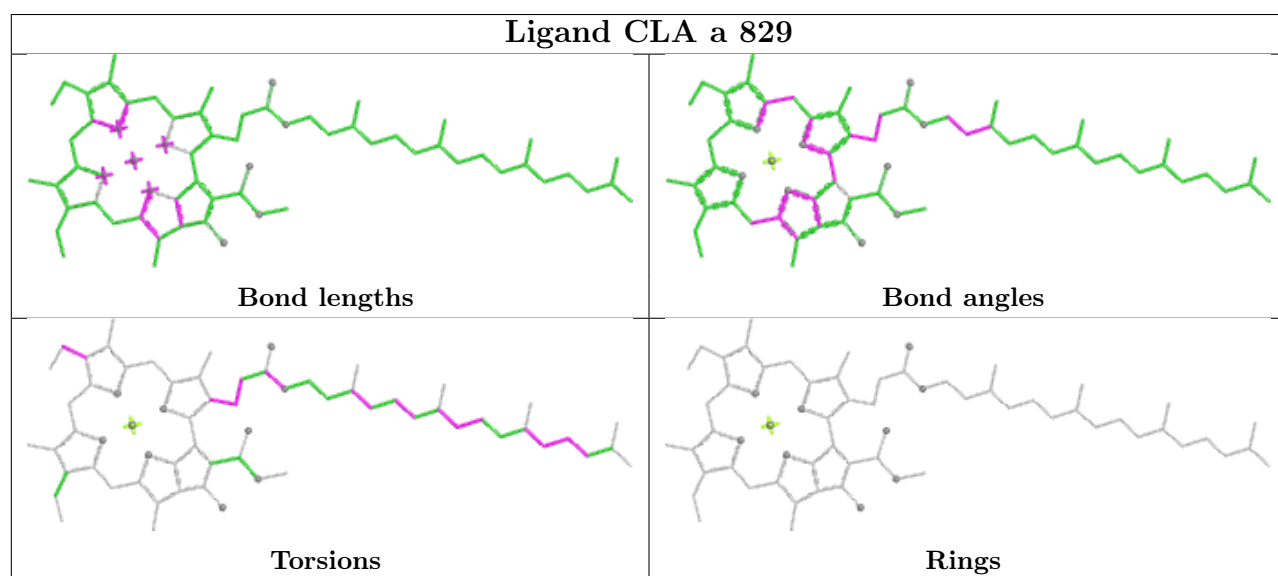
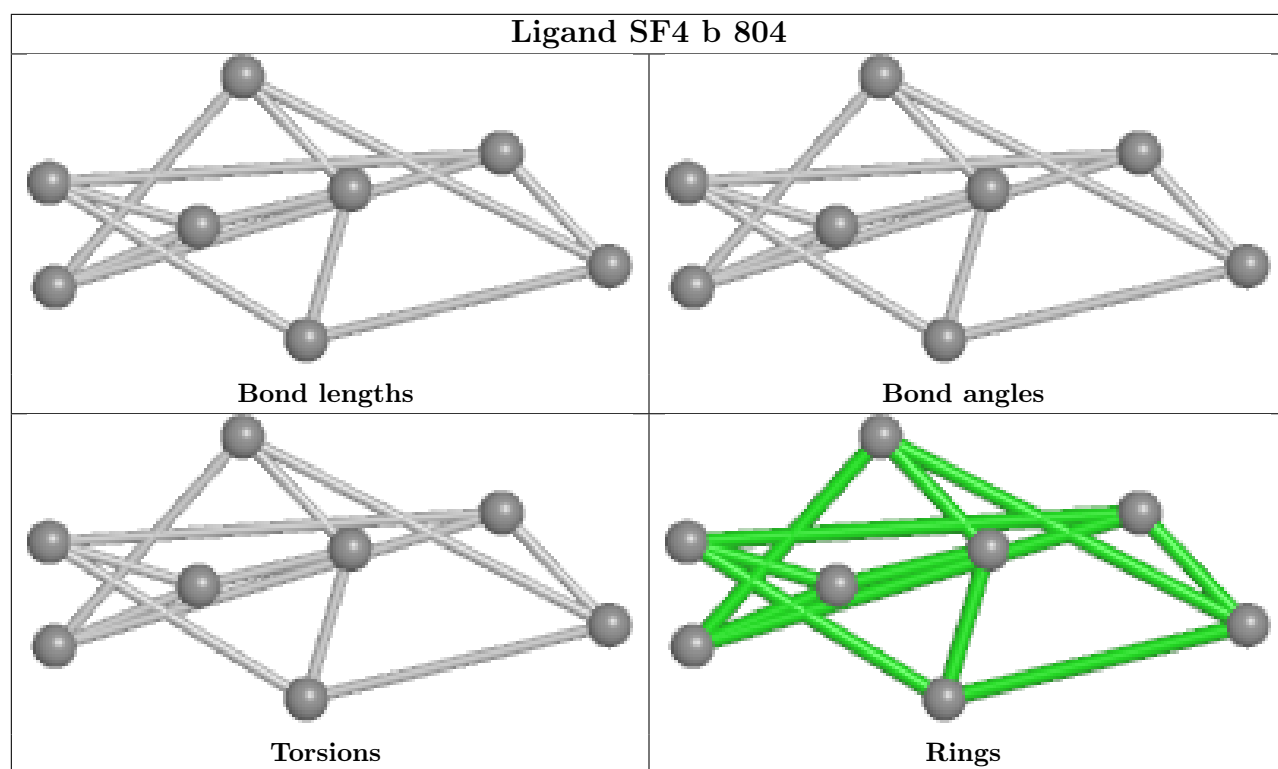
Rings

Ligand KC2 t 306

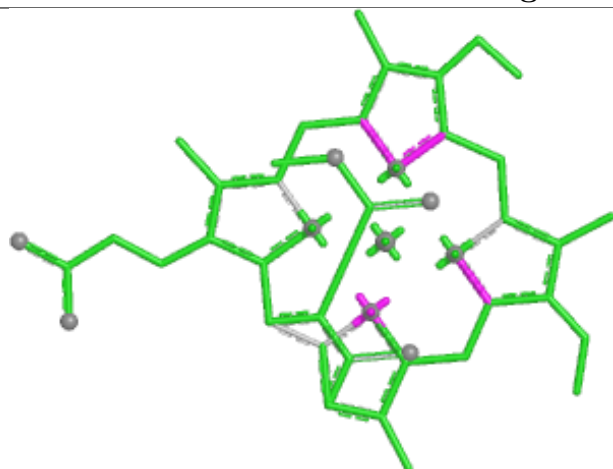


Ligand BCR m 101

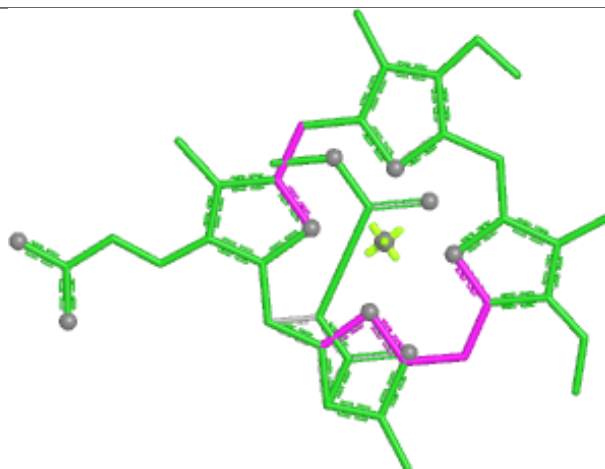




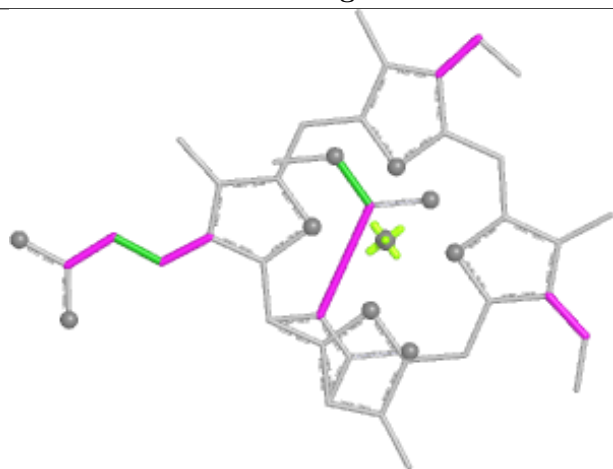
Ligand KC2 o 309



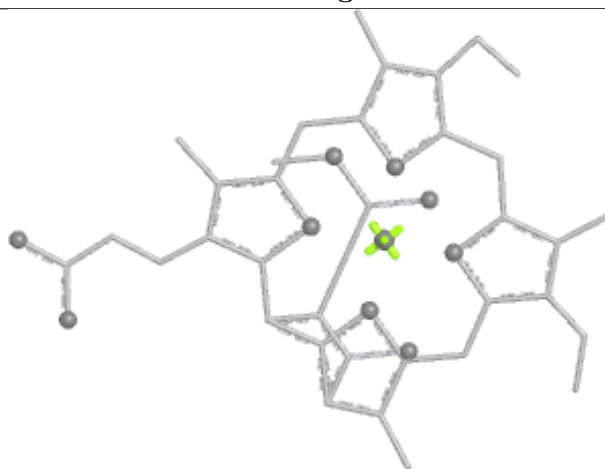
Bond lengths



Bond angles

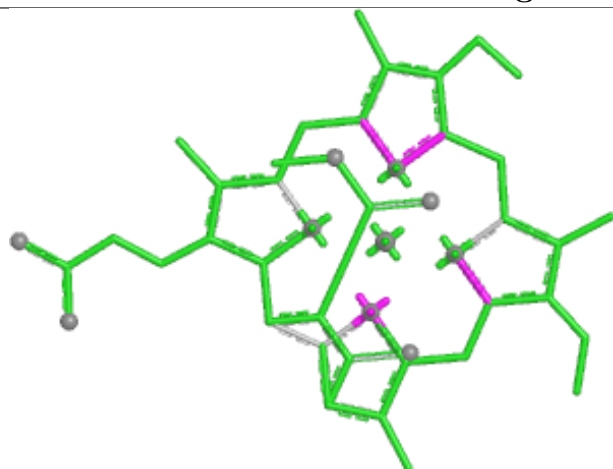


Torsions

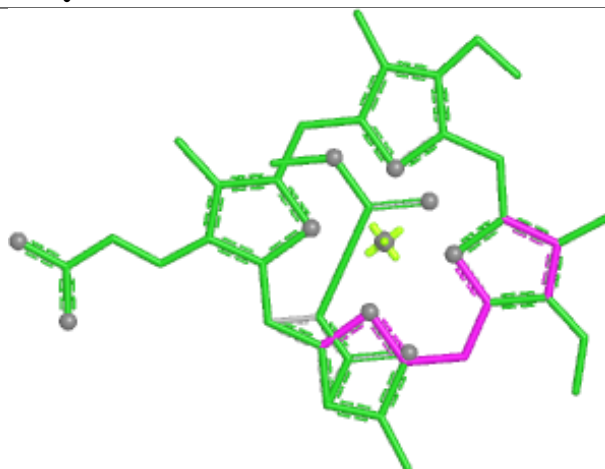


Rings

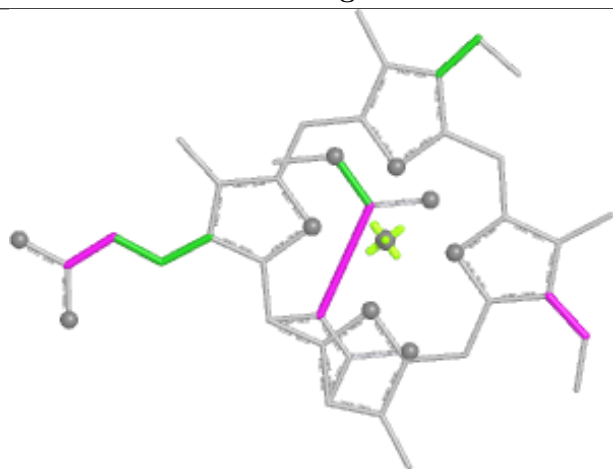
Ligand KC2 Q 201



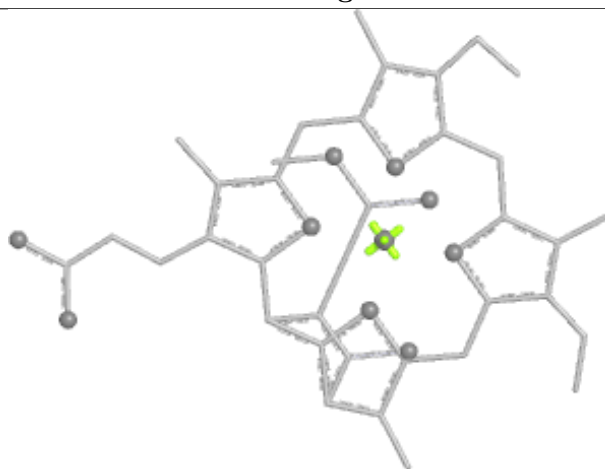
Bond lengths



Bond angles

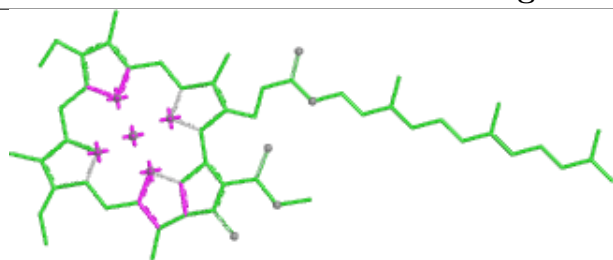


Torsions

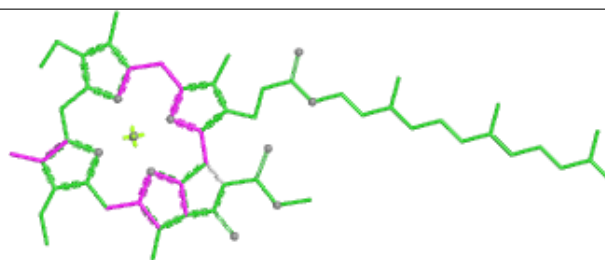


Rings

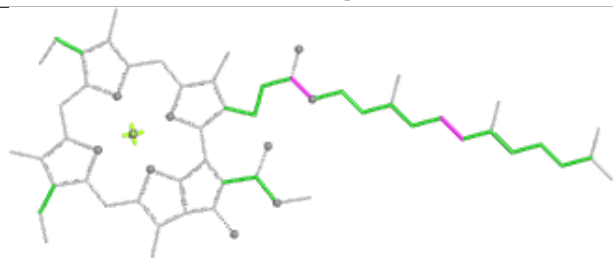
Ligand CLA v 305



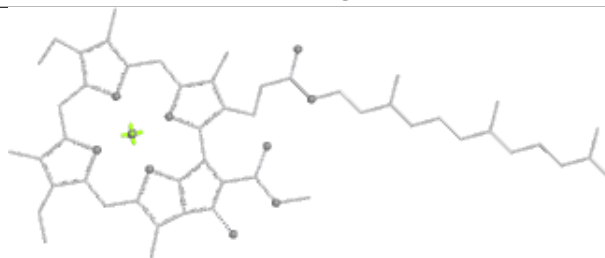
Bond lengths



Bond angles

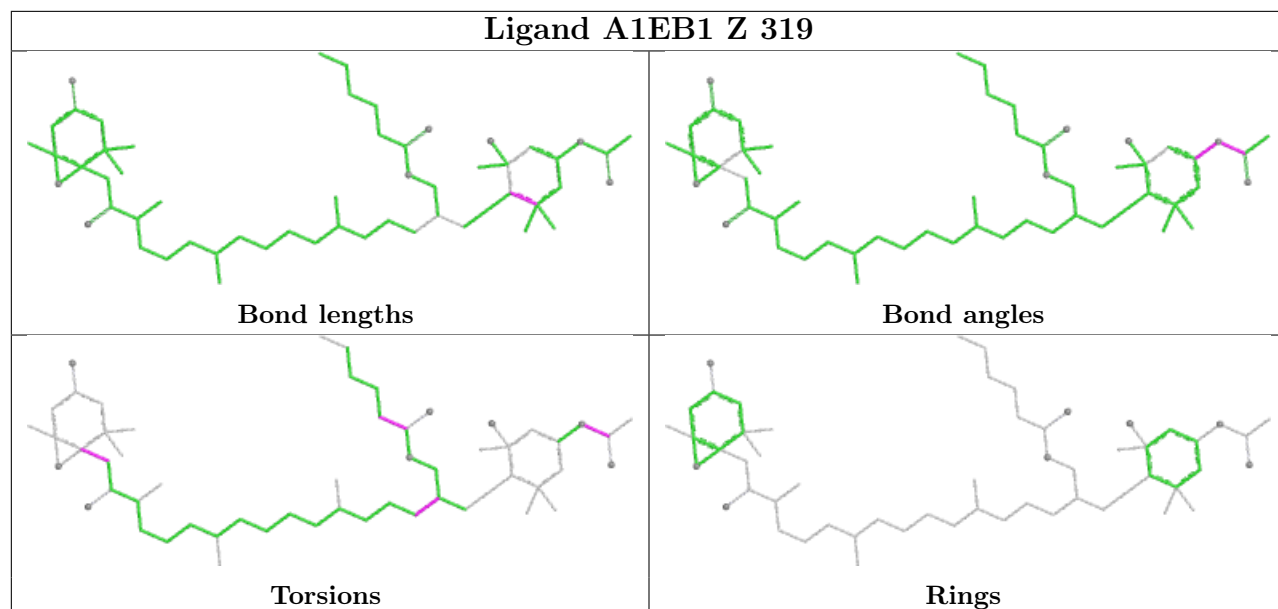


Torsions

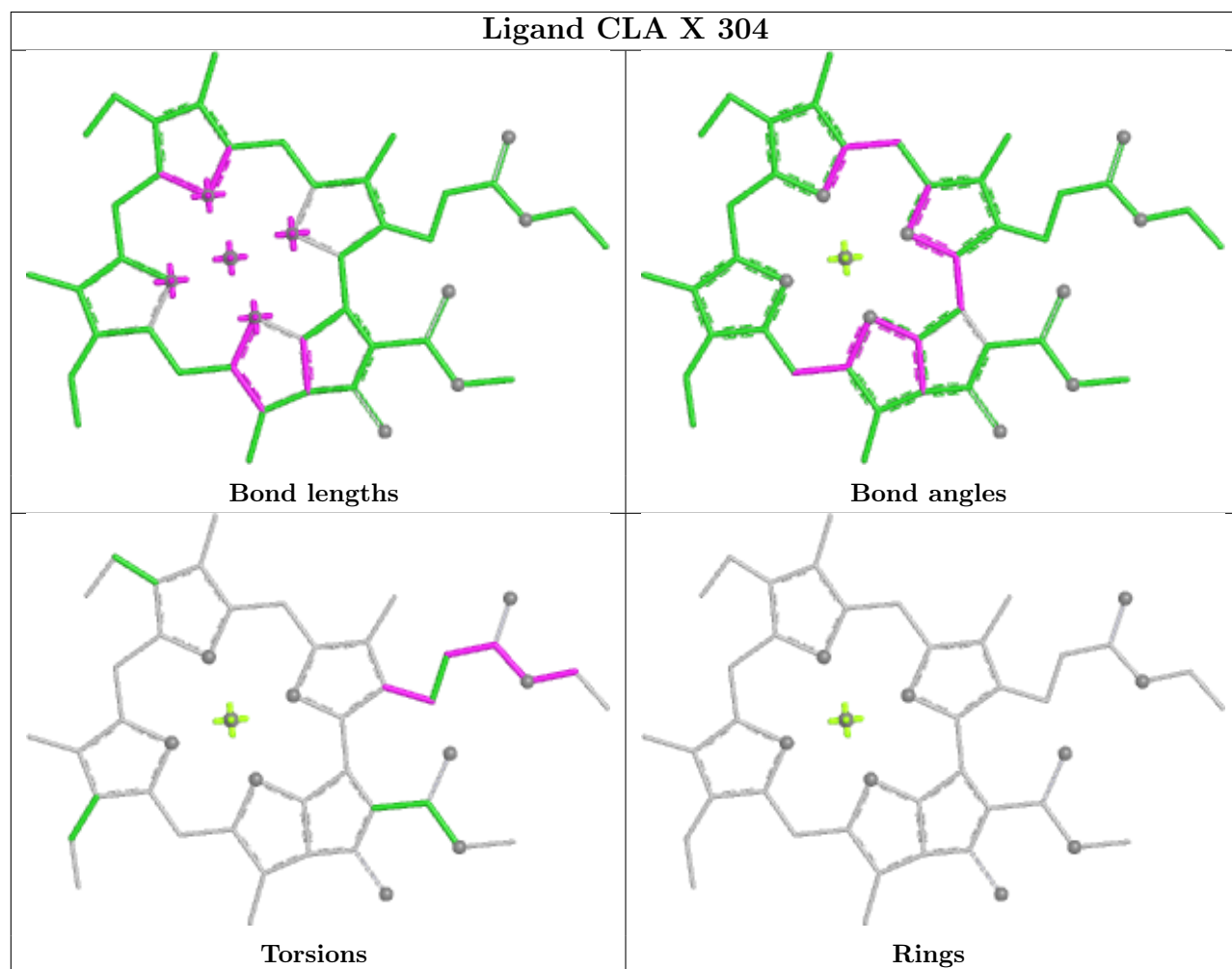


Rings

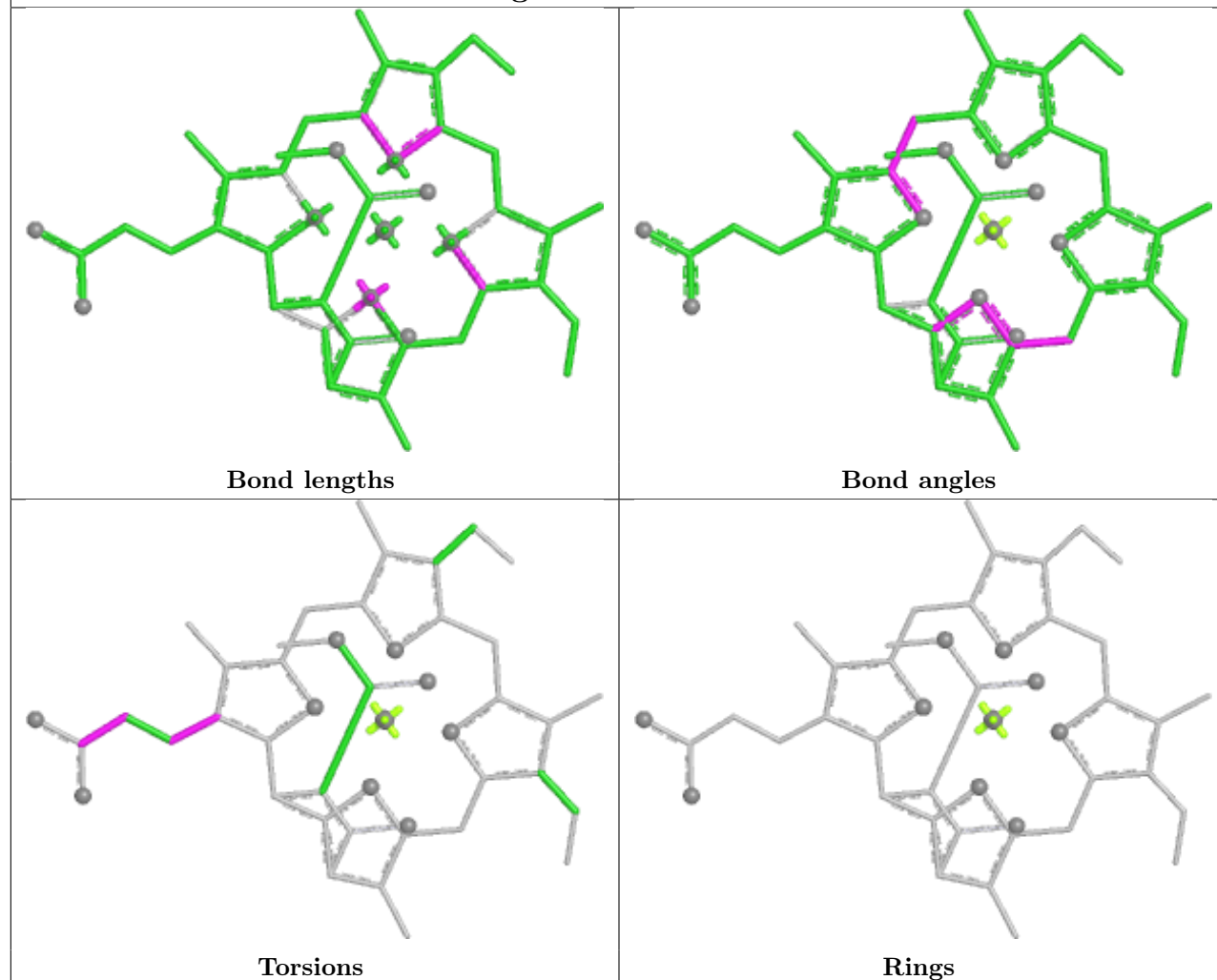
Ligand A1EB1 Z 319



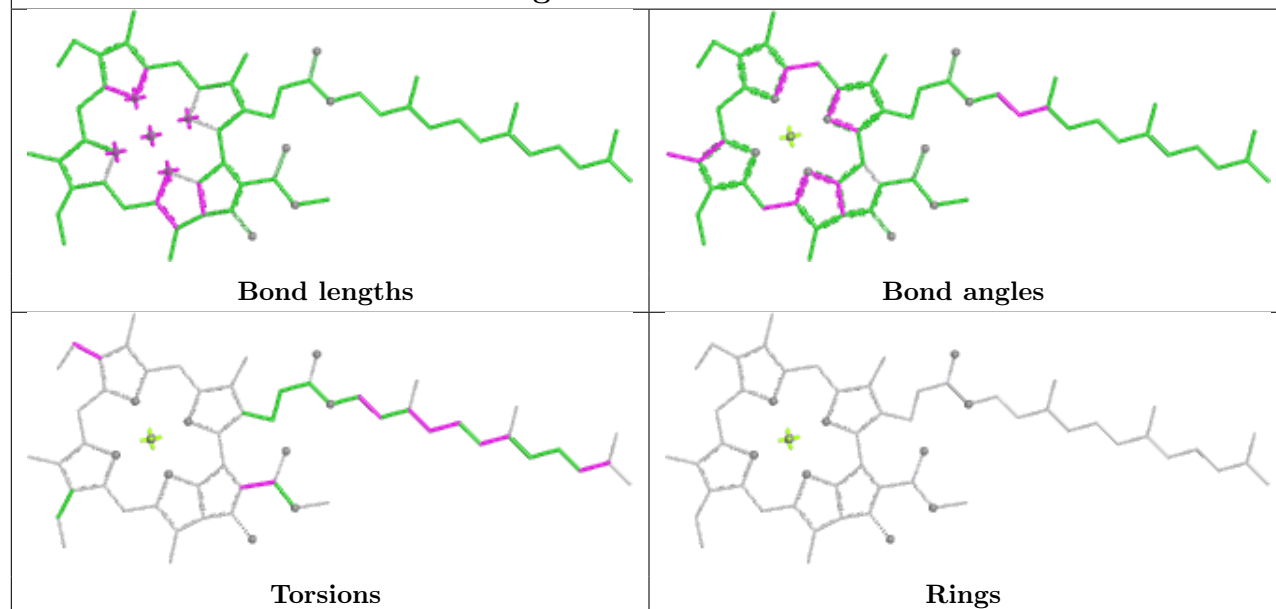
Ligand CLA X 304

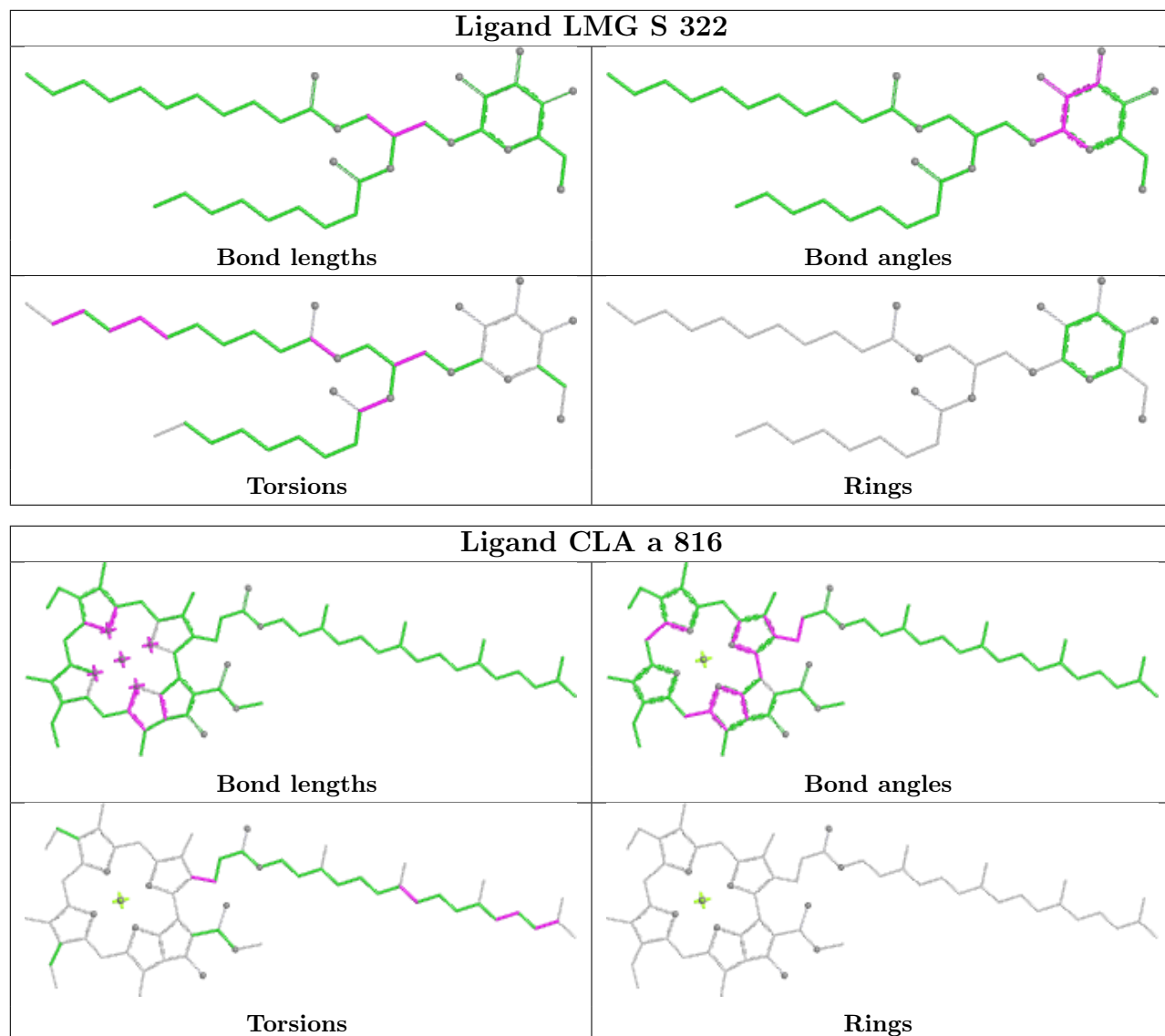


Ligand KC2 L 308

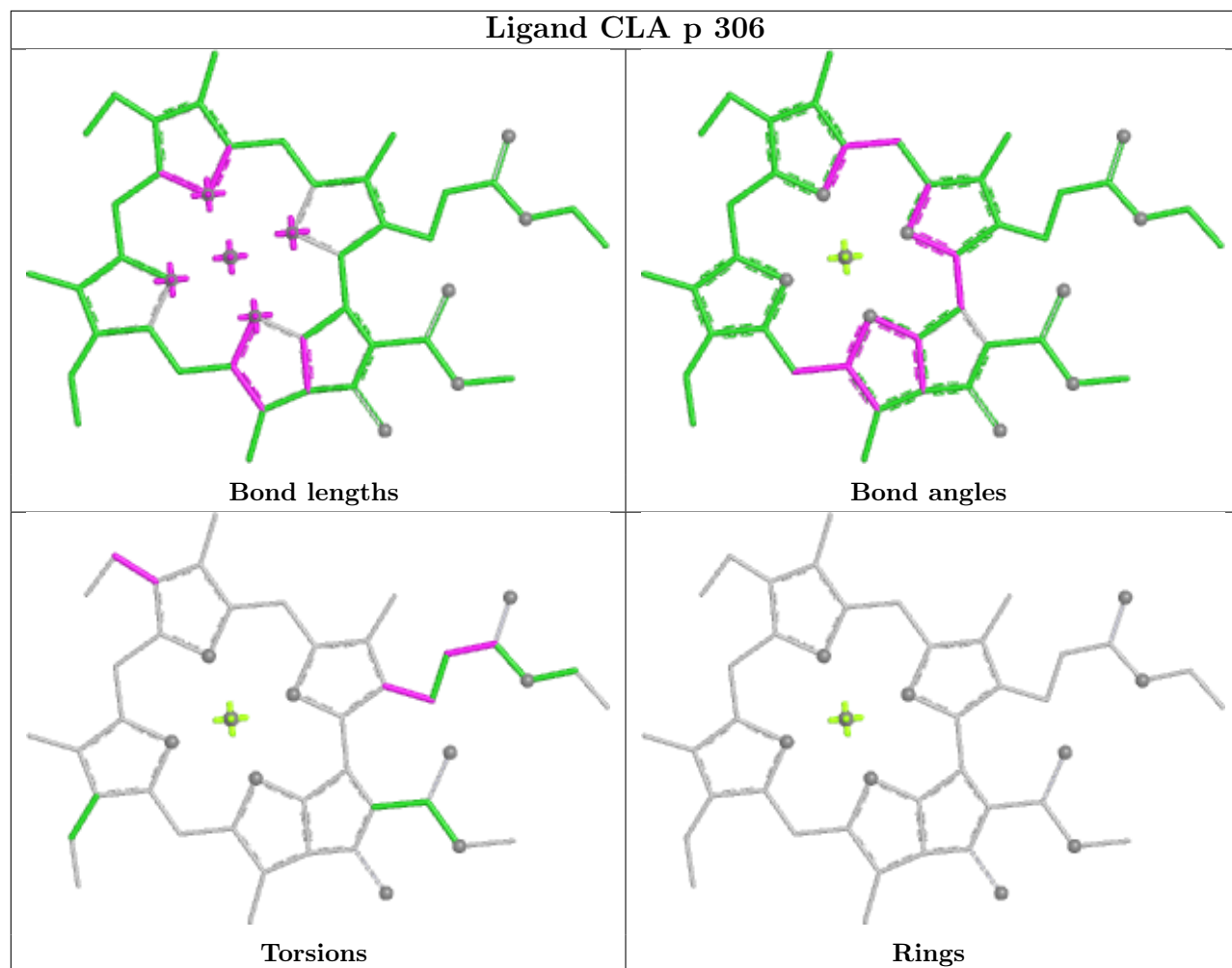


Ligand CLA P 305

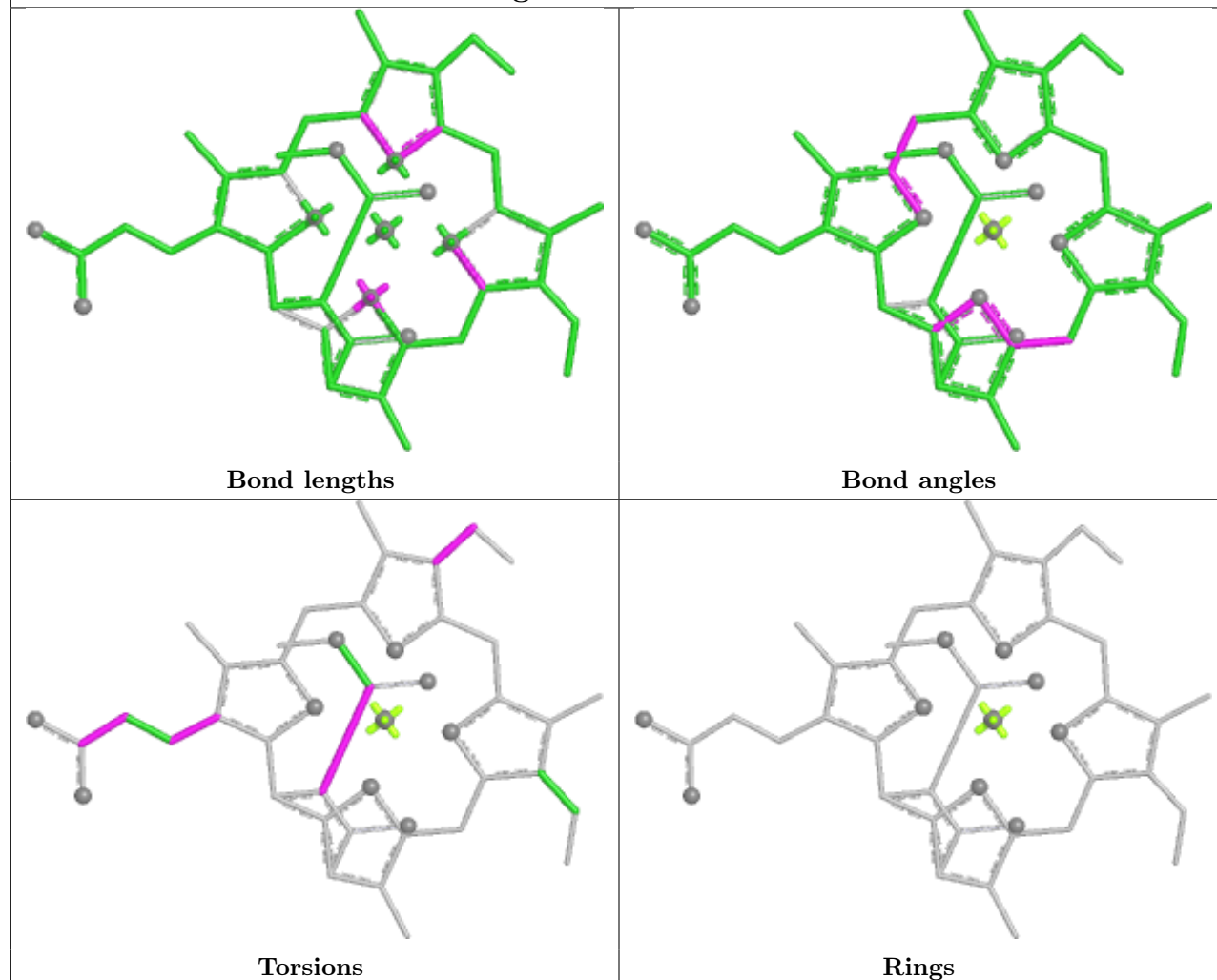




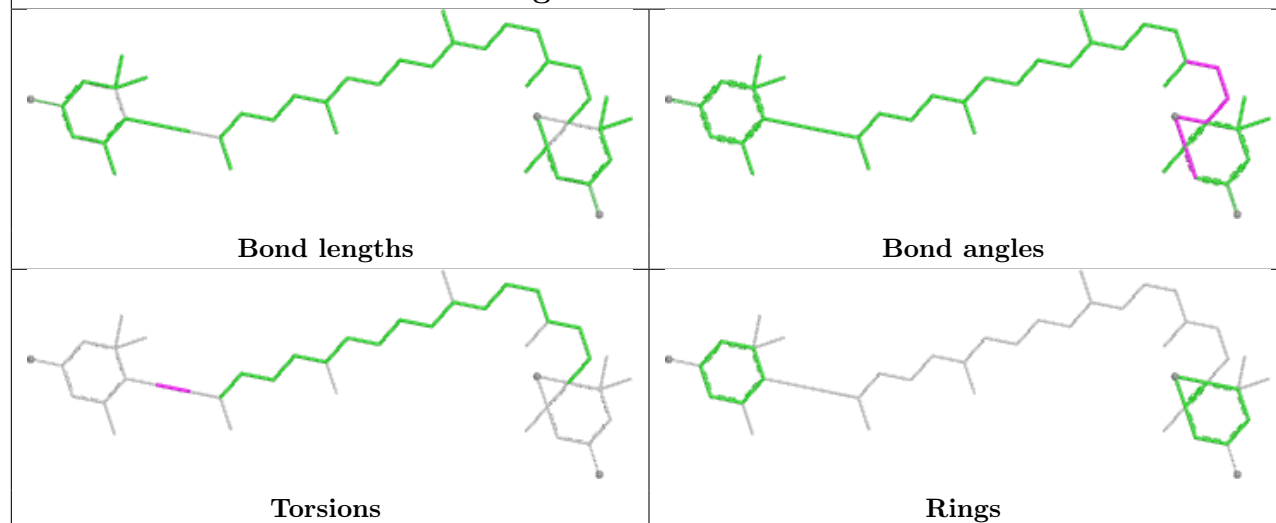
Ligand CLA p 306

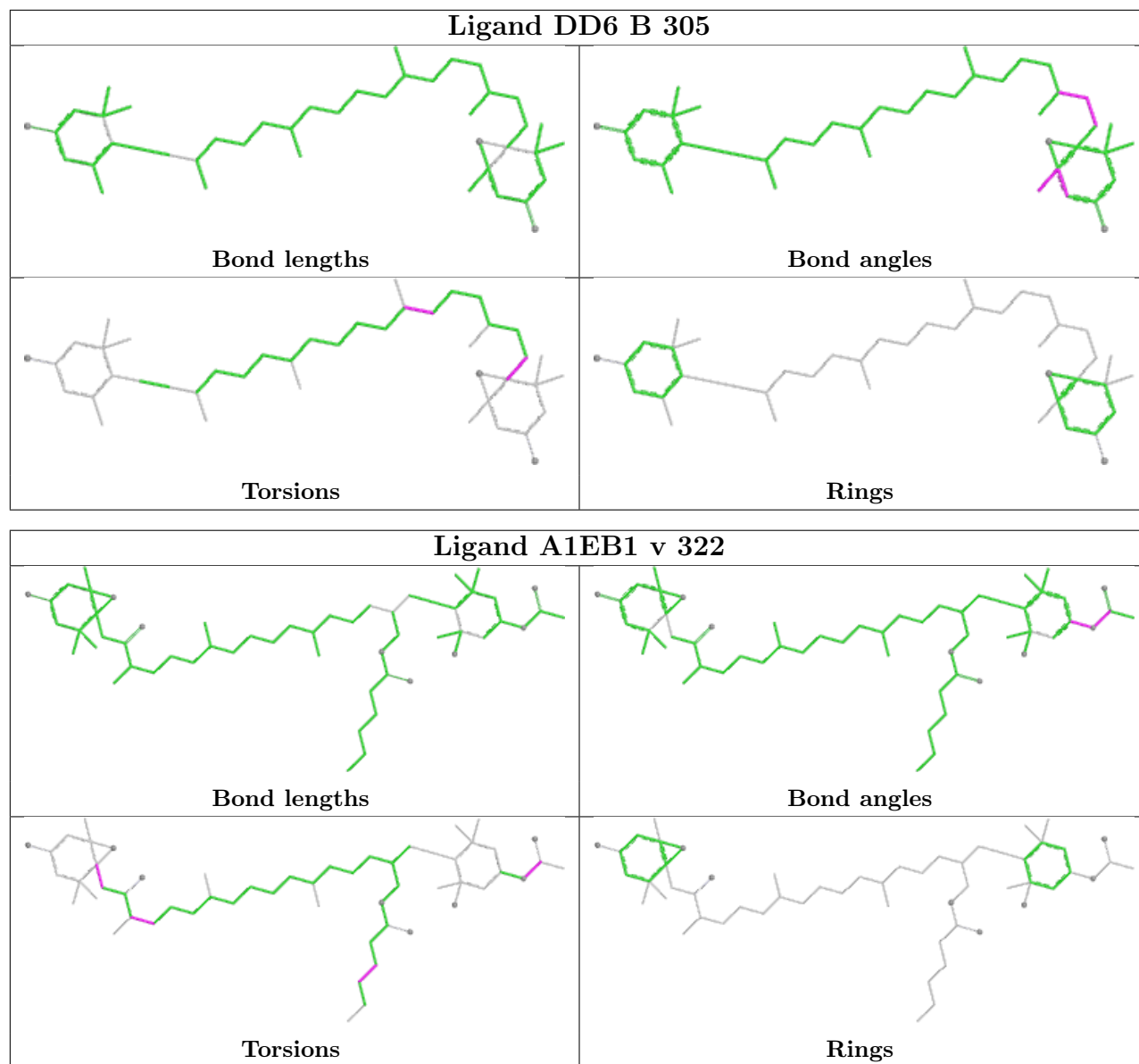


Ligand KC2 x 304

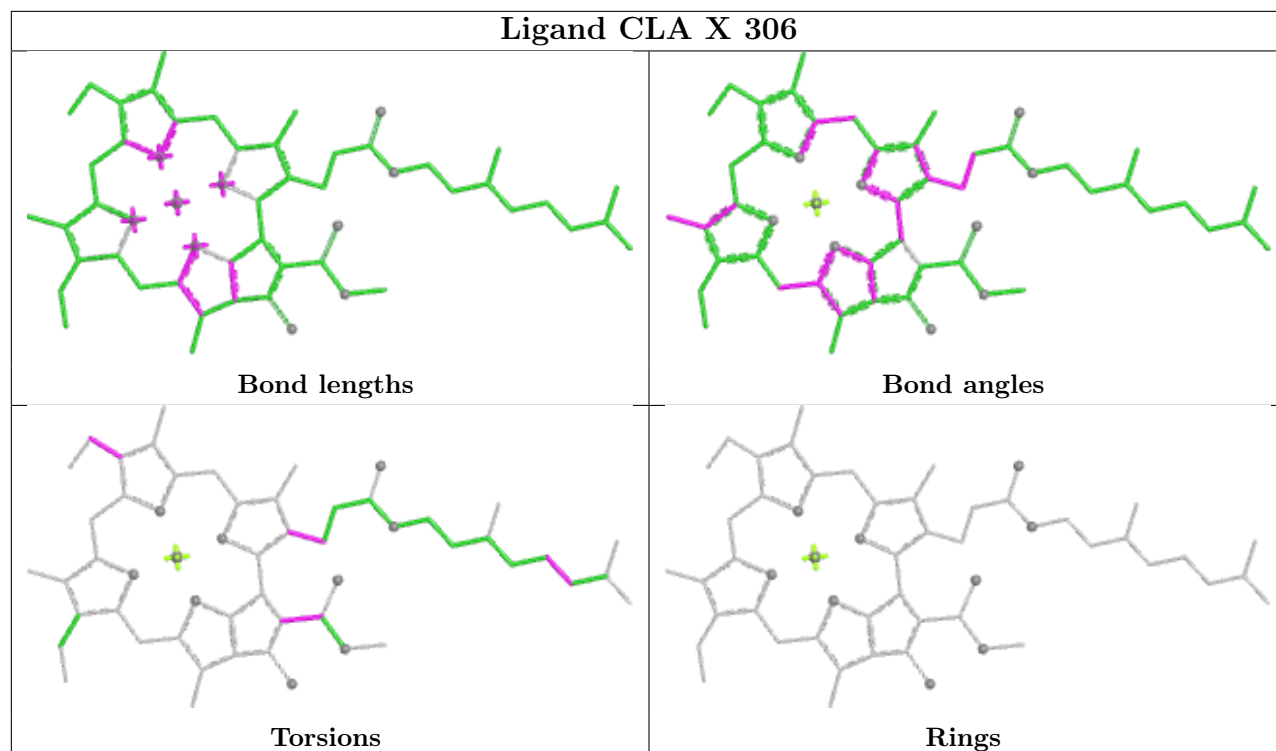


Ligand DD6 C 310

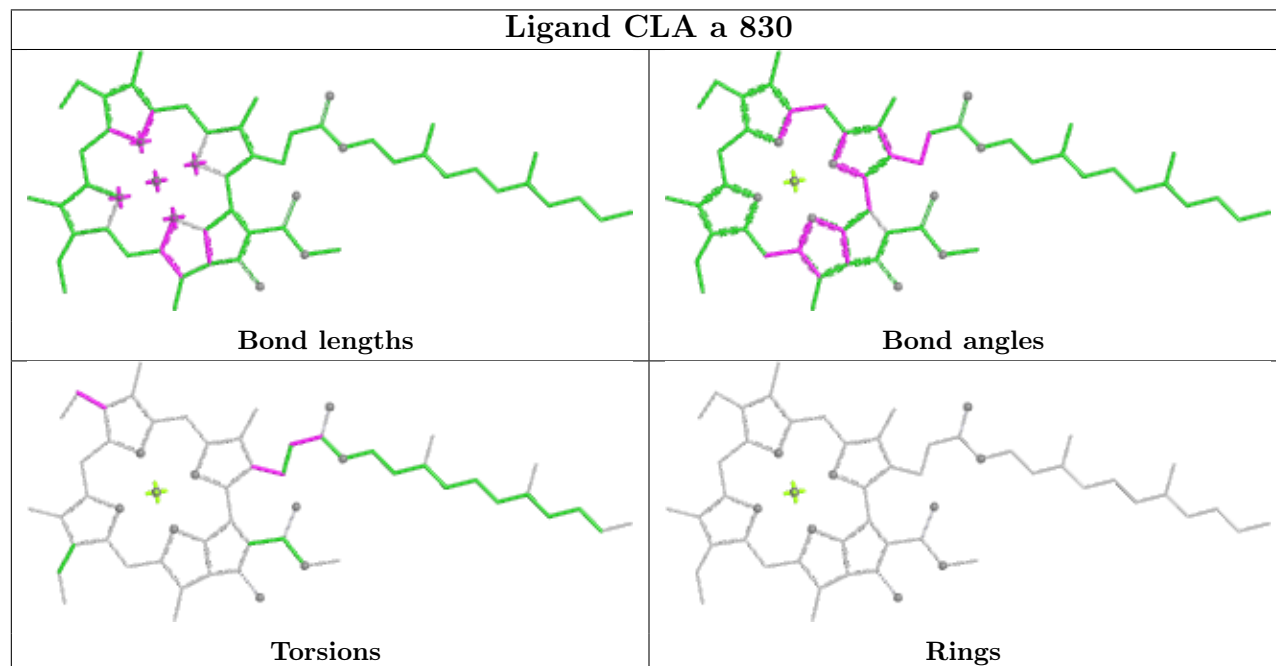


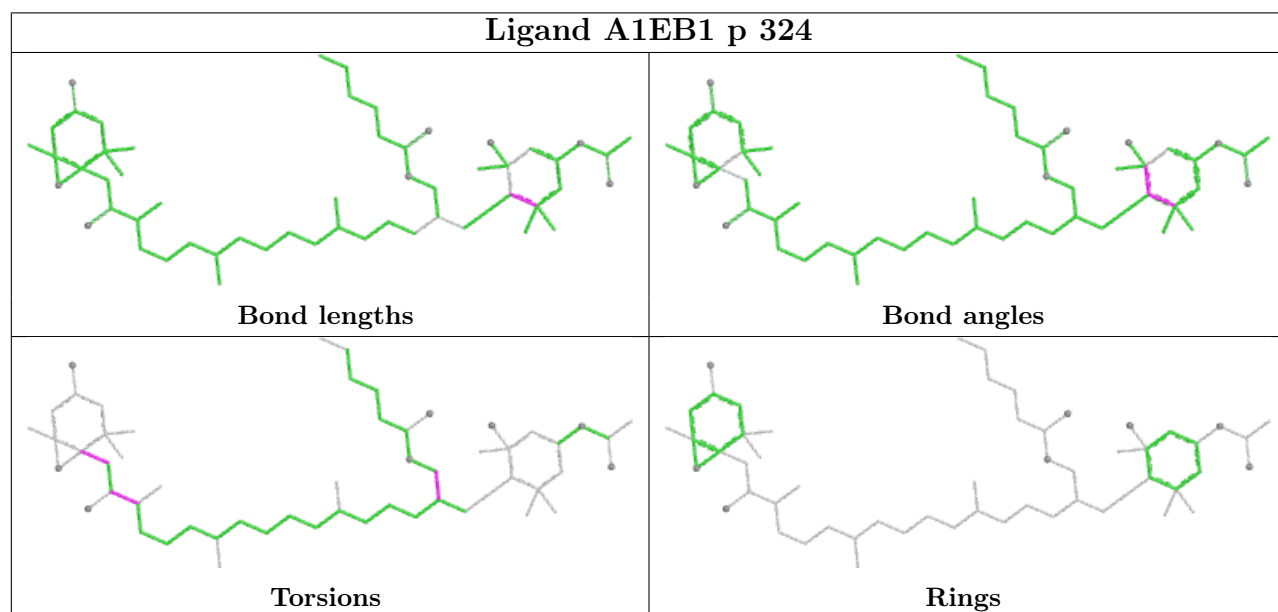
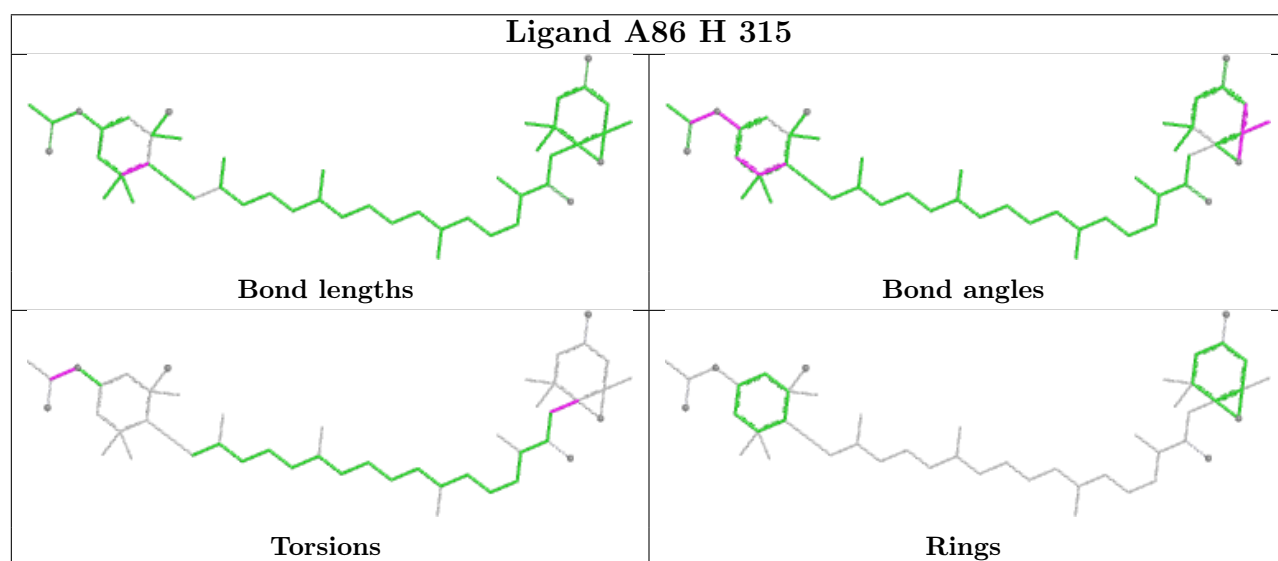
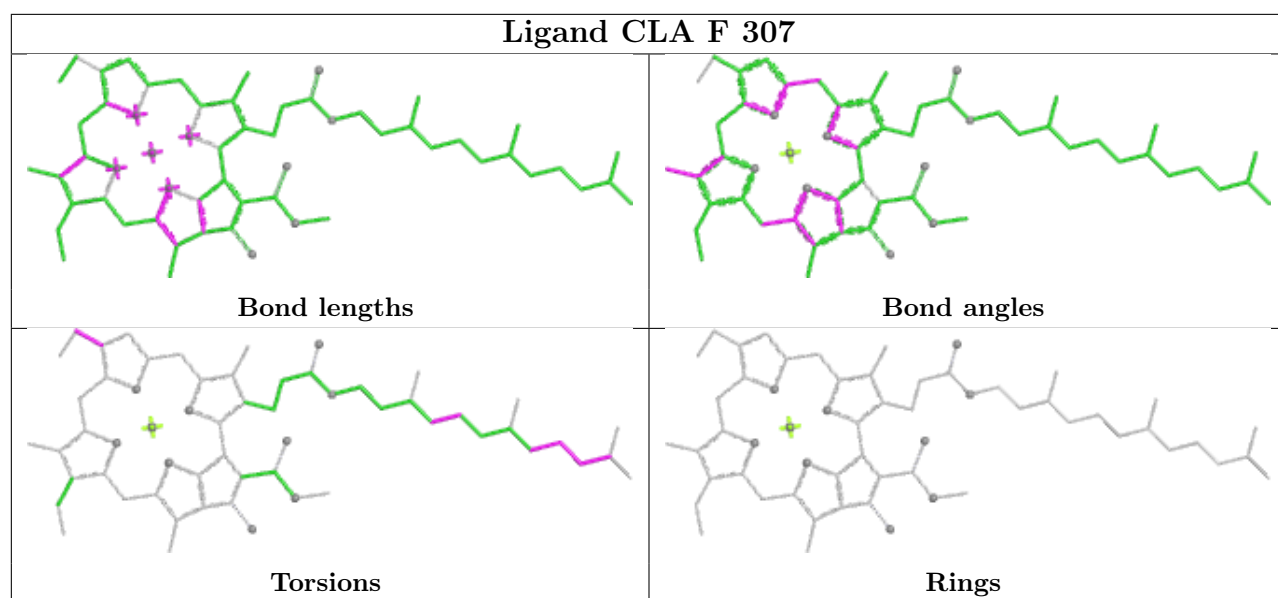


Ligand CLA X 306

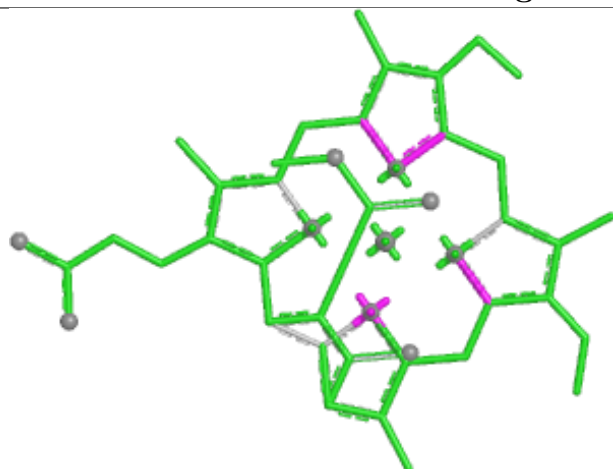


Ligand CLA a 830

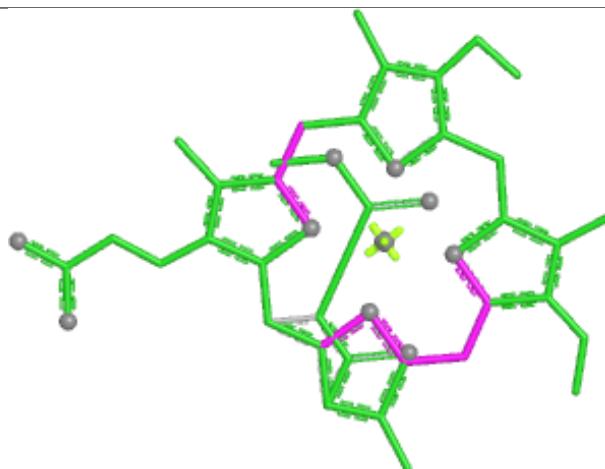




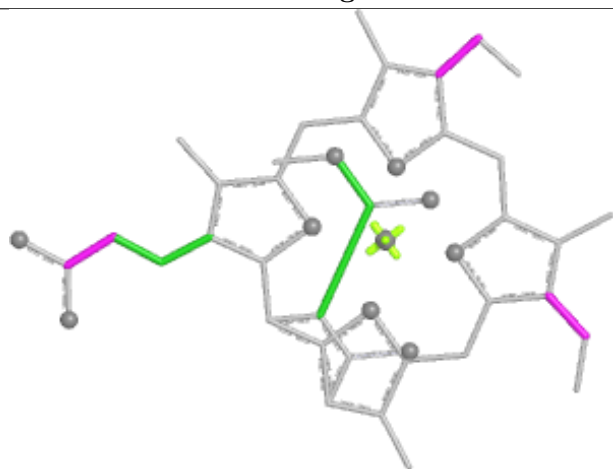
Ligand KC2 A 310



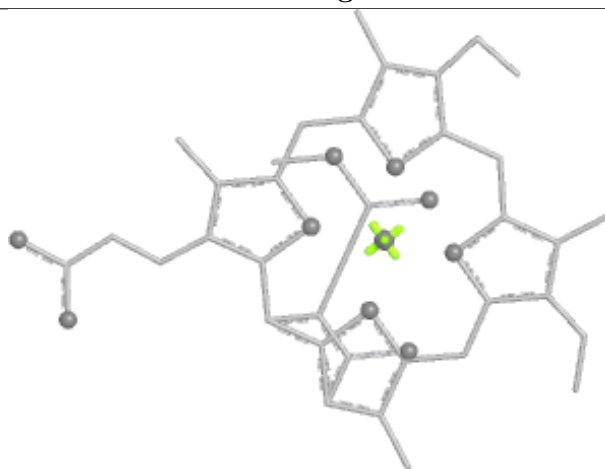
Bond lengths



Bond angles

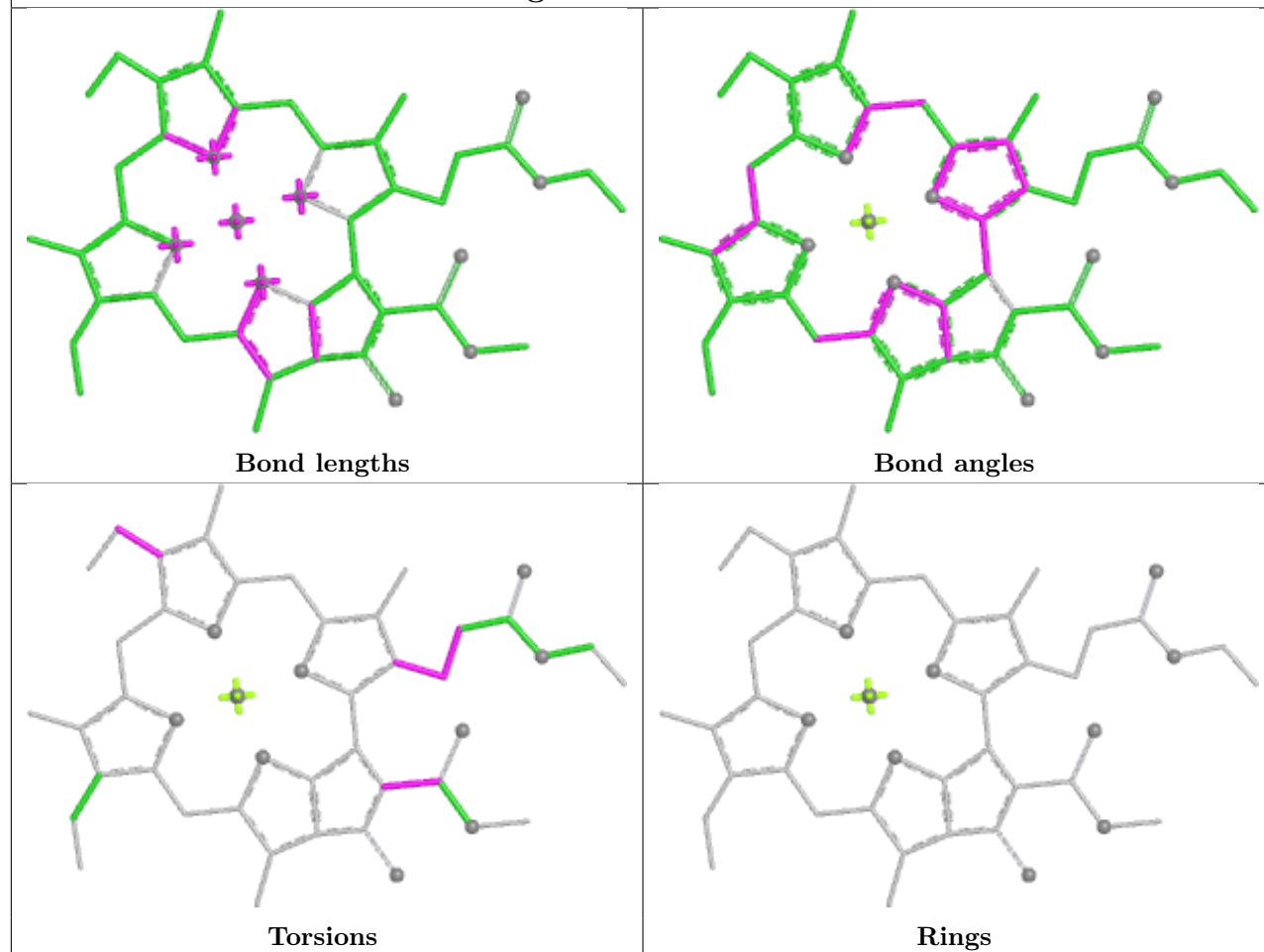


Torsions

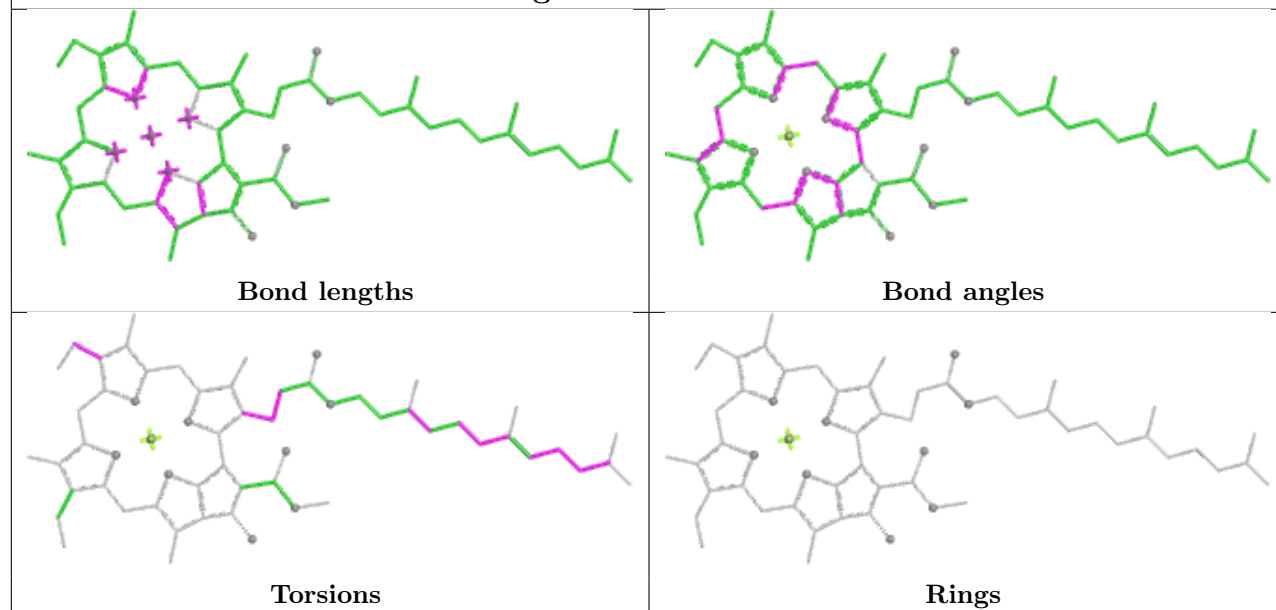


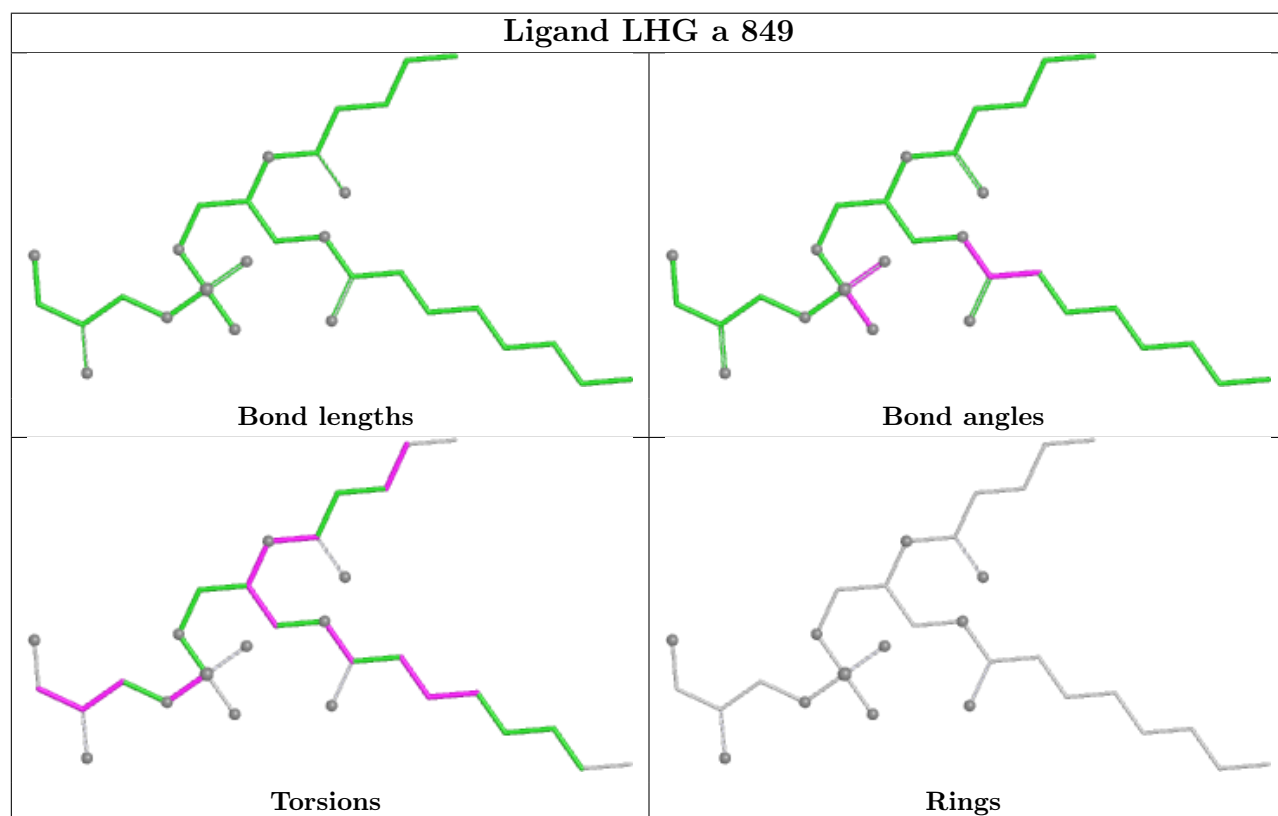
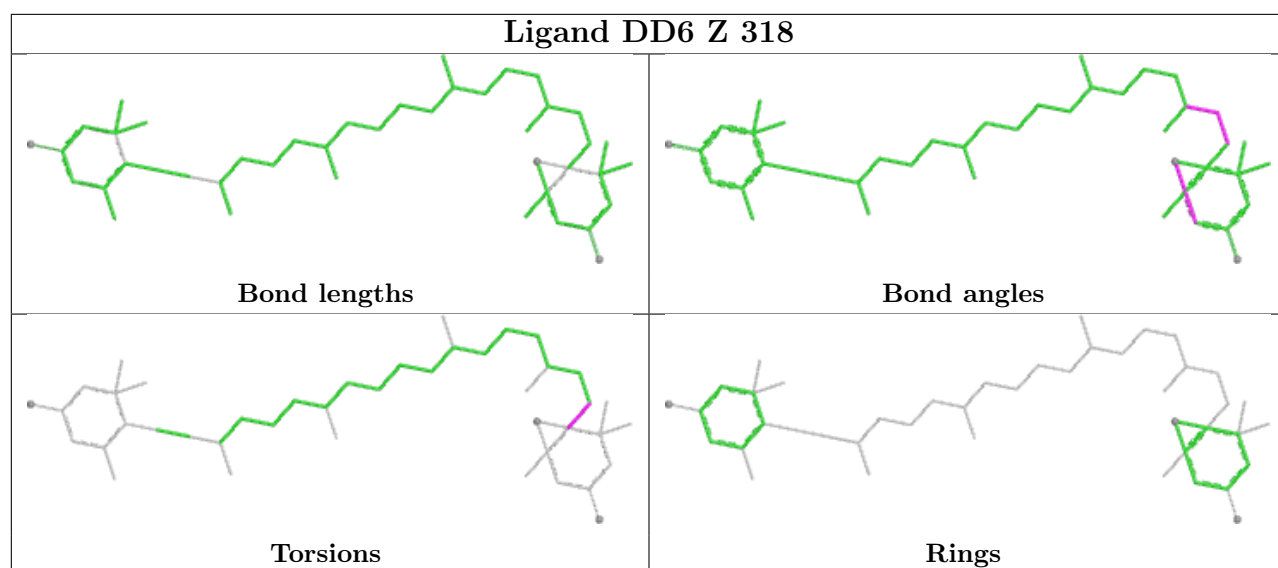
Rings

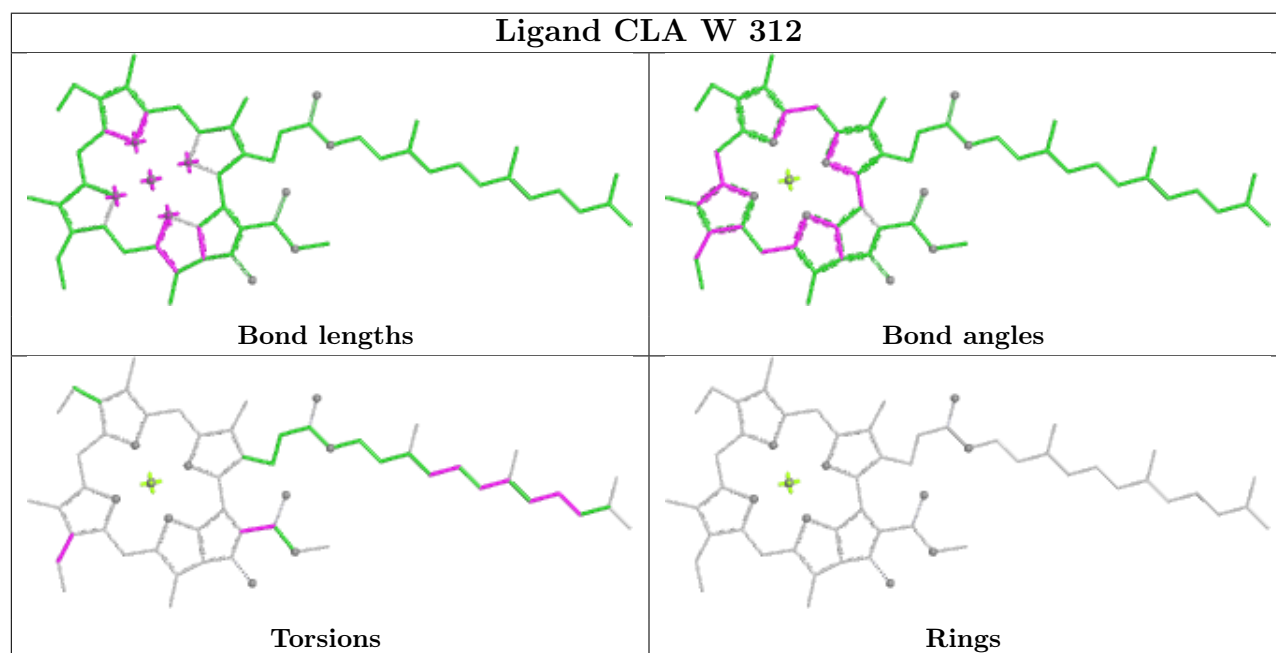
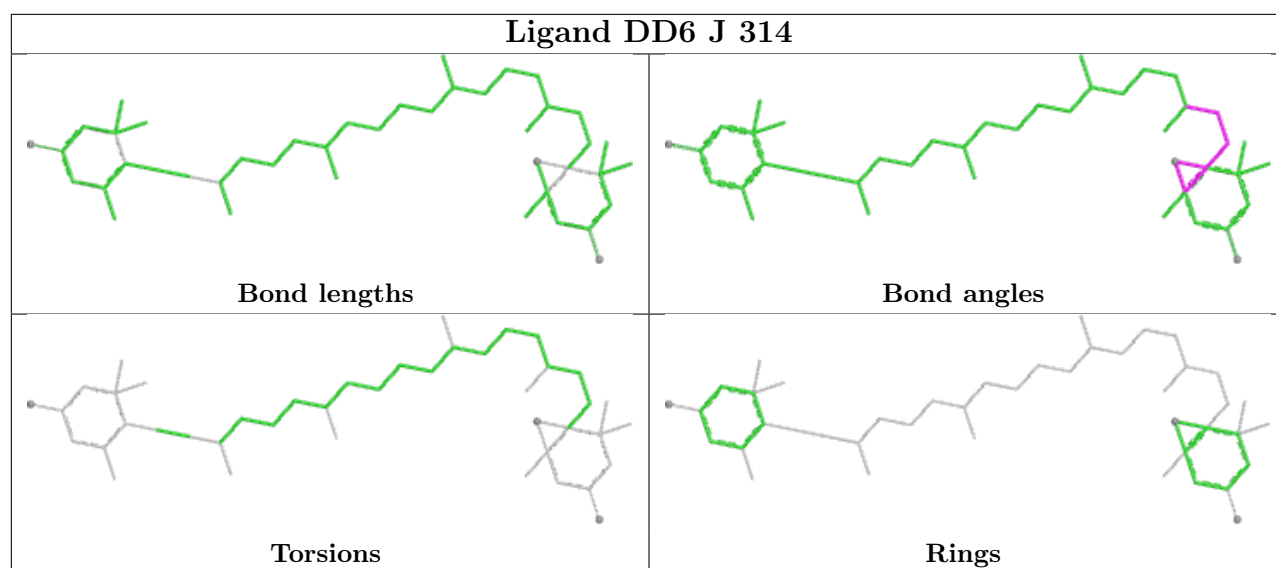
Ligand CLA B 307

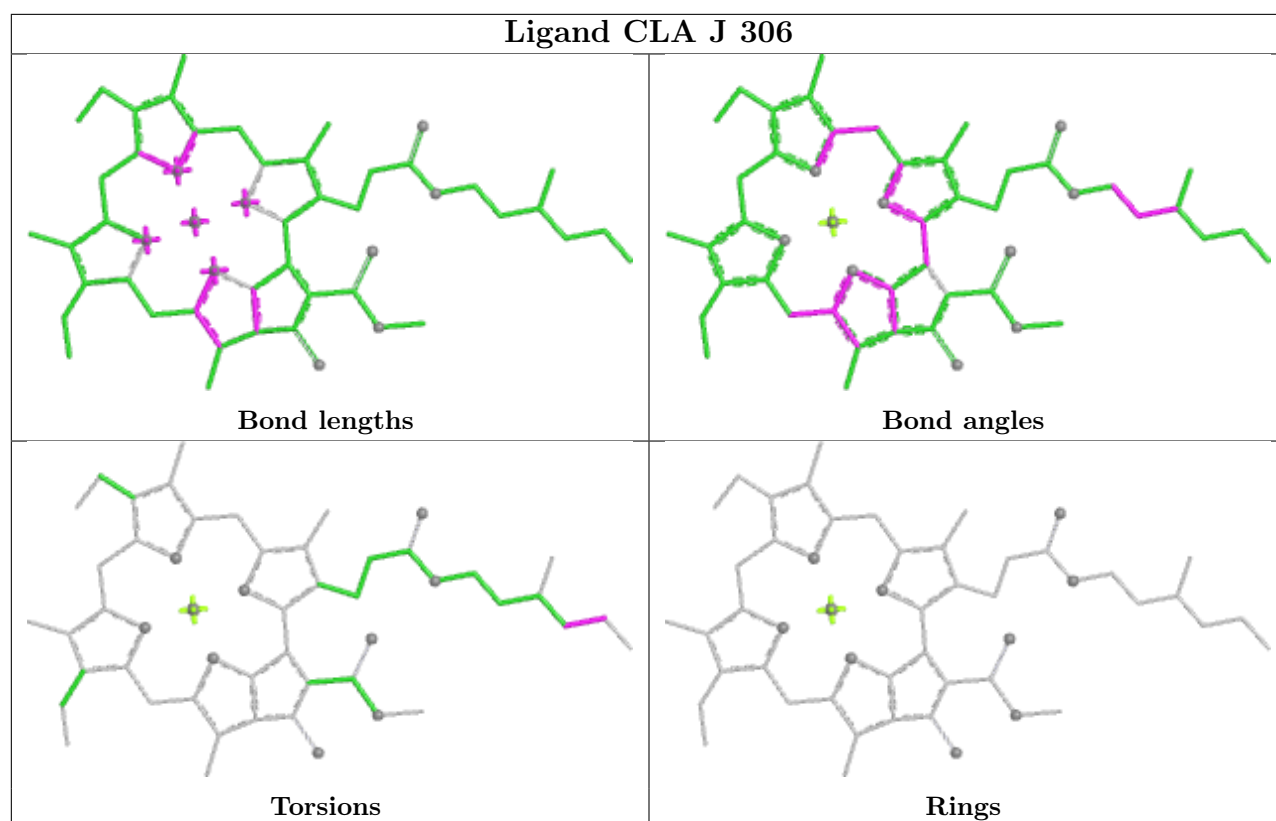


Ligand CLA P 312

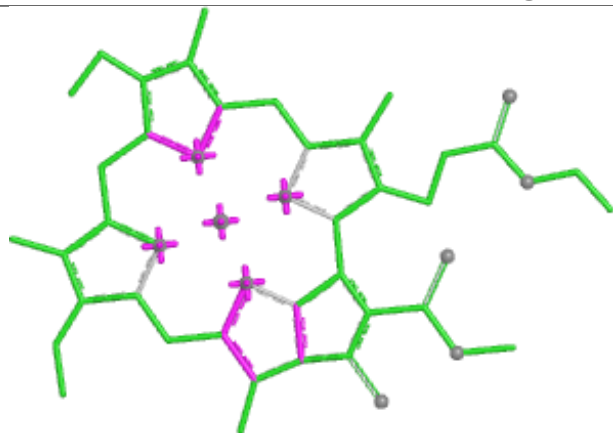




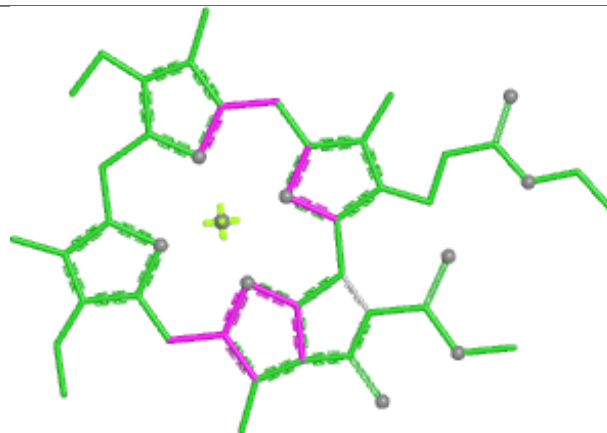




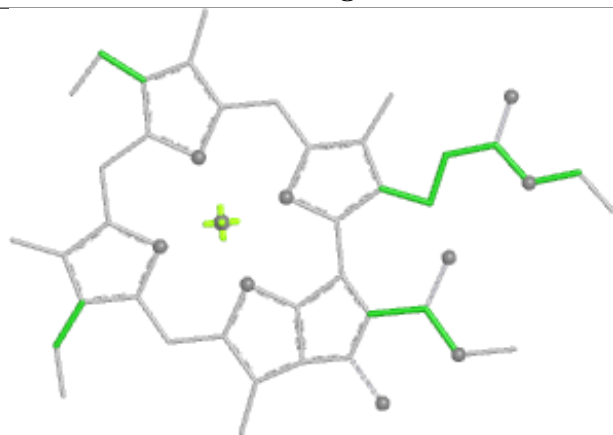
Ligand CLA t 302



Bond lengths



Bond angles

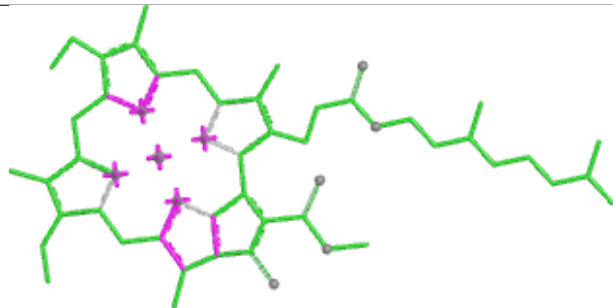


Torsions

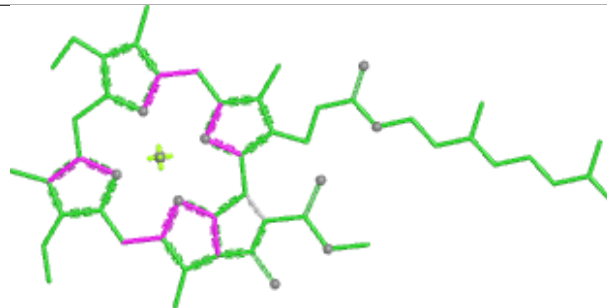


Rings

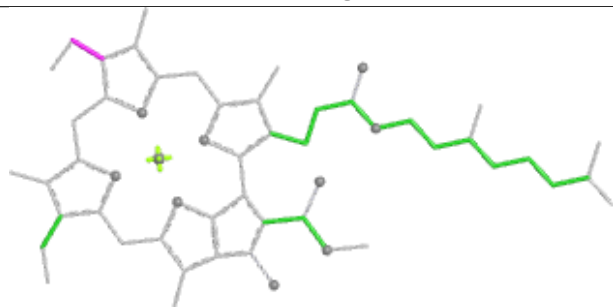
Ligand CLA p 313



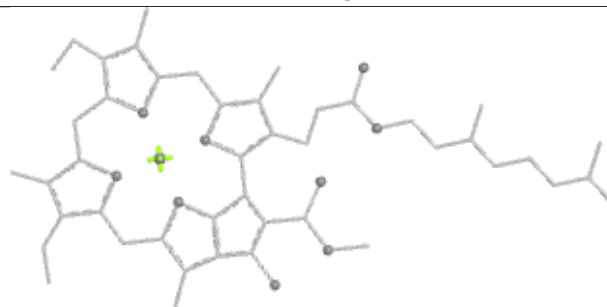
Bond lengths



Bond angles

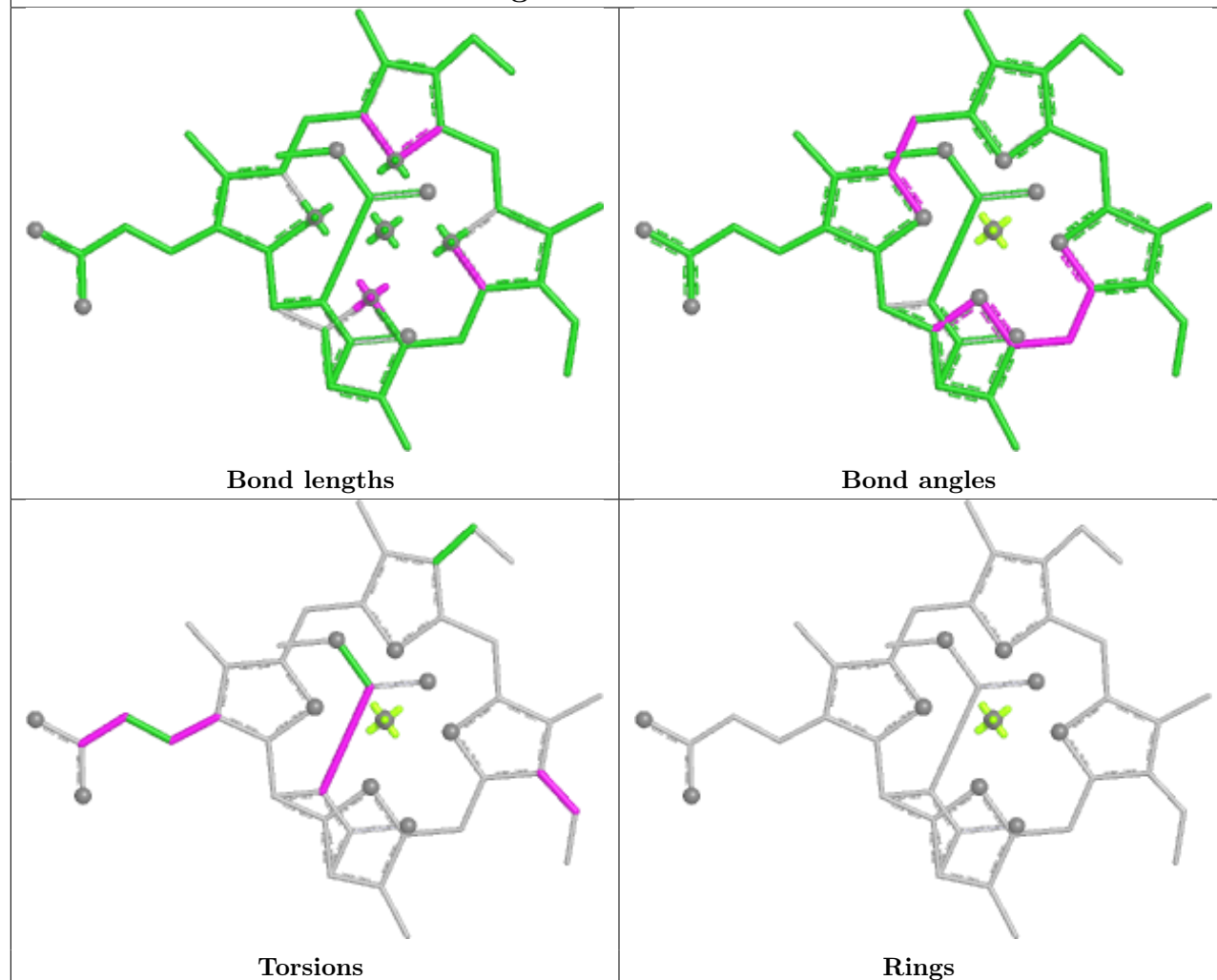


Torsions

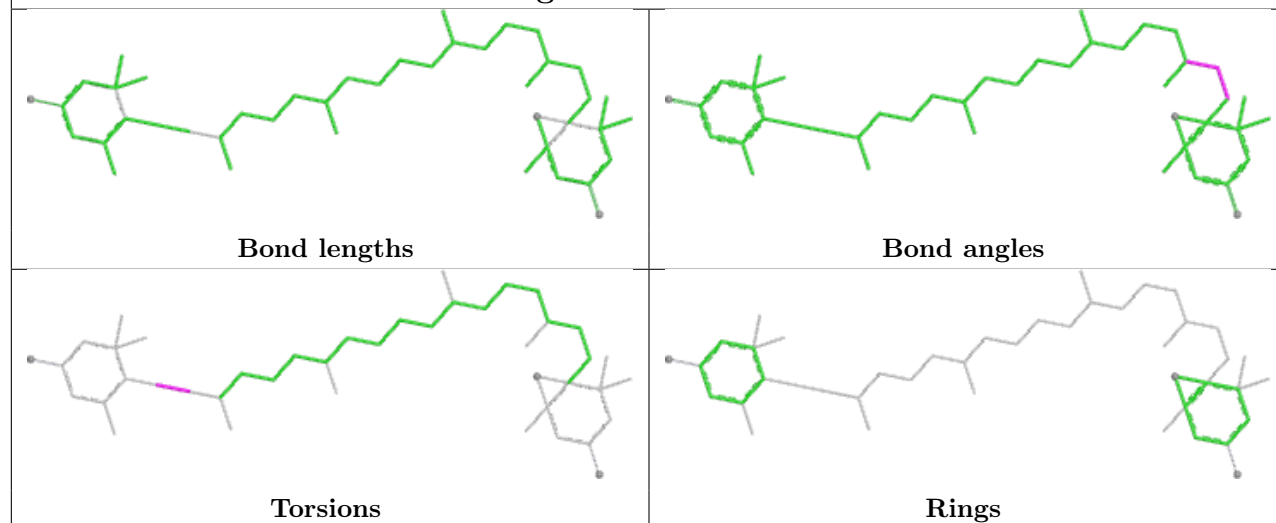


Rings

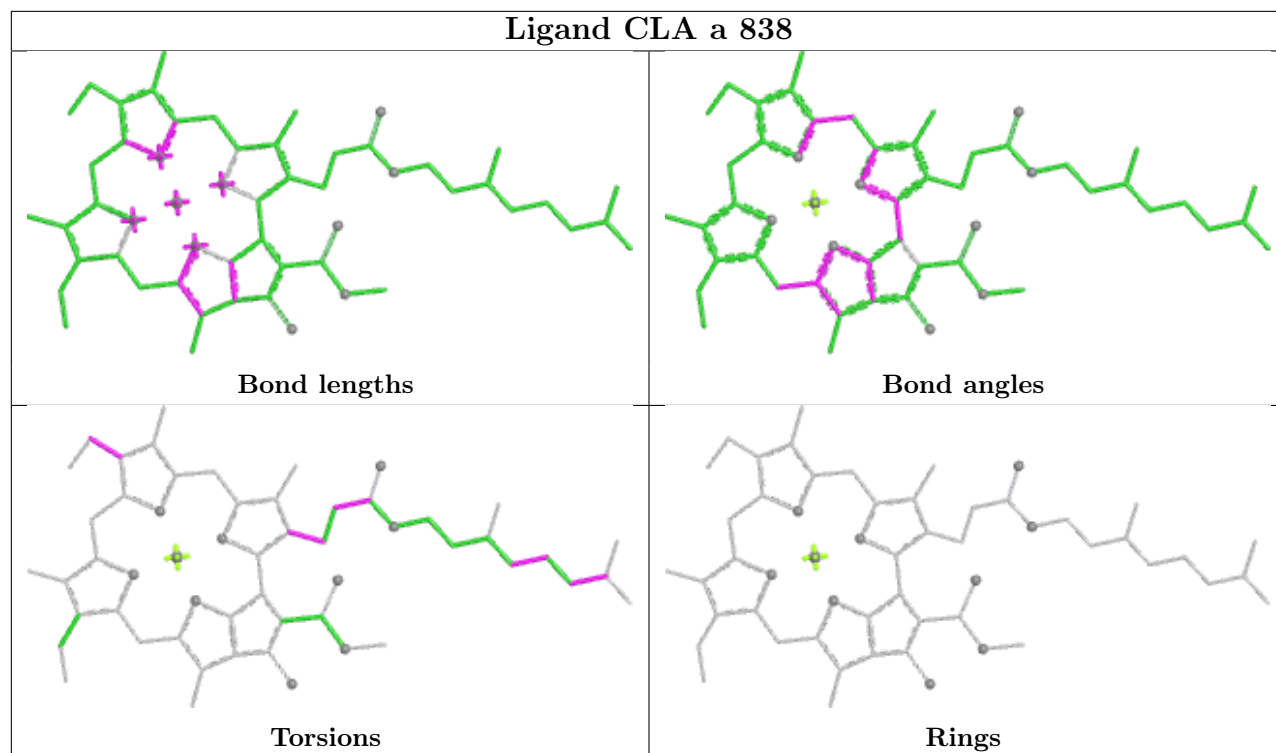
Ligand KC2 Z 302



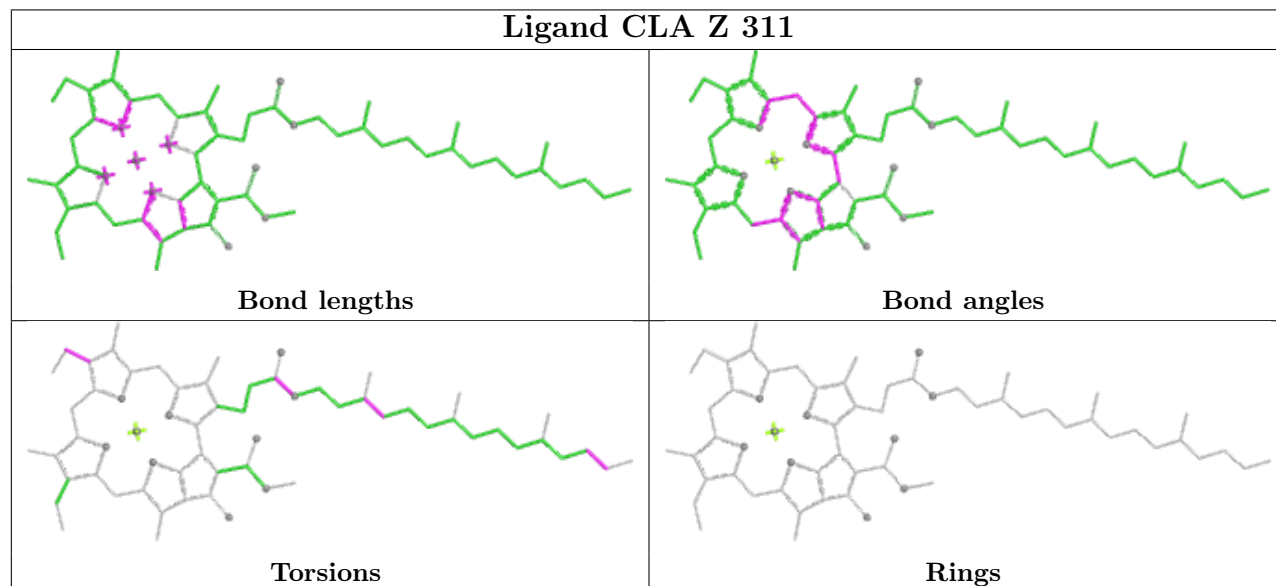
Ligand DD6 J 317

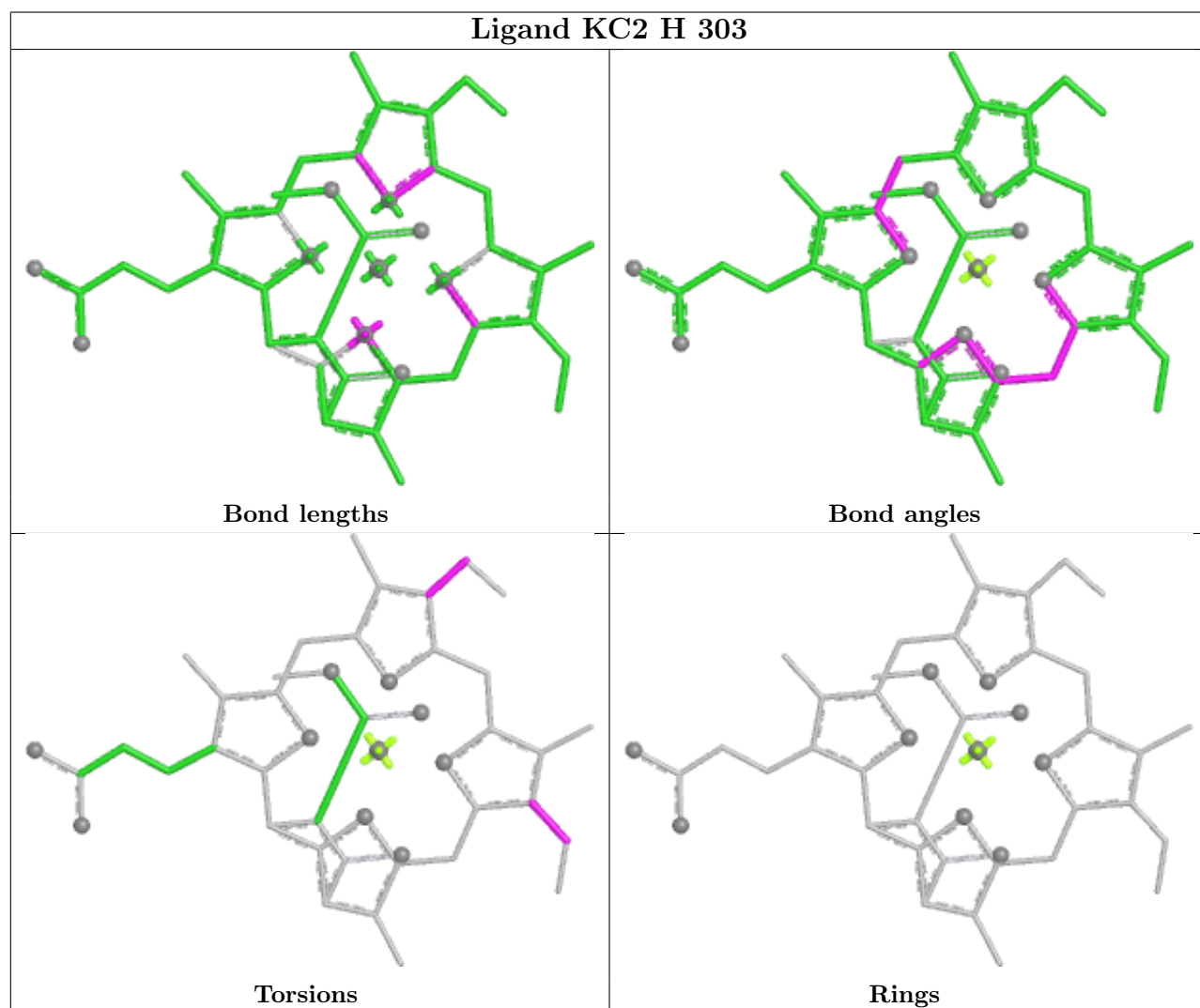
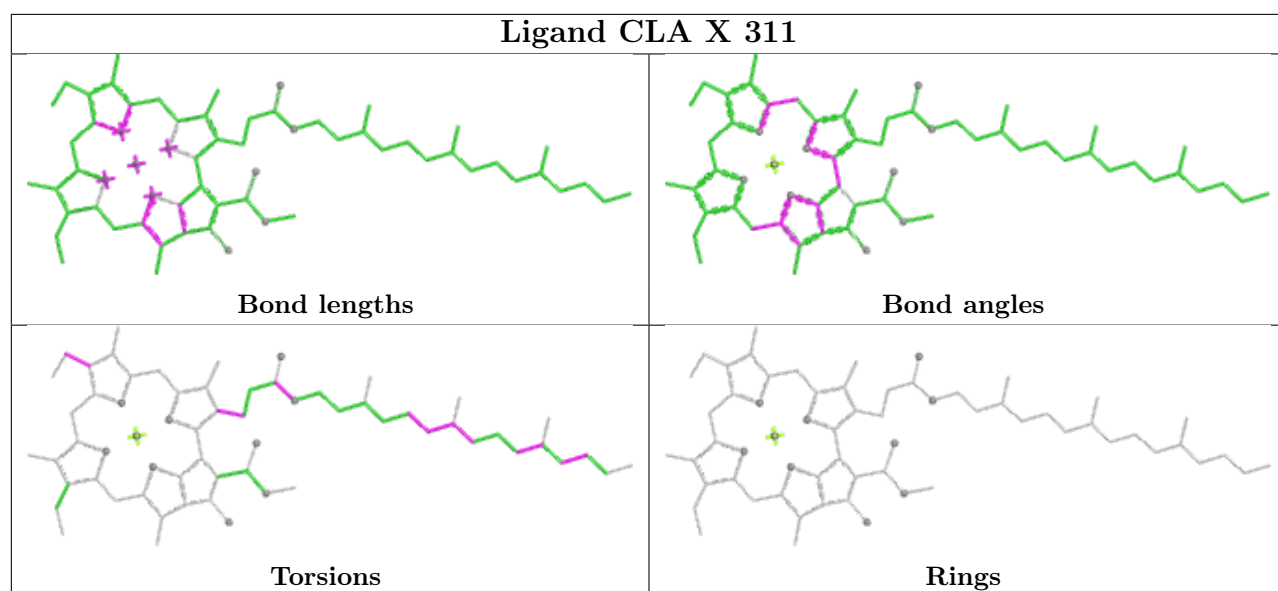


Ligand CLA a 838

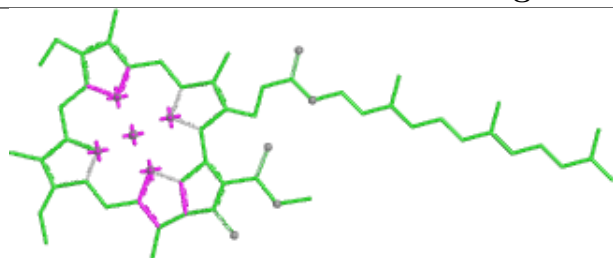


Ligand CLA Z 311

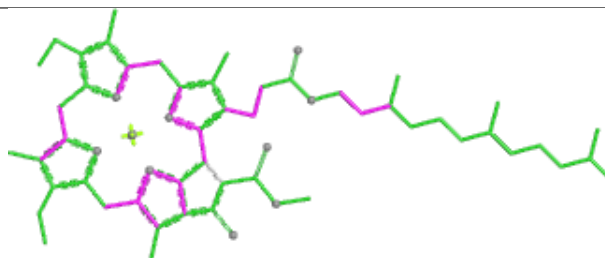




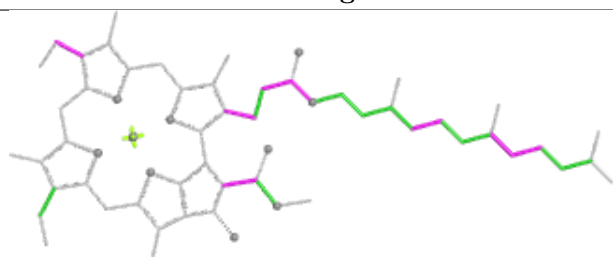
Ligand CLA H 305



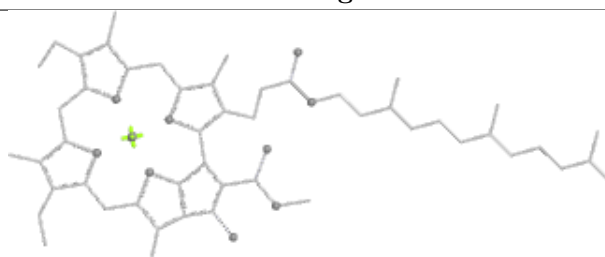
Bond lengths



Bond angles

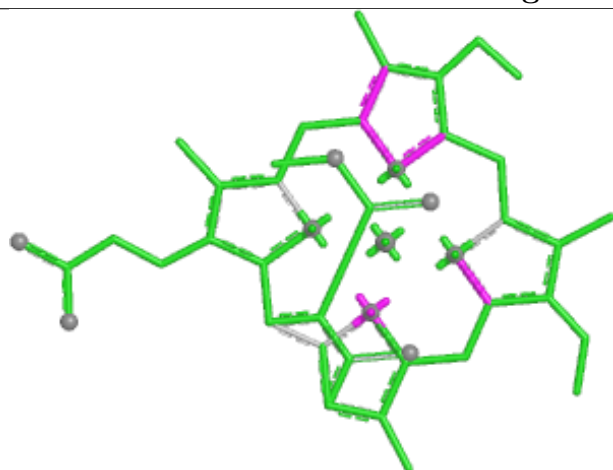


Torsions

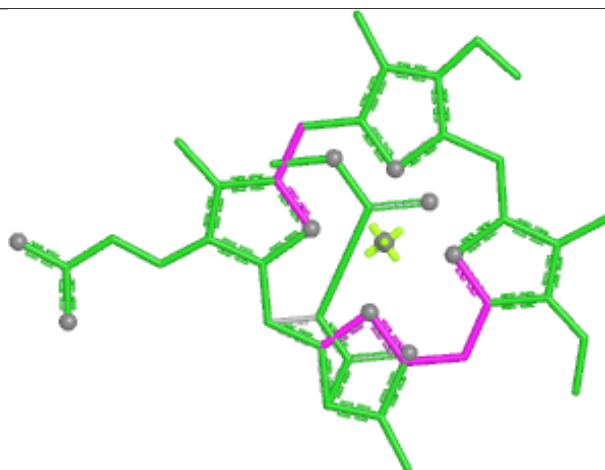


Rings

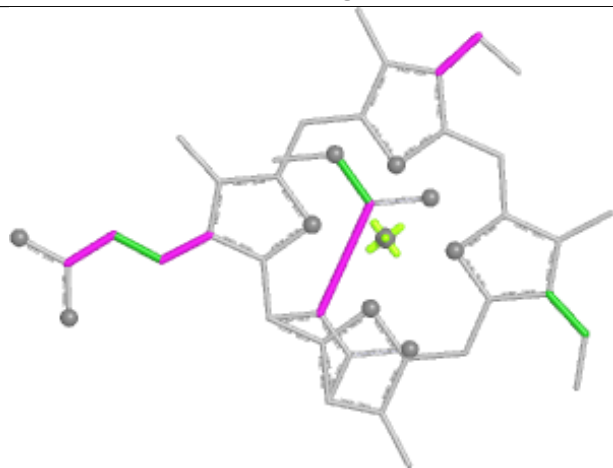
Ligand KC2 t 301



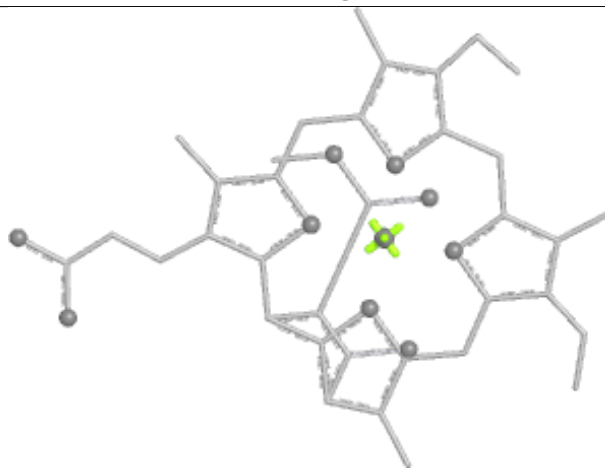
Bond lengths



Bond angles

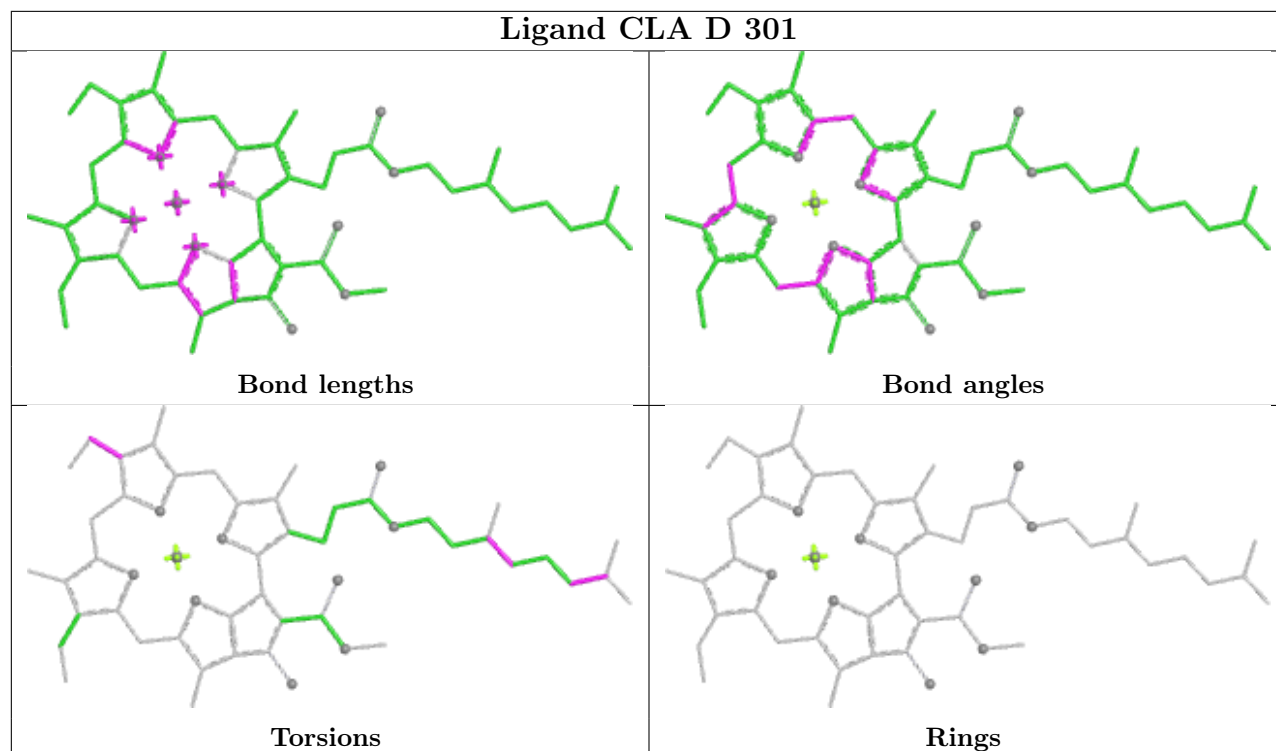


Torsions

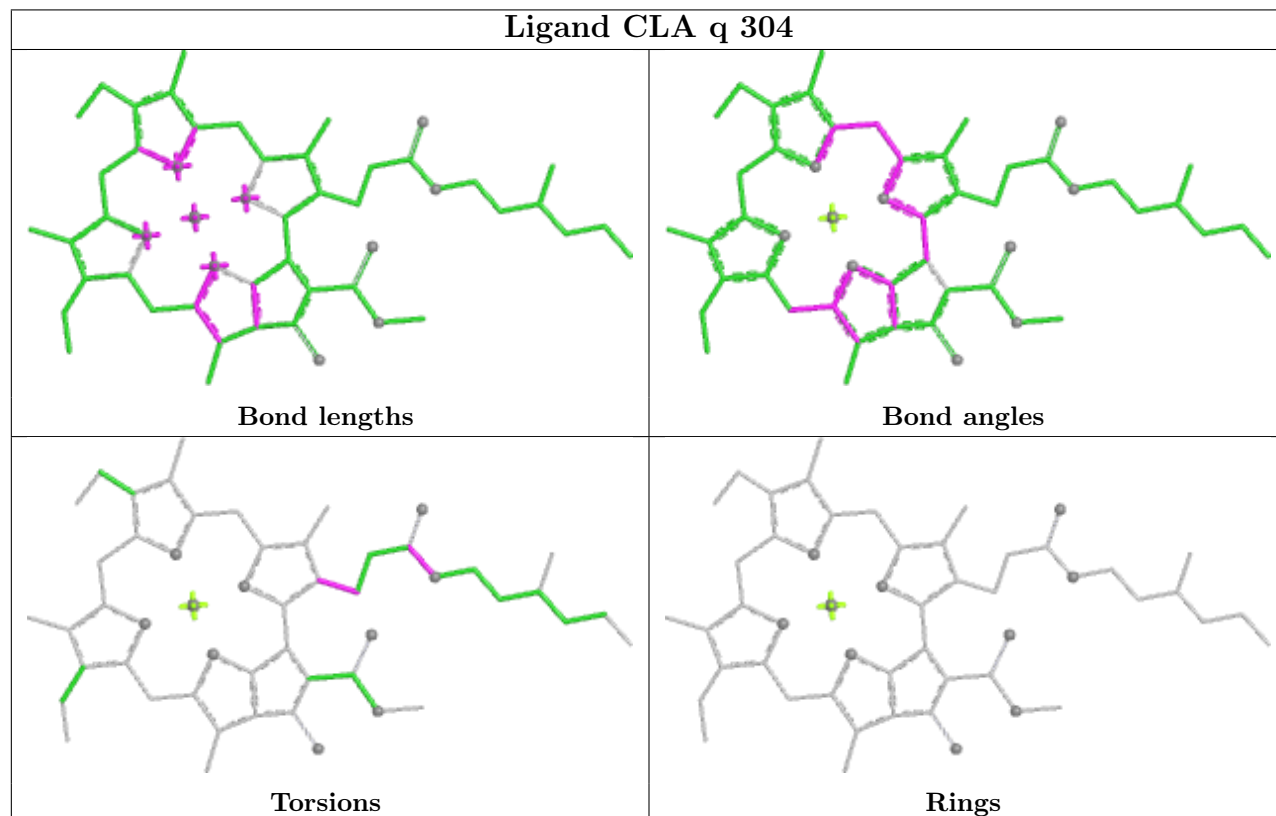


Rings

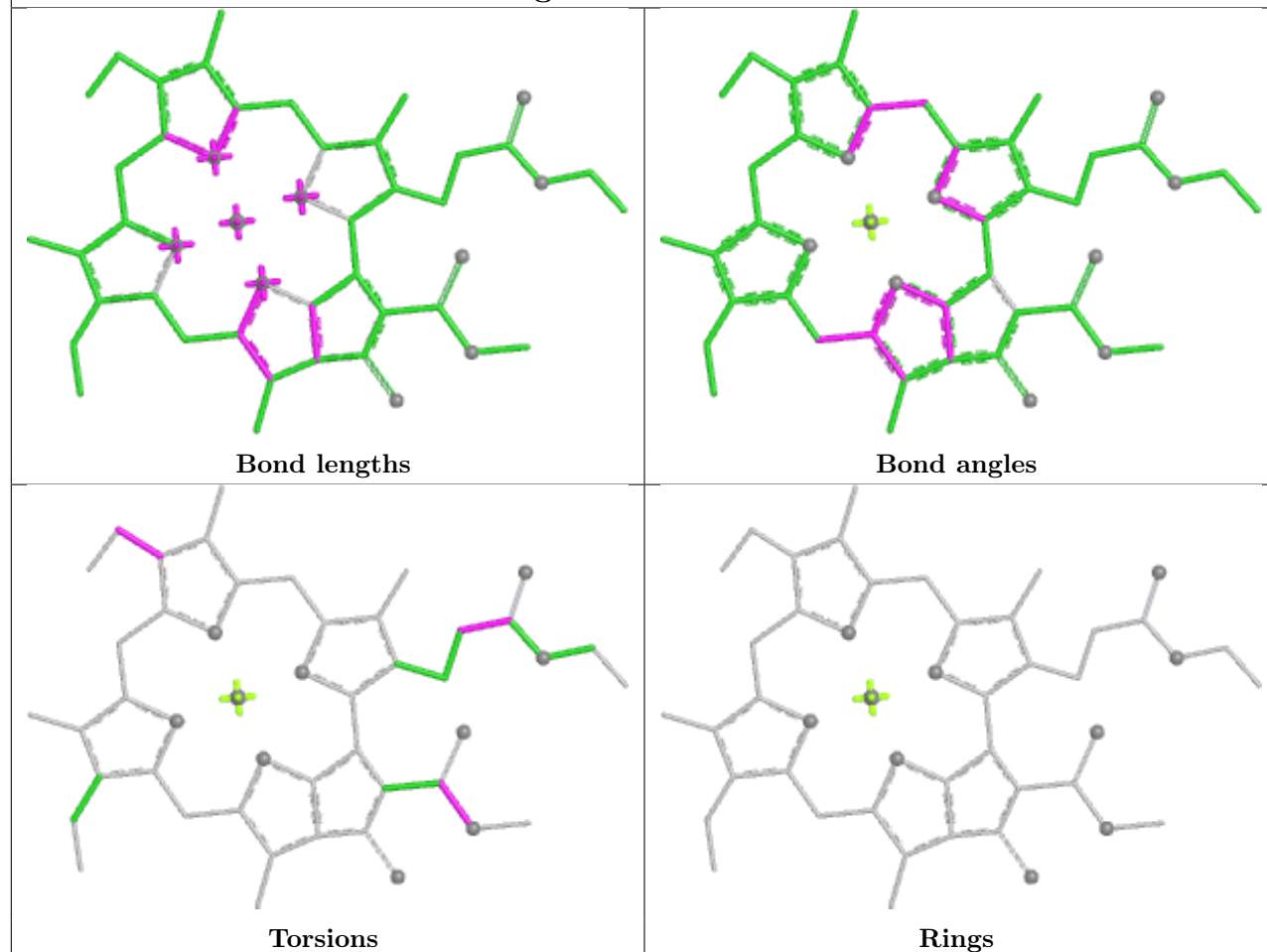
Ligand CLA D 301



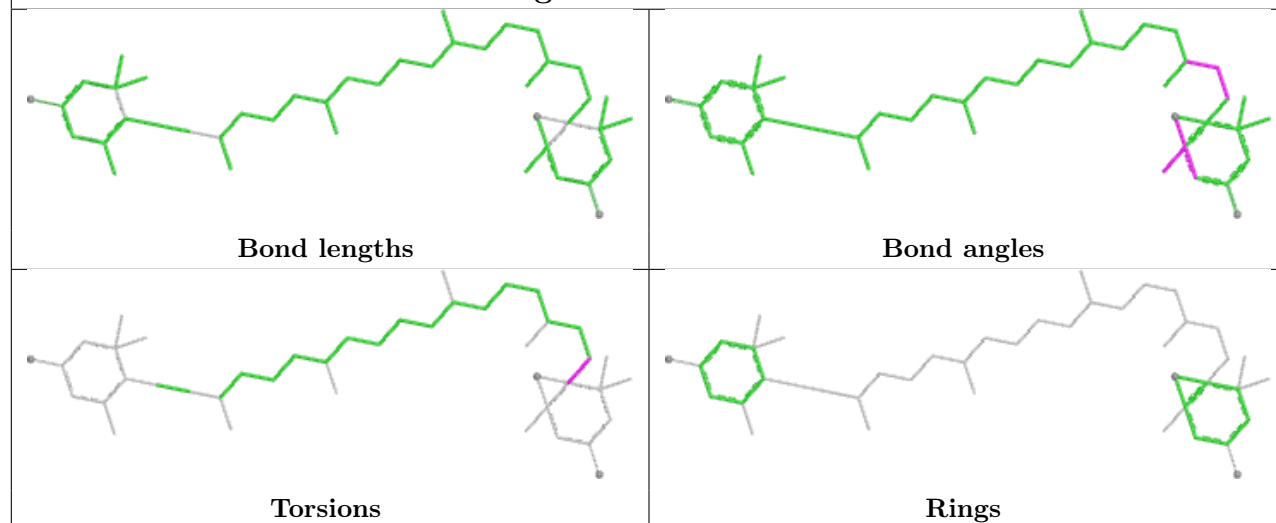
Ligand CLA q 304



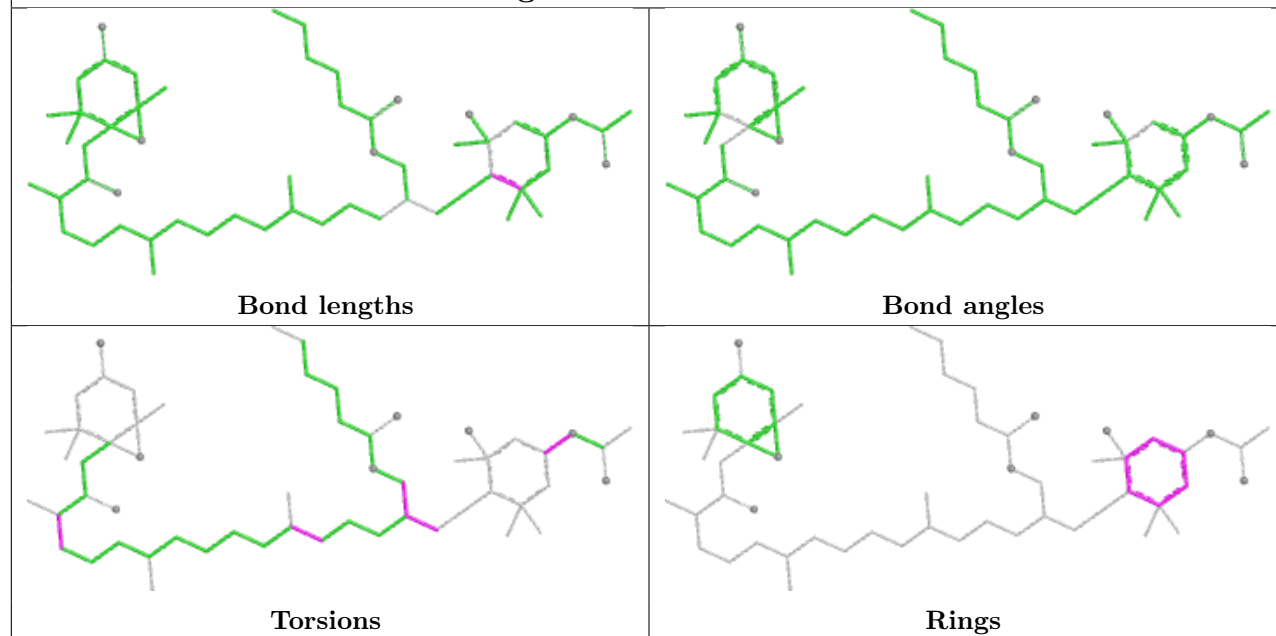
Ligand CLA t 309



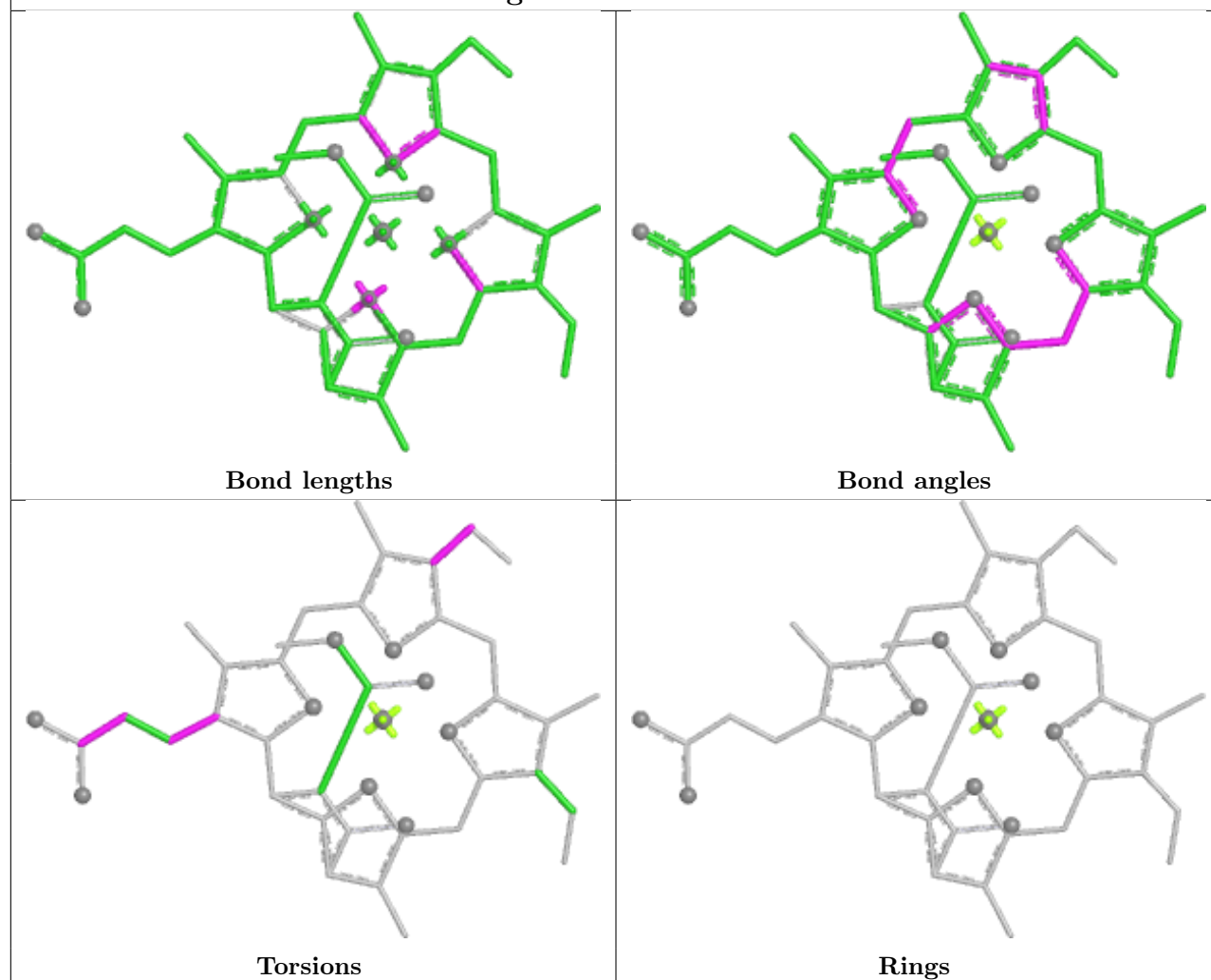
Ligand DD6 F 314



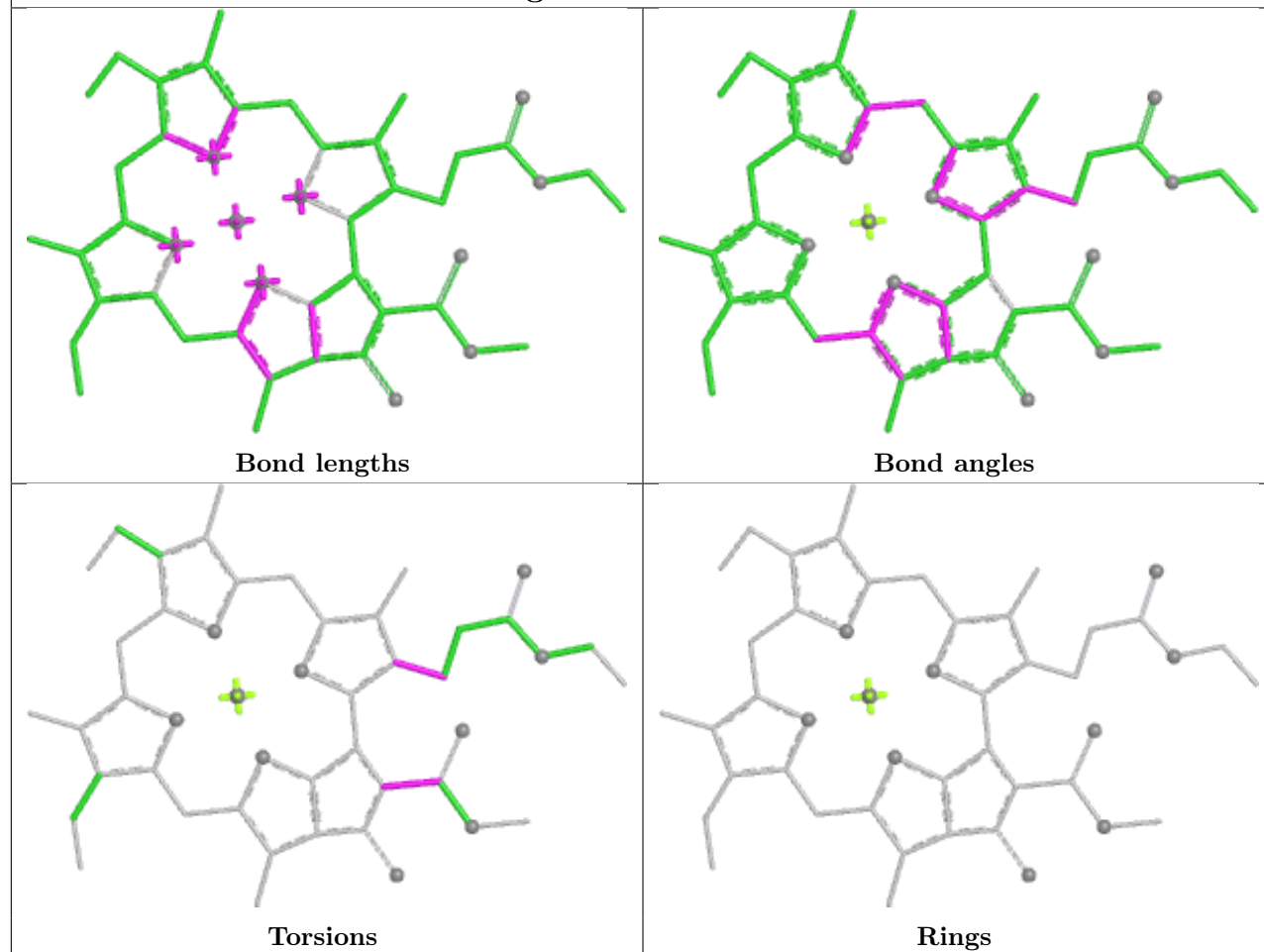
Ligand A1EB1 o 321



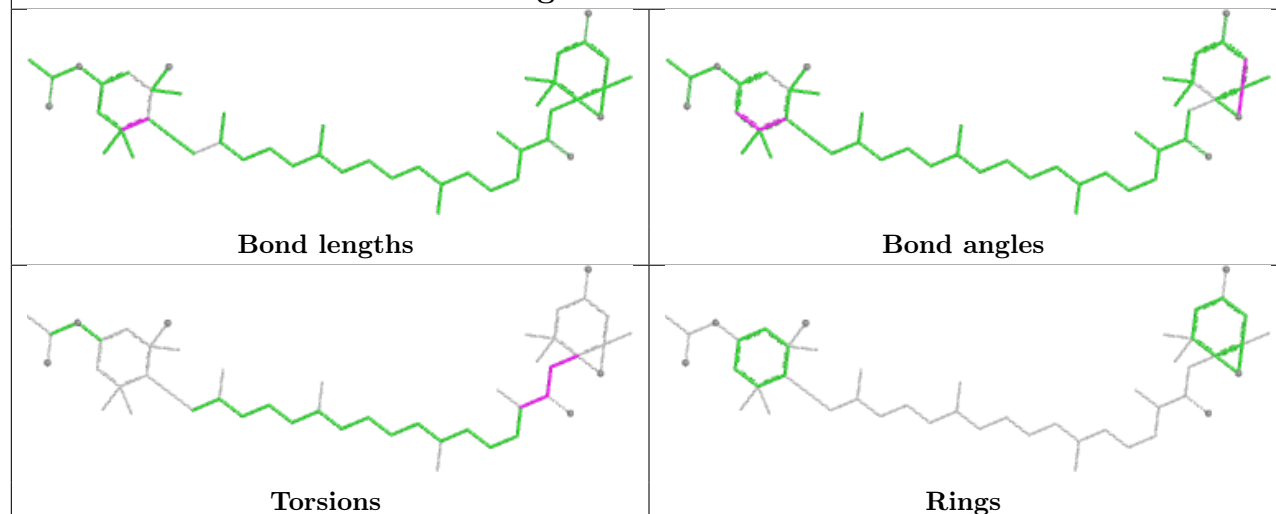
Ligand KC2 O 303

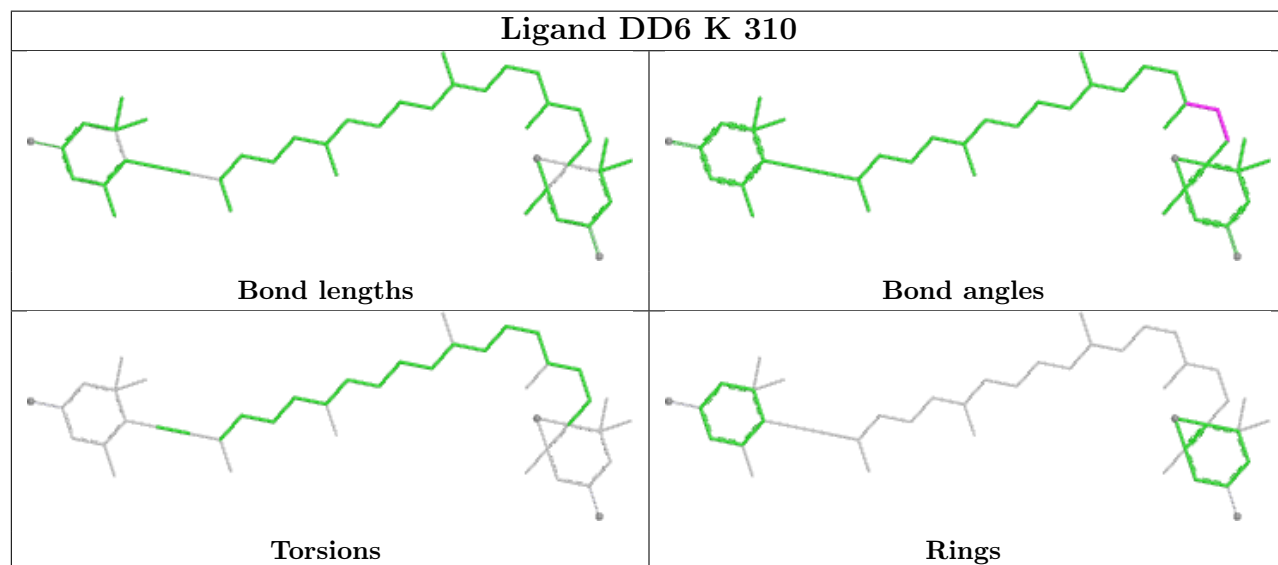
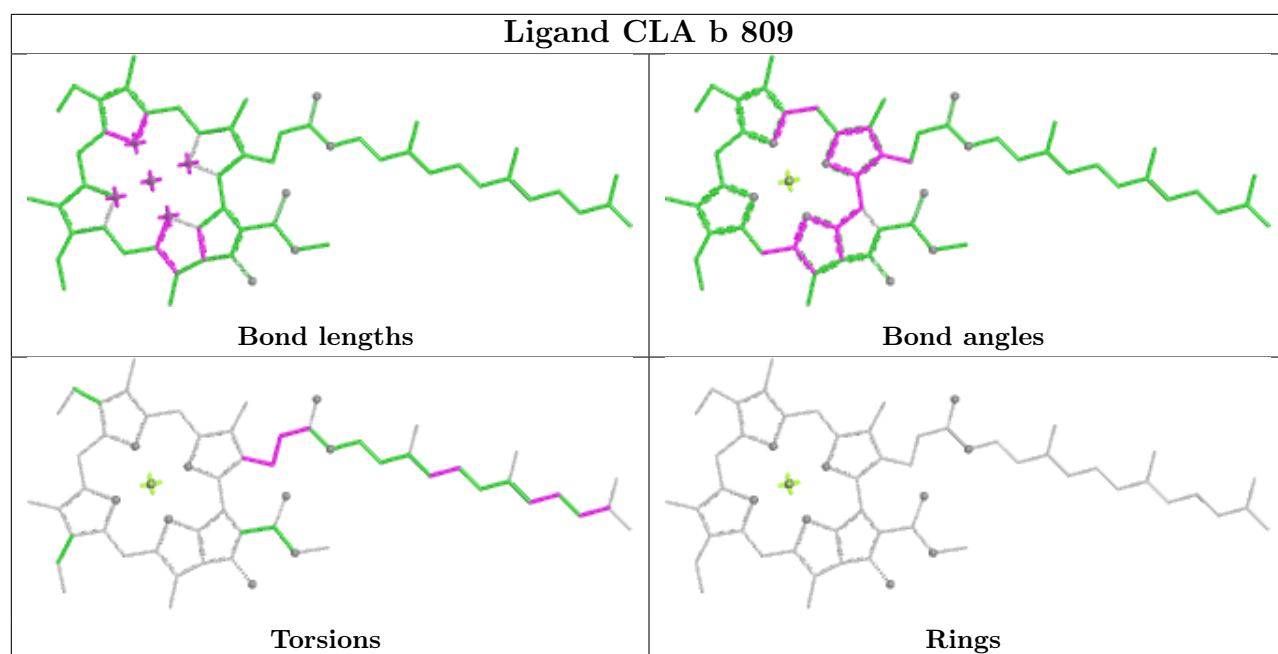


Ligand CLA D 311

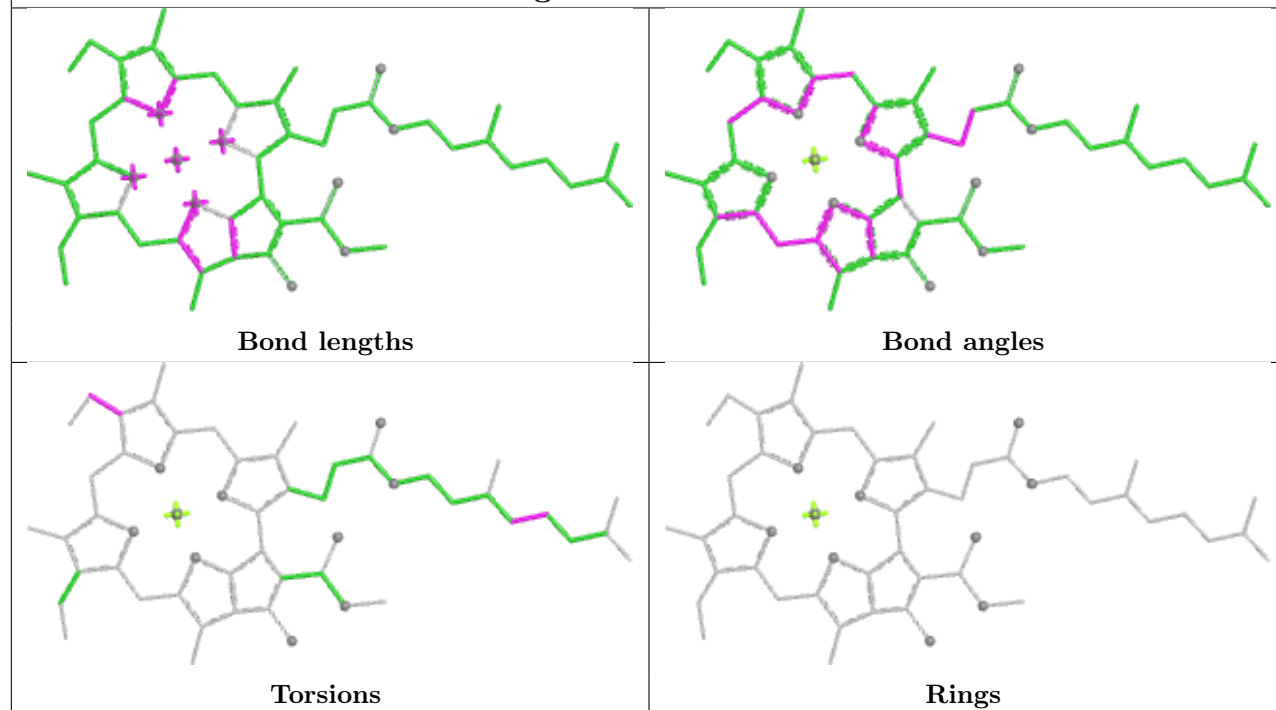


Ligand A86 X 320

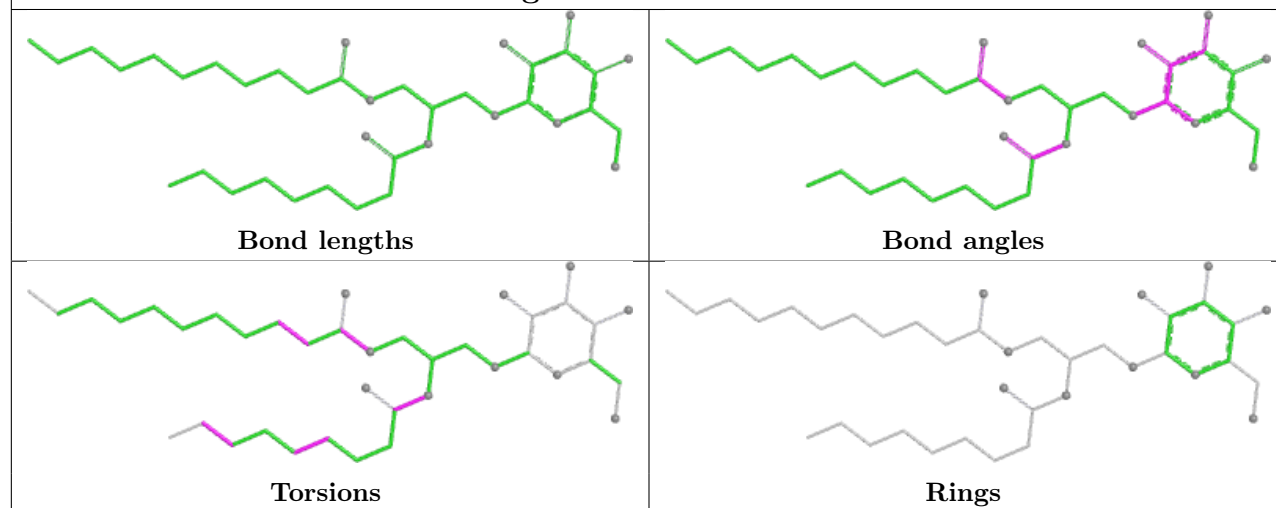




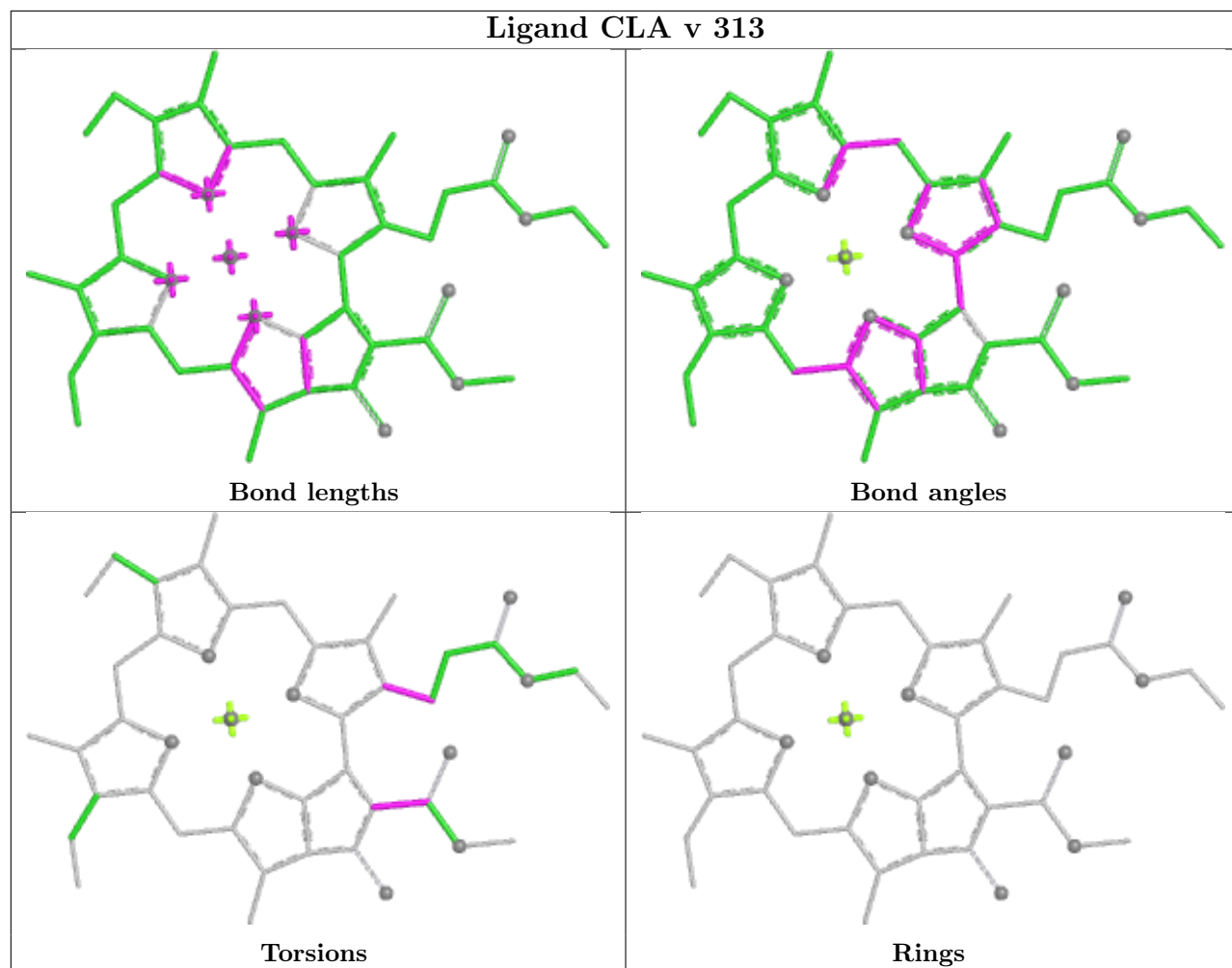
Ligand CLA F 304



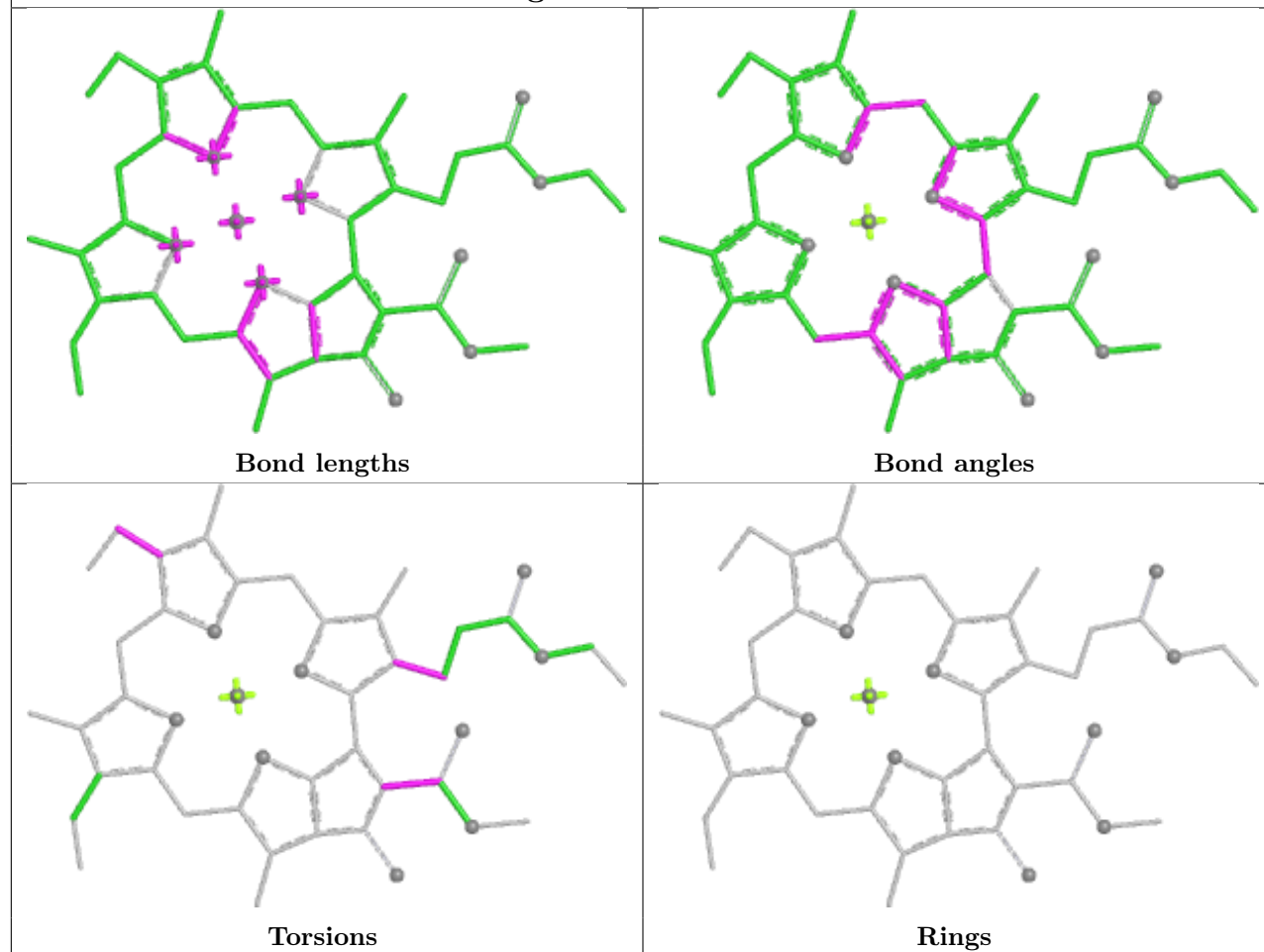
Ligand LMG W 317



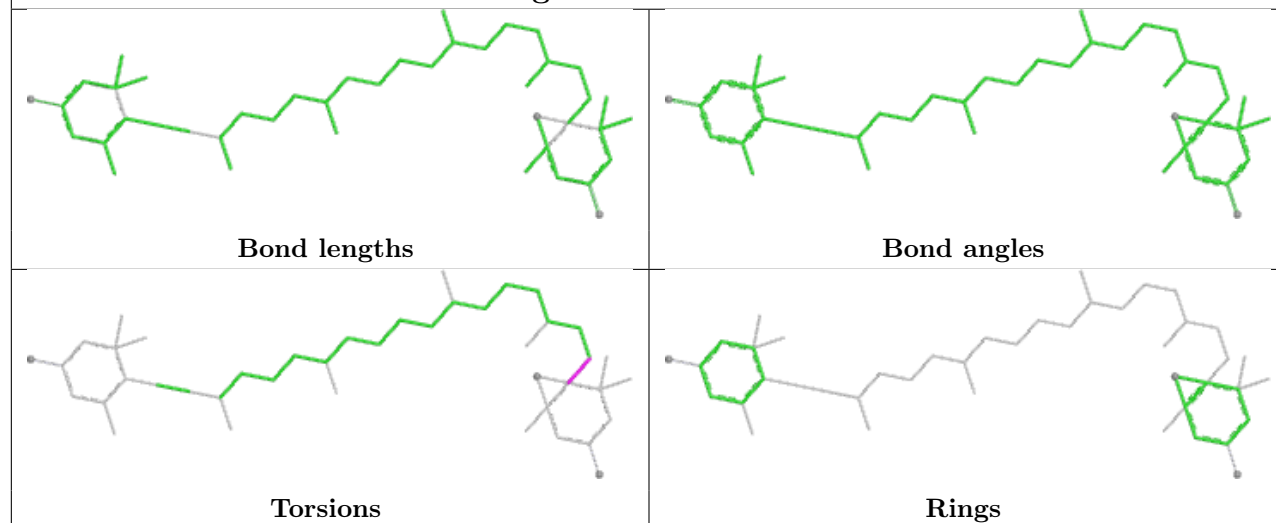
Ligand CLA v 313

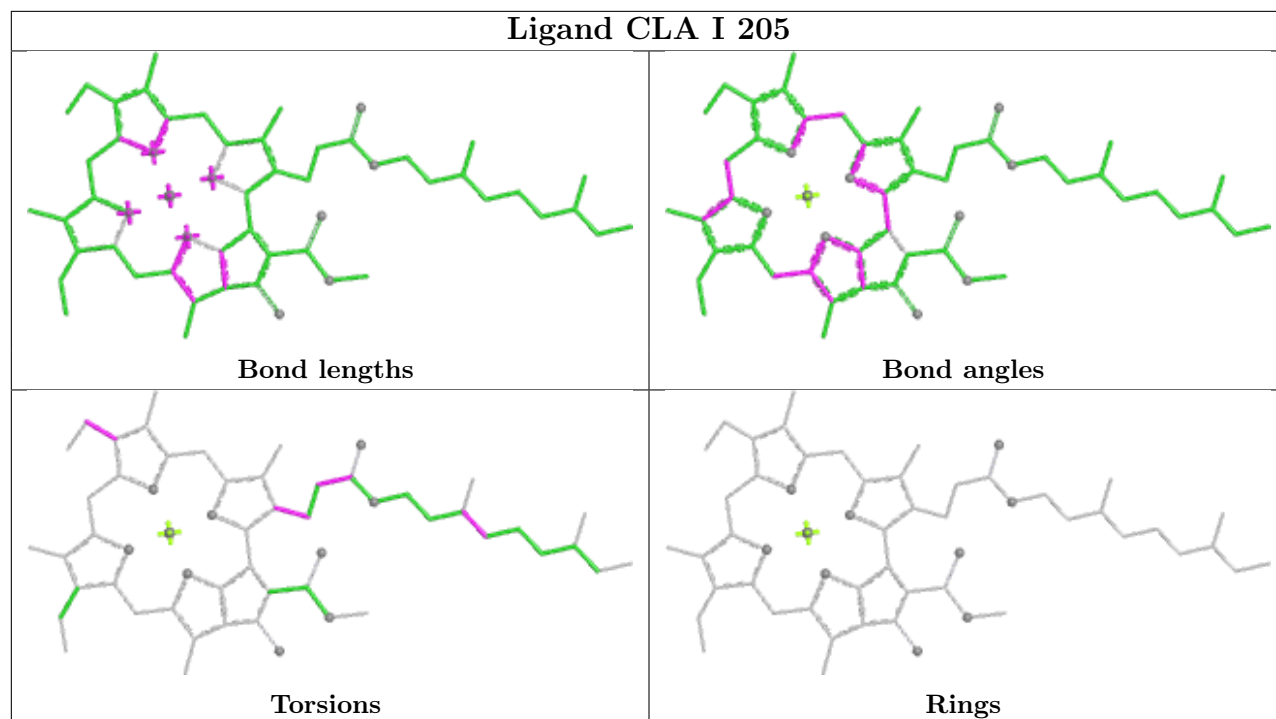
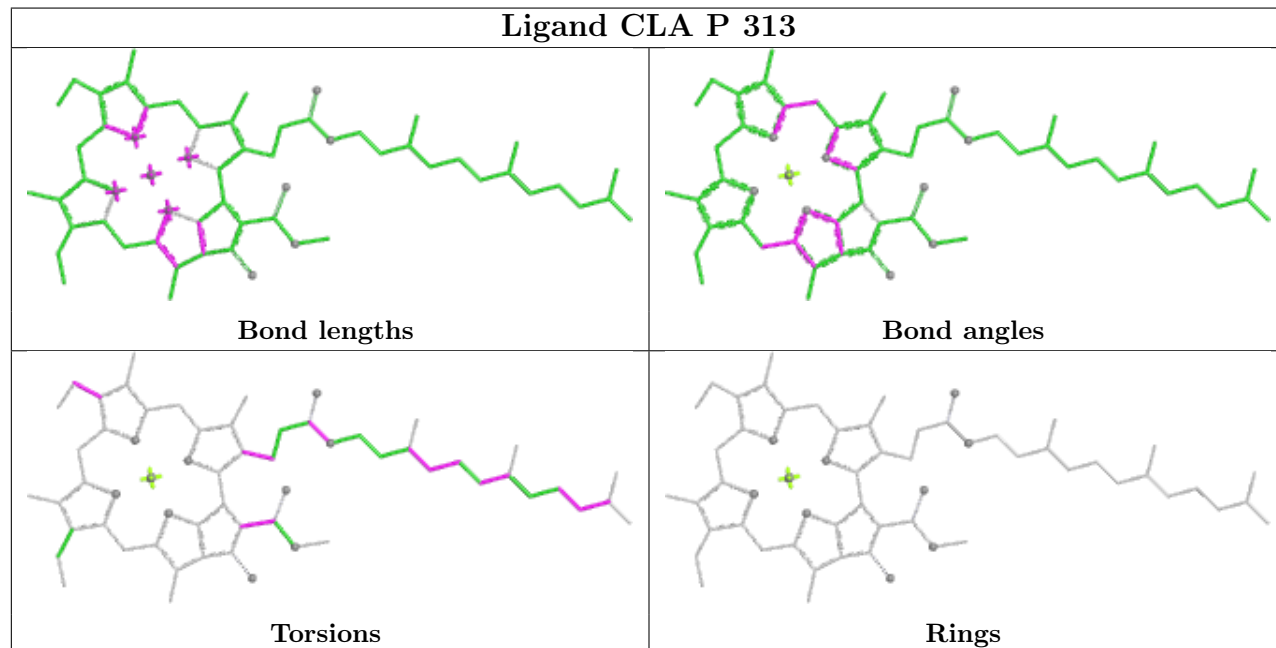


Ligand CLA C 301

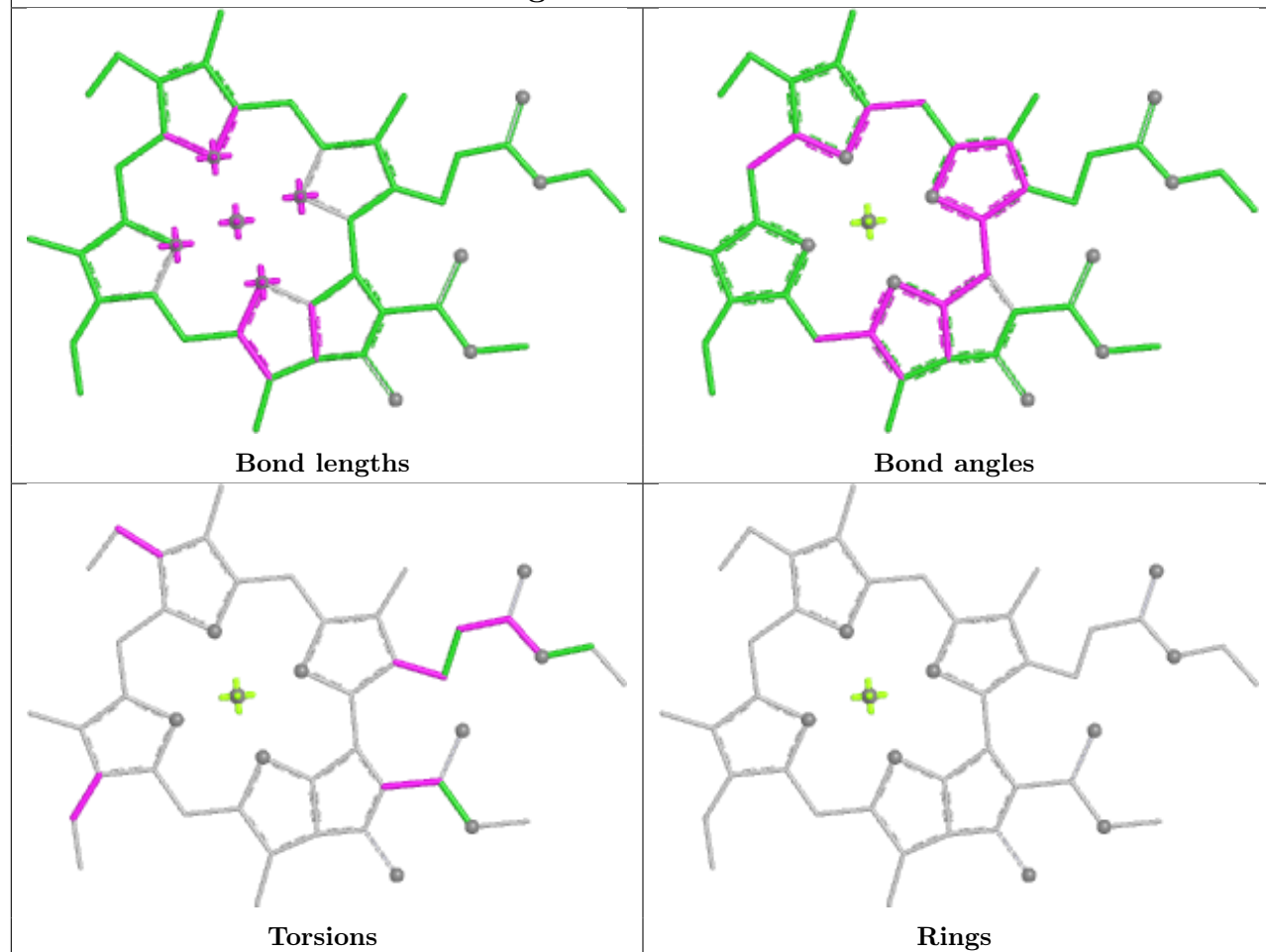


Ligand DD6 D 316

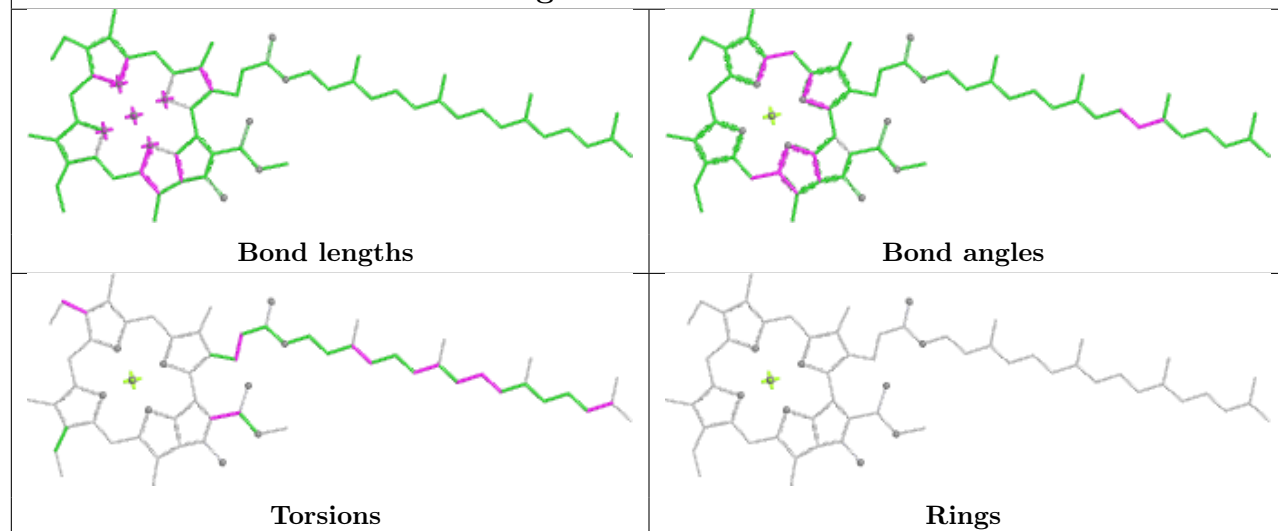


Ligand CLA I 205**Ligand CLA P 313**

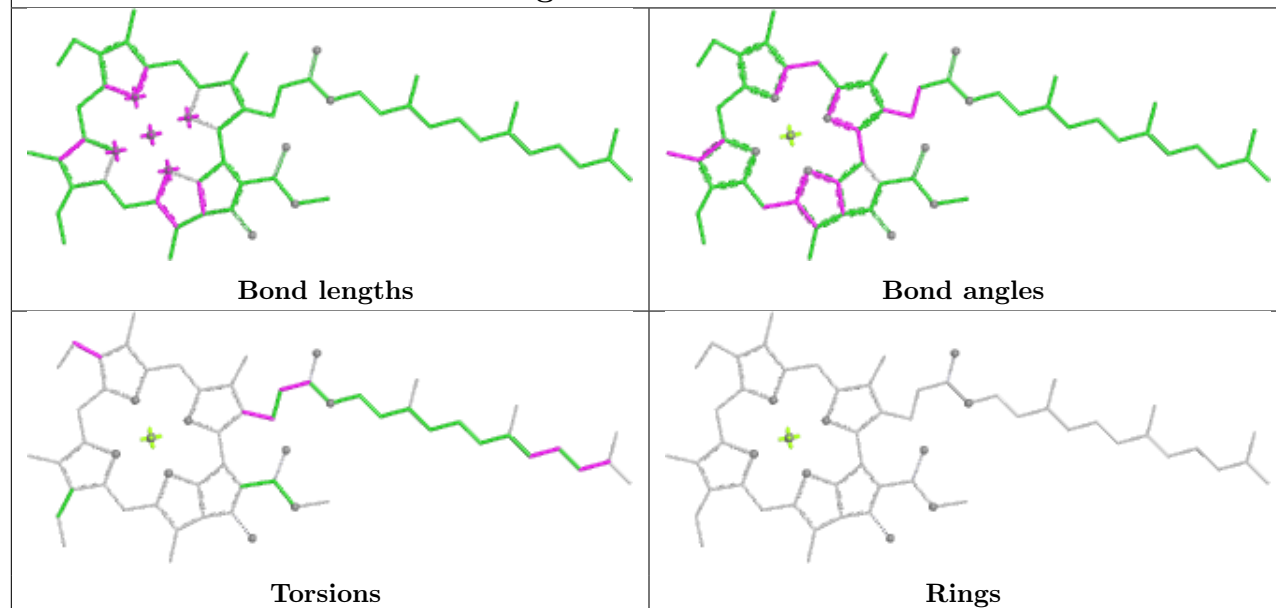
Ligand CLA E 314



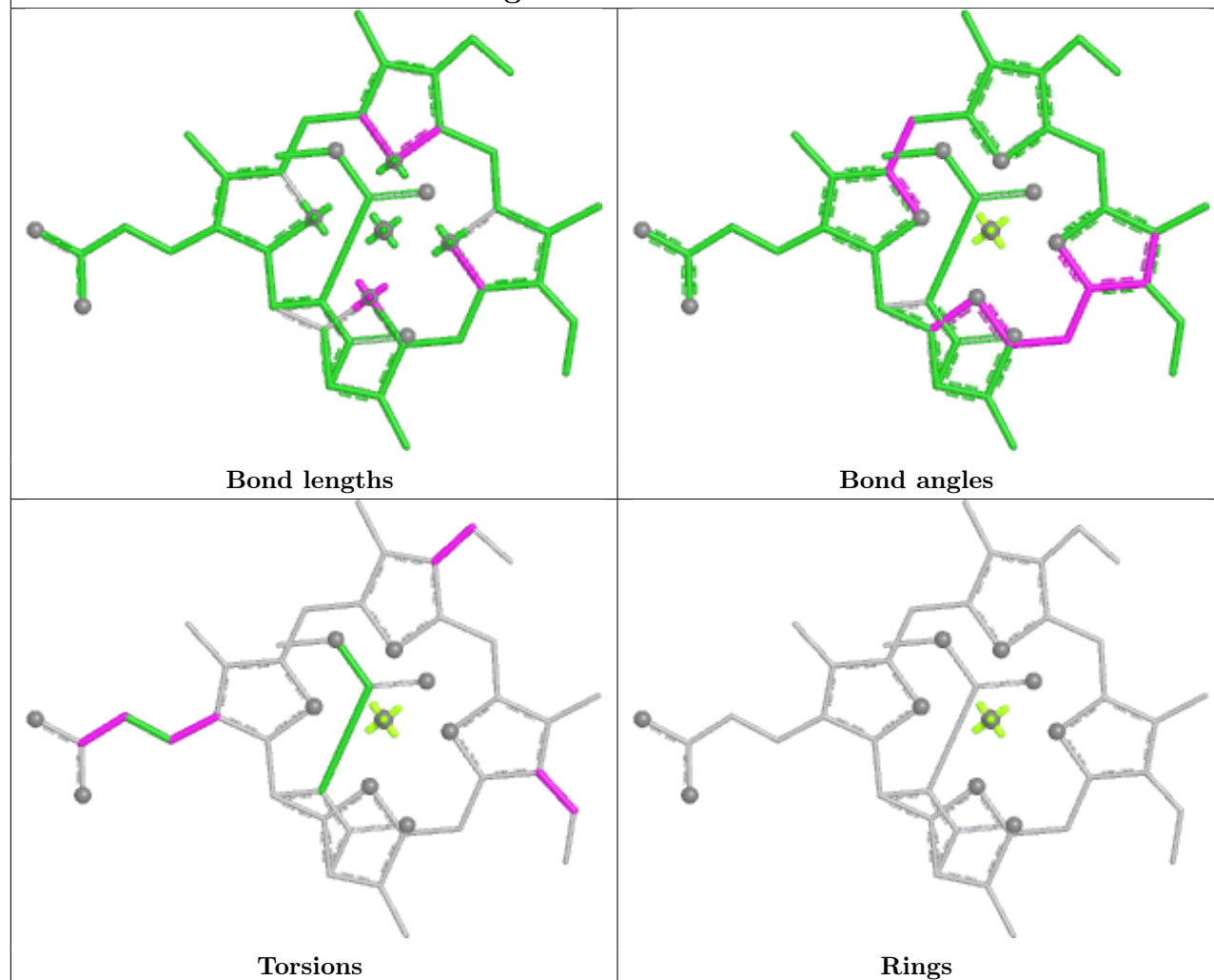
Ligand CLA a 806



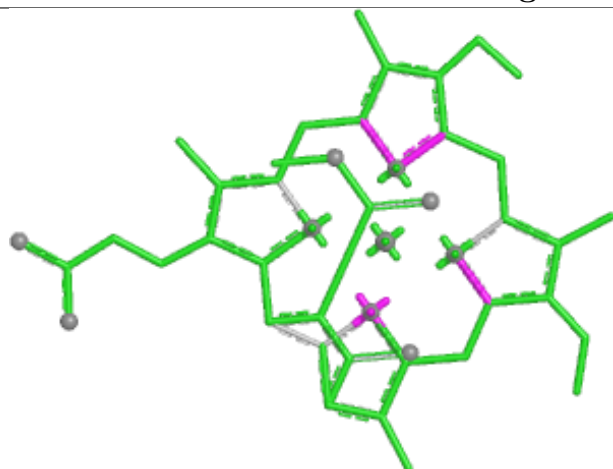
Ligand CLA o 306



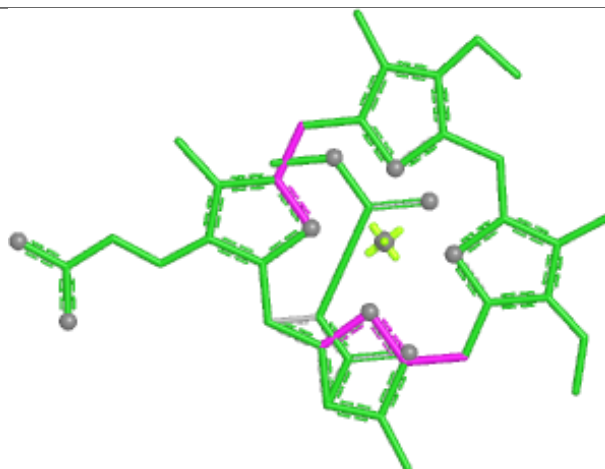
Ligand KC2 M 308



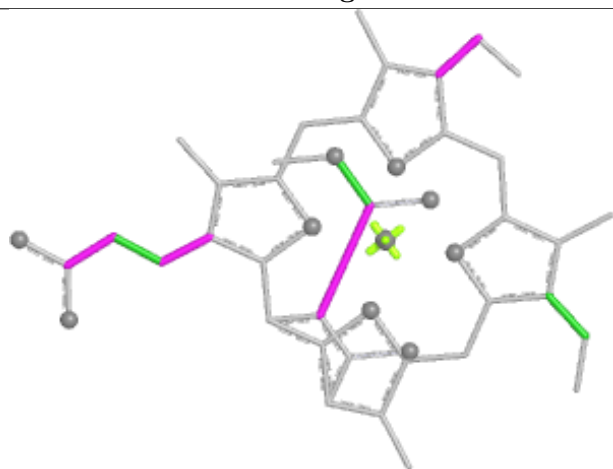
Ligand KC2 u 304



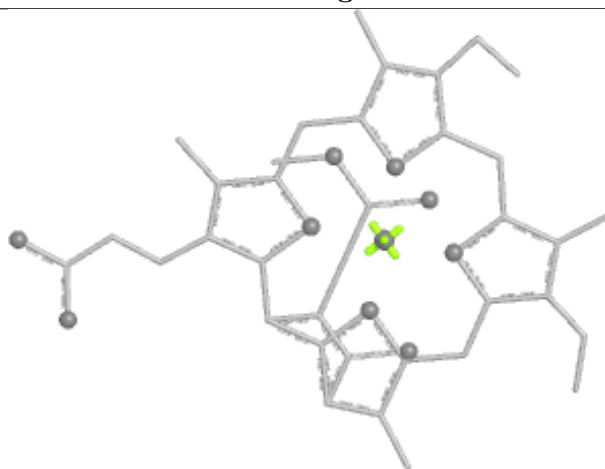
Bond lengths



Bond angles

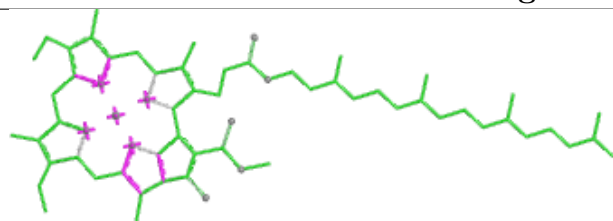


Torsions

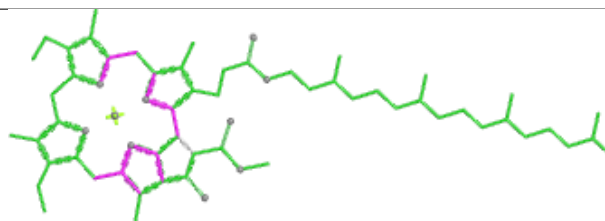


Rings

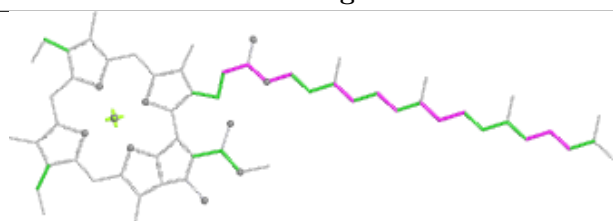
Ligand CLA a 821



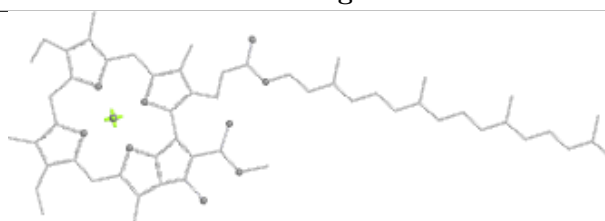
Bond lengths



Bond angles

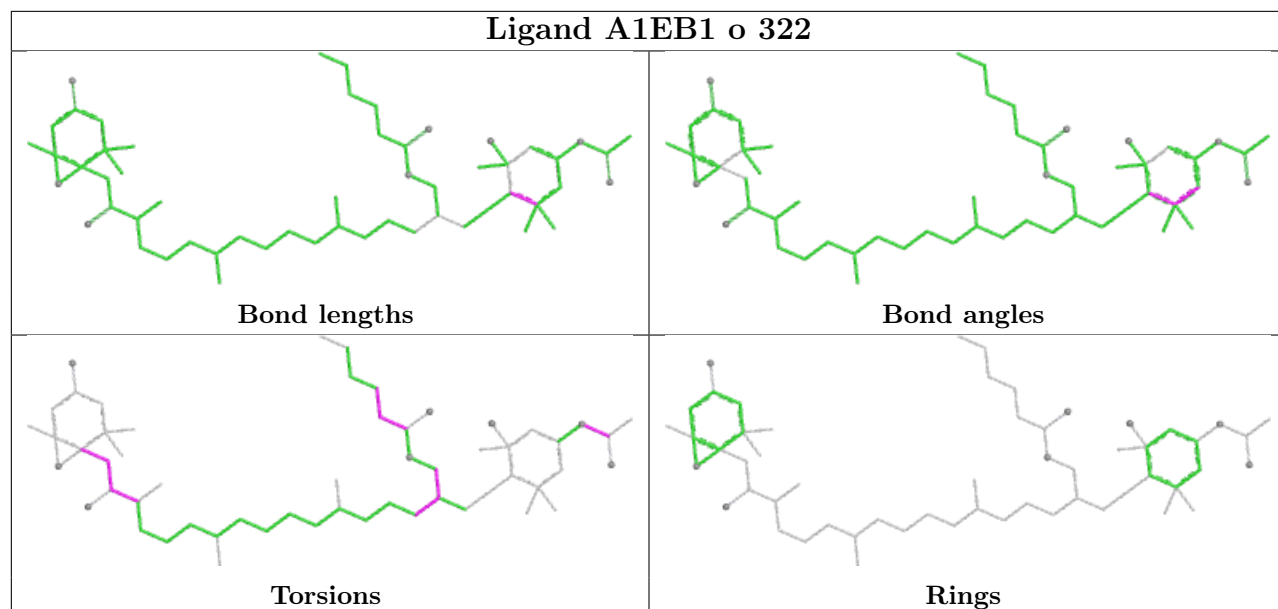


Torsions

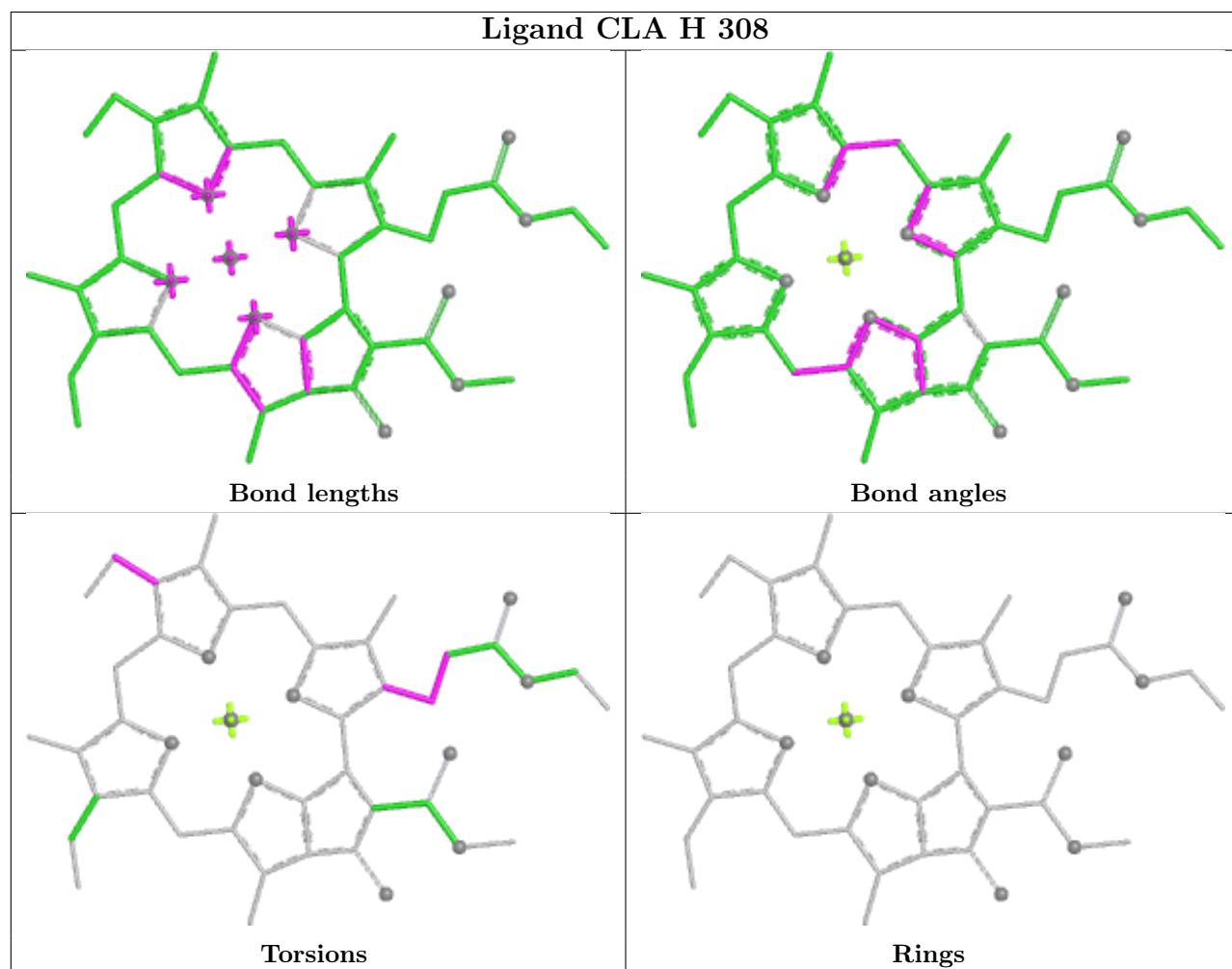


Rings

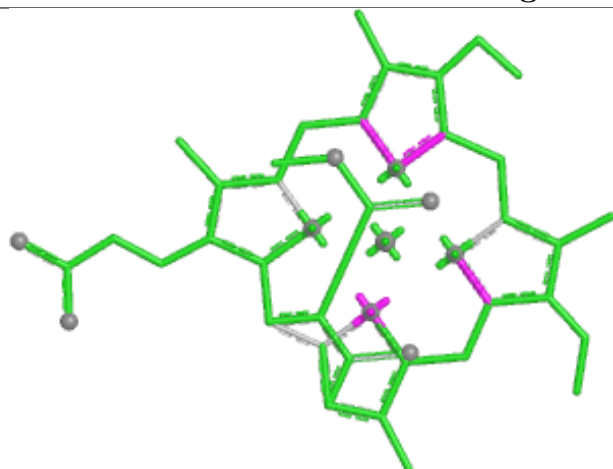
Ligand A1EB1 o 322



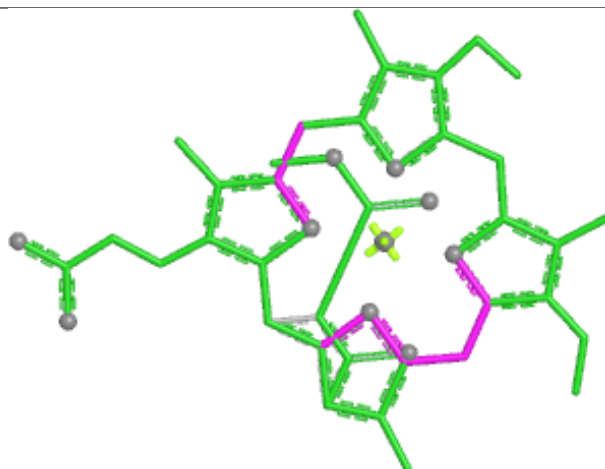
Ligand CLA H 308



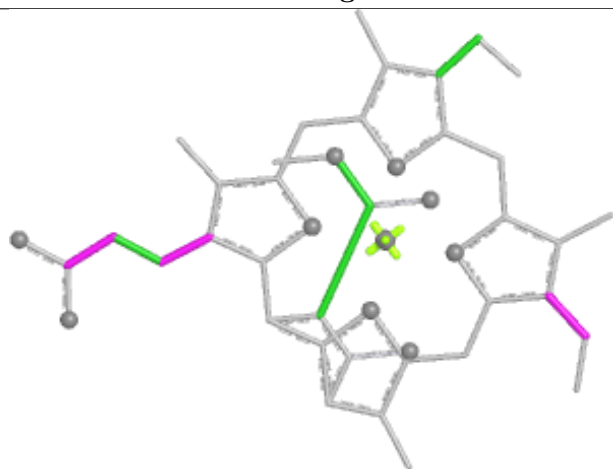
Ligand KC2 v 302



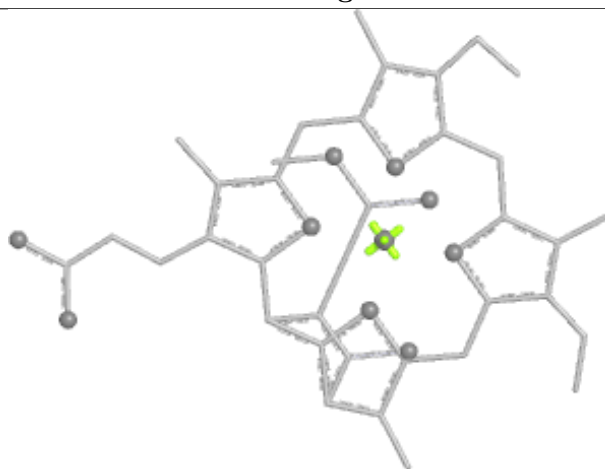
Bond lengths



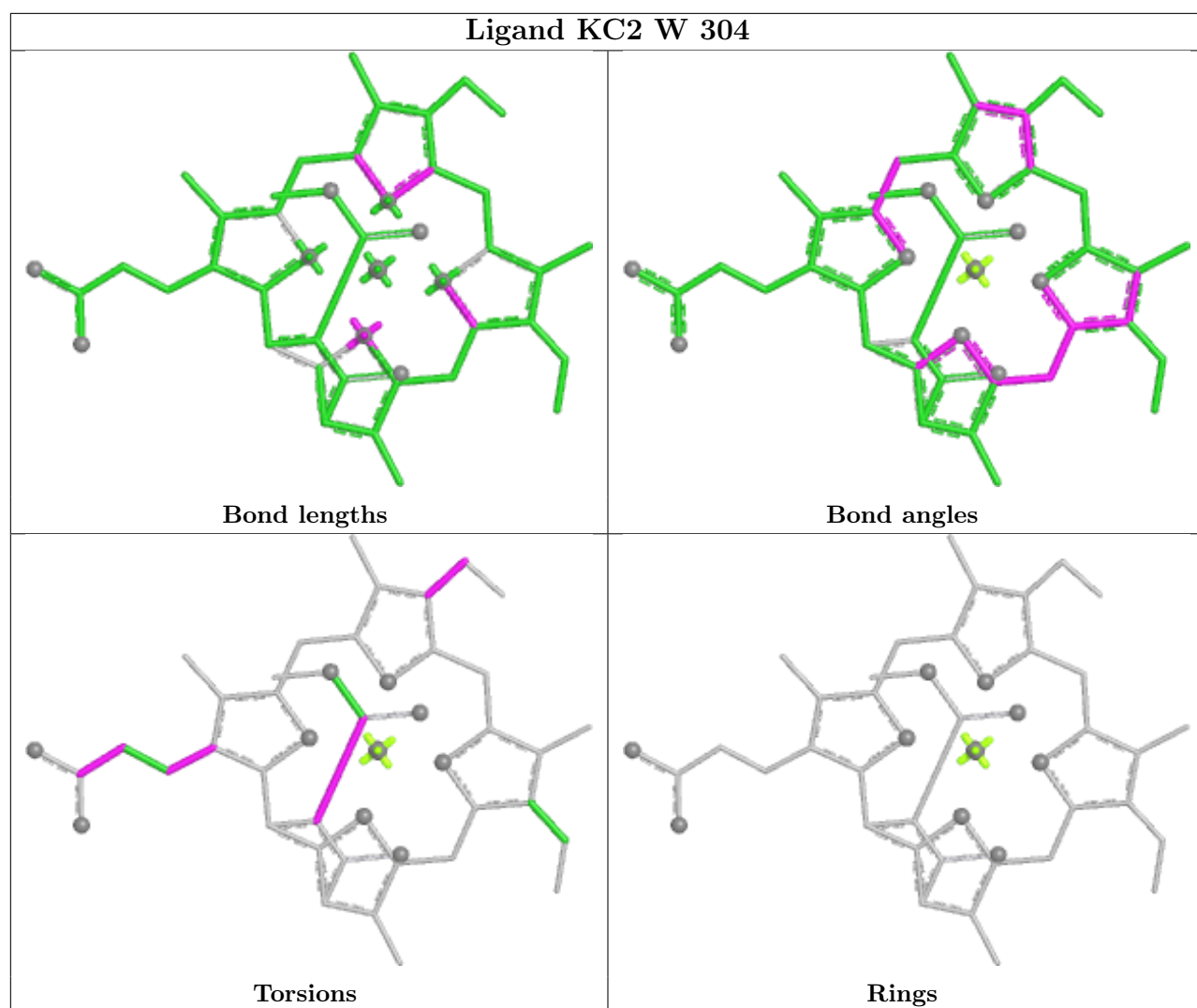
Bond angles

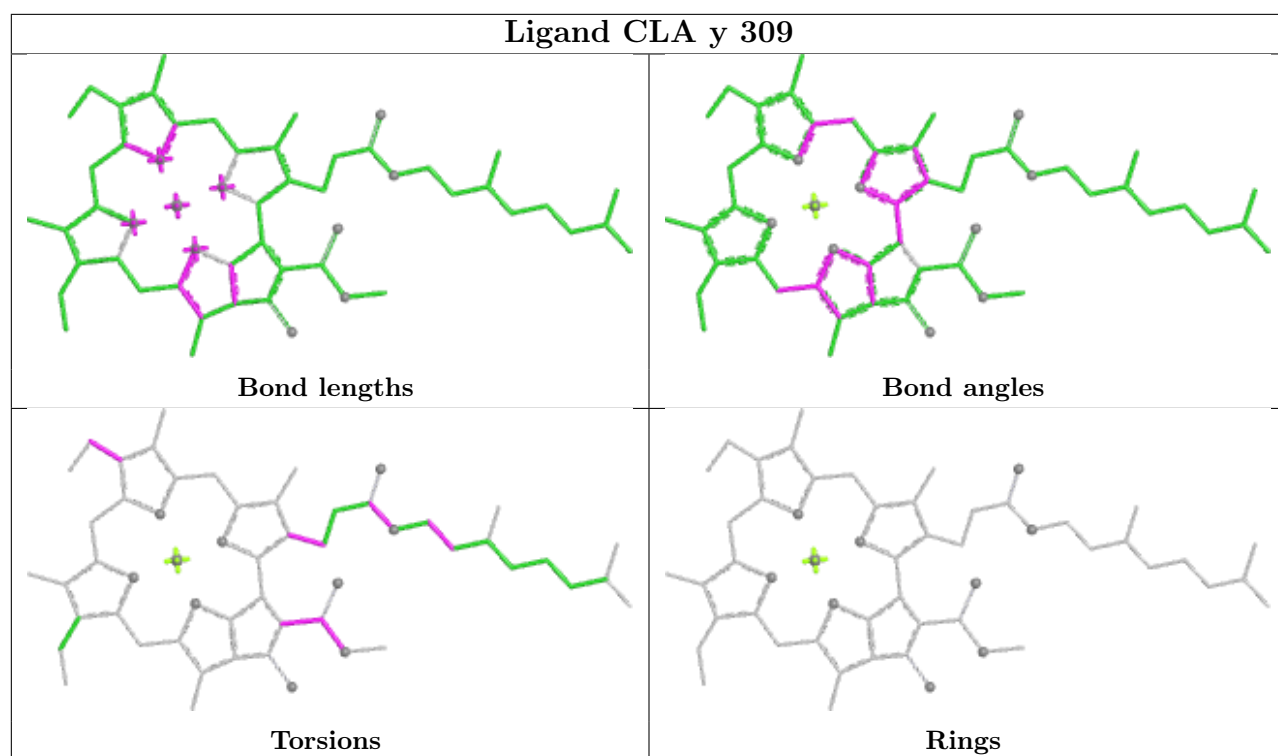


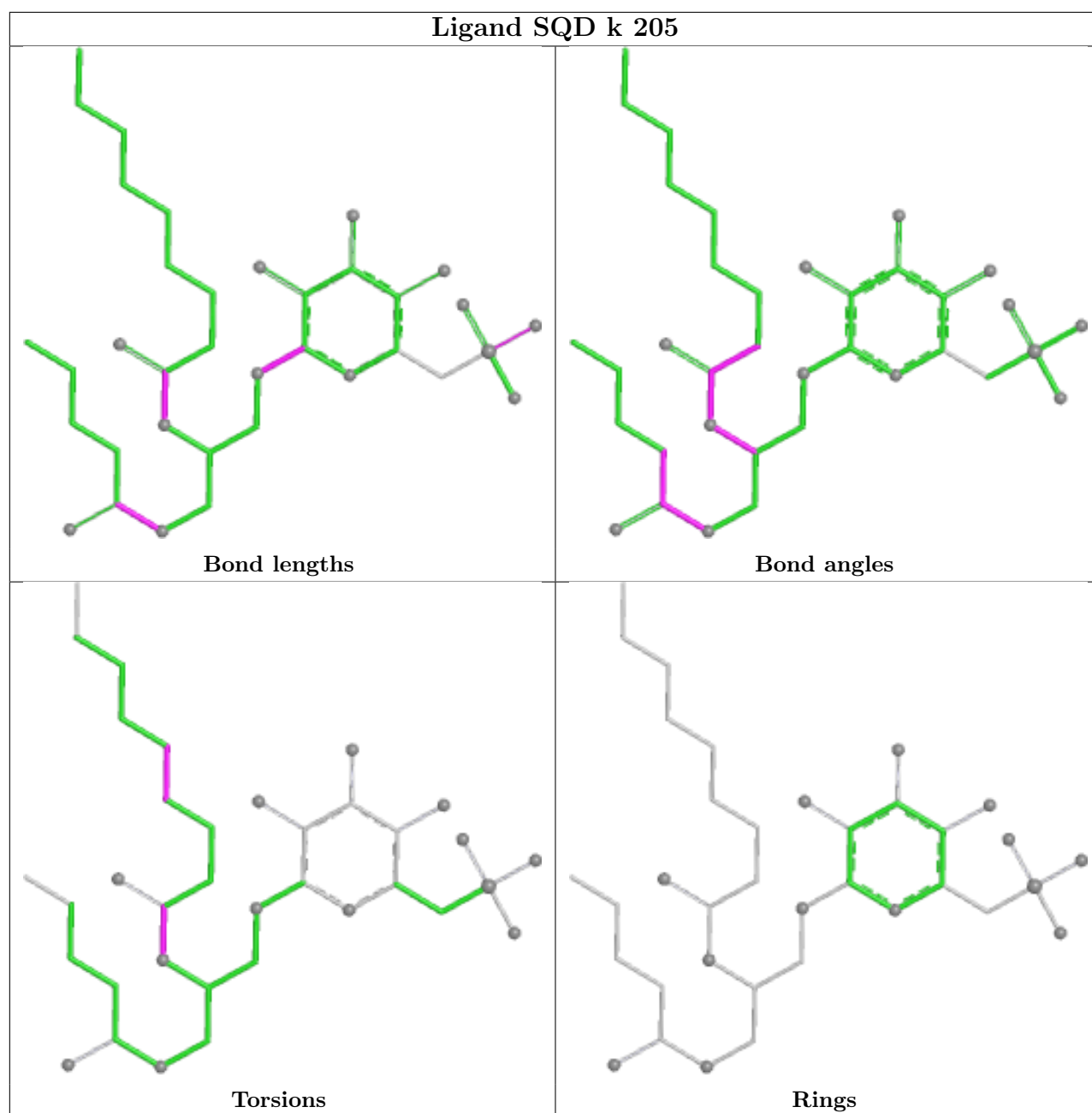
Torsions

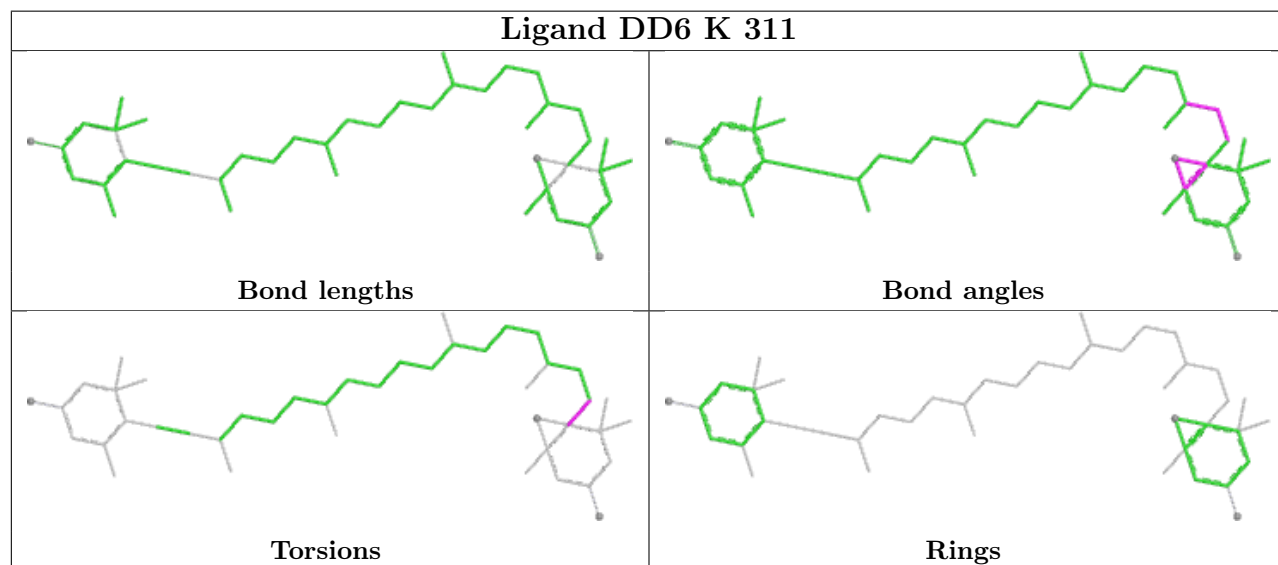
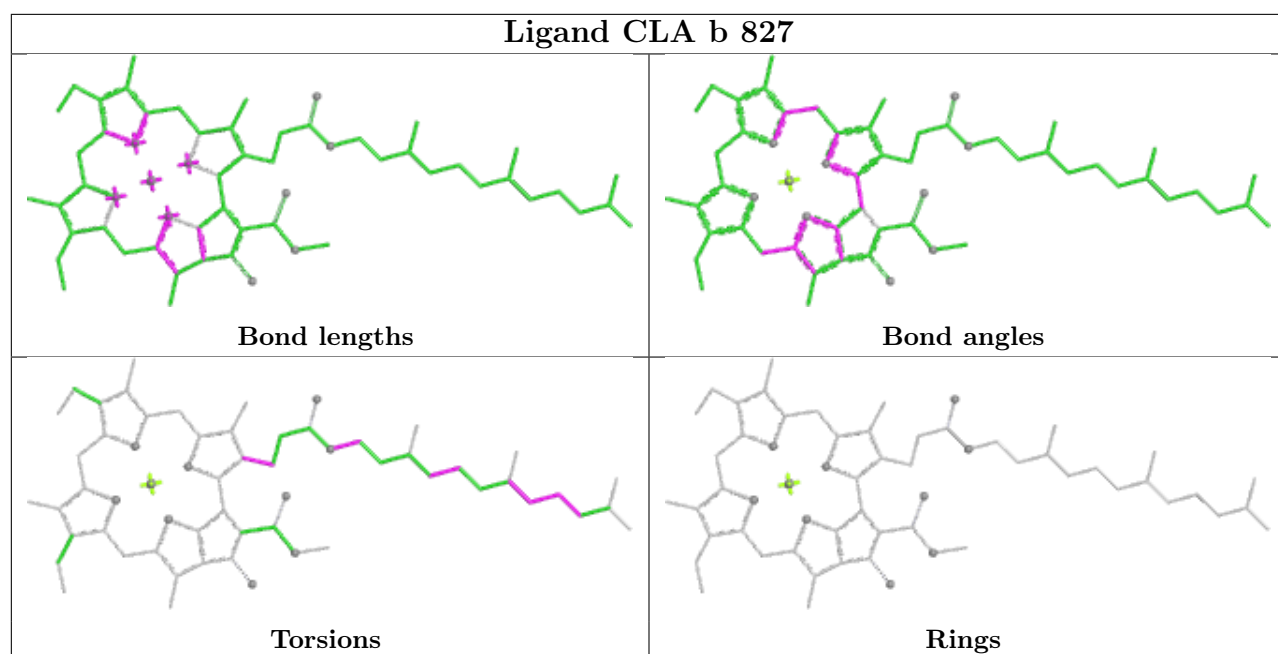


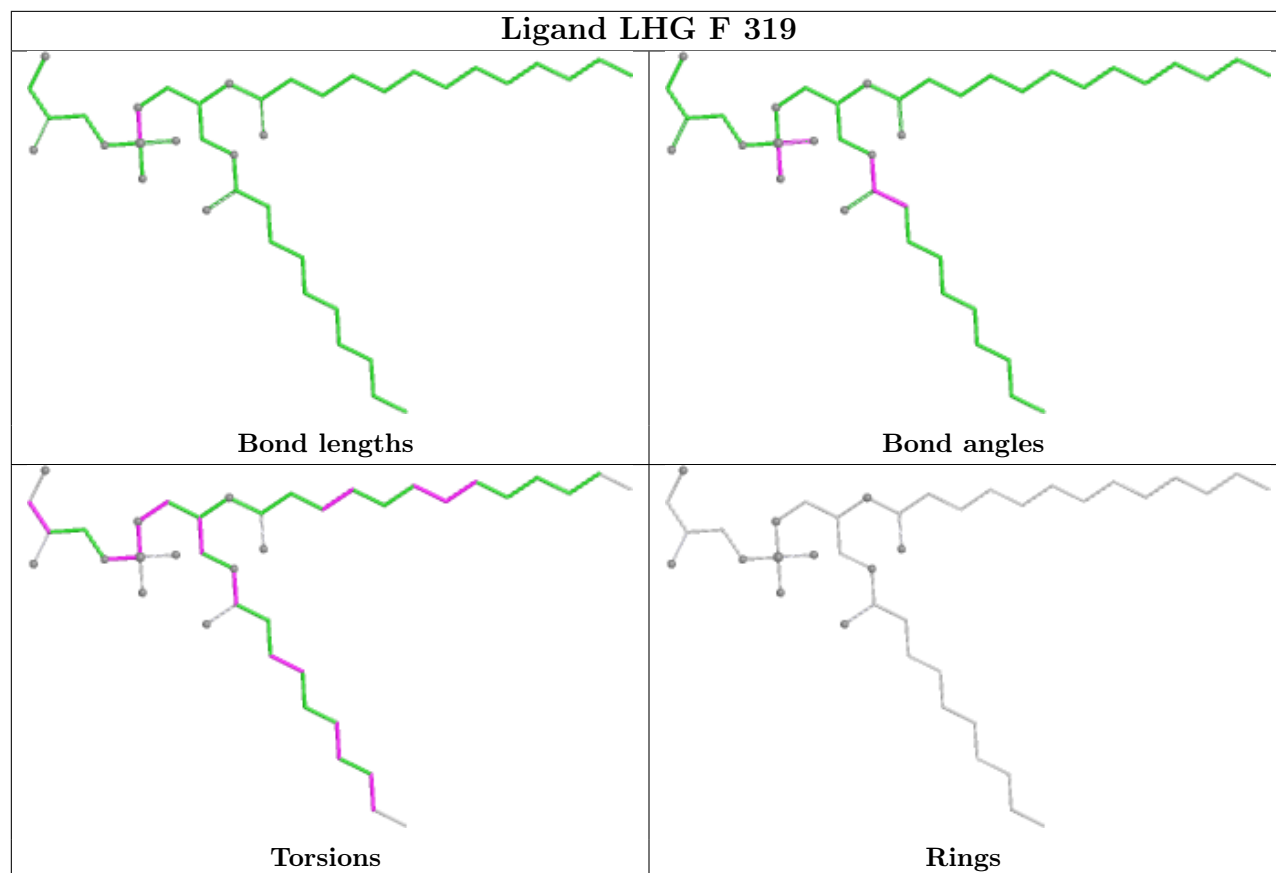
Rings



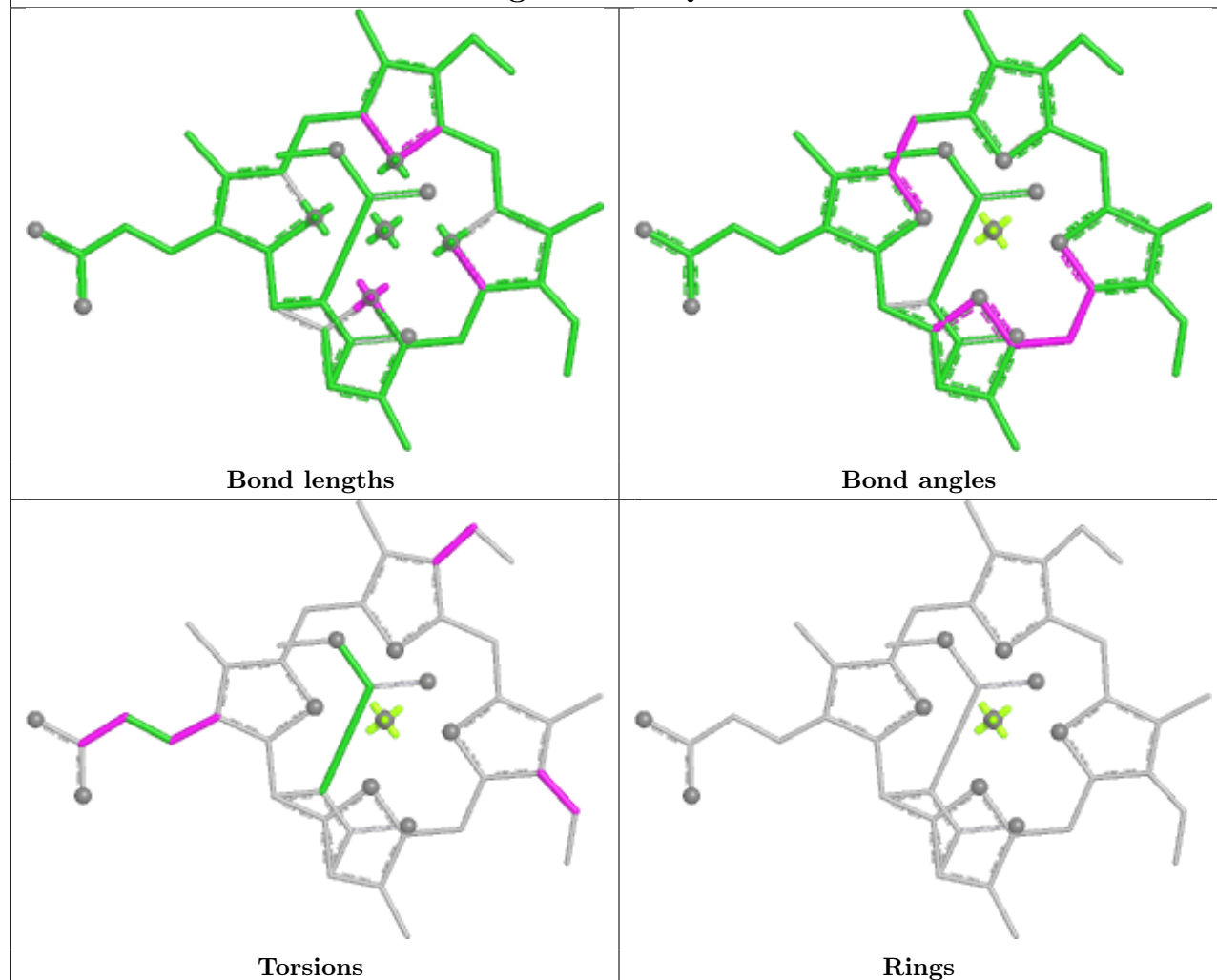




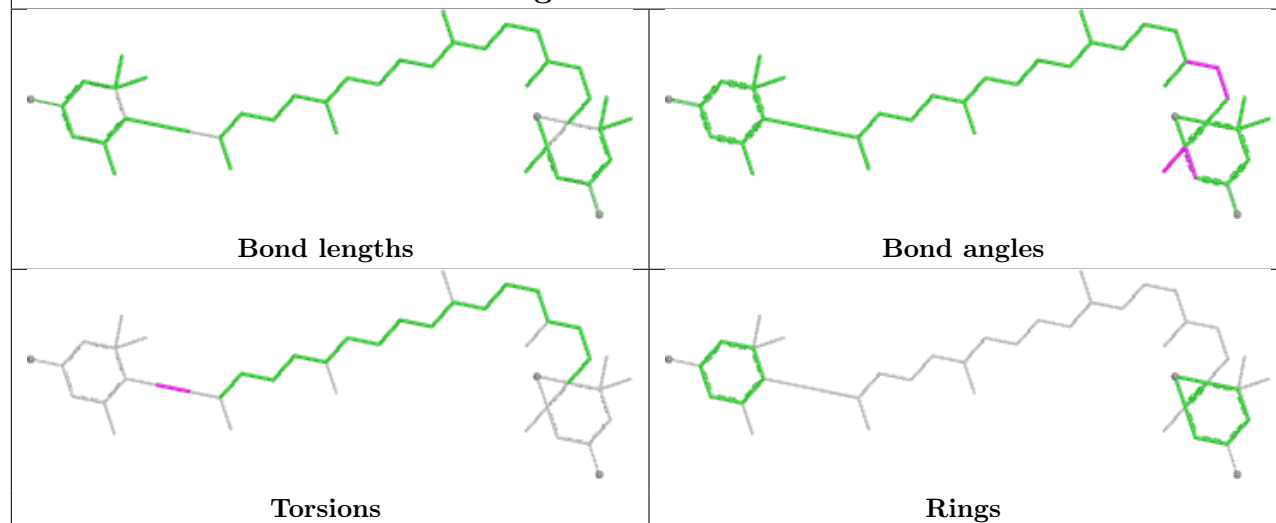


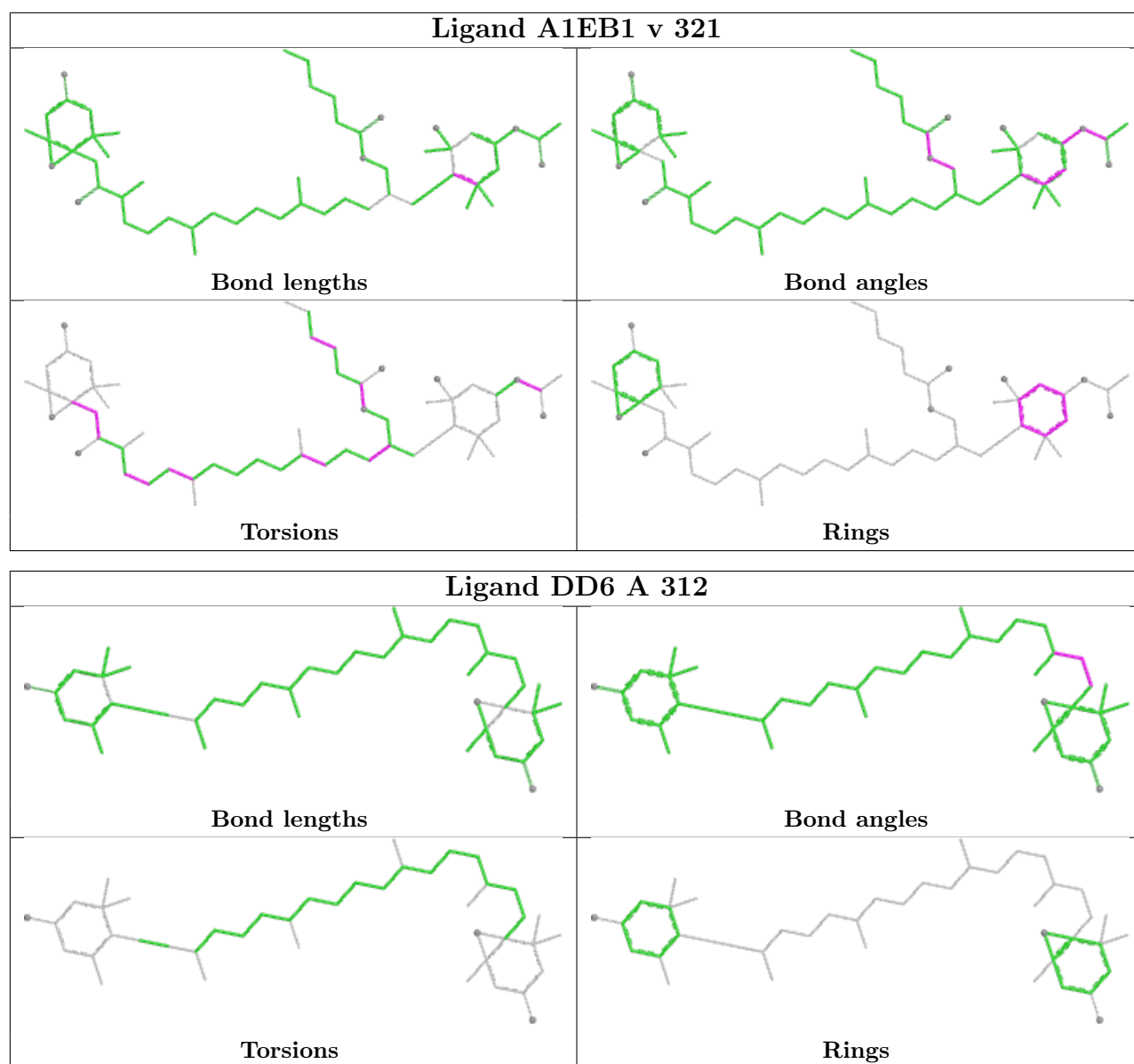


Ligand KC2 Q 216

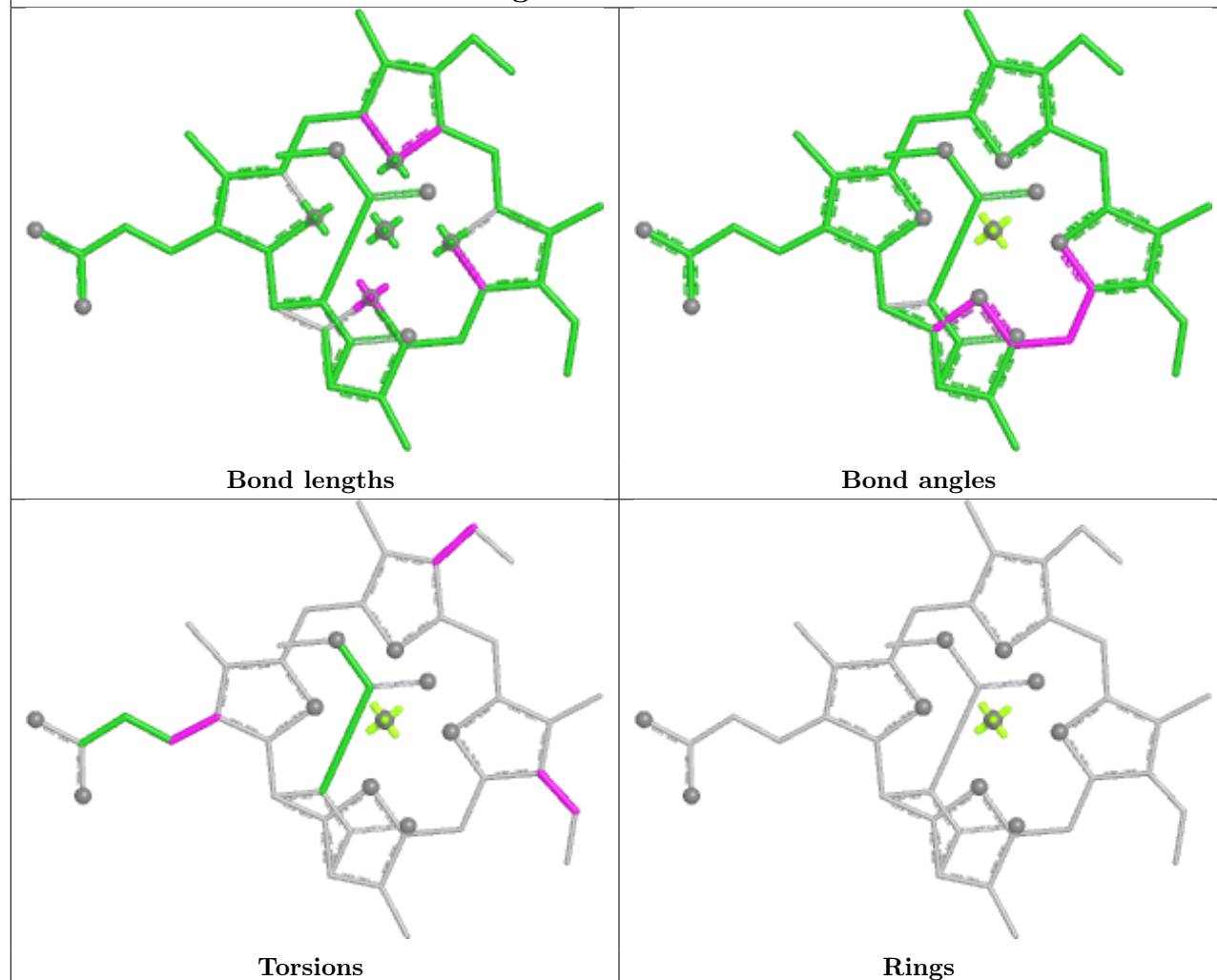


Ligand DD6 E 317

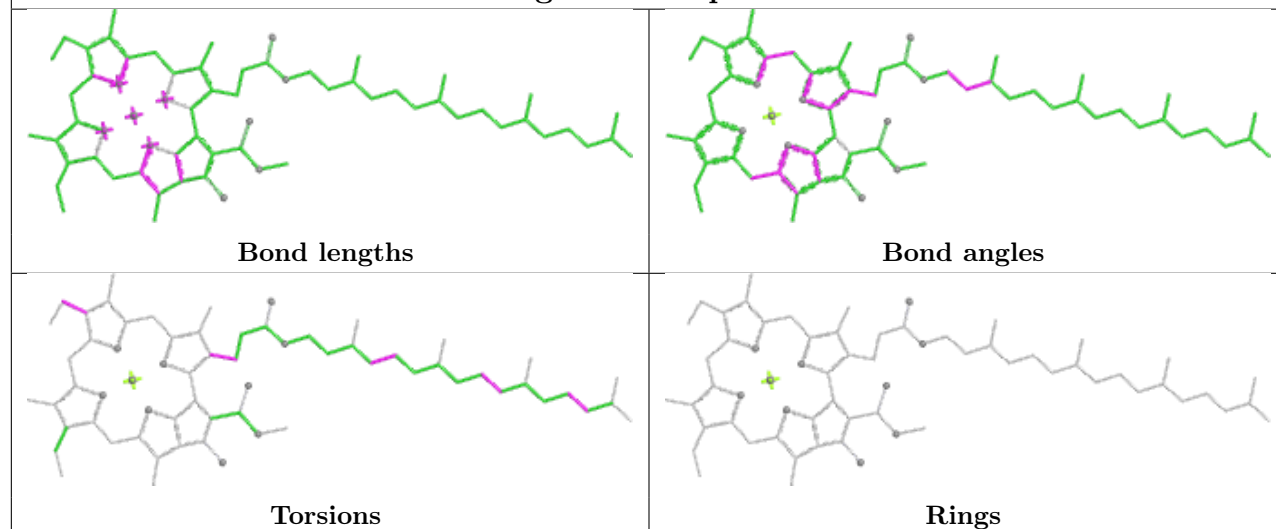




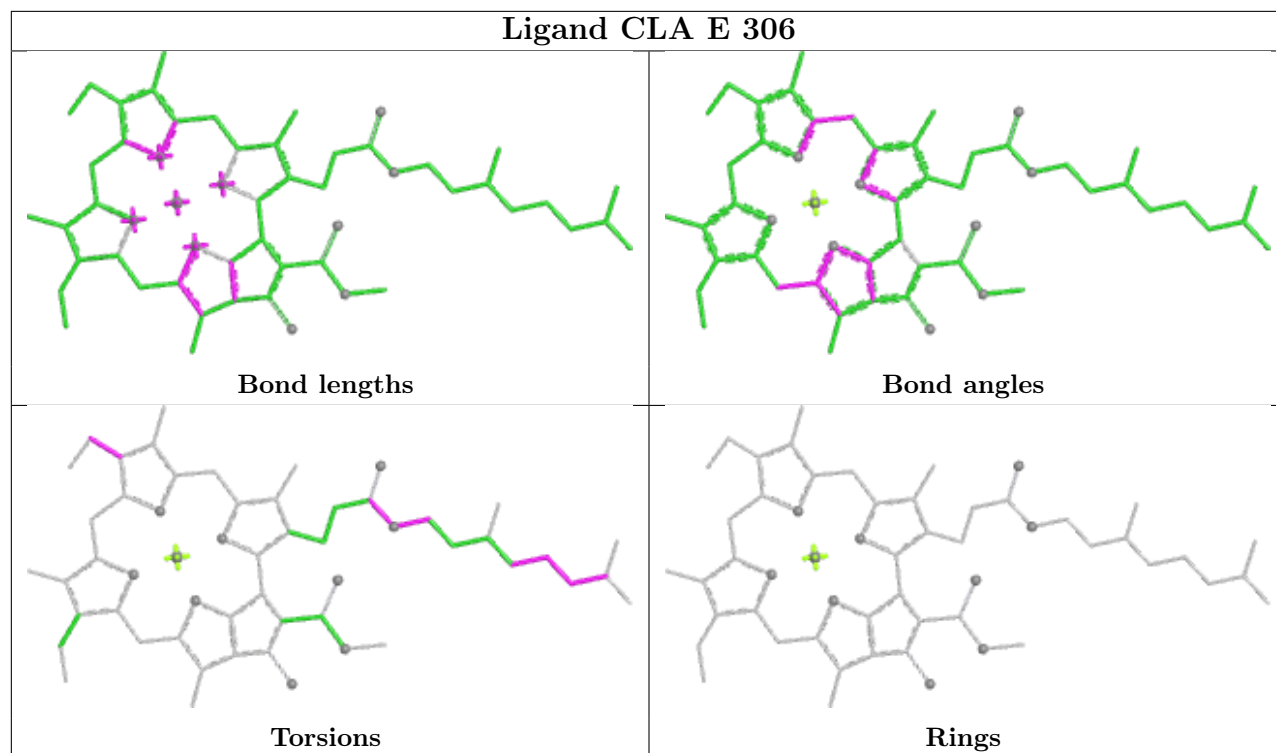
Ligand KC2 u 310



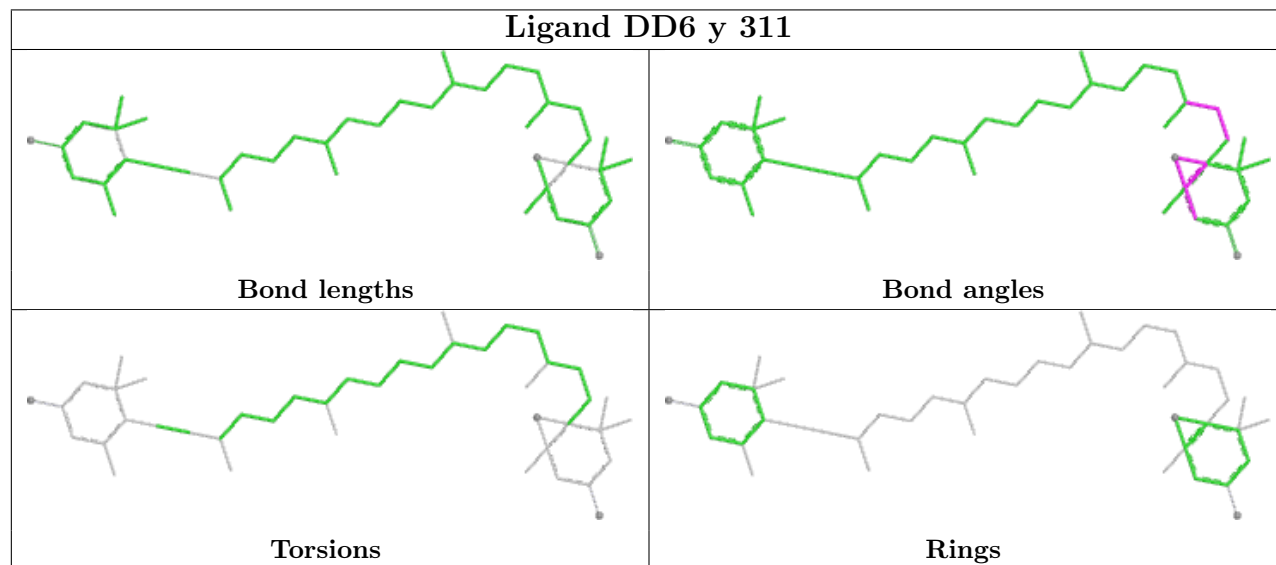
Ligand CLA p 302

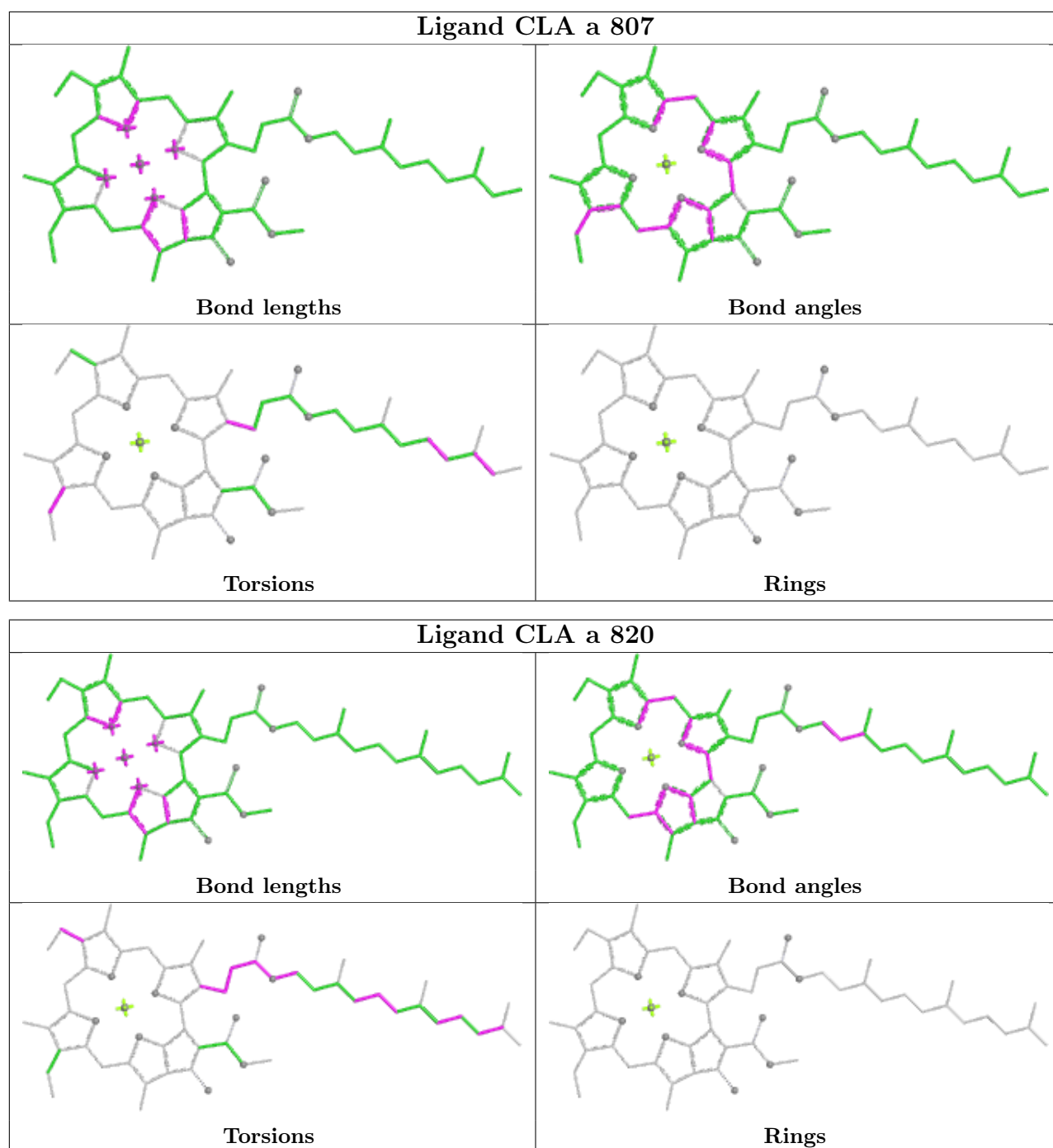


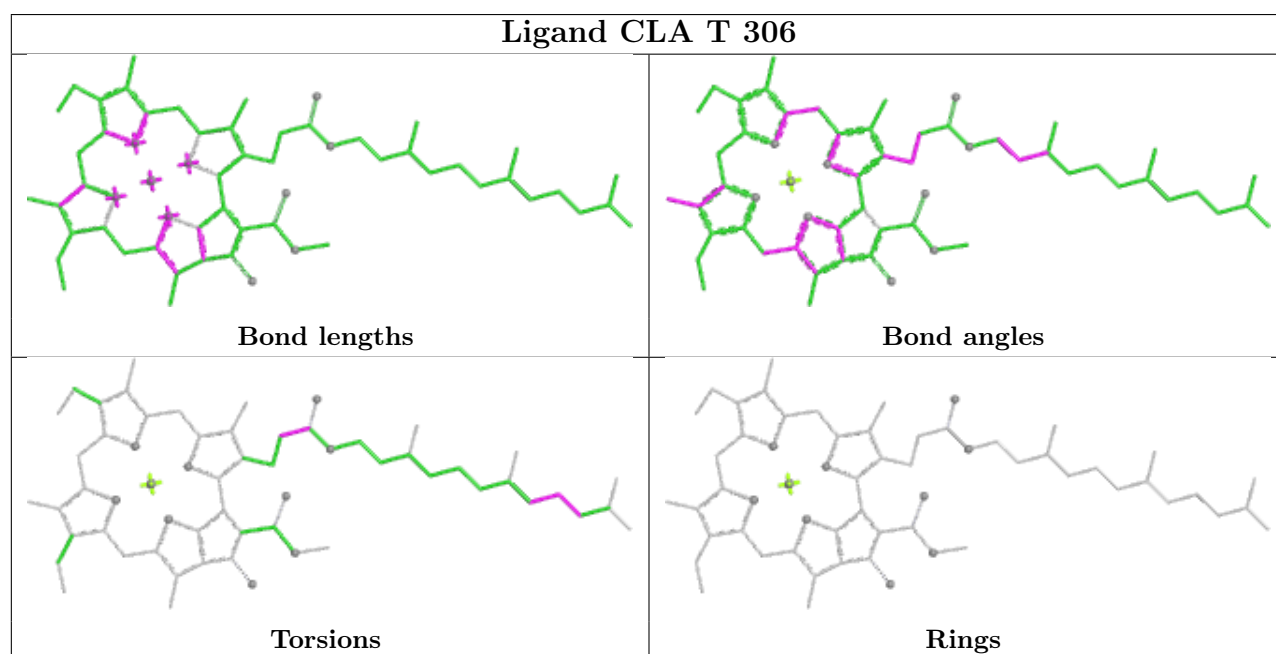
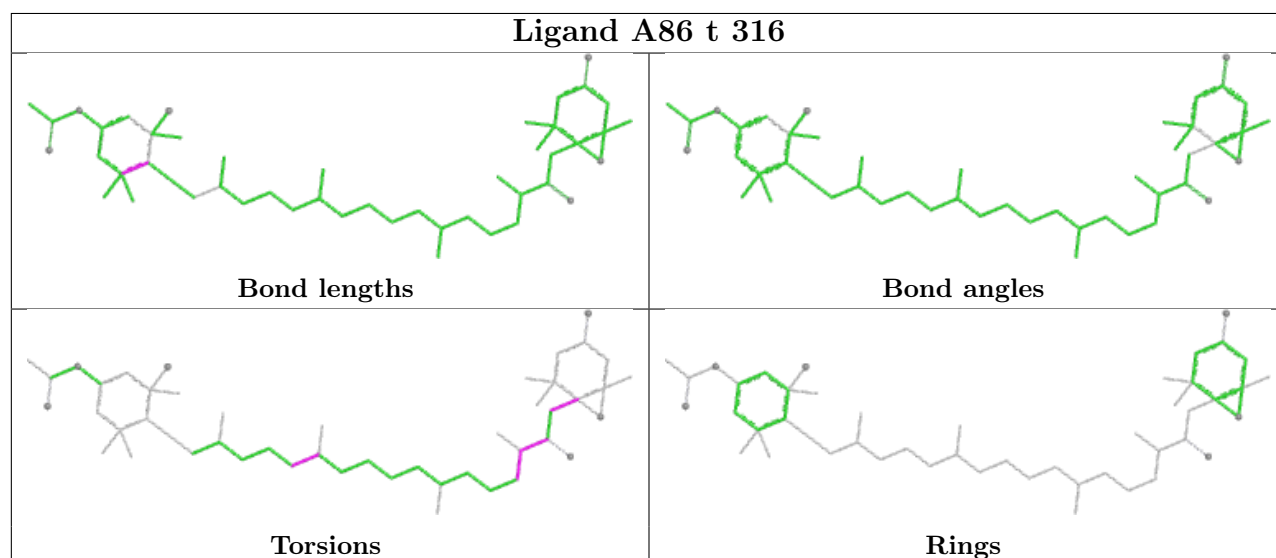
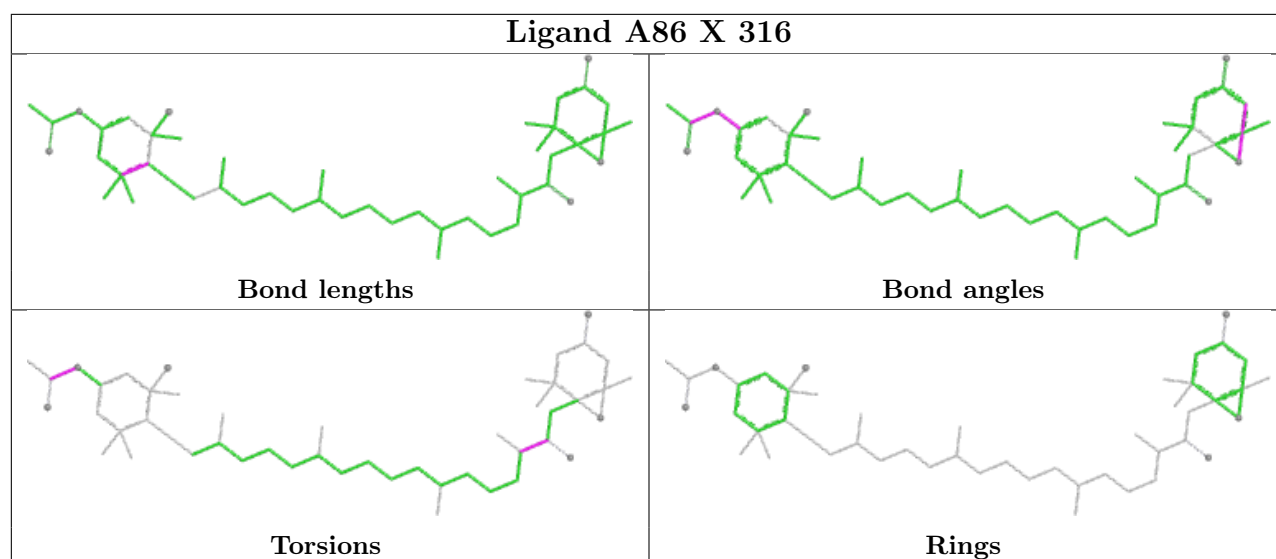
Ligand CLA E 306

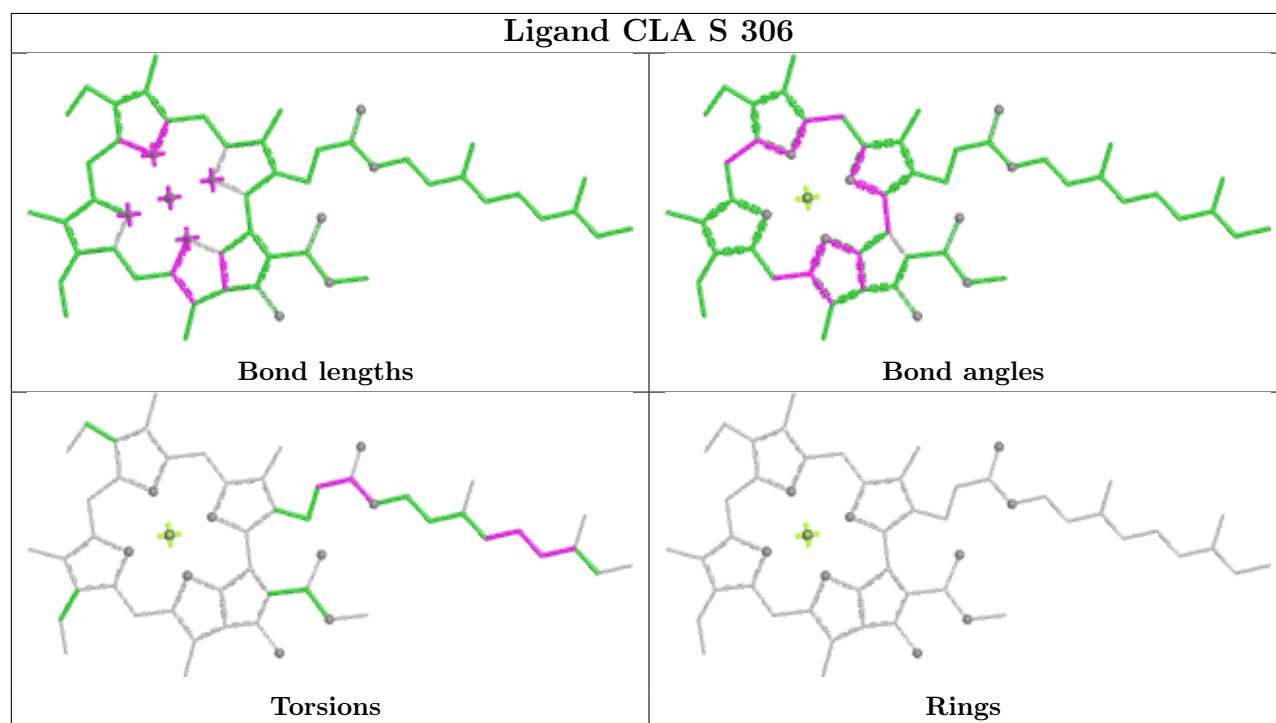
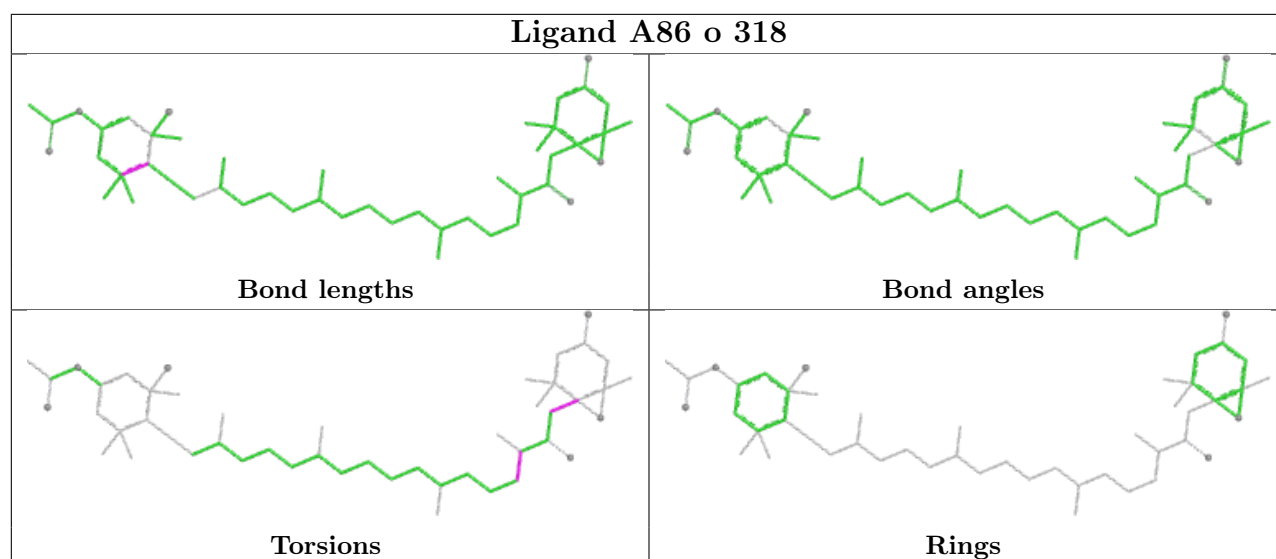


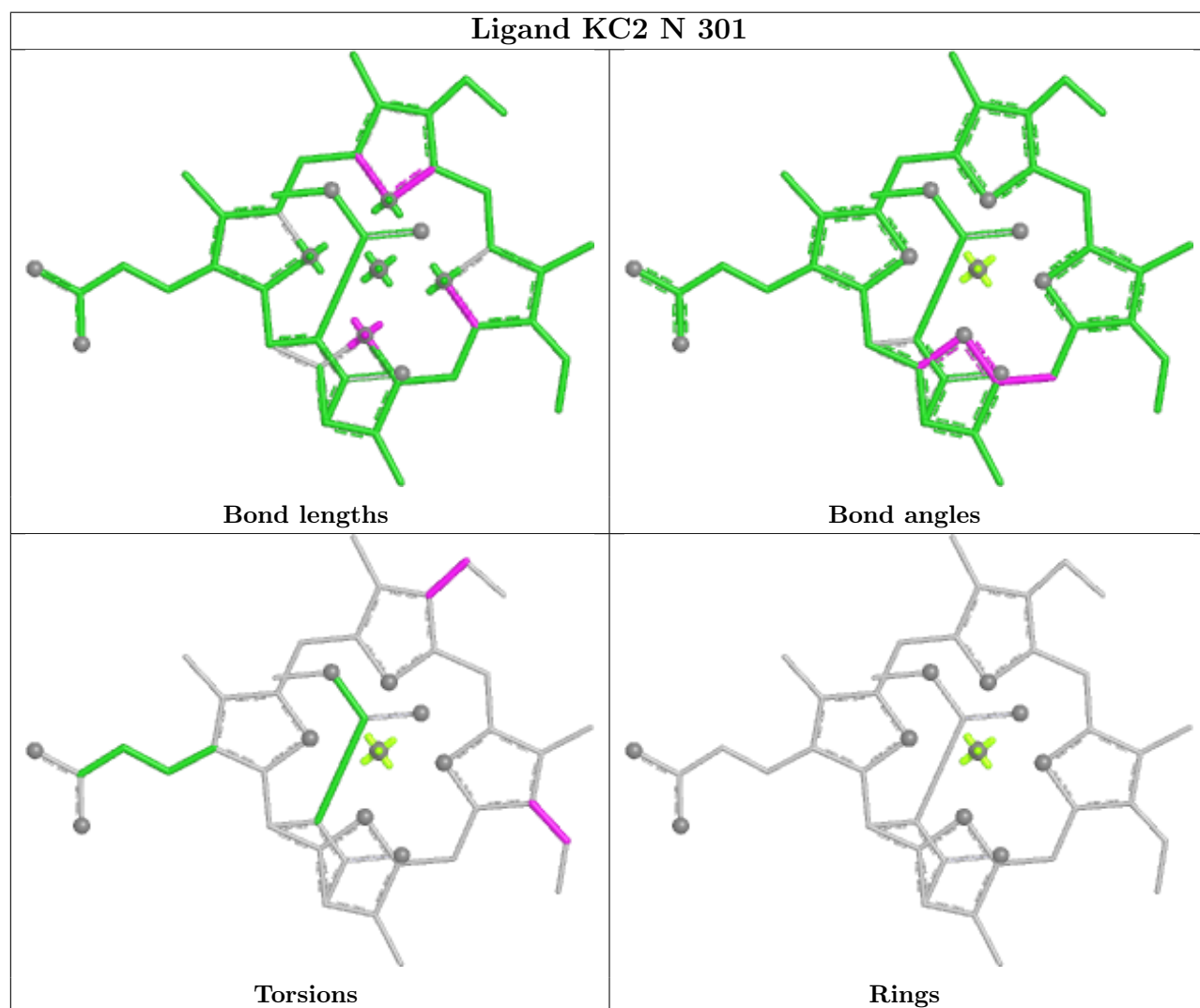
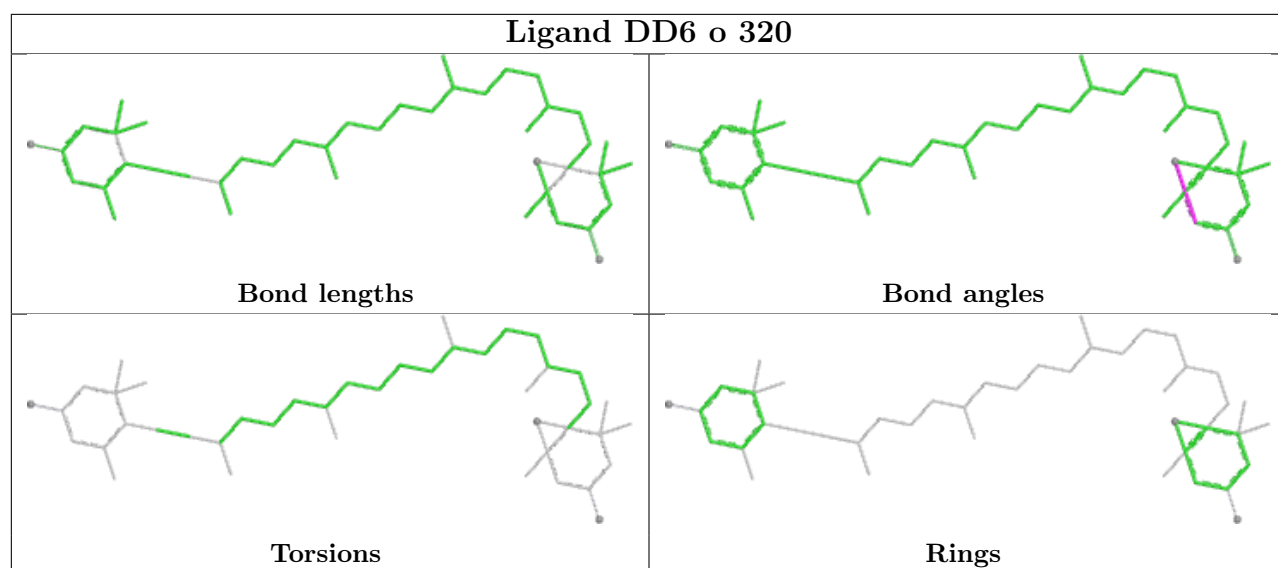
Ligand DD6 y 311

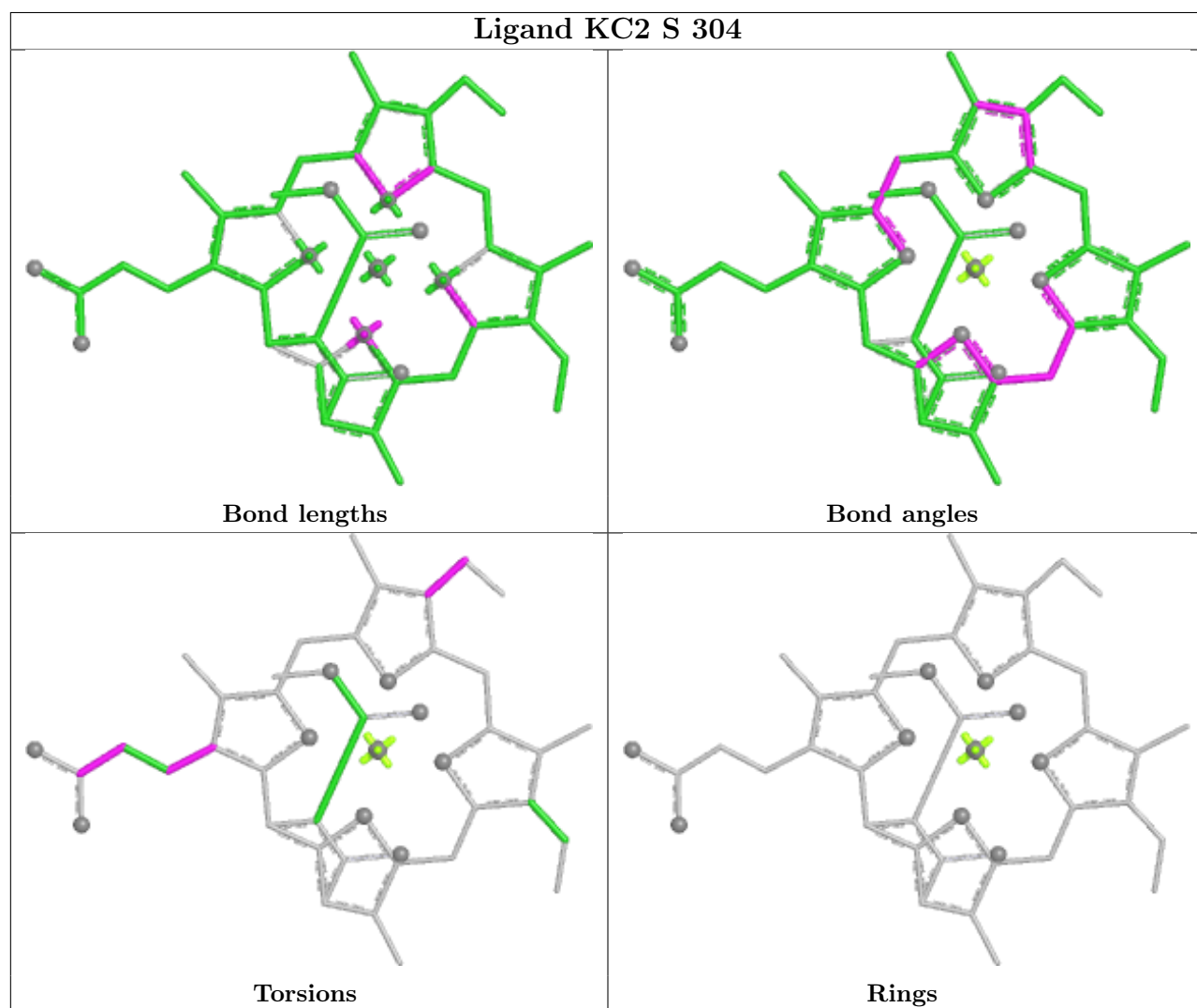
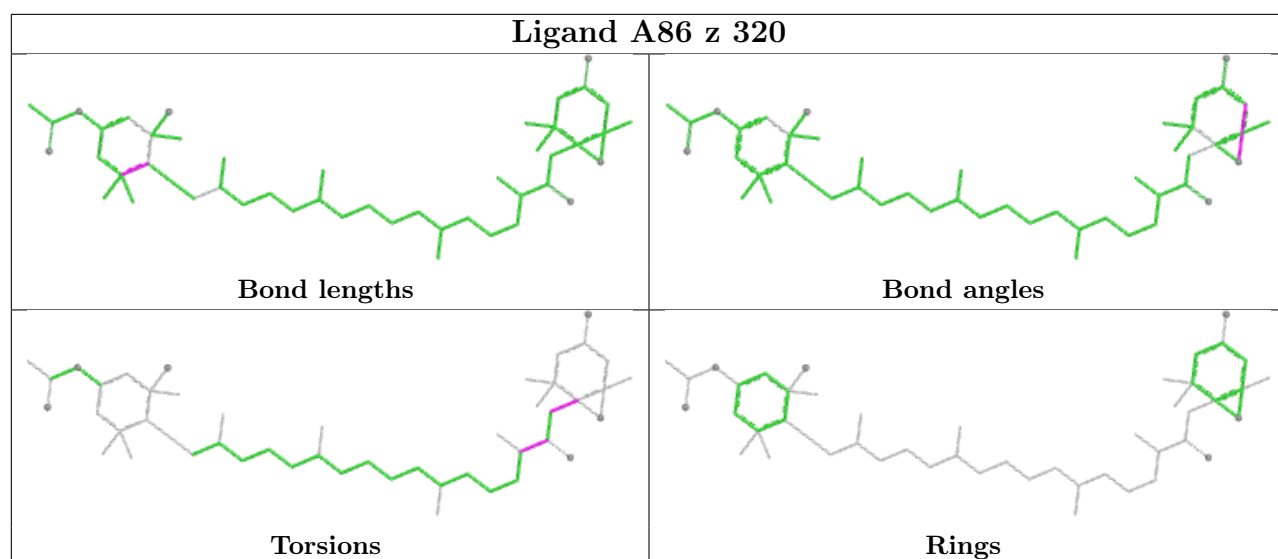




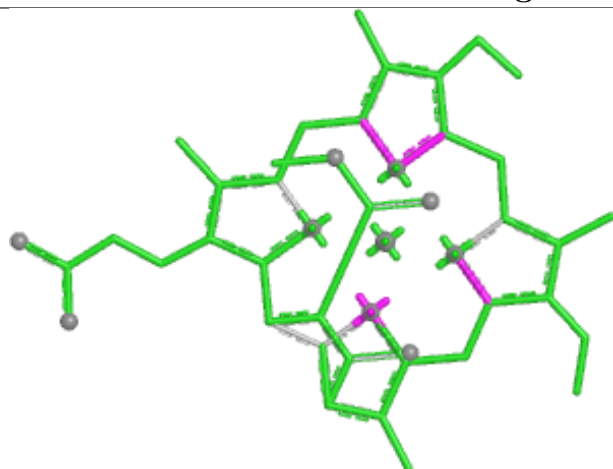




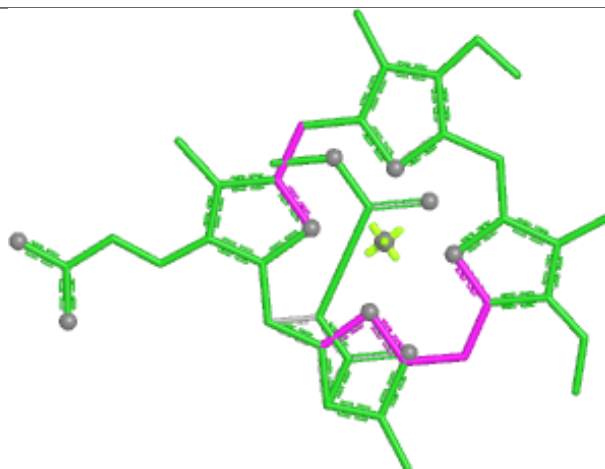




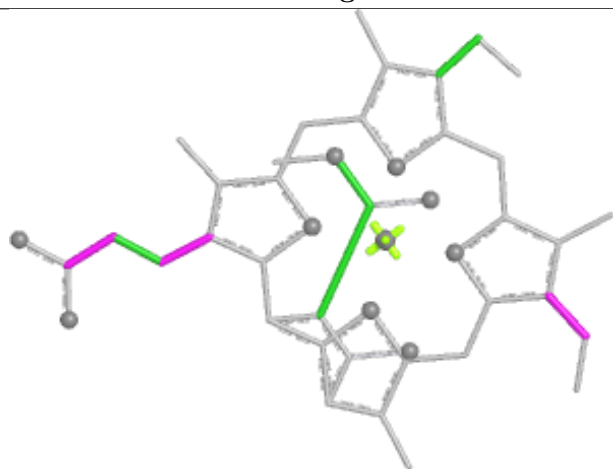
Ligand KC2 K 305



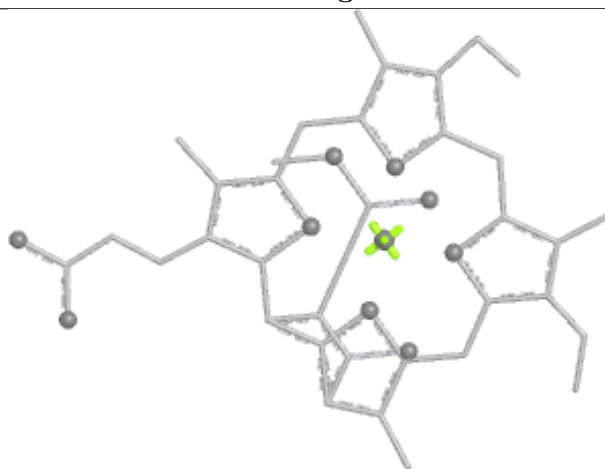
Bond lengths



Bond angles

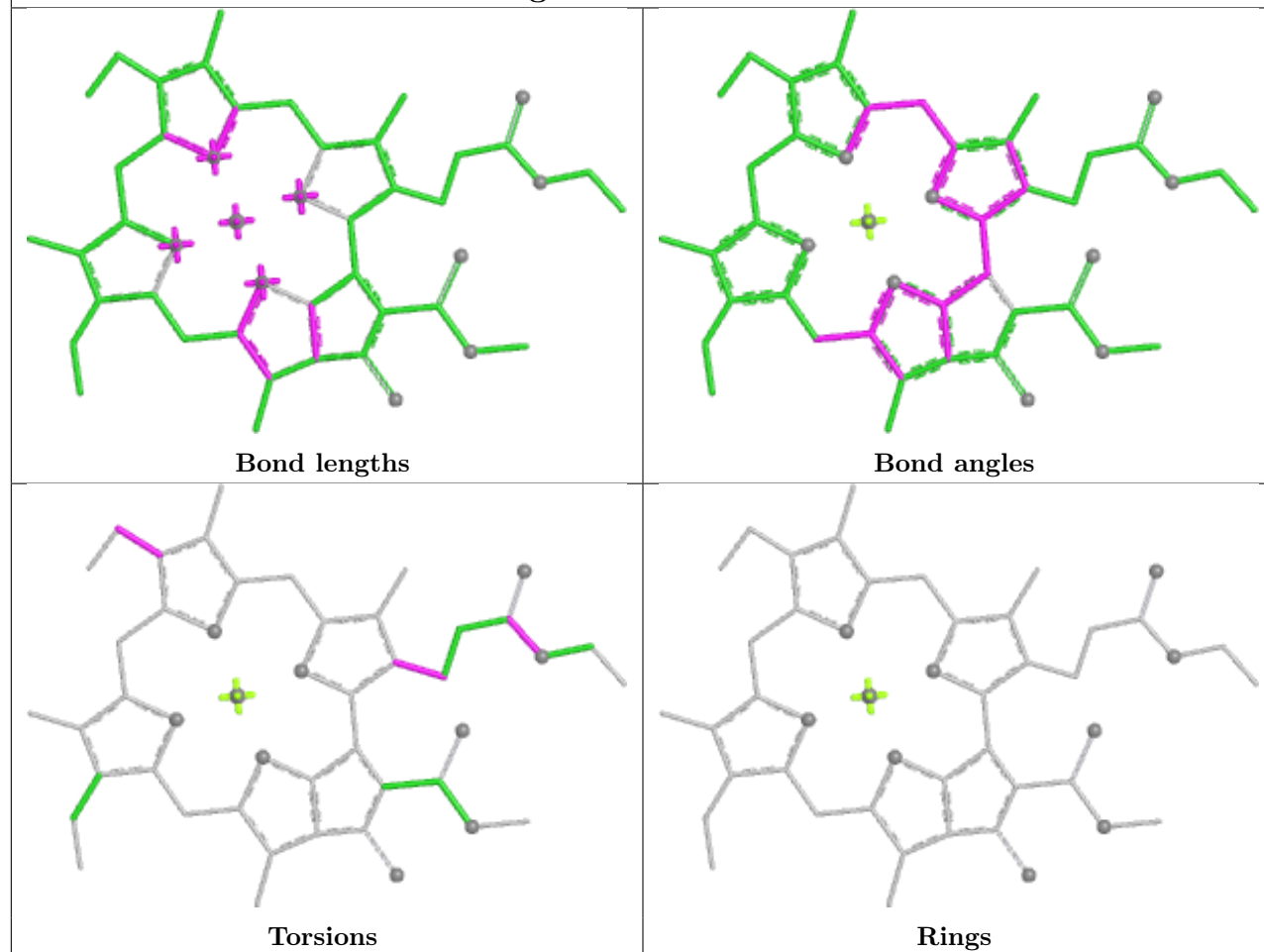


Torsions

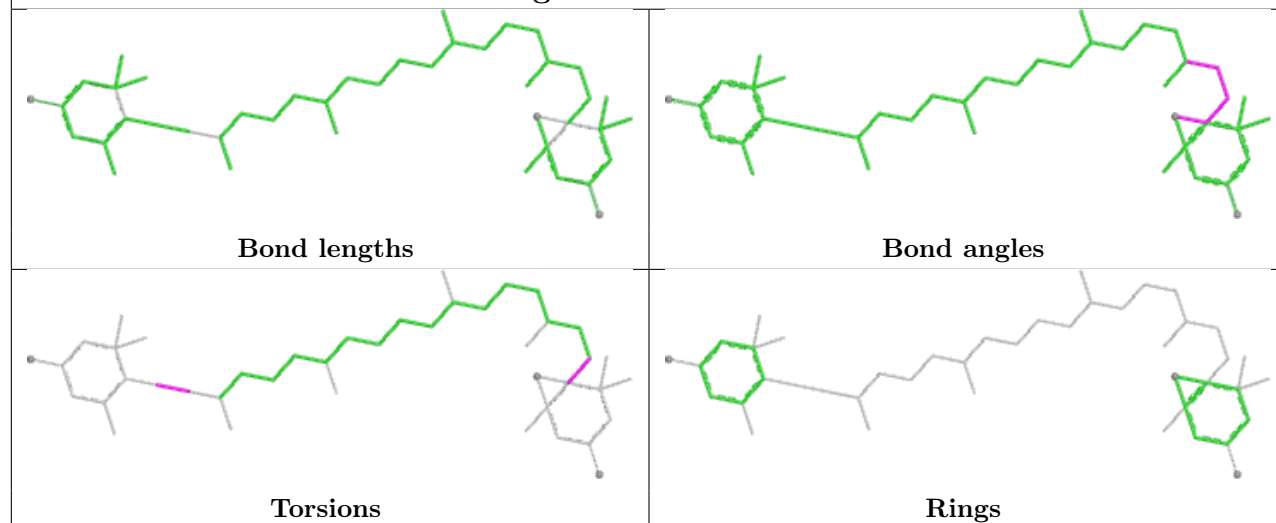


Rings

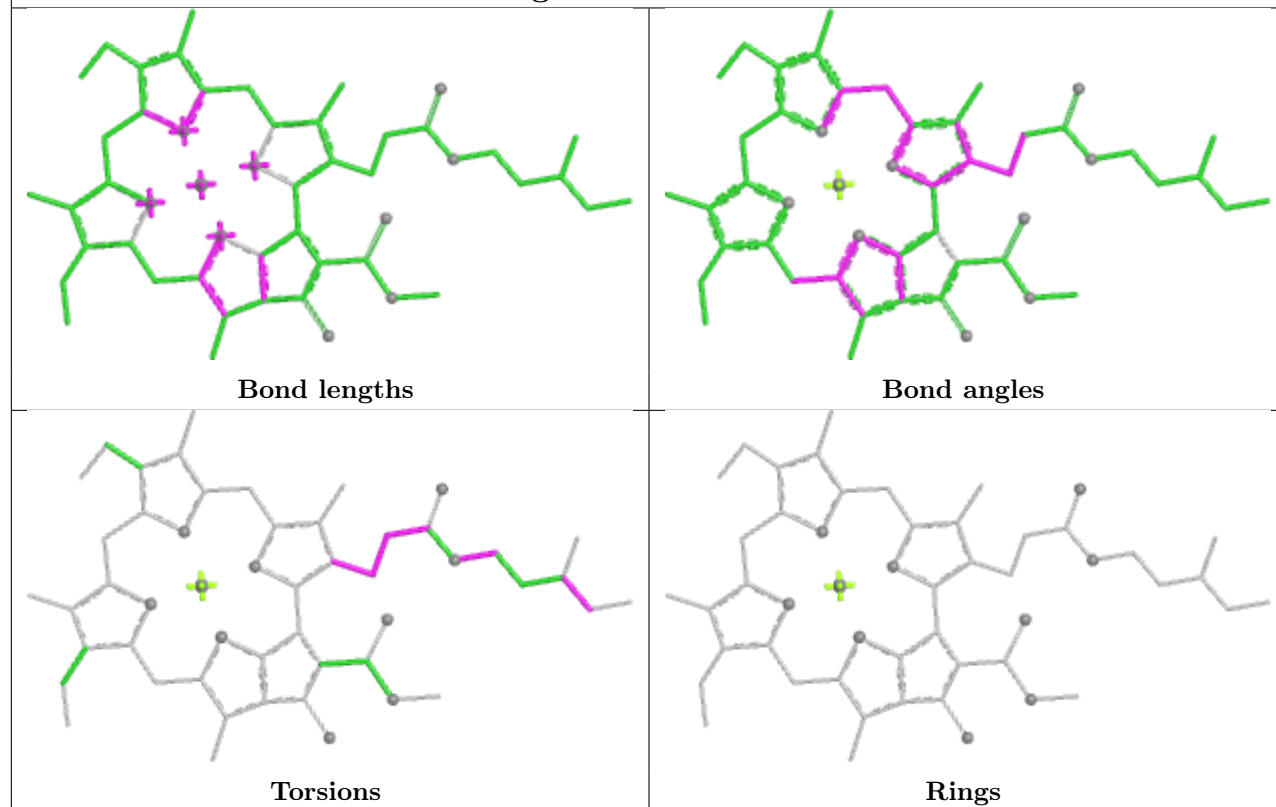
Ligand CLA L 310



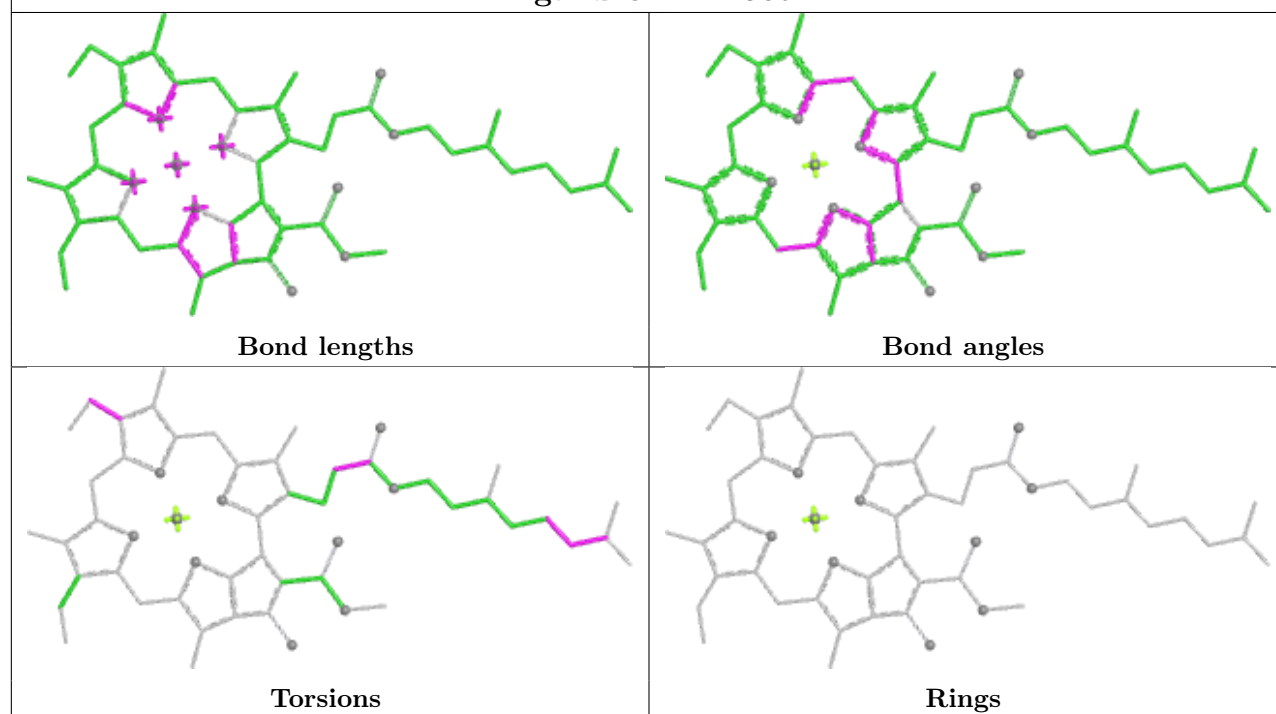
Ligand DD6 C 312

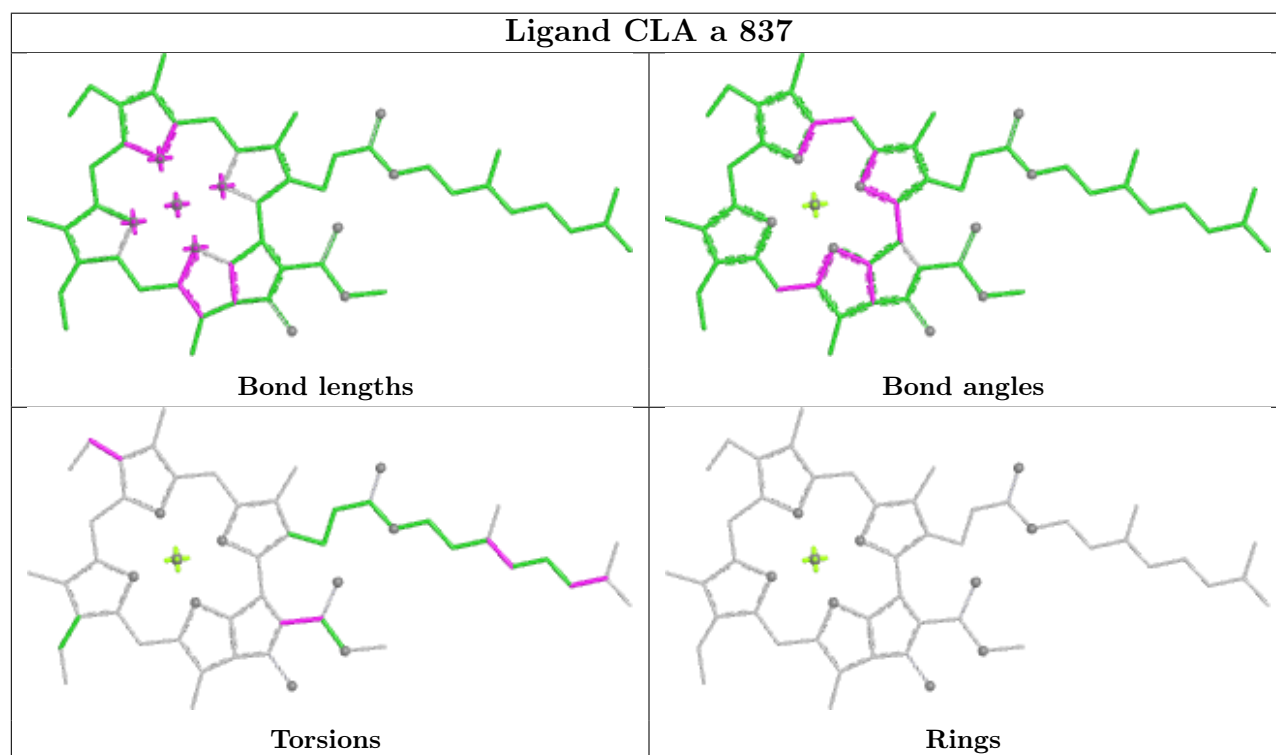
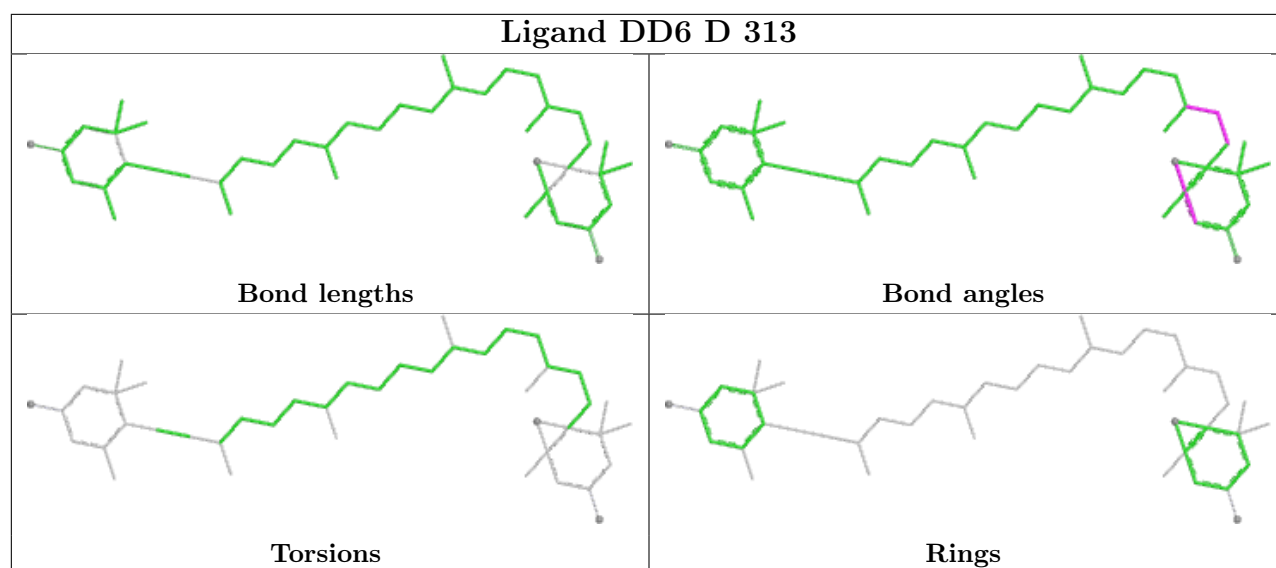


Ligand CLA R 304

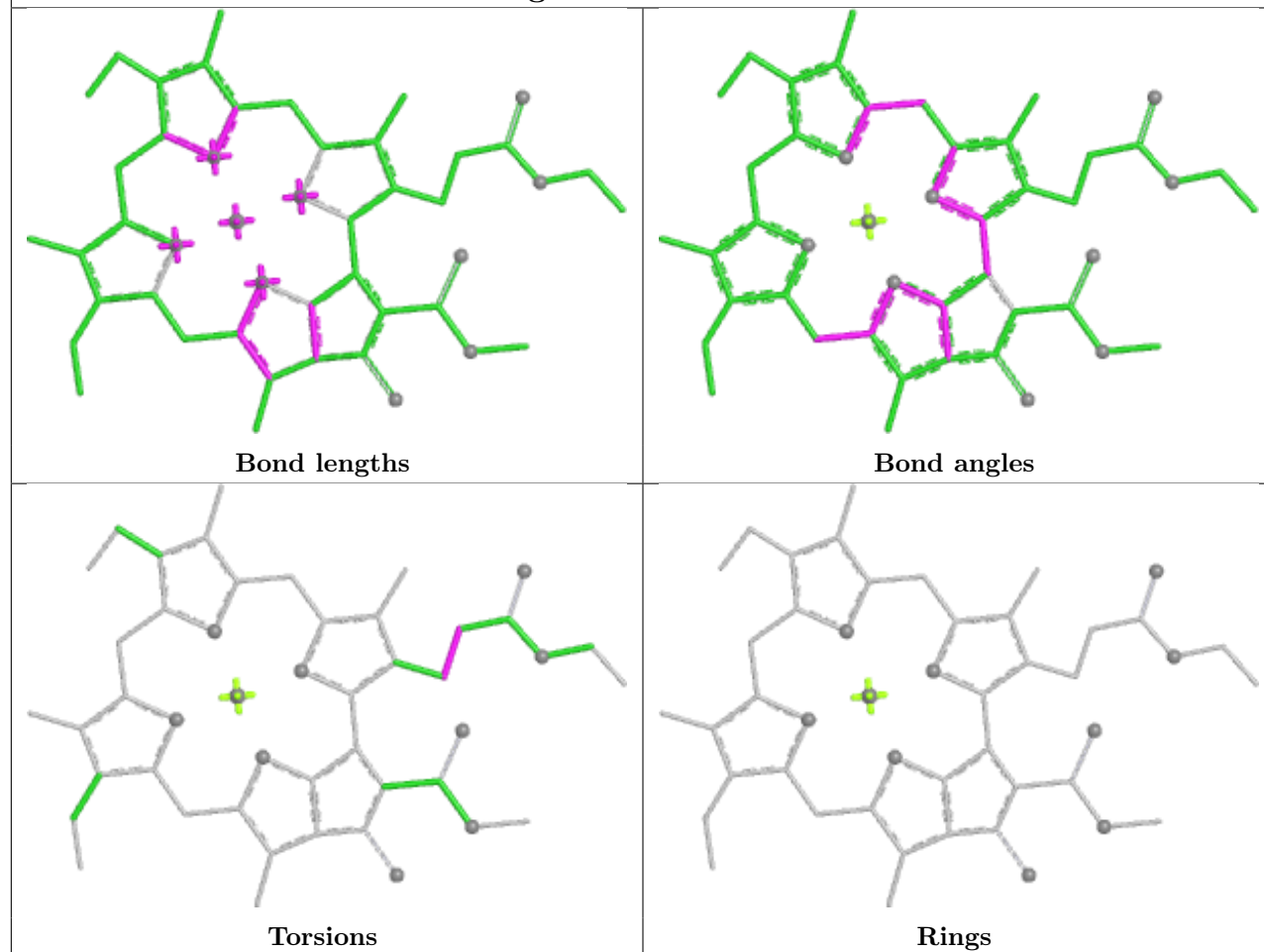


Ligand CLA Z 305

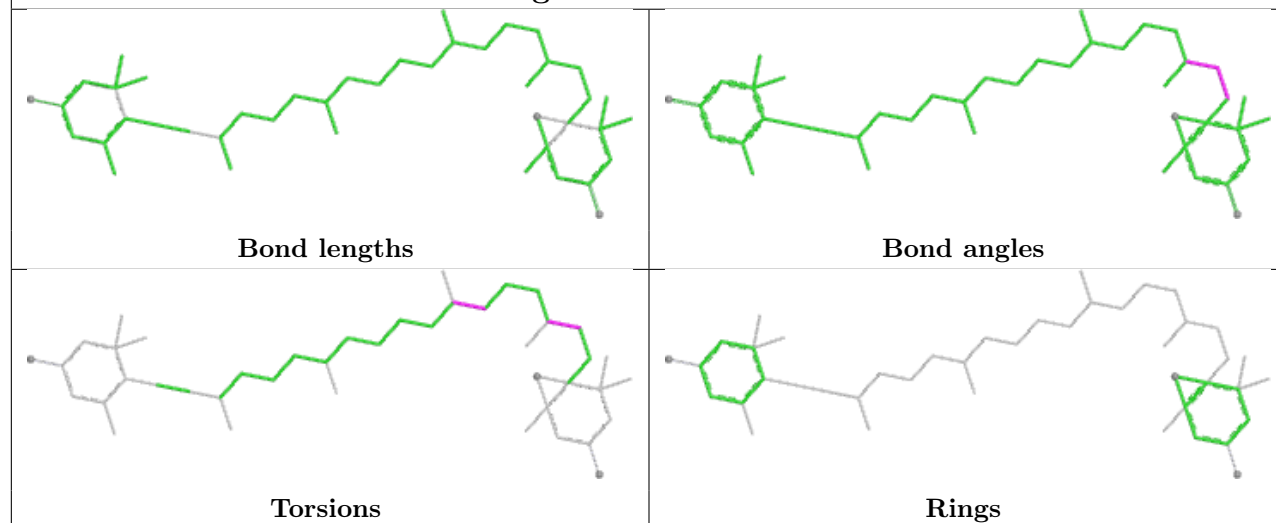


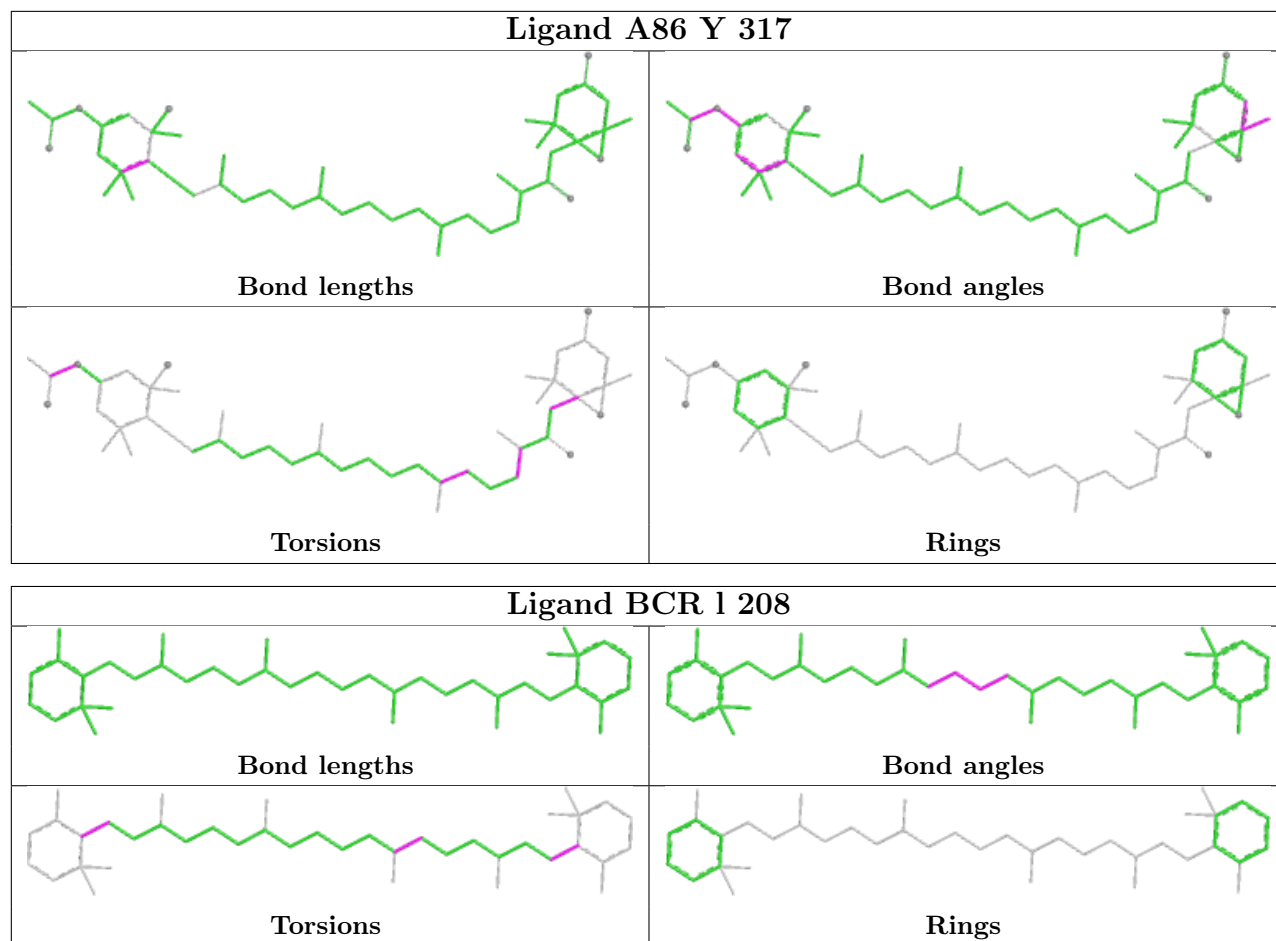


Ligand CLA E 313

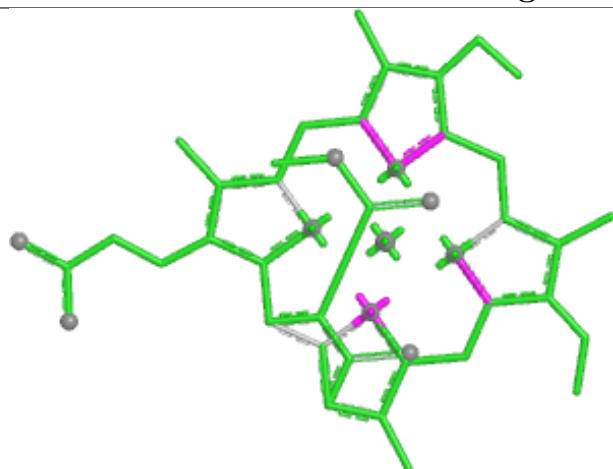


Ligand DD6 D 314

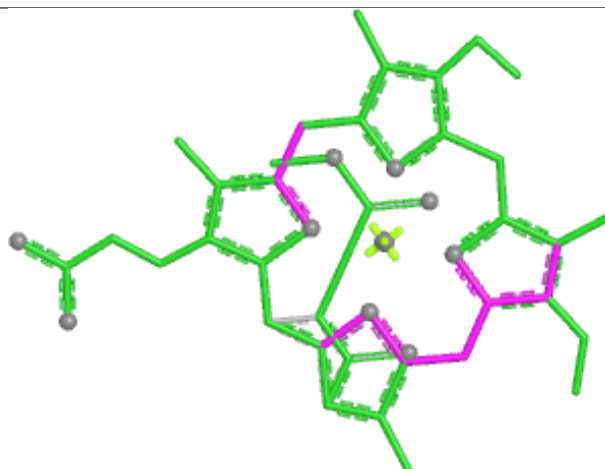




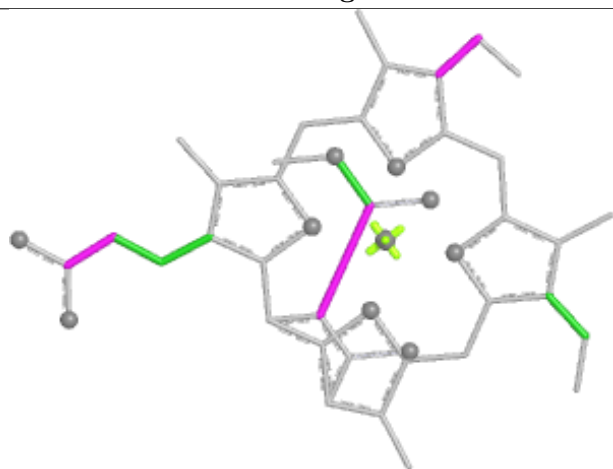
Ligand KC2 L 303



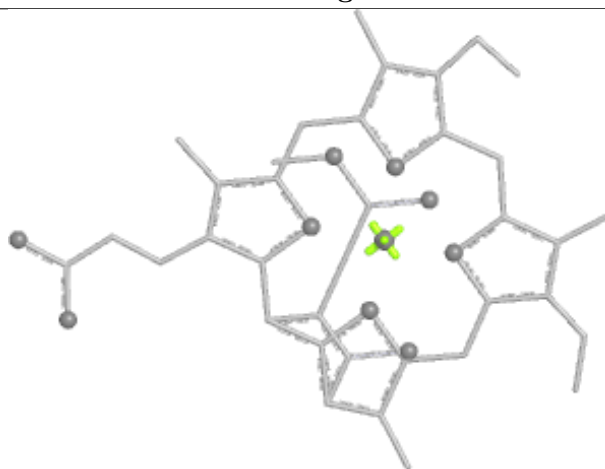
Bond lengths



Bond angles

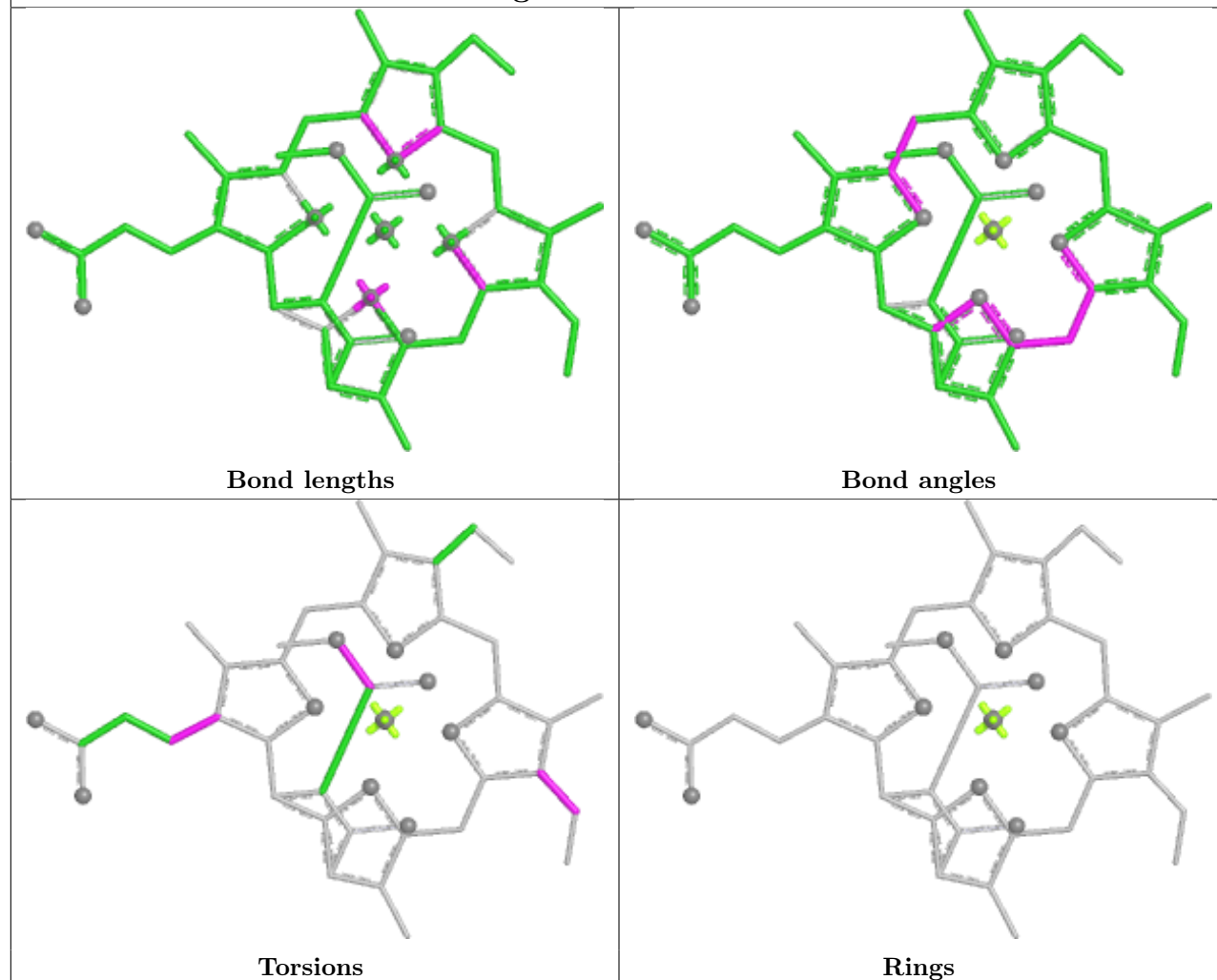


Torsions

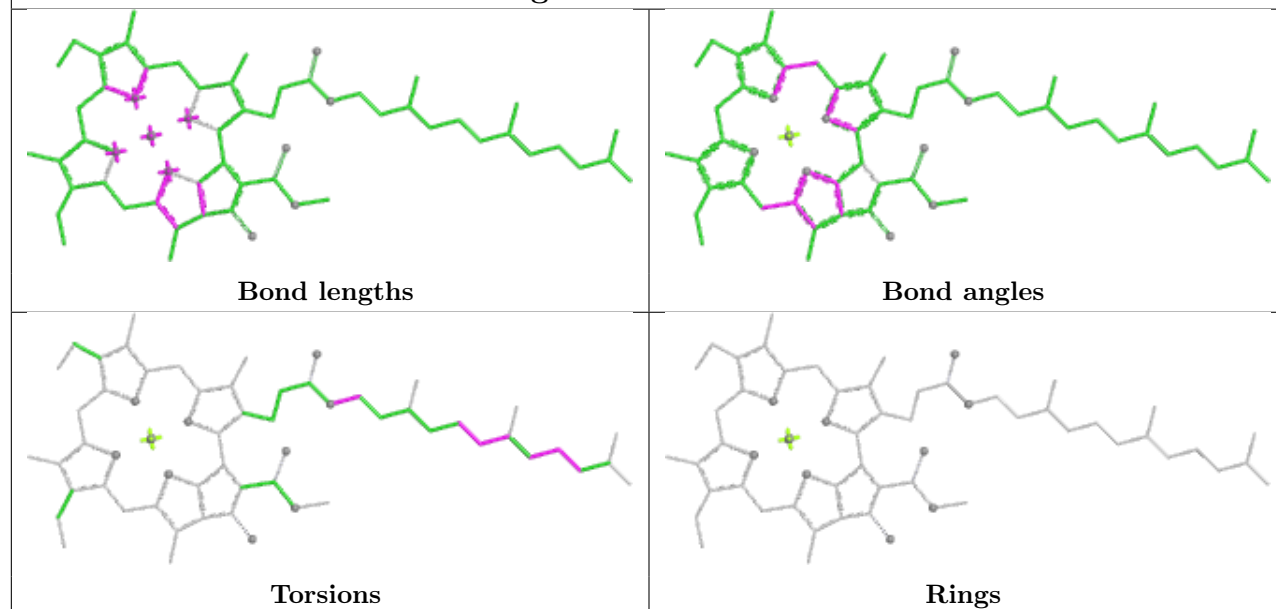


Rings

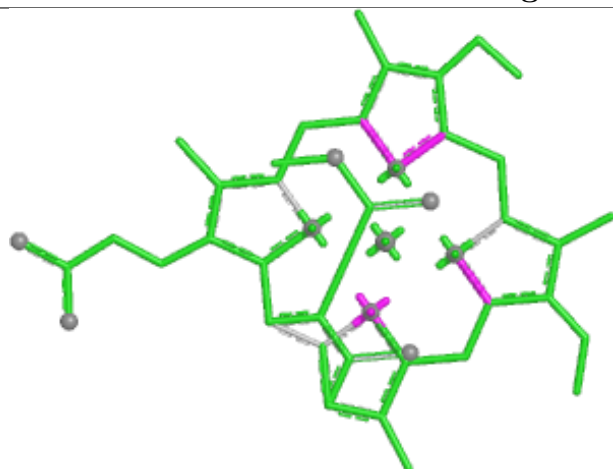
Ligand KC2 o 302



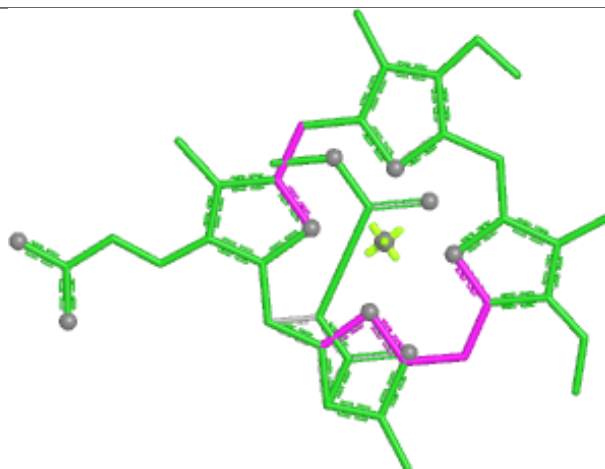
Ligand CLA K 304



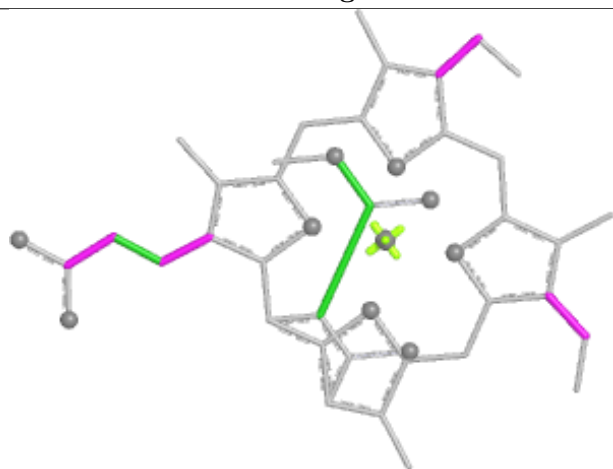
Ligand KC2 z 309



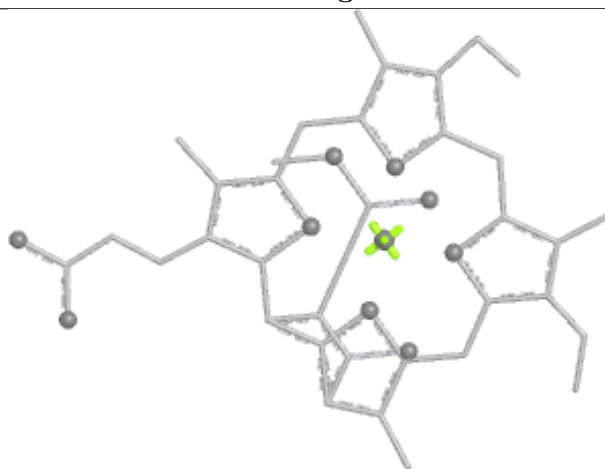
Bond lengths



Bond angles

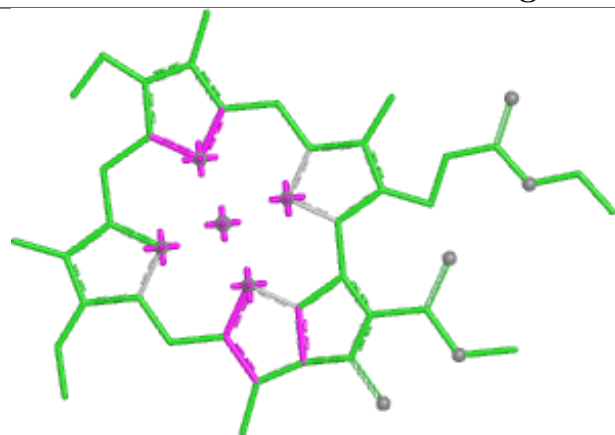


Torsions

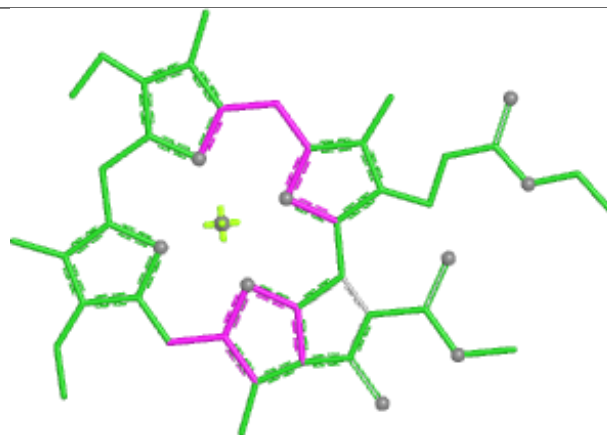


Rings

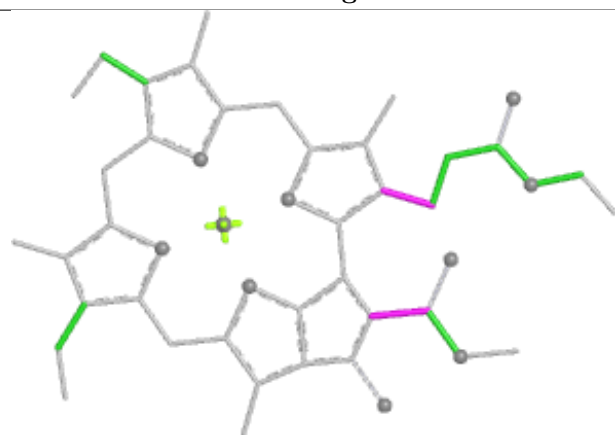
Ligand CLA S 313



Bond lengths



Bond angles

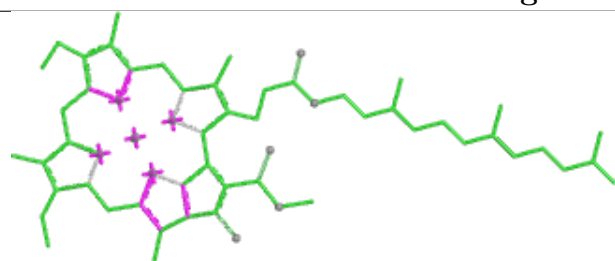


Torsions

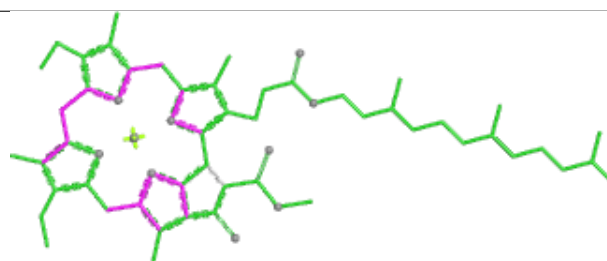


Rings

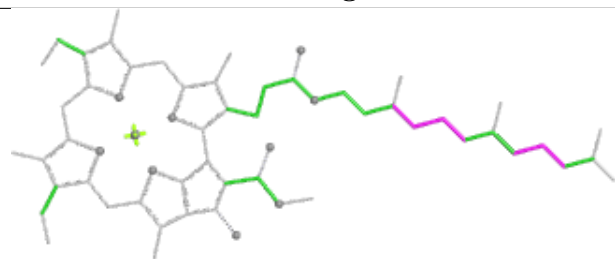
Ligand CLA a 810



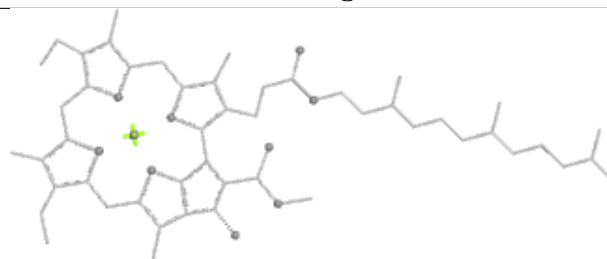
Bond lengths



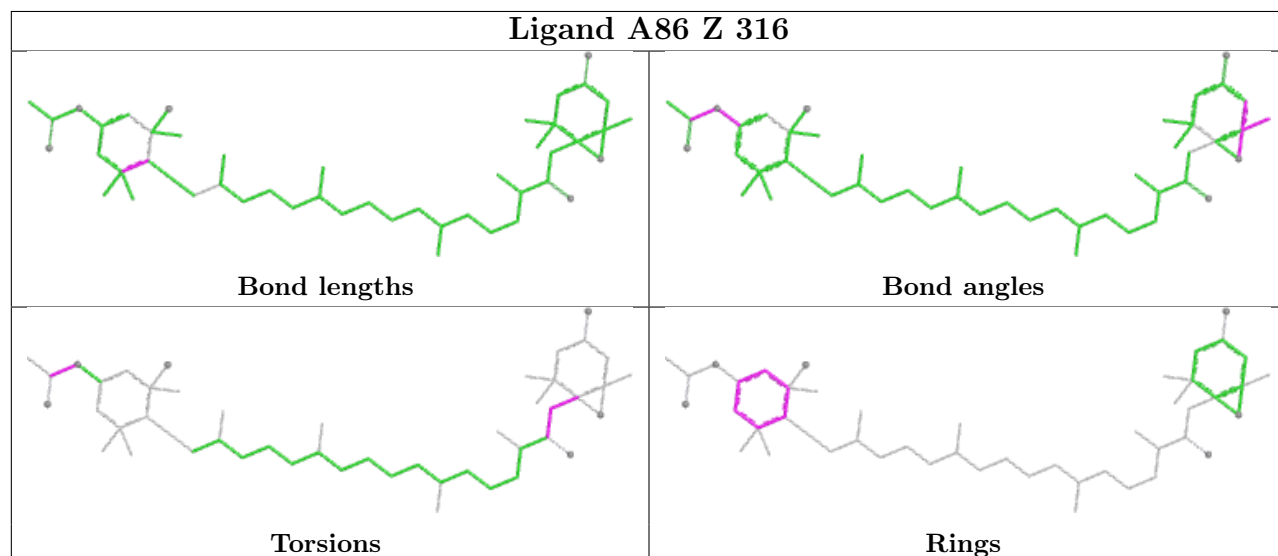
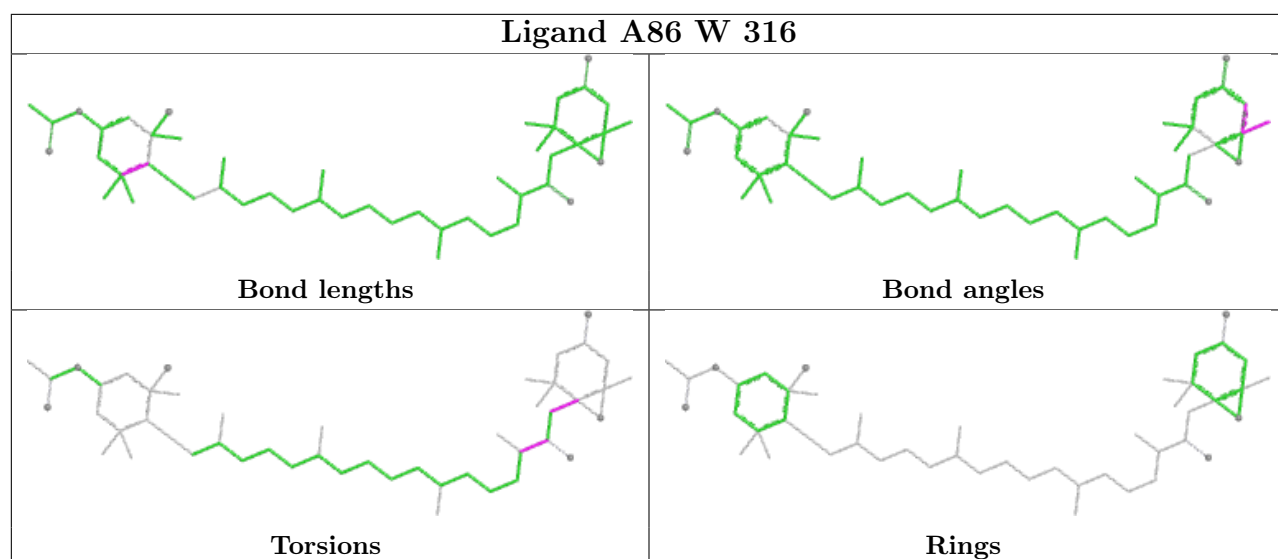
Bond angles

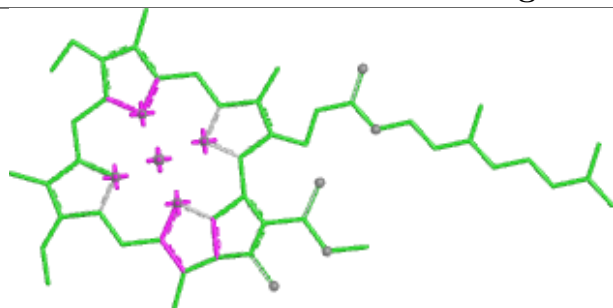


Torsions

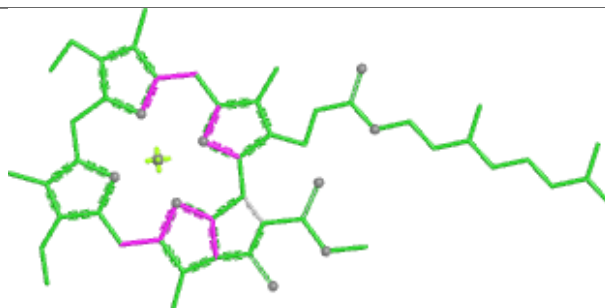


Rings

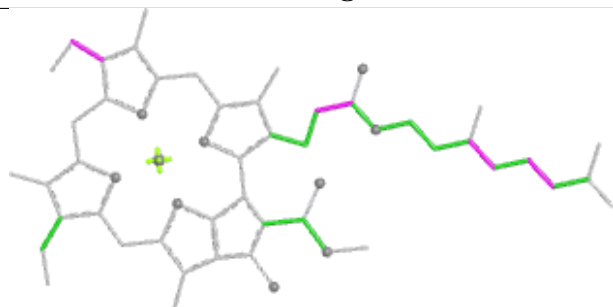


Ligand CLA a 852

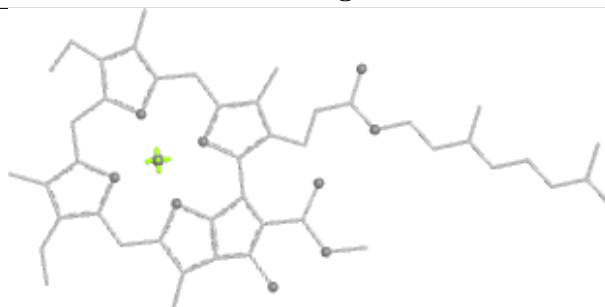
Bond lengths



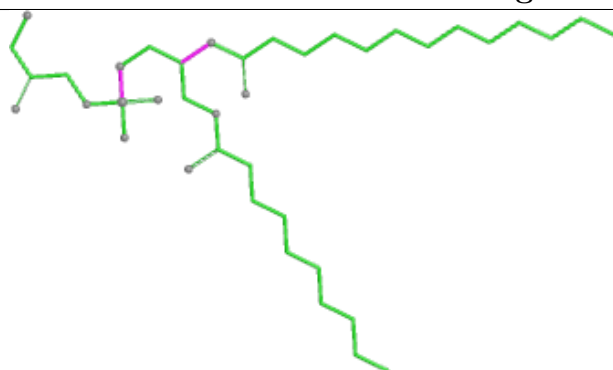
Bond angles



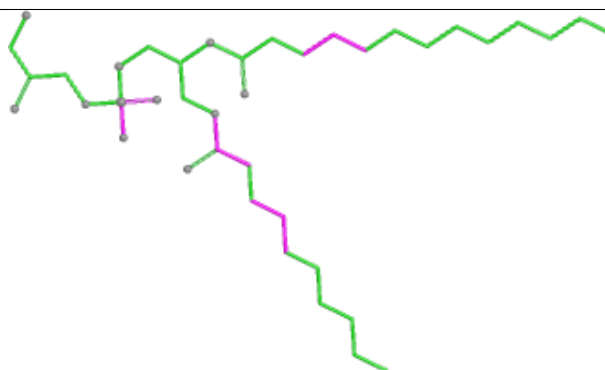
Torsions



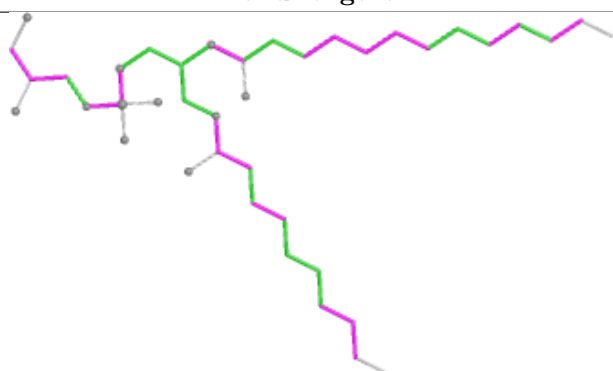
Rings

Ligand LHG S 323

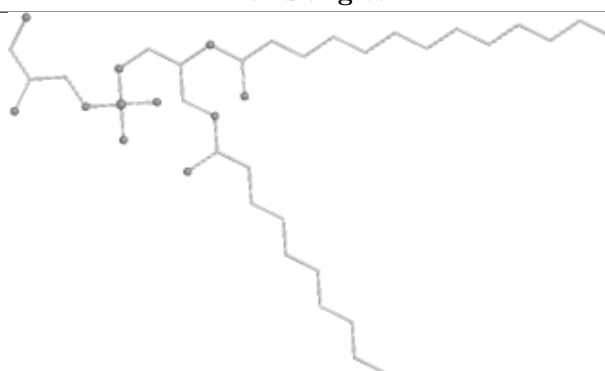
Bond lengths



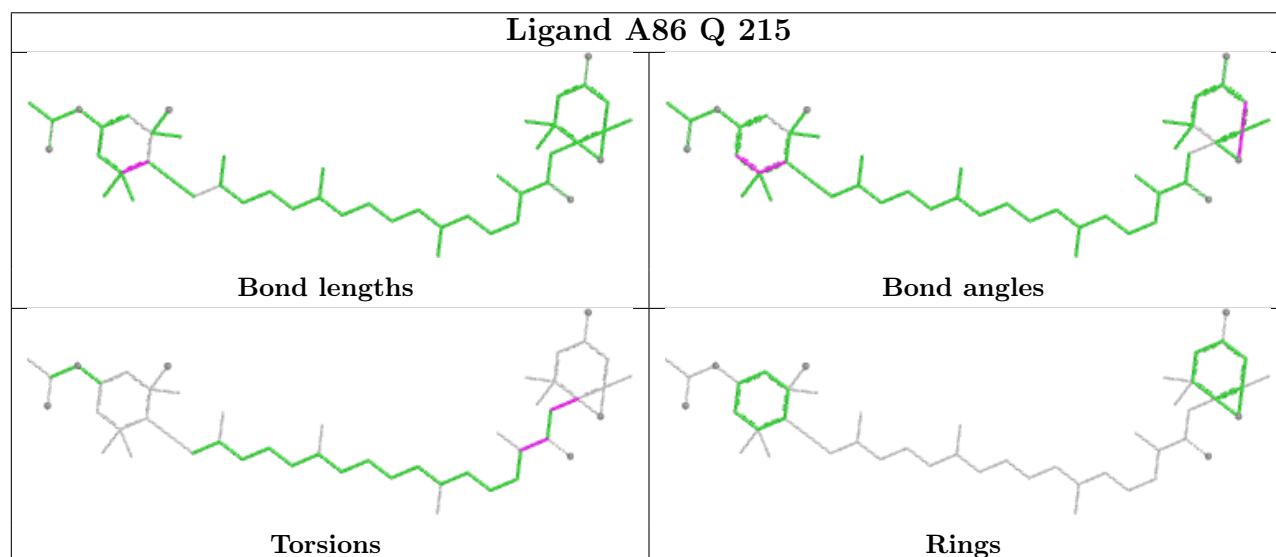
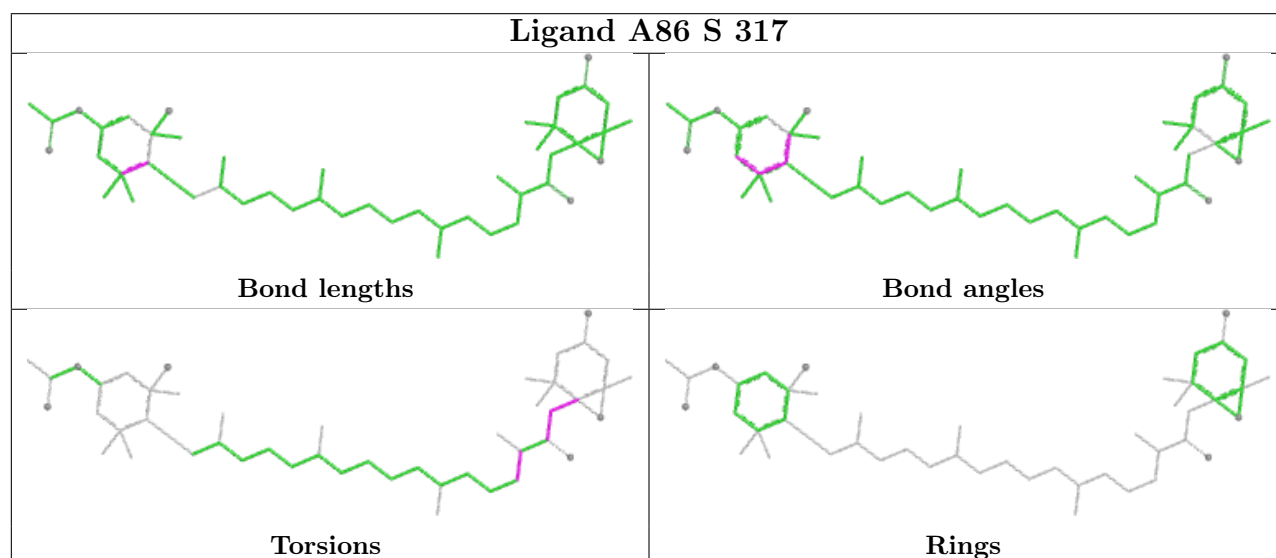
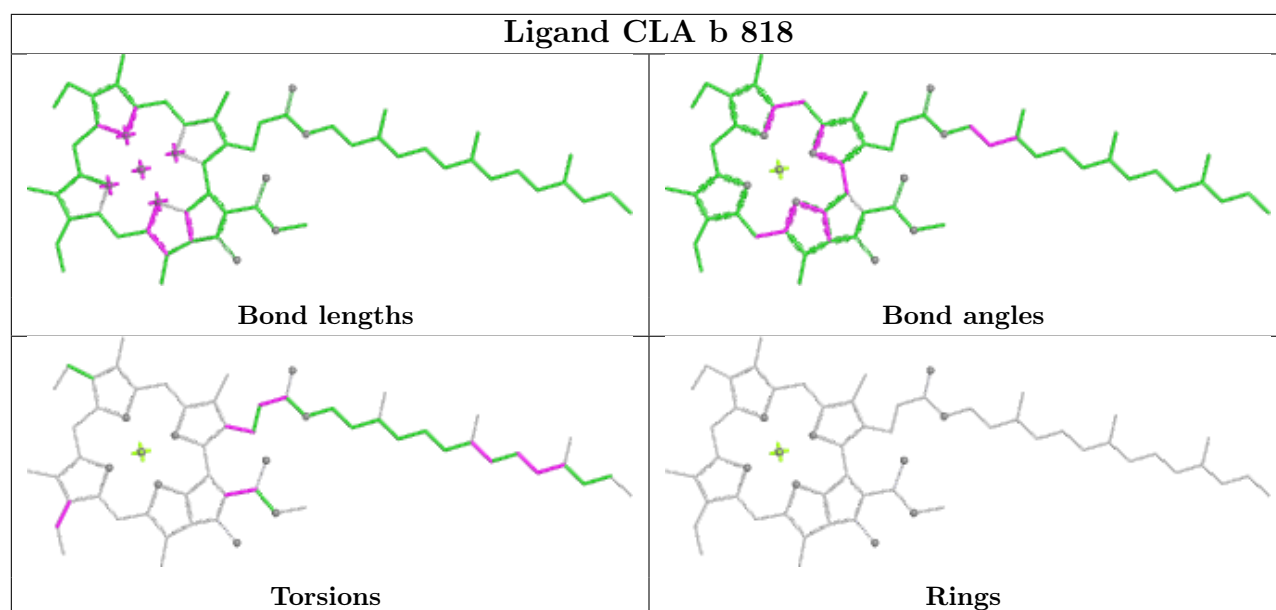
Bond angles

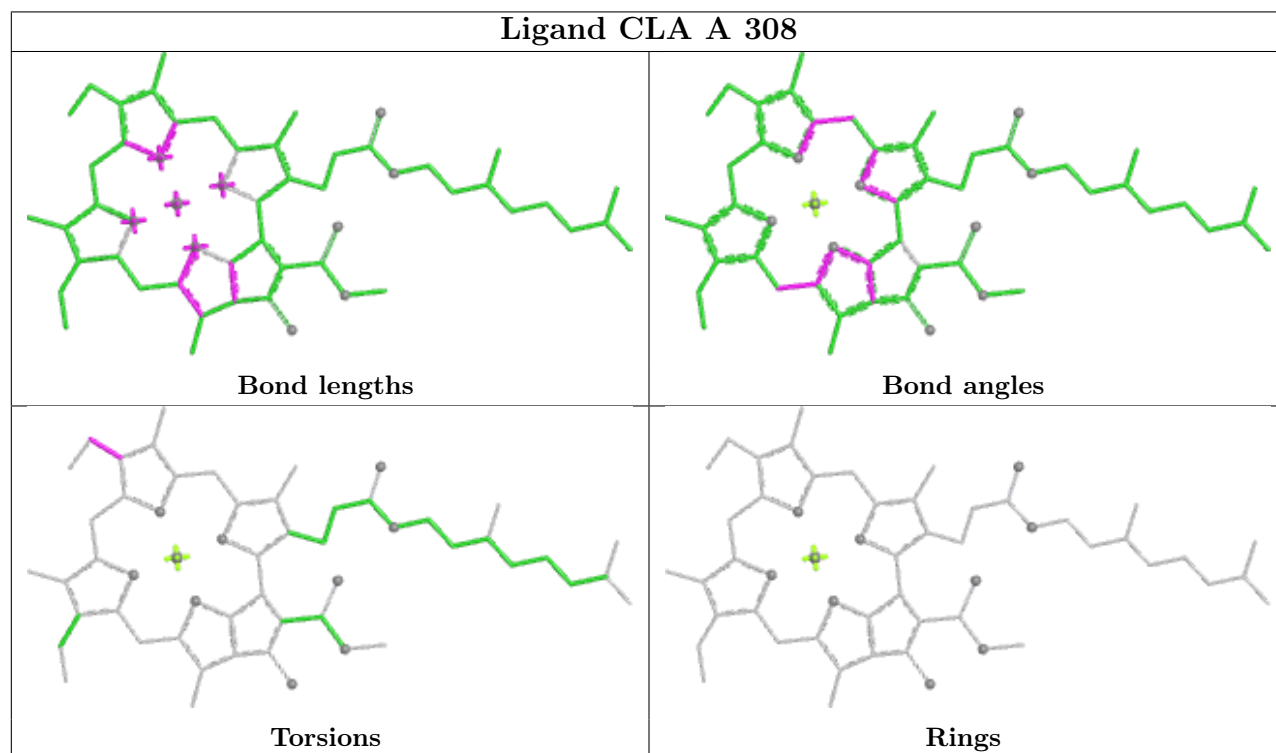
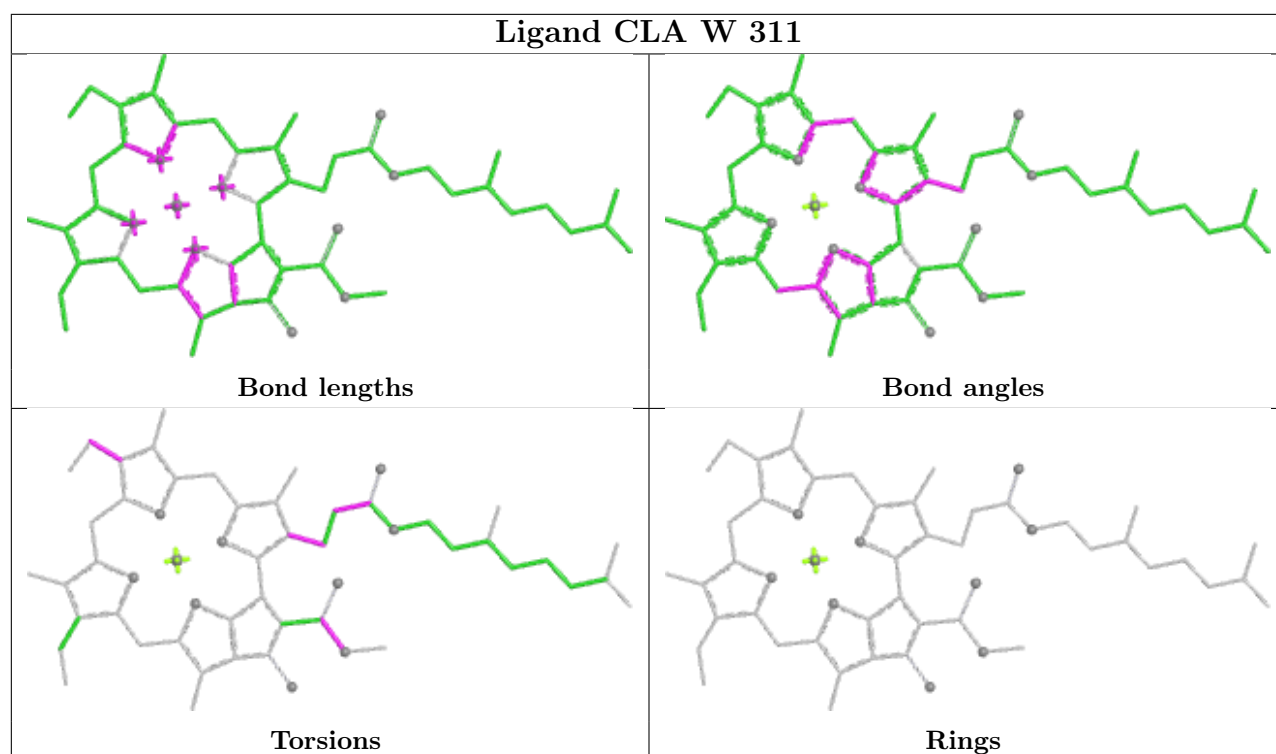


Torsions

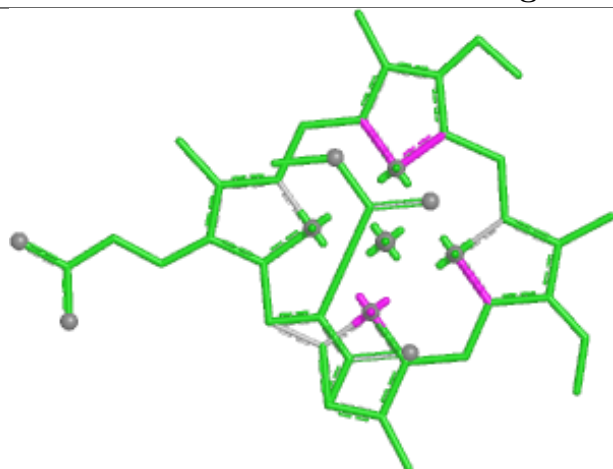


Rings

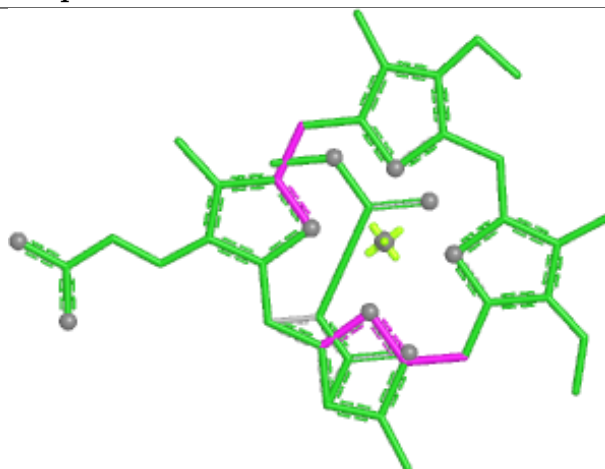




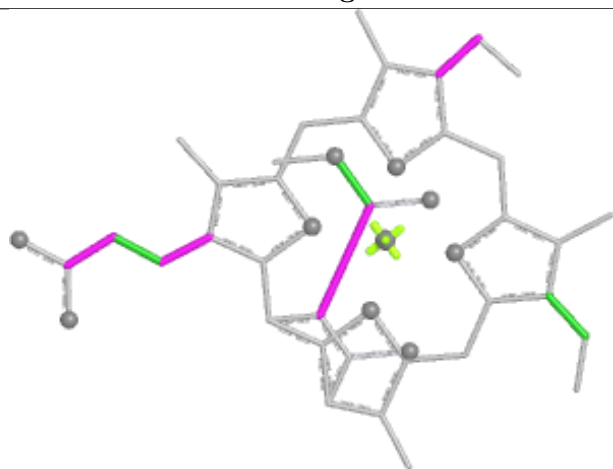
Ligand KC2 q 303



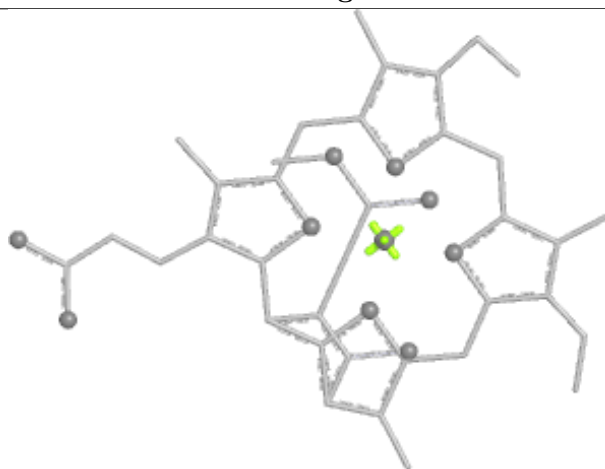
Bond lengths



Bond angles

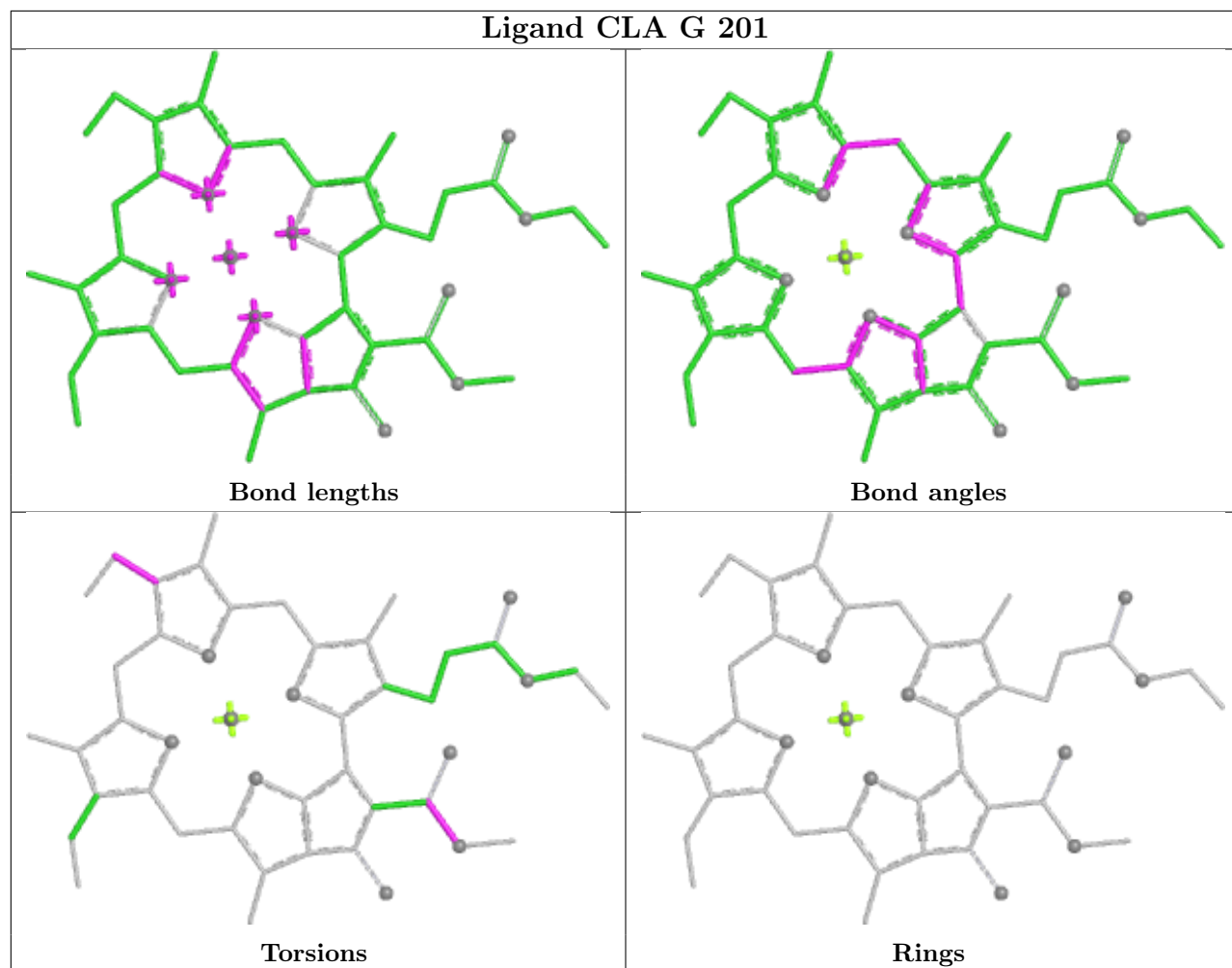


Torsions

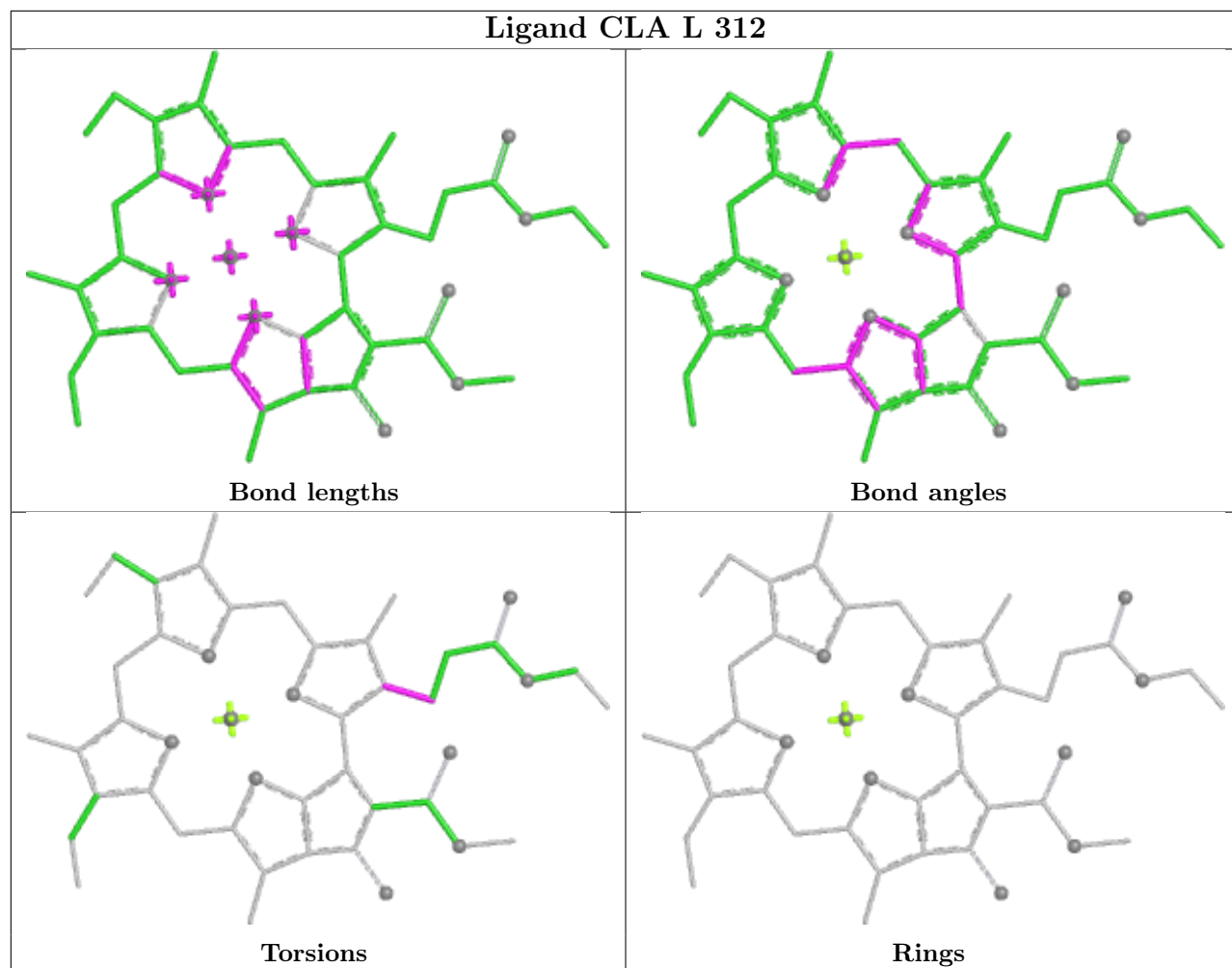


Rings

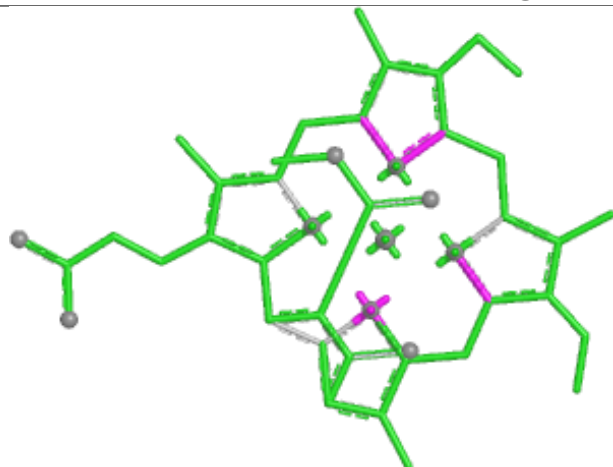
Ligand CLA G 201



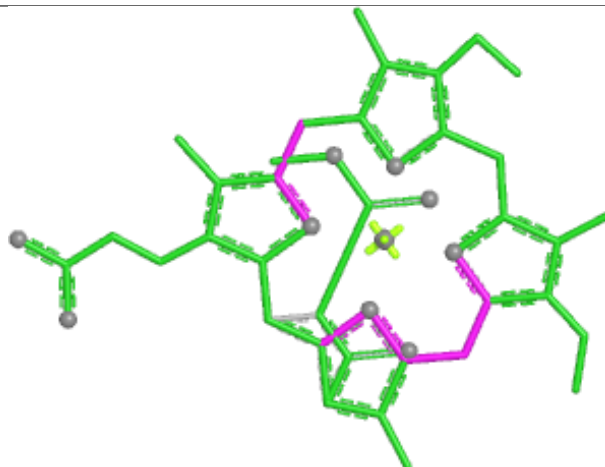
Ligand CLA L 312



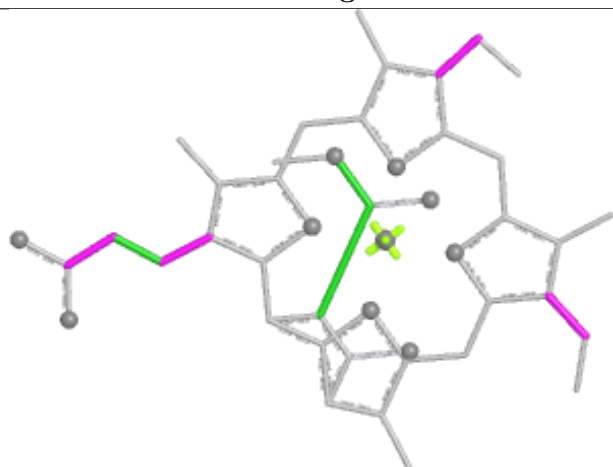
Ligand KC2 P 310



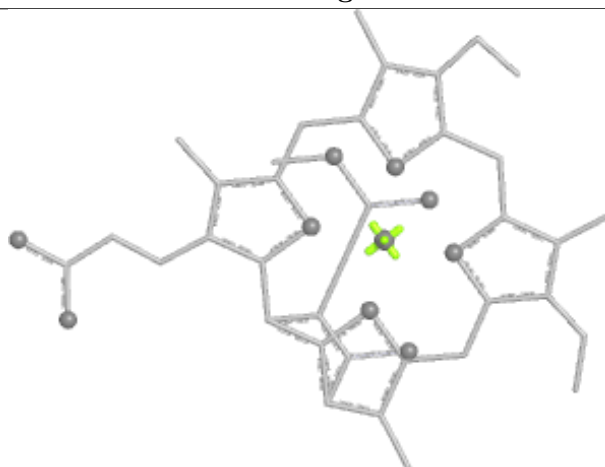
Bond lengths



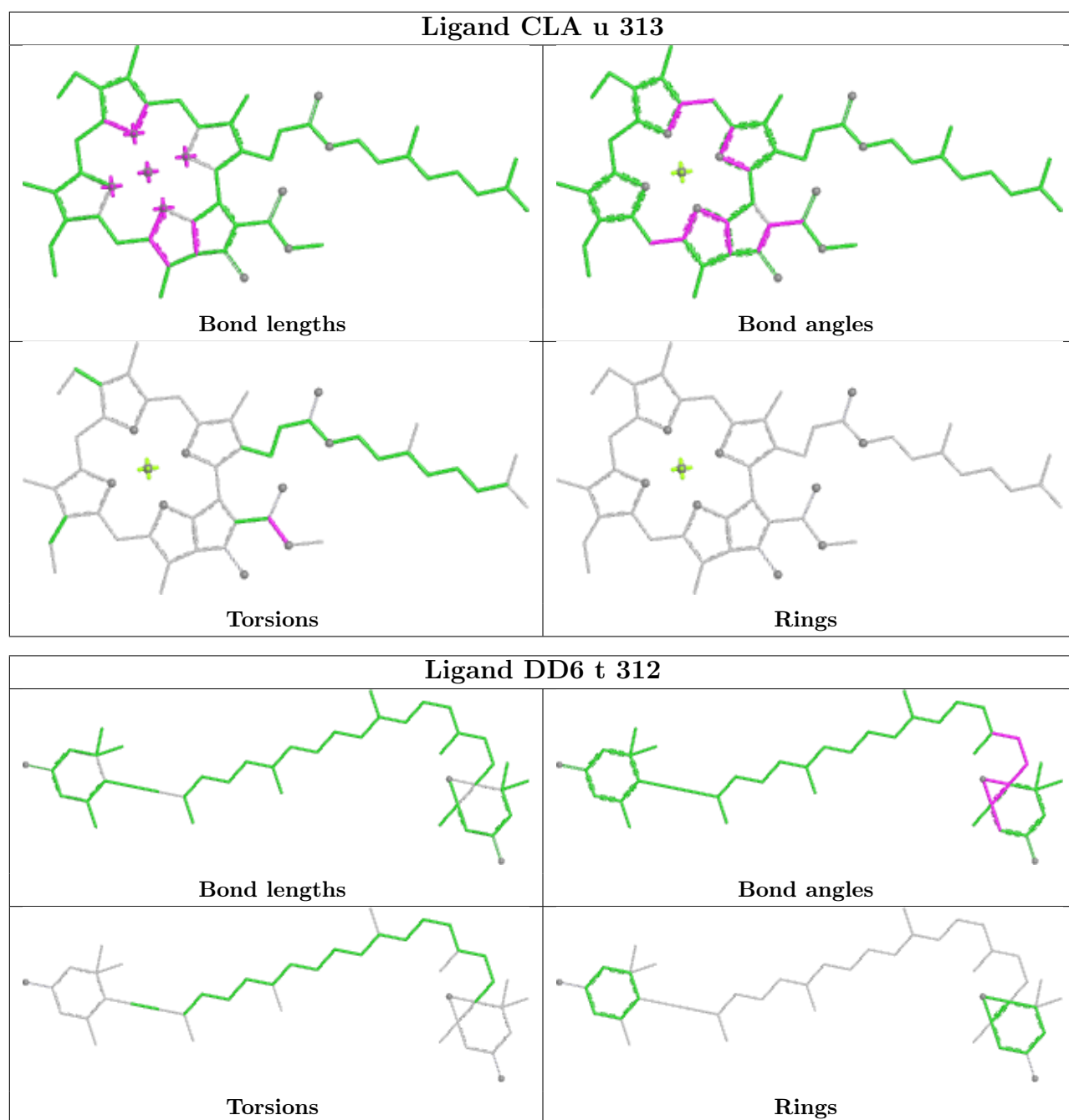
Bond angles

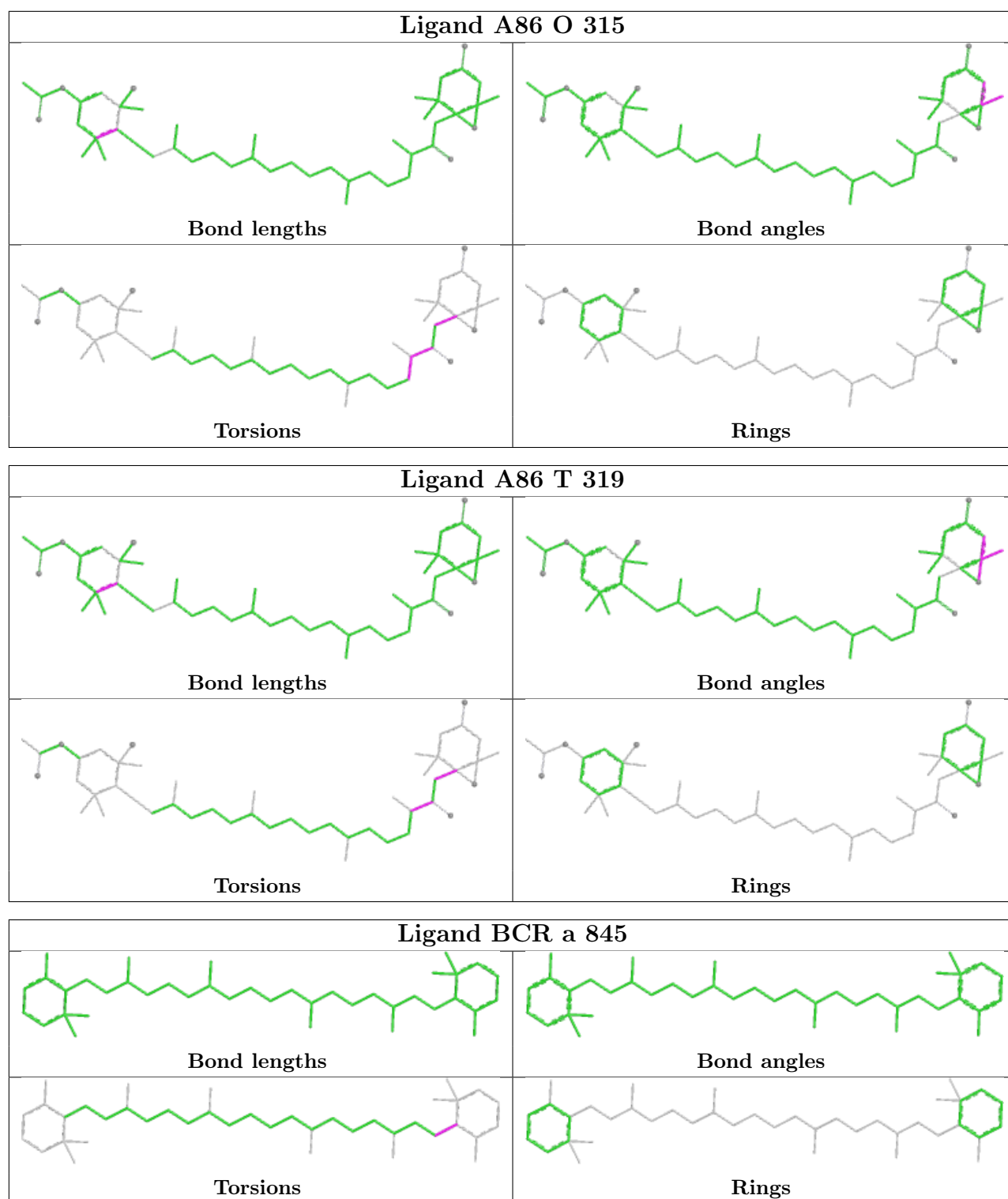


Torsions

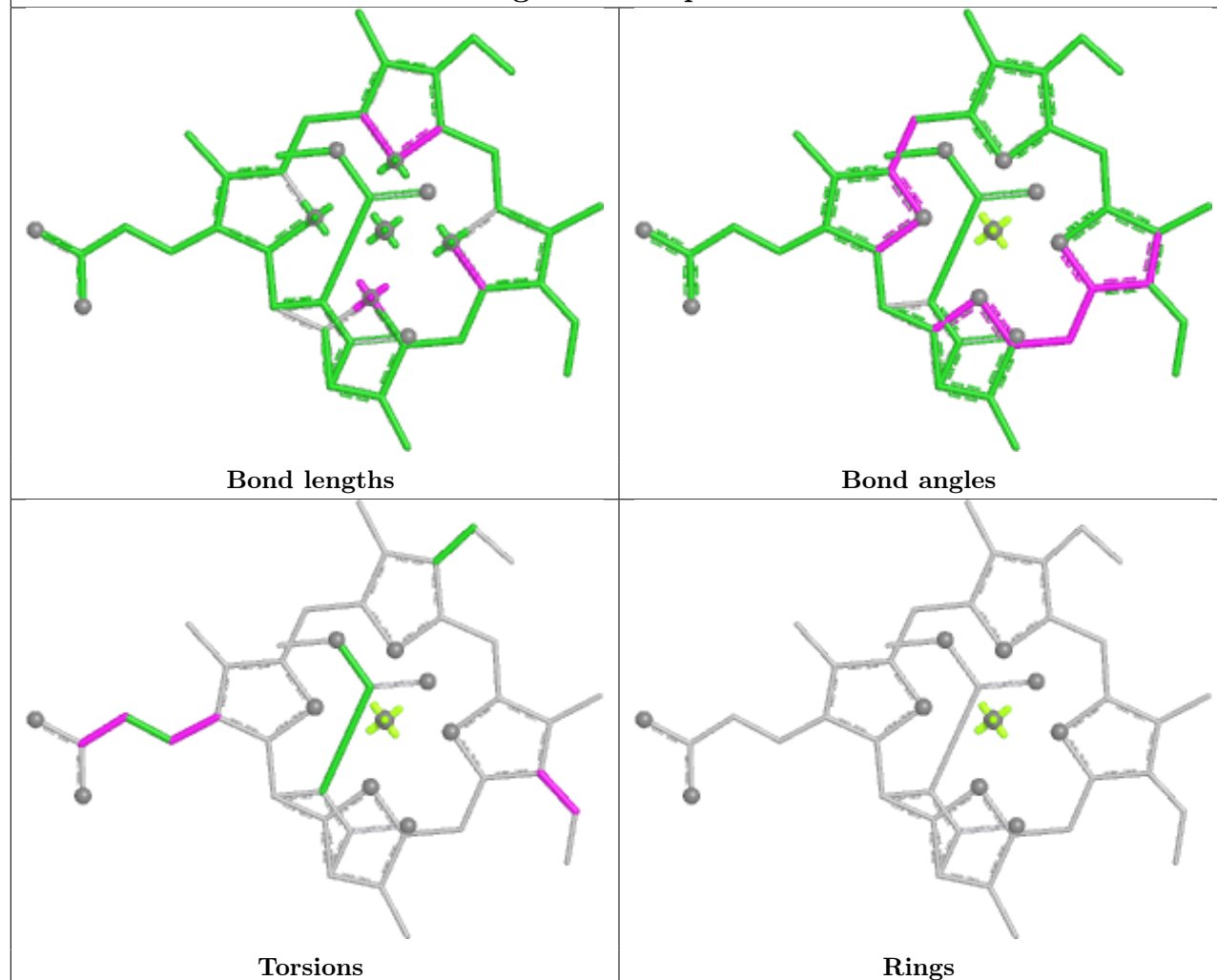


Rings

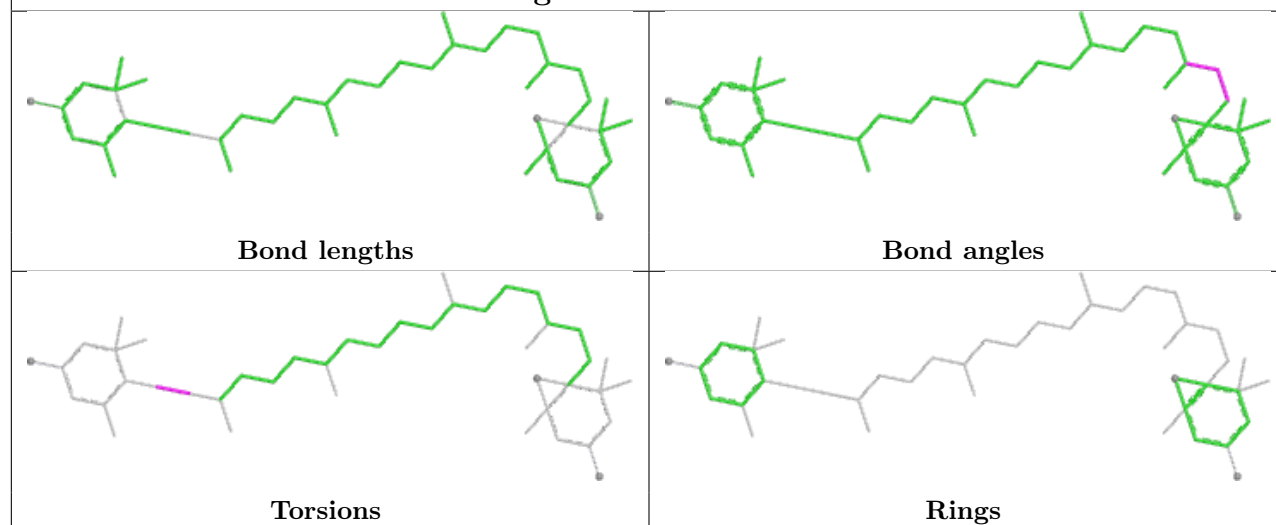




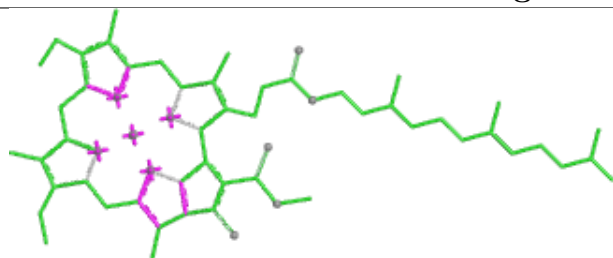
Ligand KC2 q 302



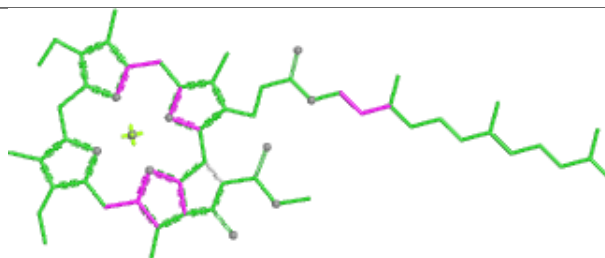
Ligand DD6 T 314



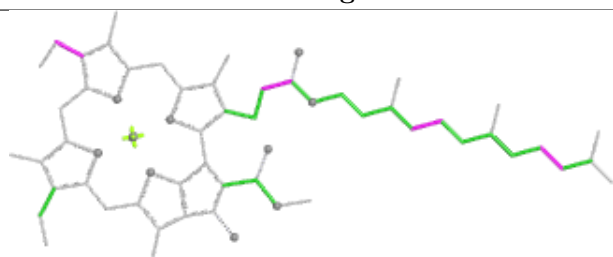
Ligand CLA R 306



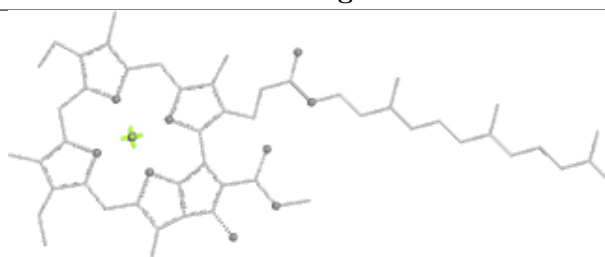
Bond lengths



Bond angles

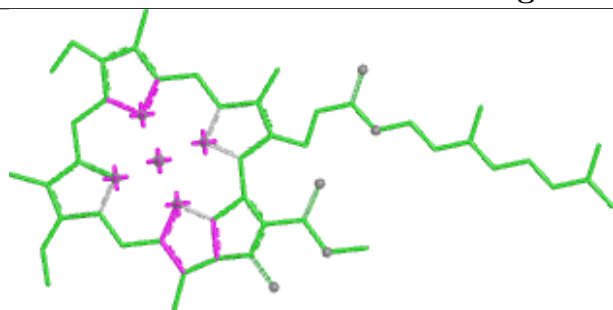


Torsions

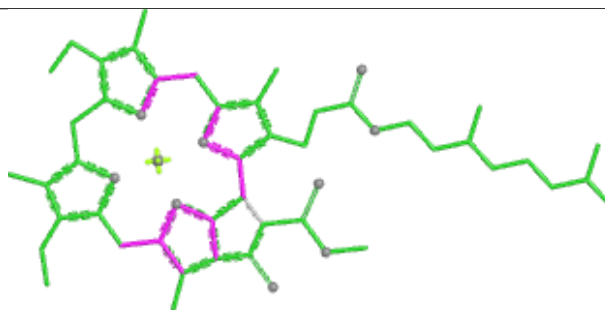


Rings

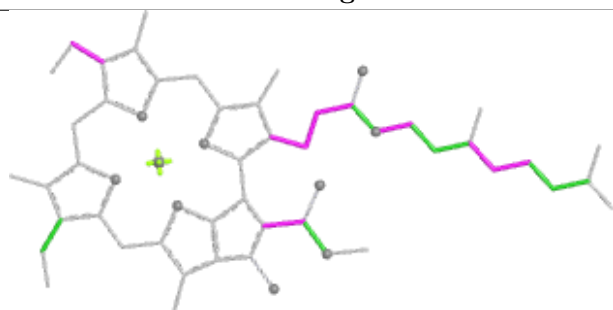
Ligand CLA S 314



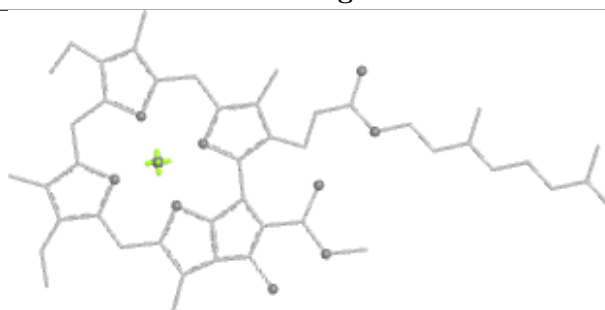
Bond lengths



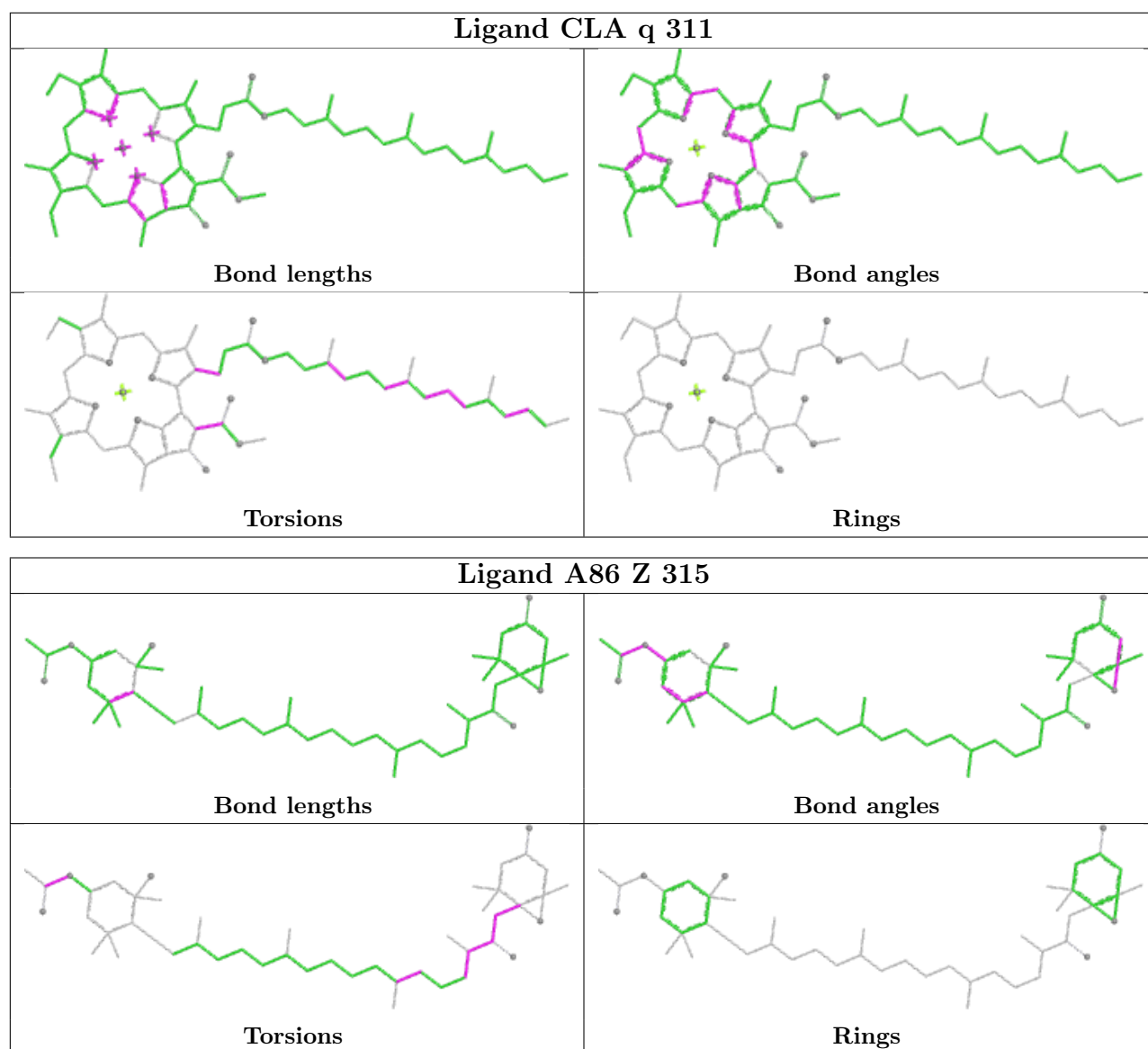
Bond angles

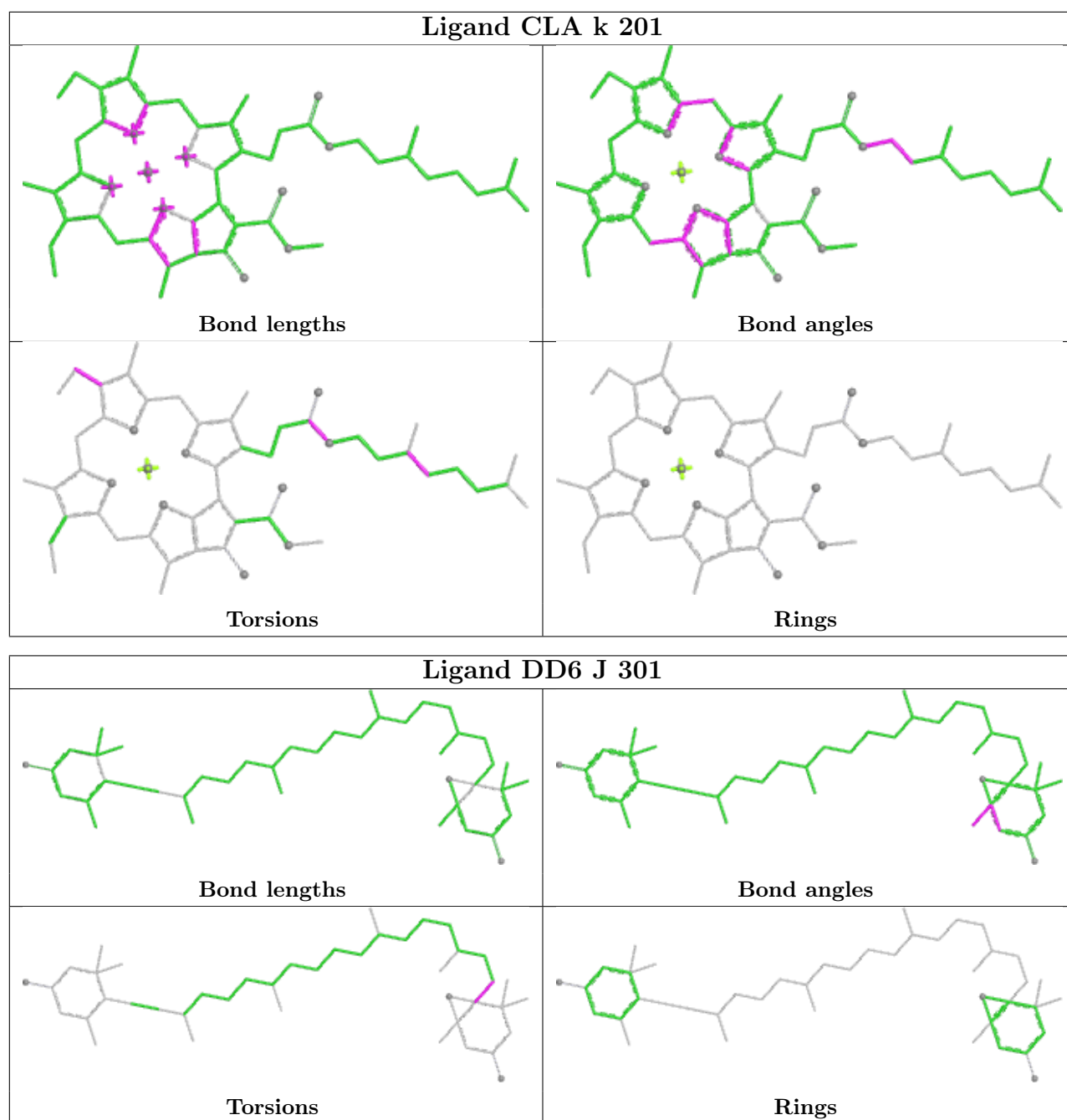


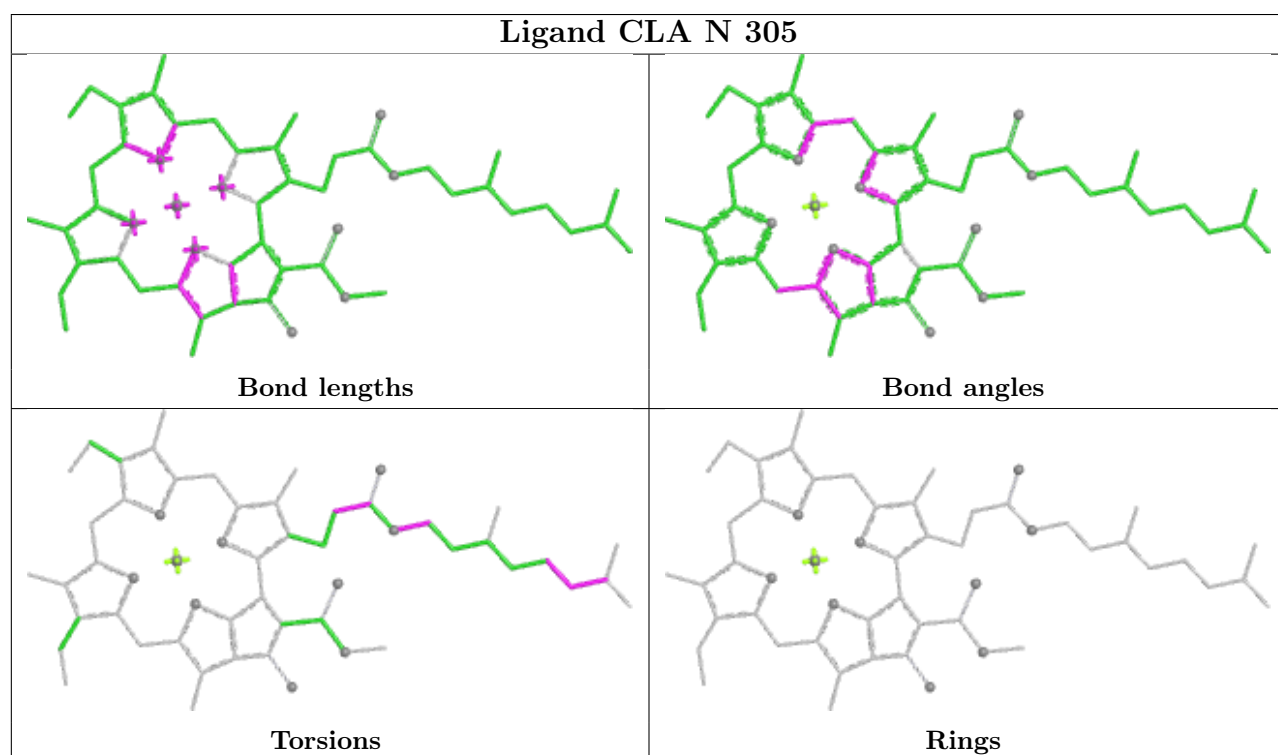
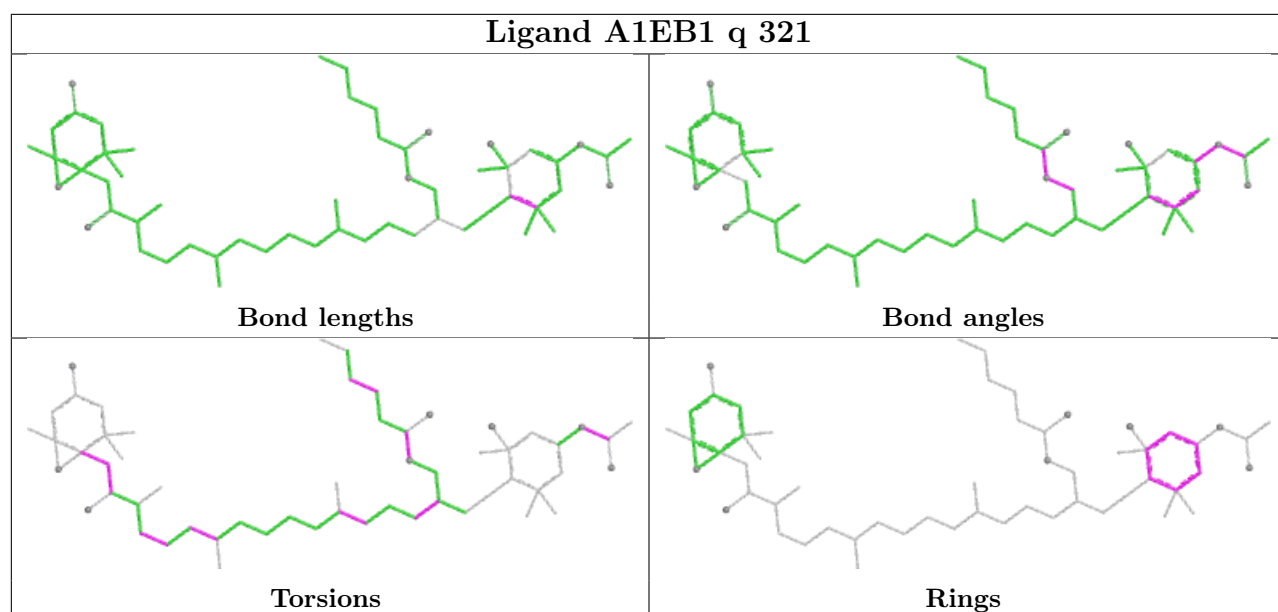
Torsions

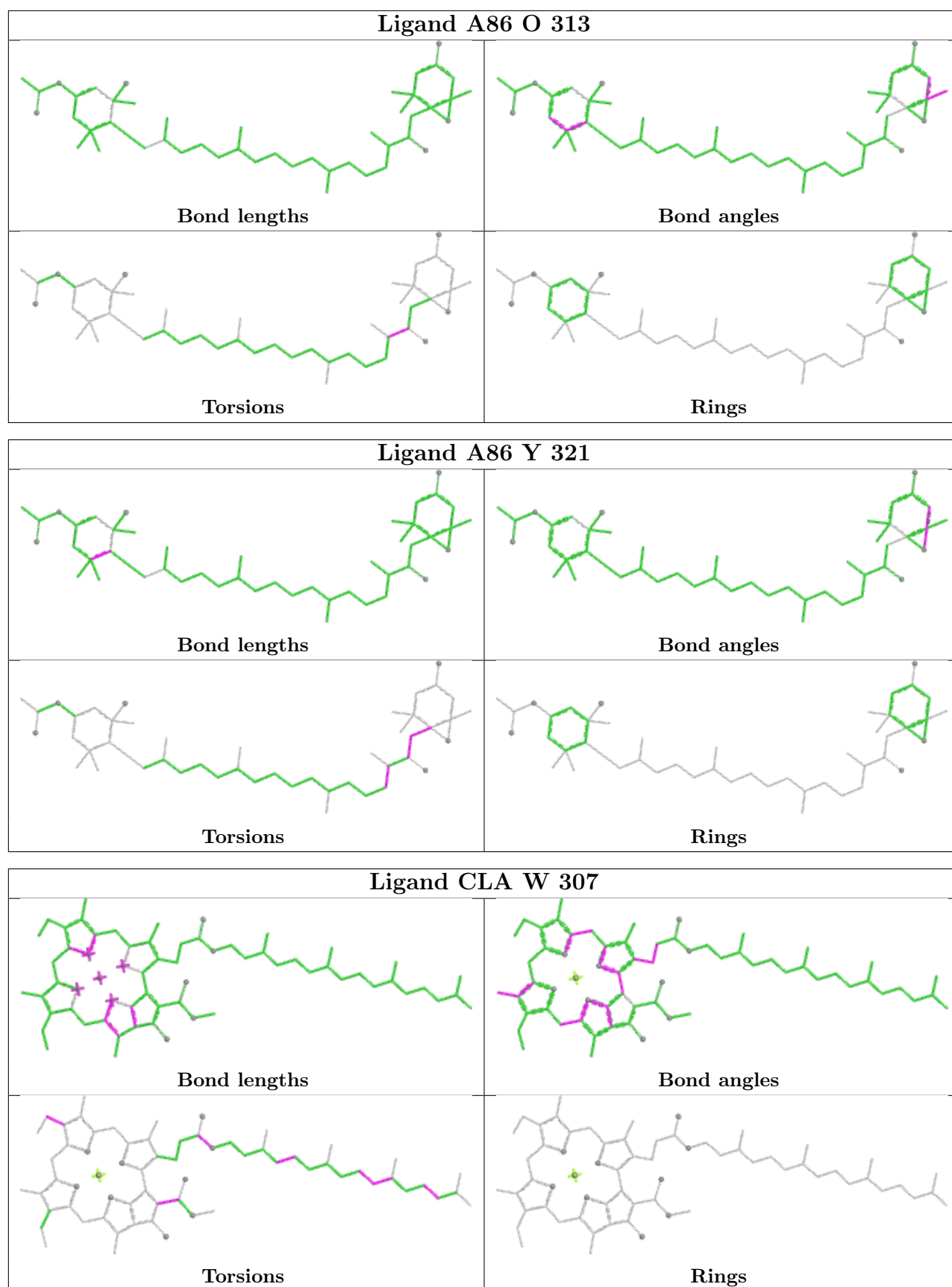


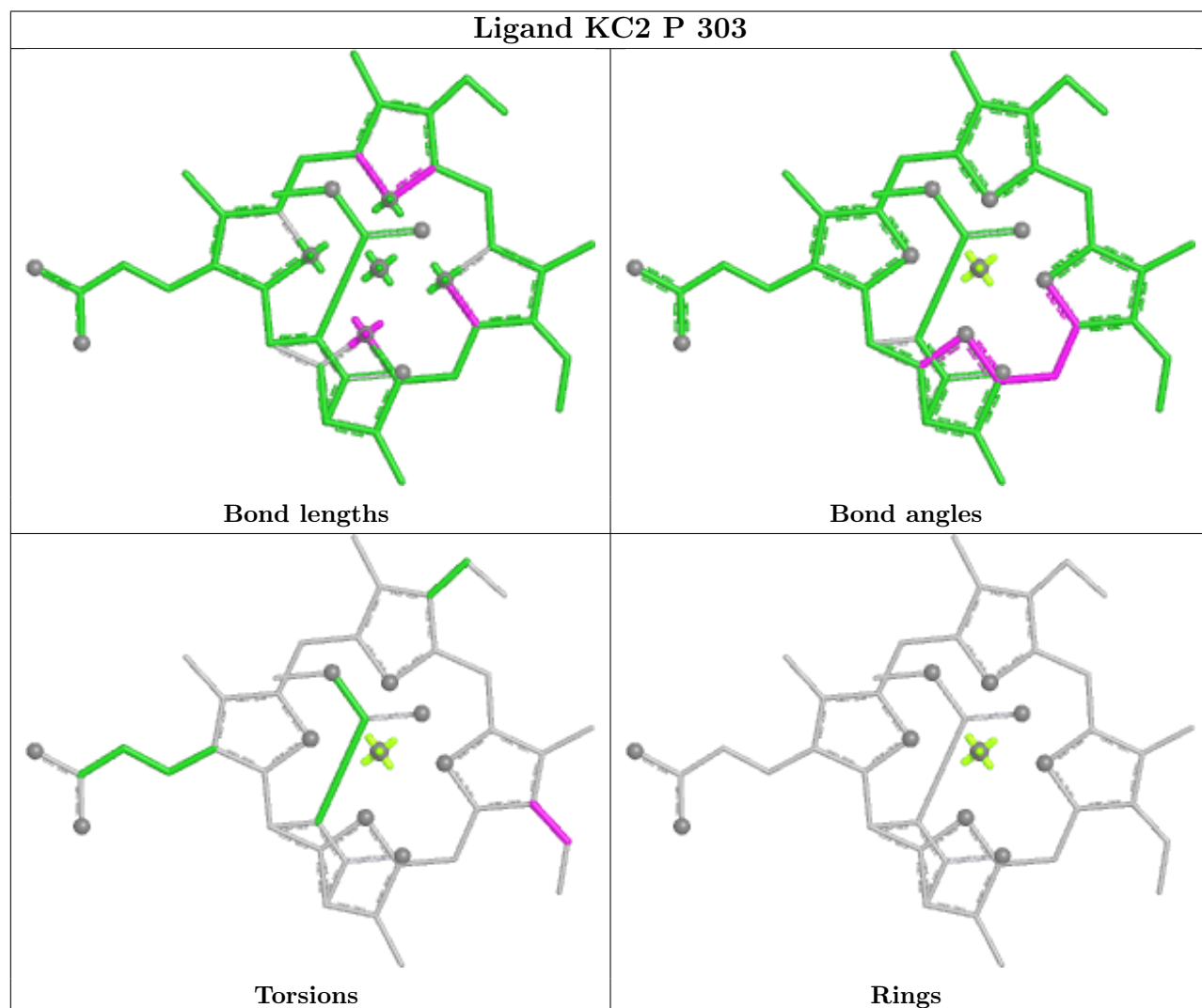
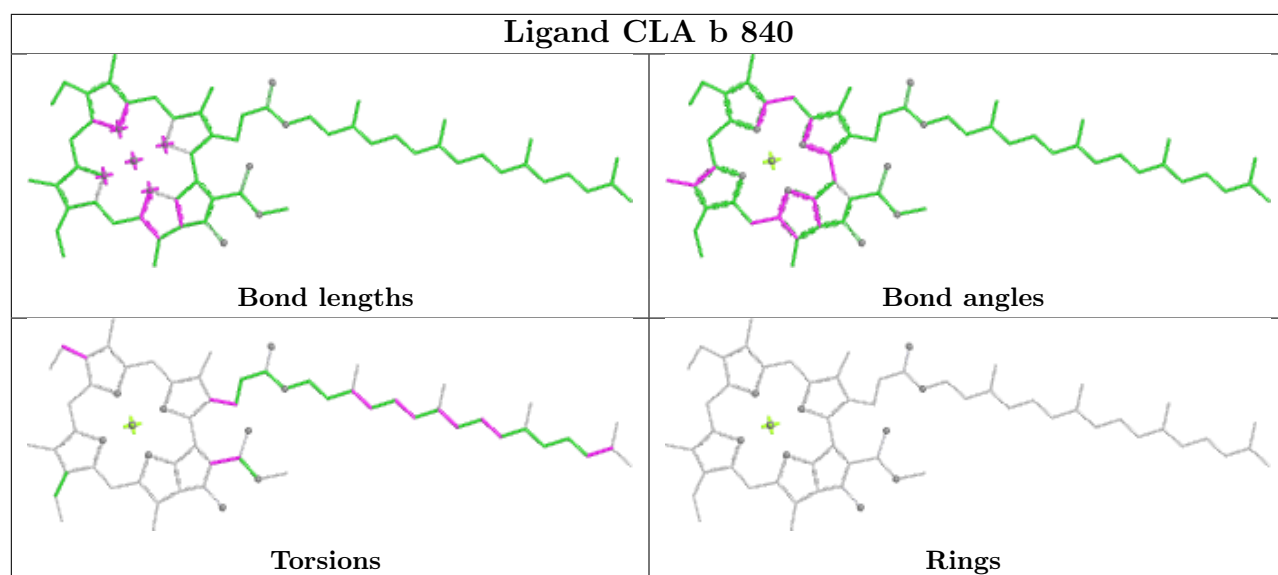
Rings



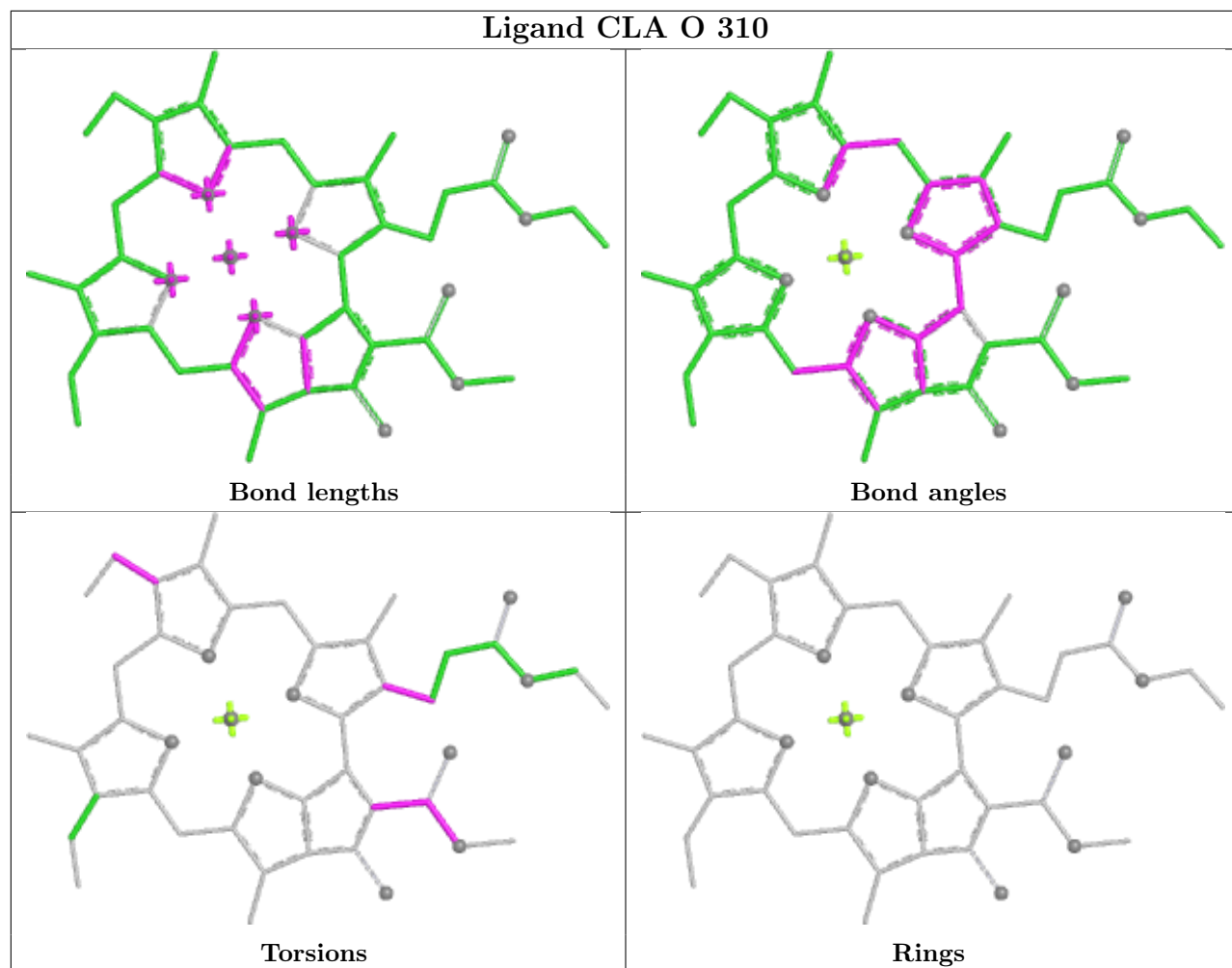




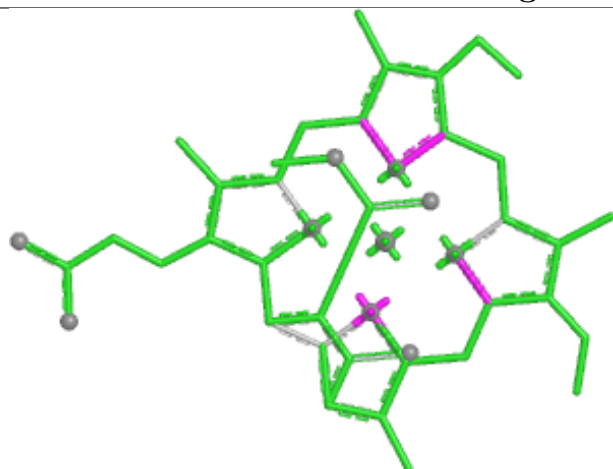




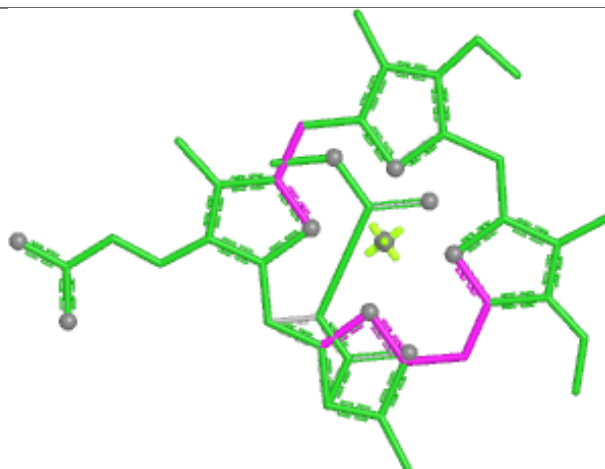
Ligand CLA O 310



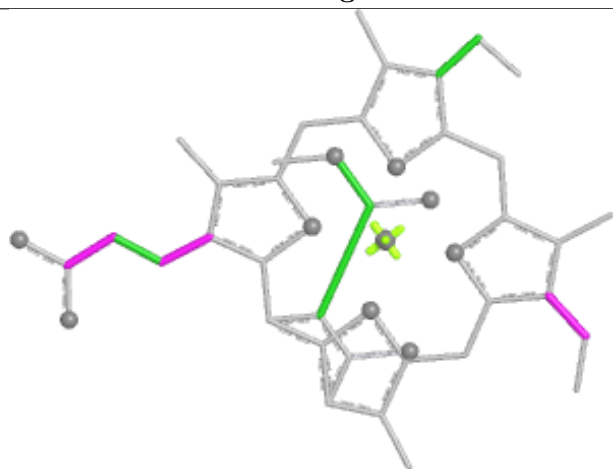
Ligand KC2 u 303



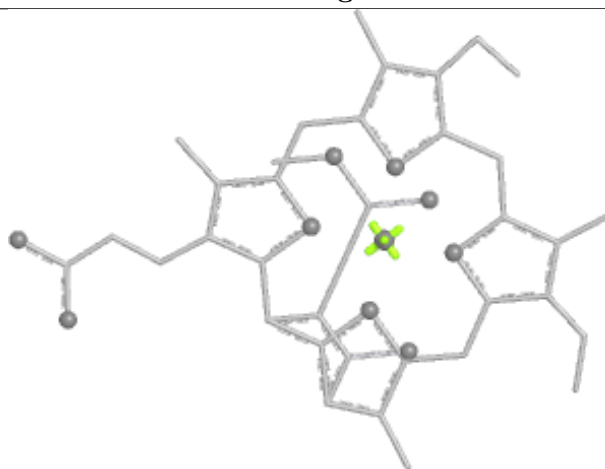
Bond lengths



Bond angles

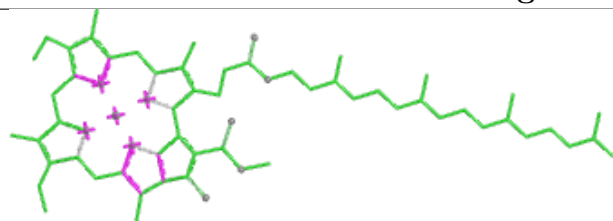


Torsions

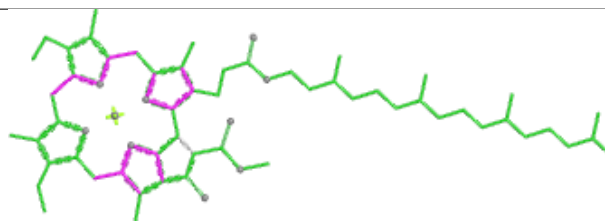


Rings

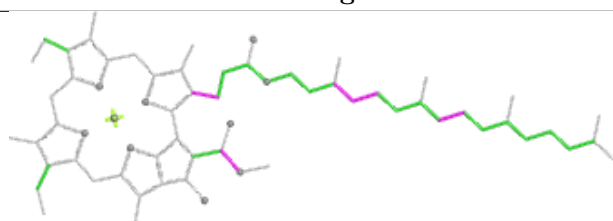
Ligand CLA b 832



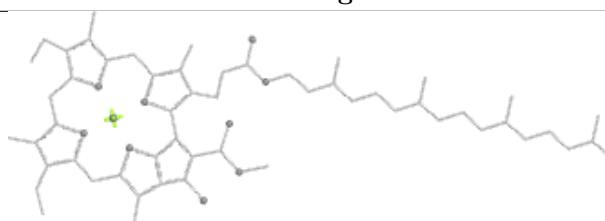
Bond lengths



Bond angles

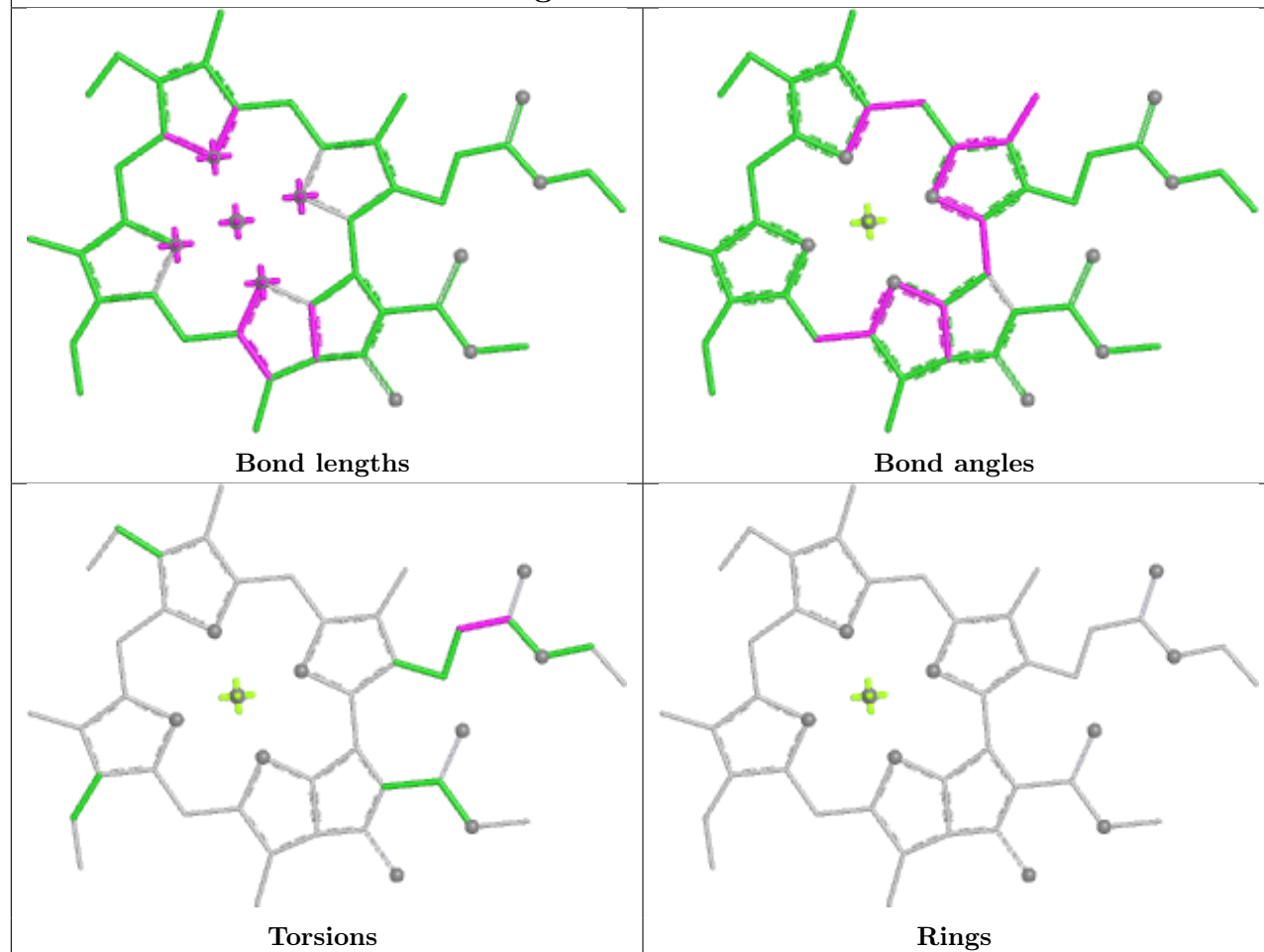


Torsions

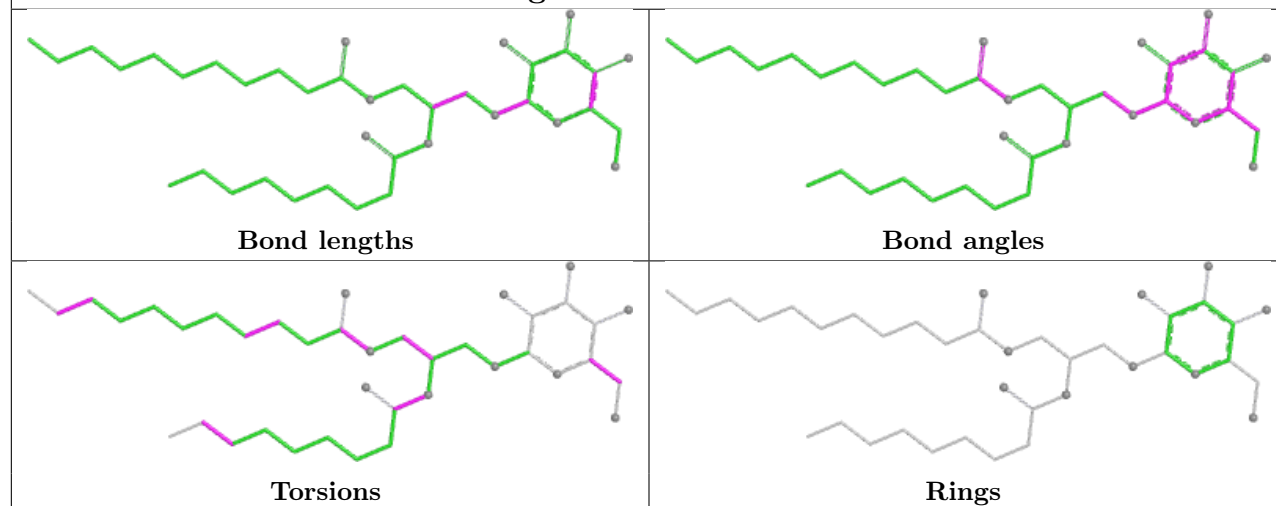


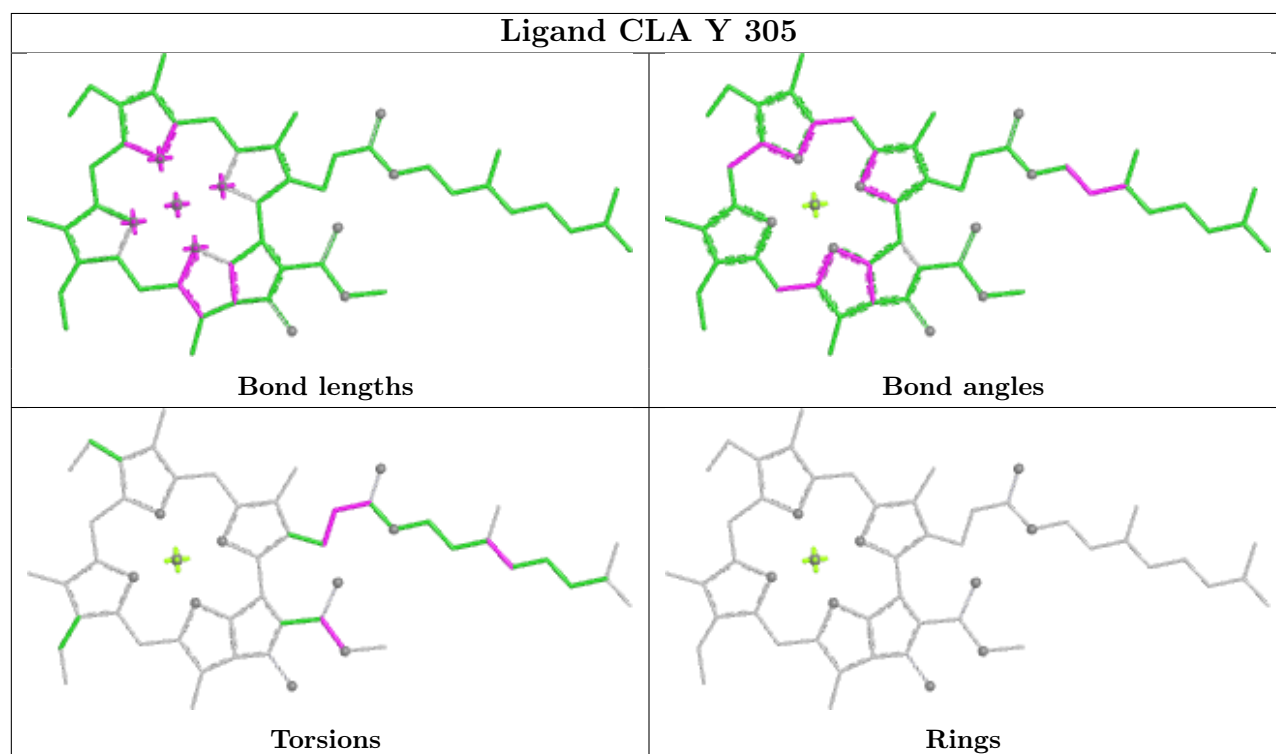
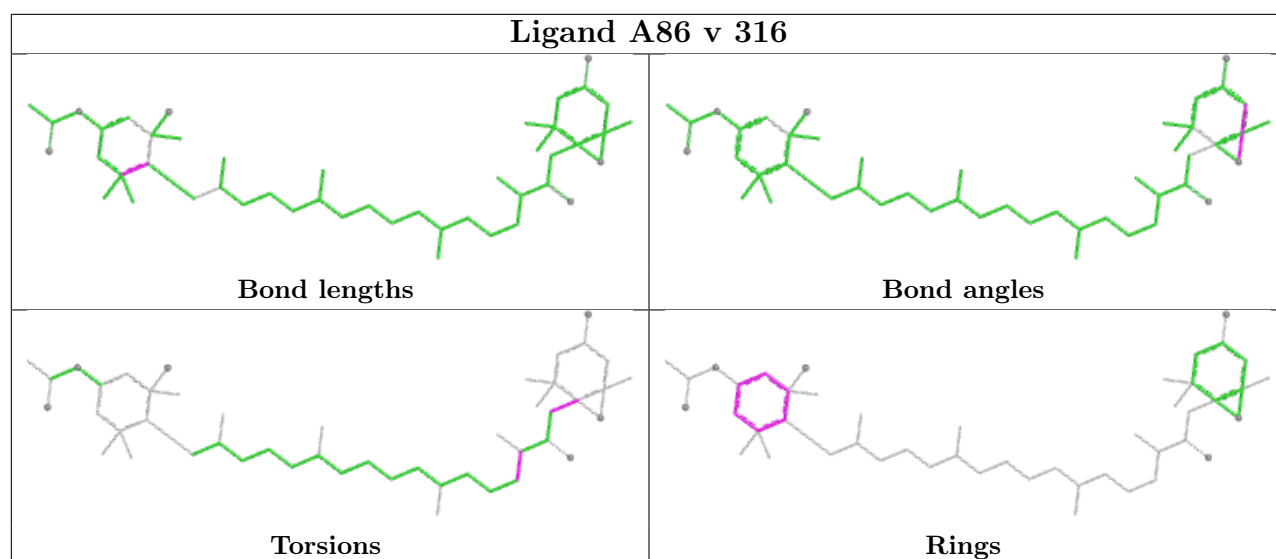
Rings

Ligand CLA f 205

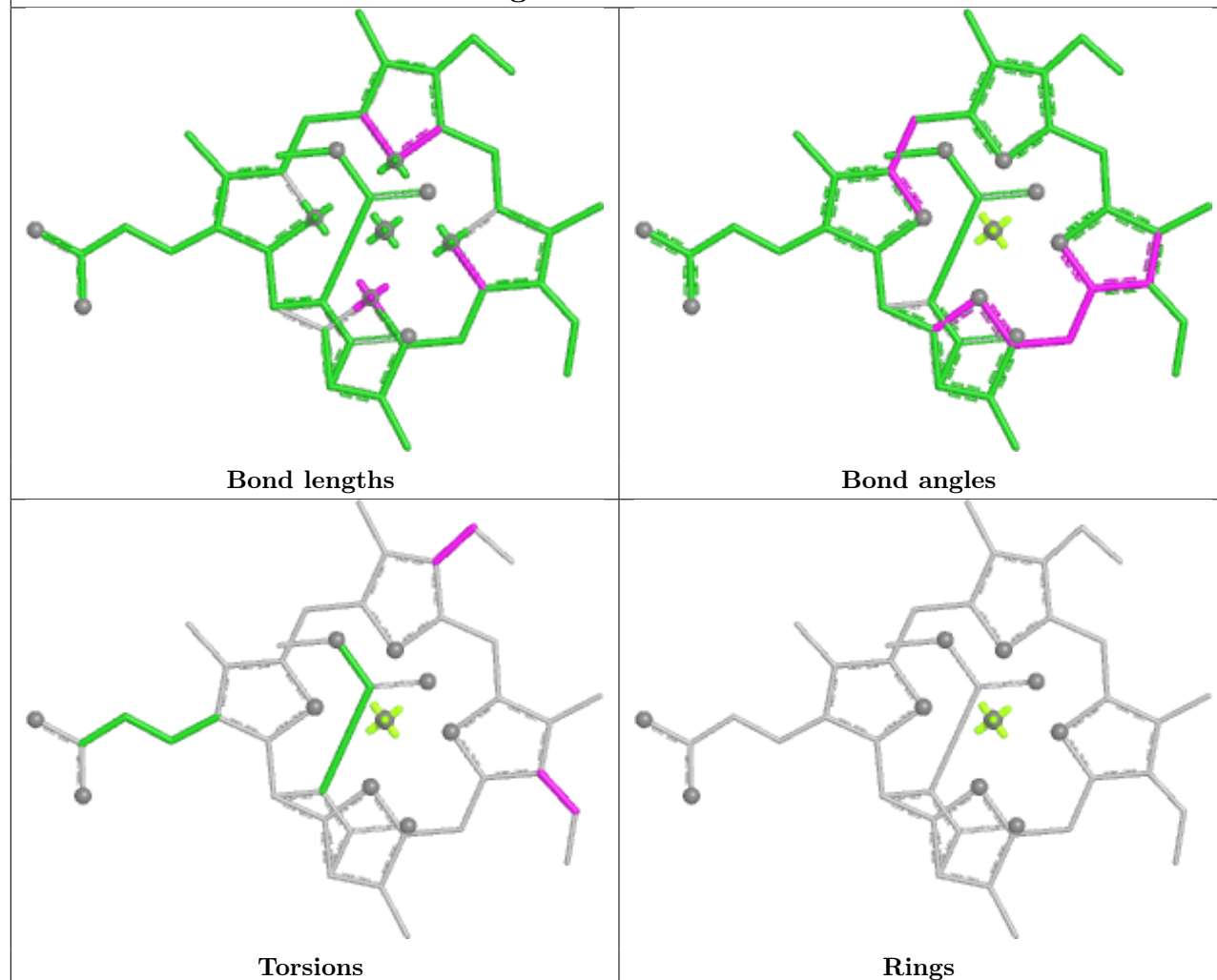


Ligand LMG P 318

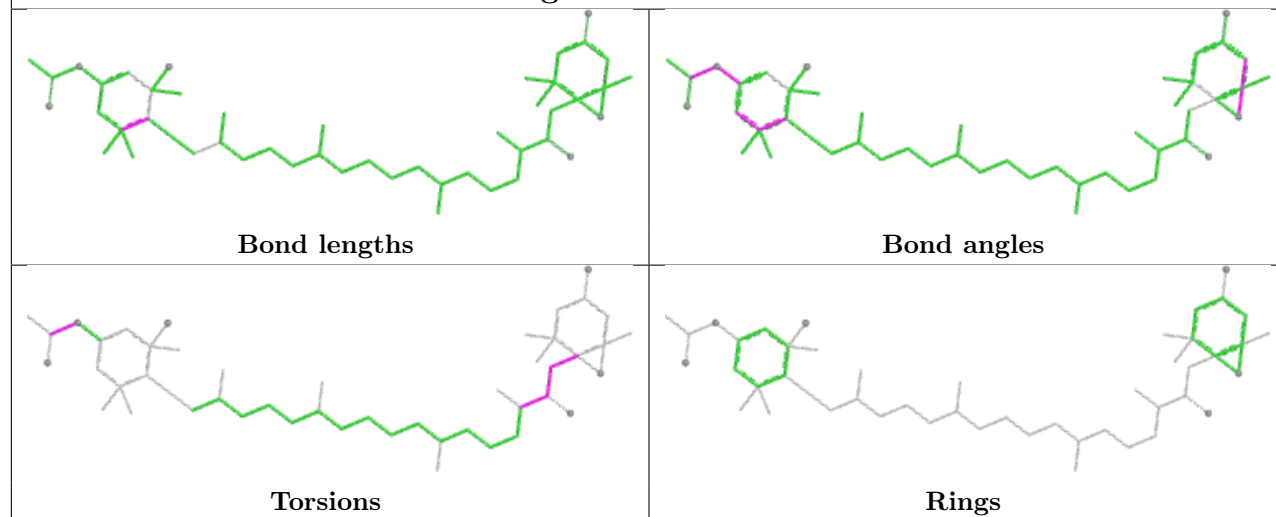




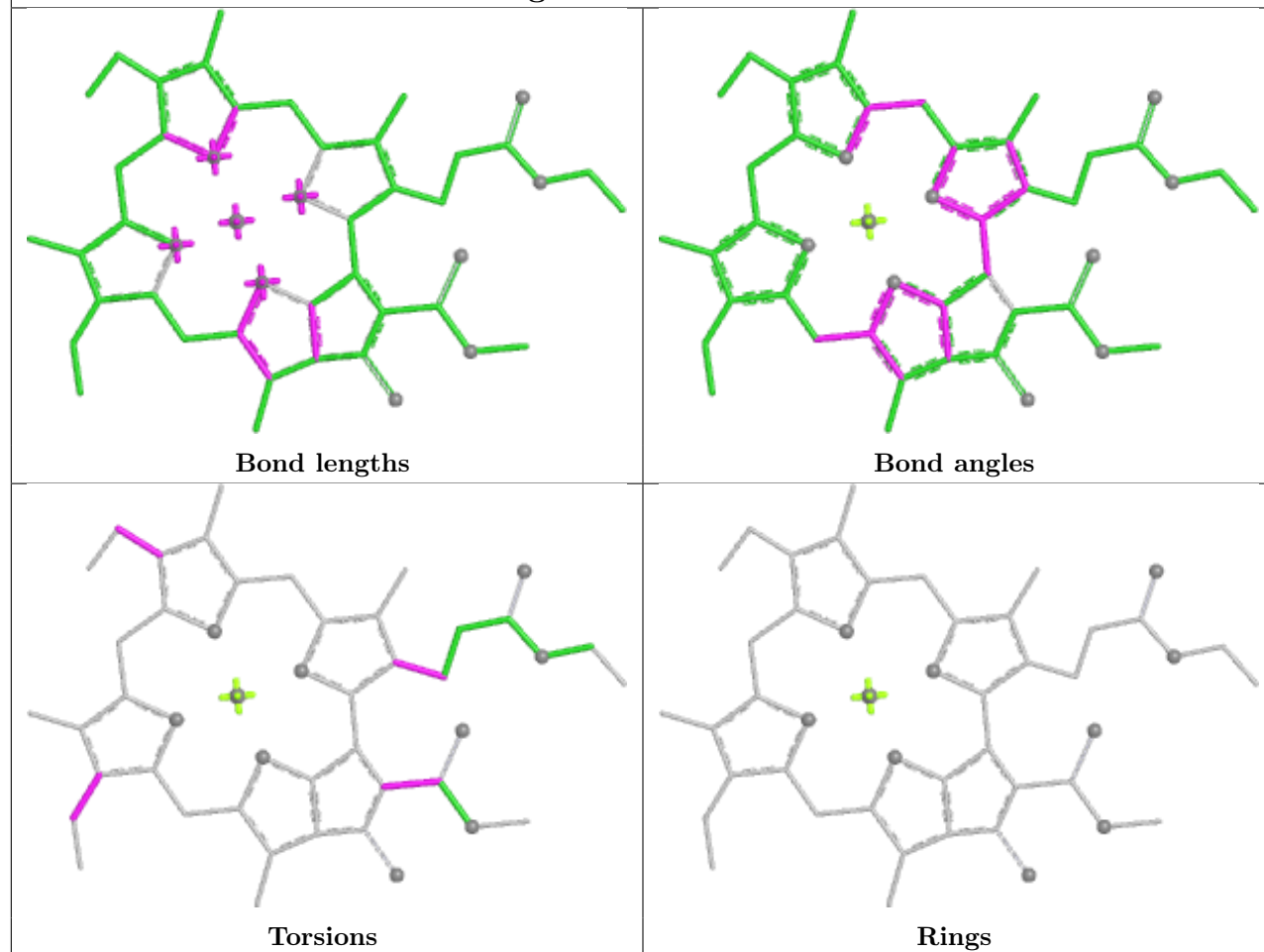
Ligand KC2 P 302



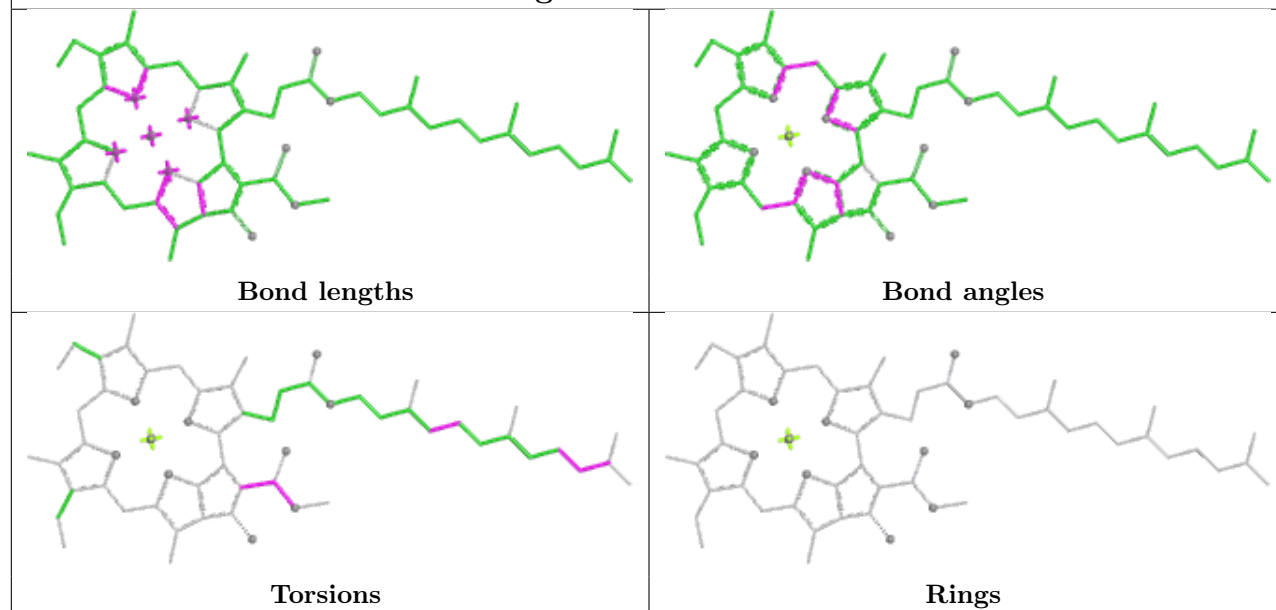
Ligand A86 u 316

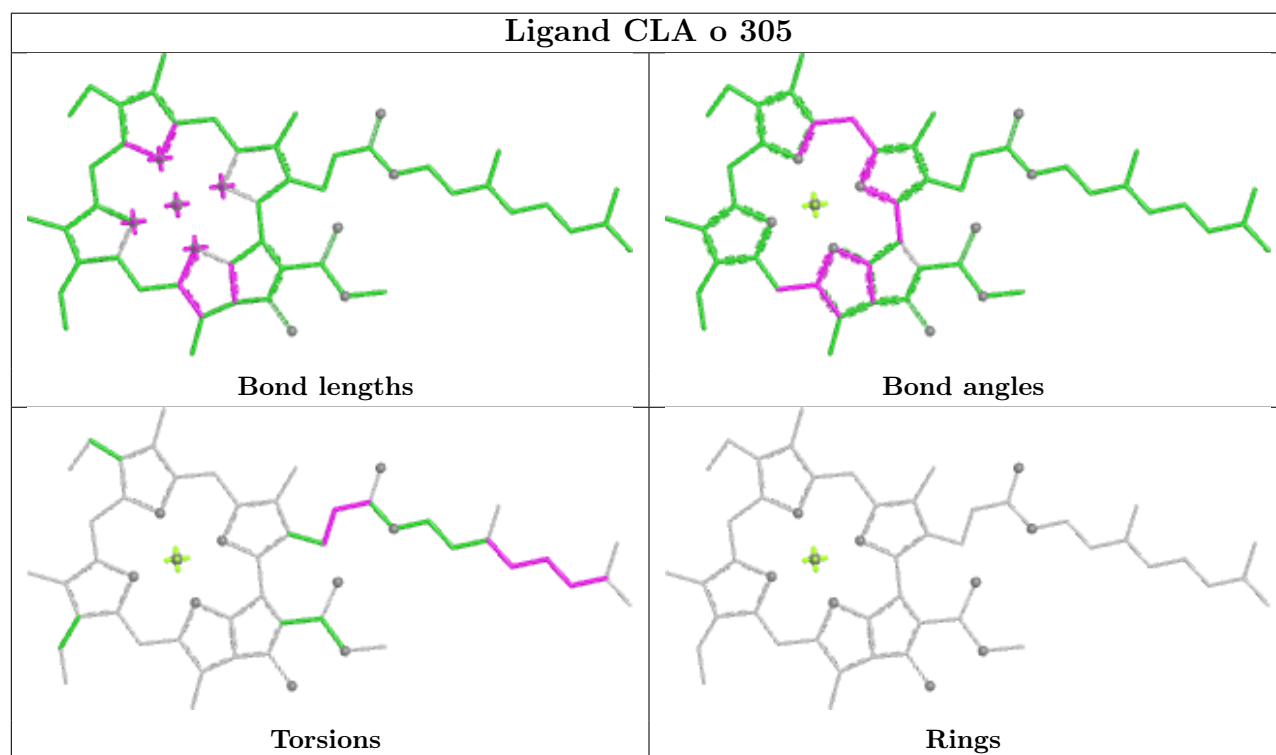
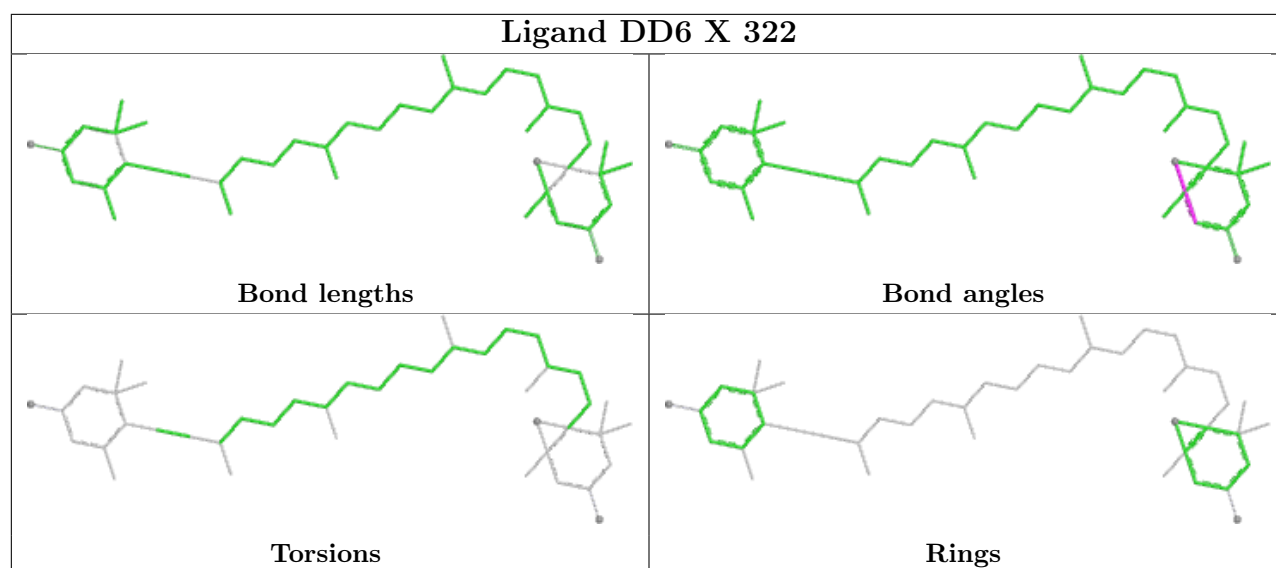


Ligand CLA E 302

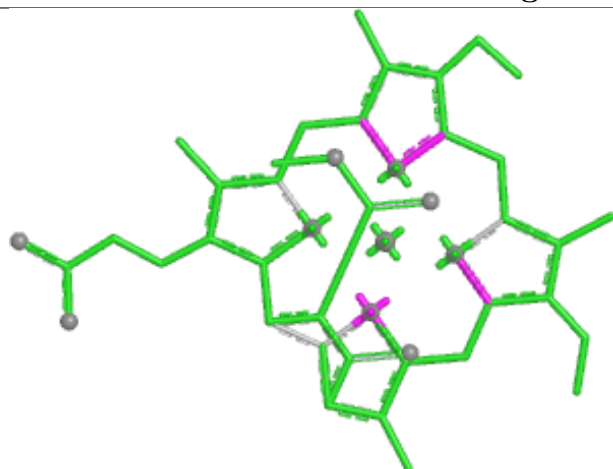


Ligand CLA u 312

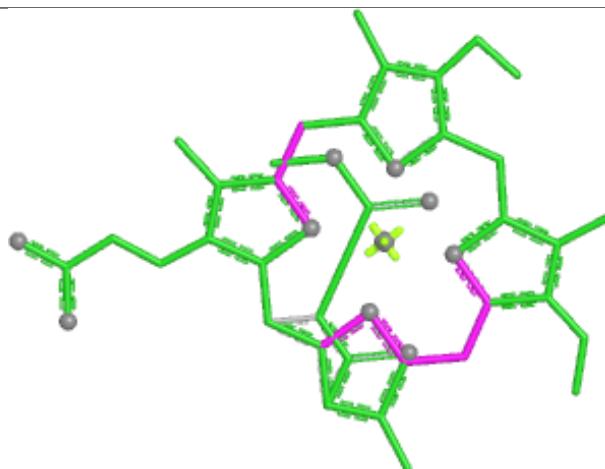




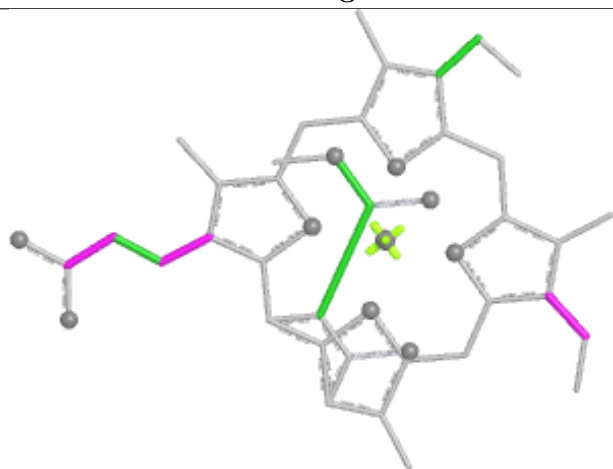
Ligand KC2 z 303



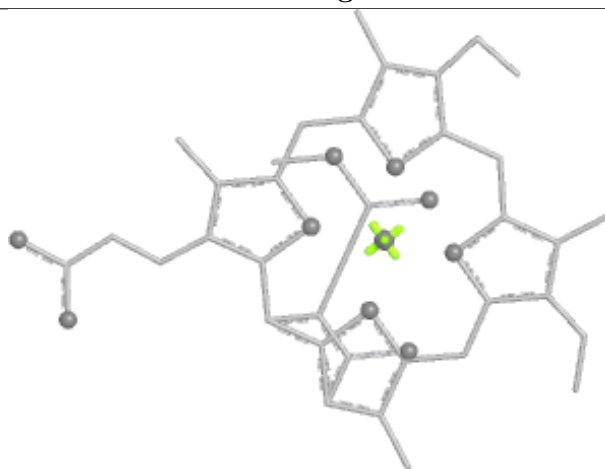
Bond lengths



Bond angles

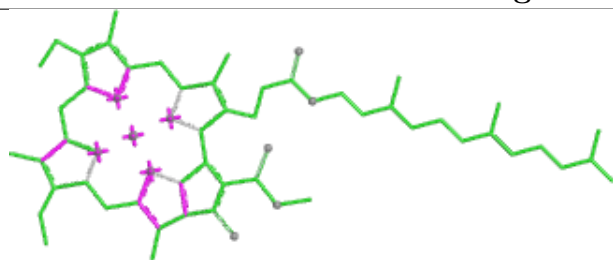


Torsions

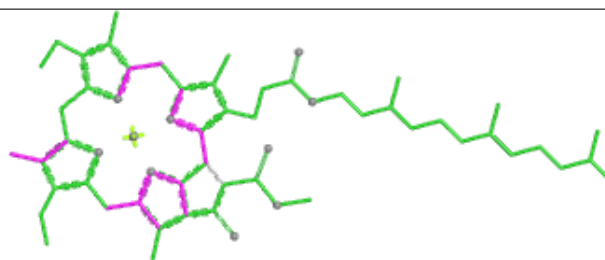


Rings

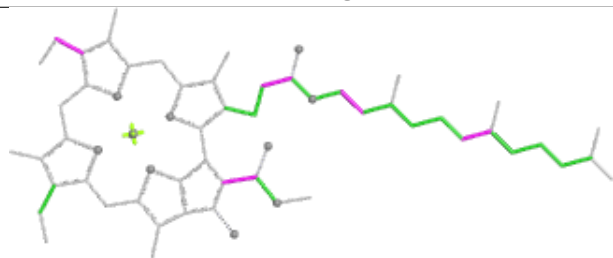
Ligand CLA A 307



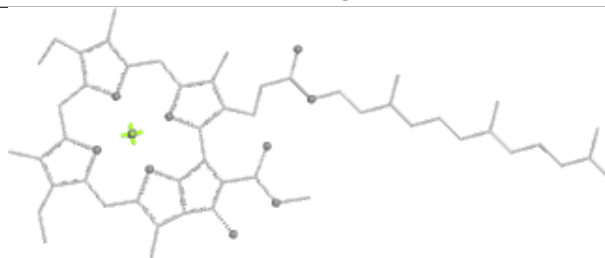
Bond lengths



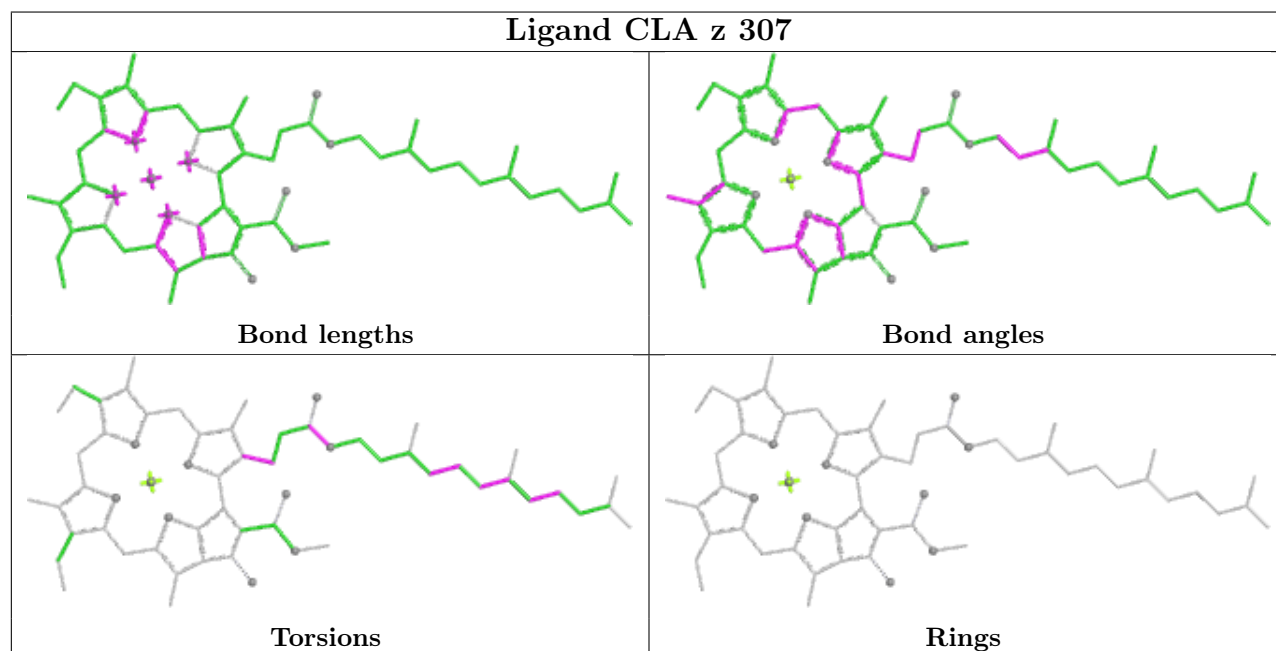
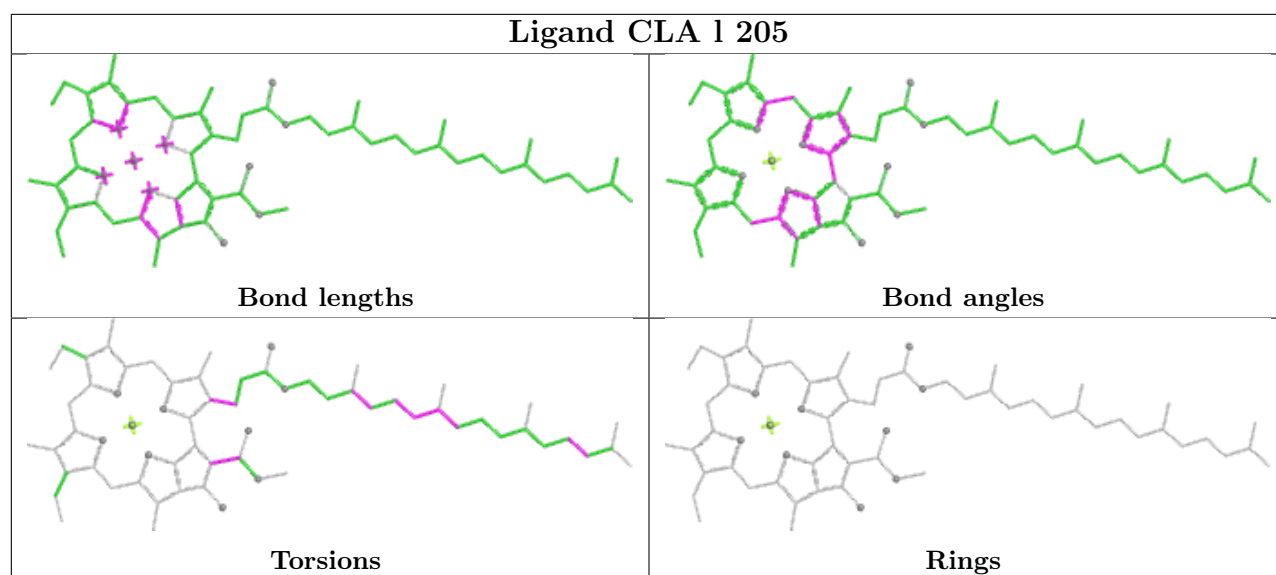
Bond angles



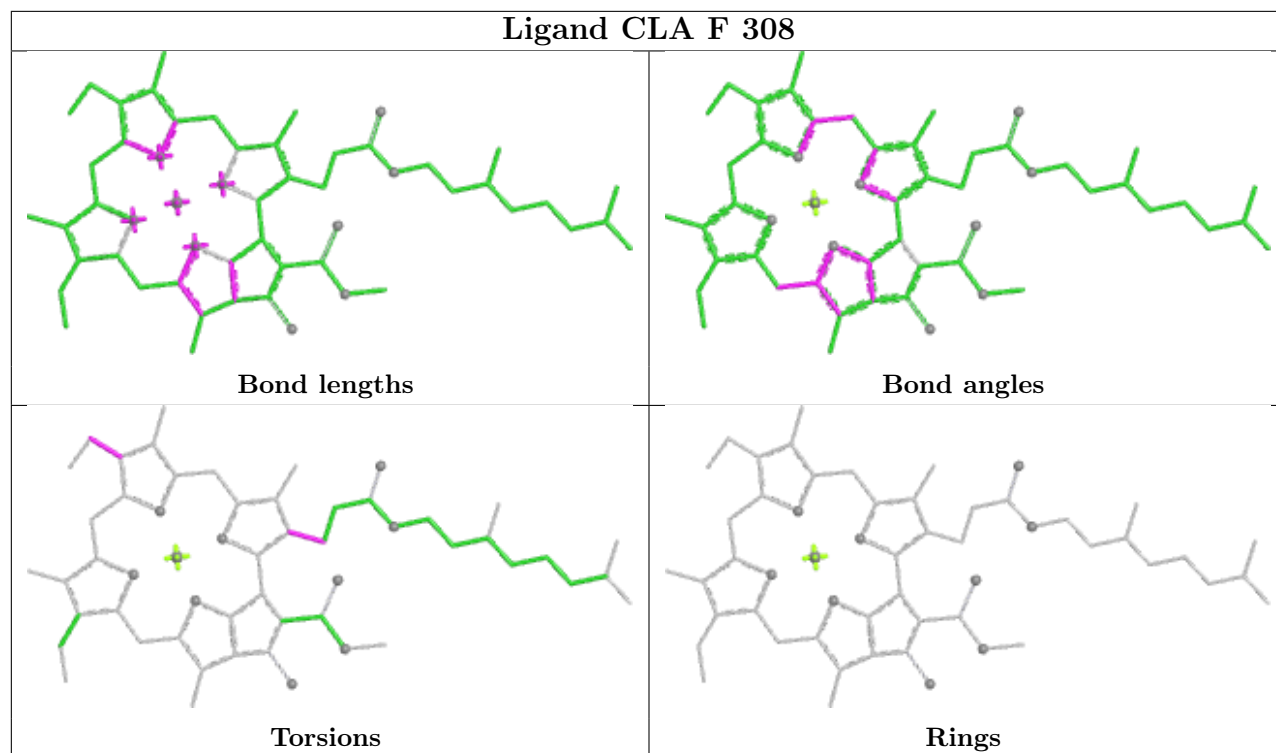
Torsions



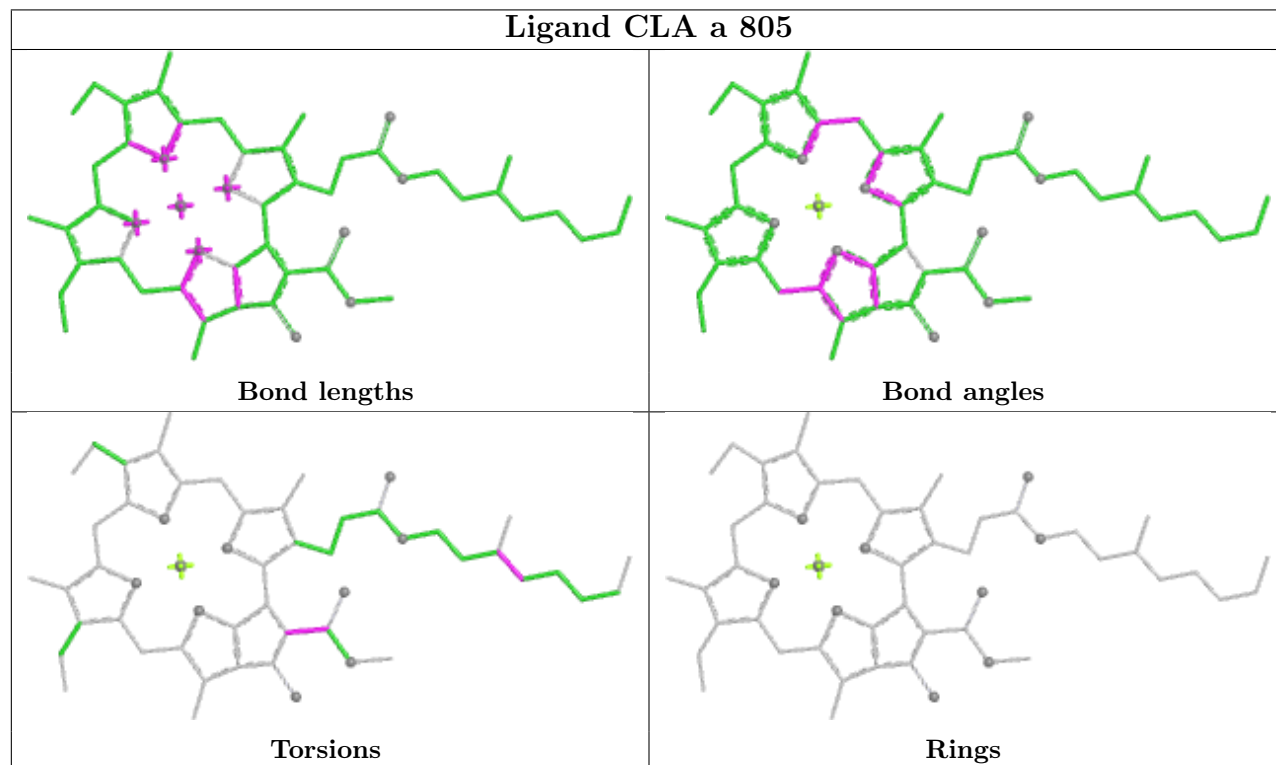
Rings

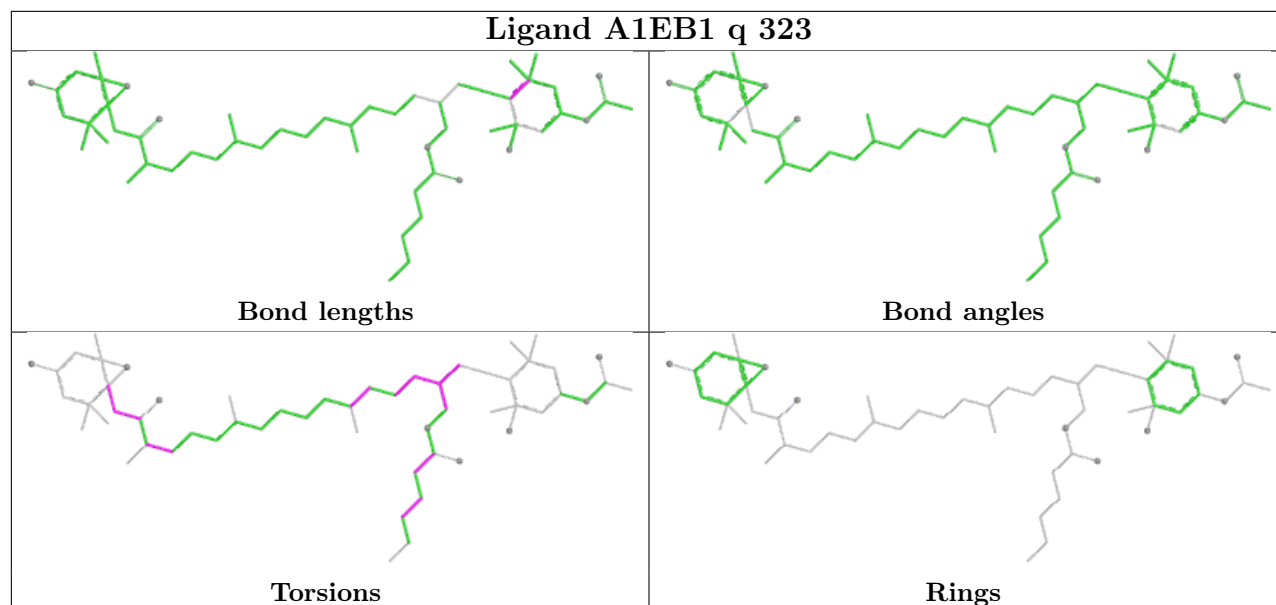
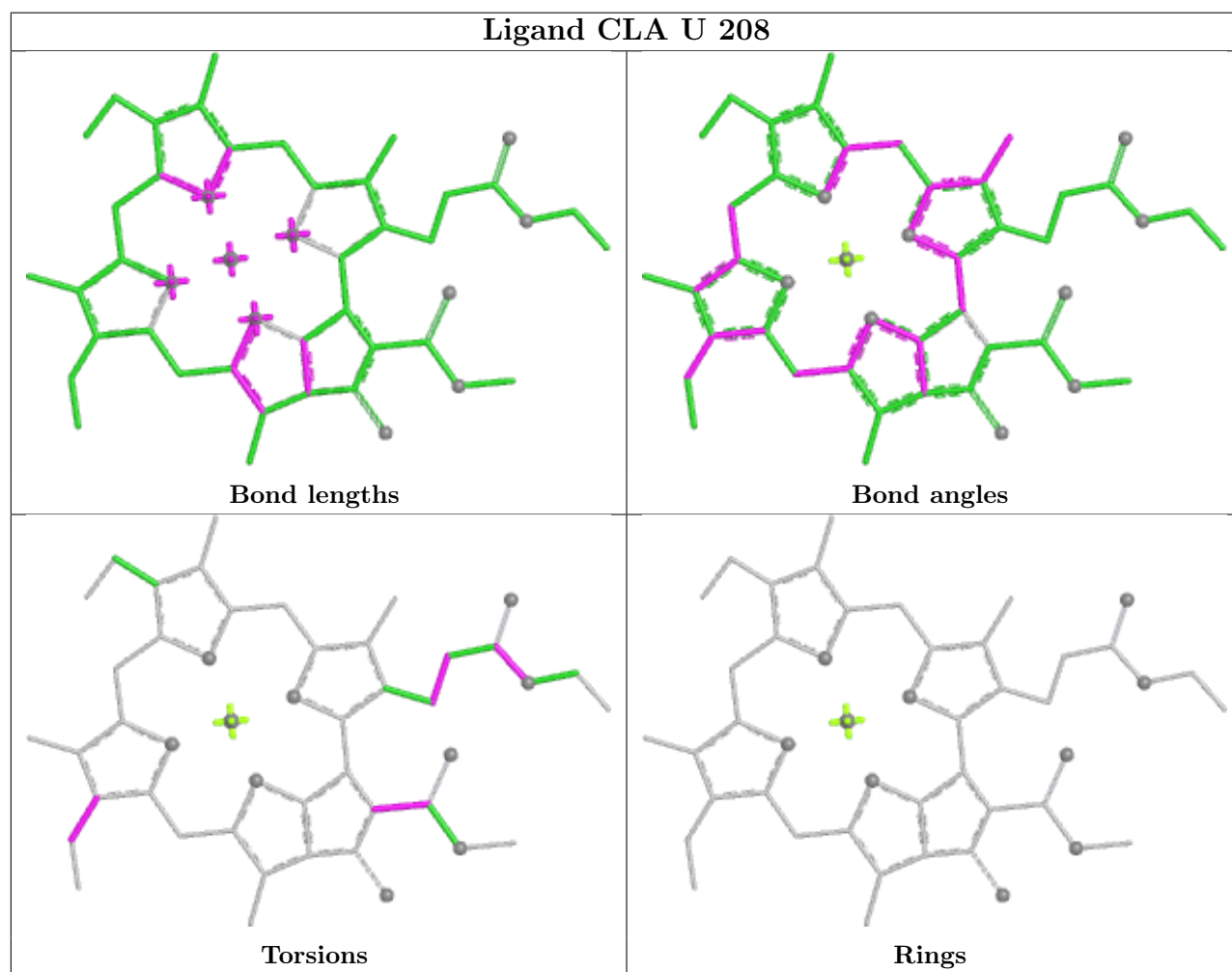


Ligand CLA F 308

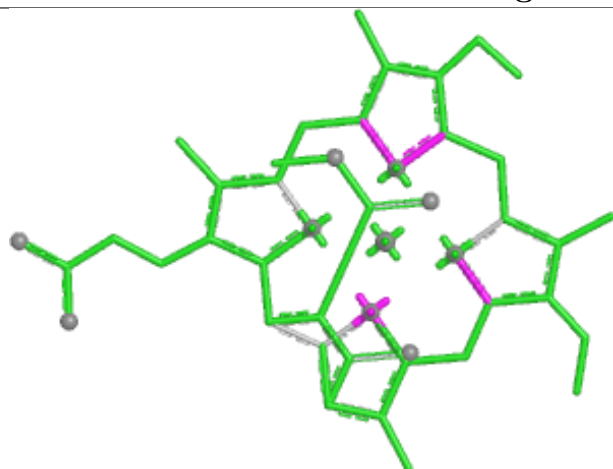


Ligand CLA a 805

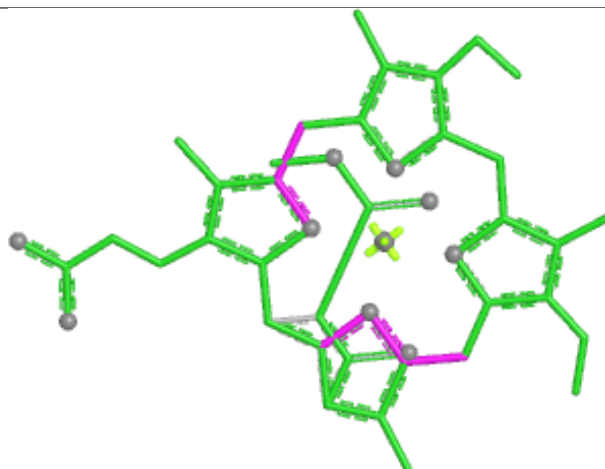


Ligand A1EB1 q 323**Ligand CLA U 208**

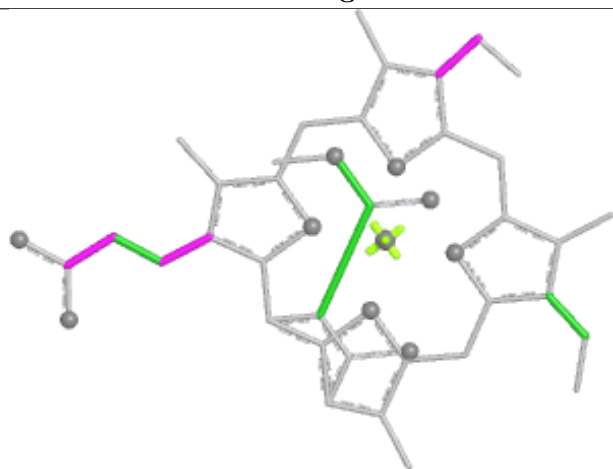
Ligand KC2 X 308



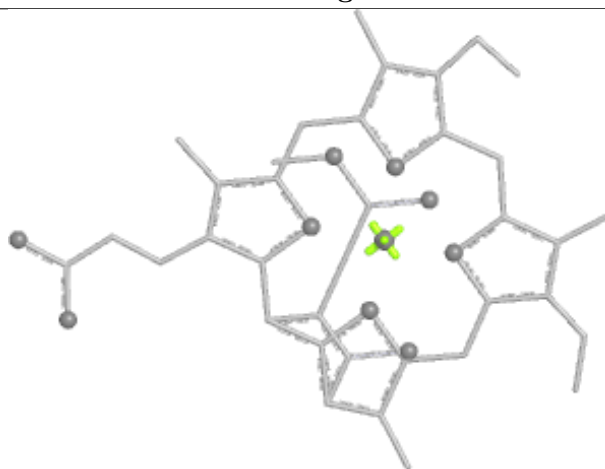
Bond lengths



Bond angles

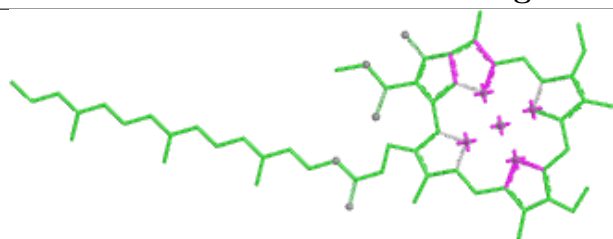


Torsions

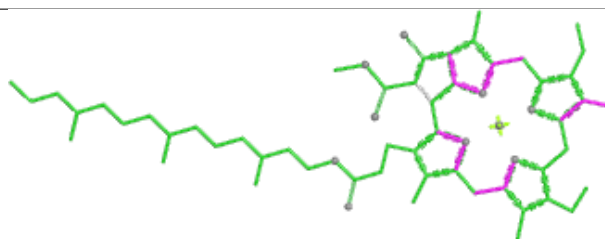


Rings

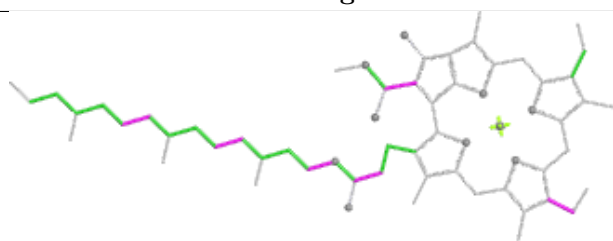
Ligand CLA O 307



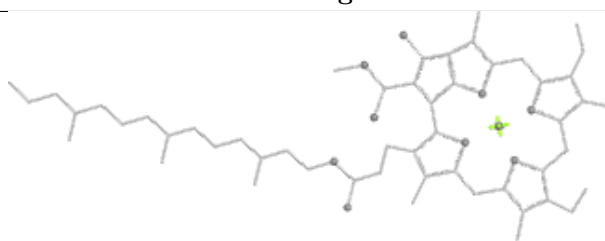
Bond lengths



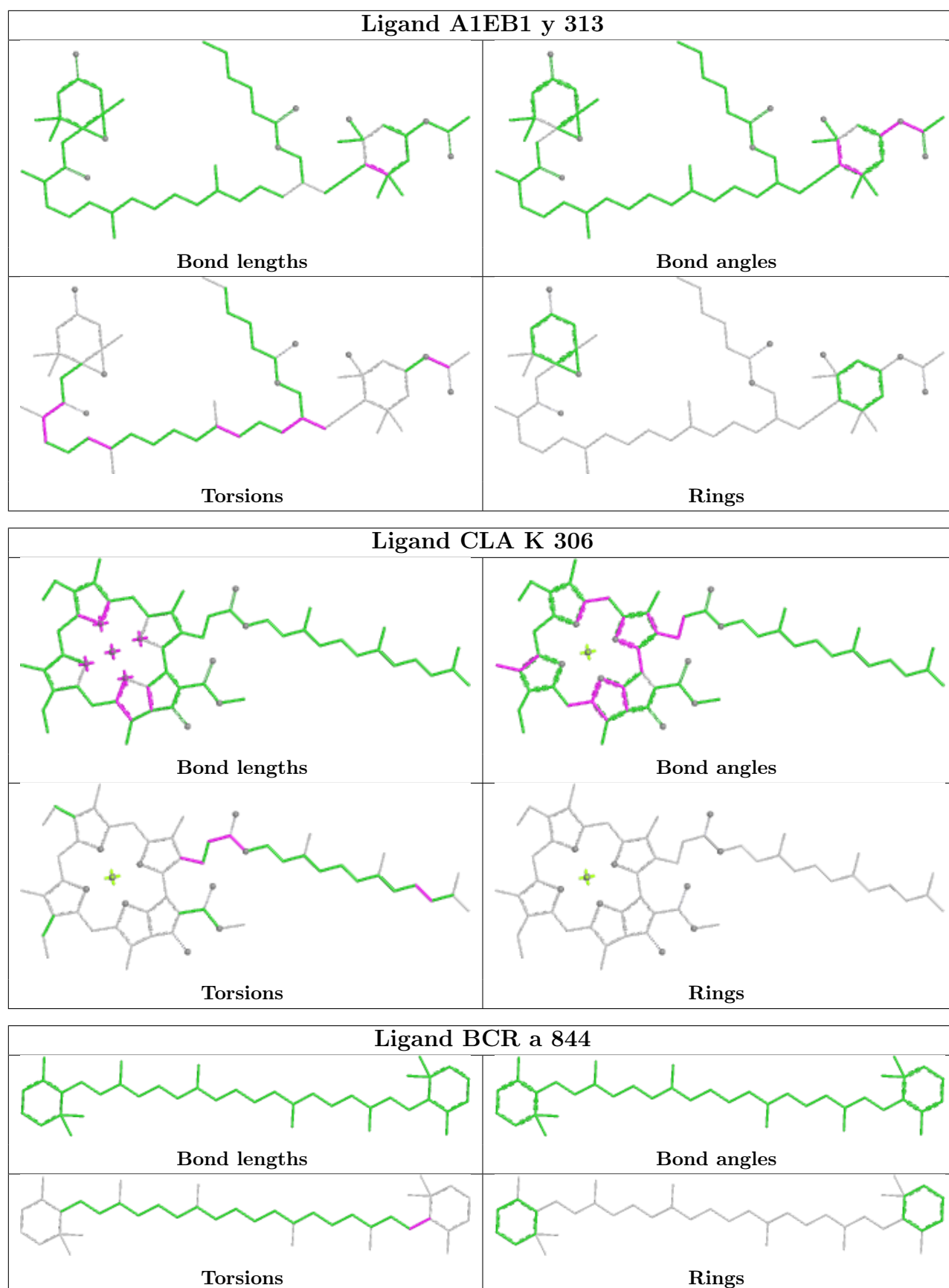
Bond angles

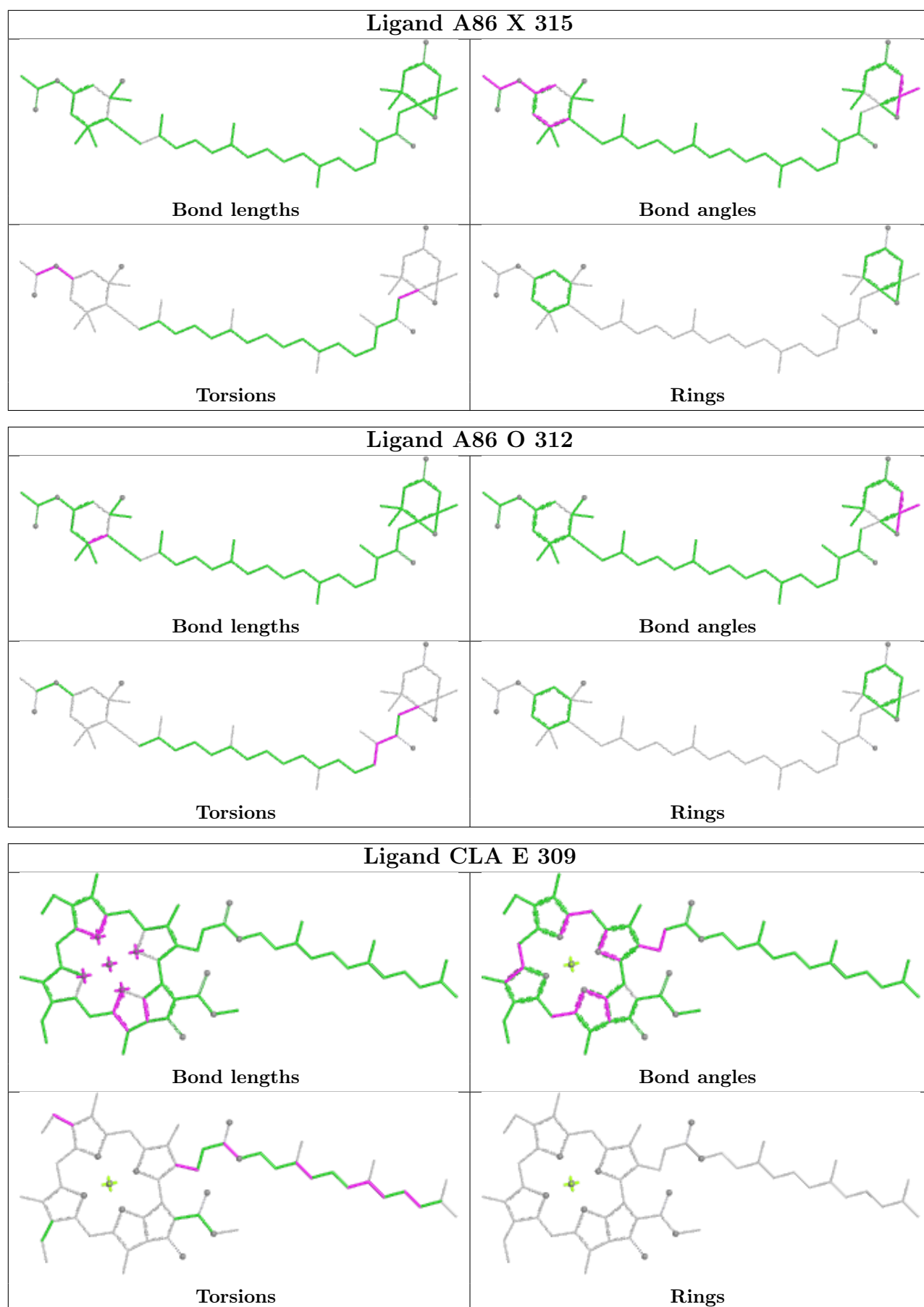


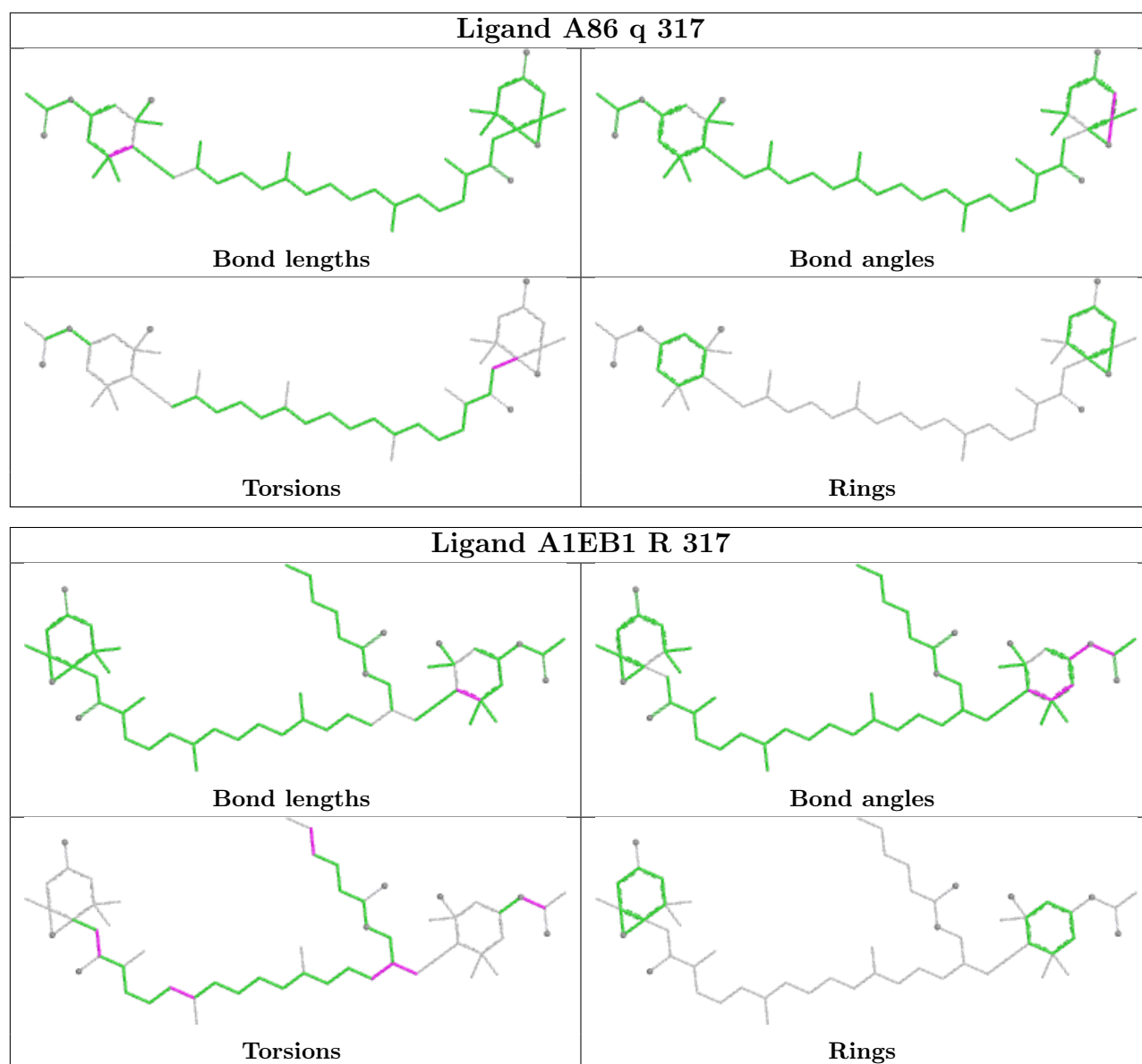
Torsions



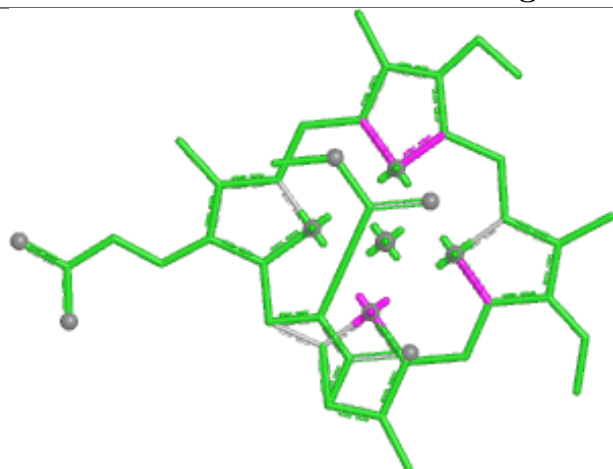
Rings



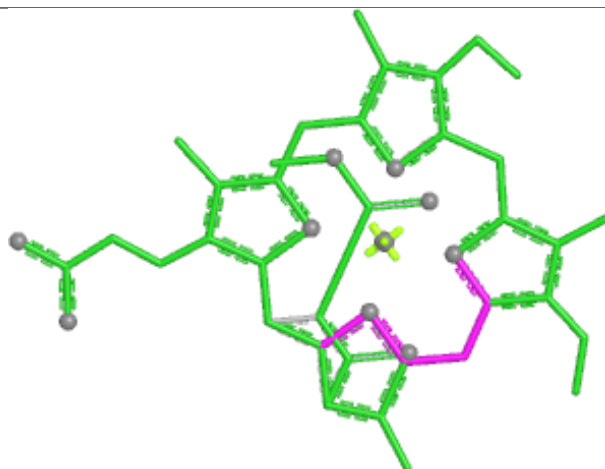




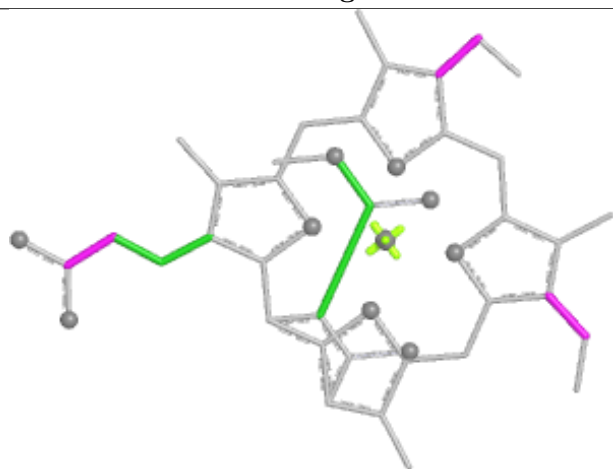
Ligand KC2 S 310



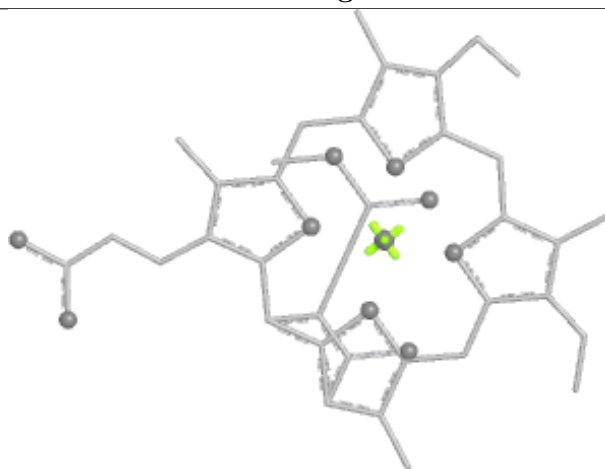
Bond lengths



Bond angles

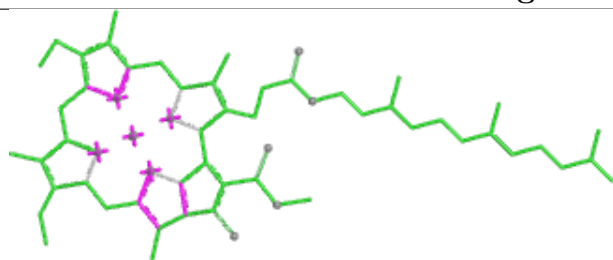


Torsions

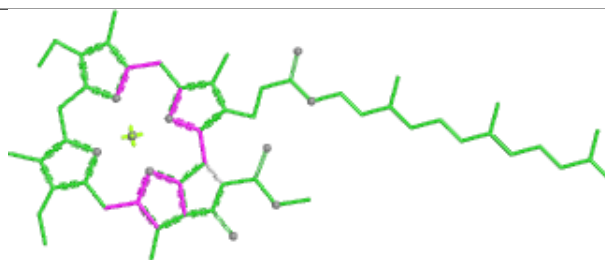


Rings

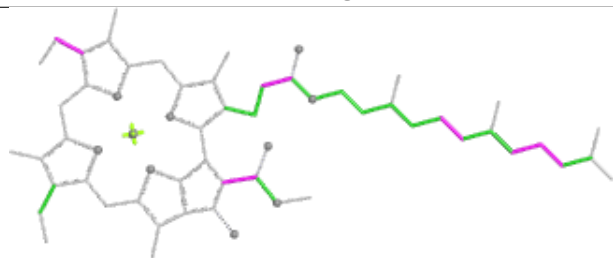
Ligand CLA u 308



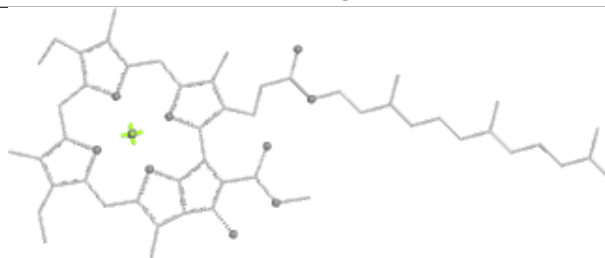
Bond lengths



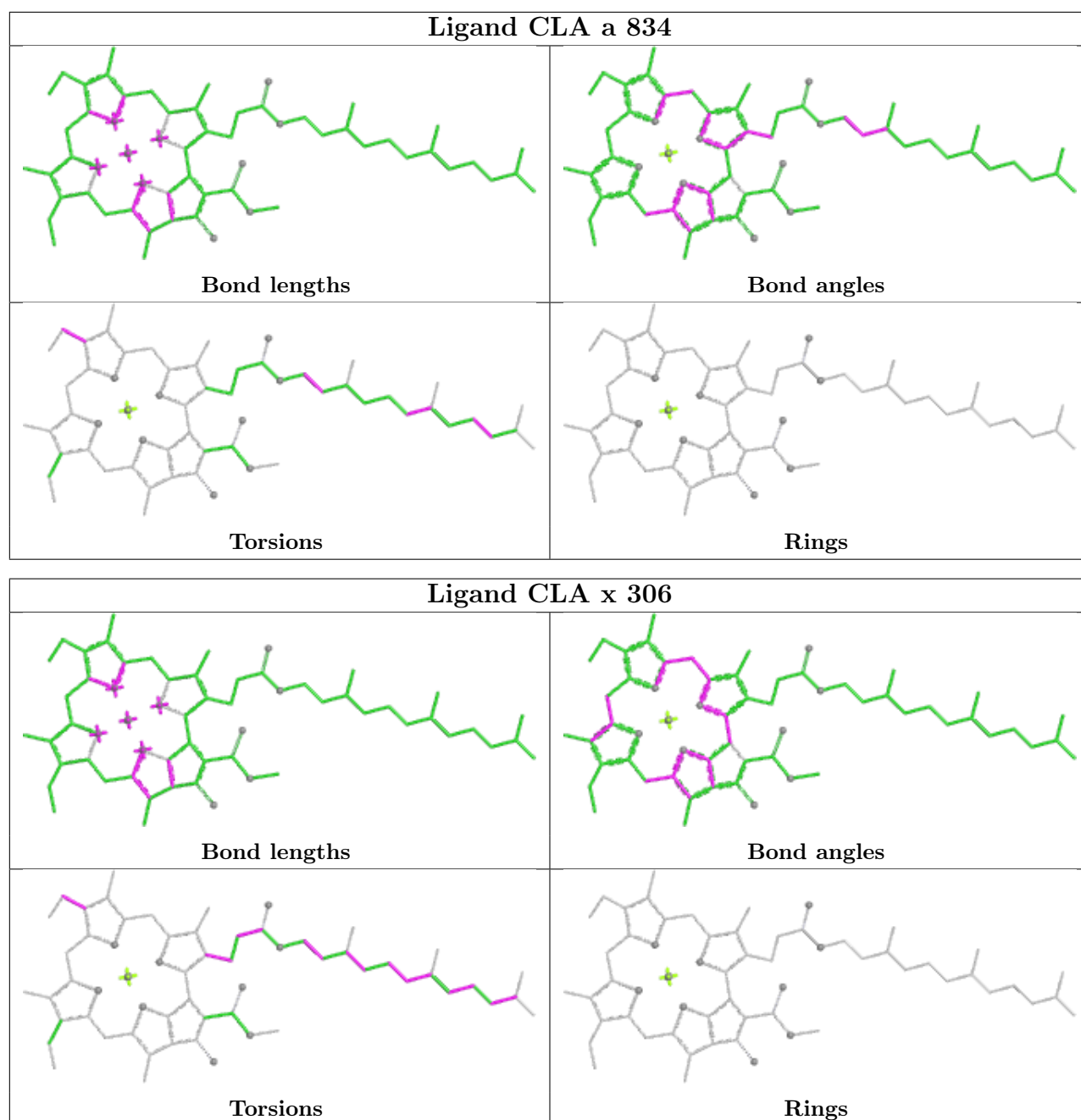
Bond angles

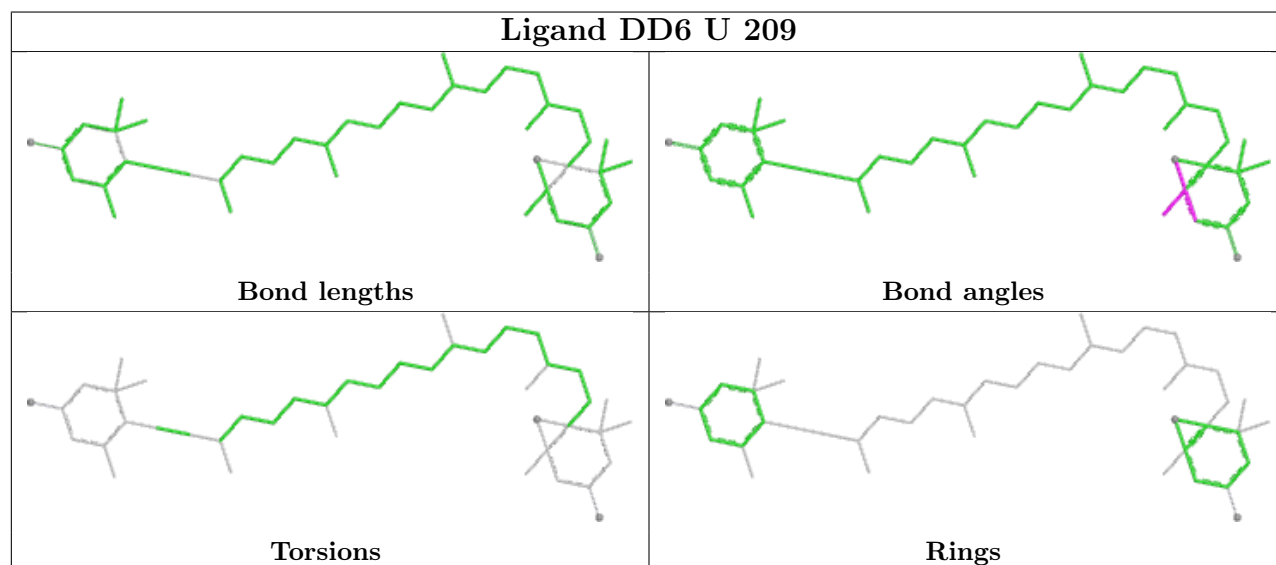
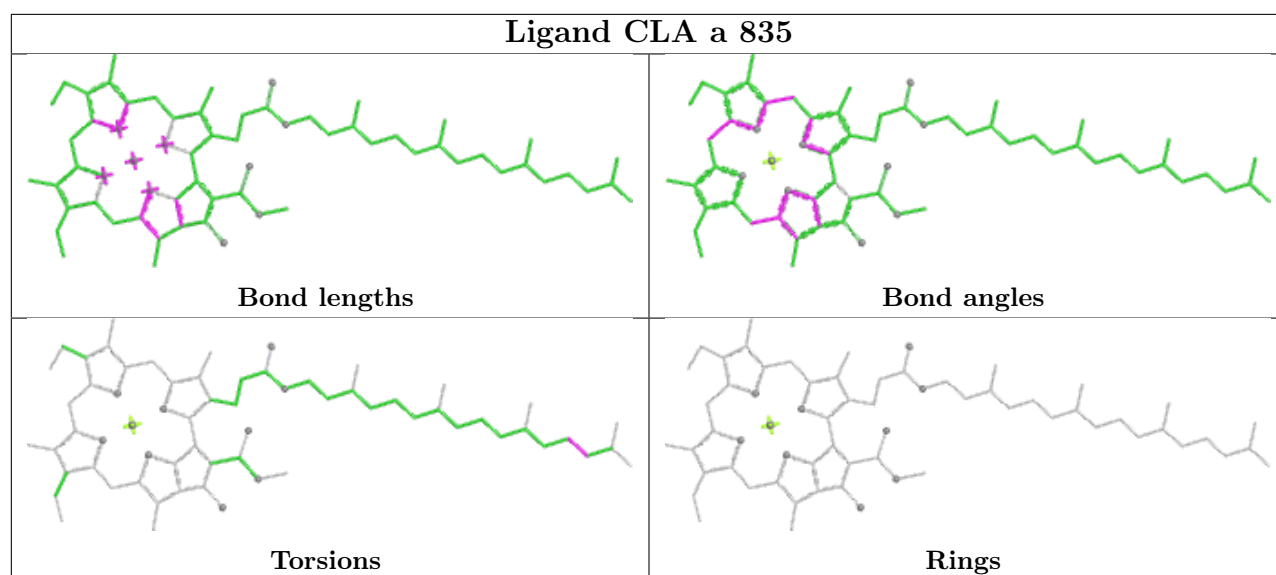


Torsions

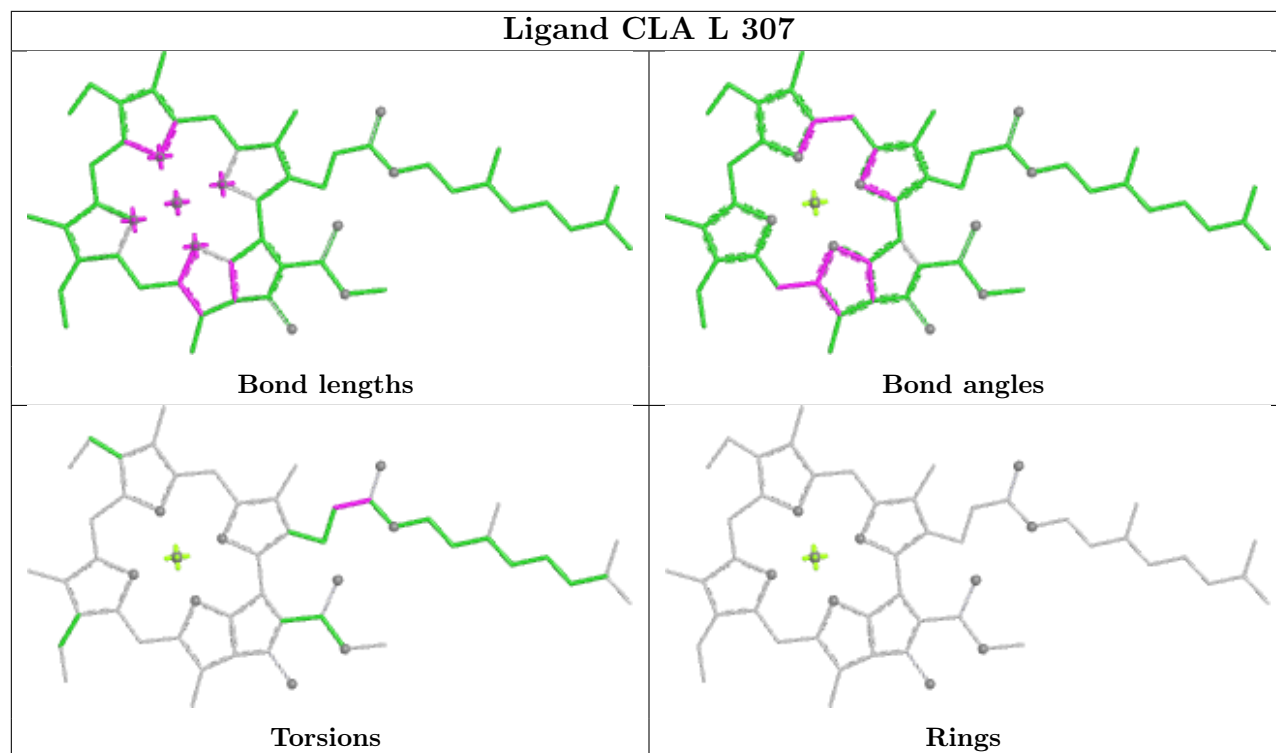


Rings

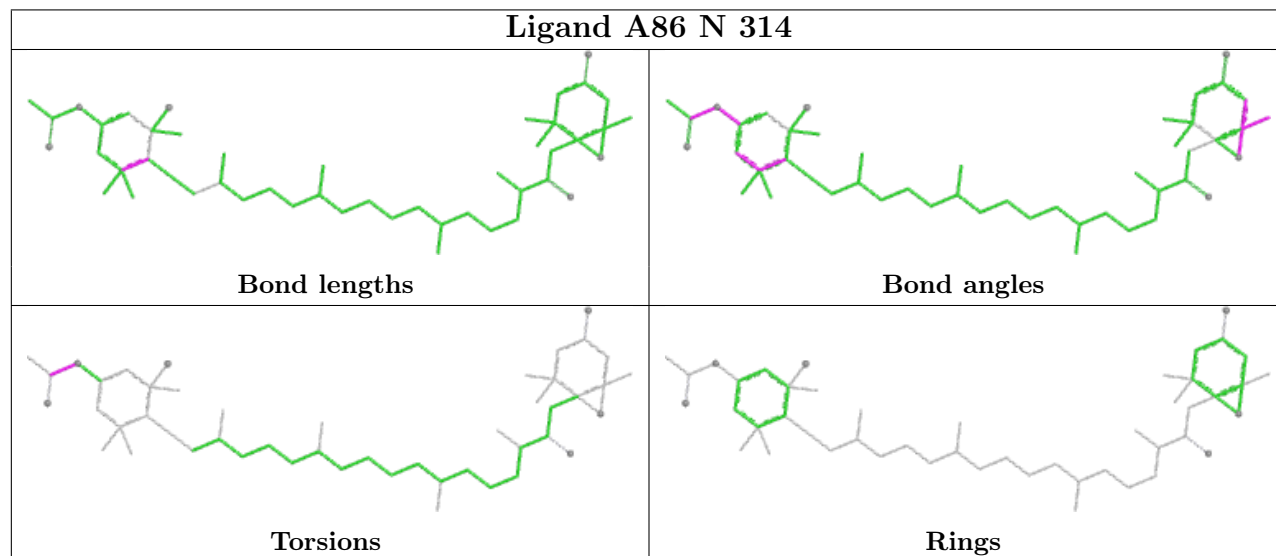




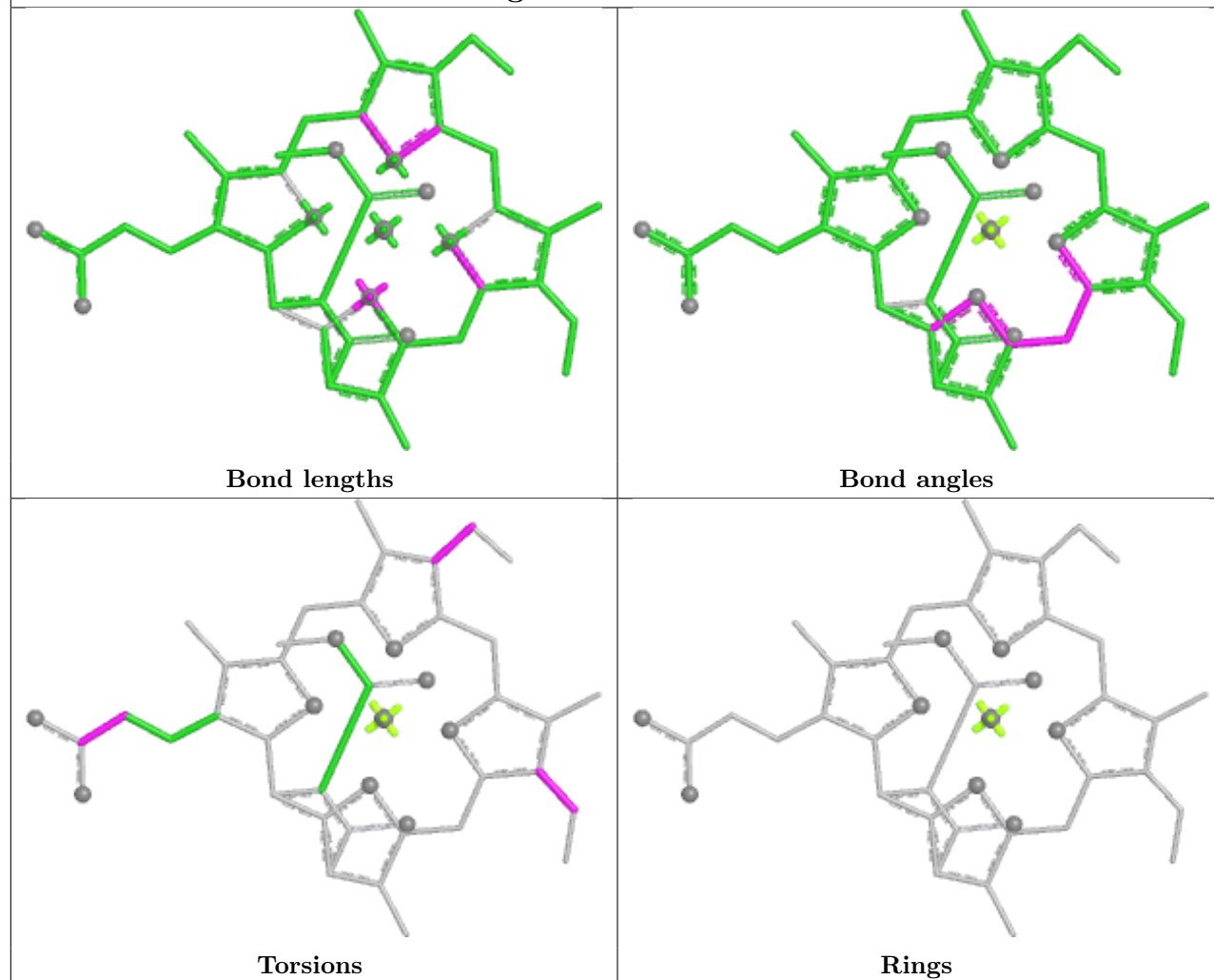
Ligand CLA L 307



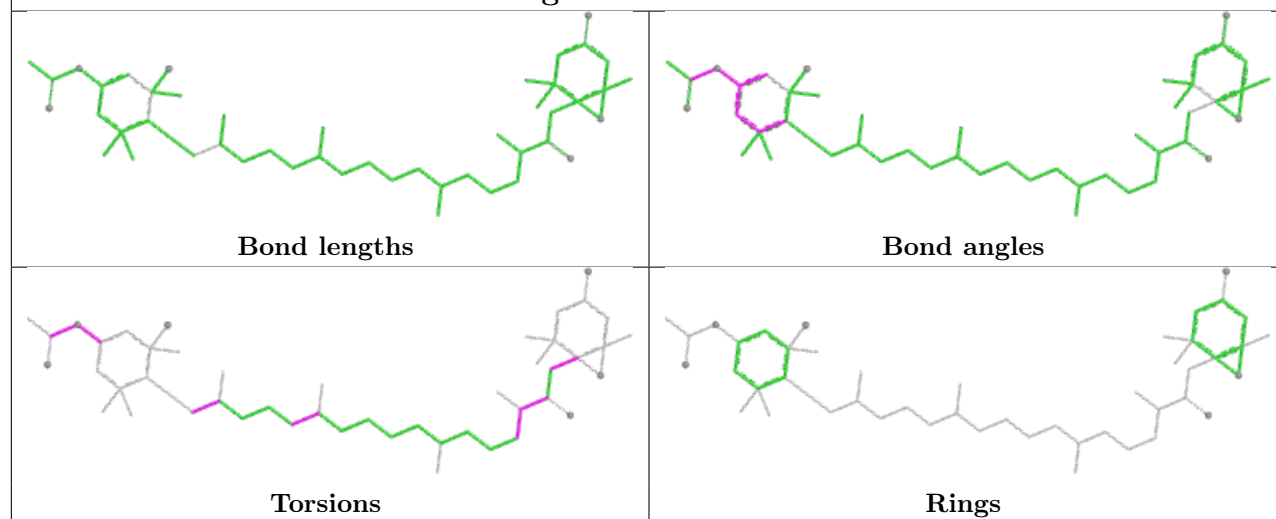
Ligand A86 N 314



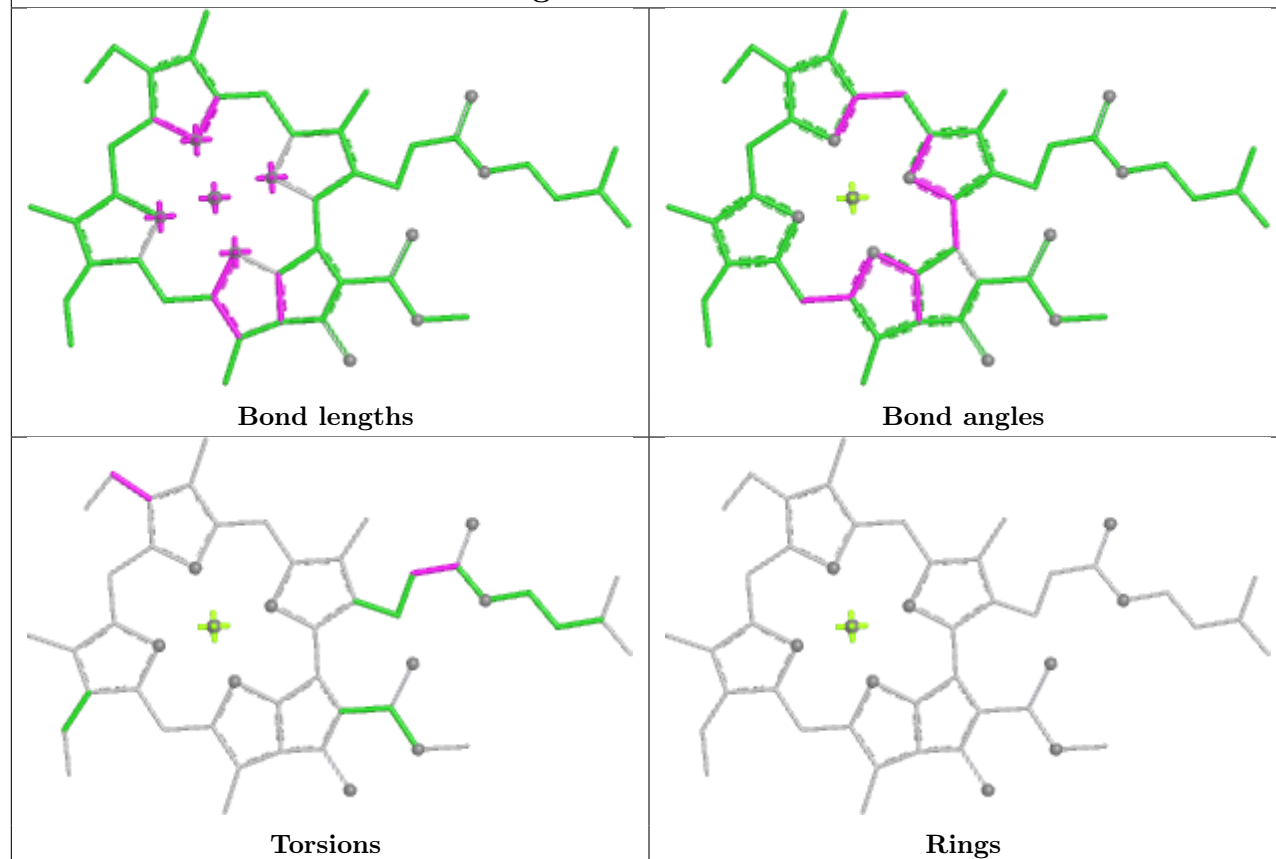
Ligand KC2 K 302



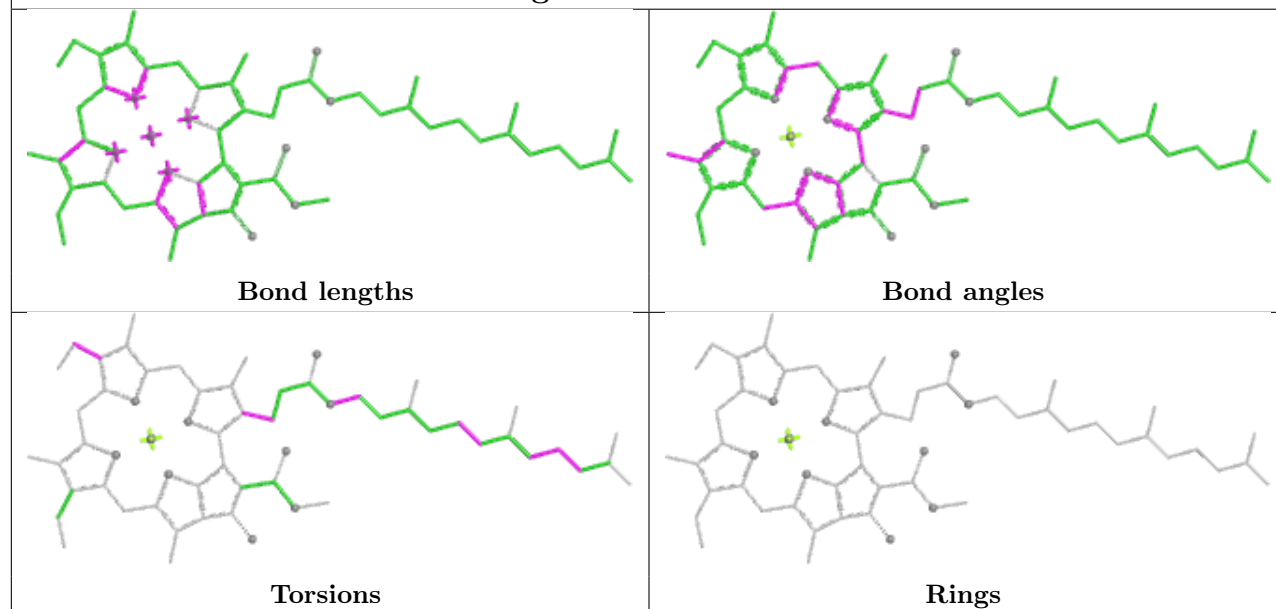
Ligand A86 v 319

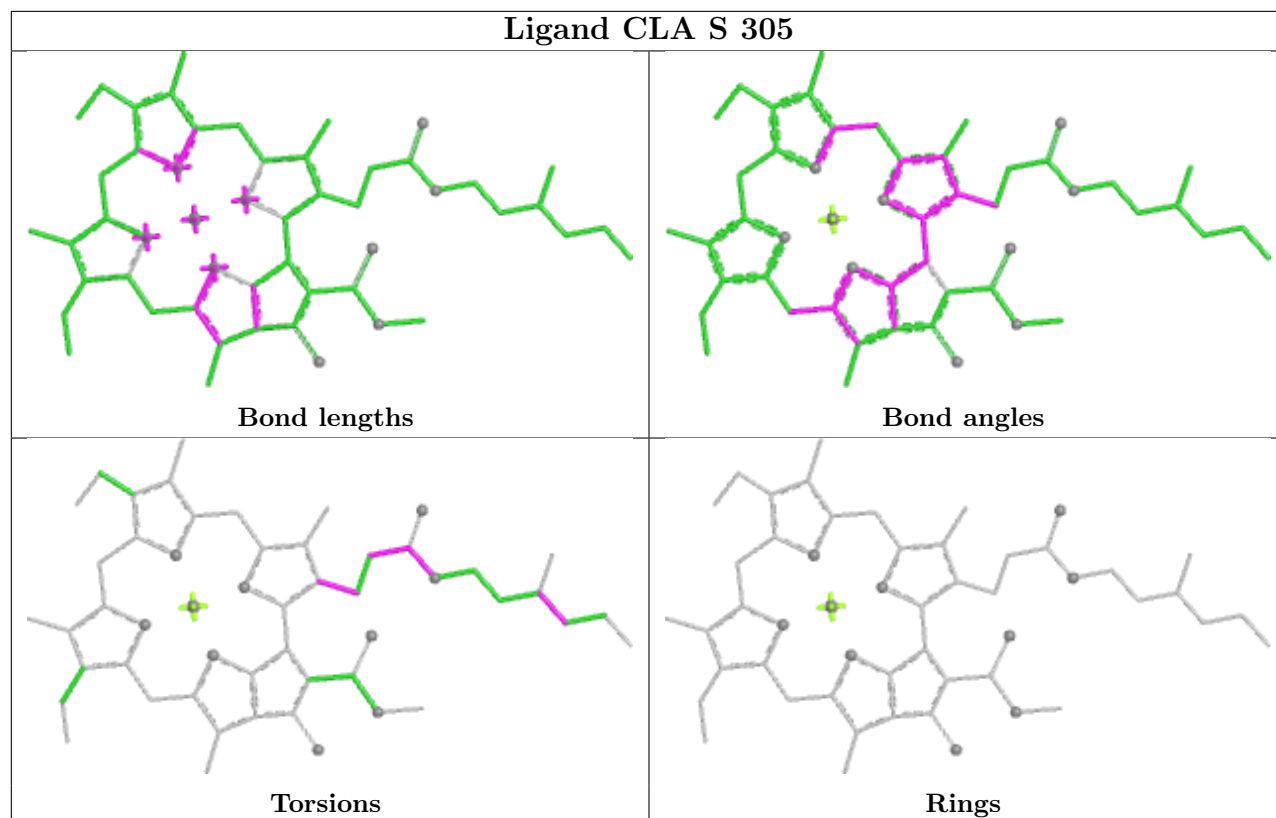


Ligand CLA T 305

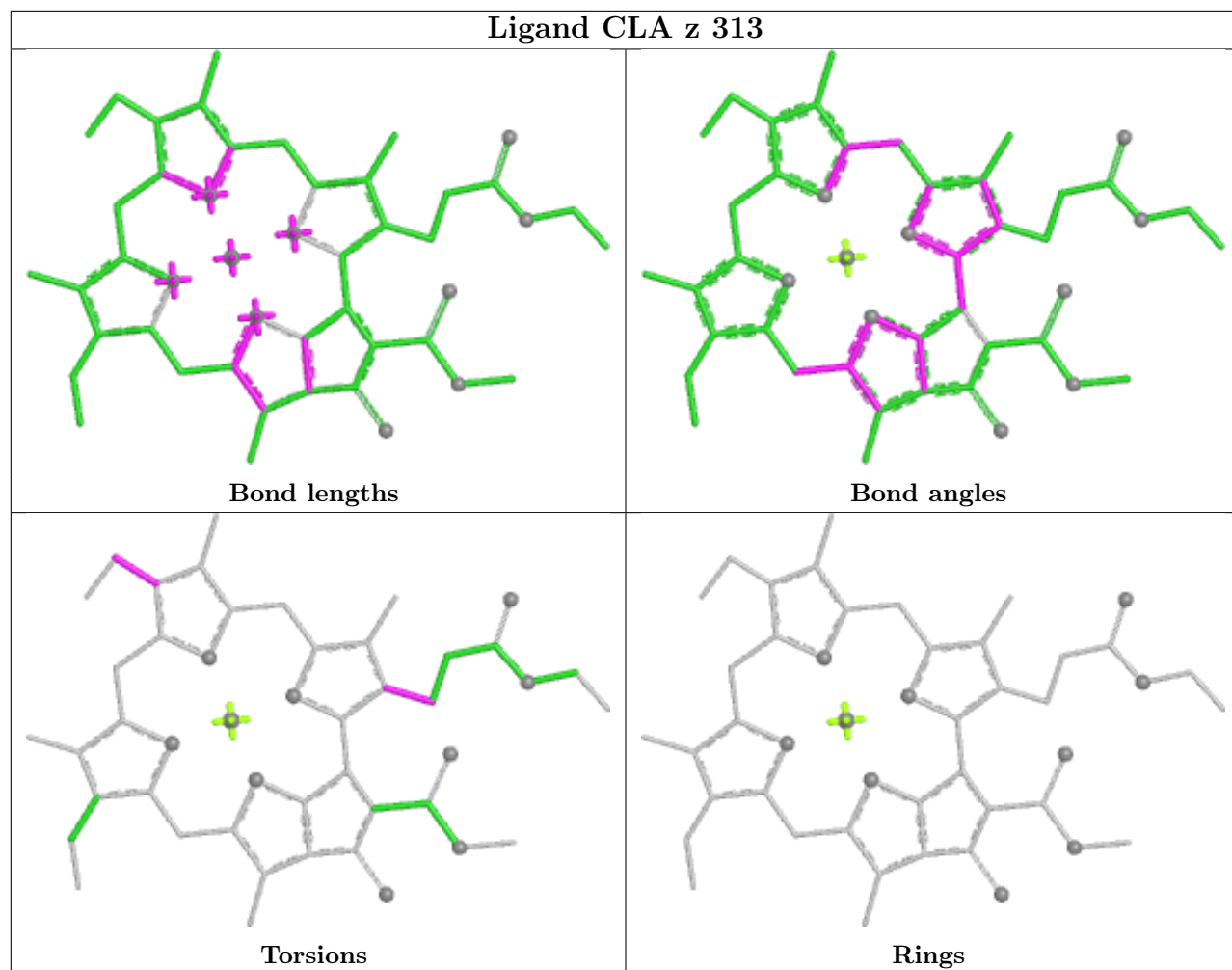


Ligand CLA Y 306

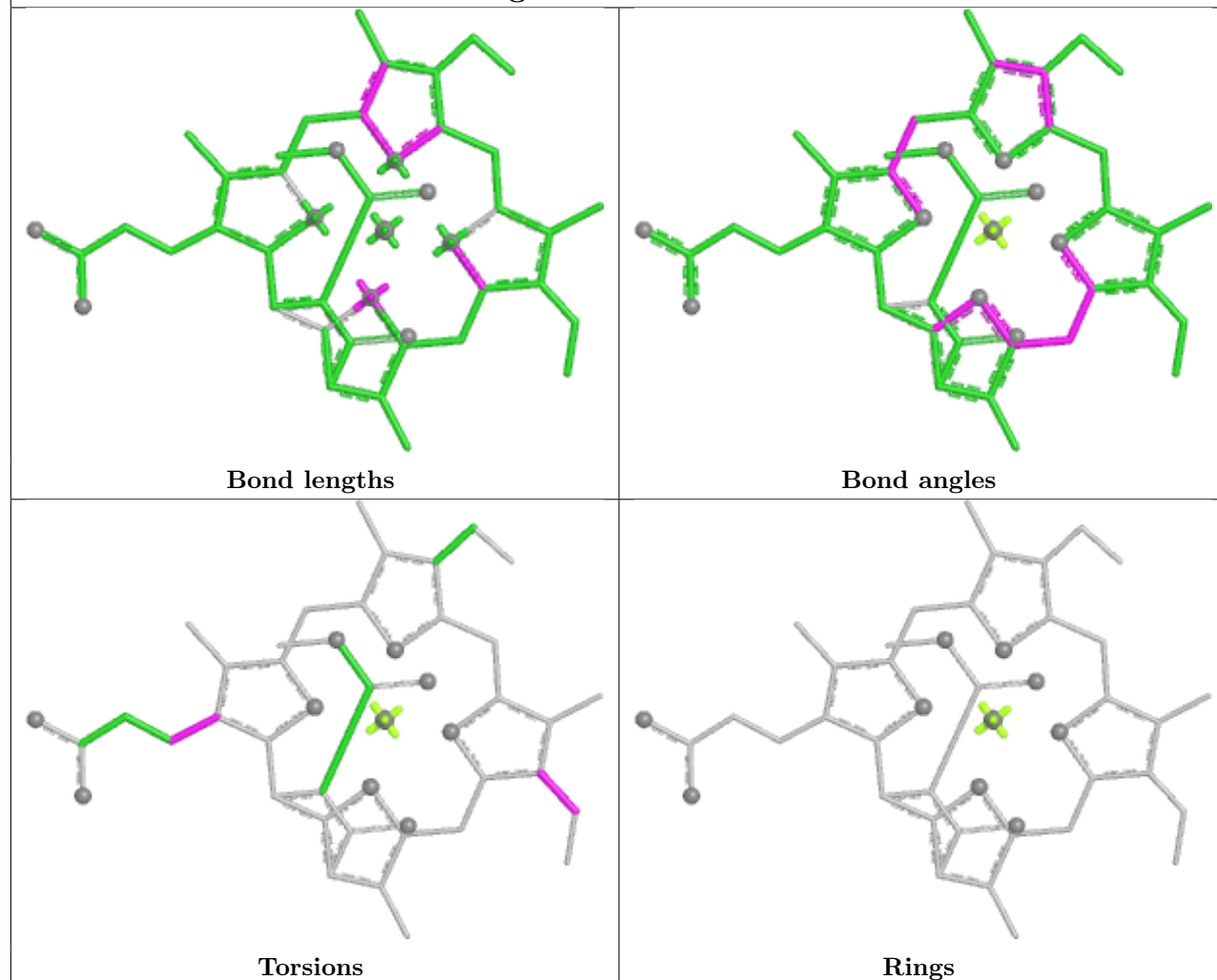




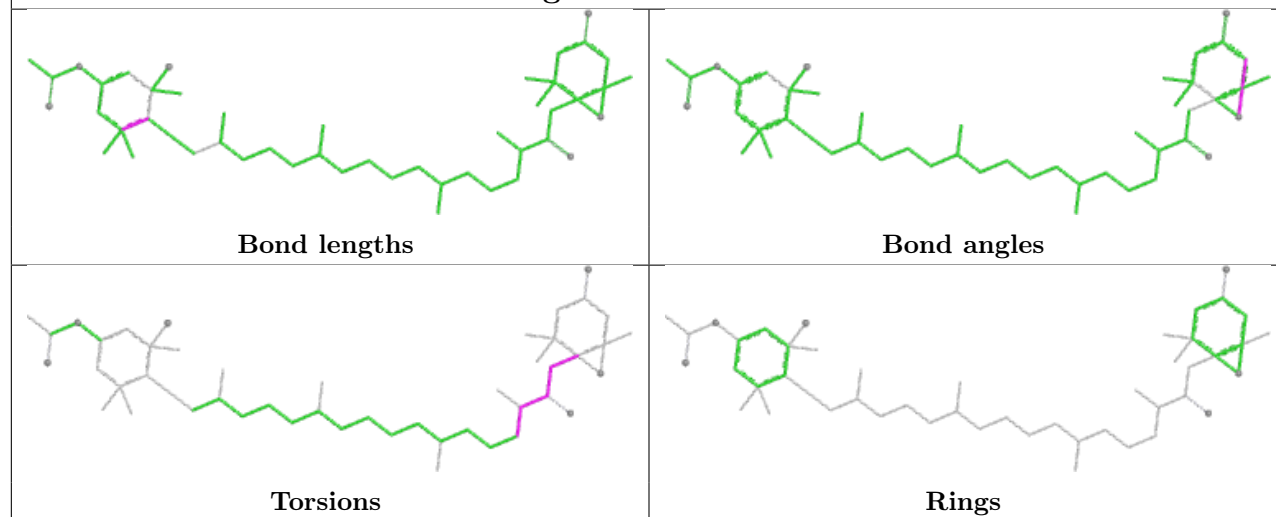
Ligand CLA z 313

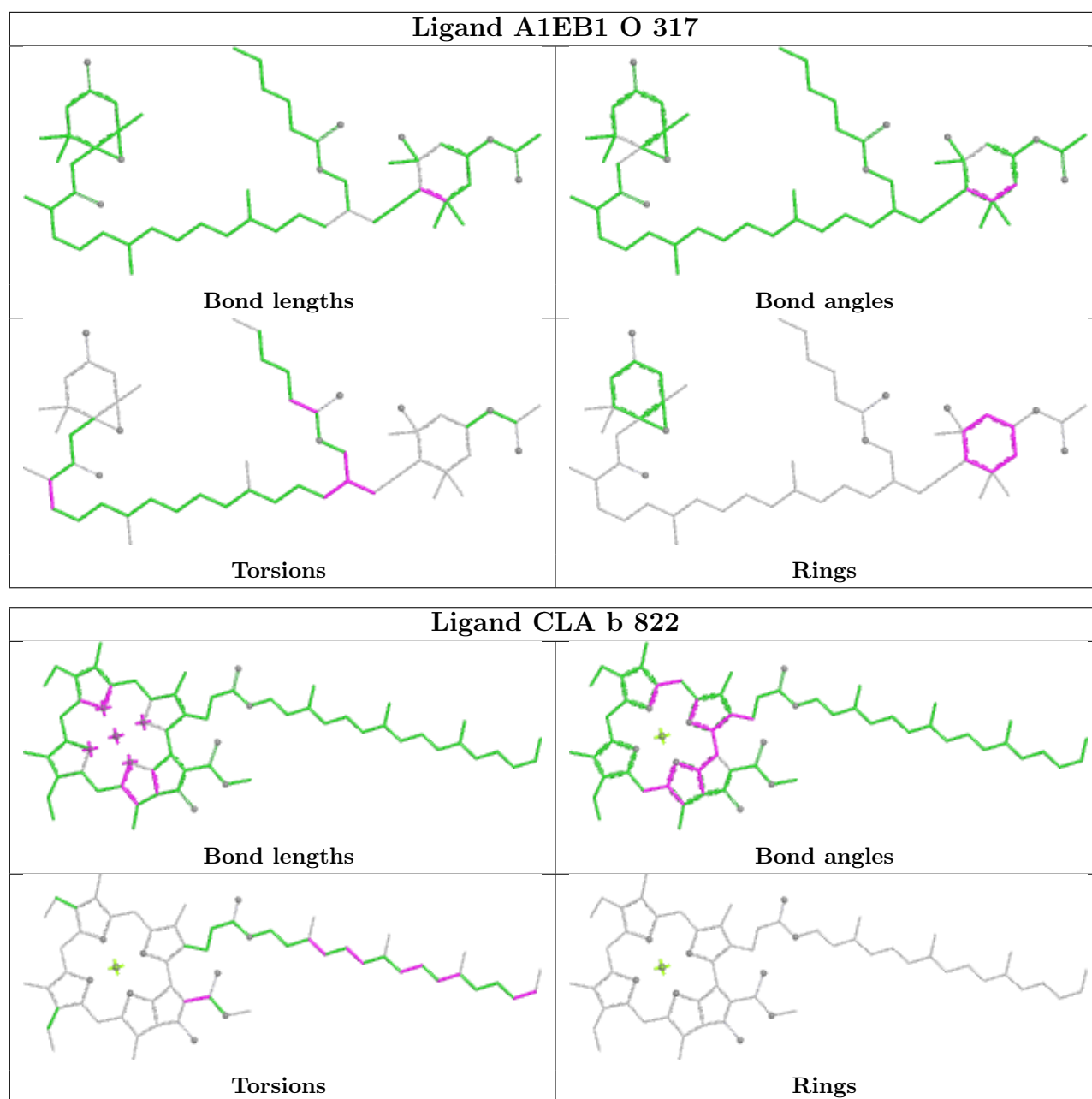


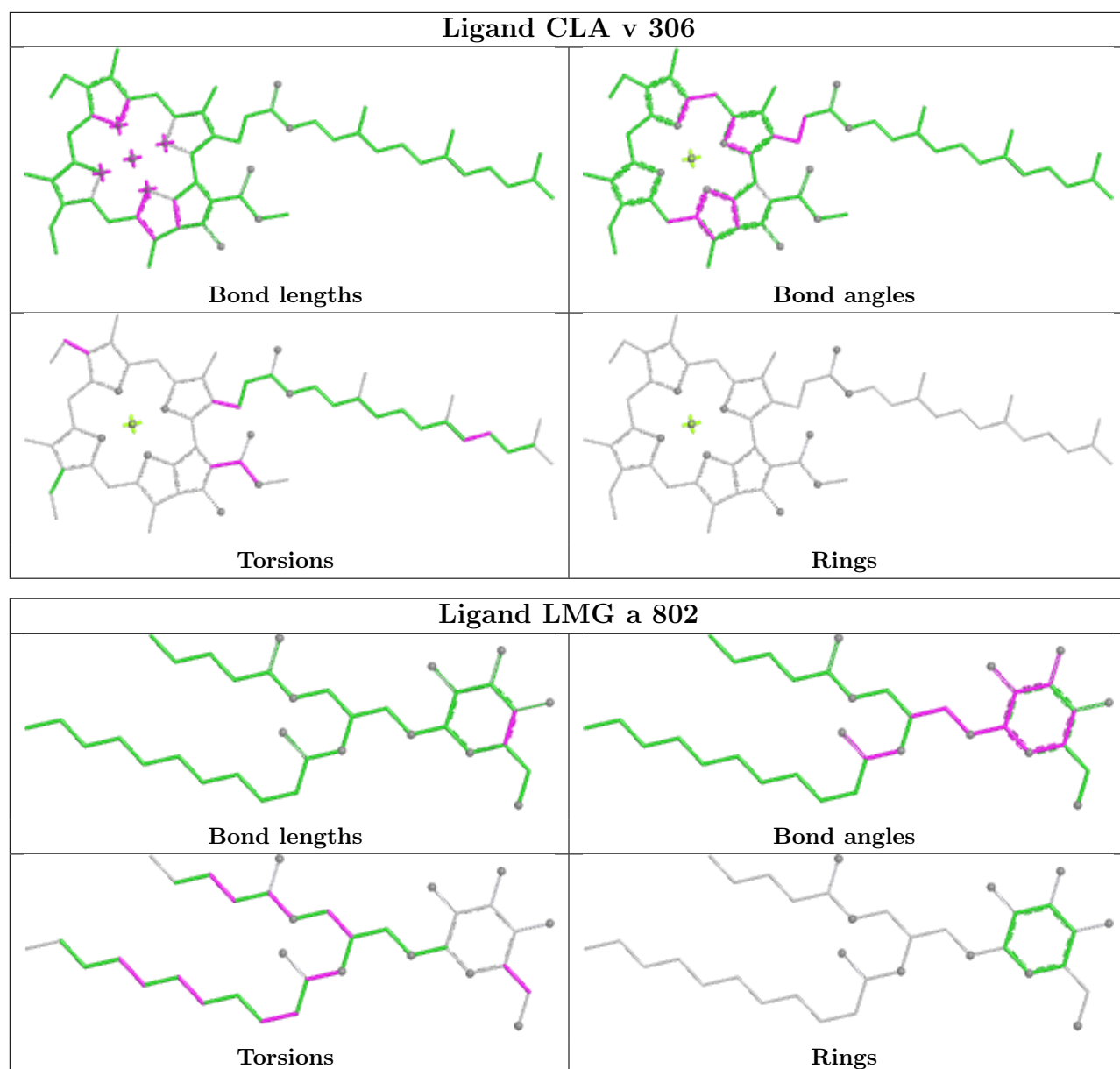
Ligand KC2 R 302

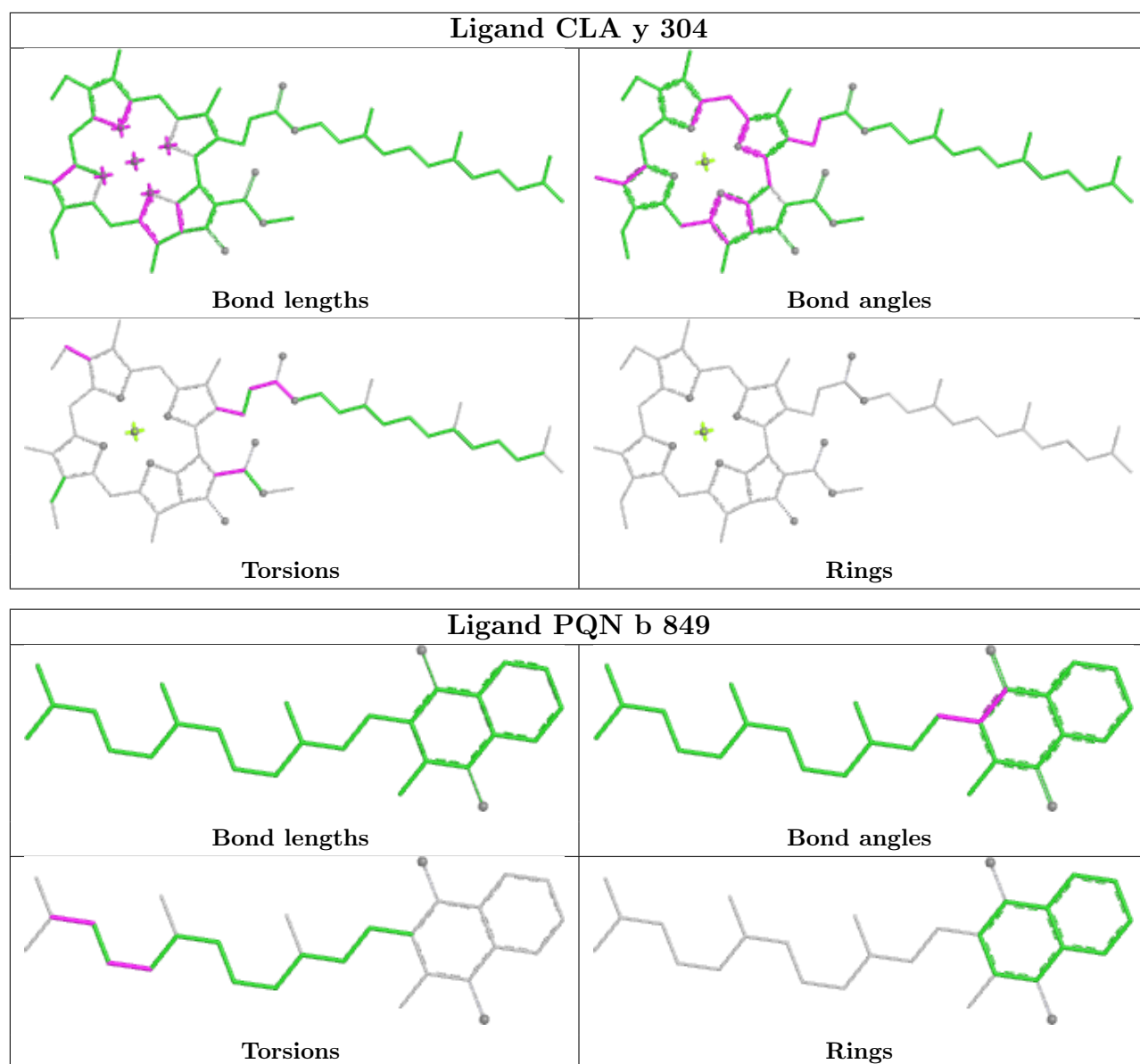


Ligand A86 z 319

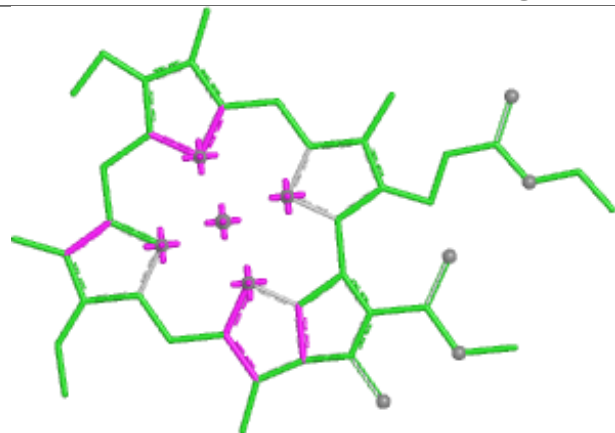




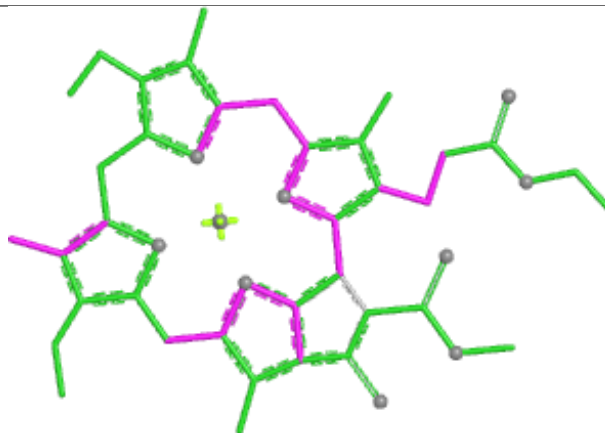




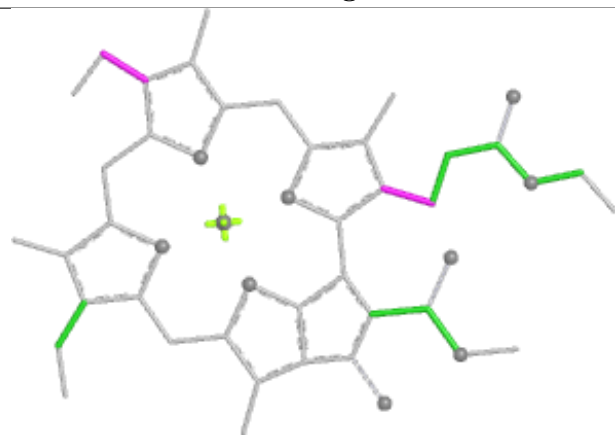
Ligand CLA H 304



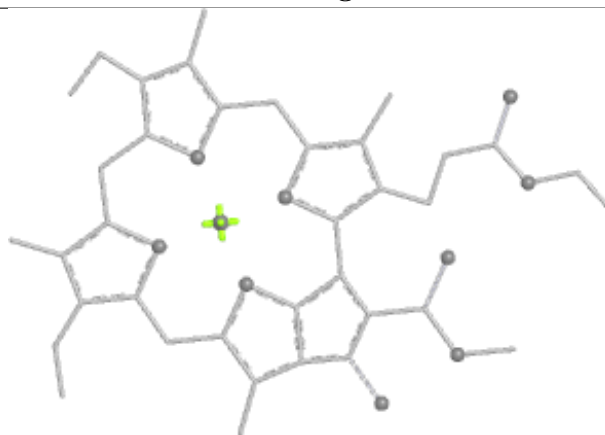
Bond lengths



Bond angles

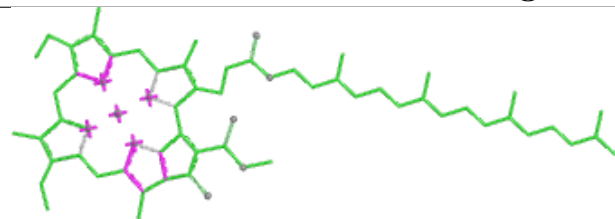


Torsions

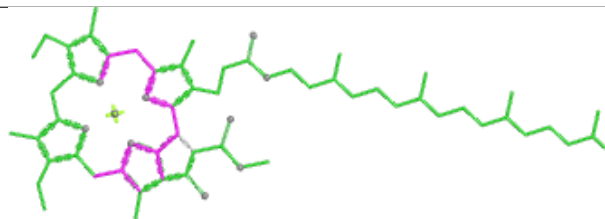


Rings

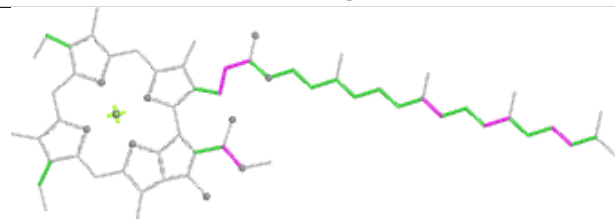
Ligand CLA b 808



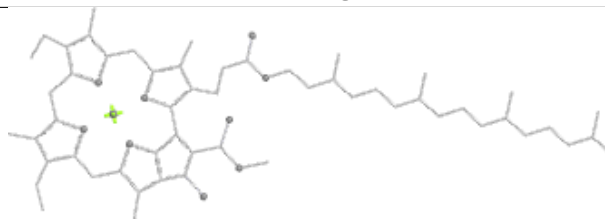
Bond lengths



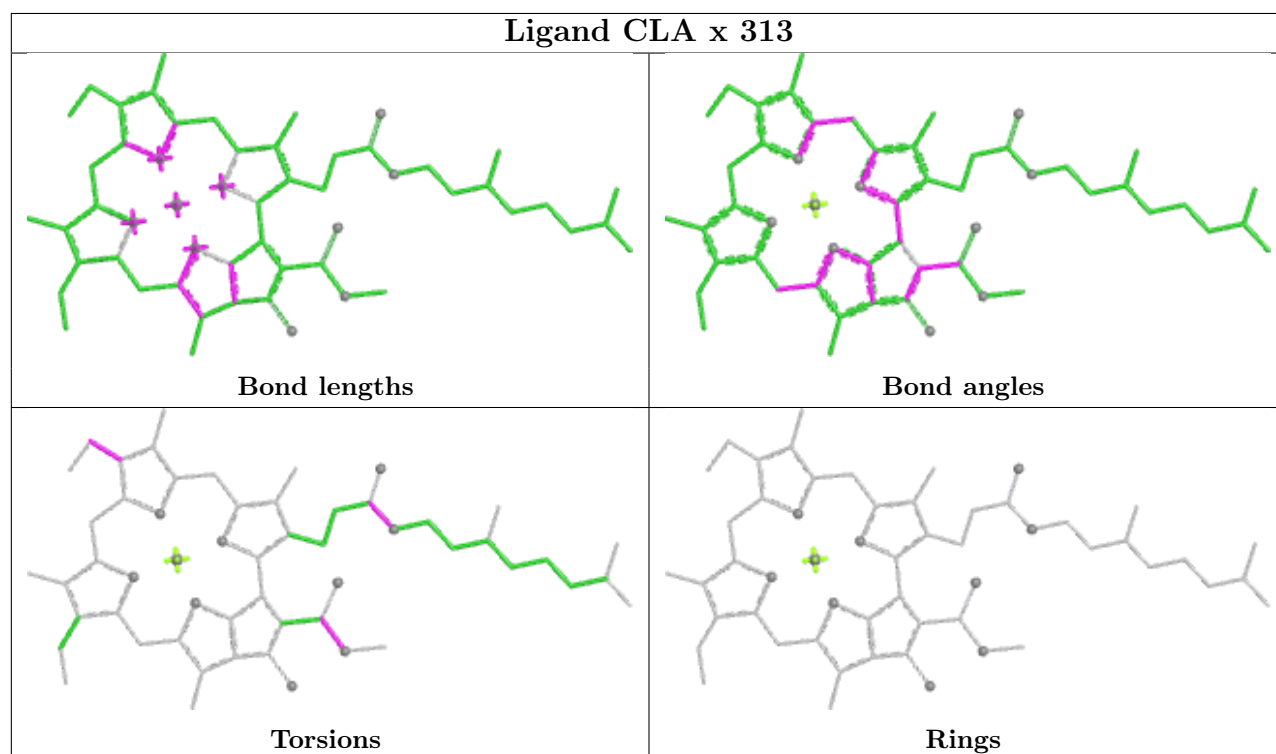
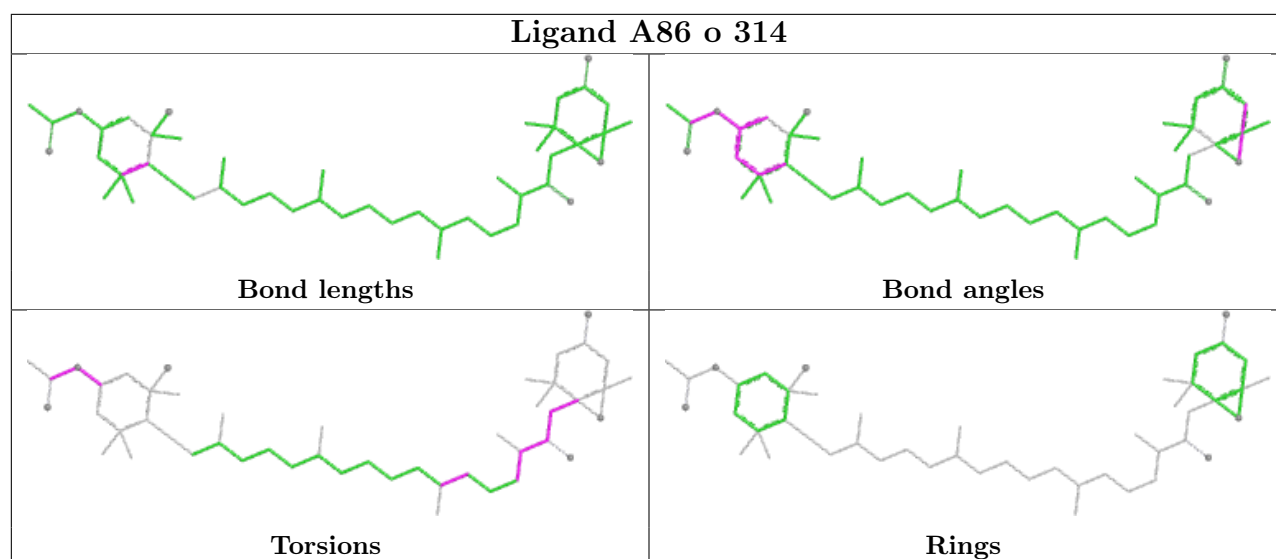
Bond angles

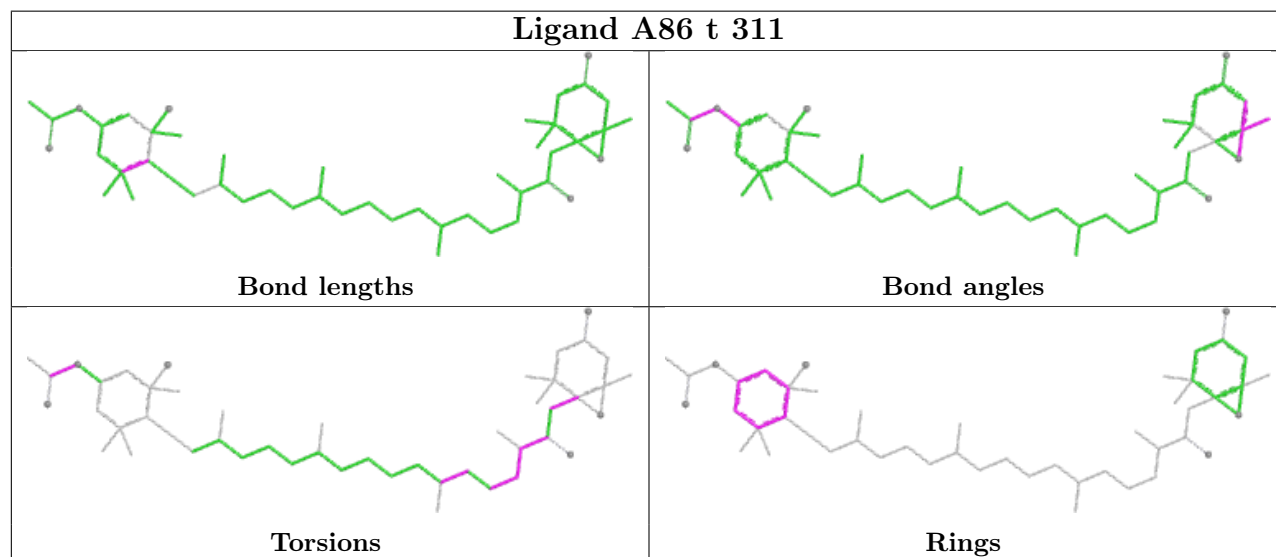
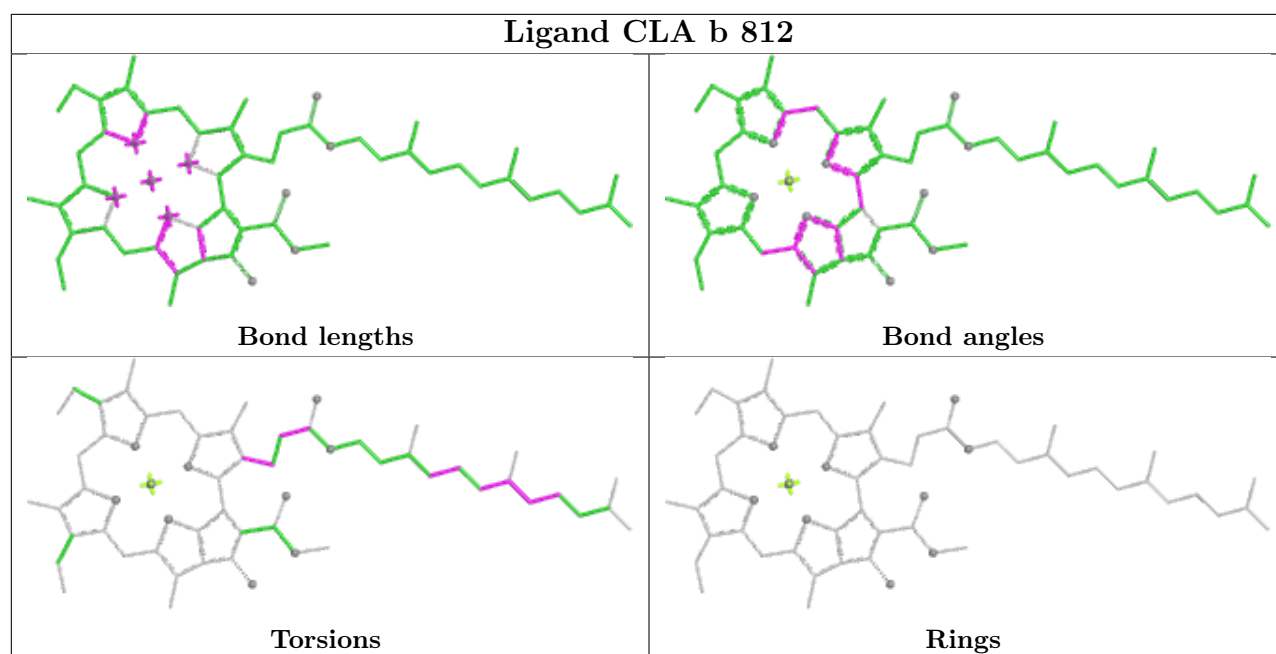


Torsions

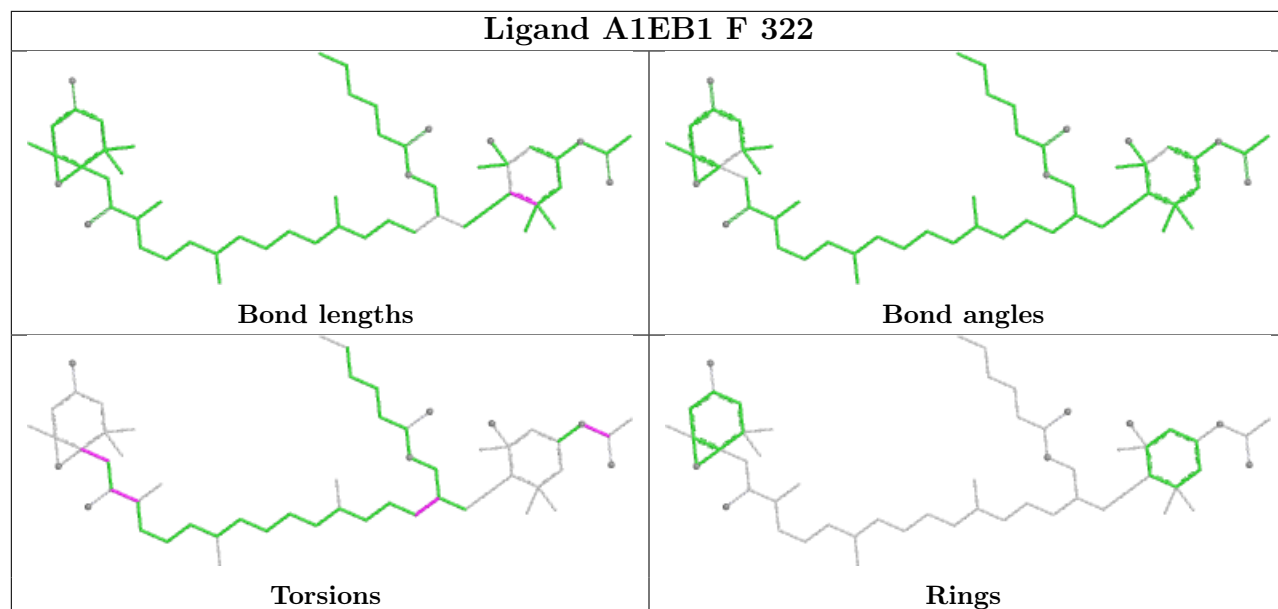


Rings

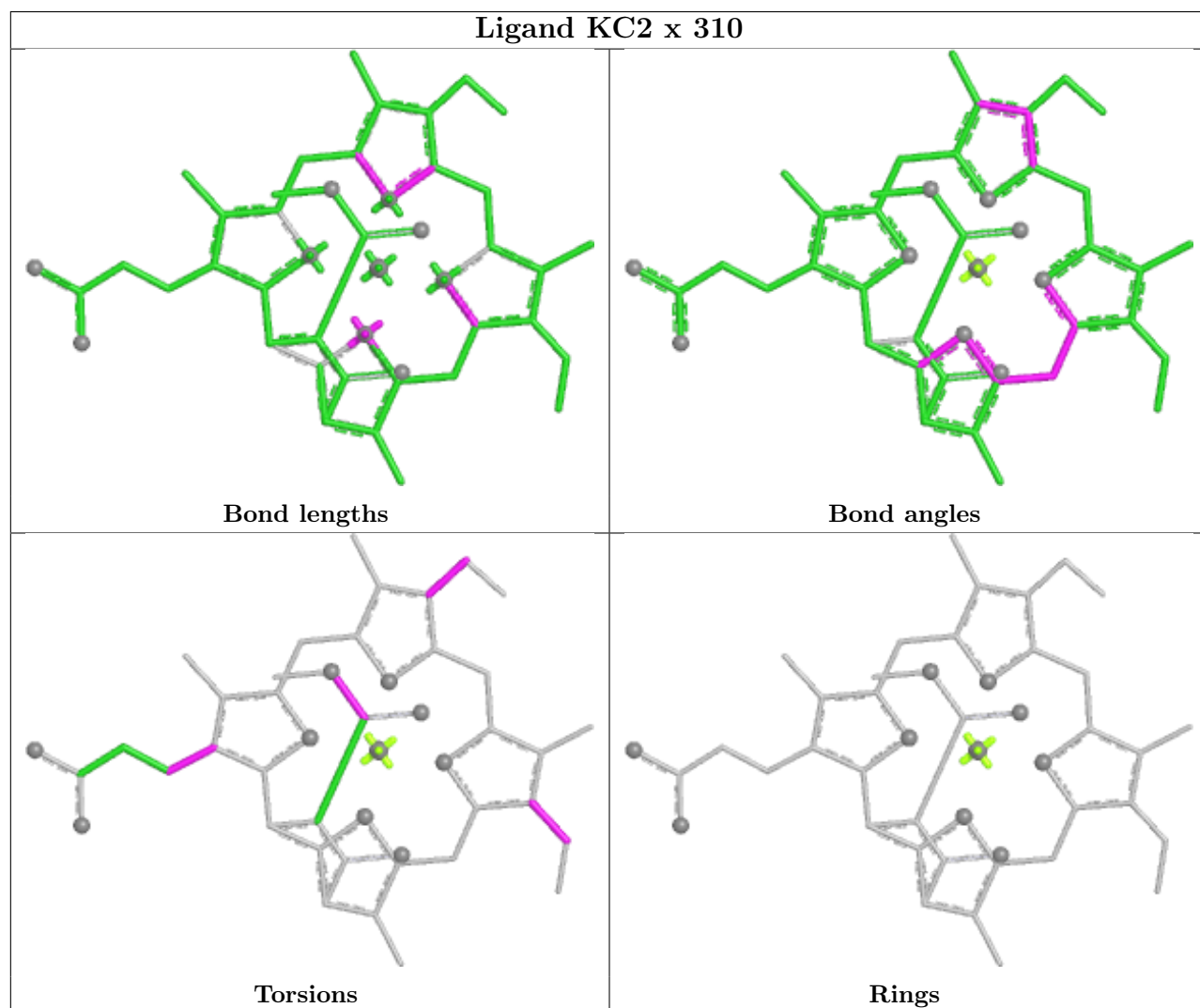




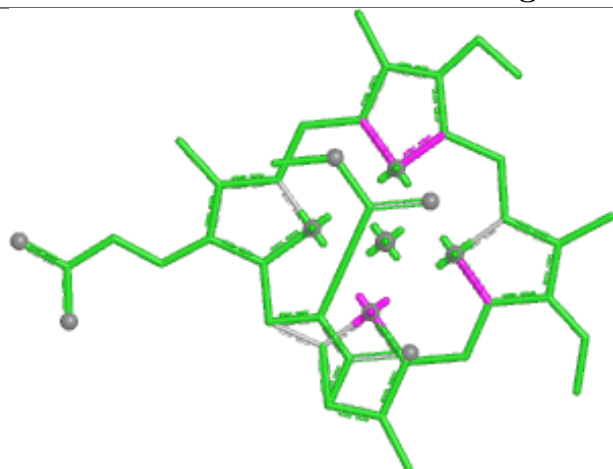
Ligand A1EB1 F 322



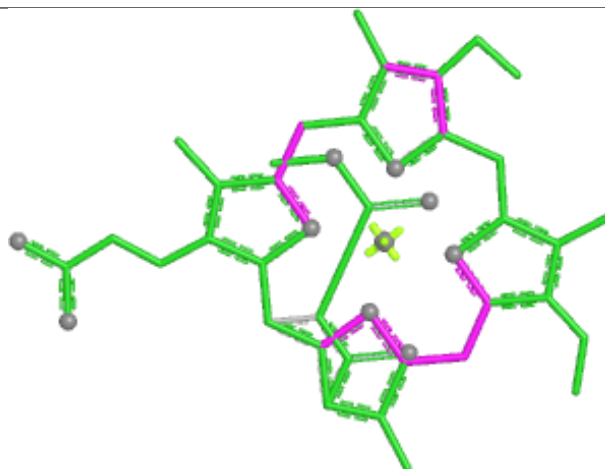
Ligand KC2 x 310



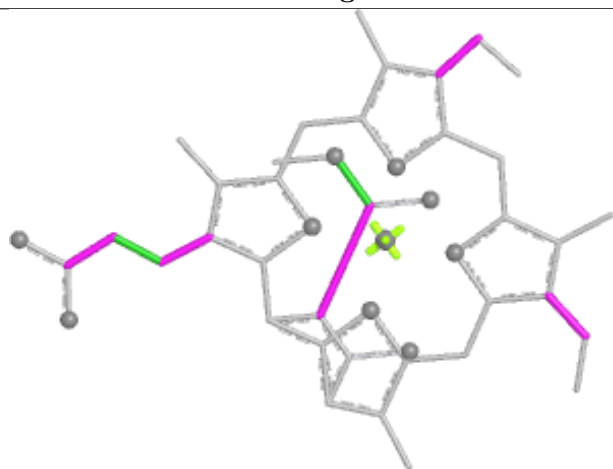
Ligand KC2 S 309



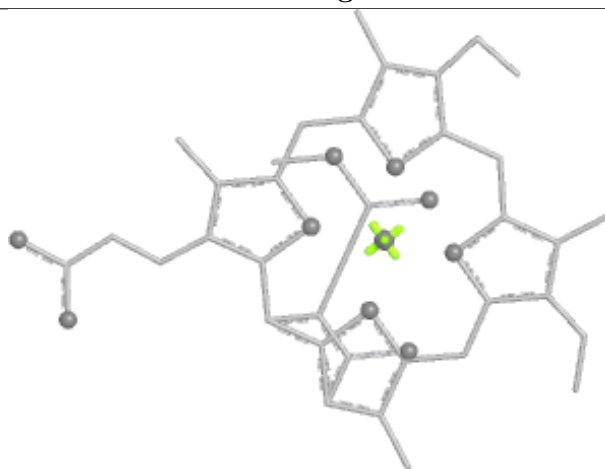
Bond lengths



Bond angles

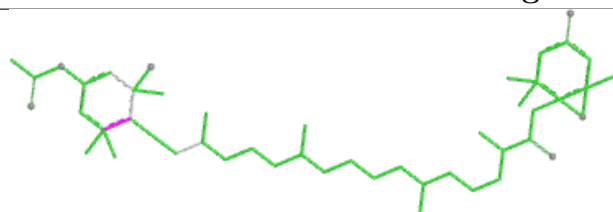


Torsions

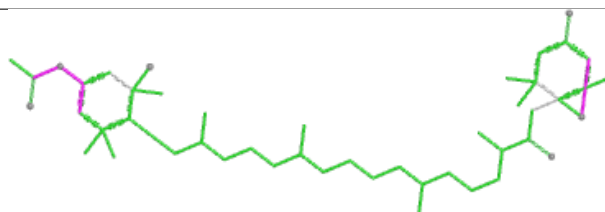


Rings

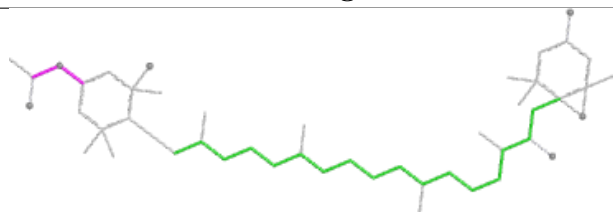
Ligand A86 Z 314



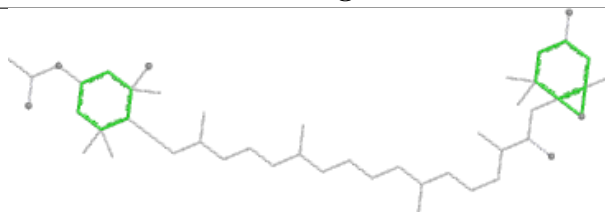
Bond lengths



Bond angles

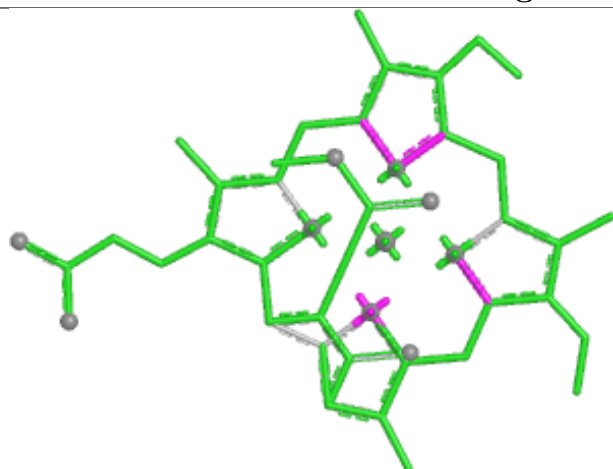


Torsions

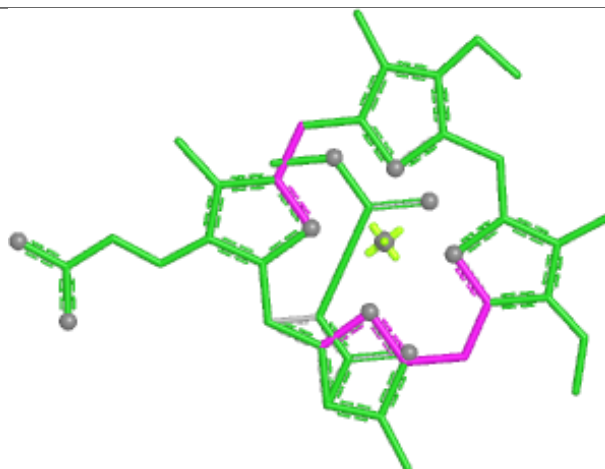


Rings

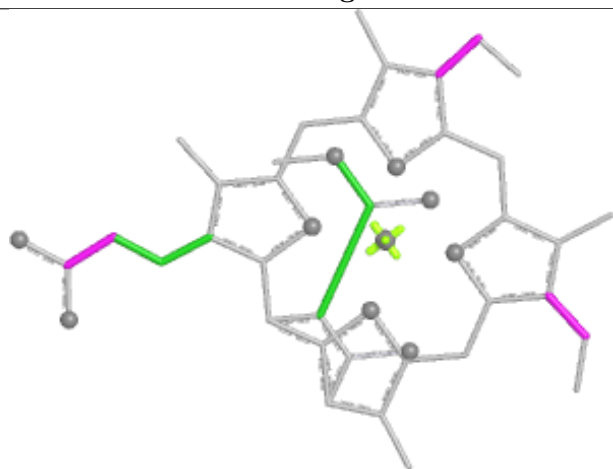
Ligand KC2 O 311



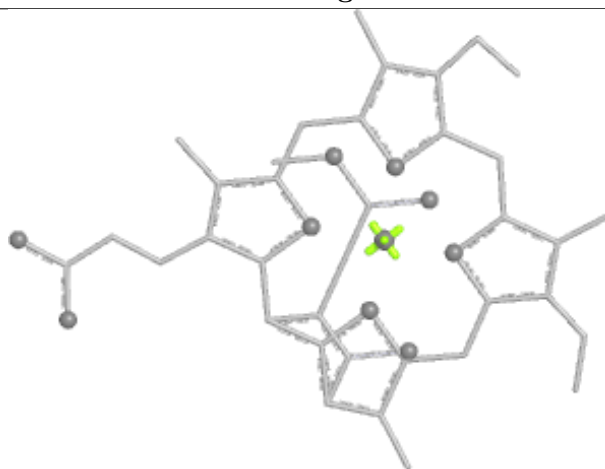
Bond lengths



Bond angles

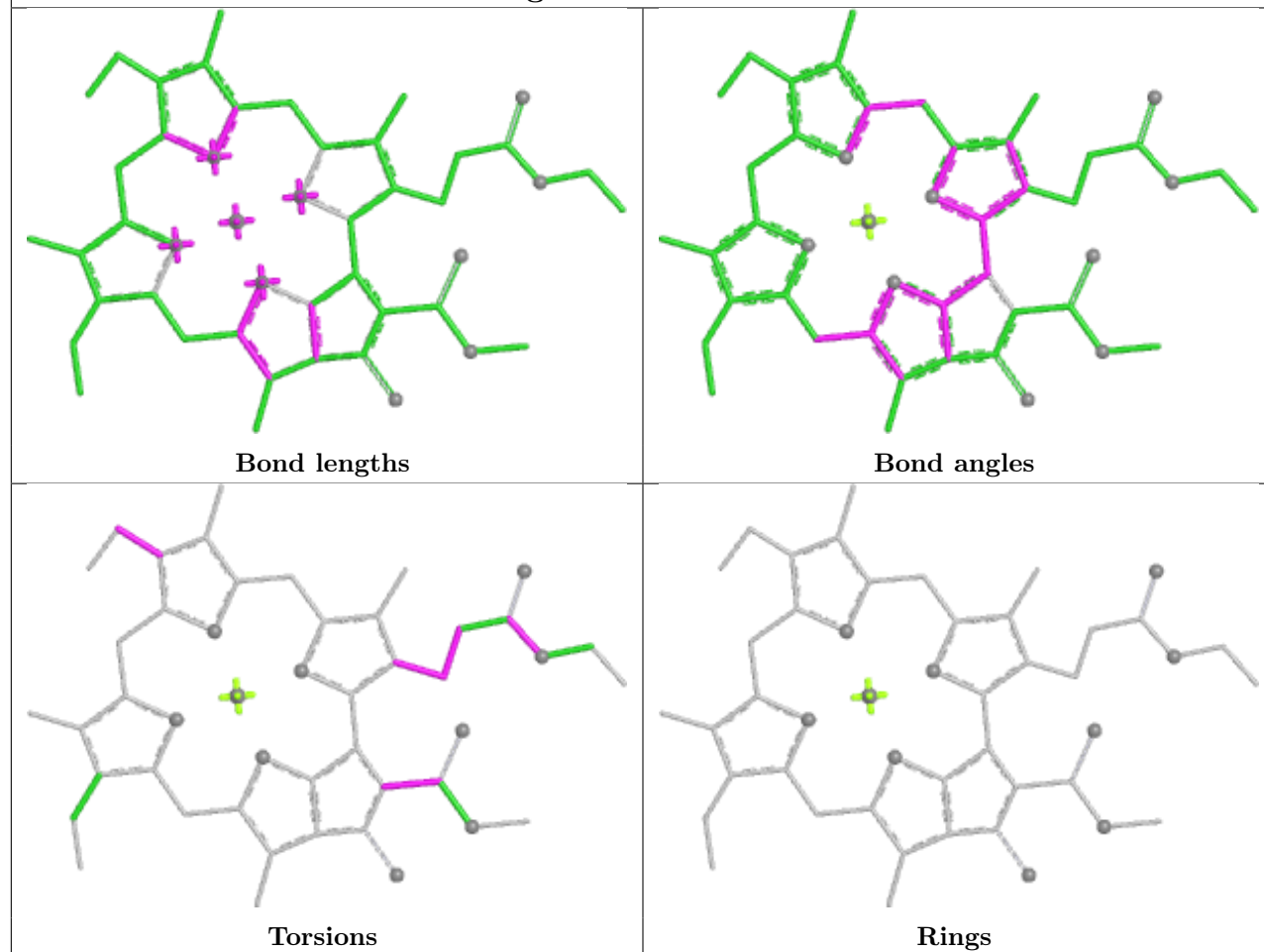


Torsions

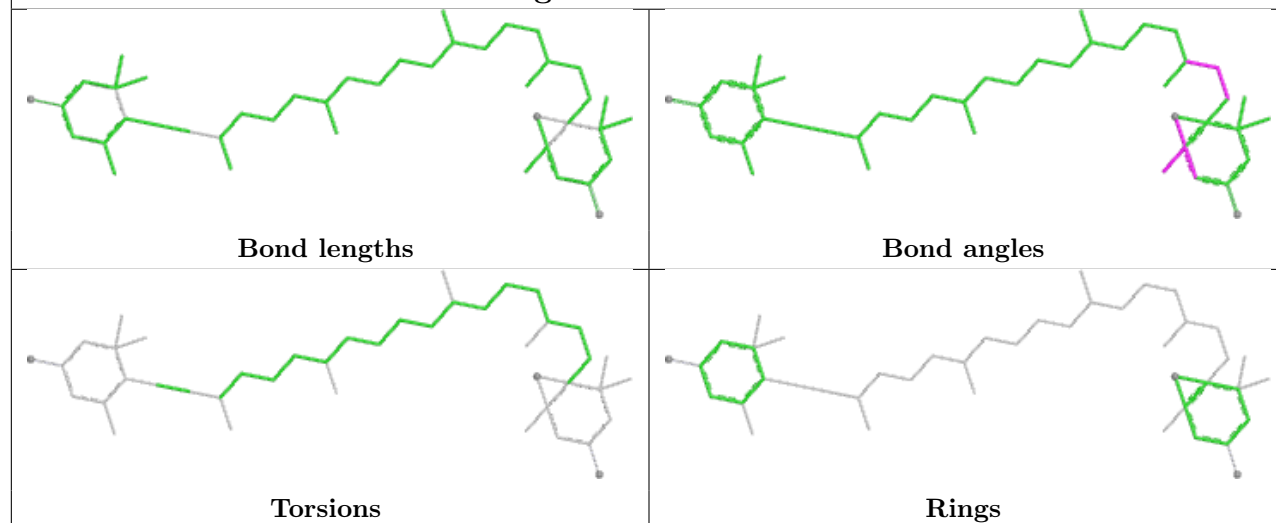


Rings

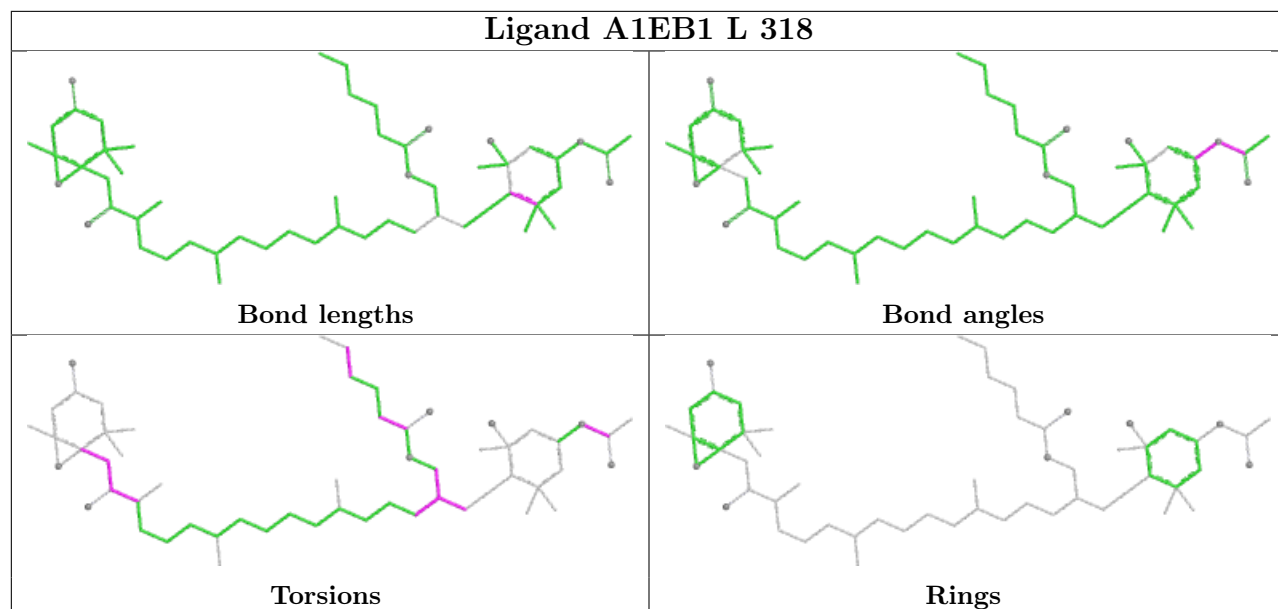
Ligand CLA Y 313



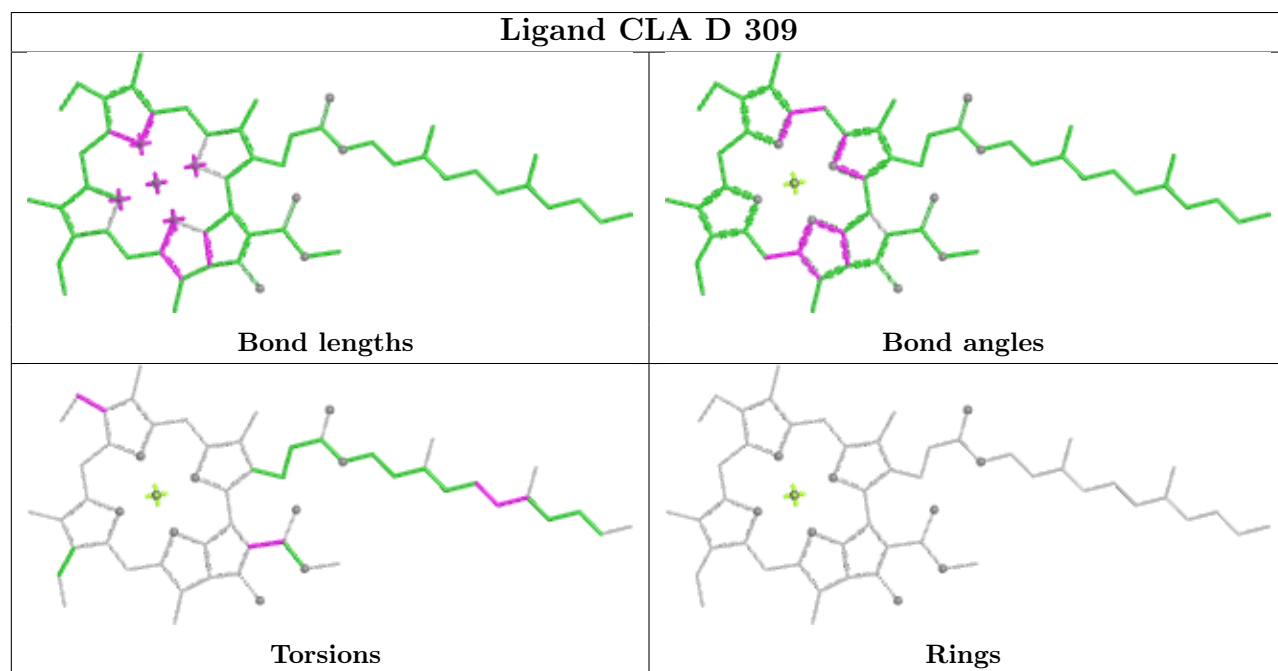
Ligand DD6 E 316

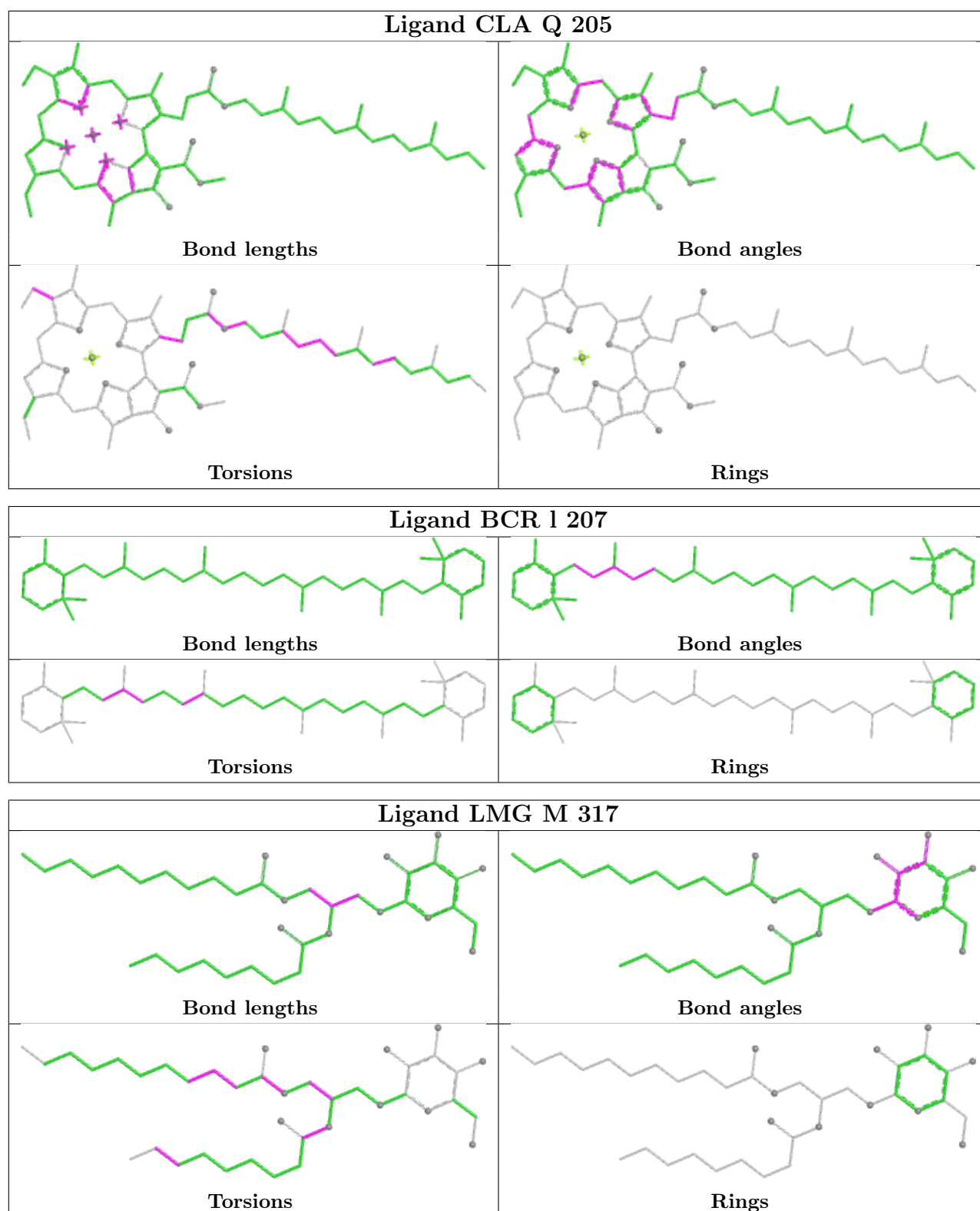


Ligand A1EB1 L 318

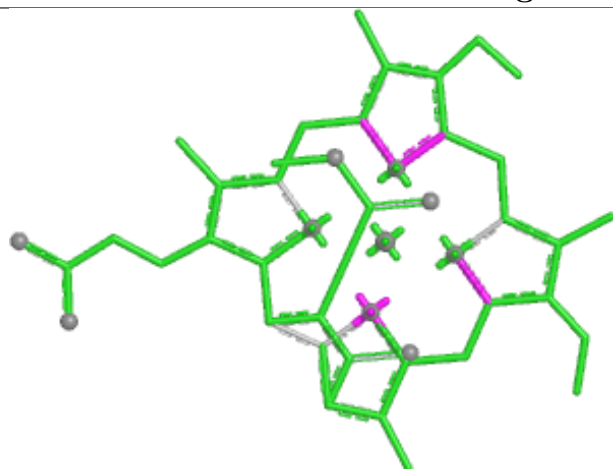


Ligand CLA D 309

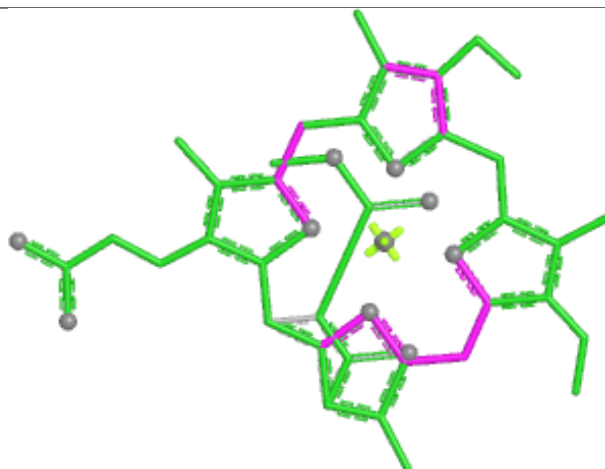




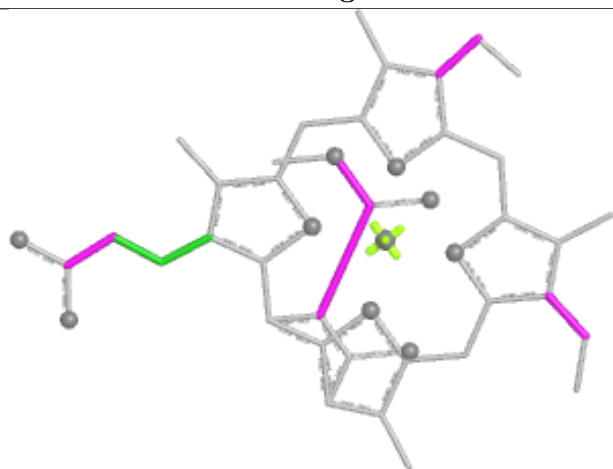
Ligand KC2 w 306



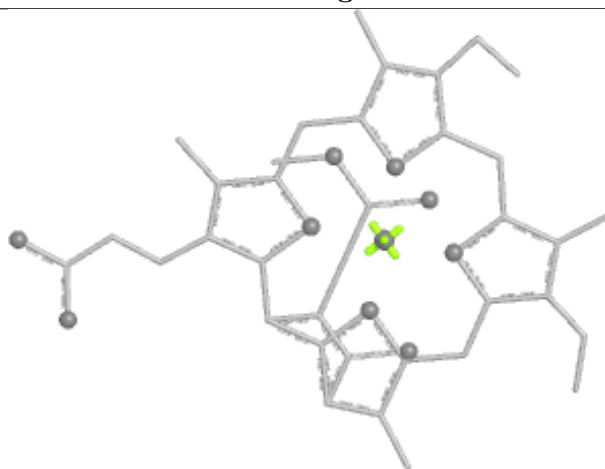
Bond lengths



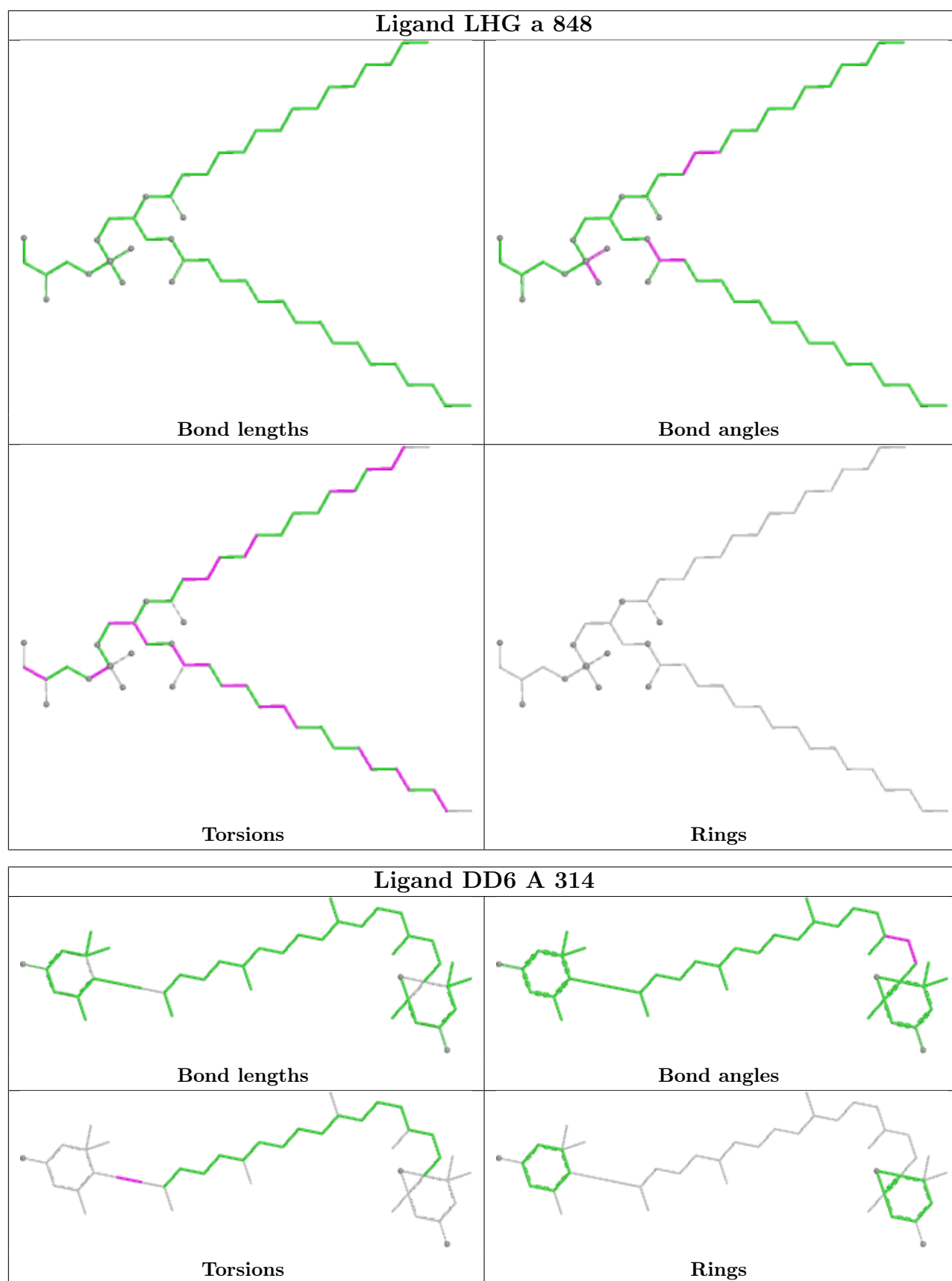
Bond angles

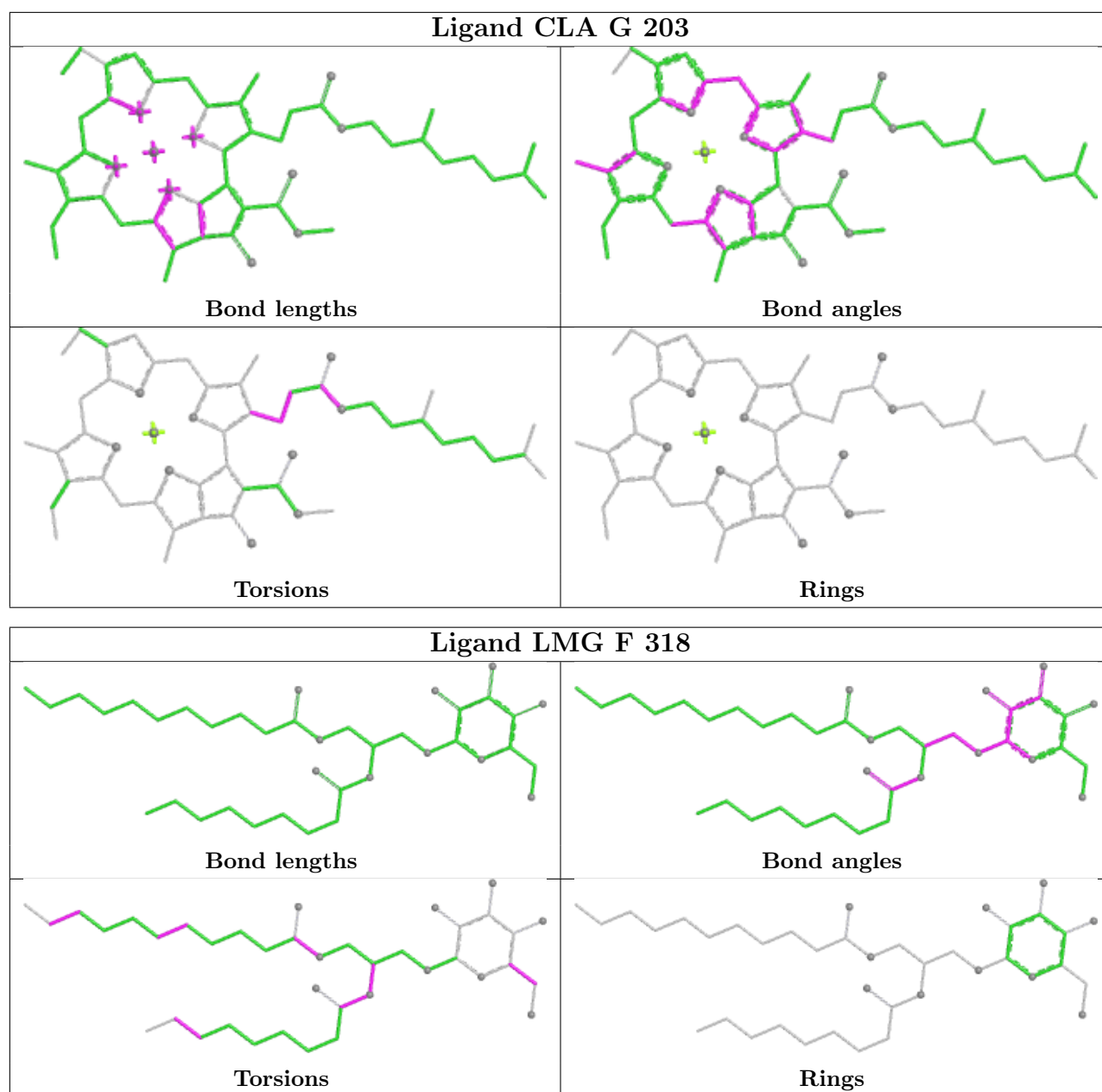


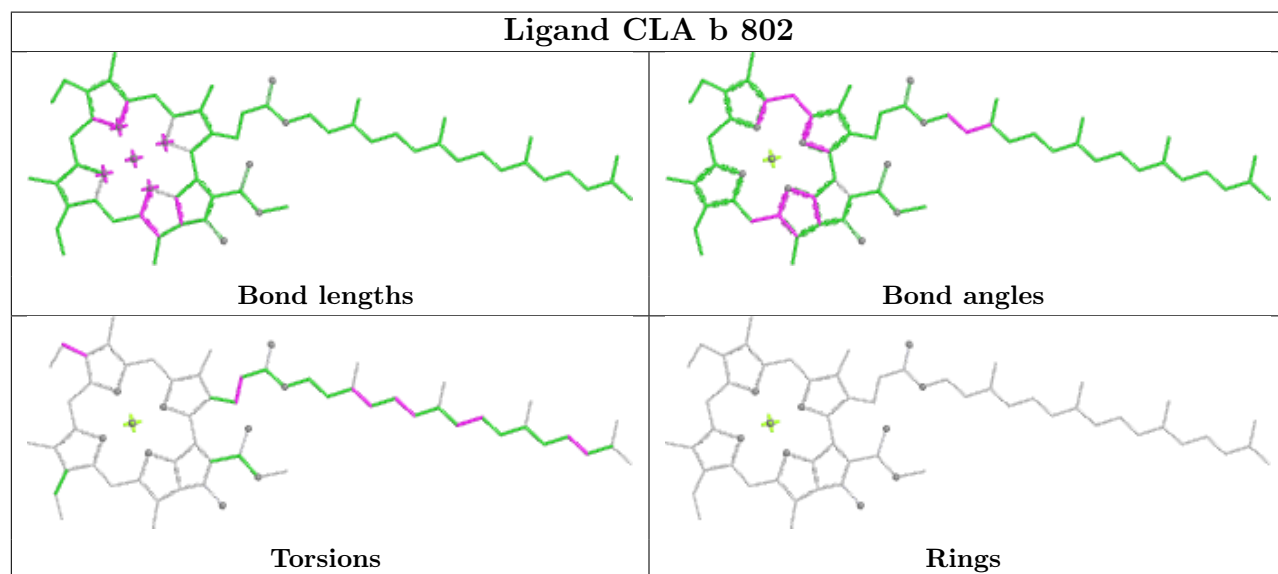
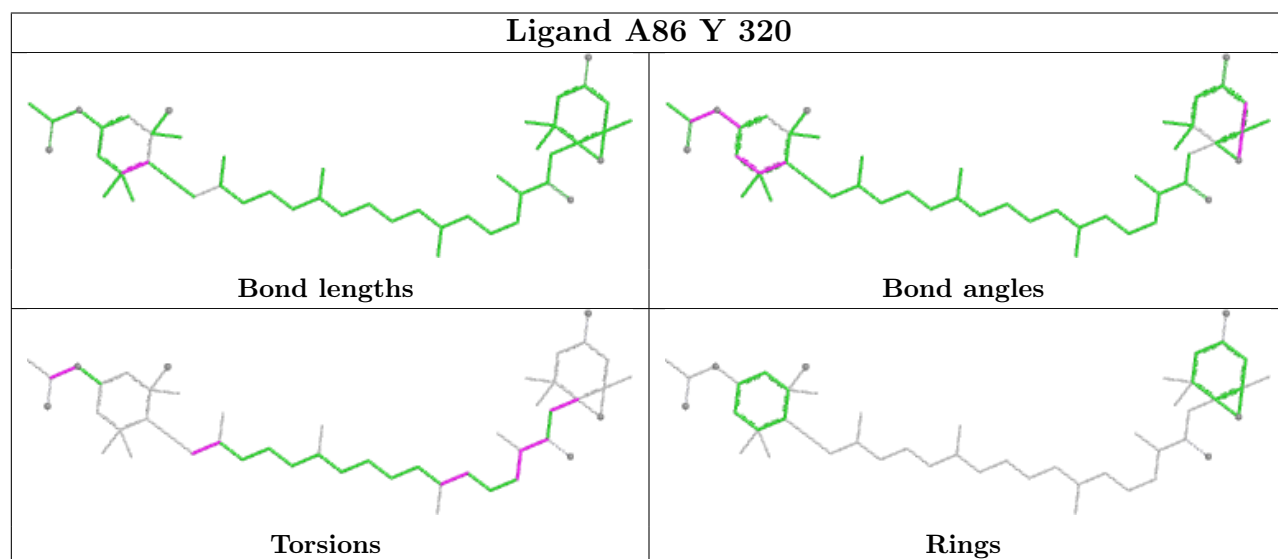
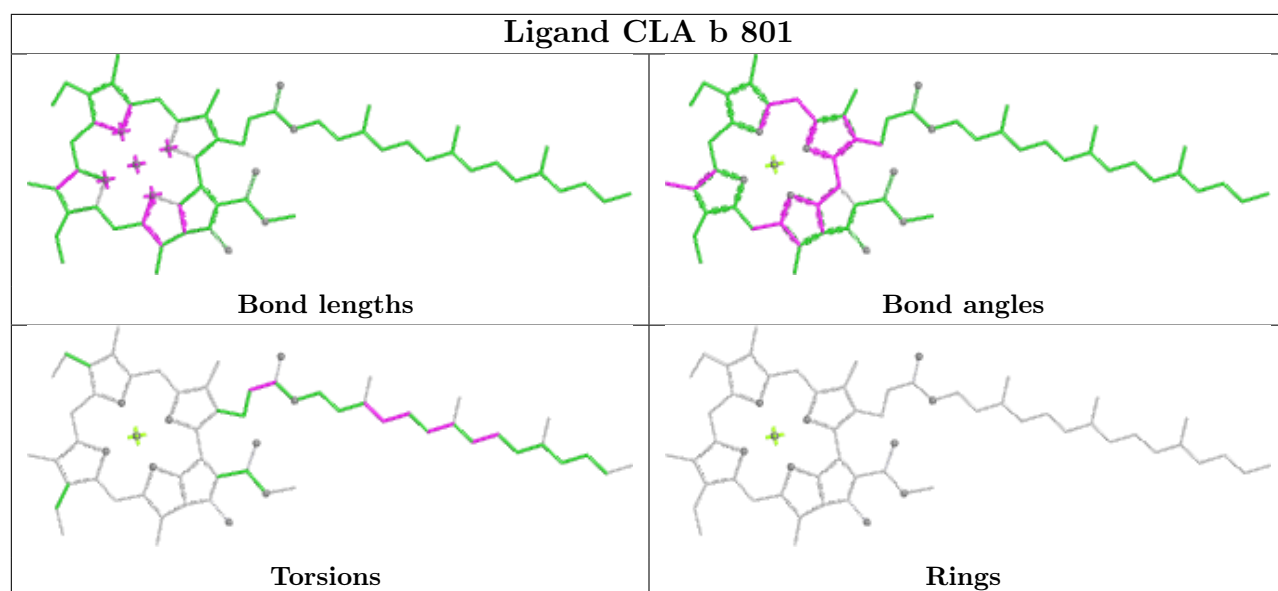
Torsions



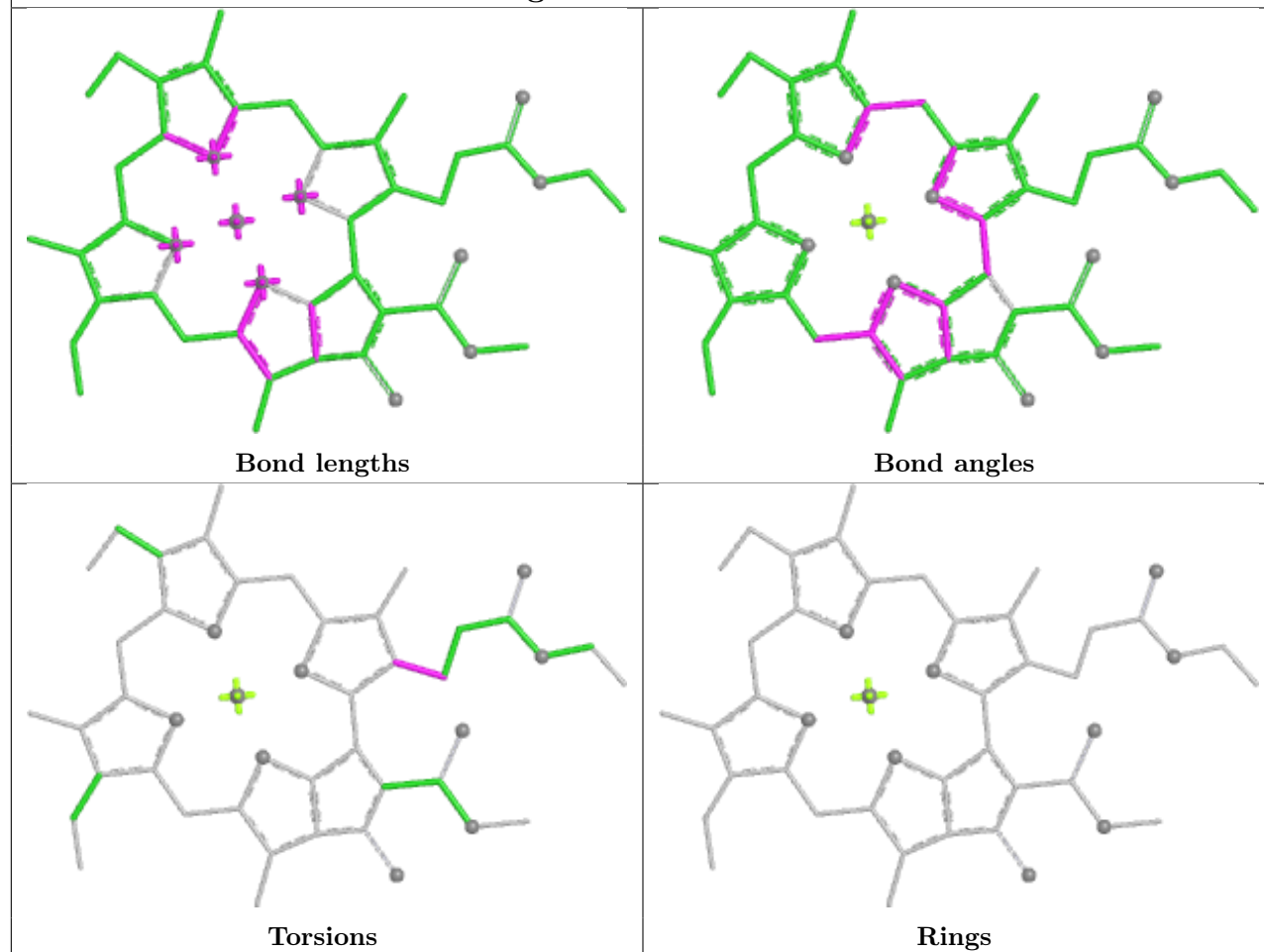
Rings



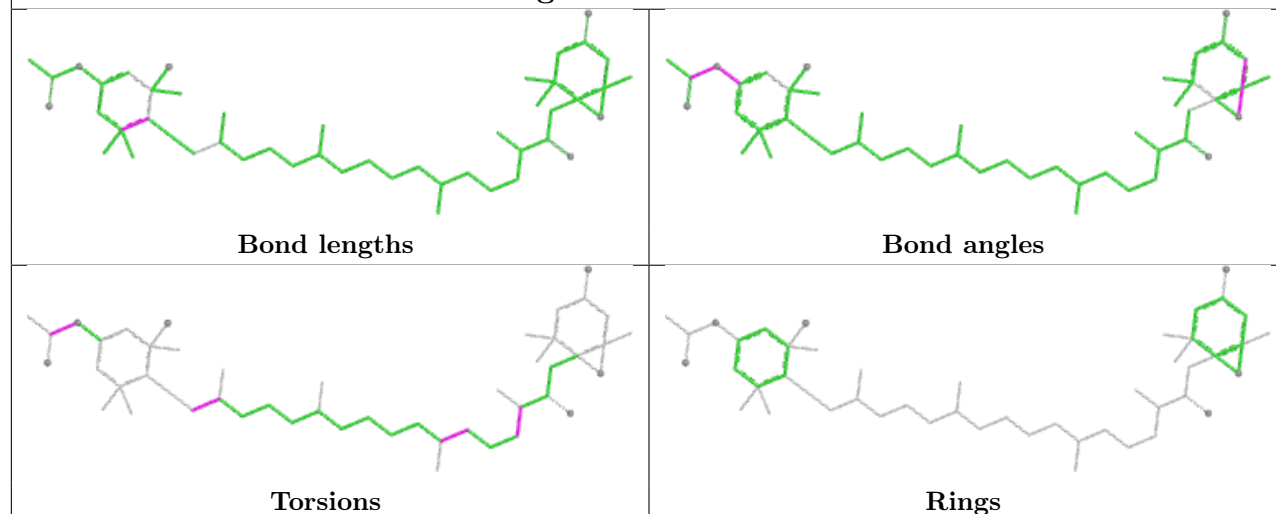


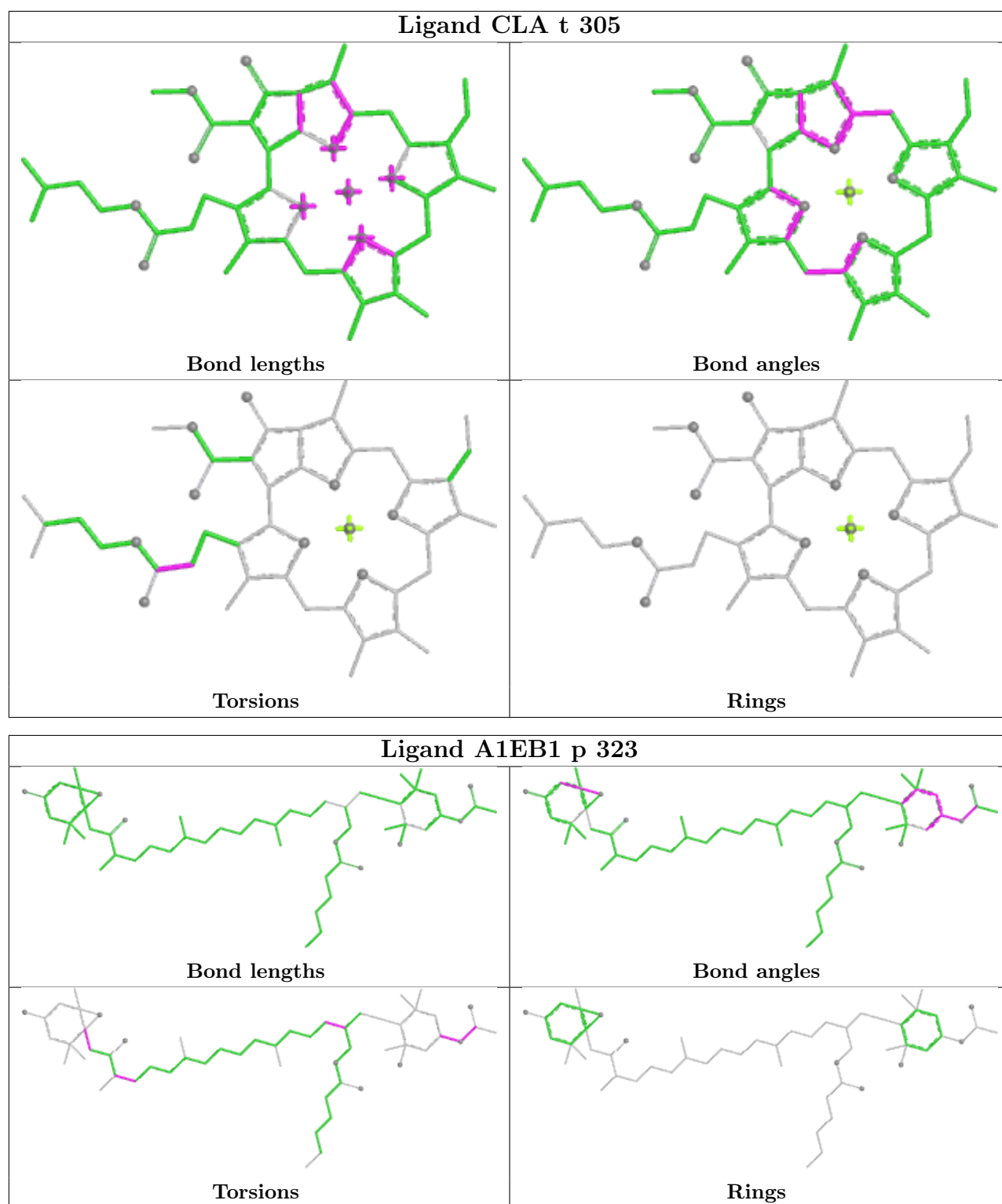


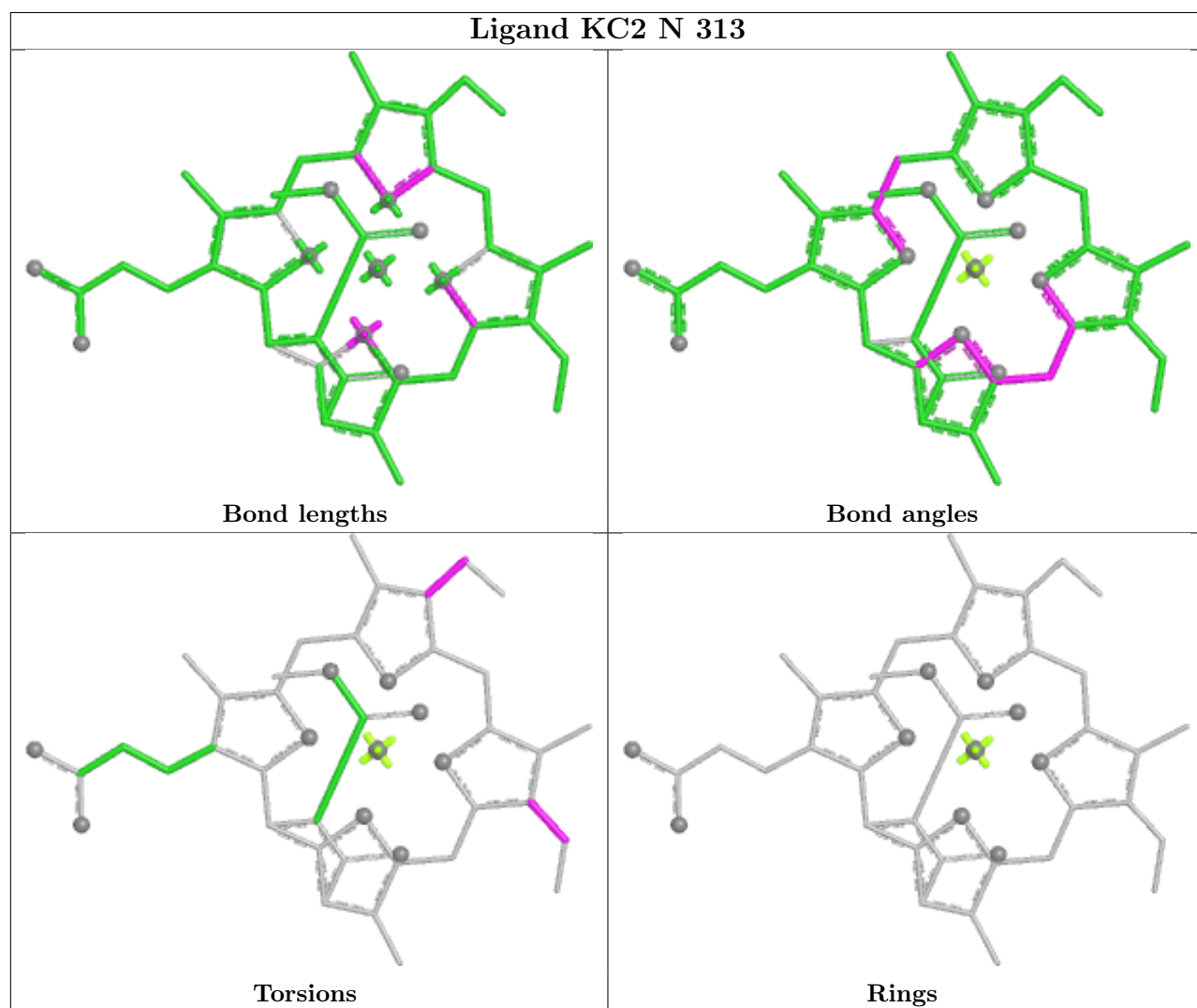
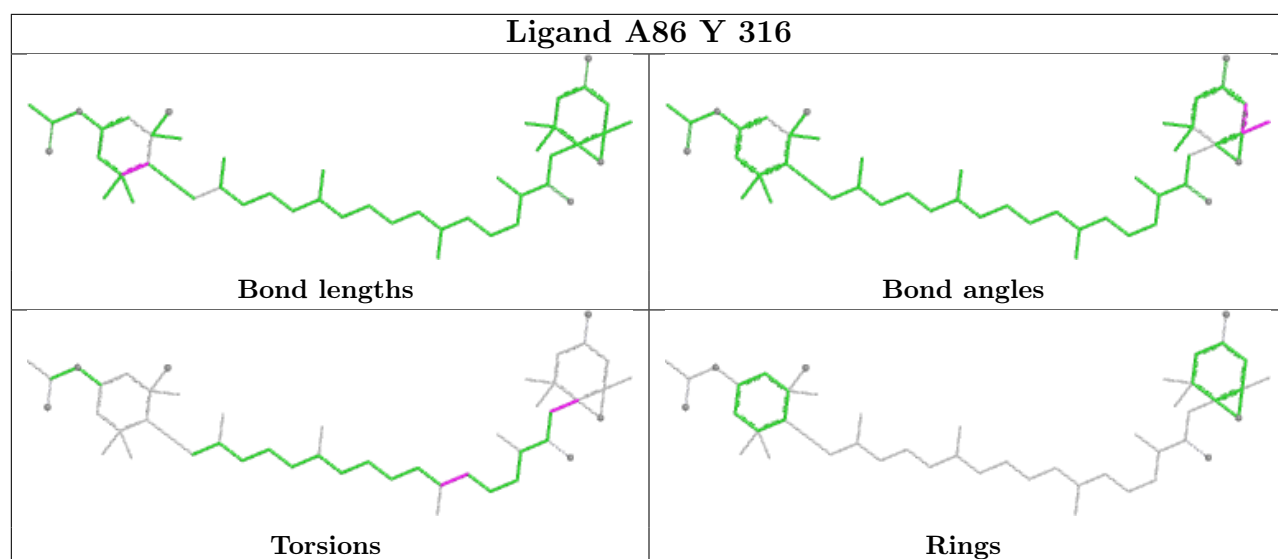
Ligand CLA C 309



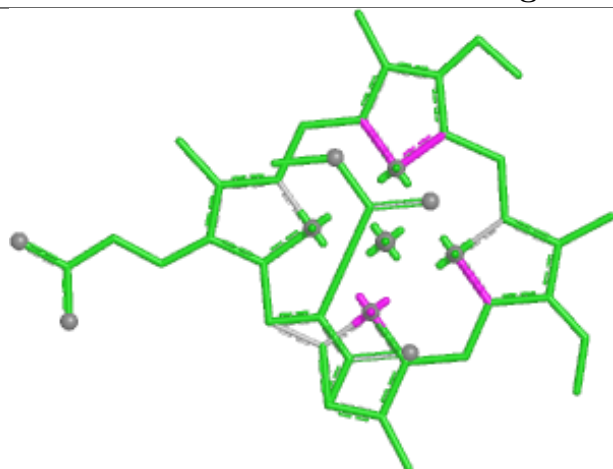
Ligand A86 N 321



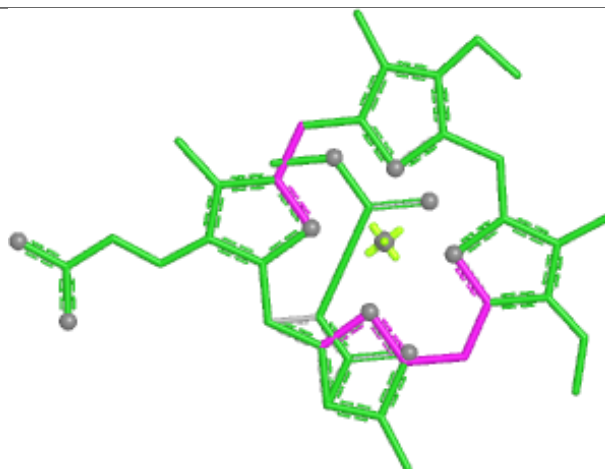




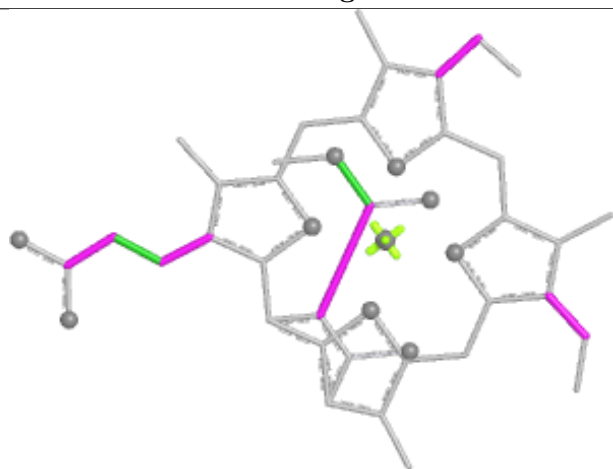
Ligand KC2 J 304



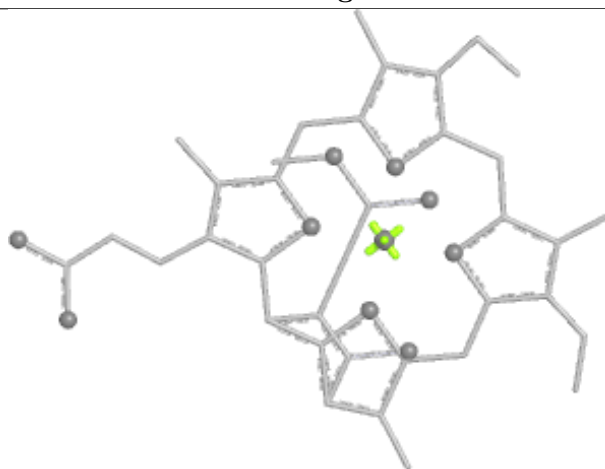
Bond lengths



Bond angles

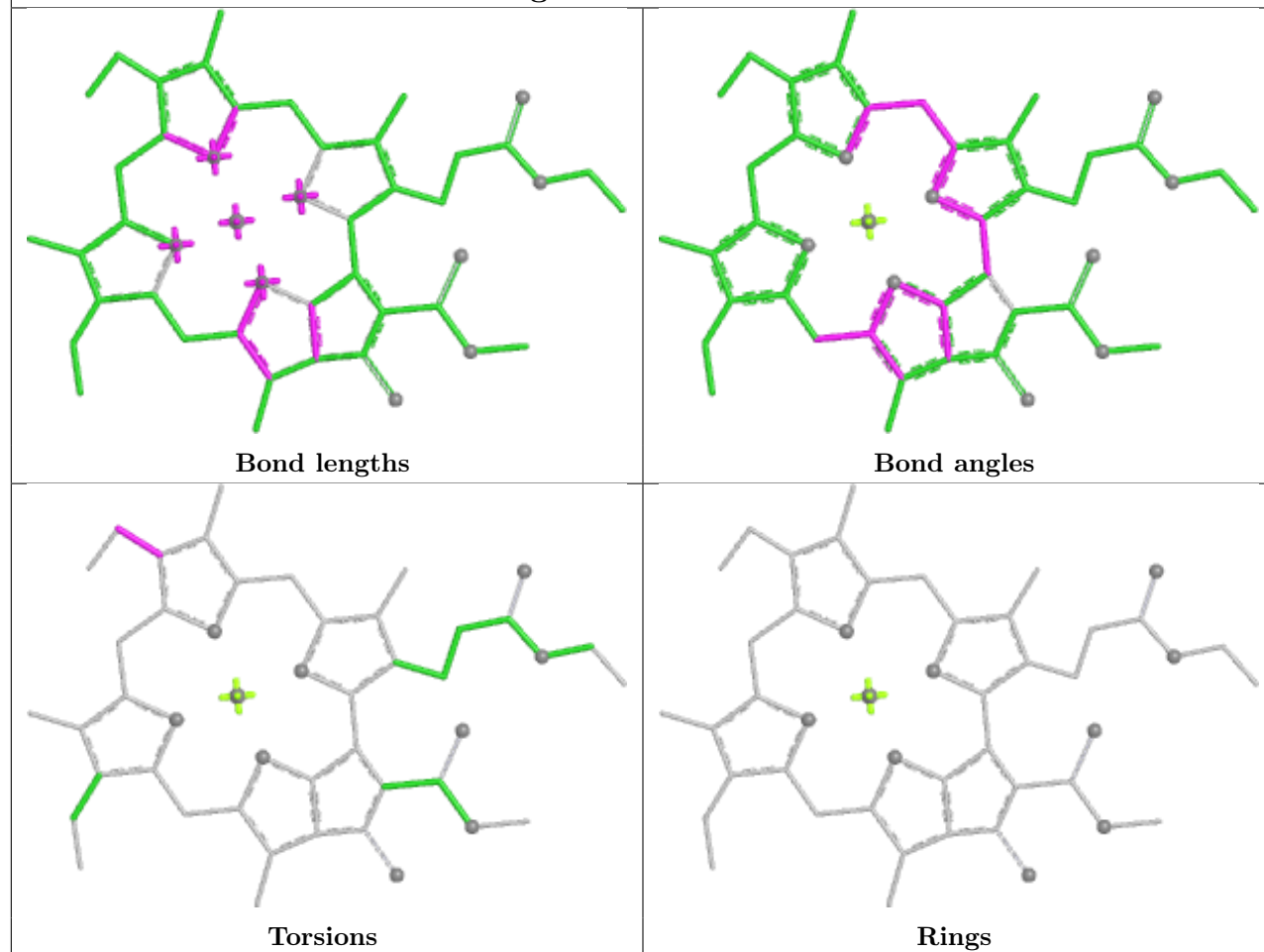


Torsions

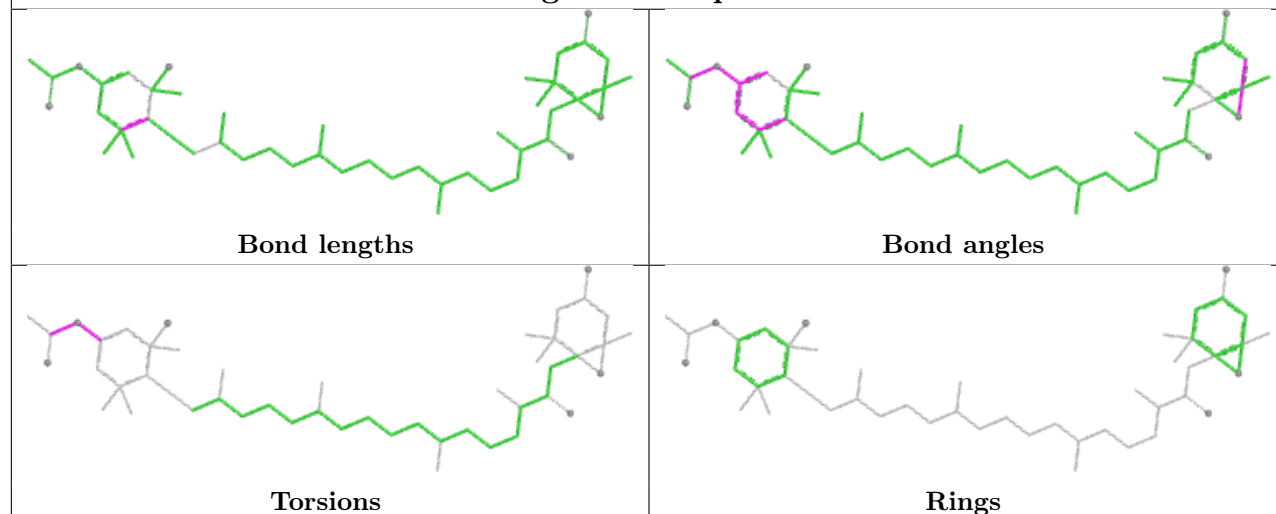


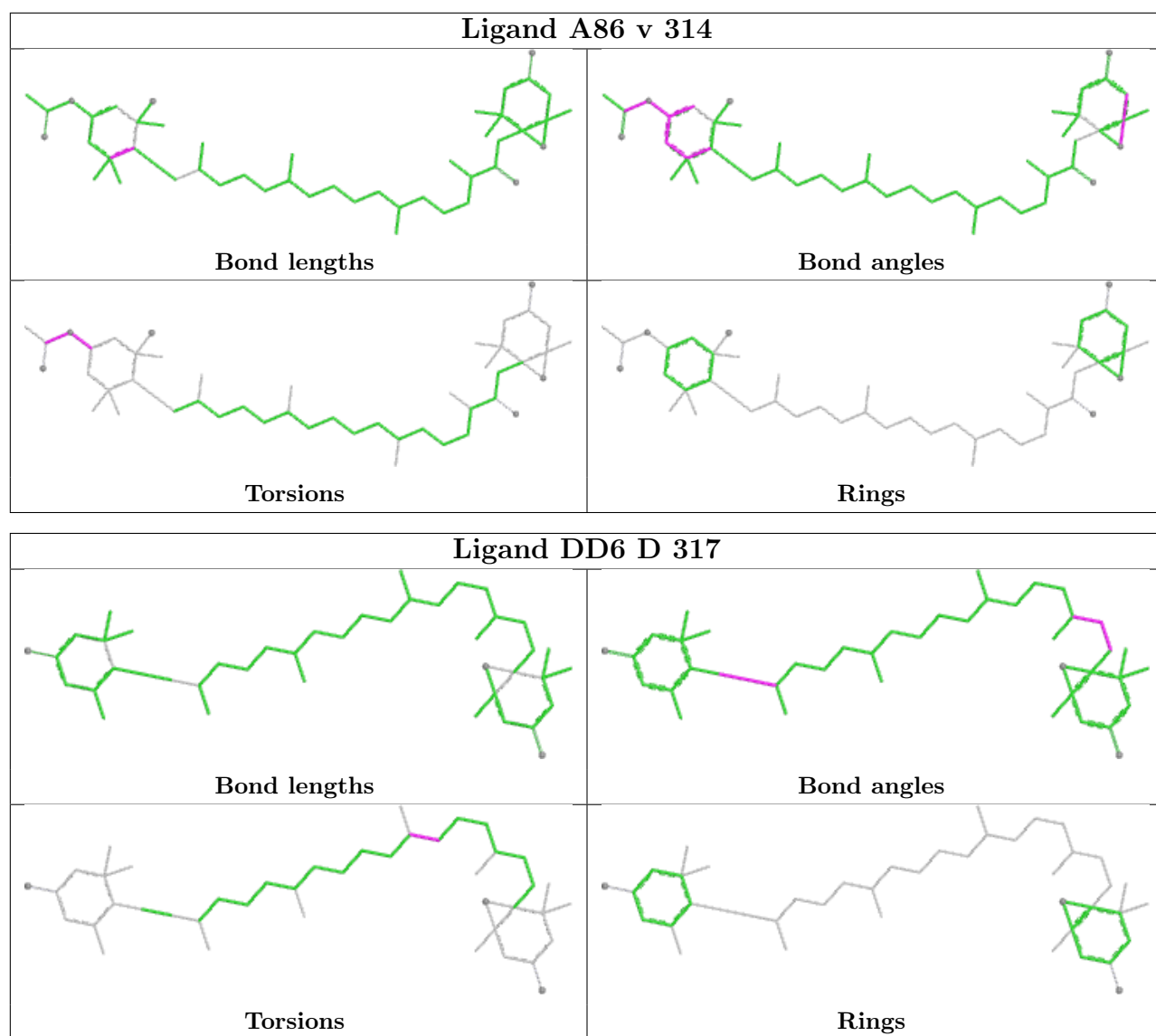
Rings

Ligand CLA b 829

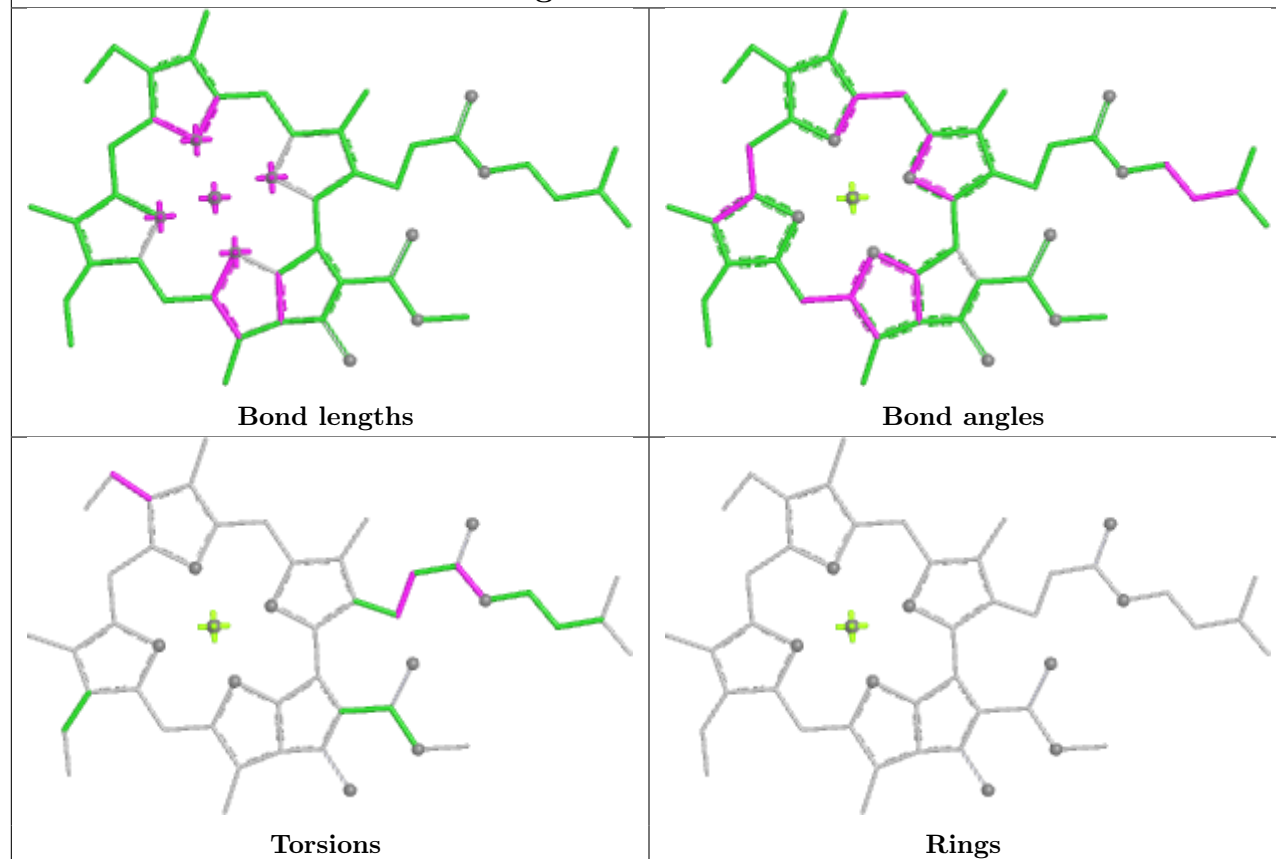


Ligand A86 q 314

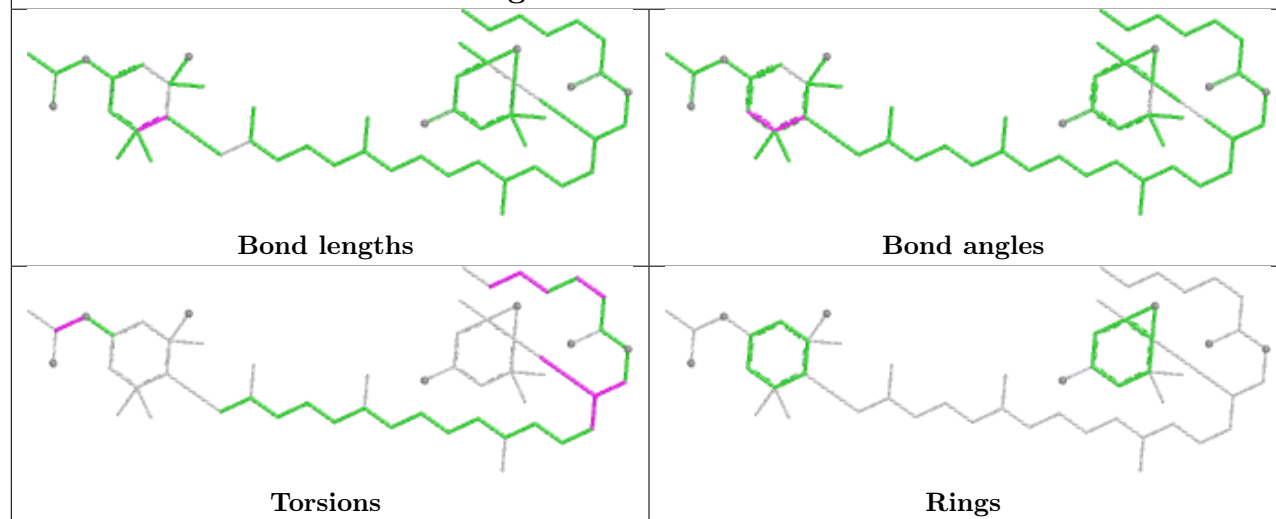


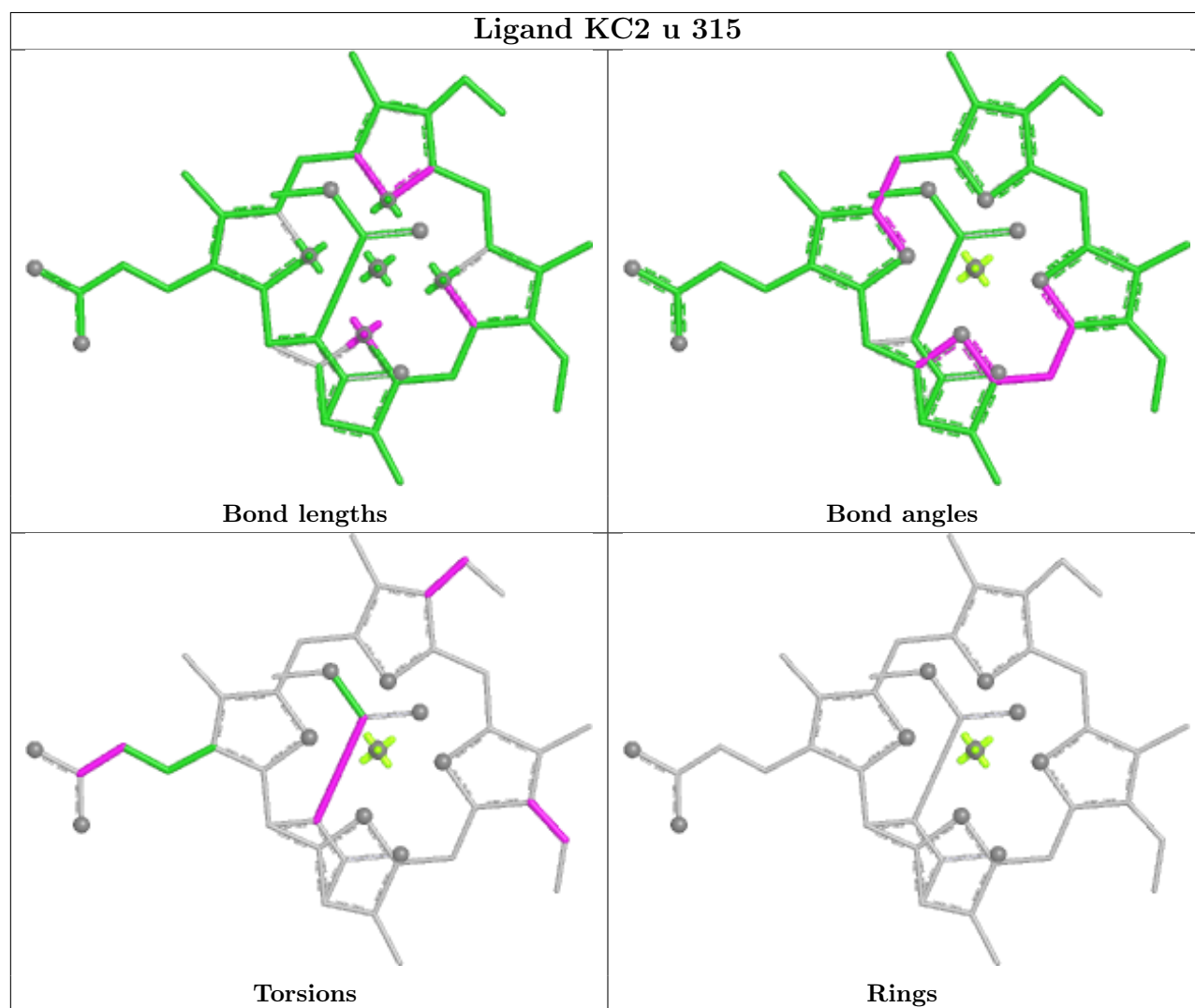
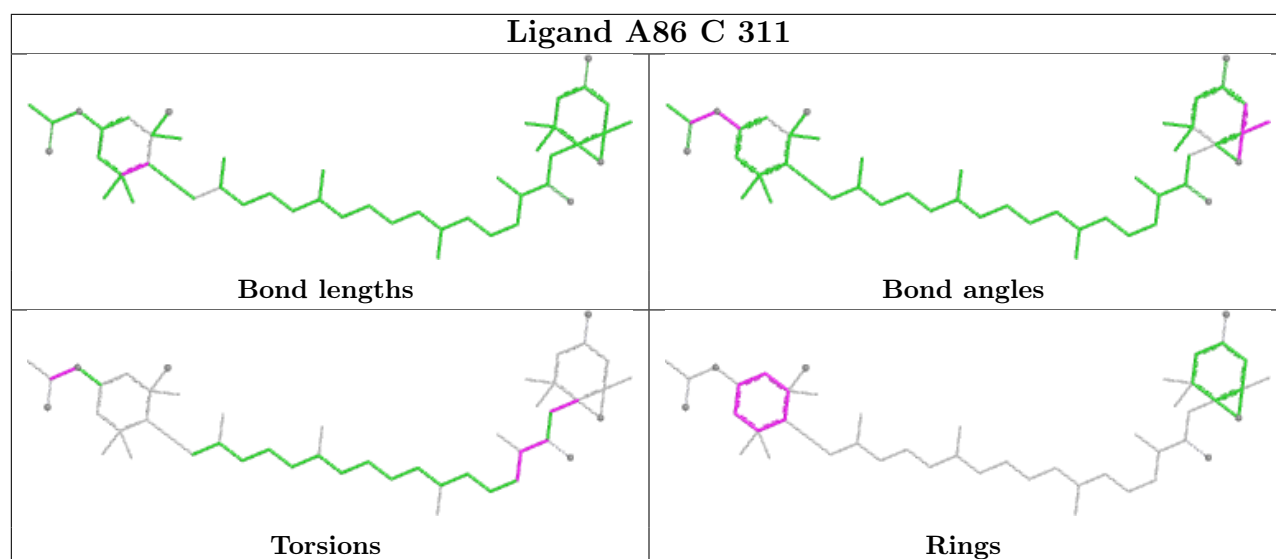


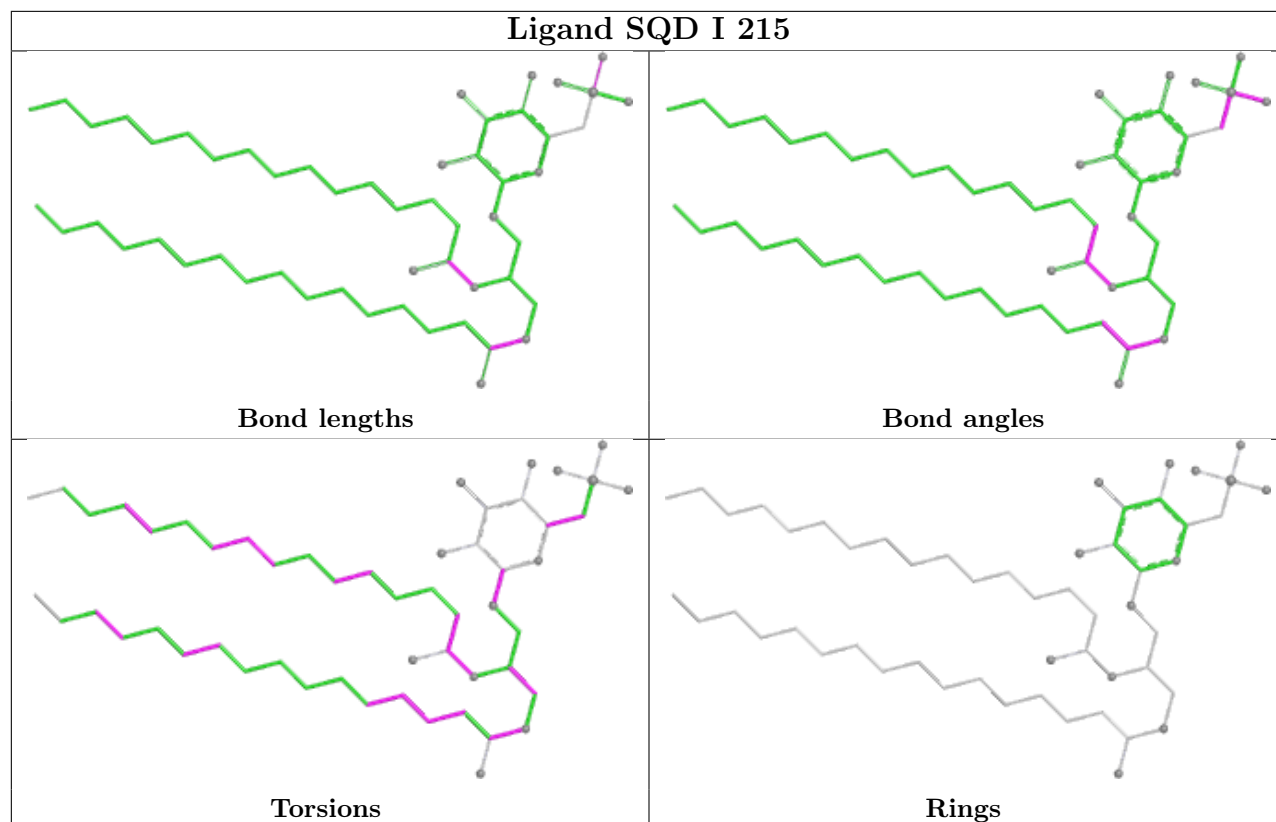
Ligand CLA b 813



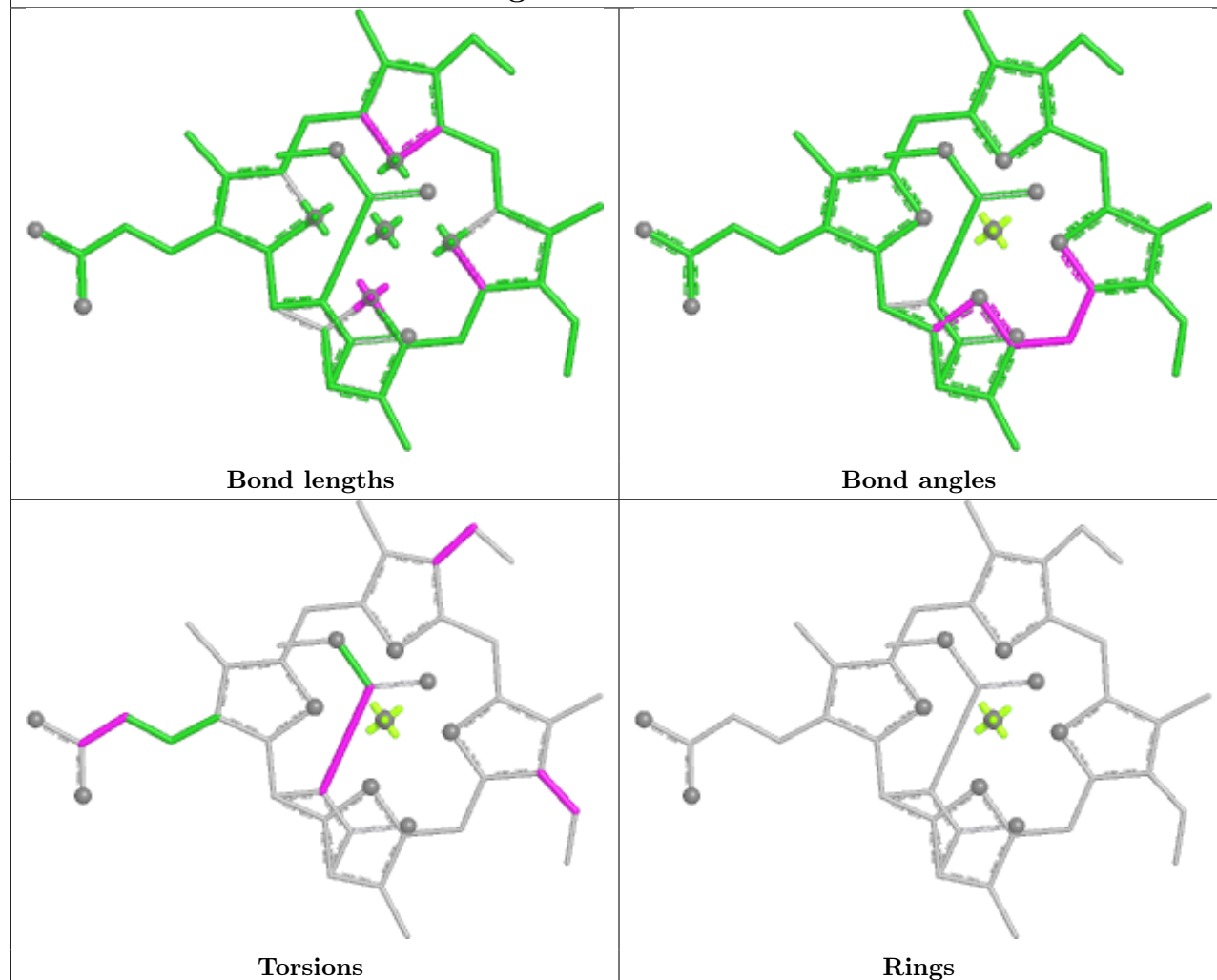
Ligand A1EB4 W 319



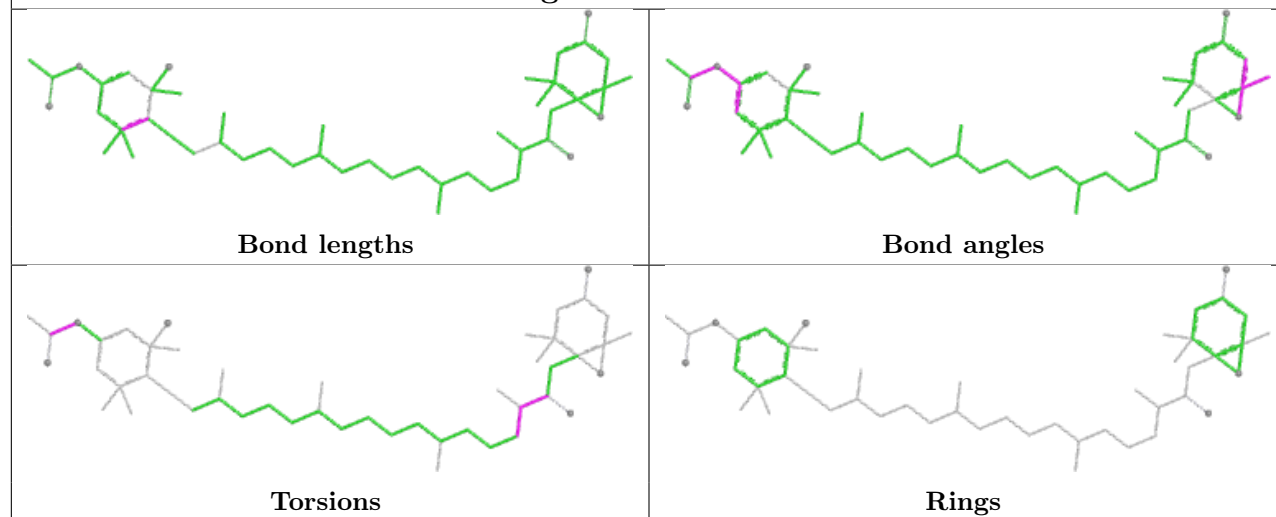


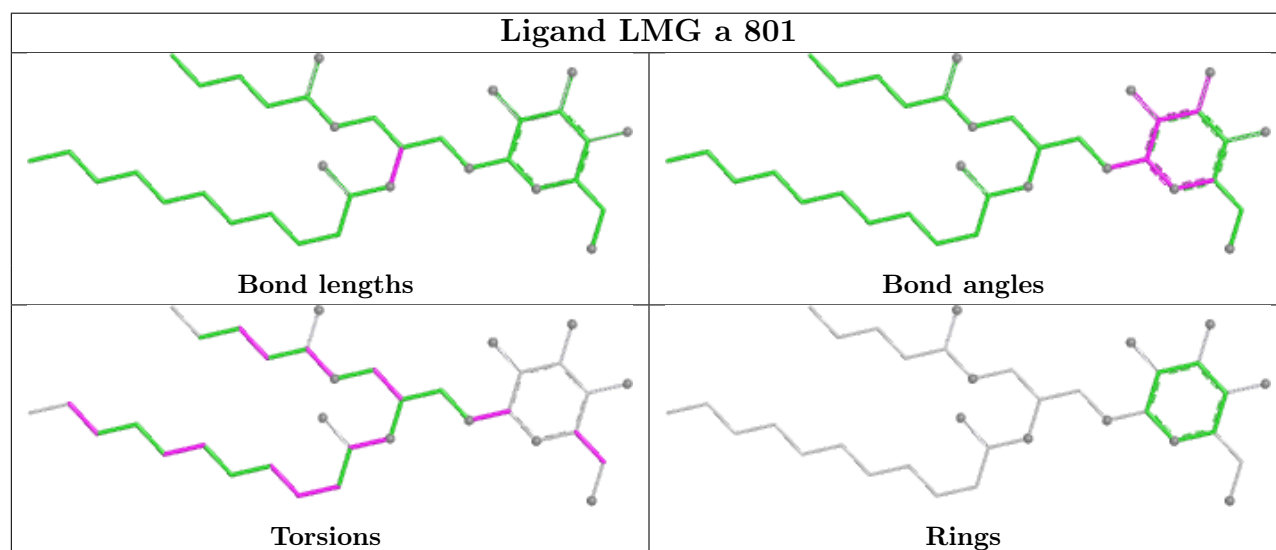
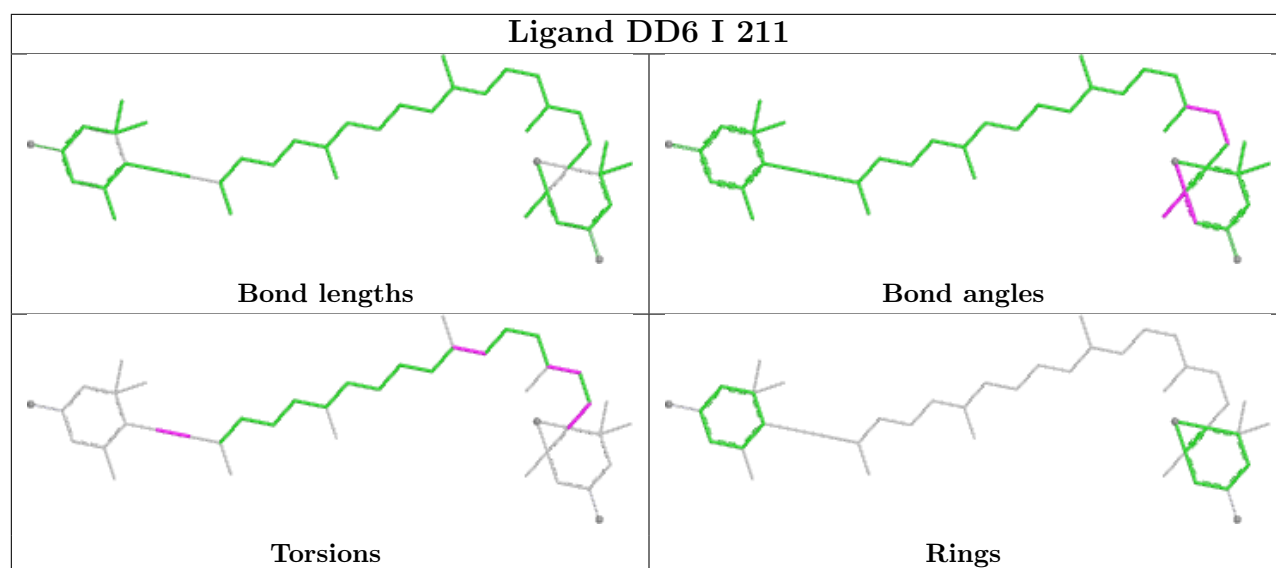


Ligand KC2 Y 309

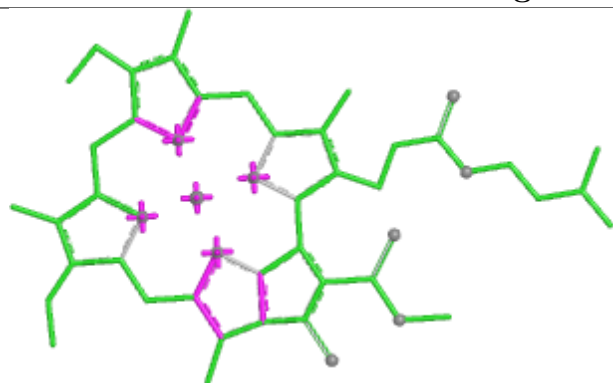


Ligand A86 S 316

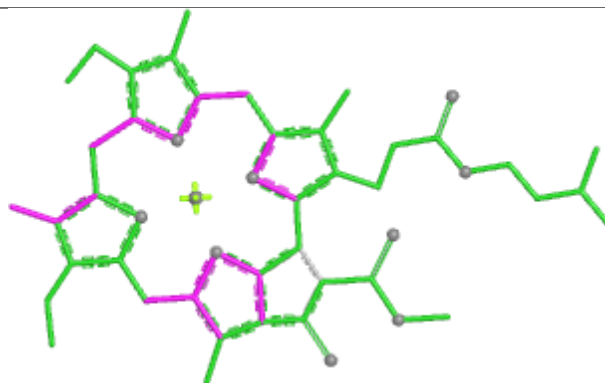




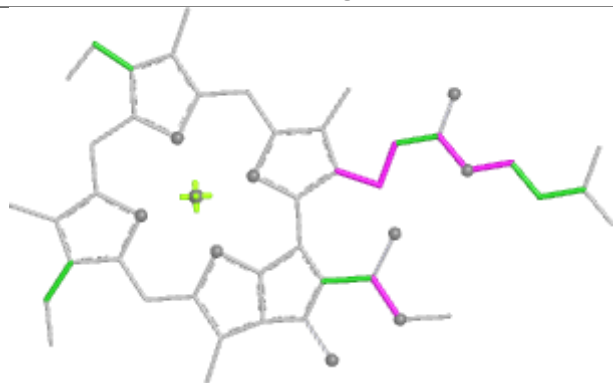
Ligand CLA X 305



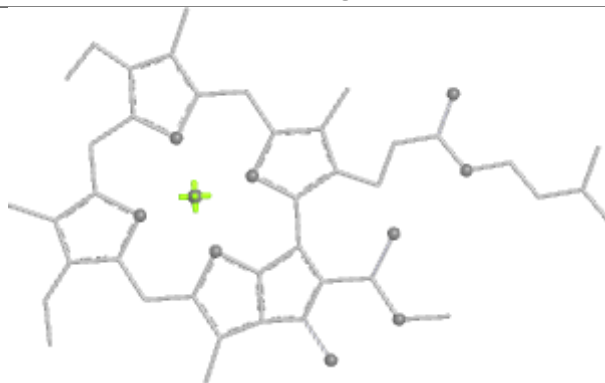
Bond lengths



Bond angles

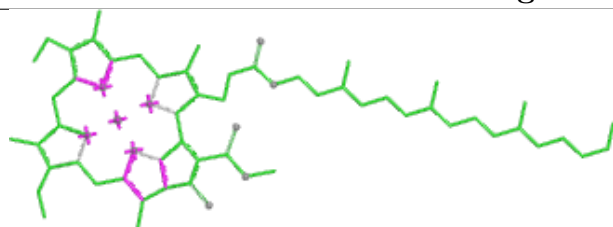


Torsions

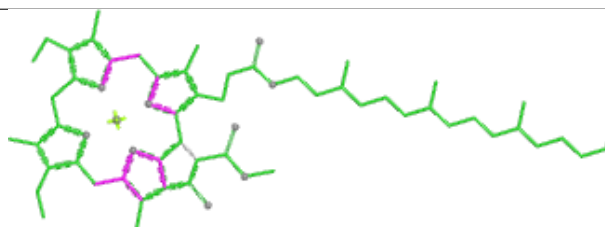


Rings

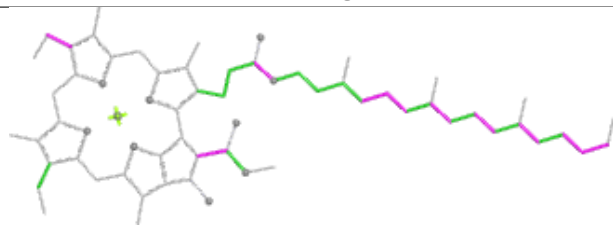
Ligand CLA b 819



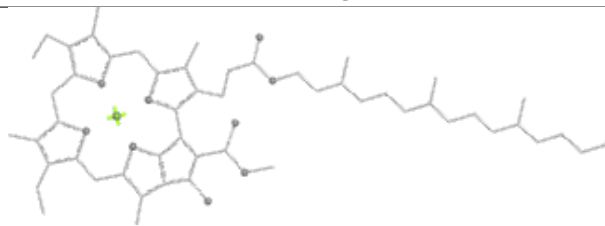
Bond lengths



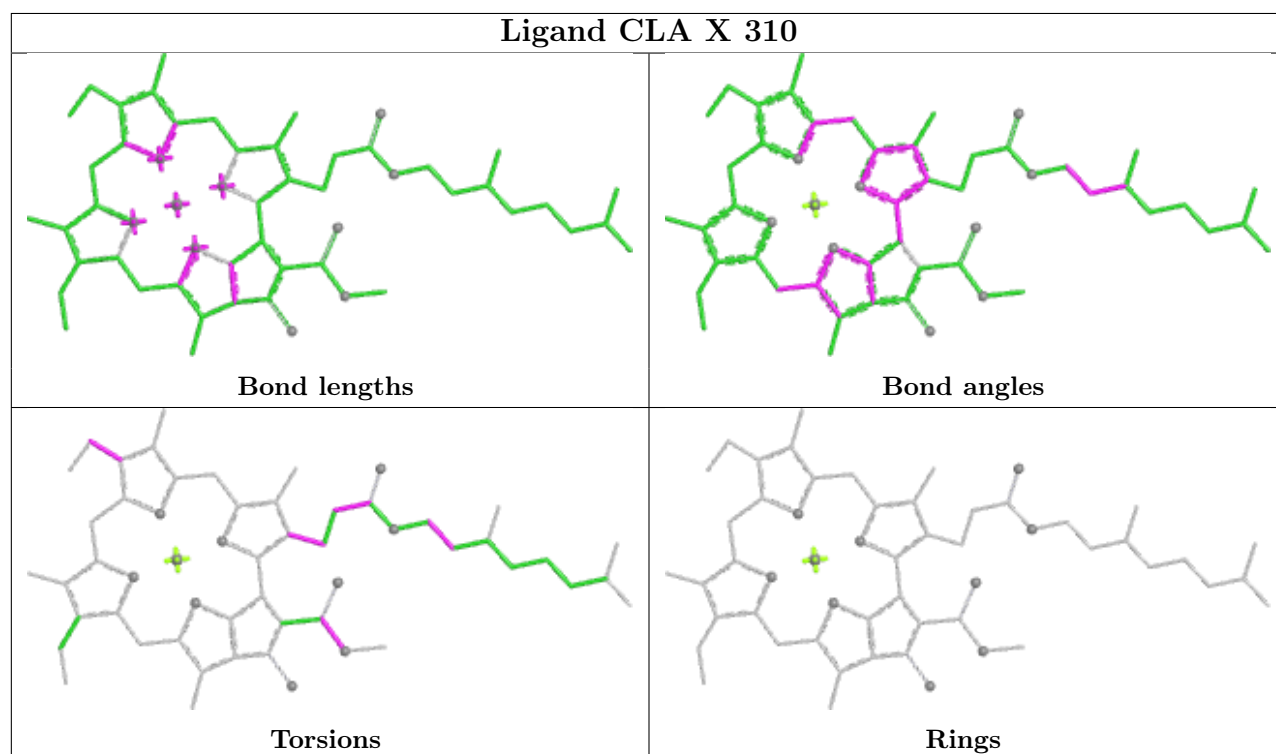
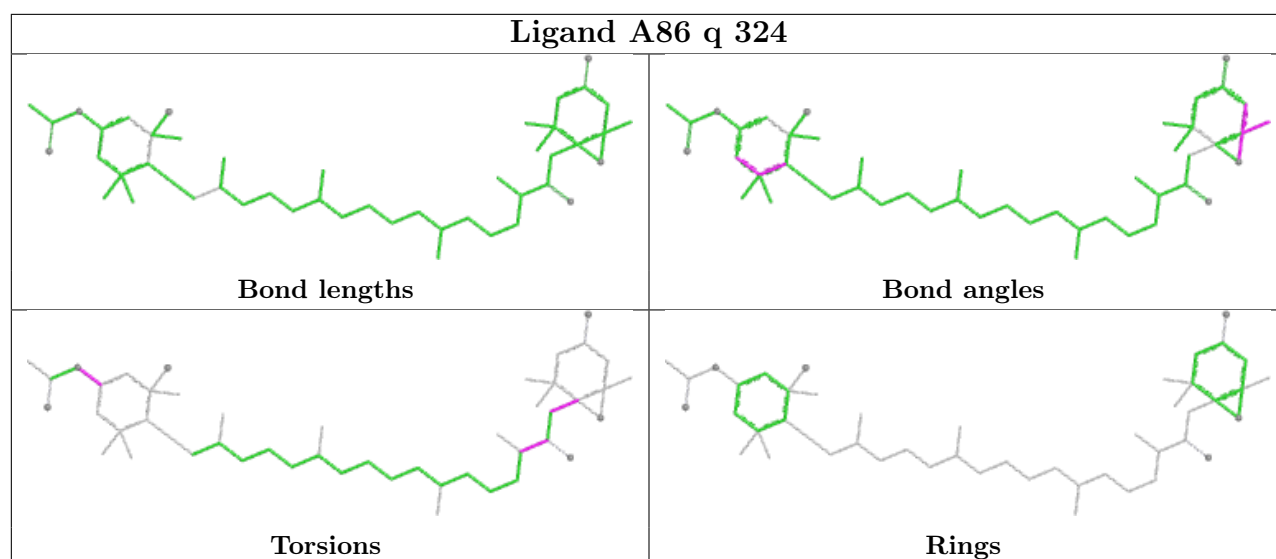
Bond angles

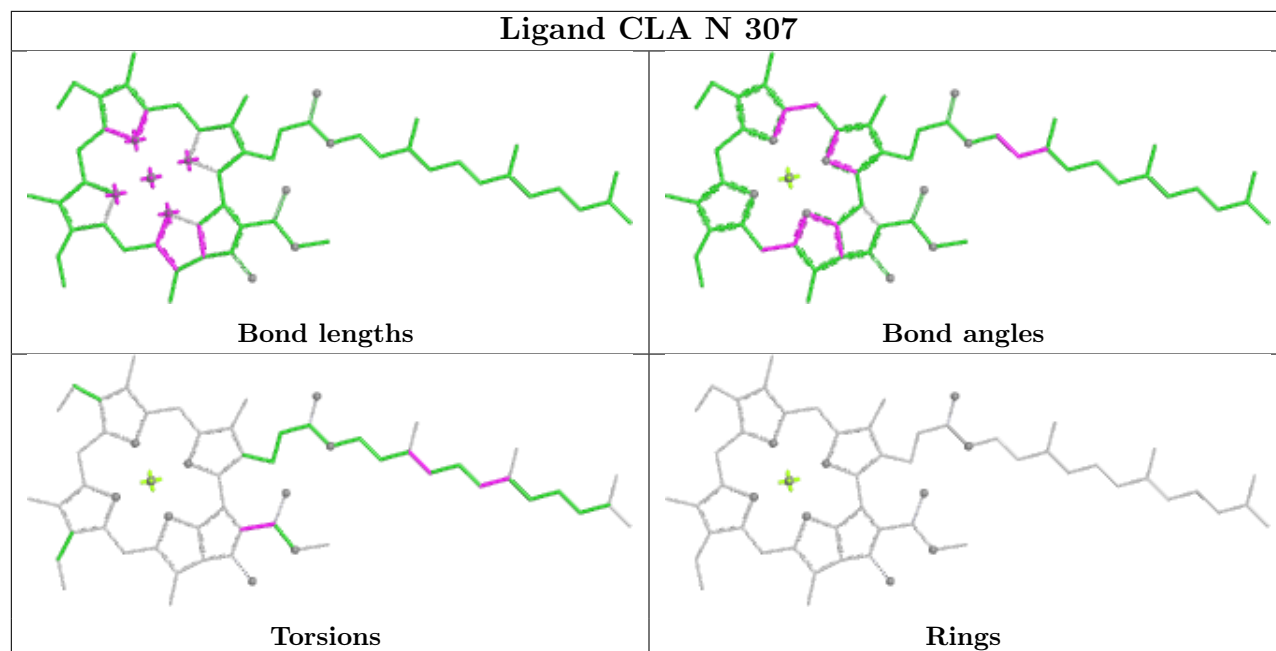
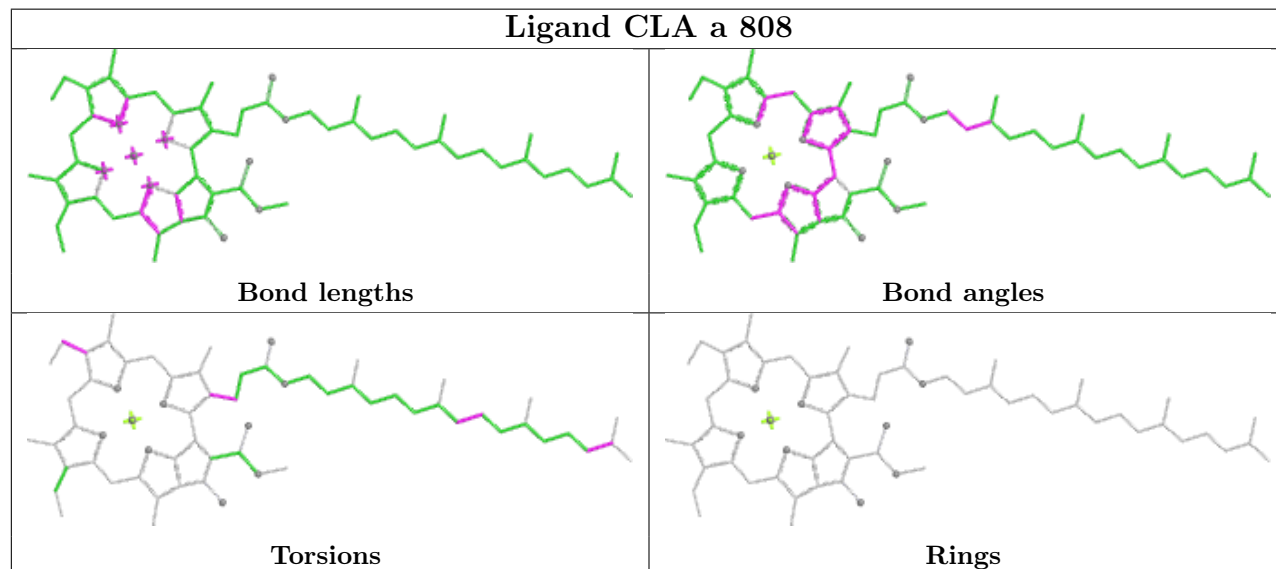


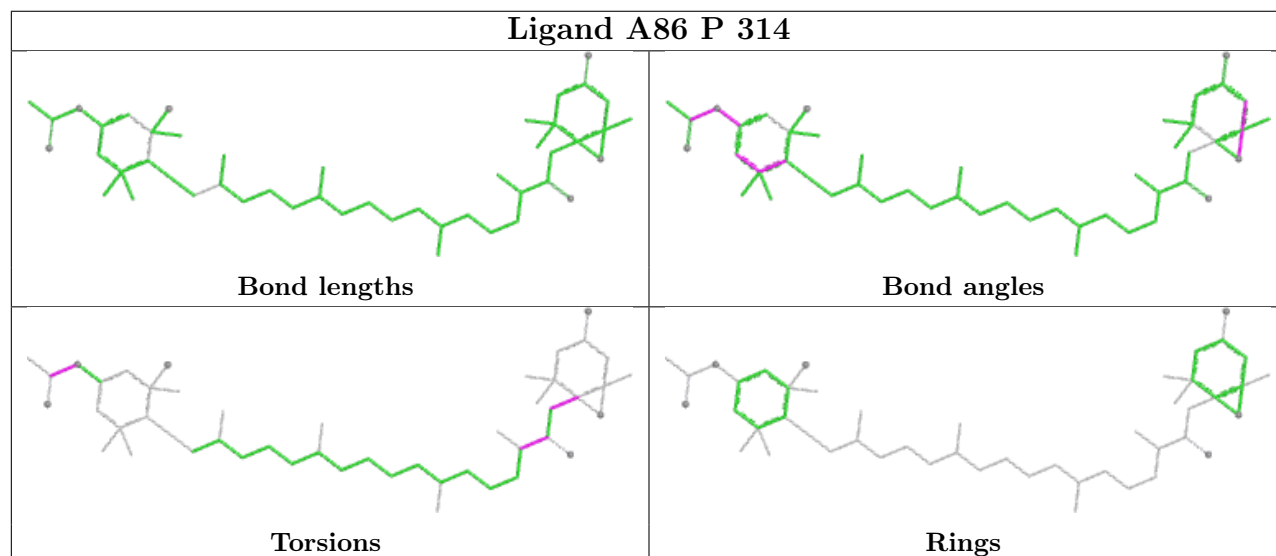
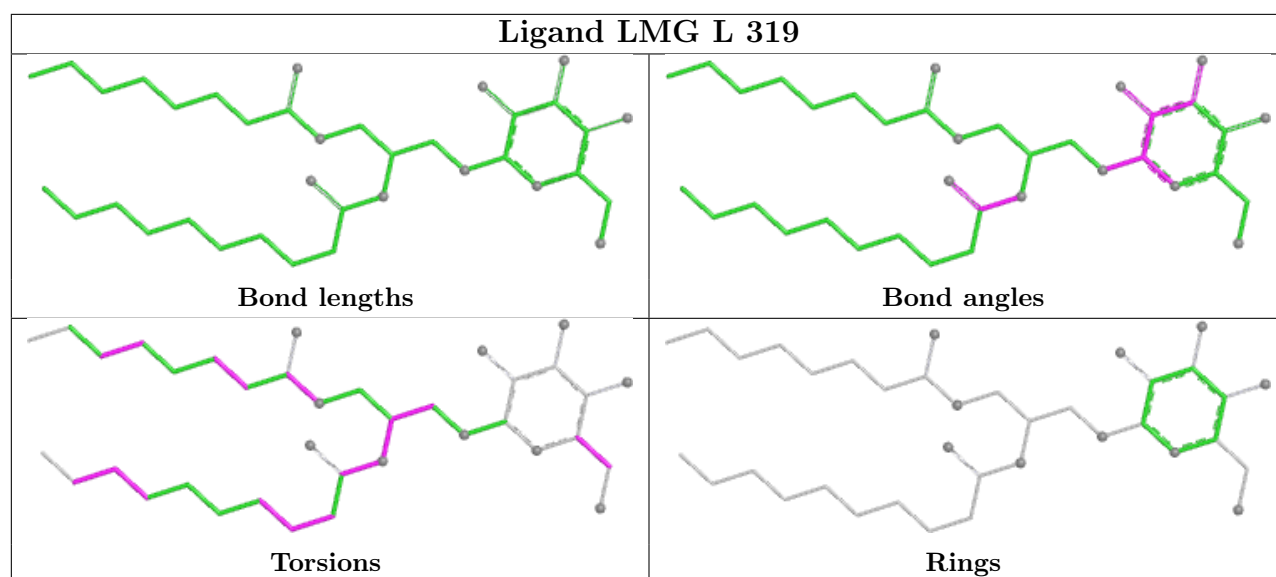
Torsions

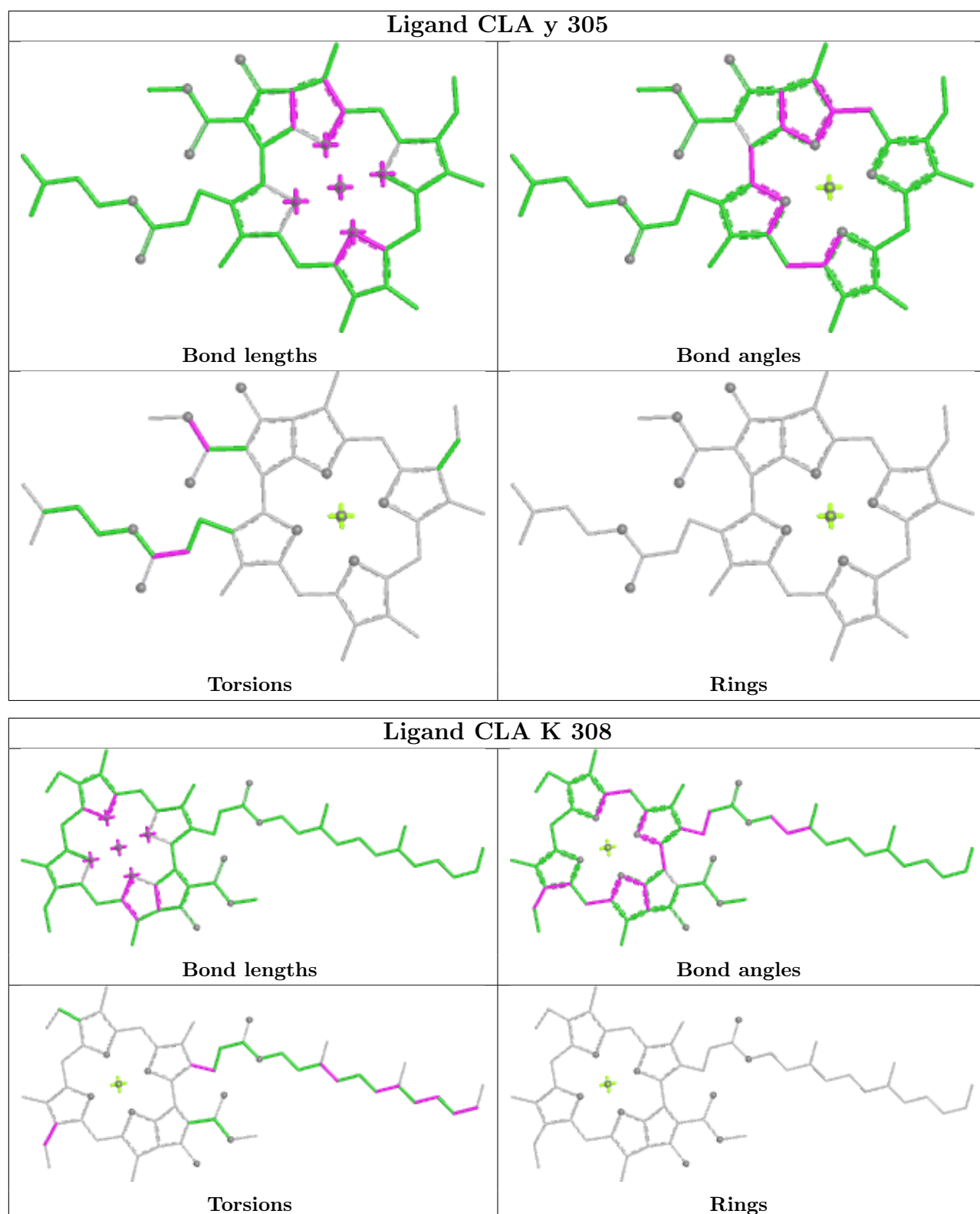


Rings

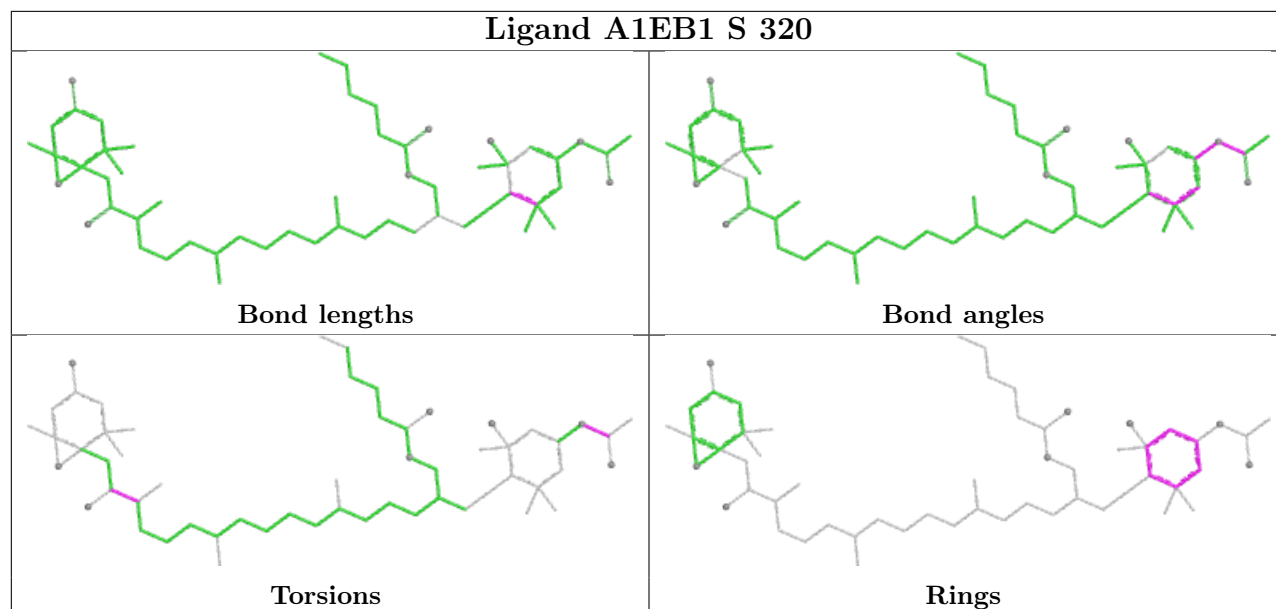


Ligand CLA N 307**Ligand CLA a 808**

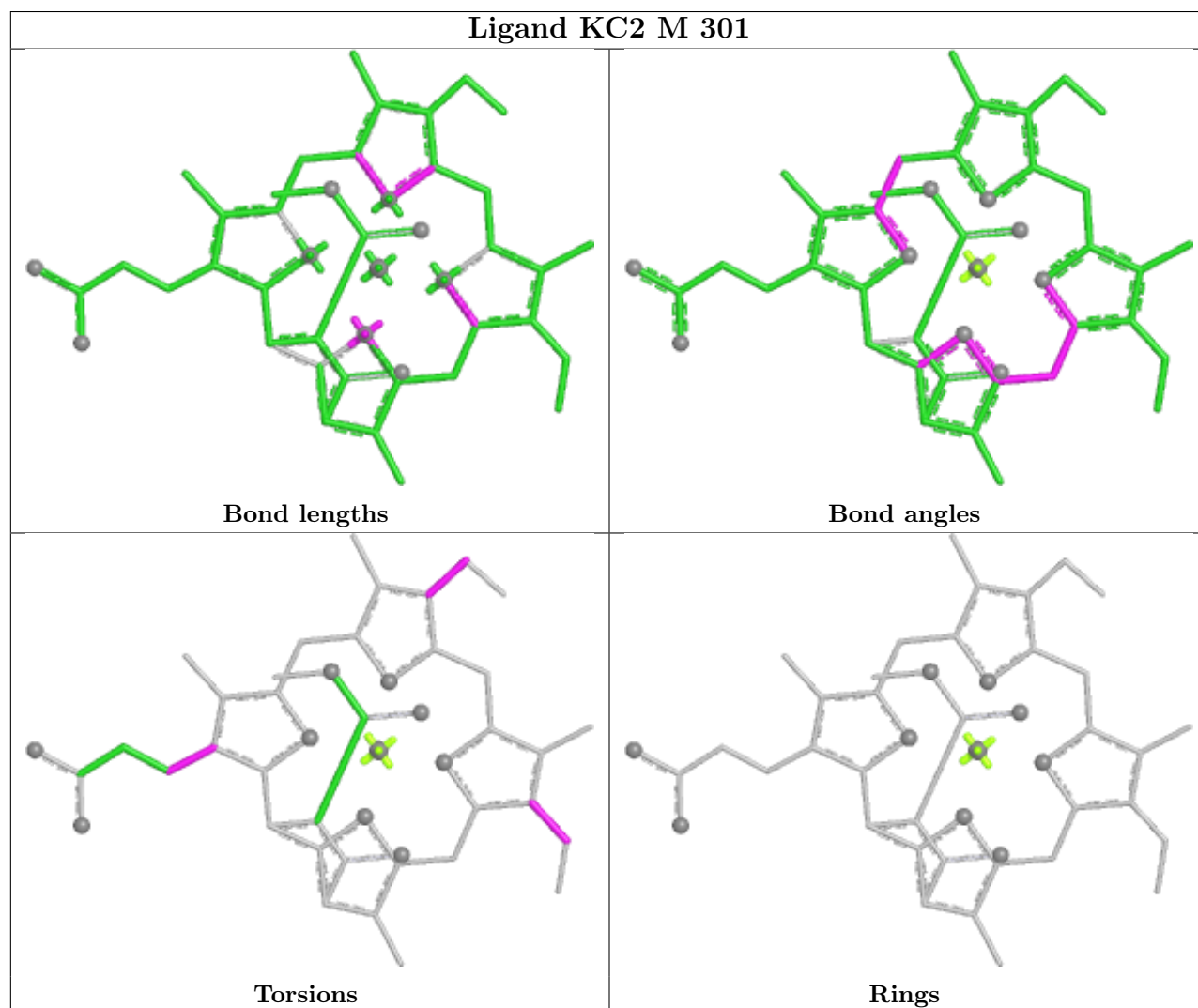




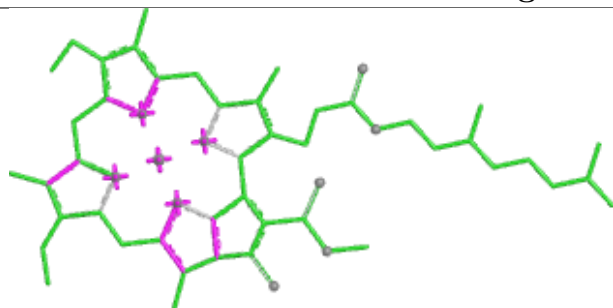
Ligand A1EB1 S 320



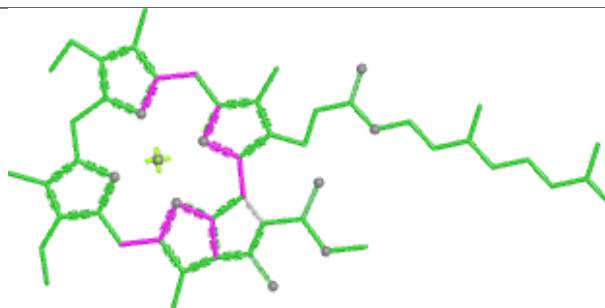
Ligand KC2 M 301



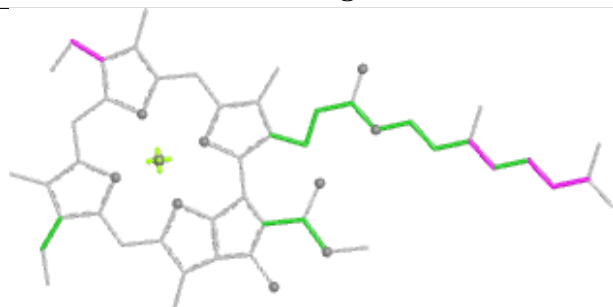
Ligand CLA J 305



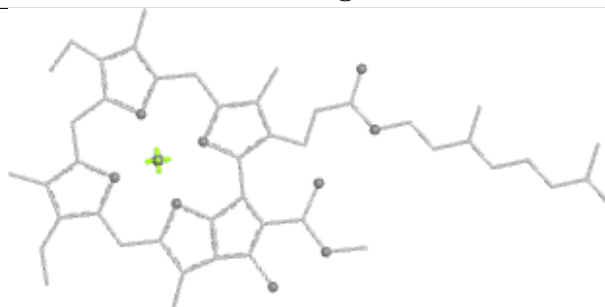
Bond lengths



Bond angles

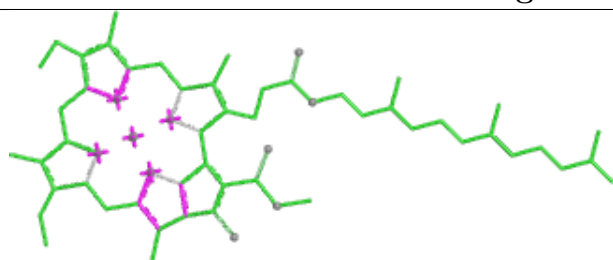


Torsions

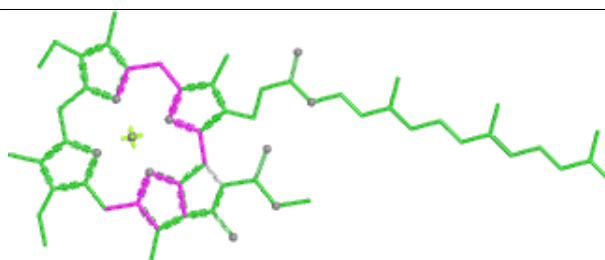


Rings

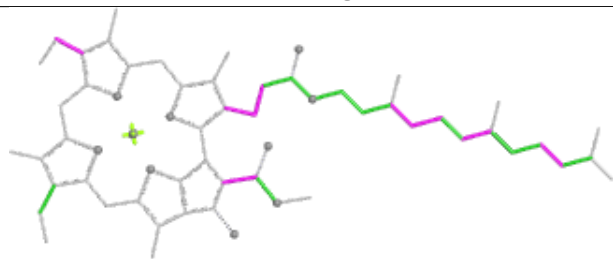
Ligand CLA F 321



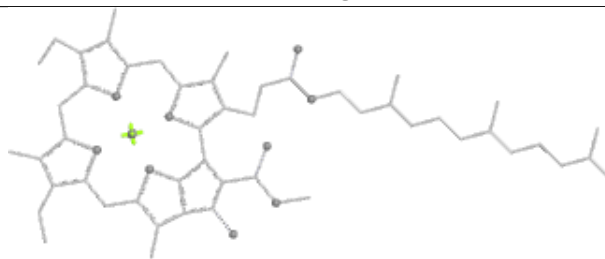
Bond lengths



Bond angles

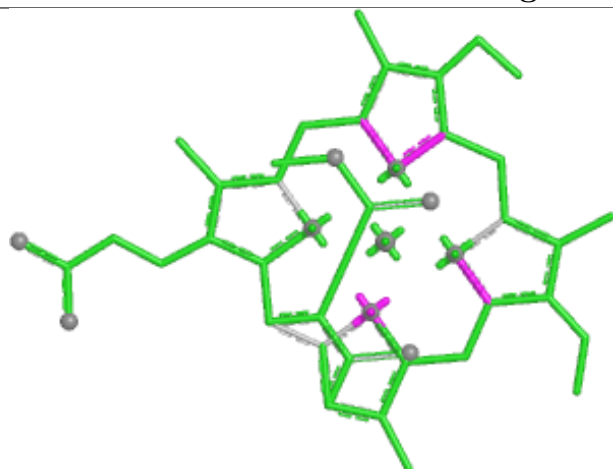


Torsions

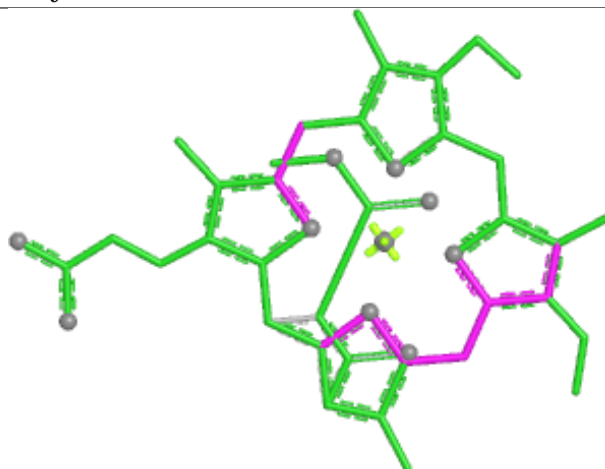


Rings

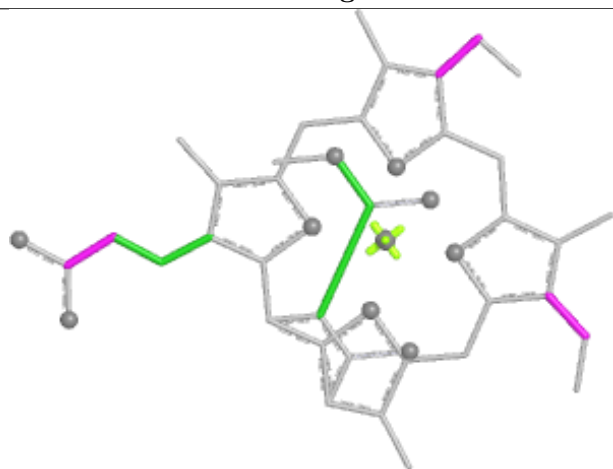
Ligand KC2 y 307



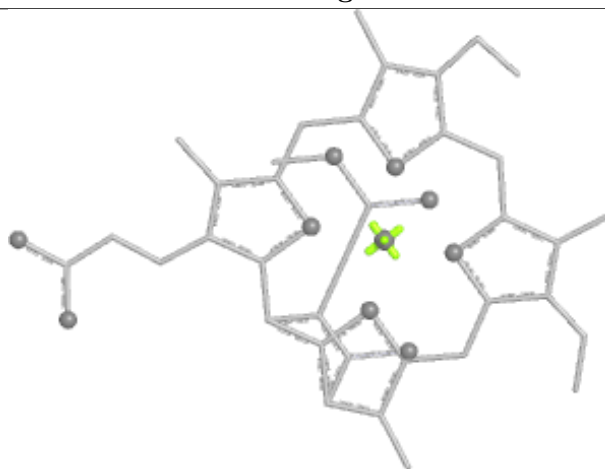
Bond lengths



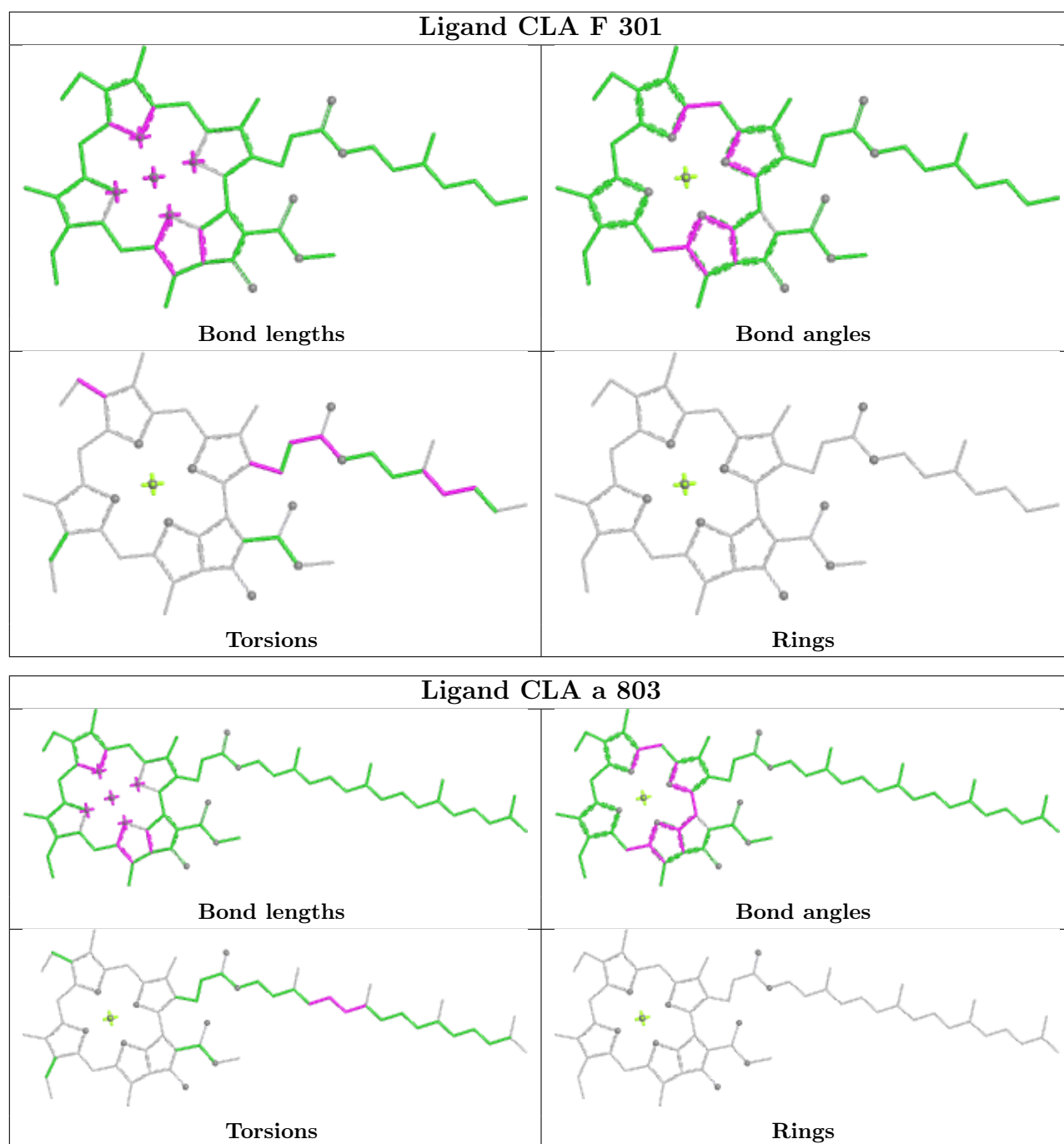
Bond angles

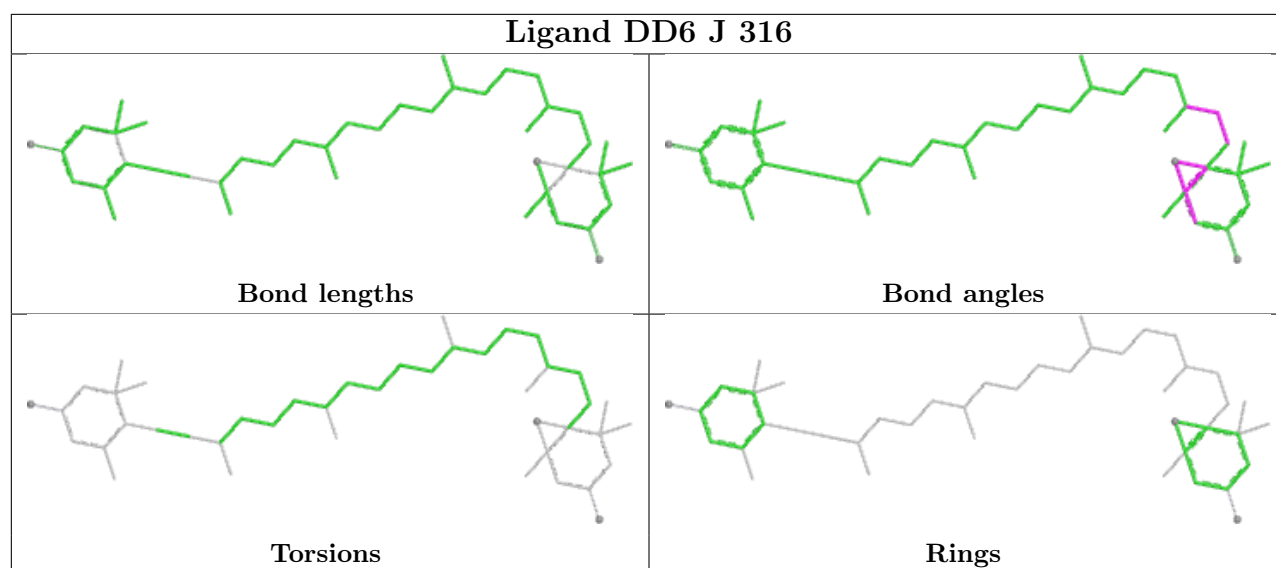


Torsions

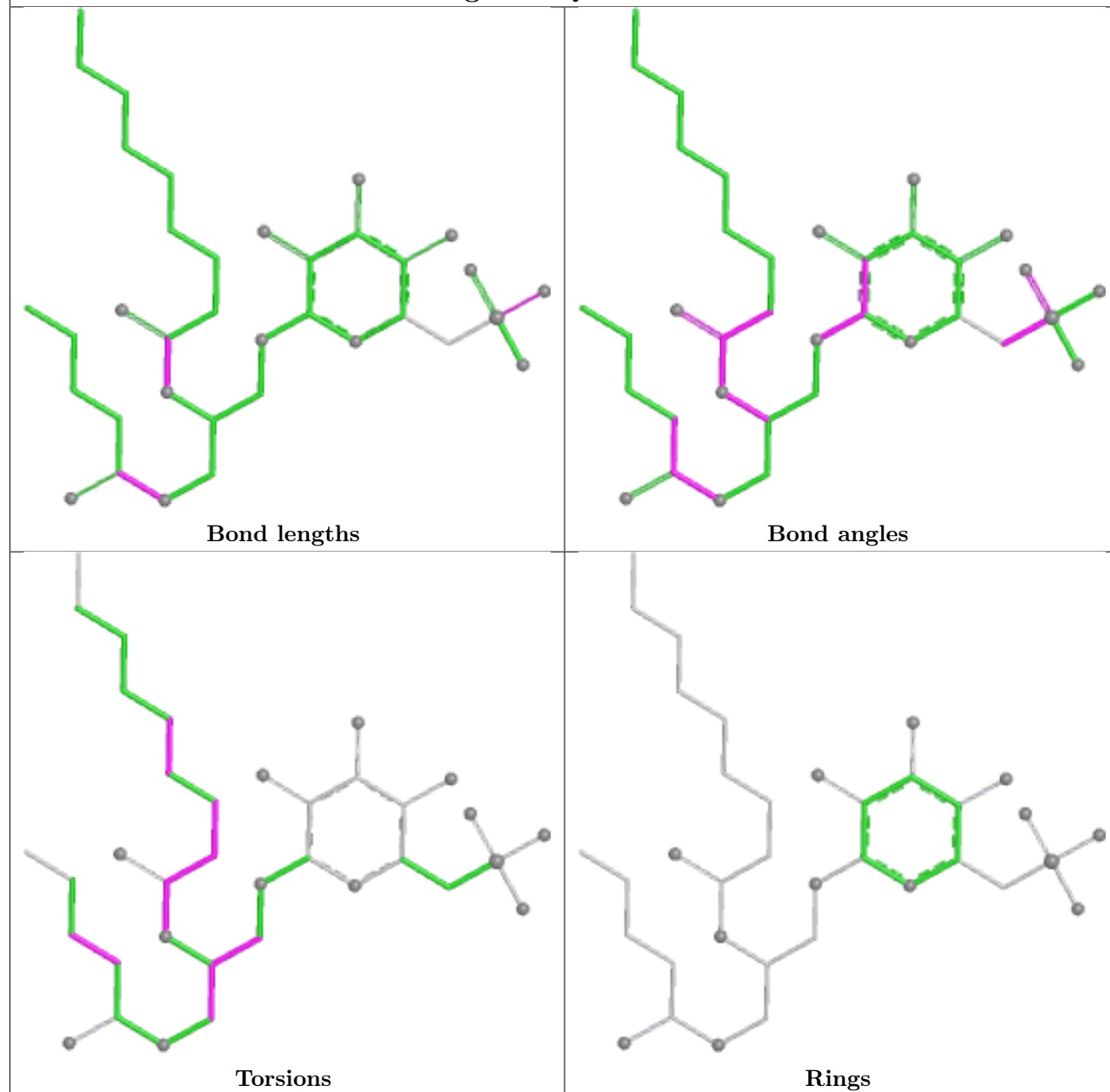


Rings

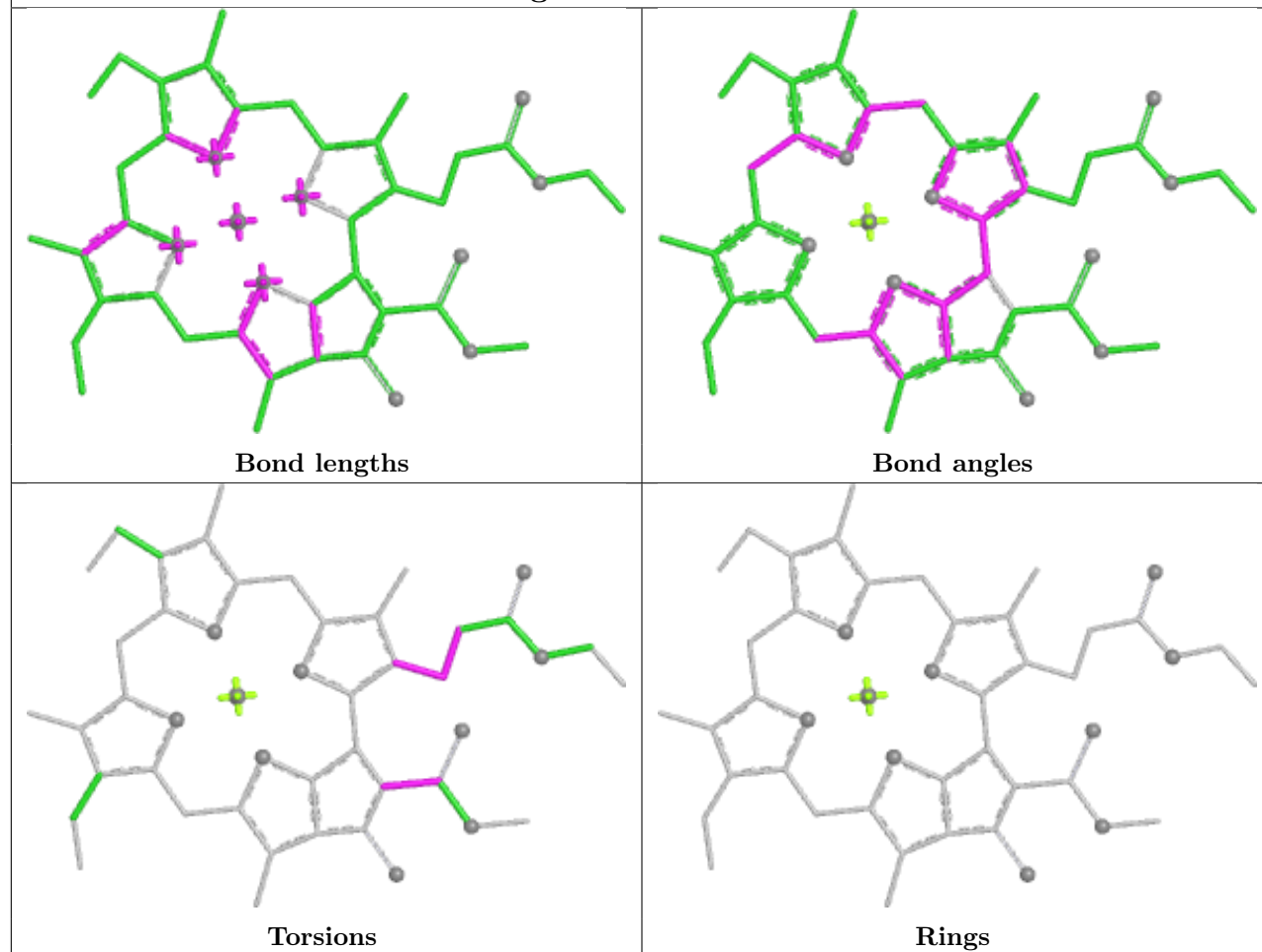




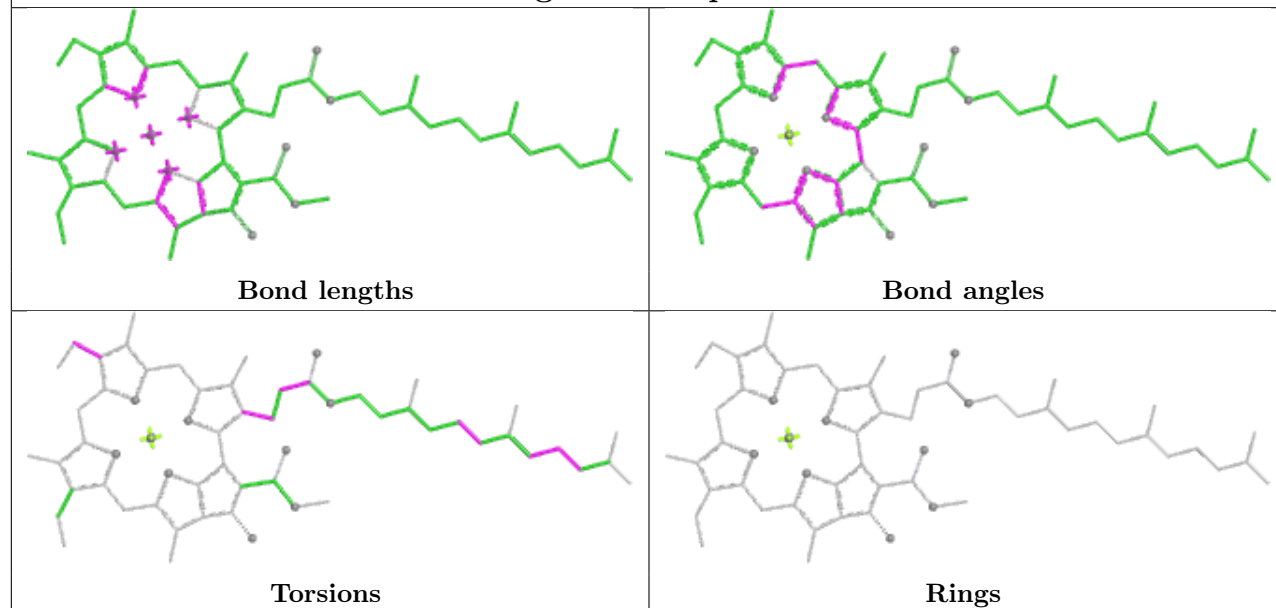
Ligand SQD F 320

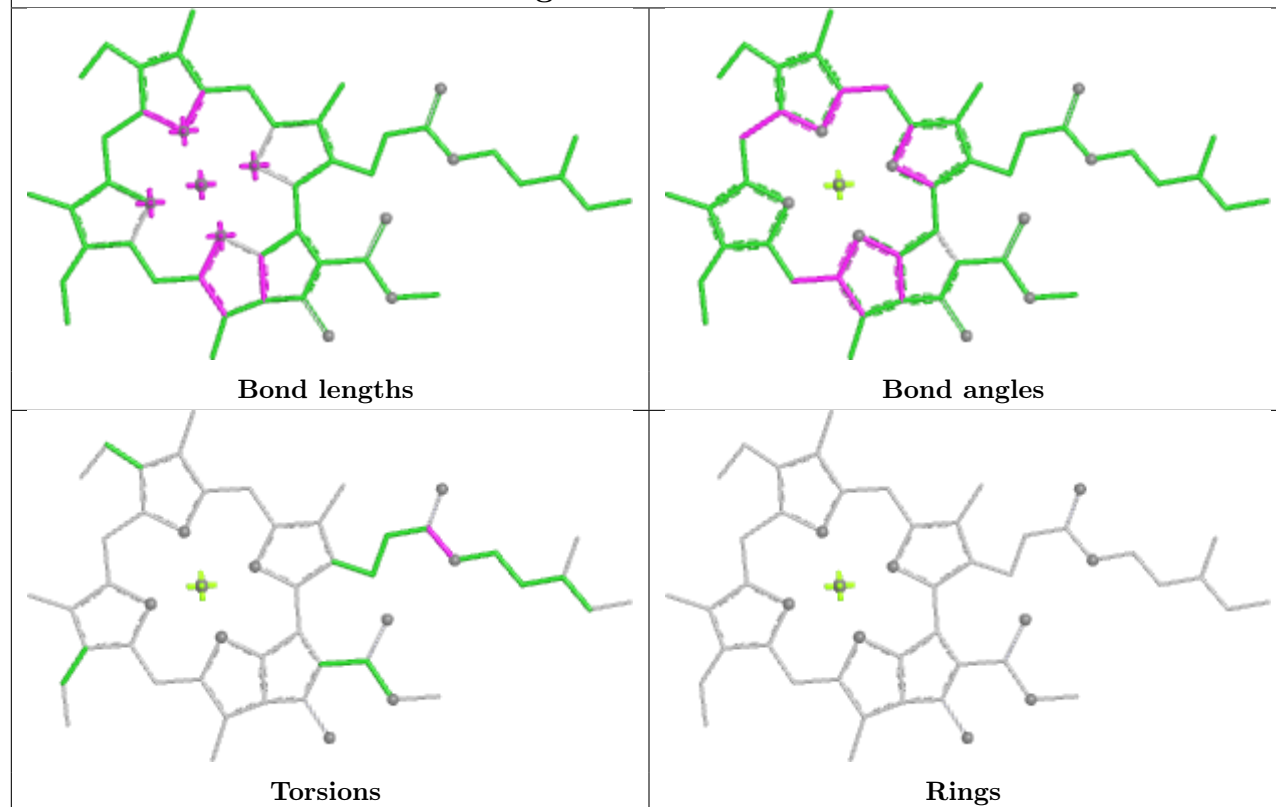
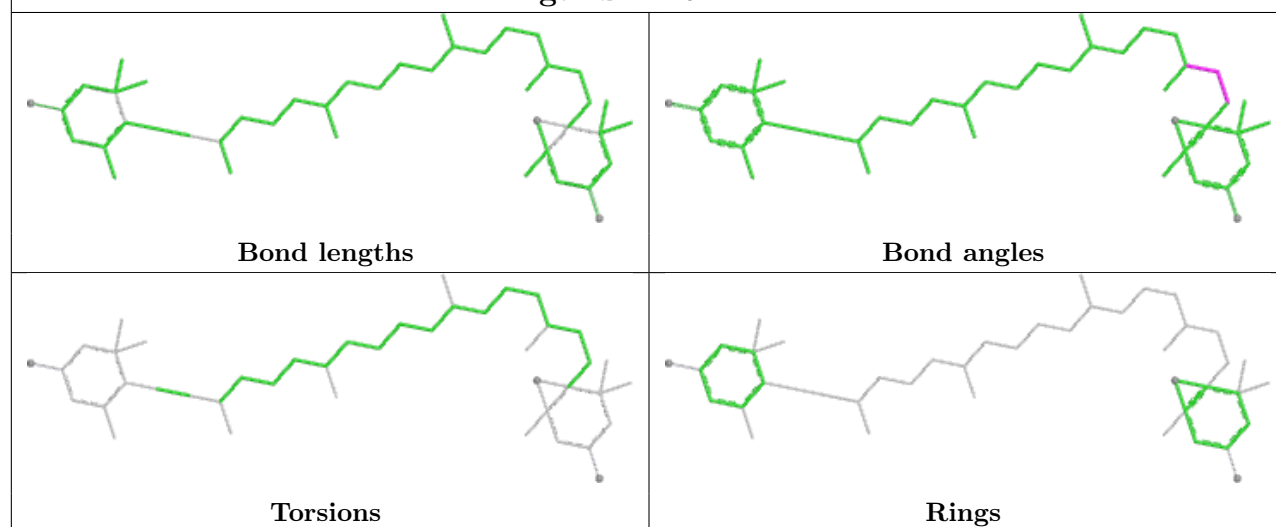


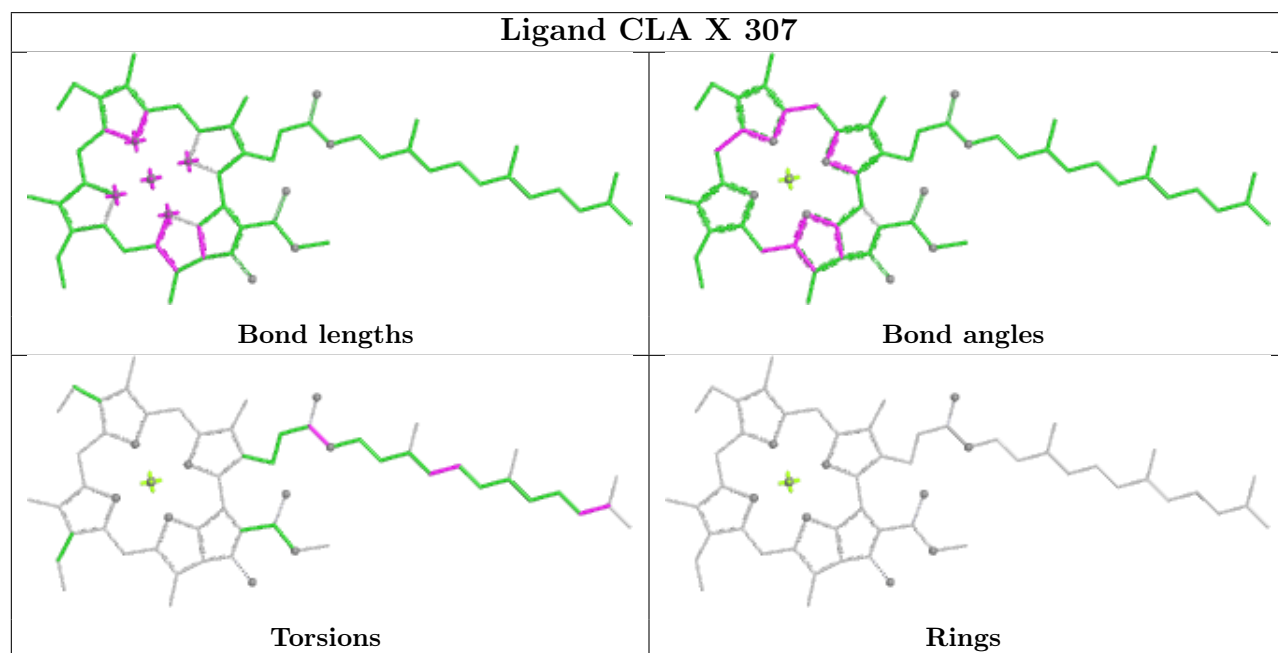
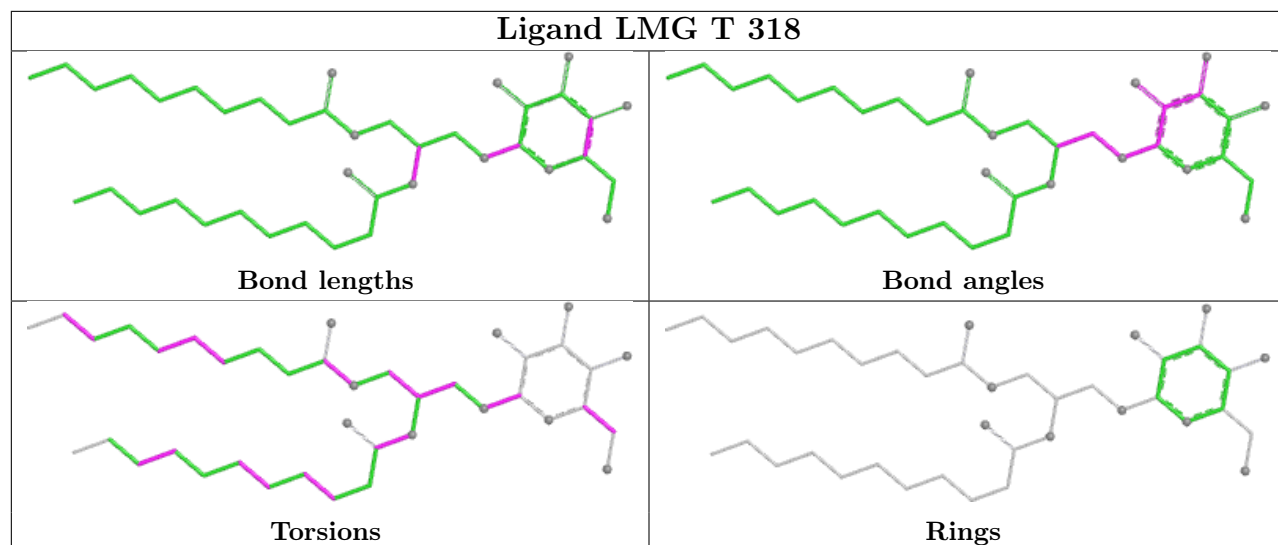
Ligand CLA o 313

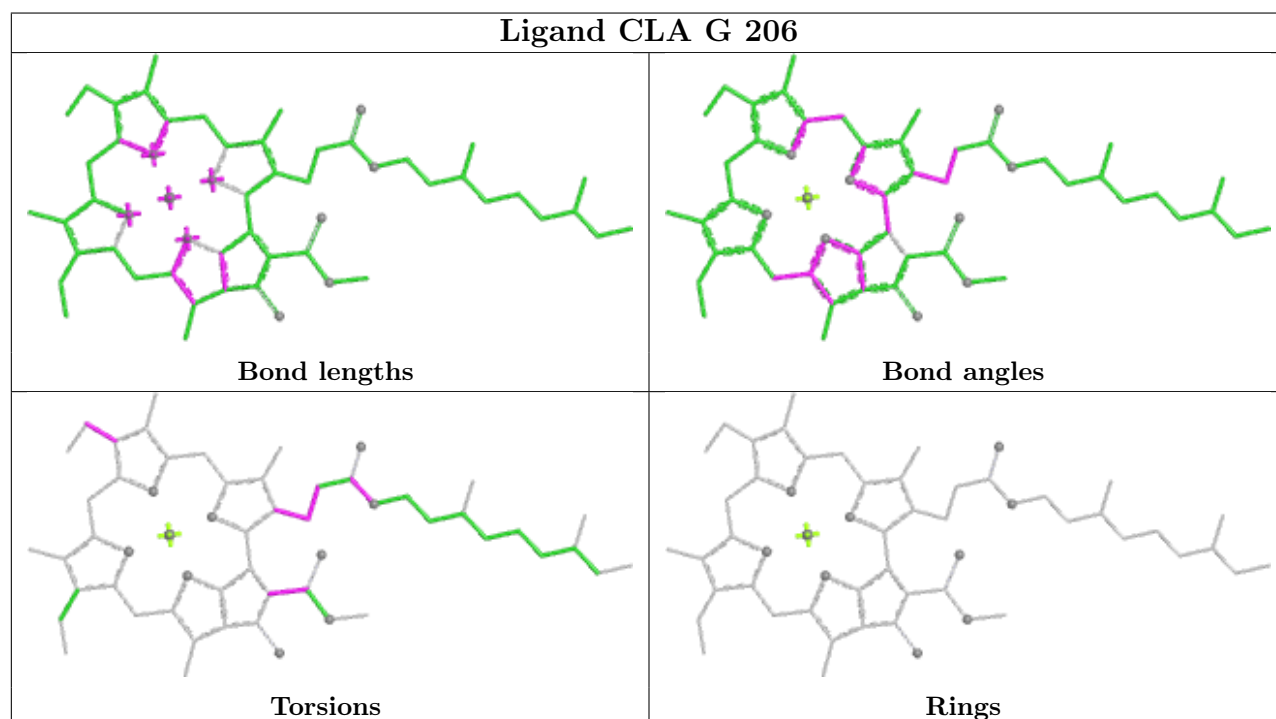
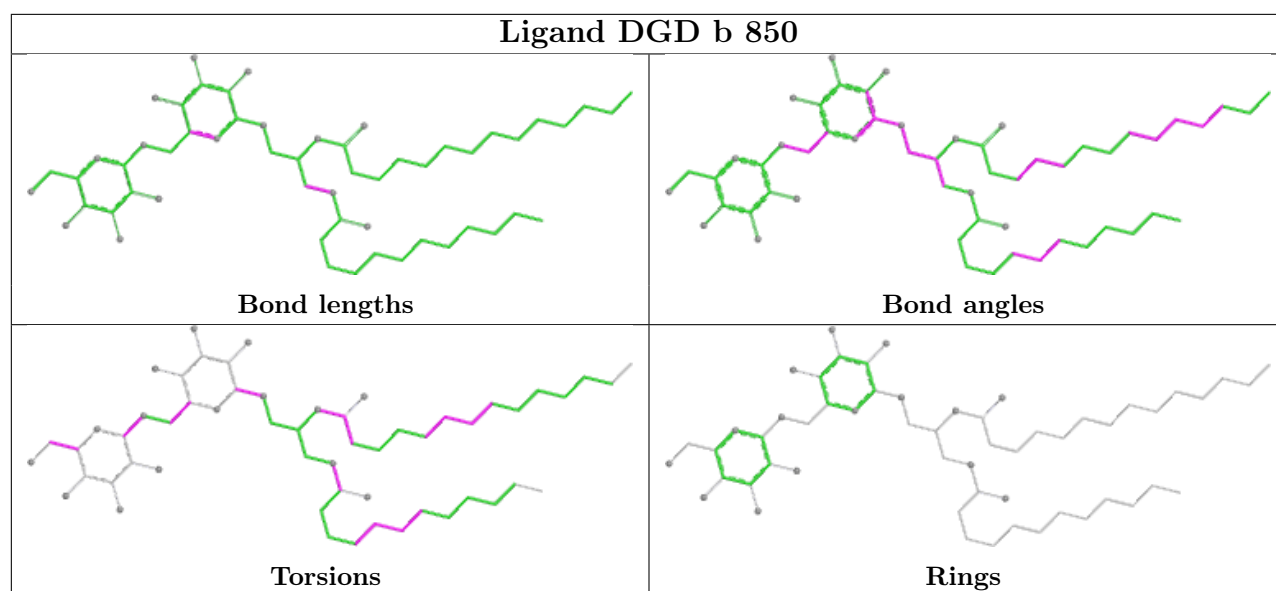


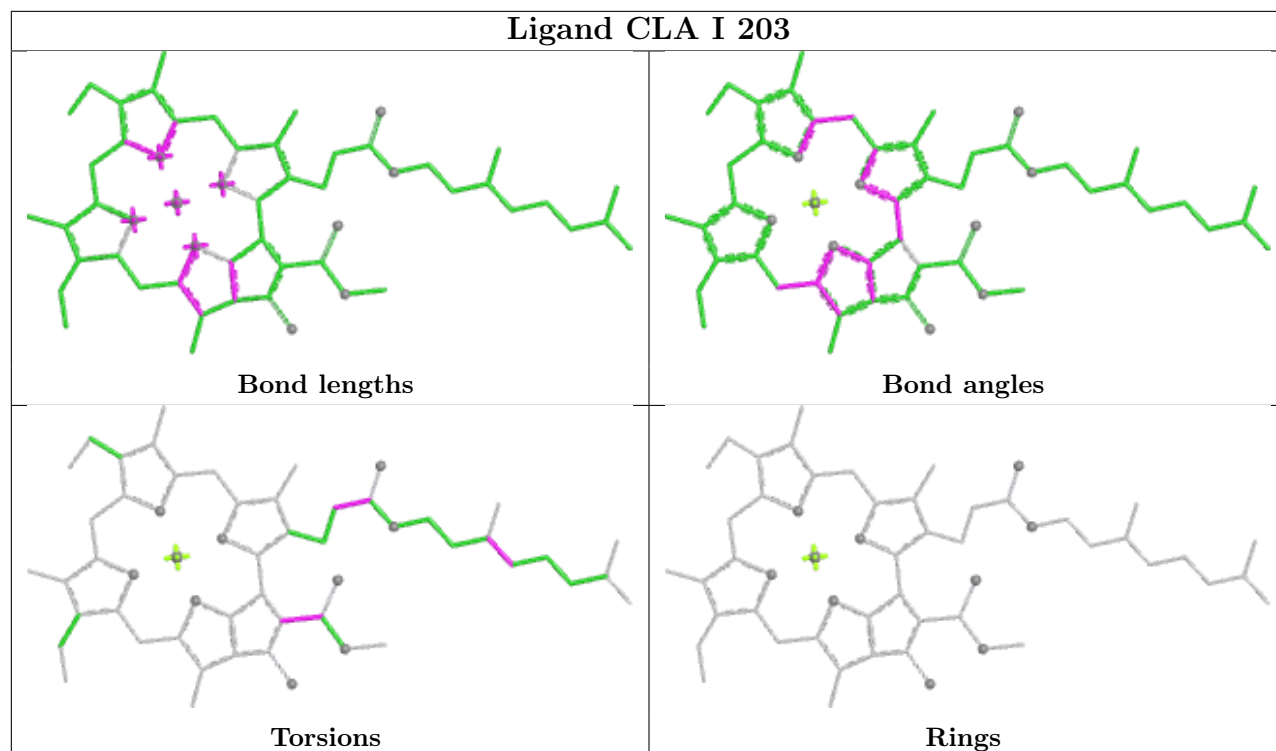
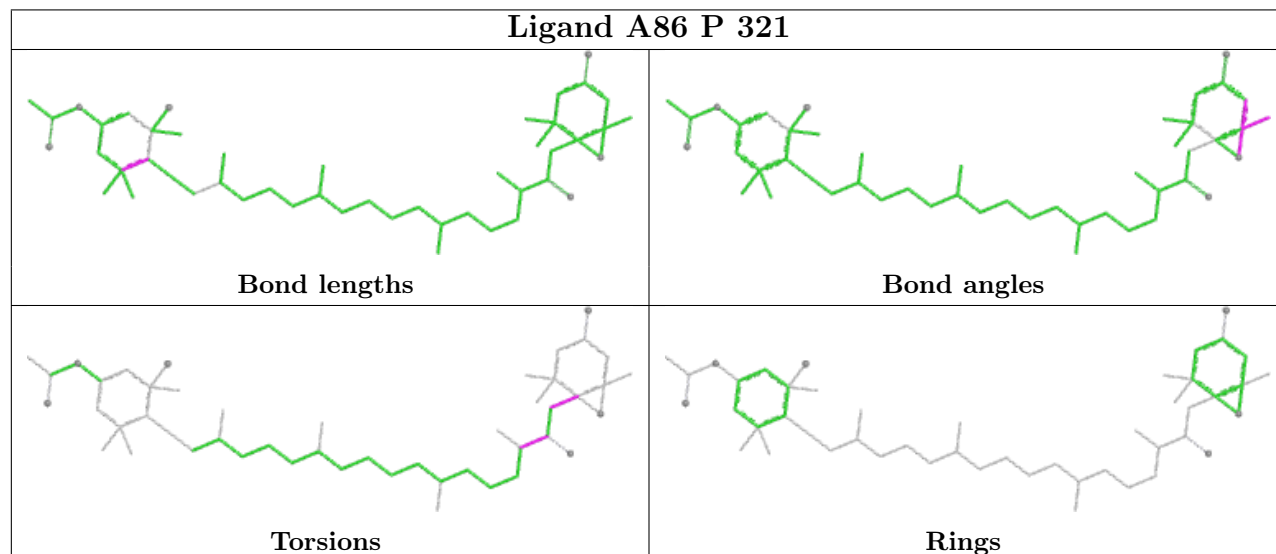
Ligand CLA p 308

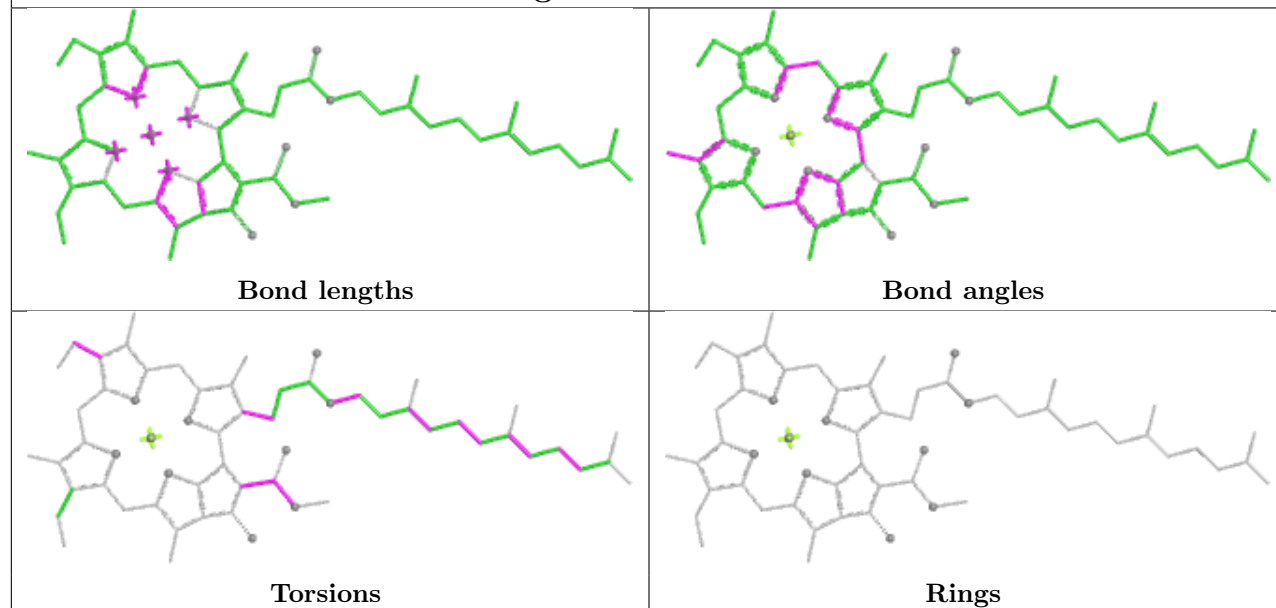
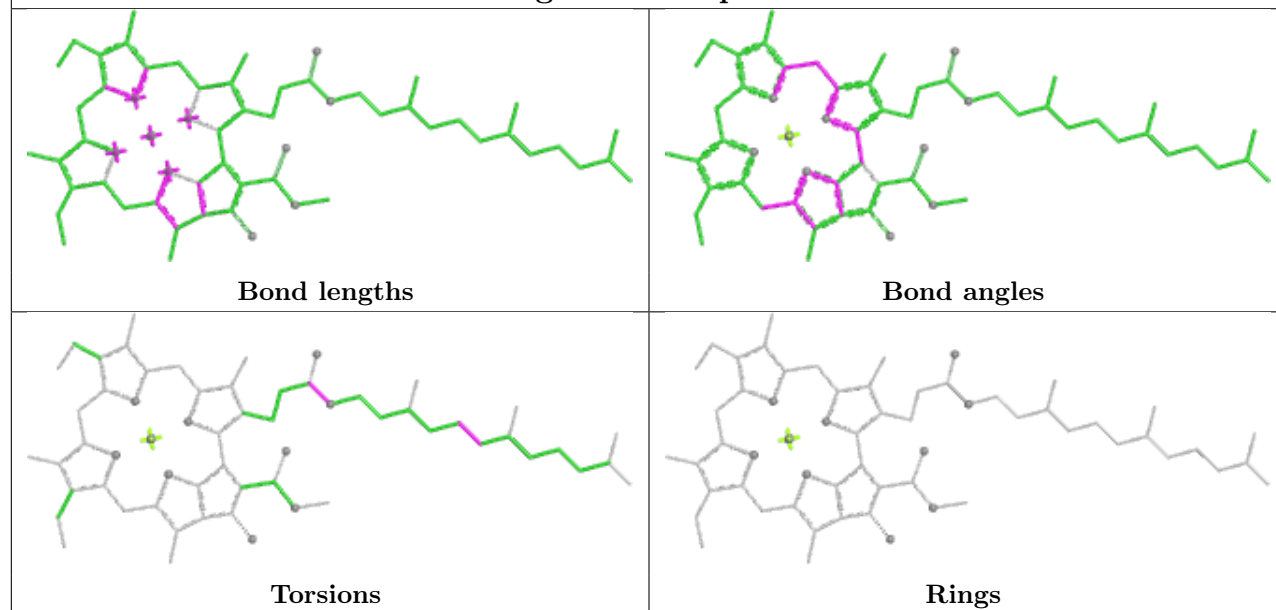


Ligand CLA x 305**Ligand DD6 I 212**

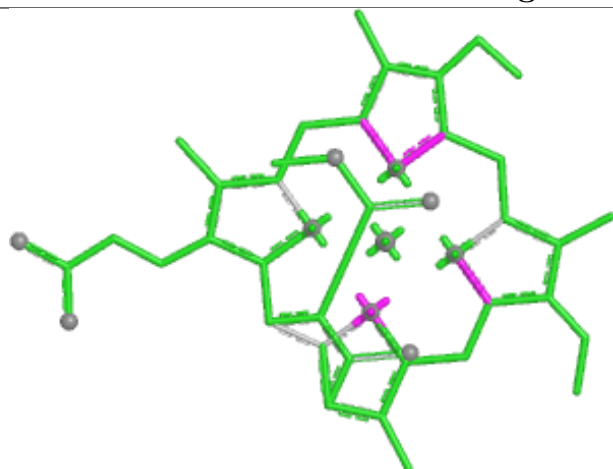




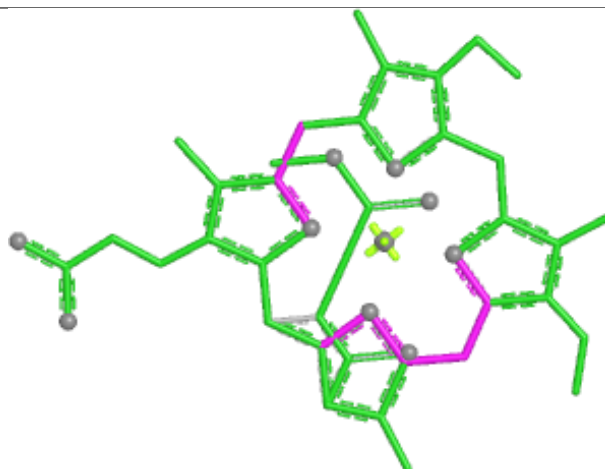
Ligand CLA I 203**Ligand A86 P 321**

Ligand CLA Z 306**Ligand CLA q 305**

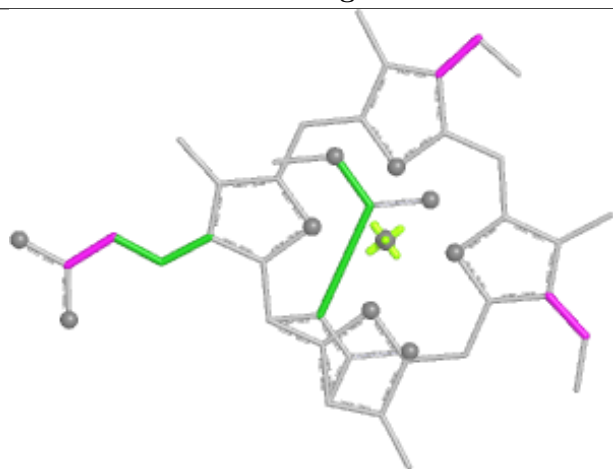
Ligand KC2 Z 308



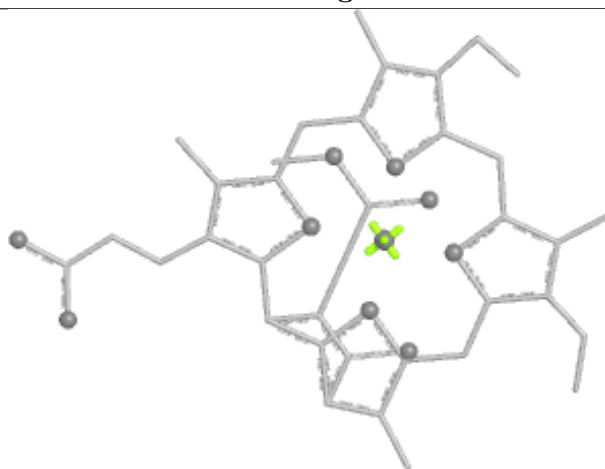
Bond lengths



Bond angles

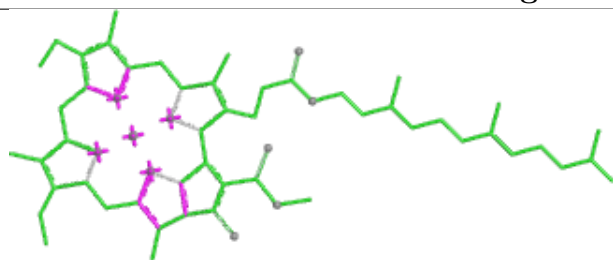


Torsions

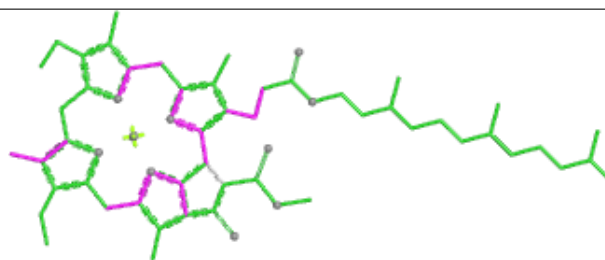


Rings

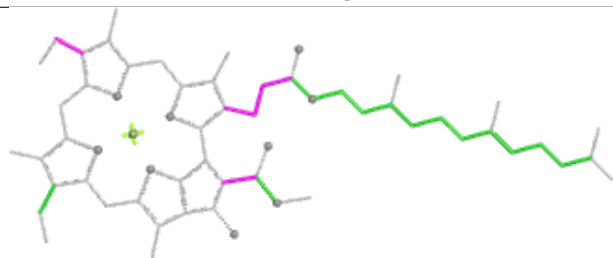
Ligand CLA t 304



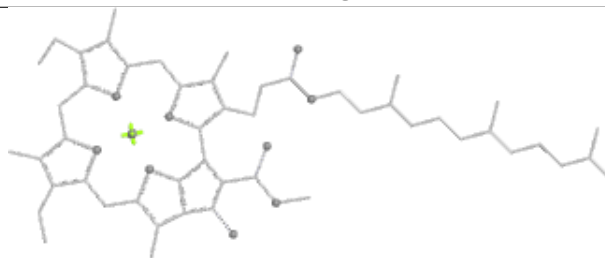
Bond lengths



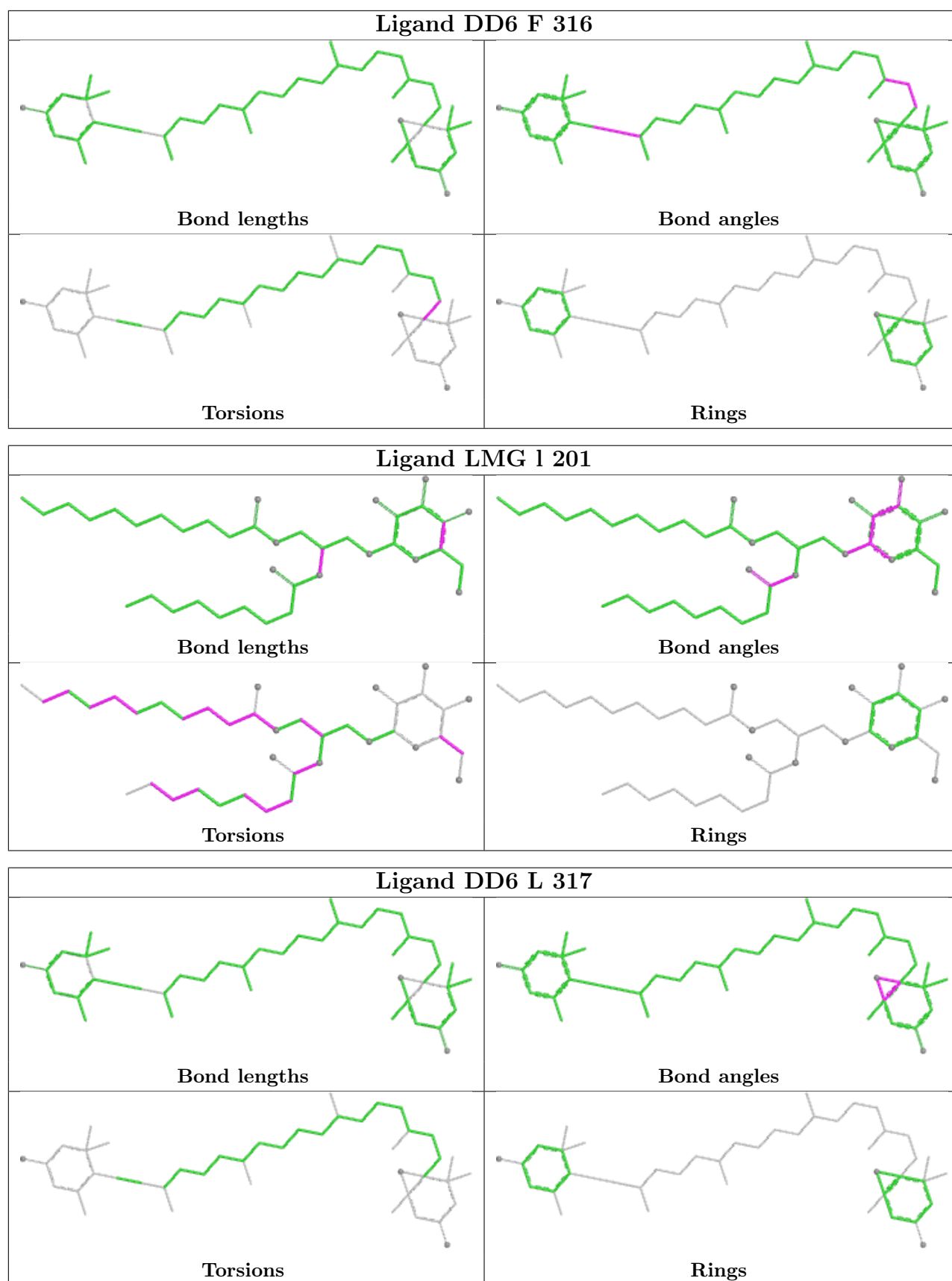
Bond angles



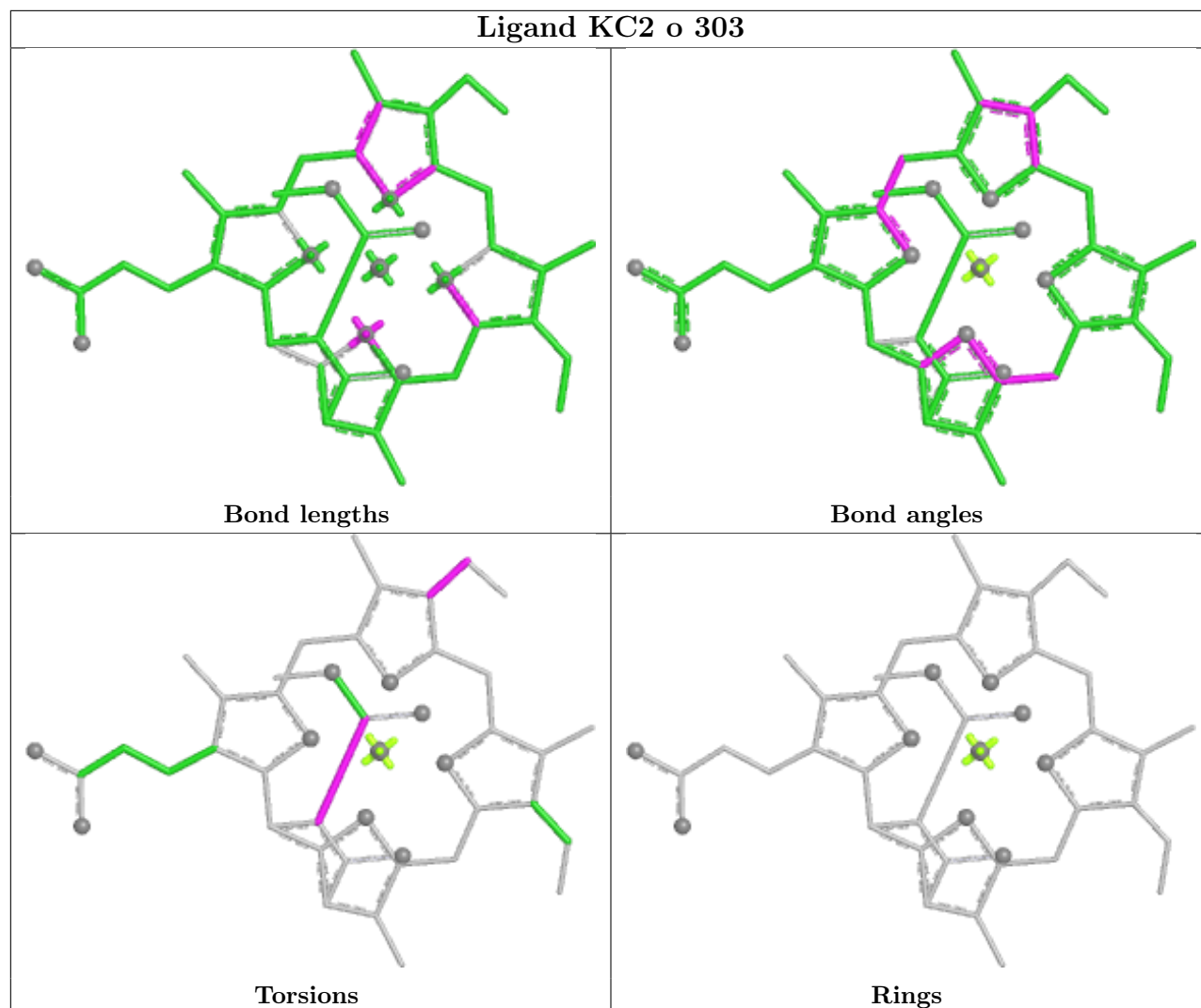
Torsions



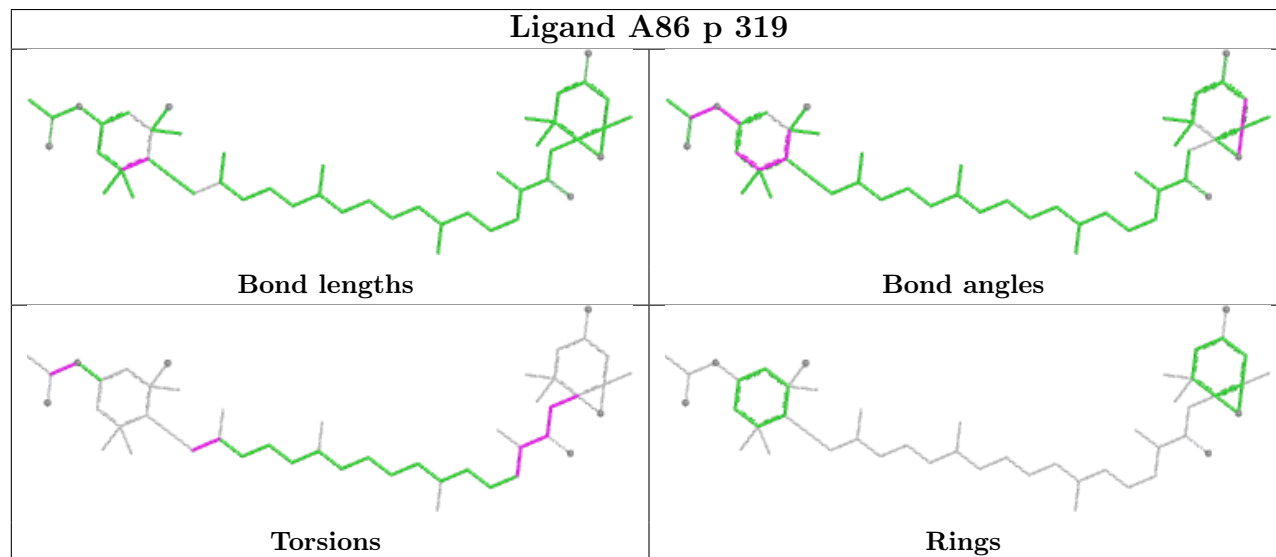
Rings

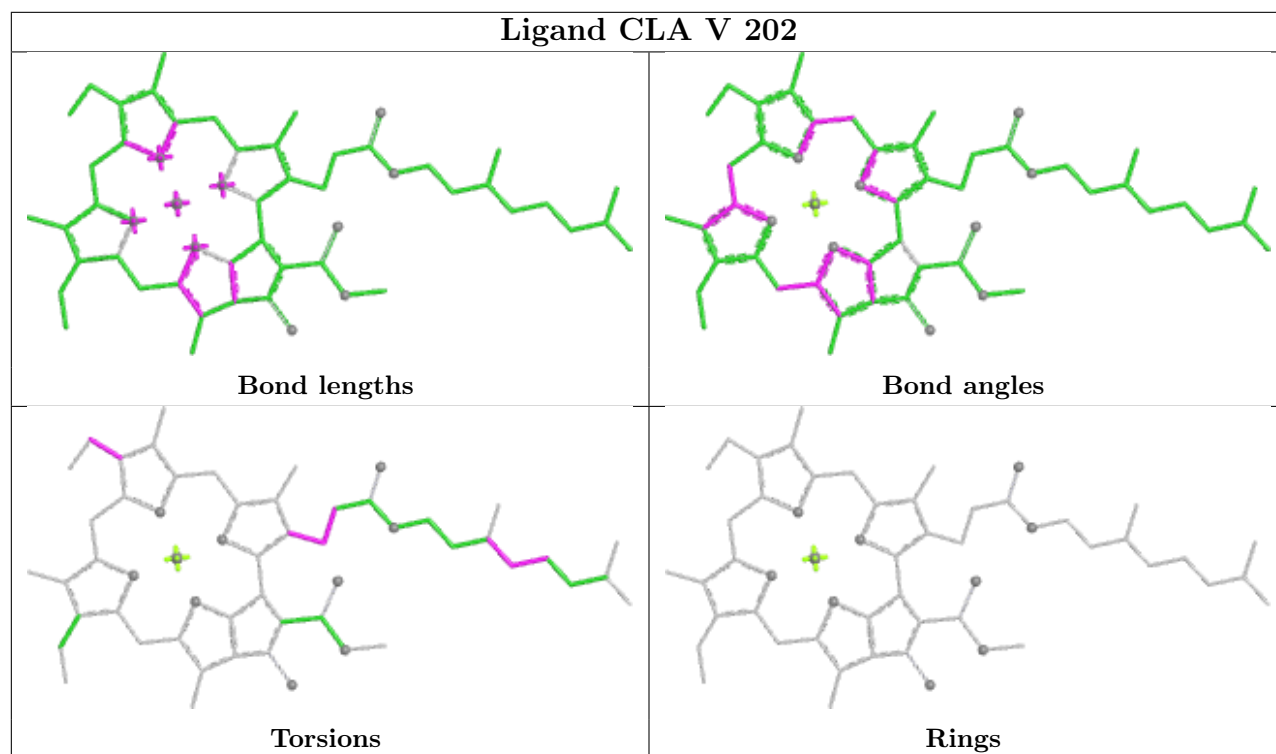
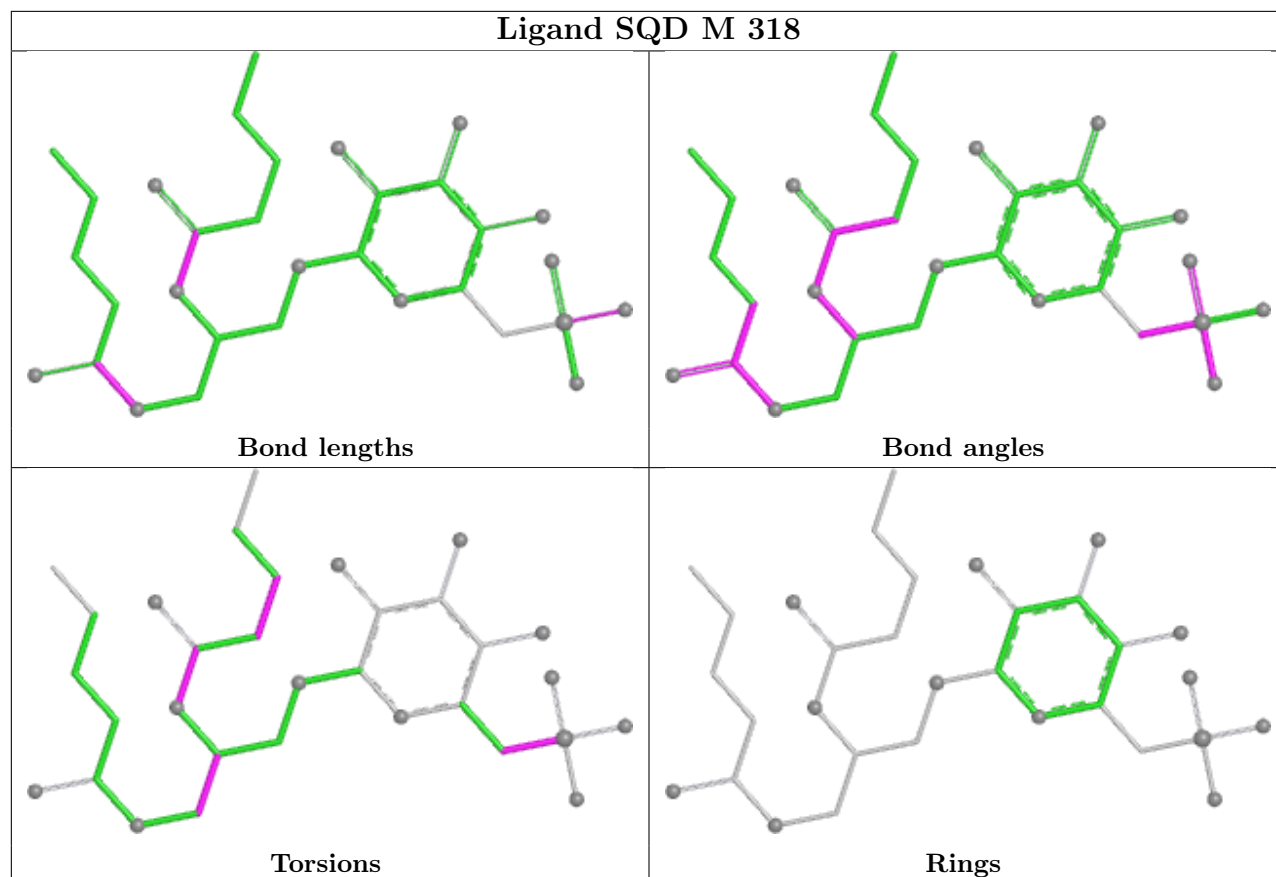


Ligand KC2 o 303

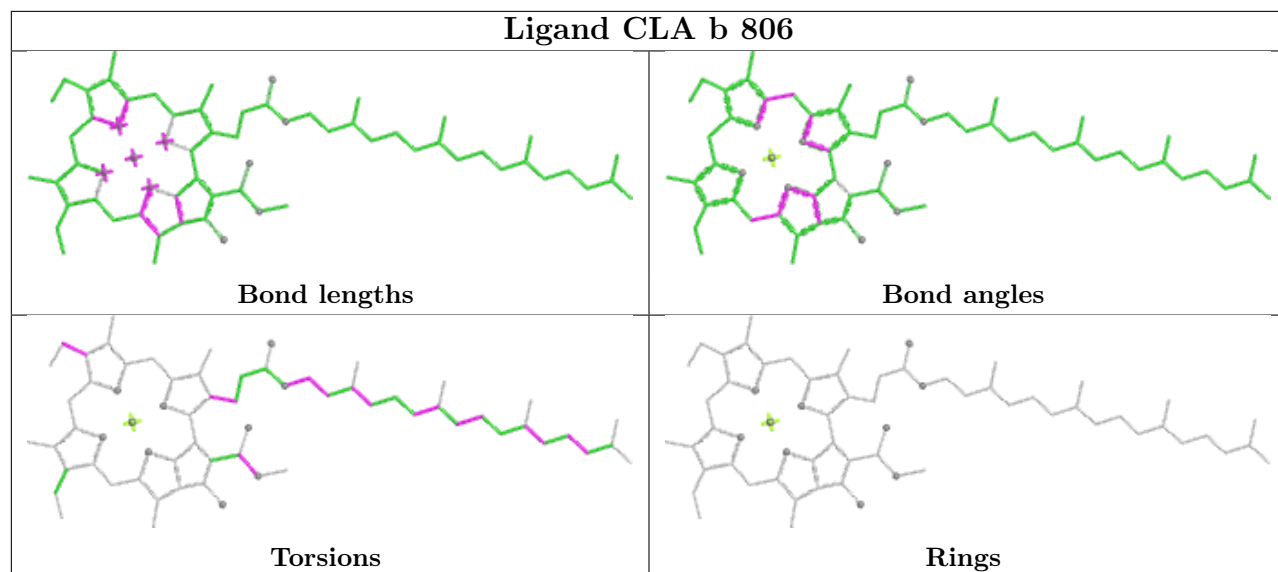


Ligand A86 p 319

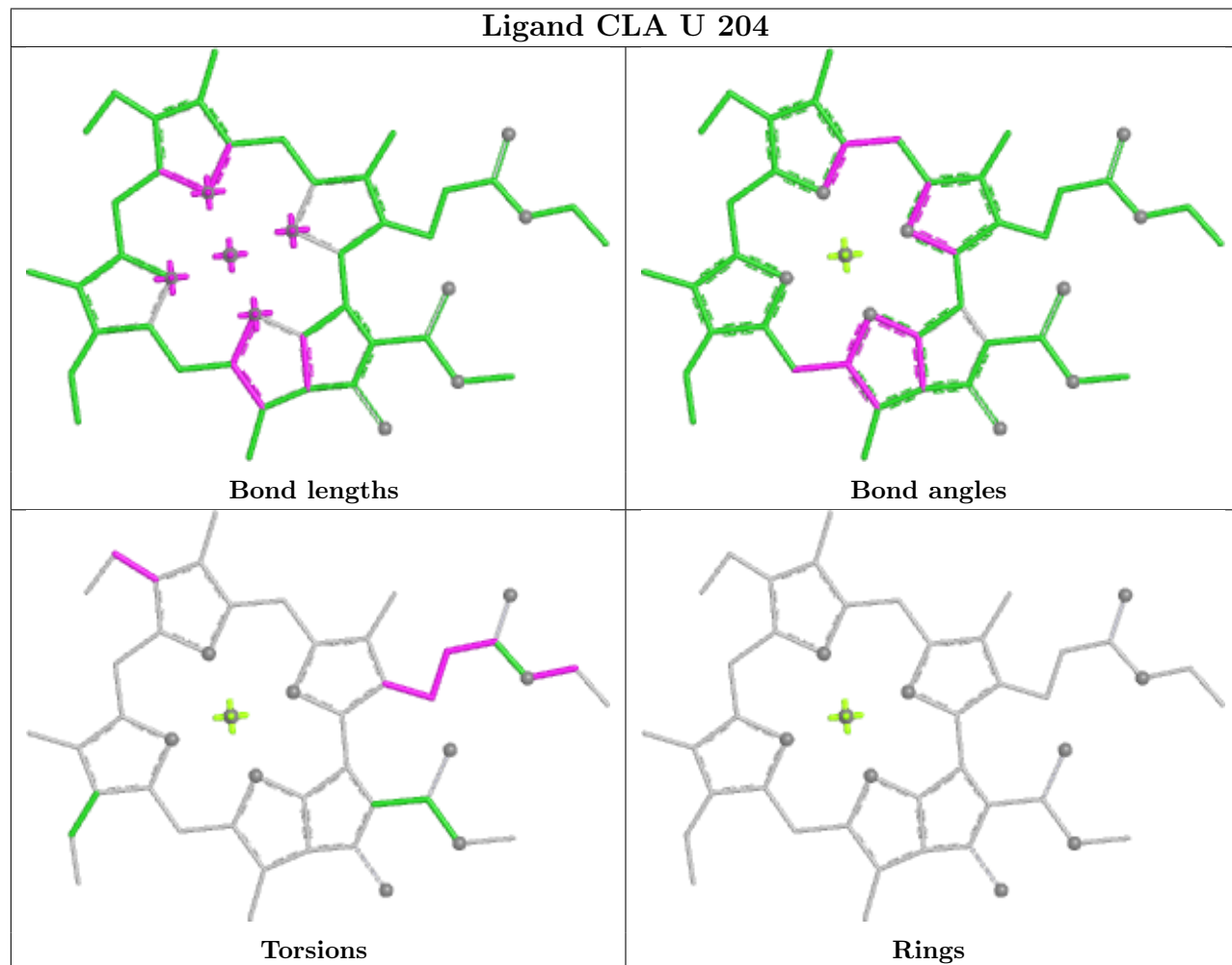


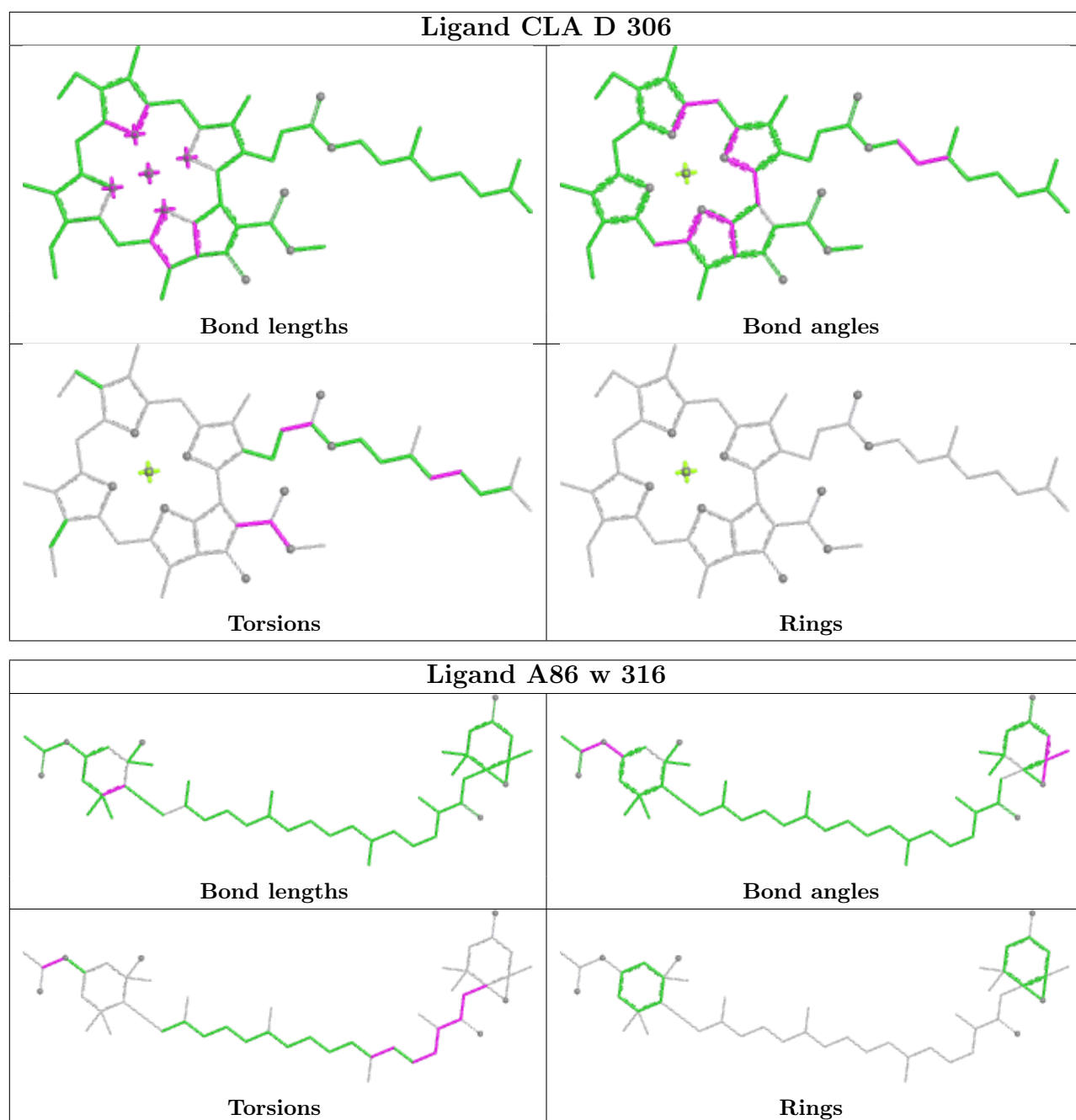


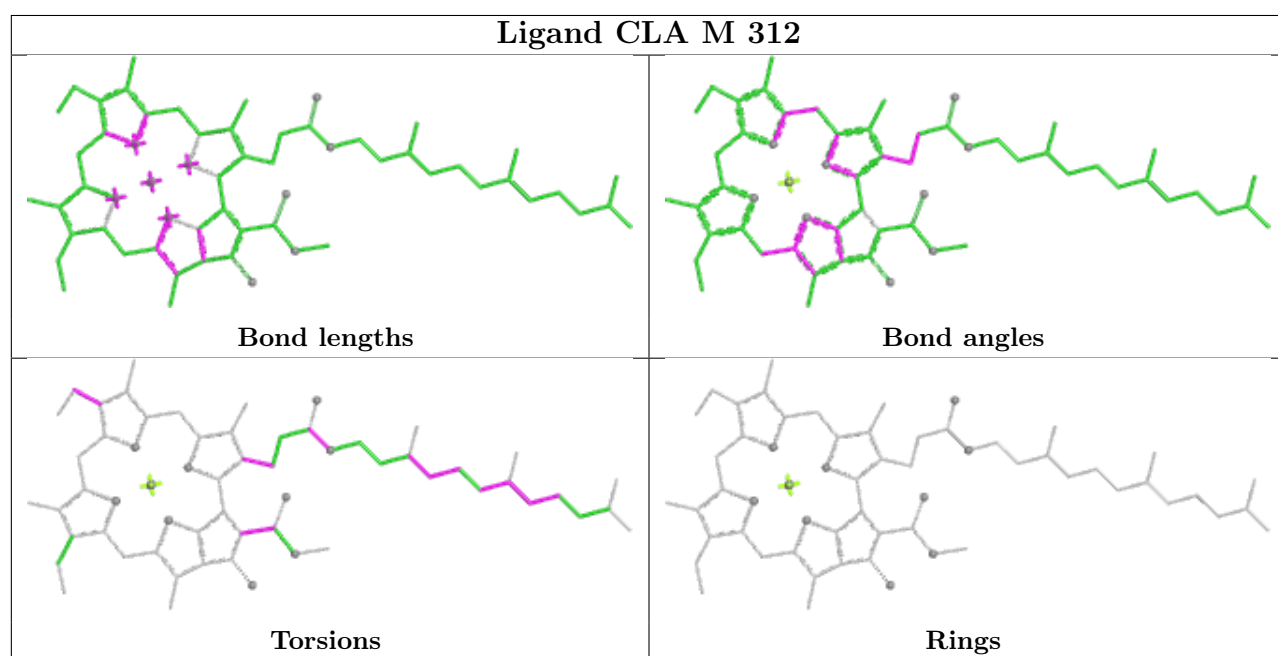
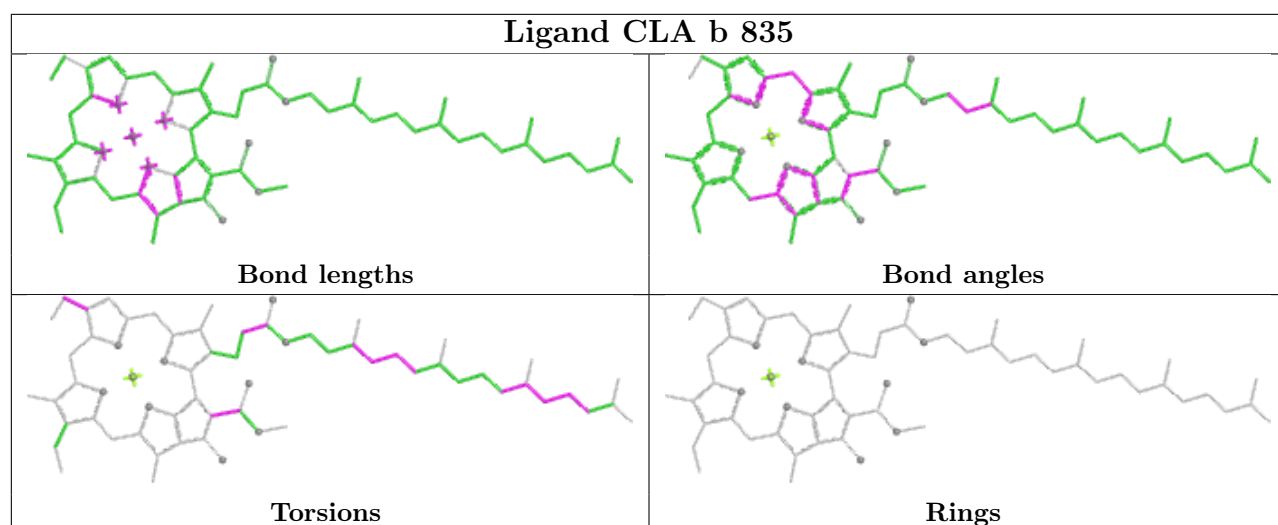
Ligand CLA b 806



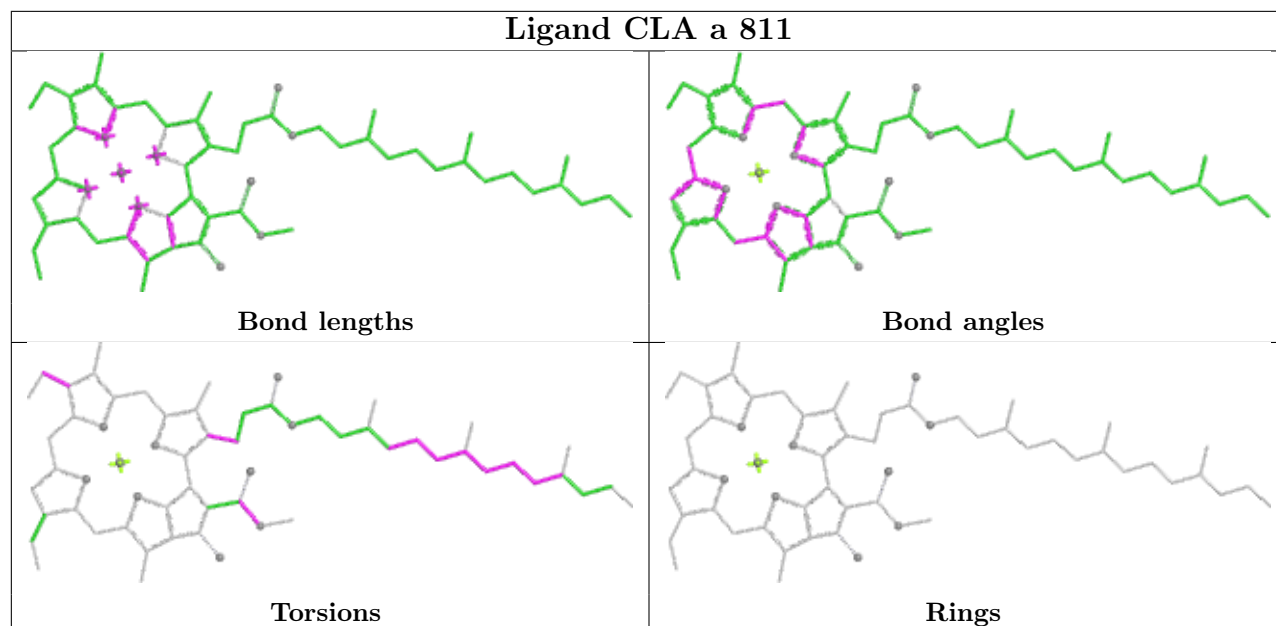
Ligand CLA U 204



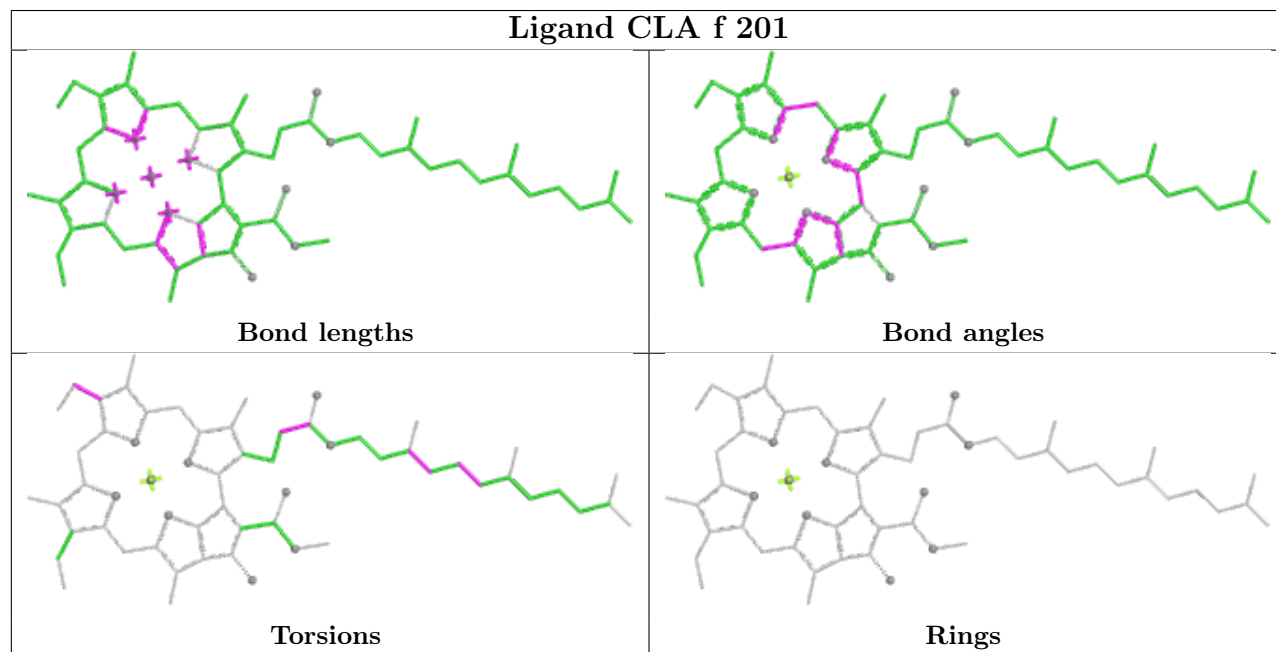


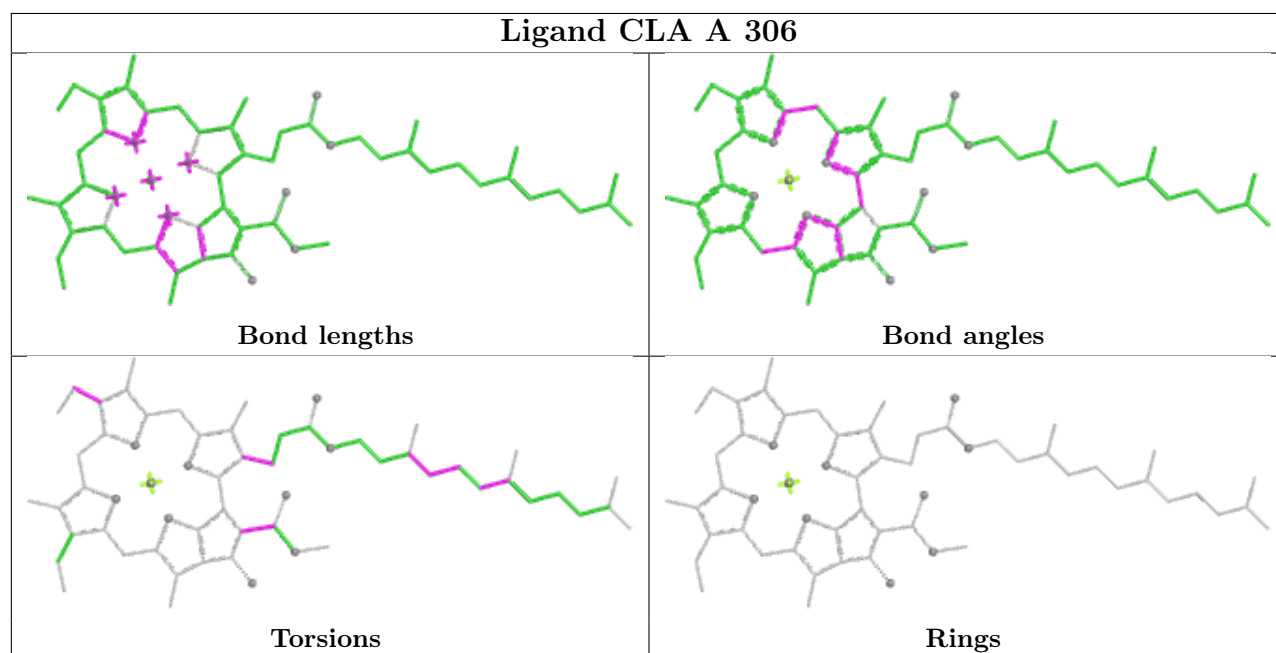
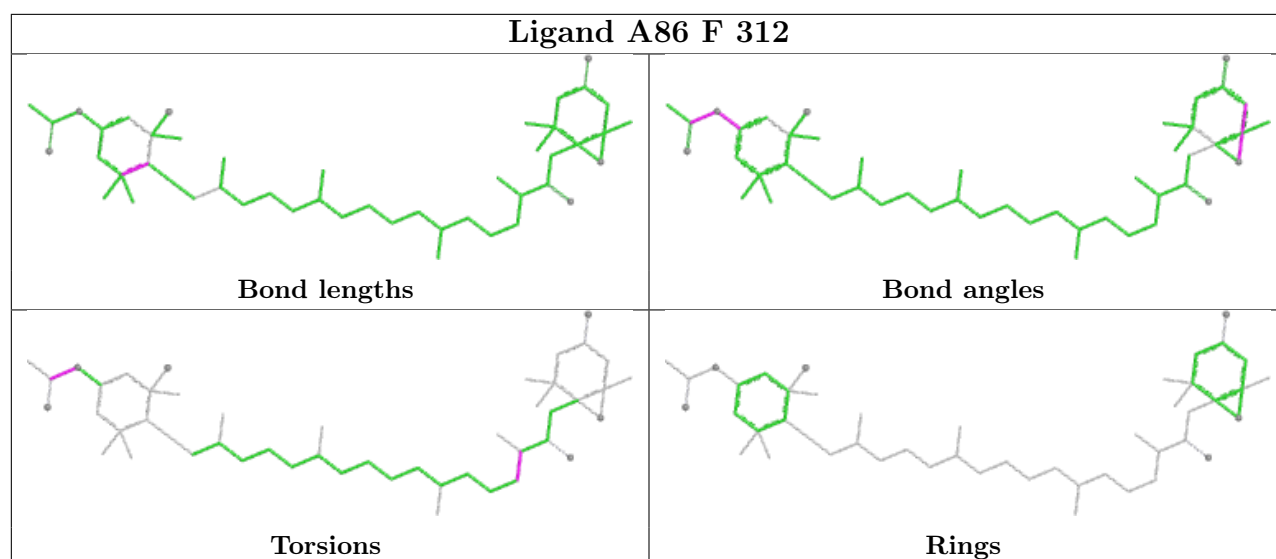


Ligand CLA a 811

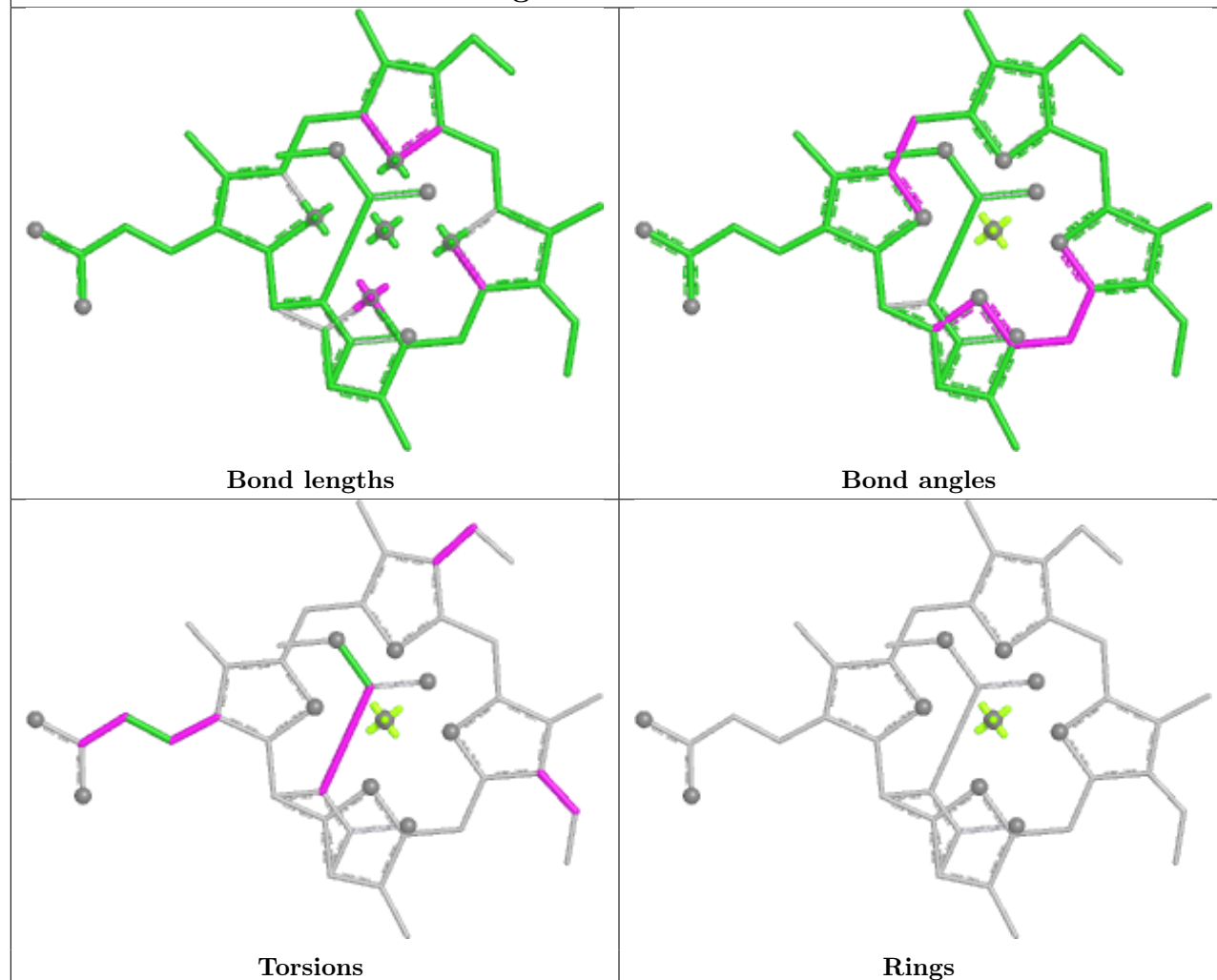


Ligand CLA f 201

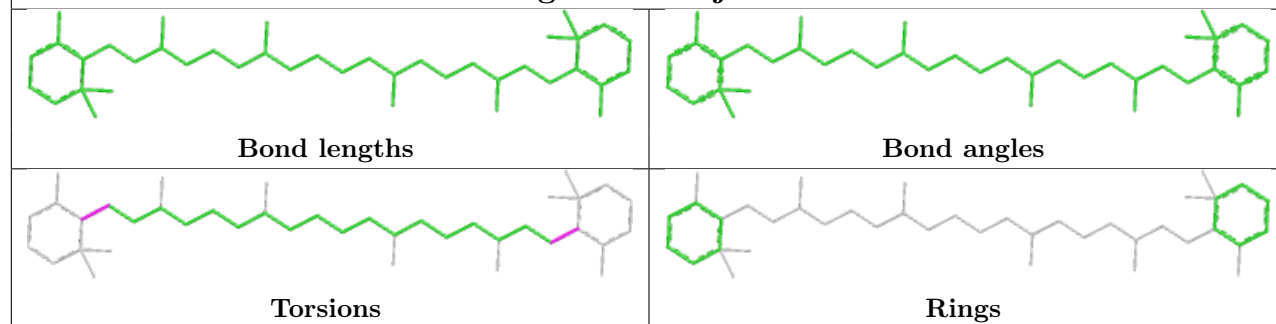




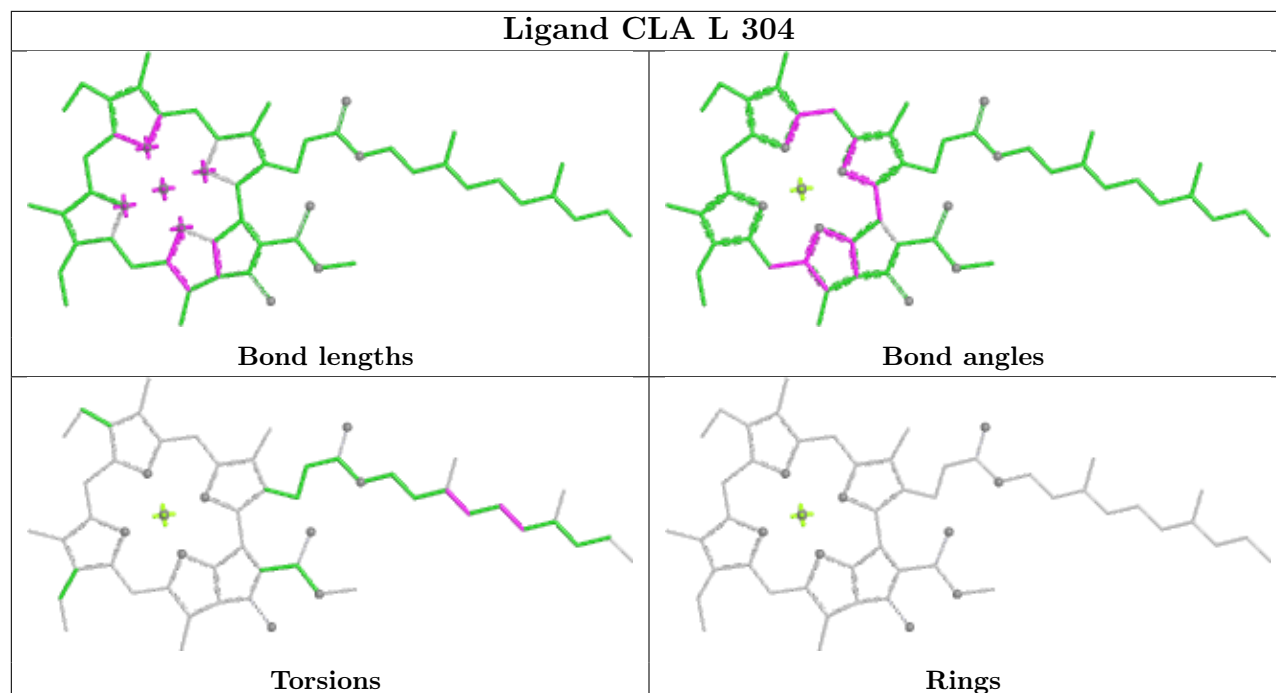
Ligand KC2 v 308



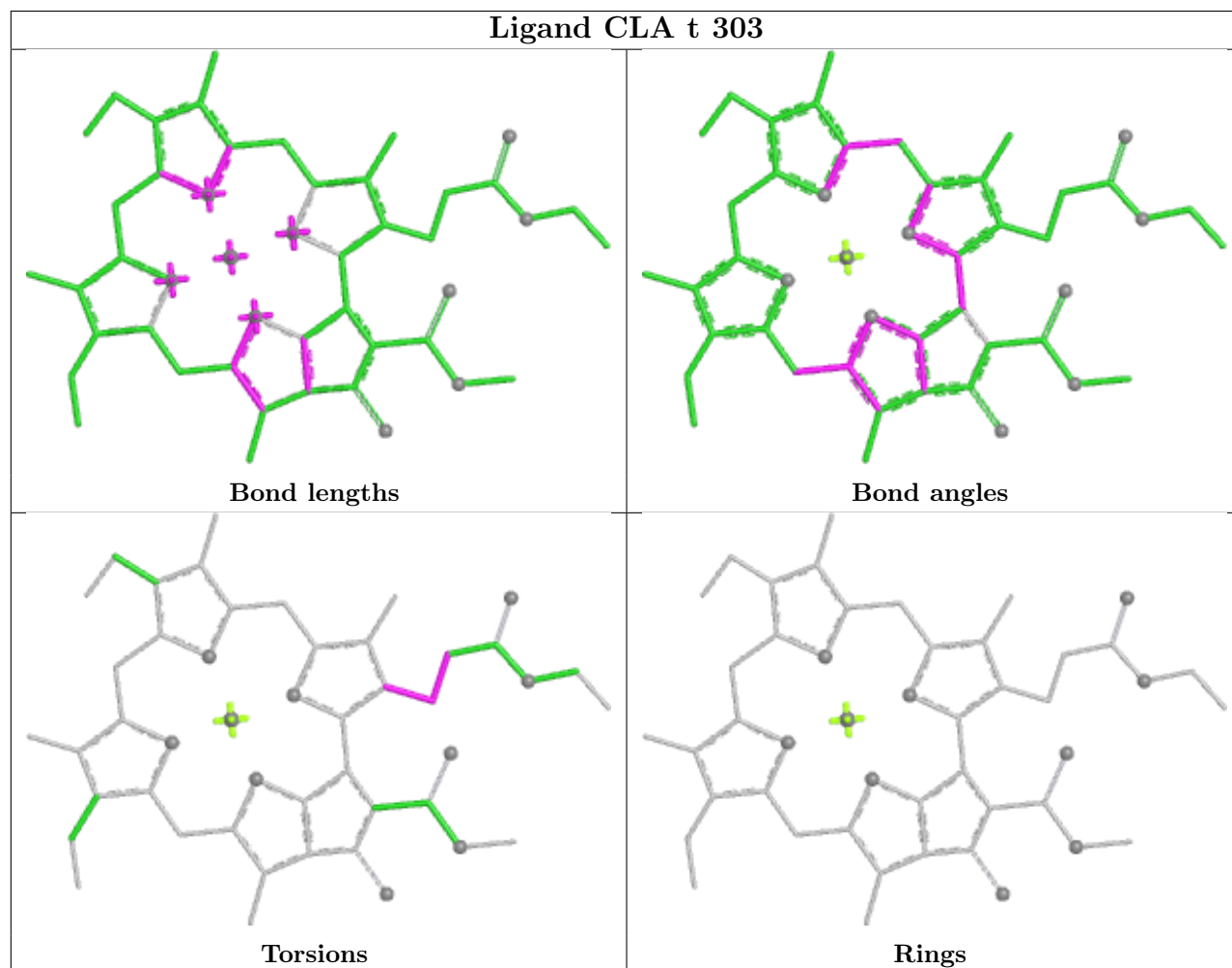
Ligand BCR j 103



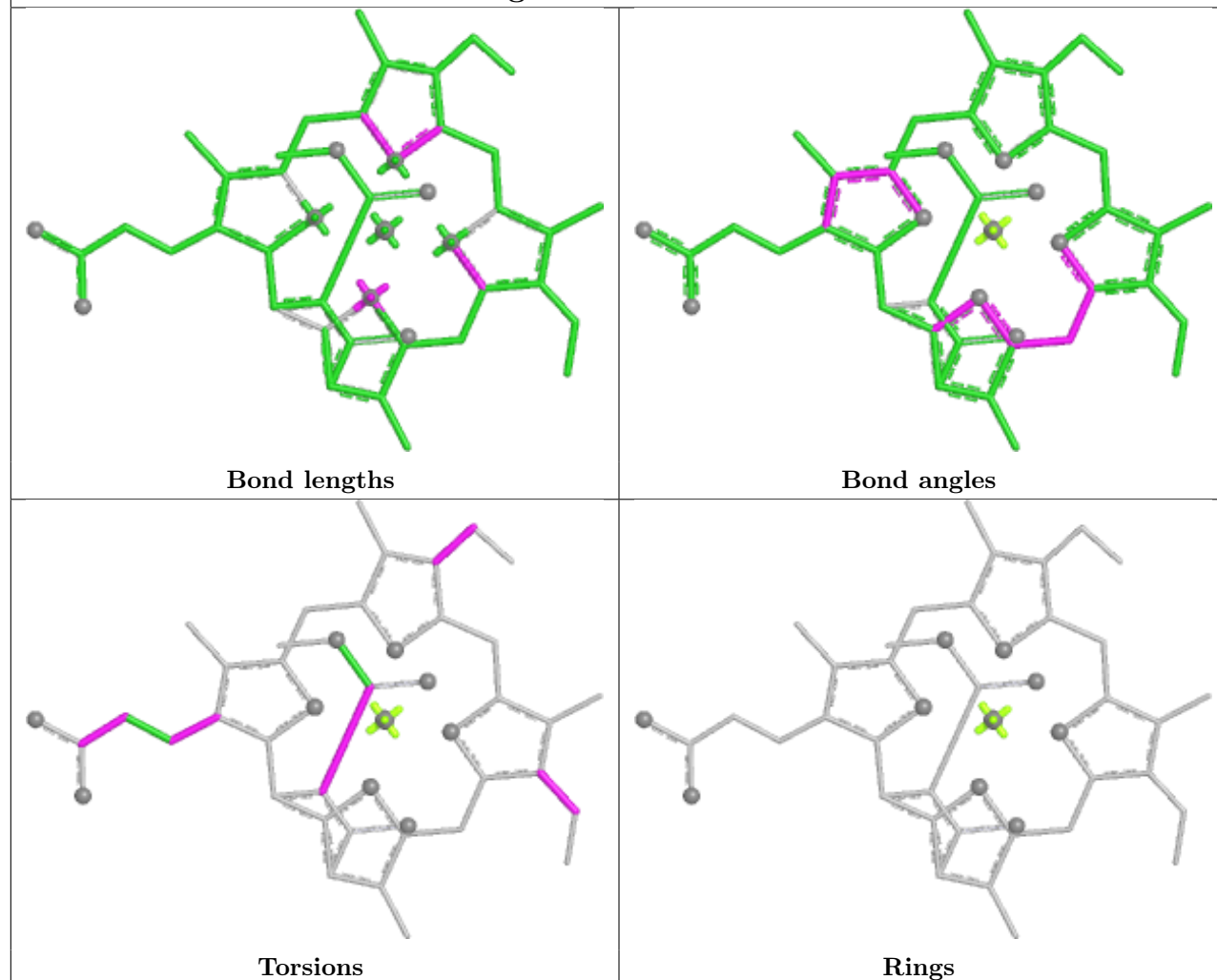
Ligand CLA L 304



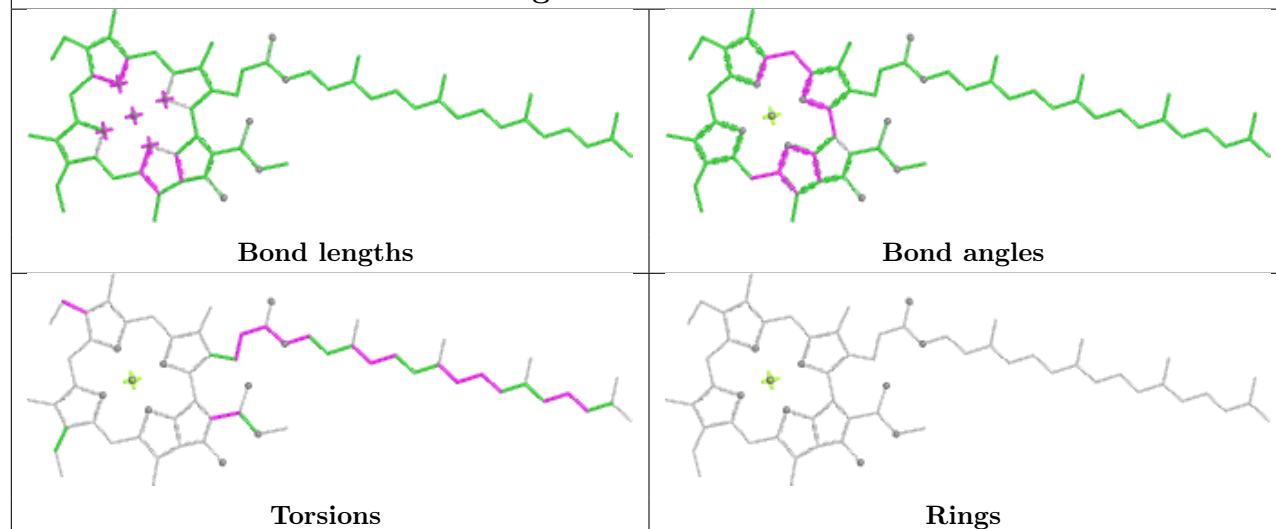
Ligand CLA t 303



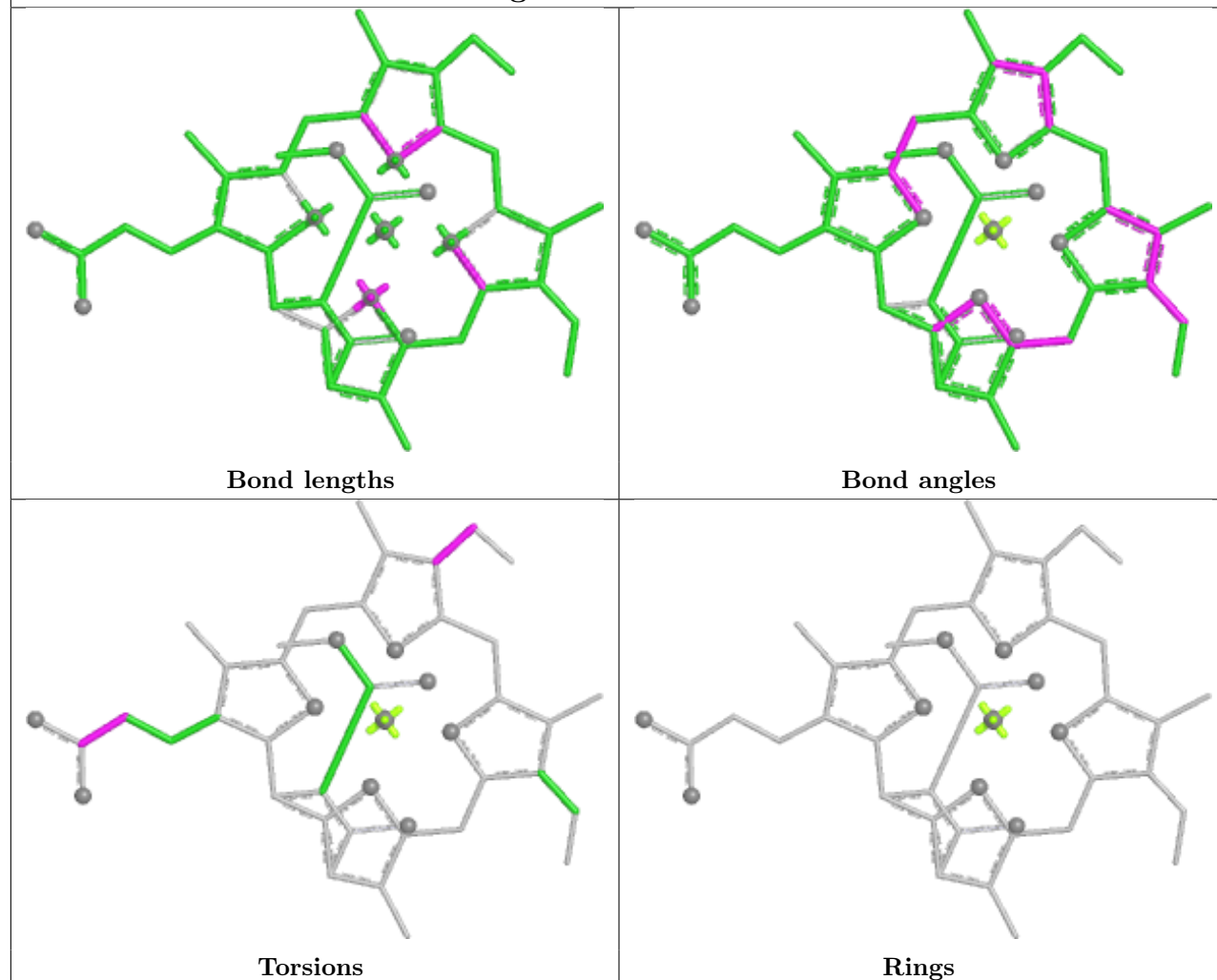
Ligand KC2 G 202



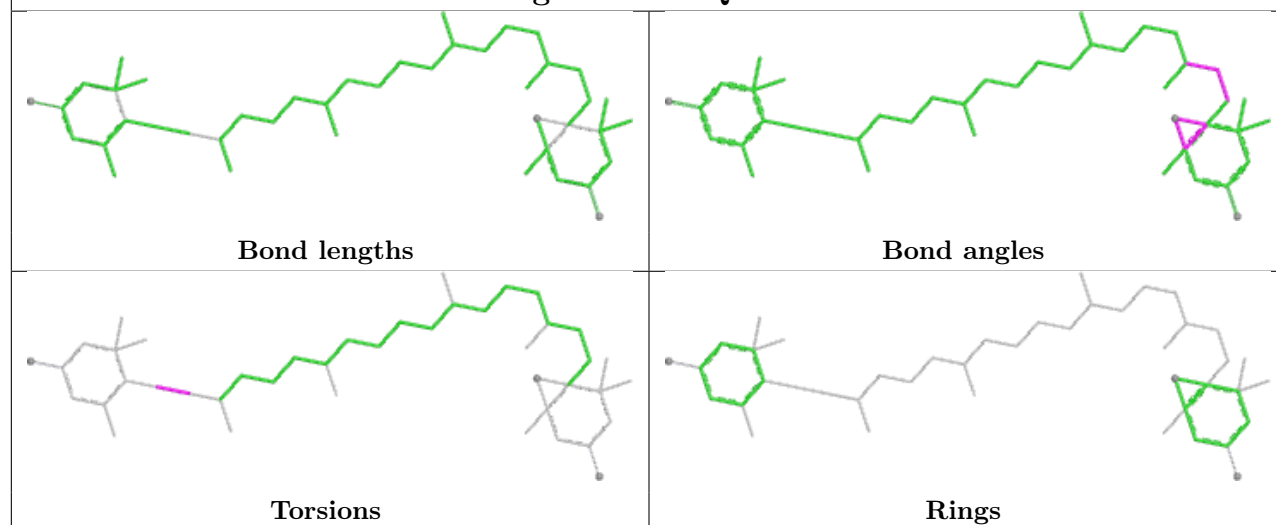
Ligand CLA C 306

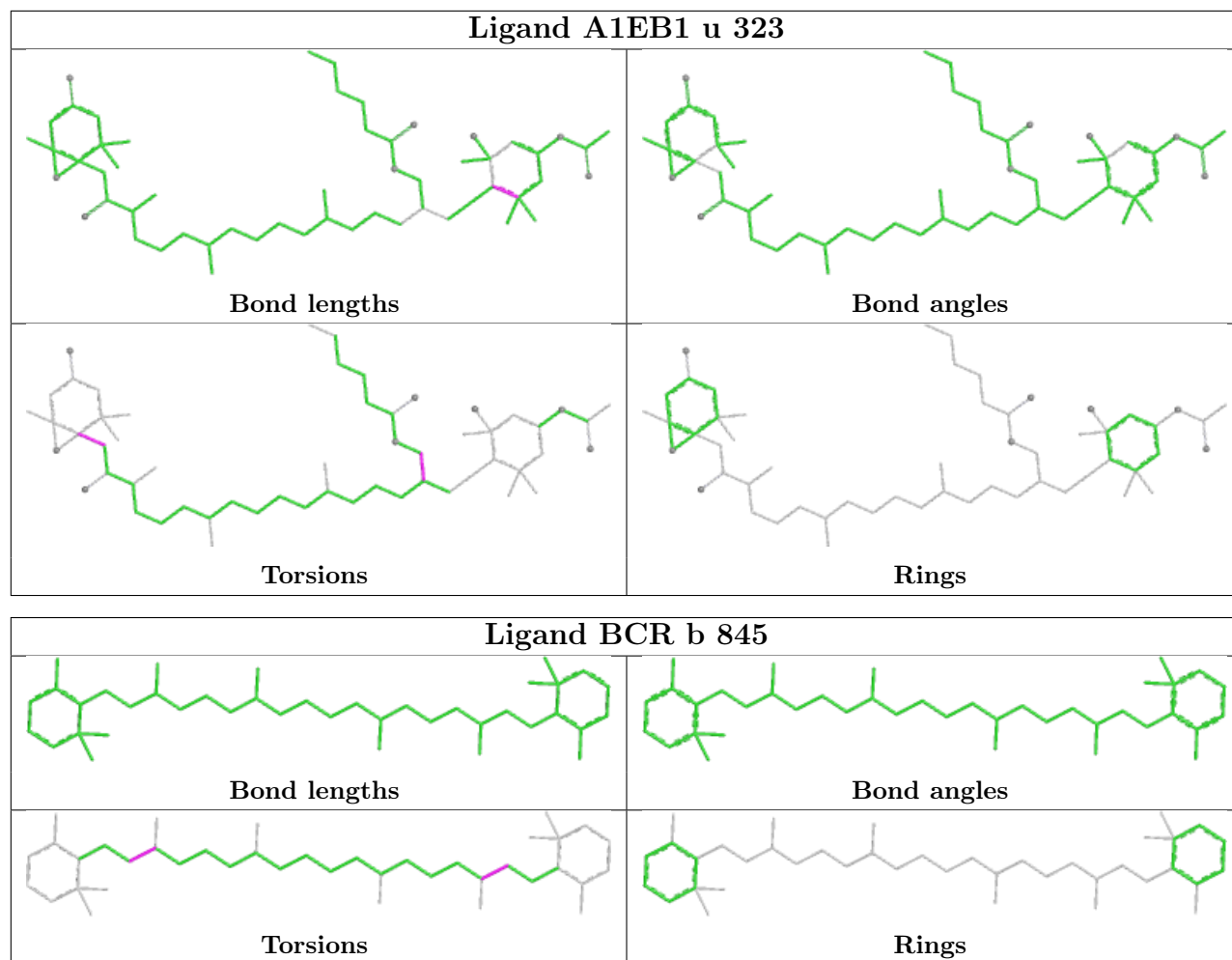


Ligand KC2 T 303

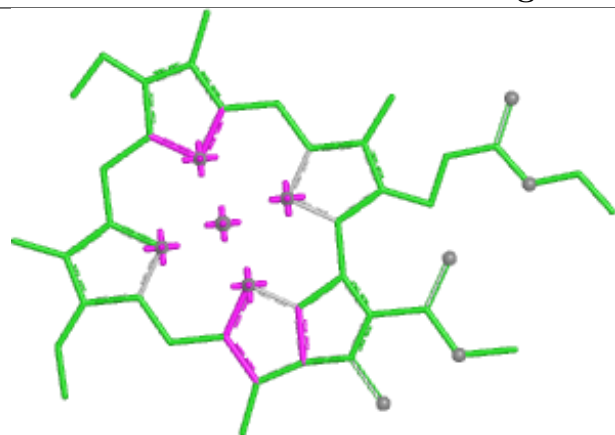


Ligand DD6 Q 212

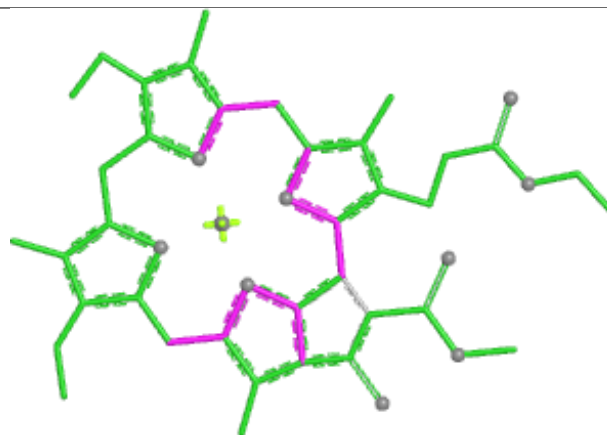




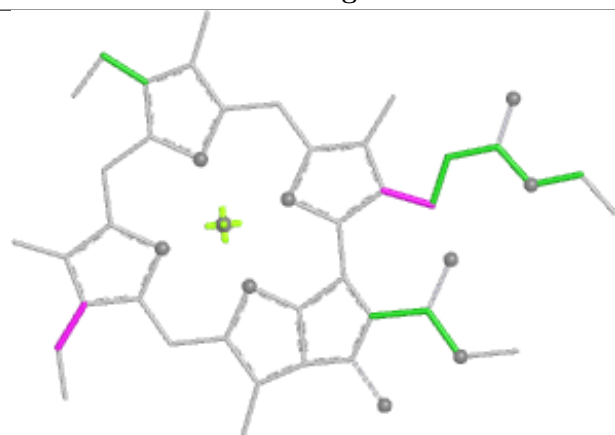
Ligand CLA E 312



Bond lengths



Bond angles

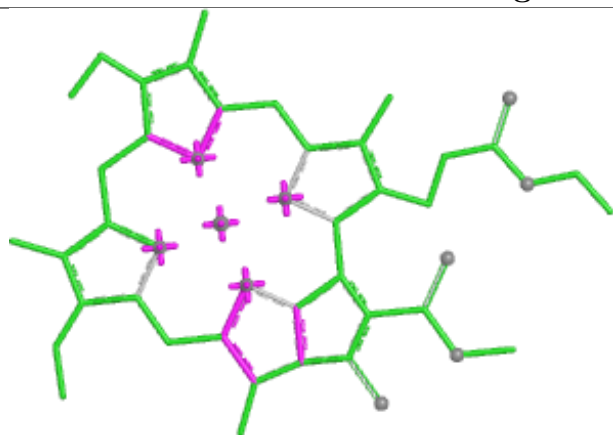


Torsions

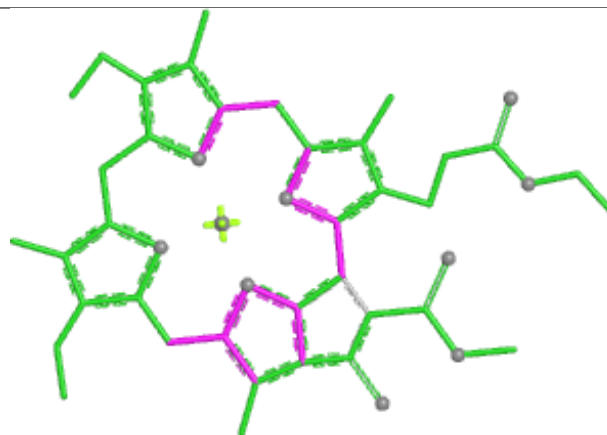


Rings

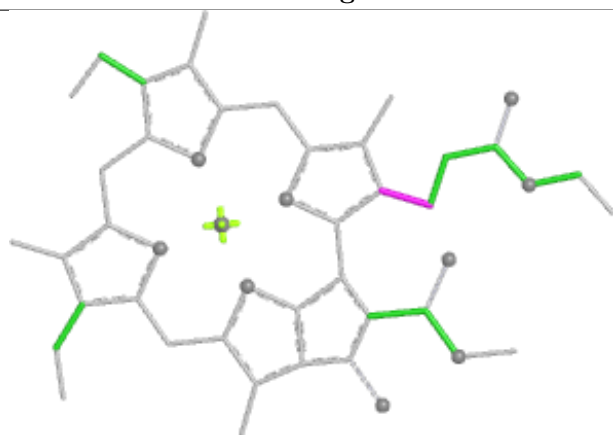
Ligand CLA Y 304



Bond lengths



Bond angles

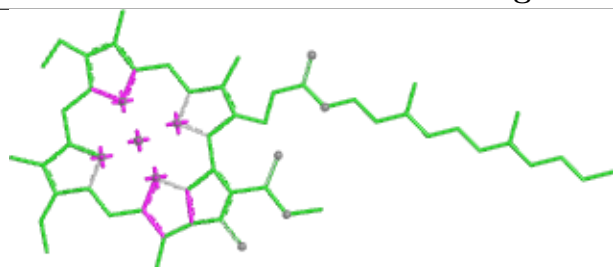


Torsions

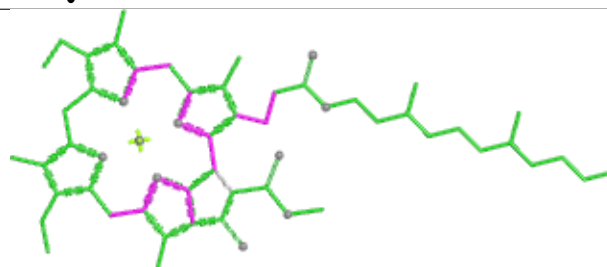


Rings

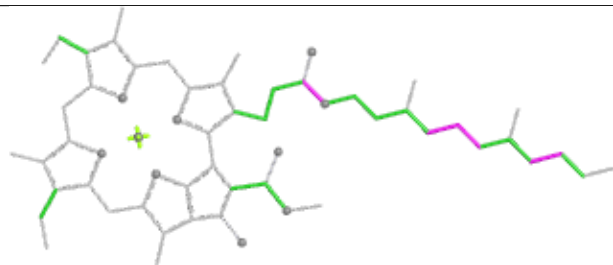
Ligand CLA Q 202



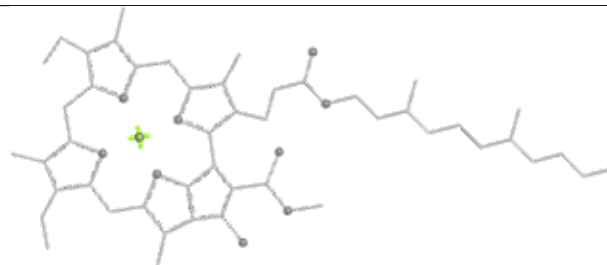
Bond lengths



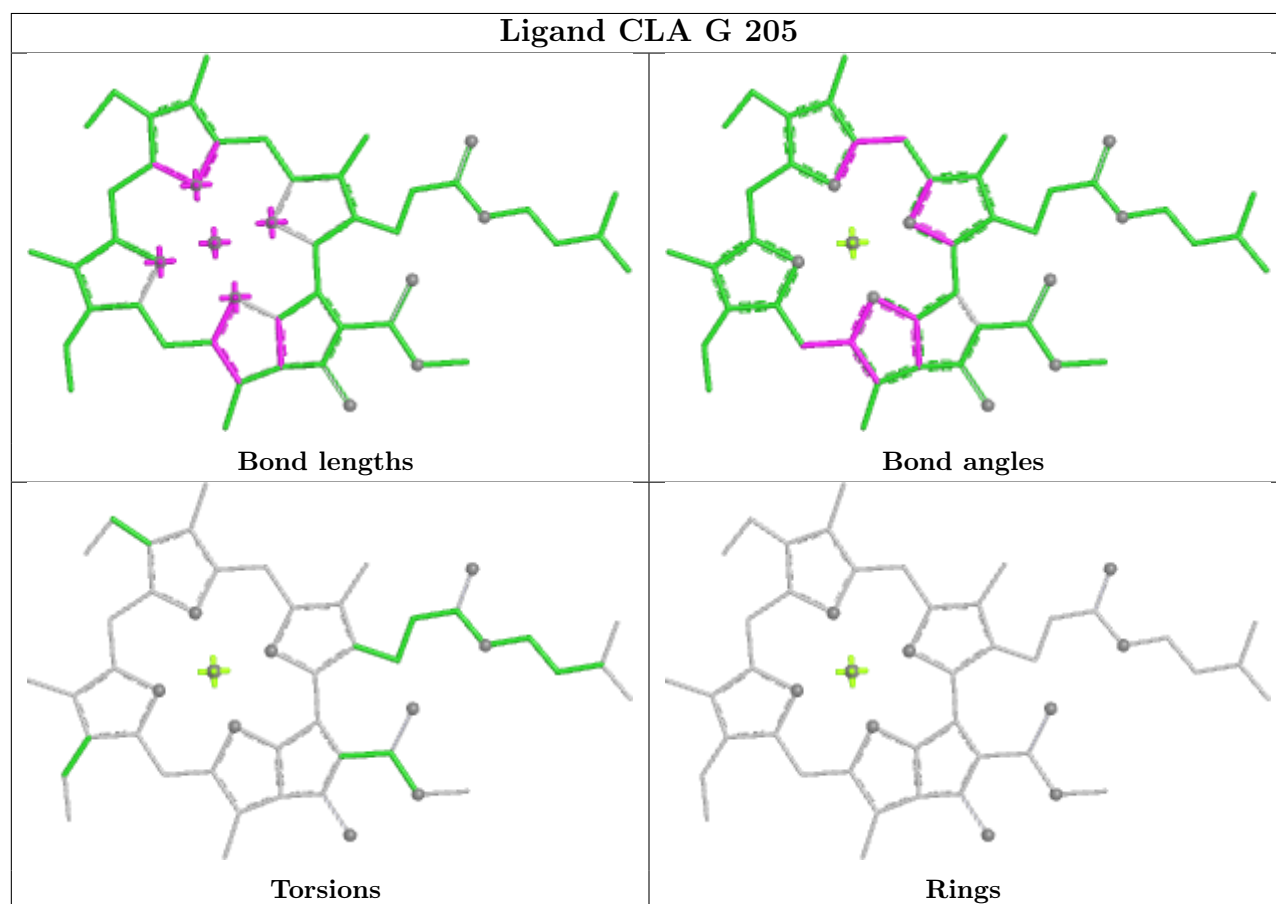
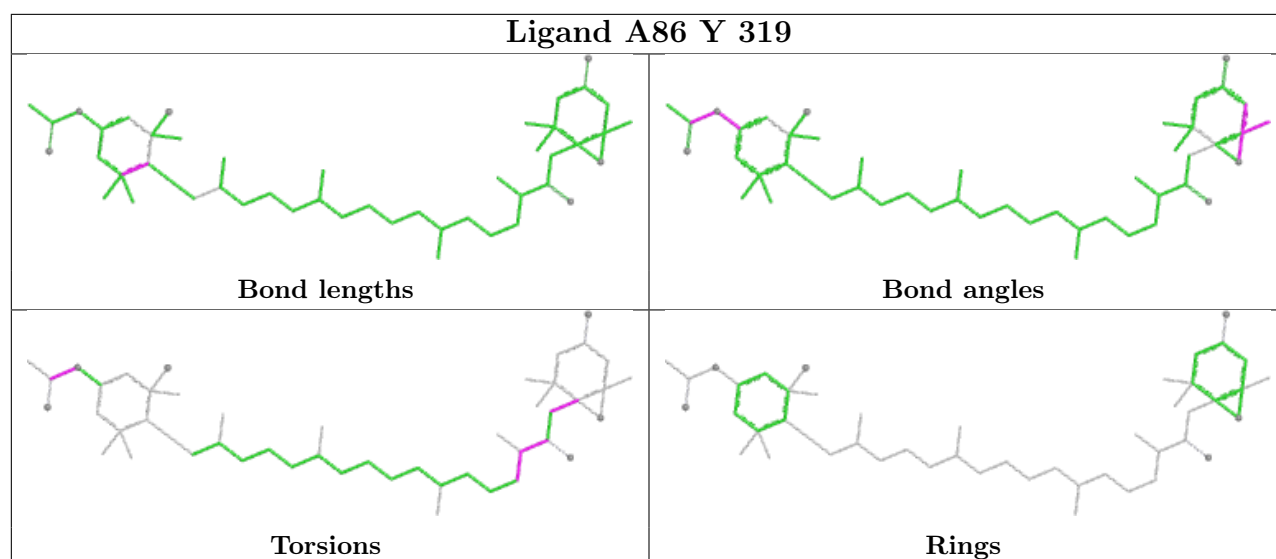
Bond angles

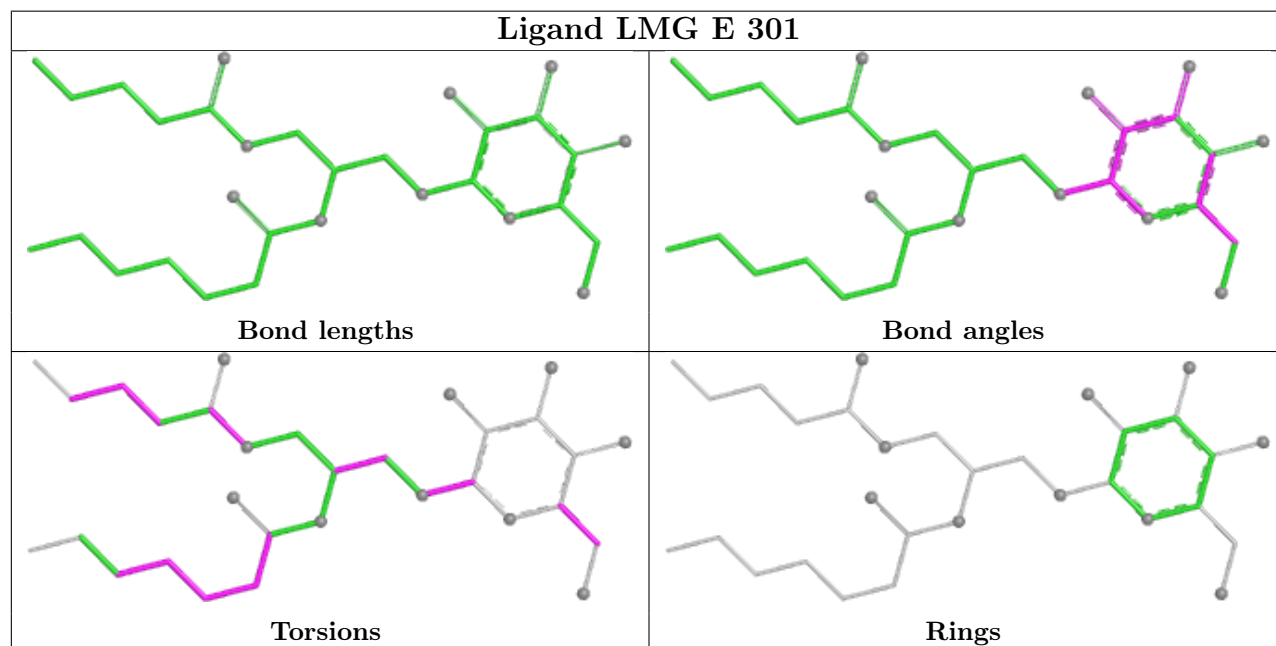
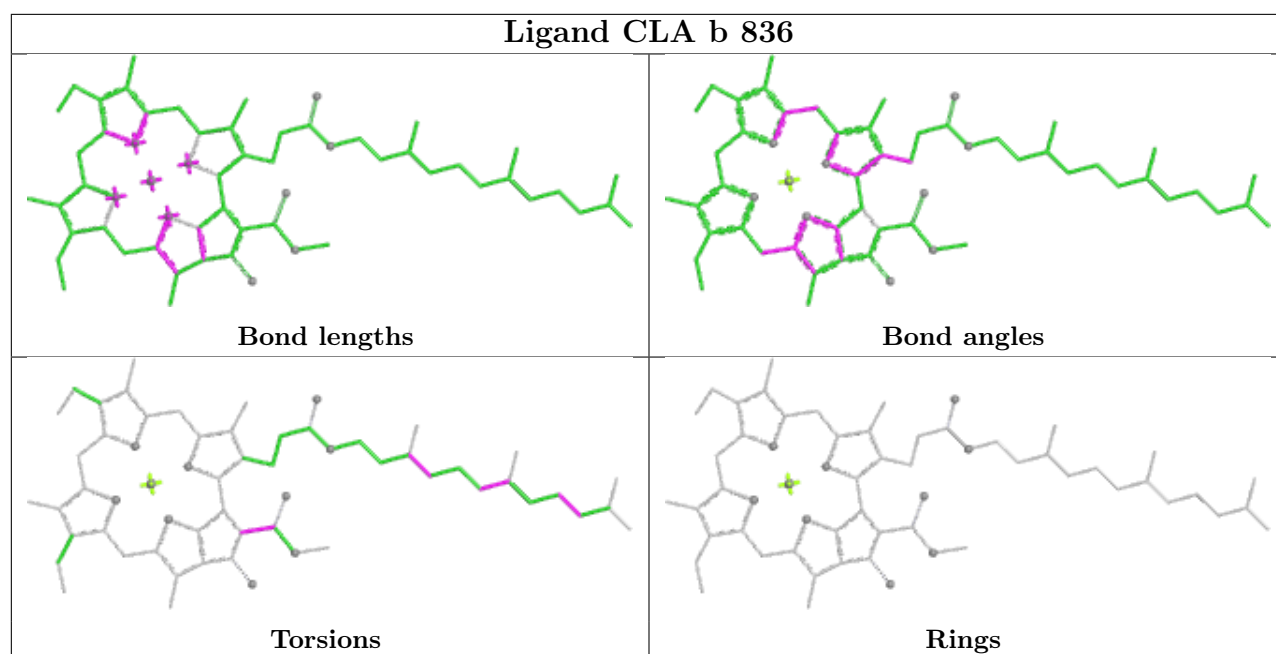


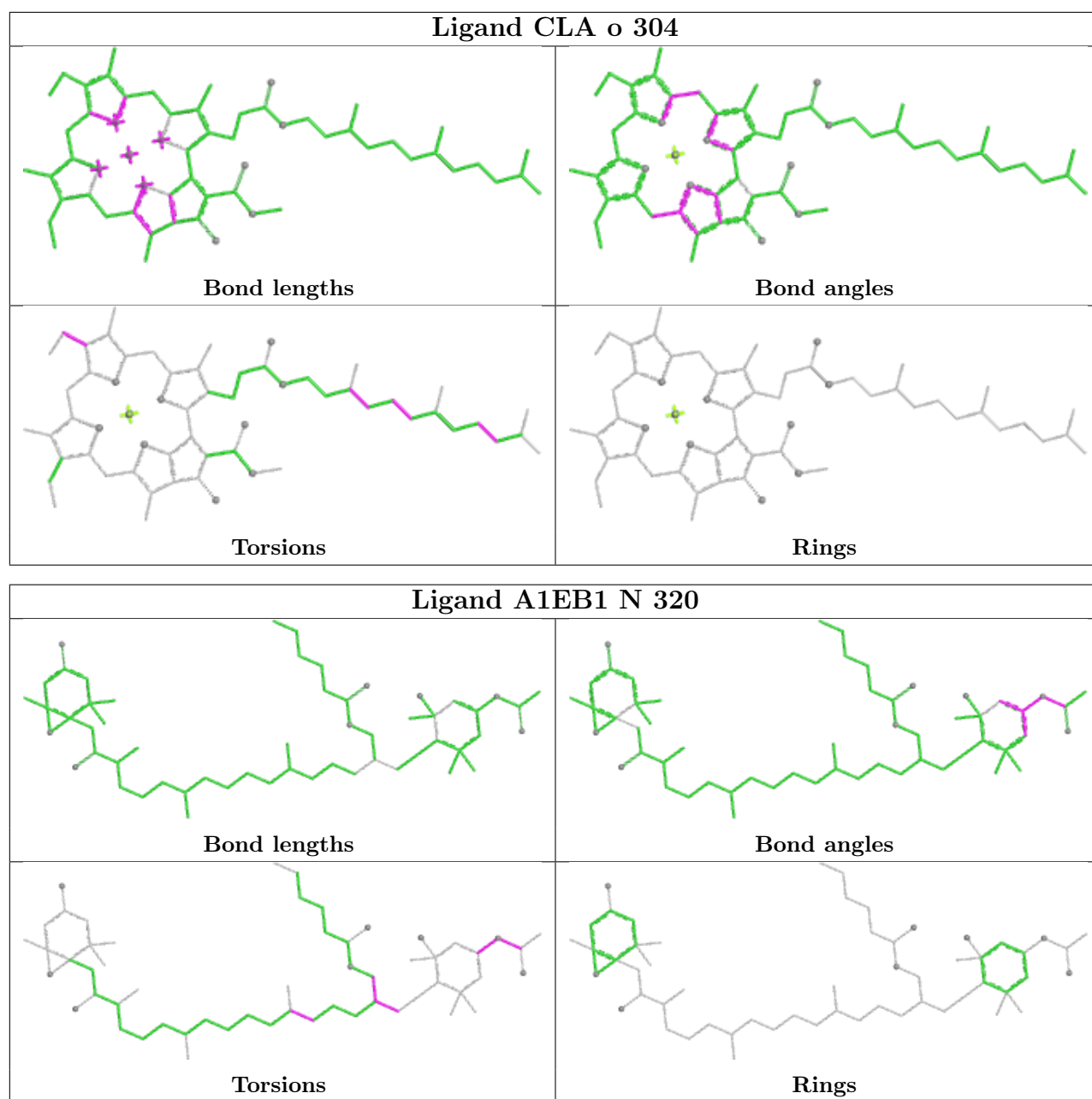
Torsions



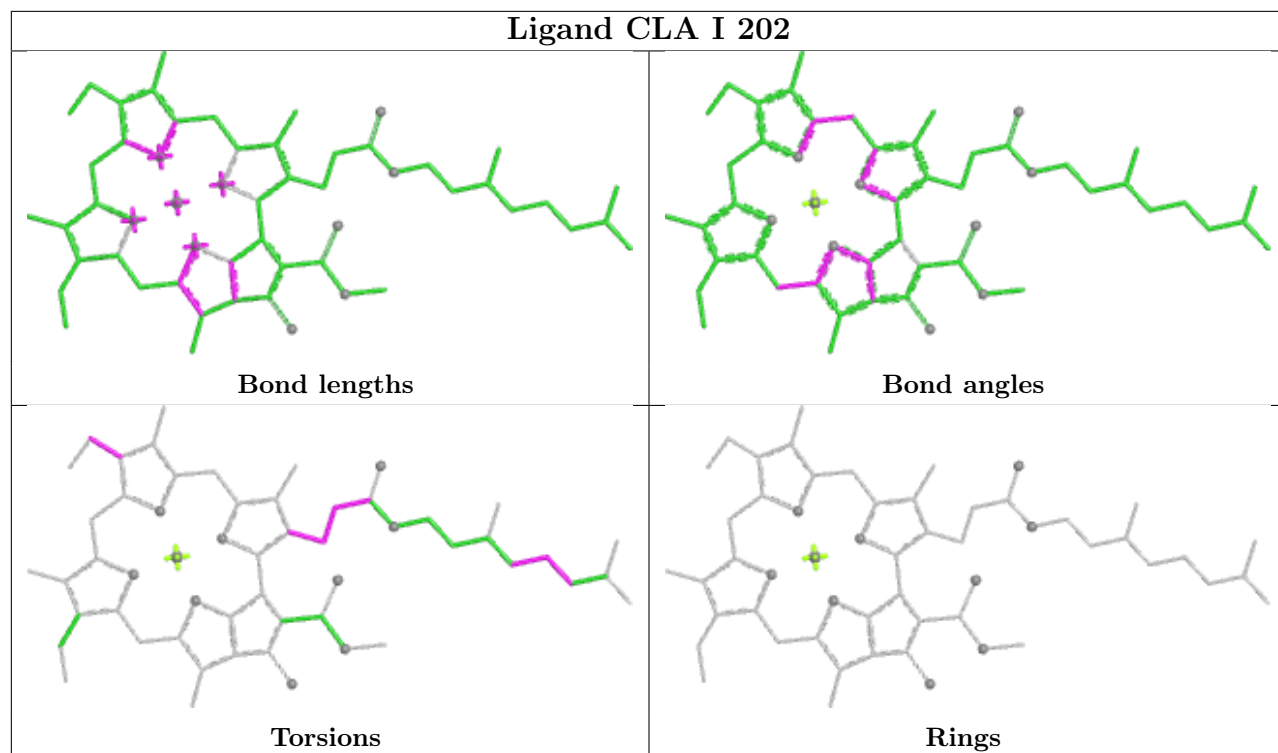
Rings



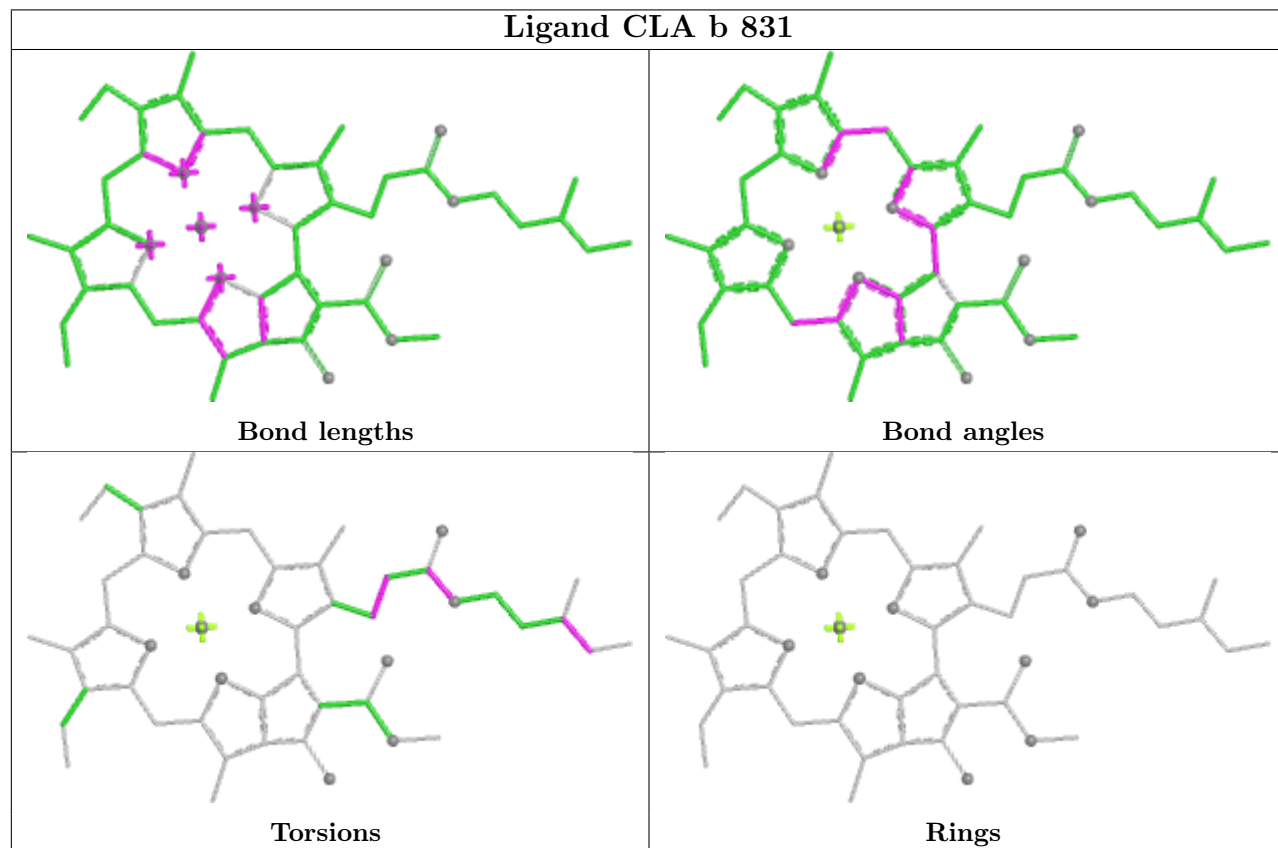


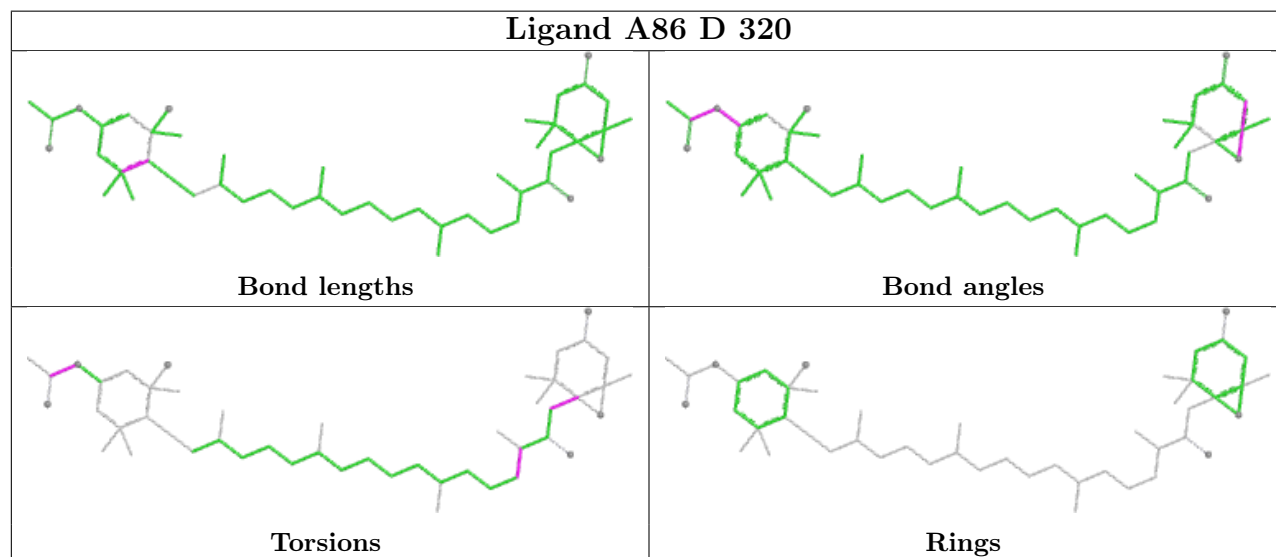
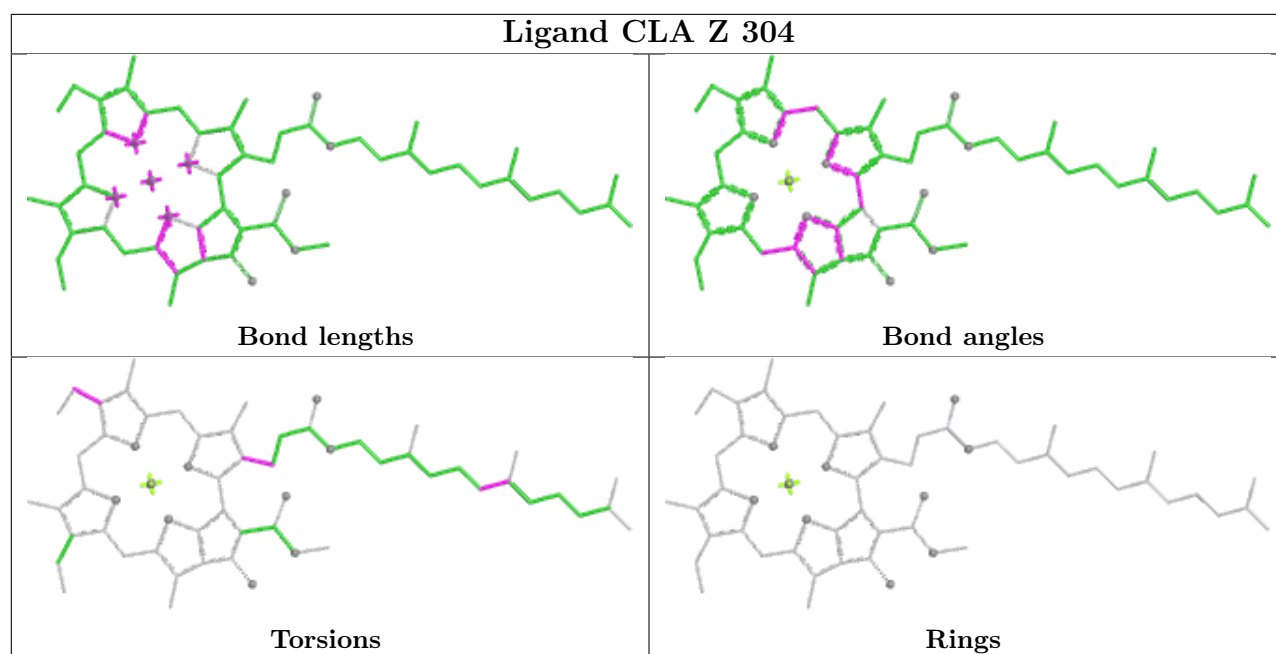


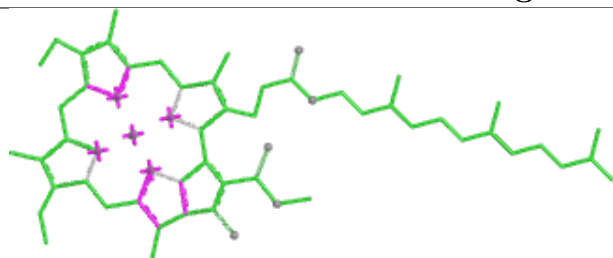
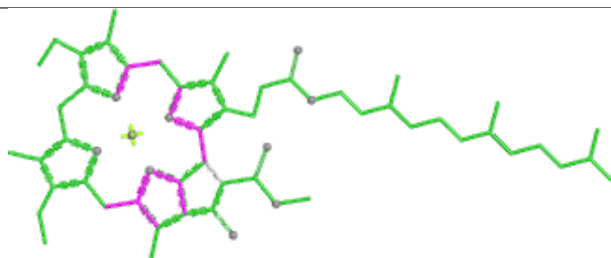
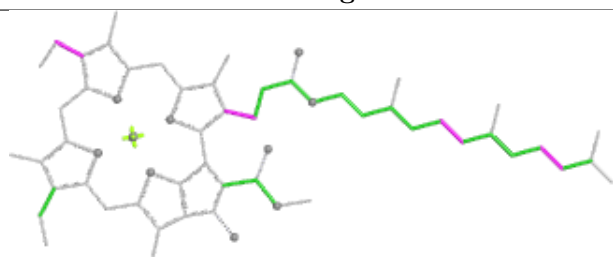
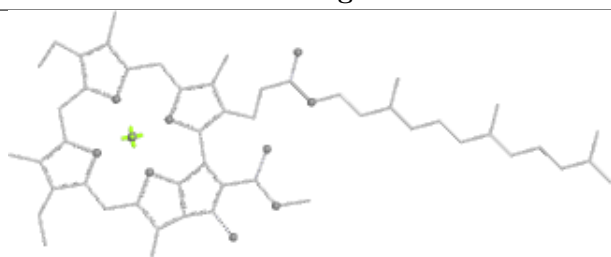
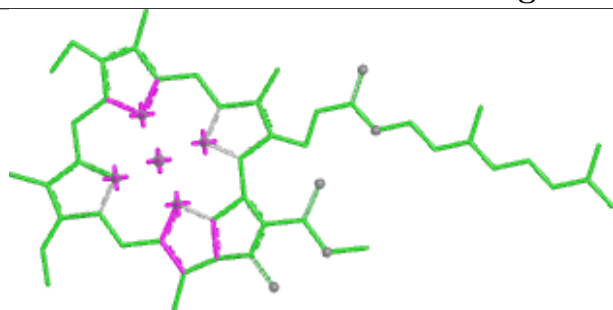
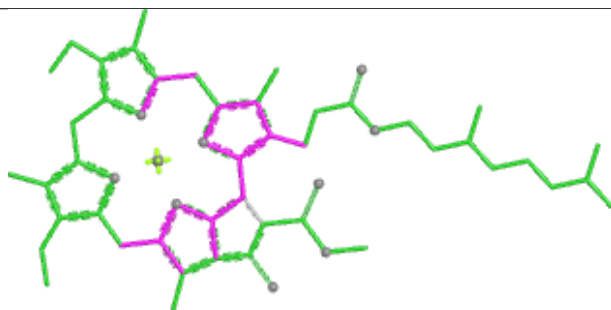
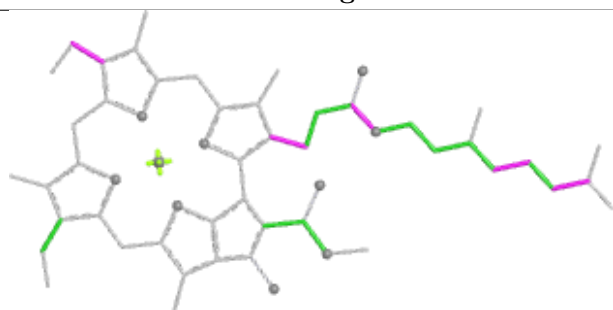
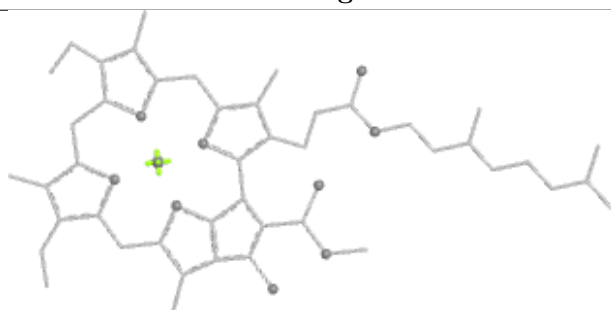
Ligand CLA I 202

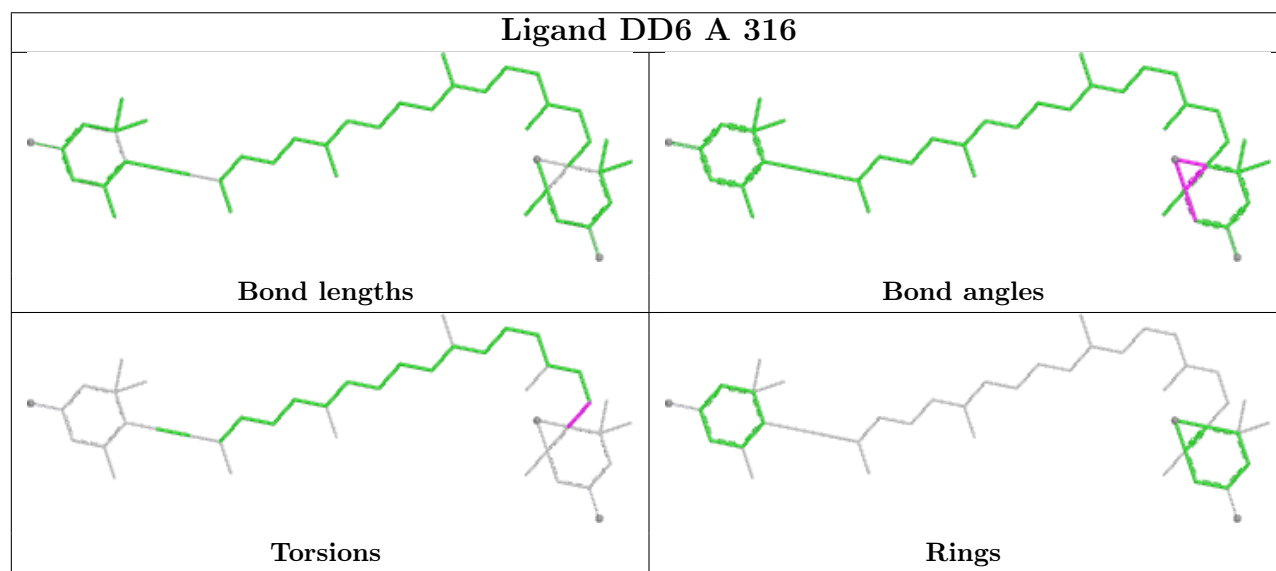
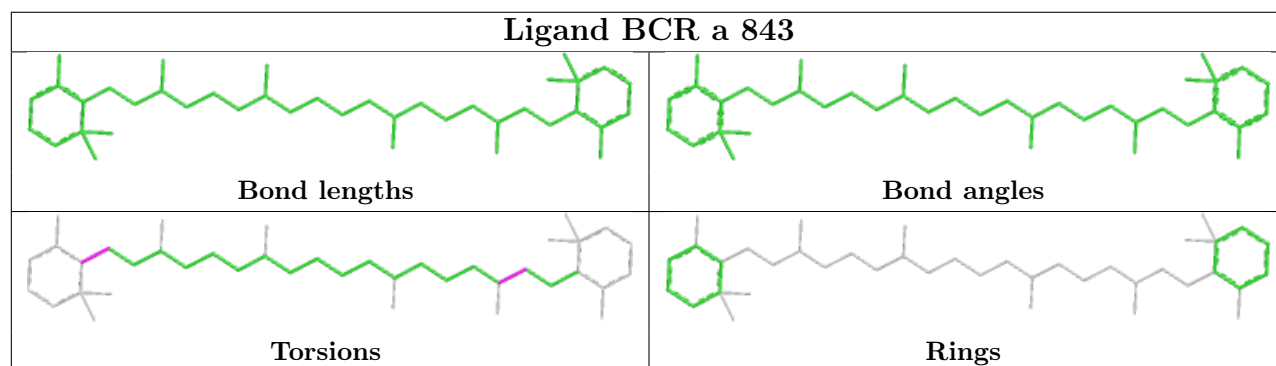
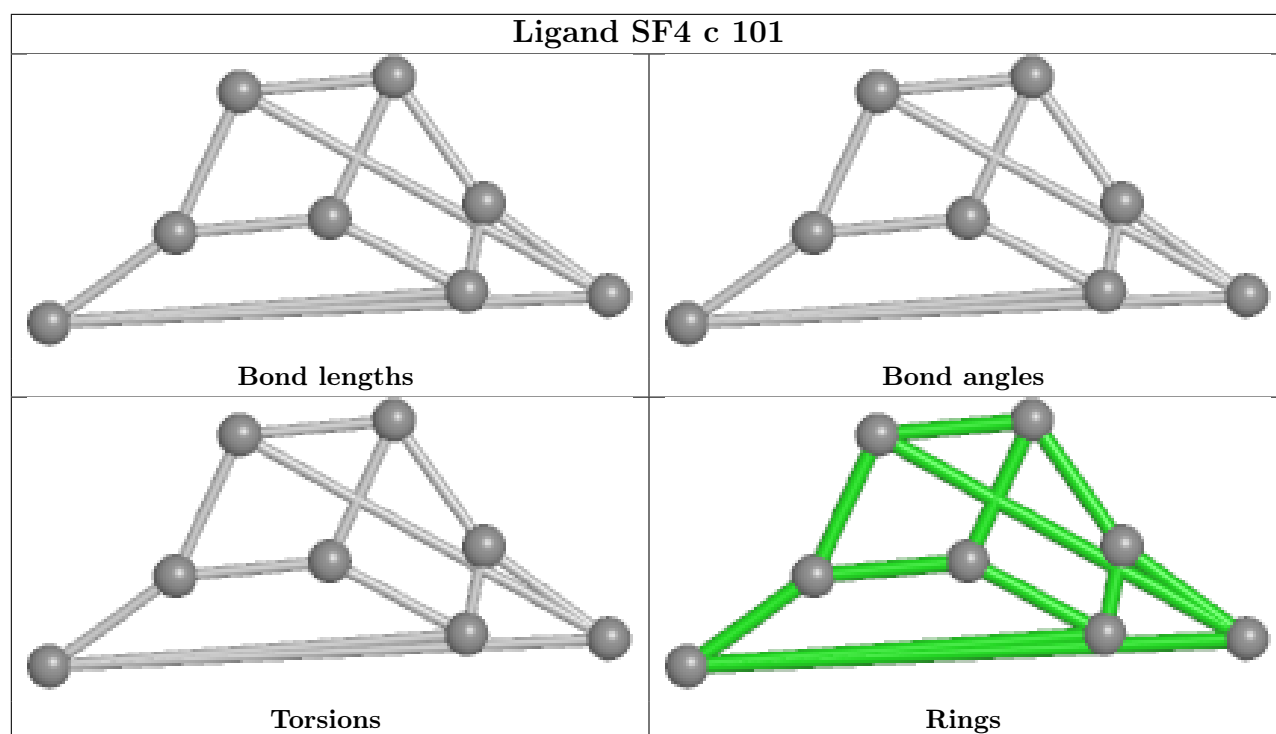


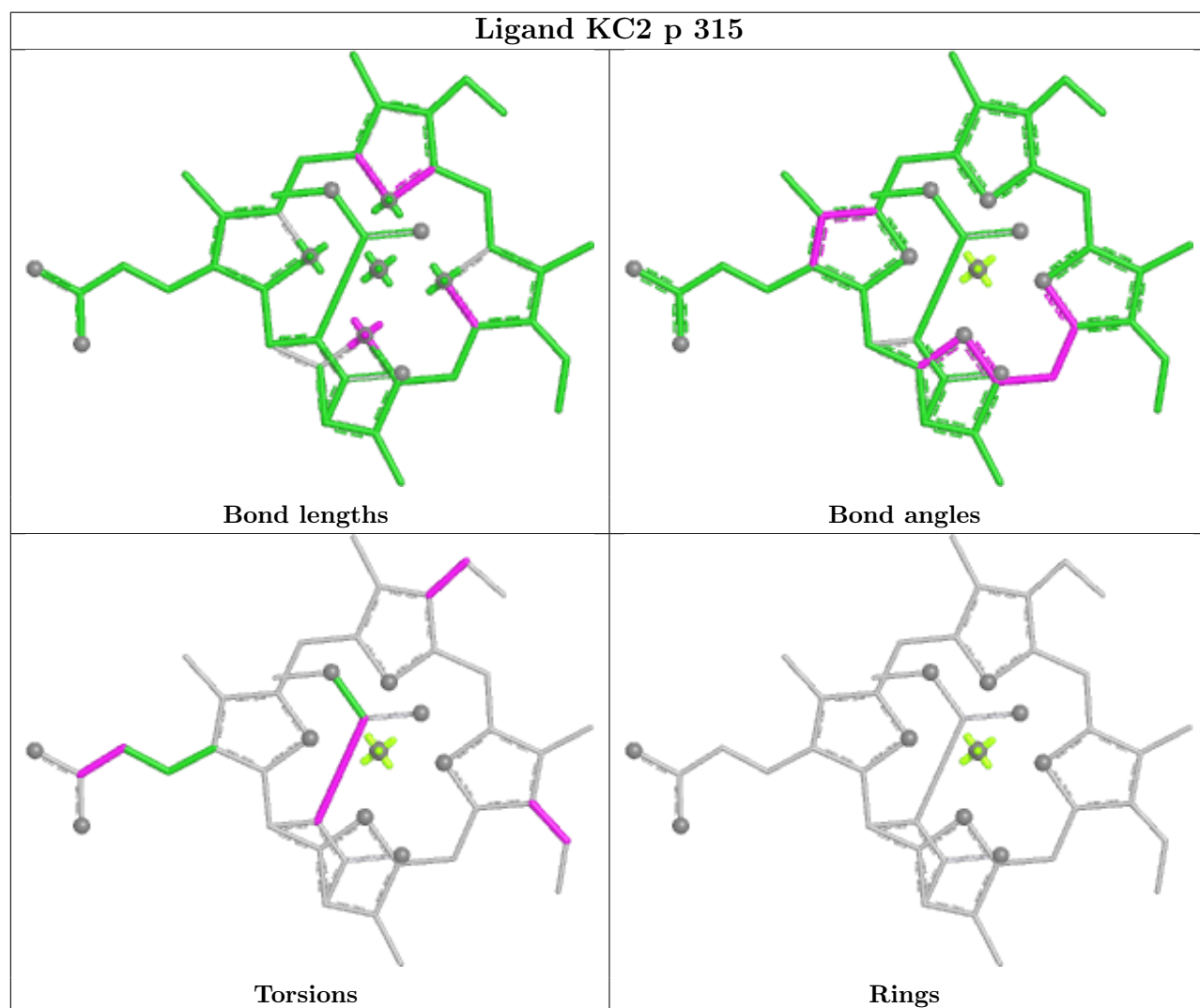
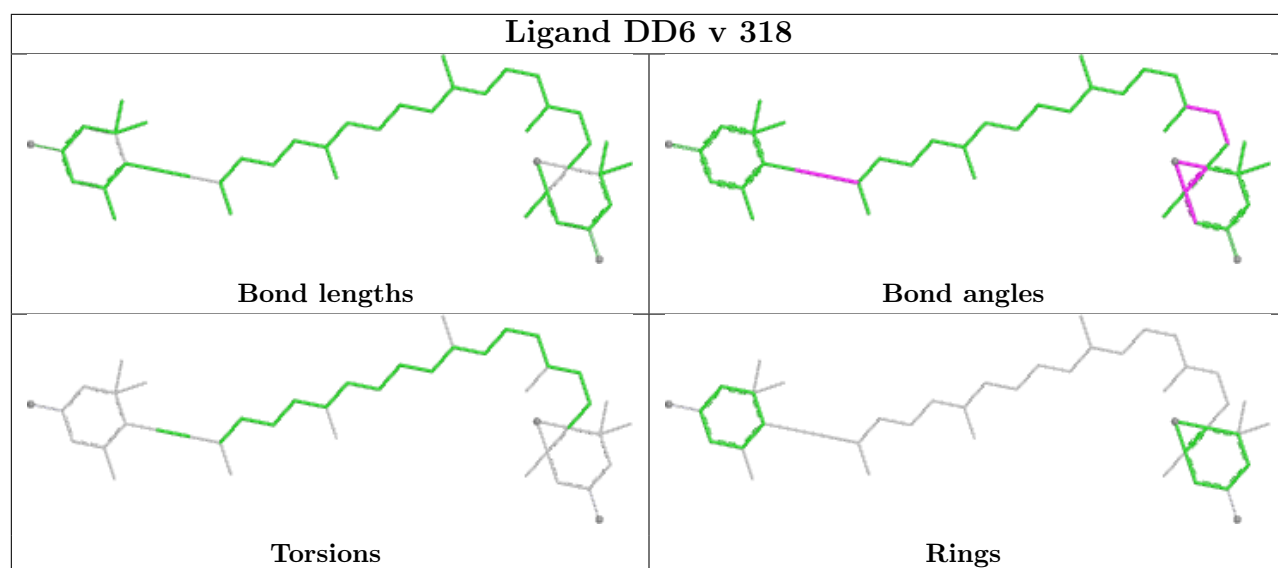
Ligand CLA b 831



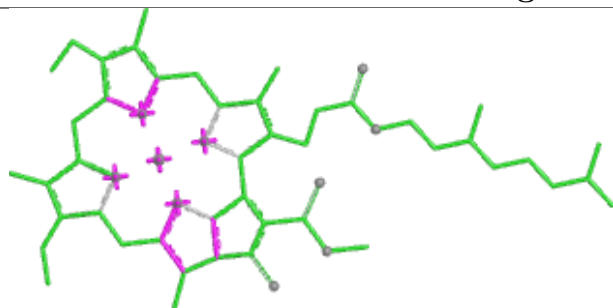


Ligand CLA E 303**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA o 310****Bond lengths****Bond angles****Torsions****Rings**

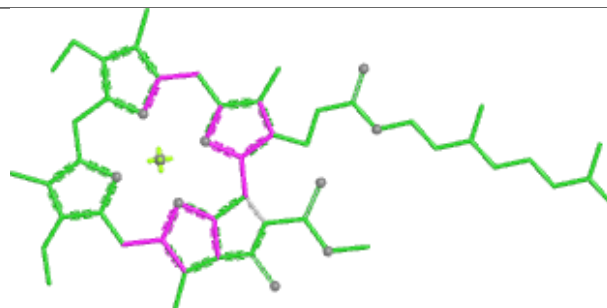




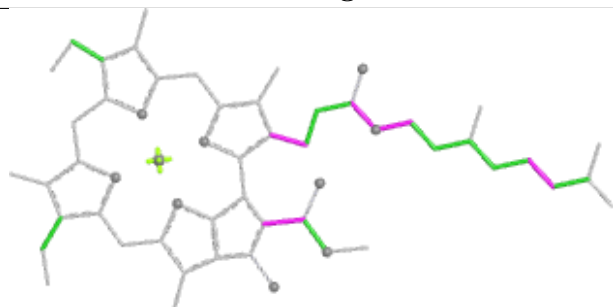
Ligand CLA u 307



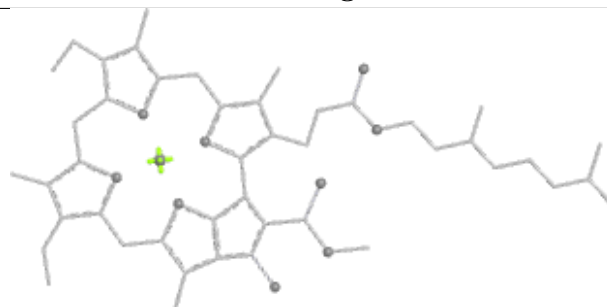
Bond lengths



Bond angles

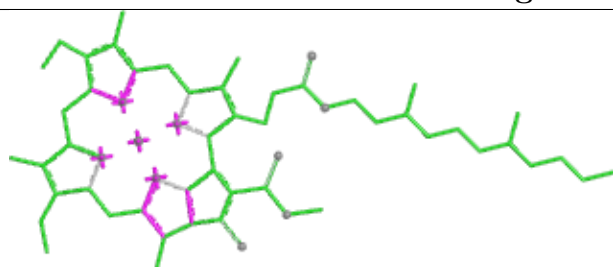


Torsions

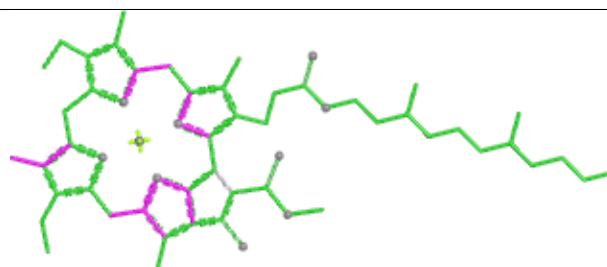


Rings

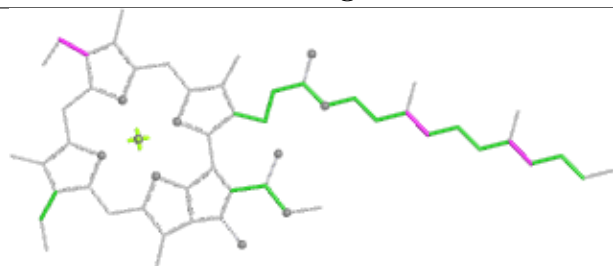
Ligand CLA E 308



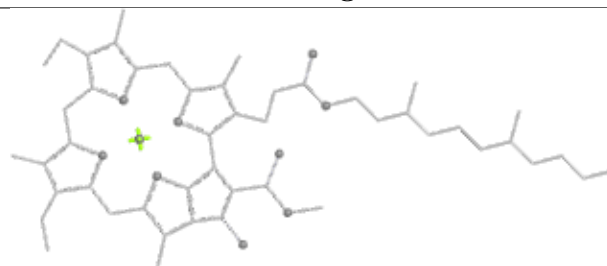
Bond lengths



Bond angles

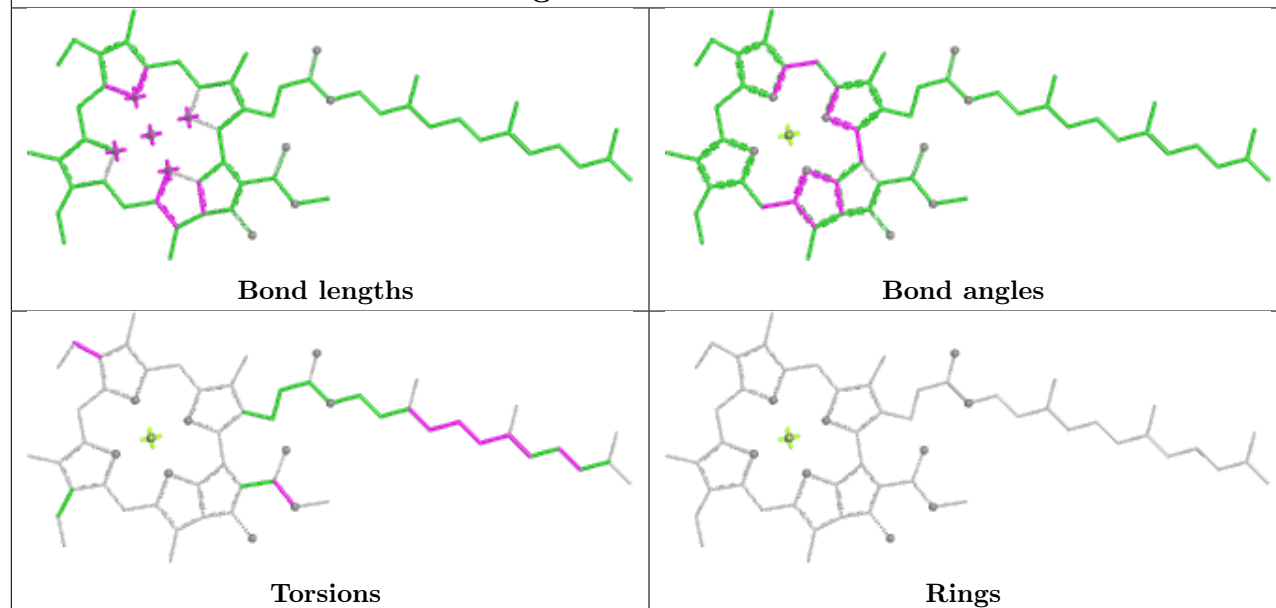


Torsions

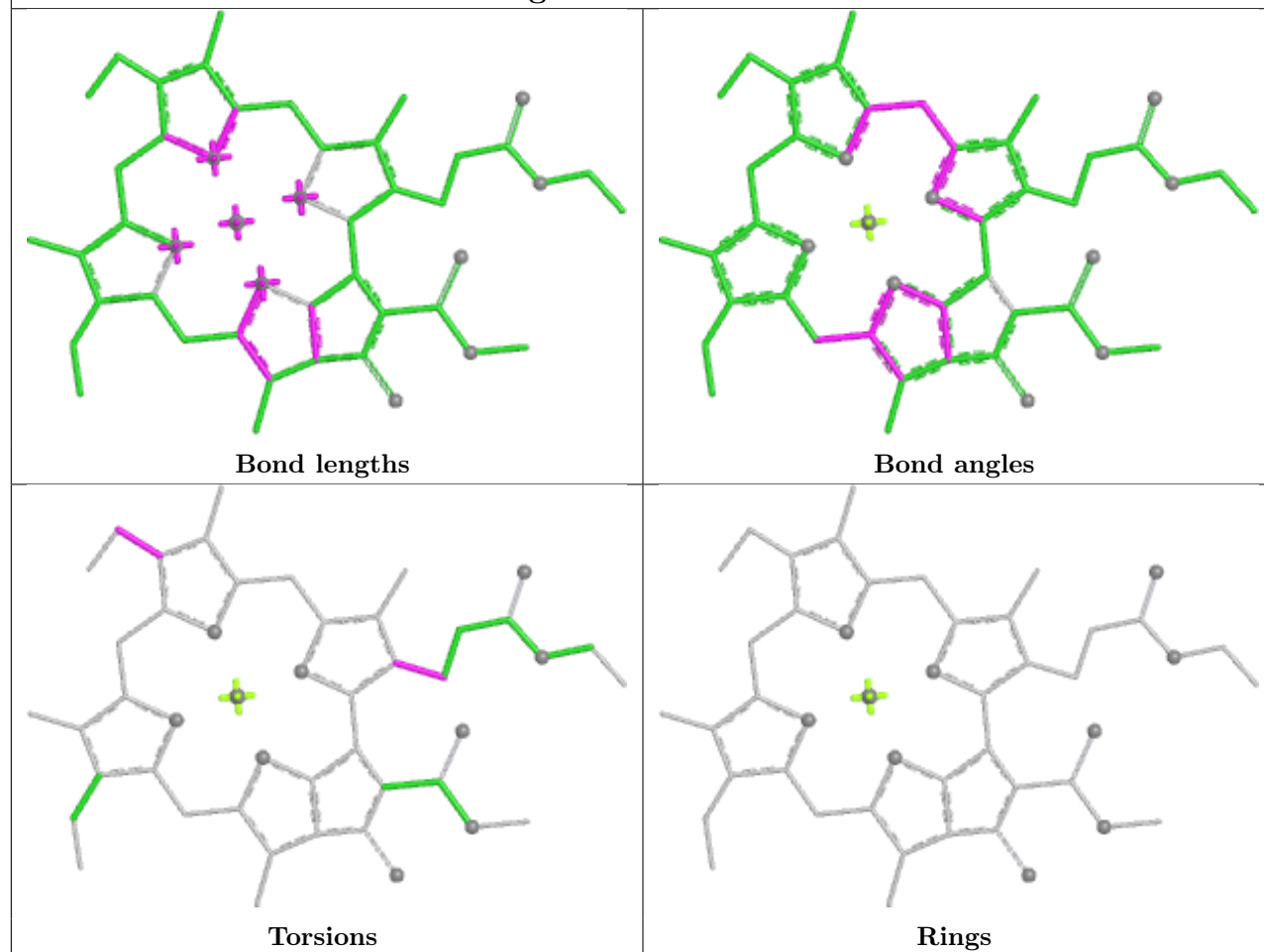


Rings

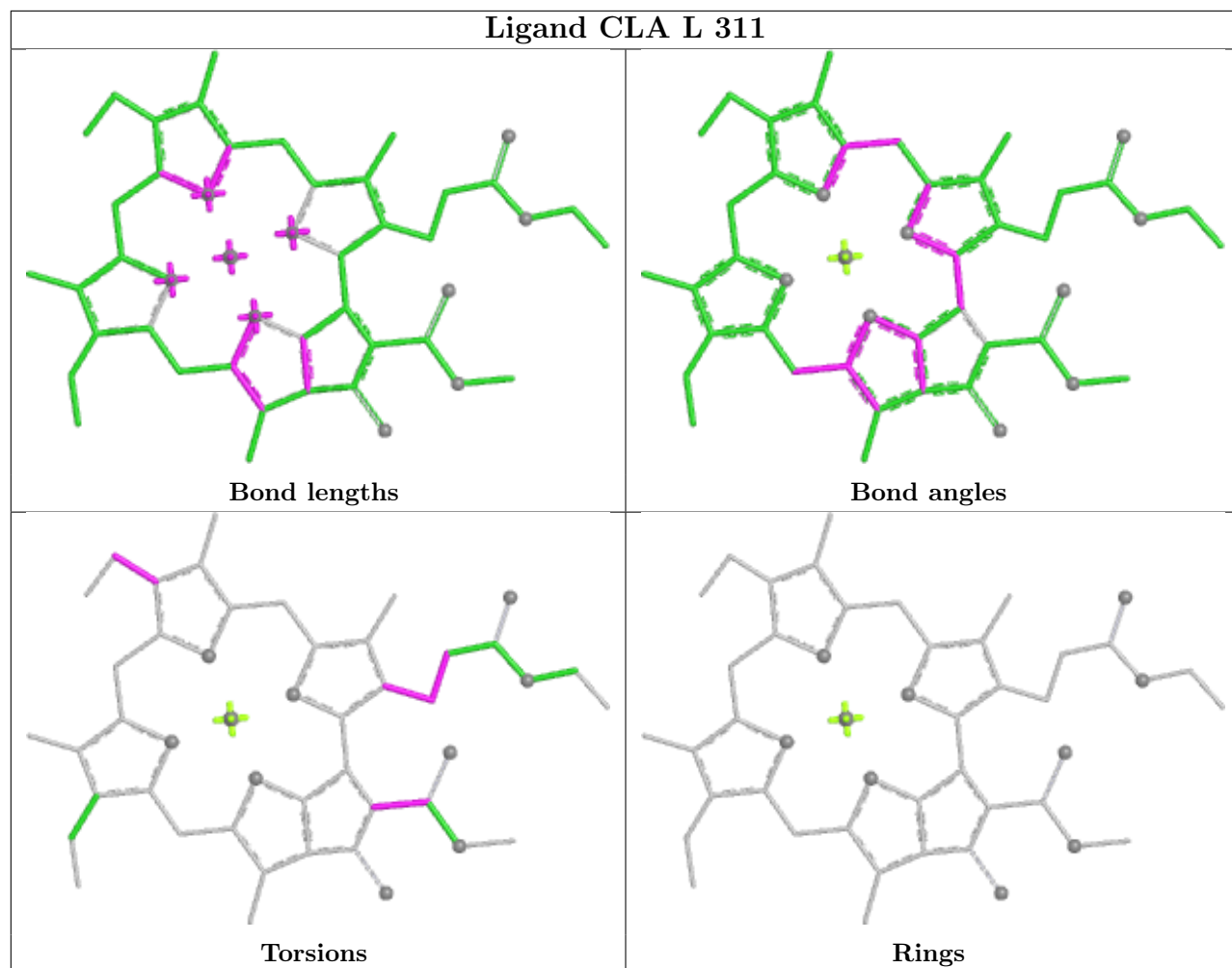
Ligand CLA P 308

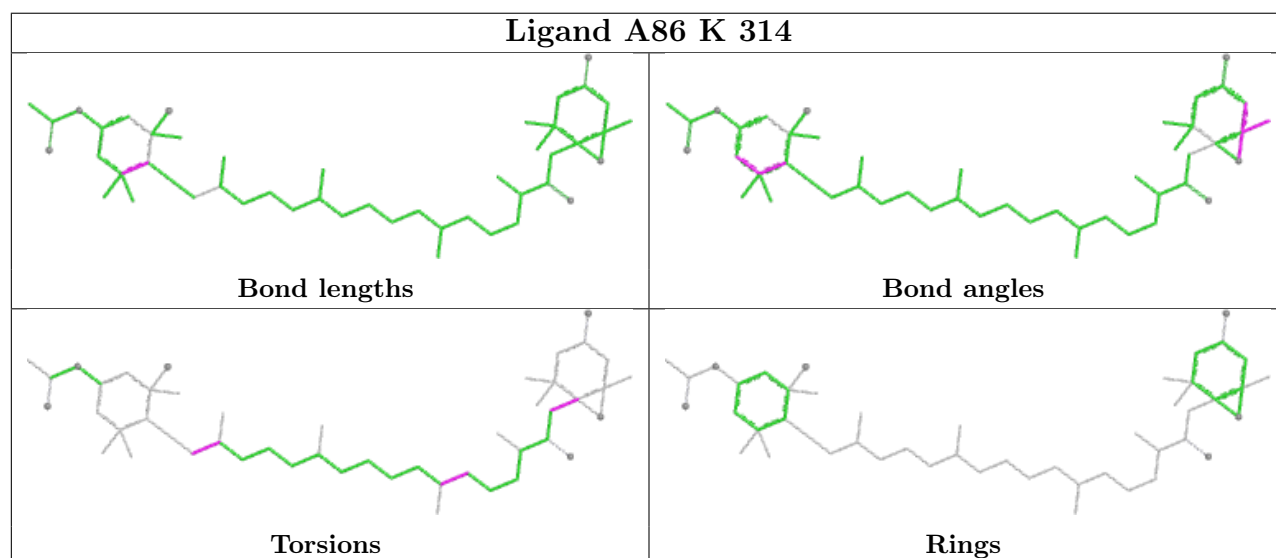
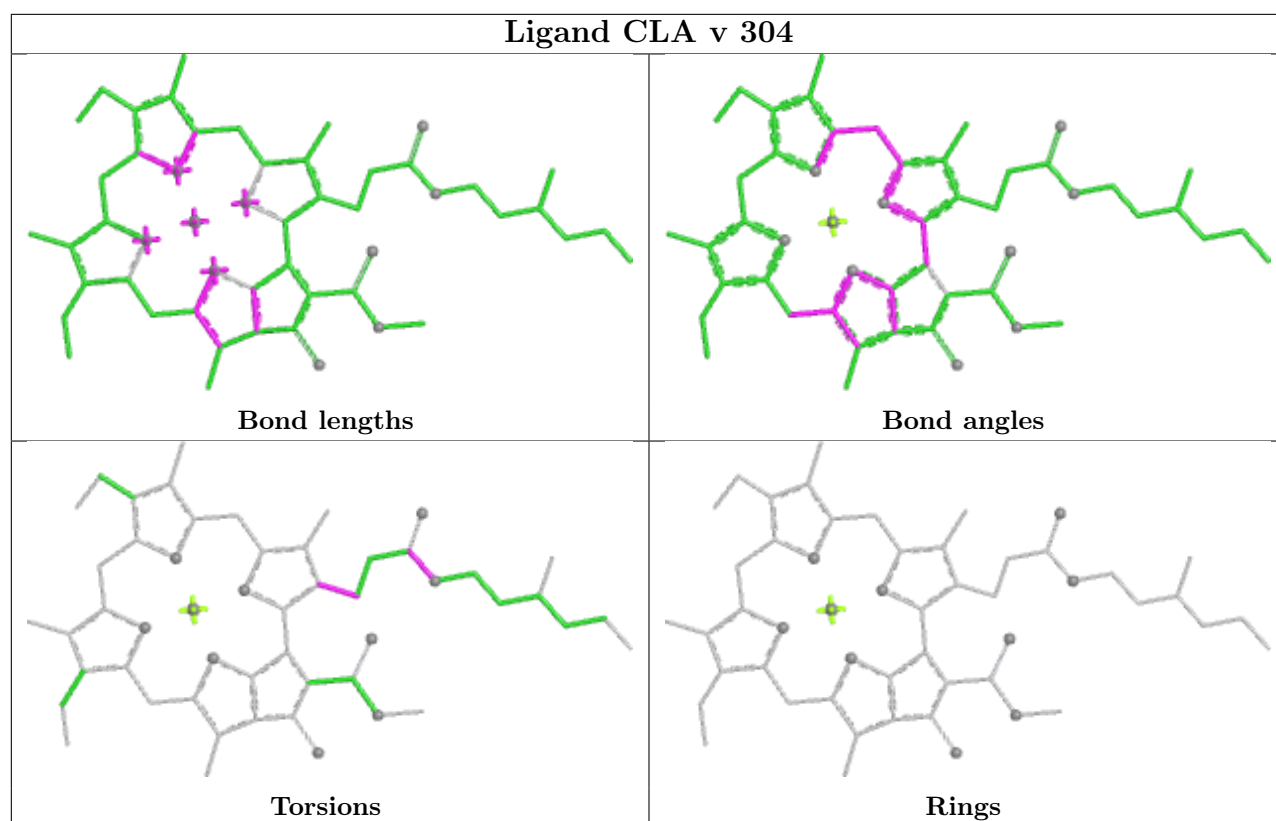


Ligand CLA F 305

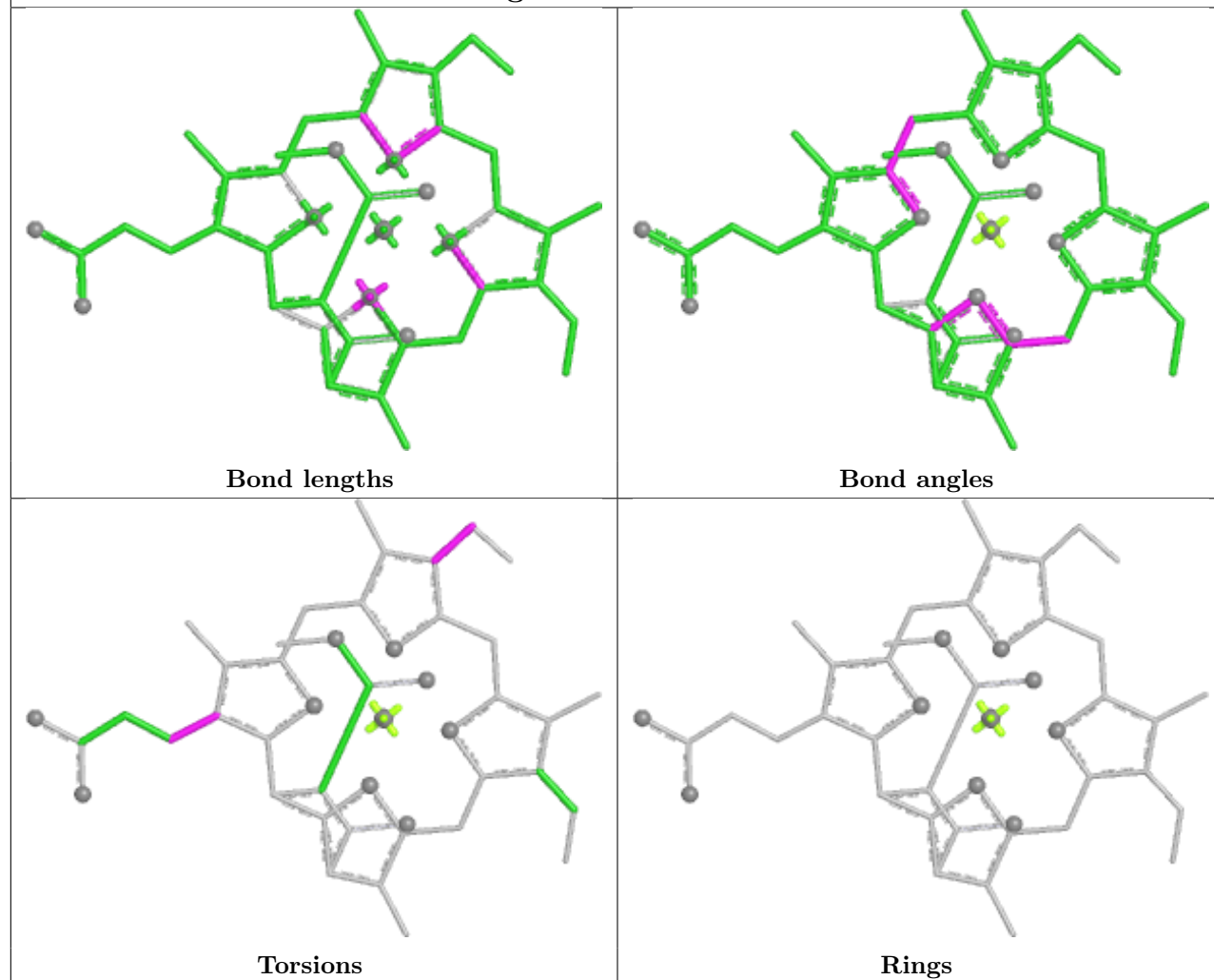


Ligand CLA L 311

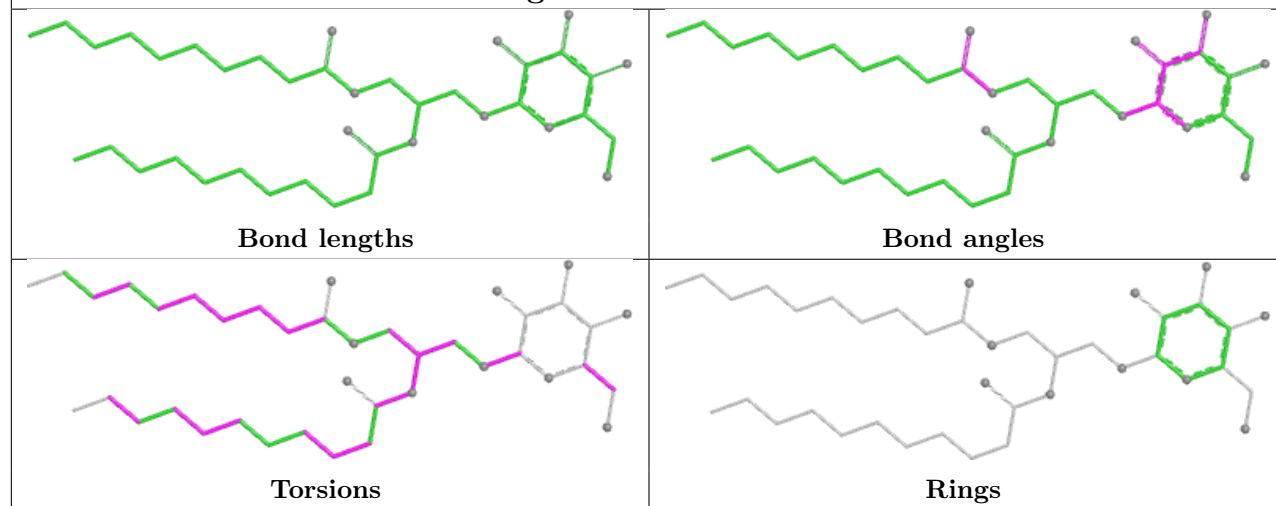


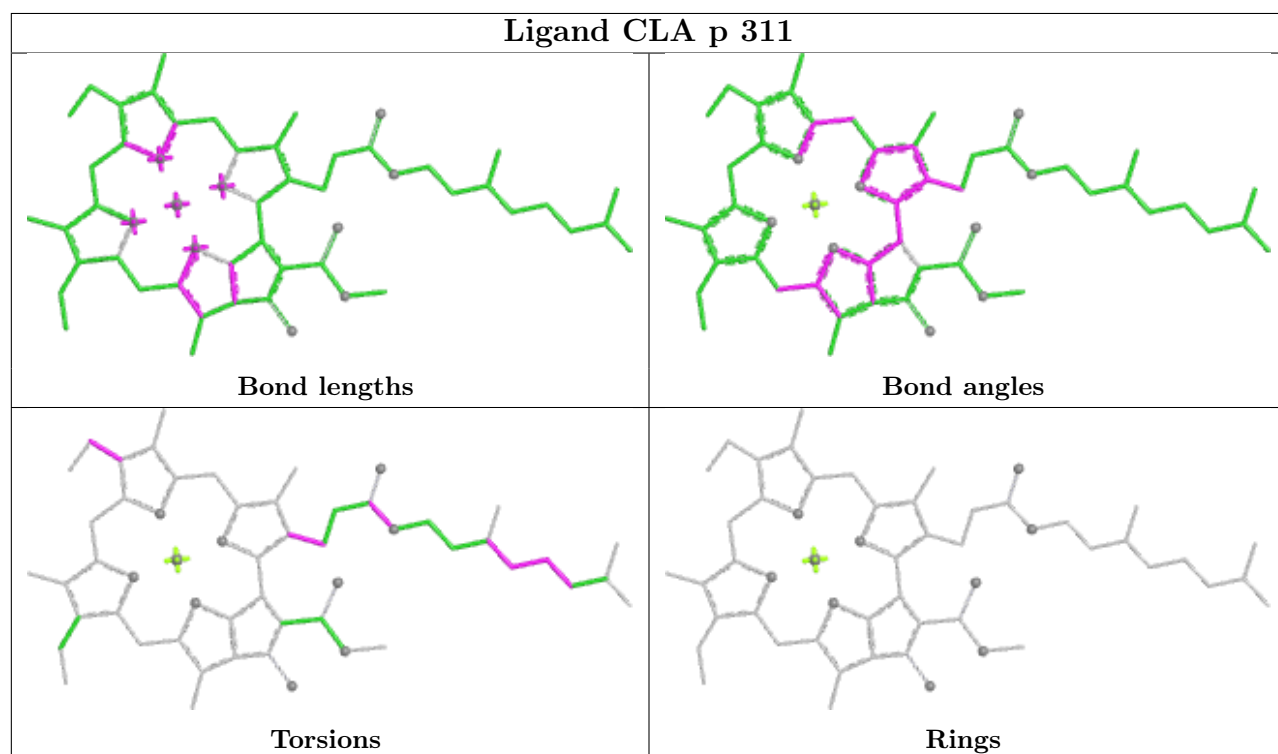
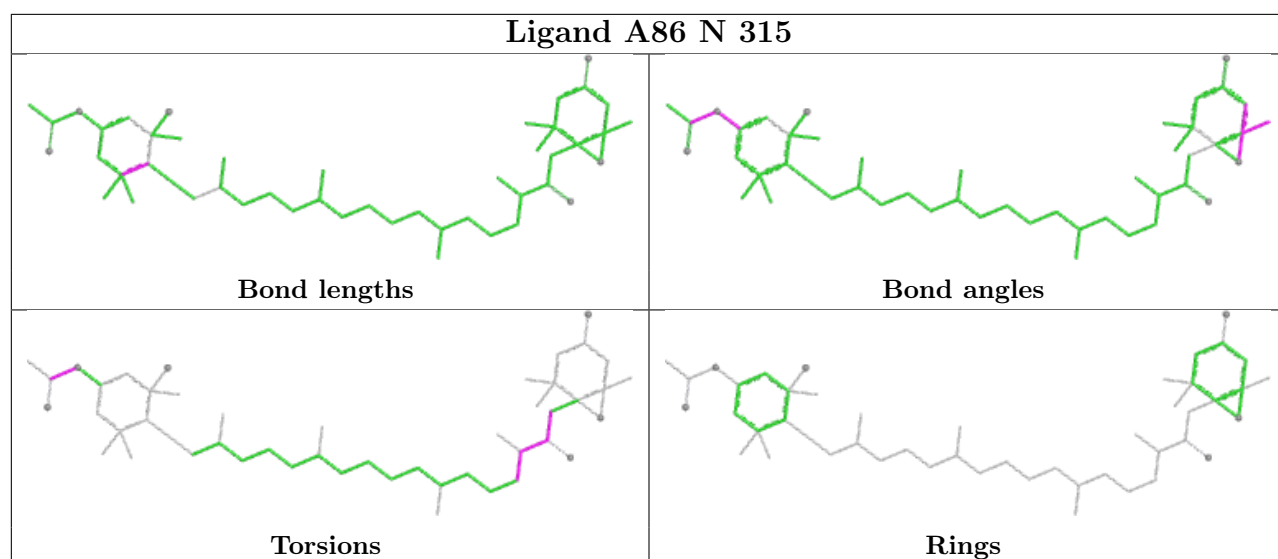


Ligand KC2 G 208

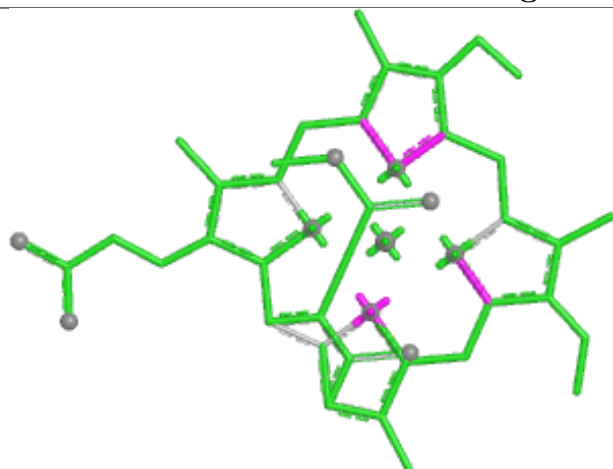


Ligand LMG A 317

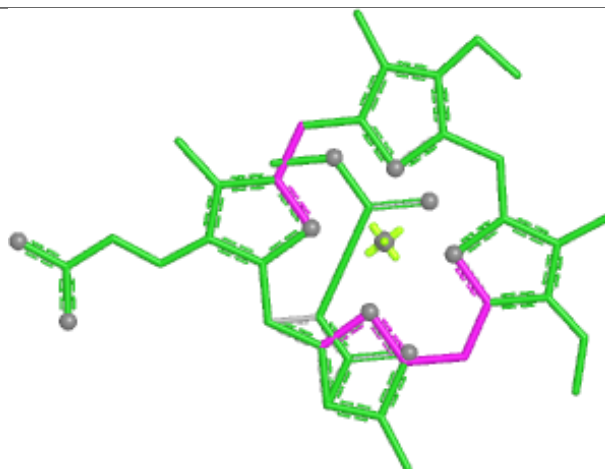




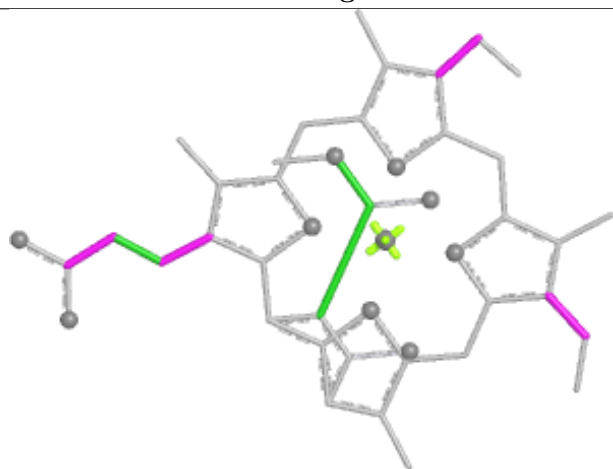
Ligand KC2 o 308



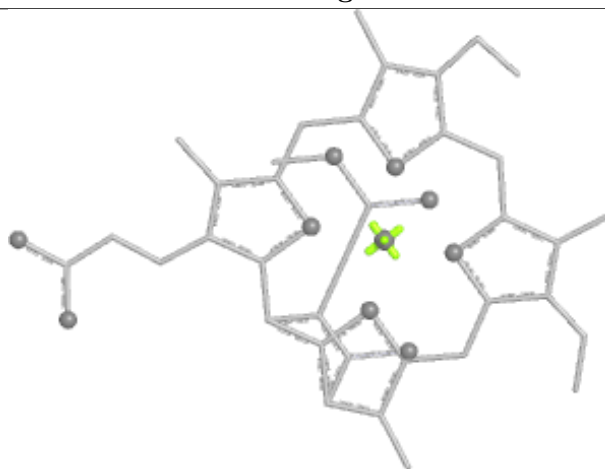
Bond lengths



Bond angles

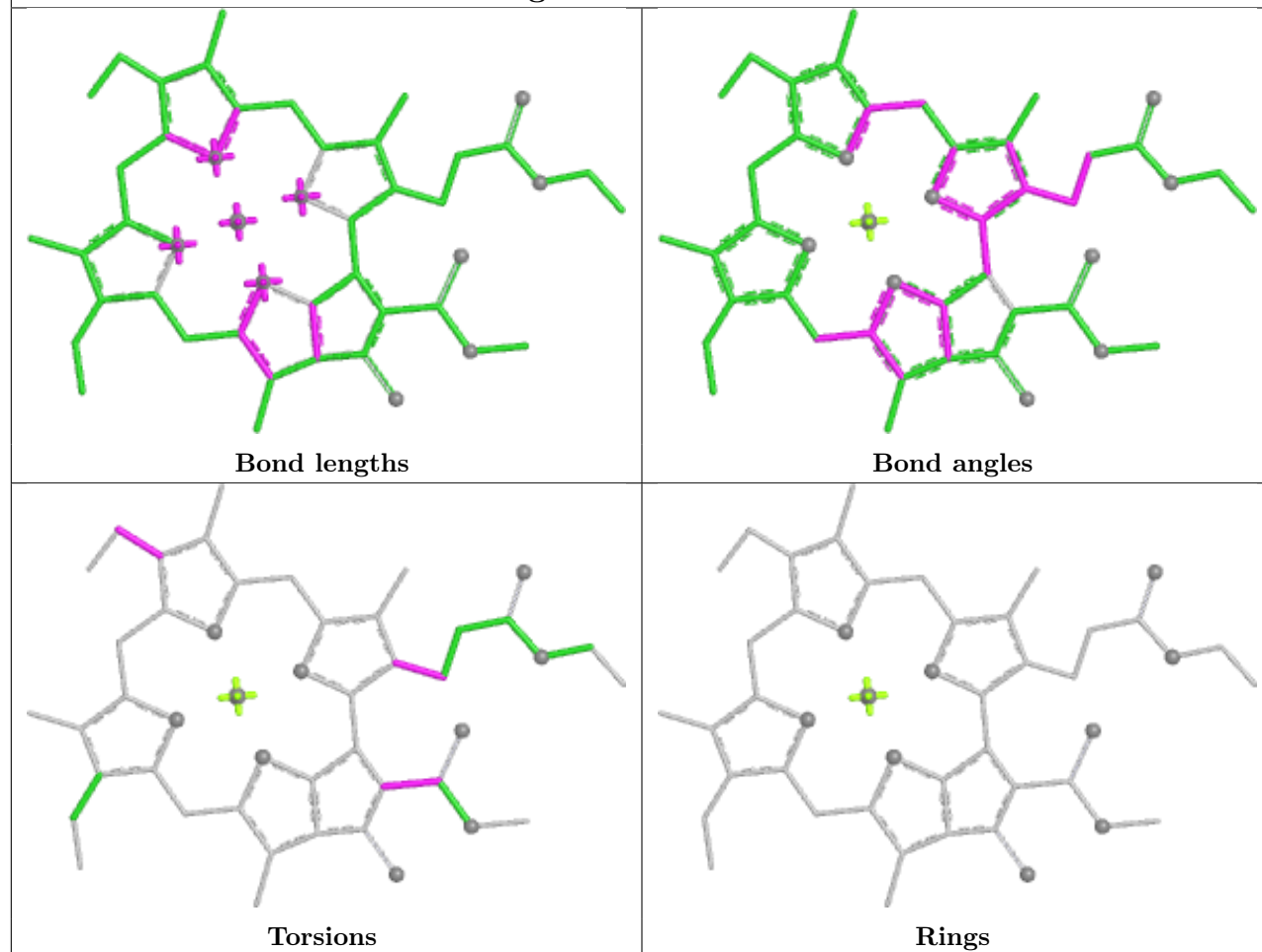


Torsions

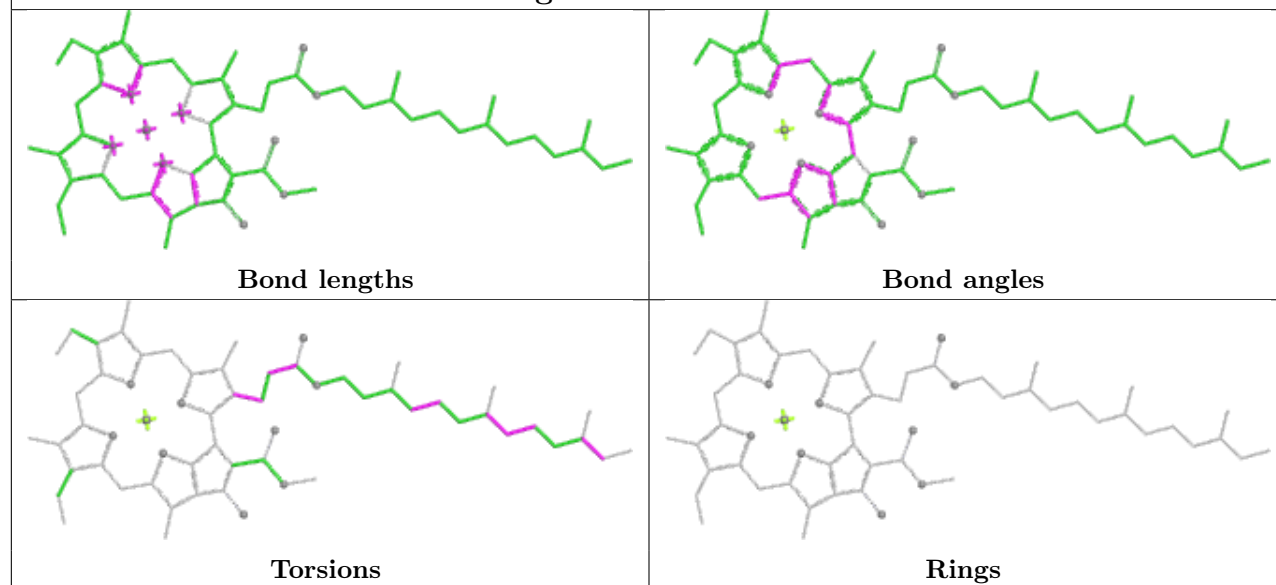


Rings

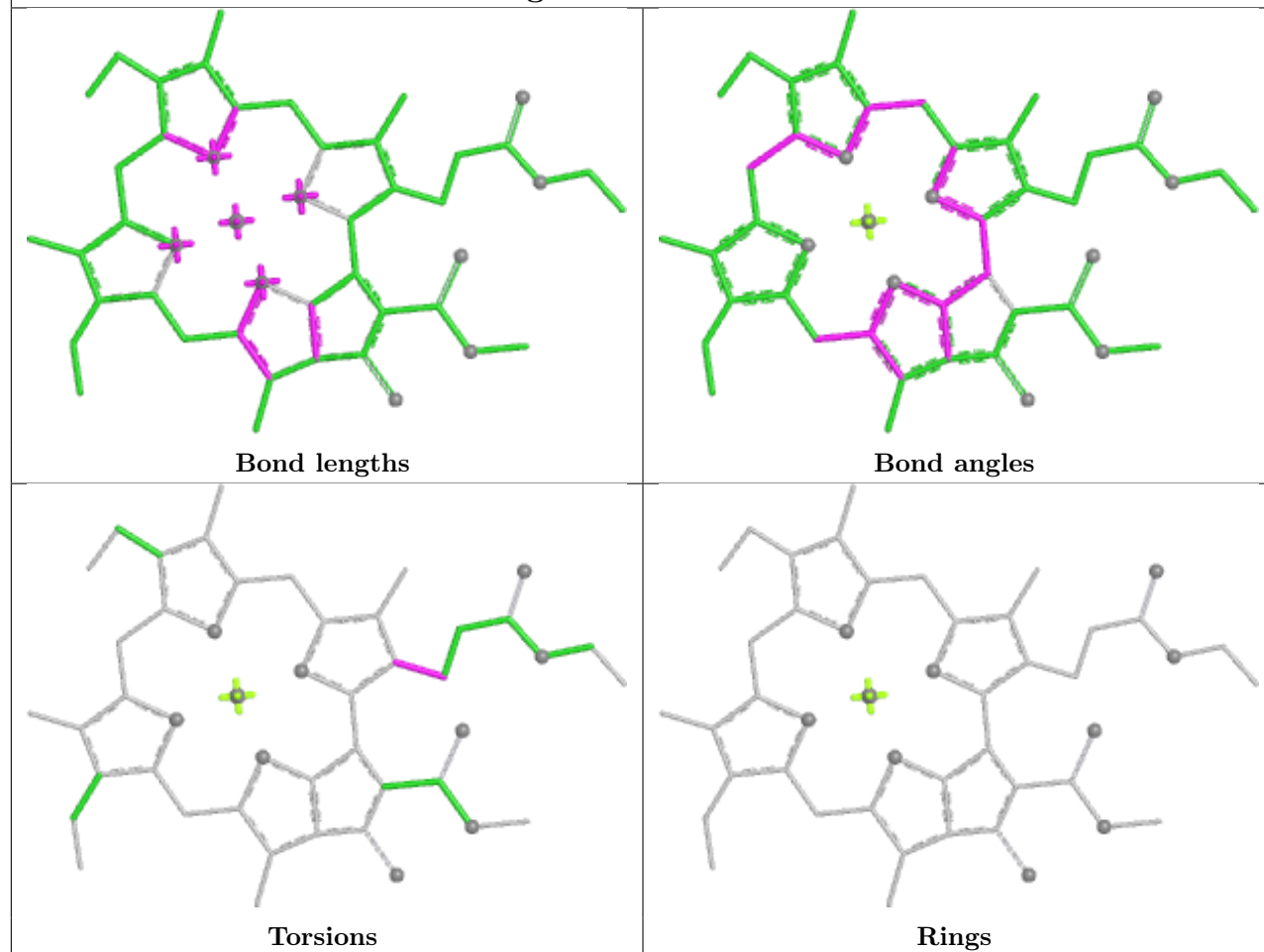
Ligand CLA Z 313



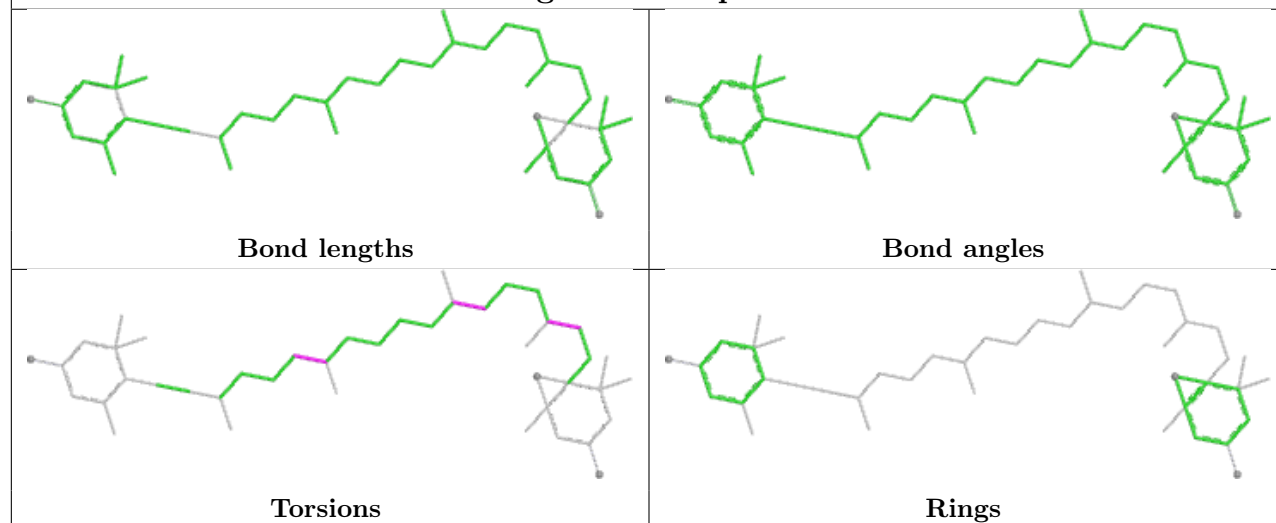
Ligand CLA b 842

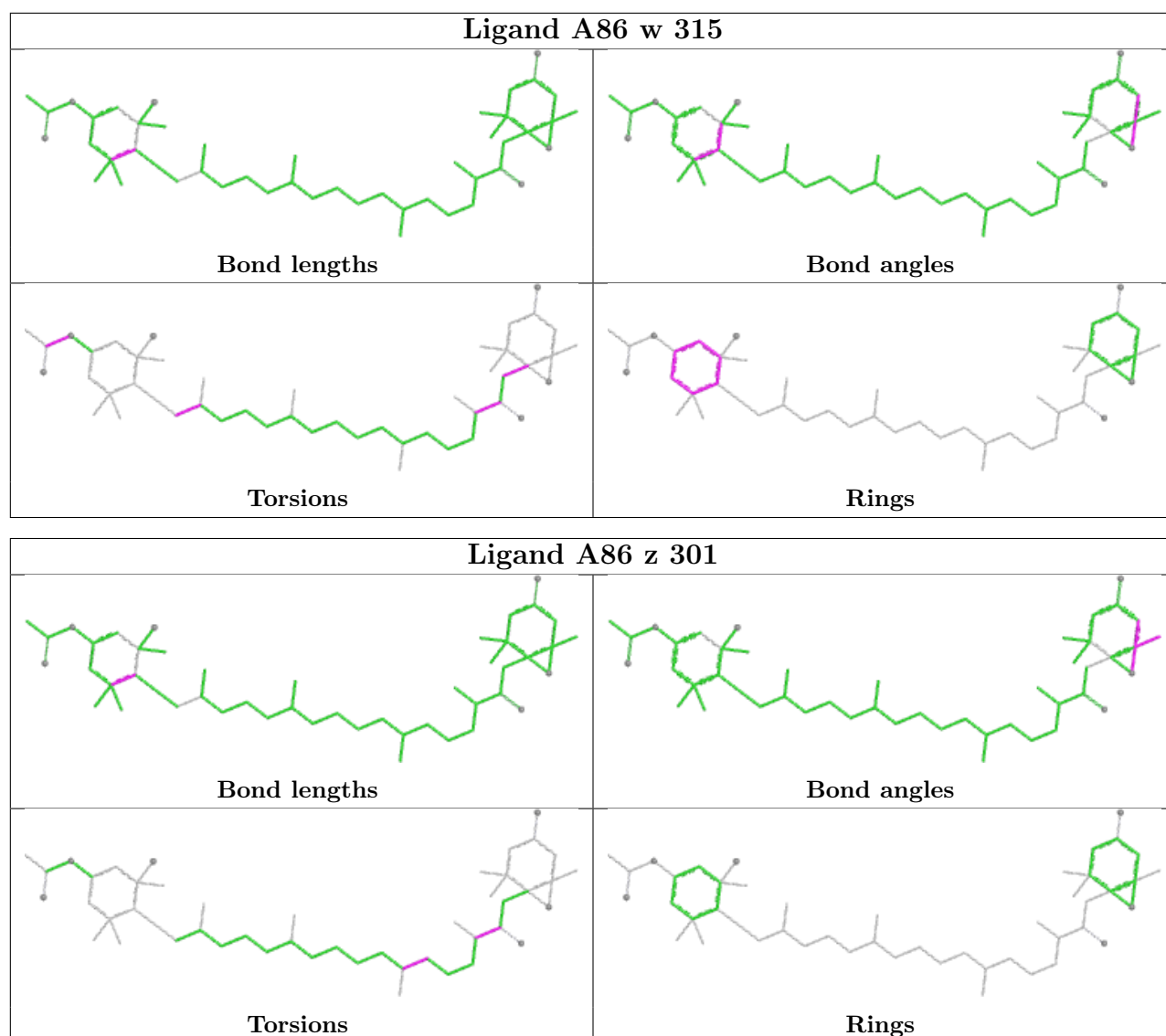


Ligand CLA X 313

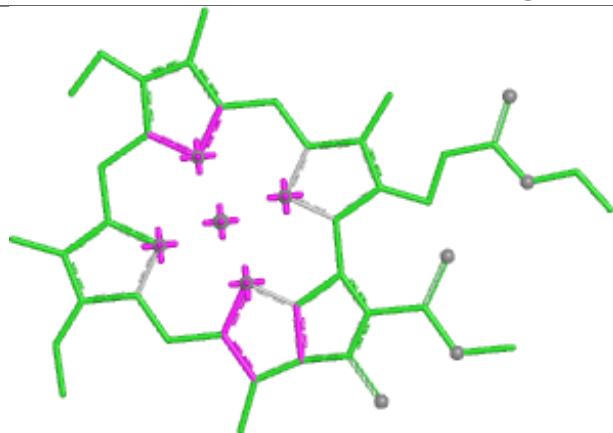


Ligand DD6 q 320

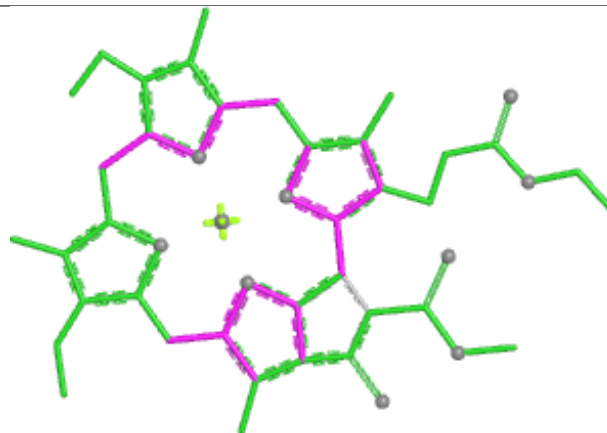




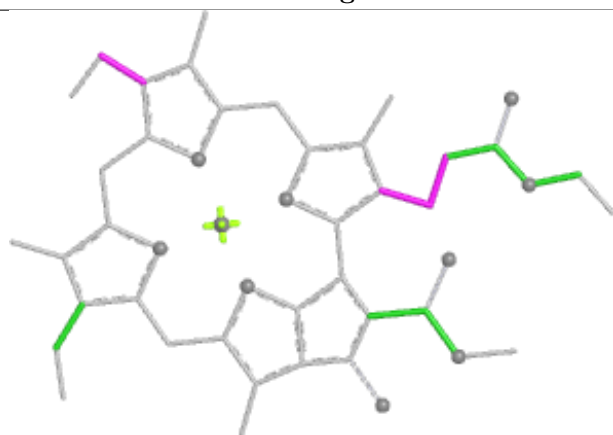
Ligand CLA z 314



Bond lengths



Bond angles

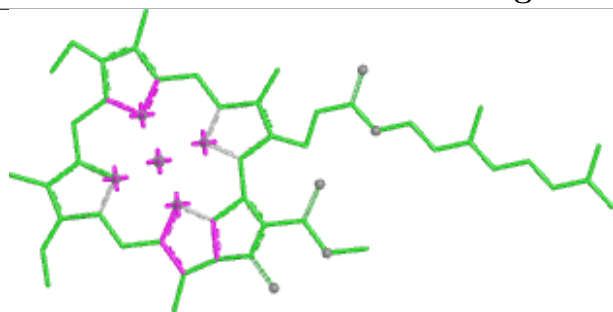


Torsions

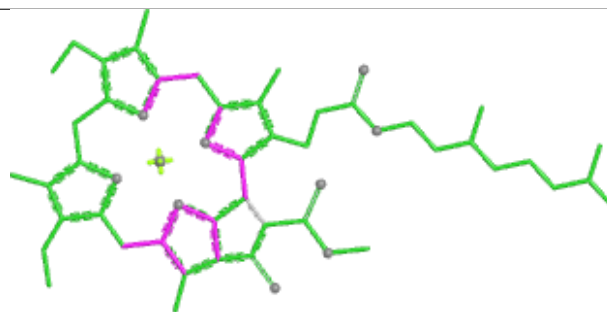


Rings

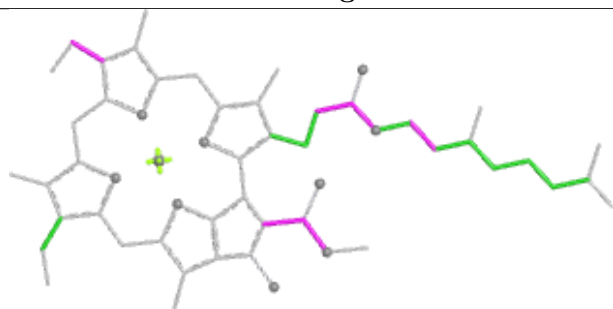
Ligand CLA w 309



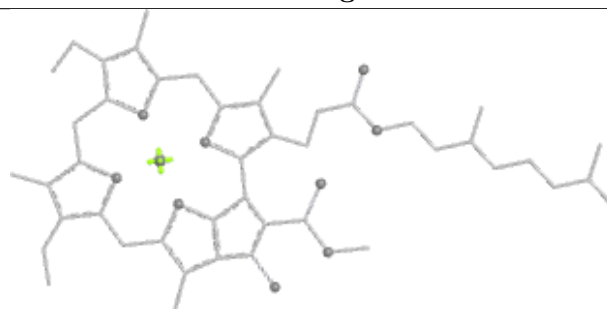
Bond lengths



Bond angles

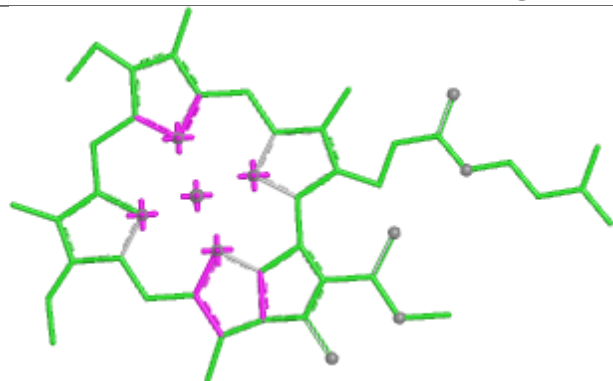


Torsions

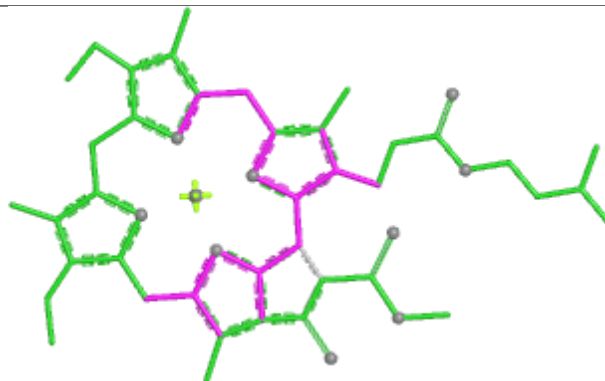


Rings

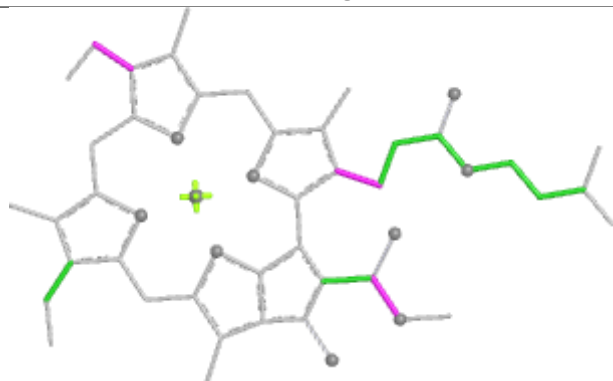
Ligand CLA N 310



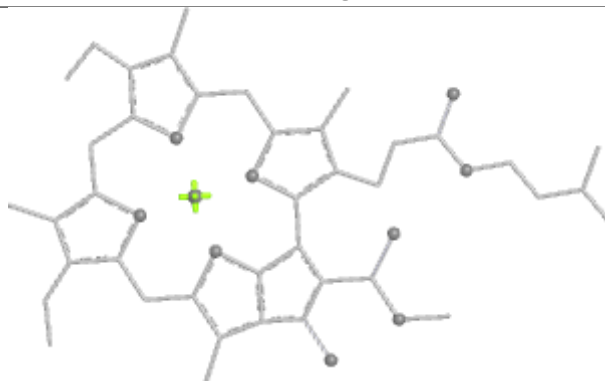
Bond lengths



Bond angles

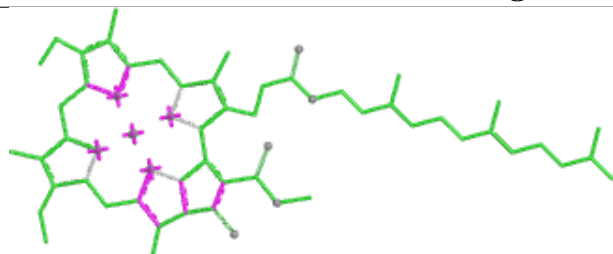


Torsions

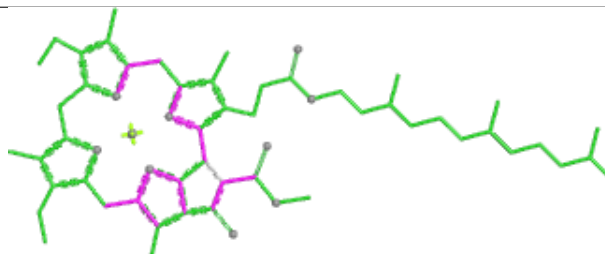


Rings

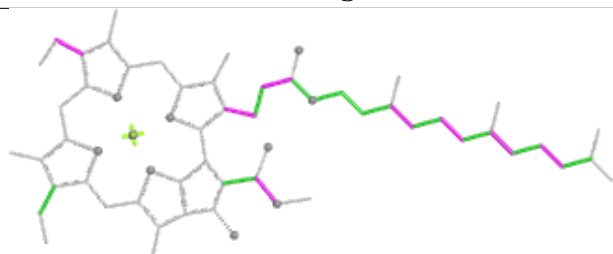
Ligand CLA W 306



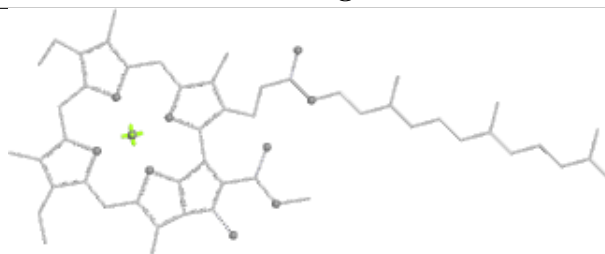
Bond lengths



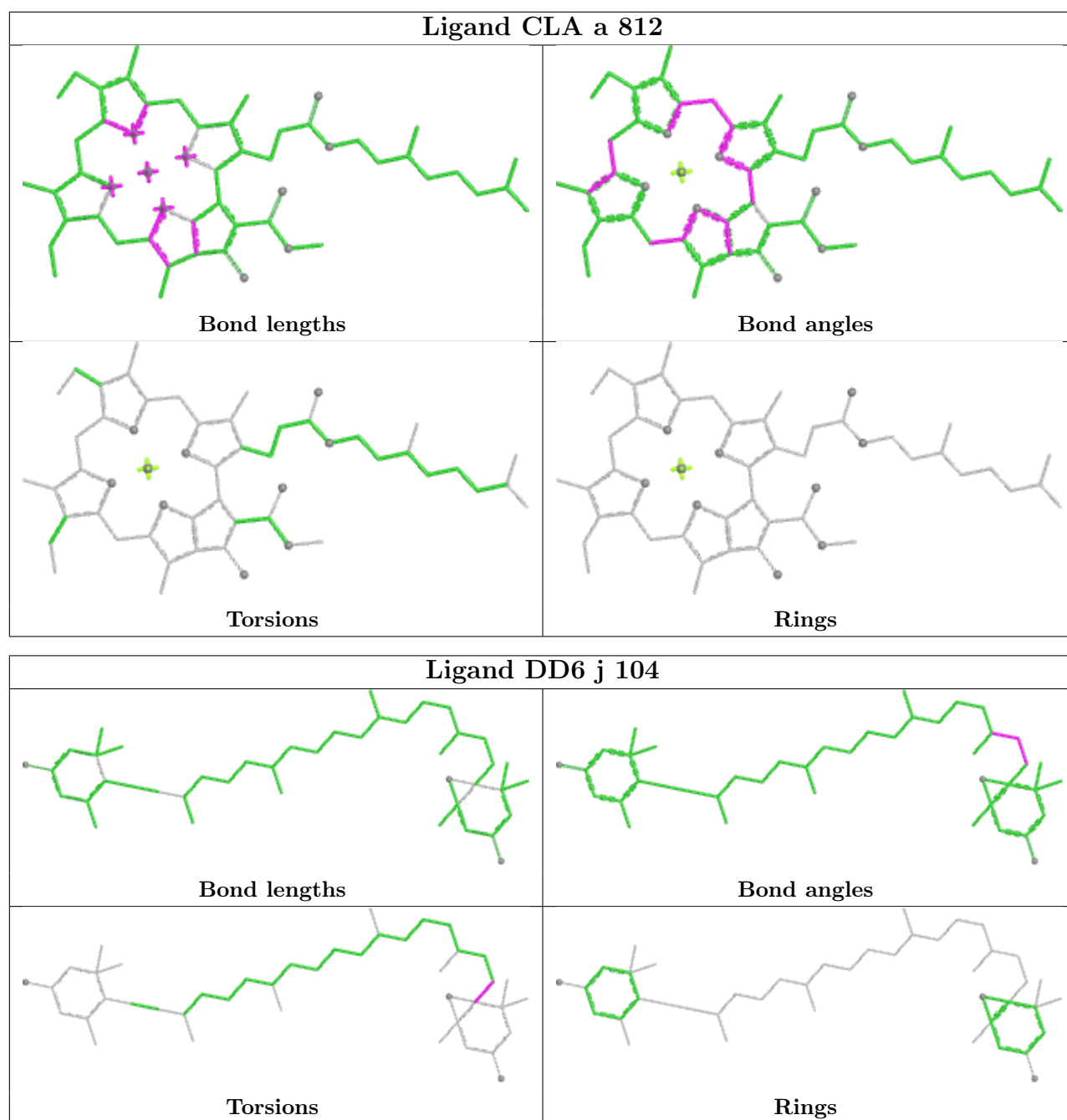
Bond angles



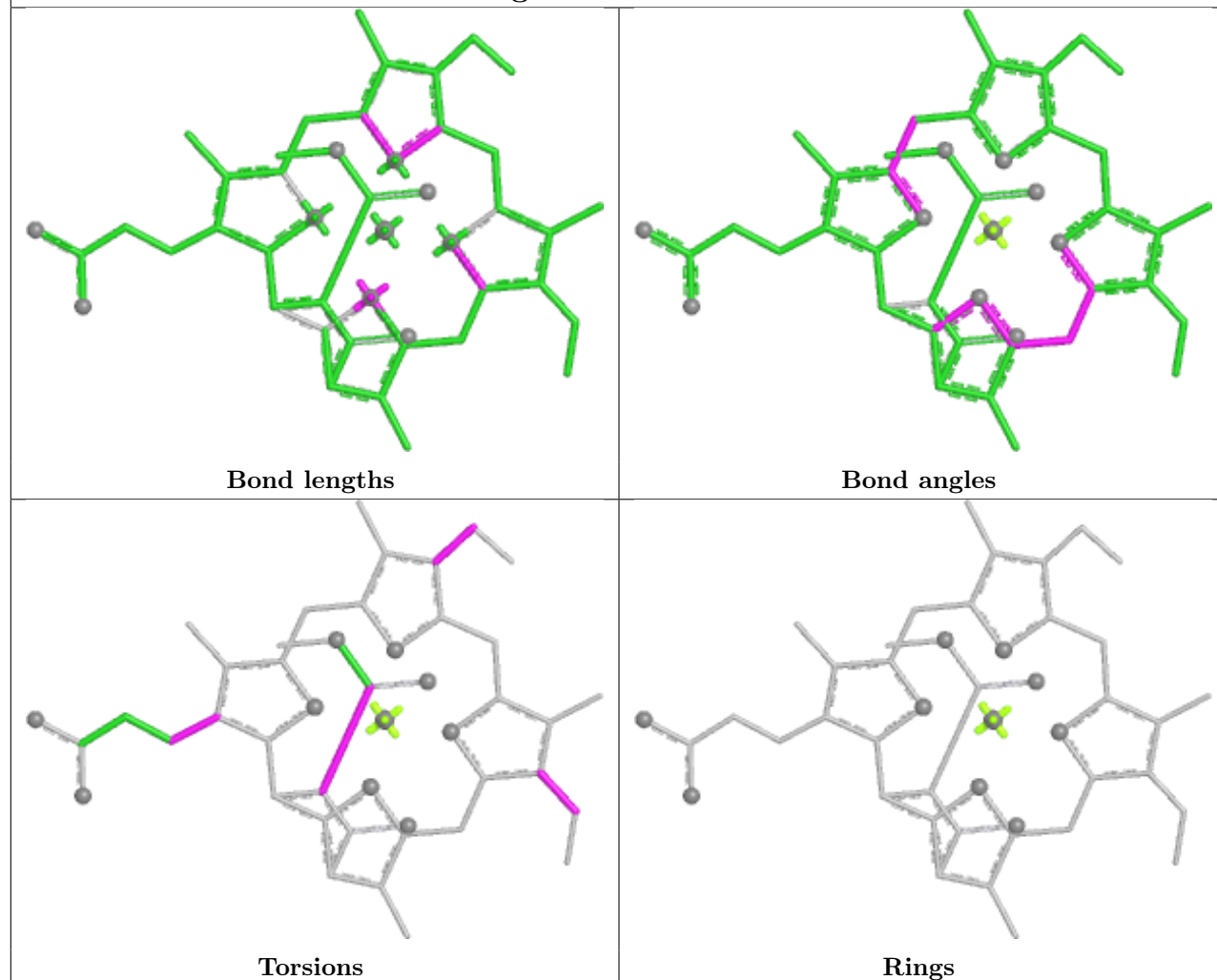
Torsions



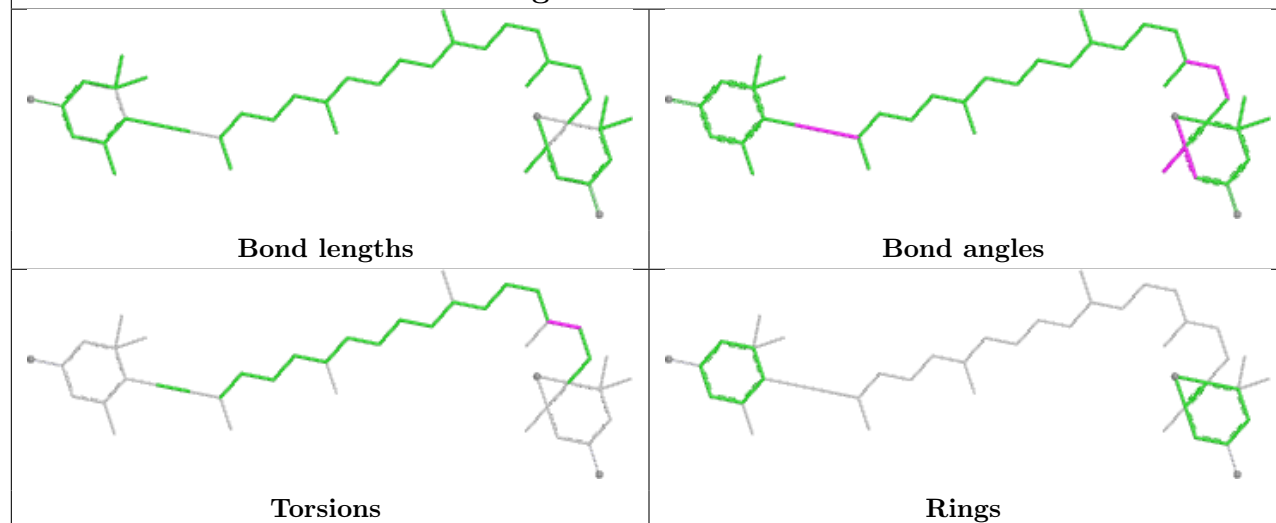
Rings

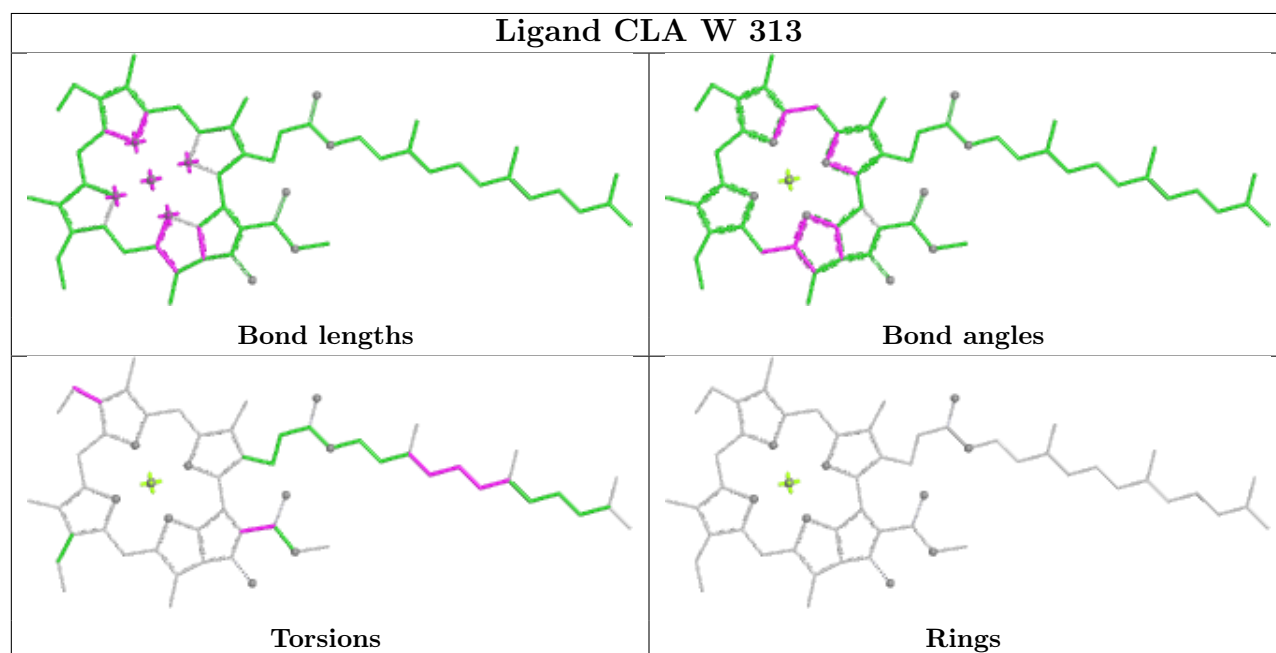
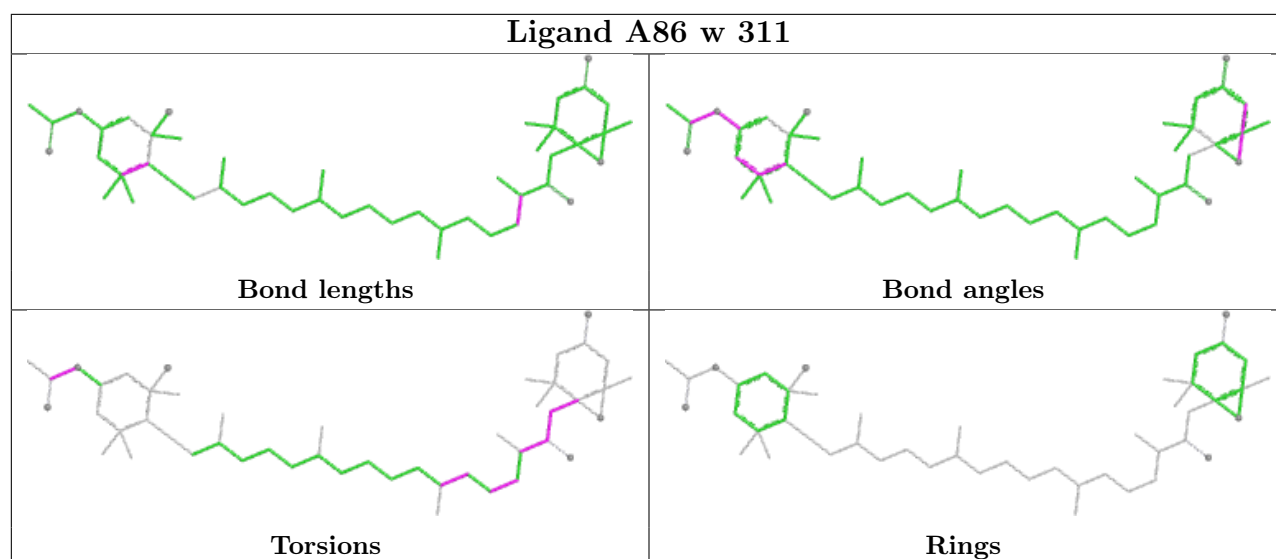


Ligand KC2 L 313

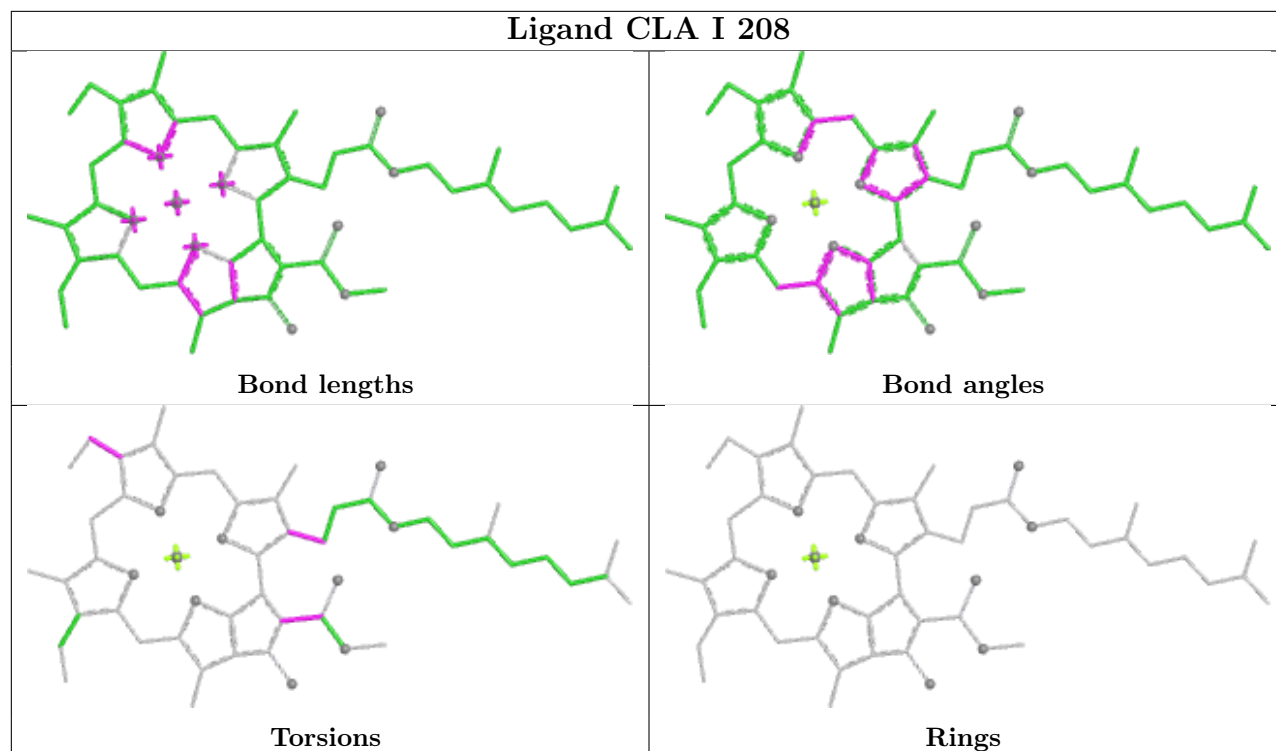


Ligand DD6 H 314

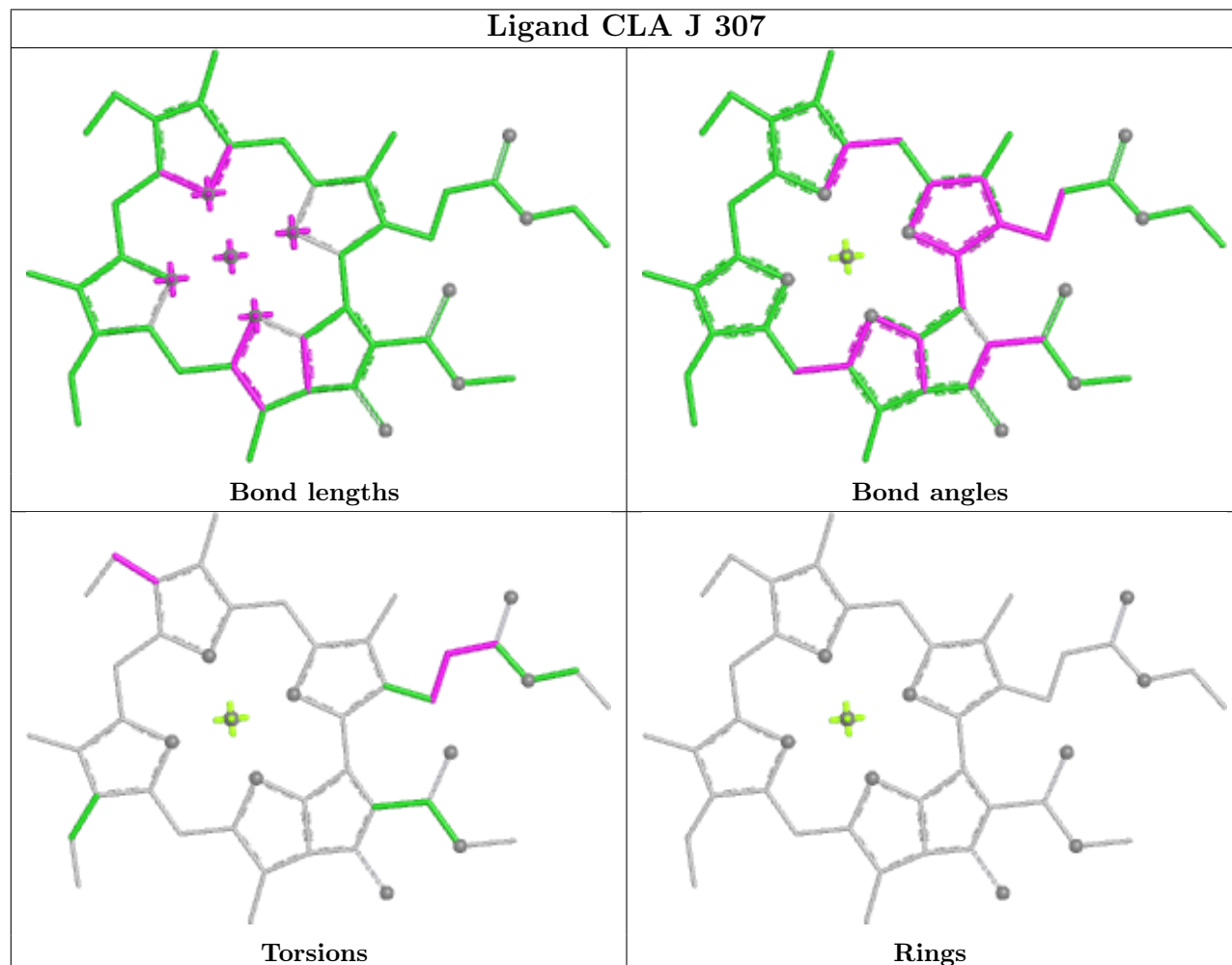


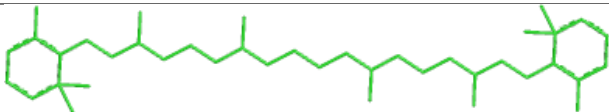
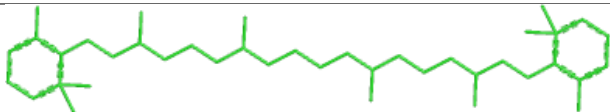
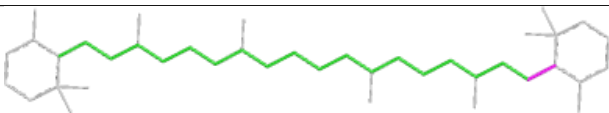
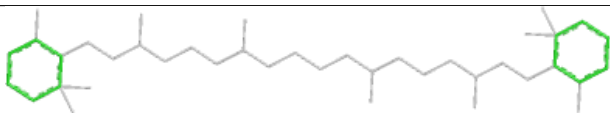
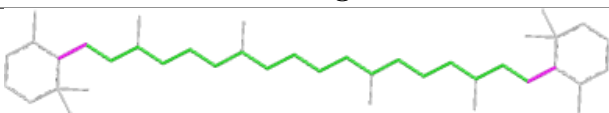
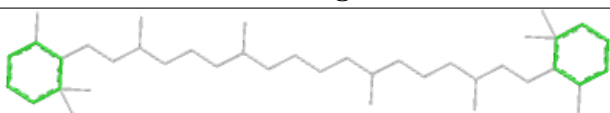


Ligand CLA I 208

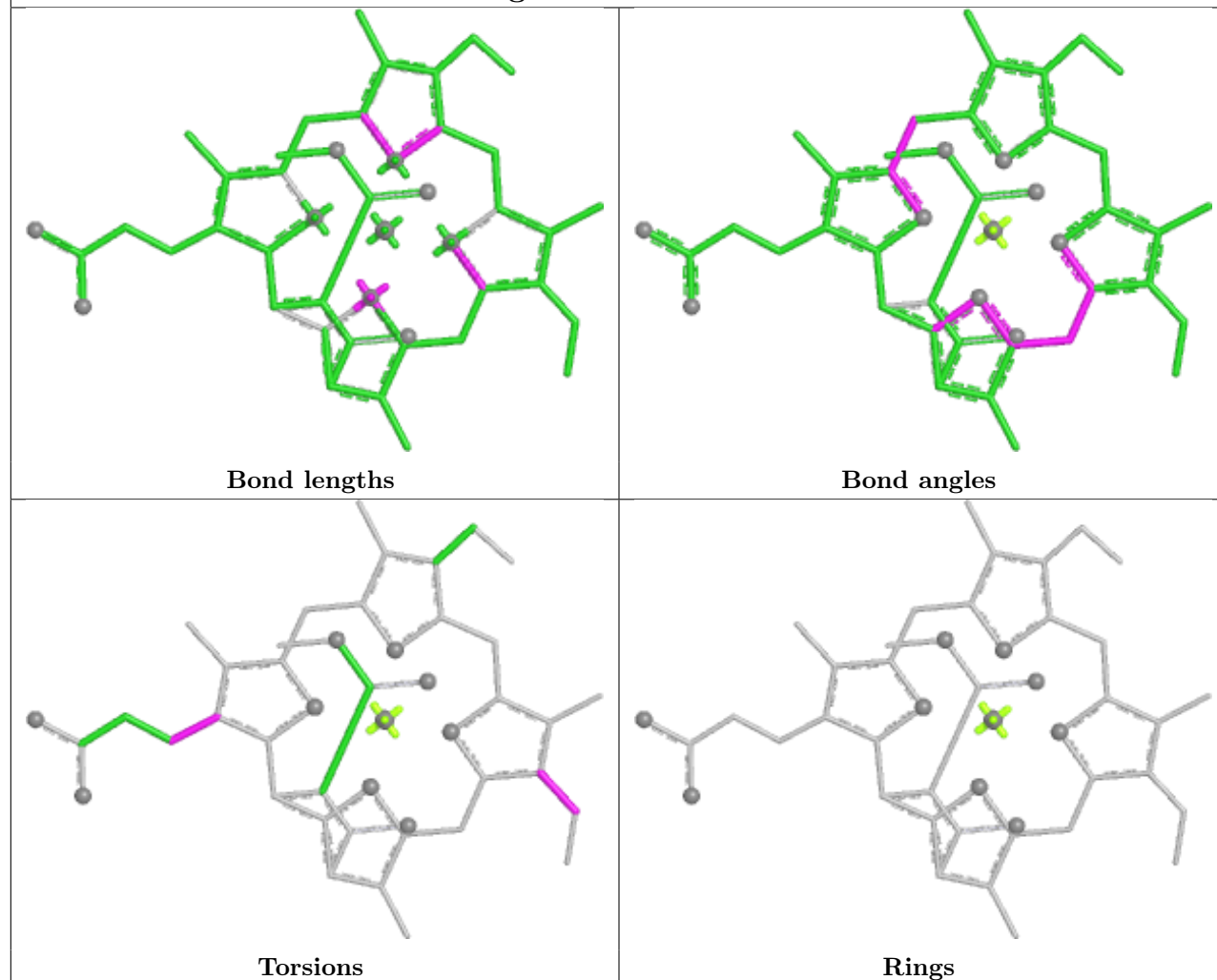


Ligand CLA J 307

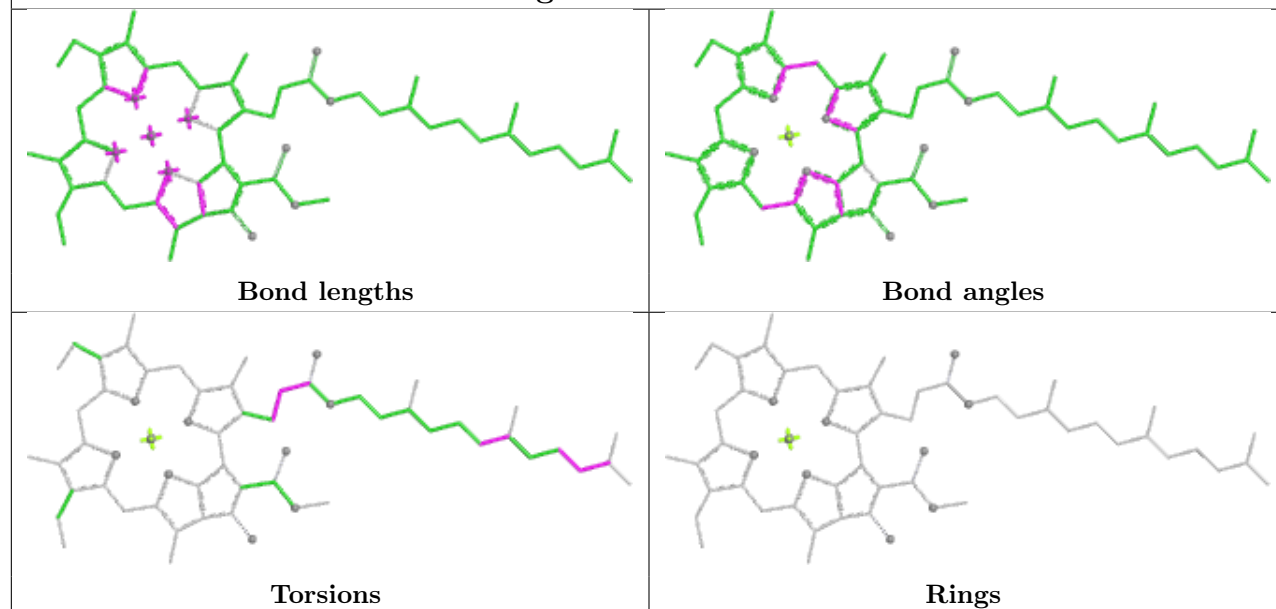


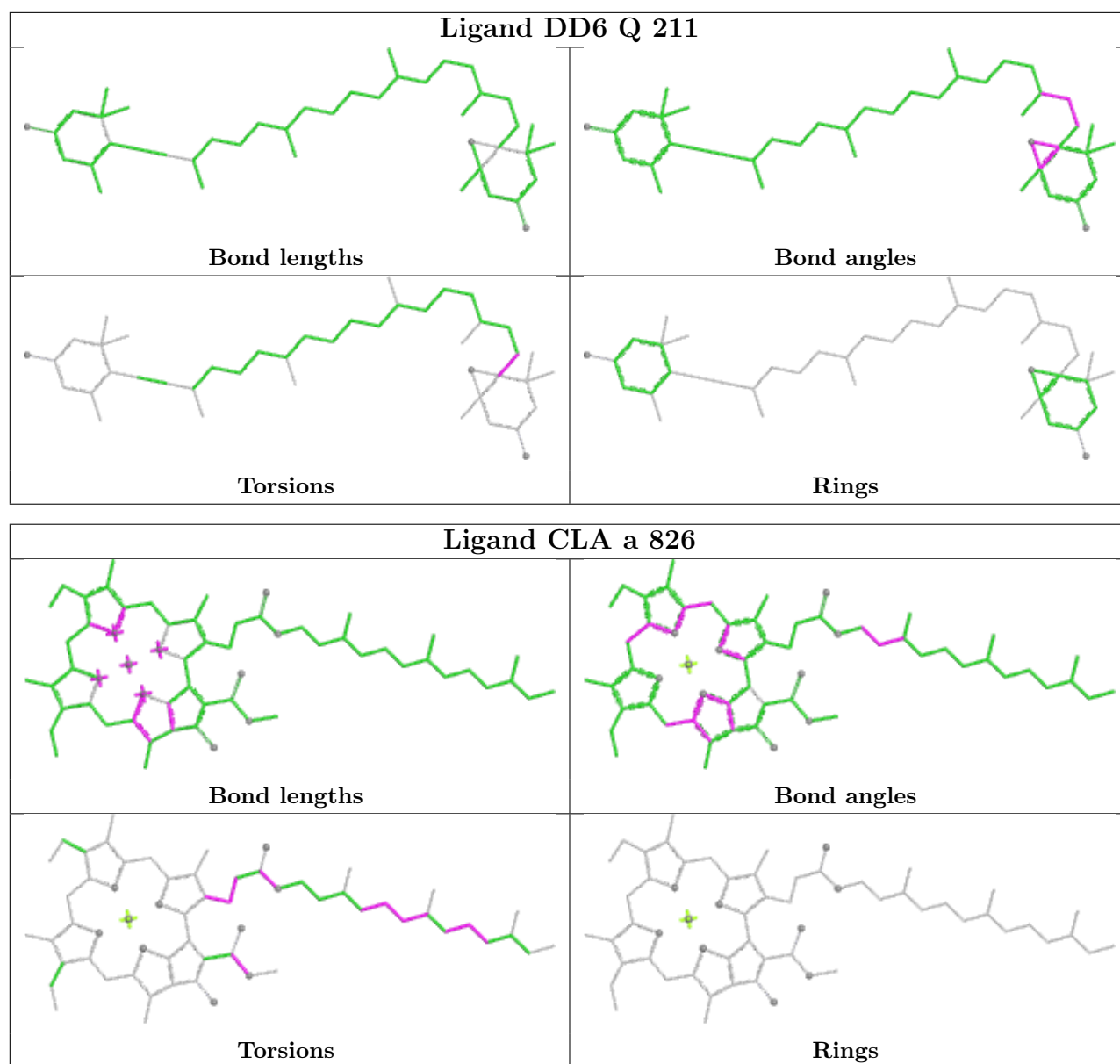
Ligand BCR a 846			
	Bond lengths		
	Torsions		
Ligand BCR i 102			
	Bond lengths		
	Torsions		

Ligand KC2 X 302

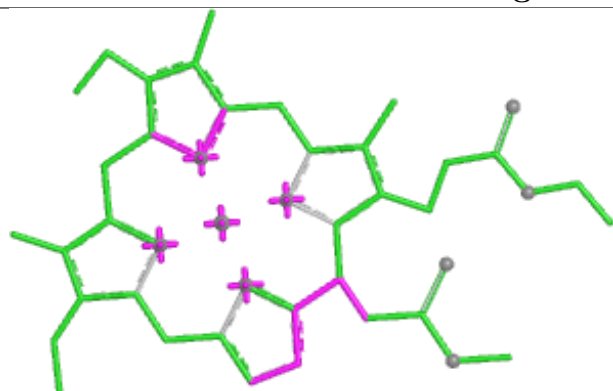


Ligand CLA a 831

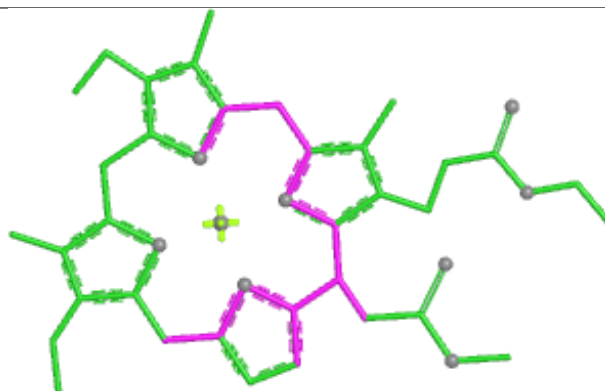




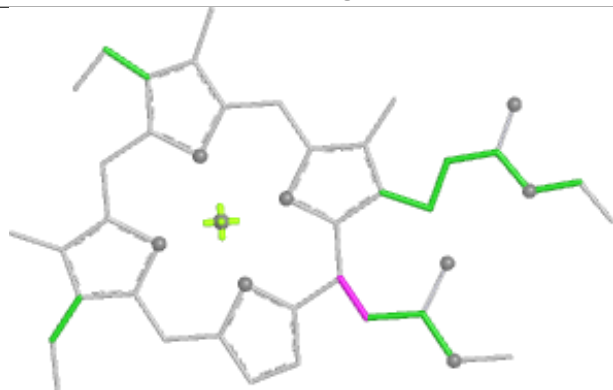
Ligand CLA D 305



Bond lengths



Bond angles

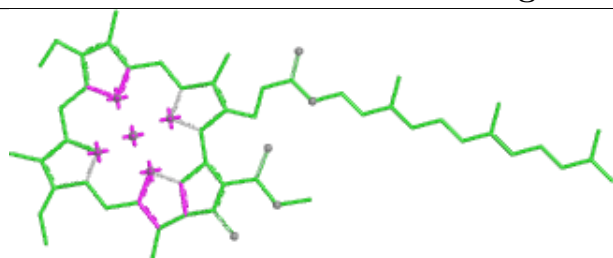


Torsions

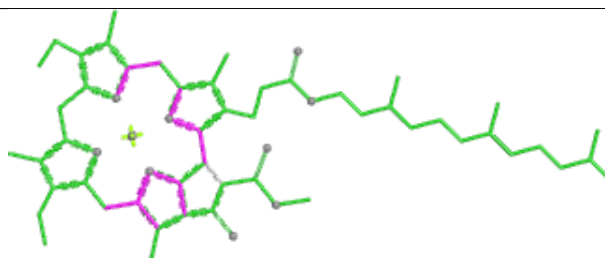


Rings

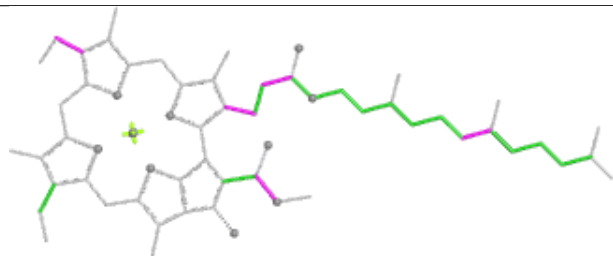
Ligand CLA a 813



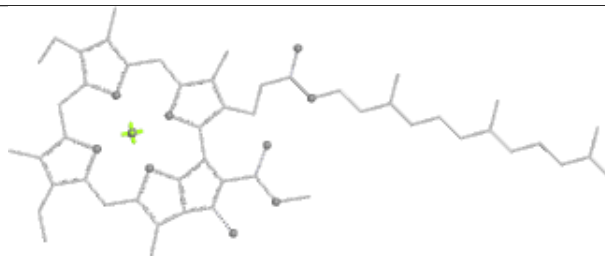
Bond lengths



Bond angles

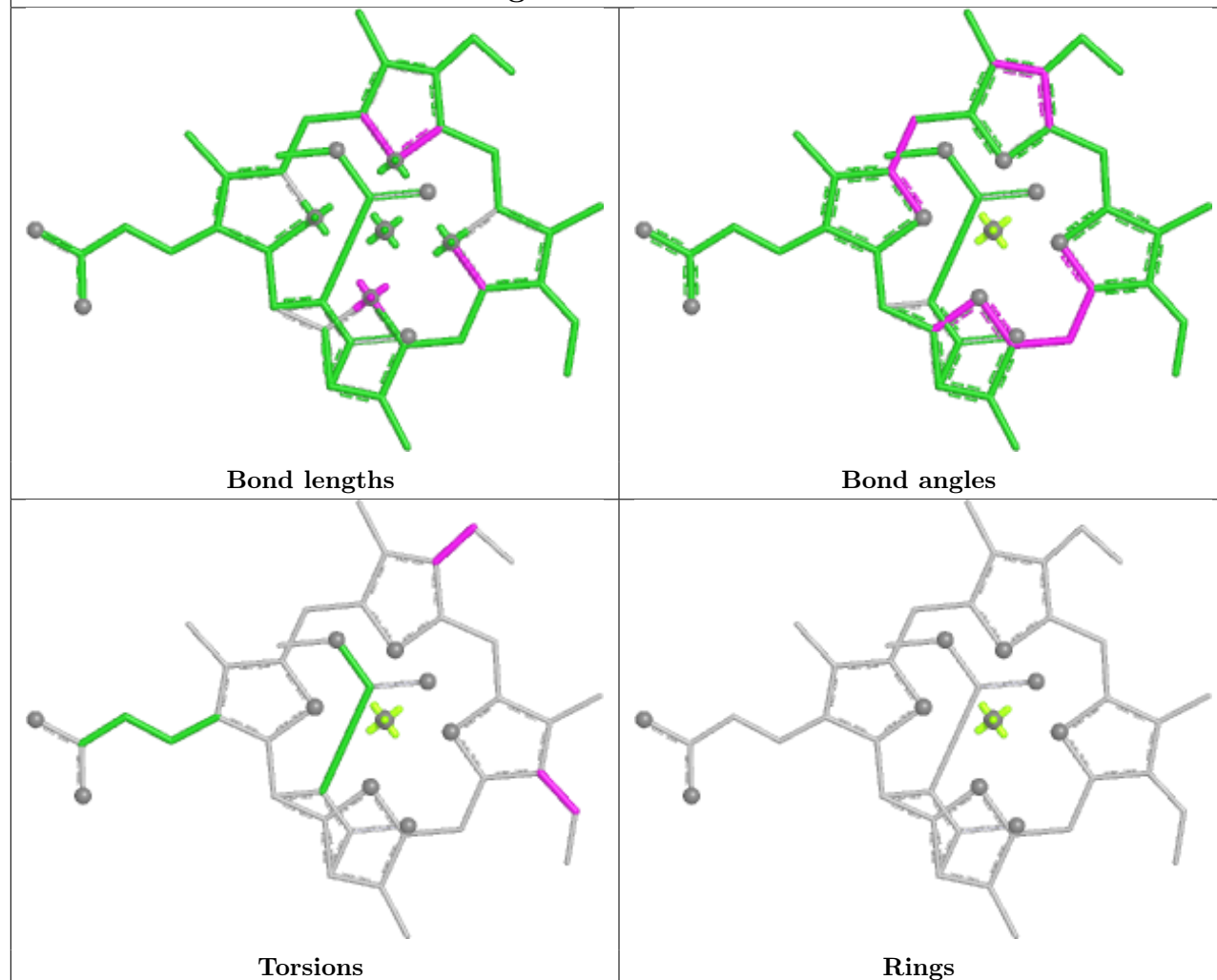


Torsions

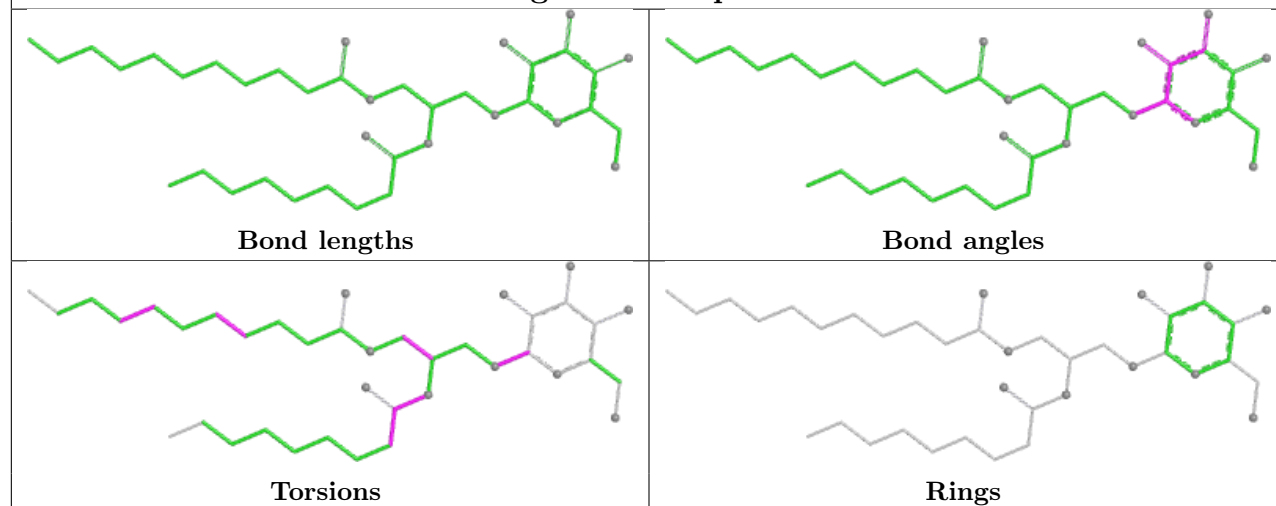


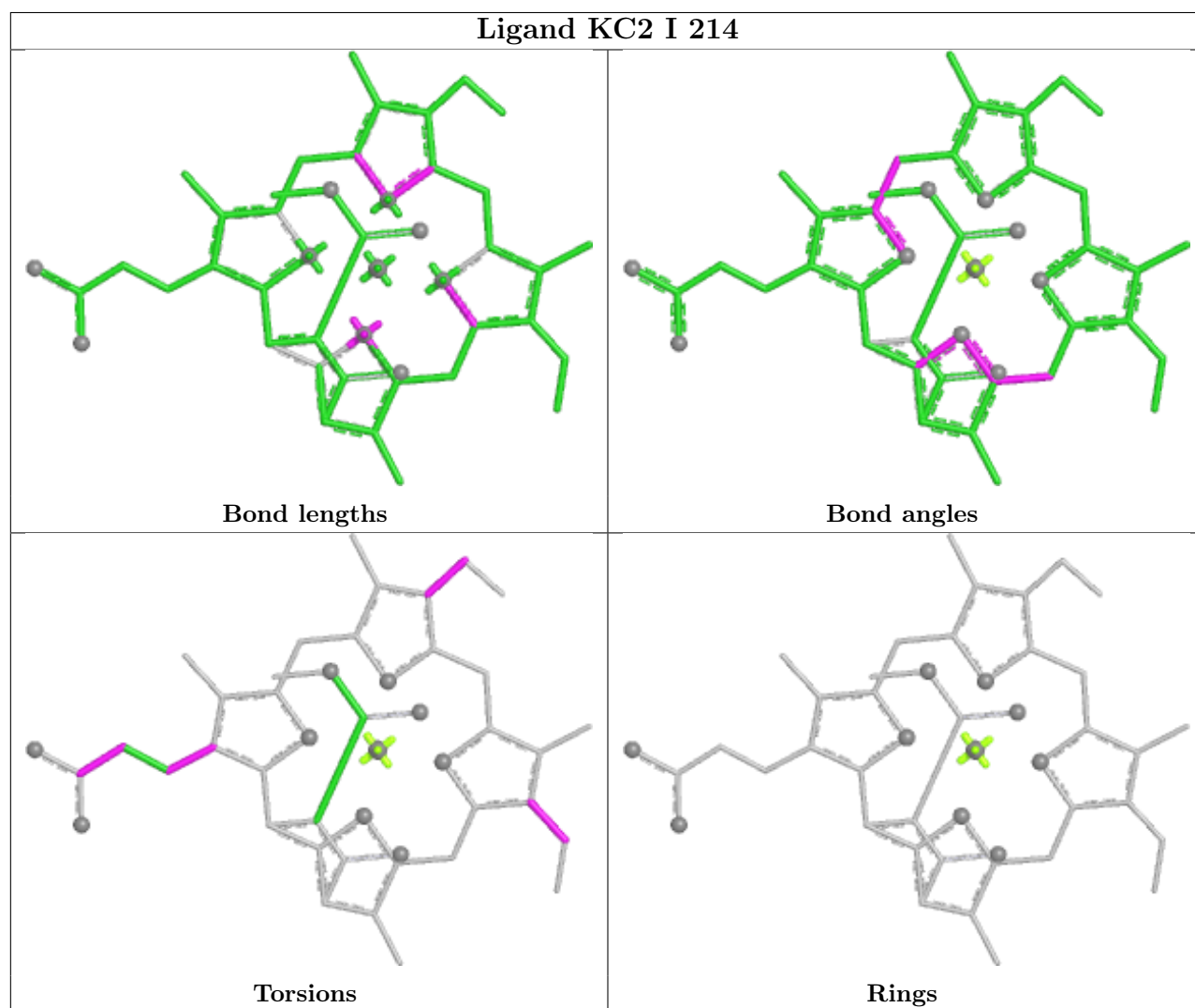
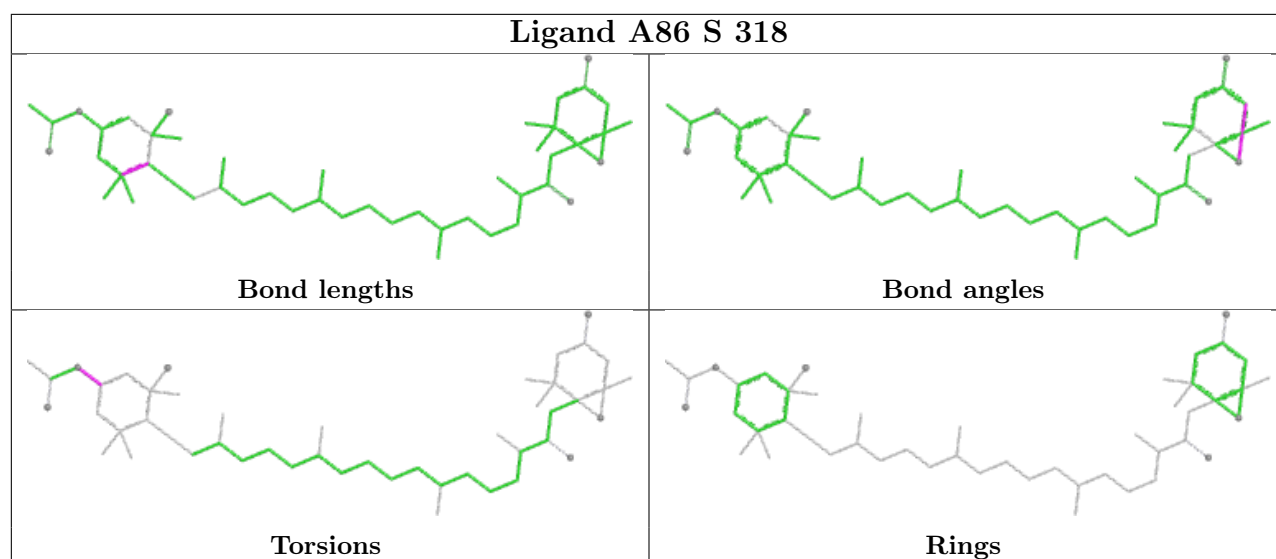
Rings

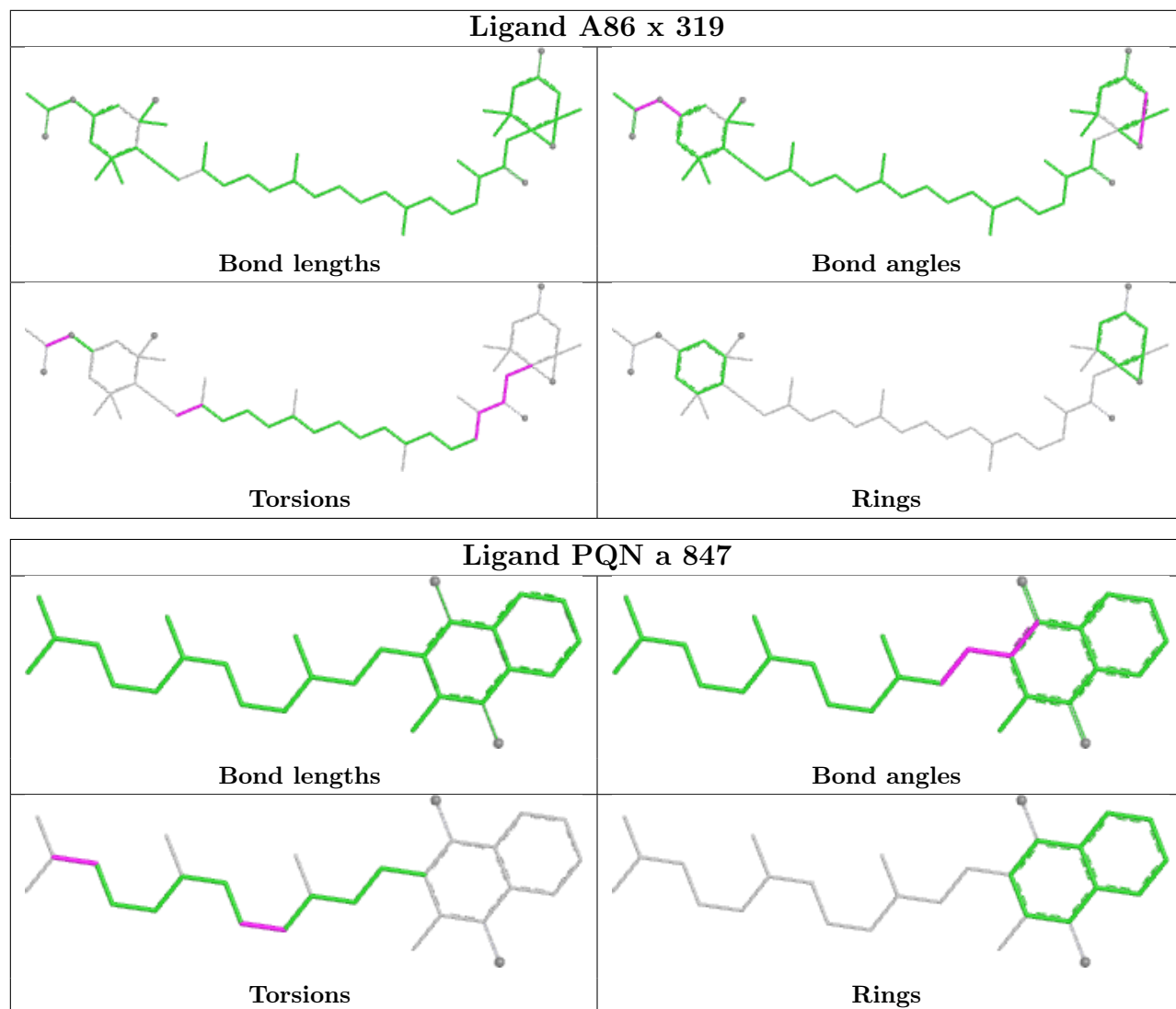
Ligand KC2 N 309



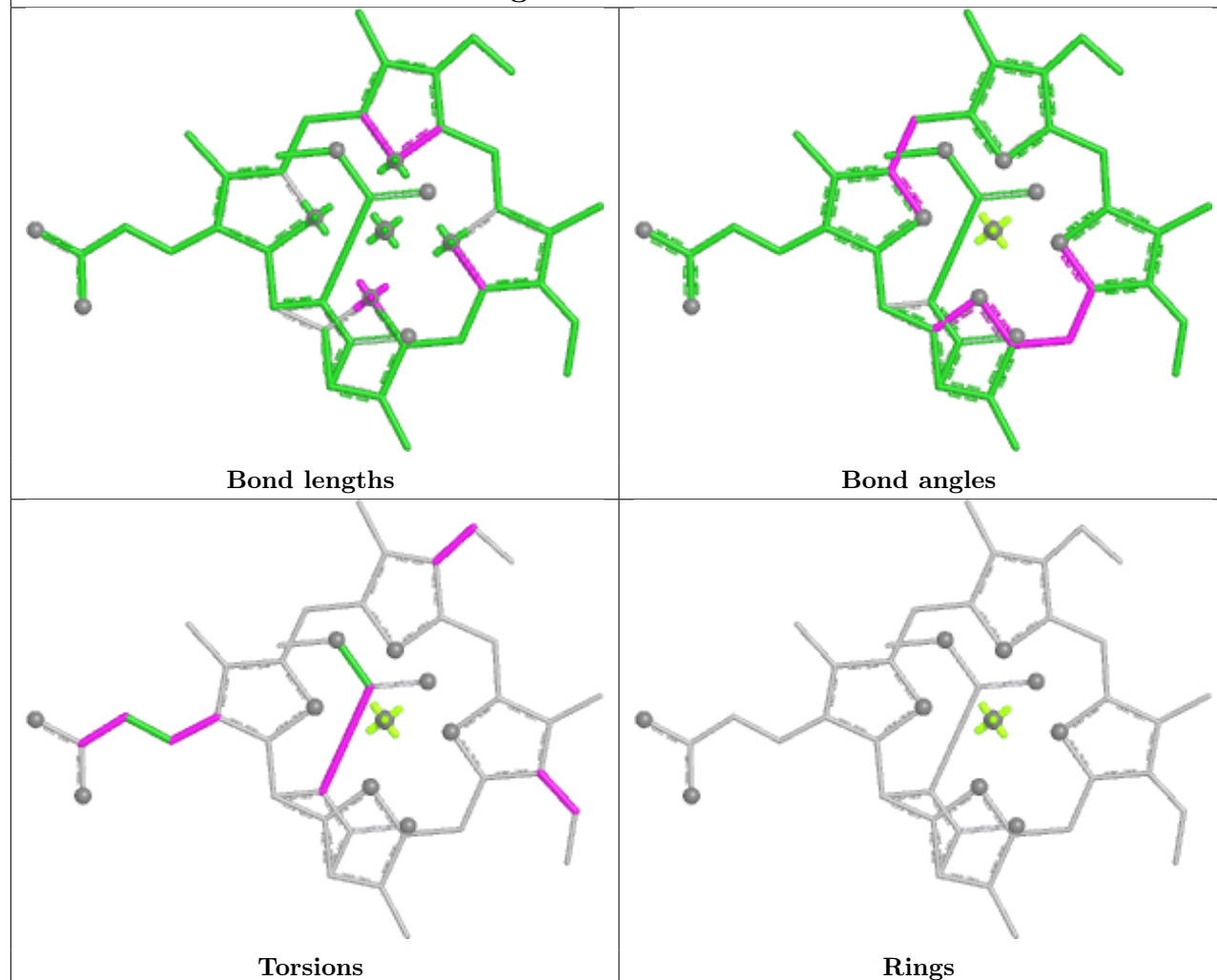
Ligand LMG p 301



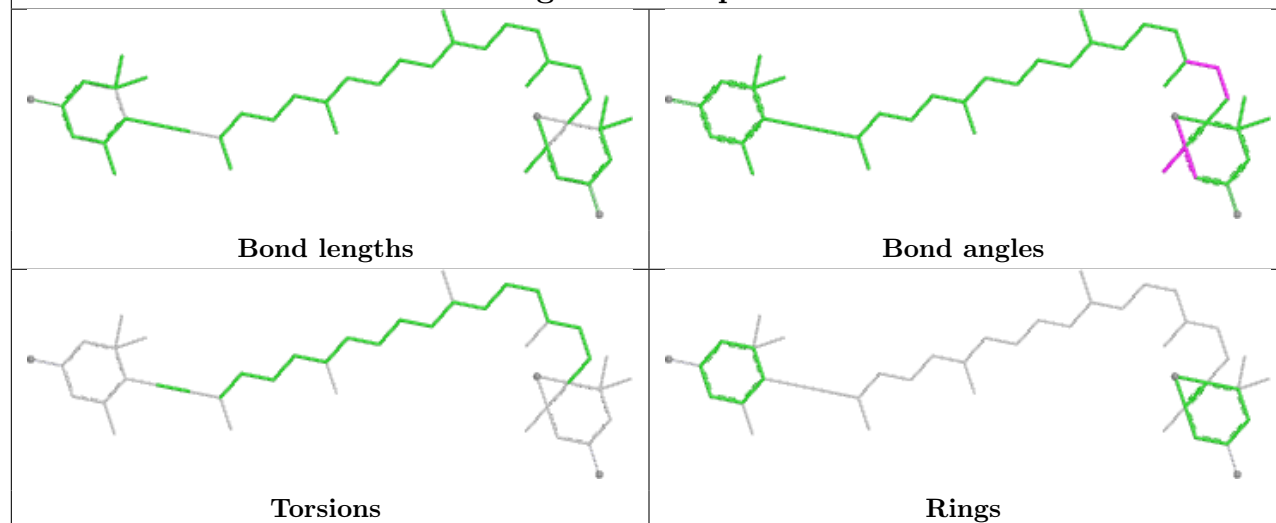


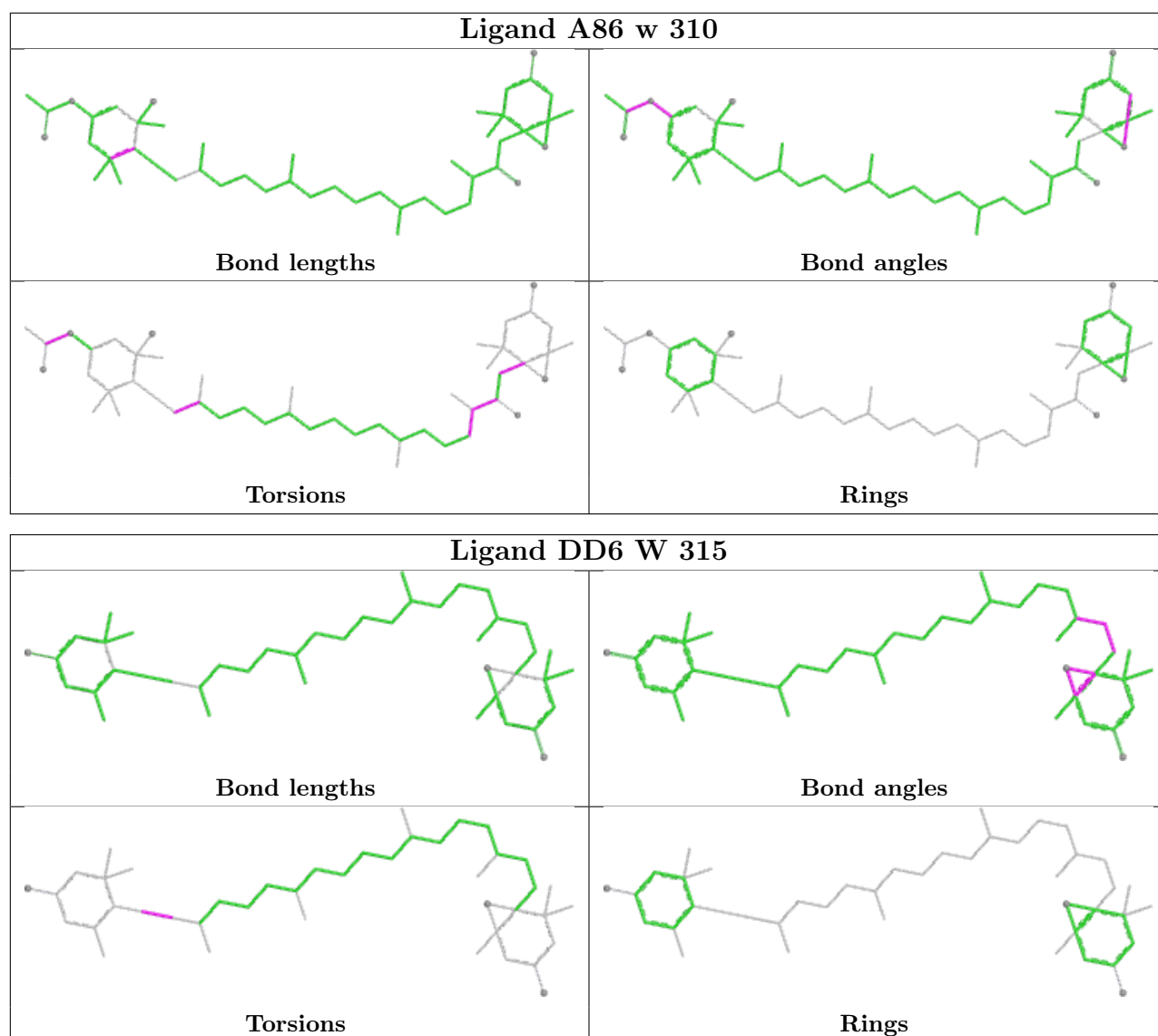


Ligand KC2 E 319

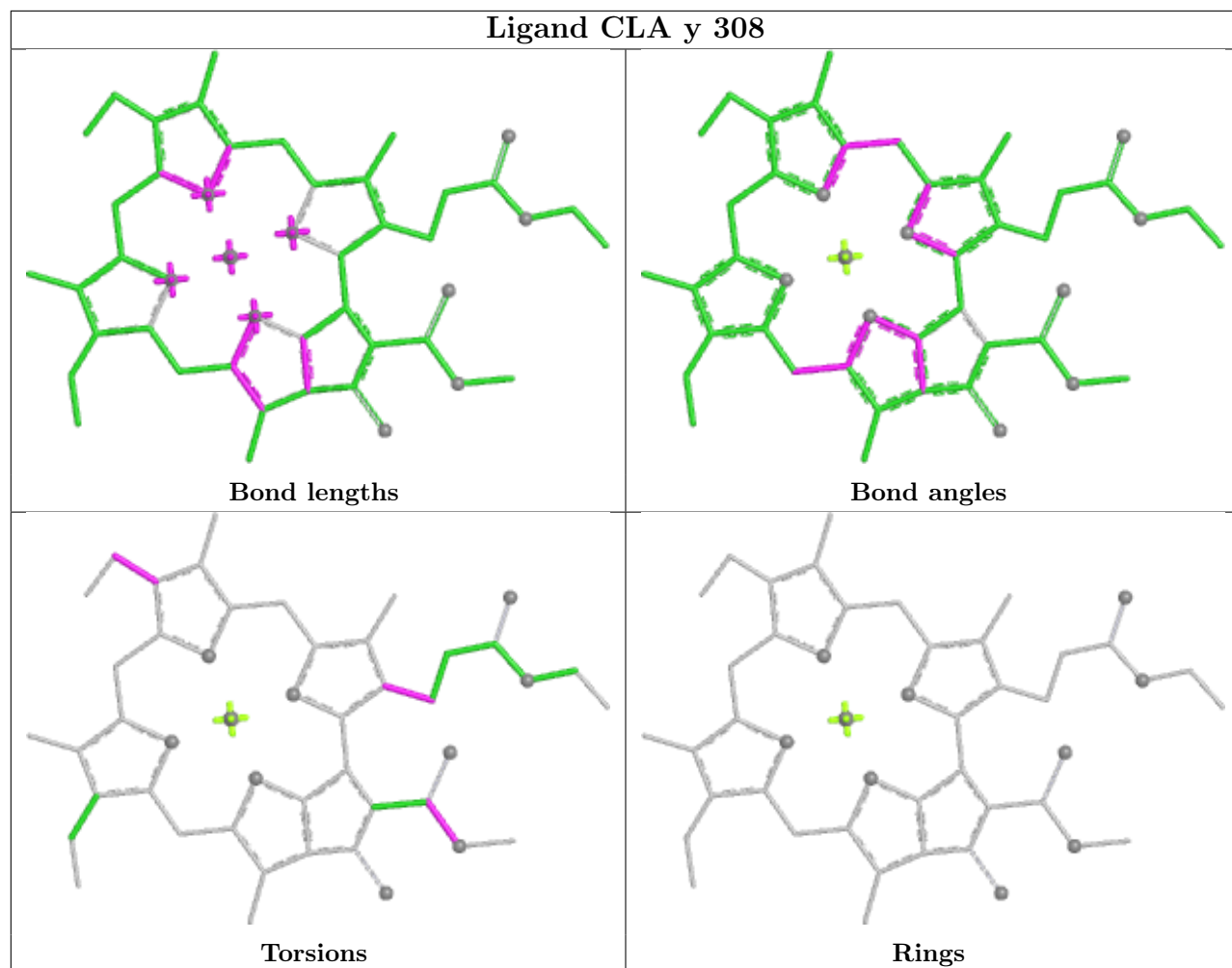


Ligand DD6 q 318

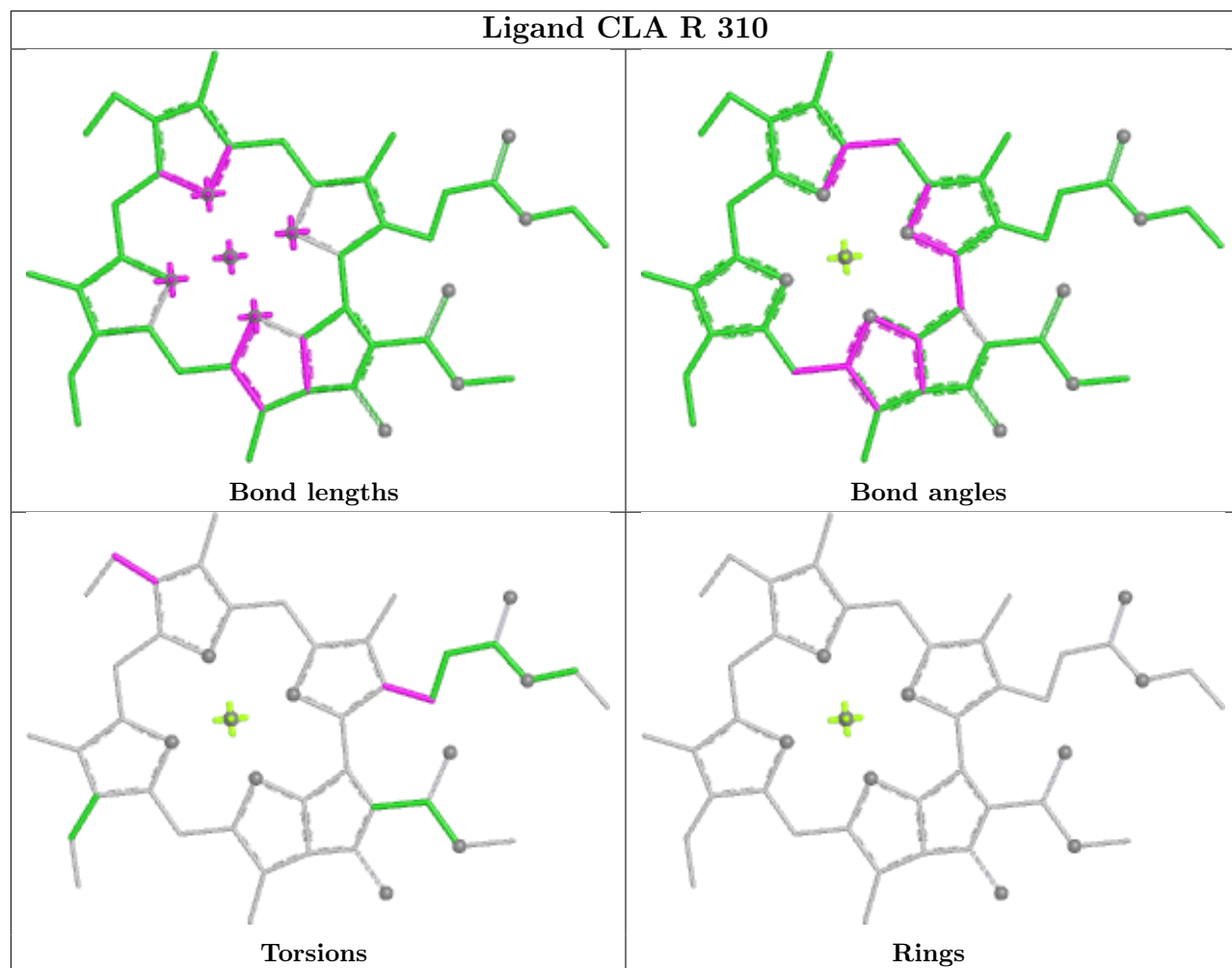




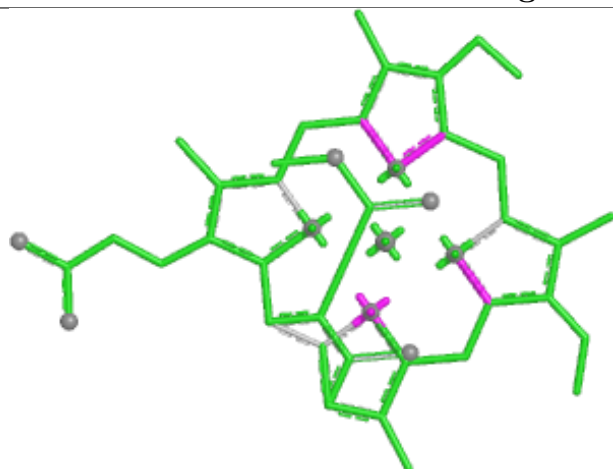
Ligand CLA y 308



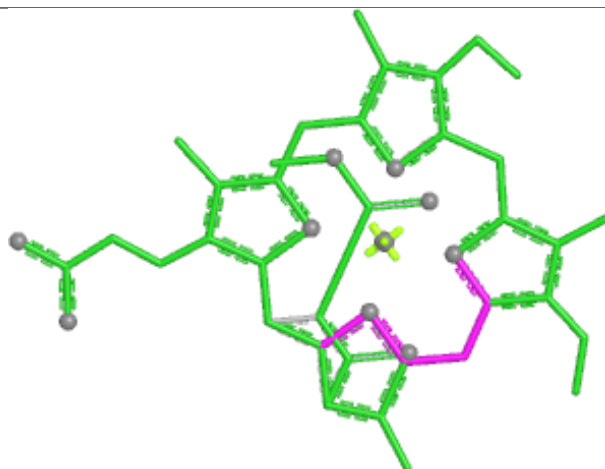
Ligand CLA R 310



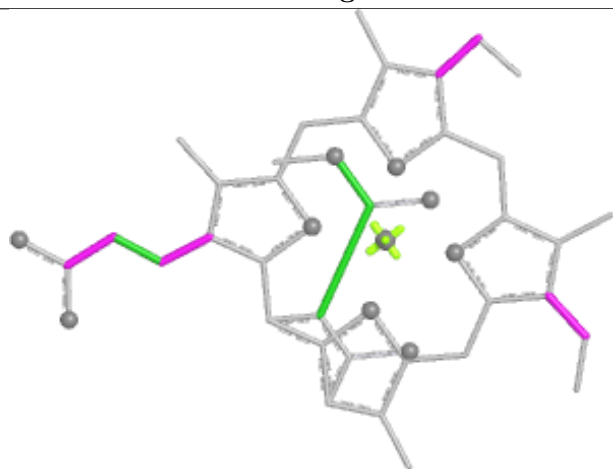
Ligand KC2 L 309



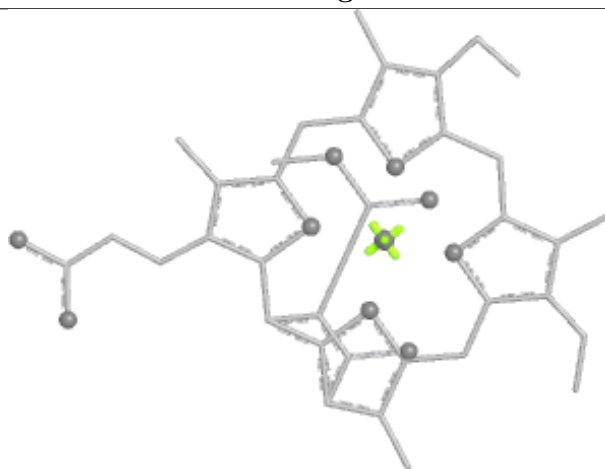
Bond lengths



Bond angles

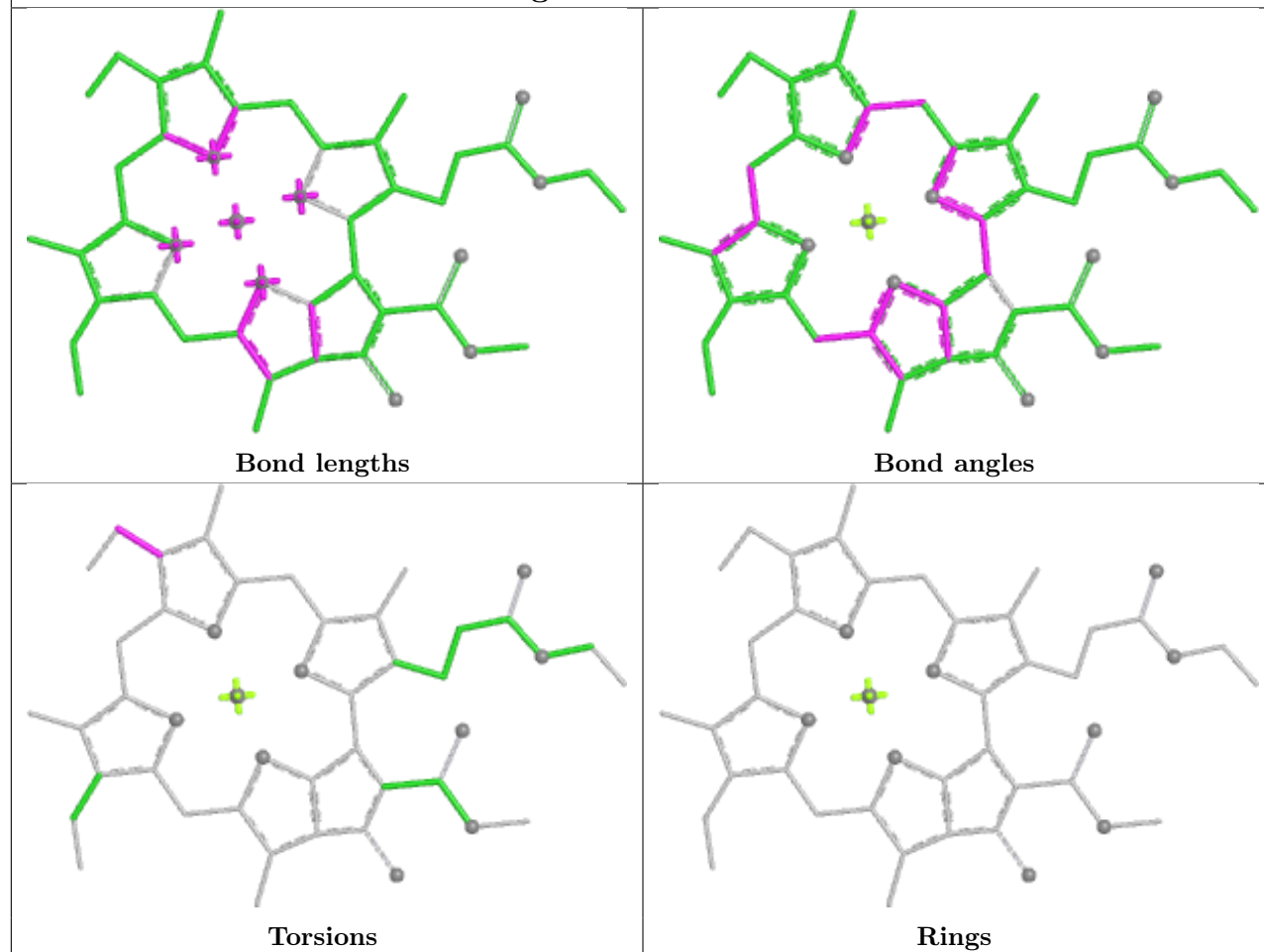


Torsions

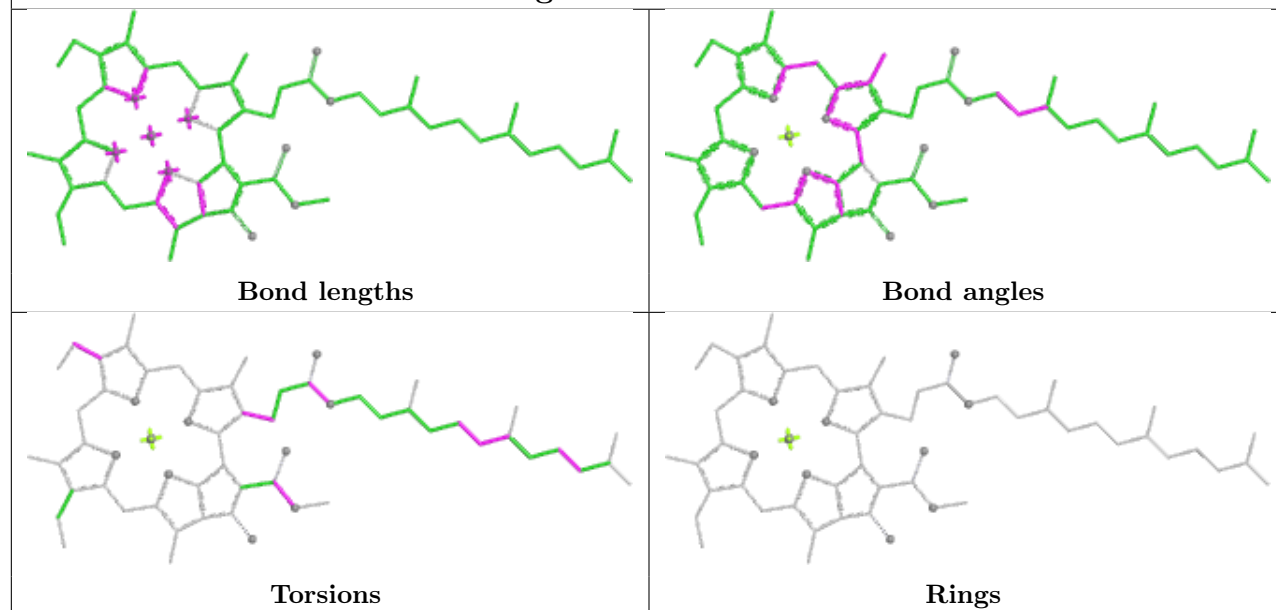


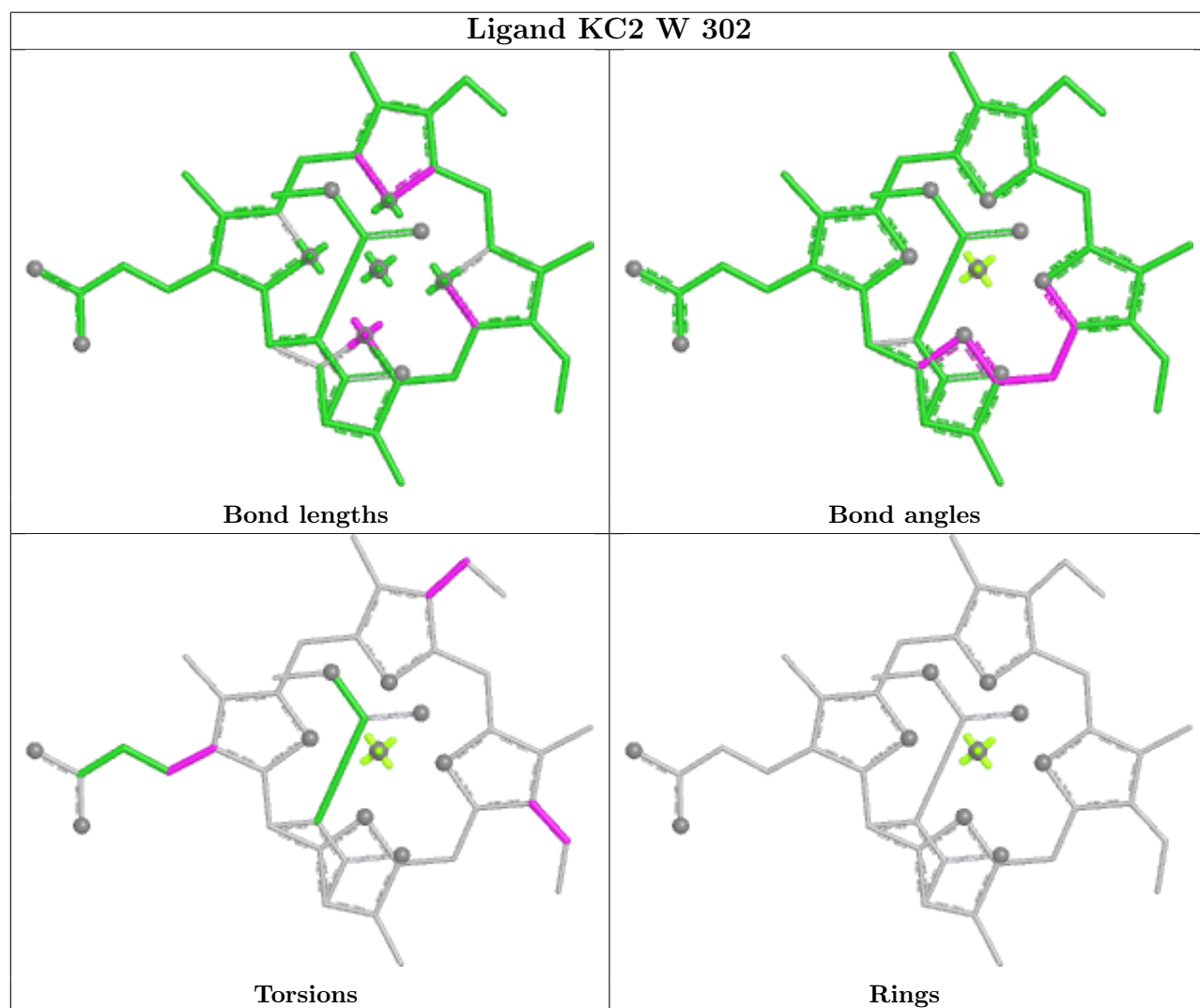
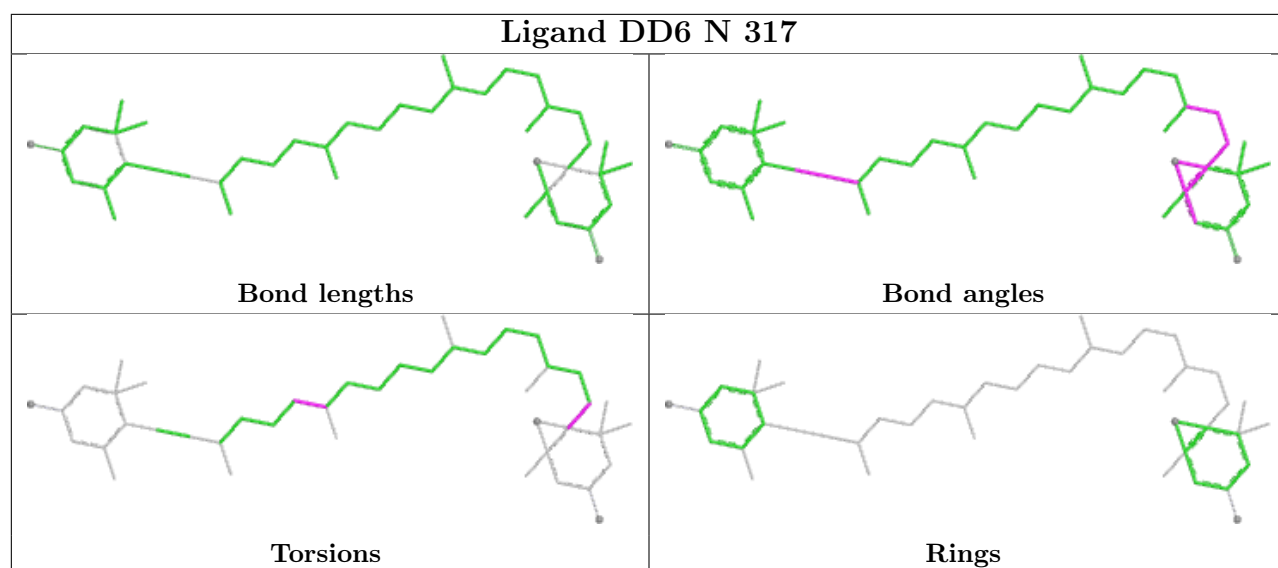
Rings

Ligand CLA a 818

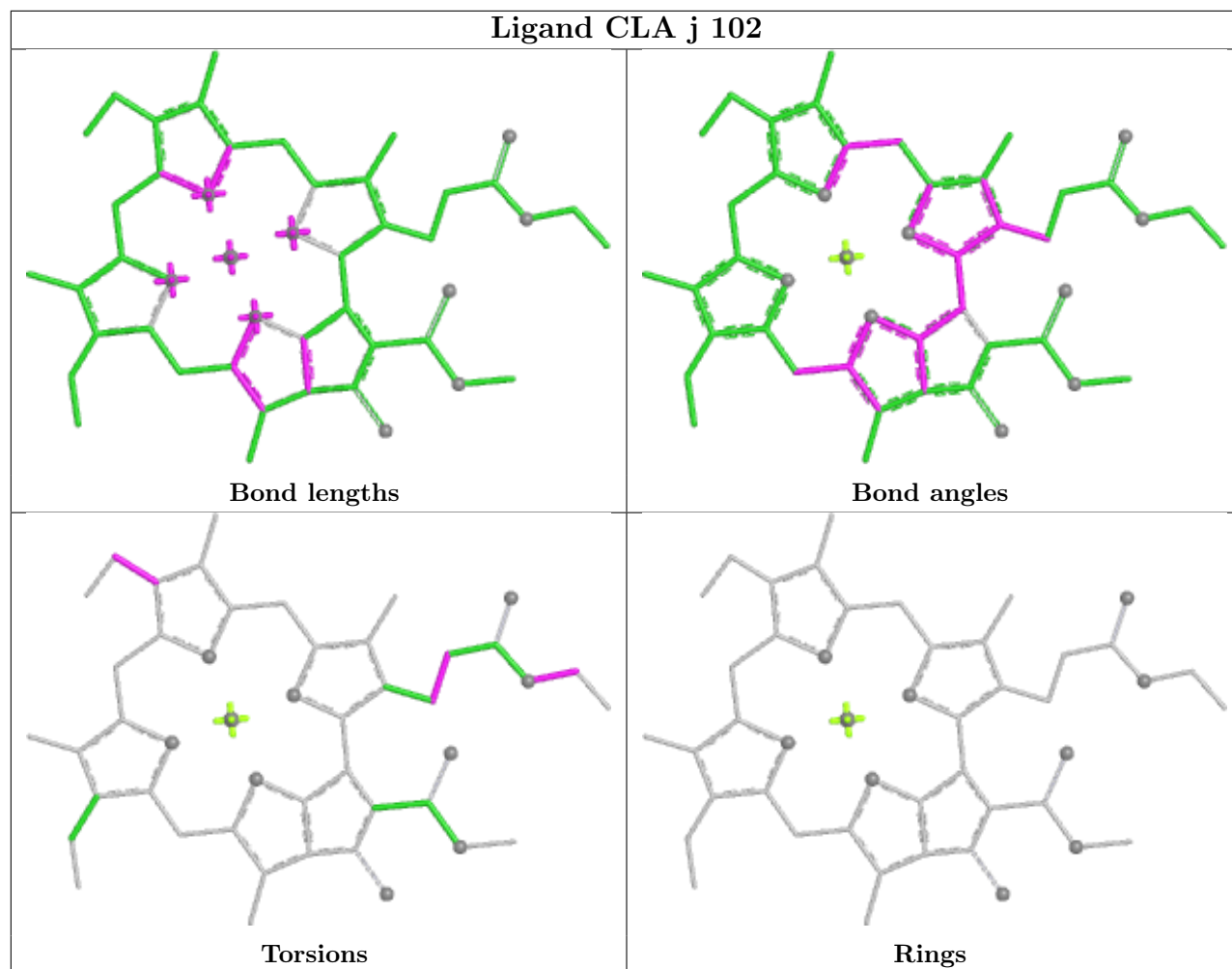


Ligand CLA x 312

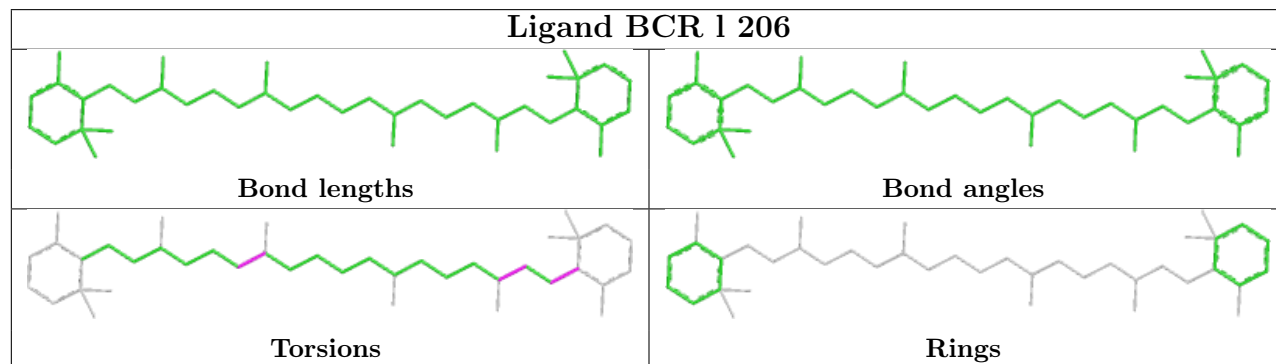




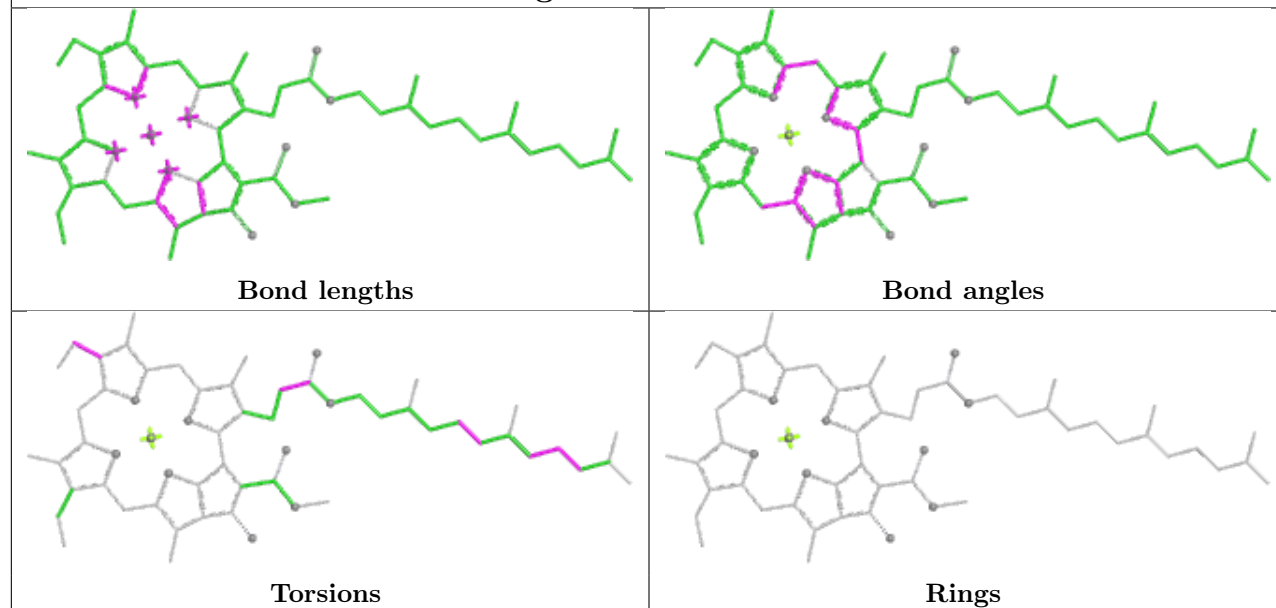
Ligand CLA j 102



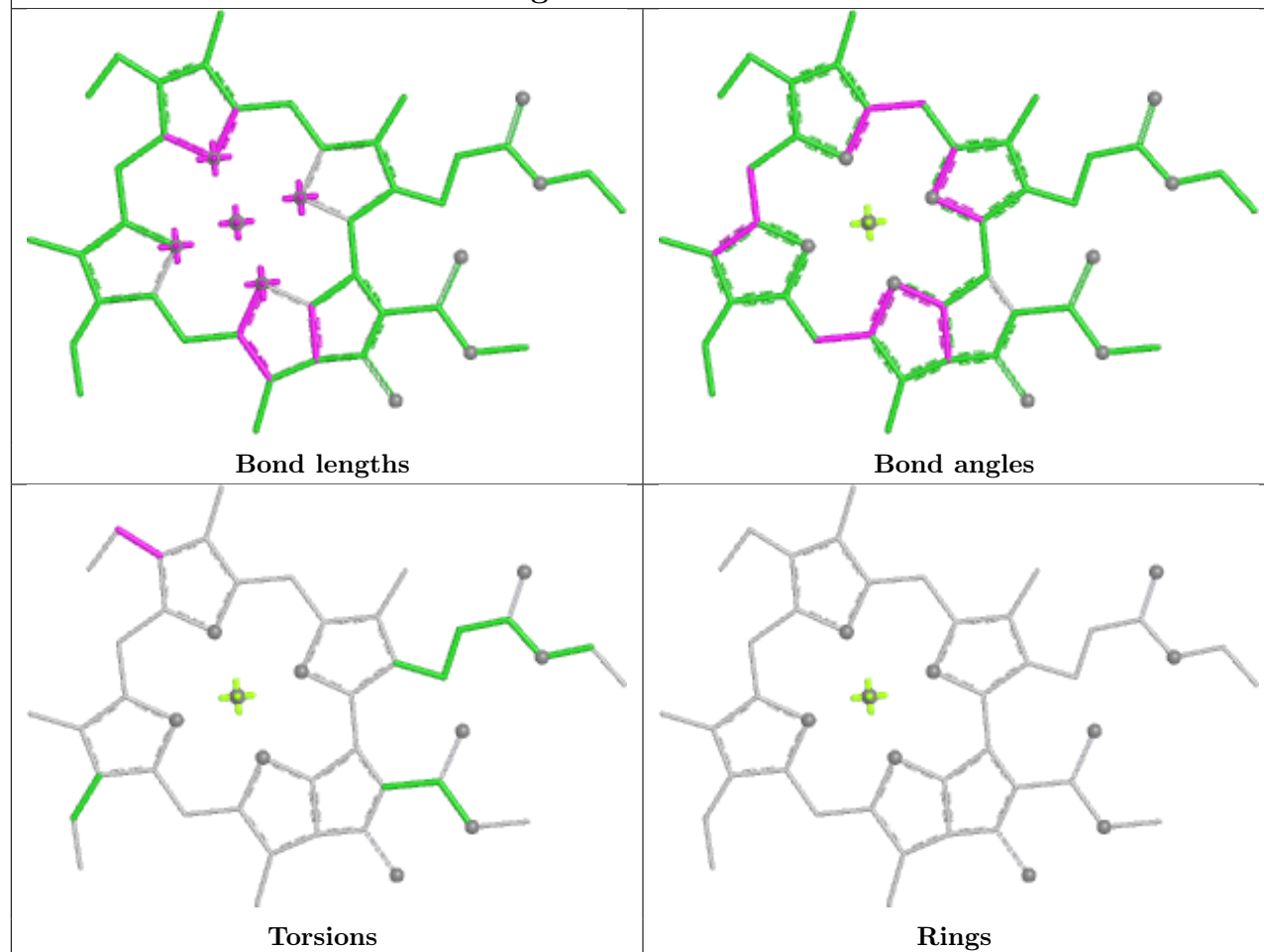
Ligand BCR l 206

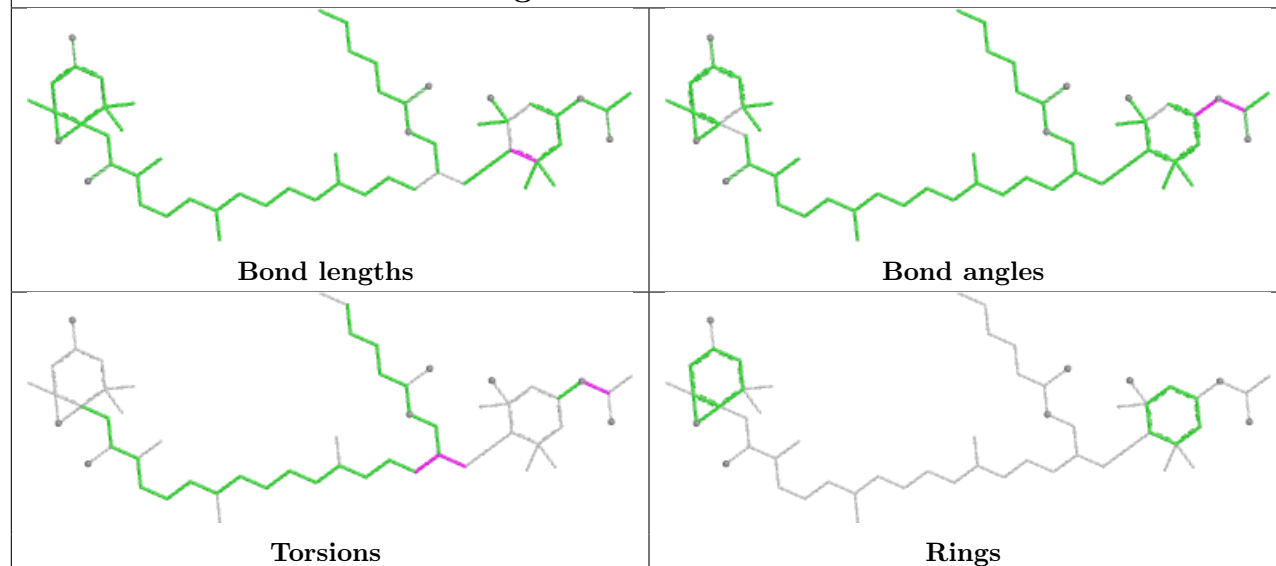
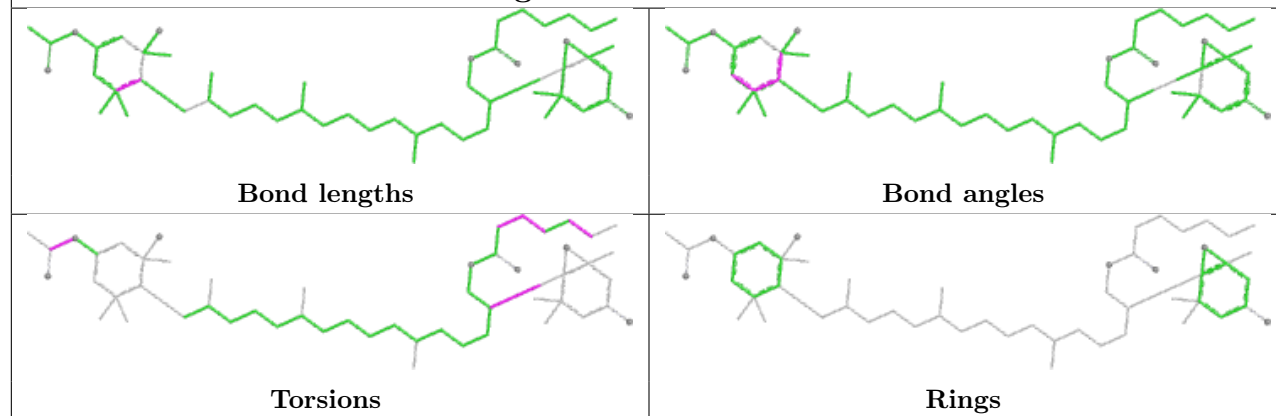


Ligand CLA x 308

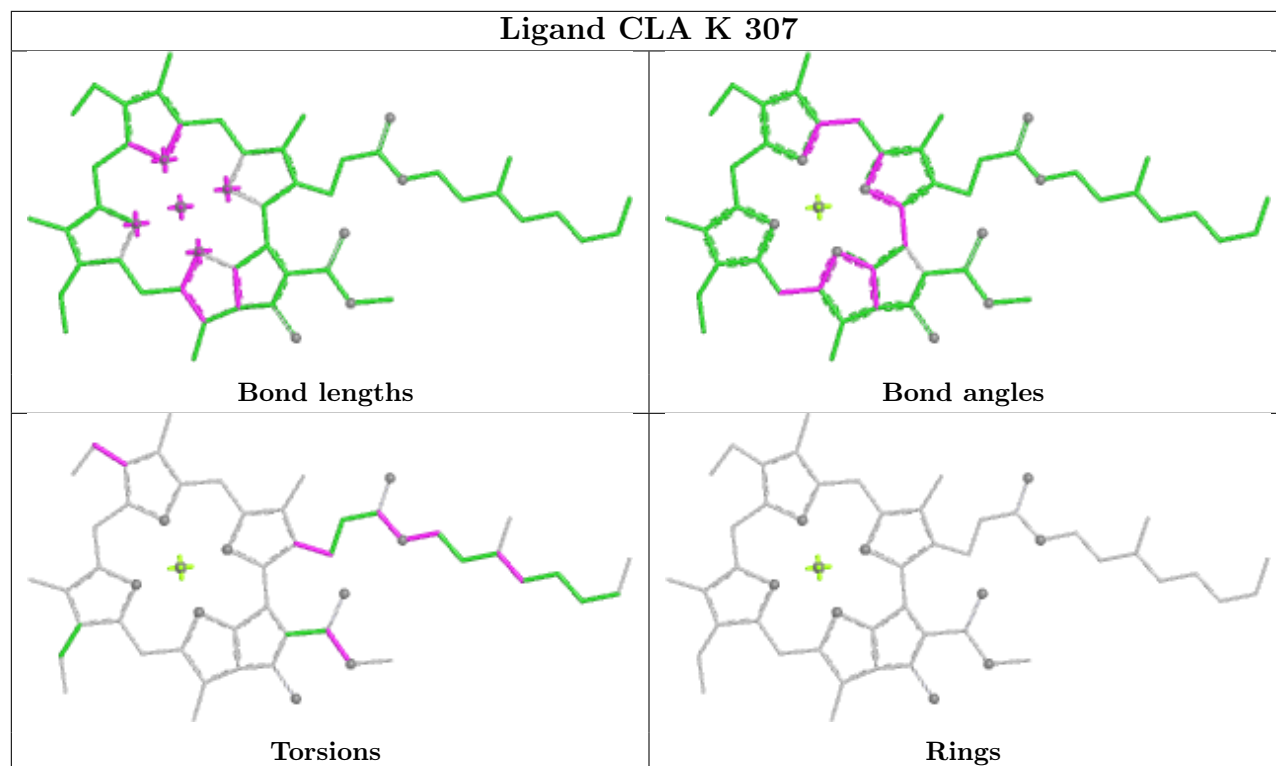


Ligand CLA J 309

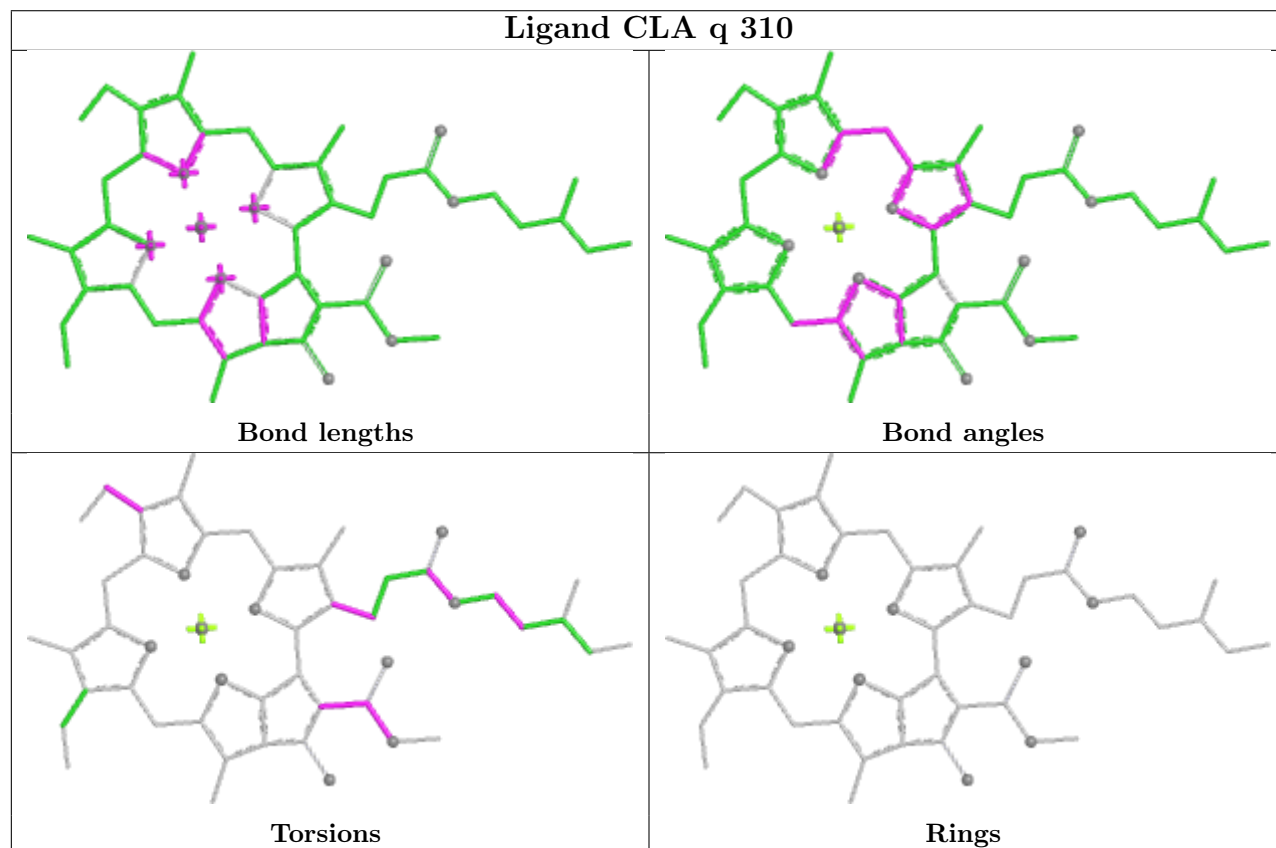


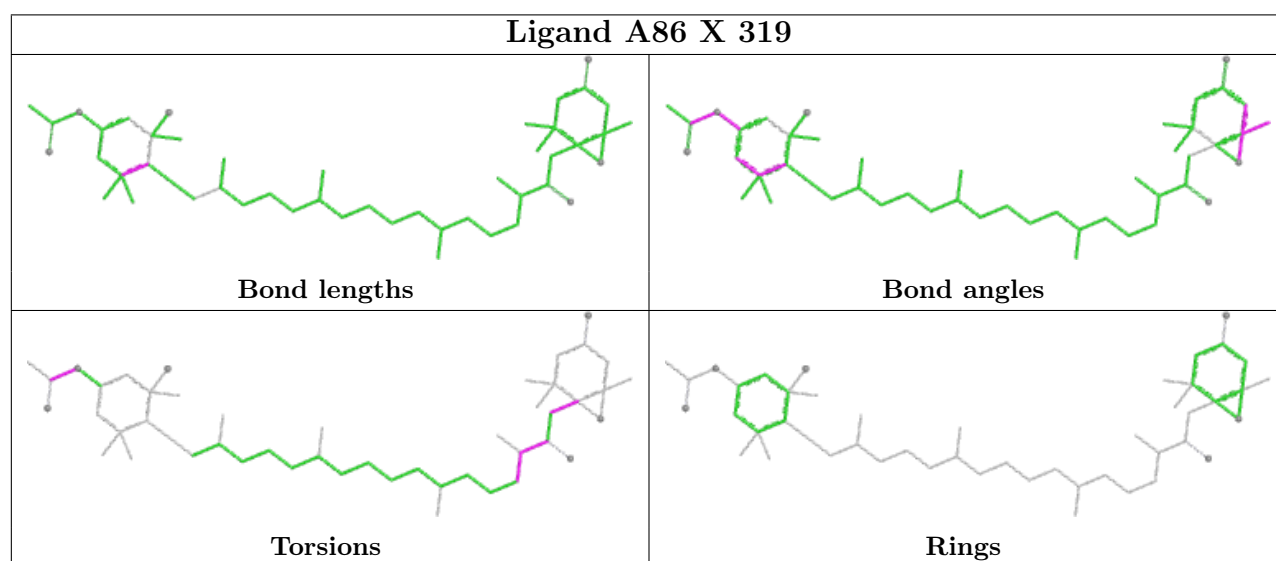
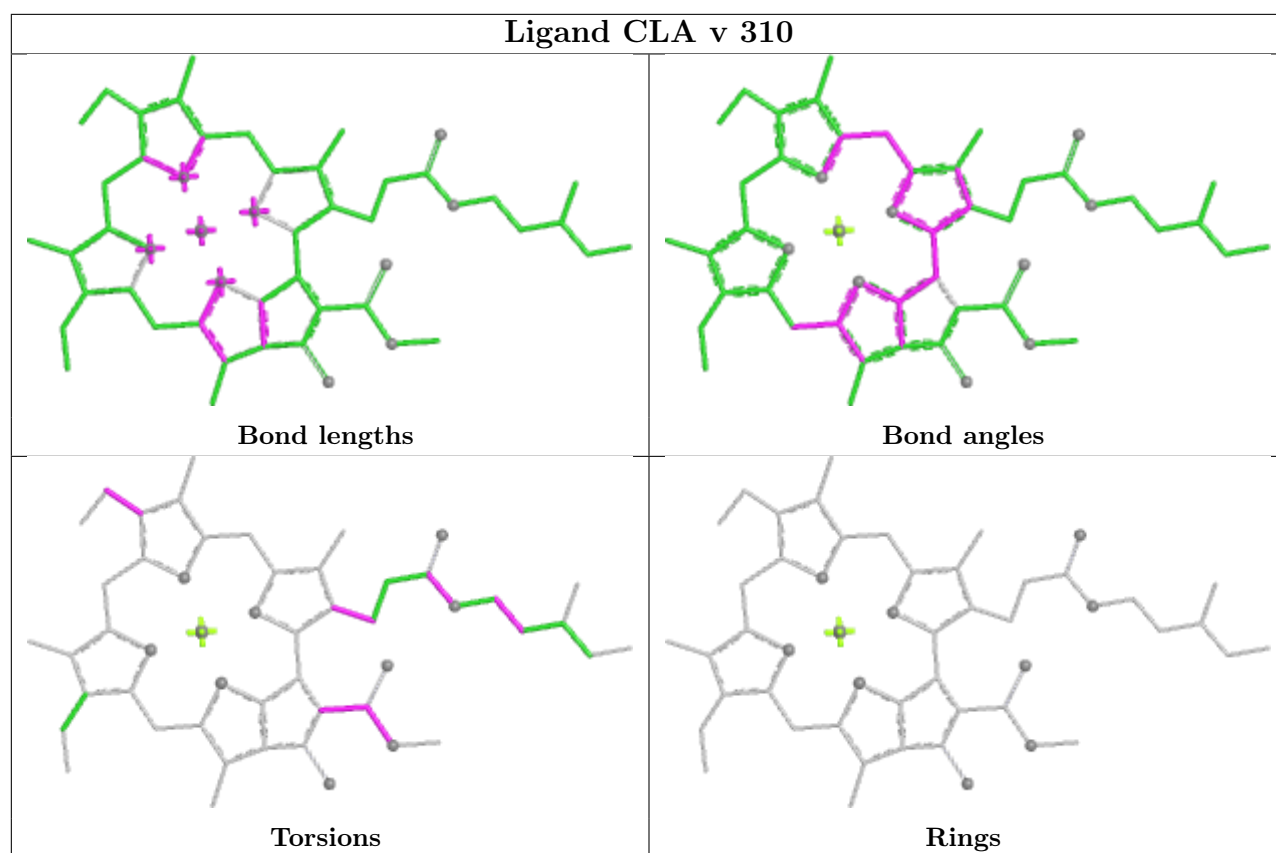
Ligand A1EB1 T 316**Ligand A1EB4 P 320**

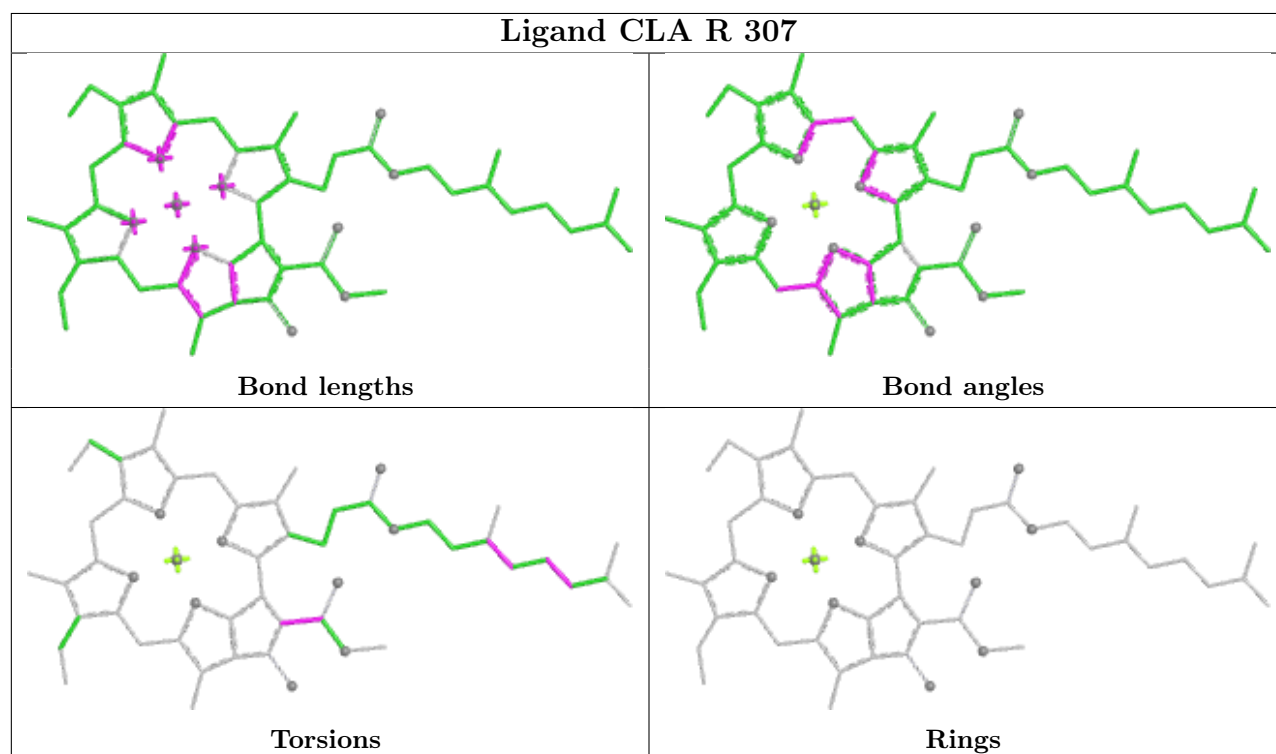
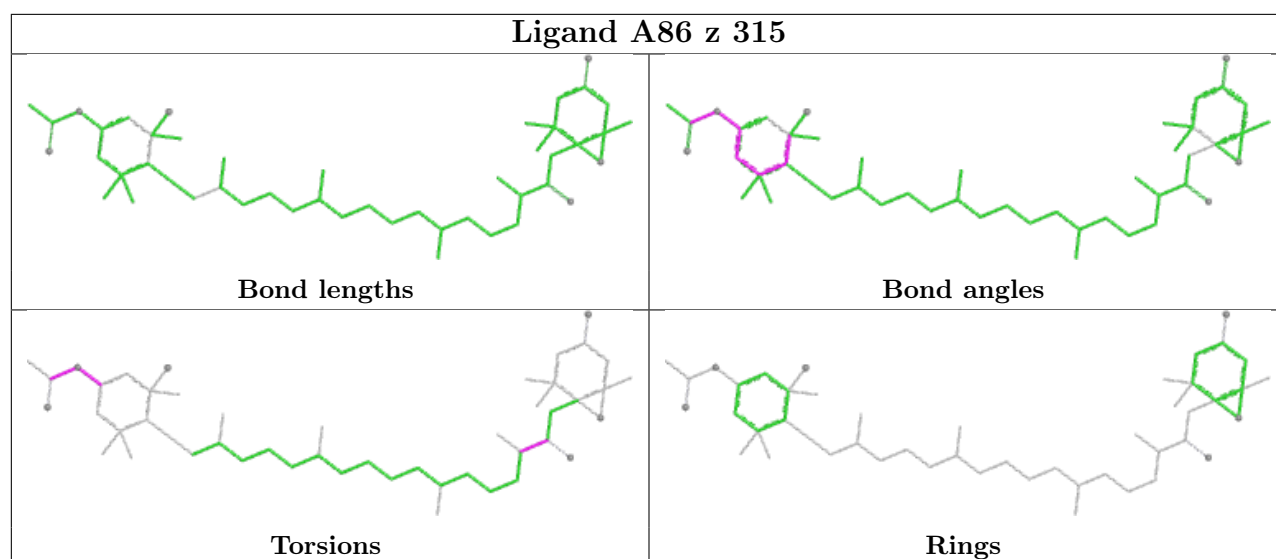
Ligand CLA K 307



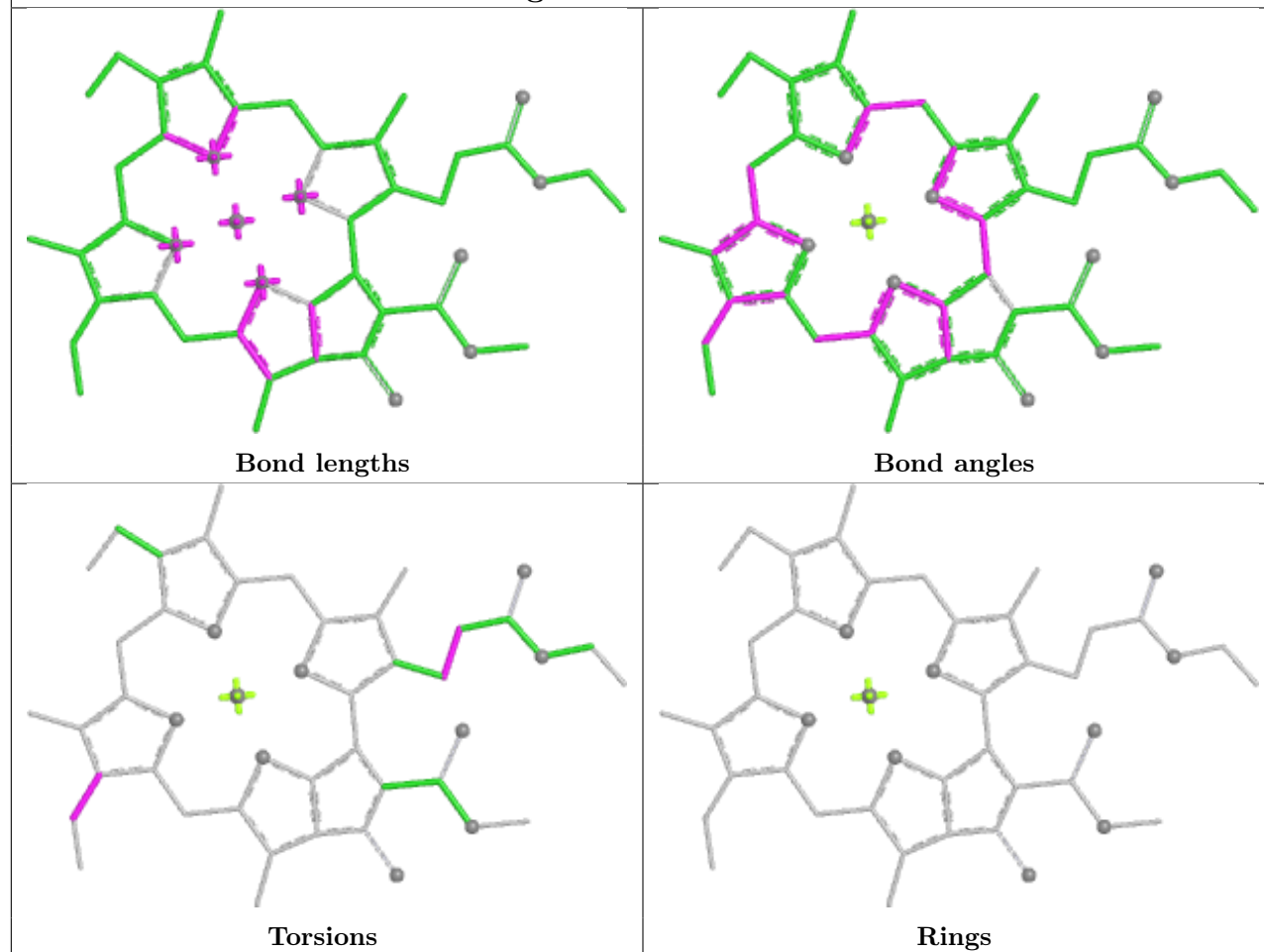
Ligand CLA q 310



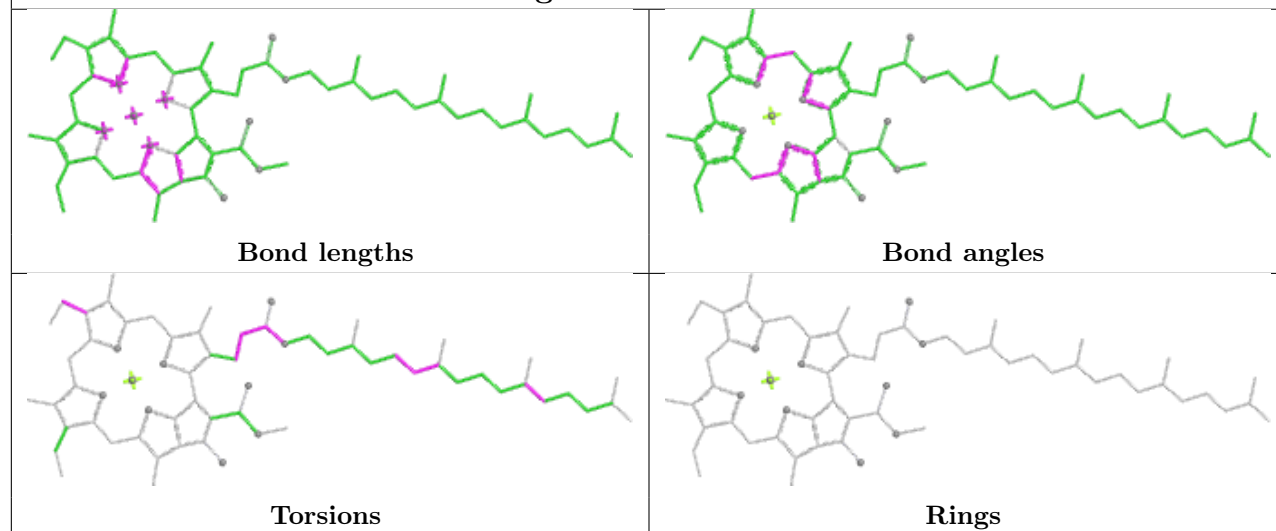


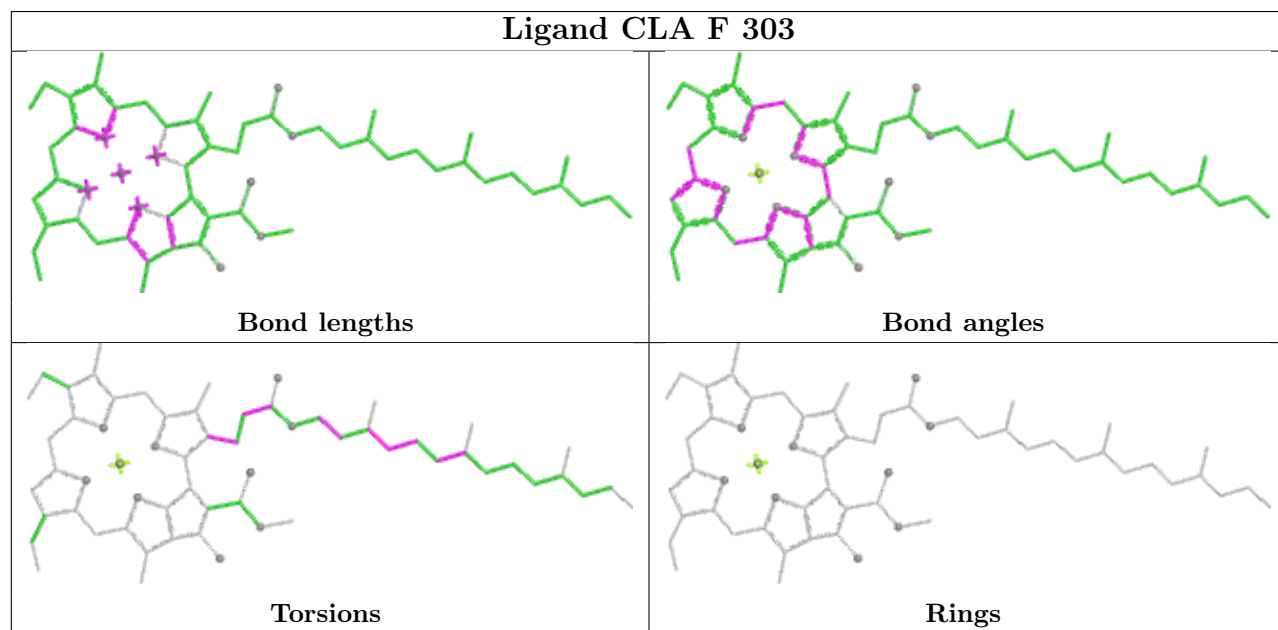
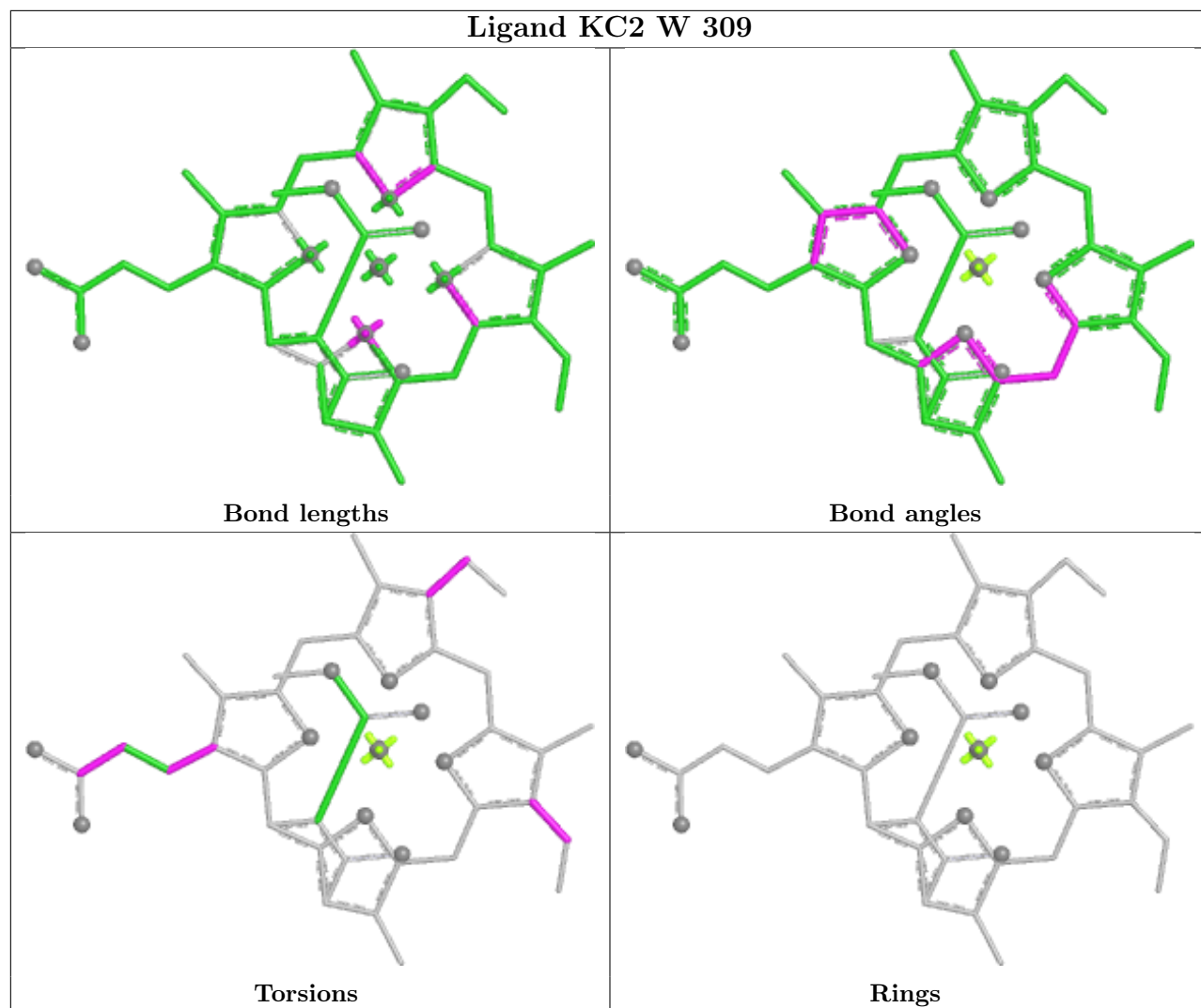


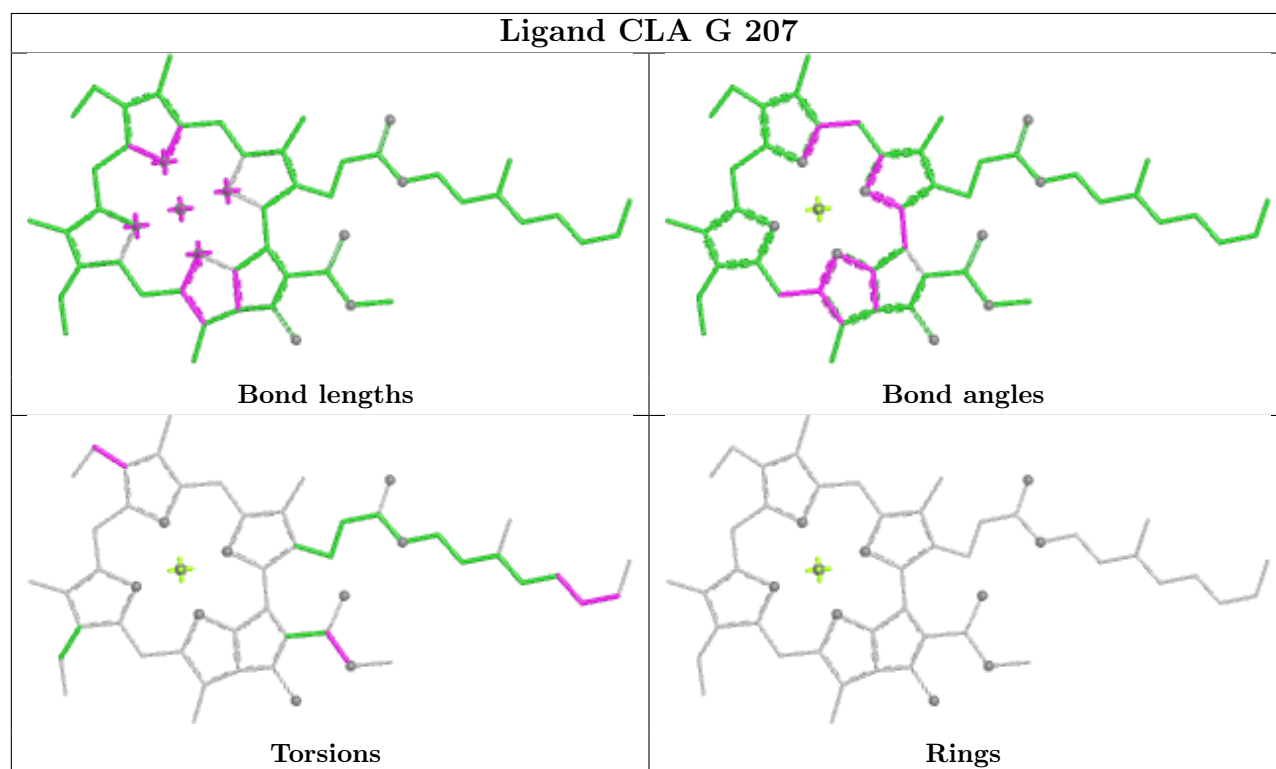
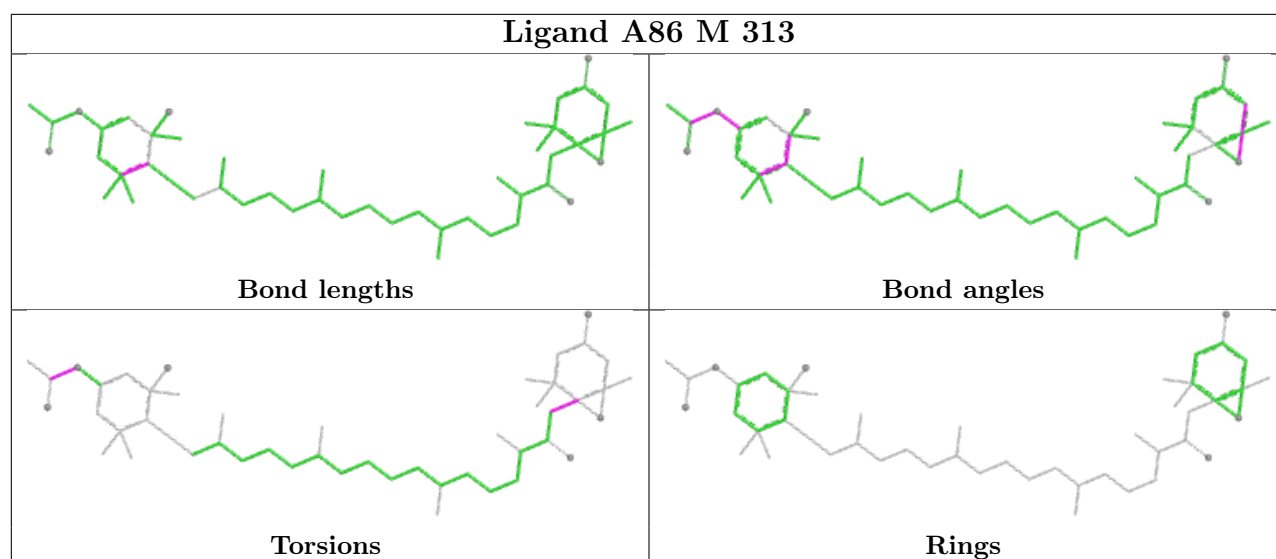
Ligand CLA A 301



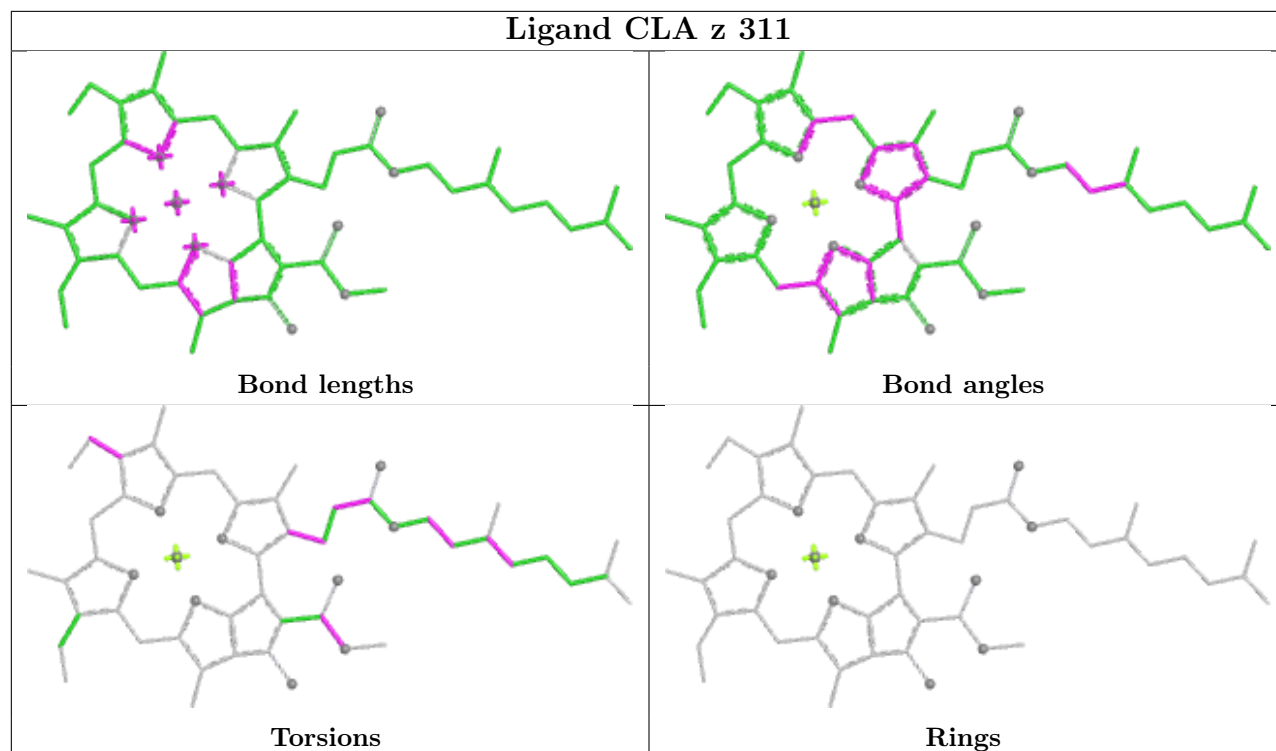
Ligand CLA b 814



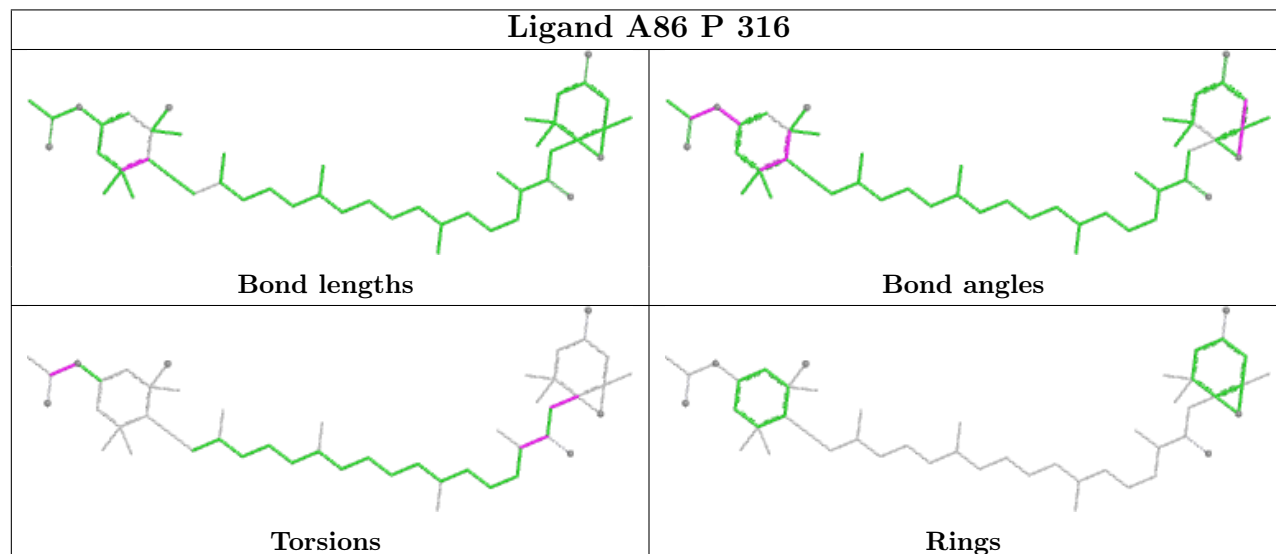




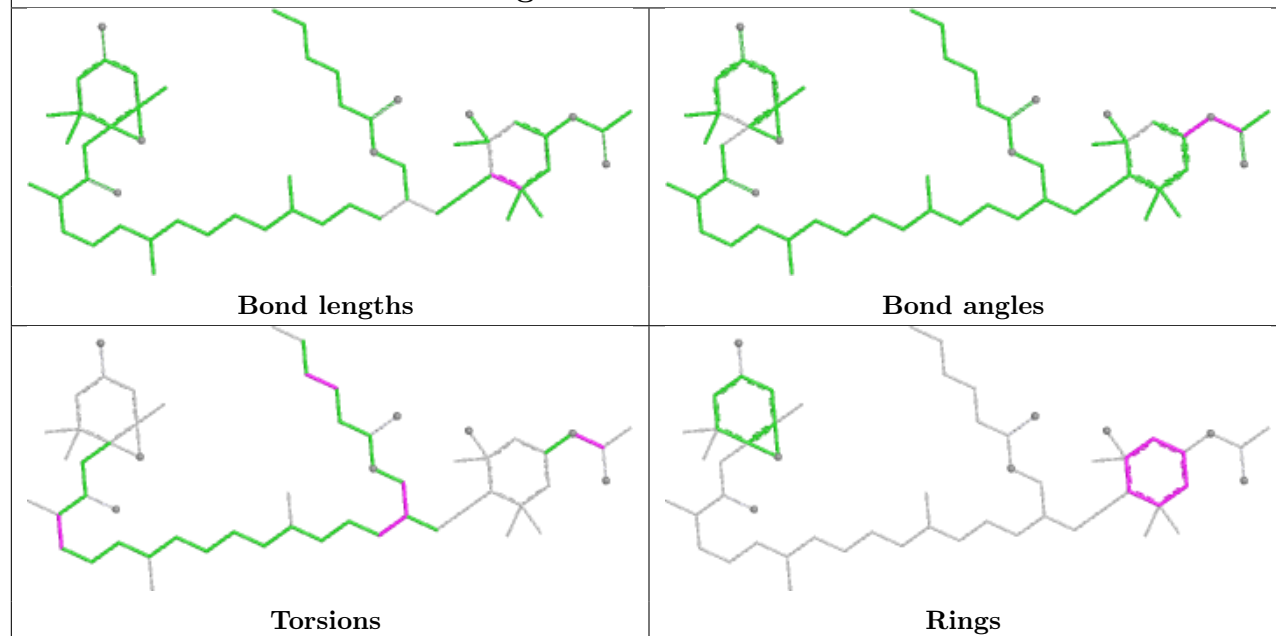
Ligand CLA z 311



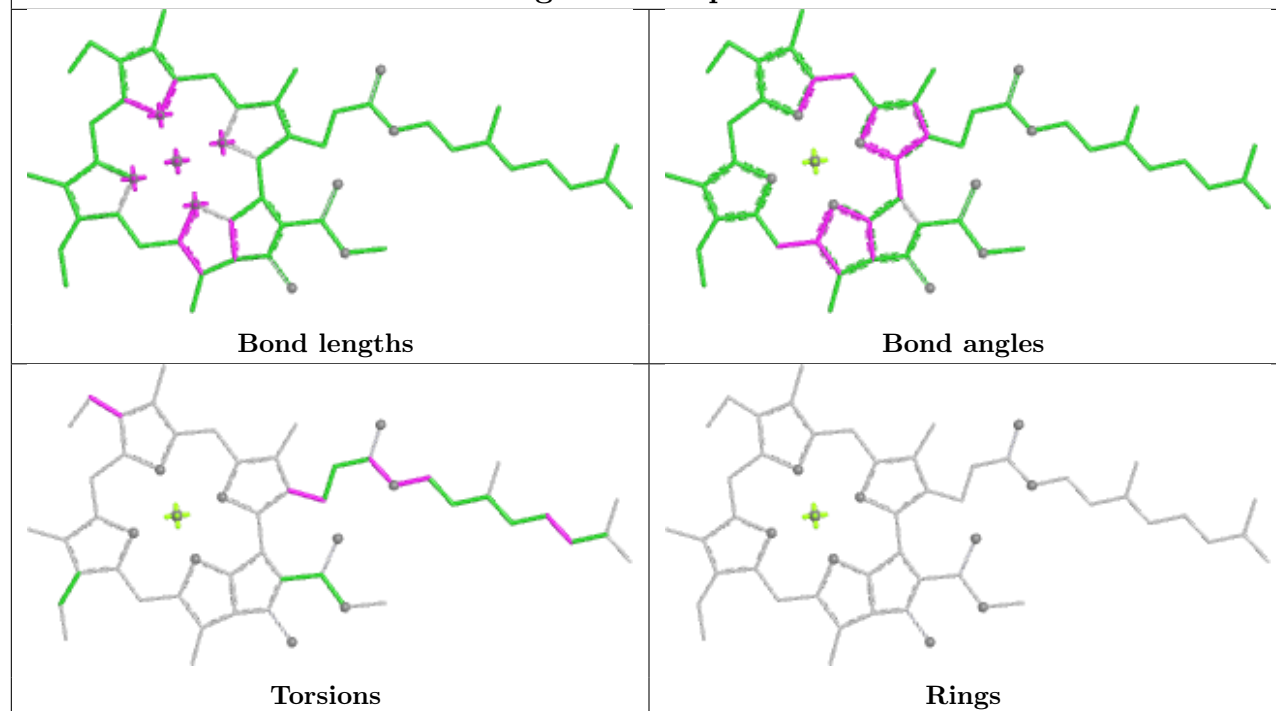
Ligand A86 P 316



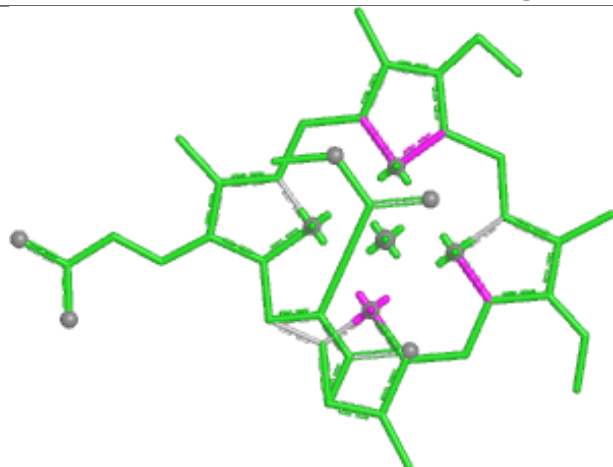
Ligand A1EB1 S 321



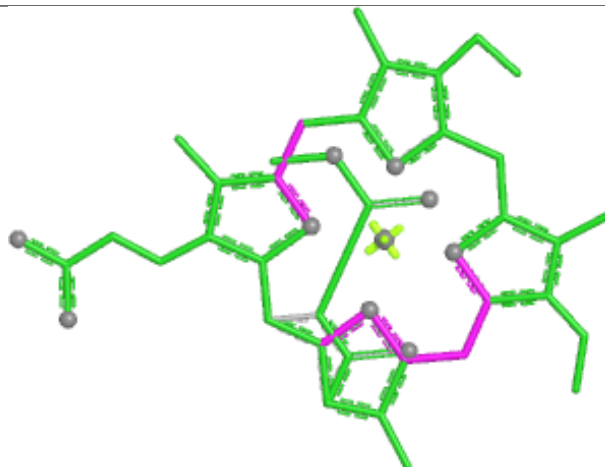
Ligand CLA p 307



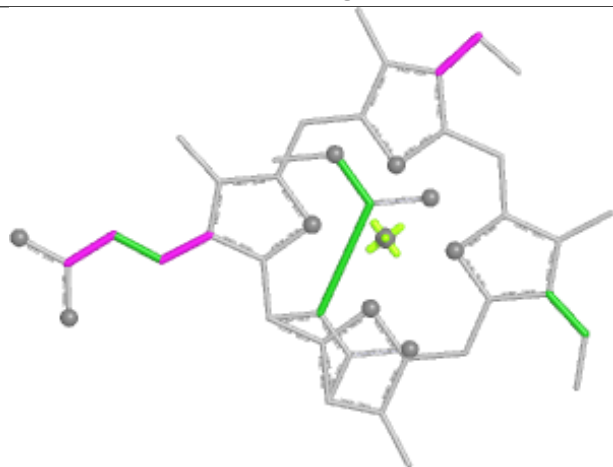
Ligand KC2 F 309



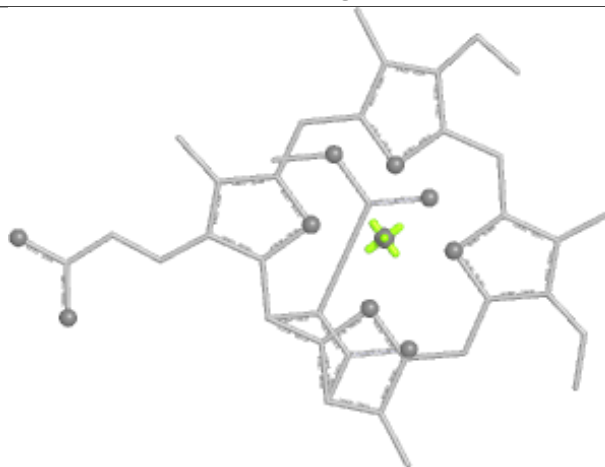
Bond lengths



Bond angles

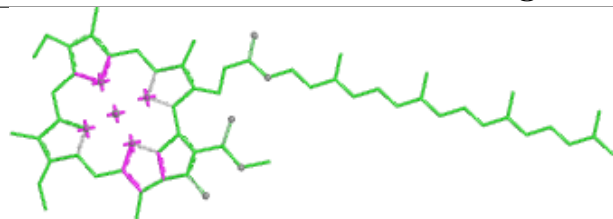


Torsions

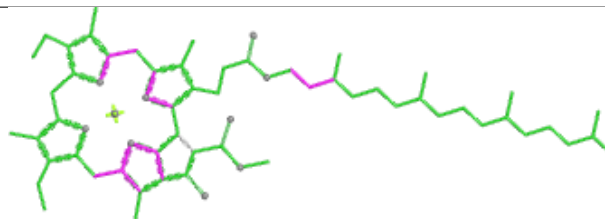


Rings

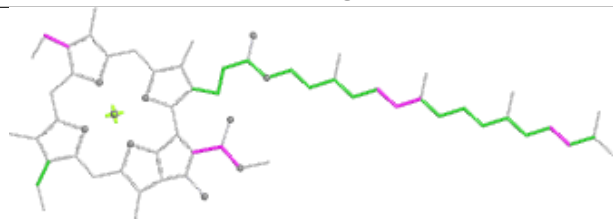
Ligand CLA a 841



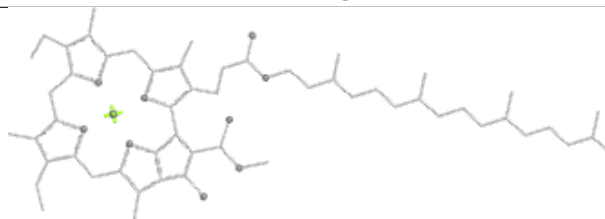
Bond lengths



Bond angles

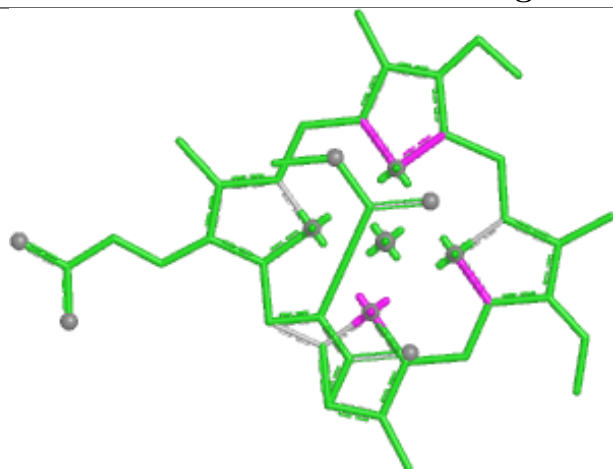


Torsions

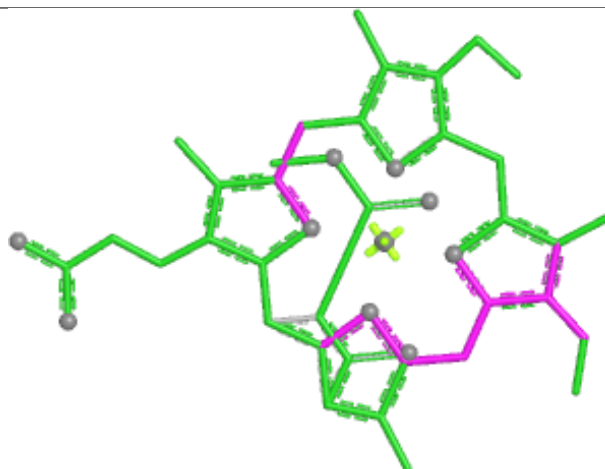


Rings

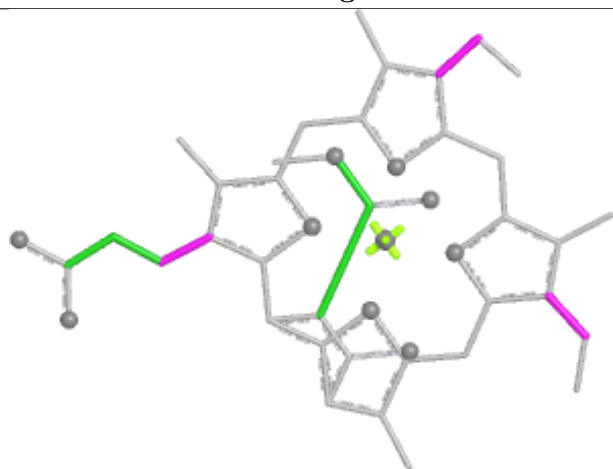
Ligand KC2 N 303



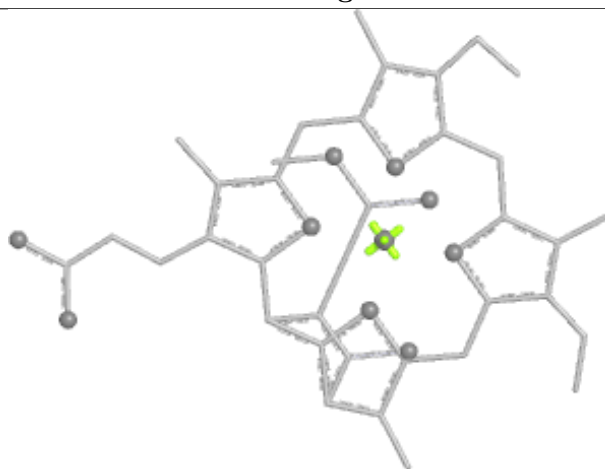
Bond lengths



Bond angles

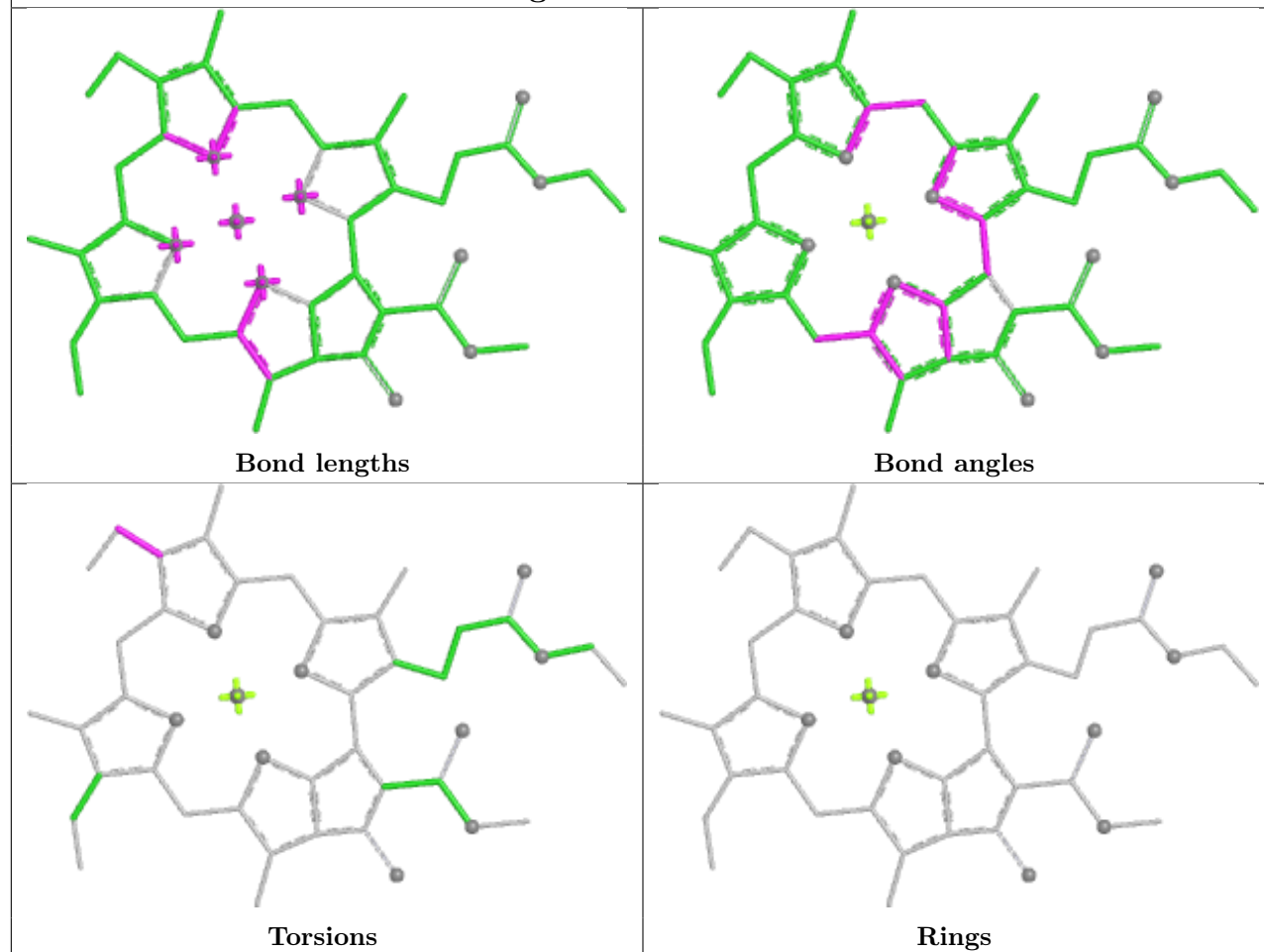


Torsions

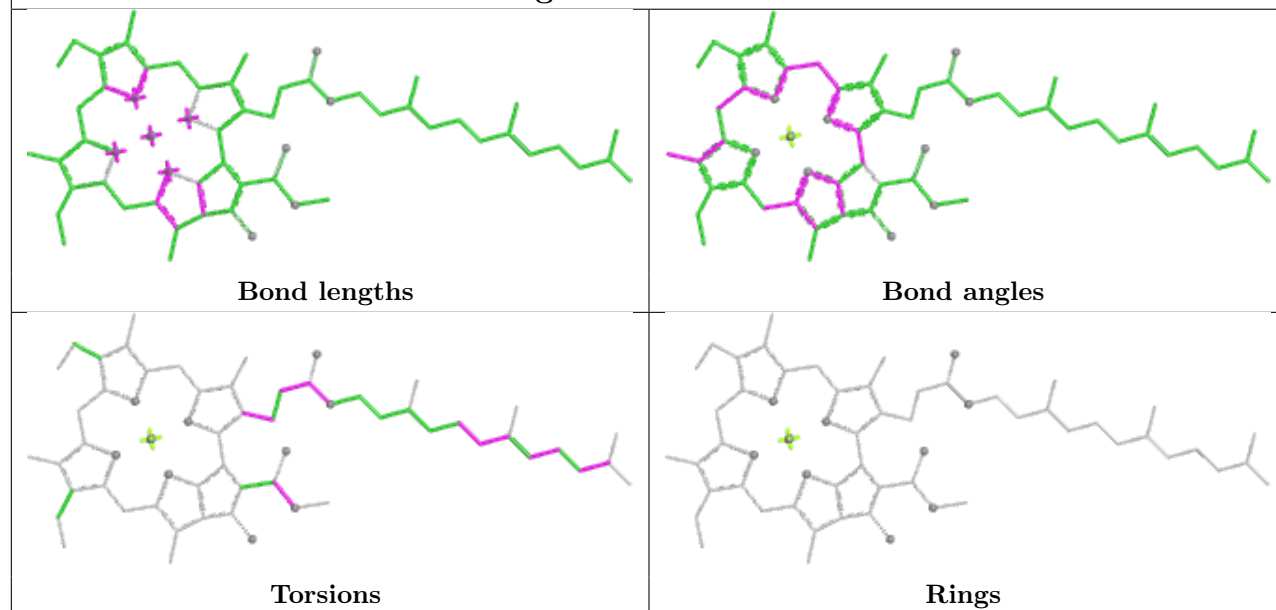


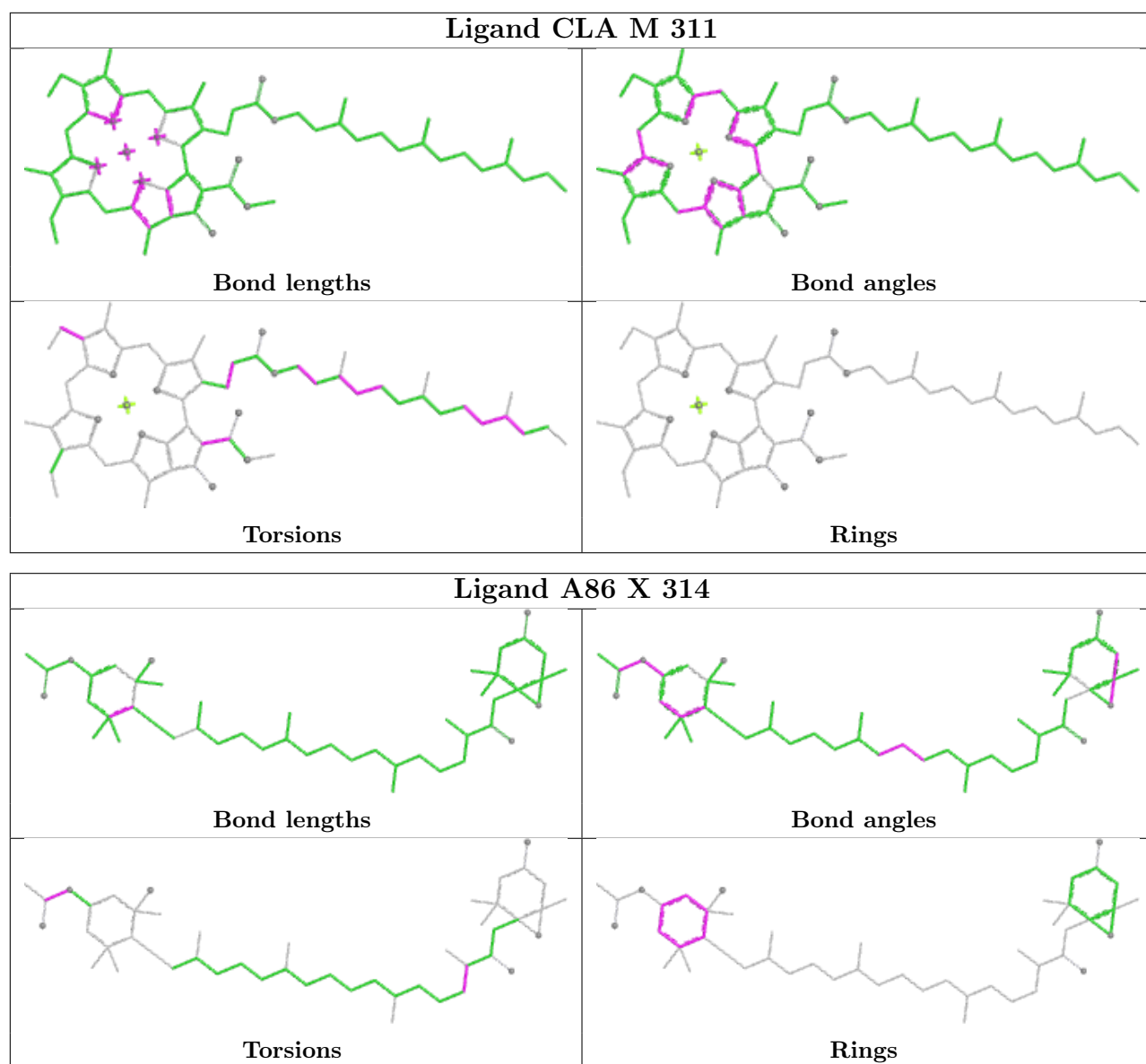
Rings

Ligand CLA L 301

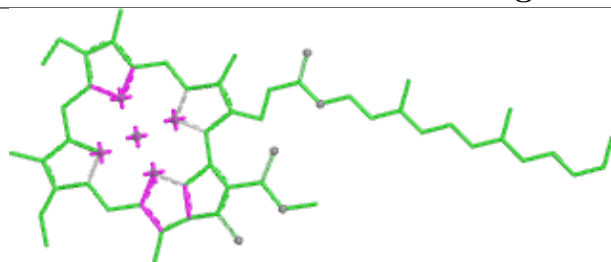


Ligand CLA v 307

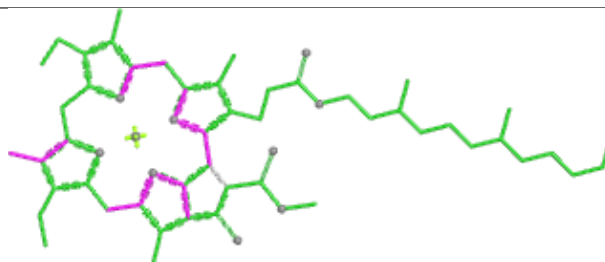




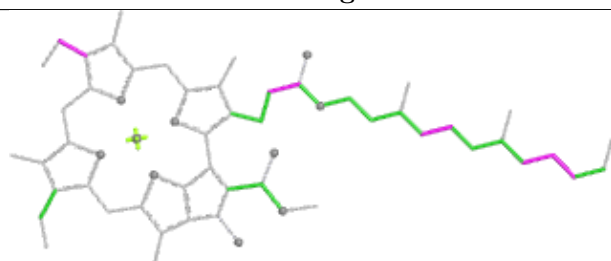
Ligand CLA P 307



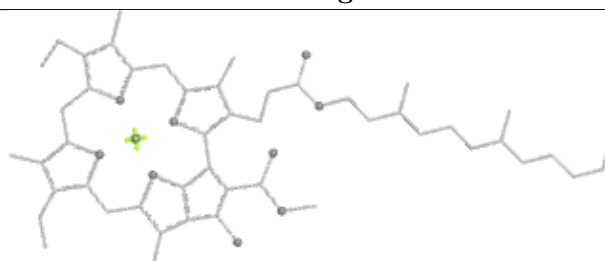
Bond lengths



Bond angles

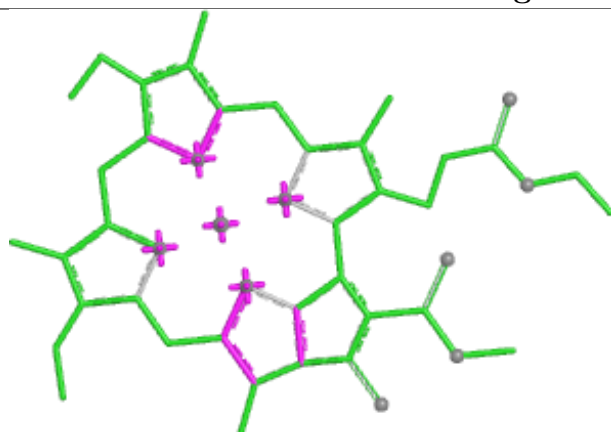


Torsions

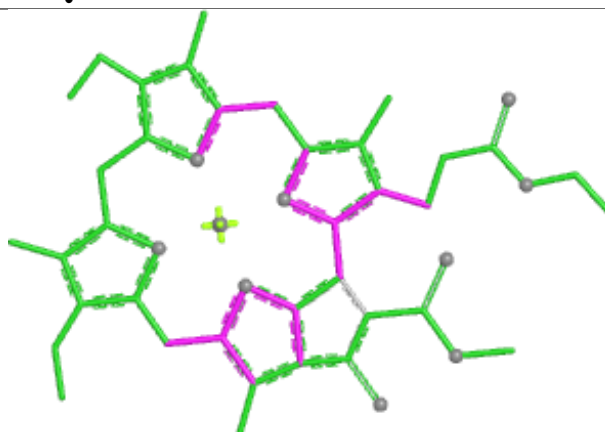


Rings

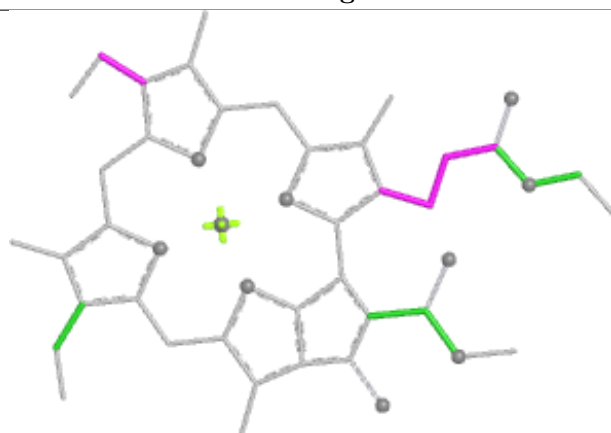
Ligand CLA Q 209



Bond lengths



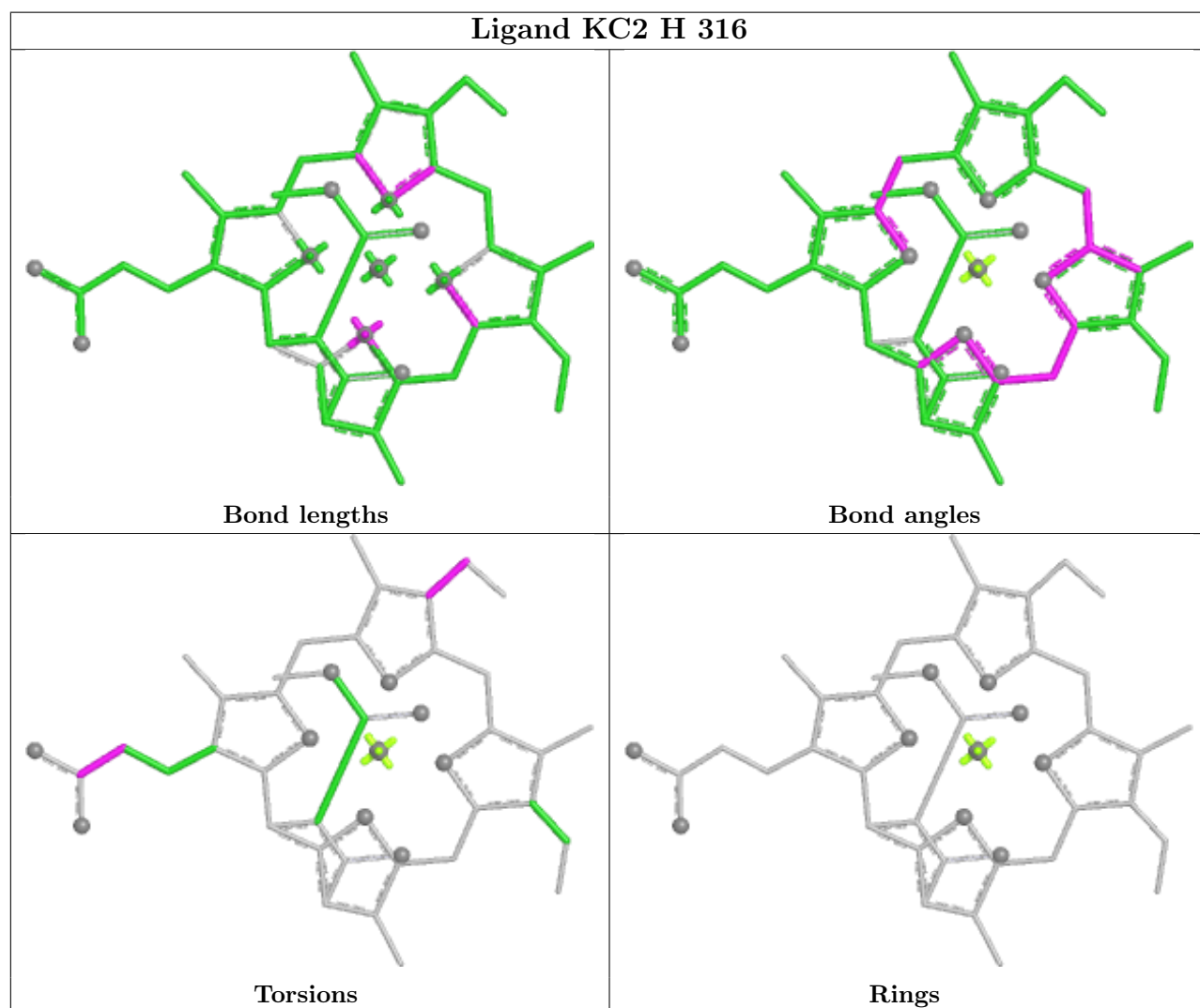
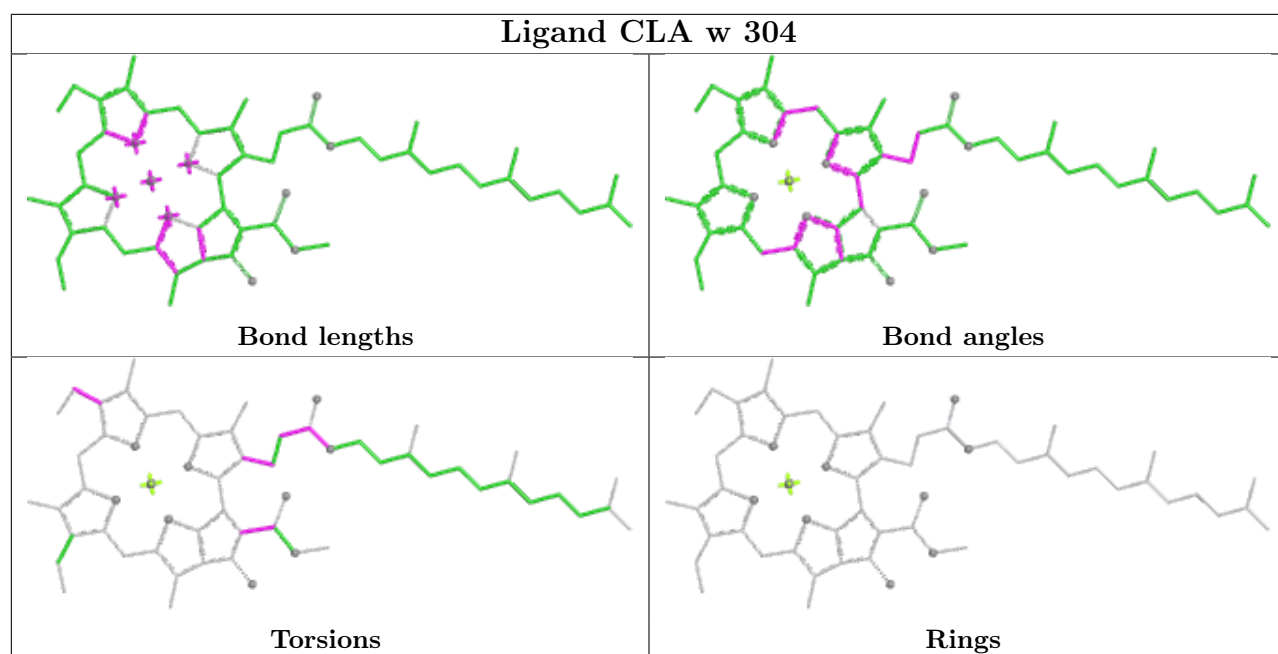
Bond angles

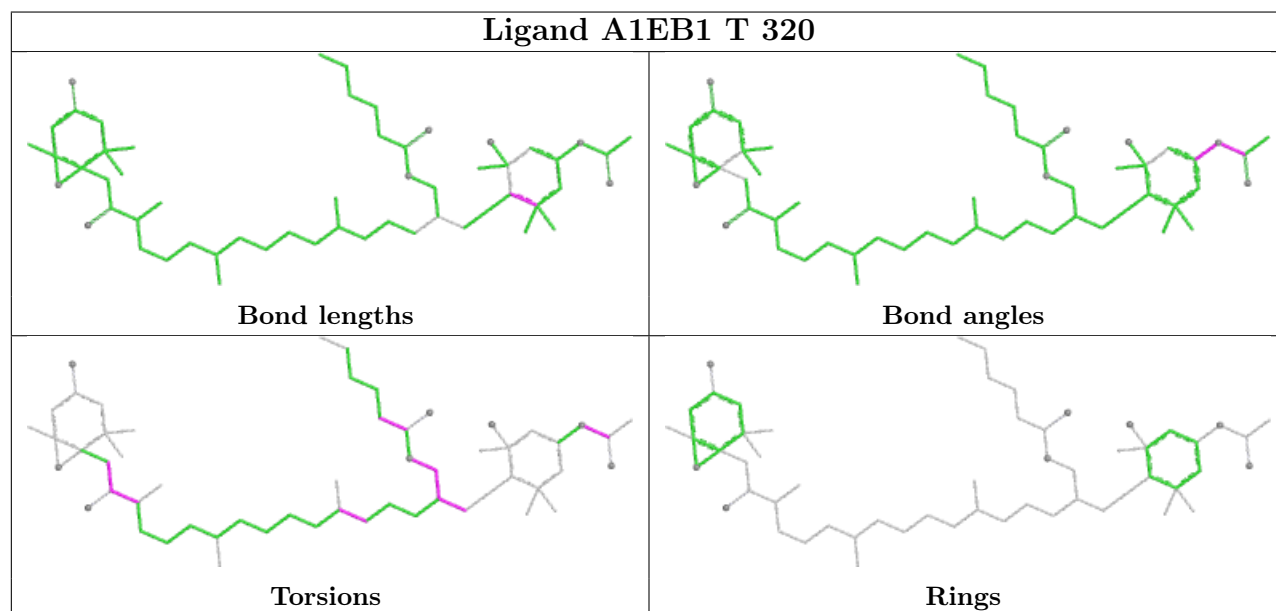
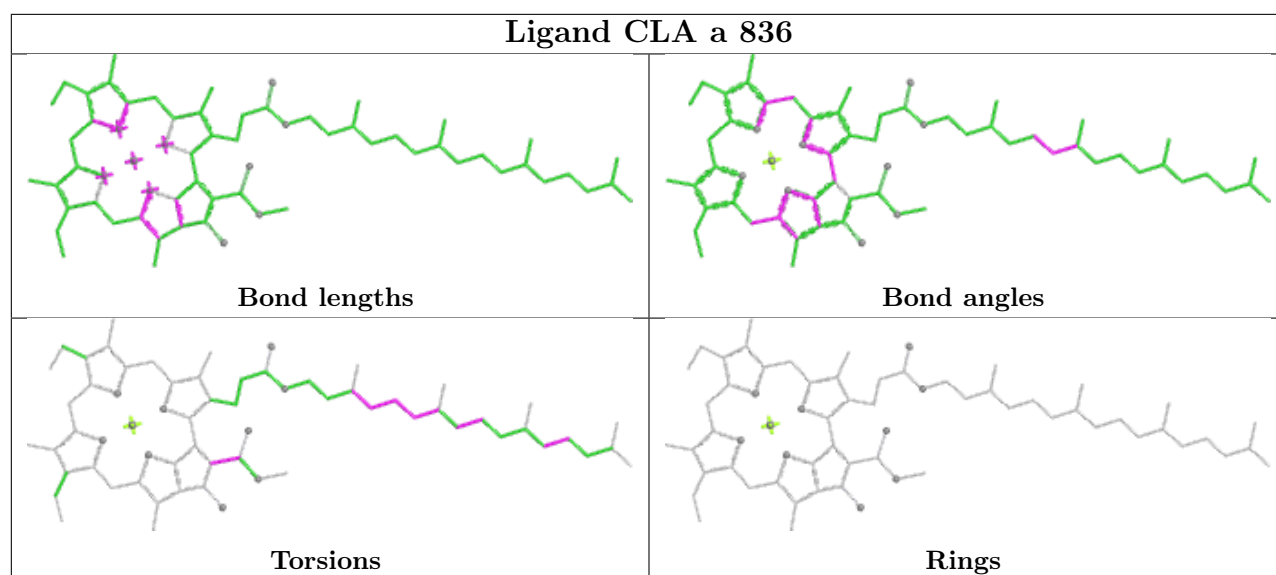


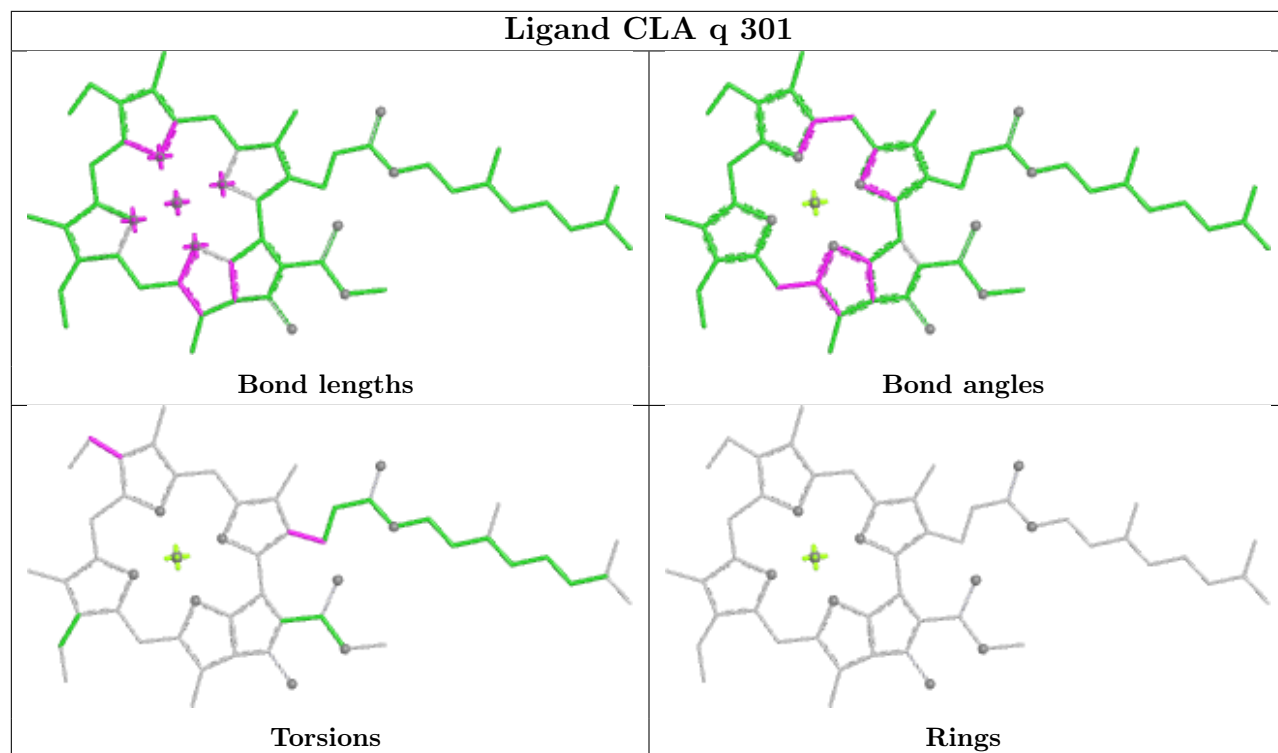
Torsions

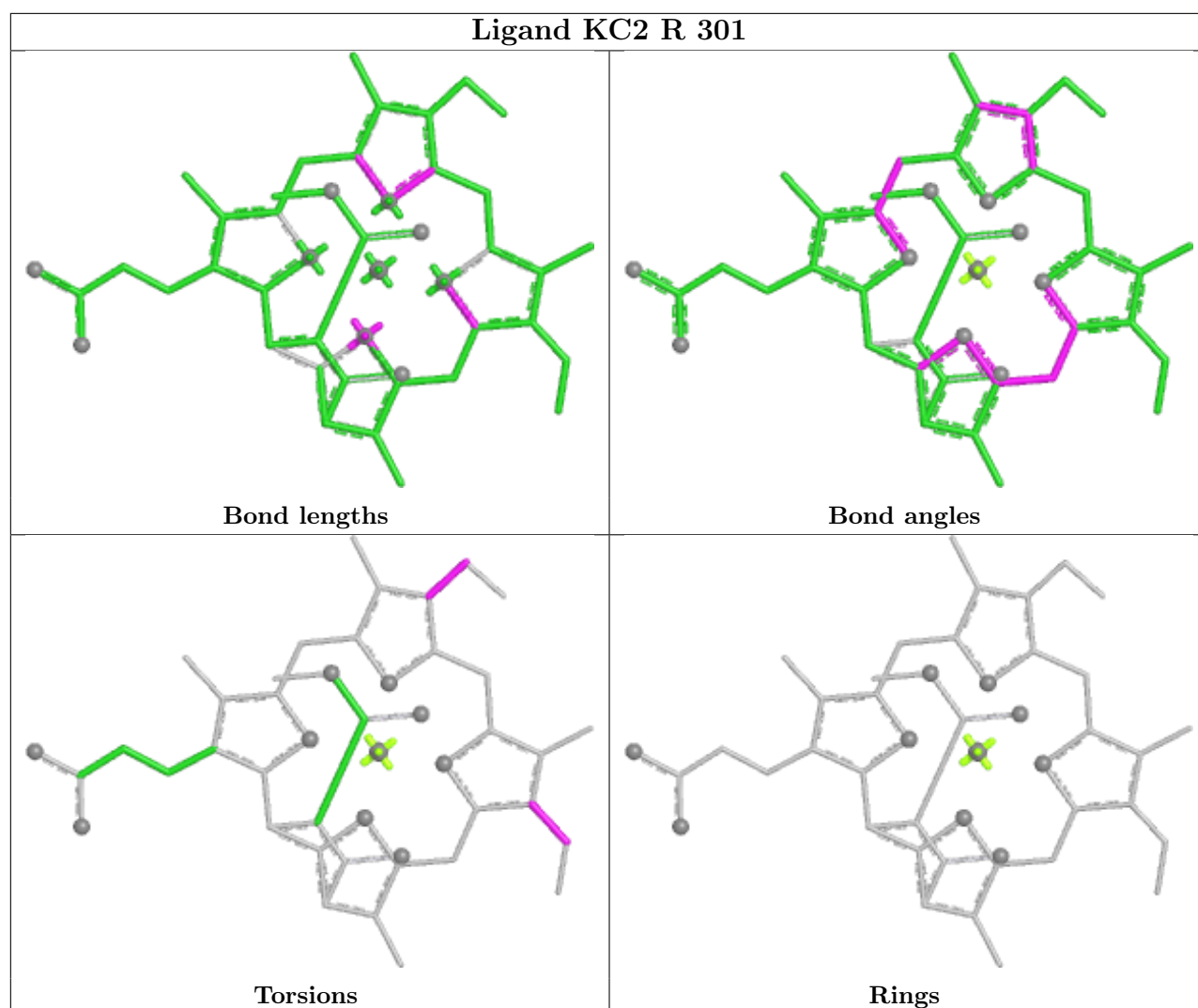


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

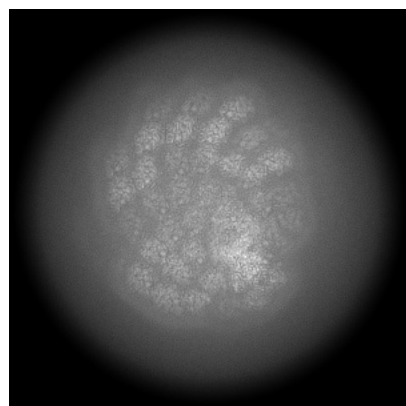
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64087. These allow visual inspection of the internal detail of the map and identification of artifacts.

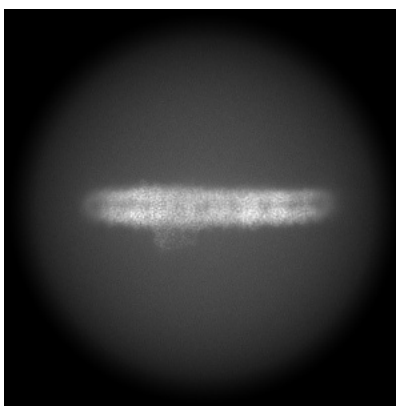
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

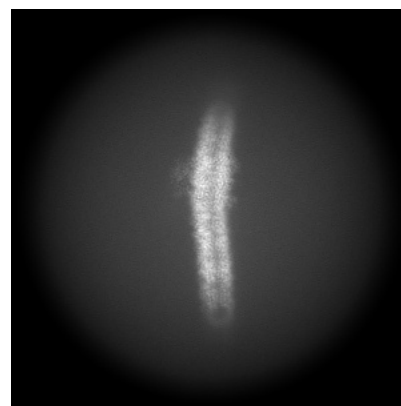
6.1.1 Primary map



X

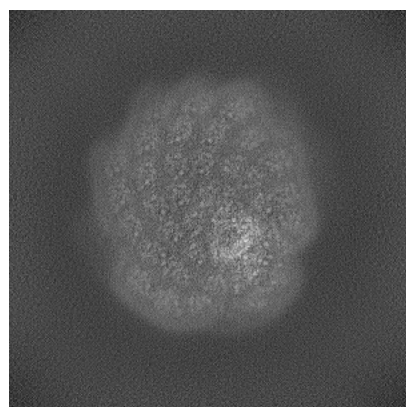


Y

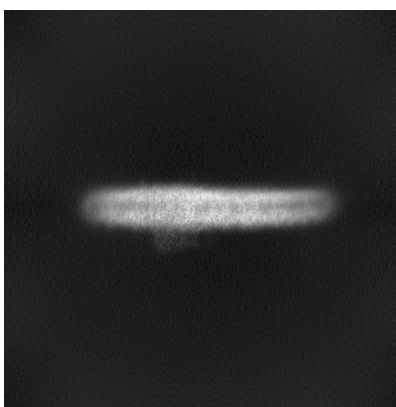


Z

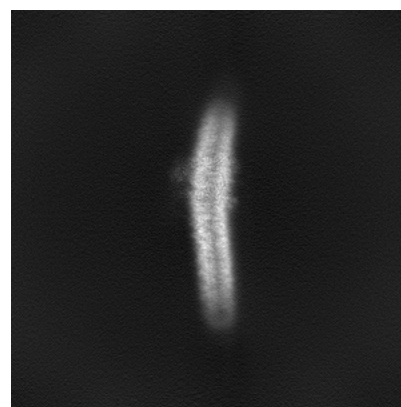
6.1.2 Raw map



X



Y

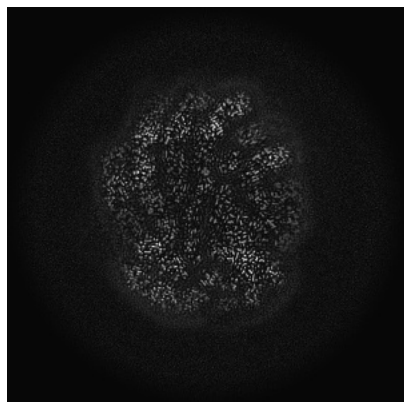


Z

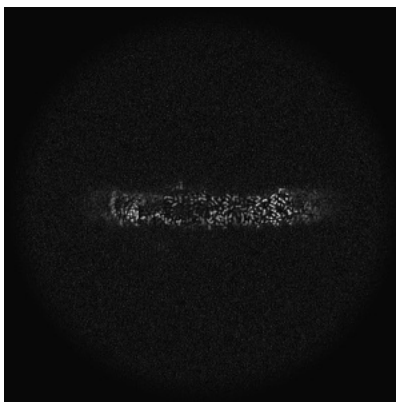
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

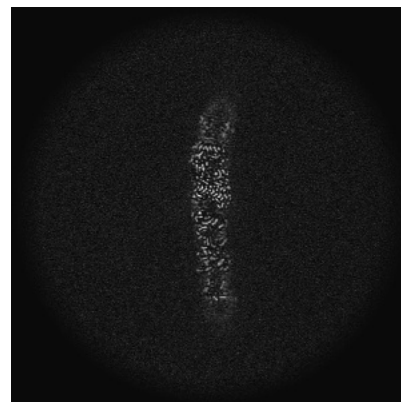
6.2.1 Primary map



X Index: 250

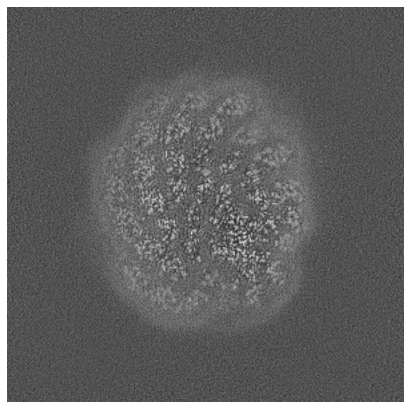


Y Index: 250

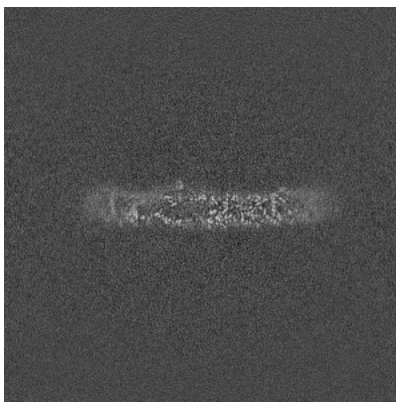


Z Index: 250

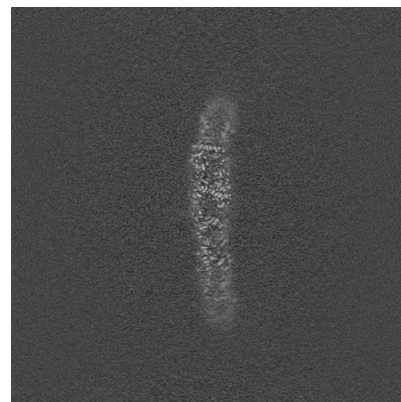
6.2.2 Raw map



X Index: 250



Y Index: 250

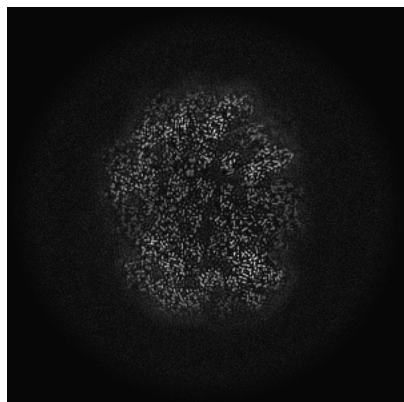


Z Index: 250

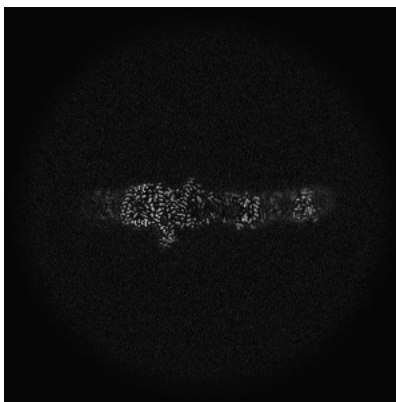
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

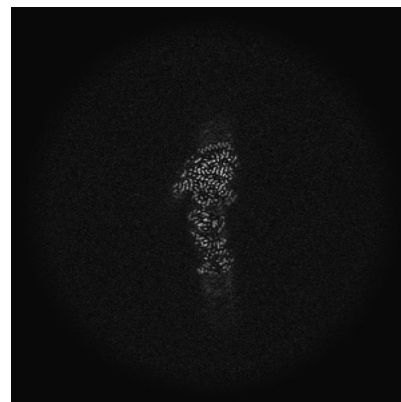
6.3.1 Primary map



X Index: 244

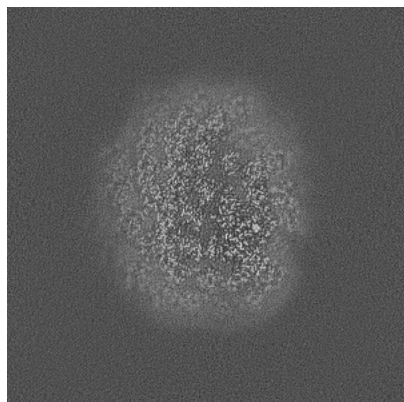


Y Index: 285



Z Index: 191

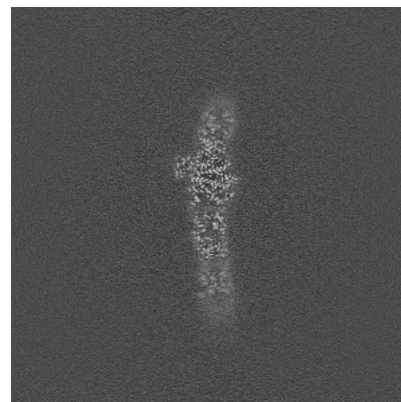
6.3.2 Raw map



X Index: 242



Y Index: 295

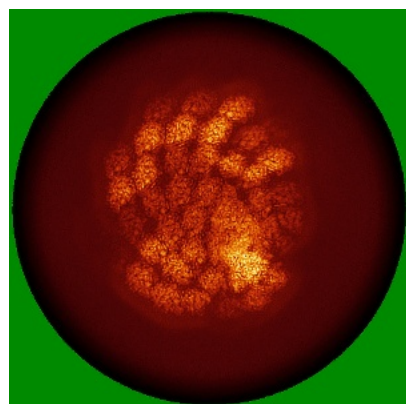


Z Index: 230

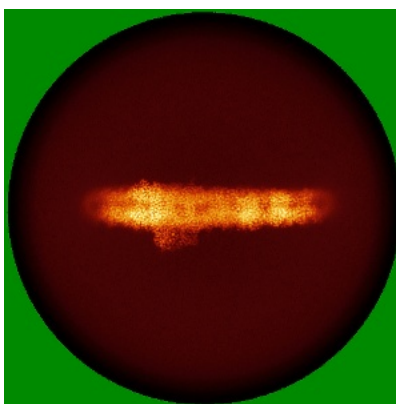
The images above show the largest variance slices of the map in three orthogonal directions.

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

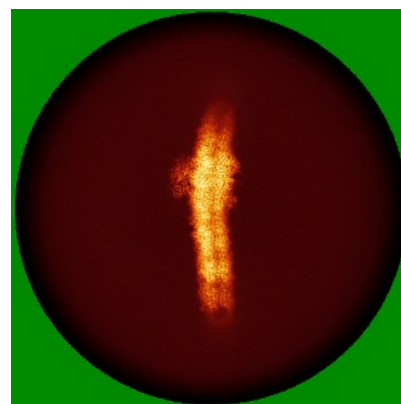
6.4.1 Primary map



X

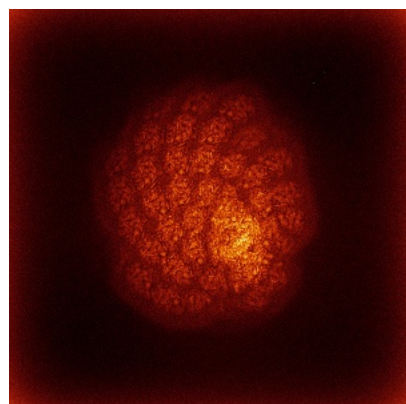


Y

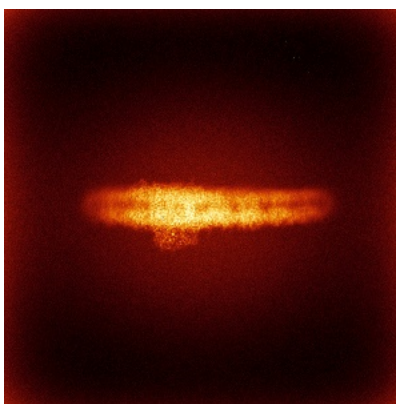


Z

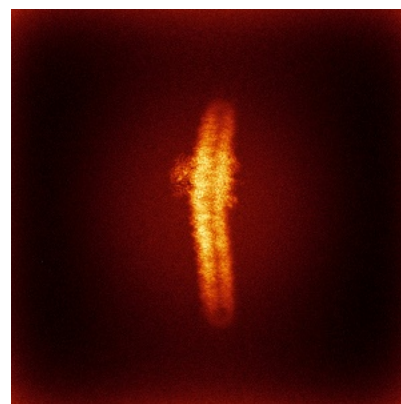
6.4.2 Raw map



X



Y

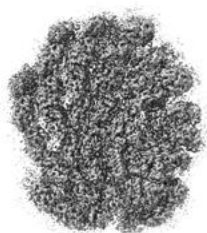


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



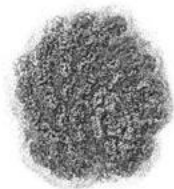
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

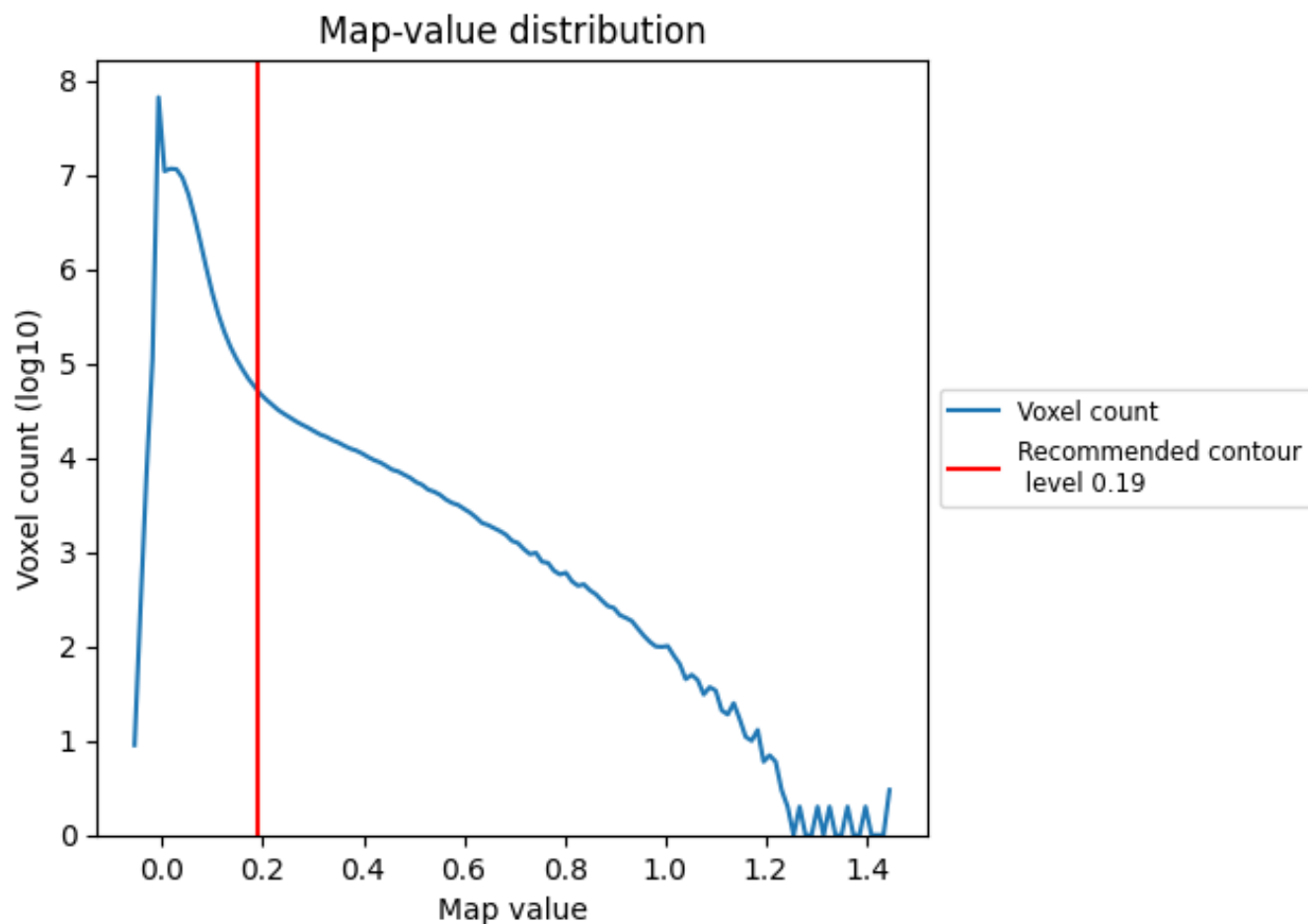
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

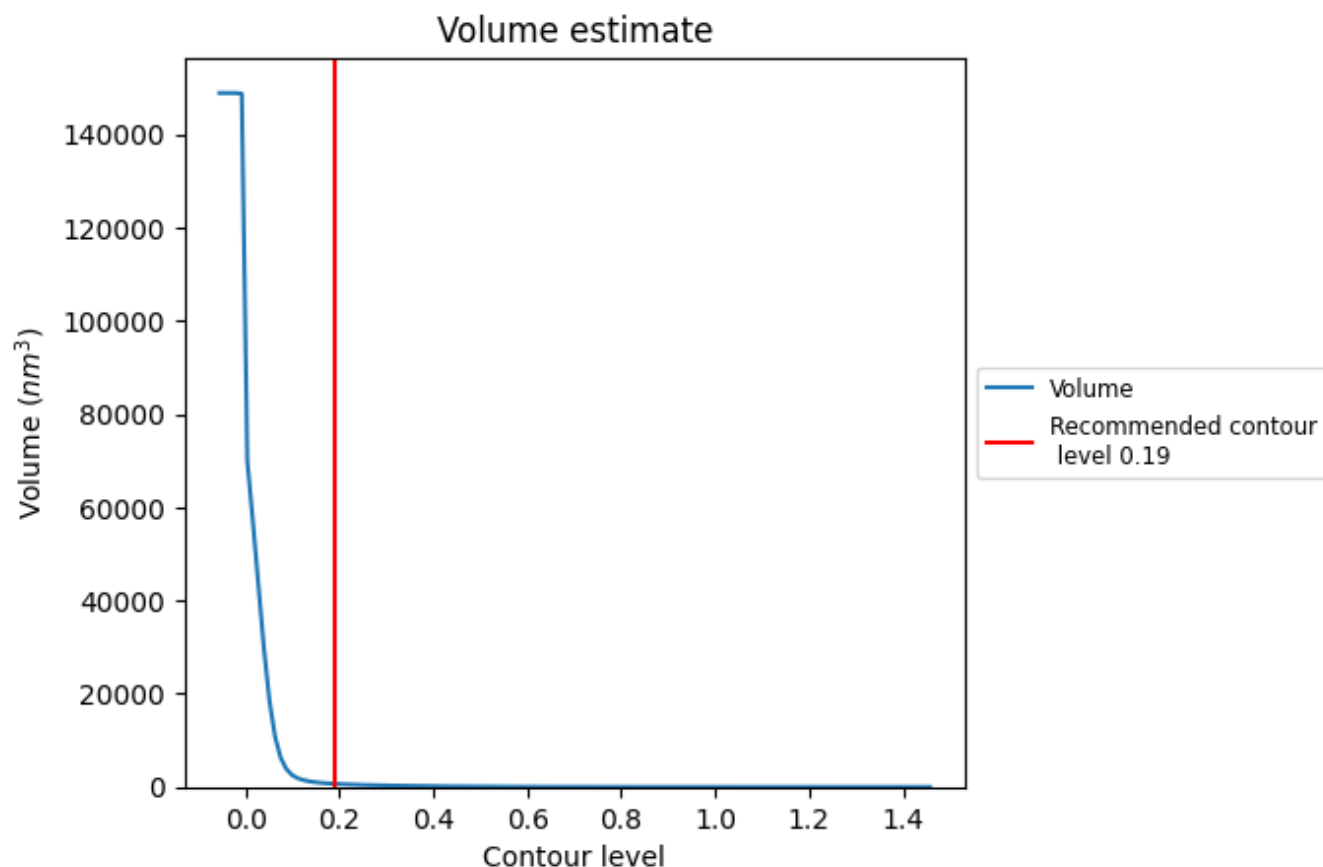
This section contains the results of statistical analysis of the map.

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.

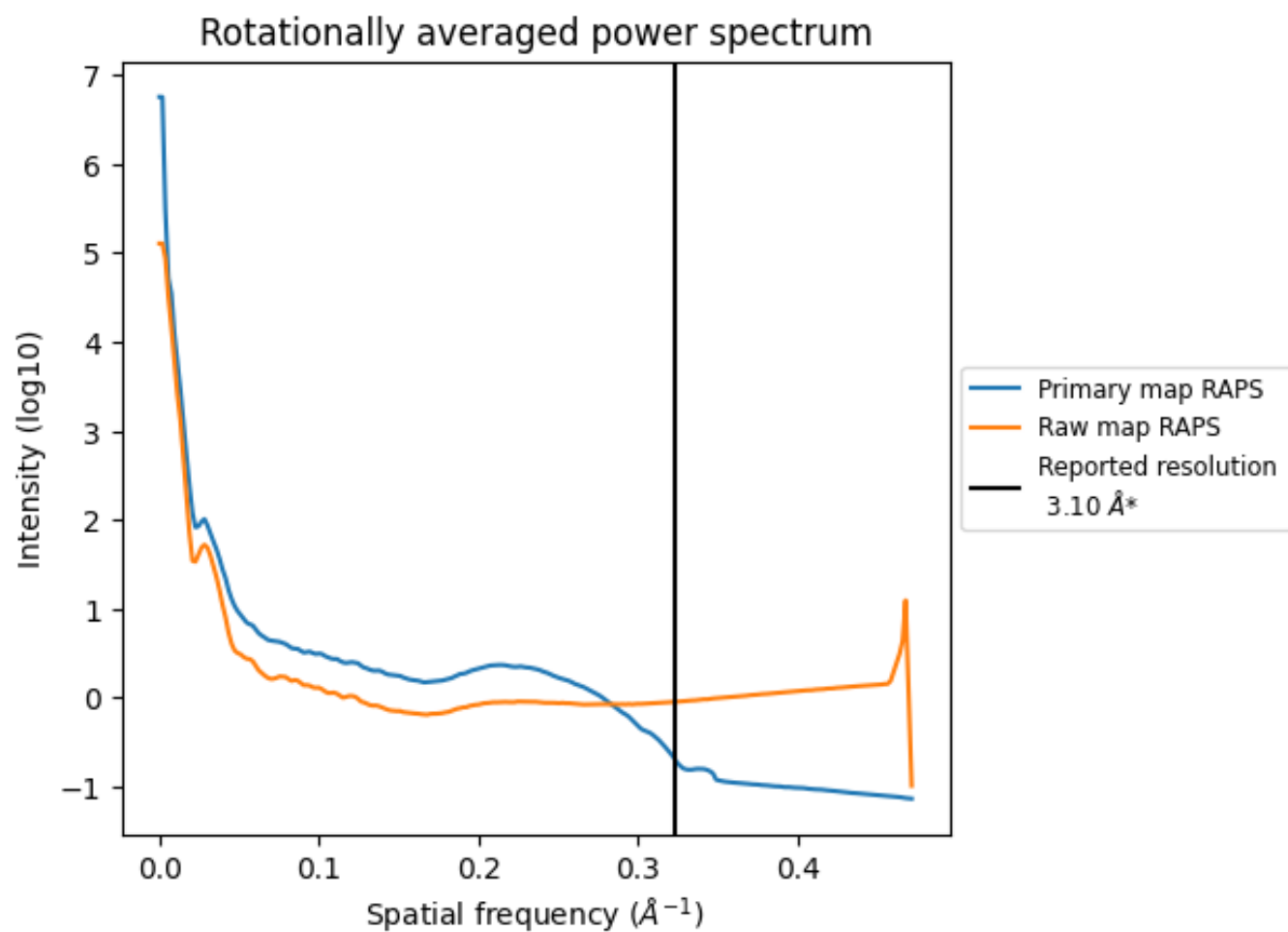
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 675 nm^3 ; this corresponds to an approximate mass of 610 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 ⓘ

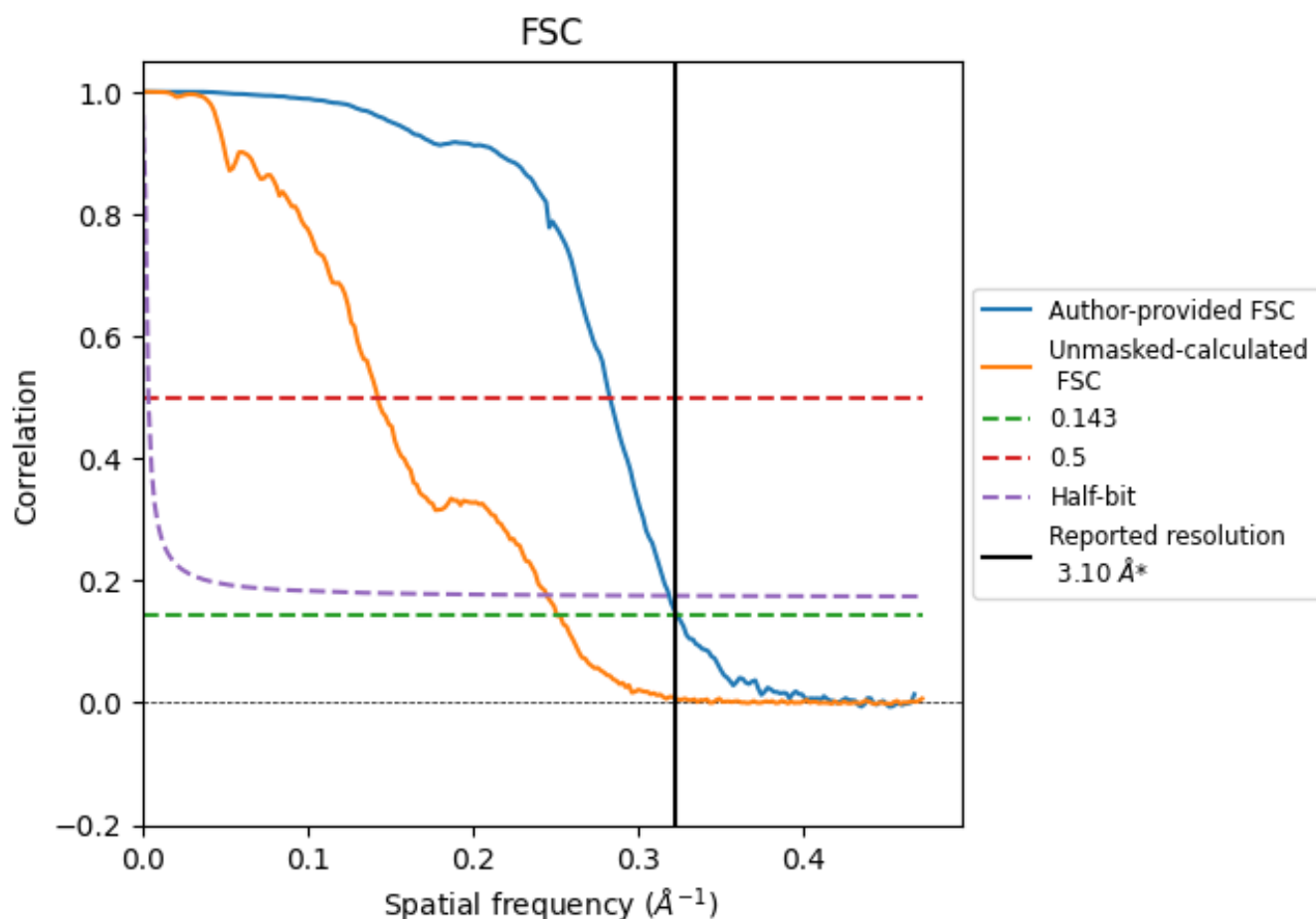


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

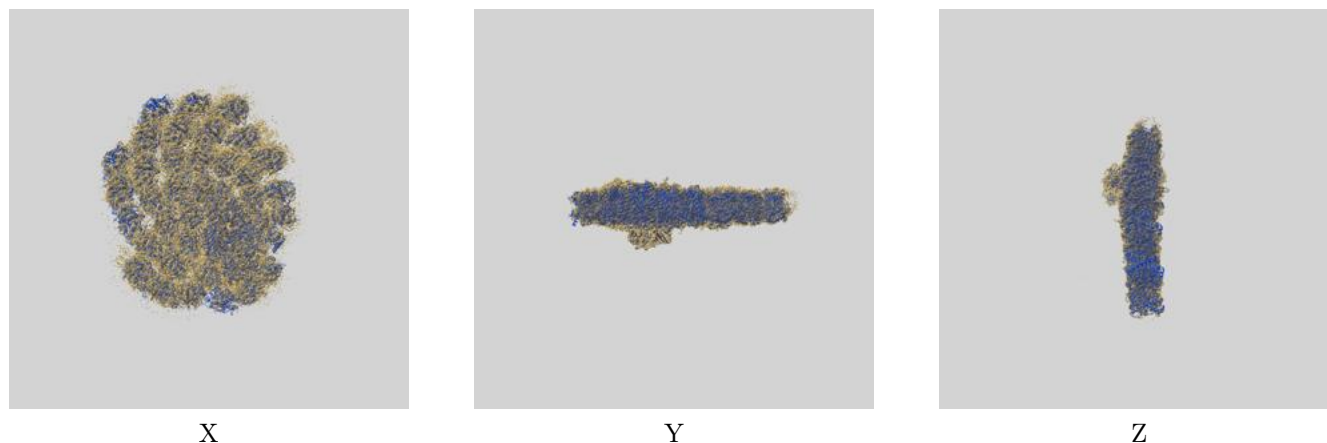
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.54	3.14
Unmasked-calculated*	3.99	7.02	4.09

*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 3.99 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

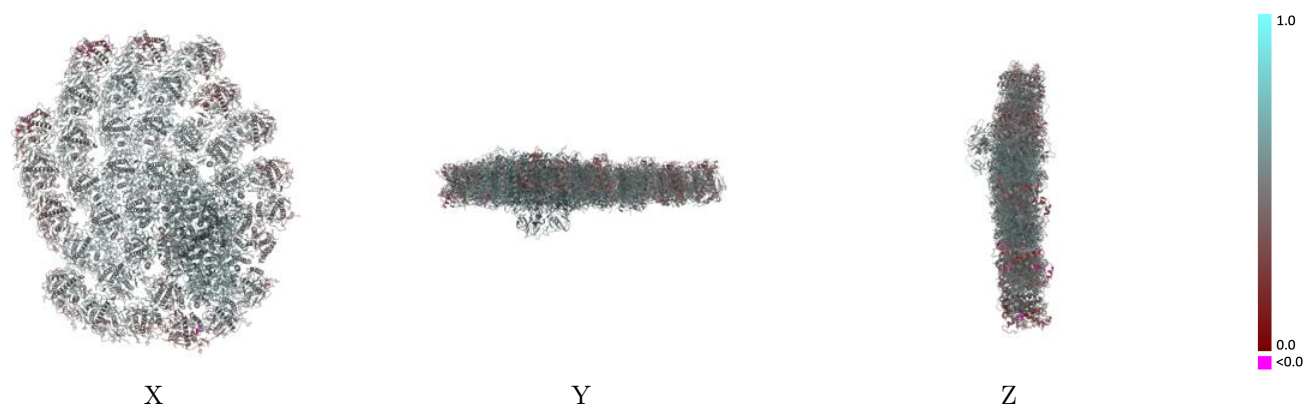
This section contains information regarding the fit between EMDB map EMD-64087 and PDB model 9UEN. Per-residue inclusion information can be found in section [3](#) on page [66](#).

9.1 Map-model overlay [i](#)



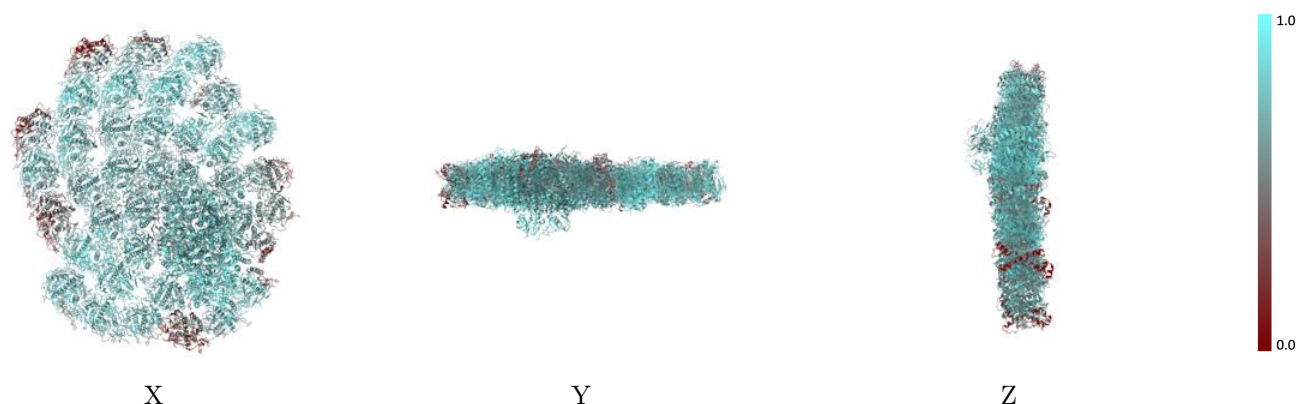
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



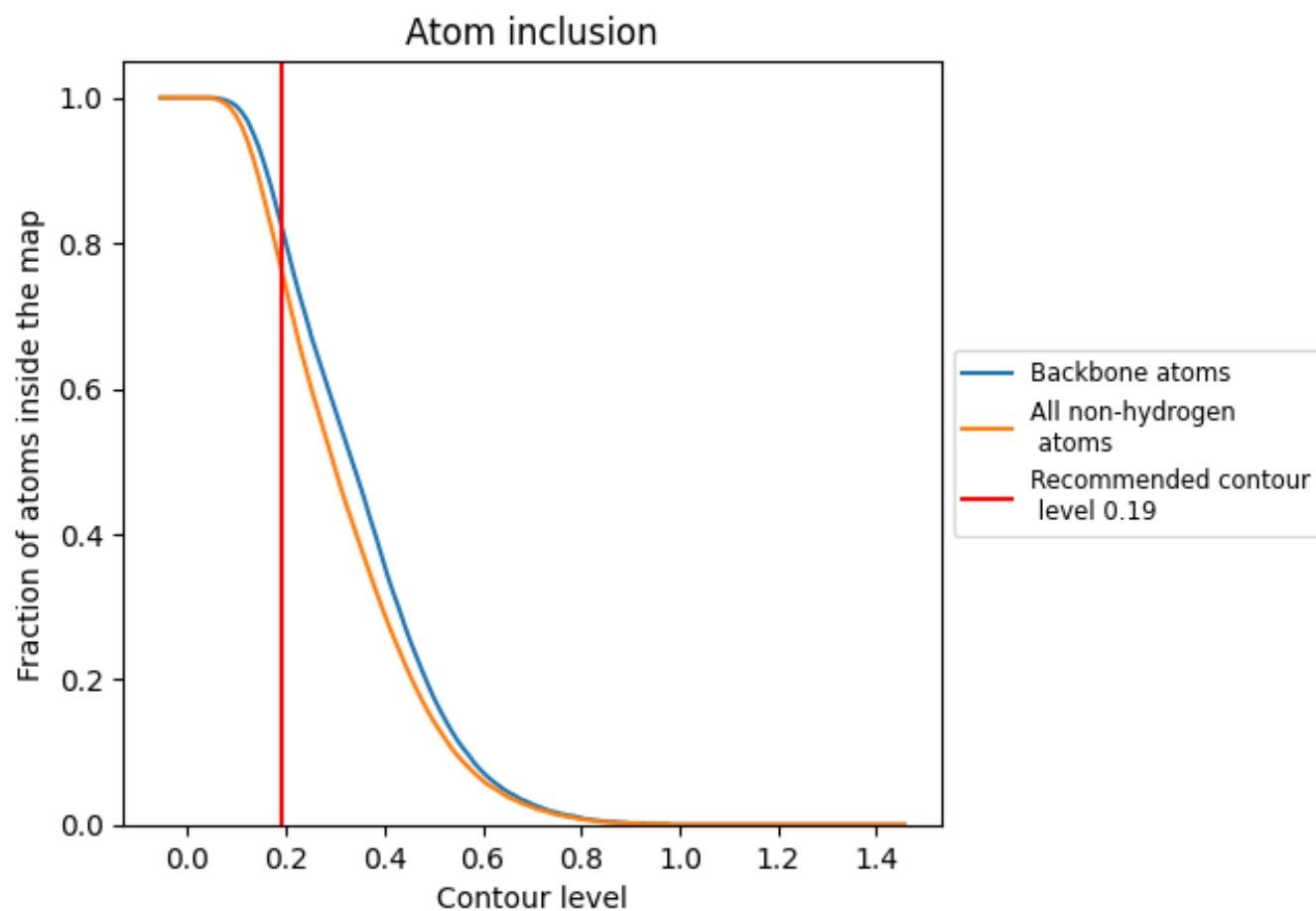
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5070
A	 0.8540	 0.5430
B	 0.5090	 0.4400
C	 0.7470	 0.4950
D	 0.8110	 0.5570
E	 0.8030	 0.5560
F	 0.8020	 0.4930
G	 0.8550	 0.5160
H	 0.7410	 0.4910
I	 0.7790	 0.5340
J	 0.3120	 0.3700
K	 0.8660	 0.5290
L	 0.5510	 0.4440
M	 0.7940	 0.5510
N	 0.8930	 0.5440
O	 0.7300	 0.5150
P	 0.8450	 0.5380
Q	 0.7710	 0.4710
R	 0.7610	 0.5210
S	 0.7700	 0.4820
T	 0.8420	 0.5370
U	 0.5700	 0.4500
V	 0.6860	 0.5350
W	 0.8160	 0.5330
X	 0.8200	 0.4800
Y	 0.6790	 0.3930
Z	 0.8280	 0.4820
a	 0.8520	 0.5670
b	 0.9260	 0.5770
c	 0.8680	 0.5250
d	 0.7420	 0.5330
e	 0.8640	 0.5520
f	 0.8090	 0.5240
i	 0.8080	 0.5410
j	 0.7870	 0.5320



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Chain	Atom inclusion	Q-score
k	 0.7620	 0.5340
l	 0.7870	 0.5340
m	 0.7740	 0.5160
o	 0.7600	 0.4860
p	 0.4340	 0.4220
q	 0.7230	 0.4690
r	 0.8990	 0.5550
t	 0.4880	 0.3920
u	 0.8180	 0.5080
v	 0.8360	 0.5130
w	 0.3790	 0.3720
x	 0.8920	 0.5460
y	 0.5790	 0.4230
z	 0.9090	 0.5450