



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2025 – 03:07 PM JST

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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 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) : 2.46

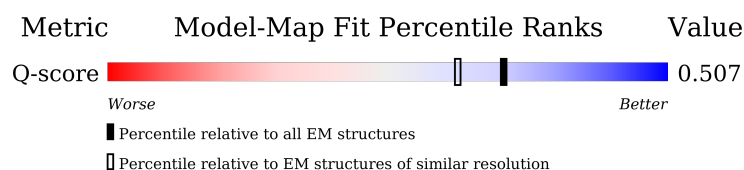
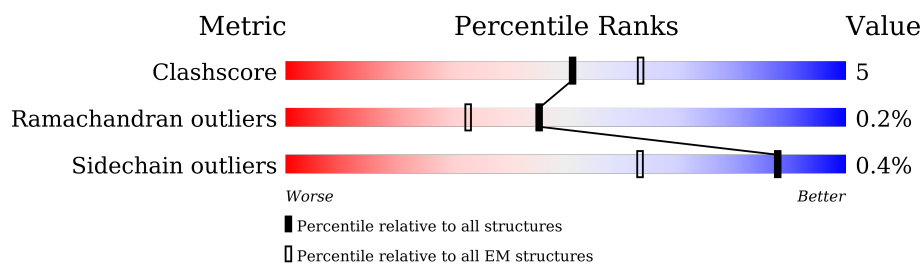
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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


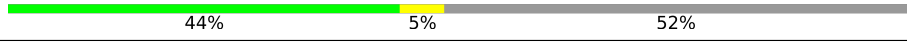
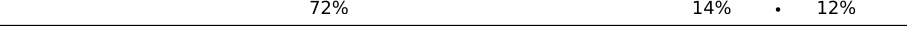
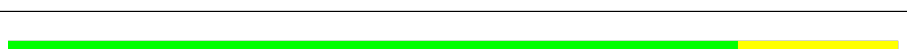

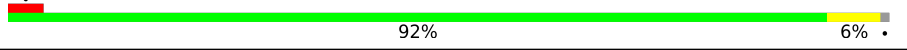

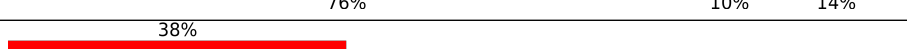
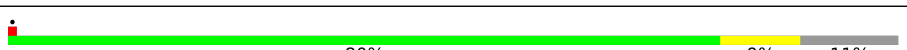


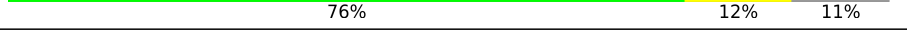

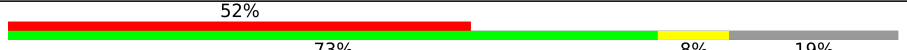



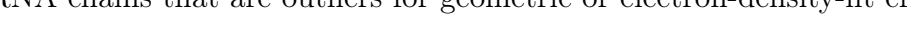
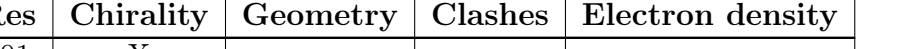
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Mol	Chain	Length	Quality of chain
5	E	217	
6	F	239	
7	G	198	
8	H	199	
9	I	196	
10	J	208	
11	K	204	
12	L	228	
13	M	224	
13	P	224	
13	W	224	
14	N	225	
15	O	210	
15	R	210	
15	T	210	
16	Q	187	
17	S	245	
18	U	198	
19	V	123	
20	X	253	
21	Y	244	
22	Z	254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

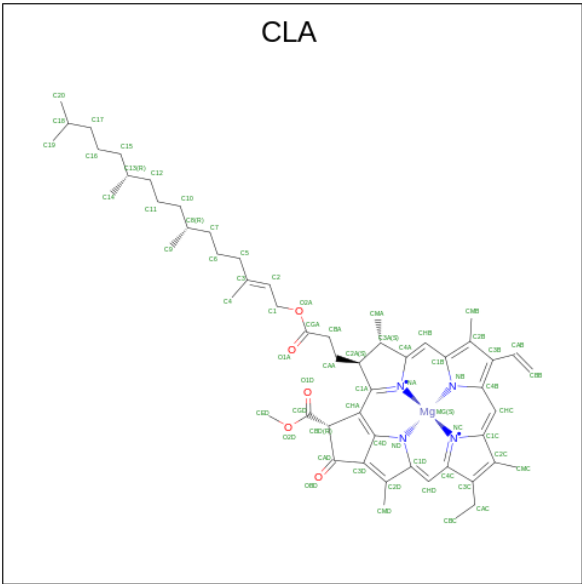
- Molecule 38 is a protein called Light harvesting protein.

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

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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	C	Mg	N	O	0
			50	40	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
			55	45	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
			50	40	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
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			47	37	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
			60	50	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
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			62	52	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	
40	a	1	Total	C	Mg	N	O	0
			65	55	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
			65	55	1	4	5	

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

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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 60	C 50	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	z	1	Total 47	C 37	Mg 1	N 4	O 5	0

- ## KC2

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



WORLD WIDE
PDB
PROTEIN DATA BANK

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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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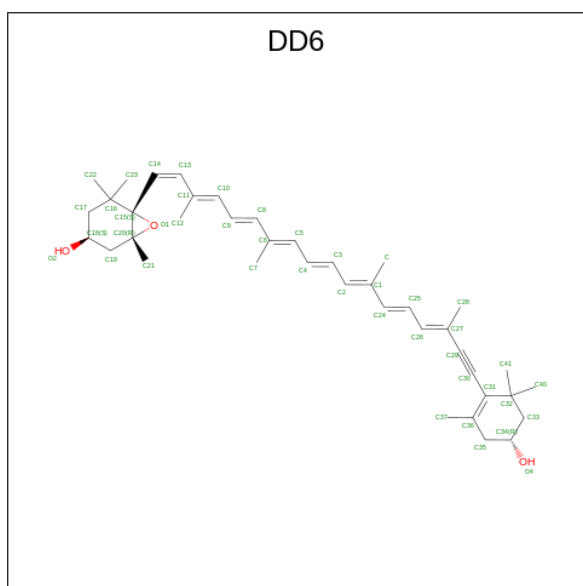
Mol	Chain	Residues	Atoms					AltConf
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 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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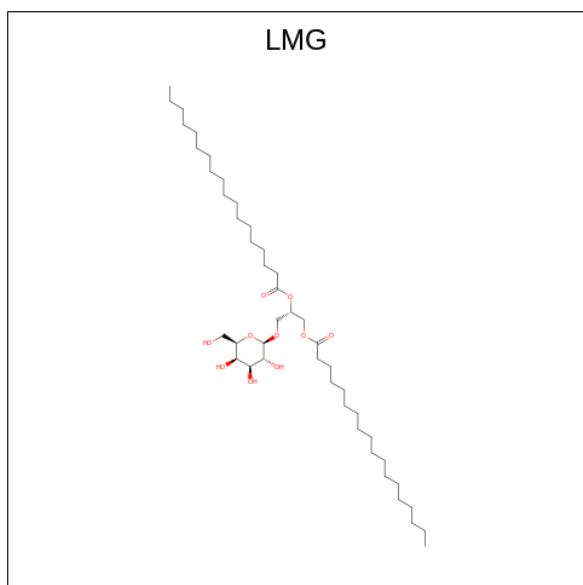
Mol	Chain	Residues	Atoms			AltConf
42	O	1	Total 43	C 40	O 3	0
42	P	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	R	1	Total 43	C 40	O 3	0
42	T	1	Total 43	C 40	O 3	0
42	U	1	Total 43	C 40	O 3	0
42	U	1	Total 43	C 40	O 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).



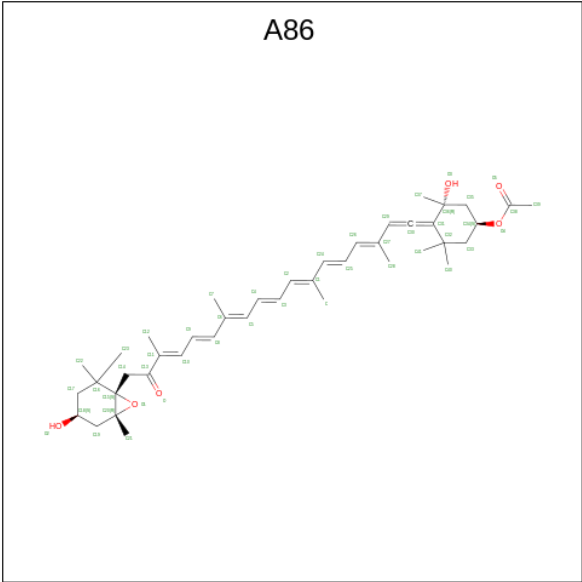
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			40	30	10	
43	D	1	Total	C	O	0
			40	30	10	

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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	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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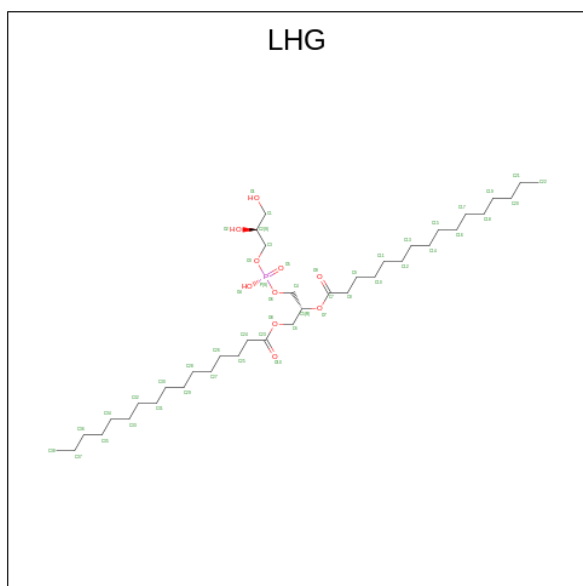
Mol	Chain	Residues	Atoms			AltConf
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			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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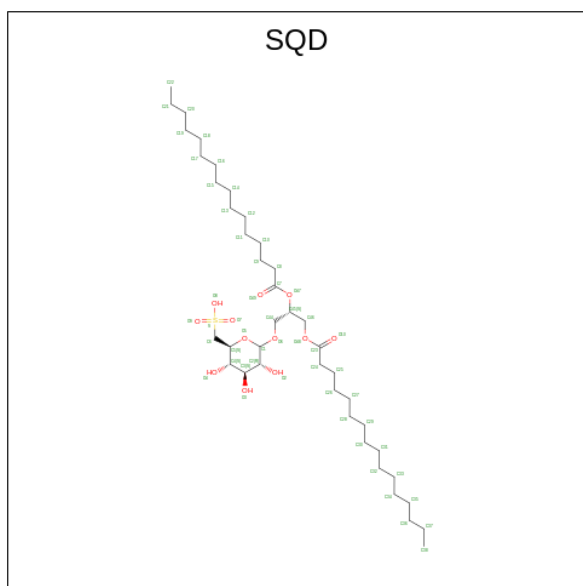
Mol	Chain	Residues	Atoms			AltConf
44	x	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	
44	y	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			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: $C_{38}H_{75}O_{10}P$) (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	

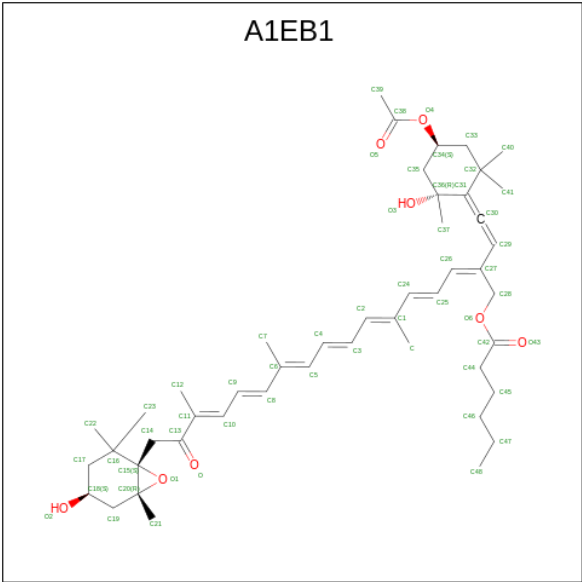
- Molecule 46 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



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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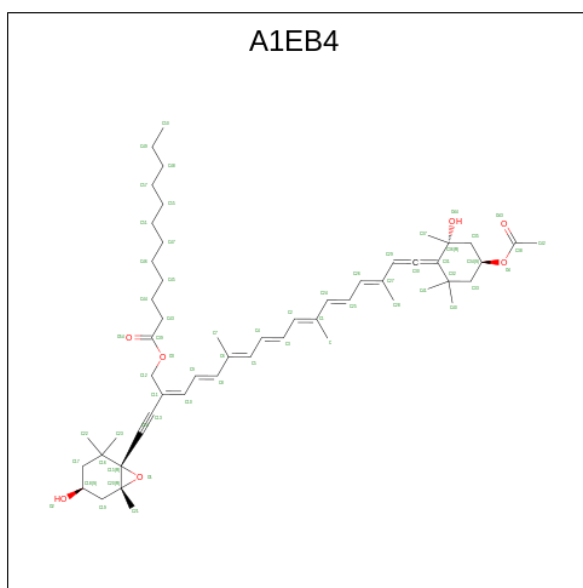
Mol	Chain	Residues	Atoms			AltConf
47	S	1	Total	C	O	0
			56	48	8	
47	T	1	Total	C	O	0
			56	48	8	
47	T	1	Total	C	O	0
			56	48	8	
47	Y	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	o	1	Total	C	O	0
			56	48	8	
47	o	1	Total	C	O	0
			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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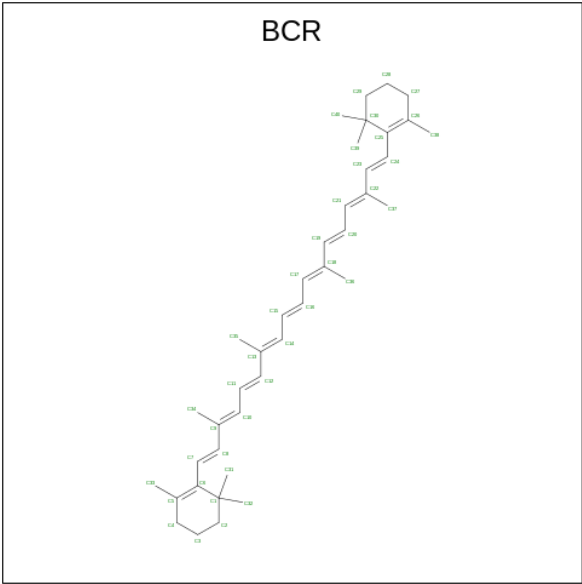
Mol	Chain	Residues	Atoms			AltConf
47	v	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	
47	w	1	Total	C	O	0
			56	48	8	
47	w	1	Total	C	O	0
			56	48	8	
47	x	1	Total	C	O	0
			56	48	8	
47	x	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			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).



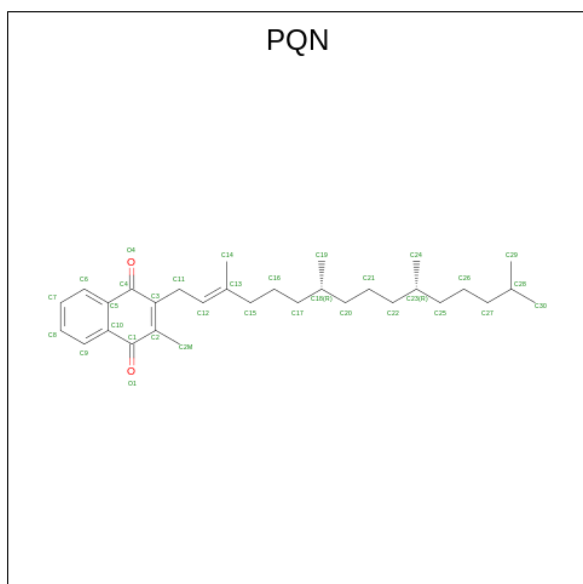
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	

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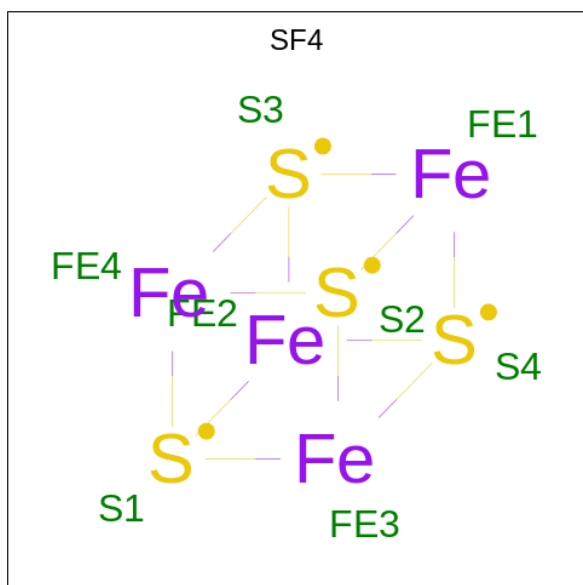
Mol	Chain	Residues	Atoms	AltConf
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	i	1	Total C 40 40	0
49	j	1	Total C 40 40	0
49	k	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	m	1	Total C 40 40	0
49	r	1	Total C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

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



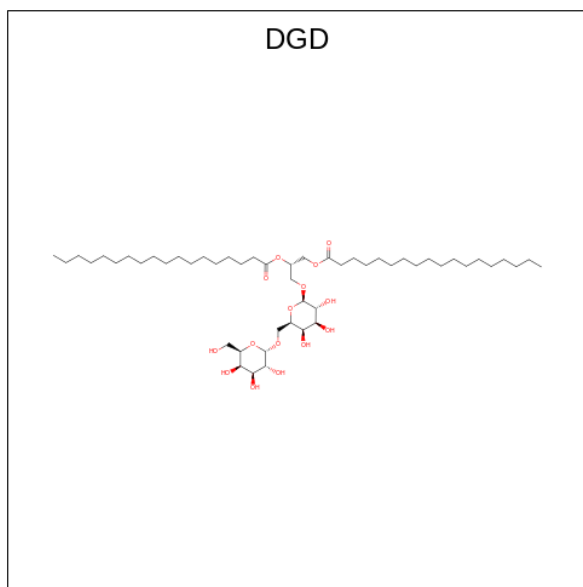
Mol	Chain	Residues	Atoms			AltConf
50	a	1	Total	C	O	0
			28	26	2	
50	b	1	Total	C	O	0
			28	26	2	

- 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.

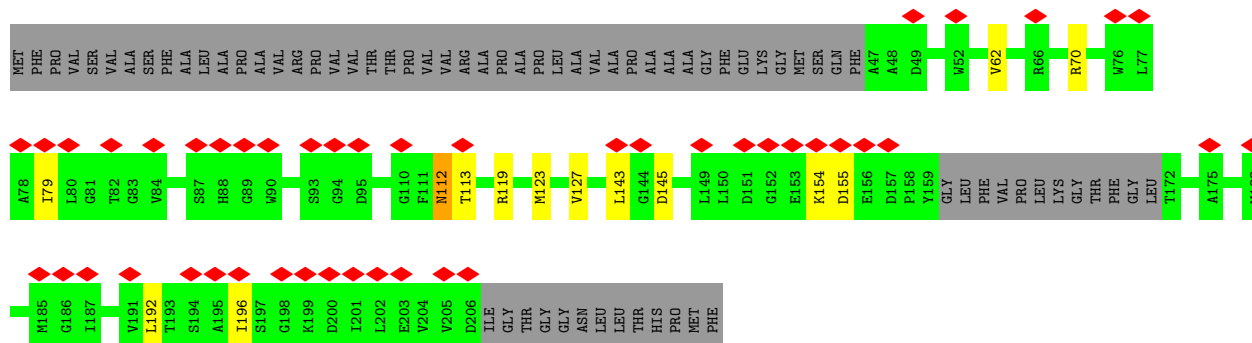
- Molecule 1: Light harvesting protein

Chain A: 




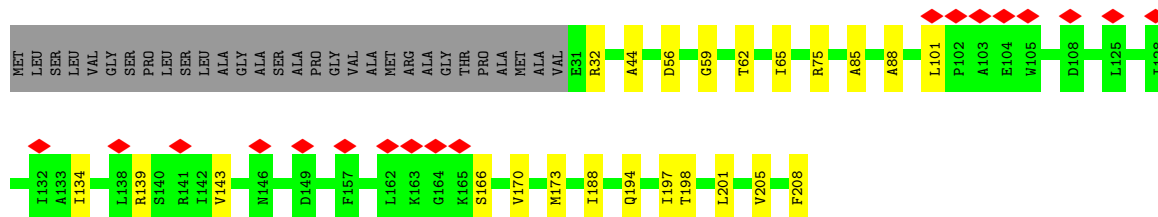
- Molecule 2: EFCPI-1

Chain B: 



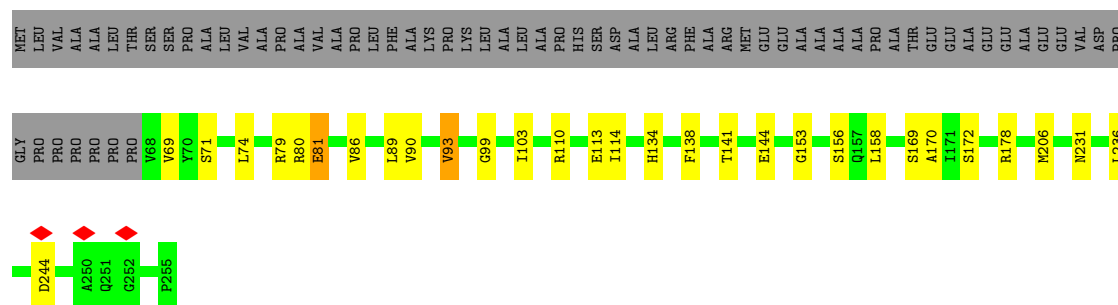
- Molecule 3: Light harvesting protein

Chain C: 



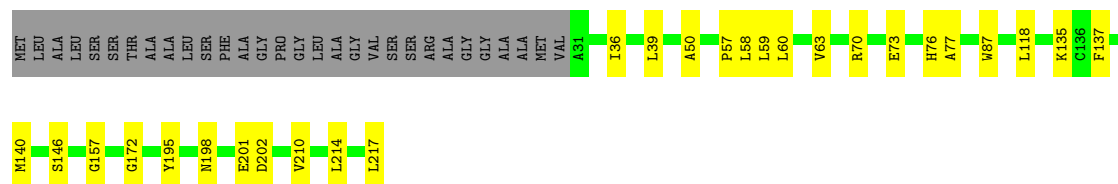
- Molecule 4: EFCPI-6

Chain D: 



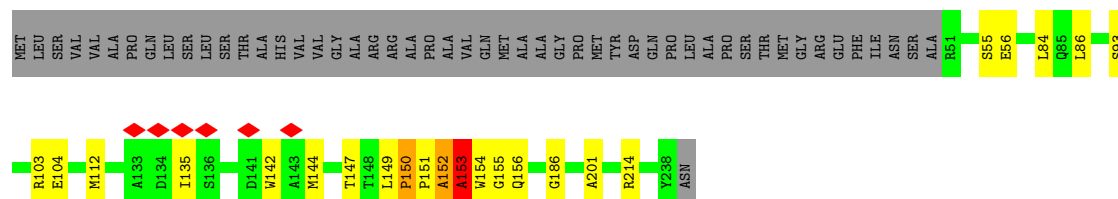
• Molecule 5: Light harvesting protein

Chain E: 74% 12% 14%



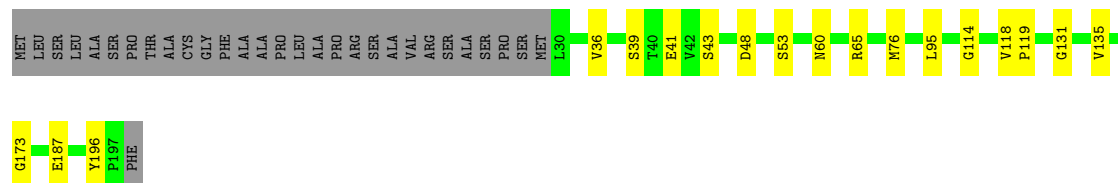
• Molecule 6: Light harvesting protein

Chain F: 69% 8% 21%



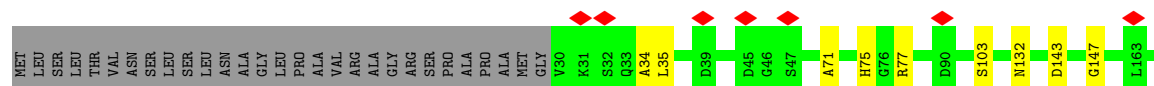
• Molecule 7: Light harvesting protein

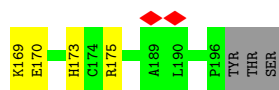
Chain G: 76% 9% 15%



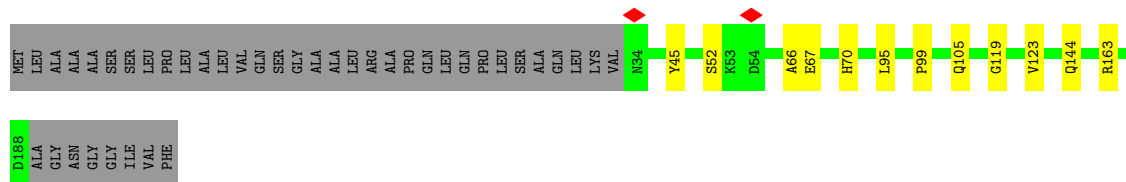
• Molecule 8: Light harvesting protein

Chain H: 5% 77% 7% 16%

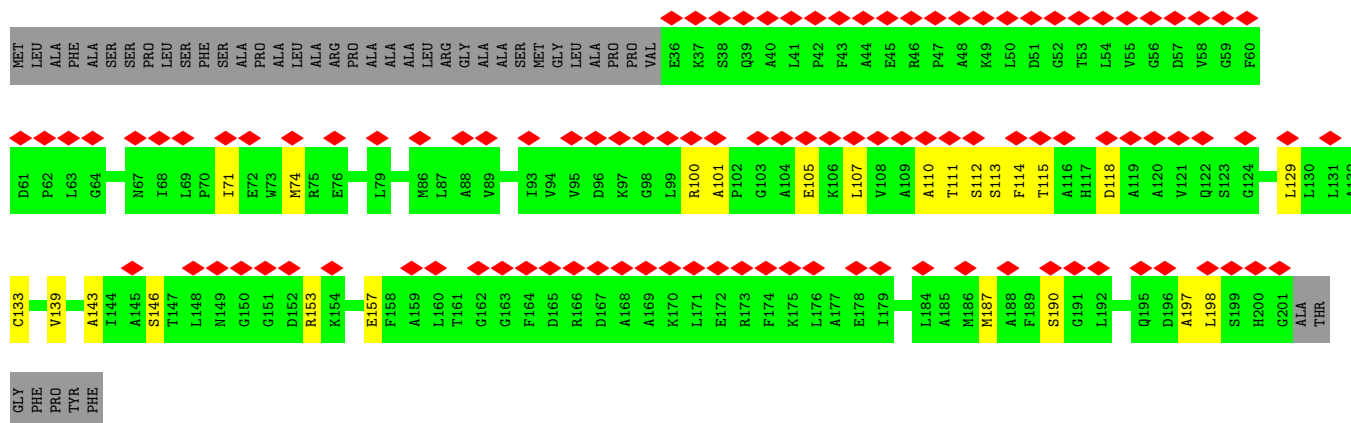




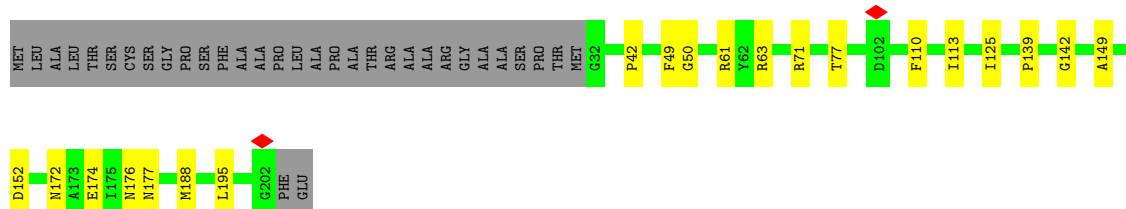
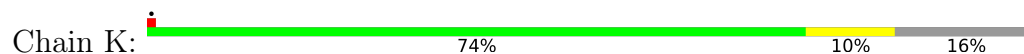
- Molecule 9: Light harvesting protein



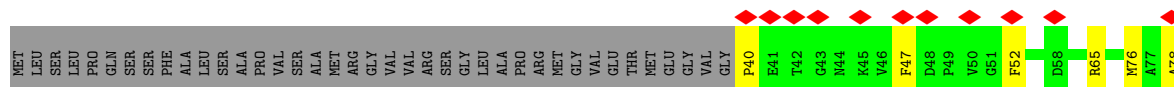
- Molecule 10: Light harvesting protein

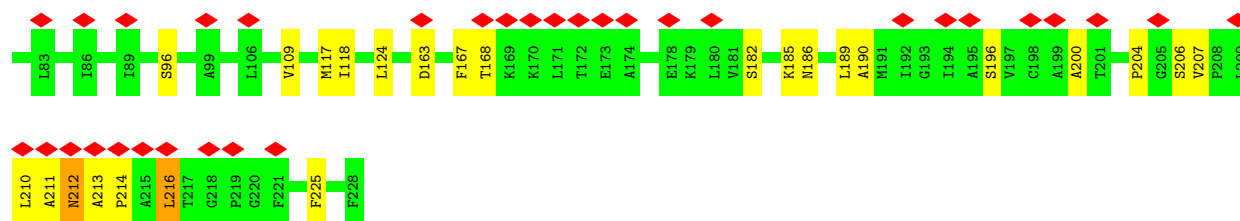


- Molecule 11: Light harvesting protein



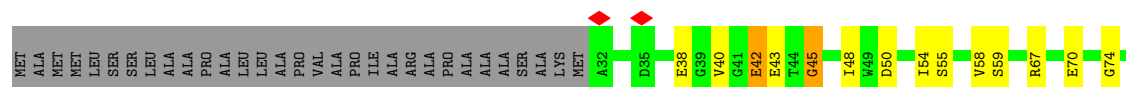
- Molecule 12: EFCPI-12





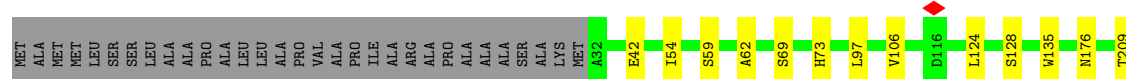
- Molecule 13: Light harvesting protein

Chain M: 74% 12% 14%



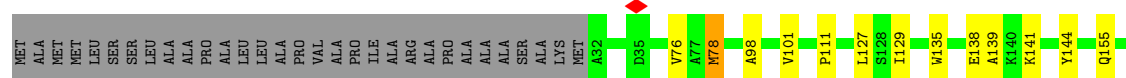
- Molecule 13: Light harvesting protein

Chain P: 79% 7% 14%



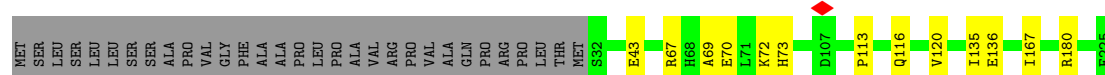
- Molecule 13: Light harvesting protein

Chain W: 76% 9% 14%



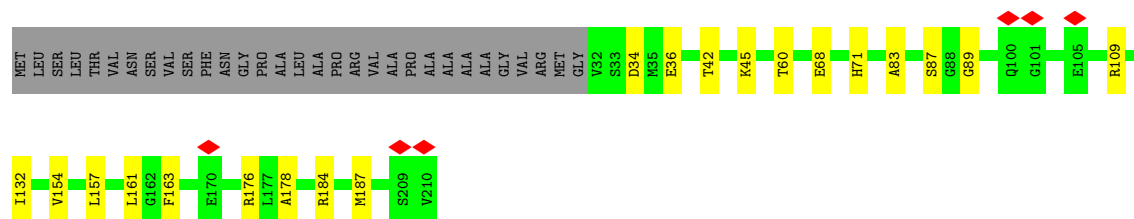
- Molecule 14: EFCPI-17

Chain N: 80% 6% 14%

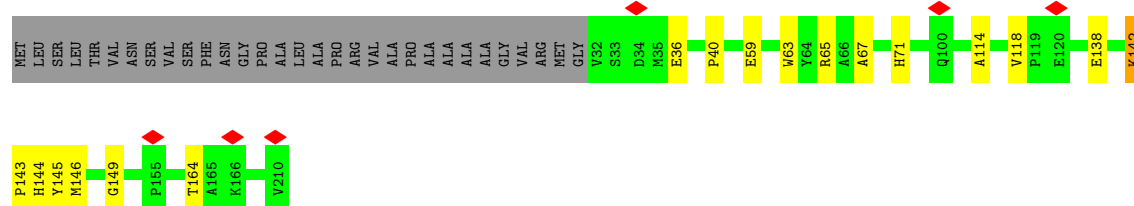
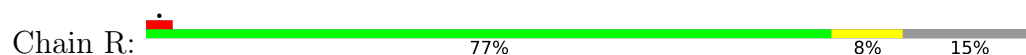


- Molecule 15: Light harvesting protein

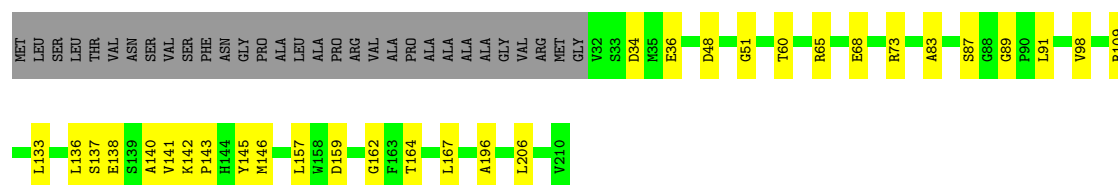
Chain O: 76% 10% 15%



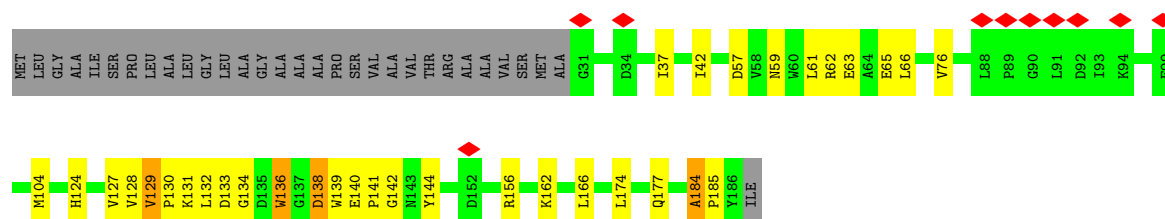
- Molecule 15: Light harvesting protein



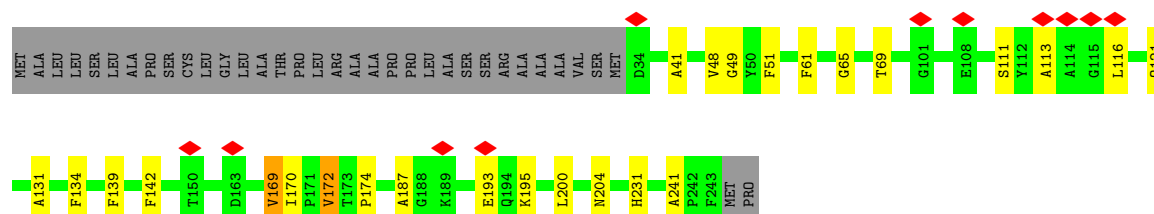
- Molecule 15: Light harvesting protein



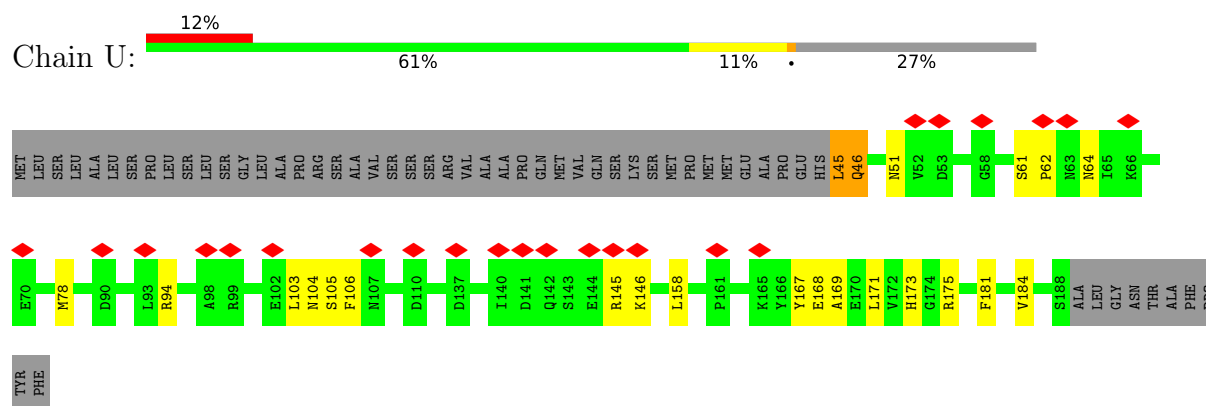
- Molecule 16: EFCPI-18



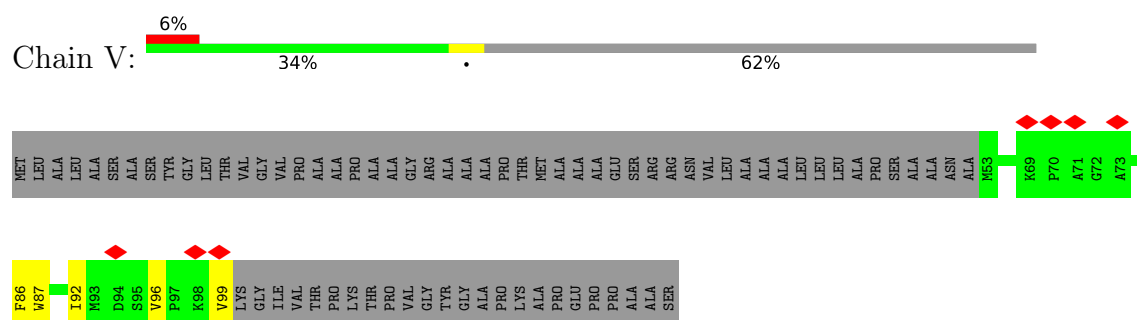
- Molecule 17: EFCPI-22



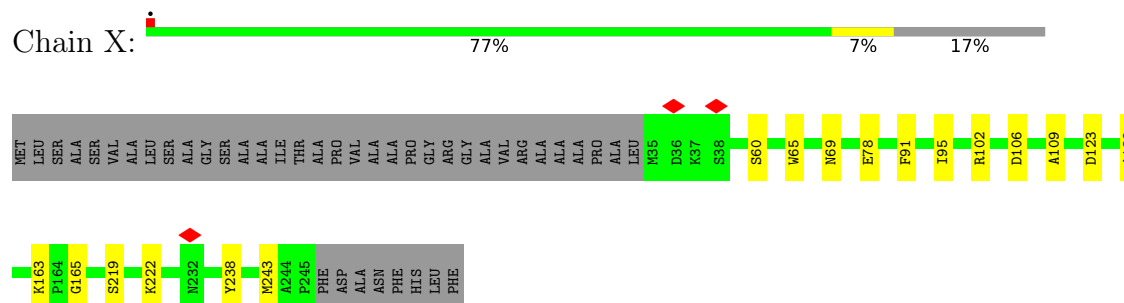
- Molecule 18: Light harvesting protein



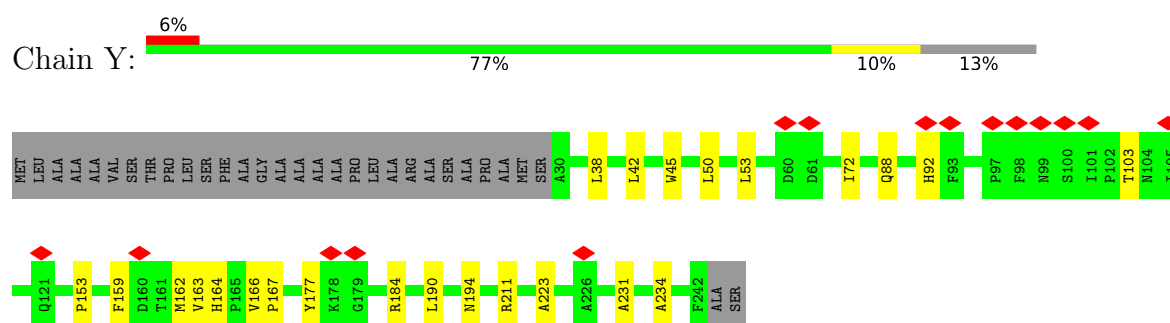
- Molecule 19: LEFP



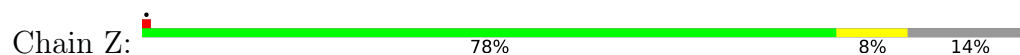
- Molecule 20: Light harvesting protein

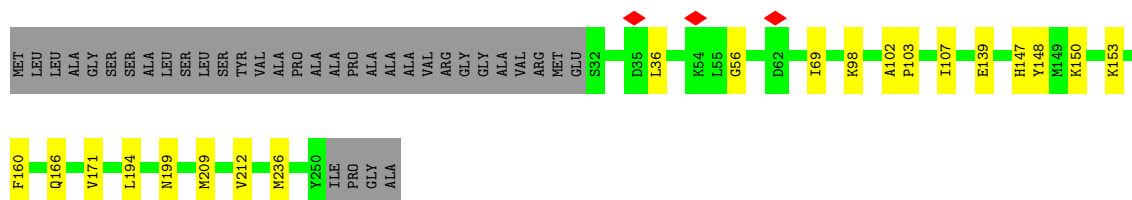


- Molecule 21: Light harvesting protein



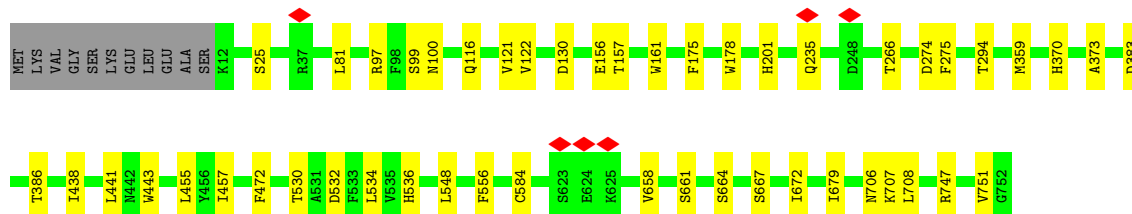
- Molecule 22: Light harvesting protein





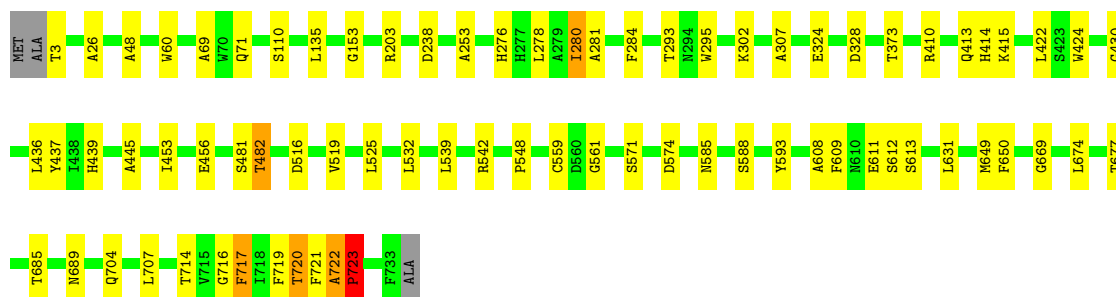
- Molecule 23: Photosystem I P700 chlorophyll a apoprotein A1

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% .



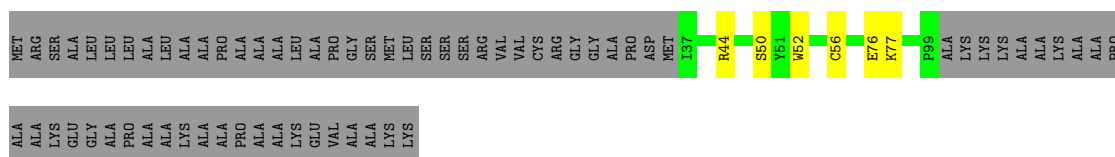
- Molecule 26: Photosystem I reaction center subunit II

Chain d: 91% 7% ..

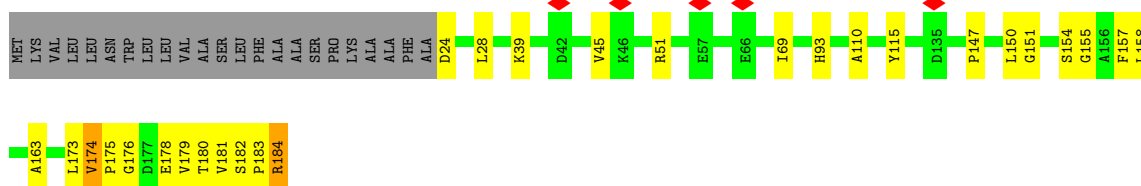


- Molecule 27: Photosystem I reaction center subunit IV

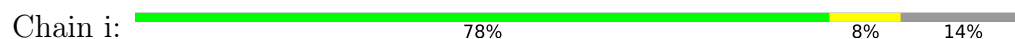
Chain e: 44% 5% 52%



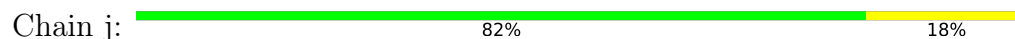
- Molecule 28: Photosystem I reaction center subunit III



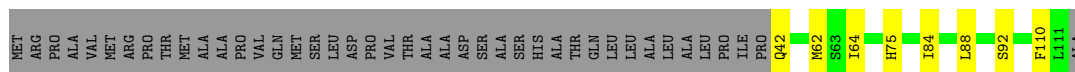
- Molecule 29: Photosystem I reaction center subunit VIII



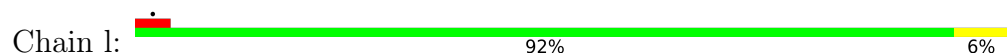
- Molecule 30: Photosystem I reaction center subunit IX



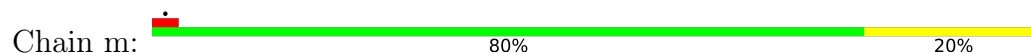
- Molecule 31: PSI-K

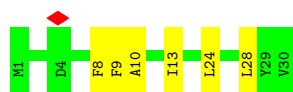


- Molecule 32: Photosystem I reaction center subunit XI

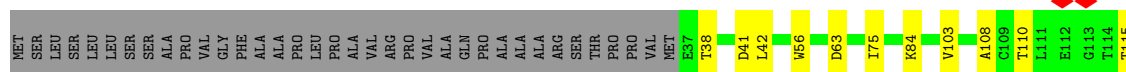


- Molecule 33: Photosystem I reaction center subunit XII

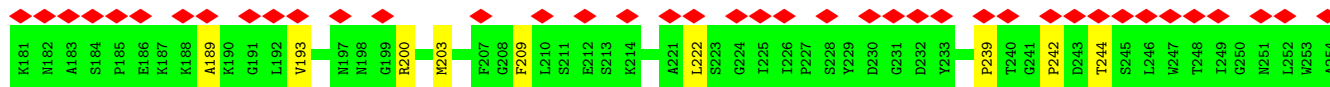
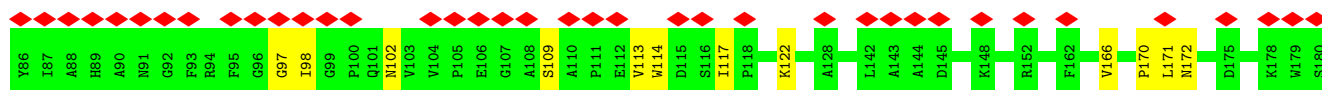
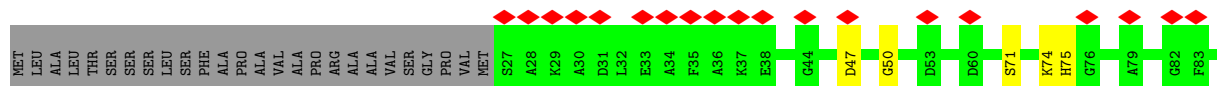
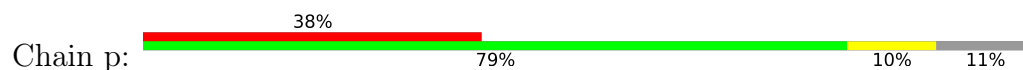




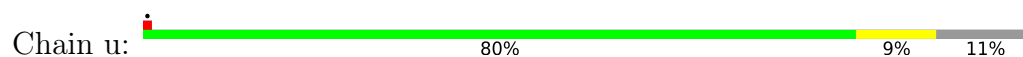
- Molecule 34: EFCPI-30



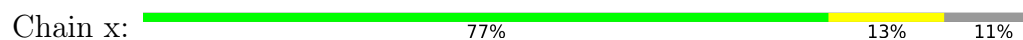
- Molecule 35: Light harvesting protein



- Molecule 35: Light harvesting protein

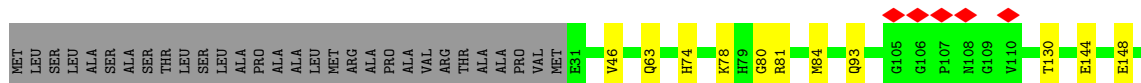
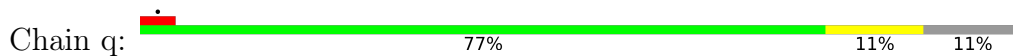


- Molecule 35: Light harvesting protein

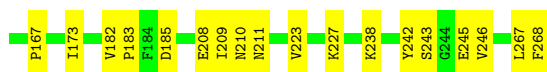
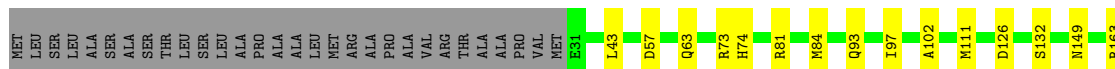
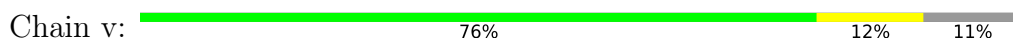




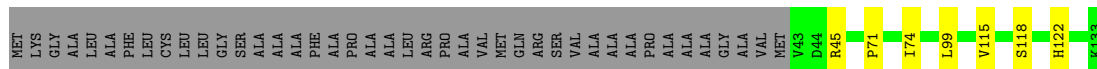
- Molecule 36: Light harvesting protein



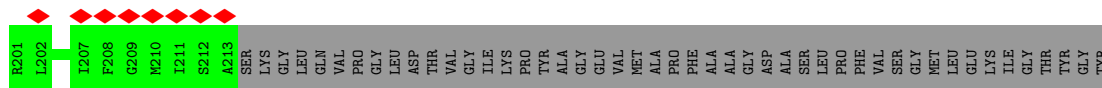
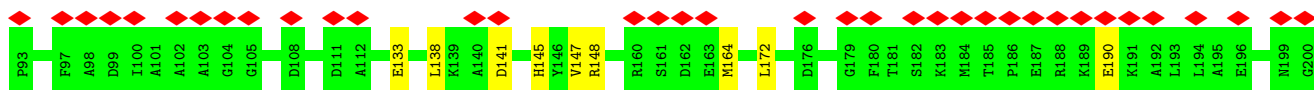
- Molecule 36: Light harvesting protein



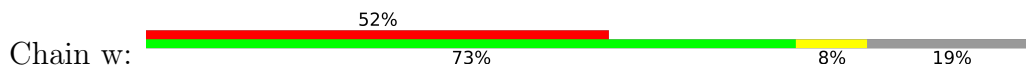
- Molecule 37: PsaR

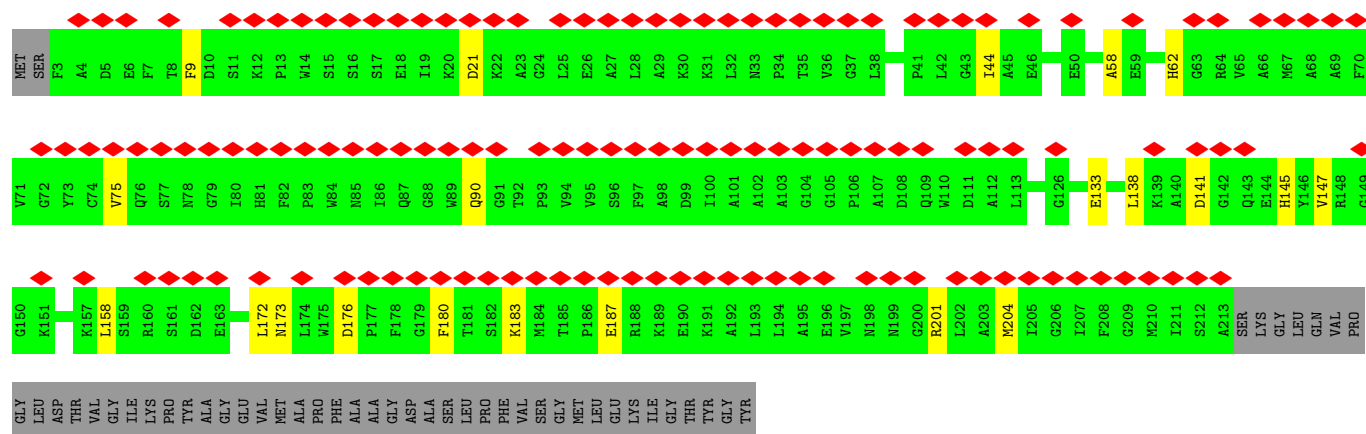


- Molecule 38: Light harvesting protein

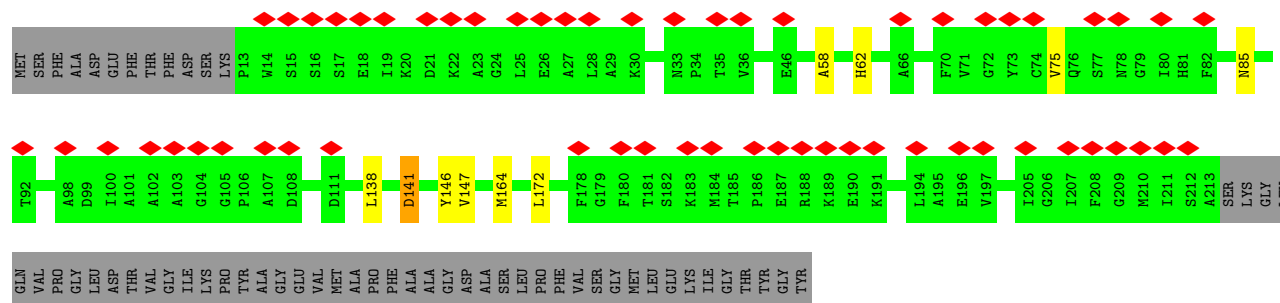
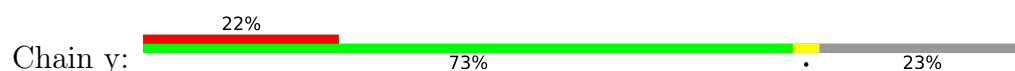


- Molecule 38: Light harvesting protein

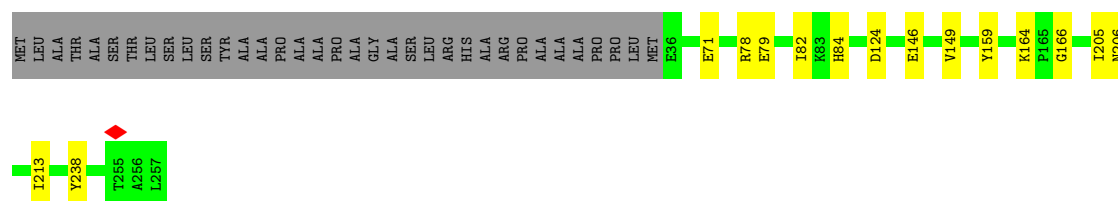
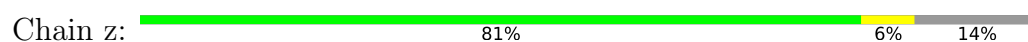




• Molecule 38: Light harvesting protein



• 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: DGD, BCR, A1EB4, LHG, A1EB1, DD6, PQN, SQD, CLA, A86, KC2, SF4, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	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%)	19	51
3	C	176/208 (85%)	166 (94%)	9 (5%)	1 (1%)	22	53
4	D	187/255 (73%)	178 (95%)	8 (4%)	1 (0%)	25	58
5	E	185/217 (85%)	176 (95%)	8 (4%)	1 (0%)	25	58
6	F	186/239 (78%)	175 (94%)	10 (5%)	1 (0%)	25	58
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%)	22	53
11	K	169/204 (83%)	158 (94%)	10 (6%)	1 (1%)	22	53
12	L	187/228 (82%)	173 (92%)	12 (6%)	2 (1%)	12	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%)	22	53
16	Q	154/187 (82%)	141 (92%)	10 (6%)	3 (2%)	6	27
17	S	208/245 (85%)	189 (91%)	18 (9%)	1 (0%)	25	58
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%)	25	58

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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	79
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	33
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	63
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%)	45	74

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%)	81	90
4	D	146/193 (76%)	145 (99%)	1 (1%)	81	90
5	E	146/163 (90%)	146 (100%)	0	100	100
6	F	140/180 (78%)	138 (99%)	2 (1%)	62	81
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%)	81	90
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%)	62	81
14	N	149/174 (86%)	148 (99%)	1 (1%)	81	90
15	O	136/157 (87%)	136 (100%)	0	100	100
15	R	136/157 (87%)	135 (99%)	1 (1%)	81	90
15	T	136/157 (87%)	135 (99%)	1 (1%)	81	90
16	Q	123/141 (87%)	122 (99%)	1 (1%)	79	89
17	S	163/188 (87%)	163 (100%)	0	100	100
18	U	118/162 (73%)	116 (98%)	2 (2%)	56	78
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%)	81	90
25	c	68/69 (99%)	68 (100%)	0	100	100
26	d	120/122 (98%)	119 (99%)	1 (1%)	79	89
27	e	51/90 (57%)	51 (100%)	0	100	100
28	f	127/144 (88%)	123 (97%)	4 (3%)	35	63
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%)	70	84
35	p	179/199 (90%)	179 (100%)	0	100	100
35	u	179/199 (90%)	178 (99%)	1 (1%)	84	91
35	x	179/199 (90%)	179 (100%)	0	100	100
36	q	183/204 (90%)	182 (100%)	1 (0%)	86	92
36	v	183/204 (90%)	182 (100%)	1 (0%)	86	92
37	r	71/94 (76%)	70 (99%)	1 (1%)	62	81
38	t	168/204 (82%)	168 (100%)	0	100	100
38	w	168/204 (82%)	167 (99%)	1 (1%)	84	91
38	y	159/204 (78%)	158 (99%)	1 (1%)	84	91
39	z	177/199 (89%)	177 (100%)	0	100	100
All	All	7210/8293 (87%)	7180 (100%)	30 (0%)	88	94

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	L	304	12	57,65,73	2.38	8 (14%)	66,103,113	1.56	6 (9%)
41	KC2	P	304	13	48,53,53	1.55	8 (16%)	54,89,89	1.04	5 (9%)
44	A86	v	317	-	44,50,50	0.46	1 (2%)	51,76,76	0.87	1 (1%)
45	LHG	a	848	-	47,47,48	0.61	0	50,53,54	1.11	3 (6%)
40	CLA	M	311	13	62,70,73	2.25	8 (12%)	72,109,113	1.42	7 (9%)
44	A86	v	314	-	44,50,50	0.55	1 (2%)	51,76,76	1.65	5 (9%)
40	CLA	L	305	12	47,55,73	2.67	8 (17%)	54,91,113	1.63	4 (7%)
40	CLA	T	305	15	50,58,73	2.47	8 (16%)	58,95,113	1.53	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	u	319	-	44,50,50	0.39	1 (2%)	51,76,76	1.40	4 (7%)
49	BCR	m	101	-	41,41,41	0.17	0	56,56,56	0.34	0
42	DD6	E	315	-	39,45,45	0.20	0	52,67,67	0.97	3 (5%)
43	LMG	P	318	-	39,39,55	1.00	3 (7%)	47,47,63	1.32	6 (12%)
40	CLA	o	304	34	60,68,73	2.27	8 (13%)	70,107,113	1.44	5 (7%)
42	DD6	Q	214	-	39,45,45	0.18	0	52,67,67	0.77	1 (1%)
40	CLA	A	305	1	61,69,73	2.27	8 (13%)	71,108,113	1.49	5 (7%)
40	CLA	G	206	7	56,64,73	2.37	8 (14%)	65,102,113	1.49	7 (10%)
40	CLA	G	213	-	47,55,73	2.59	8 (17%)	54,91,113	1.77	8 (14%)
44	A86	p	316	-	44,50,50	0.42	0	51,76,76	1.18	3 (5%)
40	CLA	a	825	-	65,73,73	2.15	8 (12%)	76,113,113	1.36	6 (7%)
40	CLA	b	803	-	65,73,73	2.12	8 (12%)	76,113,113	1.44	7 (9%)
42	DD6	Q	211	-	39,45,45	0.20	0	52,67,67	0.80	2 (3%)
47	A1EB1	u	323	-	51,58,58	0.50	1 (1%)	60,85,85	0.46	0
41	KC2	o	309	34	48,53,53	1.54	8 (16%)	54,89,89	1.02	4 (7%)
40	CLA	N	311	14	60,68,73	2.28	8 (13%)	70,107,113	1.57	6 (8%)
46	SQD	k	205	-	35,36,54	1.47	5 (14%)	44,47,65	1.28	5 (11%)
41	KC2	u	303	-	48,53,53	1.66	8 (16%)	54,89,89	1.01	3 (5%)
40	CLA	t	305	-	49,57,73	2.61	9 (18%)	61,94,113	1.64	6 (9%)
41	KC2	Y	303	21	48,53,53	1.50	7 (14%)	54,89,89	0.98	3 (5%)
40	CLA	b	802	-	65,73,73	2.16	8 (12%)	76,113,113	1.37	5 (6%)
40	CLA	F	303	6	61,69,73	2.33	9 (14%)	71,107,113	1.82	8 (11%)
40	CLA	x	307	-	55,63,73	2.40	8 (14%)	64,101,113	1.78	7 (10%)
40	CLA	O	307	-	62,70,73	2.30	8 (12%)	72,109,113	1.43	5 (6%)
40	CLA	a	836	23	65,73,73	2.18	8 (12%)	76,113,113	1.37	6 (7%)
41	KC2	y	307	-	48,53,53	1.58	8 (16%)	54,89,89	1.07	6 (11%)
40	CLA	T	306	15	60,68,73	2.28	9 (15%)	70,107,113	1.45	7 (10%)
41	KC2	F	302	6	48,53,53	1.58	8 (16%)	54,89,89	1.04	6 (11%)
41	KC2	W	310	13	48,53,53	1.57	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	J	306	10	52,60,73	2.55	8 (15%)	60,97,113	1.62	7 (11%)
40	CLA	a	823	23	55,63,73	2.41	8 (14%)	64,101,113	1.47	5 (7%)
42	DD6	E	316	-	39,45,45	0.22	0	52,67,67	0.91	3 (5%)
44	A86	F	312	-	44,50,50	0.52	1 (2%)	51,76,76	0.88	2 (3%)
41	KC2	Z	309	-	48,53,53	1.53	8 (16%)	54,89,89	1.02	3 (5%)
44	A86	w	311	-	44,50,50	0.55	2 (4%)	51,76,76	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	LMG	E	320	-	31,31,55	0.99	1 (3%)	39,39,63	1.17	2 (5%)
40	CLA	D	306	4	55,63,73	2.39	8 (14%)	64,101,113	1.50	7 (10%)
41	KC2	u	309	-	48,53,53	1.51	8 (16%)	54,89,89	1.07	6 (11%)
40	CLA	X	301	-	60,68,73	2.31	8 (13%)	70,107,113	1.45	5 (7%)
40	CLA	T	317	47	47,55,73	2.62	7 (14%)	54,91,113	1.50	6 (11%)
44	A86	W	301	-	44,50,50	0.44	1 (2%)	51,76,76	0.60	1 (1%)
40	CLA	u	311	-	55,63,73	2.43	8 (14%)	64,101,113	1.83	10 (15%)
40	CLA	z	324	-	47,55,73	2.63	8 (17%)	54,91,113	1.70	8 (14%)
40	CLA	p	313	-	55,63,73	2.35	8 (14%)	64,101,113	1.41	5 (7%)
40	CLA	a	829	-	65,73,73	2.21	8 (12%)	76,113,113	1.51	7 (9%)
40	CLA	F	301	-	53,61,73	2.49	8 (15%)	61,98,113	1.54	5 (8%)
42	DD6	v	320	-	39,45,45	0.20	0	52,67,67	0.83	1 (1%)
44	A86	F	317	-	44,50,50	0.42	1 (2%)	51,76,76	0.84	2 (3%)
40	CLA	F	311	-	47,55,73	2.66	8 (17%)	54,91,113	1.62	5 (9%)
40	CLA	b	814	24	65,73,73	2.15	8 (12%)	76,113,113	1.36	5 (6%)
40	CLA	x	314	35	47,55,73	2.61	8 (17%)	54,91,113	1.66	6 (11%)
40	CLA	b	806	24	65,73,73	2.19	8 (12%)	76,113,113	1.35	5 (6%)
40	CLA	A	304	1	65,73,73	2.18	8 (12%)	76,113,113	1.53	9 (11%)
40	CLA	C	302	-	47,55,73	2.65	8 (17%)	54,91,113	1.80	6 (11%)
40	CLA	k	202	-	55,63,73	2.36	8 (14%)	64,101,113	1.50	6 (9%)
41	KC2	X	309	-	48,53,53	1.51	7 (14%)	54,89,89	1.04	3 (5%)
44	A86	M	313	-	44,50,50	0.42	1 (2%)	51,76,76	2.18	3 (5%)
40	CLA	J	303	-	47,55,73	2.70	7 (14%)	54,91,113	1.71	7 (12%)
40	CLA	p	312	-	47,55,73	2.69	8 (17%)	54,91,113	1.64	6 (11%)
40	CLA	R	310	-	47,55,73	2.62	8 (17%)	54,91,113	1.68	6 (11%)
40	CLA	b	821	-	65,73,73	2.14	8 (12%)	76,113,113	1.30	7 (9%)
41	KC2	u	310	-	48,53,53	1.54	7 (14%)	54,89,89	1.02	4 (7%)
47	A1EB1	y	312	-	51,58,58	0.44	1 (1%)	60,85,85	0.67	1 (1%)
42	DD6	L	315	-	39,45,45	0.15	0	52,67,67	0.57	2 (3%)
42	DD6	U	209	-	39,45,45	0.27	0	52,67,67	0.80	2 (3%)
40	CLA	J	302	10	47,55,73	2.61	8 (17%)	54,91,113	1.55	5 (9%)
40	CLA	W	305	13	65,73,73	2.21	8 (12%)	76,113,113	1.37	8 (10%)
40	CLA	a	810	-	60,68,73	2.34	8 (13%)	70,107,113	1.49	5 (7%)
40	CLA	E	308	5	58,66,73	2.31	8 (13%)	67,104,113	1.54	6 (8%)
40	CLA	a	818	-	47,55,73	2.48	8 (17%)	54,91,113	1.73	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	q	310	-	51,59,73	2.47	8 (15%)	59,96,113	1.68	7 (11%)
40	CLA	b	832	24	65,73,73	2.23	8 (12%)	76,113,113	1.53	6 (7%)
40	CLA	u	307	35	55,63,73	2.38	8 (14%)	64,101,113	1.75	7 (10%)
40	CLA	R	304	15	51,59,73	2.52	8 (15%)	59,96,113	1.69	9 (15%)
40	CLA	Z	306	22	60,68,73	2.34	8 (13%)	70,107,113	1.56	7 (10%)
40	CLA	b	819	24	64,72,73	2.23	8 (12%)	74,111,113	1.40	4 (5%)
40	CLA	Z	312	-	47,55,73	2.63	8 (17%)	54,91,113	1.82	13 (24%)
40	CLA	J	309	-	47,55,73	2.70	8 (17%)	54,91,113	1.53	6 (11%)
40	CLA	X	312	-	47,55,73	2.67	8 (17%)	54,91,113	1.68	7 (12%)
40	CLA	a	835	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	5 (6%)
41	KC2	O	308	15	48,53,53	1.61	8 (16%)	54,89,89	1.11	6 (11%)
40	CLA	R	305	15	60,68,73	2.27	8 (13%)	70,107,113	1.46	4 (5%)
40	CLA	K	307	11	54,62,73	2.42	8 (14%)	62,99,113	1.41	6 (9%)
40	CLA	a	804	23	61,69,73	2.36	9 (14%)	71,107,113	1.84	9 (12%)
40	CLA	Z	304	-	60,68,73	2.26	8 (13%)	70,107,113	1.42	6 (8%)
43	LMG	A	317	-	40,40,55	0.84	0	48,48,63	1.22	4 (8%)
40	CLA	u	313	-	55,63,73	2.39	8 (14%)	64,101,113	1.40	5 (7%)
40	CLA	x	302	-	65,73,73	2.21	8 (12%)	76,113,113	1.55	6 (7%)
41	KC2	F	309	6	48,53,53	1.60	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	H	302	-	47,55,73	2.65	8 (17%)	54,91,113	1.65	7 (12%)
42	DD6	Z	318	-	39,45,45	0.21	0	52,67,67	1.05	3 (5%)
44	A86	o	315	-	44,50,50	0.55	1 (2%)	51,76,76	1.10	3 (5%)
45	LHG	F	319	-	39,39,48	0.67	1 (2%)	42,45,54	1.16	2 (4%)
41	KC2	p	303	-	48,53,53	1.68	8 (16%)	54,89,89	1.01	3 (5%)
40	CLA	N	306	-	60,68,73	2.29	8 (13%)	70,107,113	1.39	5 (7%)
41	KC2	Z	308	22	48,53,53	1.55	8 (16%)	54,89,89	1.01	5 (9%)
41	KC2	M	302	13	48,53,53	1.61	7 (14%)	54,89,89	1.03	2 (3%)
40	CLA	Z	305	22	55,63,73	2.39	8 (14%)	64,101,113	1.38	4 (6%)
40	CLA	a	809	-	50,58,73	2.56	8 (16%)	58,95,113	1.56	7 (12%)
44	A86	o	314	-	44,50,50	0.48	1 (2%)	51,76,76	1.40	5 (9%)
40	CLA	X	310	-	55,63,73	2.44	7 (12%)	64,101,113	1.86	9 (14%)
47	A1EB1	P	301	-	51,58,58	0.54	1 (1%)	60,85,85	0.57	0
40	CLA	a	817	23	50,58,73	2.52	8 (16%)	58,95,113	1.55	5 (8%)
40	CLA	a	831	-	60,68,73	2.34	8 (13%)	70,107,113	1.43	4 (5%)
40	CLA	Q	207	-	47,55,73	2.68	8 (17%)	54,91,113	1.86	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	L	309	12	48,53,53	1.59	8 (16%)	54,89,89	1.02	5 (9%)
41	KC2	W	304	13	48,53,53	1.54	7 (14%)	54,89,89	1.04	6 (11%)
41	KC2	K	303	11	48,53,53	1.52	7 (14%)	54,89,89	1.03	5 (9%)
44	A86	q	317	-	44,50,50	0.47	1 (2%)	51,76,76	1.06	1 (1%)
40	CLA	f	205	-	47,55,73	2.58	8 (17%)	54,91,113	1.54	7 (12%)
40	CLA	U	202	18	55,63,73	2.46	8 (14%)	64,101,113	1.70	8 (12%)
51	SF4	c	101	-	0,12,12	-	-	-	-	-
40	CLA	x	311	-	55,63,73	2.43	8 (14%)	64,101,113	1.87	11 (17%)
40	CLA	K	312	-	47,55,73	2.58	8 (17%)	54,91,113	1.58	5 (9%)
40	CLA	b	816	24	47,55,73	2.56	8 (17%)	54,91,113	1.77	8 (14%)
40	CLA	X	307	20	60,68,73	2.30	8 (13%)	70,107,113	1.49	6 (8%)
42	DD6	D	313	-	39,45,45	0.19	0	52,67,67	0.88	2 (3%)
40	CLA	o	312	-	47,55,73	2.66	8 (17%)	54,91,113	1.75	6 (11%)
42	DD6	D	315	-	39,45,45	0.17	0	52,67,67	0.98	3 (5%)
41	KC2	y	306	-	48,53,53	1.56	7 (14%)	54,89,89	0.98	5 (9%)
40	CLA	S	302	-	60,68,73	2.30	8 (13%)	70,107,113	1.41	7 (10%)
40	CLA	x	312	-	60,68,73	2.32	8 (13%)	70,107,113	1.46	6 (8%)
40	CLA	X	305	-	50,58,73	2.54	8 (16%)	58,95,113	1.55	6 (10%)
40	CLA	b	815	-	57,65,73	2.38	8 (14%)	66,103,113	1.49	5 (7%)
40	CLA	b	826	24	64,72,73	2.17	8 (12%)	74,111,113	1.39	4 (5%)
44	A86	z	317	-	44,50,50	0.58	1 (2%)	51,76,76	1.72	2 (3%)
40	CLA	a	833	23	60,68,73	2.33	8 (13%)	70,107,113	1.47	6 (8%)
40	CLA	G	201	7	47,55,73	2.61	8 (17%)	54,91,113	1.57	6 (11%)
51	SF4	c	102	-	0,12,12	-	-	-	-	-
40	CLA	W	308	-	60,68,73	2.36	8 (13%)	70,107,113	1.63	9 (12%)
40	CLA	l	204	-	65,73,73	2.21	8 (12%)	76,113,113	1.28	5 (6%)
44	A86	Q	215	-	44,50,50	0.44	1 (2%)	51,76,76	1.39	2 (3%)
40	CLA	M	310	-	56,64,73	2.32	8 (14%)	65,102,113	1.41	8 (12%)
41	KC2	K	302	11	48,53,53	1.58	8 (16%)	54,89,89	1.04	5 (9%)
40	CLA	f	204	28	47,55,73	2.60	8 (17%)	54,91,113	1.62	5 (9%)
40	CLA	D	301	4	55,63,73	2.37	8 (14%)	64,101,113	1.48	6 (9%)
40	CLA	a	821	23	65,73,73	2.17	8 (12%)	76,113,113	1.35	5 (6%)
43	LMG	W	317	-	39,39,55	0.85	0	47,47,63	1.29	6 (12%)
40	CLA	P	307	13	59,67,73	2.32	8 (13%)	68,105,113	1.52	6 (8%)
40	CLA	l	202	-	65,73,73	2.21	8 (12%)	76,113,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	Q	205	16	61,69,73	2.34	9 (14%)	71,107,113	1.83	10 (14%)
49	BCR	l	206	-	41,41,41	0.14	0	56,56,56	0.41	0
44	A86	S	317	-	44,50,50	0.46	1 (2%)	51,76,76	0.93	2 (3%)
40	CLA	v	305	-	60,68,73	2.28	8 (13%)	70,107,113	1.53	8 (11%)
43	LMG	j	101	-	30,30,55	0.91	1 (3%)	38,38,63	1.30	3 (7%)
40	CLA	S	311	-	47,55,73	2.70	8 (17%)	54,91,113	1.92	9 (16%)
40	CLA	L	310	-	47,55,73	2.67	8 (17%)	54,91,113	1.77	8 (14%)
44	A86	T	315	-	44,50,50	0.66	1 (2%)	51,76,76	1.16	1 (1%)
40	CLA	p	308	-	60,68,73	2.33	8 (13%)	70,107,113	1.57	6 (8%)
40	CLA	K	304	11	60,68,73	2.26	8 (13%)	70,107,113	1.48	5 (7%)
43	LMG	D	318	-	40,40,55	0.81	0	48,48,63	1.23	5 (10%)
40	CLA	S	314	17	55,63,73	2.41	8 (14%)	64,101,113	1.65	6 (9%)
41	KC2	G	208	-	48,53,53	1.57	8 (16%)	54,89,89	0.98	3 (5%)
42	DD6	A	312	-	39,45,45	0.20	0	52,67,67	0.91	2 (3%)
43	LMG	a	802	-	35,35,55	0.89	1 (2%)	43,43,63	1.30	7 (16%)
40	CLA	q	311	-	63,71,73	2.26	8 (12%)	73,110,113	1.49	7 (9%)
40	CLA	x	308	35	60,68,73	2.27	8 (13%)	70,107,113	1.52	6 (8%)
40	CLA	L	312	-	47,55,73	2.66	8 (17%)	54,91,113	1.61	6 (11%)
40	CLA	a	834	-	60,68,73	2.29	8 (13%)	70,107,113	1.55	7 (10%)
42	DD6	w	312	-	39,45,45	0.18	0	52,67,67	1.06	5 (9%)
43	LMG	T	318	-	40,40,55	0.93	3 (7%)	48,48,63	1.25	4 (8%)
41	KC2	N	303	14	48,53,53	1.53	8 (16%)	54,89,89	1.09	6 (11%)
44	A86	Y	318	-	44,50,50	0.66	1 (2%)	51,76,76	0.94	3 (5%)
41	KC2	L	313	12	48,53,53	1.60	7 (14%)	54,89,89	1.07	4 (7%)
44	A86	P	321	-	44,50,50	0.51	1 (2%)	51,76,76	1.31	2 (3%)
40	CLA	y	302	38	47,55,73	2.64	8 (17%)	54,91,113	1.74	7 (12%)
40	CLA	L	307	-	55,63,73	2.42	8 (14%)	64,101,113	1.52	5 (7%)
47	A1EB1	Z	321	-	51,58,58	0.53	1 (1%)	60,85,85	0.35	0
44	A86	X	320	-	44,50,50	0.51	1 (2%)	51,76,76	1.01	2 (3%)
40	CLA	v	311	-	63,71,73	2.24	8 (12%)	73,110,113	1.47	7 (9%)
43	LMG	p	301	-	39,39,55	0.80	0	47,47,63	1.18	3 (6%)
40	CLA	b	822	-	64,72,73	2.23	8 (12%)	74,111,113	1.51	7 (9%)
40	CLA	v	310	-	51,59,73	2.46	8 (15%)	59,96,113	1.68	8 (13%)
44	A86	z	318	-	44,50,50	0.57	1 (2%)	51,76,76	0.93	2 (3%)
40	CLA	Q	206	-	61,68,73	2.47	11 (18%)	73,105,113	1.78	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	C	308	-	47,55,73	2.70	8 (17%)	54,91,113	1.81	9 (16%)
41	KC2	E	319	-	48,53,53	1.58	7 (14%)	54,89,89	1.04	4 (7%)
42	DD6	A	313	-	39,45,45	0.16	0	52,67,67	0.66	2 (3%)
41	KC2	Y	302	-	48,53,53	1.67	7 (14%)	54,89,89	1.00	4 (7%)
49	BCR	k	203	-	41,41,41	0.18	0	56,56,56	0.46	1 (1%)
40	CLA	J	305	10	55,63,73	2.43	9 (16%)	64,101,113	1.52	5 (7%)
42	DD6	J	313	-	39,45,45	0.20	0	52,67,67	0.74	1 (1%)
41	KC2	Q	216	-	48,53,53	1.59	7 (14%)	54,89,89	1.06	5 (9%)
42	DD6	N	319	-	39,45,45	0.15	0	52,67,67	1.04	3 (5%)
40	CLA	I	202	9	55,63,73	2.43	8 (14%)	64,101,113	1.47	5 (7%)
40	CLA	X	313	20	47,55,73	2.69	8 (17%)	54,91,113	1.80	7 (12%)
40	CLA	H	311	-	47,55,73	2.67	8 (17%)	54,91,113	1.61	5 (9%)
40	CLA	a	827	23	65,73,73	2.20	8 (12%)	76,113,113	1.35	4 (5%)
41	KC2	y	301	38	48,53,53	1.59	8 (16%)	54,89,89	1.03	5 (9%)
40	CLA	D	305	4	43,51,73	2.66	9 (20%)	50,82,113	2.45	8 (16%)
40	CLA	X	304	-	47,55,73	2.52	8 (17%)	54,91,113	1.59	5 (9%)
41	KC2	w	301	38	48,53,53	1.57	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	x	306	35	60,68,73	2.20	8 (13%)	70,107,113	1.42	8 (11%)
40	CLA	a	813	23	60,68,73	2.31	8 (13%)	70,107,113	1.48	6 (8%)
41	KC2	I	209	9	48,53,53	1.57	8 (16%)	54,89,89	1.08	6 (11%)
41	KC2	w	306	38	48,53,53	1.58	7 (14%)	54,89,89	1.03	6 (11%)
40	CLA	L	301	-	47,55,73	2.67	7 (14%)	54,91,113	1.63	6 (11%)
40	CLA	b	842	-	61,69,73	2.27	8 (13%)	71,108,113	1.45	6 (8%)
47	A1EB1	v	324	-	51,58,58	0.63	1 (1%)	60,85,85	1.16	4 (6%)
41	KC2	S	309	17	48,53,53	1.54	7 (14%)	54,89,89	1.08	6 (11%)
40	CLA	G	203	7	55,62,73	2.42	10 (18%)	66,99,113	1.59	11 (16%)
47	A1EB1	o	322	-	51,58,58	0.56	1 (1%)	60,85,85	0.66	1 (1%)
40	CLA	H	307	-	60,68,73	2.31	8 (13%)	70,107,113	1.60	8 (11%)
40	CLA	a	837	23	55,63,73	2.43	8 (14%)	64,101,113	1.49	6 (9%)
40	CLA	S	313	-	47,55,73	2.60	8 (17%)	54,91,113	1.55	6 (11%)
41	KC2	P	302	-	48,53,53	1.54	8 (16%)	54,89,89	1.04	5 (9%)
40	CLA	U	208	-	47,55,73	2.54	7 (14%)	54,91,113	1.55	8 (14%)
50	PQN	a	847	-	29,29,34	0.42	0	36,39,45	0.74	1 (2%)
49	BCR	f	203	-	41,41,41	0.22	0	56,56,56	0.40	0
40	CLA	O	304	15	65,73,73	2.23	8 (12%)	76,113,113	1.42	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	N	316	-	39,45,45	0.22	0	52,67,67	1.07	3 (5%)
40	CLA	b	829	-	47,55,73	2.61	8 (17%)	54,91,113	1.57	7 (12%)
40	CLA	b	811	24	47,55,73	2.44	8 (17%)	54,91,113	1.66	8 (14%)
42	DD6	D	316	-	39,45,45	0.21	0	52,67,67	0.62	0
40	CLA	K	308	11	59,67,73	2.24	8 (13%)	68,105,113	1.56	8 (11%)
42	DD6	J	301	-	39,45,45	0.22	0	52,67,67	0.75	3 (5%)
44	A86	M	320	-	44,50,50	0.37	1 (2%)	51,76,76	0.59	0
40	CLA	S	301	-	60,68,73	2.34	8 (13%)	70,107,113	1.47	5 (7%)
40	CLA	H	305	8	60,68,73	2.24	8 (13%)	70,107,113	1.44	9 (12%)
44	A86	T	319	-	44,50,50	0.62	1 (2%)	51,76,76	0.79	2 (3%)
44	A86	N	318	-	44,50,50	0.68	1 (2%)	51,76,76	0.46	0
41	KC2	M	308	13	48,53,53	1.56	8 (16%)	54,89,89	1.08	6 (11%)
40	CLA	z	302	-	60,68,73	2.28	8 (13%)	70,107,113	1.38	5 (7%)
41	KC2	N	312	14	48,53,53	1.57	8 (16%)	54,89,89	1.05	6 (11%)
40	CLA	a	815	23	65,73,73	2.25	8 (12%)	76,113,113	1.46	7 (9%)
40	CLA	y	303	-	47,55,73	2.69	8 (17%)	54,91,113	1.79	7 (12%)
40	CLA	B	303	-	47,55,73	2.62	8 (17%)	54,91,113	1.60	5 (9%)
40	CLA	z	313	-	47,55,73	2.65	8 (17%)	54,91,113	1.78	7 (12%)
41	KC2	U	201	-	48,53,53	1.63	8 (16%)	54,89,89	1.06	4 (7%)
44	A86	W	316	-	44,50,50	0.42	1 (2%)	51,76,76	0.68	1 (1%)
44	A86	Y	319	-	44,50,50	0.45	1 (2%)	51,76,76	1.15	4 (7%)
44	A86	w	310	-	44,50,50	0.45	1 (2%)	51,76,76	1.25	2 (3%)
44	A86	S	315	-	44,50,50	0.38	1 (2%)	51,76,76	1.25	2 (3%)
40	CLA	w	304	-	60,68,73	2.31	8 (13%)	70,107,113	1.42	6 (8%)
42	DD6	A	315	-	39,45,45	0.17	0	52,67,67	0.74	1 (1%)
40	CLA	E	302	5	47,55,73	2.63	8 (17%)	54,91,113	1.86	7 (12%)
40	CLA	a	819	23	61,69,73	2.31	8 (13%)	71,108,113	1.54	7 (9%)
40	CLA	b	805	-	61,69,73	2.27	8 (13%)	71,108,113	1.44	5 (7%)
44	A86	q	314	-	44,50,50	0.60	1 (2%)	51,76,76	1.49	5 (9%)
48	A1EB4	P	320	-	51,58,63	0.80	1 (1%)	60,84,89	1.23	2 (3%)
40	CLA	K	306	-	60,68,73	2.24	8 (13%)	70,107,113	1.49	9 (12%)
47	A1EB1	q	322	-	51,58,58	0.36	0	60,85,85	0.81	2 (3%)
47	A1EB1	v	321	-	51,58,58	0.51	1 (1%)	60,85,85	0.90	4 (6%)
40	CLA	u	306	35	47,55,73	2.57	8 (17%)	54,91,113	1.61	6 (11%)
41	KC2	L	308	12	48,53,53	1.60	8 (16%)	54,89,89	0.96	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A1EB4	M	319	-	51,58,63	0.62	1 (1%)	60,84,89	0.61	1 (1%)
40	CLA	T	304	15	60,68,73	2.29	8 (13%)	70,107,113	1.47	5 (7%)
40	CLA	D	312	4	55,63,73	2.47	8 (14%)	64,101,113	1.54	6 (9%)
40	CLA	I	201	-	65,73,73	2.21	8 (12%)	76,113,113	1.40	5 (6%)
41	KC2	T	311	15	48,53,53	1.62	8 (16%)	54,89,89	1.02	5 (9%)
42	DD6	T	314	-	39,45,45	0.21	0	52,67,67	0.72	1 (1%)
40	CLA	E	309	-	60,68,73	2.29	8 (13%)	70,107,113	1.43	7 (10%)
40	CLA	D	308	4	55,63,73	2.43	8 (14%)	64,101,113	1.51	6 (9%)
41	KC2	H	303	-	48,53,53	1.60	8 (16%)	54,89,89	1.04	4 (7%)
40	CLA	t	302	38	47,55,73	2.62	8 (17%)	54,91,113	1.63	5 (9%)
41	KC2	S	303	17	48,53,53	1.62	7 (14%)	54,89,89	1.10	5 (9%)
40	CLA	w	308	-	47,55,73	2.64	8 (17%)	54,91,113	1.56	5 (9%)
40	CLA	D	307	4	65,73,73	2.23	8 (12%)	76,113,113	1.47	9 (11%)
40	CLA	E	311	-	50,58,73	2.56	8 (16%)	58,95,113	1.63	5 (8%)
44	A86	Z	316	-	44,50,50	0.59	1 (2%)	51,76,76	1.23	3 (5%)
44	A86	v	316	-	44,50,50	0.58	1 (2%)	51,76,76	1.51	1 (1%)
40	CLA	O	310	-	47,55,73	2.62	8 (17%)	54,91,113	1.85	10 (18%)
44	A86	z	301	-	44,50,50	0.49	1 (2%)	51,76,76	1.08	2 (3%)
40	CLA	E	314	5	47,55,73	2.59	8 (17%)	54,91,113	2.11	10 (18%)
40	CLA	G	205	7	50,58,73	2.51	8 (16%)	58,95,113	1.55	5 (8%)
42	DD6	A	316	-	39,45,45	0.16	0	52,67,67	0.63	2 (3%)
40	CLA	a	822	-	65,73,73	2.17	8 (12%)	76,113,113	1.44	8 (10%)
44	A86	R	313	-	44,50,50	0.62	1 (2%)	51,76,76	0.64	0
40	CLA	b	838	-	65,73,73	2.11	8 (12%)	76,113,113	1.50	6 (7%)
44	A86	p	321	-	44,50,50	0.34	0	51,76,76	1.04	3 (5%)
41	KC2	W	309	-	48,53,53	1.57	7 (14%)	54,89,89	1.14	7 (12%)
40	CLA	b	837	24	60,68,73	2.21	8 (13%)	70,107,113	1.49	5 (7%)
41	KC2	O	309	15	48,53,53	1.56	7 (14%)	54,89,89	1.11	4 (7%)
42	DD6	x	320	-	39,45,45	0.18	0	52,67,67	0.65	0
40	CLA	z	308	39	60,68,73	2.20	8 (13%)	70,107,113	1.56	8 (11%)
49	BCR	f	206	-	41,41,41	0.21	0	56,56,56	0.53	0
47	A1EB1	Z	320	-	51,58,58	0.30	0	60,85,85	0.61	0
40	CLA	b	839	24	65,73,73	2.19	8 (12%)	76,113,113	1.53	6 (7%)
40	CLA	b	810	24	65,73,73	2.14	8 (12%)	76,113,113	1.35	6 (7%)
40	CLA	Y	312	-	47,55,73	2.69	8 (17%)	54,91,113	1.91	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	U	211	-	39,45,45	0.20	0	52,67,67	0.82	2 (3%)
40	CLA	M	306	13	62,70,73	2.23	8 (12%)	72,109,113	1.39	4 (5%)
41	KC2	p	304	35	48,53,53	1.55	8 (16%)	54,89,89	1.03	5 (9%)
41	KC2	u	304	35	48,53,53	1.53	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	C	307	3	60,68,73	2.29	8 (13%)	70,107,113	1.64	7 (10%)
40	CLA	E	313	5	47,55,73	2.63	8 (17%)	54,91,113	1.61	5 (9%)
40	CLA	A	308	-	55,63,73	2.43	8 (14%)	64,101,113	1.45	4 (6%)
40	CLA	Y	307	21	60,68,73	2.34	8 (13%)	70,107,113	1.57	7 (10%)
41	KC2	x	304	35	48,53,53	1.52	8 (16%)	54,89,89	0.98	3 (5%)
44	A86	p	320	-	44,50,50	0.33	0	51,76,76	1.10	4 (7%)
40	CLA	A	307	1	60,68,73	2.31	9 (15%)	70,107,113	1.54	7 (10%)
42	DD6	F	316	-	39,45,45	0.19	0	52,67,67	0.83	2 (3%)
44	A86	w	315	-	44,50,50	0.62	1 (2%)	51,76,76	0.71	2 (3%)
40	CLA	Y	310	-	55,63,73	2.39	8 (14%)	64,101,113	1.53	5 (7%)
44	A86	S	316	-	44,50,50	0.55	1 (2%)	51,76,76	1.13	4 (7%)
44	A86	Z	315	-	44,50,50	0.49	1 (2%)	51,76,76	1.16	3 (5%)
40	CLA	a	808	-	65,73,73	2.22	8 (12%)	76,113,113	1.65	8 (10%)
40	CLA	b	825	-	65,73,73	2.11	8 (12%)	76,113,113	1.37	5 (6%)
40	CLA	W	311	-	55,63,73	2.40	8 (14%)	64,101,113	1.61	6 (9%)
41	KC2	K	309	11	48,53,53	1.57	8 (16%)	54,89,89	1.07	5 (9%)
41	KC2	o	308	34	48,53,53	1.57	8 (16%)	54,89,89	1.02	5 (9%)
44	A86	o	317	-	44,50,50	0.47	1 (2%)	51,76,76	1.00	3 (5%)
40	CLA	a	811	40,23	61,69,73	2.31	9 (14%)	71,107,113	1.76	8 (11%)
40	CLA	O	305	15	47,55,73	2.60	8 (17%)	54,91,113	1.66	6 (11%)
40	CLA	b	809	24	60,68,73	2.31	8 (13%)	70,107,113	1.68	9 (12%)
40	CLA	L	306	12	47,55,73	2.63	8 (17%)	54,91,113	1.88	9 (16%)
40	CLA	E	306	5	55,63,73	2.39	8 (14%)	64,101,113	1.52	5 (7%)
40	CLA	b	820	-	65,73,73	2.21	8 (12%)	76,113,113	1.43	7 (9%)
44	A86	p	318	-	44,50,50	0.48	1 (2%)	51,76,76	1.25	3 (5%)
43	LMG	S	322	-	39,39,55	0.95	2 (5%)	47,47,63	1.22	4 (8%)
40	CLA	M	304	13	60,68,73	2.26	8 (13%)	70,107,113	1.43	5 (7%)
40	CLA	U	206	-	47,55,73	2.65	8 (17%)	54,91,113	1.51	6 (11%)
40	CLA	A	306	1	60,68,73	2.29	8 (13%)	70,107,113	1.38	6 (8%)
40	CLA	F	304	6	55,63,73	2.48	8 (14%)	64,101,113	1.58	8 (12%)
47	A1EB1	t	315	-	51,58,58	0.46	1 (1%)	60,85,85	0.74	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	C	304	3	56,64,73	2.39	9 (16%)	65,102,113	1.51	9 (13%)
40	CLA	E	310	-	60,68,73	2.31	8 (13%)	70,107,113	1.50	6 (8%)
49	BCR	b	848	-	41,41,41	0.15	0	56,56,56	0.33	0
40	CLA	a	851	-	65,73,73	2.19	8 (12%)	76,113,113	1.41	6 (7%)
40	CLA	b	807	-	65,73,73	2.08	8 (12%)	76,113,113	1.30	6 (7%)
44	A86	w	316	-	44,50,50	0.59	1 (2%)	51,76,76	1.15	3 (5%)
40	CLA	a	832	23	65,73,73	2.23	8 (12%)	76,113,113	1.37	6 (7%)
42	DD6	Q	213	-	39,45,45	0.22	0	52,67,67	0.73	2 (3%)
43	LMG	F	318	-	39,39,55	0.80	0	47,47,63	1.33	6 (12%)
42	DD6	C	312	-	39,45,45	0.15	0	52,67,67	0.95	1 (1%)
44	A86	X	321	-	44,50,50	0.81	1 (2%)	51,76,76	1.18	3 (5%)
40	CLA	C	309	-	47,55,73	2.65	8 (17%)	54,91,113	1.69	6 (11%)
41	KC2	I	214	-	48,53,53	1.62	8 (16%)	54,89,89	1.03	4 (7%)
42	DD6	G	210	-	39,45,45	0.23	0	52,67,67	0.73	2 (3%)
46	SQD	W	318	-	31,32,54	1.56	5 (16%)	40,43,65	1.33	5 (12%)
40	CLA	t	307	-	55,63,73	2.43	8 (14%)	64,101,113	1.70	7 (10%)
47	A1EB1	T	320	-	51,58,58	0.43	1 (1%)	60,85,85	0.67	1 (1%)
47	A1EB1	u	322	-	51,58,58	0.35	0	60,85,85	1.33	6 (10%)
44	A86	x	316	-	44,50,50	0.45	1 (2%)	51,76,76	1.23	3 (5%)
42	DD6	A	314	-	39,45,45	0.16	0	52,67,67	0.72	1 (1%)
44	A86	K	314	-	44,50,50	0.47	1 (2%)	51,76,76	1.07	3 (5%)
40	CLA	p	305	35	47,55,73	2.55	8 (17%)	54,91,113	1.70	6 (11%)
40	CLA	I	205	9	56,64,73	2.37	8 (14%)	65,102,113	1.46	7 (10%)
41	KC2	p	315	-	48,53,53	1.60	7 (14%)	54,89,89	1.12	6 (11%)
41	KC2	R	308	15	48,53,53	1.59	8 (16%)	54,89,89	1.01	5 (9%)
40	CLA	z	306	-	55,63,73	2.36	8 (14%)	64,101,113	1.48	6 (9%)
40	CLA	u	312	-	60,68,73	2.33	8 (13%)	70,107,113	1.40	5 (7%)
41	KC2	p	309	-	48,53,53	1.57	7 (14%)	54,89,89	1.10	6 (11%)
49	BCR	b	846	-	41,41,41	0.13	0	56,56,56	0.65	1 (1%)
49	BCR	j	103	-	41,41,41	0.23	0	56,56,56	0.53	0
41	KC2	q	302	36	48,53,53	1.65	7 (14%)	54,89,89	1.14	5 (9%)
40	CLA	U	203	-	55,63,73	2.39	8 (14%)	64,101,113	1.58	9 (14%)
43	LMG	E	321	-	40,40,55	0.87	1 (2%)	48,48,63	1.27	7 (14%)
43	LMG	a	801	-	35,35,55	0.96	0	43,43,63	1.17	4 (9%)
47	A1EB1	T	316	40	51,58,58	0.49	1 (1%)	60,85,85	0.75	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	b	801	-	63,71,73	2.25	9 (14%)	73,110,113	1.54	11 (15%)
44	A86	o	318	-	44,50,50	0.60	1 (2%)	51,76,76	0.50	0
41	KC2	O	303	15	48,53,53	1.59	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	a	838	23	55,63,73	2.43	8 (14%)	64,101,113	1.68	6 (9%)
40	CLA	B	301	2	47,55,73	2.67	8 (17%)	54,91,113	1.90	8 (14%)
40	CLA	a	805	40,23	54,62,73	2.37	8 (14%)	62,99,113	1.53	5 (8%)
41	KC2	t	306	-	48,53,53	1.55	7 (14%)	54,89,89	0.99	4 (7%)
40	CLA	w	303	38	47,55,73	2.65	8 (17%)	54,91,113	1.65	5 (9%)
42	DD6	o	320	-	39,45,45	0.18	0	52,67,67	0.61	1 (1%)
42	DD6	H	313	-	39,45,45	0.24	0	52,67,67	0.98	4 (7%)
40	CLA	E	305	5	60,68,73	2.28	8 (13%)	70,107,113	1.48	6 (8%)
40	CLA	b	827	24	60,68,73	2.28	8 (13%)	70,107,113	1.57	6 (8%)
41	KC2	M	309	-	48,53,53	1.62	7 (14%)	54,89,89	1.02	5 (9%)
47	A1EB1	Y	323	-	51,58,58	0.39	1 (1%)	60,85,85	0.82	2 (3%)
40	CLA	a	839	45	65,73,73	2.19	8 (12%)	76,113,113	1.40	5 (6%)
44	A86	Y	315	-	44,50,50	0.59	1 (2%)	51,76,76	1.13	2 (3%)
42	DD6	L	317	-	39,45,45	0.15	0	52,67,67	0.71	2 (3%)
40	CLA	a	852	-	55,63,73	2.43	8 (14%)	64,101,113	1.48	5 (7%)
40	CLA	B	302	2	47,55,73	2.47	8 (17%)	54,91,113	1.51	5 (9%)
41	KC2	t	308	-	48,53,53	1.62	7 (14%)	54,89,89	1.10	6 (11%)
40	CLA	C	301	3	47,55,73	2.65	8 (17%)	54,91,113	1.68	6 (11%)
47	A1EB1	t	314	-	51,58,58	0.62	1 (1%)	60,85,85	0.90	3 (5%)
40	CLA	R	306	15	60,68,73	2.31	8 (13%)	70,107,113	1.48	6 (8%)
42	DD6	Y	322	-	39,45,45	0.17	0	52,67,67	0.78	3 (5%)
40	CLA	a	824	-	62,70,73	2.22	8 (12%)	72,109,113	1.38	7 (9%)
40	CLA	G	207	-	54,62,73	2.43	8 (14%)	62,99,113	1.53	7 (11%)
40	CLA	E	303	-	60,68,73	2.36	8 (13%)	70,107,113	1.55	6 (8%)
45	LHG	S	323	-	39,39,48	0.68	0	42,45,54	1.26	4 (9%)
40	CLA	N	304	14	60,68,73	2.32	8 (13%)	70,107,113	1.46	5 (7%)
40	CLA	Z	301	-	60,68,73	2.32	8 (13%)	70,107,113	1.40	5 (7%)
44	A86	q	324	-	44,50,50	0.34	0	51,76,76	1.07	3 (5%)
40	CLA	p	307	35	55,63,73	2.46	8 (14%)	64,101,113	1.74	7 (10%)
42	DD6	D	317	-	39,45,45	0.18	0	52,67,67	0.83	3 (5%)
40	CLA	D	304	4	56,64,73	2.39	9 (16%)	65,102,113	1.61	6 (9%)
42	DD6	z	322	-	39,45,45	0.22	0	52,67,67	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	v	325	-	44,50,50	0.34	0	51,76,76	1.05	2 (3%)
41	KC2	N	308	14	48,53,53	1.60	7 (14%)	54,89,89	1.02	4 (7%)
44	A86	o	316	-	44,50,50	0.56	1 (2%)	51,76,76	1.03	3 (5%)
41	KC2	v	302	-	48,53,53	1.64	8 (16%)	54,89,89	1.06	4 (7%)
47	A1EB1	O	317	40	51,58,58	0.56	1 (1%)	60,85,85	0.80	1 (1%)
44	A86	C	311	-	44,50,50	0.70	1 (2%)	51,76,76	1.02	3 (5%)
41	KC2	x	303	-	48,53,53	1.64	8 (16%)	54,89,89	0.98	3 (5%)
40	CLA	F	307	6	60,67,73	2.41	11 (18%)	72,105,113	1.53	8 (11%)
42	DD6	P	315	-	39,45,45	0.39	0	52,67,67	1.02	2 (3%)
47	A1EB1	Z	319	-	51,58,58	0.51	1 (1%)	60,85,85	0.68	1 (1%)
41	KC2	q	308	36	48,53,53	1.56	8 (16%)	54,89,89	1.09	5 (9%)
41	KC2	Z	303	22	48,53,53	1.55	8 (16%)	54,89,89	0.99	5 (9%)
40	CLA	j	102	30	47,55,73	2.66	8 (17%)	54,91,113	1.77	9 (16%)
40	CLA	F	310	-	47,55,73	2.56	8 (17%)	54,91,113	1.64	10 (18%)
42	DD6	Q	212	-	39,45,45	0.20	0	52,67,67	0.73	2 (3%)
42	DD6	R	314	-	39,45,45	0.18	0	52,67,67	1.05	3 (5%)
44	A86	W	314	-	44,50,50	0.66	1 (2%)	51,76,76	0.93	2 (3%)
40	CLA	M	312	13	60,68,73	2.33	8 (13%)	70,107,113	1.51	7 (10%)
41	KC2	O	311	-	48,53,53	1.61	8 (16%)	54,89,89	1.03	5 (9%)
40	CLA	a	807	-	56,64,73	2.36	8 (14%)	65,102,113	1.56	6 (9%)
40	CLA	X	306	20	55,63,73	2.40	8 (14%)	64,101,113	1.66	9 (14%)
41	KC2	C	303	-	48,53,53	1.62	7 (14%)	54,89,89	1.06	4 (7%)
42	DD6	E	317	-	39,45,45	0.18	0	52,67,67	0.68	2 (3%)
41	KC2	u	315	-	48,53,53	1.55	7 (14%)	54,89,89	1.08	6 (11%)
47	A1EB1	S	320	-	51,58,58	0.50	1 (1%)	60,85,85	0.81	2 (3%)
40	CLA	U	207	-	47,55,73	2.71	8 (17%)	54,91,113	1.73	5 (9%)
42	DD6	X	322	-	39,45,45	0.18	0	52,67,67	0.73	2 (3%)
40	CLA	U	204	18	47,55,73	2.67	8 (17%)	54,91,113	1.62	5 (9%)
40	CLA	u	314	35	47,55,73	2.68	8 (17%)	54,91,113	1.84	7 (12%)
42	DD6	J	315	-	39,45,45	0.22	0	52,67,67	0.89	3 (5%)
40	CLA	k	201	31	55,63,73	2.46	8 (14%)	64,101,113	1.58	6 (9%)
40	CLA	J	312	-	58,66,73	2.37	8 (13%)	67,104,113	1.41	5 (7%)
40	CLA	b	828	24	55,63,73	2.41	8 (14%)	64,101,113	1.56	7 (10%)
41	KC2	H	316	-	48,53,53	1.49	7 (14%)	54,89,89	1.08	7 (12%)
42	DD6	I	212	-	39,45,45	0.19	0	52,67,67	0.73	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	Z	317	-	44,50,50	0.59	1 (2%)	51,76,76	0.92	1 (1%)
40	CLA	a	840	23	55,63,73	2.37	8 (14%)	64,101,113	1.51	6 (9%)
40	CLA	v	306	36	60,68,73	2.26	8 (13%)	70,107,113	1.46	7 (10%)
40	CLA	O	306	15	60,68,73	2.29	9 (15%)	70,107,113	1.57	7 (10%)
40	CLA	y	305	-	49,57,73	2.59	9 (18%)	61,94,113	1.63	7 (11%)
41	KC2	X	308	20	48,53,53	1.54	8 (16%)	54,89,89	0.98	5 (9%)
44	A86	z	315	-	44,50,50	0.41	0	51,76,76	1.43	5 (9%)
47	A1EB1	S	321	-	51,58,58	0.46	1 (1%)	60,85,85	0.75	1 (1%)
40	CLA	Y	304	-	47,55,73	2.68	8 (17%)	54,91,113	1.63	6 (11%)
40	CLA	J	307	10	47,55,73	2.57	8 (17%)	54,91,113	1.69	9 (16%)
41	KC2	R	302	15	48,53,53	1.62	9 (18%)	54,89,89	1.04	6 (11%)
49	BCR	b	845	-	41,41,41	0.18	0	56,56,56	0.39	0
49	BCR	i	102	-	41,41,41	0.37	0	56,56,56	0.68	0
44	A86	R	312	-	44,50,50	0.77	1 (2%)	51,76,76	1.28	3 (5%)
40	CLA	J	310	-	47,55,73	2.71	8 (17%)	54,91,113	1.79	7 (12%)
44	A86	M	315	-	44,50,50	0.56	1 (2%)	51,76,76	1.24	3 (5%)
41	KC2	Q	201	16	48,53,53	1.62	7 (14%)	54,89,89	1.08	4 (7%)
49	BCR	a	844	-	41,41,41	0.17	0	56,56,56	0.47	0
40	CLA	J	318	10	47,55,73	2.65	8 (17%)	54,91,113	1.62	7 (12%)
40	CLA	a	814	-	50,58,73	2.55	8 (16%)	58,95,113	1.58	5 (8%)
44	A86	Z	314	-	44,50,50	0.51	1 (2%)	51,76,76	1.39	3 (5%)
44	A86	G	209	-	44,50,50	0.55	1 (2%)	51,76,76	1.18	3 (5%)
40	CLA	U	205	-	47,55,73	2.64	8 (17%)	54,91,113	1.69	6 (11%)
40	CLA	B	306	-	52,60,73	2.51	8 (15%)	60,97,113	1.60	7 (11%)
40	CLA	p	311	-	55,63,73	2.50	8 (14%)	64,101,113	1.82	10 (15%)
40	CLA	v	313	36	47,55,73	2.64	8 (17%)	54,91,113	1.75	7 (12%)
40	CLA	b	813	24	50,58,73	2.45	8 (16%)	58,95,113	1.58	8 (13%)
42	DD6	E	318	-	39,45,45	0.19	0	52,67,67	0.90	5 (9%)
43	LMG	L	319	-	37,37,55	0.86	0	45,45,63	1.23	4 (8%)
40	CLA	z	307	-	60,68,73	2.34	8 (13%)	70,107,113	1.58	7 (10%)
41	KC2	M	303	13	48,53,53	1.53	8 (16%)	54,89,89	1.05	5 (9%)
40	CLA	H	310	-	60,68,73	2.31	8 (13%)	70,107,113	1.49	5 (7%)
41	KC2	W	302	-	48,53,53	1.55	8 (16%)	54,89,89	0.98	4 (7%)
40	CLA	Q	203	-	49,57,73	2.62	9 (18%)	57,93,113	2.01	8 (14%)
44	A86	S	318	-	44,50,50	0.42	1 (2%)	51,76,76	1.15	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	P	308	-	60,68,73	2.30	8 (13%)	70,107,113	1.42	6 (8%)
44	A86	O	312	-	44,50,50	0.48	1 (2%)	51,76,76	1.06	2 (3%)
44	A86	D	319	-	44,50,50	0.46	1 (2%)	51,76,76	1.05	2 (3%)
41	KC2	N	313	14	48,53,53	1.56	8 (16%)	54,89,89	1.00	4 (7%)
42	DD6	C	313	-	39,45,45	0.19	0	52,67,67	0.65	2 (3%)
40	CLA	L	311	12	47,55,73	2.68	8 (17%)	54,91,113	1.70	6 (11%)
40	CLA	p	306	35	47,55,73	2.66	8 (17%)	54,91,113	1.61	6 (11%)
42	DD6	K	311	-	39,45,45	0.17	0	52,67,67	0.80	2 (3%)
40	CLA	t	304	-	60,68,73	2.31	9 (15%)	70,107,113	1.44	7 (10%)
40	CLA	I	207	9	47,55,73	2.68	8 (17%)	54,91,113	1.75	6 (11%)
40	CLA	S	312	-	47,55,73	2.69	8 (17%)	54,91,113	1.78	8 (14%)
42	DD6	K	310	-	39,45,45	0.23	0	52,67,67	0.67	2 (3%)
41	KC2	x	310	-	48,53,53	1.55	8 (16%)	54,89,89	1.03	5 (9%)
40	CLA	B	304	-	47,55,73	2.62	8 (17%)	54,91,113	1.67	6 (11%)
40	CLA	o	310	-	55,63,73	2.44	8 (14%)	64,101,113	1.69	10 (15%)
42	DD6	o	319	-	39,45,45	0.20	0	52,67,67	0.88	4 (7%)
40	CLA	a	803	-	65,73,73	2.11	8 (12%)	76,113,113	1.34	7 (9%)
40	CLA	q	306	36	60,68,73	2.28	9 (15%)	70,107,113	1.49	6 (8%)
40	CLA	H	306	8	50,58,73	2.51	8 (16%)	58,95,113	1.55	6 (10%)
48	A1EB4	W	319	-	51,58,63	0.68	1 (1%)	60,84,89	0.68	1 (1%)
41	KC2	t	301	38	48,53,53	1.58	9 (18%)	54,89,89	0.99	5 (9%)
44	A86	t	310	-	44,50,50	0.51	1 (2%)	51,76,76	0.94	3 (5%)
44	A86	u	320	-	44,50,50	0.38	1 (2%)	51,76,76	1.21	2 (3%)
41	KC2	T	301	-	48,53,53	1.57	8 (16%)	54,89,89	1.01	4 (7%)
41	KC2	v	308	36	48,53,53	1.58	7 (14%)	54,89,89	1.10	4 (7%)
40	CLA	C	306	3	65,73,73	2.20	8 (12%)	76,113,113	1.35	7 (9%)
40	CLA	l	203	-	64,72,73	2.15	9 (14%)	74,111,113	1.61	7 (9%)
44	A86	N	315	-	44,50,50	0.66	1 (2%)	51,76,76	1.21	3 (5%)
44	A86	Q	210	-	44,50,50	0.41	1 (2%)	51,76,76	0.89	1 (1%)
47	A1EB1	L	318	-	51,58,58	0.58	1 (1%)	60,85,85	0.73	1 (1%)
44	A86	T	312	-	44,50,50	0.48	1 (2%)	51,76,76	1.17	3 (5%)
42	DD6	C	310	-	39,45,45	0.19	0	52,67,67	0.94	4 (7%)
40	CLA	o	305	34	55,63,73	2.40	8 (14%)	64,101,113	1.49	7 (10%)
40	CLA	A	311	1	47,55,73	2.59	8 (17%)	54,91,113	1.61	5 (9%)
40	CLA	S	307	17	60,68,73	2.27	8 (13%)	70,107,113	1.54	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	a	850	-	65,73,73	2.05	8 (12%)	76,113,113	1.49	6 (7%)
40	CLA	p	302	-	65,73,73	2.21	8 (12%)	76,113,113	1.48	8 (10%)
40	CLA	o	311	-	63,71,73	2.26	8 (12%)	73,110,113	1.48	6 (8%)
41	KC2	O	302	15	48,53,53	1.61	9 (18%)	54,89,89	1.15	7 (12%)
44	A86	Y	321	-	44,50,50	0.65	1 (2%)	51,76,76	0.76	1 (1%)
44	A86	u	317	-	44,50,50	0.56	1 (2%)	51,76,76	1.41	2 (3%)
42	DD6	u	321	-	39,45,45	0.21	0	52,67,67	0.62	0
40	CLA	q	307	36	60,68,73	2.32	9 (15%)	70,107,113	1.61	8 (11%)
40	CLA	v	304	-	52,60,73	2.42	8 (15%)	60,97,113	1.50	7 (11%)
40	CLA	a	830	-	58,66,73	2.32	8 (13%)	67,104,113	1.52	8 (11%)
44	A86	u	316	-	44,50,50	0.42	1 (2%)	51,76,76	1.29	3 (5%)
49	BCR	l	207	-	41,41,41	0.26	0	56,56,56	0.92	3 (5%)
42	DD6	j	104	-	39,45,45	0.19	0	52,67,67	0.77	2 (3%)
44	A86	U	210	-	44,50,50	0.43	1 (2%)	51,76,76	1.08	3 (5%)
49	BCR	a	843	-	41,41,41	0.20	0	56,56,56	0.44	0
50	PQN	b	849	-	29,29,34	0.43	0	36,39,45	0.77	1 (2%)
40	CLA	F	305	-	47,55,73	2.64	8 (17%)	54,91,113	1.68	6 (11%)
41	KC2	w	307	-	48,53,53	1.61	8 (16%)	54,89,89	1.07	6 (11%)
43	LMG	E	301	40	31,31,55	0.92	0	39,39,63	1.23	5 (12%)
40	CLA	K	301	-	47,55,73	2.61	8 (17%)	54,91,113	1.56	5 (9%)
40	CLA	W	312	13	60,68,73	2.21	8 (13%)	70,107,113	1.39	8 (11%)
42	DD6	I	213	-	39,45,45	0.26	0	52,67,67	0.99	3 (5%)
47	A1EB1	o	321	-	51,58,58	0.52	1 (1%)	60,85,85	0.62	0
42	DD6	I	211	-	39,45,45	0.22	0	52,67,67	1.08	4 (7%)
40	CLA	V	202	19	55,63,73	2.37	8 (14%)	64,101,113	1.53	8 (12%)
40	CLA	a	842	-	65,73,73	2.14	8 (12%)	76,113,113	1.34	7 (9%)
41	KC2	X	302	-	48,53,53	1.64	8 (16%)	54,89,89	1.01	4 (7%)
47	A1EB1	q	323	-	51,58,58	0.56	1 (1%)	60,85,85	0.50	0
41	KC2	o	303	34	48,53,53	1.58	9 (18%)	54,89,89	1.03	5 (9%)
40	CLA	O	316	47	47,55,73	2.59	8 (17%)	54,91,113	1.48	6 (11%)
40	CLA	b	833	24	60,68,73	2.26	8 (13%)	70,107,113	1.44	7 (10%)
40	CLA	D	303	4	60,68,73	2.29	8 (13%)	70,107,113	1.48	6 (8%)
49	BCR	a	846	-	41,41,41	0.16	0	56,56,56	0.41	0
46	SQD	I	215	-	53,54,54	1.20	4 (7%)	62,65,65	1.12	5 (8%)
47	A1EB1	R	317	40	51,58,58	0.60	1 (1%)	60,85,85	1.12	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	z	314	-	47,55,73	2.59	8 (17%)	54,91,113	1.85	7 (12%)
41	KC2	T	309	15	48,53,53	1.55	8 (16%)	54,89,89	1.02	3 (5%)
40	CLA	w	305	-	49,57,73	2.59	9 (18%)	61,94,113	1.63	5 (8%)
47	A1EB1	v	323	-	51,58,58	0.53	1 (1%)	60,85,85	0.59	1 (1%)
40	CLA	t	309	-	47,55,73	2.65	8 (17%)	54,91,113	1.62	5 (9%)
47	A1EB1	z	323	-	51,58,58	0.53	1 (1%)	60,85,85	0.94	2 (3%)
40	CLA	q	304	-	52,60,73	2.43	8 (15%)	60,97,113	1.51	7 (11%)
40	CLA	P	306	13	47,55,73	2.60	8 (17%)	54,91,113	1.55	6 (11%)
40	CLA	X	311	20	63,71,73	2.23	8 (12%)	73,110,113	1.51	6 (8%)
40	CLA	b	824	24	65,73,73	2.13	8 (12%)	76,113,113	1.40	8 (10%)
40	CLA	b	812	24	60,68,73	2.20	8 (13%)	70,107,113	1.36	5 (7%)
41	KC2	R	309	15	48,53,53	1.63	8 (16%)	54,89,89	1.14	7 (12%)
40	CLA	o	313	-	47,55,73	2.77	9 (19%)	54,91,113	1.94	7 (12%)
42	DD6	H	312	-	39,45,45	0.22	0	52,67,67	1.12	4 (7%)
40	CLA	z	312	-	60,68,73	2.26	8 (13%)	70,107,113	1.47	7 (10%)
41	KC2	R	311	15	48,53,53	1.60	8 (16%)	54,89,89	1.03	6 (11%)
41	KC2	q	309	-	48,53,53	1.53	8 (16%)	54,89,89	1.04	6 (11%)
40	CLA	F	306	6	60,68,73	2.27	8 (13%)	70,107,113	1.42	7 (10%)
40	CLA	b	818	24	62,70,73	2.24	8 (12%)	72,109,113	1.44	5 (6%)
40	CLA	x	305	-	51,59,73	2.41	8 (15%)	59,96,113	1.58	5 (8%)
40	CLA	W	306	13	60,68,73	2.30	8 (13%)	70,107,113	1.50	7 (10%)
44	A86	X	317	-	44,50,50	0.49	1 (2%)	51,76,76	1.03	3 (5%)
41	KC2	L	303	12	48,53,53	1.58	8 (16%)	54,89,89	1.03	5 (9%)
40	CLA	Z	310	-	55,63,73	2.42	8 (14%)	64,101,113	1.83	10 (15%)
44	A86	v	319	-	44,50,50	0.36	0	51,76,76	1.30	4 (7%)
40	CLA	E	312	-	47,55,73	2.61	8 (17%)	54,91,113	1.77	5 (9%)
40	CLA	b	840	-	65,73,73	2.19	8 (12%)	76,113,113	1.50	7 (9%)
42	DD6	J	316	-	39,45,45	0.14	0	52,67,67	0.69	3 (5%)
44	A86	p	317	-	44,50,50	0.57	1 (2%)	51,76,76	1.31	2 (3%)
41	KC2	L	302	-	48,53,53	1.61	8 (16%)	54,89,89	1.04	6 (11%)
40	CLA	b	808	-	65,73,73	2.19	8 (12%)	76,113,113	1.30	8 (10%)
44	A86	X	319	-	44,50,50	0.44	1 (2%)	51,76,76	1.46	4 (7%)
44	A86	u	318	-	44,50,50	0.45	1 (2%)	51,76,76	1.55	3 (5%)
47	A1EB1	y	313	-	51,58,58	0.45	1 (1%)	60,85,85	0.80	2 (3%)
40	CLA	M	307	-	60,68,73	2.28	8 (13%)	70,107,113	1.45	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	R	316	47	47,55,73	2.58	7 (14%)	54,91,113	1.46	6 (11%)
40	CLA	v	301	-	55,63,73	2.37	8 (14%)	64,101,113	1.54	5 (7%)
40	CLA	W	313	13	60,68,73	2.33	8 (13%)	70,107,113	1.45	6 (8%)
41	KC2	M	301	13	48,53,53	1.56	8 (16%)	54,89,89	1.00	5 (9%)
40	CLA	A	303	1	61,69,73	2.25	8 (13%)	71,108,113	1.42	6 (8%)
46	SQD	P	319	-	31,32,54	1.54	4 (12%)	40,43,65	1.39	8 (20%)
40	CLA	Q	204	16	50,58,73	2.56	9 (18%)	58,94,113	1.98	9 (15%)
44	A86	x	319	-	44,50,50	0.30	0	51,76,76	1.41	2 (3%)
44	A86	F	313	-	44,50,50	0.43	1 (2%)	51,76,76	0.78	2 (3%)
40	CLA	T	307	-	55,63,73	2.42	8 (14%)	64,101,113	1.58	5 (7%)
42	DD6	q	320	-	39,45,45	0.19	0	52,67,67	0.79	1 (1%)
42	DD6	F	314	-	39,45,45	0.30	0	52,67,67	1.03	4 (7%)
44	A86	P	317	-	44,50,50	0.44	1 (2%)	51,76,76	0.78	2 (3%)
42	DD6	J	317	-	39,45,45	0.20	0	52,67,67	0.75	1 (1%)
41	KC2	J	304	-	48,53,53	1.60	8 (16%)	54,89,89	1.04	7 (12%)
40	CLA	Z	311	22	63,71,73	2.26	8 (12%)	73,110,113	1.51	8 (10%)
42	DD6	B	305	-	39,45,45	0.19	0	52,67,67	0.78	2 (3%)
49	BCR	b	843	-	41,41,41	0.13	0	56,56,56	0.43	0
40	CLA	V	201	-	58,66,73	2.35	8 (13%)	67,104,113	1.44	4 (5%)
41	KC2	x	315	-	48,53,53	1.56	7 (14%)	54,89,89	1.12	5 (9%)
41	KC2	N	301	14	48,53,53	1.51	8 (16%)	54,89,89	1.01	4 (7%)
40	CLA	E	307	-	65,73,73	2.17	8 (12%)	76,113,113	1.29	4 (5%)
47	A1EB1	L	316	-	51,58,58	0.55	1 (1%)	60,85,85	0.74	1 (1%)
40	CLA	q	312	-	60,68,73	2.30	8 (13%)	70,107,113	1.36	5 (7%)
41	KC2	Y	314	-	48,53,53	1.61	7 (14%)	54,89,89	1.13	9 (16%)
42	DD6	M	314	-	39,45,45	0.21	0	52,67,67	0.81	2 (3%)
41	KC2	K	305	11	48,53,53	1.52	8 (16%)	54,89,89	1.04	4 (7%)
41	KC2	v	309	-	48,53,53	1.51	8 (16%)	54,89,89	1.05	4 (7%)
40	CLA	y	308	-	47,55,73	2.63	8 (17%)	54,91,113	1.54	5 (9%)
41	KC2	G	202	-	48,53,53	1.57	8 (16%)	54,89,89	1.11	7 (12%)
40	CLA	S	305	-	52,60,73	2.51	8 (15%)	60,97,113	1.76	10 (16%)
40	CLA	q	313	36	47,55,73	2.65	8 (17%)	54,91,113	1.65	6 (11%)
41	KC2	z	309	39	48,53,53	1.50	8 (16%)	54,89,89	0.99	3 (5%)
47	A1EB1	w	313	-	51,58,58	0.44	1 (1%)	60,85,85	0.62	1 (1%)
41	KC2	Y	308	-	48,53,53	1.59	8 (16%)	54,89,89	1.06	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	I	208	-	55,63,73	2.45	8 (14%)	64,101,113	1.62	5 (7%)
40	CLA	q	301	-	55,63,73	2.40	8 (14%)	64,101,113	1.59	5 (7%)
43	LMG	x	301	-	39,39,55	0.88	1 (2%)	47,47,63	1.22	4 (8%)
40	CLA	H	301	-	47,55,73	2.59	8 (17%)	54,91,113	1.60	7 (12%)
40	CLA	S	319	-	47,55,73	2.63	8 (17%)	54,91,113	1.51	4 (7%)
44	A86	X	315	-	44,50,50	0.49	0	51,76,76	1.68	6 (11%)
42	DD6	z	321	-	39,45,45	0.22	0	52,67,67	0.91	3 (5%)
41	KC2	T	303	-	48,53,53	1.52	7 (14%)	54,89,89	1.12	6 (11%)
41	KC2	x	309	-	48,53,53	1.50	8 (16%)	54,89,89	1.14	6 (11%)
40	CLA	P	305	13	60,68,73	2.24	8 (13%)	70,107,113	1.45	6 (8%)
44	A86	R	315	-	44,50,50	0.51	1 (2%)	51,76,76	1.26	3 (5%)
41	KC2	z	304	39	48,53,53	1.58	9 (18%)	54,89,89	1.10	5 (9%)
40	CLA	P	311	-	47,55,73	2.58	8 (17%)	54,91,113	1.71	8 (14%)
42	DD6	F	315	-	39,45,45	0.21	0	52,67,67	1.02	3 (5%)
41	KC2	W	303	-	48,53,53	1.59	8 (16%)	54,89,89	1.05	6 (11%)
49	BCR	a	845	-	41,41,41	0.14	0	56,56,56	0.46	0
44	A86	q	315	-	44,50,50	0.50	1 (2%)	51,76,76	0.90	2 (3%)
40	CLA	Z	313	22	47,55,73	2.66	8 (17%)	54,91,113	1.86	8 (14%)
47	A1EB1	y	314	-	51,58,58	0.57	1 (1%)	60,85,85	0.40	0
49	BCR	b	844	-	41,41,41	0.26	0	56,56,56	0.59	1 (1%)
40	CLA	t	303	38	47,55,73	2.62	8 (17%)	54,91,113	1.64	4 (7%)
40	CLA	w	309	-	55,63,73	2.42	8 (14%)	64,101,113	1.70	6 (9%)
42	DD6	p	322	-	39,45,45	0.17	0	52,67,67	0.70	0
47	A1EB1	x	322	-	51,58,58	0.58	1 (1%)	60,85,85	0.58	1 (1%)
41	KC2	o	302	-	48,53,53	1.63	8 (16%)	54,89,89	1.07	6 (11%)
41	KC2	S	304	17	48,53,53	1.56	8 (16%)	54,89,89	1.07	5 (9%)
44	A86	q	319	-	44,50,50	0.35	0	51,76,76	1.32	5 (9%)
41	KC2	P	310	-	48,53,53	1.54	8 (16%)	54,89,89	1.00	4 (7%)
41	KC2	R	303	-	48,53,53	1.57	7 (14%)	54,89,89	1.08	6 (11%)
44	A86	D	320	-	44,50,50	0.47	1 (2%)	51,76,76	0.89	2 (3%)
41	KC2	N	302	14	48,53,53	1.56	7 (14%)	54,89,89	1.04	5 (9%)
40	CLA	b	841	24	65,73,73	2.19	8 (12%)	76,113,113	1.32	6 (7%)
47	A1EB1	F	322	-	51,58,58	0.53	1 (1%)	60,85,85	0.40	0
40	CLA	a	820	23	60,68,73	2.34	8 (13%)	70,107,113	1.59	7 (10%)
42	DD6	N	317	-	39,45,45	0.21	0	52,67,67	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	A1EB1	K	313	-	51,58,58	0.56	1 (1%)	60,85,85	1.24	2 (3%)
40	CLA	a	812	23	55,63,73	2.41	8 (14%)	64,101,113	1.45	8 (12%)
41	KC2	q	303	36	48,53,53	1.53	8 (16%)	54,89,89	0.99	4 (7%)
40	CLA	P	312	13	60,68,73	2.30	8 (13%)	70,107,113	1.41	7 (10%)
41	KC2	T	308	15	48,53,53	1.59	8 (16%)	54,89,89	1.03	4 (7%)
44	A86	G	211	-	44,50,50	0.54	1 (2%)	51,76,76	0.75	1 (1%)
43	LMG	u	301	-	39,39,55	0.84	0	47,47,63	1.28	4 (8%)
44	A86	q	316	-	44,50,50	0.56	1 (2%)	51,76,76	1.52	1 (1%)
40	CLA	b	831	24	51,59,73	2.46	8 (15%)	59,96,113	1.52	5 (8%)
41	KC2	P	309	13	48,53,53	1.58	8 (16%)	54,89,89	1.08	6 (11%)
40	CLA	D	309	-	58,66,73	2.37	8 (13%)	67,104,113	1.46	5 (7%)
40	CLA	z	305	39	60,68,73	2.22	8 (13%)	70,107,113	1.55	6 (8%)
44	A86	P	314	-	44,50,50	0.40	0	51,76,76	0.96	3 (5%)
42	DD6	J	314	-	39,45,45	0.19	0	52,67,67	0.69	2 (3%)
41	KC2	R	301	15	48,53,53	1.53	7 (14%)	54,89,89	1.06	6 (11%)
40	CLA	H	304	-	47,55,73	2.64	9 (19%)	54,91,113	1.65	8 (14%)
40	CLA	P	313	-	60,68,73	2.26	8 (13%)	70,107,113	1.44	6 (8%)
42	DD6	q	318	-	39,45,45	0.21	0	52,67,67	0.96	3 (5%)
42	DD6	D	314	-	39,45,45	0.20	0	52,67,67	0.85	1 (1%)
44	A86	N	321	-	44,50,50	0.47	1 (2%)	51,76,76	0.89	2 (3%)
40	CLA	I	206	9	65,73,73	2.23	9 (13%)	76,113,113	1.41	7 (9%)
40	CLA	p	314	35	47,55,73	2.66	8 (17%)	54,91,113	1.74	6 (11%)
40	CLA	Q	208	-	60,68,73	2.29	7 (11%)	70,107,113	1.38	8 (11%)
42	DD6	H	314	-	39,45,45	0.23	0	52,67,67	0.92	3 (5%)
40	CLA	o	301	-	60,68,73	2.35	8 (13%)	70,107,113	1.40	4 (5%)
52	DGD	b	850	-	57,57,67	0.95	2 (3%)	71,71,81	1.47	9 (12%)
44	A86	v	315	-	44,50,50	0.58	1 (2%)	51,76,76	0.83	2 (3%)
40	CLA	l	205	32	65,73,73	2.18	8 (12%)	76,113,113	1.48	7 (9%)
40	CLA	H	309	-	56,64,73	2.41	8 (14%)	65,102,113	1.78	9 (13%)
41	KC2	X	303	20	48,53,53	1.60	8 (16%)	54,89,89	1.03	6 (11%)
42	DD6	k	204	-	39,45,45	0.20	0	52,67,67	0.83	4 (7%)
40	CLA	f	202	24	65,73,73	2.11	8 (12%)	76,113,113	1.32	5 (6%)
40	CLA	z	311	-	55,63,73	2.41	8 (14%)	64,101,113	1.91	10 (15%)
40	CLA	u	308	35	60,68,73	2.29	8 (13%)	70,107,113	1.54	6 (8%)
41	KC2	p	310	-	48,53,53	1.59	8 (16%)	54,89,89	1.01	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	S	306	17	56,64,73	2.40	8 (14%)	65,102,113	1.46	5 (7%)
40	CLA	a	828	23	65,73,73	2.17	8 (12%)	76,113,113	1.37	5 (6%)
40	CLA	Y	306	21	60,68,73	2.33	9 (15%)	70,107,113	1.55	8 (11%)
40	CLA	f	201	-	60,68,73	2.32	8 (13%)	70,107,113	1.35	5 (7%)
41	KC2	z	310	39	48,53,53	1.57	8 (16%)	54,89,89	1.01	4 (7%)
47	A1EB1	v	322	-	51,58,58	0.37	0	60,85,85	0.82	2 (3%)
47	A1EB1	w	314	-	51,58,58	0.52	1 (1%)	60,85,85	0.65	1 (1%)
40	CLA	F	321	-	60,68,73	2.29	8 (13%)	70,107,113	1.50	7 (10%)
44	A86	X	316	-	44,50,50	0.52	1 (2%)	51,76,76	1.26	2 (3%)
40	CLA	b	836	24	60,68,73	2.31	8 (13%)	70,107,113	1.46	6 (8%)
44	A86	Y	320	-	44,50,50	0.64	1 (2%)	51,76,76	1.59	3 (5%)
47	A1EB1	t	313	-	51,58,58	0.42	1 (1%)	60,85,85	0.78	3 (5%)
40	CLA	F	308	-	55,63,73	2.46	8 (14%)	64,101,113	1.55	5 (7%)
44	A86	Y	316	-	44,50,50	0.44	1 (2%)	51,76,76	0.61	1 (1%)
40	CLA	b	834	-	65,73,73	2.12	8 (12%)	76,113,113	1.42	4 (5%)
40	CLA	A	302	-	60,68,73	2.33	8 (13%)	70,107,113	1.39	6 (8%)
44	A86	y	310	-	44,50,50	0.53	1 (2%)	51,76,76	1.19	4 (7%)
44	A86	O	315	-	44,50,50	0.39	1 (2%)	51,76,76	0.73	1 (1%)
40	CLA	v	312	-	60,68,73	2.29	8 (13%)	70,107,113	1.43	5 (7%)
44	A86	z	320	-	44,50,50	0.59	1 (2%)	51,76,76	0.69	1 (1%)
49	BCR	r	201	-	41,41,41	0.19	0	56,56,56	0.39	0
46	SQD	F	320	-	35,36,54	1.44	4 (11%)	44,47,65	1.39	8 (18%)
40	CLA	G	204	7	55,63,73	2.40	8 (14%)	64,101,113	1.54	6 (9%)
44	A86	z	316	-	44,50,50	0.54	1 (2%)	51,76,76	1.76	3 (5%)
44	A86	P	316	-	44,50,50	0.39	1 (2%)	51,76,76	1.02	3 (5%)
47	A1EB1	p	324	-	51,58,58	0.50	1 (1%)	60,85,85	0.41	1 (1%)
47	A1EB1	G	212	-	51,58,58	0.59	1 (1%)	60,85,85	0.71	1 (1%)
41	KC2	P	303	13	48,53,53	1.63	8 (16%)	54,89,89	1.01	4 (7%)
40	CLA	q	305	-	60,68,73	2.25	8 (13%)	70,107,113	1.52	7 (10%)
41	KC2	N	309	-	48,53,53	1.51	8 (16%)	54,89,89	1.02	6 (11%)
40	CLA	D	311	-	47,55,73	2.58	8 (17%)	54,91,113	1.79	7 (12%)
41	KC2	O	301	15	48,53,53	1.55	7 (14%)	54,89,89	1.08	5 (9%)
44	A86	M	316	-	44,50,50	0.49	1 (2%)	51,76,76	0.83	3 (5%)
40	CLA	u	305	35	47,55,73	2.60	8 (17%)	54,91,113	1.80	6 (11%)
40	CLA	Y	301	-	60,68,73	2.31	8 (13%)	70,107,113	1.41	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	J	308	10	55,63,73	2.45	9 (16%)	64,101,113	1.50	7 (10%)
40	CLA	x	313	-	55,63,73	2.38	8 (14%)	64,101,113	1.40	6 (9%)
44	A86	Y	317	41	44,50,50	0.56	1 (2%)	51,76,76	0.97	4 (7%)
40	CLA	a	841	23	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
40	CLA	A	301	1	47,55,73	2.55	8 (17%)	54,91,113	1.64	8 (14%)
40	CLA	Y	311	-	47,55,73	2.63	8 (17%)	54,91,113	1.59	6 (11%)
41	KC2	A	310	1	48,53,53	1.59	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	y	304	-	60,68,73	2.32	9 (15%)	70,107,113	1.46	8 (11%)
40	CLA	Z	307	22	60,68,73	2.29	8 (13%)	70,107,113	1.51	7 (10%)
40	CLA	E	304	5	55,63,73	2.40	8 (14%)	64,101,113	1.48	6 (9%)
42	DD6	t	312	-	39,45,45	0.16	0	52,67,67	0.99	3 (5%)
40	CLA	N	310	-	50,58,73	2.52	8 (16%)	58,95,113	1.71	9 (15%)
47	A1EB1	p	323	-	51,58,58	0.38	0	60,85,85	1.26	5 (8%)
42	DD6	O	314	-	39,45,45	0.21	0	52,67,67	0.86	3 (5%)
40	CLA	D	310	4	60,68,73	2.17	8 (13%)	70,107,113	1.44	8 (11%)
44	A86	t	311	-	44,50,50	0.63	1 (2%)	51,76,76	1.29	3 (5%)
40	CLA	w	302	38	47,55,73	2.59	8 (17%)	54,91,113	1.66	5 (9%)
40	CLA	y	309	-	55,63,73	2.41	8 (14%)	64,101,113	1.72	7 (10%)
41	KC2	S	310	-	48,53,53	1.58	8 (16%)	54,89,89	1.02	5 (9%)
40	CLA	B	307	-	47,55,73	2.56	8 (17%)	54,91,113	1.81	9 (16%)
40	CLA	a	816	23	65,73,73	2.17	8 (12%)	76,113,113	1.57	8 (10%)
44	A86	N	314	-	44,50,50	0.54	1 (2%)	51,76,76	1.08	4 (7%)
40	CLA	T	310	-	58,66,73	2.30	8 (13%)	67,104,113	1.51	7 (10%)
44	A86	x	317	-	44,50,50	0.56	1 (2%)	51,76,76	0.84	2 (3%)
44	A86	O	313	-	44,50,50	0.30	0	51,76,76	0.82	2 (3%)
40	CLA	W	307	13	65,73,73	2.21	8 (12%)	76,113,113	1.37	8 (10%)
40	CLA	H	308	8	47,55,73	2.66	8 (17%)	54,91,113	1.56	4 (7%)
40	CLA	N	307	-	60,68,73	2.32	8 (13%)	70,107,113	1.44	5 (7%)
41	KC2	T	302	-	48,53,53	1.59	9 (18%)	54,89,89	1.04	6 (11%)
44	A86	x	318	-	44,50,50	0.48	1 (2%)	51,76,76	1.30	2 (3%)
44	A86	z	319	-	44,50,50	0.54	1 (2%)	51,76,76	1.07	1 (1%)
40	CLA	b	830	24	61,69,73	2.25	8 (13%)	71,108,113	1.62	8 (11%)
42	DD6	y	311	-	39,45,45	0.19	0	52,67,67	1.02	4 (7%)
47	A1EB1	q	321	-	51,58,58	0.53	1 (1%)	60,85,85	0.94	3 (5%)
40	CLA	a	826	-	61,69,73	2.27	8 (13%)	71,108,113	1.47	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	A1EB1	x	321	-	51,58,58	0.53	1 (1%)	60,85,85	0.54	1 (1%)
47	A1EB1	K	315	-	51,58,58	0.57	1 (1%)	60,85,85	0.46	0
41	KC2	v	303	36	48,53,53	1.51	8 (16%)	54,89,89	1.05	4 (7%)
40	CLA	N	305	14	55,63,73	2.35	8 (14%)	64,101,113	1.52	5 (7%)
44	A86	H	315	-	44,50,50	0.49	1 (2%)	51,76,76	1.31	4 (7%)
40	CLA	D	302	43	58,66,73	2.35	8 (13%)	67,104,113	1.52	5 (7%)
44	A86	t	316	-	44,50,50	0.58	1 (2%)	51,76,76	0.50	0
41	KC2	z	303	39	48,53,53	1.59	8 (16%)	54,89,89	1.02	3 (5%)
43	LMG	l	201	-	39,39,55	0.85	1 (2%)	47,47,63	1.25	4 (8%)
43	LMG	M	317	-	39,39,55	0.89	2 (5%)	47,47,63	1.33	4 (8%)
40	CLA	b	817	24	65,73,73	2.09	8 (12%)	76,113,113	1.39	6 (7%)
40	CLA	i	101	-	55,63,73	2.42	8 (14%)	64,101,113	1.72	7 (10%)
40	CLA	Y	305	21	55,63,73	2.43	8 (14%)	64,101,113	1.50	5 (7%)
40	CLA	A	309	1	65,73,73	2.24	8 (12%)	76,113,113	1.37	4 (5%)
40	CLA	R	307	-	55,63,73	2.41	8 (14%)	64,101,113	1.57	5 (7%)
42	DD6	I	210	-	39,45,45	0.17	0	52,67,67	0.90	1 (1%)
51	SF4	b	804	-	0,12,12	-	-	-	-	-
41	KC2	Z	302	-	48,53,53	1.64	7 (14%)	54,89,89	1.03	4 (7%)
49	BCR	b	847	-	41,41,41	0.19	0	56,56,56	0.58	0
41	KC2	Y	309	44,21	48,53,53	1.57	8 (16%)	54,89,89	0.99	4 (7%)
42	DD6	v	318	-	39,45,45	0.23	0	52,67,67	0.84	3 (5%)
44	A86	T	313	-	44,50,50	0.41	1 (2%)	51,76,76	0.91	3 (5%)
40	CLA	Q	202	16	58,66,73	2.36	8 (13%)	67,104,113	1.59	6 (8%)
40	CLA	J	311	-	47,55,73	2.70	8 (17%)	54,91,113	1.74	6 (11%)
40	CLA	o	307	34	60,68,73	2.30	8 (13%)	70,107,113	1.61	9 (12%)
40	CLA	Y	313	21	47,55,73	2.73	8 (17%)	54,91,113	1.88	8 (14%)
40	CLA	b	823	24	55,63,73	2.37	8 (14%)	64,101,113	1.57	6 (9%)
40	CLA	v	307	36	60,68,73	2.32	8 (13%)	70,107,113	1.62	8 (11%)
47	A1EB1	N	320	-	51,58,58	0.43	0	60,85,85	1.09	3 (5%)
49	BCR	l	208	-	41,41,41	0.20	0	56,56,56	0.66	2 (3%)
45	LHG	a	849	40	29,29,48	0.78	0	32,35,54	1.19	2 (6%)
40	CLA	S	308	-	49,57,73	2.56	9 (18%)	61,94,113	1.69	10 (16%)
40	CLA	o	306	34	60,68,73	2.31	9 (15%)	70,107,113	1.49	7 (10%)
40	CLA	M	305	13	60,68,73	2.26	8 (13%)	70,107,113	1.45	6 (8%)
40	CLA	Q	209	-	47,55,73	2.65	8 (17%)	54,91,113	1.73	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	a	806	23	65,73,73	2.20	8 (12%)	76,113,113	1.56	6 (7%)
44	A86	X	318	-	44,50,50	0.64	1 (2%)	51,76,76	2.03	4 (7%)
40	CLA	b	835	24	65,72,73	2.30	10 (15%)	78,111,113	1.47	9 (11%)
40	CLA	I	203	9	55,63,73	2.41	8 (14%)	64,101,113	1.57	6 (9%)
40	CLA	I	204	9	47,55,73	2.59	8 (17%)	54,91,113	1.53	5 (9%)
44	A86	X	314	-	44,50,50	0.60	1 (2%)	51,76,76	1.13	4 (7%)
40	CLA	u	302	-	65,73,73	2.15	8 (12%)	76,113,113	1.47	7 (9%)
46	SQD	M	318	-	31,32,54	1.52	4 (12%)	40,43,65	1.22	5 (12%)
40	CLA	C	305	3	60,68,73	2.34	8 (13%)	70,107,113	1.53	7 (10%)
42	DD6	W	315	-	39,45,45	0.20	0	52,67,67	0.74	2 (3%)
44	A86	L	314	-	44,50,50	0.73	1 (2%)	51,76,76	1.17	2 (3%)
44	A86	p	319	-	44,50,50	0.41	1 (2%)	51,76,76	1.63	4 (7%)

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	L	304	12	1/1/13/20	2/28/106/115	-
41	KC2	P	304	13	-	4/15/71/71	-
44	A86	v	317	-	-	1/34/90/90	0/3/3/3
45	LHG	a	848	-	-	22/52/52/53	-
40	CLA	M	311	13	1/1/14/20	11/34/112/115	-
44	A86	v	314	-	-	3/34/90/90	0/3/3/3
40	CLA	L	305	12	1/1/11/20	6/16/94/115	-
40	CLA	T	305	15	1/1/12/20	1/19/97/115	-
44	A86	u	319	-	-	11/34/90/90	0/3/3/3
49	BCR	m	101	-	-	0/29/63/63	0/2/2/2
42	DD6	E	315	-	-	1/26/80/80	0/3/3/3
43	LMG	P	318	-	-	11/34/54/70	0/1/1/1
40	CLA	o	304	34	1/1/14/20	4/31/109/115	-
42	DD6	Q	214	-	-	1/26/80/80	0/3/3/3
40	CLA	A	305	1	1/1/14/20	5/33/111/115	-
40	CLA	G	206	7	1/1/13/20	9/27/105/115	-
40	CLA	G	213	-	1/1/11/20	6/16/94/115	-
44	A86	p	316	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	a	825	-	1/1/15/20	5/37/115/115	-
40	CLA	b	803	-	1/1/15/20	12/37/115/115	-
42	DD6	Q	211	-	-	2/26/80/80	0/3/3/3
47	A1EB1	u	323	-	-	4/42/100/100	0/3/3/3
41	KC2	o	309	34	-	10/15/71/71	-
40	CLA	N	311	14	1/1/14/20	11/31/109/115	-
46	SQD	k	205	-	-	3/31/51/69	0/1/1/1
41	KC2	u	303	-	-	6/15/71/71	-
40	CLA	t	305	-	1/1/12/20	2/19/95/115	-
41	KC2	Y	303	21	-	7/15/71/71	-
40	CLA	b	802	-	1/1/15/20	11/37/115/115	-
40	CLA	F	303	6	1/1/14/20	9/34/112/115	-
40	CLA	x	307	-	1/1/13/20	9/25/103/115	-
40	CLA	O	307	-	1/1/14/20	8/34/112/115	-
40	CLA	a	836	23	1/1/15/20	11/37/115/115	-
41	KC2	y	307	-	-	6/15/71/71	-
40	CLA	T	306	15	1/1/14/20	3/31/109/115	-
41	KC2	F	302	6	-	8/15/71/71	-
41	KC2	W	310	13	-	7/15/71/71	-
40	CLA	J	306	10	1/1/12/20	2/22/100/115	-
40	CLA	a	823	23	1/1/13/20	7/25/103/115	-
42	DD6	E	316	-	-	0/26/80/80	0/3/3/3
44	A86	F	312	-	-	4/34/90/90	0/3/3/3
41	KC2	Z	309	-	-	8/15/71/71	-
44	A86	w	311	-	-	9/34/90/90	0/3/3/3
43	LMG	E	320	-	-	14/26/46/70	0/1/1/1
40	CLA	D	306	4	1/1/13/20	6/25/103/115	-
41	KC2	u	309	-	-	6/15/71/71	-
40	CLA	X	301	-	1/1/14/20	6/31/109/115	-
40	CLA	T	317	47	1/1/11/20	2/16/94/115	-
44	A86	W	301	-	-	1/34/90/90	0/3/3/3
40	CLA	u	311	-	1/1/13/20	9/25/103/115	-
40	CLA	z	324	-	1/1/11/20	3/16/94/115	-
40	CLA	p	313	-	1/1/13/20	2/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	a	829	-	1/1/15/20	14/37/115/115	-
40	CLA	F	301	-	1/1/12/20	9/23/101/115	-
42	DD6	v	320	-	-	7/26/80/80	0/3/3/3
44	A86	F	317	-	-	9/34/90/90	0/3/3/3
40	CLA	F	311	-	1/1/11/20	3/16/94/115	-
40	CLA	b	814	24	1/1/15/20	11/37/115/115	-
40	CLA	x	314	35	1/1/11/20	3/16/94/115	-
40	CLA	b	806	24	1/1/15/20	13/37/115/115	-
40	CLA	A	304	1	1/1/15/20	15/37/115/115	-
40	CLA	C	302	-	1/1/11/20	5/16/94/115	-
40	CLA	k	202	-	1/1/13/20	4/25/103/115	-
41	KC2	X	309	-	-	6/15/71/71	-
44	A86	M	313	-	-	3/34/90/90	0/3/3/3
40	CLA	J	303	-	1/1/11/20	2/16/94/115	-
40	CLA	p	312	-	1/1/11/20	3/16/94/115	-
40	CLA	R	310	-	1/1/11/20	3/16/94/115	-
40	CLA	b	821	-	1/1/15/20	7/37/115/115	-
41	KC2	u	310	-	-	6/15/71/71	-
47	A1EB1	y	312	-	-	11/42/100/100	0/3/3/3
42	DD6	L	315	-	-	0/26/80/80	0/3/3/3
42	DD6	U	209	-	-	1/26/80/80	0/3/3/3
40	CLA	J	302	10	1/1/11/20	6/16/94/115	-
40	CLA	W	305	13	1/1/15/20	6/37/115/115	-
40	CLA	a	810	-	1/1/14/20	6/31/109/115	-
40	CLA	E	308	5	1/1/13/20	6/29/107/115	-
40	CLA	a	818	-	1/1/11/20	0/16/94/115	-
40	CLA	q	310	-	1/1/12/20	10/21/99/115	-
40	CLA	b	832	24	1/1/15/20	6/37/115/115	-
40	CLA	u	307	35	1/1/13/20	8/25/103/115	-
40	CLA	R	304	15	1/1/12/20	9/21/99/115	-
40	CLA	Z	306	22	1/1/14/20	14/31/109/115	-
40	CLA	b	819	24	1/1/14/20	14/36/114/115	-
40	CLA	Z	312	-	1/1/11/20	5/16/94/115	-
40	CLA	J	309	-	1/1/11/20	0/16/94/115	-
40	CLA	X	312	-	1/1/11/20	5/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	a	835	-	1/1/15/20	2/37/115/115	-
41	KC2	O	308	15	-	8/15/71/71	-
40	CLA	R	305	15	1/1/14/20	6/31/109/115	-
40	CLA	K	307	11	1/1/12/20	11/24/102/115	-
40	CLA	a	804	23	1/1/14/20	10/34/112/115	-
40	CLA	Z	304	-	1/1/14/20	2/31/109/115	-
43	LMG	A	317	-	-	22/35/55/70	0/1/1/1
40	CLA	u	313	-	1/1/13/20	1/25/103/115	-
40	CLA	x	302	-	1/1/15/20	8/37/115/115	-
41	KC2	F	309	6	-	6/15/71/71	-
40	CLA	H	302	-	1/1/11/20	5/16/94/115	-
42	DD6	Z	318	-	-	1/26/80/80	0/3/3/3
44	A86	o	315	-	-	9/34/90/90	0/3/3/3
45	LHG	F	319	-	-	18/44/44/53	-
41	KC2	p	303	-	-	6/15/71/71	-
40	CLA	N	306	-	1/1/14/20	0/31/109/115	-
41	KC2	Z	308	22	-	4/15/71/71	-
41	KC2	M	302	13	-	2/15/71/71	-
40	CLA	Z	305	22	1/1/13/20	7/25/103/115	-
40	CLA	a	809	-	1/1/12/20	3/19/97/115	-
44	A86	o	314	-	-	12/34/90/90	0/3/3/3
40	CLA	X	310	-	1/1/13/20	7/25/103/115	-
47	A1EB1	P	301	-	-	14/42/100/100	0/3/3/3
40	CLA	a	817	23	1/1/12/20	1/19/97/115	-
40	CLA	a	831	-	1/1/14/20	8/31/109/115	-
40	CLA	Q	207	-	1/1/11/20	3/16/94/115	-
41	KC2	L	309	12	-	7/15/71/71	-
41	KC2	W	304	13	-	5/15/71/71	-
41	KC2	K	303	11	-	9/15/71/71	-
44	A86	q	317	-	-	1/34/90/90	0/3/3/3
40	CLA	f	205	-	1/1/11/20	3/16/94/115	-
40	CLA	U	202	18	1/1/13/20	7/25/103/115	-
51	SF4	c	101	-	-	-	0/6/5/5
40	CLA	x	311	-	1/1/13/20	9/25/103/115	-
40	CLA	K	312	-	1/1/11/20	3/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	b	816	24	1/1/11/20	5/16/94/115	-
40	CLA	X	307	20	1/1/14/20	7/31/109/115	-
42	DD6	D	313	-	-	0/26/80/80	0/3/3/3
40	CLA	o	312	-	1/1/11/20	6/16/94/115	-
42	DD6	D	315	-	-	0/26/80/80	0/3/3/3
41	KC2	y	306	-	-	7/15/71/71	-
40	CLA	S	302	-	1/1/14/20	11/31/109/115	-
40	CLA	x	312	-	1/1/14/20	8/31/109/115	-
40	CLA	X	305	-	1/1/12/20	8/19/97/115	-
40	CLA	b	815	-	1/1/13/20	4/28/106/115	-
40	CLA	b	826	24	1/1/14/20	8/36/114/115	-
44	A86	z	317	-	-	6/34/90/90	0/3/3/3
40	CLA	a	833	23	1/1/14/20	6/31/109/115	-
40	CLA	G	201	7	1/1/11/20	2/16/94/115	-
51	SF4	c	102	-	-	-	0/6/5/5
40	CLA	W	308	-	1/1/14/20	12/31/109/115	-
40	CLA	l	204	-	1/1/15/20	8/37/115/115	-
44	A86	Q	215	-	-	3/34/90/90	0/3/3/3
40	CLA	M	310	-	1/1/13/20	4/27/105/115	-
41	KC2	K	302	11	-	6/15/71/71	-
40	CLA	f	204	28	1/1/11/20	0/16/94/115	-
40	CLA	D	301	4	1/1/13/20	6/25/103/115	-
40	CLA	a	821	23	1/1/15/20	16/37/115/115	-
43	LMG	W	317	-	-	7/34/54/70	0/1/1/1
40	CLA	P	307	13	1/1/13/20	6/30/108/115	-
40	CLA	l	202	-	1/1/15/20	13/37/115/115	-
40	CLA	Q	205	16	1/1/14/20	9/34/112/115	-
49	BCR	l	206	-	-	6/29/63/63	0/2/2/2
44	A86	S	317	-	-	5/34/90/90	0/3/3/3
40	CLA	v	305	-	1/1/14/20	4/31/109/115	-
43	LMG	j	101	-	-	10/25/45/70	0/1/1/1
40	CLA	S	311	-	1/1/11/20	4/16/94/115	-
40	CLA	L	310	-	1/1/11/20	4/16/94/115	-
44	A86	T	315	-	-	11/34/90/90	1/3/3/3
40	CLA	p	308	-	1/1/14/20	6/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	K	304	11	1/1/14/20	7/31/109/115	-
43	LMG	D	318	-	-	16/35/55/70	0/1/1/1
40	CLA	S	314	17	1/1/13/20	10/25/103/115	-
41	KC2	G	208	-	-	5/15/71/71	-
42	DD6	A	312	-	-	0/26/80/80	0/3/3/3
43	LMG	a	802	-	-	12/30/50/70	0/1/1/1
40	CLA	q	311	-	1/1/14/20	11/35/113/115	-
40	CLA	x	308	35	1/1/14/20	4/31/109/115	-
40	CLA	L	312	-	1/1/11/20	2/16/94/115	-
40	CLA	a	834	-	1/1/14/20	4/31/109/115	-
42	DD6	w	312	-	-	1/26/80/80	0/3/3/3
43	LMG	T	318	-	-	16/35/55/70	0/1/1/1
41	KC2	N	303	14	-	4/15/71/71	-
44	A86	Y	318	-	-	9/34/90/90	0/3/3/3
41	KC2	L	313	12	-	8/15/71/71	-
44	A86	P	321	-	-	6/34/90/90	0/3/3/3
40	CLA	y	302	38	1/1/11/20	2/16/94/115	-
40	CLA	L	307	-	1/1/13/20	3/25/103/115	-
47	A1EB1	Z	321	-	-	9/42/100/100	0/3/3/3
44	A86	X	320	-	-	6/34/90/90	0/3/3/3
40	CLA	v	311	-	1/1/14/20	10/35/113/115	-
43	LMG	p	301	-	-	9/34/54/70	0/1/1/1
40	CLA	b	822	-	1/1/14/20	9/36/114/115	-
40	CLA	v	310	-	1/1/12/20	10/21/99/115	-
44	A86	z	318	-	-	4/34/90/90	1/3/3/3
40	CLA	Q	206	-	1/1/14/20	7/34/112/115	-
40	CLA	C	308	-	1/1/11/20	7/16/94/115	-
41	KC2	E	319	-	-	10/15/71/71	-
42	DD6	A	313	-	-	1/26/80/80	0/3/3/3
41	KC2	Y	302	-	-	5/15/71/71	-
49	BCR	k	203	-	-	4/29/63/63	0/2/2/2
40	CLA	J	305	10	1/1/13/20	7/25/103/115	-
42	DD6	J	313	-	-	1/26/80/80	0/3/3/3
41	KC2	Q	216	-	-	7/15/71/71	-
42	DD6	N	319	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	I	202	9	1/1/13/20	6/25/103/115	-
40	CLA	X	313	20	1/1/11/20	2/16/94/115	-
40	CLA	H	311	-	1/1/11/20	1/16/94/115	-
40	CLA	a	827	23	1/1/15/20	2/37/115/115	-
41	KC2	y	301	38	-	9/15/71/71	-
40	CLA	D	305	4	1/1/9/20	0/16/82/115	-
40	CLA	X	304	-	1/1/11/20	6/16/94/115	-
41	KC2	w	301	38	-	7/15/71/71	-
40	CLA	x	306	35	1/1/14/20	13/31/109/115	-
40	CLA	a	813	23	1/1/14/20	5/31/109/115	-
41	KC2	I	209	9	-	8/15/71/71	-
41	KC2	w	306	38	-	8/15/71/71	-
40	CLA	L	301	-	1/1/11/20	0/16/94/115	-
40	CLA	b	842	-	1/1/14/20	10/33/111/115	-
47	A1EB1	v	324	-	-	12/42/100/100	0/3/3/3
41	KC2	S	309	17	-	10/15/71/71	-
40	CLA	G	203	7	1/1/13/20	8/25/103/115	-
47	A1EB1	o	322	-	-	14/42/100/100	0/3/3/3
40	CLA	H	307	-	1/1/14/20	17/31/109/115	-
40	CLA	a	837	23	1/1/13/20	6/25/103/115	-
40	CLA	S	313	-	1/1/11/20	5/16/94/115	-
41	KC2	P	302	-	-	4/15/71/71	-
40	CLA	U	208	-	1/1/11/20	7/16/94/115	-
50	PQN	a	847	-	-	4/17/37/43	0/2/2/2
49	BCR	f	203	-	-	0/29/63/63	0/2/2/2
40	CLA	O	304	15	1/1/15/20	7/37/115/115	-
42	DD6	N	316	-	-	2/26/80/80	0/3/3/3
40	CLA	b	829	-	1/1/11/20	1/16/94/115	-
40	CLA	b	811	24	1/1/11/20	4/16/94/115	-
42	DD6	D	316	-	-	1/26/80/80	0/3/3/3
40	CLA	K	308	11	1/1/13/20	10/30/108/115	-
42	DD6	J	301	-	-	2/26/80/80	0/3/3/3
44	A86	M	320	-	-	5/34/90/90	0/3/3/3
40	CLA	S	301	-	1/1/14/20	6/31/109/115	-
40	CLA	H	305	8	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	T	319	-	-	6/34/90/90	0/3/3/3
44	A86	N	318	-	-	2/34/90/90	0/3/3/3
41	KC2	M	308	13	-	6/15/71/71	-
40	CLA	z	302	-	1/1/14/20	6/31/109/115	-
41	KC2	N	312	14	-	8/15/71/71	-
40	CLA	a	815	23	1/1/15/20	7/37/115/115	-
40	CLA	y	303	-	1/1/11/20	3/16/94/115	-
40	CLA	B	303	-	1/1/11/20	1/16/94/115	-
40	CLA	z	313	-	1/1/11/20	3/16/94/115	-
41	KC2	U	201	-	-	5/15/71/71	-
44	A86	W	316	-	-	5/34/90/90	0/3/3/3
44	A86	Y	319	-	-	6/34/90/90	0/3/3/3
44	A86	w	310	-	-	9/34/90/90	0/3/3/3
44	A86	S	315	-	-	9/34/90/90	0/3/3/3
40	CLA	w	304	-	1/1/14/20	7/31/109/115	-
42	DD6	A	315	-	-	0/26/80/80	0/3/3/3
40	CLA	E	302	5	1/1/11/20	7/16/94/115	-
40	CLA	a	819	23	1/1/14/20	8/33/111/115	-
40	CLA	b	805	-	1/1/14/20	7/33/111/115	-
44	A86	q	314	-	-	3/34/90/90	0/3/3/3
48	A1EB4	P	320	-	-	6/37/98/103	0/3/3/3
40	CLA	K	306	-	1/1/14/20	6/31/109/115	-
47	A1EB1	q	322	-	-	8/42/100/100	0/3/3/3
47	A1EB1	v	321	-	-	16/42/100/100	1/3/3/3
40	CLA	u	306	35	1/1/11/20	6/16/94/115	-
41	KC2	L	308	12	-	4/15/71/71	-
48	A1EB4	M	319	-	-	5/37/98/103	0/3/3/3
40	CLA	T	304	15	1/1/14/20	6/31/109/115	-
40	CLA	D	312	4	1/1/13/20	7/25/103/115	-
40	CLA	I	201	-	1/1/15/20	8/37/115/115	-
41	KC2	T	311	15	-	8/15/71/71	-
42	DD6	T	314	-	-	1/26/80/80	0/3/3/3
40	CLA	E	309	-	1/1/14/20	9/31/109/115	-
40	CLA	D	308	4	1/1/13/20	1/25/103/115	-
41	KC2	H	303	-	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	t	302	38	1/1/11/20	2/16/94/115	-
41	KC2	S	303	17	-	5/15/71/71	-
40	CLA	w	308	-	1/1/11/20	4/16/94/115	-
40	CLA	D	307	4	1/1/15/20	6/37/115/115	-
40	CLA	E	311	-	1/1/12/20	5/19/97/115	-
44	A86	Z	316	-	-	5/34/90/90	1/3/3/3
44	A86	v	316	-	-	3/34/90/90	1/3/3/3
40	CLA	O	310	-	1/1/11/20	4/16/94/115	-
44	A86	z	301	-	-	7/34/90/90	0/3/3/3
40	CLA	E	314	5	1/1/11/20	11/16/94/115	-
40	CLA	G	205	7	1/1/12/20	1/19/97/115	-
42	DD6	A	316	-	-	1/26/80/80	0/3/3/3
40	CLA	a	822	-	1/1/15/20	10/37/115/115	-
44	A86	R	313	-	-	6/34/90/90	0/3/3/3
40	CLA	b	838	-	1/1/15/20	9/37/115/115	-
44	A86	p	321	-	-	7/34/90/90	0/3/3/3
41	KC2	W	309	-	-	6/15/71/71	-
40	CLA	b	837	24	1/1/14/20	10/31/109/115	-
41	KC2	O	309	15	-	9/15/71/71	-
42	DD6	x	320	-	-	0/26/80/80	0/3/3/3
40	CLA	z	308	39	1/1/14/20	11/31/109/115	-
49	BCR	f	206	-	-	4/29/63/63	0/2/2/2
47	A1EB1	Z	320	-	-	7/42/100/100	0/3/3/3
40	CLA	b	839	24	1/1/15/20	12/37/115/115	-
40	CLA	b	810	24	1/1/15/20	13/37/115/115	-
40	CLA	Y	312	-	1/1/11/20	4/16/94/115	-
42	DD6	U	211	-	-	0/26/80/80	0/3/3/3
40	CLA	M	306	13	1/1/14/20	3/34/112/115	-
41	KC2	p	304	35	-	8/15/71/71	-
41	KC2	u	304	35	-	8/15/71/71	-
40	CLA	C	307	3	1/1/14/20	7/31/109/115	-
40	CLA	E	313	5	1/1/11/20	3/16/94/115	-
40	CLA	A	308	-	1/1/13/20	0/25/103/115	-
40	CLA	Y	307	21	1/1/14/20	7/31/109/115	-
41	KC2	x	304	35	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	p	320	-	-	7/34/90/90	0/3/3/3
40	CLA	A	307	1	1/1/14/20	4/31/109/115	-
42	DD6	F	316	-	-	2/26/80/80	0/3/3/3
44	A86	w	315	-	-	8/34/90/90	1/3/3/3
40	CLA	Y	310	-	1/1/13/20	8/25/103/115	-
44	A86	S	316	-	-	8/34/90/90	0/3/3/3
44	A86	Z	315	-	-	12/34/90/90	0/3/3/3
40	CLA	a	808	-	1/1/15/20	6/37/115/115	-
40	CLA	b	825	-	1/1/15/20	7/37/115/115	-
40	CLA	W	311	-	1/1/13/20	7/25/103/115	-
41	KC2	K	309	11	-	8/15/71/71	-
41	KC2	o	308	34	-	8/15/71/71	-
44	A86	o	317	-	-	7/34/90/90	0/3/3/3
40	CLA	a	811	40,23	1/1/14/20	12/34/112/115	-
40	CLA	O	305	15	1/1/11/20	2/16/94/115	-
40	CLA	b	809	24	1/1/14/20	10/31/109/115	-
40	CLA	L	306	12	1/1/11/20	4/16/94/115	-
40	CLA	E	306	5	1/1/13/20	7/25/103/115	-
40	CLA	b	820	-	1/1/15/20	9/37/115/115	-
44	A86	p	318	-	-	10/34/90/90	0/3/3/3
43	LMG	S	322	-	-	9/34/54/70	0/1/1/1
40	CLA	M	304	13	1/1/14/20	8/31/109/115	-
40	CLA	U	206	-	1/1/11/20	1/16/94/115	-
40	CLA	A	306	1	1/1/14/20	8/31/109/115	-
40	CLA	F	304	6	1/1/13/20	1/25/103/115	-
47	A1EB1	t	315	-	-	12/42/100/100	0/3/3/3
40	CLA	C	304	3	1/1/13/20	3/27/105/115	-
40	CLA	E	310	-	1/1/14/20	6/31/109/115	-
49	BCR	b	848	-	-	4/29/63/63	0/2/2/2
40	CLA	a	851	-	1/1/15/20	13/37/115/115	-
40	CLA	b	807	-	1/1/15/20	10/37/115/115	-
44	A86	w	316	-	-	12/34/90/90	0/3/3/3
40	CLA	a	832	23	1/1/15/20	15/37/115/115	-
42	DD6	Q	213	-	-	1/26/80/80	0/3/3/3
43	LMG	F	318	-	-	10/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	C	312	-	-	2/26/80/80	0/3/3/3
44	A86	X	321	-	-	5/34/90/90	0/3/3/3
40	CLA	C	309	-	1/1/11/20	2/16/94/115	-
41	KC2	I	214	-	-	6/15/71/71	-
42	DD6	G	210	-	-	1/26/80/80	0/3/3/3
46	SQD	W	318	-	-	7/27/47/69	0/1/1/1
40	CLA	t	307	-	1/1/13/20	10/25/103/115	-
47	A1EB1	T	320	-	-	11/42/100/100	0/3/3/3
47	A1EB1	u	322	-	-	10/42/100/100	0/3/3/3
44	A86	x	316	-	-	5/34/90/90	0/3/3/3
42	DD6	A	314	-	-	1/26/80/80	0/3/3/3
44	A86	K	314	-	-	4/34/90/90	0/3/3/3
40	CLA	p	305	35	1/1/11/20	4/16/94/115	-
40	CLA	I	205	9	1/1/13/20	6/27/105/115	-
41	KC2	p	315	-	-	8/15/71/71	-
41	KC2	R	308	15	-	6/15/71/71	-
40	CLA	z	306	-	1/1/13/20	5/25/103/115	-
40	CLA	u	312	-	1/1/14/20	8/31/109/115	-
41	KC2	p	309	-	-	7/15/71/71	-
49	BCR	b	846	-	-	4/29/63/63	0/2/2/2
49	BCR	j	103	-	-	4/29/63/63	0/2/2/2
41	KC2	q	302	36	-	7/15/71/71	-
40	CLA	U	203	-	1/1/13/20	9/25/103/115	-
43	LMG	E	321	-	-	12/35/55/70	0/1/1/1
43	LMG	a	801	-	-	13/30/50/70	0/1/1/1
47	A1EB1	T	316	40	-	4/42/100/100	0/3/3/3
40	CLA	b	801	-	1/1/14/20	7/35/113/115	-
44	A86	o	318	-	-	3/34/90/90	0/3/3/3
41	KC2	O	303	15	-	6/15/71/71	-
40	CLA	a	838	23	1/1/13/20	7/25/103/115	-
40	CLA	B	301	2	1/1/11/20	7/16/94/115	-
40	CLA	a	805	40,23	1/1/12/20	4/24/102/115	-
41	KC2	t	306	-	-	9/15/71/71	-
40	CLA	w	303	38	1/1/11/20	5/16/94/115	-
42	DD6	o	320	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	H	313	-	-	5/26/80/80	0/3/3/3
40	CLA	E	305	5	1/1/14/20	3/31/109/115	-
40	CLA	b	827	24	1/1/14/20	9/31/109/115	-
41	KC2	M	309	-	-	4/15/71/71	-
47	A1EB1	Y	323	-	-	3/42/100/100	0/3/3/3
40	CLA	a	839	45	1/1/15/20	10/37/115/115	-
44	A86	Y	315	-	-	8/34/90/90	0/3/3/3
42	DD6	L	317	-	-	0/26/80/80	0/3/3/3
40	CLA	a	852	-	1/1/13/20	5/25/103/115	-
40	CLA	B	302	2	1/1/11/20	2/16/94/115	-
41	KC2	t	308	-	-	6/15/71/71	-
40	CLA	C	301	3	1/1/11/20	4/16/94/115	-
47	A1EB1	t	314	-	-	17/42/100/100	1/3/3/3
40	CLA	R	306	15	1/1/14/20	3/31/109/115	-
42	DD6	Y	322	-	-	3/26/80/80	0/3/3/3
40	CLA	a	824	-	1/1/14/20	13/34/112/115	-
40	CLA	G	207	-	1/1/12/20	5/24/102/115	-
40	CLA	E	303	-	1/1/14/20	3/31/109/115	-
45	LHG	S	323	-	-	23/44/44/53	-
40	CLA	N	304	14	1/1/14/20	10/31/109/115	-
40	CLA	Z	301	-	1/1/14/20	4/31/109/115	-
44	A86	q	324	-	-	7/34/90/90	0/3/3/3
40	CLA	p	307	35	1/1/13/20	7/25/103/115	-
42	DD6	D	317	-	-	1/26/80/80	0/3/3/3
40	CLA	D	304	4	1/1/13/20	5/27/105/115	-
42	DD6	z	322	-	-	3/26/80/80	0/3/3/3
44	A86	v	325	-	-	7/34/90/90	0/3/3/3
41	KC2	N	308	14	-	7/15/71/71	-
44	A86	o	316	-	-	11/34/90/90	0/3/3/3
41	KC2	v	302	-	-	7/15/71/71	-
47	A1EB1	O	317	40	-	8/42/100/100	1/3/3/3
44	A86	C	311	-	-	9/34/90/90	1/3/3/3
41	KC2	x	303	-	-	7/15/71/71	-
40	CLA	F	307	6	1/1/14/20	7/31/109/115	-
42	DD6	P	315	-	1/1/12/24	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	A1EB1	Z	319	-	-	7/42/100/100	0/3/3/3
41	KC2	q	308	36	-	10/15/71/71	-
41	KC2	Z	303	22	-	3/15/71/71	-
40	CLA	j	102	30	1/1/11/20	3/16/94/115	-
40	CLA	F	310	-	1/1/11/20	4/16/94/115	-
42	DD6	Q	212	-	-	1/26/80/80	0/3/3/3
42	DD6	R	314	-	-	0/26/80/80	0/3/3/3
44	A86	W	314	-	-	6/34/90/90	0/3/3/3
40	CLA	M	312	13	1/1/14/20	13/31/109/115	-
41	KC2	O	311	-	-	7/15/71/71	-
40	CLA	a	807	-	1/1/13/20	9/27/105/115	-
40	CLA	X	306	20	1/1/13/20	4/25/103/115	-
41	KC2	C	303	-	-	8/15/71/71	-
42	DD6	E	317	-	-	1/26/80/80	0/3/3/3
41	KC2	u	315	-	-	7/15/71/71	-
47	A1EB1	S	320	-	-	7/42/100/100	1/3/3/3
40	CLA	U	207	-	1/1/11/20	4/16/94/115	-
42	DD6	X	322	-	-	0/26/80/80	0/3/3/3
40	CLA	U	204	18	1/1/11/20	7/16/94/115	-
40	CLA	u	314	35	1/1/11/20	7/16/94/115	-
42	DD6	J	315	-	-	1/26/80/80	0/3/3/3
40	CLA	k	201	31	1/1/13/20	5/25/103/115	-
40	CLA	J	312	-	1/1/13/20	10/29/107/115	-
40	CLA	b	828	24	1/1/13/20	2/25/103/115	-
41	KC2	H	316	-	-	5/15/71/71	-
42	DD6	I	212	-	-	0/26/80/80	0/3/3/3
44	A86	Z	317	-	-	2/34/90/90	1/3/3/3
40	CLA	a	840	23	1/1/13/20	6/25/103/115	-
40	CLA	v	306	36	1/1/14/20	8/31/109/115	-
40	CLA	O	306	15	1/1/14/20	10/31/109/115	-
40	CLA	y	305	-	1/1/12/20	3/19/95/115	-
41	KC2	X	308	20	-	5/15/71/71	-
44	A86	z	315	-	-	7/34/90/90	0/3/3/3
47	A1EB1	S	321	-	-	9/42/100/100	1/3/3/3
40	CLA	Y	304	-	1/1/11/20	2/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	J	307	10	1/1/11/20	3/16/94/115	-
41	KC2	R	302	15	-	5/15/71/71	-
49	BCR	b	845	-	-	2/29/63/63	0/2/2/2
49	BCR	i	102	-	-	4/29/63/63	0/2/2/2
44	A86	R	312	-	-	5/34/90/90	0/3/3/3
40	CLA	J	310	-	1/1/11/20	2/16/94/115	-
44	A86	M	315	-	-	5/34/90/90	1/3/3/3
41	KC2	Q	201	16	-	5/15/71/71	-
49	BCR	a	844	-	-	2/29/63/63	0/2/2/2
40	CLA	J	318	10	1/1/11/20	1/16/94/115	-
40	CLA	a	814	-	1/1/12/20	1/19/97/115	-
44	A86	Z	314	-	-	3/34/90/90	0/3/3/3
44	A86	G	209	-	-	9/34/90/90	0/3/3/3
40	CLA	U	205	-	1/1/11/20	3/16/94/115	-
40	CLA	B	306	-	1/1/12/20	7/22/100/115	-
40	CLA	p	311	-	1/1/13/20	10/25/103/115	-
40	CLA	v	313	36	1/1/11/20	4/16/94/115	-
40	CLA	b	813	24	1/1/12/20	6/19/97/115	-
42	DD6	E	318	-	-	3/26/80/80	0/3/3/3
43	LMG	L	319	-	-	15/32/52/70	0/1/1/1
40	CLA	z	307	-	1/1/14/20	7/31/109/115	-
41	KC2	M	303	13	-	4/15/71/71	-
40	CLA	H	310	-	1/1/14/20	4/31/109/115	-
41	KC2	W	302	-	-	5/15/71/71	-
40	CLA	Q	203	-	1/1/12/20	2/19/97/115	-
44	A86	S	318	-	-	2/34/90/90	0/3/3/3
40	CLA	P	308	-	1/1/14/20	15/31/109/115	-
44	A86	O	312	-	-	6/34/90/90	0/3/3/3
44	A86	D	319	-	-	4/34/90/90	0/3/3/3
41	KC2	N	313	14	-	4/15/71/71	-
42	DD6	C	313	-	-	2/26/80/80	0/3/3/3
40	CLA	L	311	12	1/1/11/20	3/16/94/115	-
40	CLA	p	306	35	1/1/11/20	6/16/94/115	-
42	DD6	K	311	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	t	304	-	1/1/14/20	8/31/109/115	-
40	CLA	I	207	9	1/1/11/20	5/16/94/115	-
40	CLA	S	312	-	1/1/11/20	3/16/94/115	-
42	DD6	K	310	-	-	0/26/80/80	0/3/3/3
41	KC2	x	310	-	-	6/15/71/71	-
40	CLA	B	304	-	1/1/11/20	6/16/94/115	-
40	CLA	o	310	-	1/1/13/20	8/25/103/115	-
42	DD6	o	319	-	-	1/26/80/80	0/3/3/3
40	CLA	a	803	-	1/1/15/20	7/37/115/115	-
40	CLA	q	306	36	1/1/14/20	4/31/109/115	-
40	CLA	H	306	8	1/1/12/20	0/19/97/115	-
48	A1EB4	W	319	-	-	10/37/98/103	0/3/3/3
41	KC2	t	301	38	-	7/15/71/71	-
44	A86	t	310	-	-	7/34/90/90	0/3/3/3
44	A86	u	320	-	-	5/34/90/90	0/3/3/3
41	KC2	T	301	-	-	4/15/71/71	-
41	KC2	v	308	36	-	10/15/71/71	-
40	CLA	C	306	3	1/1/15/20	15/37/115/115	-
40	CLA	l	203	-	1/1/14/20	12/36/114/115	-
44	A86	N	315	-	-	9/34/90/90	0/3/3/3
44	A86	Q	210	-	-	5/34/90/90	0/3/3/3
47	A1EB1	L	318	-	-	15/42/100/100	0/3/3/3
44	A86	T	312	-	-	4/34/90/90	0/3/3/3
42	DD6	C	310	-	-	1/26/80/80	0/3/3/3
40	CLA	o	305	34	1/1/13/20	9/25/103/115	-
40	CLA	A	311	1	1/1/11/20	5/16/94/115	-
40	CLA	S	307	17	1/1/14/20	10/31/109/115	-
40	CLA	a	850	-	1/1/15/20	4/37/115/115	-
40	CLA	p	302	-	1/1/15/20	5/37/115/115	-
40	CLA	o	311	-	1/1/14/20	8/35/113/115	-
41	KC2	O	302	15	-	10/15/71/71	-
44	A86	Y	321	-	-	5/34/90/90	0/3/3/3
44	A86	u	317	-	-	1/34/90/90	0/3/3/3
42	DD6	u	321	-	-	1/26/80/80	0/3/3/3
40	CLA	q	307	36	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	v	304	-	1/1/12/20	4/22/100/115	-
40	CLA	a	830	-	1/1/13/20	5/29/107/115	-
44	A86	u	316	-	-	6/34/90/90	0/3/3/3
49	BCR	l	207	-	-	6/29/63/63	0/2/2/2
42	DD6	j	104	-	-	1/26/80/80	0/3/3/3
44	A86	U	210	-	-	2/34/90/90	0/3/3/3
49	BCR	a	843	-	-	4/29/63/63	0/2/2/2
50	PQN	b	849	-	-	3/17/37/43	0/2/2/2
40	CLA	F	305	-	1/1/11/20	2/16/94/115	-
41	KC2	w	307	-	-	4/15/71/71	-
43	LMG	E	301	40	-	14/26/46/70	0/1/1/1
40	CLA	K	301	-	1/1/11/20	4/16/94/115	-
40	CLA	W	312	13	1/1/14/20	9/31/109/115	-
42	DD6	I	213	-	-	1/26/80/80	0/3/3/3
47	A1EB1	o	321	-	-	8/42/100/100	1/3/3/3
42	DD6	I	211	-	-	5/26/80/80	0/3/3/3
40	CLA	V	202	19	1/1/13/20	8/25/103/115	-
40	CLA	a	842	-	1/1/15/20	13/37/115/115	-
41	KC2	X	302	-	-	4/15/71/71	-
47	A1EB1	q	323	-	-	13/42/100/100	0/3/3/3
41	KC2	o	303	34	-	4/15/71/71	-
40	CLA	O	316	47	1/1/11/20	1/16/94/115	-
40	CLA	b	833	24	1/1/14/20	12/31/109/115	-
40	CLA	D	303	4	1/1/14/20	10/31/109/115	-
49	BCR	a	846	-	-	3/29/63/63	0/2/2/2
46	SQD	I	215	-	-	17/49/69/69	0/1/1/1
47	A1EB1	R	317	40	-	9/42/100/100	0/3/3/3
40	CLA	z	314	-	1/1/11/20	3/16/94/115	-
41	KC2	T	309	15	-	5/15/71/71	-
40	CLA	w	305	-	1/1/12/20	3/19/95/115	-
47	A1EB1	v	323	-	-	13/42/100/100	1/3/3/3
40	CLA	t	309	-	1/1/11/20	2/16/94/115	-
47	A1EB1	z	323	-	-	8/42/100/100	0/3/3/3
40	CLA	q	304	-	1/1/12/20	4/22/100/115	-
40	CLA	P	306	13	1/1/11/20	1/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	X	311	20	1/1/14/20	9/35/113/115	-
40	CLA	b	824	24	1/1/15/20	13/37/115/115	-
40	CLA	b	812	24	1/1/14/20	8/31/109/115	-
41	KC2	R	309	15	-	7/15/71/71	-
40	CLA	o	313	-	1/1/11/20	4/16/94/115	-
42	DD6	H	312	-	-	0/26/80/80	0/3/3/3
40	CLA	z	312	-	1/1/14/20	9/31/109/115	-
41	KC2	R	311	15	-	10/15/71/71	-
41	KC2	q	309	-	-	8/15/71/71	-
40	CLA	F	306	6	1/1/14/20	7/31/109/115	-
40	CLA	b	818	24	1/1/14/20	13/34/112/115	-
40	CLA	x	305	-	1/1/12/20	2/21/99/115	-
40	CLA	W	306	13	1/1/14/20	10/31/109/115	-
44	A86	X	317	-	-	6/34/90/90	0/3/3/3
41	KC2	L	303	12	-	6/15/71/71	-
40	CLA	Z	310	-	1/1/13/20	8/25/103/115	-
44	A86	v	319	-	-	13/34/90/90	0/3/3/3
40	CLA	E	312	-	1/1/11/20	4/16/94/115	-
40	CLA	b	840	-	1/1/15/20	11/37/115/115	-
42	DD6	J	316	-	-	0/26/80/80	0/3/3/3
44	A86	p	317	-	-	1/34/90/90	0/3/3/3
41	KC2	L	302	-	-	6/15/71/71	-
40	CLA	b	808	-	1/1/15/20	13/37/115/115	-
44	A86	X	319	-	-	8/34/90/90	0/3/3/3
44	A86	u	318	-	-	12/34/90/90	0/3/3/3
47	A1EB1	y	313	-	-	13/42/100/100	0/3/3/3
40	CLA	M	307	-	1/1/14/20	9/31/109/115	-
40	CLA	R	316	47	1/1/11/20	0/16/94/115	-
40	CLA	v	301	-	1/1/13/20	6/25/103/115	-
40	CLA	W	313	13	1/1/14/20	9/31/109/115	-
41	KC2	M	301	13	-	7/15/71/71	-
40	CLA	A	303	1	1/1/14/20	11/33/111/115	-
46	SQD	P	319	-	-	8/27/47/69	0/1/1/1
40	CLA	Q	204	16	1/1/12/20	2/21/99/115	-
44	A86	x	319	-	-	12/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	F	313	-	-	7/34/90/90	0/3/3/3
40	CLA	T	307	-	1/1/13/20	2/25/103/115	-
42	DD6	q	320	-	-	6/26/80/80	0/3/3/3
42	DD6	F	314	-	-	1/26/80/80	0/3/3/3
44	A86	P	317	-	-	3/34/90/90	0/3/3/3
42	DD6	J	317	-	-	1/26/80/80	0/3/3/3
41	KC2	J	304	-	-	8/15/71/71	-
40	CLA	Z	311	22	1/1/14/20	8/35/113/115	-
42	DD6	B	305	-	-	3/26/80/80	0/3/3/3
49	BCR	b	843	-	-	2/29/63/63	0/2/2/2
40	CLA	V	201	-	1/1/13/20	6/29/107/115	-
41	KC2	x	315	-	-	7/15/71/71	-
41	KC2	N	301	14	-	5/15/71/71	-
40	CLA	E	307	-	1/1/15/20	8/37/115/115	-
47	A1EB1	L	316	-	-	7/42/100/100	0/3/3/3
40	CLA	q	312	-	1/1/14/20	7/31/109/115	-
41	KC2	Y	314	-	-	9/15/71/71	-
42	DD6	M	314	-	-	1/26/80/80	0/3/3/3
41	KC2	K	305	11	-	5/15/71/71	-
41	KC2	v	309	-	-	8/15/71/71	-
40	CLA	y	308	-	1/1/11/20	4/16/94/115	-
41	KC2	G	202	-	-	10/15/71/71	-
40	CLA	S	305	-	1/1/12/20	7/22/100/115	-
40	CLA	q	313	36	1/1/11/20	7/16/94/115	-
41	KC2	z	309	39	-	5/15/71/71	-
47	A1EB1	w	313	-	-	13/42/100/100	0/3/3/3
41	KC2	Y	308	-	-	7/15/71/71	-
40	CLA	I	208	-	1/1/13/20	6/25/103/115	-
40	CLA	q	301	-	1/1/13/20	2/25/103/115	-
43	LMG	x	301	-	-	15/34/54/70	0/1/1/1
40	CLA	H	301	-	1/1/11/20	5/16/94/115	-
40	CLA	S	319	-	1/1/11/20	5/16/94/115	-
44	A86	X	315	-	-	5/34/90/90	0/3/3/3
42	DD6	z	321	-	-	1/26/80/80	0/3/3/3
41	KC2	T	303	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	x	309	-	-	5/15/71/71	-
40	CLA	P	305	13	1/1/14/20	7/31/109/115	-
44	A86	R	315	-	-	7/34/90/90	0/3/3/3
41	KC2	z	304	39	-	3/15/71/71	-
40	CLA	P	311	-	1/1/11/20	4/16/94/115	-
42	DD6	F	315	-	-	3/26/80/80	0/3/3/3
41	KC2	W	303	-	-	7/15/71/71	-
49	BCR	a	845	-	-	3/29/63/63	0/2/2/2
44	A86	q	315	-	-	6/34/90/90	0/3/3/3
40	CLA	Z	313	22	1/1/11/20	3/16/94/115	-
47	A1EB1	y	314	-	-	9/42/100/100	0/3/3/3
49	BCR	b	844	-	-	6/29/63/63	0/2/2/2
40	CLA	t	303	38	1/1/11/20	4/16/94/115	-
40	CLA	w	309	-	1/1/13/20	7/25/103/115	-
42	DD6	p	322	-	-	3/26/80/80	0/3/3/3
47	A1EB1	x	322	-	-	4/42/100/100	0/3/3/3
41	KC2	o	302	-	-	6/15/71/71	-
41	KC2	S	304	17	-	6/15/71/71	-
44	A86	q	319	-	-	13/34/90/90	0/3/3/3
41	KC2	P	310	-	-	7/15/71/71	-
41	KC2	R	303	-	-	9/15/71/71	-
44	A86	D	320	-	-	5/34/90/90	0/3/3/3
41	KC2	N	302	14	-	5/15/71/71	-
40	CLA	b	841	24	1/1/15/20	5/37/115/115	-
47	A1EB1	F	322	-	-	9/42/100/100	0/3/3/3
40	CLA	a	820	23	1/1/14/20	11/31/109/115	-
42	DD6	N	317	-	-	3/26/80/80	0/3/3/3
47	A1EB1	K	313	-	-	4/42/100/100	0/3/3/3
40	CLA	a	812	23	1/1/13/20	1/25/103/115	-
41	KC2	q	303	36	-	6/15/71/71	-
40	CLA	P	312	13	1/1/14/20	12/31/109/115	-
41	KC2	T	308	15	-	8/15/71/71	-
44	A86	G	211	-	-	8/34/90/90	0/3/3/3
43	LMG	u	301	-	-	15/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	q	316	-	-	3/34/90/90	1/3/3/3
40	CLA	b	831	24	1/1/12/20	5/21/99/115	-
41	KC2	P	309	13	-	4/15/71/71	-
40	CLA	D	309	-	1/1/13/20	6/29/107/115	-
40	CLA	z	305	39	1/1/14/20	12/31/109/115	-
44	A86	P	314	-	-	7/34/90/90	0/3/3/3
42	DD6	J	314	-	-	0/26/80/80	0/3/3/3
41	KC2	R	301	15	-	5/15/71/71	-
40	CLA	H	304	-	1/1/11/20	3/16/94/115	-
40	CLA	P	313	-	1/1/14/20	11/31/109/115	-
42	DD6	q	318	-	-	0/26/80/80	0/3/3/3
42	DD6	D	314	-	-	3/26/80/80	0/3/3/3
44	A86	N	321	-	-	8/34/90/90	0/3/3/3
40	CLA	I	206	9	1/1/15/20	6/37/115/115	-
40	CLA	p	314	35	1/1/11/20	6/16/94/115	-
40	CLA	Q	208	-	1/1/14/20	7/31/109/115	-
42	DD6	H	314	-	-	2/26/80/80	0/3/3/3
40	CLA	o	301	-	1/1/14/20	4/31/109/115	-
52	DGD	b	850	-	-	19/45/85/95	0/2/2/2
44	A86	v	315	-	-	6/34/90/90	0/3/3/3
40	CLA	l	205	32	1/1/15/20	13/37/115/115	-
40	CLA	H	309	-	1/1/13/20	6/27/105/115	-
41	KC2	X	303	20	-	1/15/71/71	-
42	DD6	k	204	-	-	1/26/80/80	0/3/3/3
40	CLA	f	202	24	1/1/15/20	7/37/115/115	-
40	CLA	z	311	-	1/1/13/20	7/25/103/115	-
40	CLA	u	308	35	1/1/14/20	5/31/109/115	-
41	KC2	p	310	-	-	6/15/71/71	-
40	CLA	S	306	17	1/1/13/20	8/27/105/115	-
40	CLA	a	828	23	1/1/15/20	13/37/115/115	-
40	CLA	Y	306	21	1/1/14/20	8/31/109/115	-
40	CLA	f	201	-	1/1/14/20	7/31/109/115	-
41	KC2	z	310	39	-	9/15/71/71	-
47	A1EB1	v	322	-	-	7/42/100/100	0/3/3/3
47	A1EB1	w	314	-	-	10/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	F	321	-	1/1/14/20	11/31/109/115	-
44	A86	X	316	-	-	4/34/90/90	0/3/3/3
40	CLA	b	836	24	1/1/14/20	6/31/109/115	-
44	A86	Y	320	-	-	10/34/90/90	0/3/3/3
47	A1EB1	t	313	-	-	15/42/100/100	0/3/3/3
40	CLA	F	308	-	1/1/13/20	1/25/103/115	-
44	A86	Y	316	-	-	3/34/90/90	0/3/3/3
40	CLA	b	834	-	1/1/15/20	8/37/115/115	-
40	CLA	A	302	-	1/1/14/20	7/31/109/115	-
44	A86	y	310	-	-	7/34/90/90	0/3/3/3
44	A86	O	315	-	-	8/34/90/90	0/3/3/3
40	CLA	v	312	-	1/1/14/20	5/31/109/115	-
44	A86	z	320	-	-	1/34/90/90	0/3/3/3
49	BCR	r	201	-	-	2/29/63/63	0/2/2/2
46	SQD	F	320	-	-	9/31/51/69	0/1/1/1
40	CLA	G	204	7	1/1/13/20	2/25/103/115	-
44	A86	z	316	-	-	8/34/90/90	1/3/3/3
44	A86	P	316	-	-	7/34/90/90	0/3/3/3
47	A1EB1	p	324	-	-	5/42/100/100	0/3/3/3
47	A1EB1	G	212	-	-	15/42/100/100	0/3/3/3
41	KC2	P	303	13	-	3/15/71/71	-
40	CLA	q	305	-	1/1/14/20	4/31/109/115	-
41	KC2	N	309	-	-	5/15/71/71	-
40	CLA	D	311	-	1/1/11/20	4/16/94/115	-
41	KC2	O	301	15	-	8/15/71/71	-
44	A86	M	316	-	-	2/34/90/90	0/3/3/3
40	CLA	u	305	35	1/1/11/20	1/16/94/115	-
40	CLA	Y	301	-	1/1/14/20	8/31/109/115	-
40	CLA	J	308	10	1/1/13/20	8/25/103/115	-
40	CLA	x	313	-	1/1/13/20	2/25/103/115	-
44	A86	Y	317	41	-	6/34/90/90	0/3/3/3
40	CLA	a	841	23	1/1/15/20	6/37/115/115	-
40	CLA	A	301	1	1/1/11/20	4/16/94/115	-
40	CLA	Y	311	-	1/1/11/20	4/16/94/115	-
41	KC2	A	310	1	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	y	304	-	1/1/14/20	6/31/109/115	-
40	CLA	Z	307	22	1/1/14/20	11/31/109/115	-
40	CLA	E	304	5	1/1/13/20	1/25/103/115	-
42	DD6	t	312	-	-	0/26/80/80	0/3/3/3
40	CLA	N	310	-	1/1/12/20	3/19/97/115	-
47	A1EB1	p	323	-	-	10/42/100/100	0/3/3/3
42	DD6	O	314	-	-	1/26/80/80	0/3/3/3
40	CLA	D	310	4	1/1/14/20	9/31/109/115	-
44	A86	t	311	-	-	12/34/90/90	1/3/3/3
40	CLA	w	302	38	1/1/11/20	0/16/94/115	-
40	CLA	y	309	-	1/1/13/20	7/25/103/115	-
41	KC2	S	310	-	-	8/15/71/71	-
40	CLA	B	307	-	1/1/11/20	6/16/94/115	-
40	CLA	a	816	23	1/1/15/20	6/37/115/115	-
44	A86	N	314	-	-	2/34/90/90	0/3/3/3
40	CLA	T	310	-	1/1/13/20	7/29/107/115	-
44	A86	x	317	-	-	6/34/90/90	0/3/3/3
44	A86	O	313	-	-	3/34/90/90	0/3/3/3
40	CLA	W	307	13	1/1/15/20	13/37/115/115	-
40	CLA	H	308	8	1/1/11/20	5/16/94/115	-
40	CLA	N	307	-	1/1/14/20	7/31/109/115	-
41	KC2	T	302	-	-	3/15/71/71	-
44	A86	x	318	-	-	8/34/90/90	0/3/3/3
44	A86	z	319	-	-	8/34/90/90	0/3/3/3
40	CLA	b	830	24	1/1/14/20	4/33/111/115	-
42	DD6	y	311	-	-	0/26/80/80	0/3/3/3
47	A1EB1	q	321	-	-	16/42/100/100	1/3/3/3
40	CLA	a	826	-	1/1/14/20	11/33/111/115	-
47	A1EB1	x	321	-	-	2/42/100/100	0/3/3/3
47	A1EB1	K	315	-	-	15/42/100/100	1/3/3/3
41	KC2	v	303	36	-	5/15/71/71	-
40	CLA	N	305	14	1/1/13/20	6/25/103/115	-
44	A86	H	315	-	-	5/34/90/90	0/3/3/3
40	CLA	D	302	43	1/1/13/20	9/29/107/115	-
44	A86	t	316	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	z	303	39	-	6/15/71/71	-
43	LMG	l	201	-	-	19/34/54/70	0/1/1/1
43	LMG	M	317	-	-	9/34/54/70	0/1/1/1
40	CLA	b	817	24	1/1/15/20	6/37/115/115	-
40	CLA	i	101	-	1/1/13/20	10/25/103/115	-
40	CLA	Y	305	21	1/1/13/20	7/25/103/115	-
40	CLA	A	309	1	1/1/15/20	11/37/115/115	-
40	CLA	R	307	-	1/1/13/20	6/25/103/115	-
42	DD6	I	210	-	-	0/26/80/80	0/3/3/3
51	SF4	b	804	-	-	-	0/6/5/5
41	KC2	Z	302	-	-	7/15/71/71	-
49	BCR	b	847	-	-	4/29/63/63	0/2/2/2
41	KC2	Y	309	44,21	-	8/15/71/71	-
42	DD6	v	318	-	-	0/26/80/80	0/3/3/3
44	A86	T	313	-	-	2/34/90/90	0/3/3/3
40	CLA	Q	202	16	1/1/13/20	5/29/107/115	-
40	CLA	J	311	-	1/1/11/20	4/16/94/115	-
40	CLA	o	307	34	1/1/14/20	16/31/109/115	-
40	CLA	Y	313	21	1/1/11/20	8/16/94/115	-
40	CLA	b	823	24	1/1/13/20	4/25/103/115	-
40	CLA	v	307	36	1/1/14/20	13/31/109/115	-
47	A1EB1	N	320	-	-	7/42/100/100	0/3/3/3
49	BCR	l	208	-	-	5/29/63/63	0/2/2/2
45	LHG	a	849	40	-	17/34/34/53	-
40	CLA	S	308	-	1/1/12/20	5/19/95/115	-
40	CLA	o	306	34	1/1/14/20	8/31/109/115	-
40	CLA	M	305	13	1/1/14/20	10/31/109/115	-
40	CLA	Q	209	-	1/1/11/20	4/16/94/115	-
40	CLA	a	806	23	1/1/15/20	11/37/115/115	-
44	A86	X	318	-	-	5/34/90/90	0/3/3/3
40	CLA	b	835	24	1/1/15/20	12/37/115/115	-
40	CLA	I	203	9	1/1/13/20	6/25/103/115	-
40	CLA	I	204	9	1/1/11/20	3/16/94/115	-
44	A86	X	314	-	-	4/34/90/90	1/3/3/3
40	CLA	u	302	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SQD	M	318	-	-	8/27/47/69	0/1/1/1
40	CLA	C	305	3	1/1/14/20	3/31/109/115	-
42	DD6	W	315	-	-	1/26/80/80	0/3/3/3
44	A86	L	314	-	-	5/34/90/90	0/3/3/3
44	A86	p	319	-	-	11/34/90/90	0/3/3/3

The worst 5 of 4248 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	o	313	CLA	C1B-NB	11.25	1.45	1.35
40	J	311	CLA	C1B-NB	11.10	1.45	1.35
40	Y	313	CLA	C1B-NB	11.08	1.45	1.35
40	J	309	CLA	C1B-NB	11.05	1.45	1.35
40	p	311	CLA	C1B-NB	11.02	1.45	1.35

The worst 5 of 3783 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	M	313	A86	O1-C20-C19	-14.27	102.66	113.38
44	X	318	A86	O1-C20-C19	11.95	122.36	113.38
44	z	317	A86	O1-C20-C19	-10.89	105.20	113.38
44	z	316	A86	O1-C20-C19	10.85	121.53	113.38
40	F	303	CLA	C1C-NC-C4C	-10.00	102.21	106.71

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 4910 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	A	303	CLA	C1A-C2A-CAA-CBA
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	B	301	CLA	C1A-C2A-CAA-CBA

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	M	311	CLA	1	0
40	L	305	CLA	1	0
40	T	305	CLA	1	0
49	m	101	BCR	4	0
42	Q	214	DD6	1	0
40	A	305	CLA	3	0
40	G	213	CLA	2	0
40	b	803	CLA	1	0
47	u	323	A1EB1	1	0
46	k	205	SQD	3	0
40	t	305	CLA	1	0
40	b	802	CLA	2	0
41	y	307	KC2	1	0
41	W	310	KC2	1	0
40	a	823	CLA	1	0
41	Z	309	KC2	1	0
43	E	320	LMG	2	0
40	D	306	CLA	1	0
44	W	301	A86	1	0
40	F	301	CLA	7	0
42	v	320	DD6	1	0
40	b	814	CLA	3	0
40	b	806	CLA	3	0
40	C	302	CLA	1	0
40	k	202	CLA	16	0
42	L	315	DD6	15	0
40	W	305	CLA	1	0
40	E	308	CLA	4	0
40	b	832	CLA	2	0
40	Z	306	CLA	1	0
40	b	819	CLA	1	0
40	J	309	CLA	12	0
40	a	835	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	R	305	CLA	1	0
40	K	307	CLA	1	0
44	o	315	A86	1	0
40	N	306	CLA	1	0
40	Z	305	CLA	1	0
40	a	809	CLA	1	0
47	P	301	A1EB1	9	0
40	a	817	CLA	1	0
40	Q	207	CLA	1	0
40	f	205	CLA	4	0
40	o	312	CLA	2	0
41	y	306	KC2	7	0
40	x	312	CLA	1	0
40	b	826	CLA	1	0
40	G	201	CLA	1	0
40	l	202	CLA	2	0
43	j	101	LMG	13	0
43	D	318	LMG	1	0
40	S	314	CLA	1	0
43	a	802	LMG	1	0
40	q	311	CLA	2	0
40	L	312	CLA	1	0
42	w	312	DD6	26	0
40	y	302	CLA	1	0
40	L	307	CLA	1	0
47	Z	321	A1EB1	1	0
40	v	311	CLA	1	0
40	Q	206	CLA	9	0
41	Q	216	KC2	8	0
40	D	305	CLA	1	0
40	X	304	CLA	2	0
40	x	306	CLA	1	0
41	w	306	KC2	12	0
47	v	324	A1EB1	4	0
40	G	203	CLA	1	0
40	H	307	CLA	1	0
40	S	313	CLA	1	0
50	a	847	PQN	1	0
42	N	316	DD6	1	0
40	b	829	CLA	2	0
40	K	308	CLA	2	0
40	S	301	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	z	302	CLA	1	0
40	a	815	CLA	12	0
44	Y	319	A86	1	0
40	E	302	CLA	1	0
40	a	819	CLA	21	0
48	P	320	A1EB4	4	0
40	K	306	CLA	1	0
47	q	322	A1EB1	1	0
40	w	308	CLA	5	0
40	D	307	CLA	1	0
40	E	311	CLA	6	0
44	Z	316	A86	1	0
42	A	316	DD6	10	0
42	x	320	DD6	2	0
49	f	206	BCR	4	0
40	b	839	CLA	1	0
40	b	810	CLA	2	0
40	C	307	CLA	2	0
40	A	308	CLA	4	0
40	a	808	CLA	1	0
40	W	311	CLA	1	0
41	o	308	KC2	1	0
40	b	809	CLA	3	0
40	L	306	CLA	7	0
40	E	306	CLA	8	0
40	b	820	CLA	1	0
44	p	318	A86	1	0
40	A	306	CLA	12	0
47	t	315	A1EB1	1	0
40	b	807	CLA	1	0
44	w	316	A86	1	0
40	a	832	CLA	2	0
46	W	318	SQD	4	0
47	T	320	A1EB1	1	0
47	u	322	A1EB1	1	0
40	p	305	CLA	1	0
40	z	306	CLA	1	0
49	b	846	BCR	1	0
40	U	203	CLA	1	0
43	E	321	LMG	3	0
43	a	801	LMG	2	0
41	t	306	KC2	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	o	320	DD6	2	0
40	b	827	CLA	1	0
44	Y	315	A86	1	0
42	L	317	DD6	17	0
41	t	308	KC2	1	0
47	t	314	A1EB1	1	0
40	R	306	CLA	1	0
42	Y	322	DD6	9	0
40	a	824	CLA	1	0
40	E	303	CLA	4	0
45	S	323	LHG	2	0
40	N	304	CLA	1	0
42	D	317	DD6	1	0
40	D	304	CLA	1	0
40	F	307	CLA	4	0
42	P	315	DD6	5	0
41	Z	303	KC2	1	0
40	j	102	CLA	2	0
44	W	314	A86	1	0
41	C	303	KC2	1	0
42	J	315	DD6	1	0
40	k	201	CLA	1	0
40	b	828	CLA	1	0
42	I	212	DD6	1	0
40	y	305	CLA	1	0
49	i	102	BCR	3	0
44	M	315	A86	1	0
41	Q	201	KC2	2	0
40	J	318	CLA	2	0
40	a	814	CLA	1	0
44	G	209	A86	3	0
40	b	813	CLA	2	0
41	M	303	KC2	1	0
40	P	308	CLA	6	0
44	D	319	A86	1	0
40	p	306	CLA	1	0
40	S	312	CLA	6	0
48	W	319	A1EB4	7	0
44	t	310	A86	1	0
41	T	301	KC2	1	0
41	v	308	KC2	1	0
40	C	306	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	l	203	CLA	1	0
44	N	315	A86	7	0
44	Q	210	A86	1	0
42	C	310	DD6	1	0
40	A	311	CLA	3	0
40	a	850	CLA	1	0
40	o	311	CLA	1	0
42	u	321	DD6	1	0
40	a	830	CLA	1	0
49	l	207	BCR	3	0
49	a	843	BCR	5	0
50	b	849	PQN	2	0
40	F	305	CLA	1	0
41	w	307	KC2	1	0
43	E	301	LMG	1	0
40	K	301	CLA	2	0
40	W	312	CLA	2	0
40	V	202	CLA	4	0
40	a	842	CLA	1	0
40	b	833	CLA	1	0
40	D	303	CLA	1	0
49	a	846	BCR	1	0
46	I	215	SQD	2	0
40	w	305	CLA	1	0
40	P	306	CLA	1	0
40	b	824	CLA	2	0
42	H	312	DD6	1	0
40	F	306	CLA	1	0
40	x	305	CLA	1	0
40	W	306	CLA	1	0
44	X	317	A86	3	0
41	L	303	KC2	1	0
42	J	316	DD6	15	0
47	y	313	A1EB1	4	0
40	M	307	CLA	1	0
40	v	301	CLA	1	0
41	M	301	KC2	1	0
46	P	319	SQD	5	0
40	Q	204	CLA	1	0
42	q	320	DD6	1	0
42	F	314	DD6	1	0
44	P	317	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	B	305	DD6	1	0
40	V	201	CLA	2	0
40	E	307	CLA	12	0
42	M	314	DD6	1	0
40	y	308	CLA	5	0
40	S	305	CLA	5	0
41	Y	308	KC2	9	0
43	x	301	LMG	5	0
40	H	301	CLA	1	0
40	S	319	CLA	1	0
41	T	303	KC2	1	0
40	P	305	CLA	3	0
41	z	304	KC2	1	0
49	a	845	BCR	1	0
42	p	322	DD6	1	0
47	x	322	A1EB1	1	0
41	N	302	KC2	1	0
41	T	308	KC2	1	0
43	u	301	LMG	1	0
40	z	305	CLA	3	0
40	P	313	CLA	1	0
42	q	318	DD6	6	0
40	o	301	CLA	1	0
52	b	850	DGD	7	0
40	l	205	CLA	1	0
41	X	303	KC2	1	0
40	f	202	CLA	3	0
47	v	322	A1EB1	1	0
44	Y	320	A86	1	0
40	b	834	CLA	2	0
40	A	302	CLA	2	0
44	y	310	A86	1	0
40	v	312	CLA	2	0
49	r	201	BCR	1	0
46	F	320	SQD	2	0
47	p	324	A1EB1	1	0
41	P	303	KC2	1	0
40	D	311	CLA	2	0
41	O	301	KC2	1	0
40	a	841	CLA	2	0
42	t	312	DD6	29	0
40	N	310	CLA	1	0

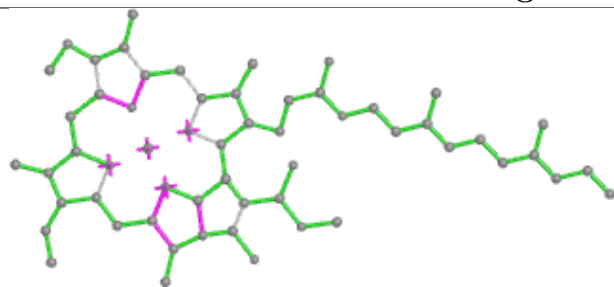
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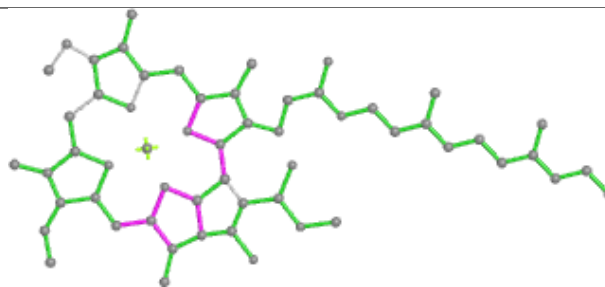
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	p	323	A1EB1	1	0
42	O	314	DD6	1	0
40	B	307	CLA	3	0
40	a	816	CLA	1	0
44	z	319	A86	1	0
42	y	311	DD6	17	0
47	x	321	A1EB1	1	0
47	K	315	A1EB1	1	0
40	N	305	CLA	1	0
40	i	101	CLA	4	0
42	I	210	DD6	1	0
49	b	847	BCR	1	0
42	v	318	DD6	4	0
40	o	307	CLA	1	0
49	l	208	BCR	1	0
40	S	308	CLA	3	0
40	M	305	CLA	1	0
40	b	835	CLA	3	0
46	M	318	SQD	1	0
42	W	315	DD6	1	0
44	L	314	A86	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.

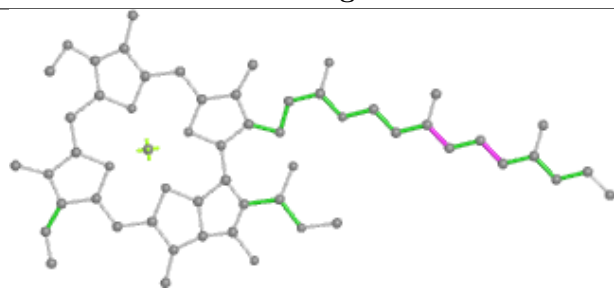
Ligand CLA L 304



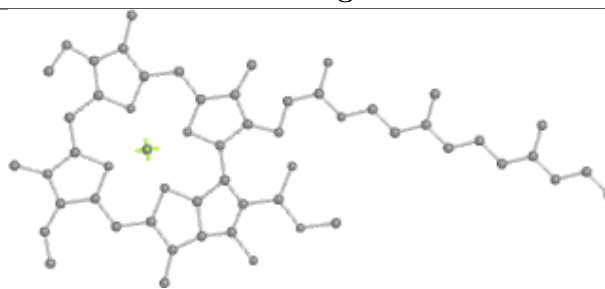
Bond lengths



Bond angles

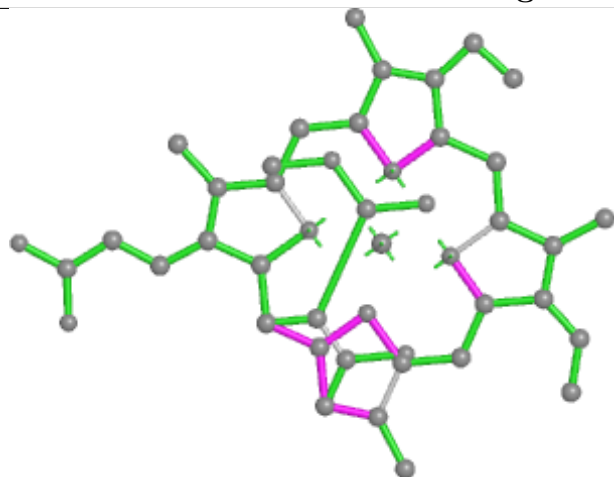


Torsions

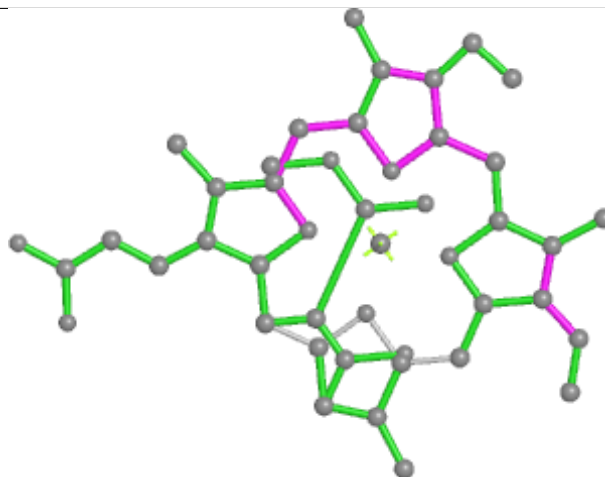


Rings

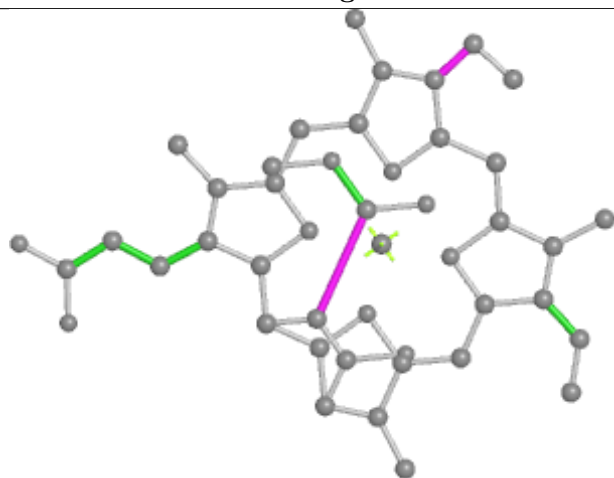
Ligand KC2 P 304



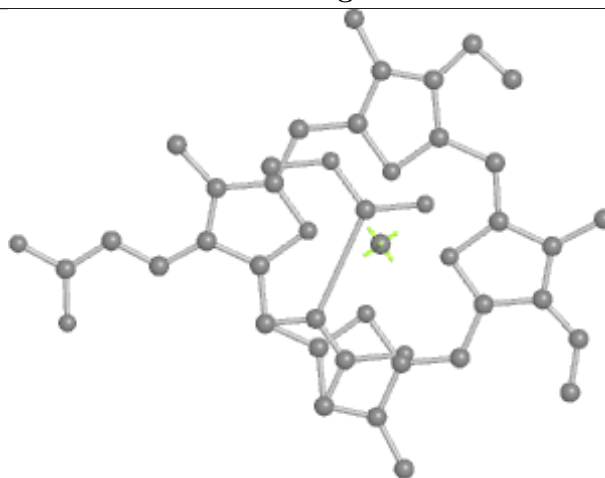
Bond lengths



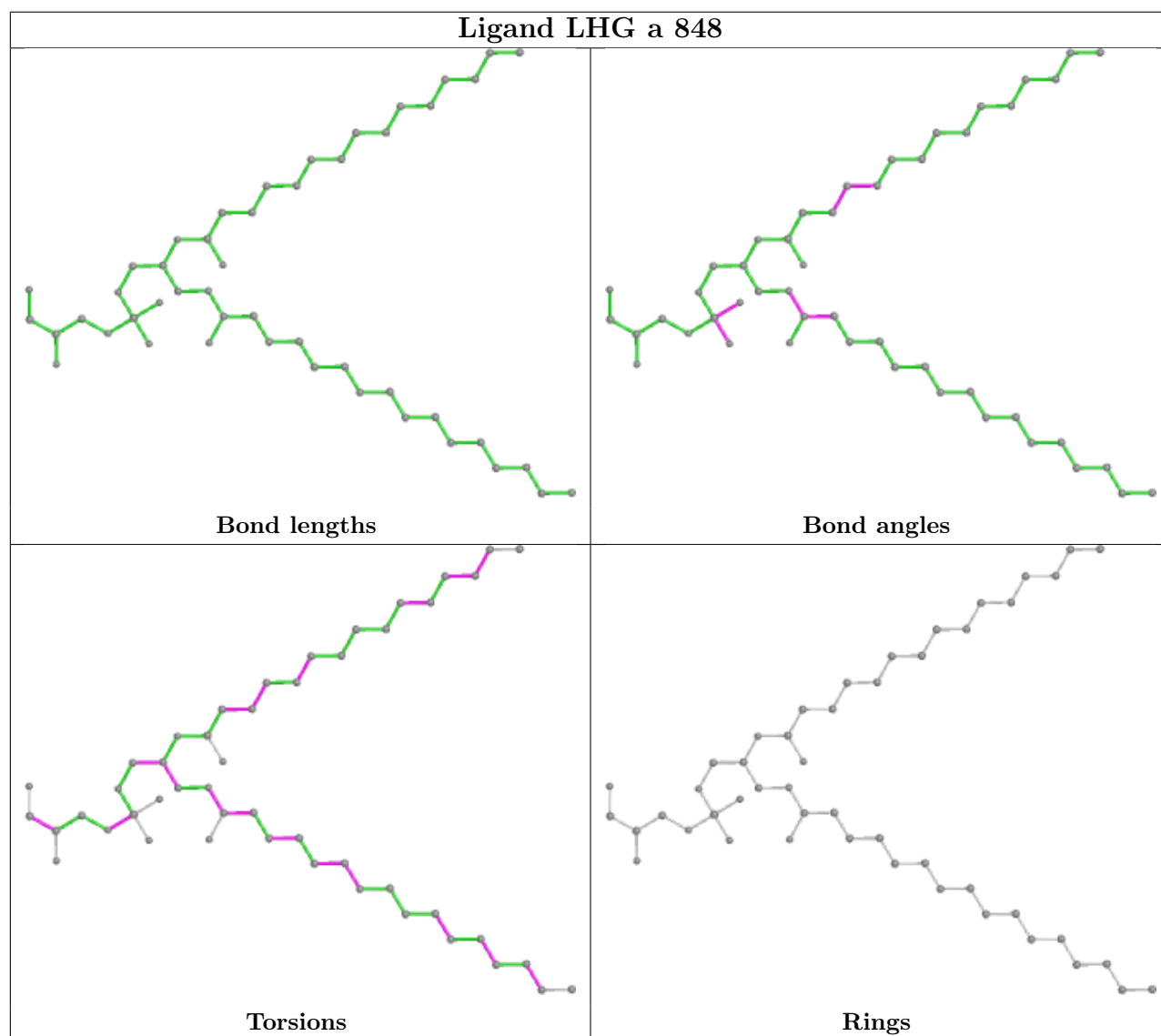
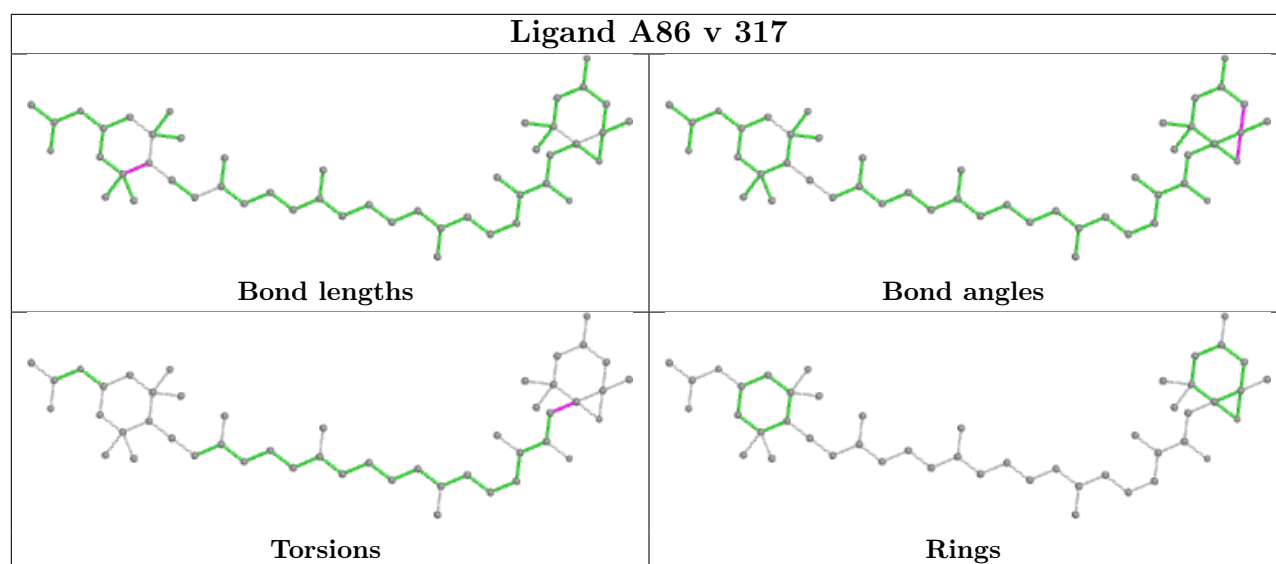
Bond angles

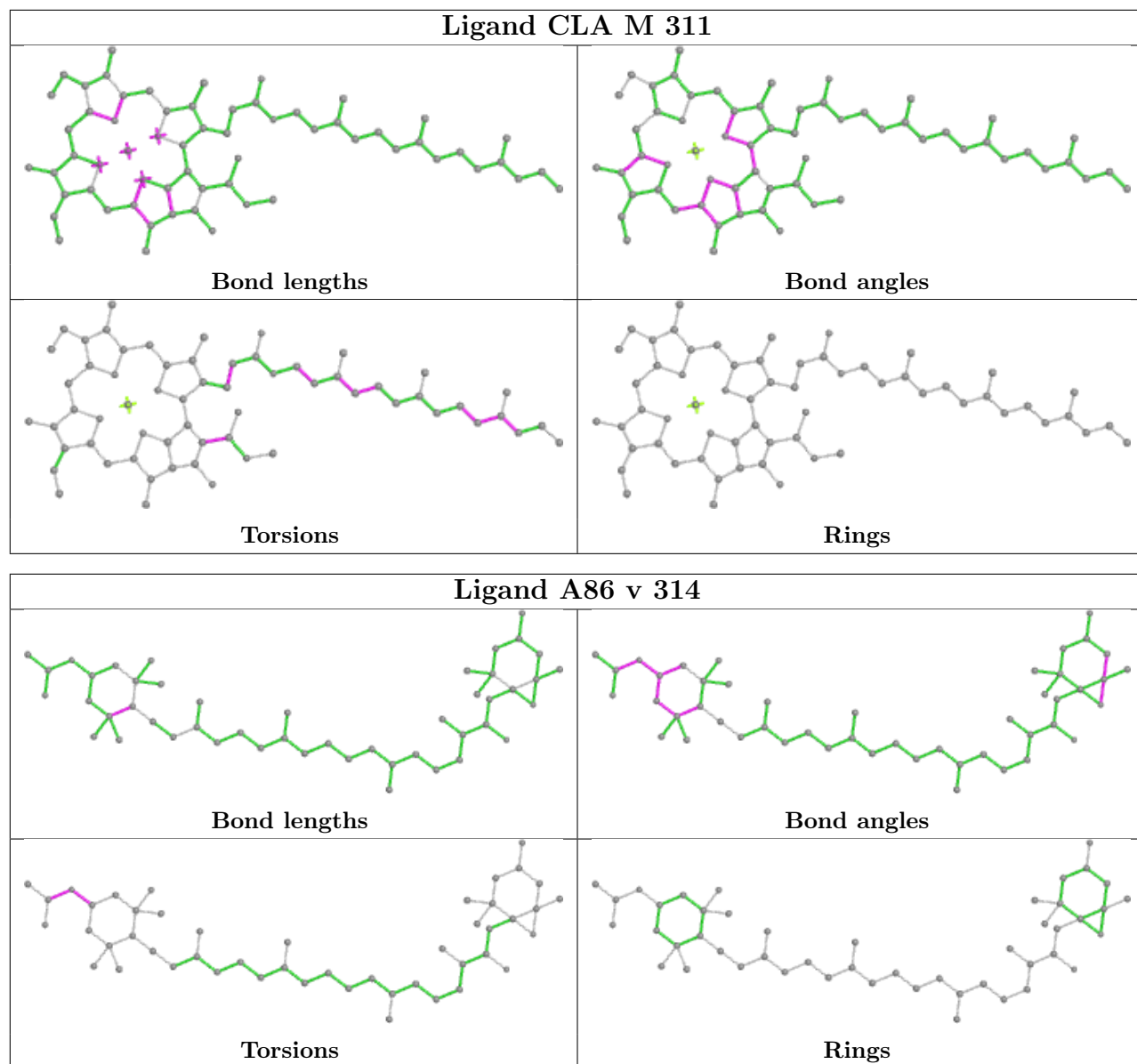


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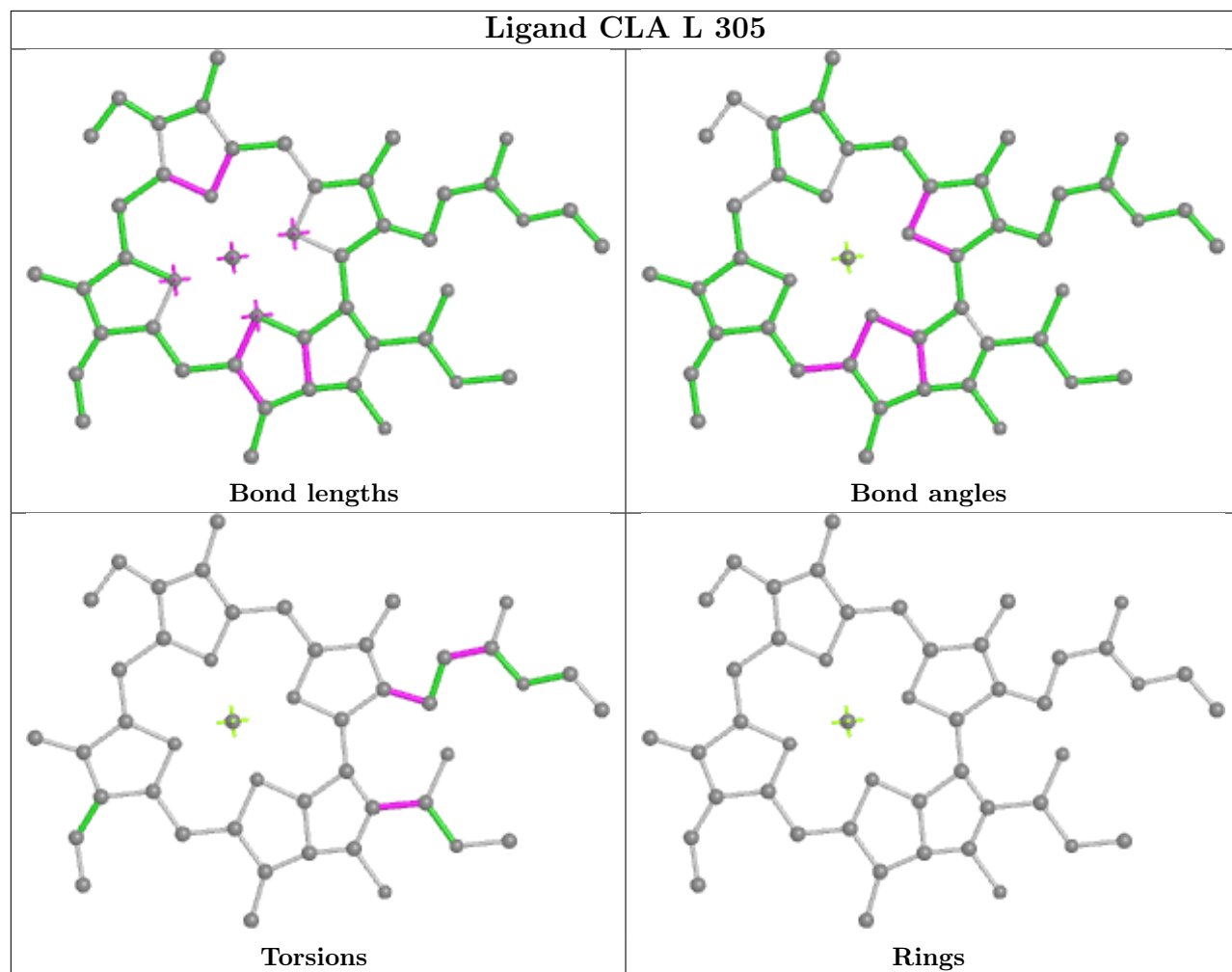


Rings

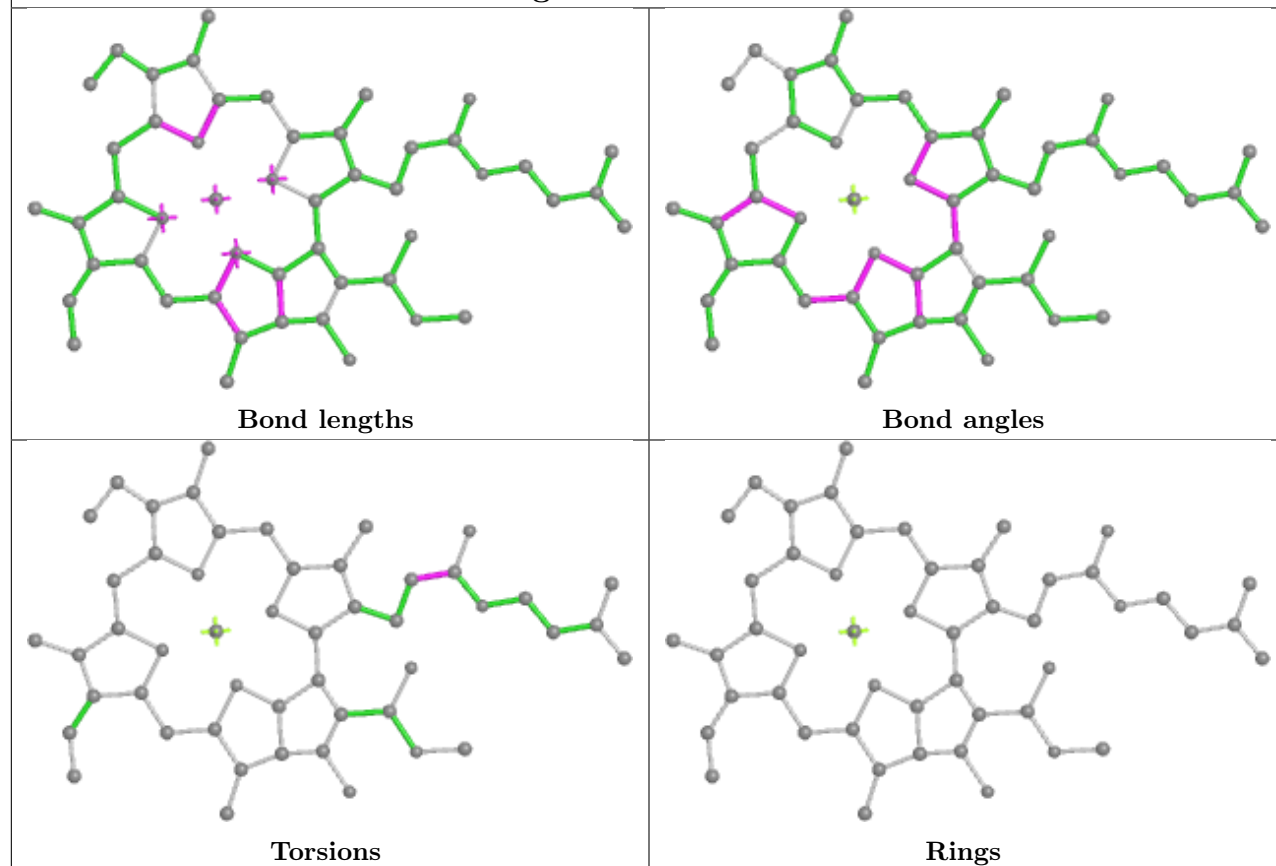




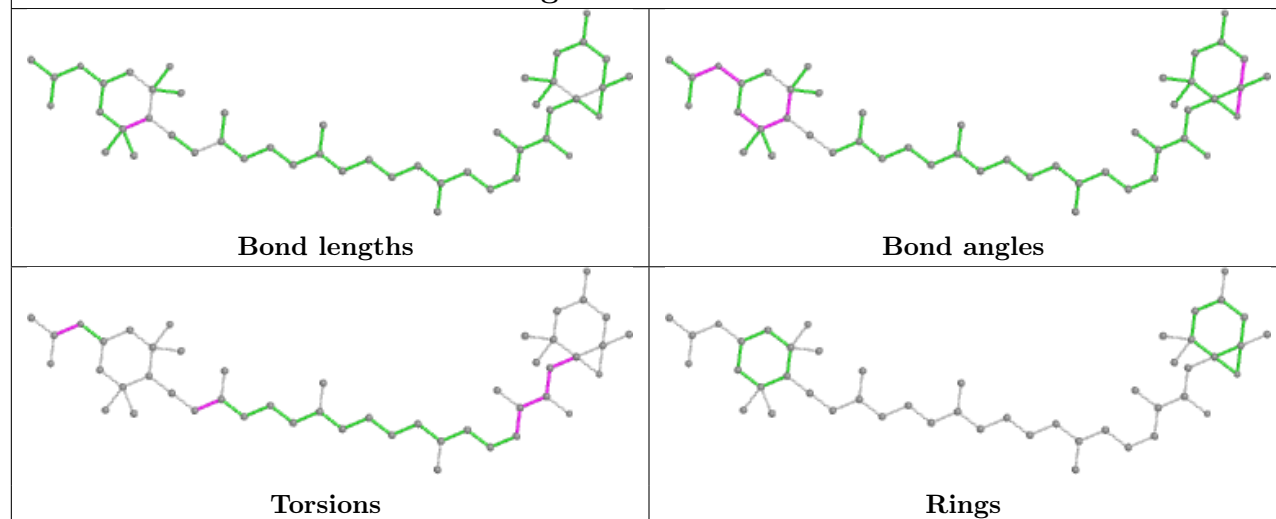
Ligand CLA L 305

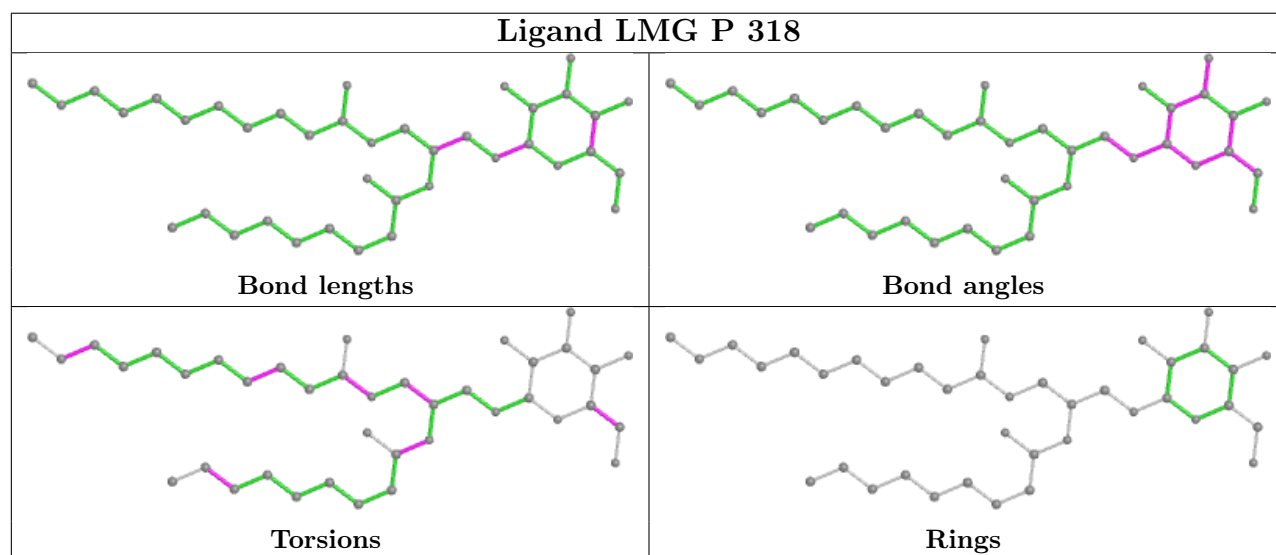
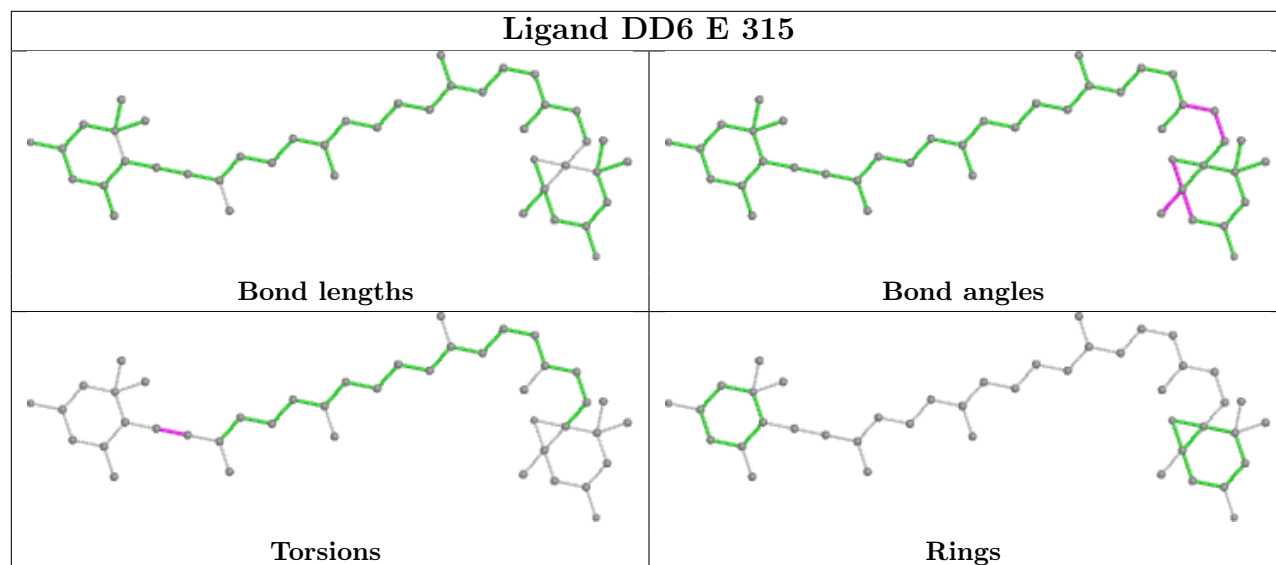
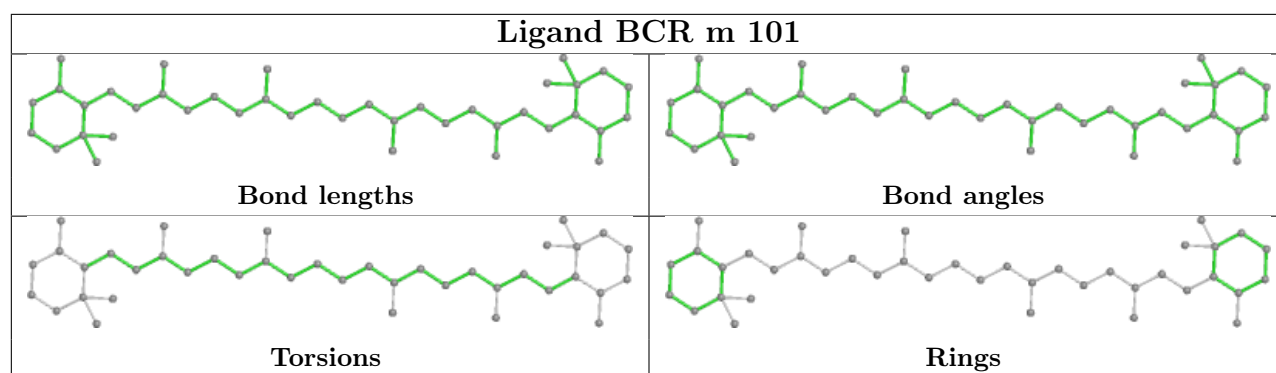


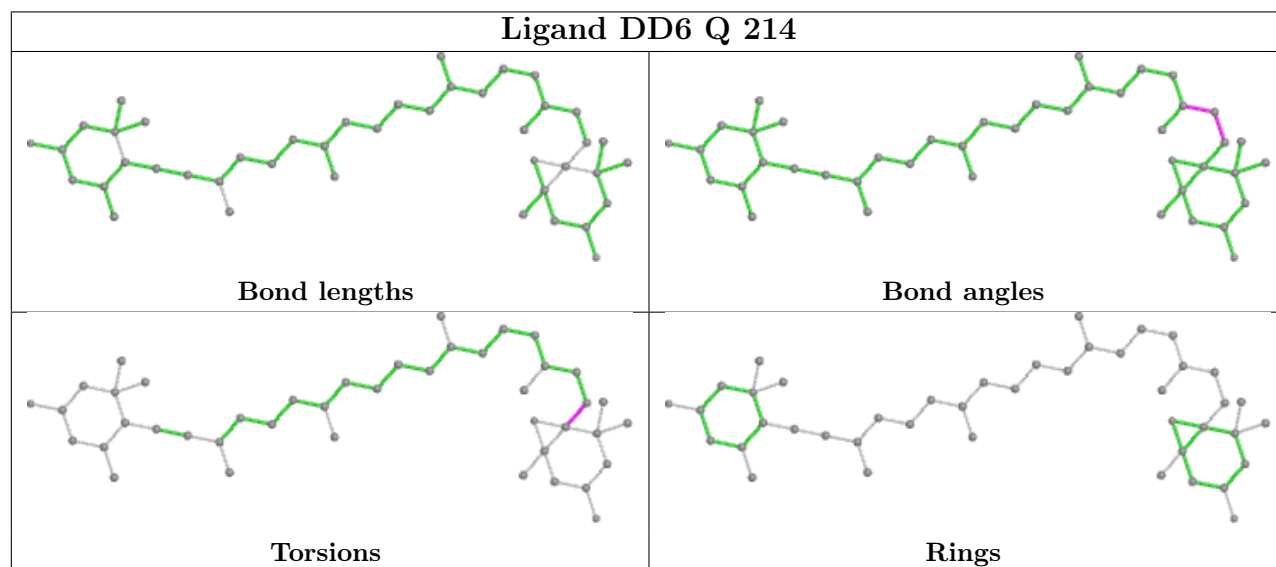
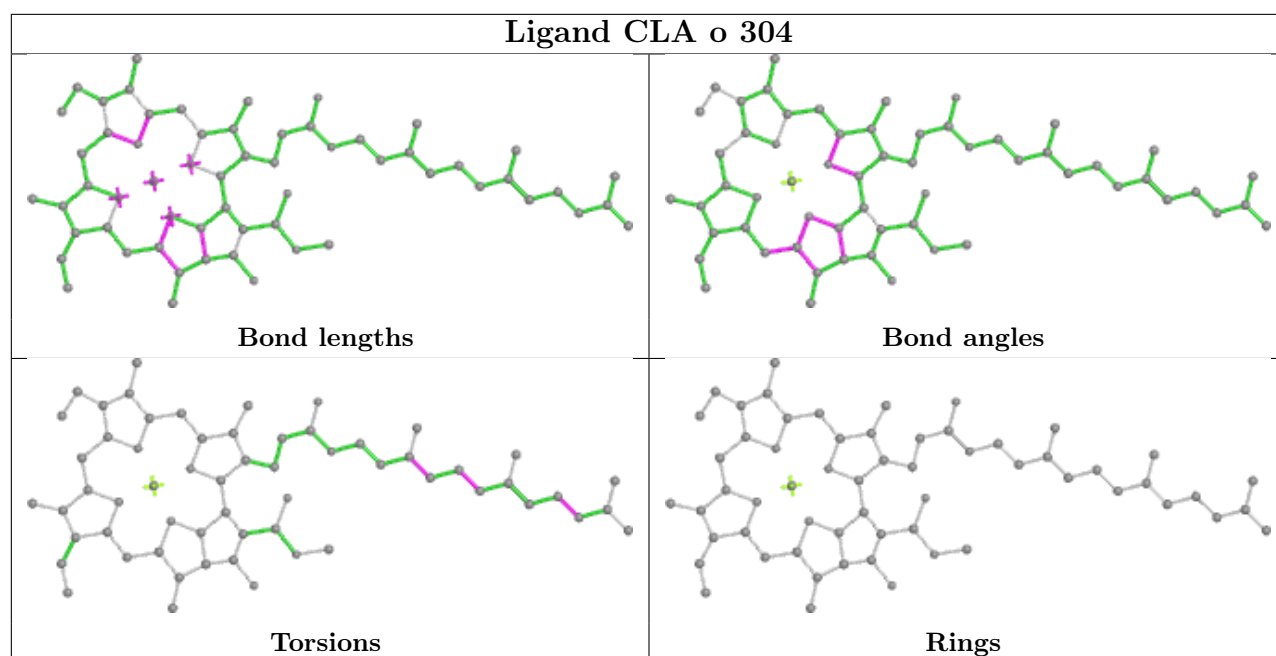
Ligand CLA T 305

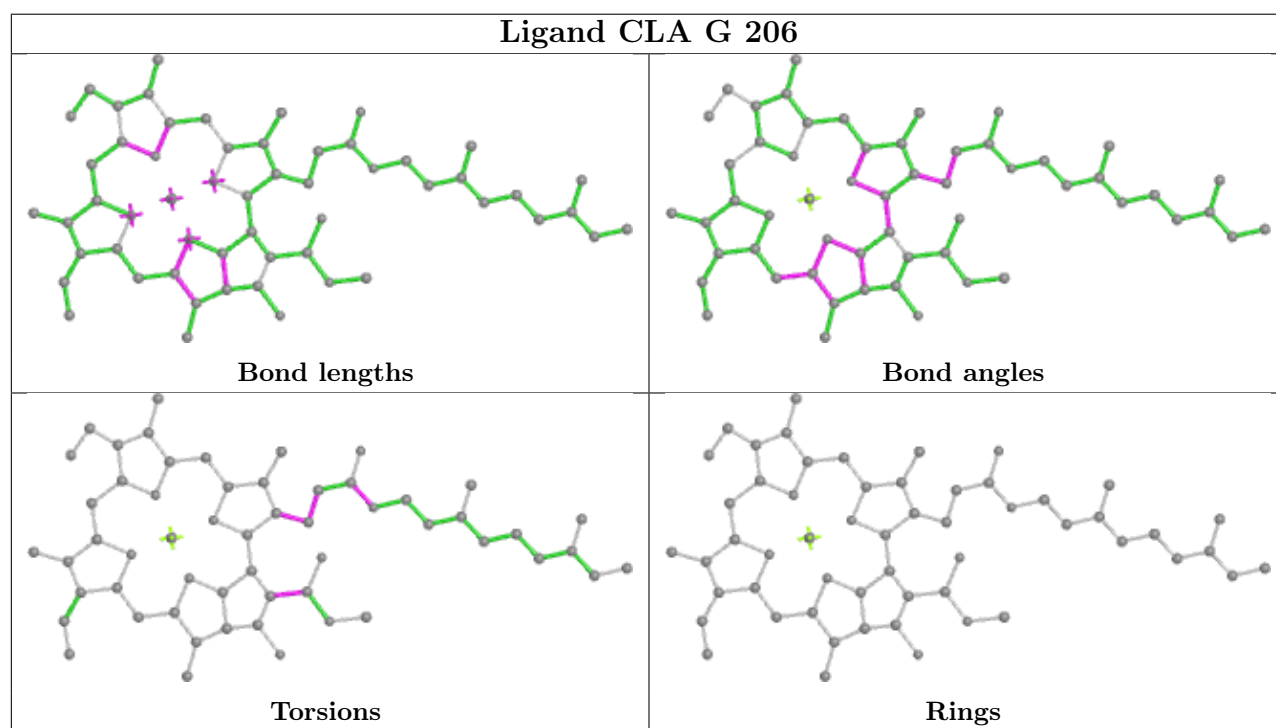
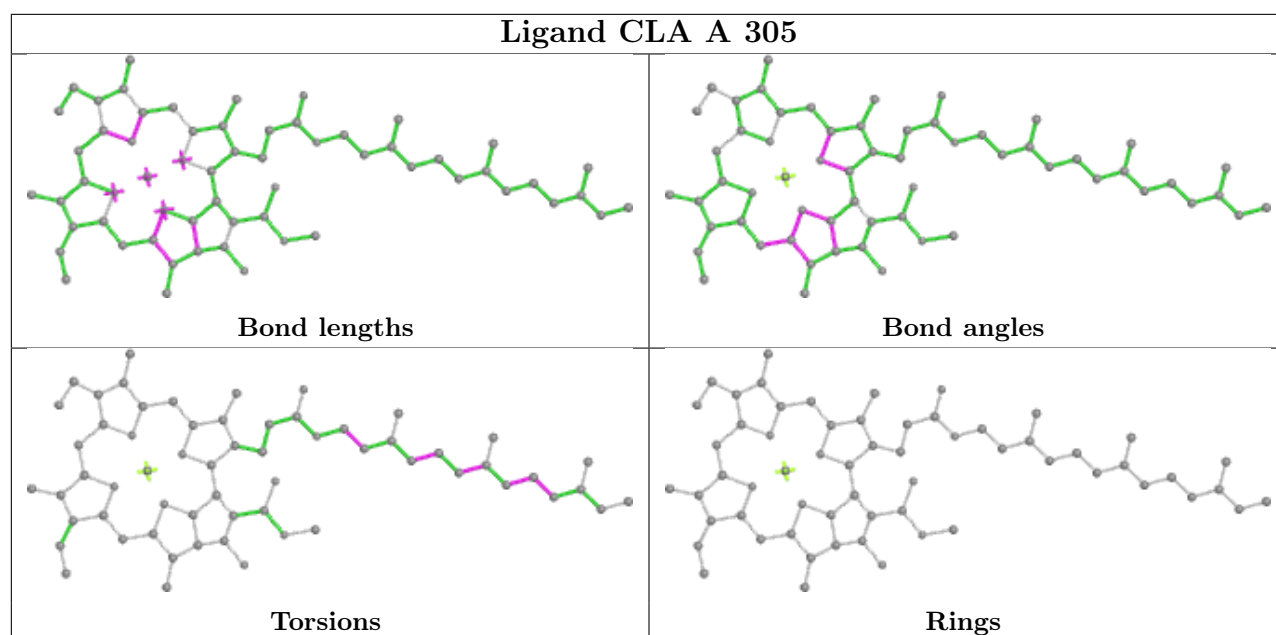


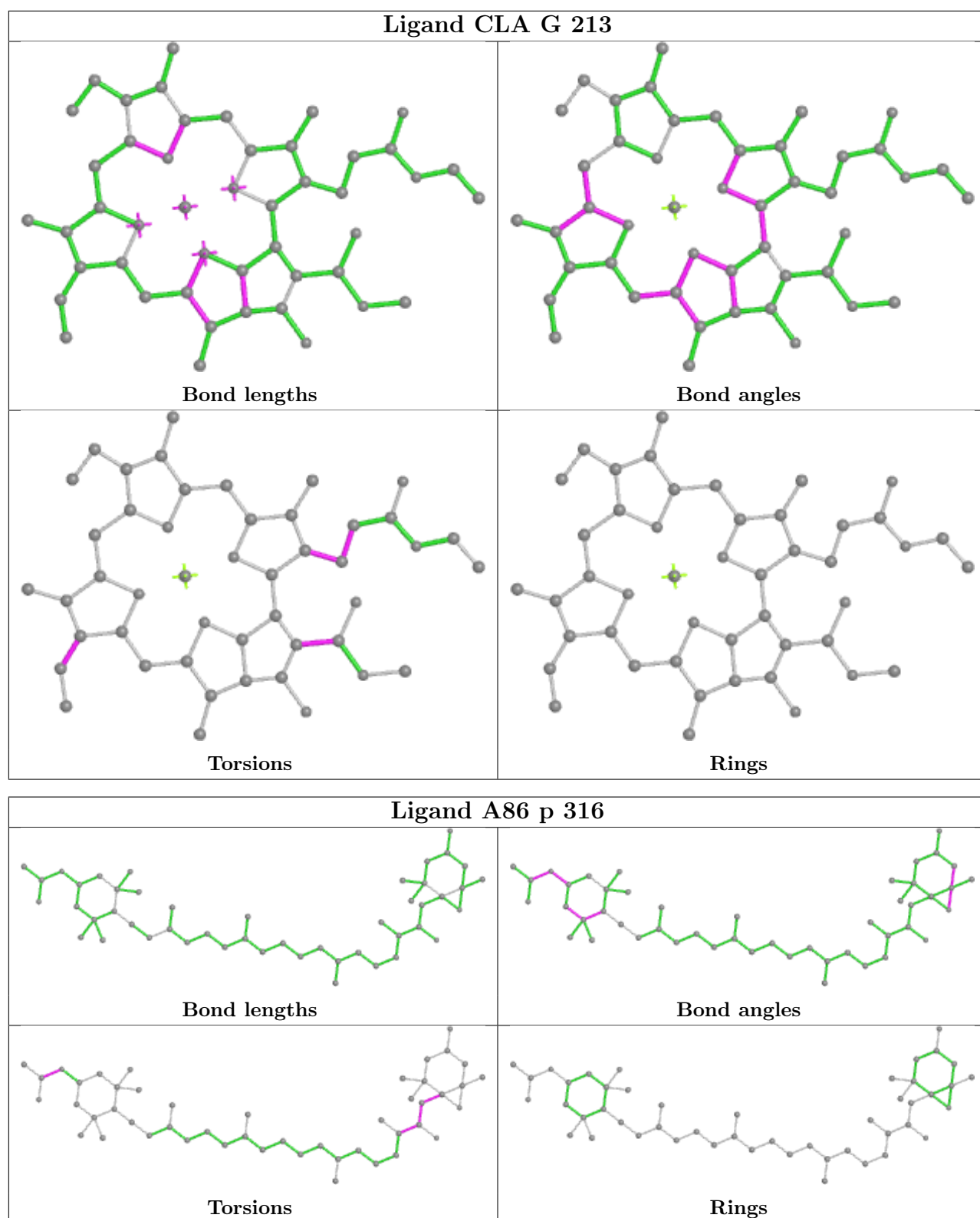
Ligand A86 u 319

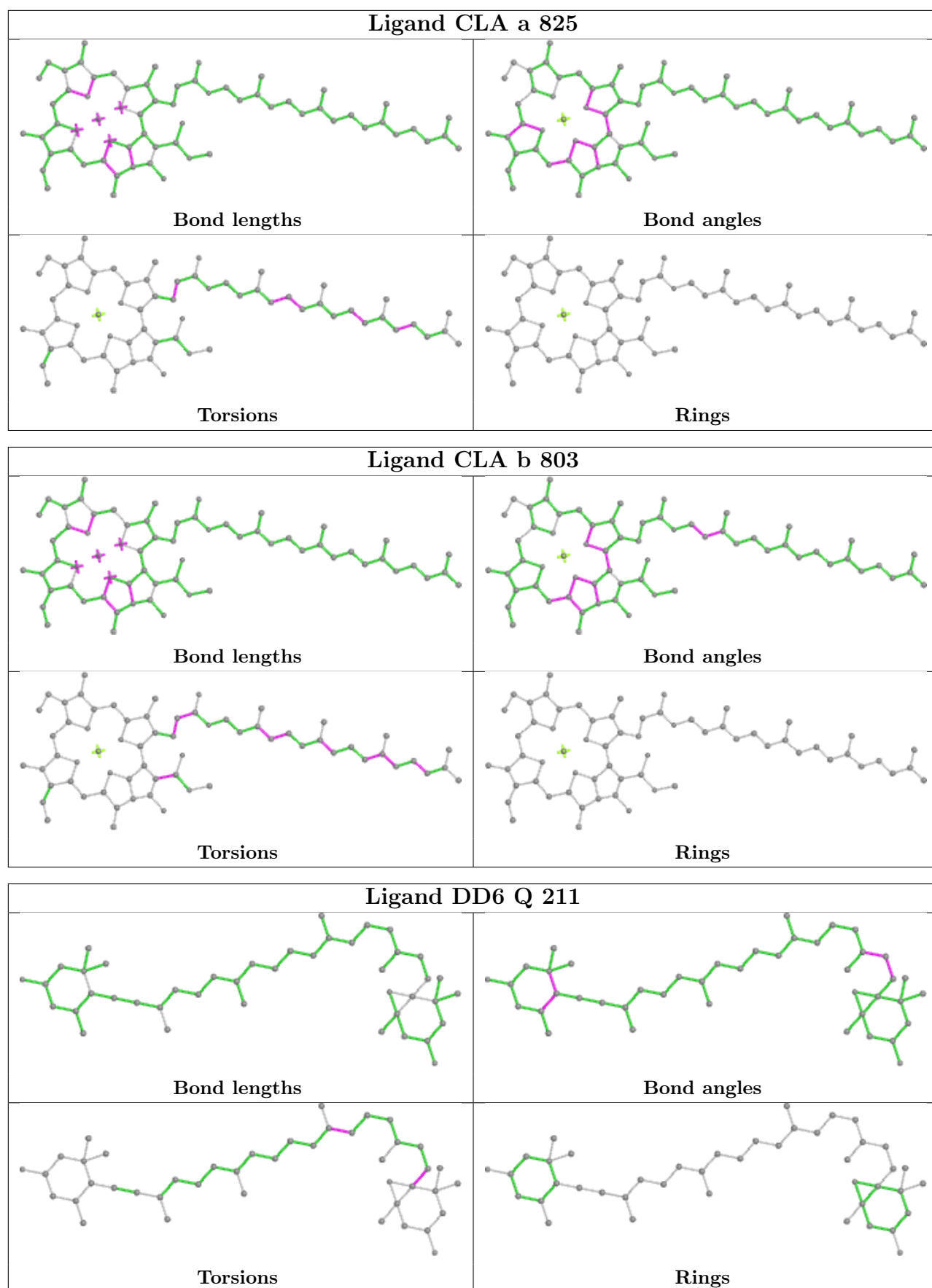




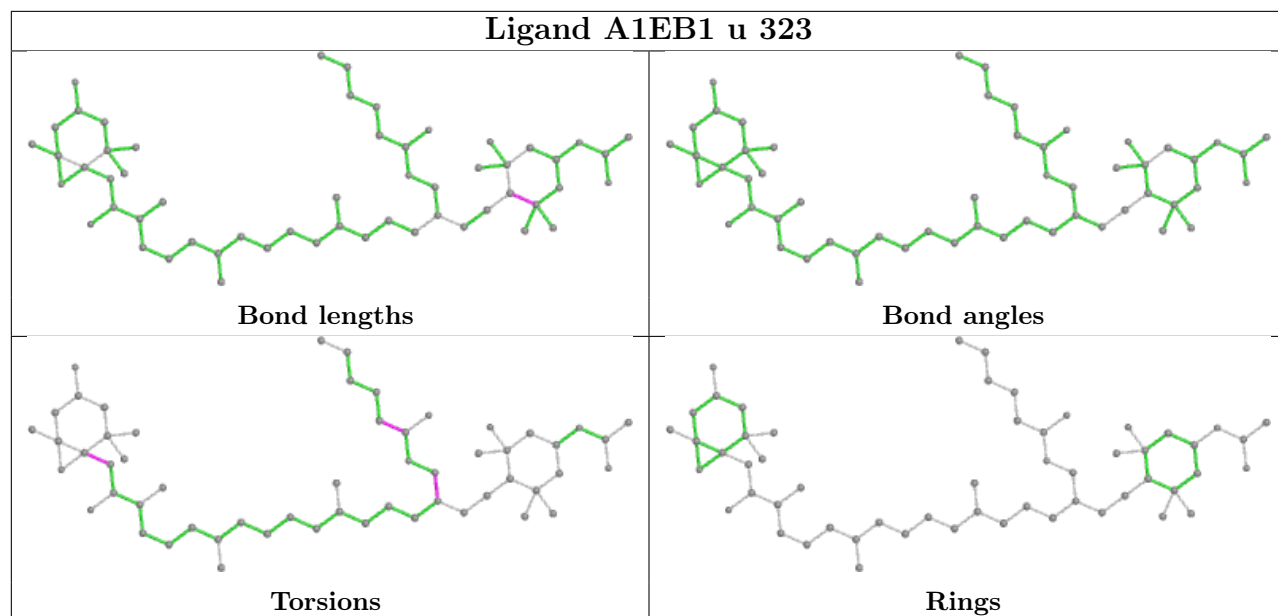




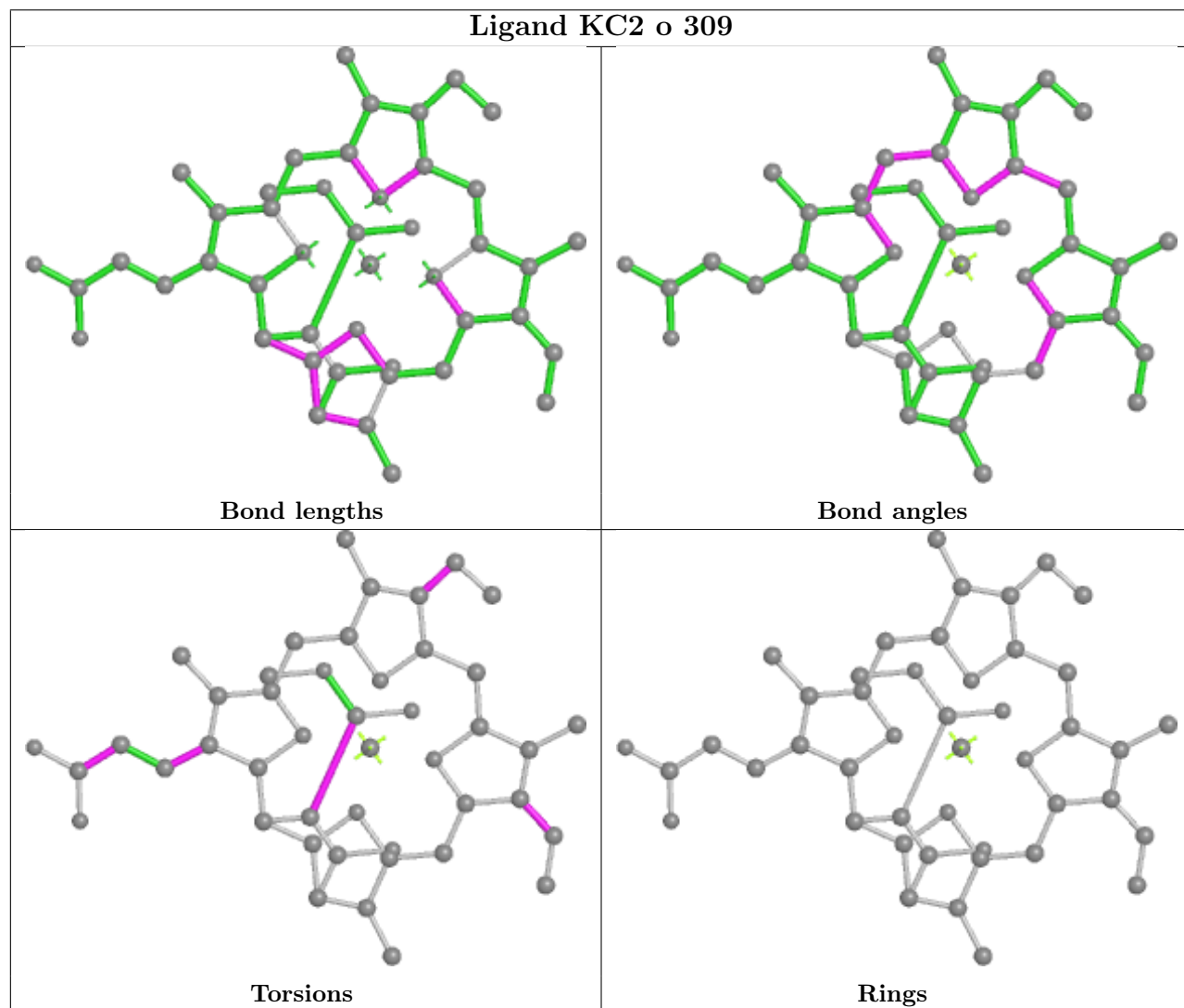


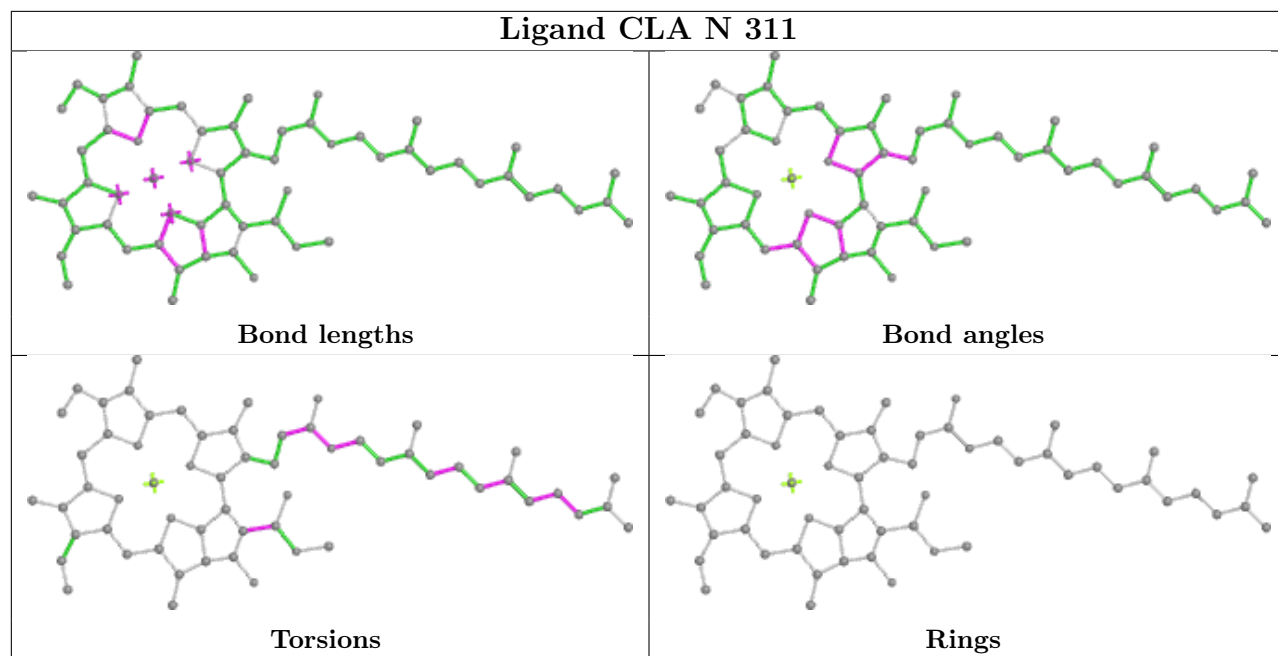


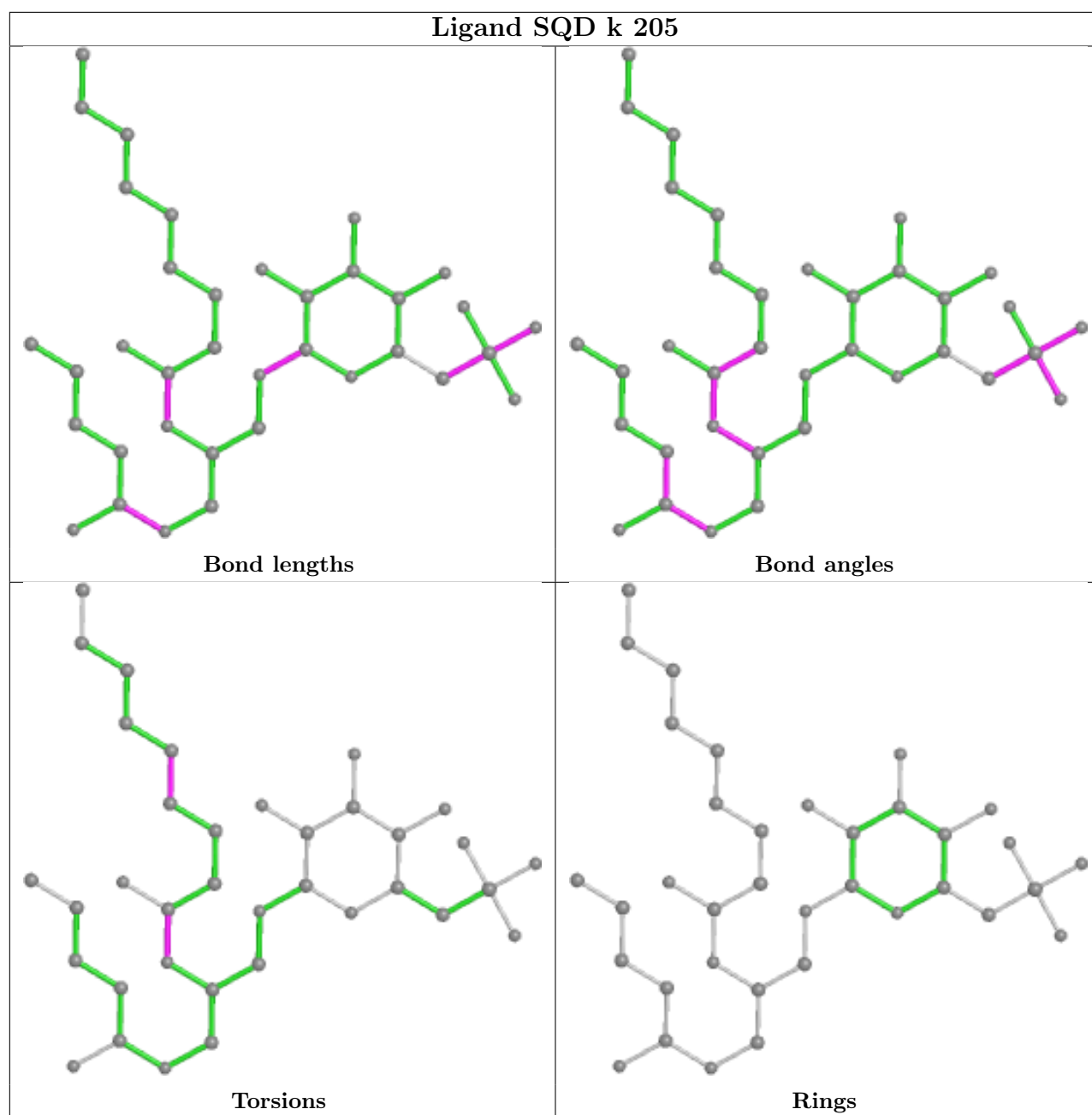
Ligand A1EB1 u 323



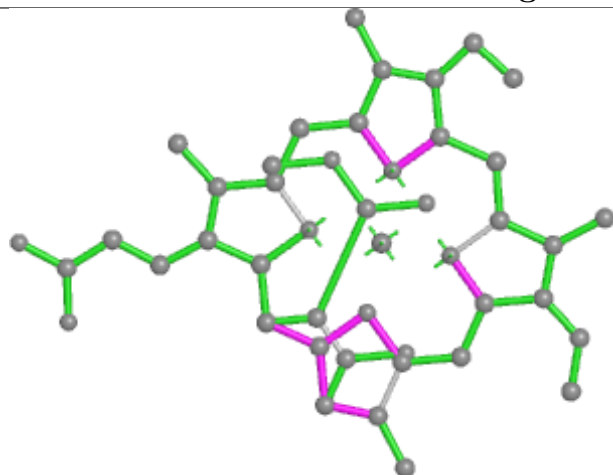
Ligand KC2 o 309



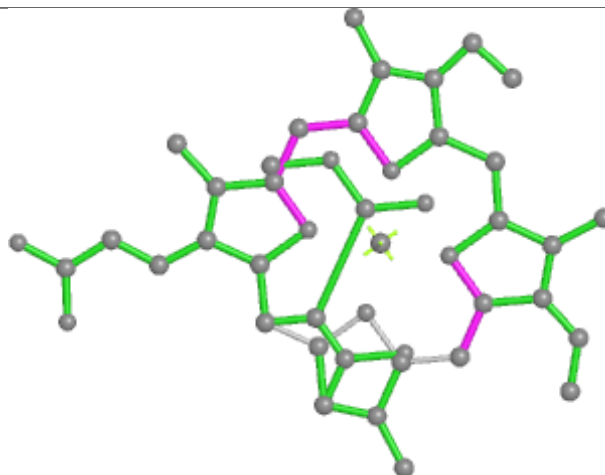




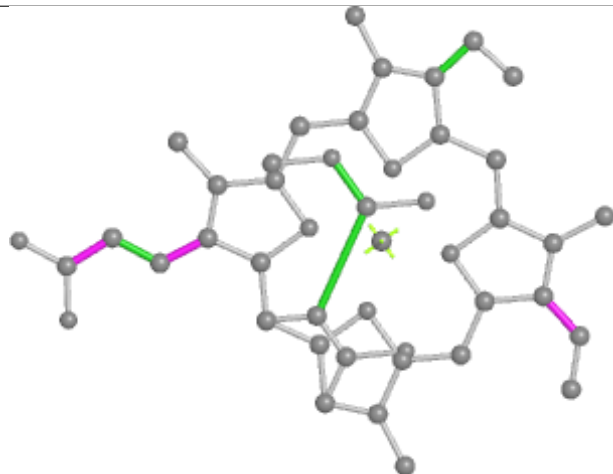
Ligand KC2 u 303



Bond lengths



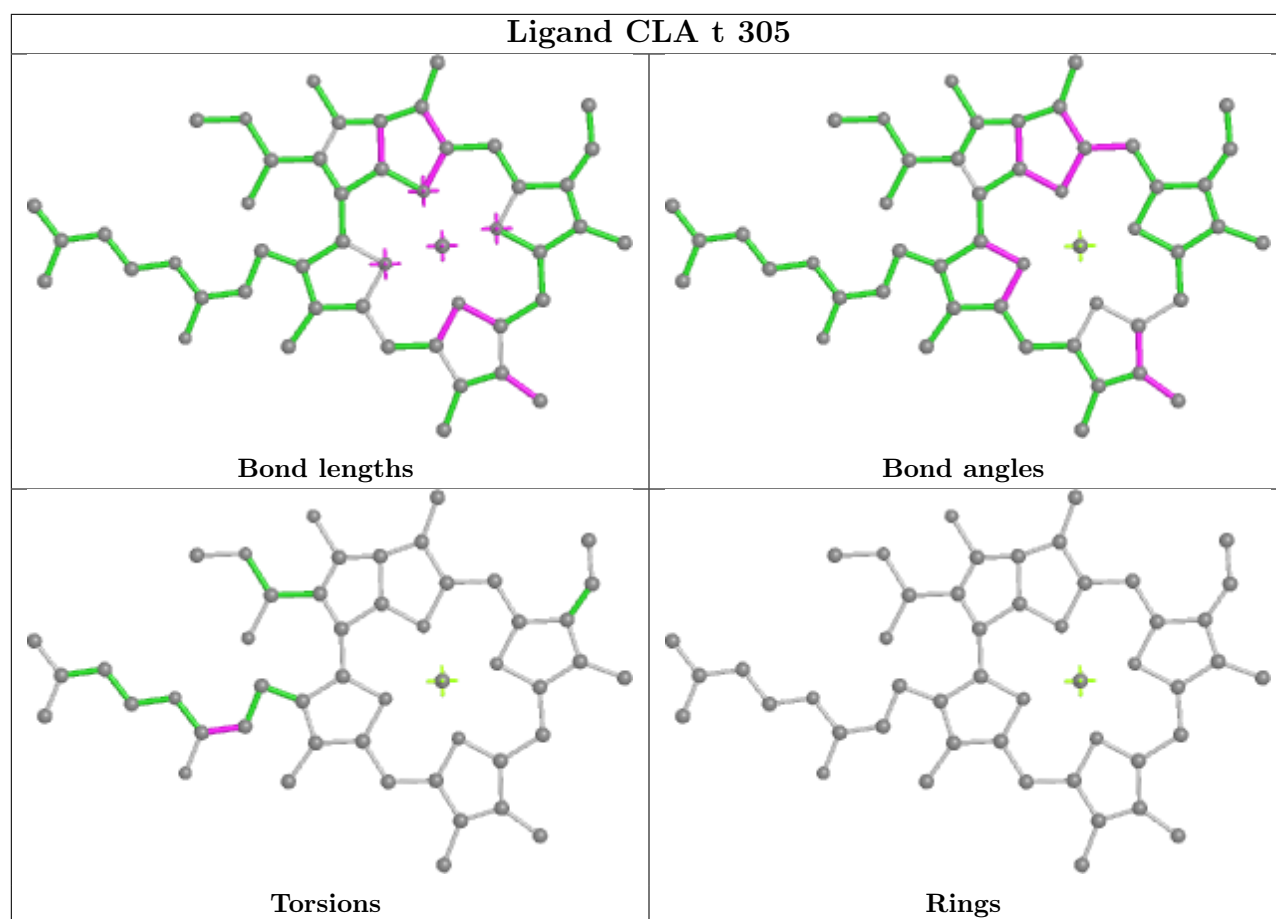
Bond angles



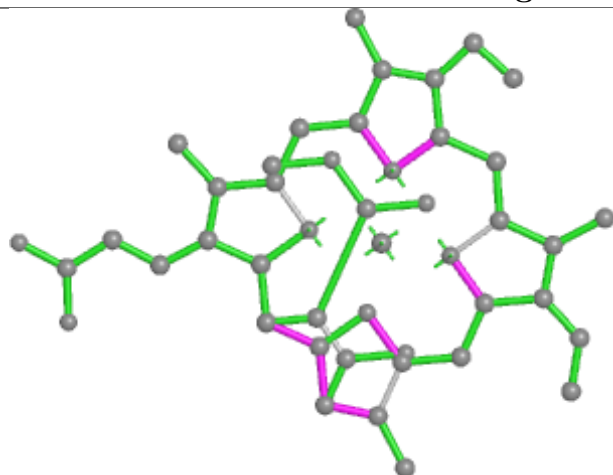
Torsions



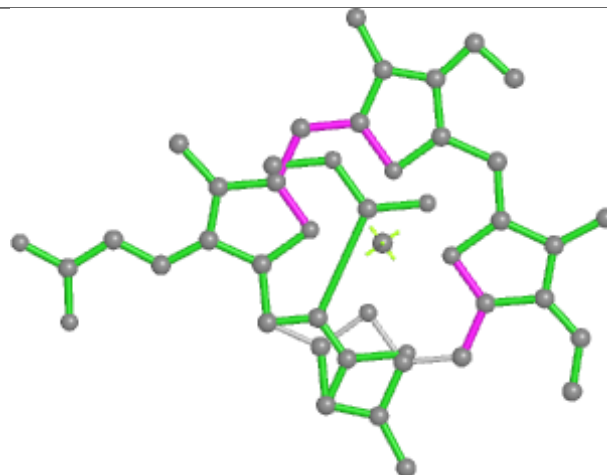
Rings



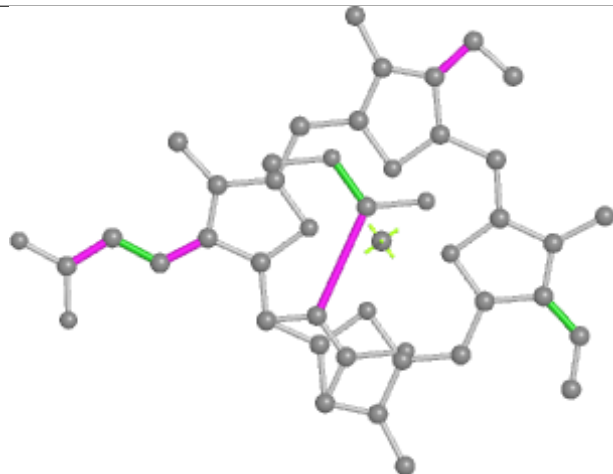
Ligand KC2 Y 303



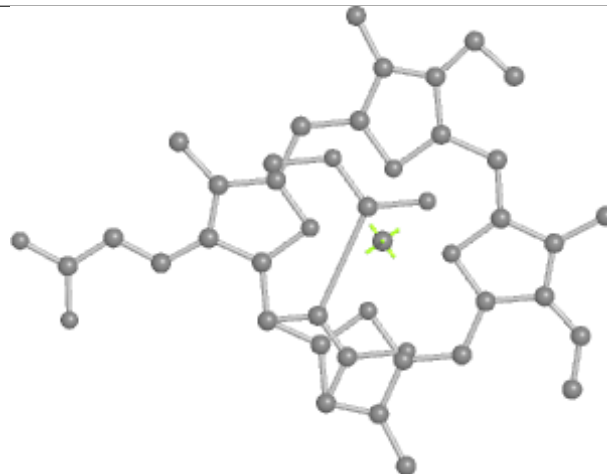
Bond lengths



Bond angles

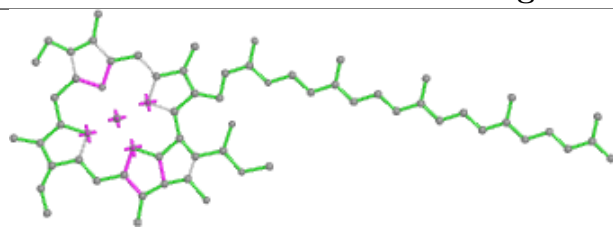


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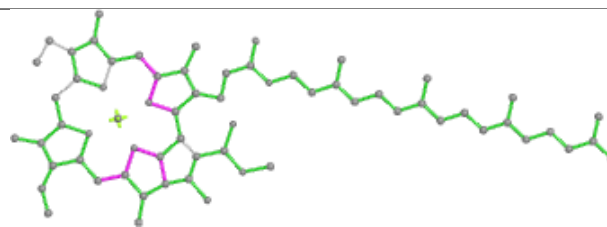


Rings

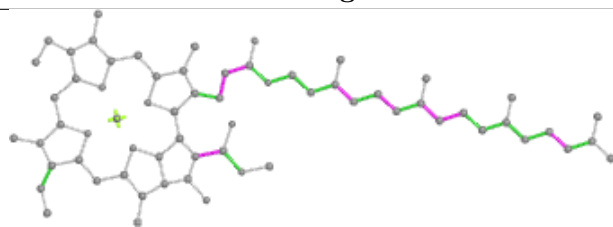
Ligand CLA b 802



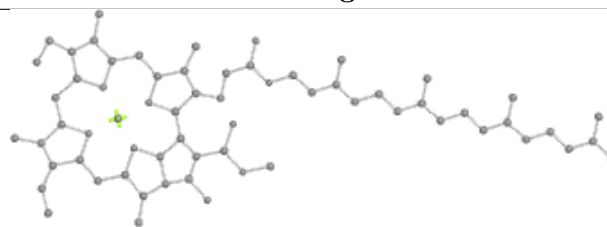
Bond lengths



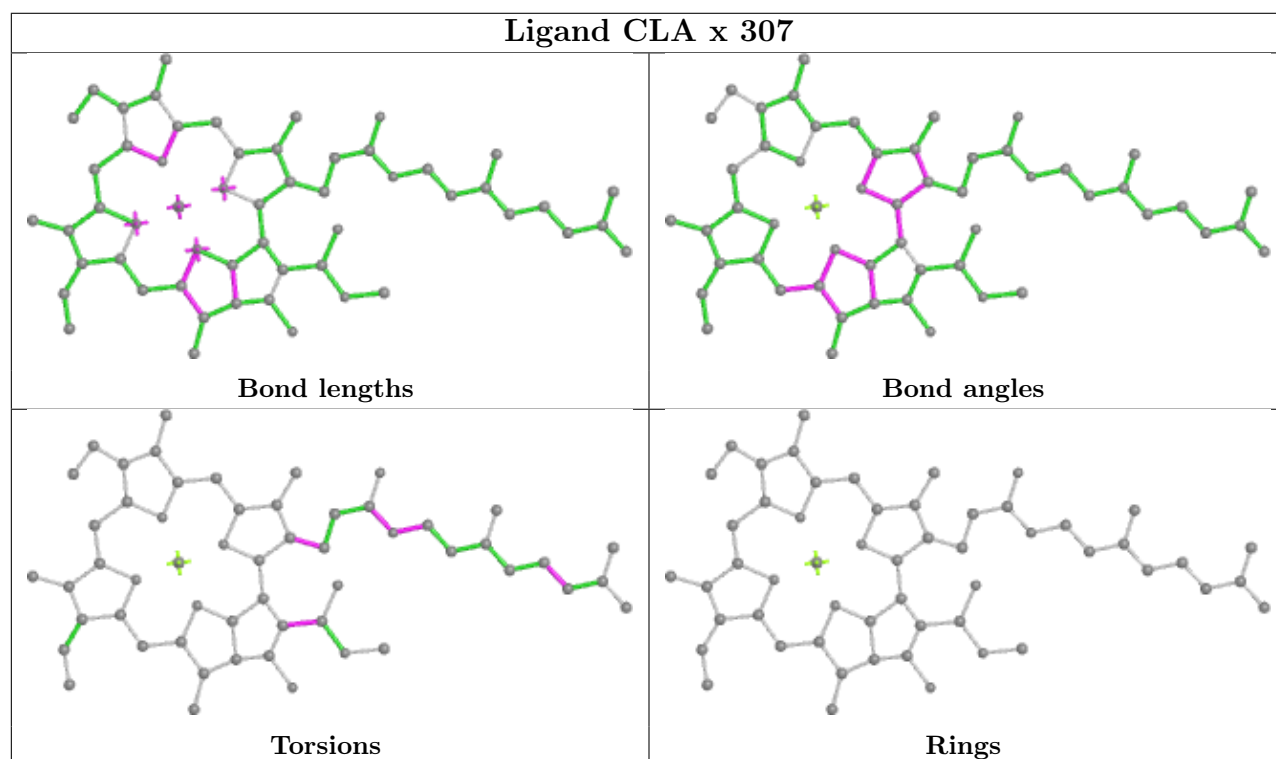
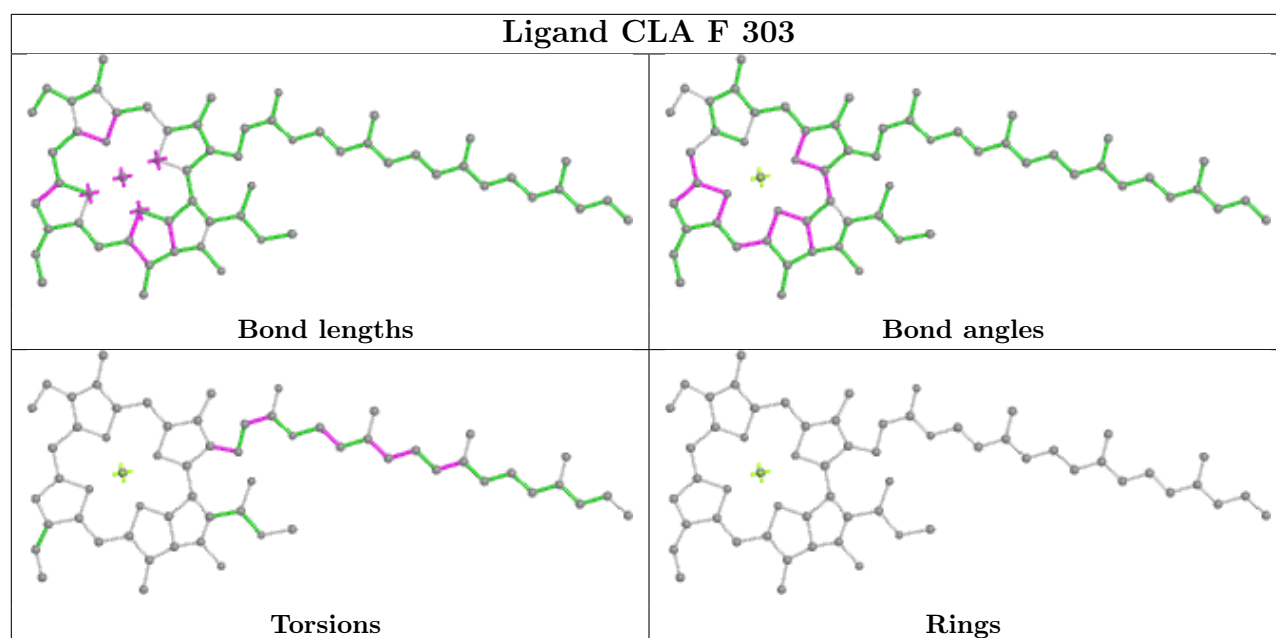
Bond angles

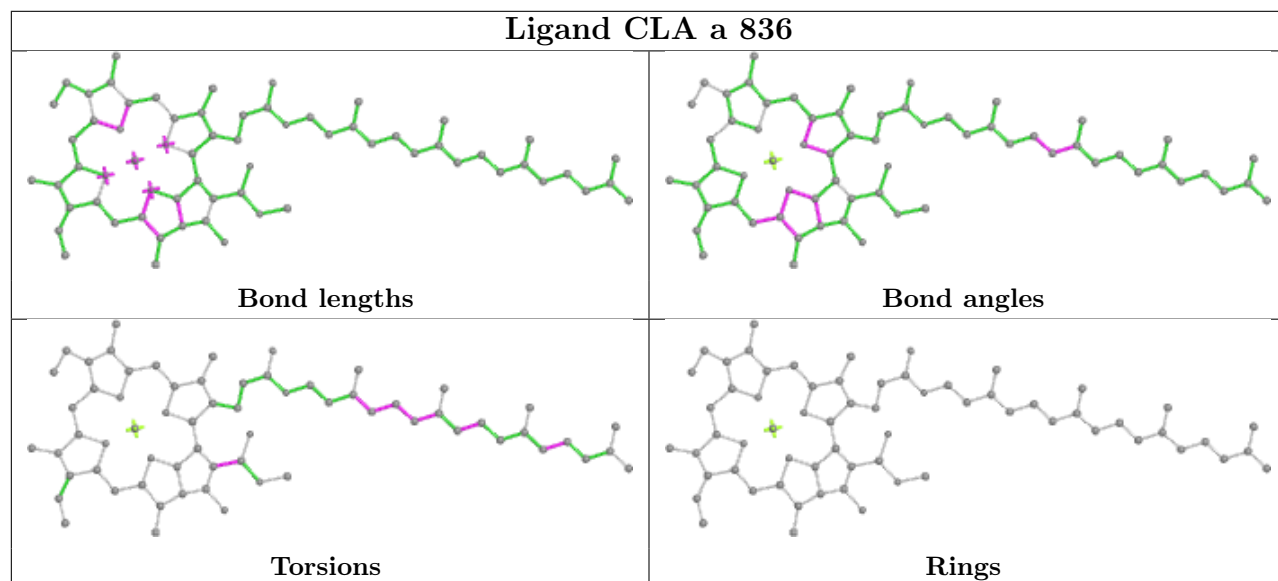
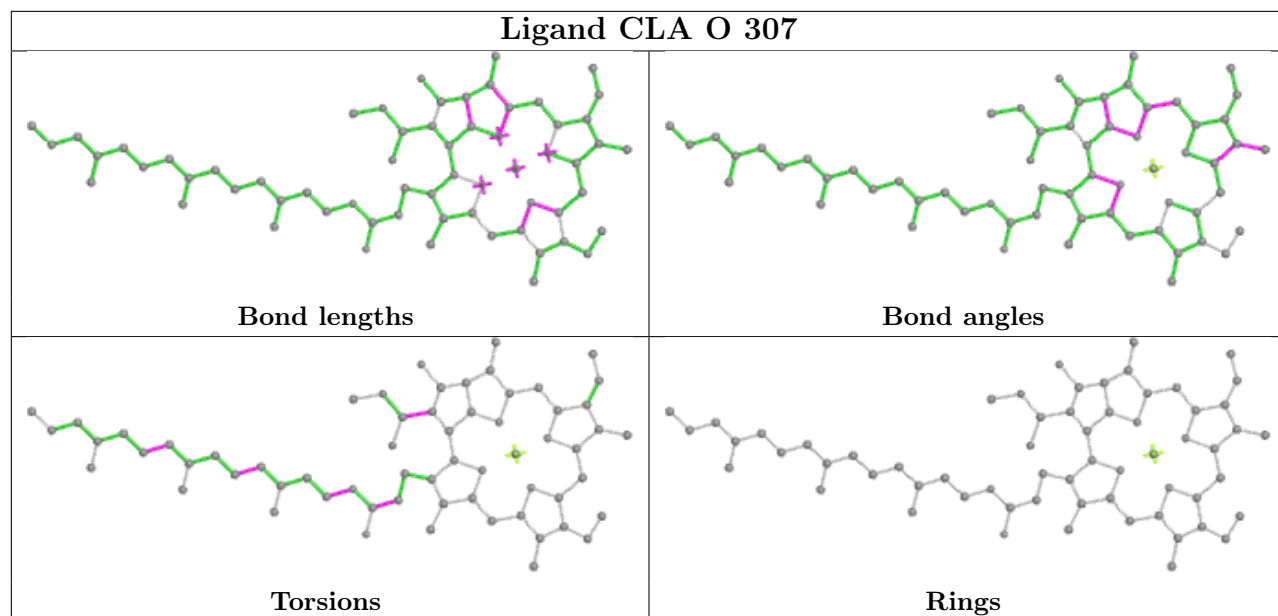


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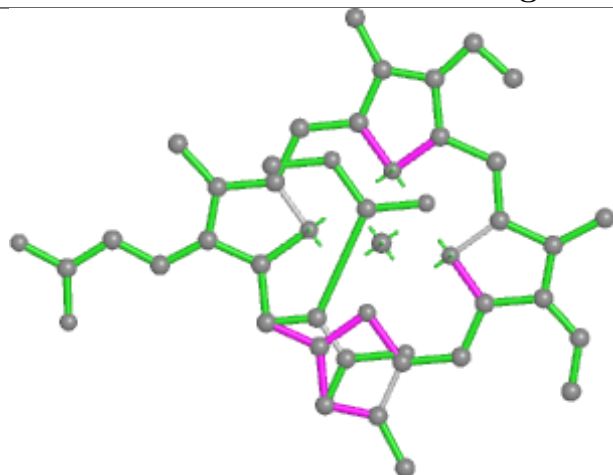


Rings

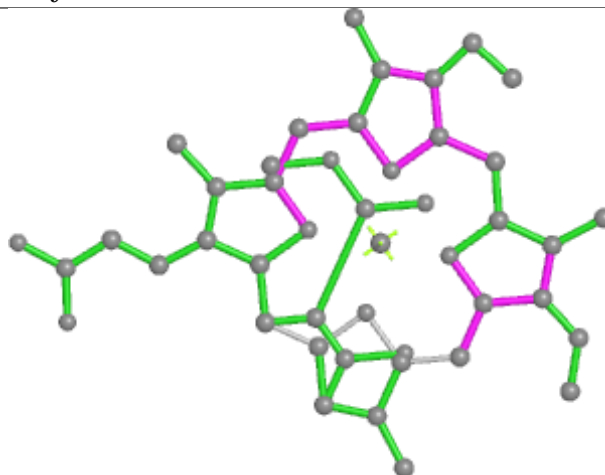




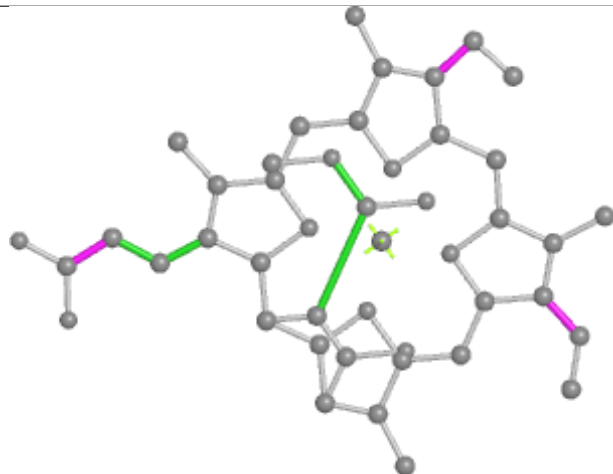
Ligand KC2 y 307



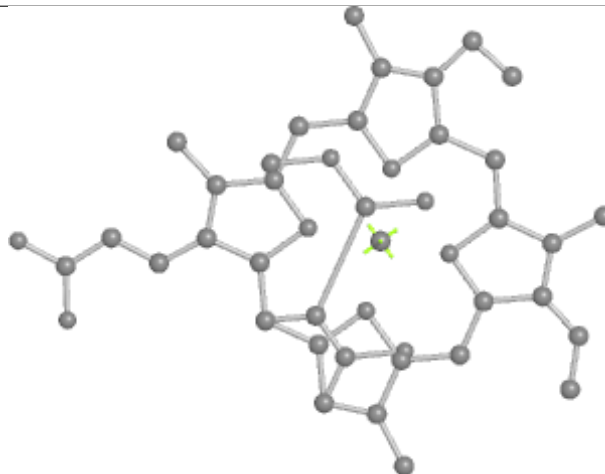
Bond lengths



Bond angles

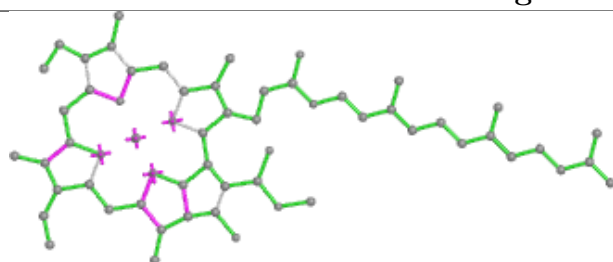


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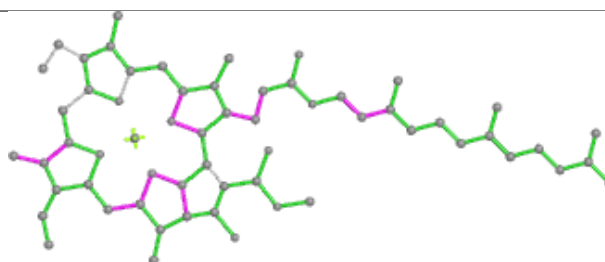


Rings

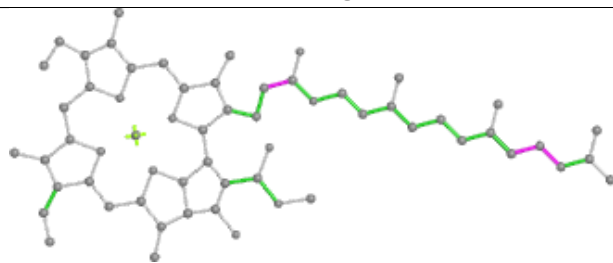
Ligand CLA T 306



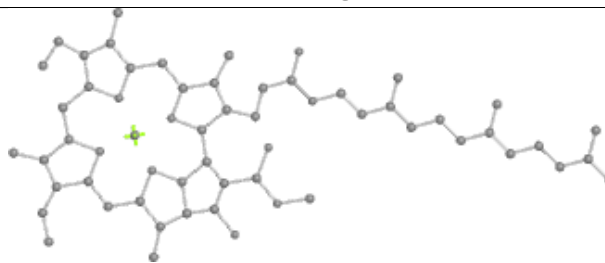
Bond lengths



Bond angles

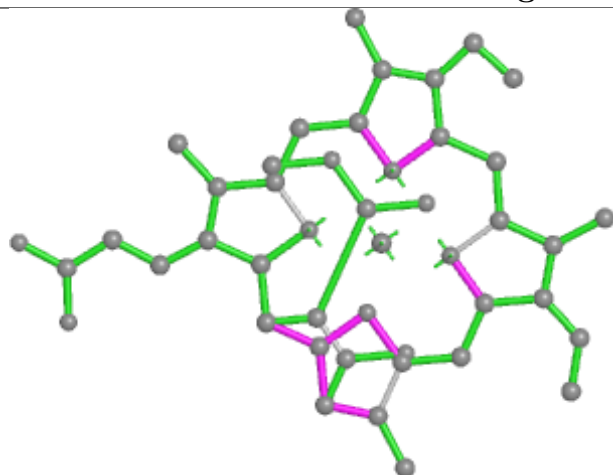


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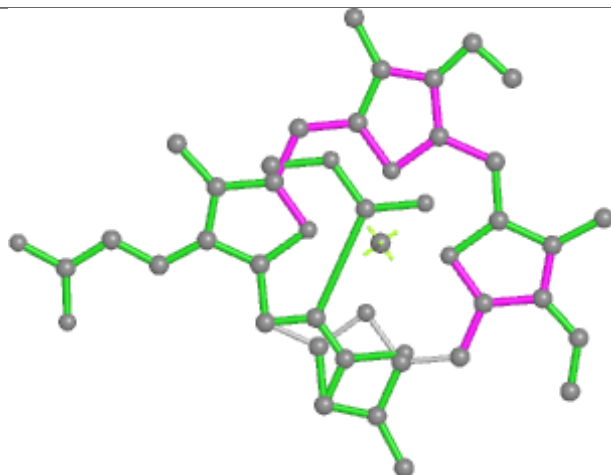


Rings

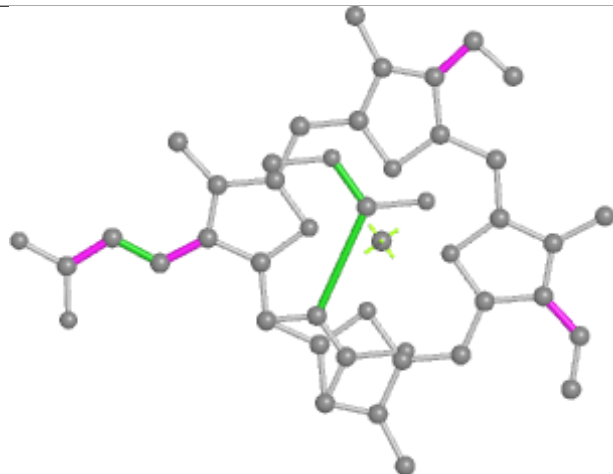
Ligand KC2 F 302



Bond lengths



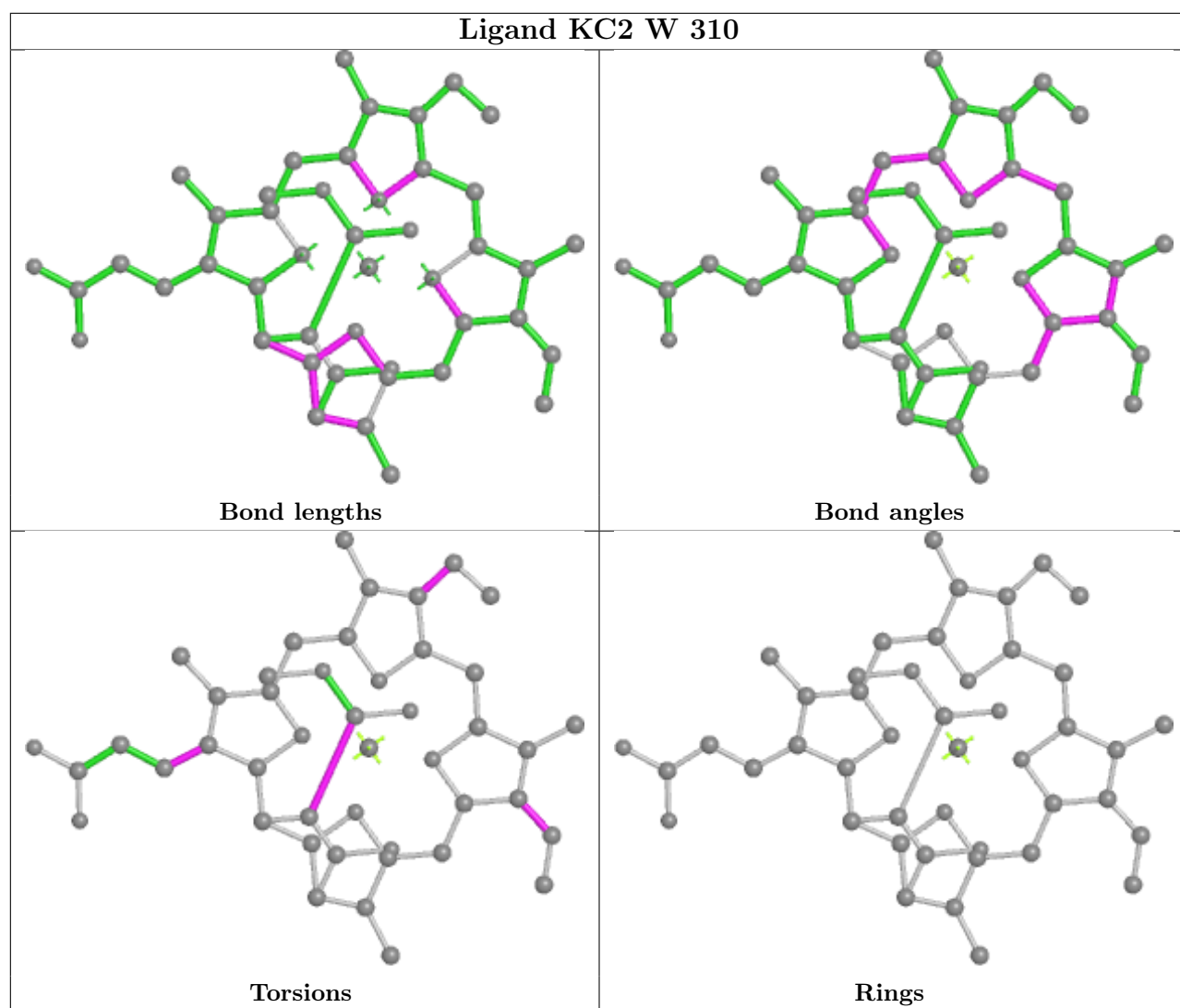
Bond angles



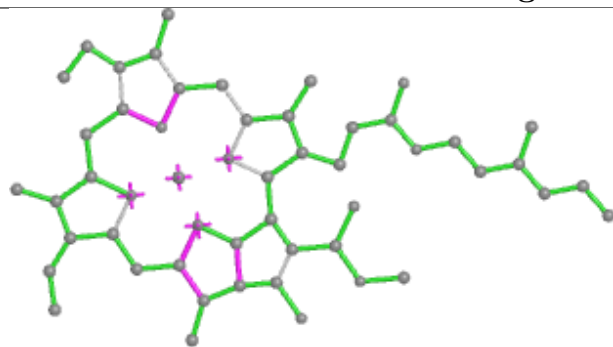
Torsions



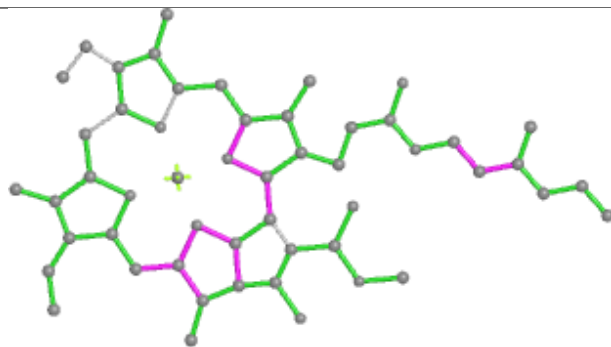
Rings



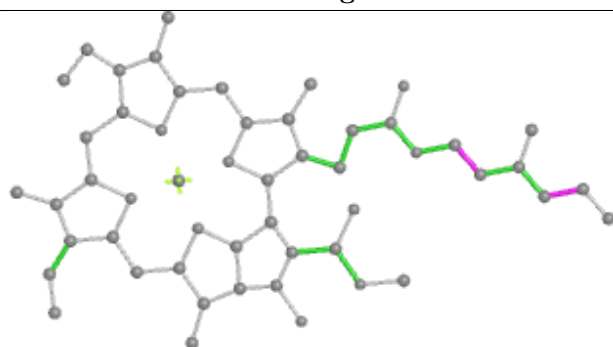
Ligand CLA J 306



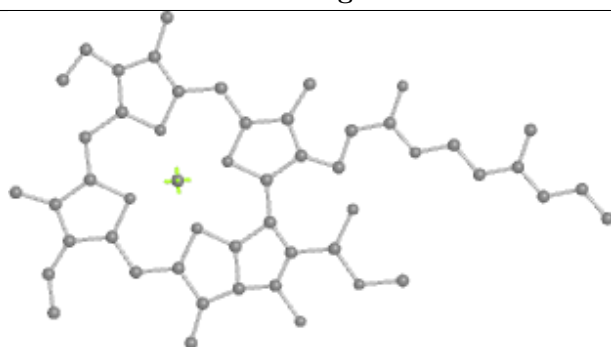
Bond lengths



Bond angles

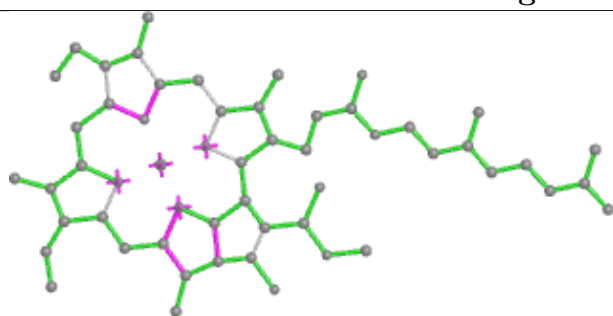


Torsions

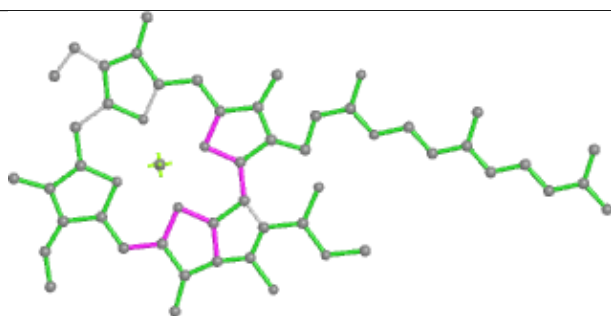


Rings

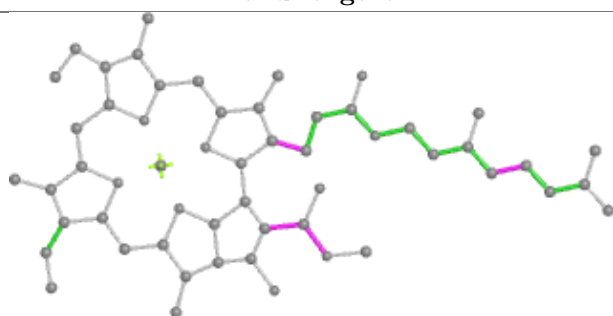
Ligand CLA a 823



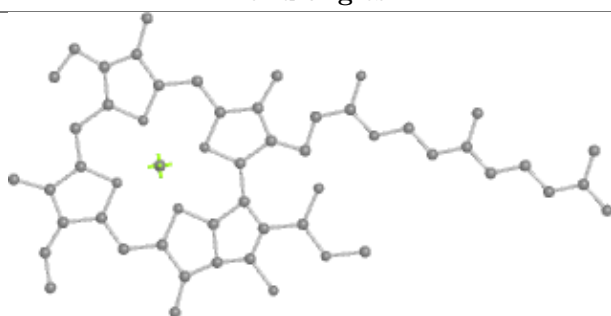
Bond lengths



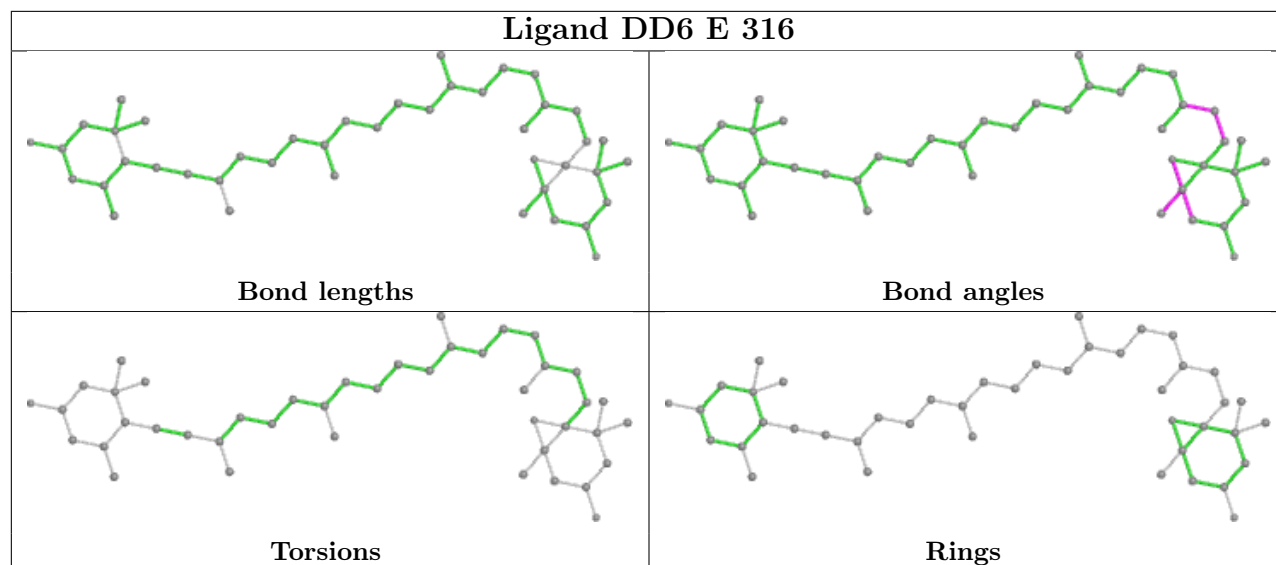
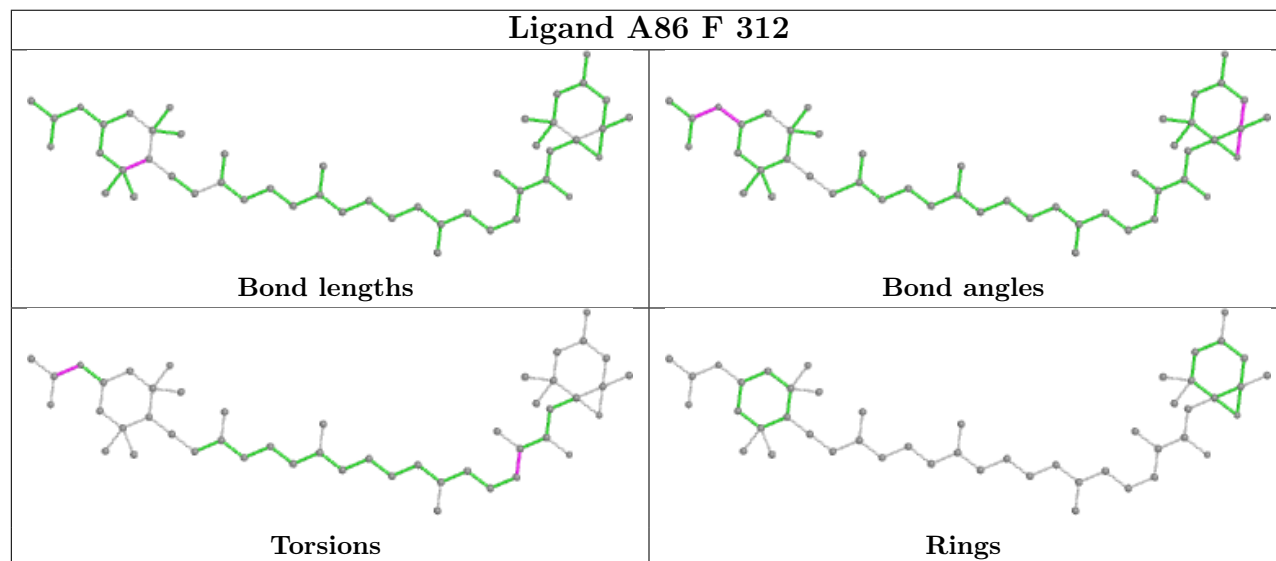
Bond angles



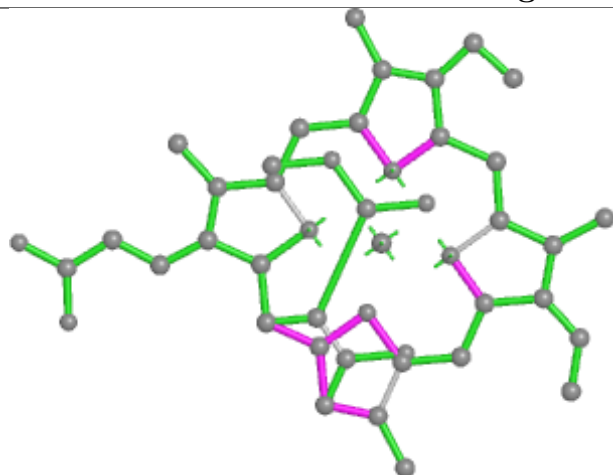
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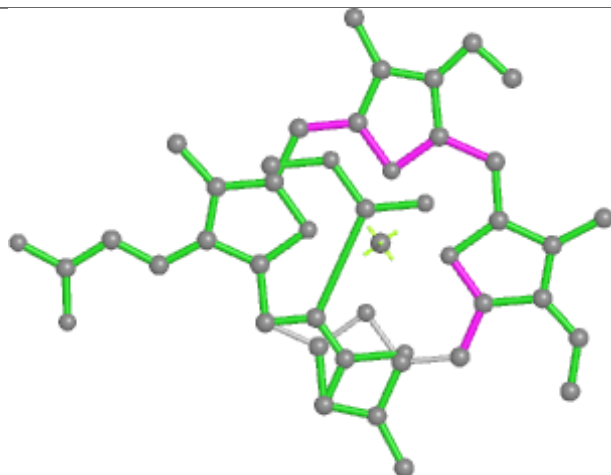
Rings

Ligand DD6 E 316**Ligand A86 F 312**

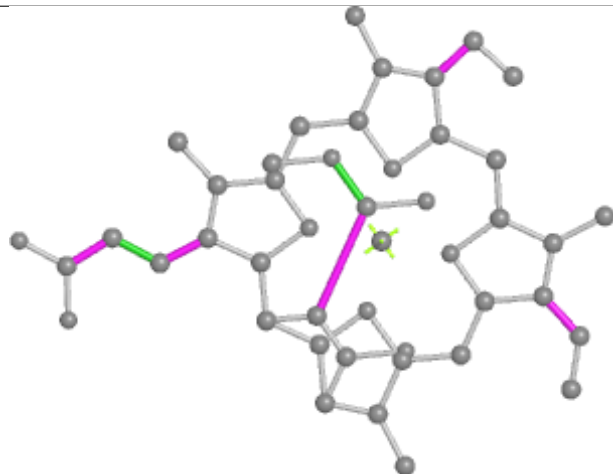
Ligand KC2 Z 309



Bond lengths



Bond angles

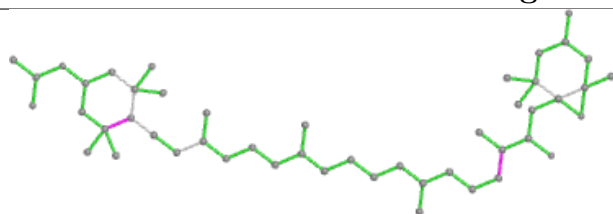


Torsions

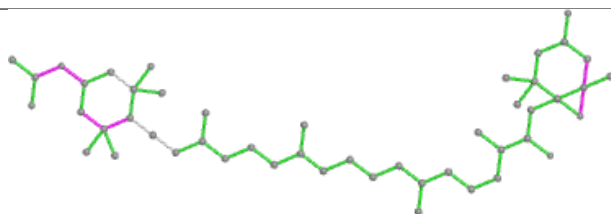


Rings

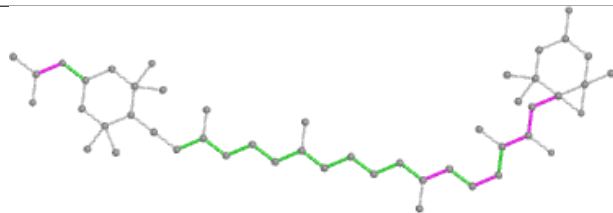
Ligand A86 w 311



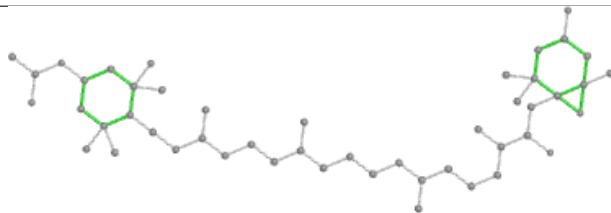
Bond lengths



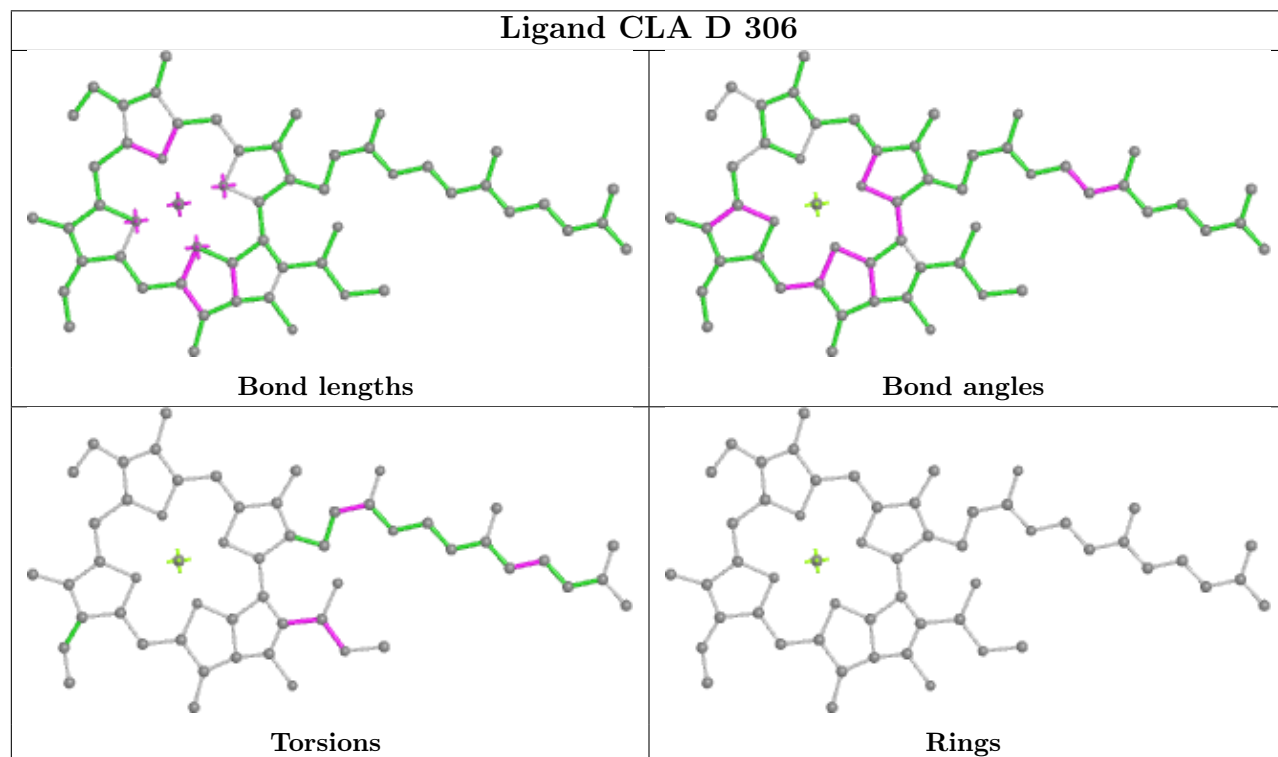
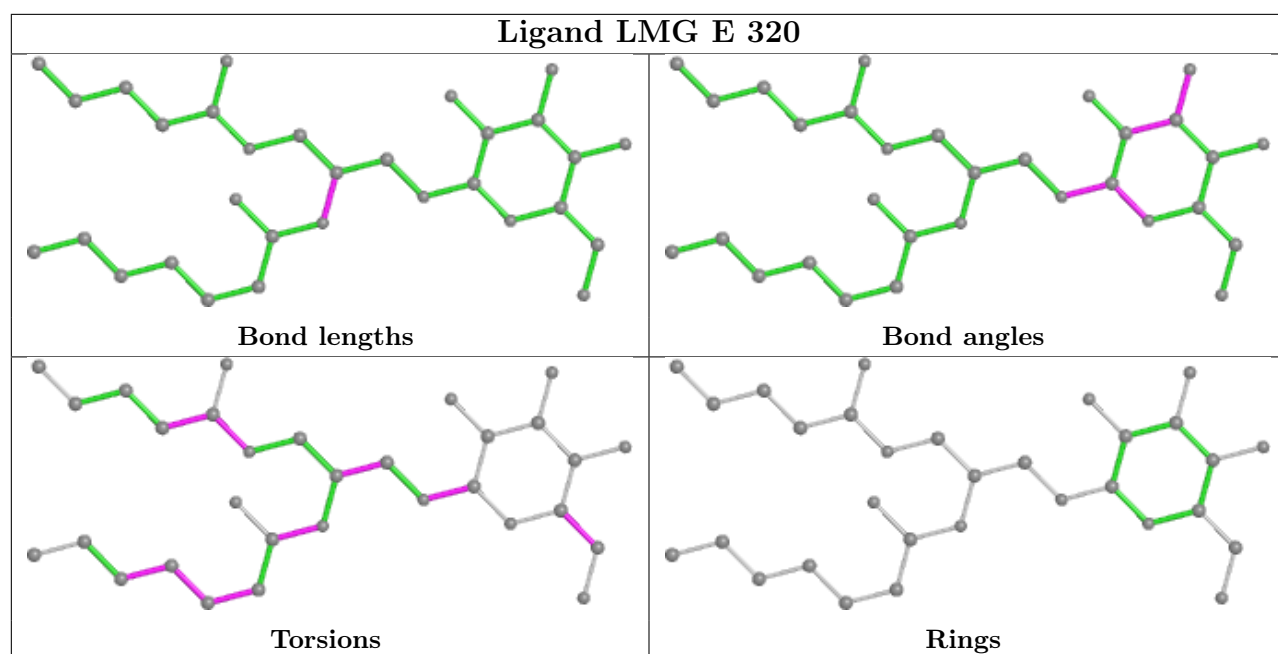
Bond angles



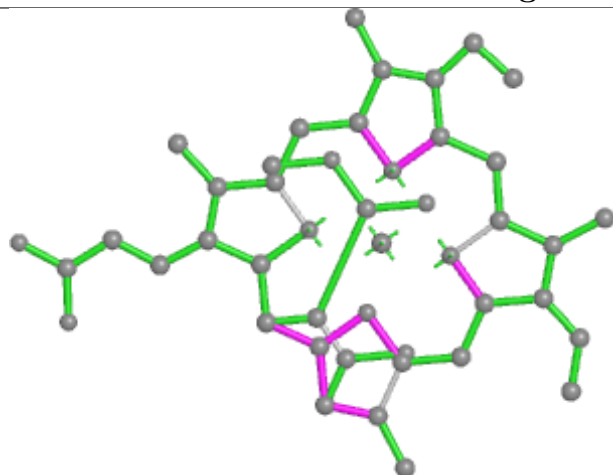
Torsions



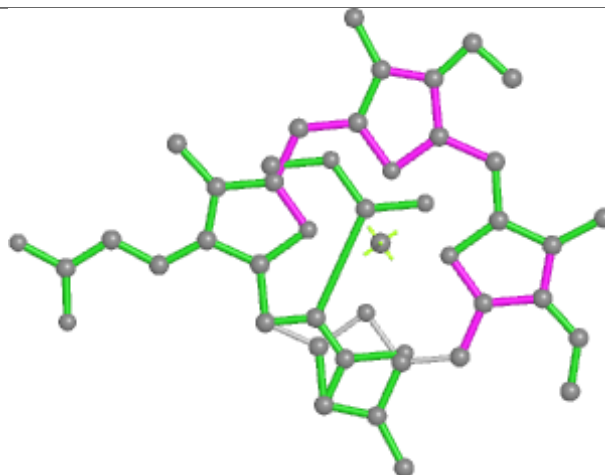
Rings



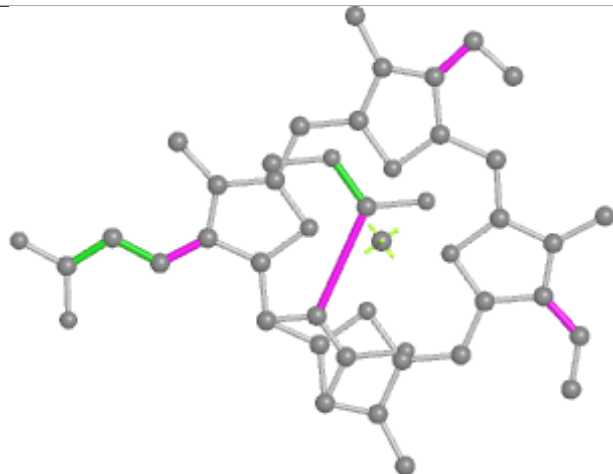
Ligand KC2 u 309



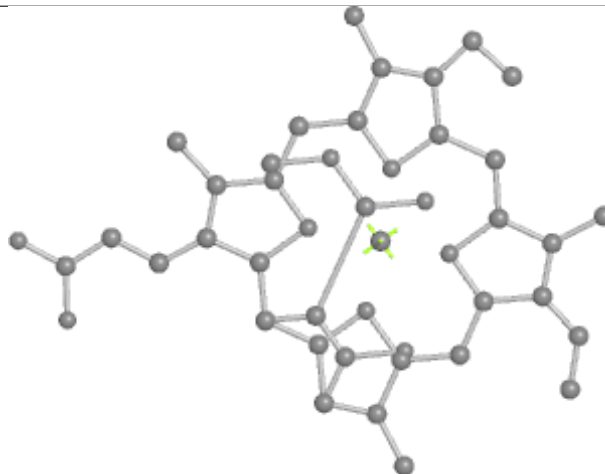
Bond lengths



Bond angles

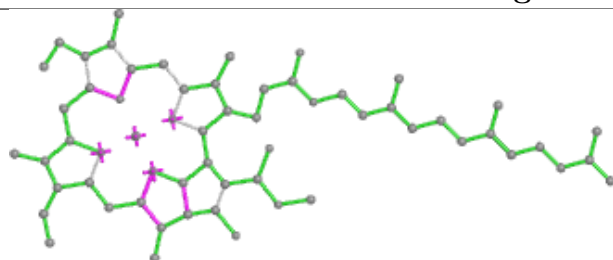


Torsions

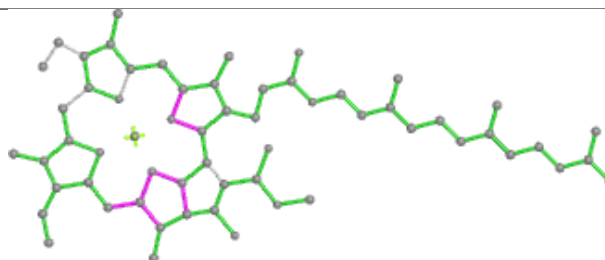


Rings

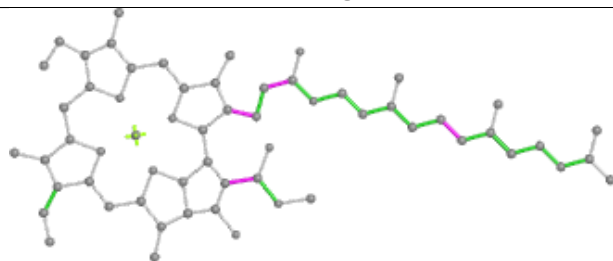
Ligand CLA X 301



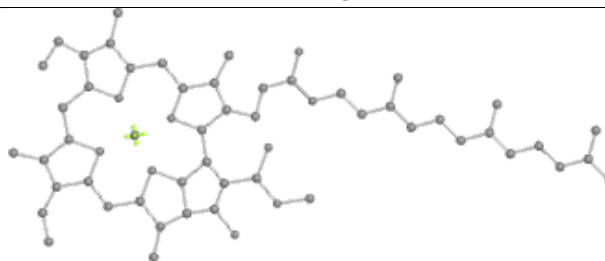
Bond lengths



Bond angles

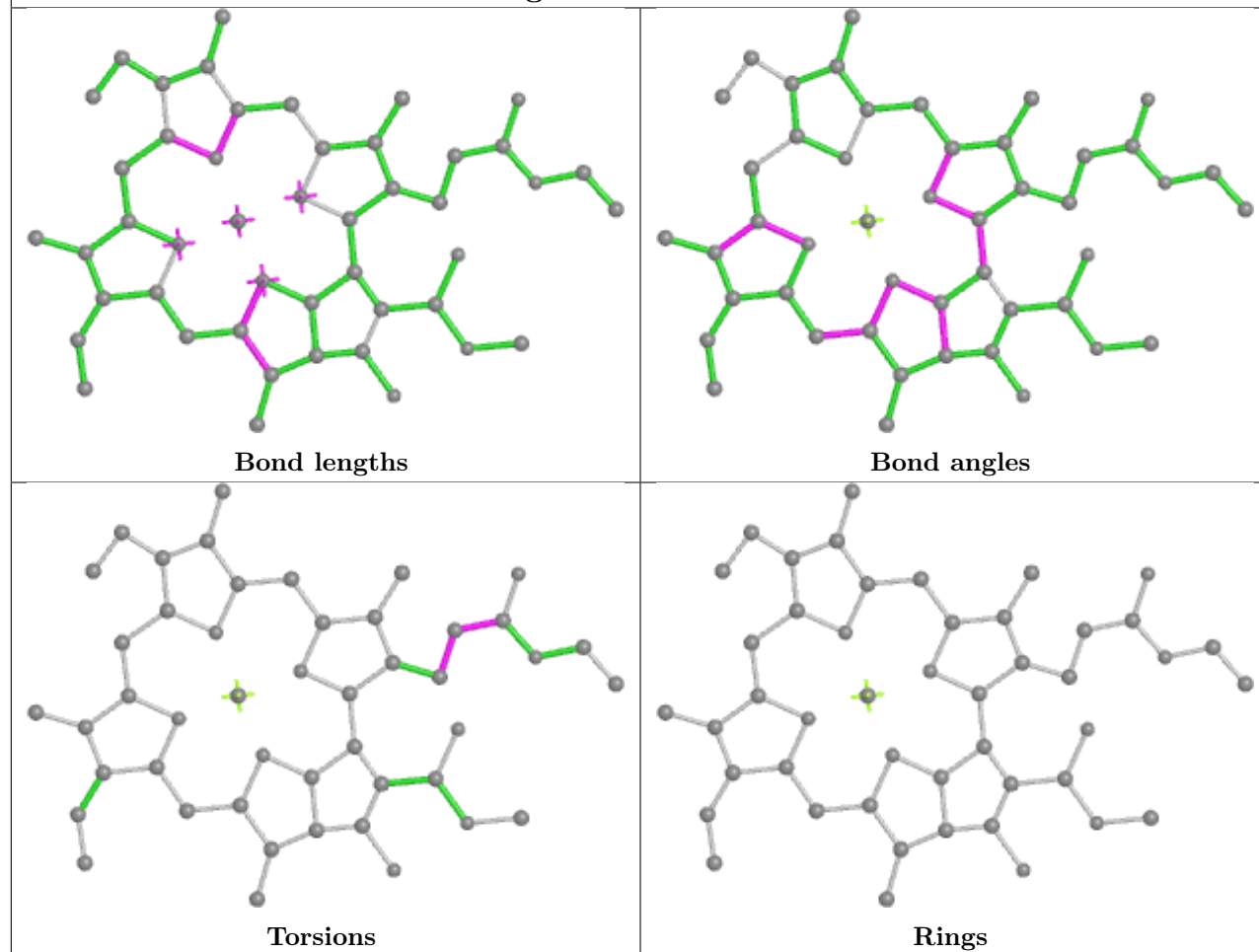


Torsions

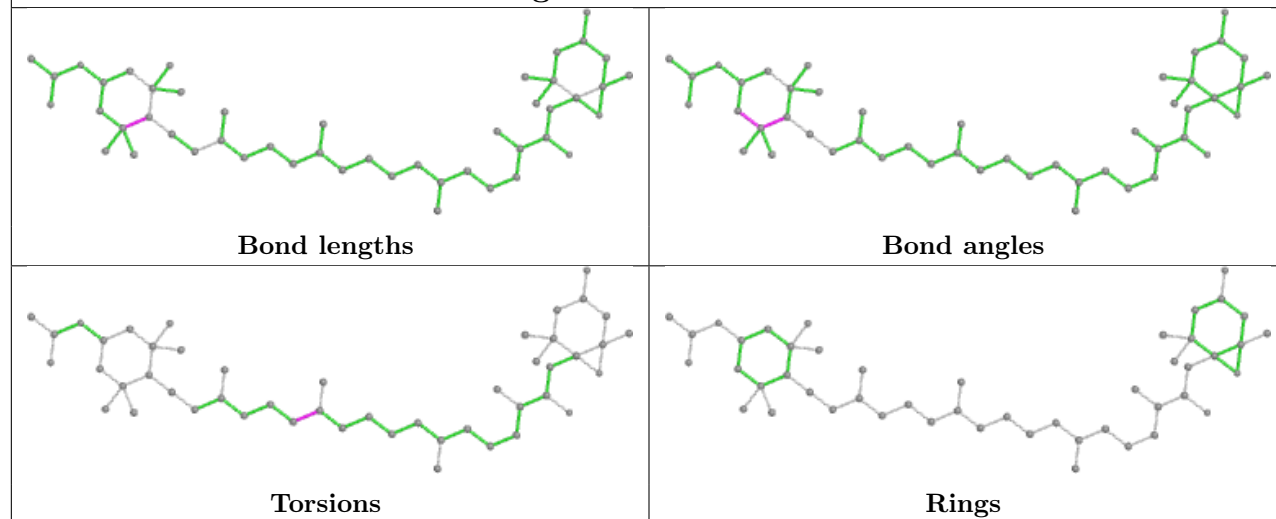


Rings

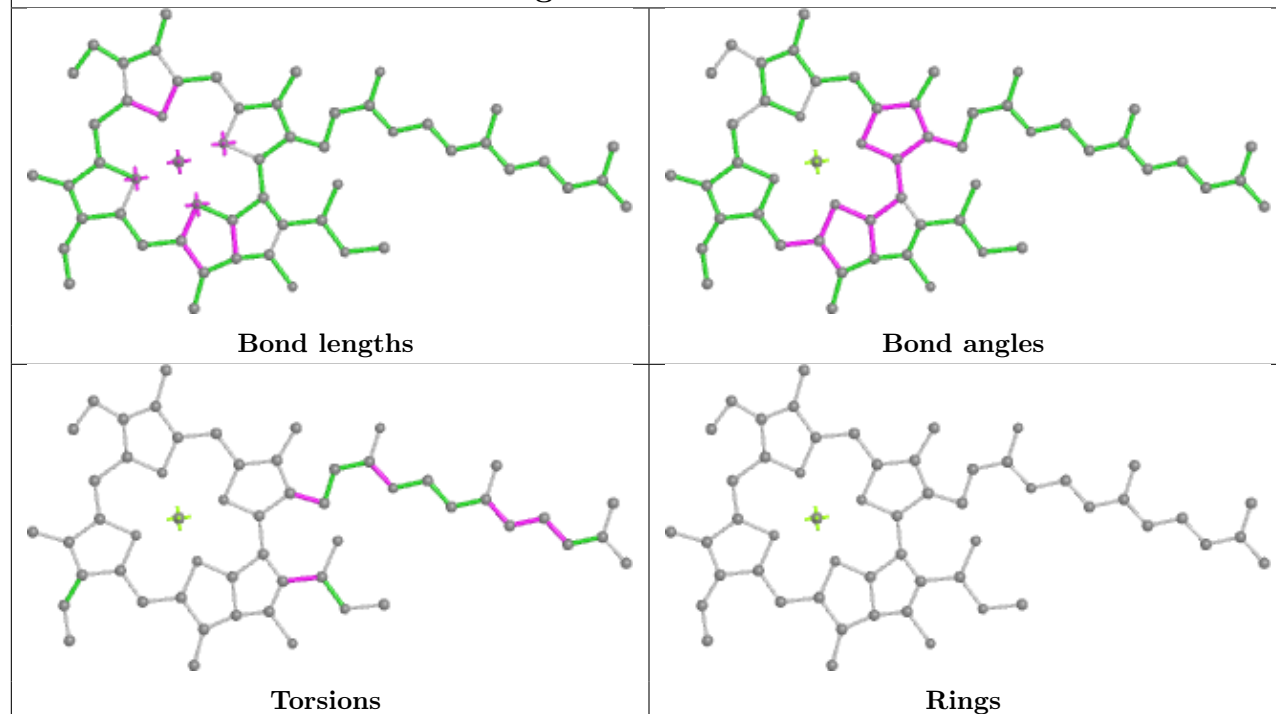
Ligand CLA T 317



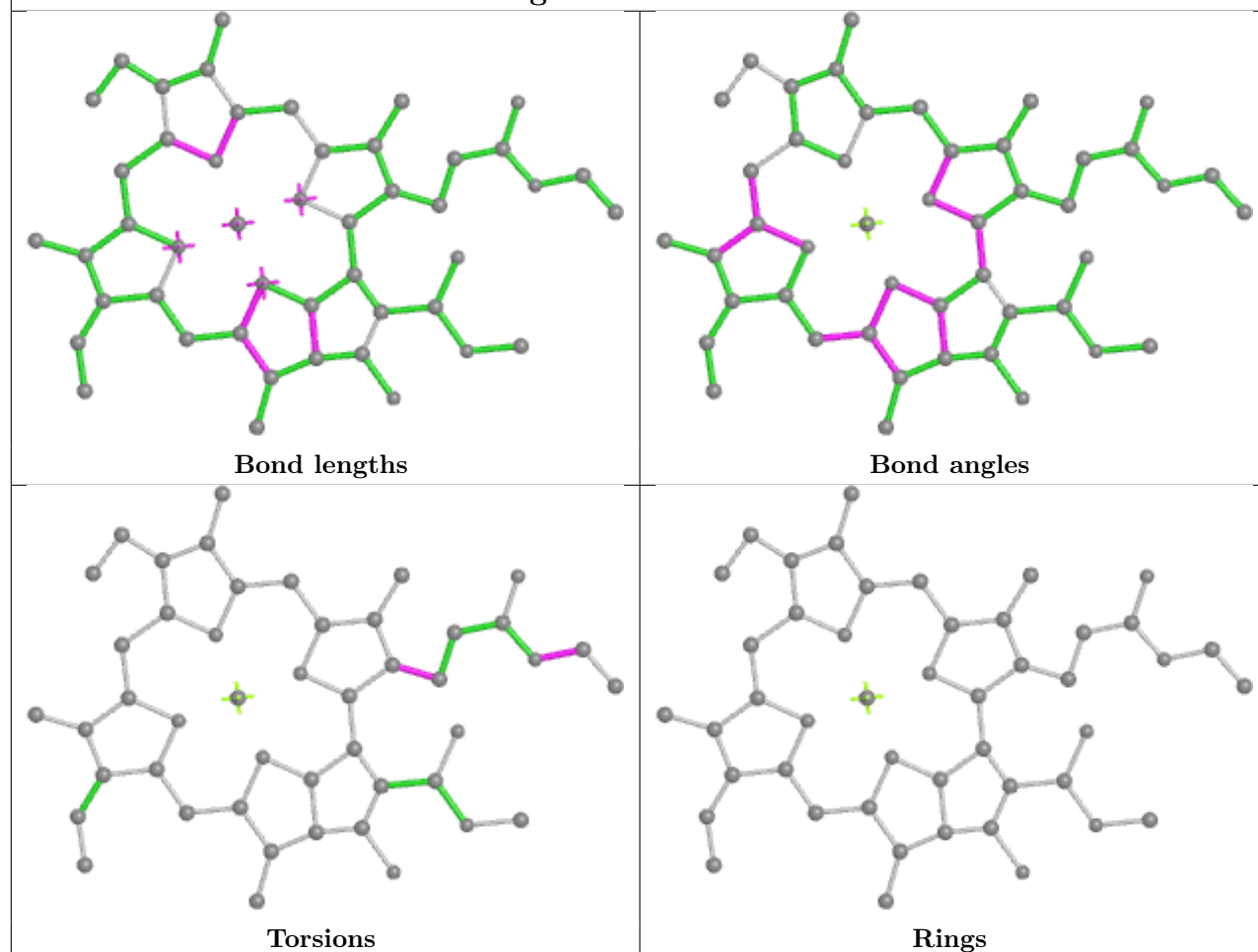
Ligand A86 W 301



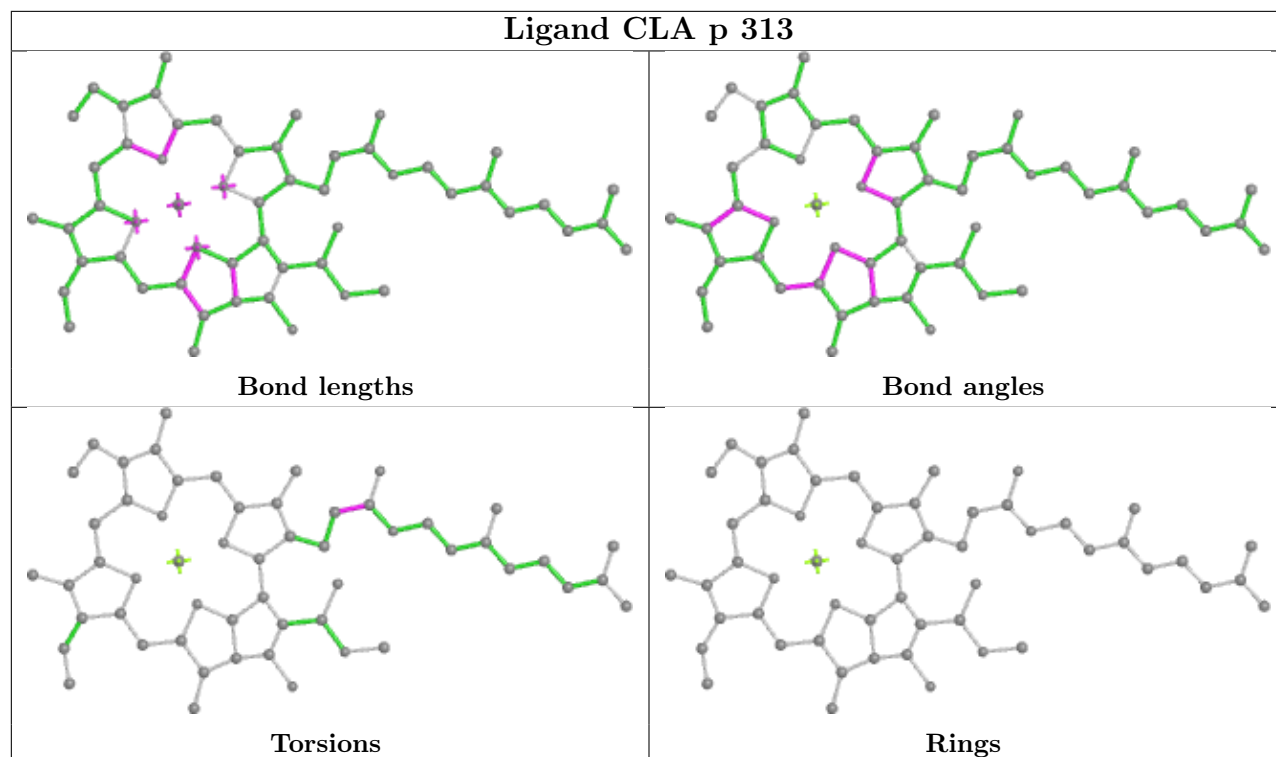
Ligand CLA u 311



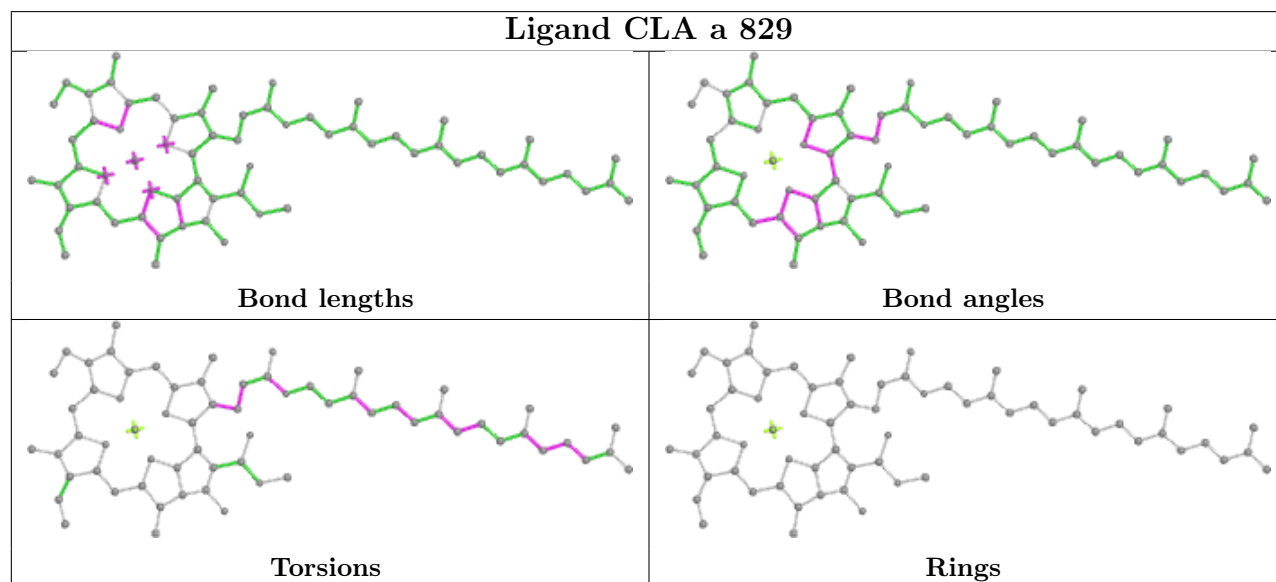
Ligand CLA z 324

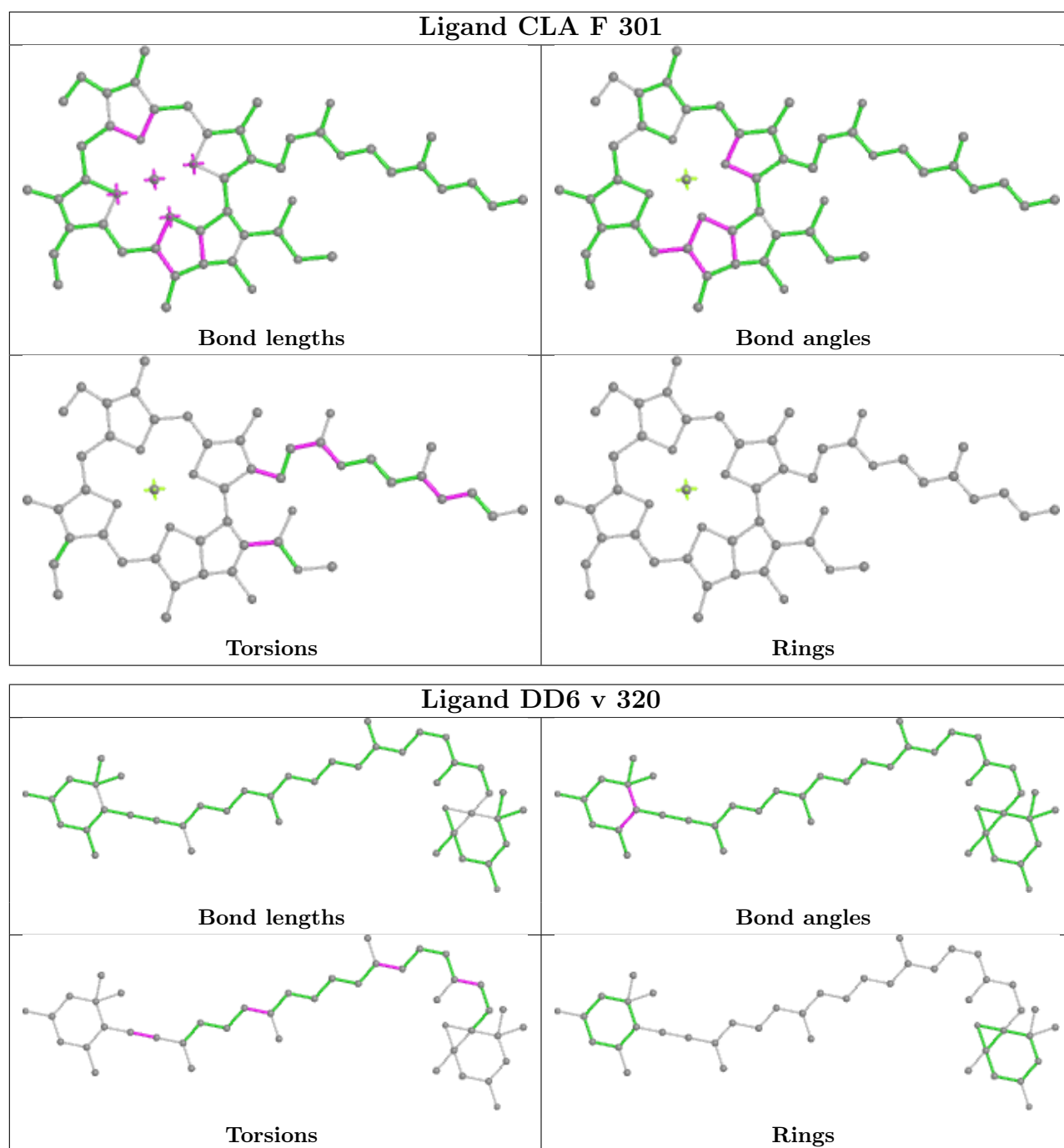


Ligand CLA p 313

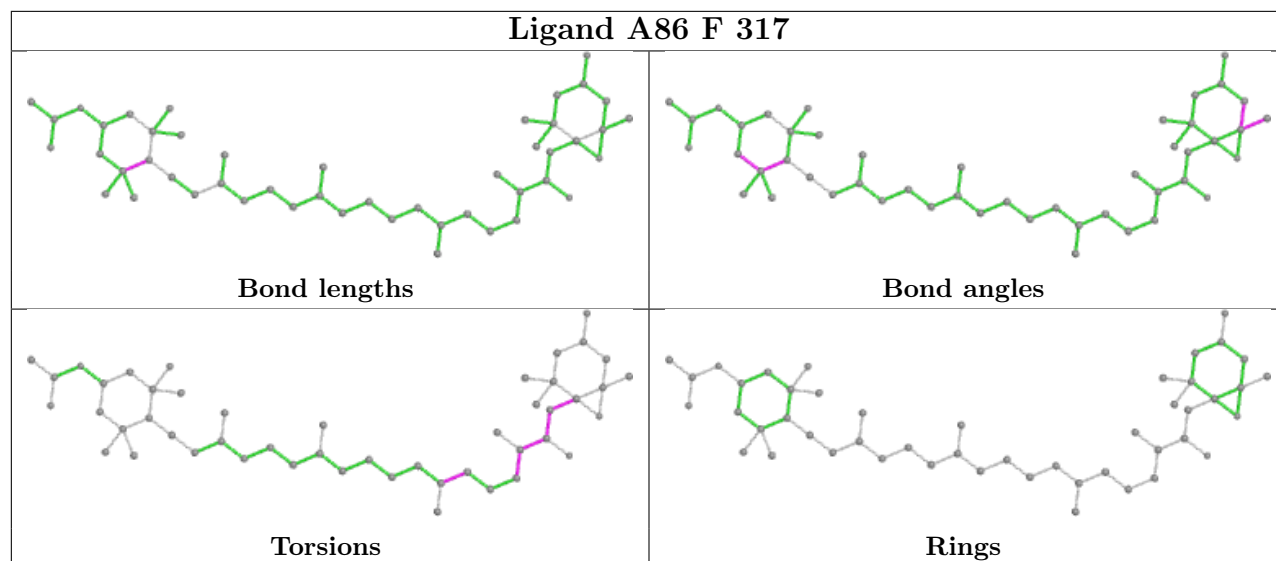


Ligand CLA a 829

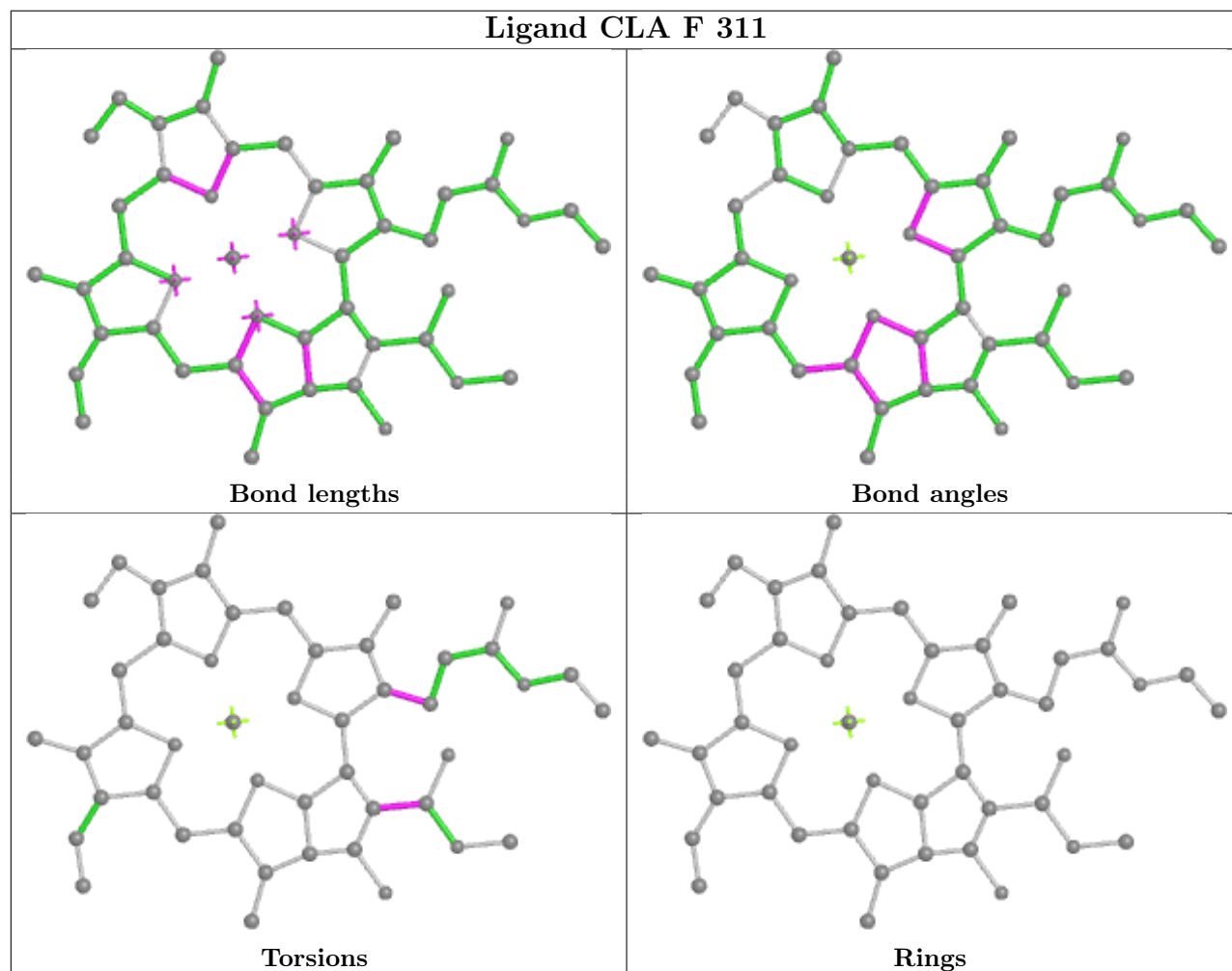




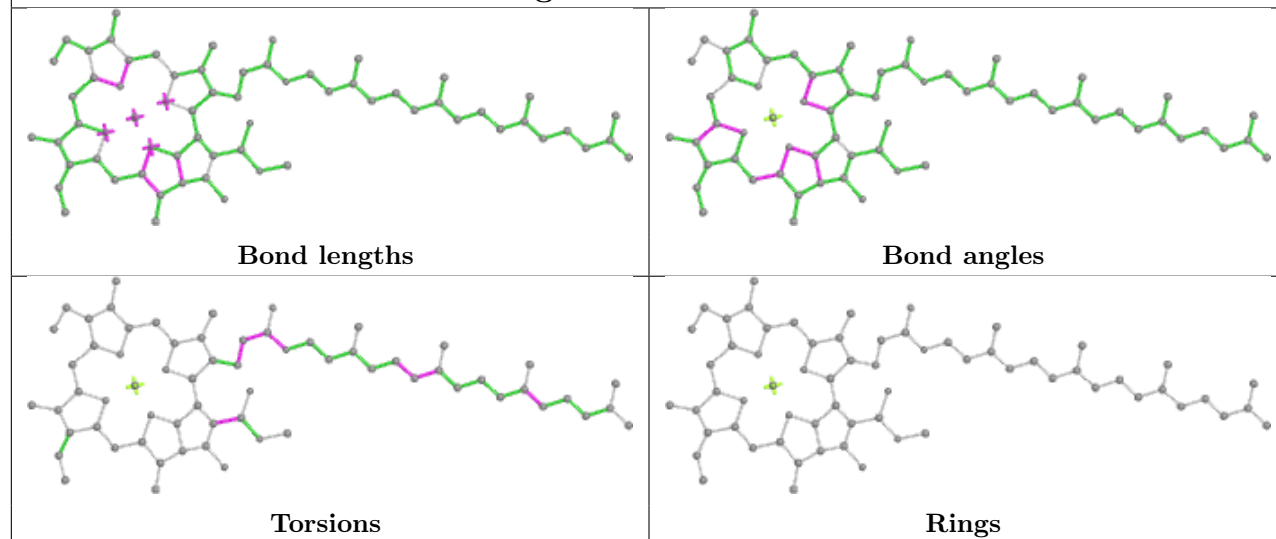
Ligand A86 F 317



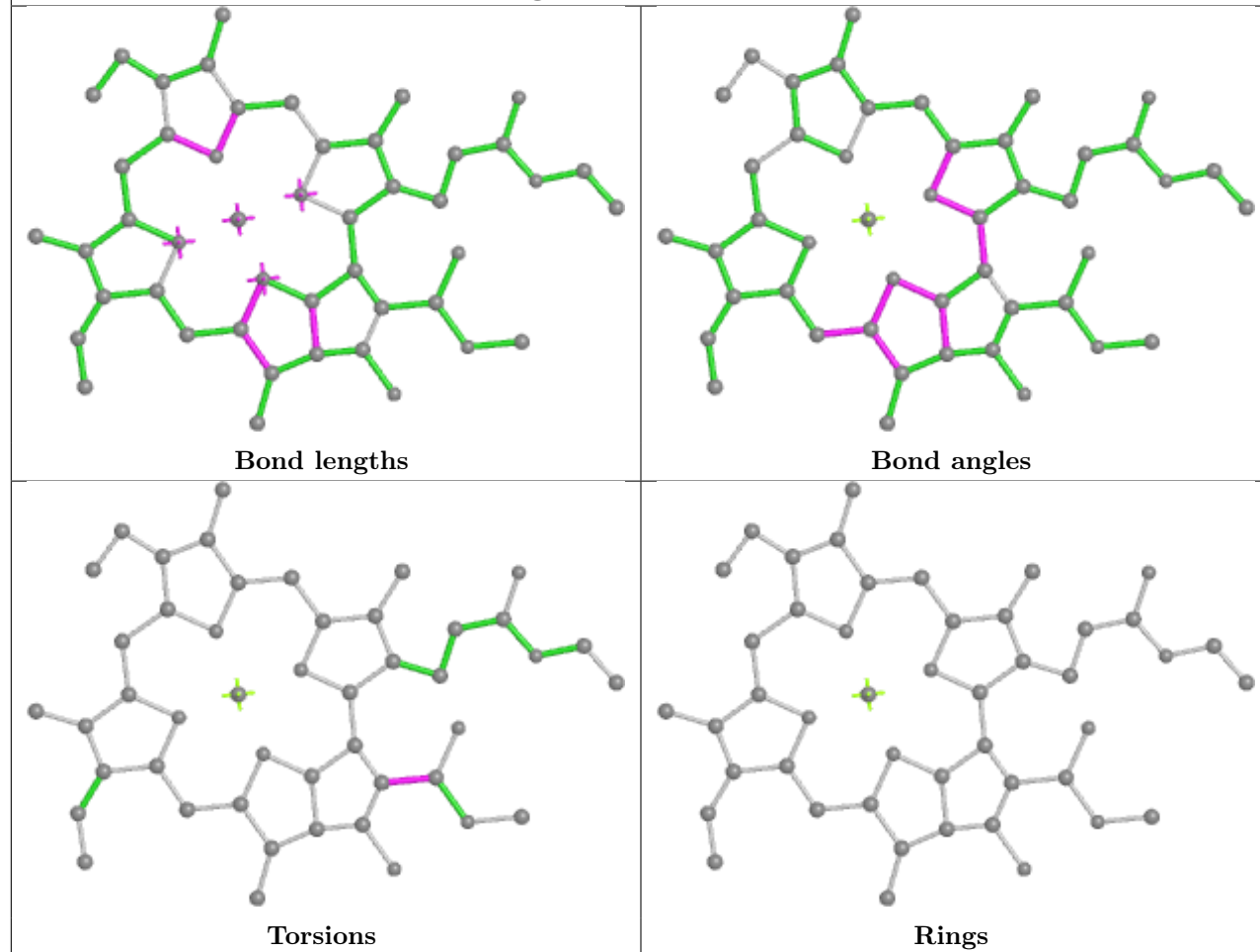
Ligand CLA F 311

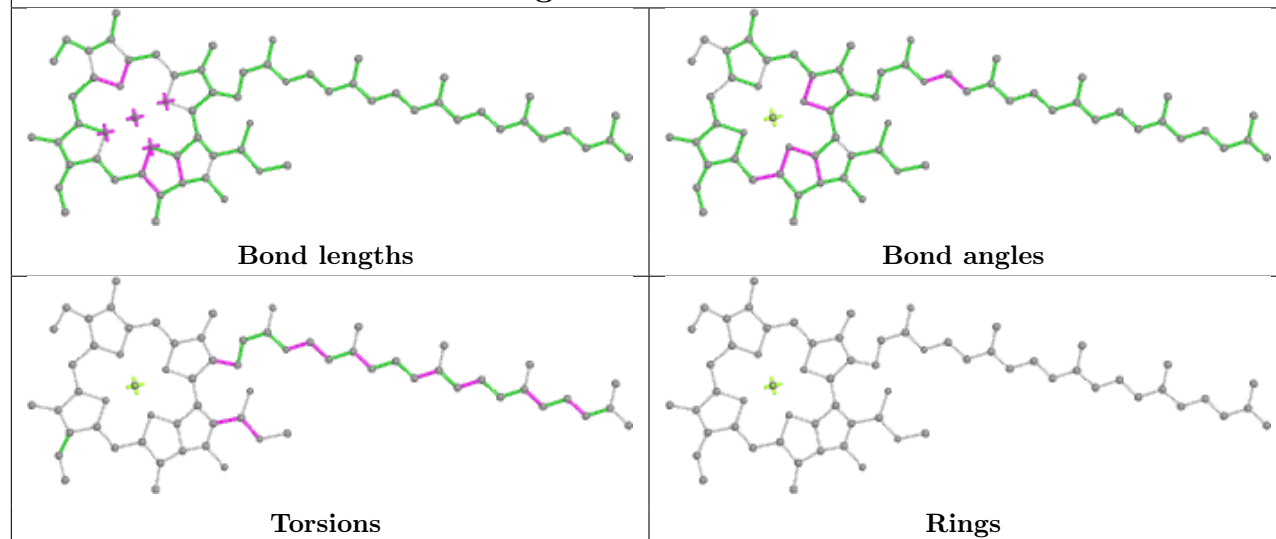
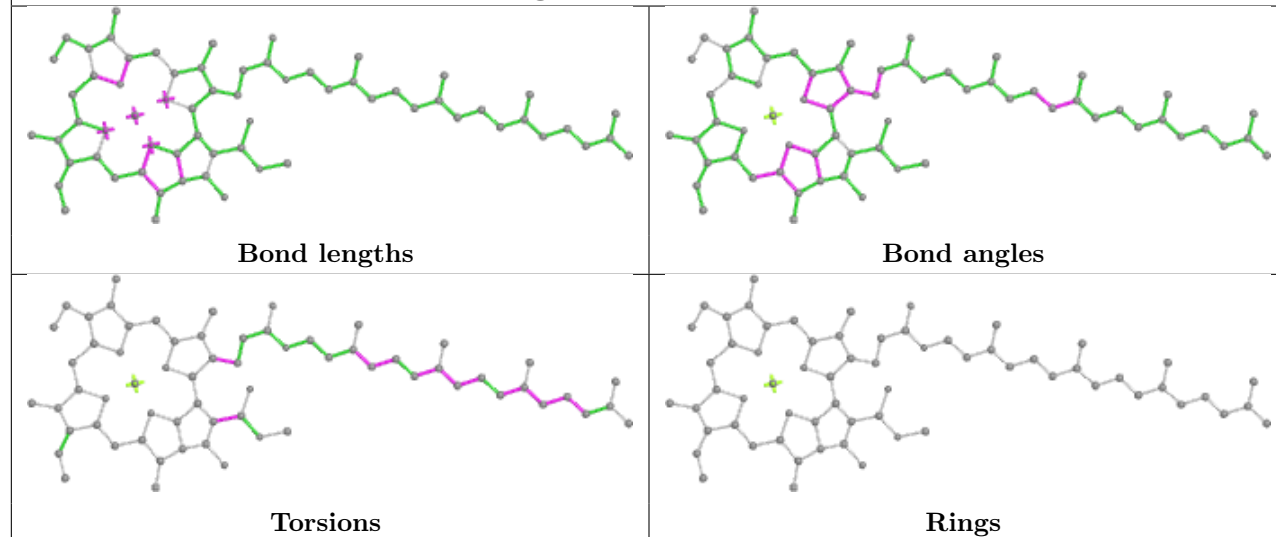


Ligand CLA b 814

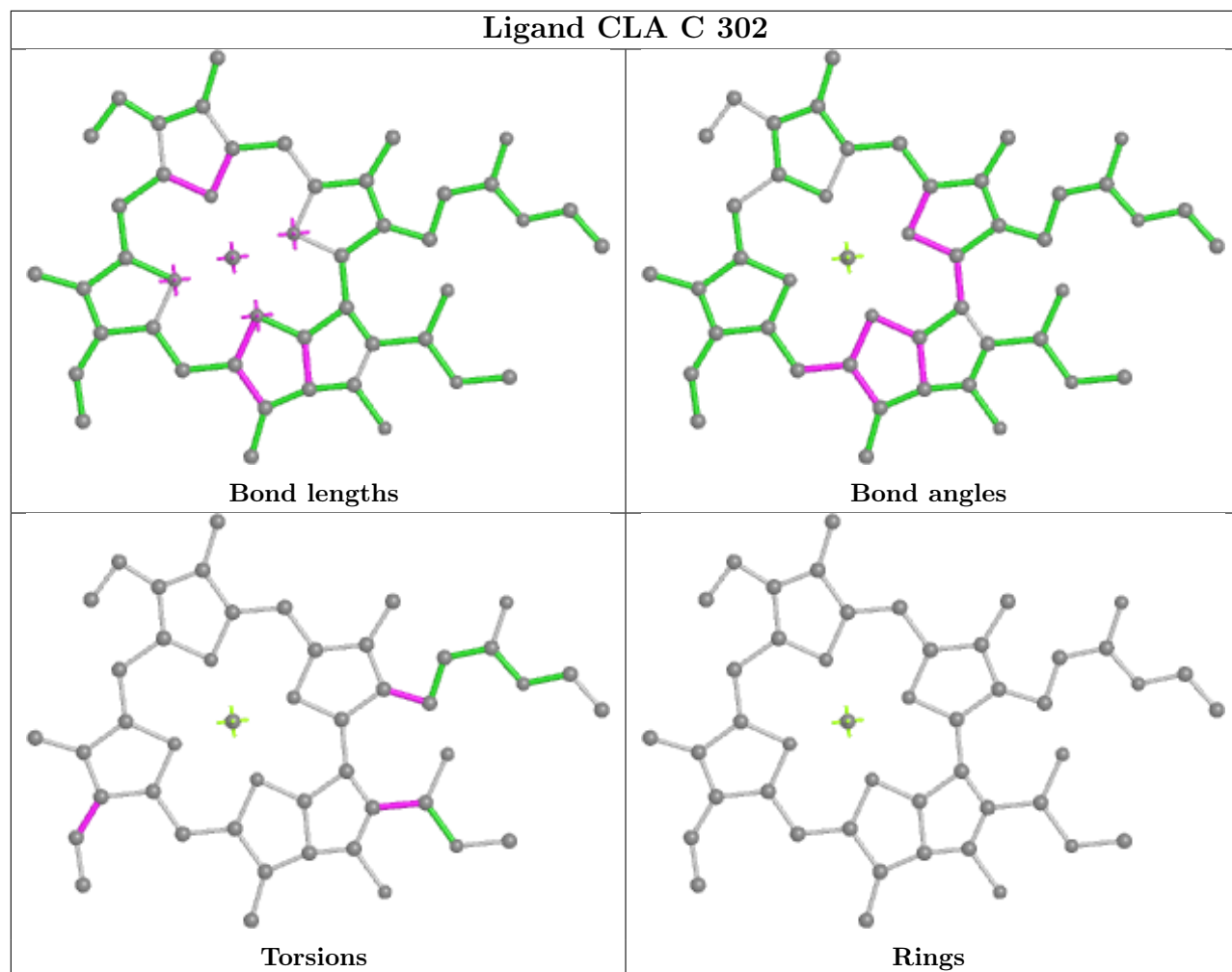


Ligand CLA x 314

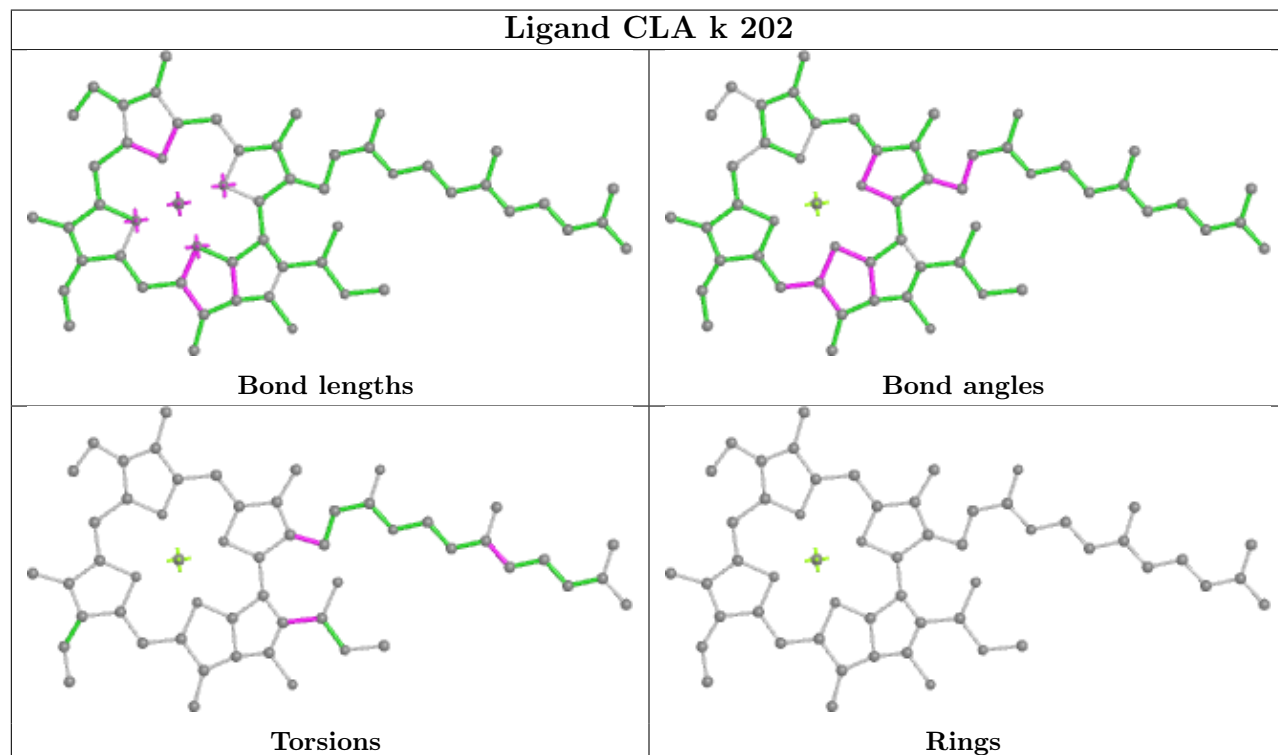


Ligand CLA b 806**Ligand CLA A 304**

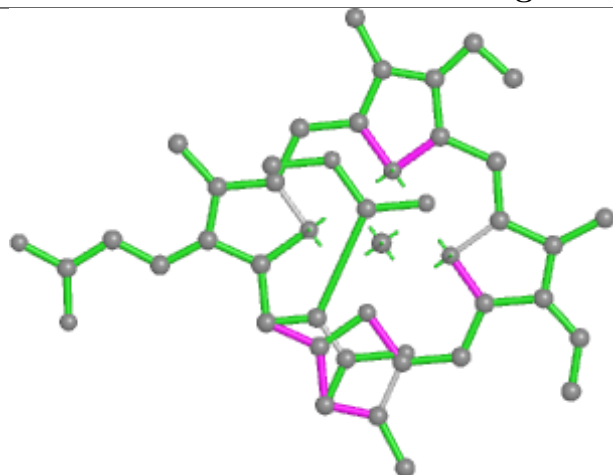
Ligand CLA C 302



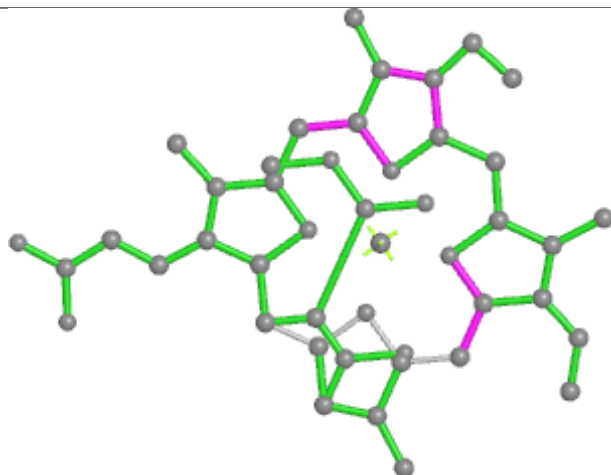
Ligand CLA k 202



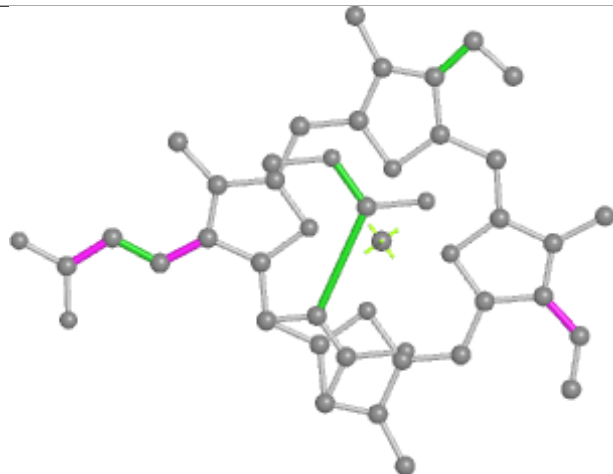
Ligand KC2 X 309



Bond lengths



Bond angles

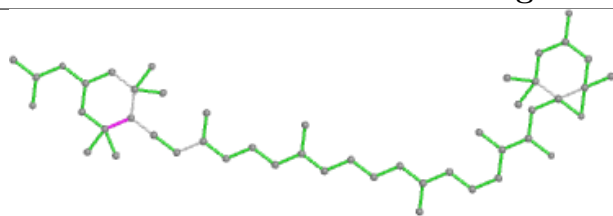


Torsions

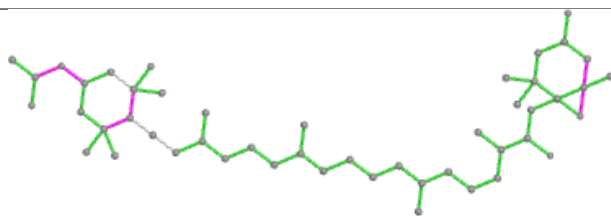


Rings

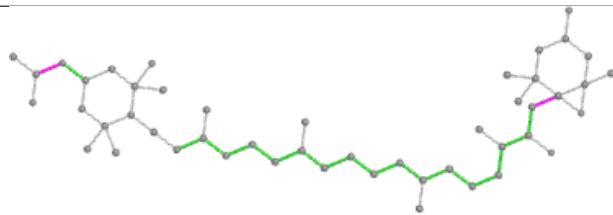
Ligand A86 M 313



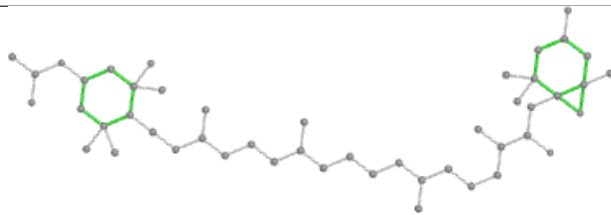
Bond lengths



Bond angles

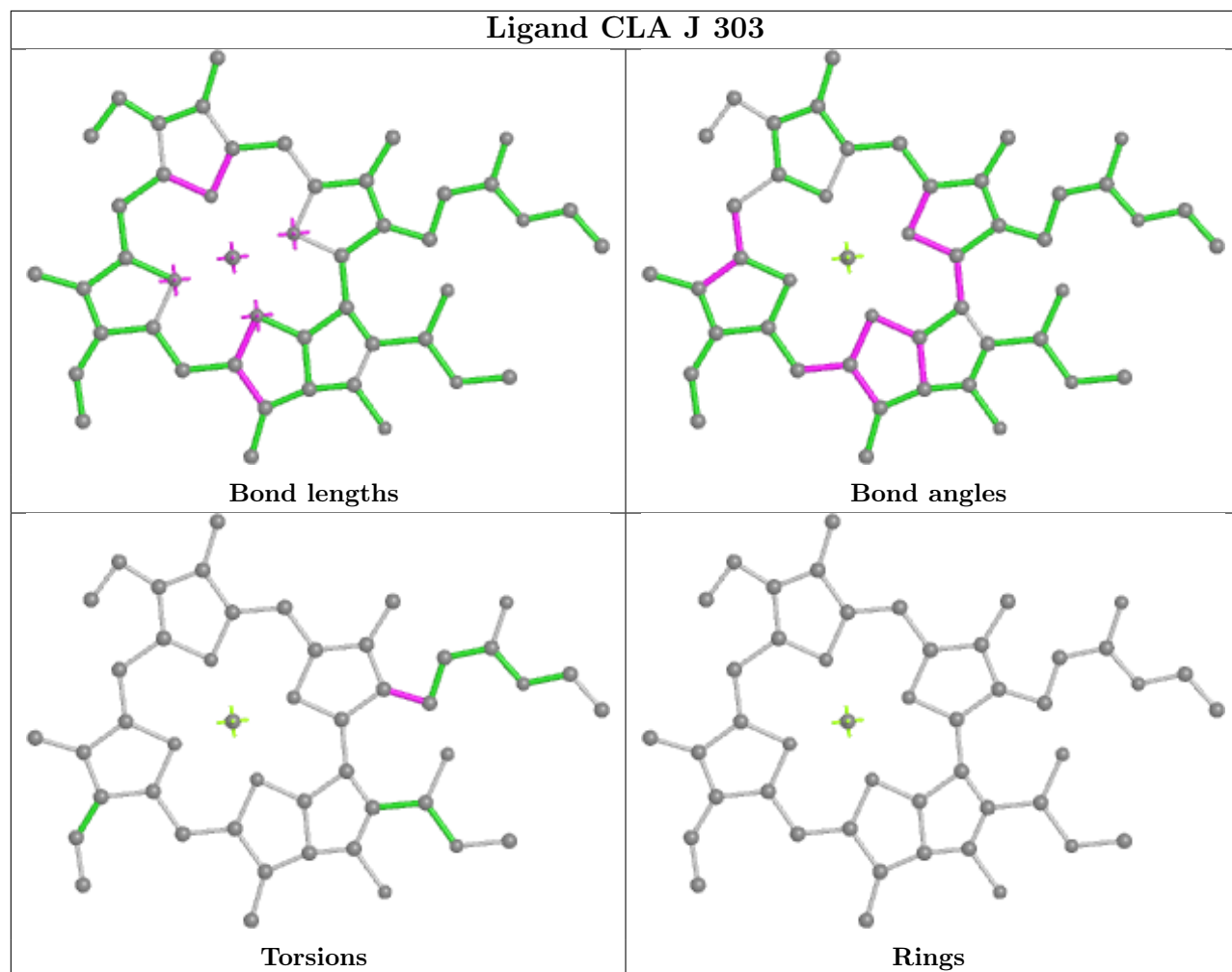


Torsions

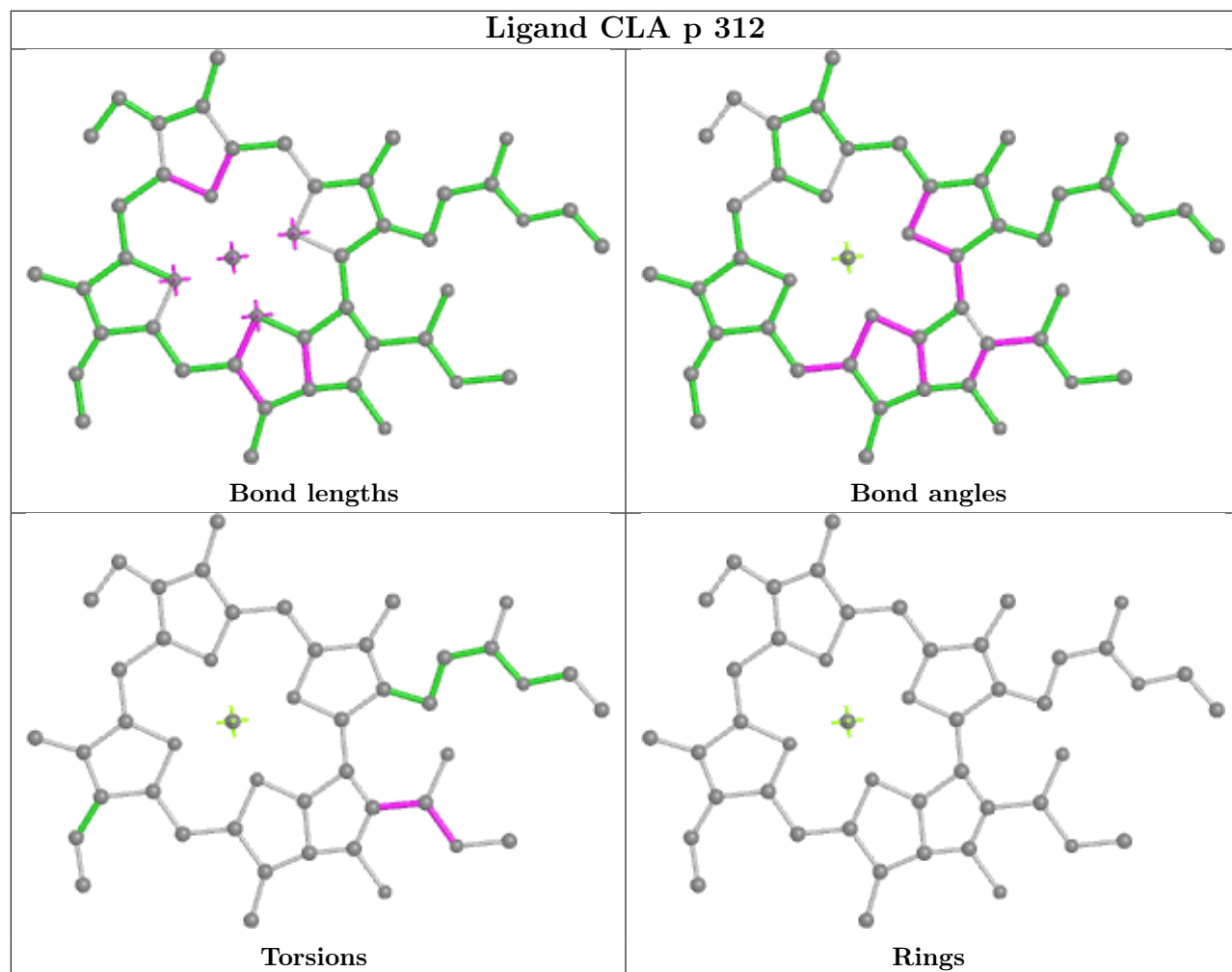


Rings

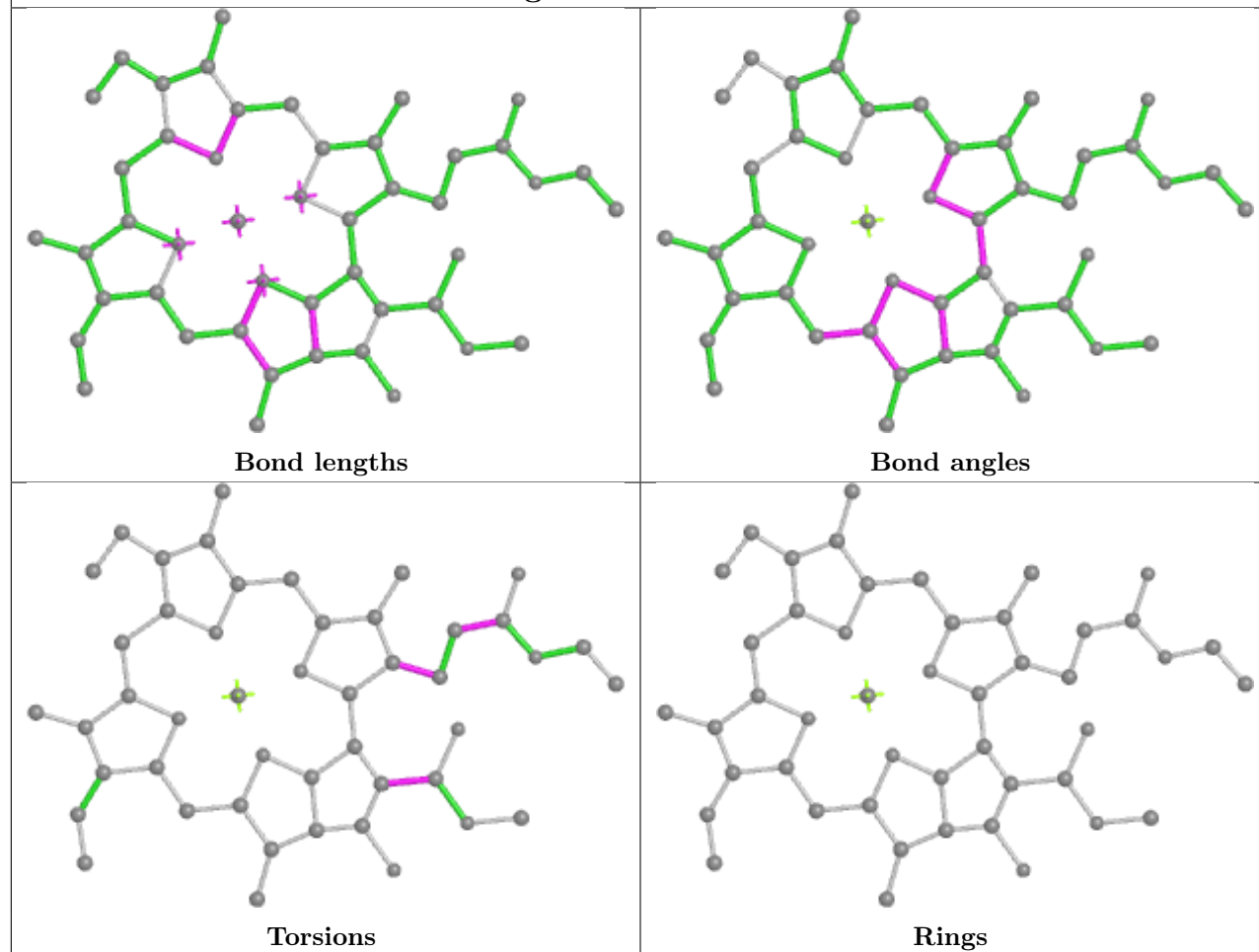
Ligand CLA J 303



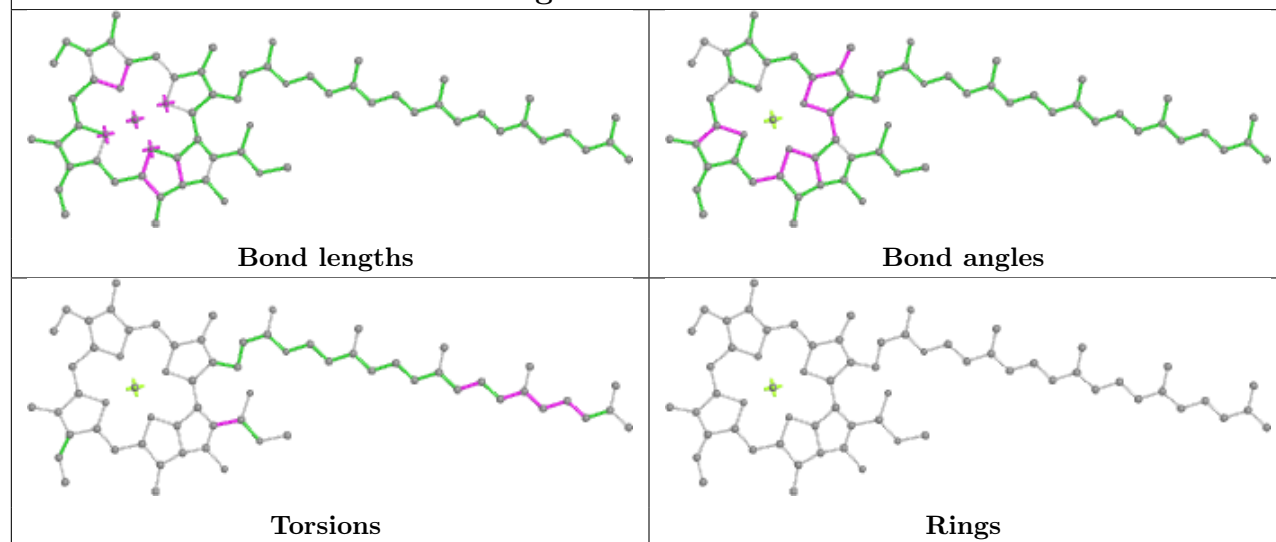
Ligand CLA p 312



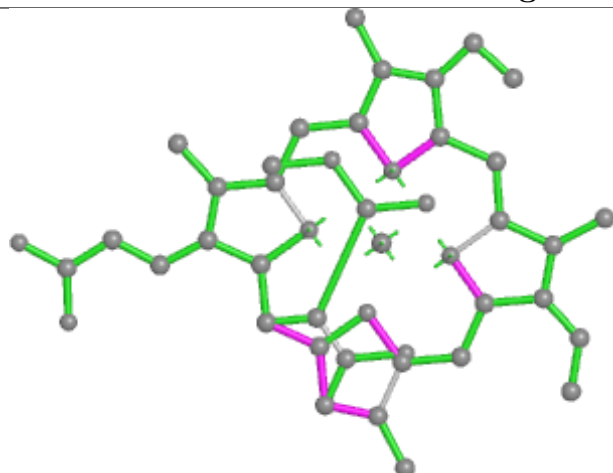
Ligand CLA R 310



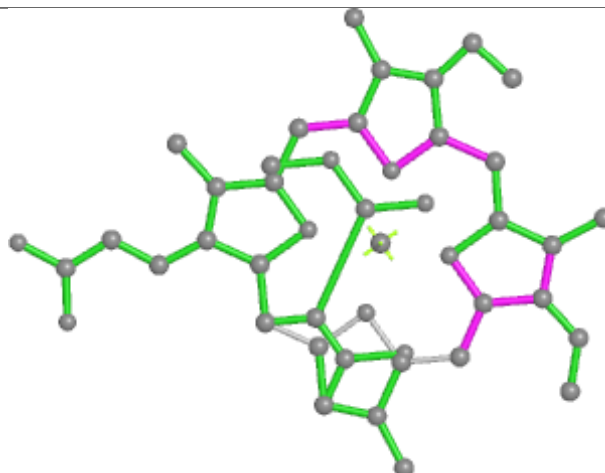
Ligand CLA b 821



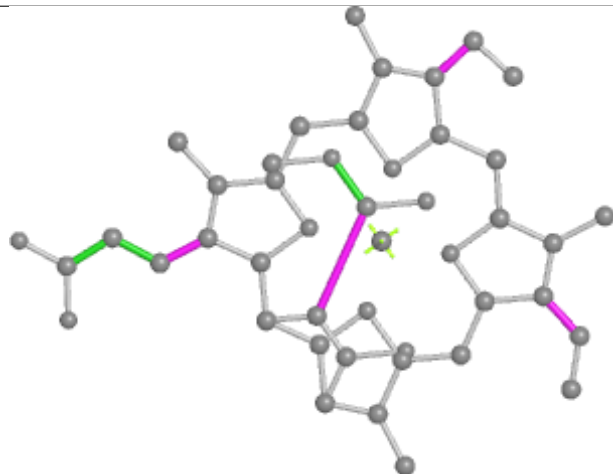
Ligand KC2 u 310



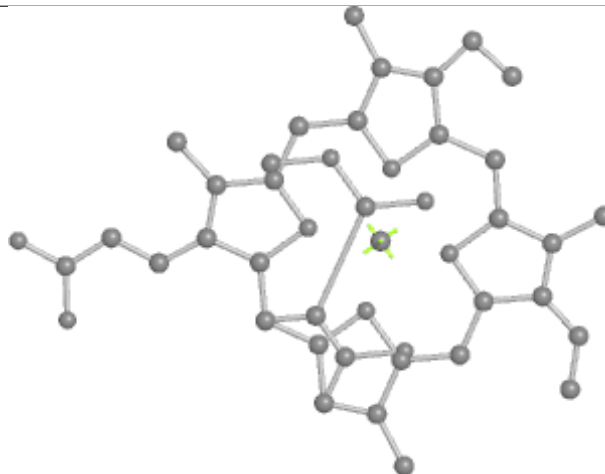
Bond lengths



Bond angles

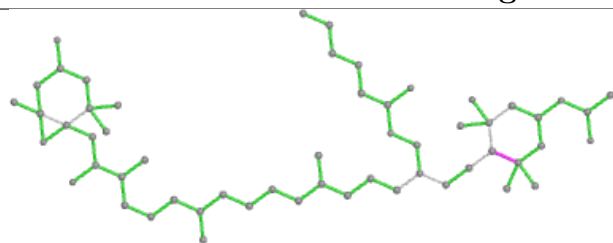


Torsions

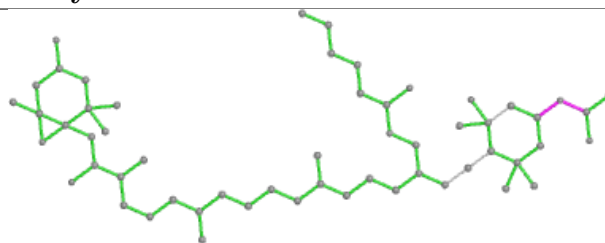


Rings

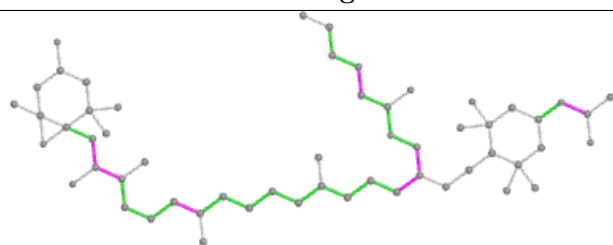
Ligand A1EB1 y 312



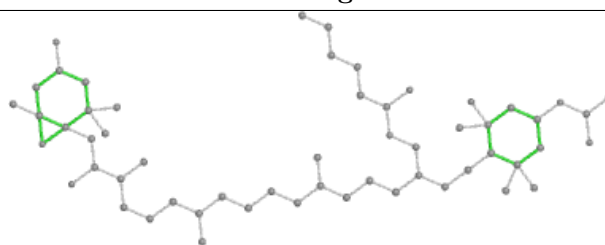
Bond lengths



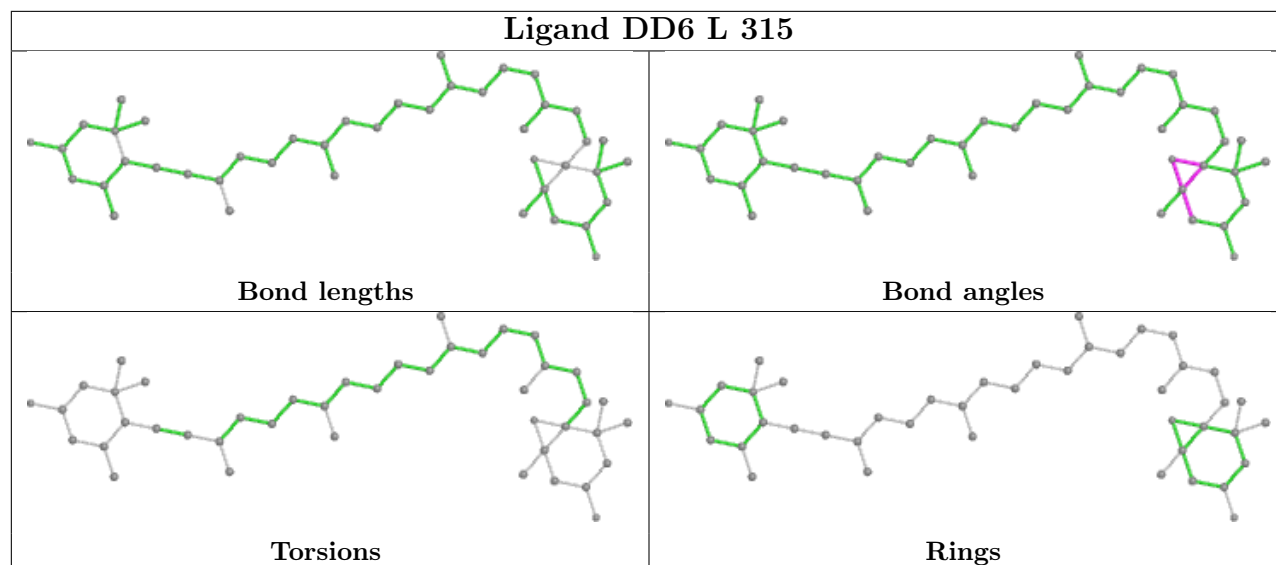
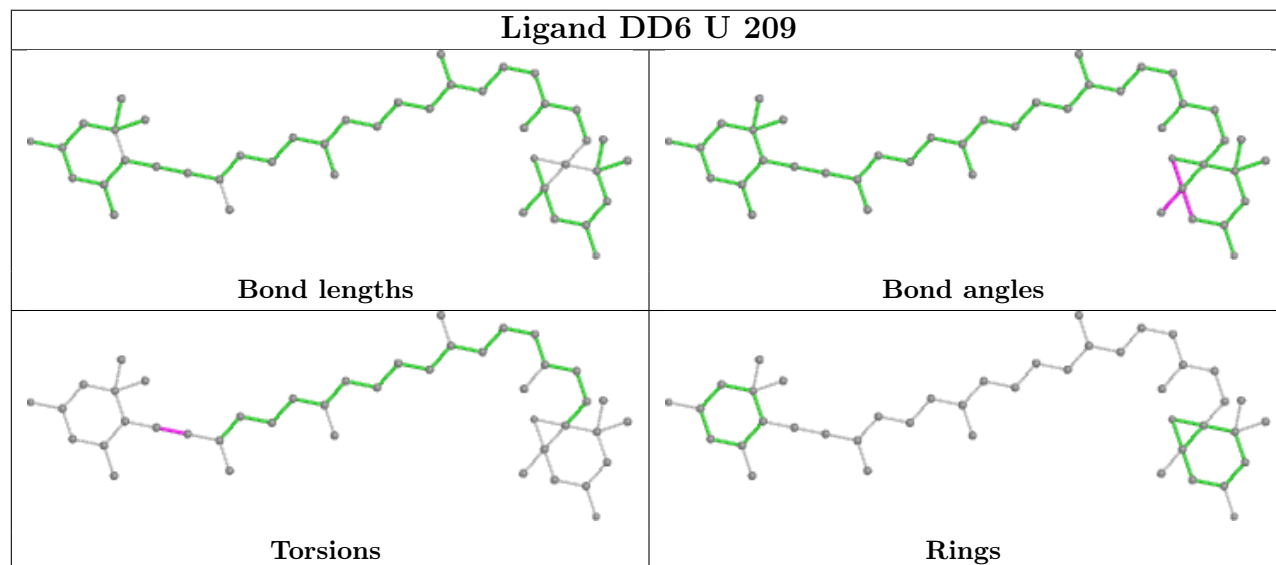
Bond angles



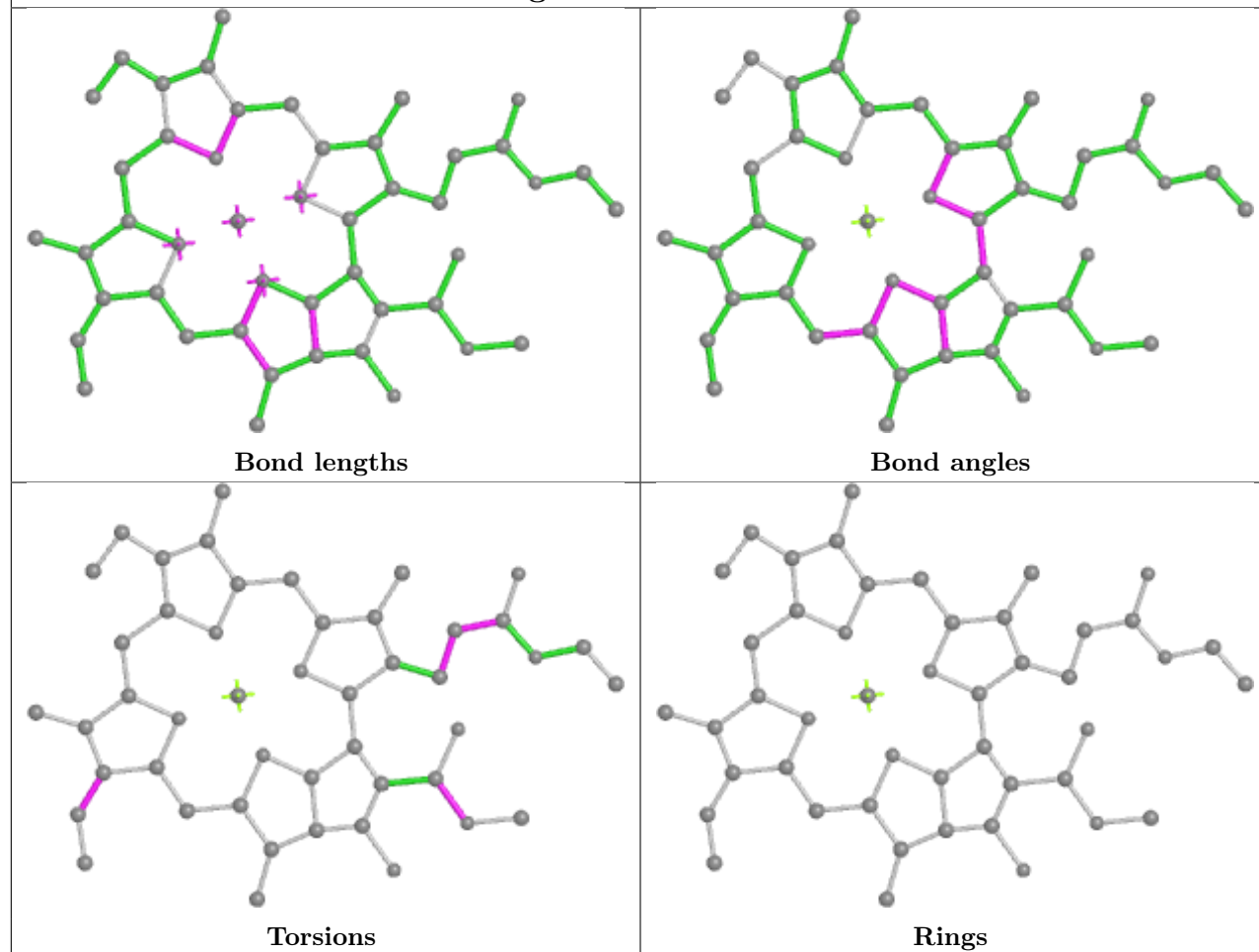
Torsions



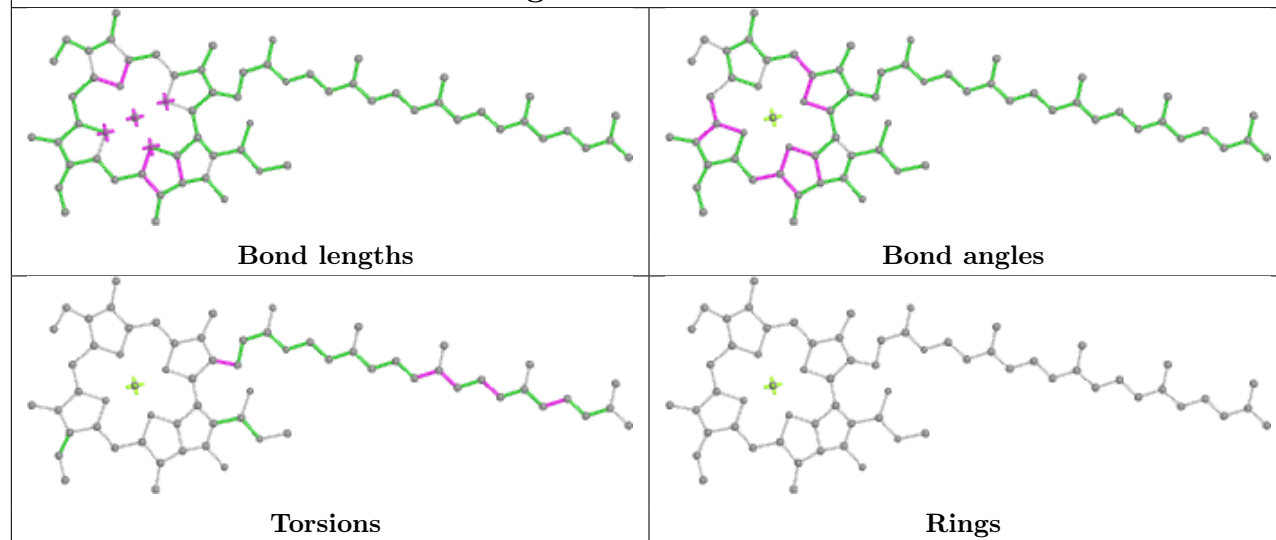
Rings

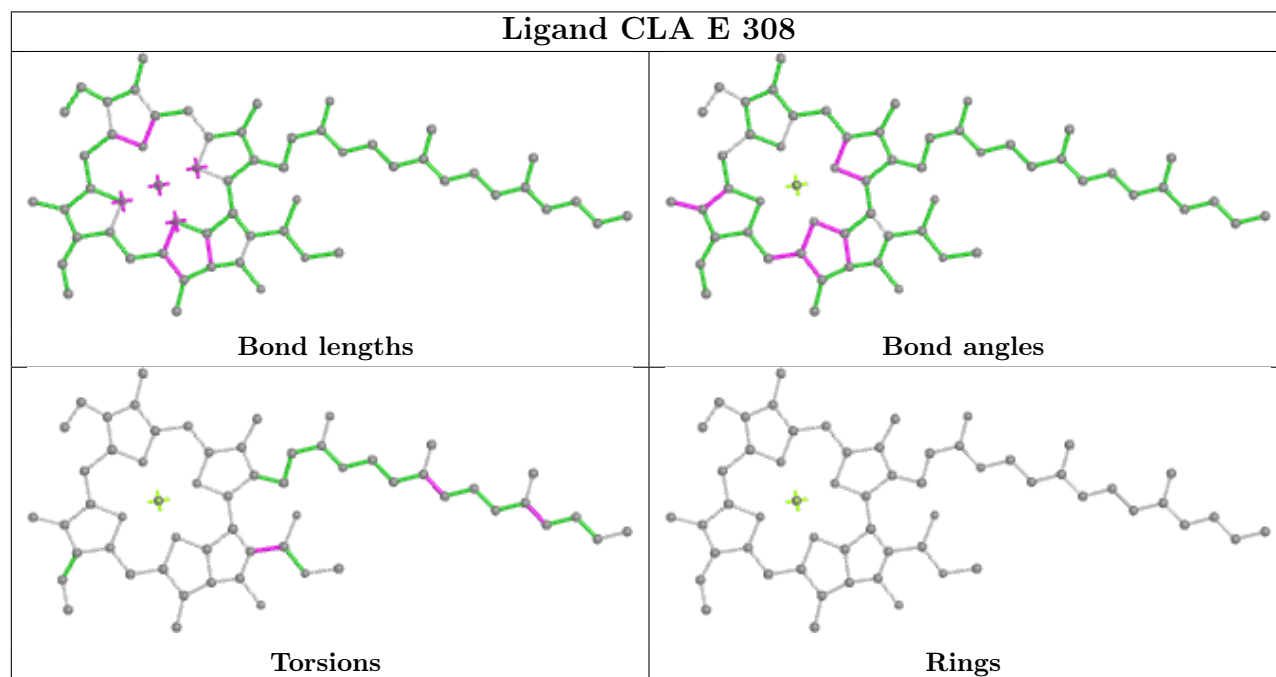
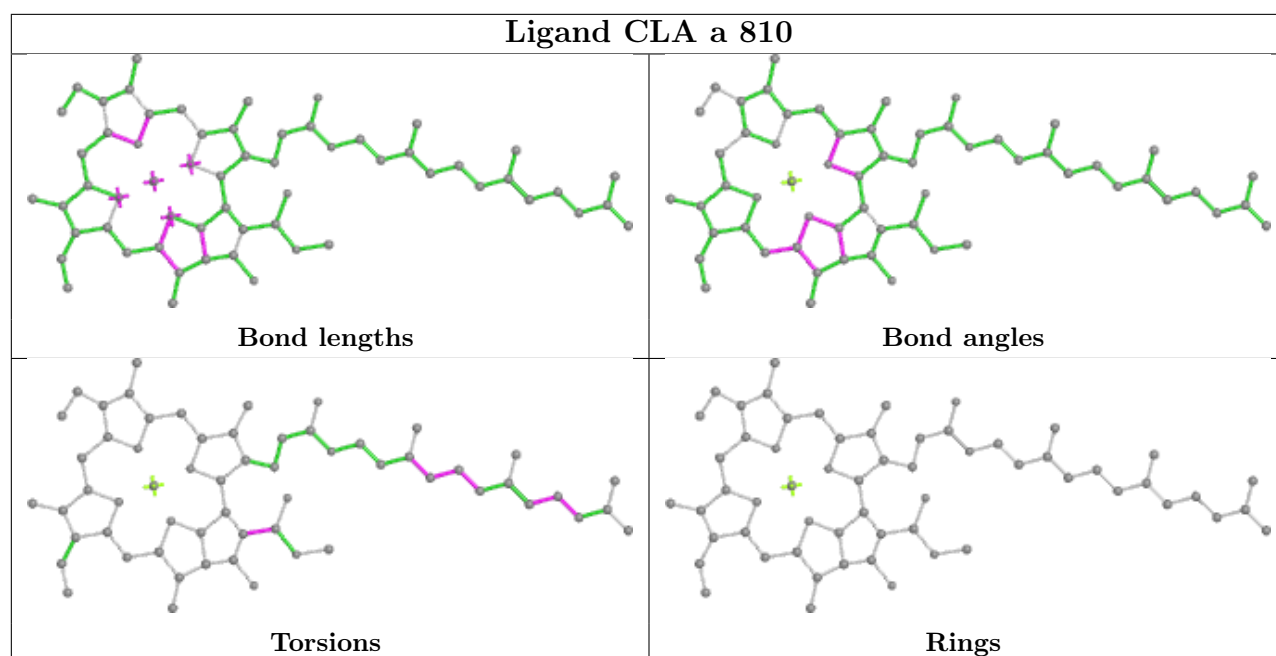
Ligand DD6 L 315**Ligand DD6 U 209**

Ligand CLA J 302

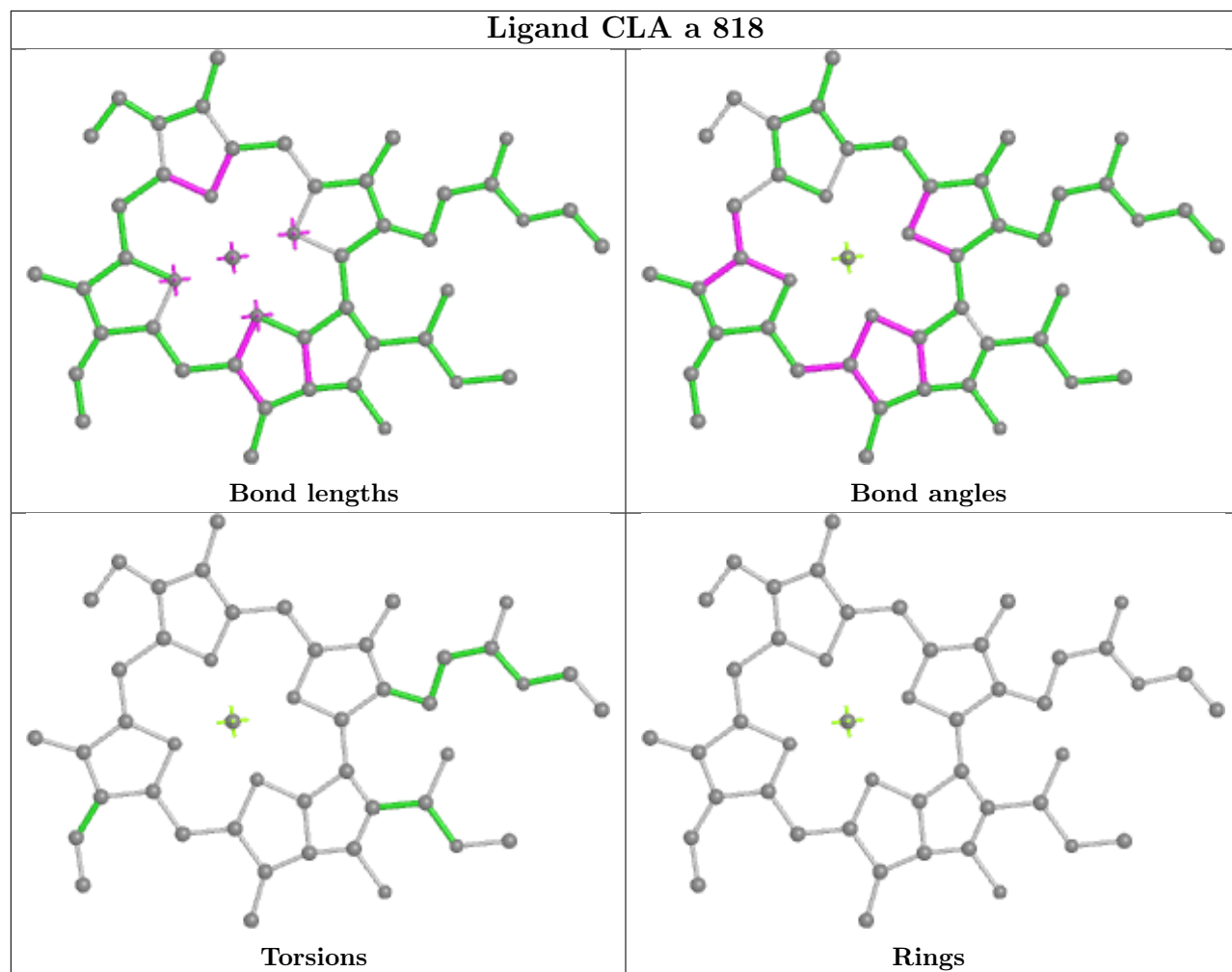


Ligand CLA W 305

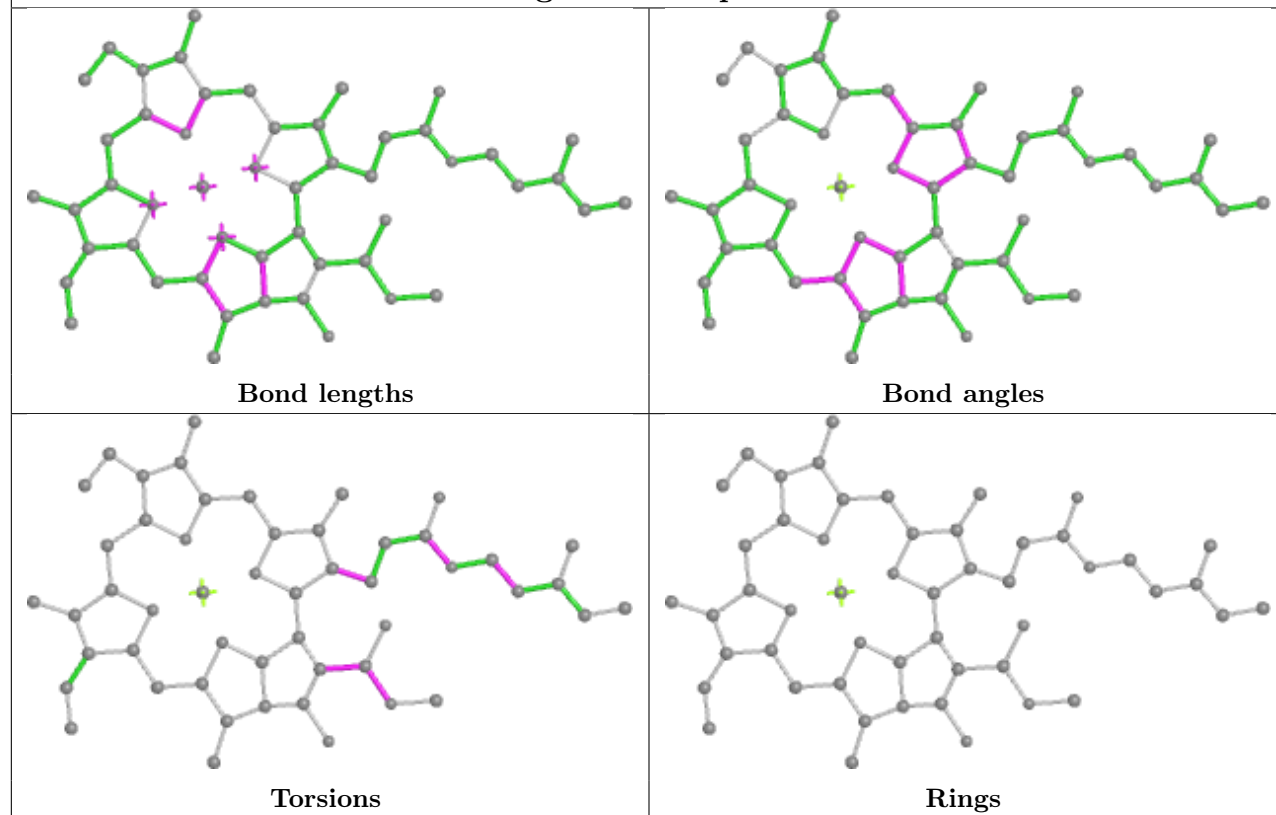




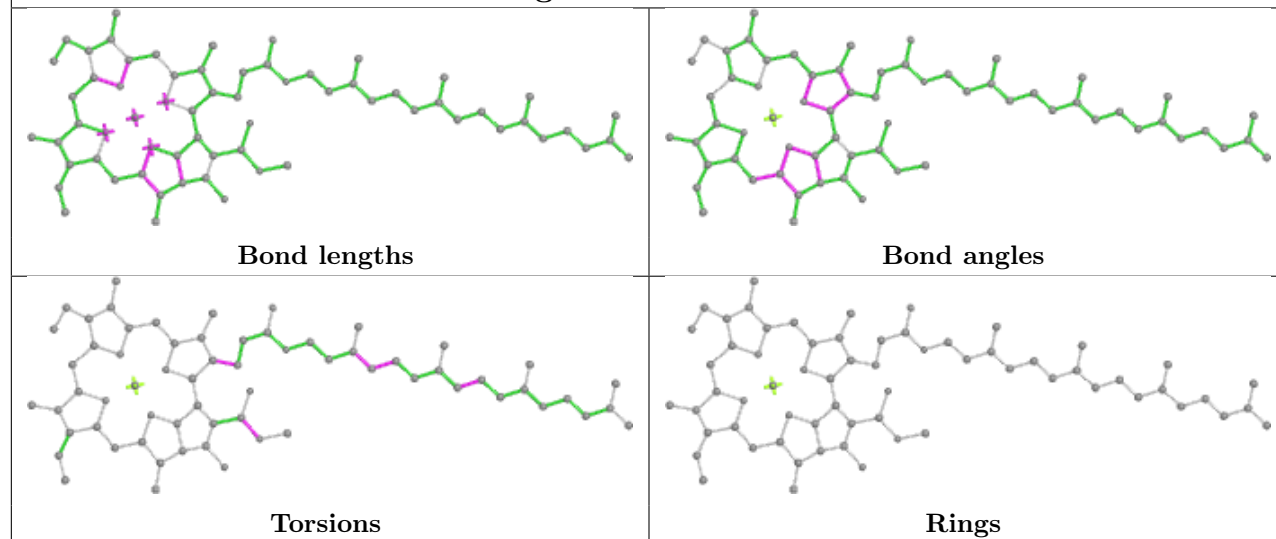
Ligand CLA a 818



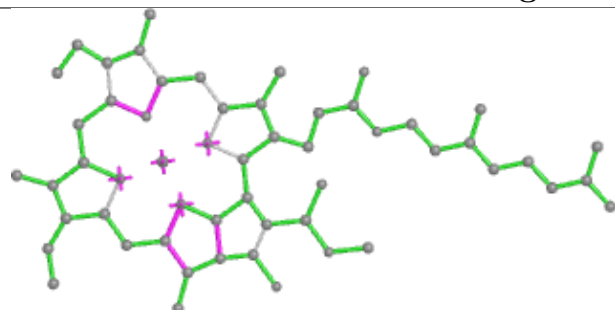
Ligand CLA q 310



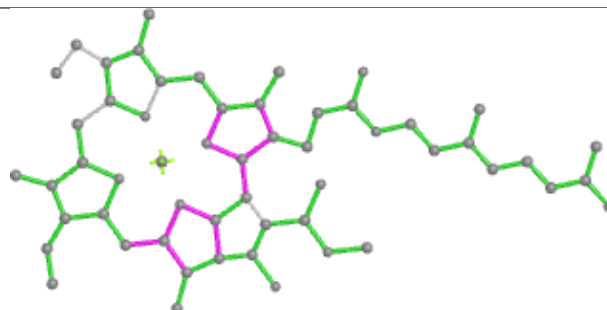
Ligand CLA b 832



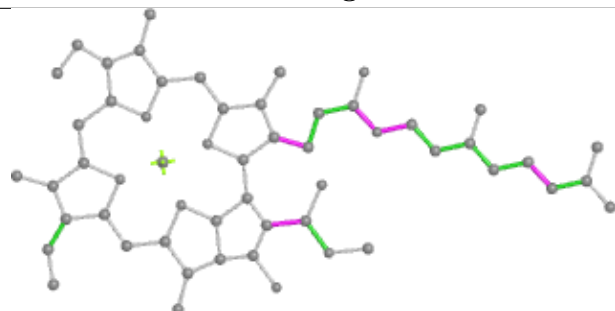
Ligand CLA u 307



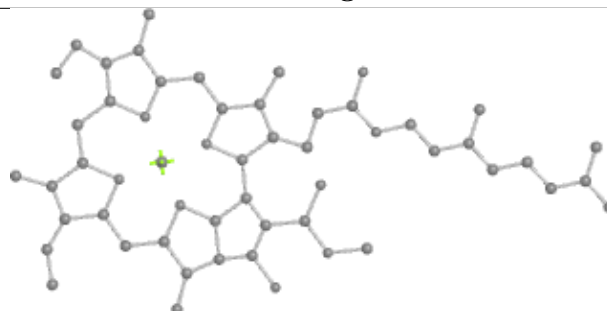
Bond lengths



Bond angles

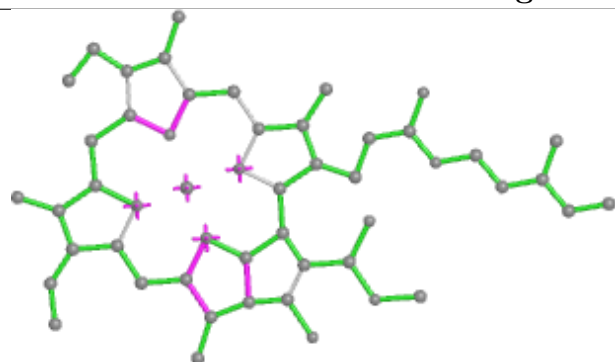


Torsions

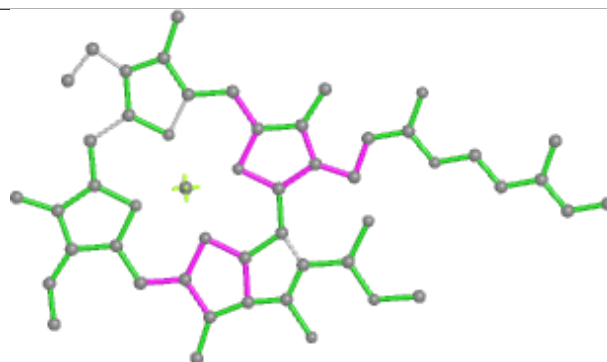


Rings

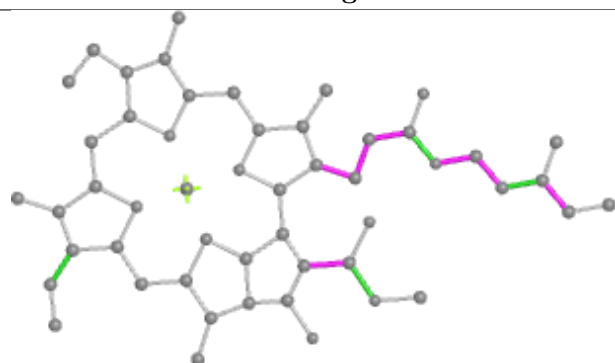
Ligand CLA R 304



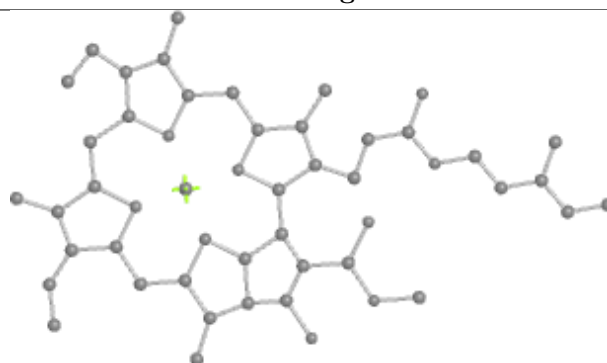
Bond lengths



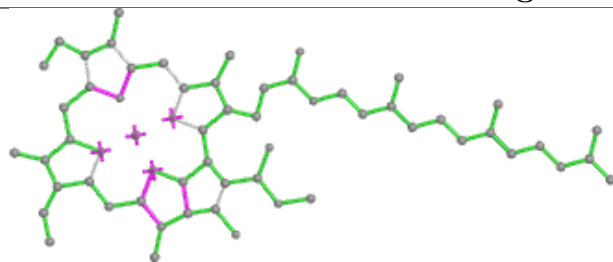
Bond angles



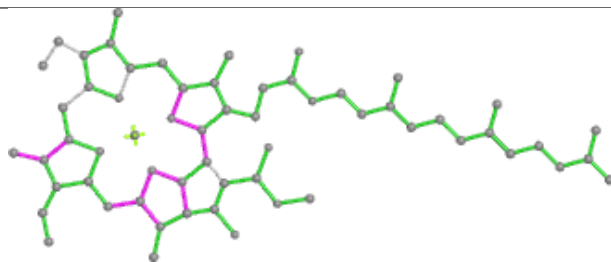
Torsions



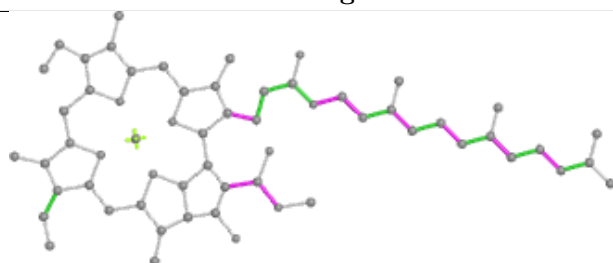
Rings

Ligand CLA Z 306

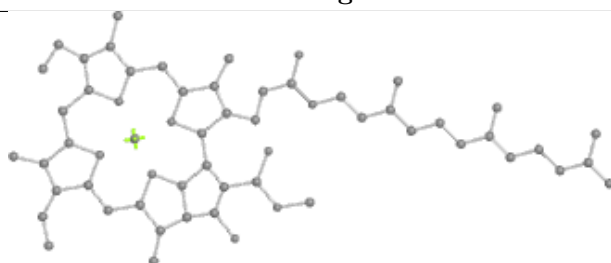
Bond lengths



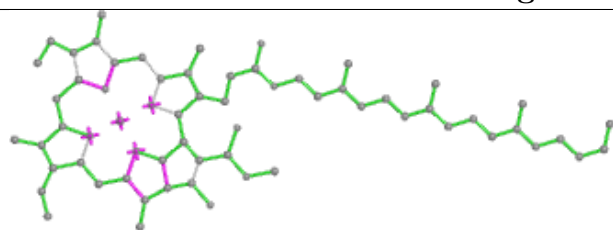
Bond angles



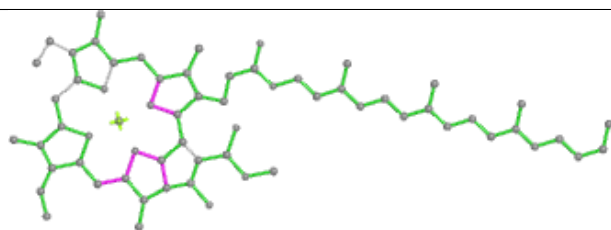
Torsions



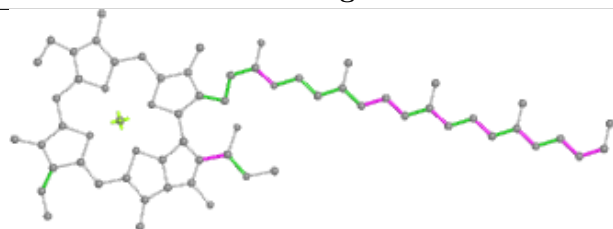
Rings

Ligand CLA b 819

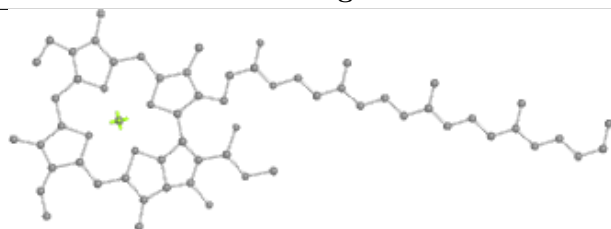
Bond lengths



Bond angles

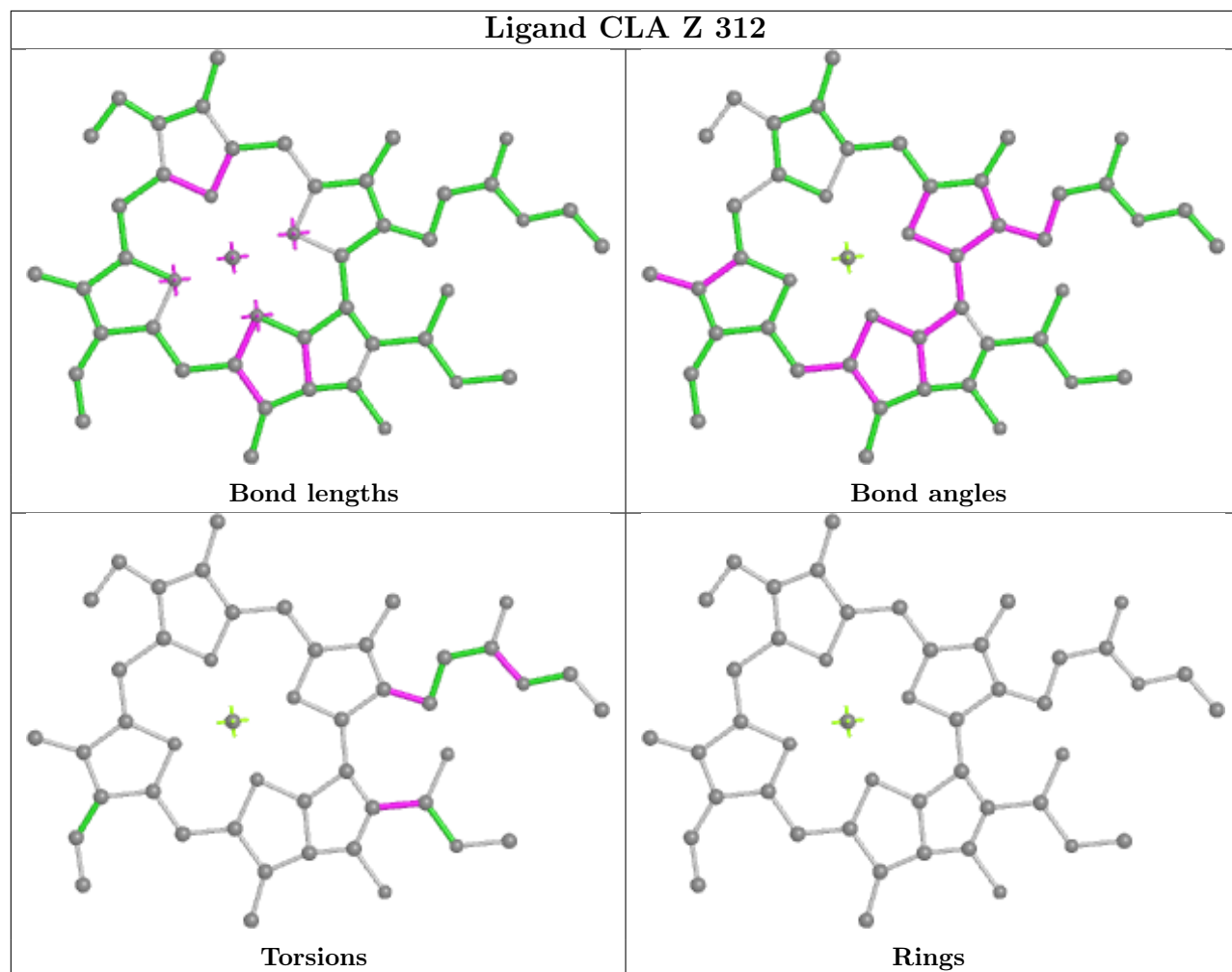


Torsions

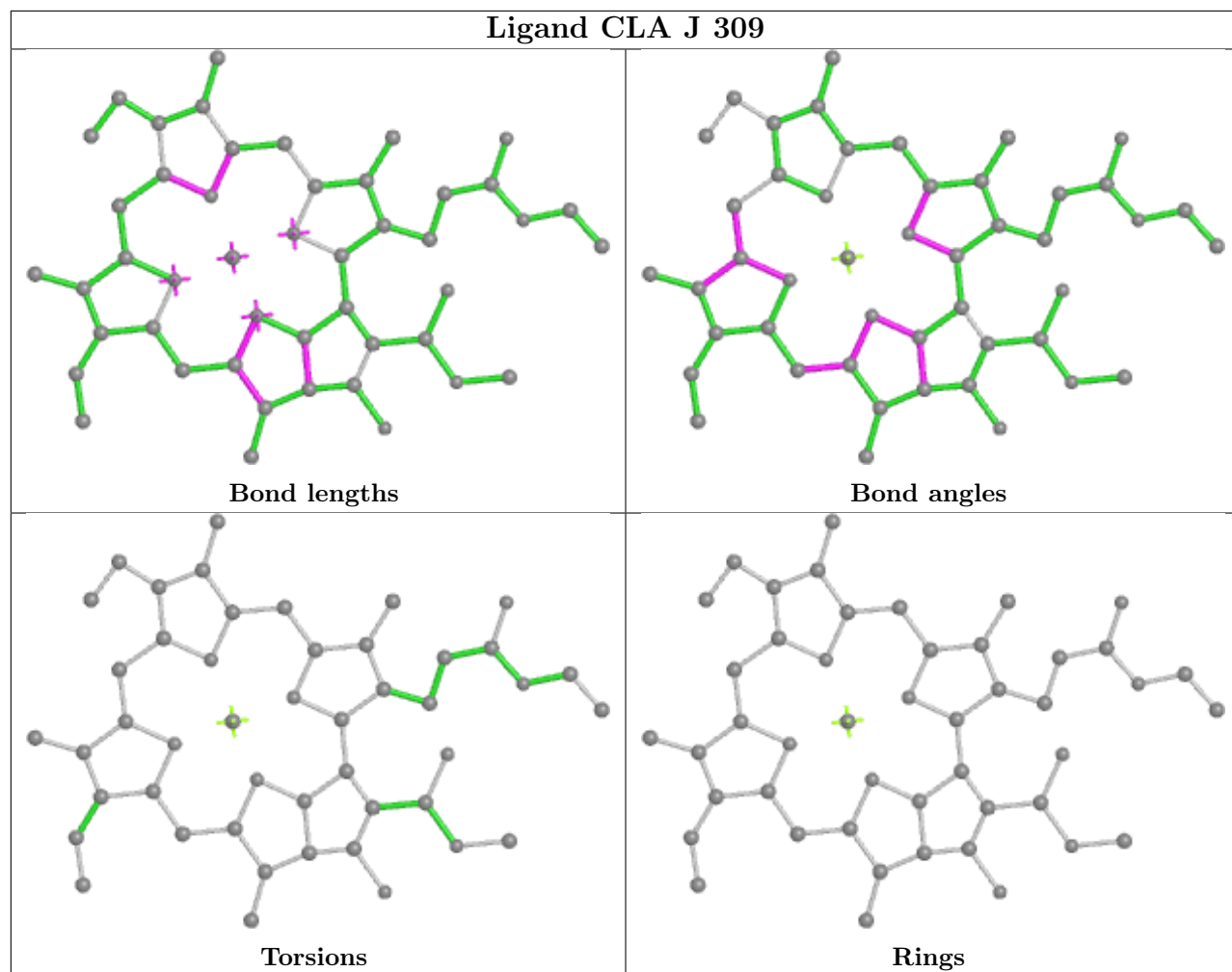


Rings

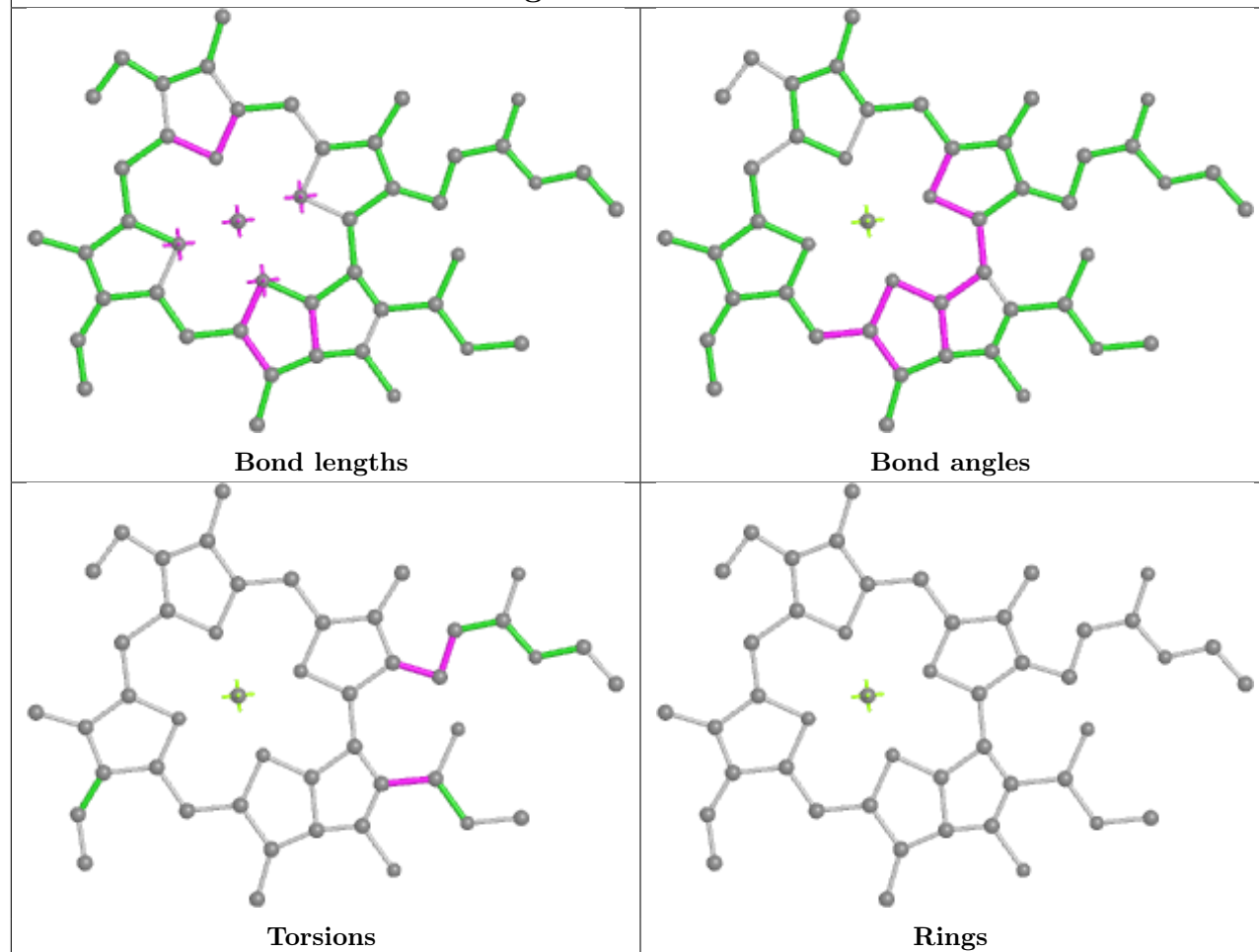
Ligand CLA Z 312



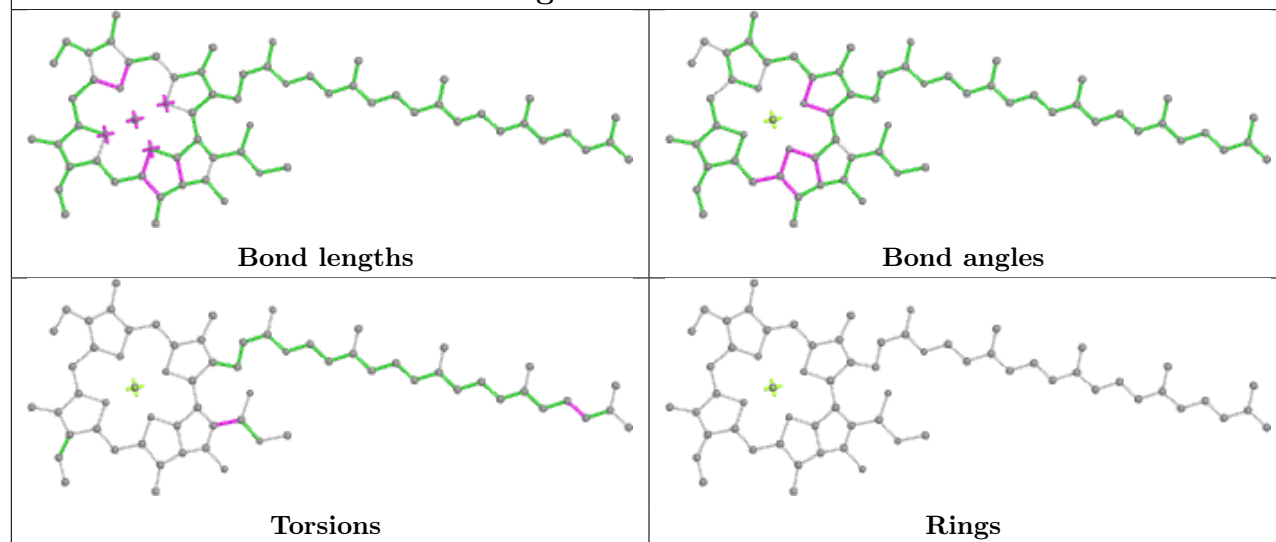
Ligand CLA J 309



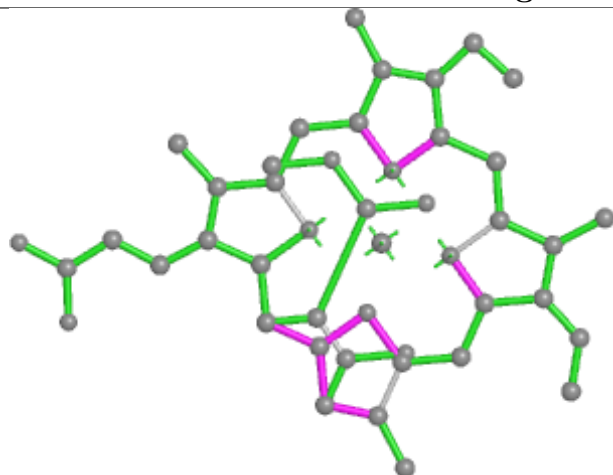
Ligand CLA X 312



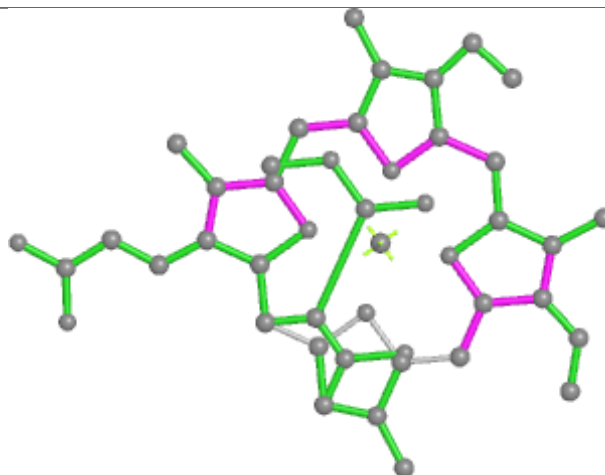
Ligand CLA a 835



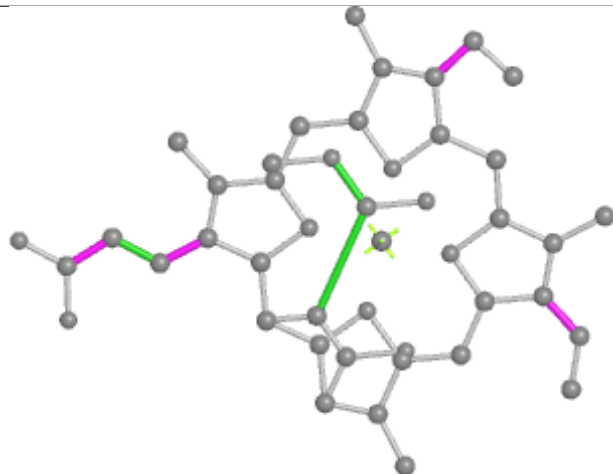
Ligand KC2 O 308



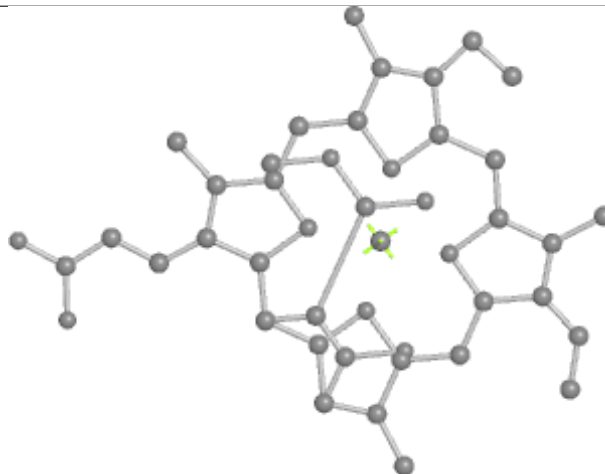
Bond lengths



Bond angles

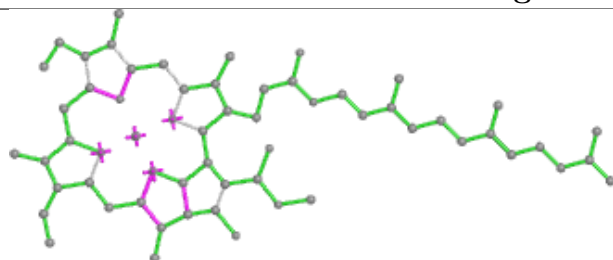


Torsions

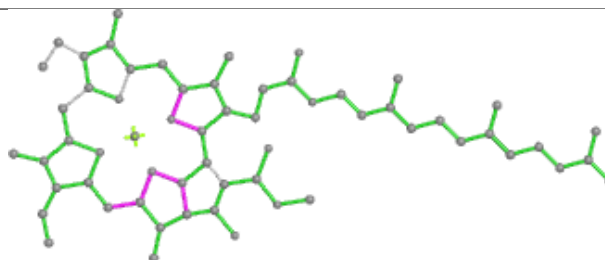


Rings

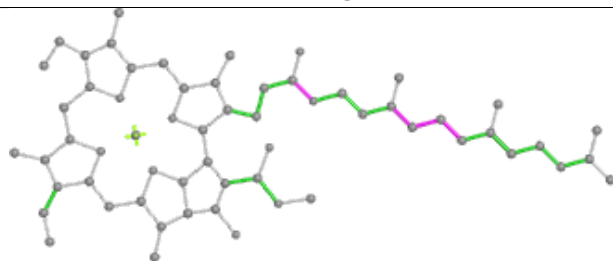
Ligand CLA R 305



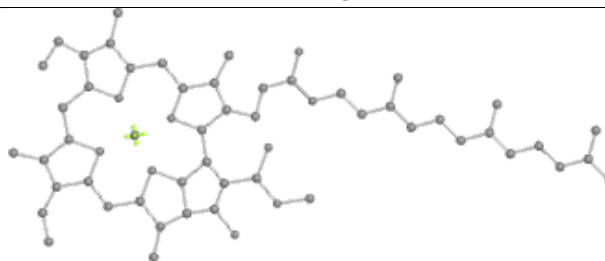
Bond lengths



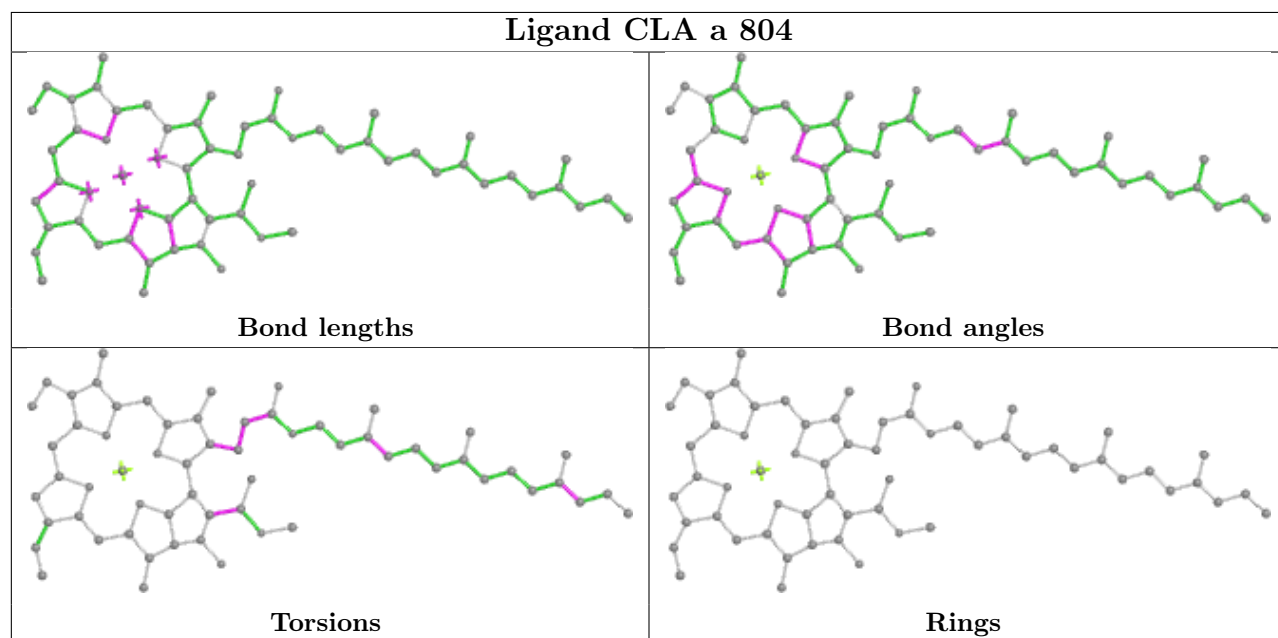
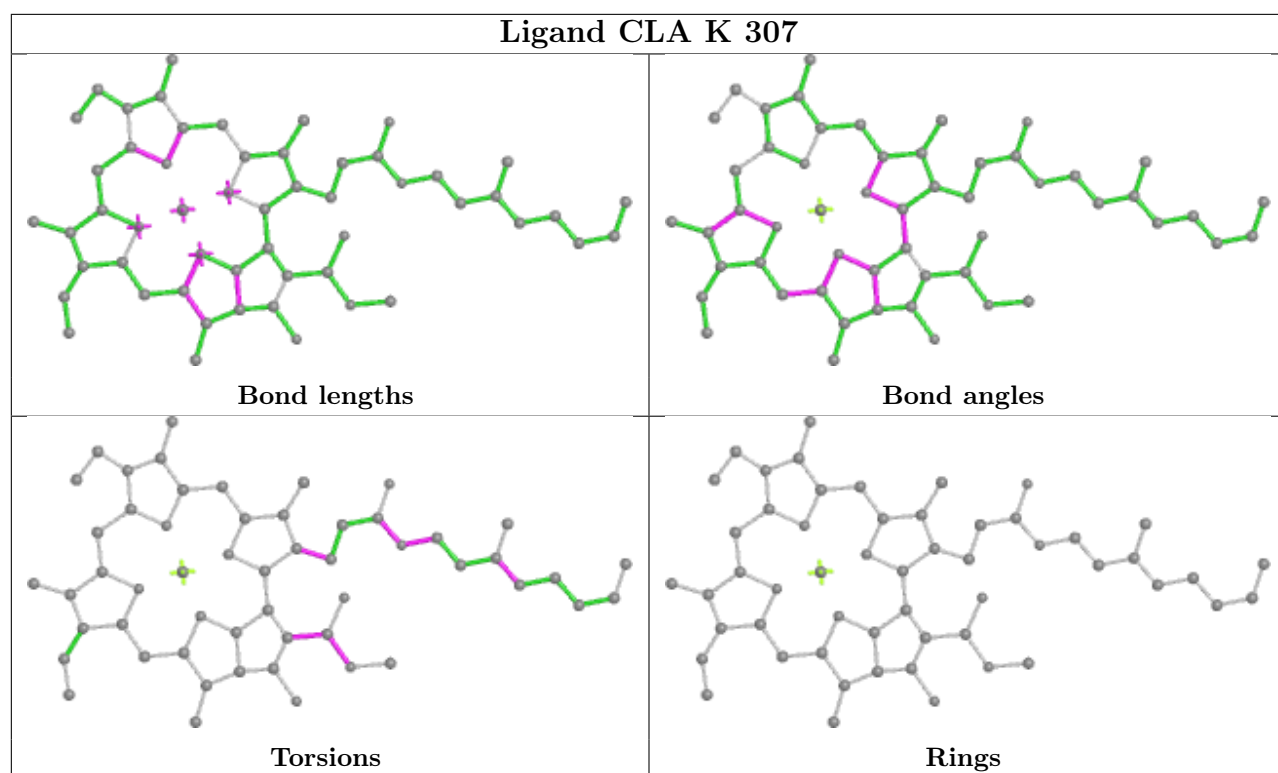
Bond angles

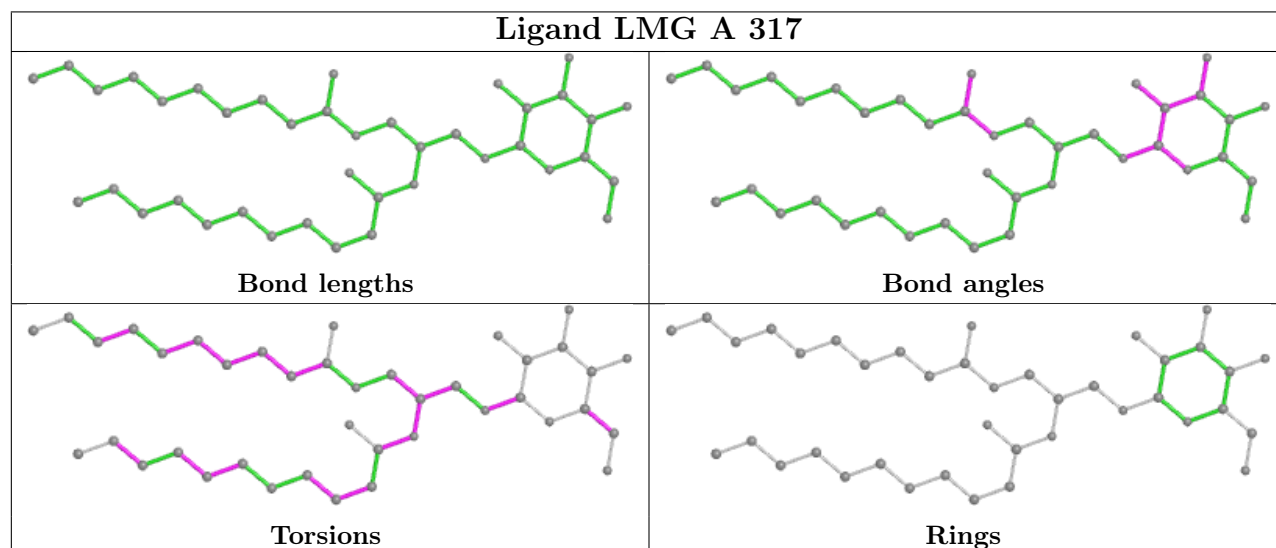
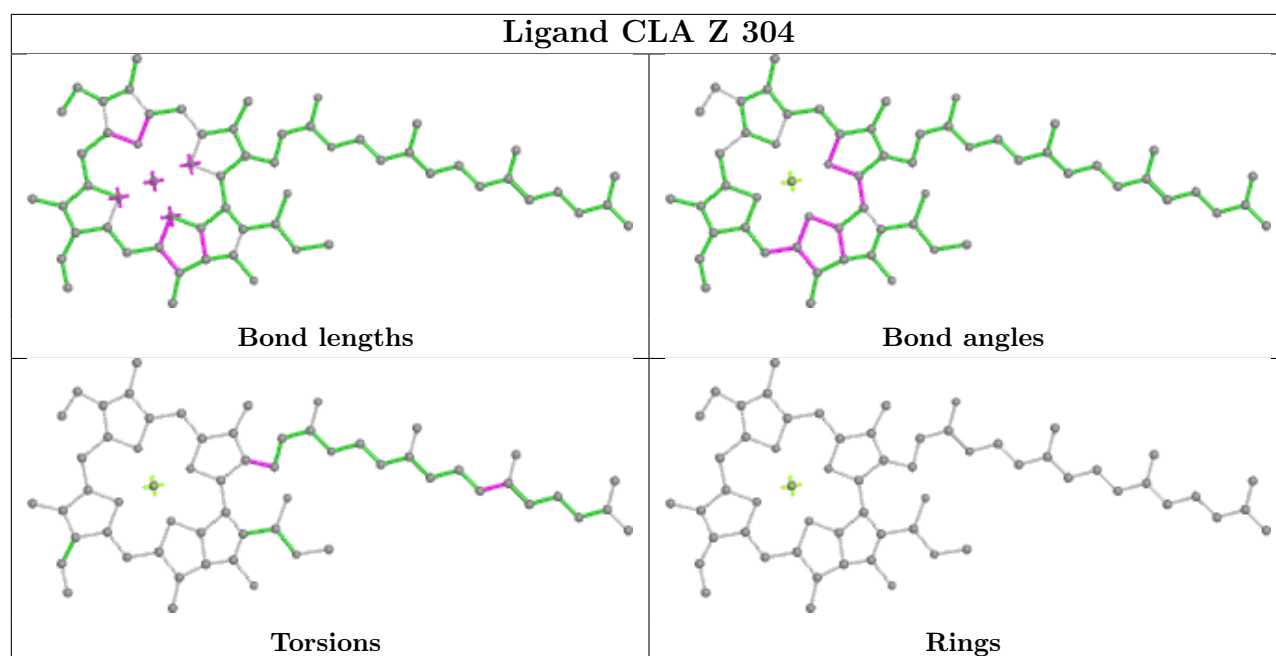


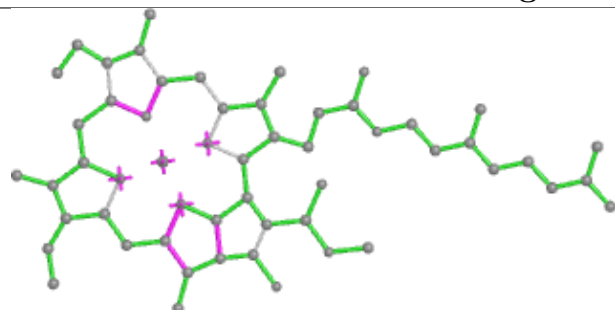
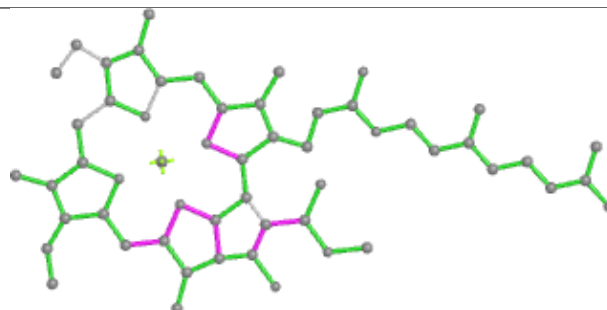
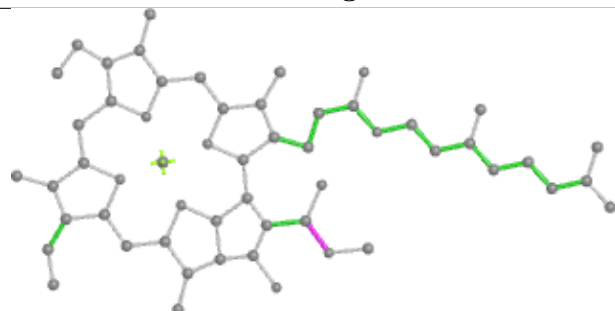
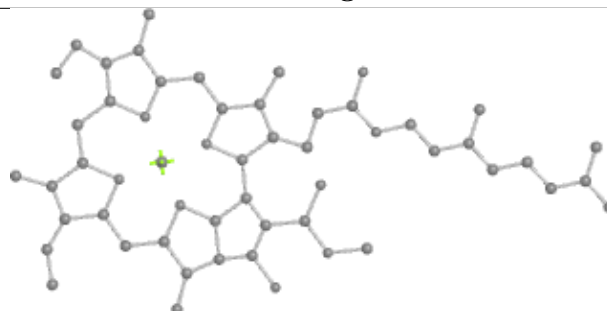
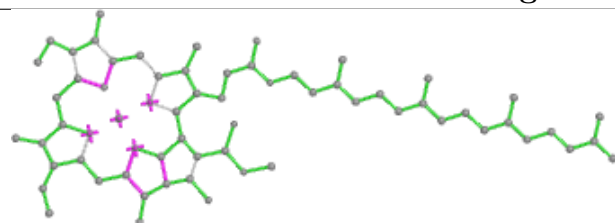
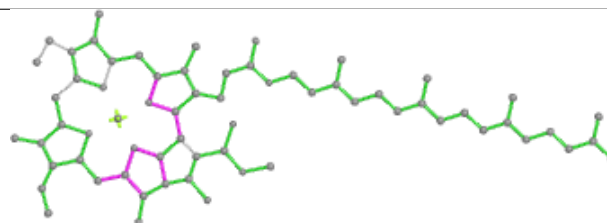
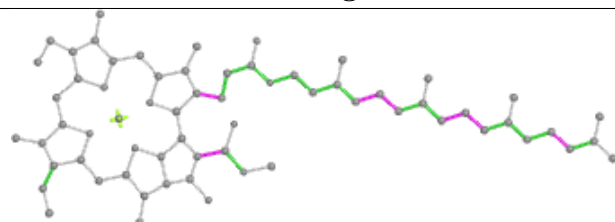
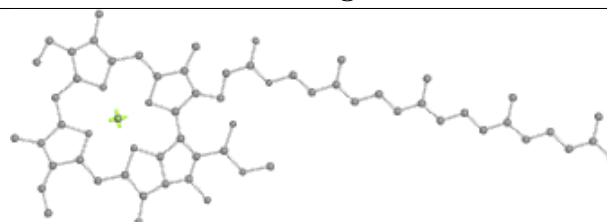
Torsions



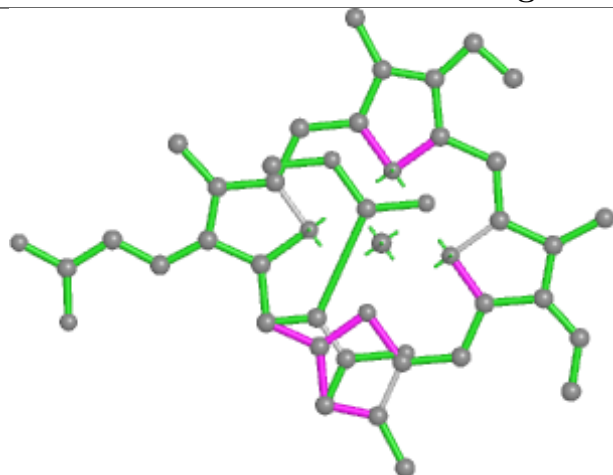
Rings



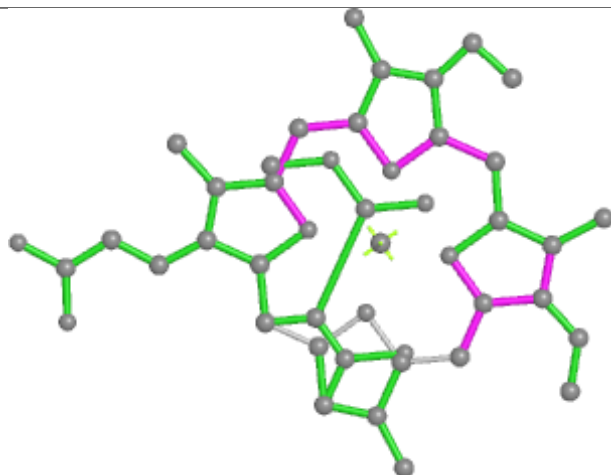


Ligand CLA u 313**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA x 302****Bond lengths****Bond angles****Torsions****Rings**

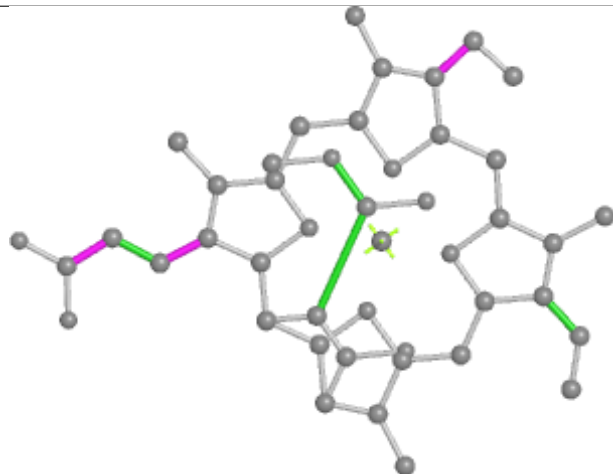
Ligand KC2 F 309



Bond lengths



Bond angles

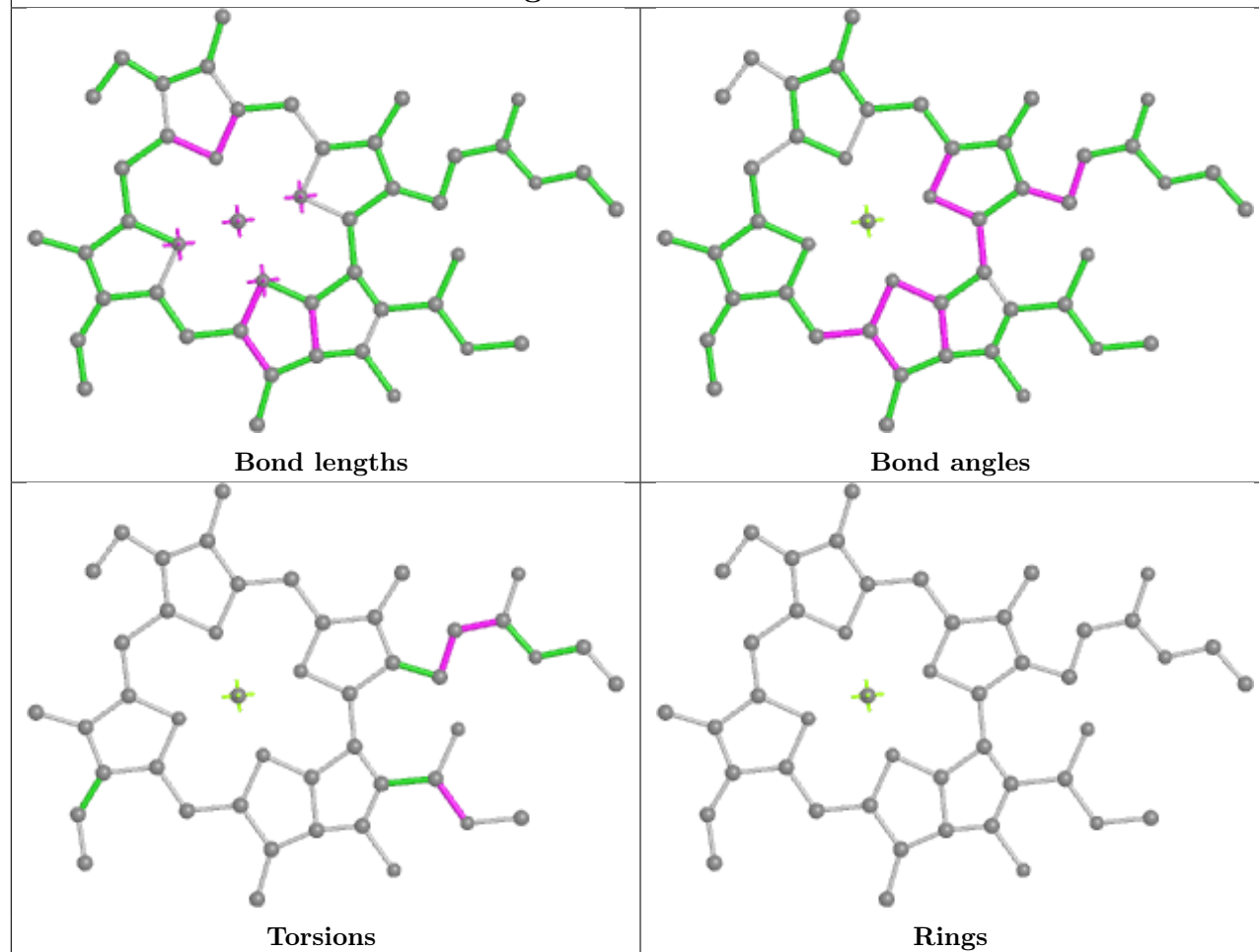


Torsions

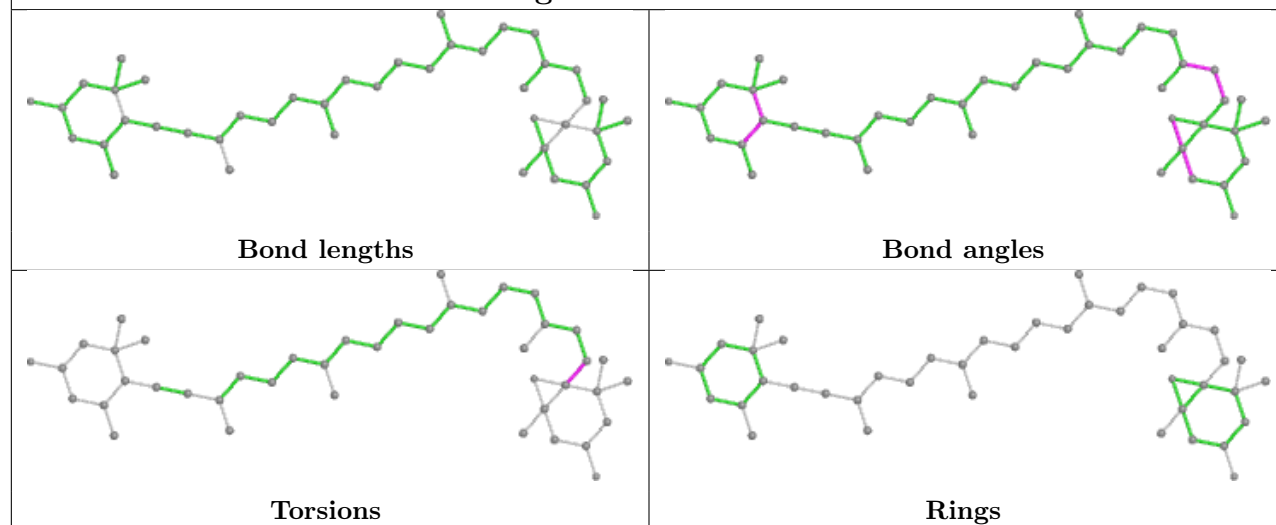


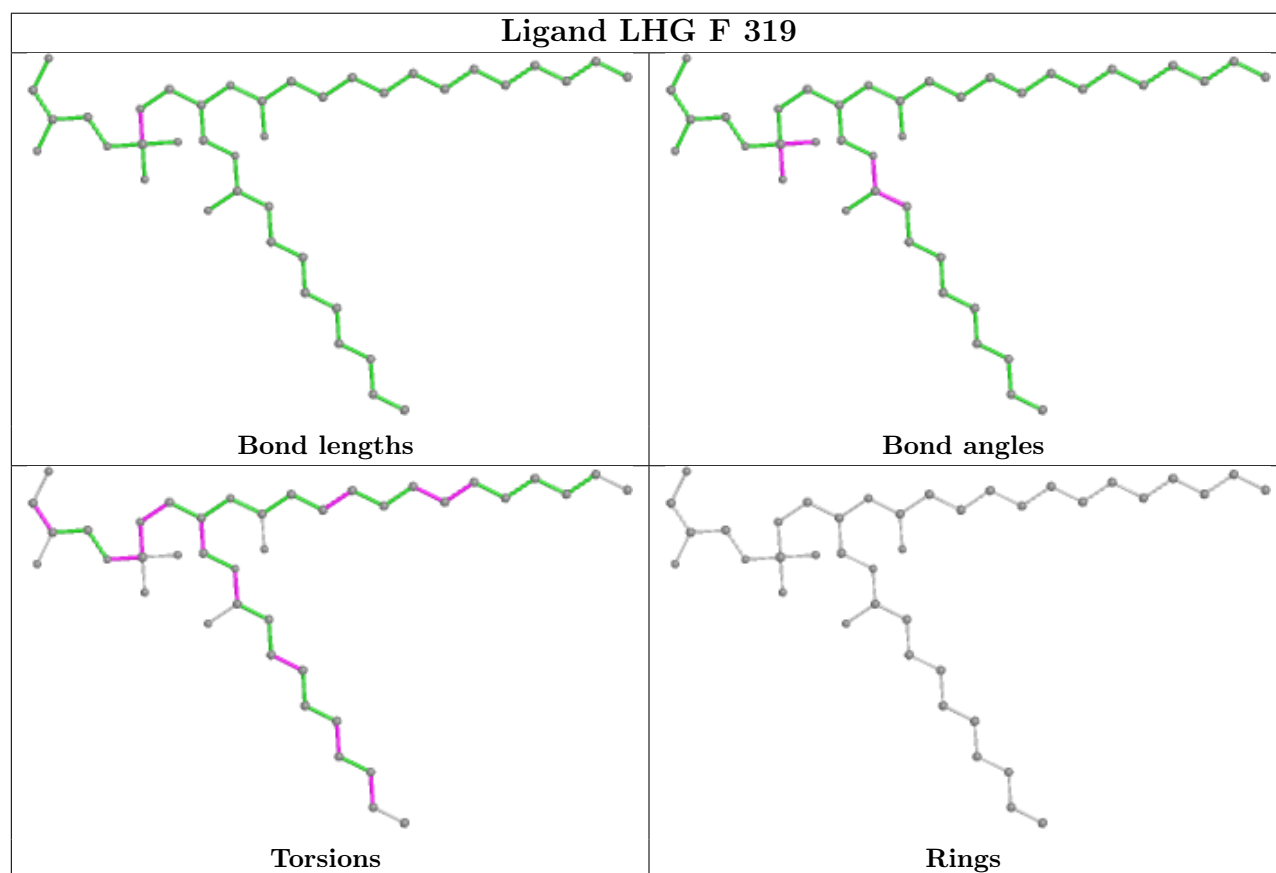
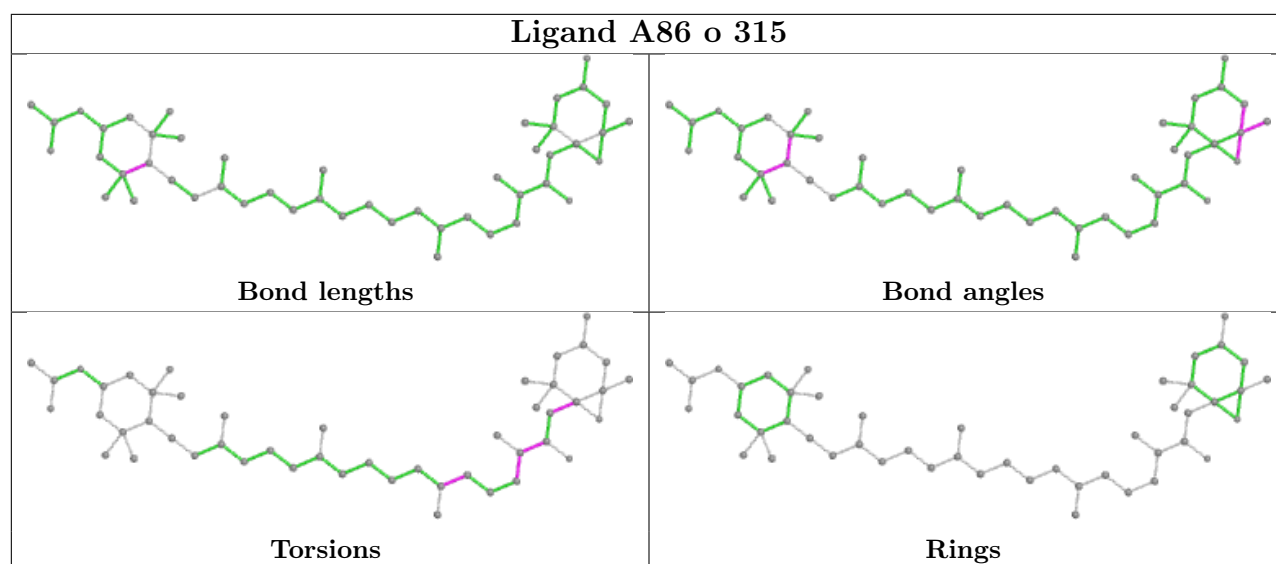
Rings

Ligand CLA H 302

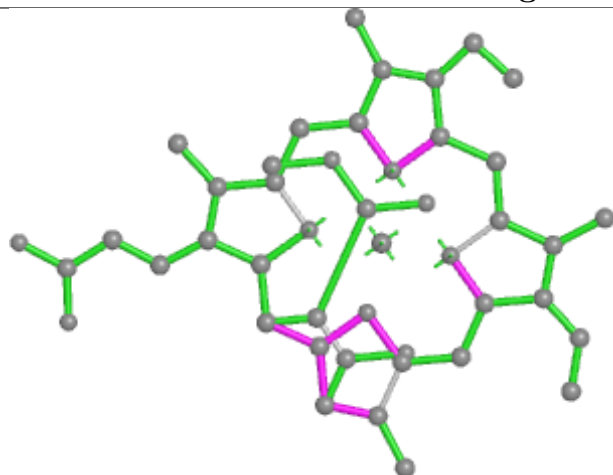


Ligand DD6 Z 318

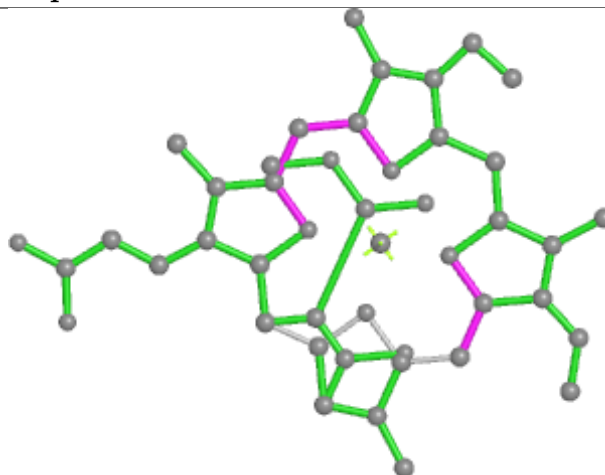




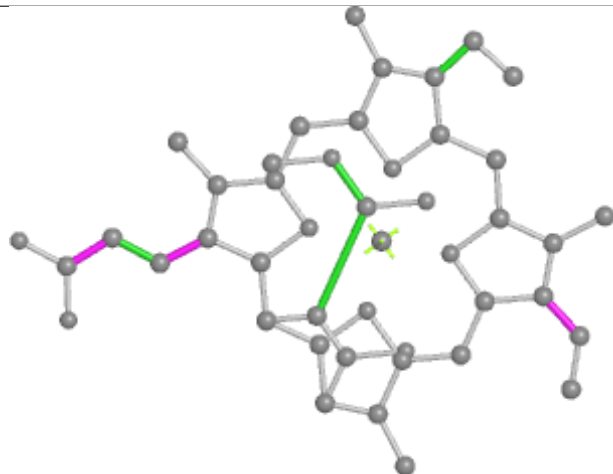
Ligand KC2 p 303



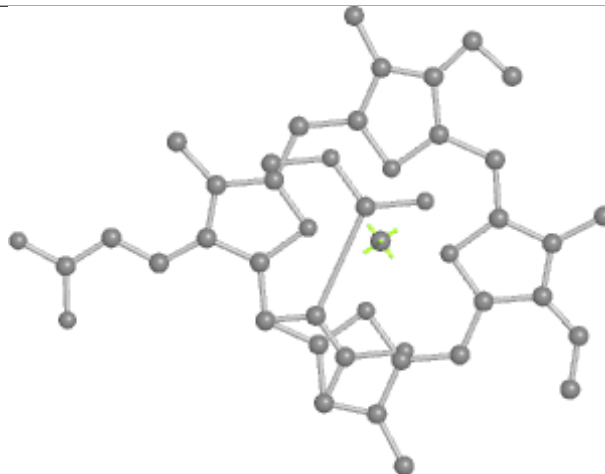
Bond lengths



Bond angles

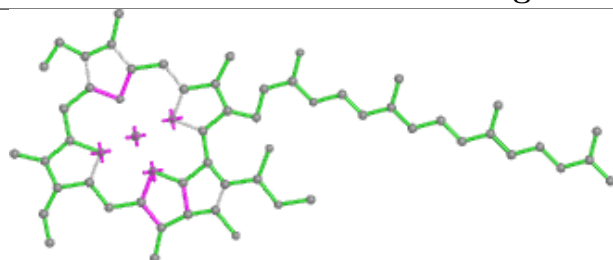


Torsions

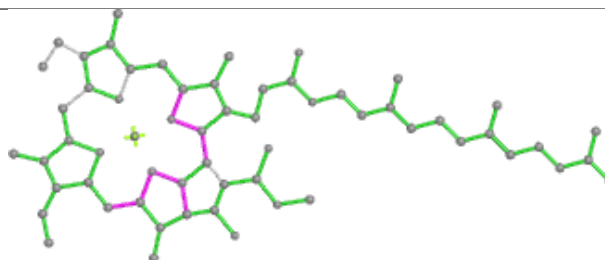


Rings

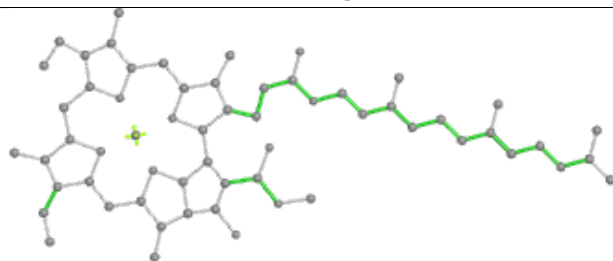
Ligand CLA N 306



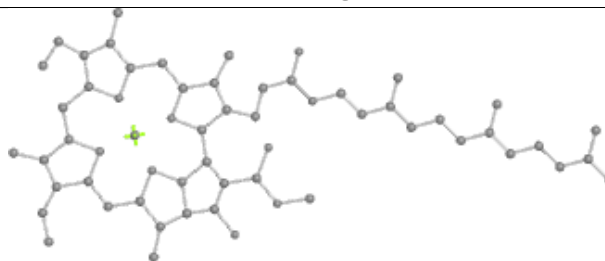
Bond lengths



Bond angles

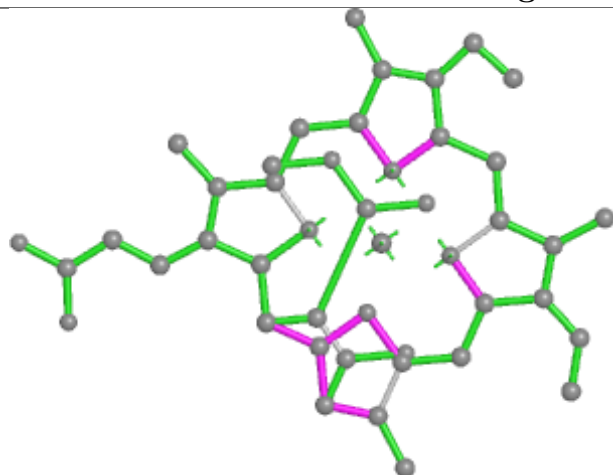


Torsions

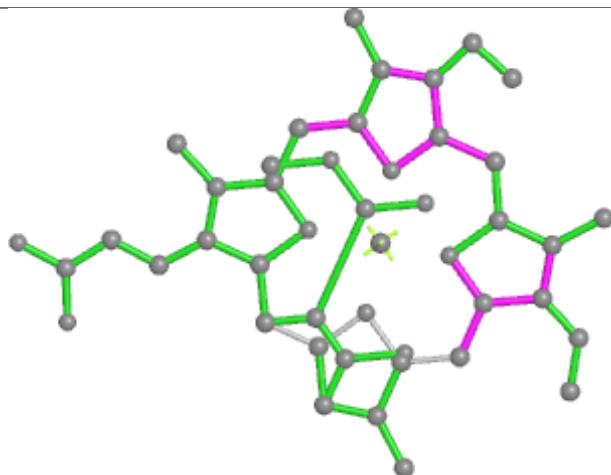


Rings

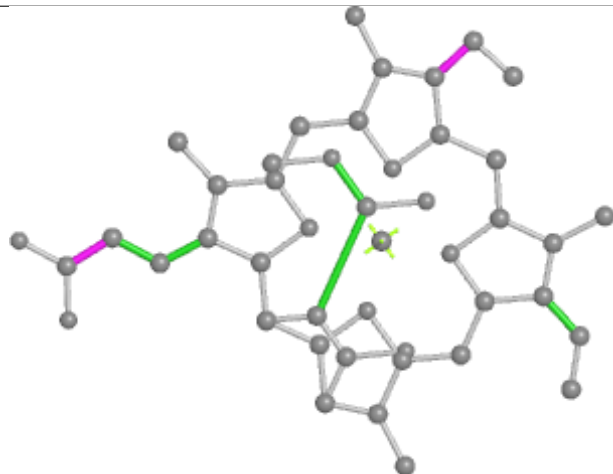
Ligand KC2 Z 308



Bond lengths



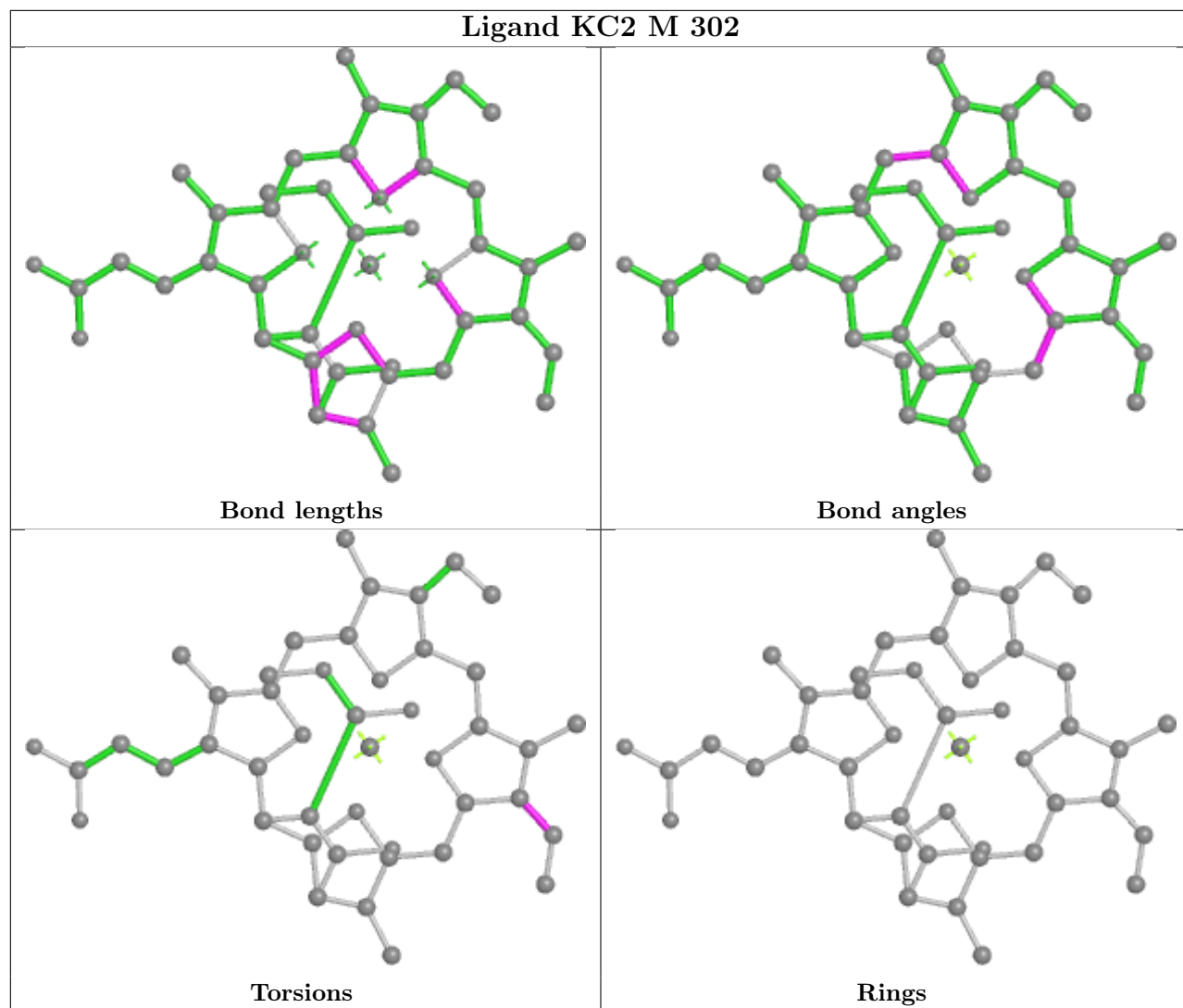
Bond angles



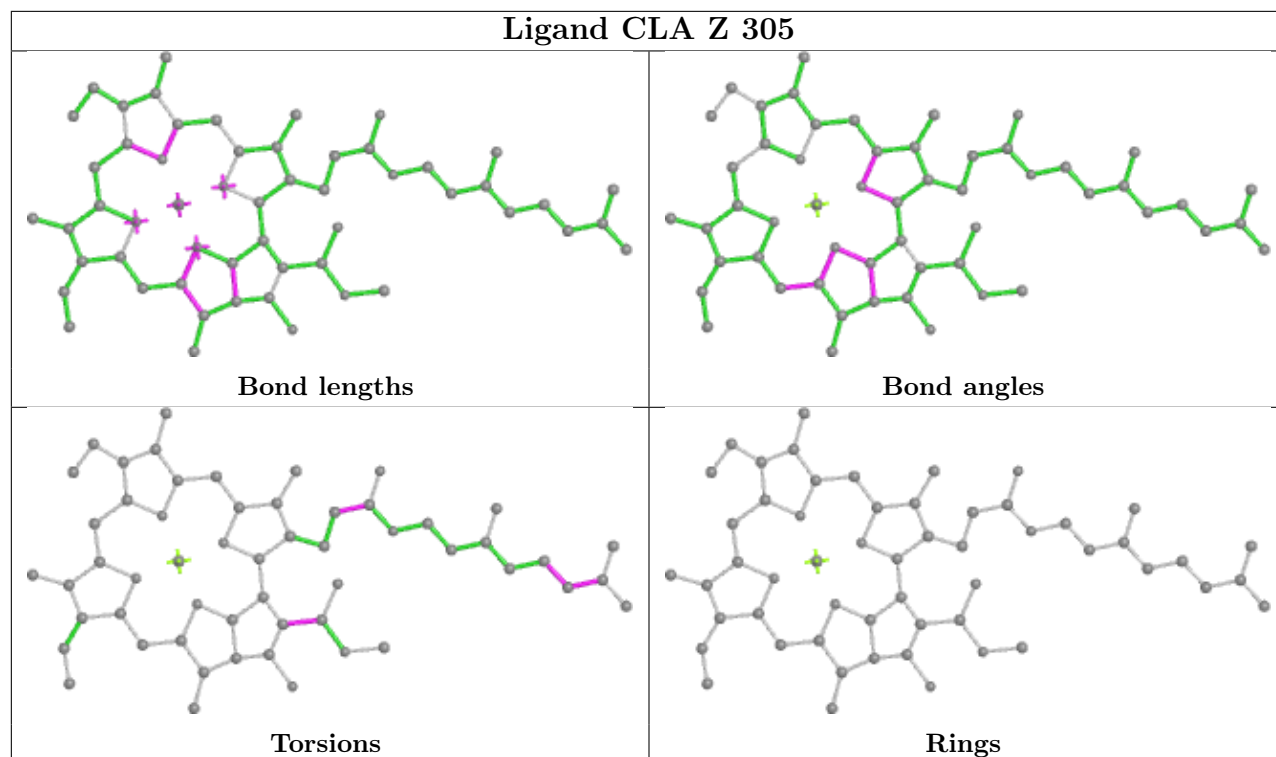
Torsions



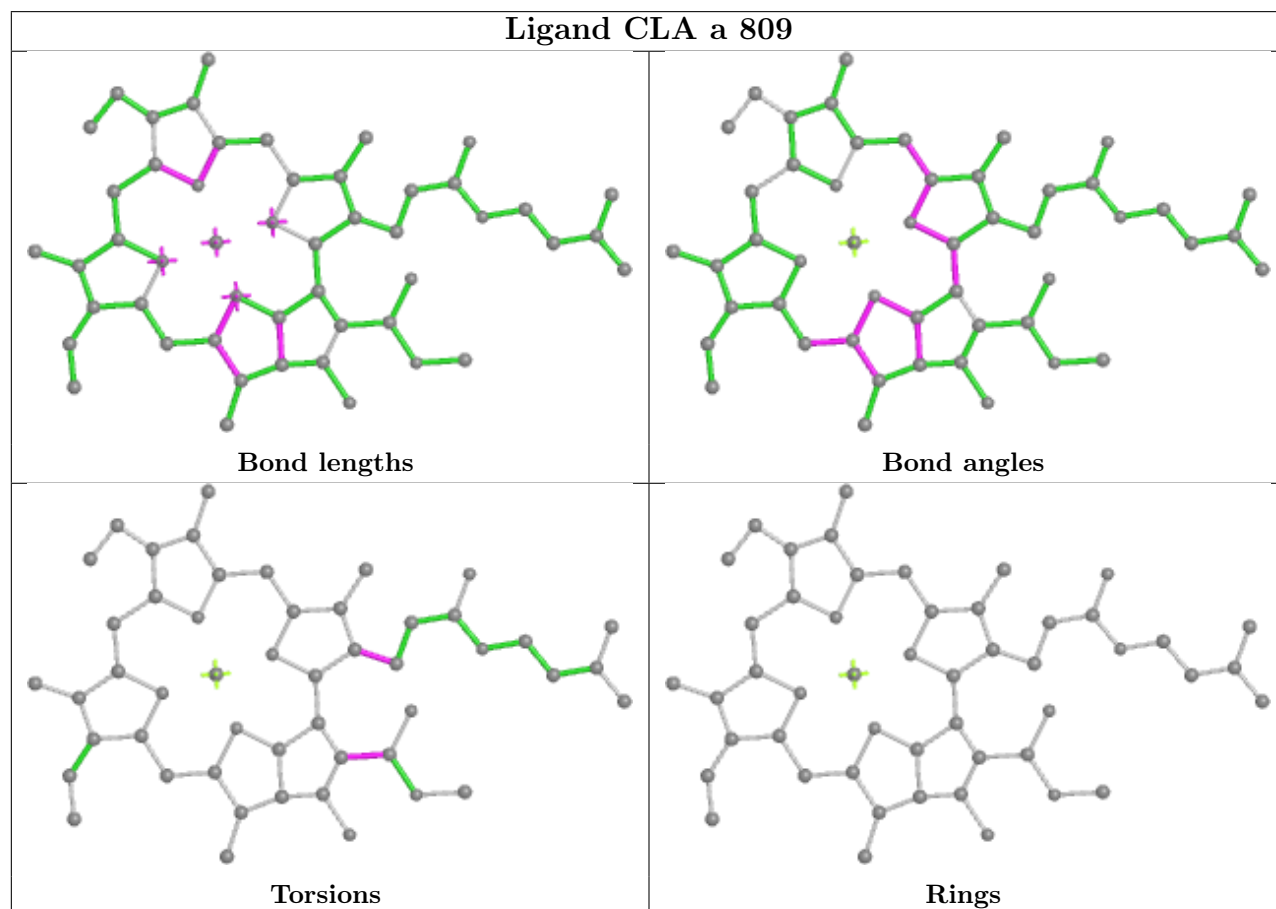
Rings

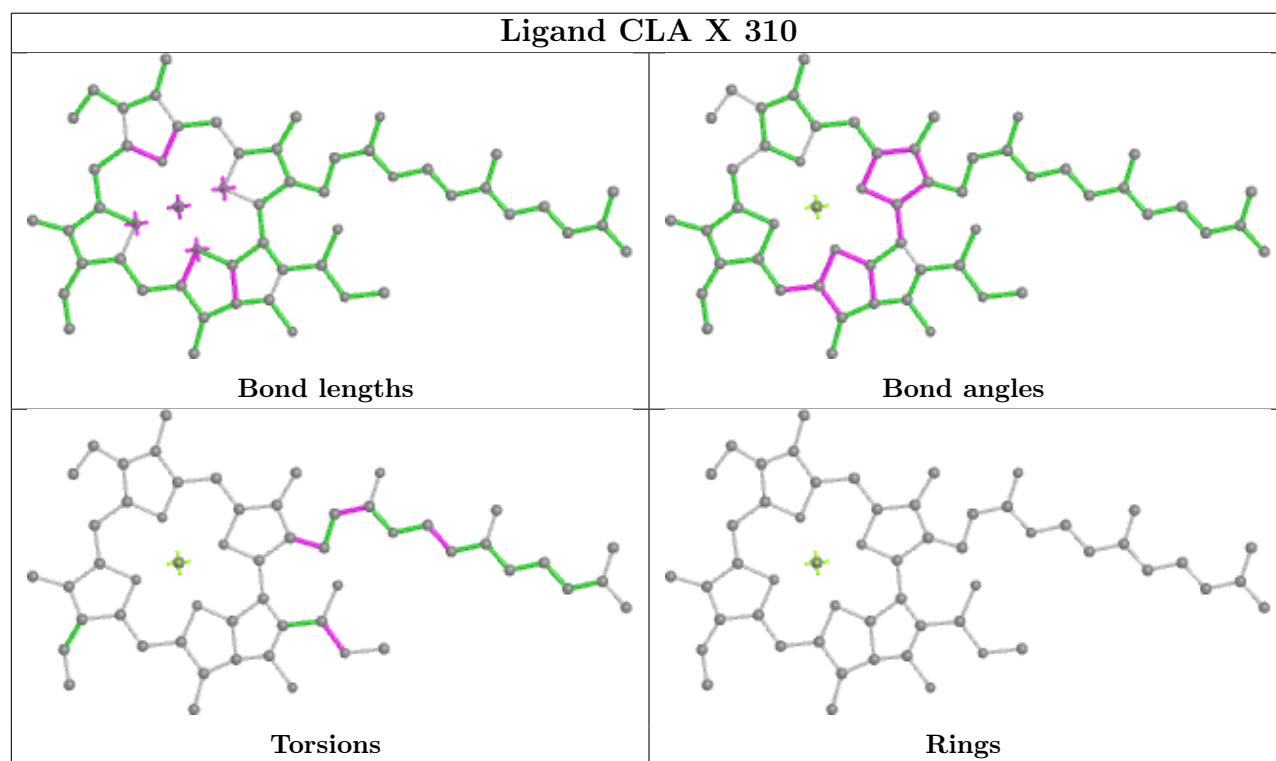
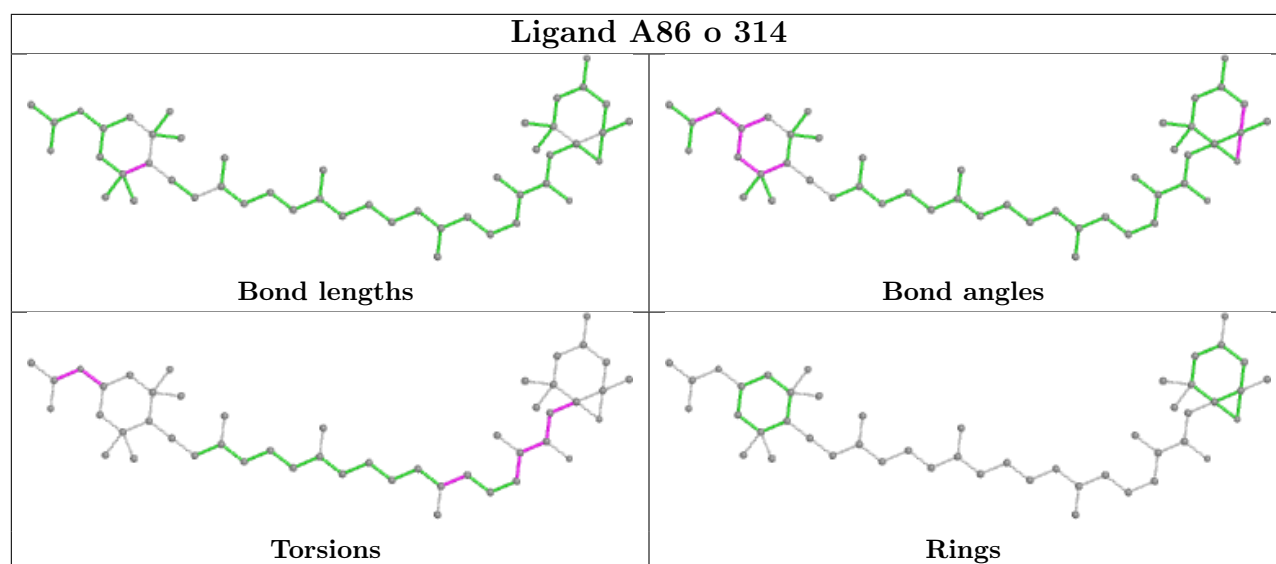


Ligand CLA Z 305

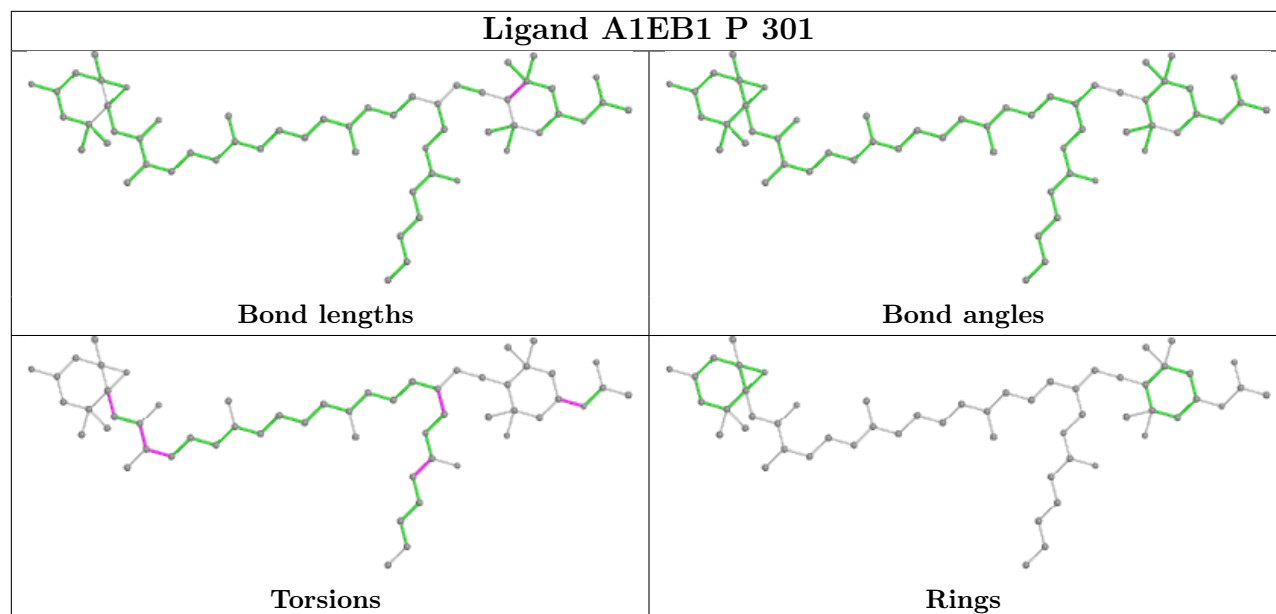


Ligand CLA a 809

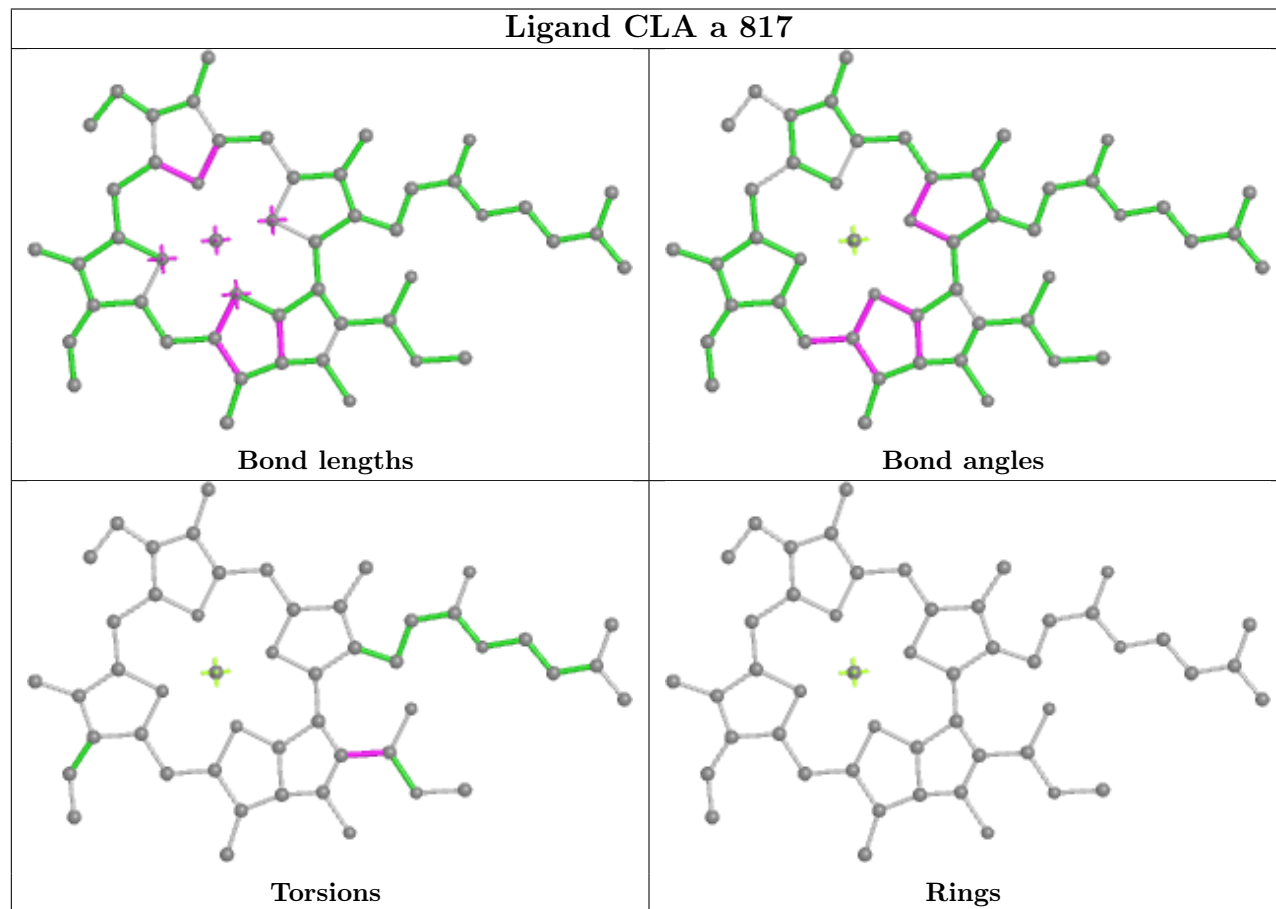




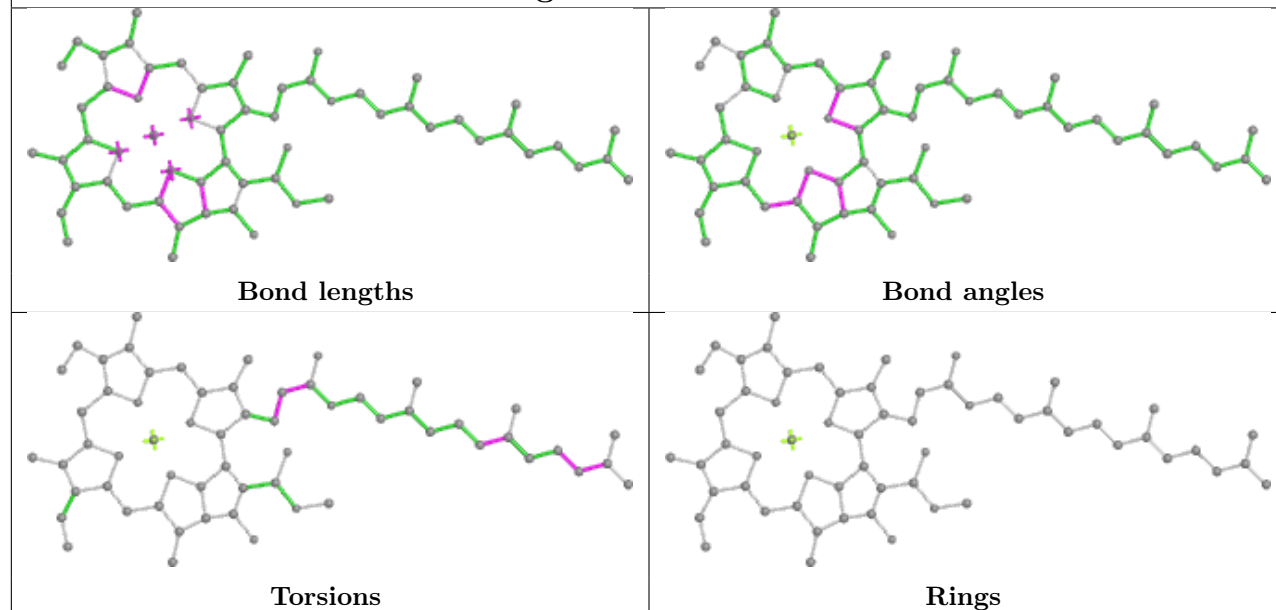
Ligand A1EB1 P 301



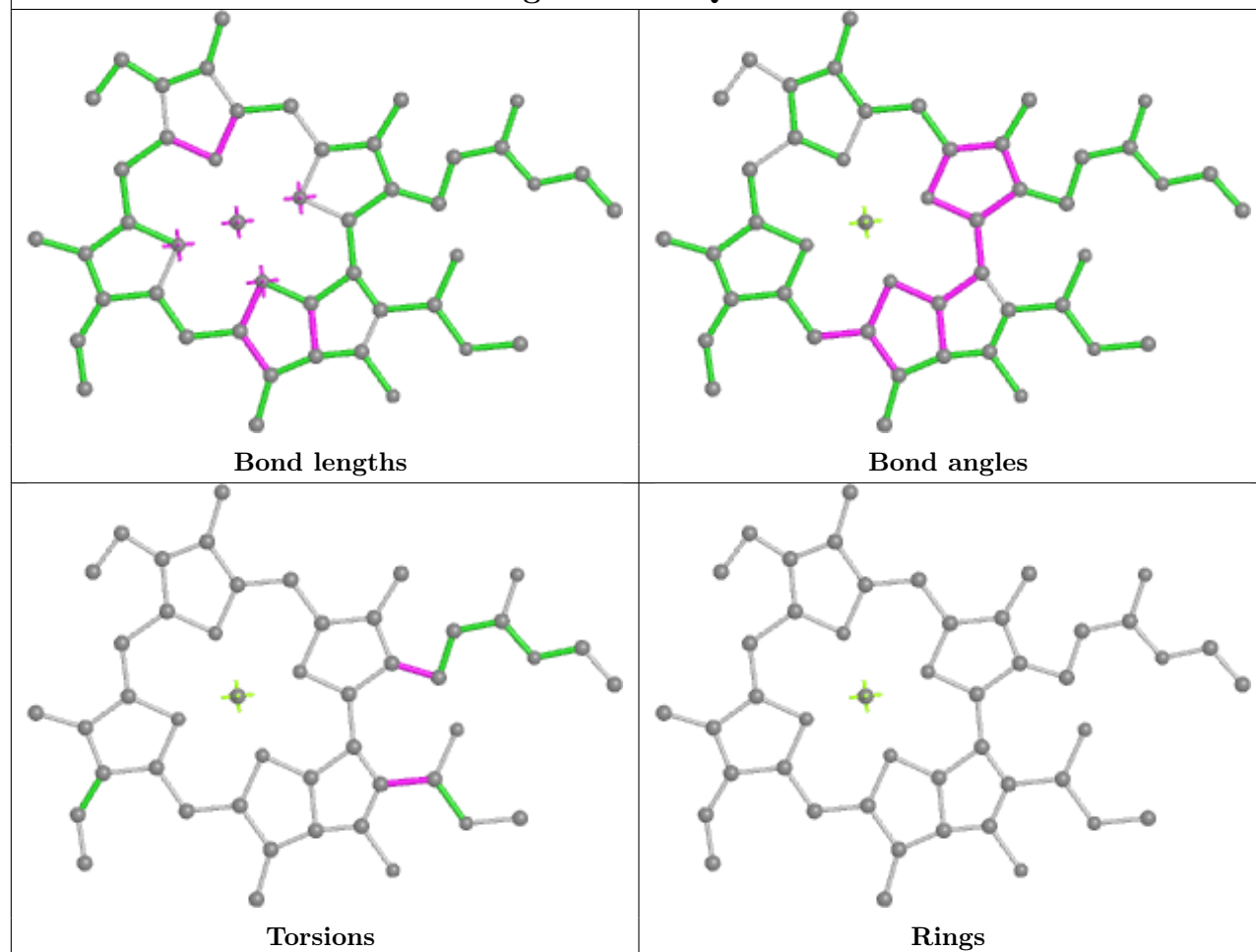
Ligand CLA a 817



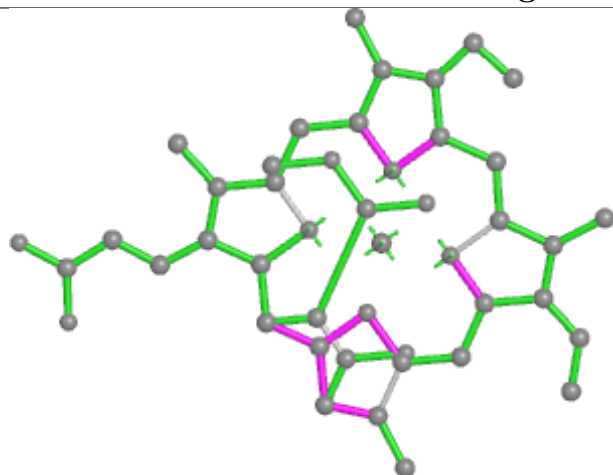
Ligand CLA a 831



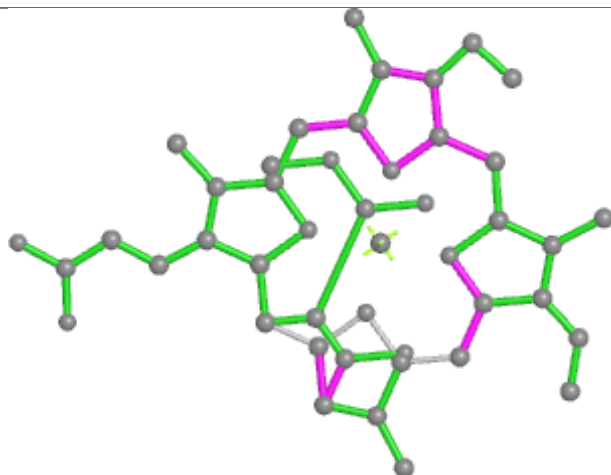
Ligand CLA Q 207



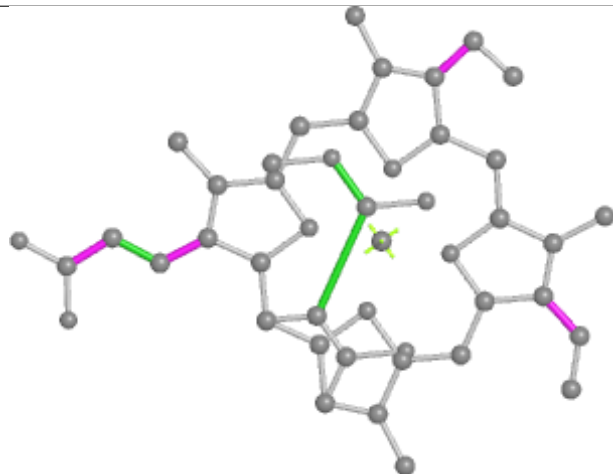
Ligand KC2 L 309



Bond lengths



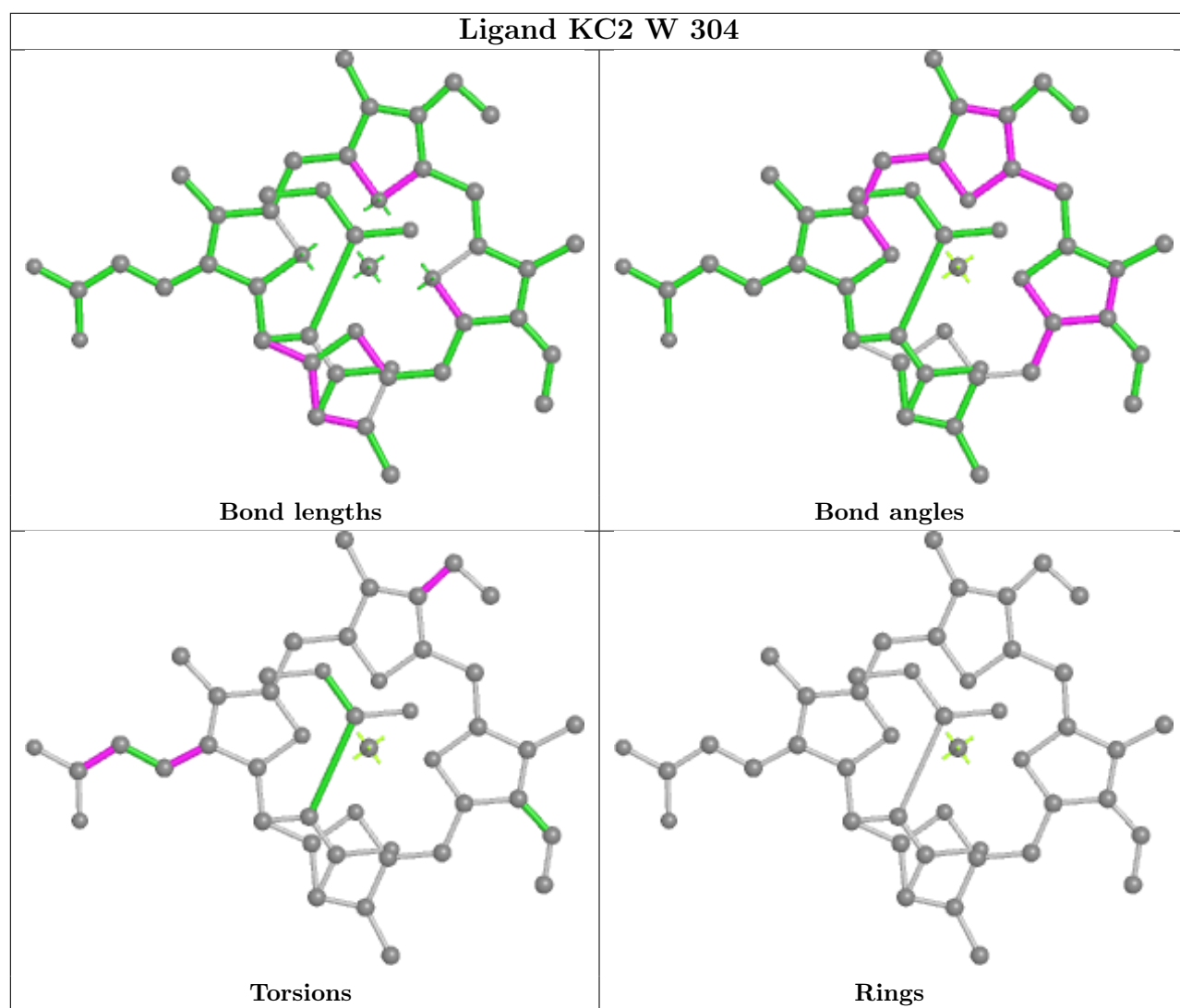
Bond angles



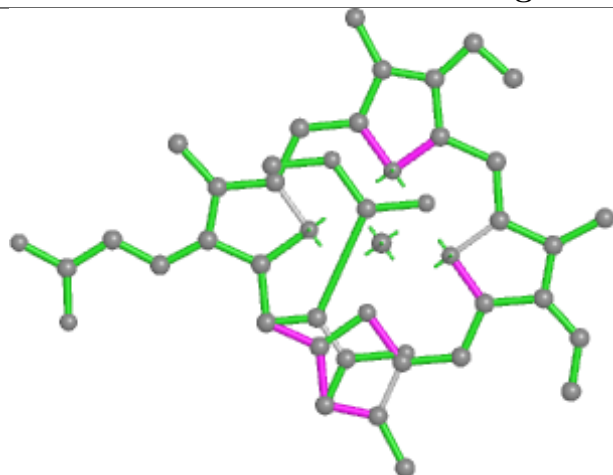
Torsions



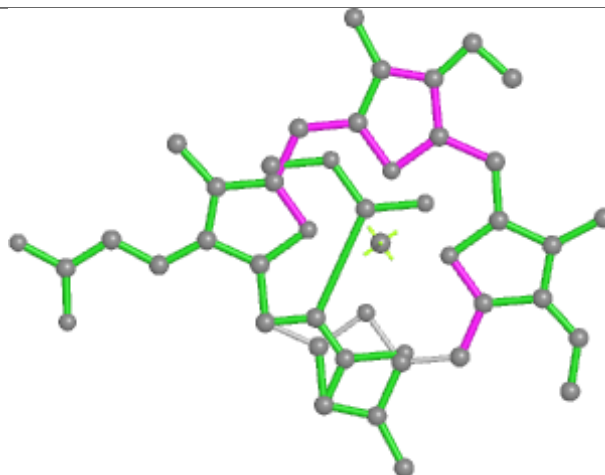
Rings



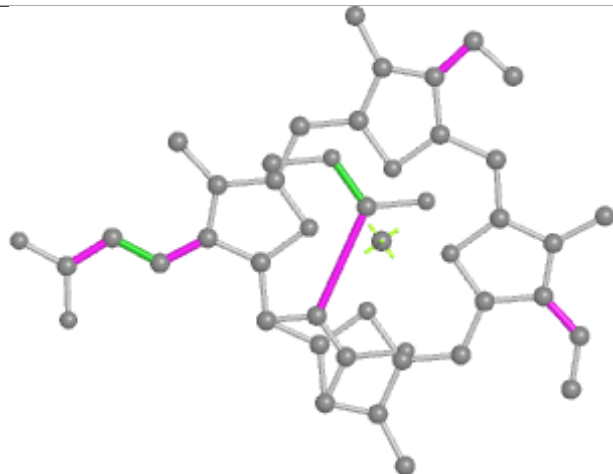
Ligand KC2 K 303



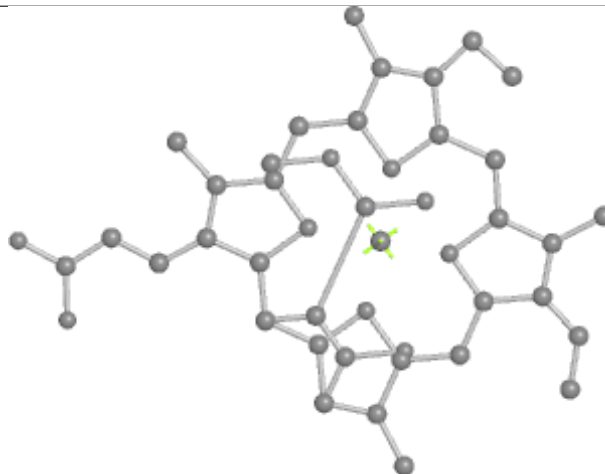
Bond lengths



Bond angles

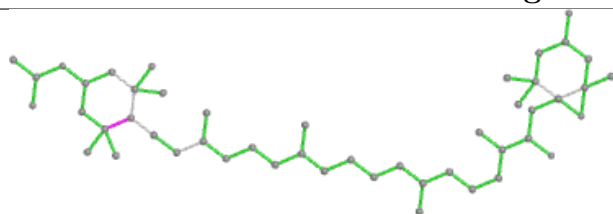


Torsions

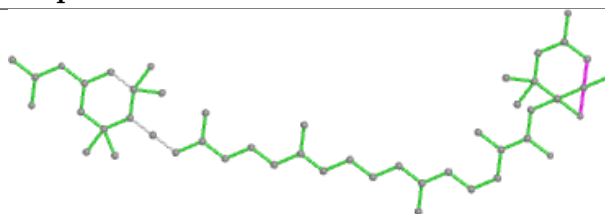


Rings

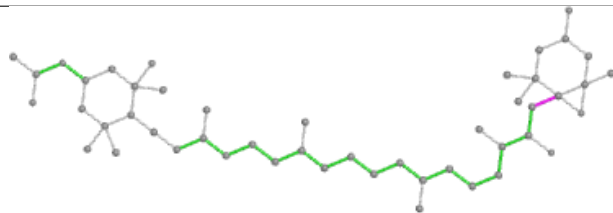
Ligand A86 q 317



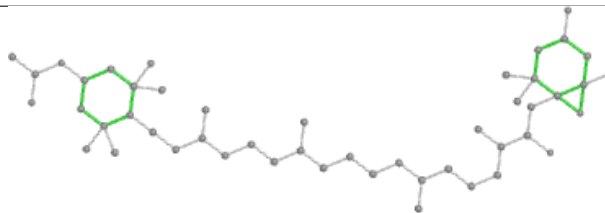
Bond lengths



Bond angles

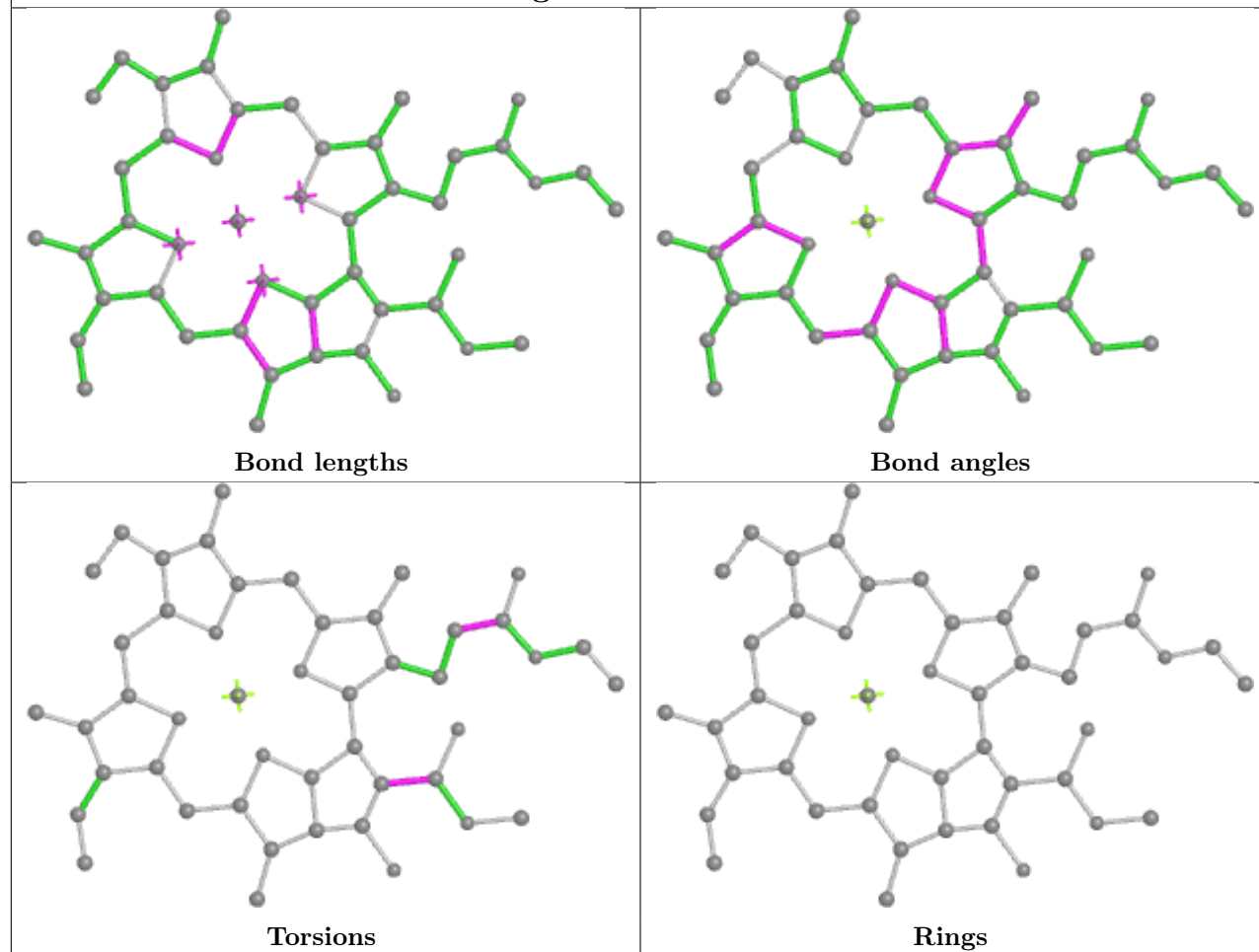


Torsions

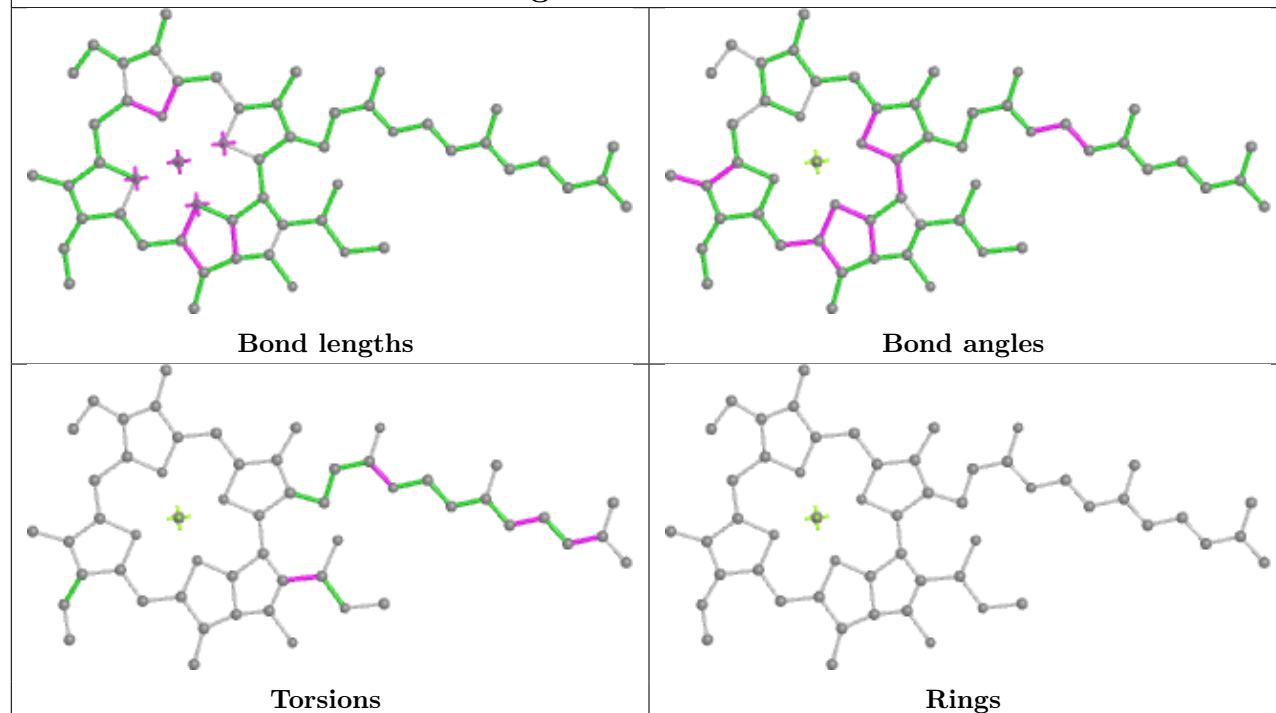


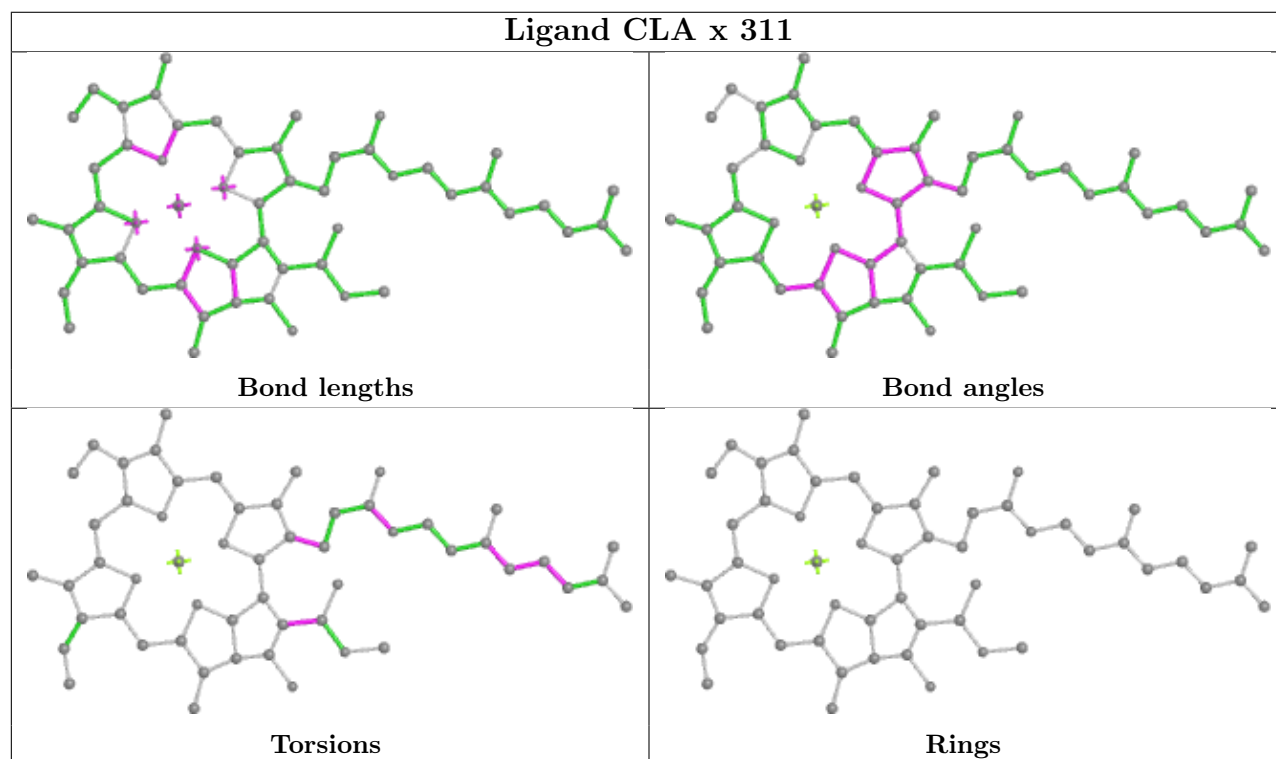
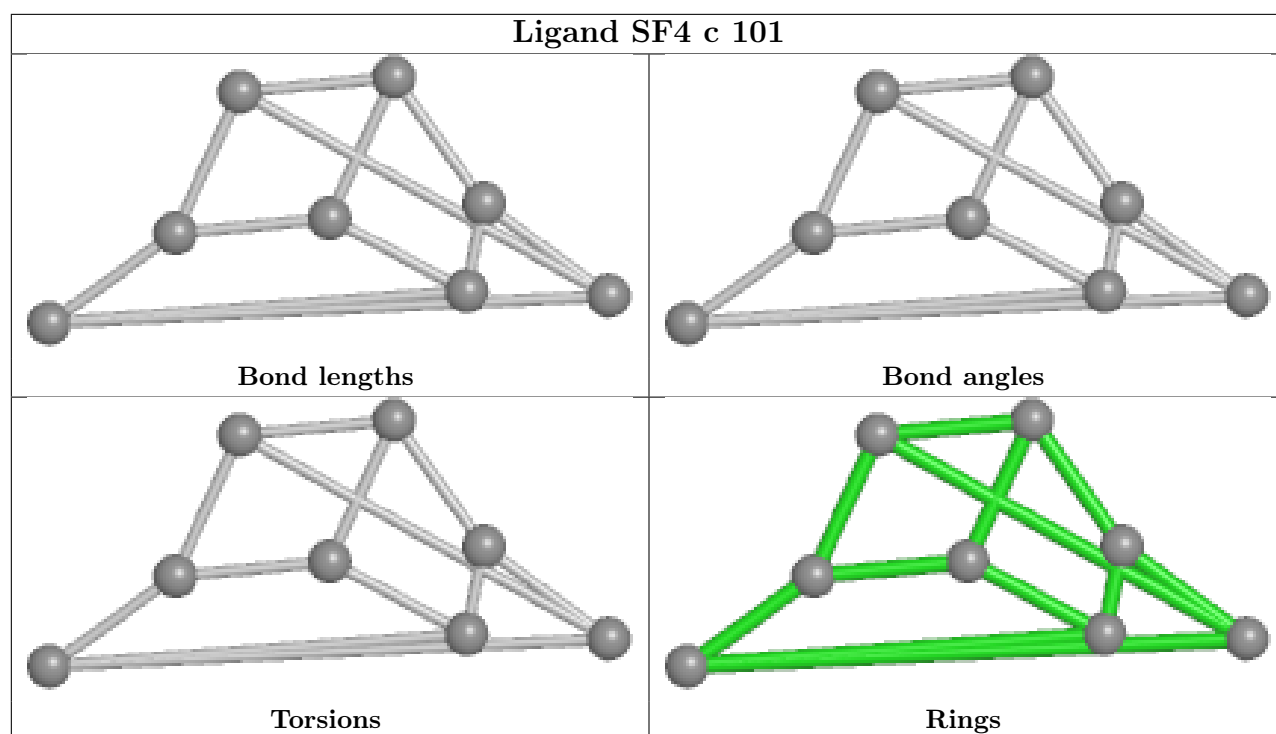
Rings

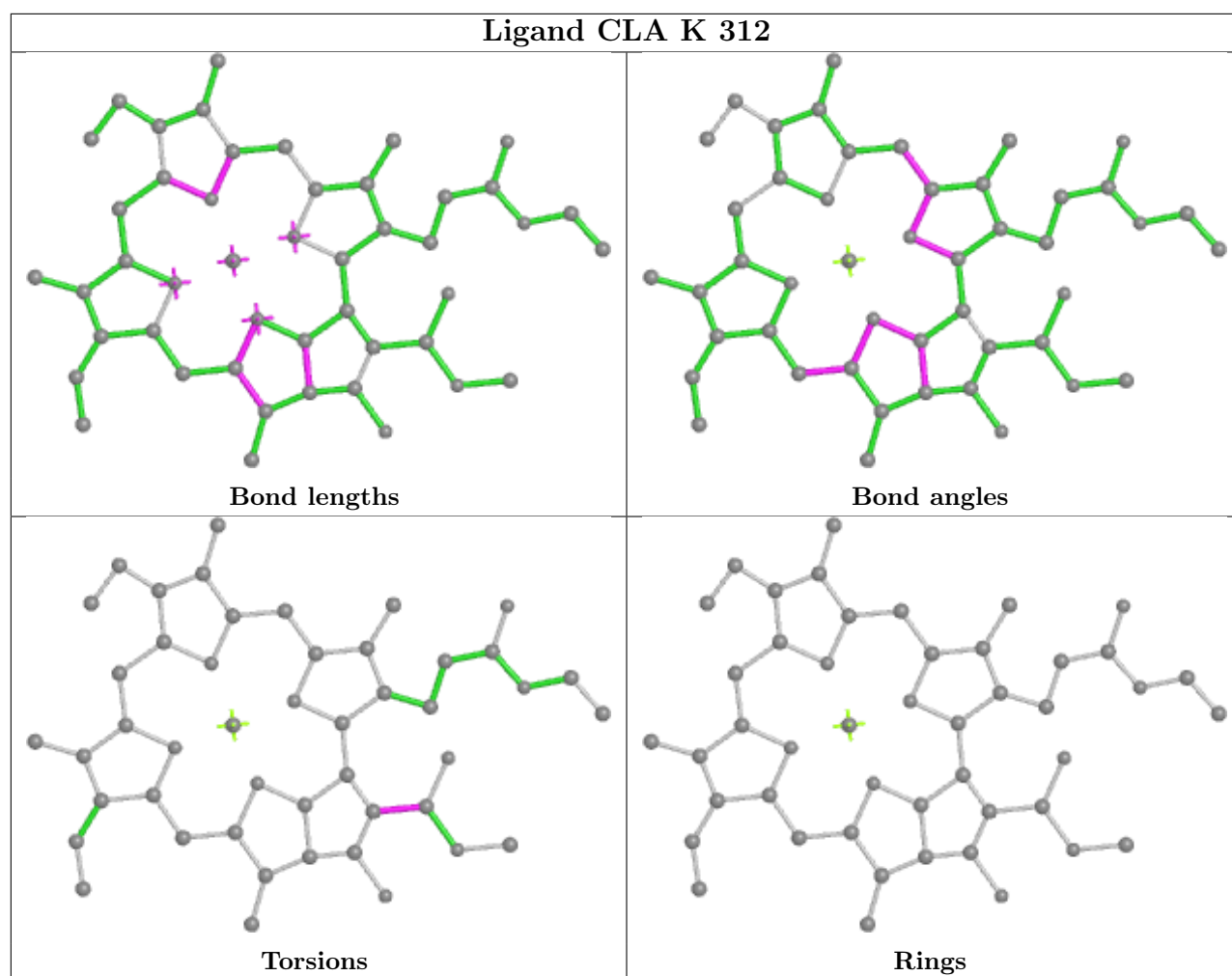
Ligand CLA f 205



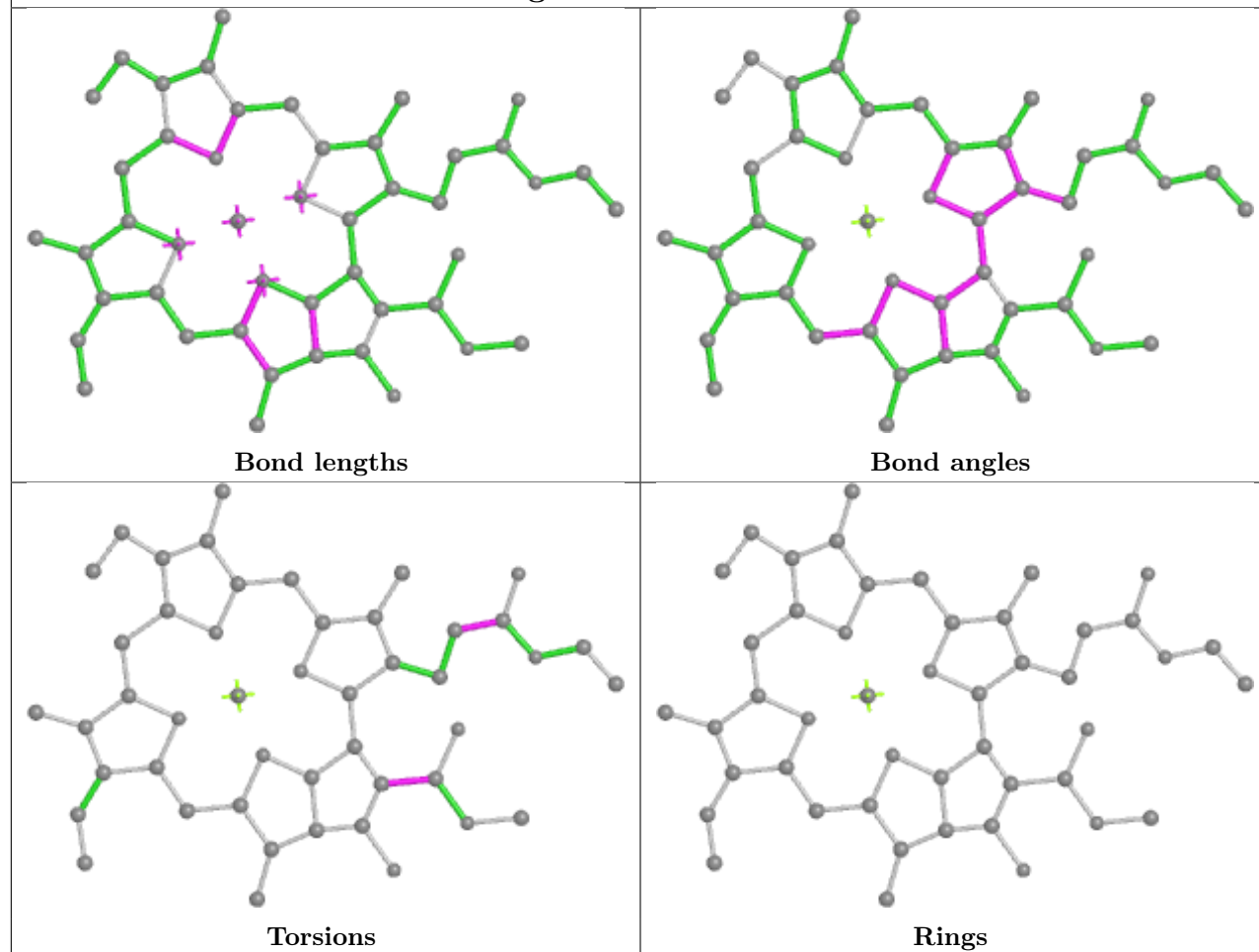
Ligand CLA U 202



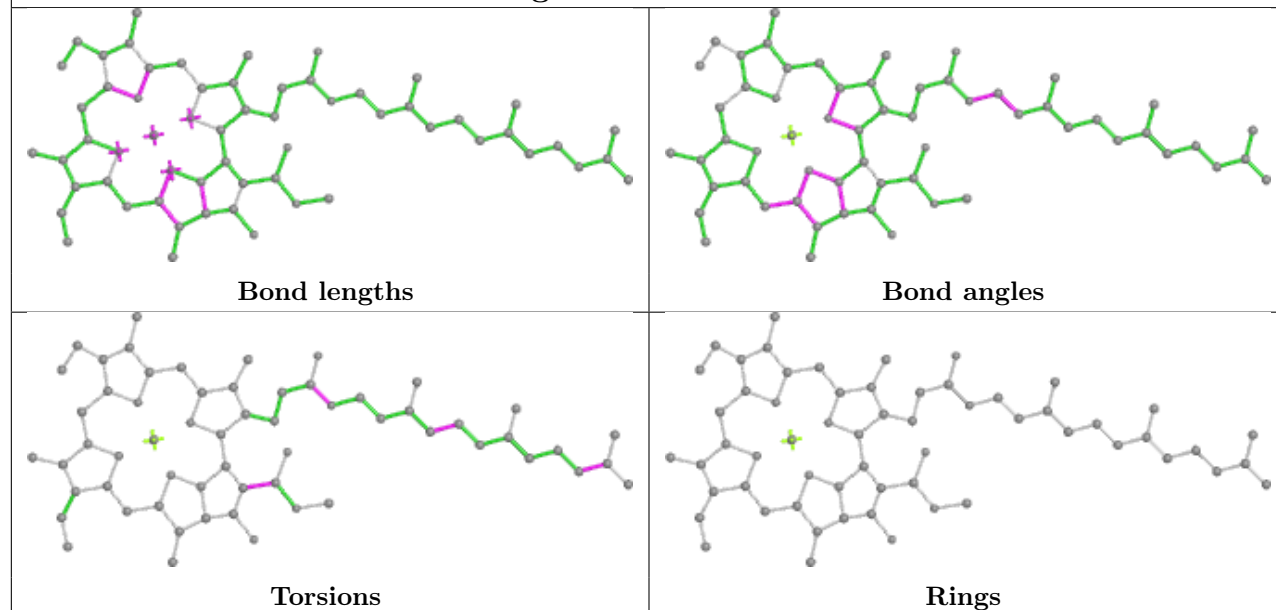


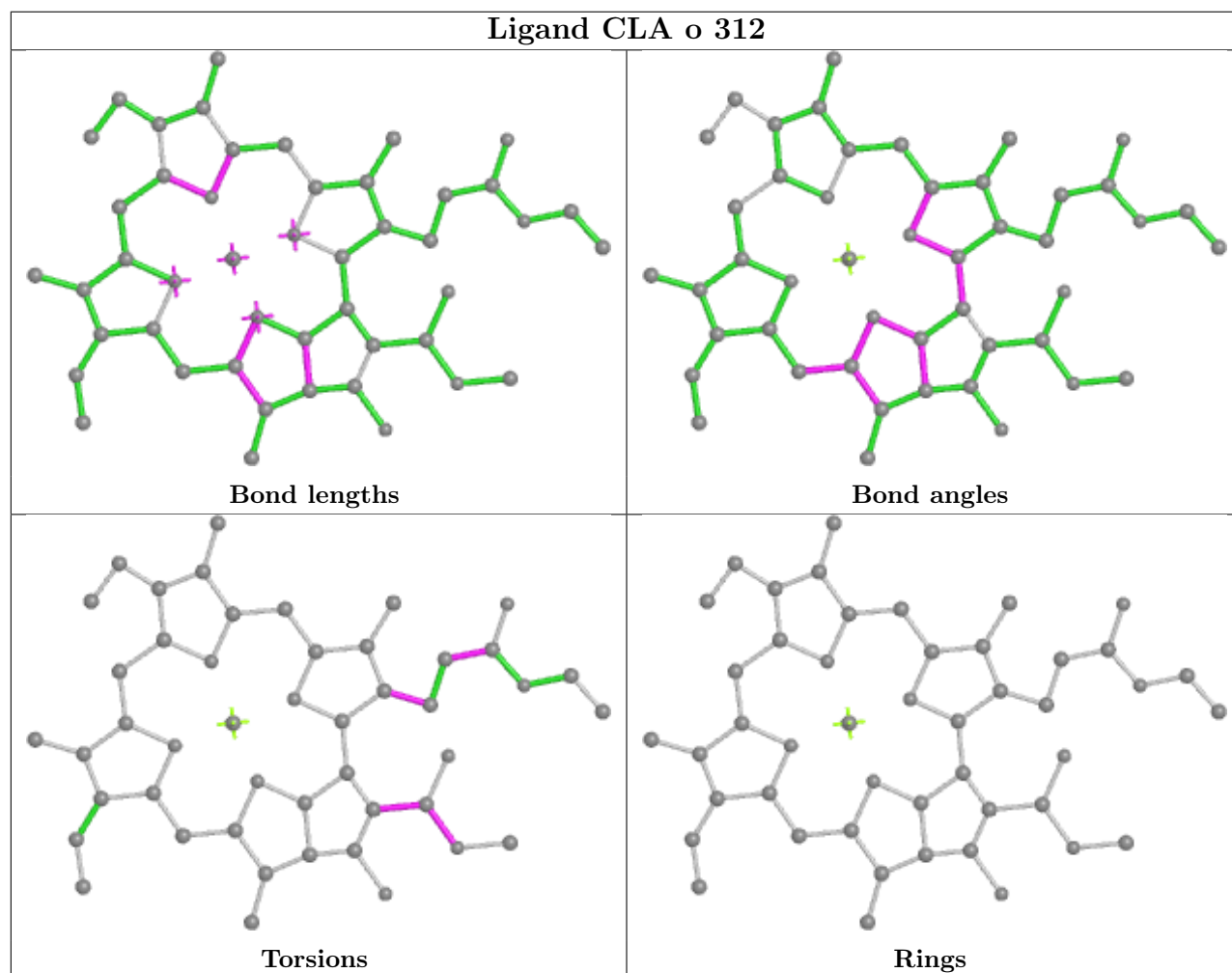
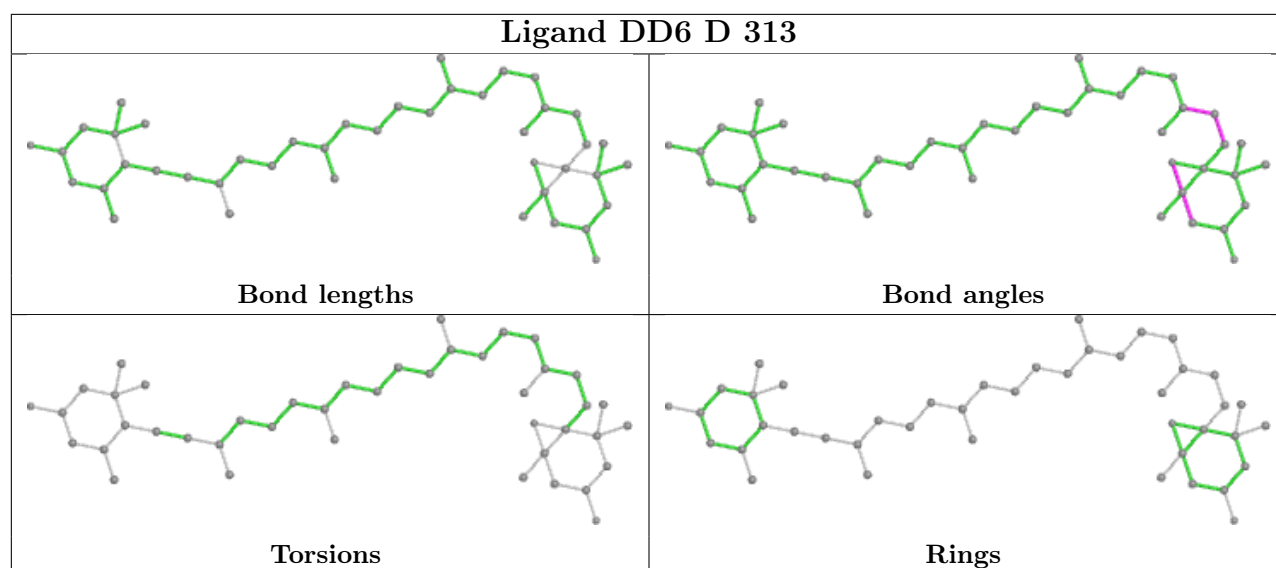


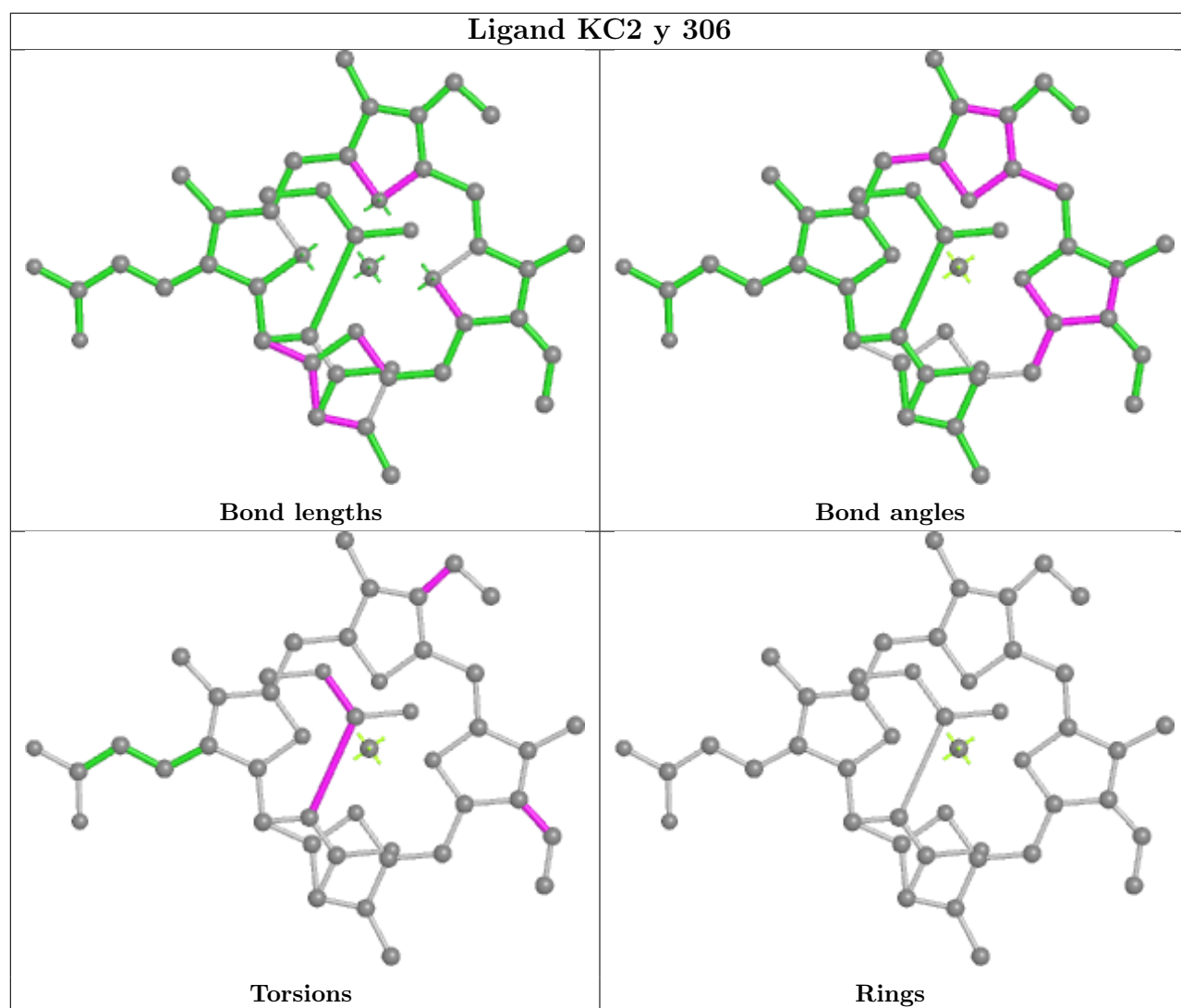
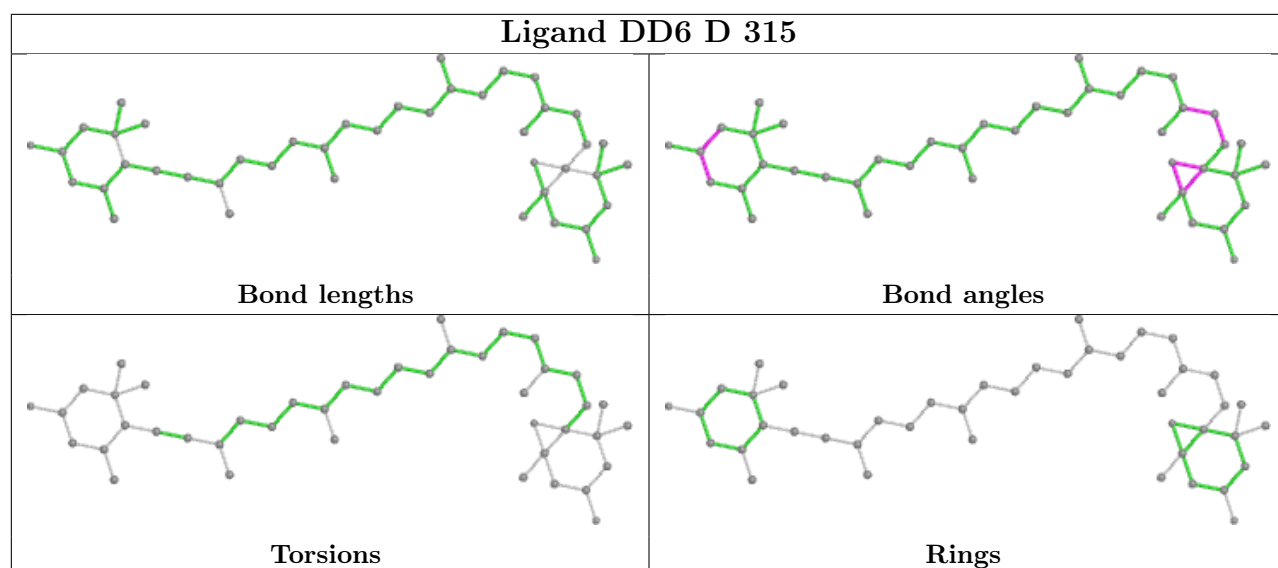
Ligand CLA b 816

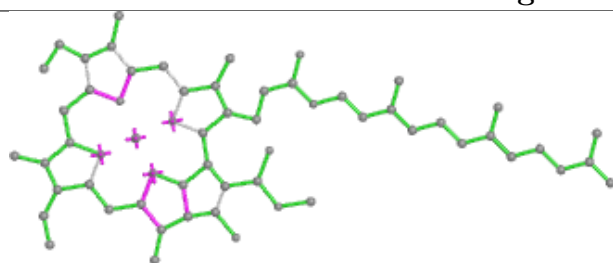
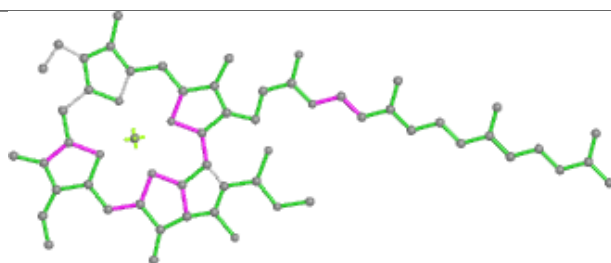
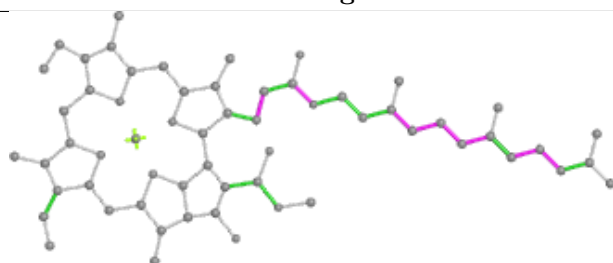
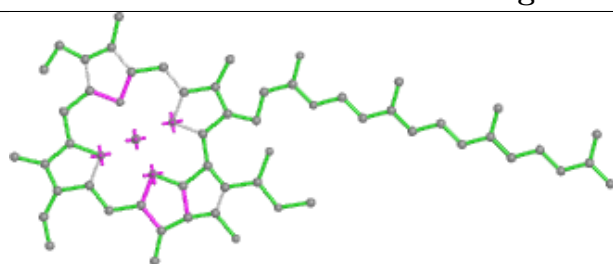
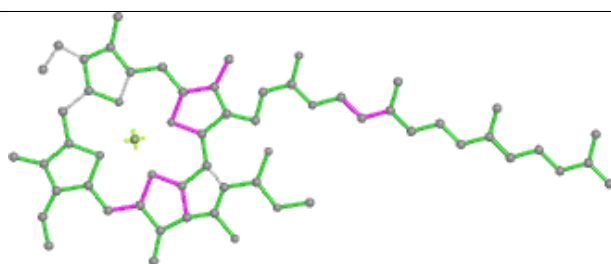
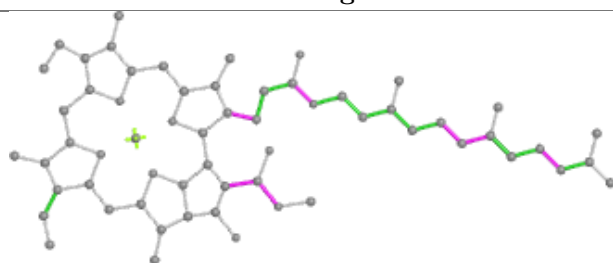
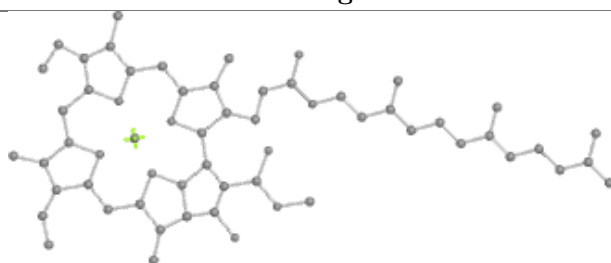


Ligand CLA X 307

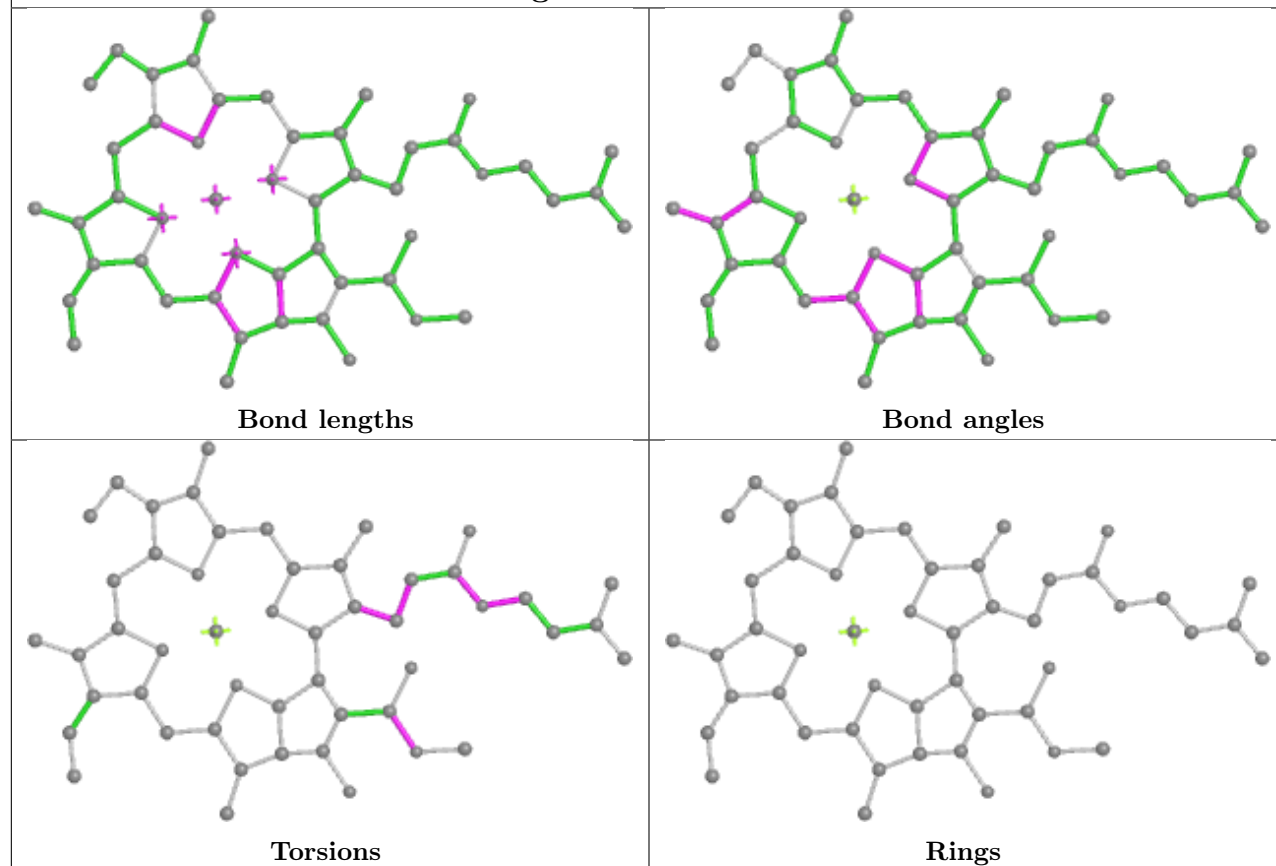




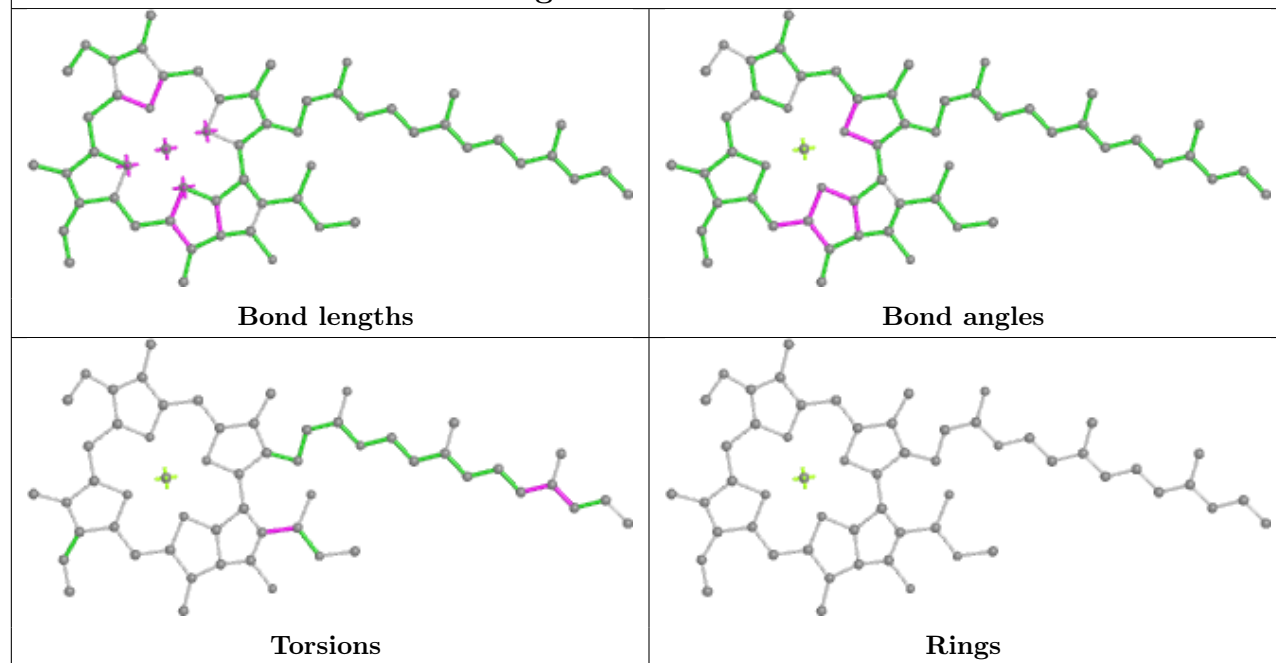


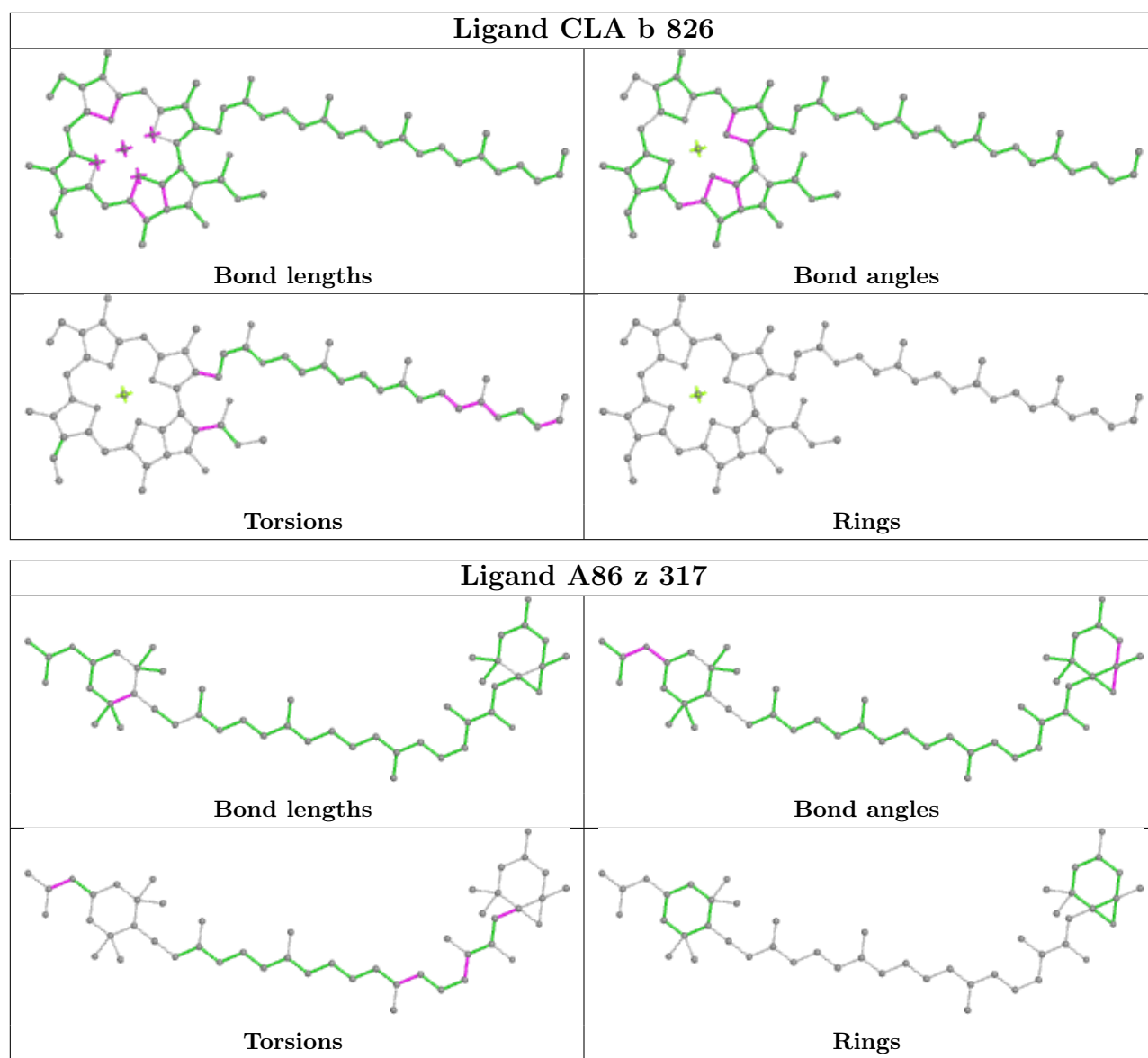
Ligand CLA S 302**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA x 312****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA X 305

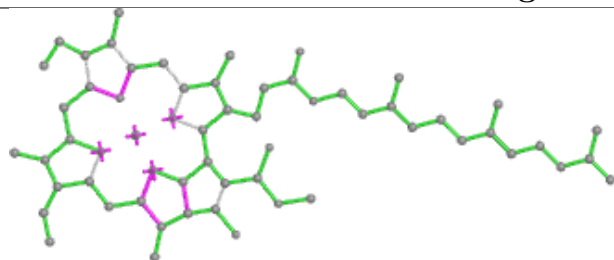


Ligand CLA b 815

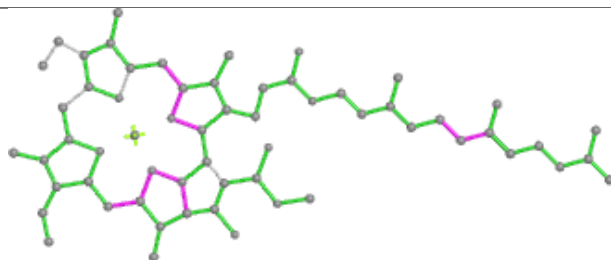




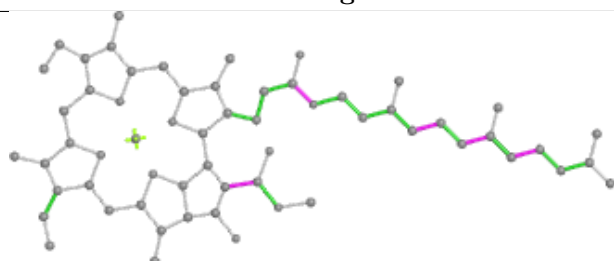
Ligand CLA a 833



Bond lengths



Bond angles

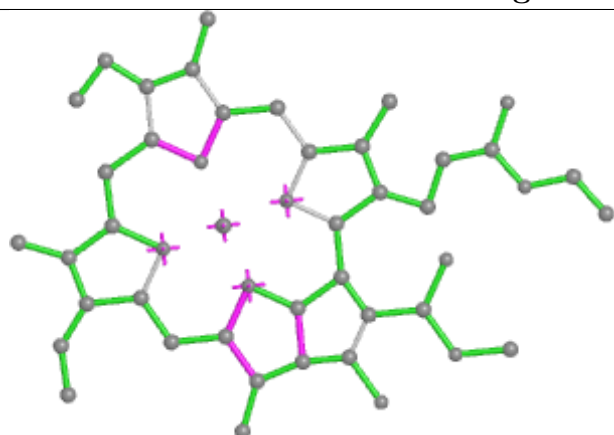


Torsions

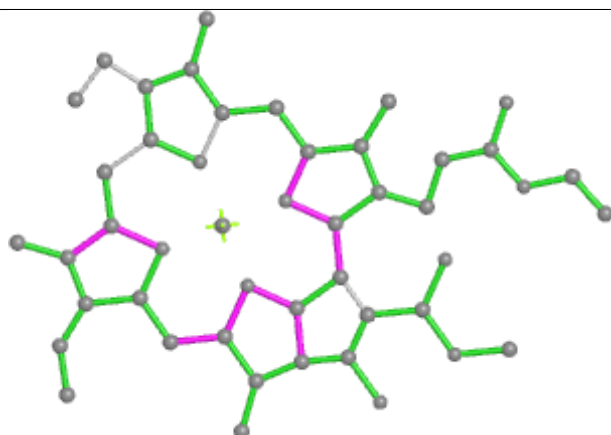


Rings

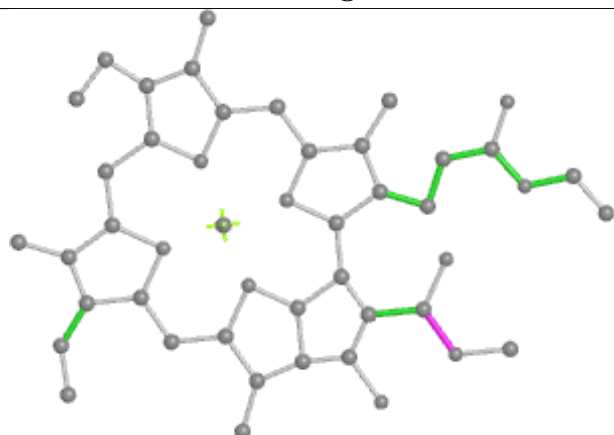
Ligand CLA G 201



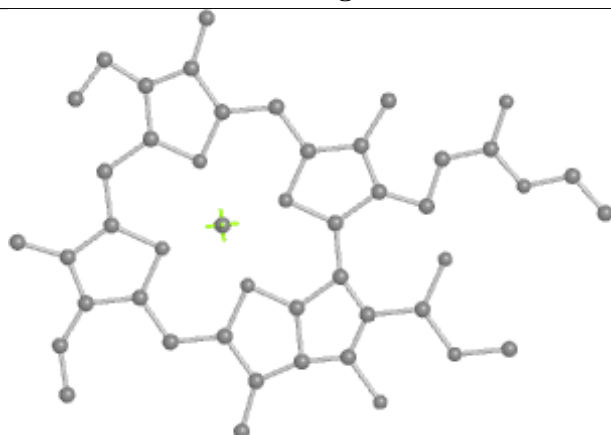
Bond lengths



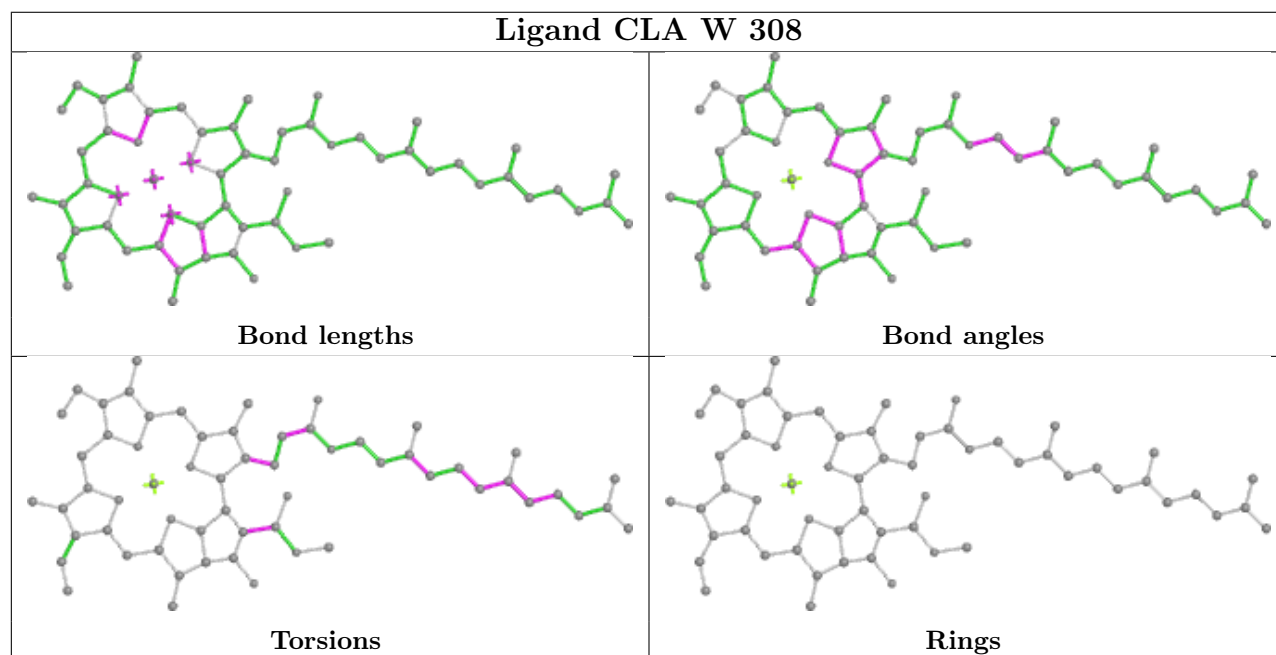
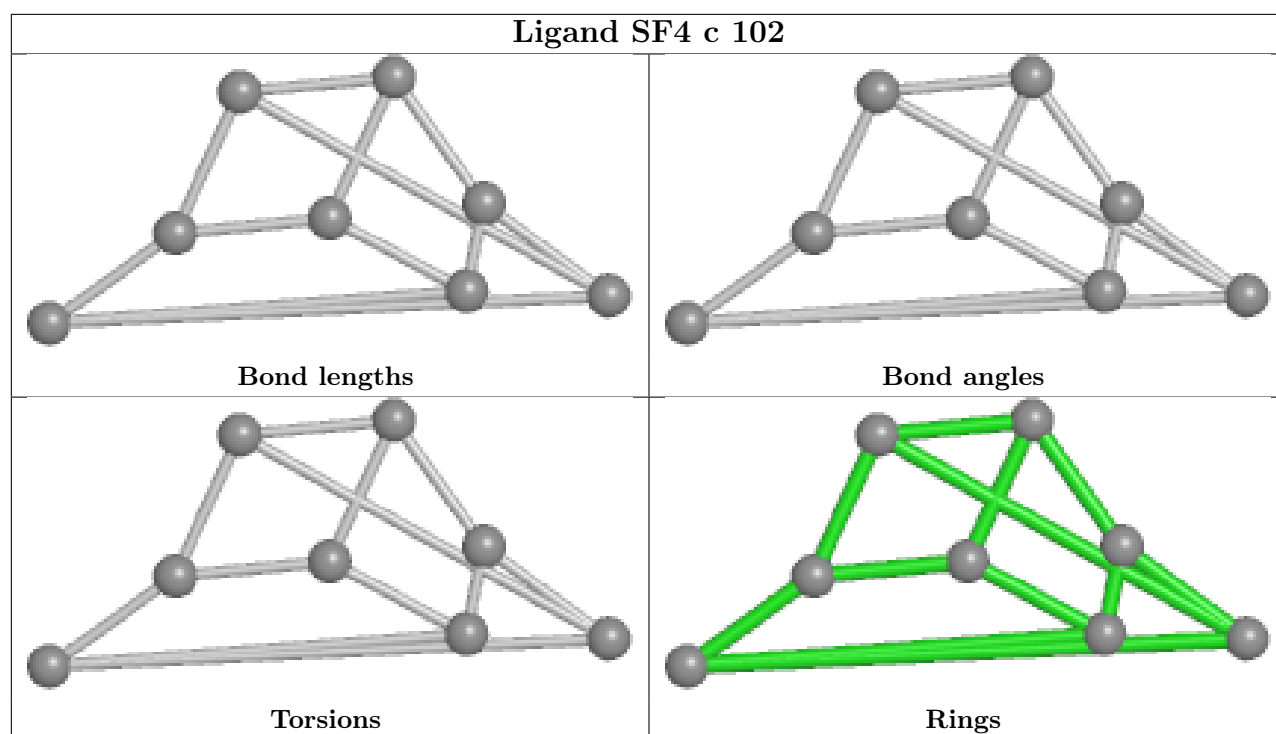
Bond angles

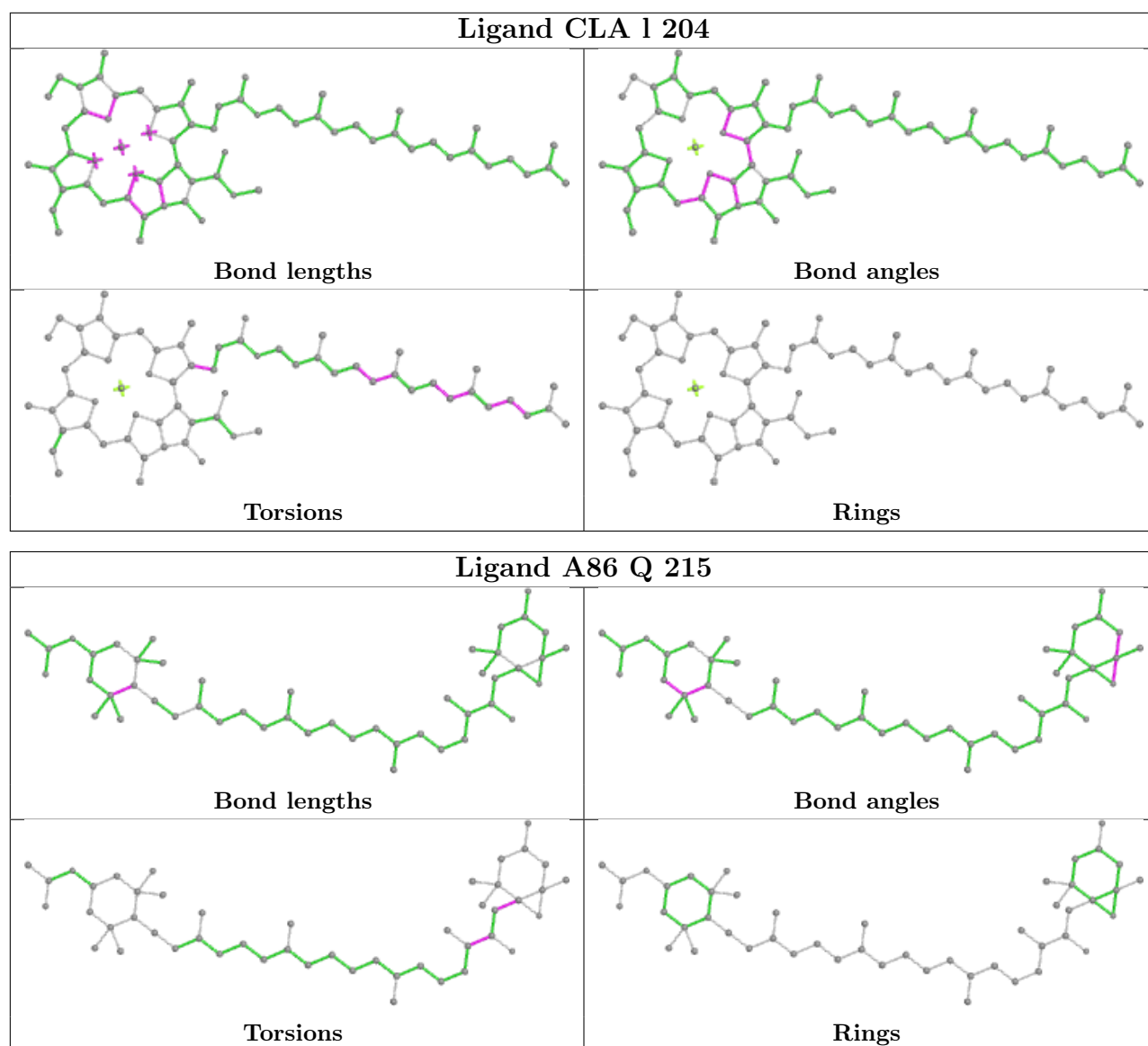


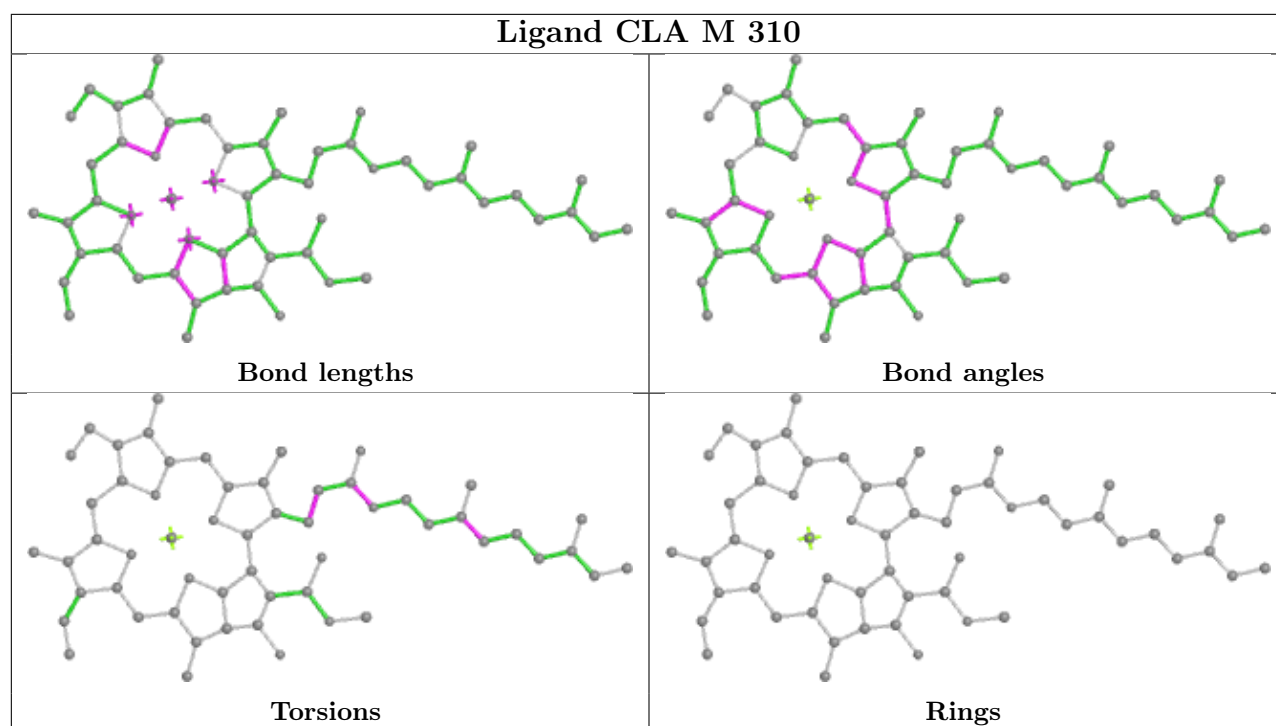
Torsions



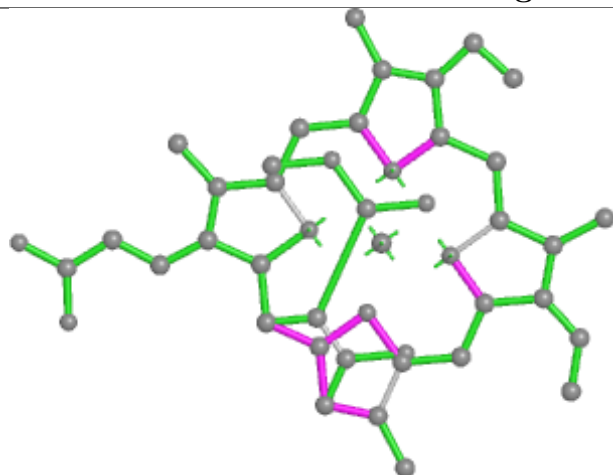
Rings



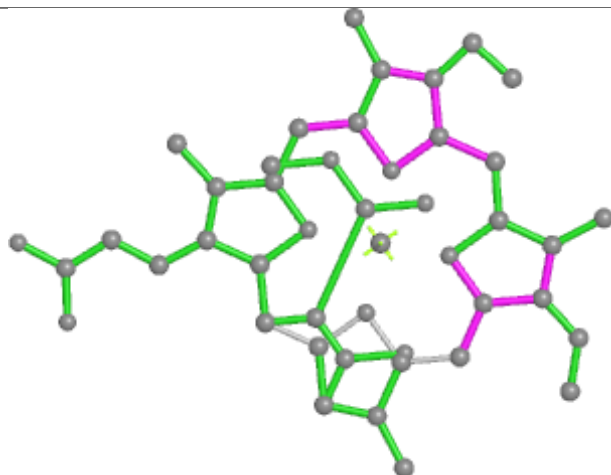




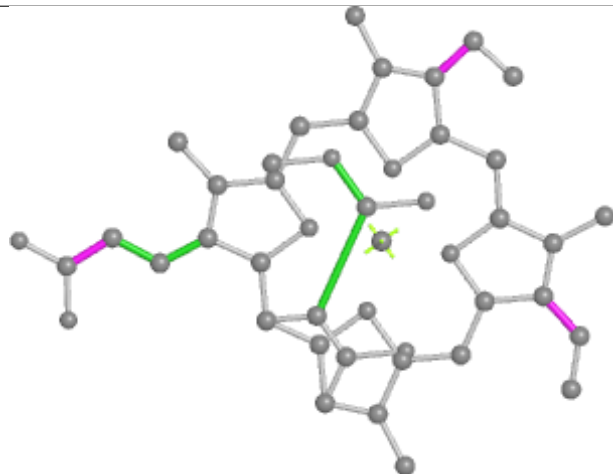
Ligand KC2 K 302



Bond lengths



Bond angles

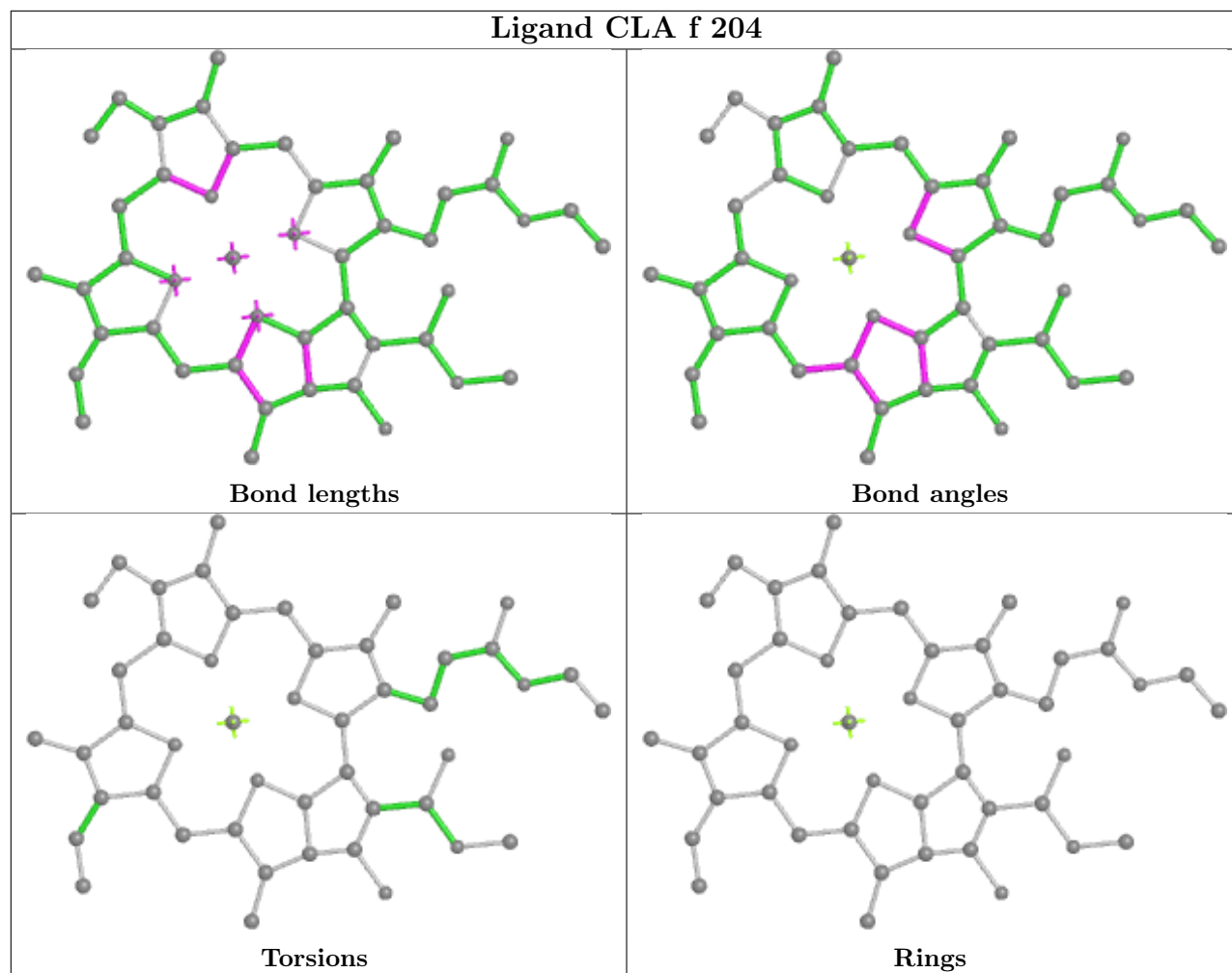


Torsions

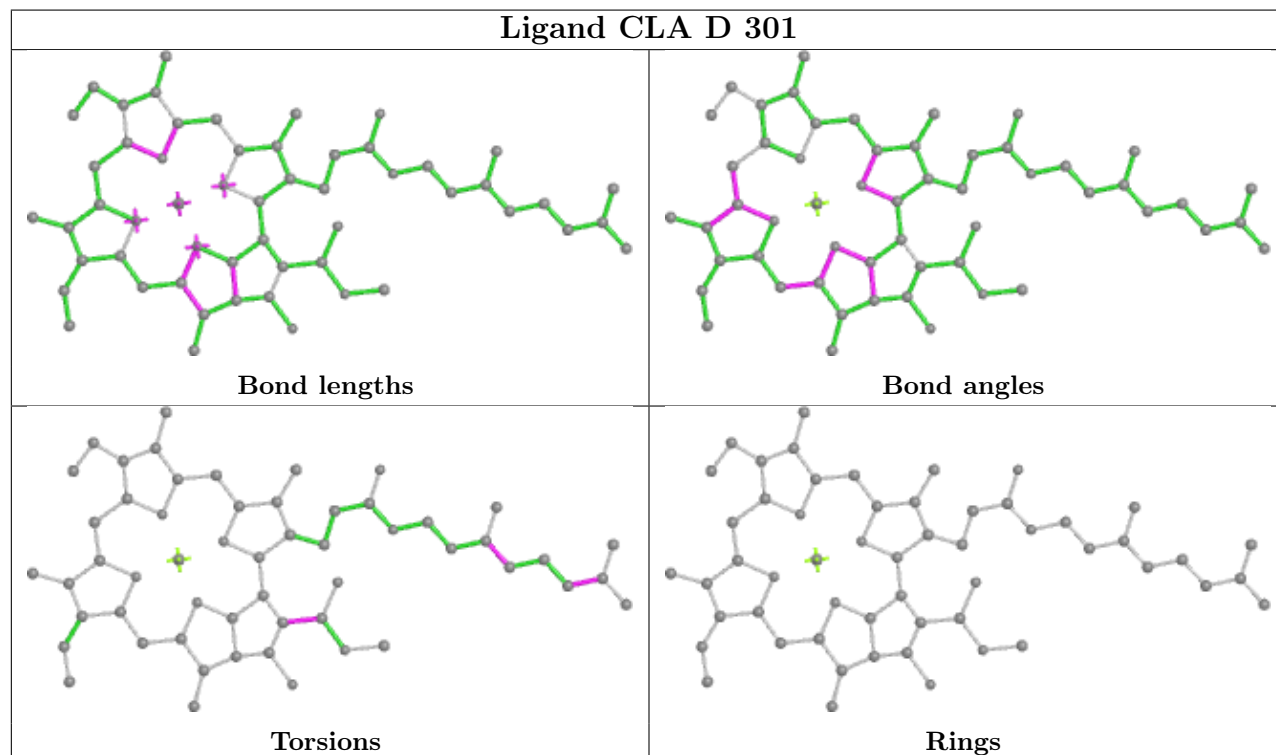


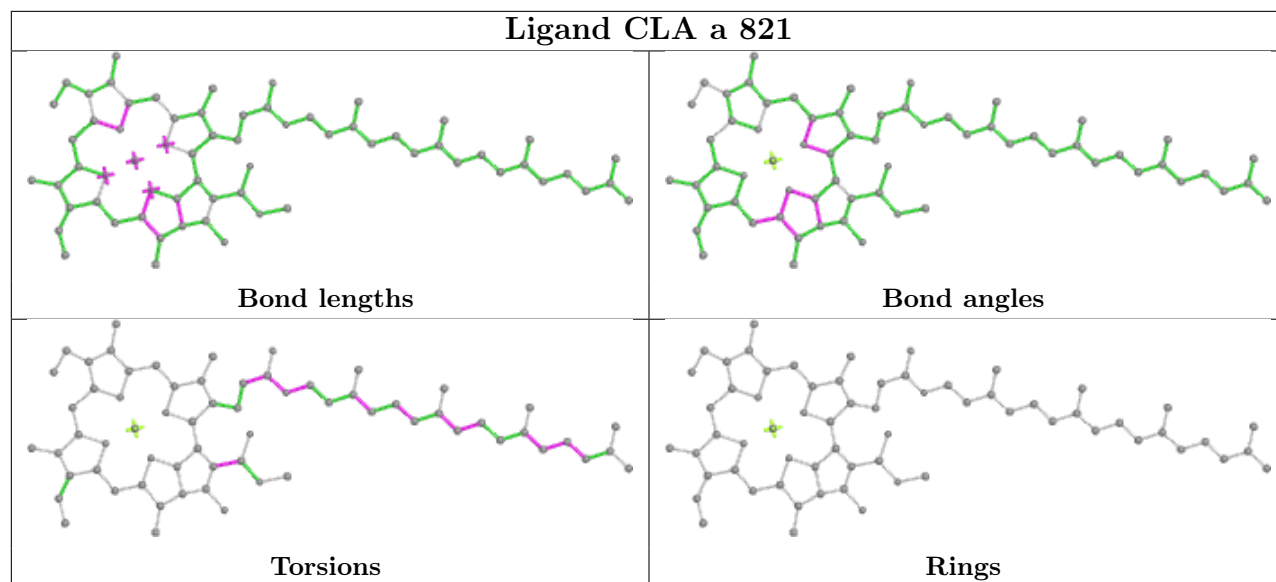
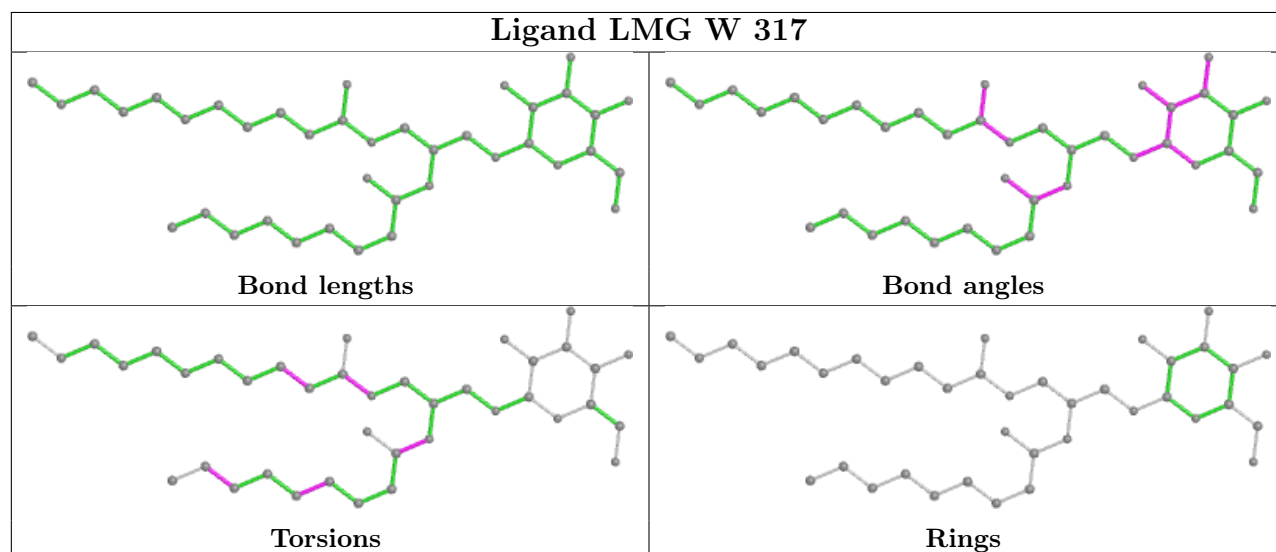
Rings

Ligand CLA f 204

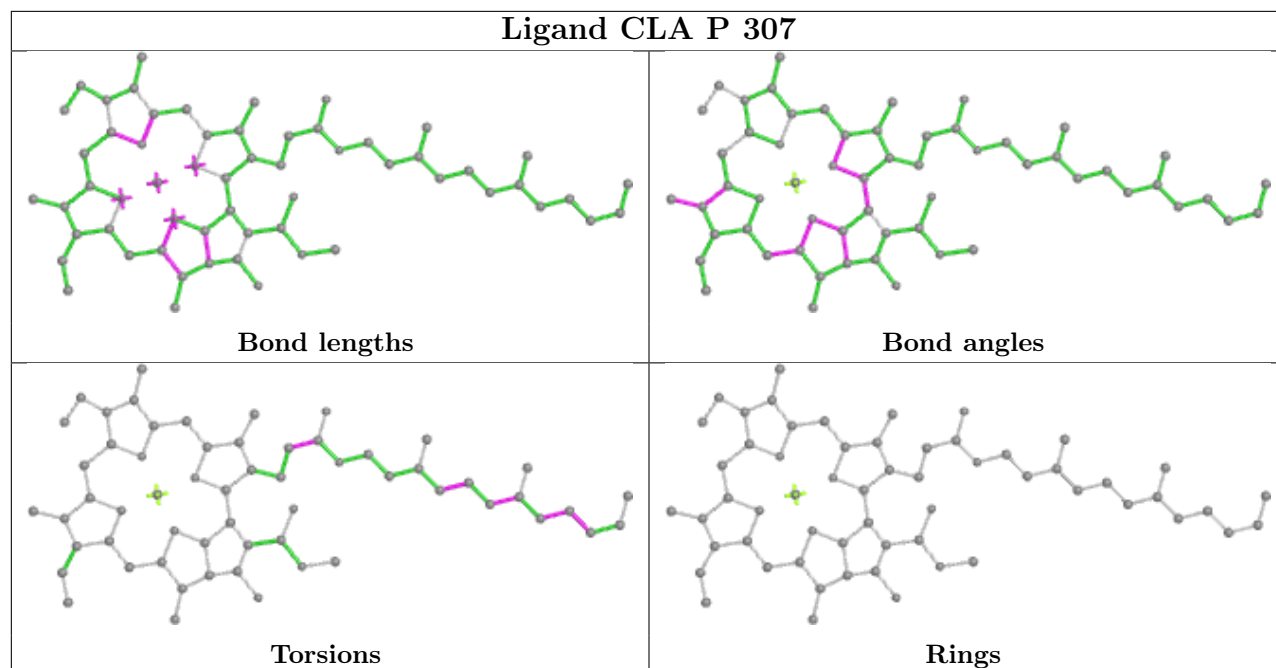


Ligand CLA D 301

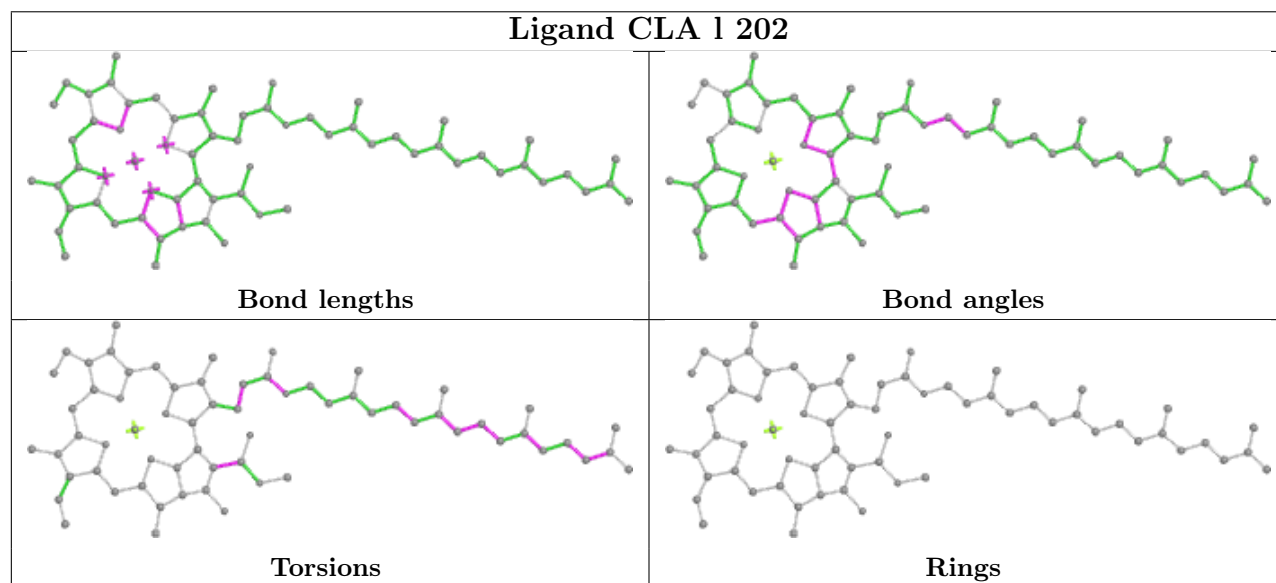


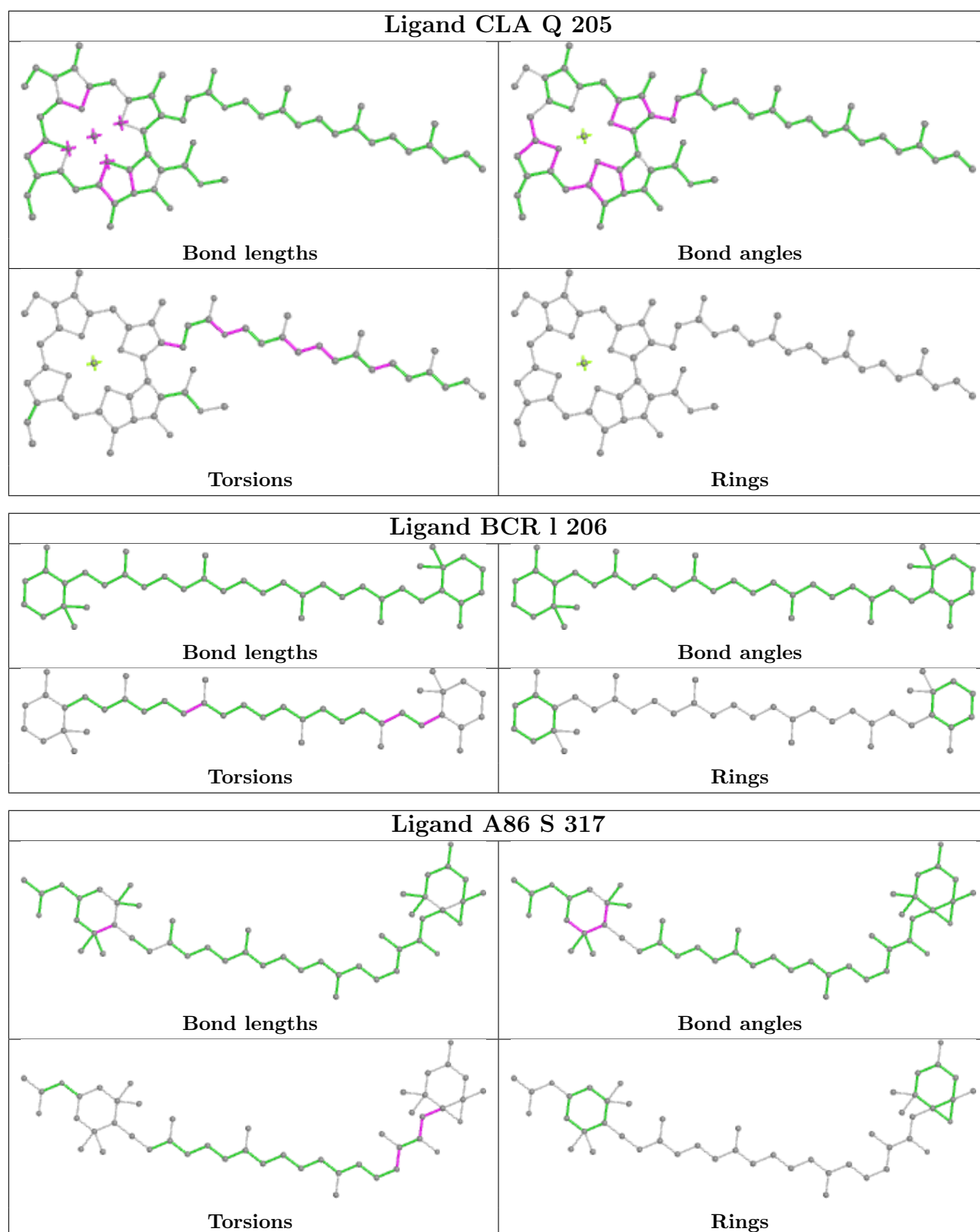
Ligand CLA a 821**Ligand LMG W 317**

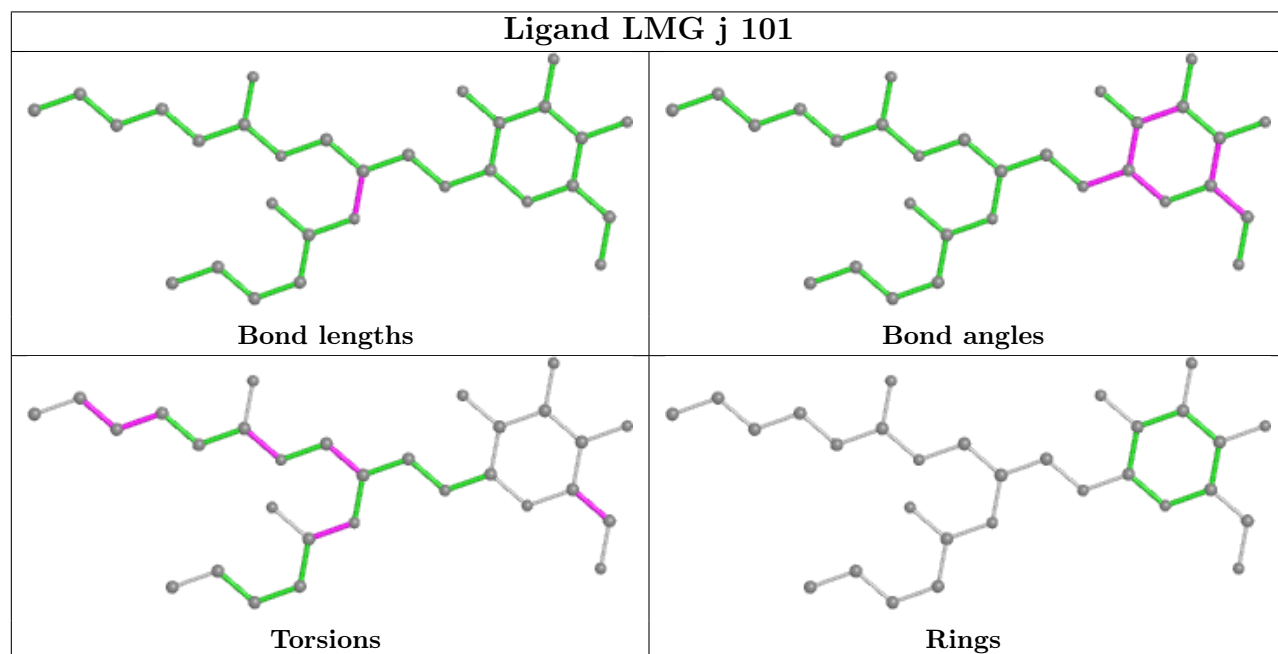
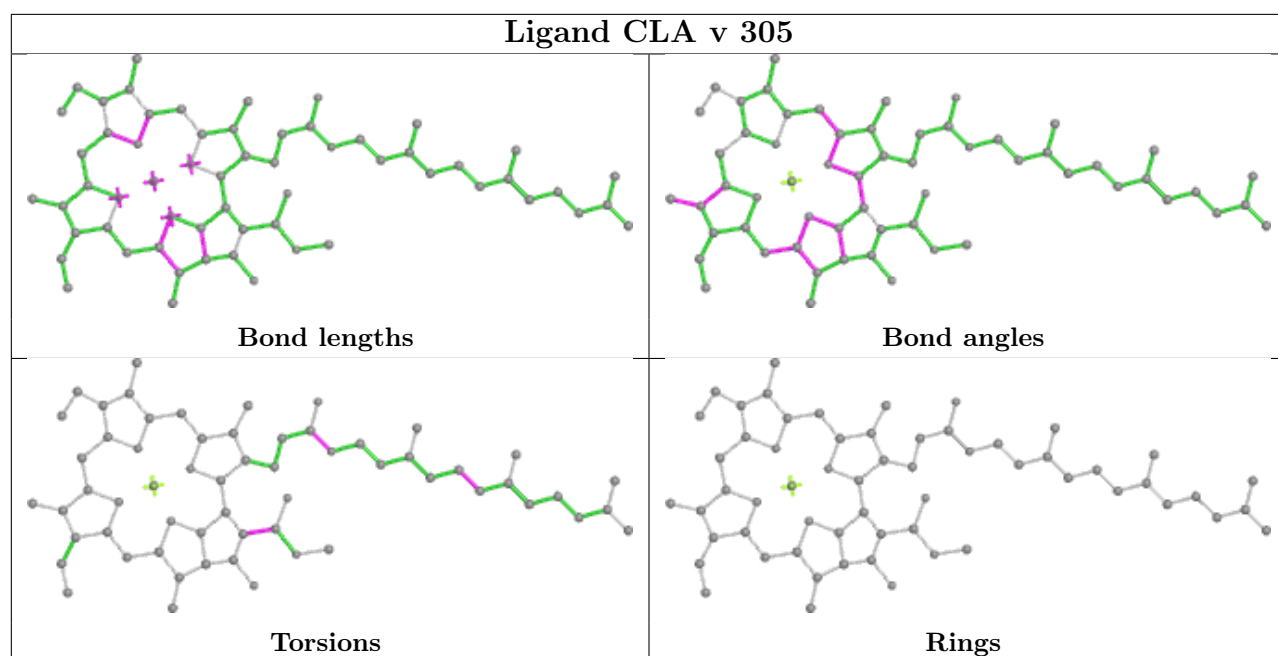
Ligand CLA P 307



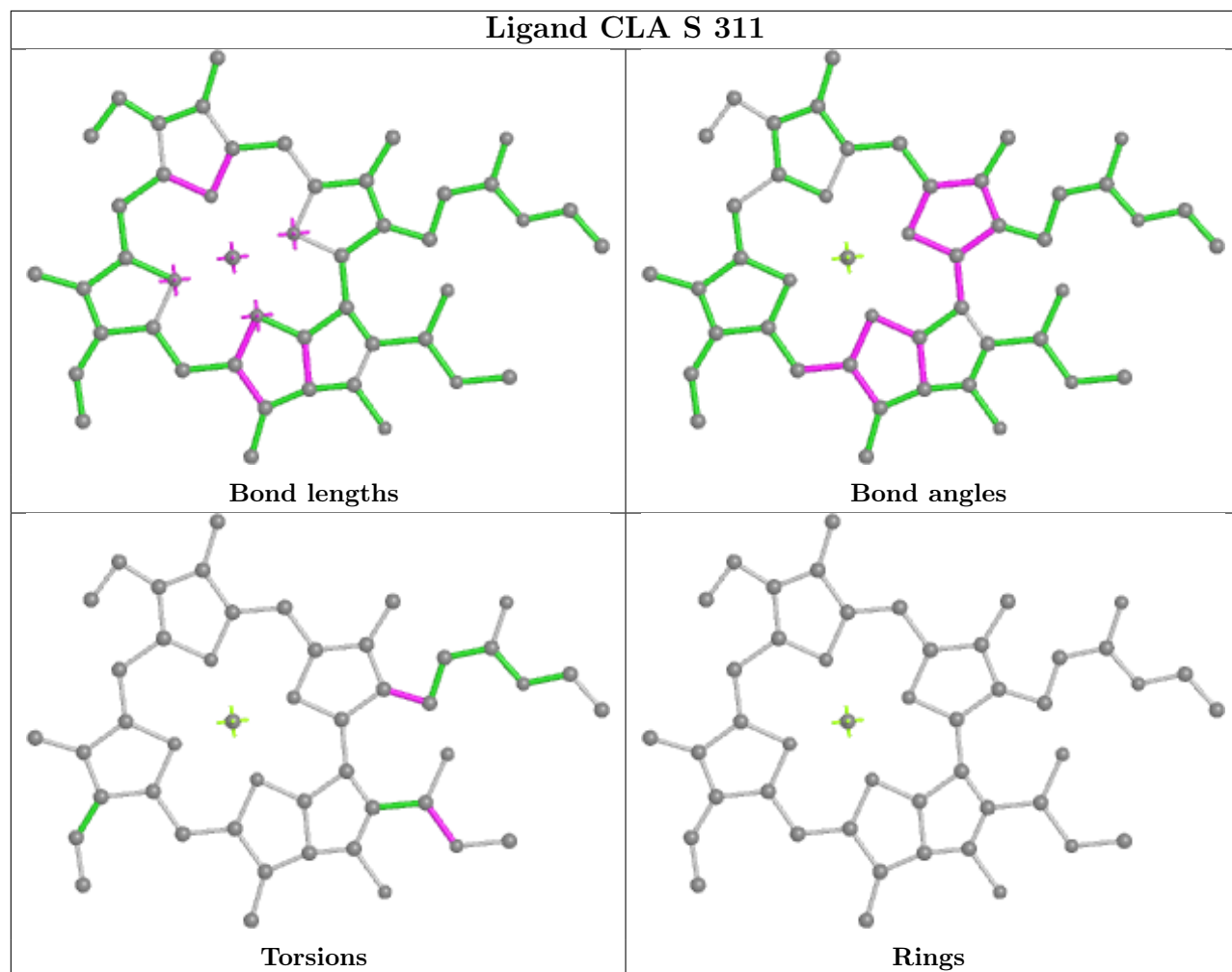
Ligand CLA I 202



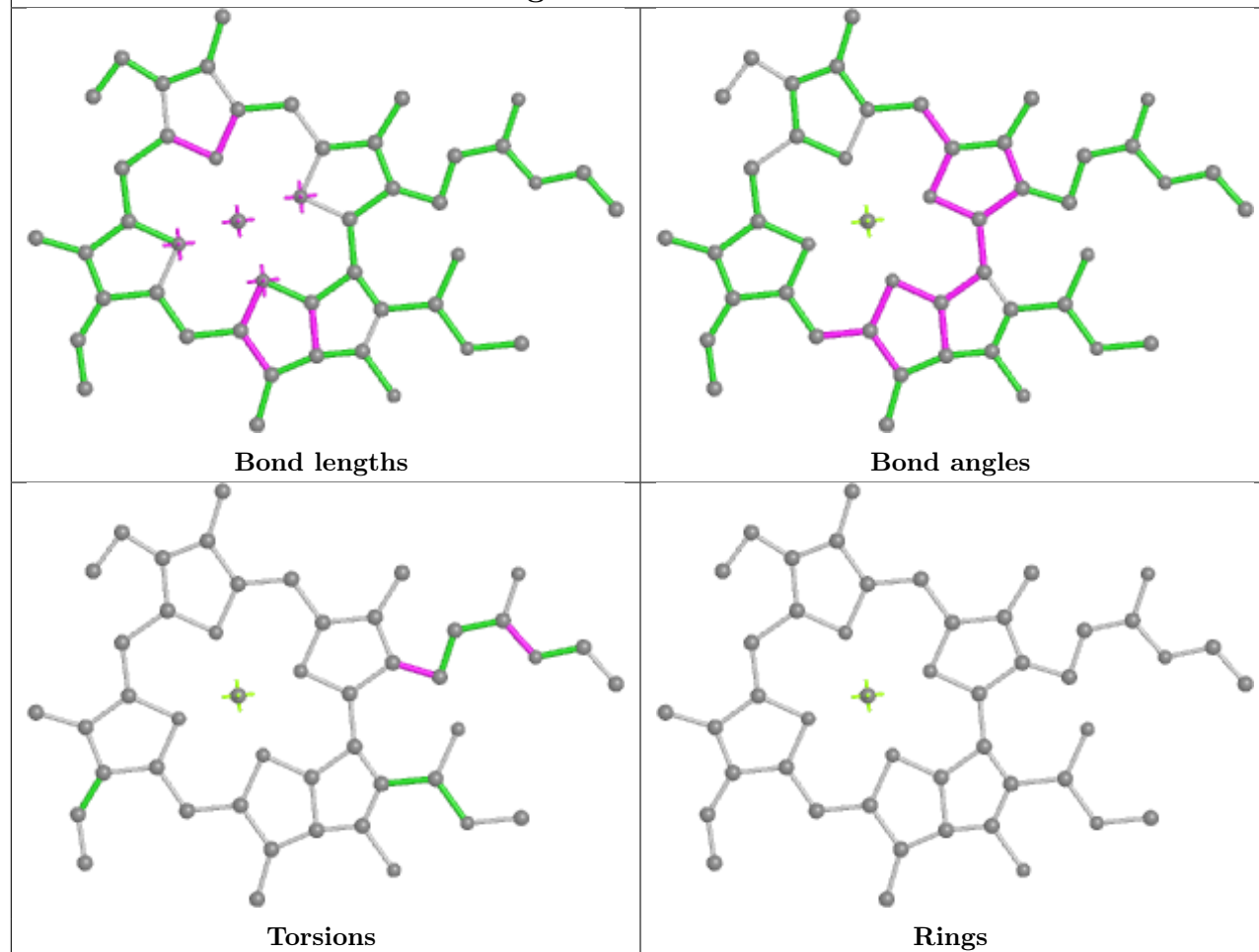




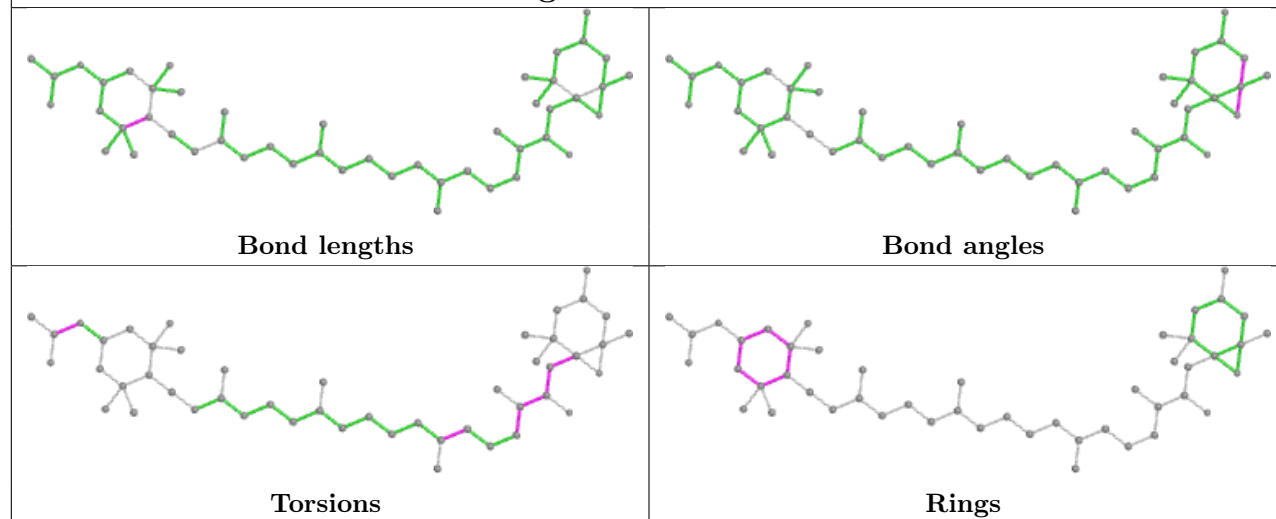
Ligand CLA S 311



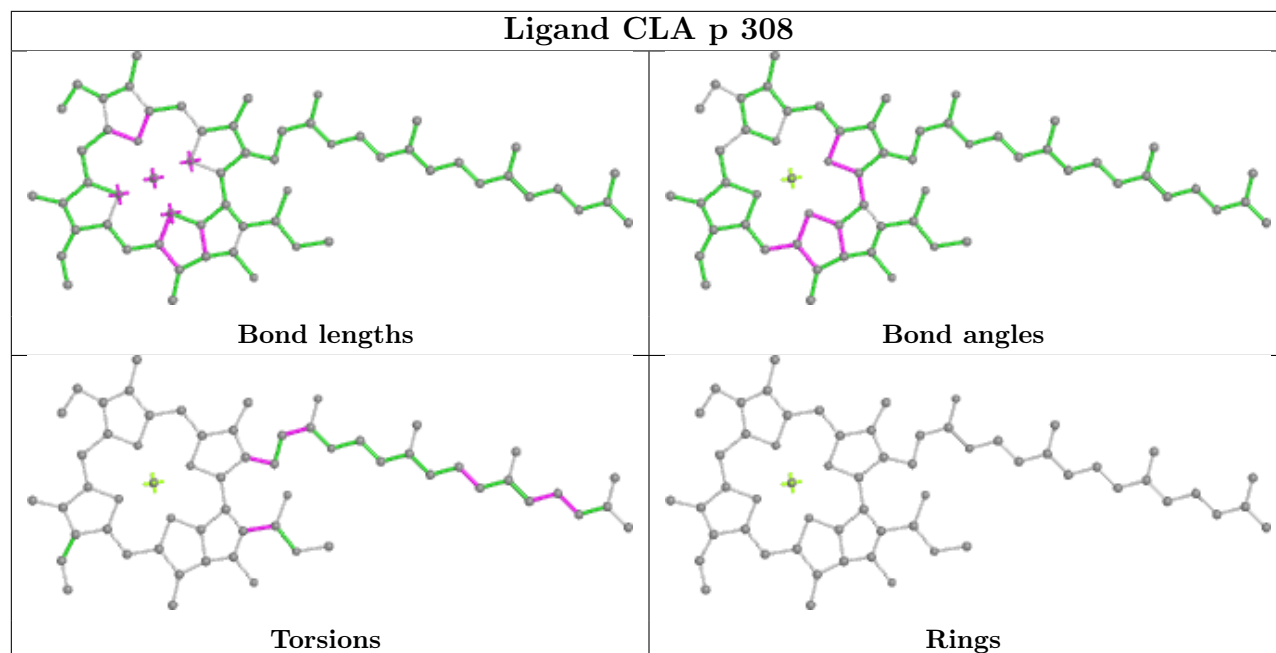
Ligand CLA L 310



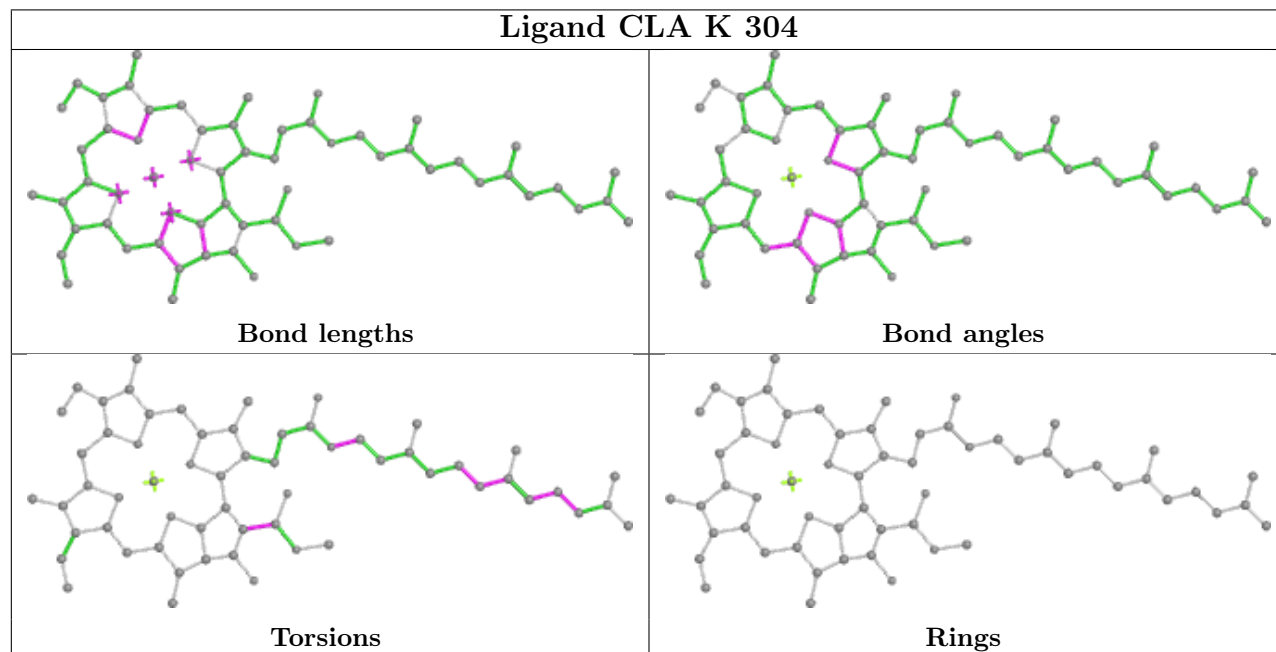
Ligand A86 T 315

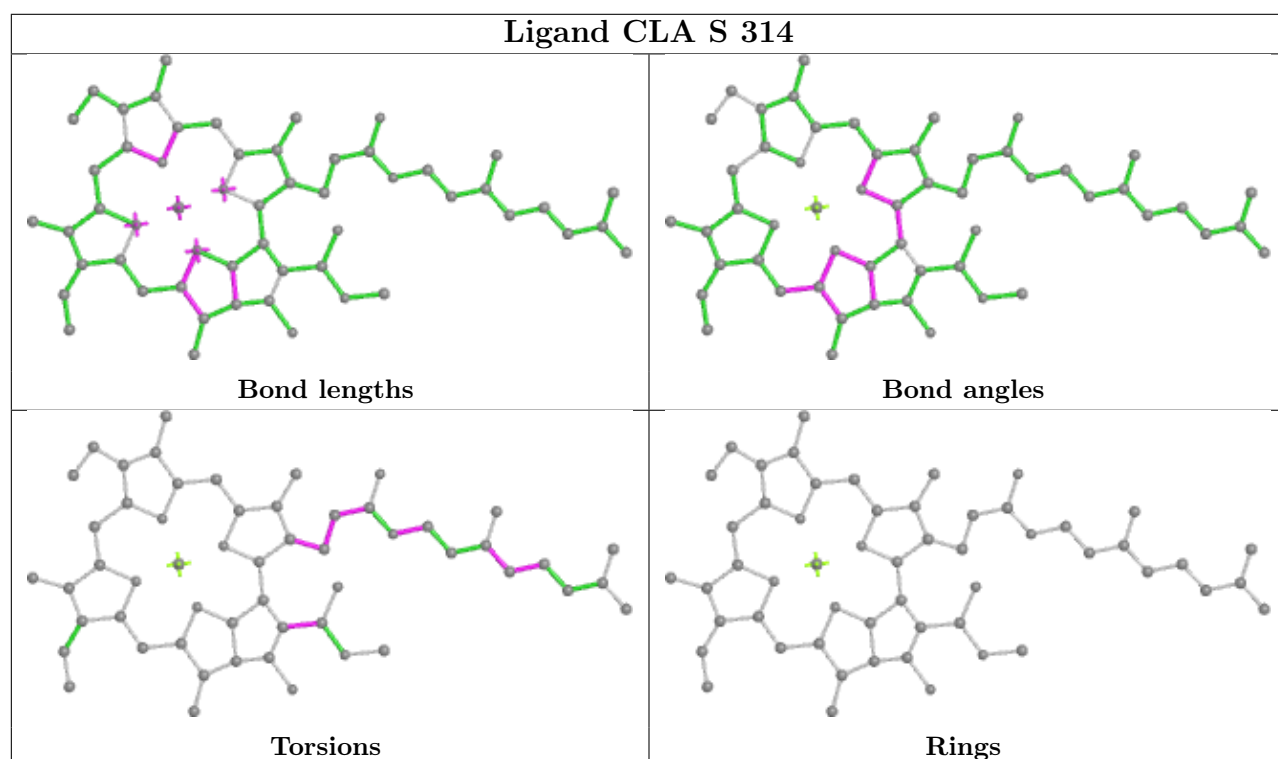
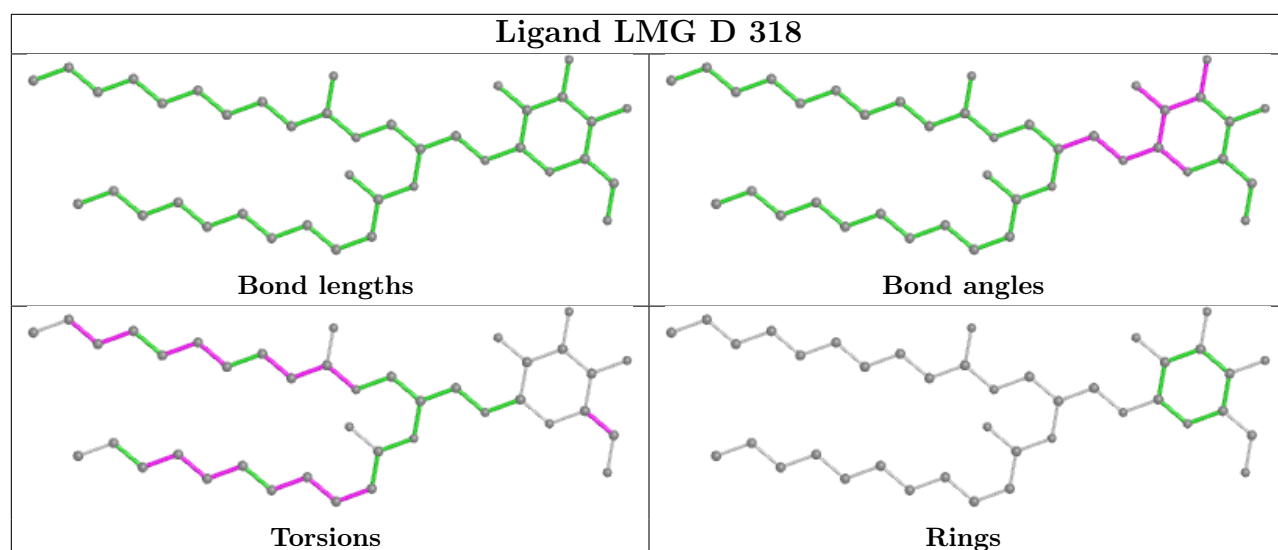


Ligand CLA p 308

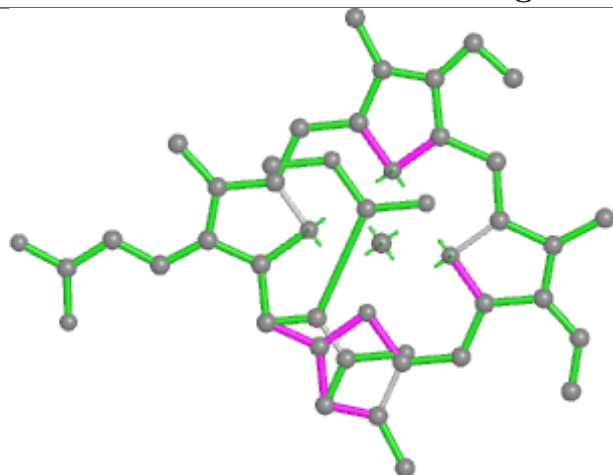


Ligand CLA K 304

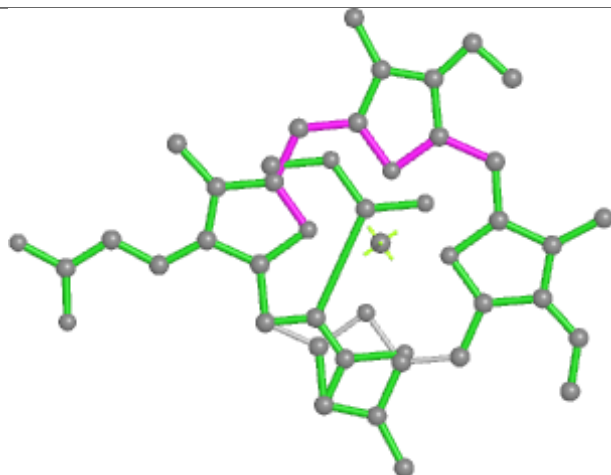




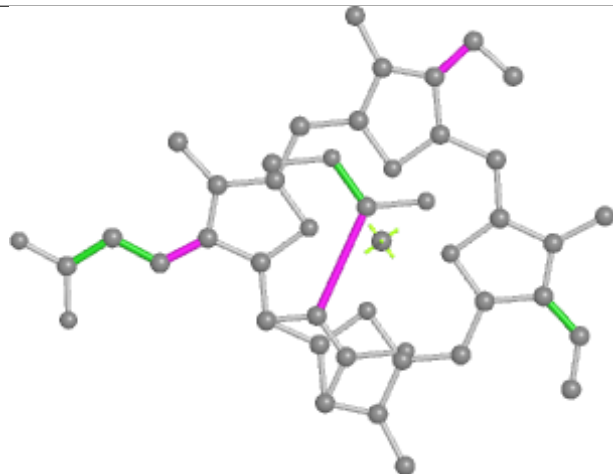
Ligand KC2 G 208



Bond lengths



Bond angles

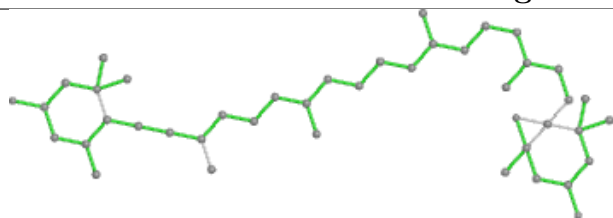


Torsions

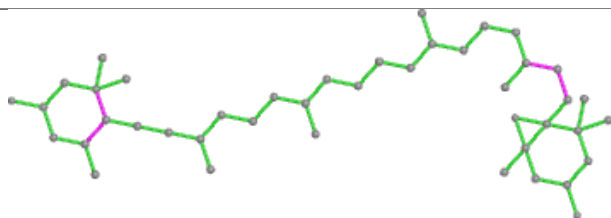


Rings

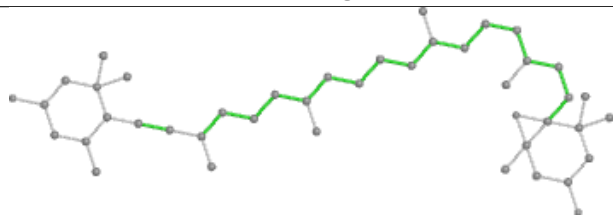
Ligand DD6 A 312



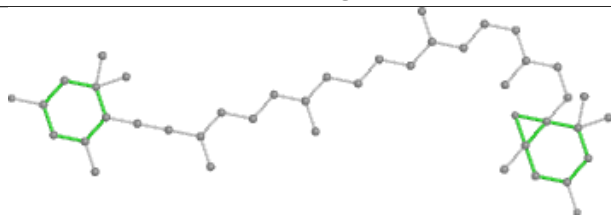
Bond lengths



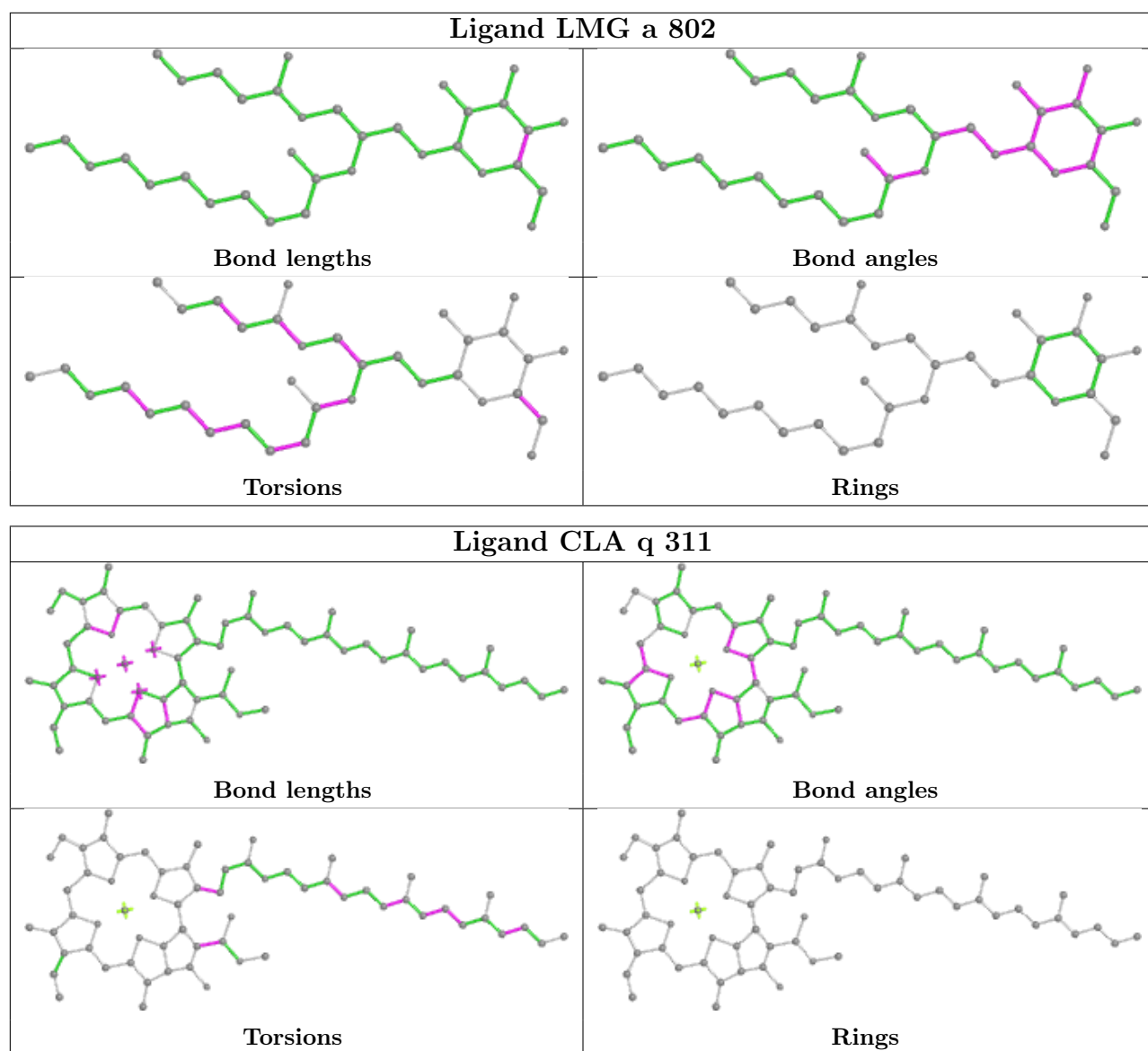
Bond angles



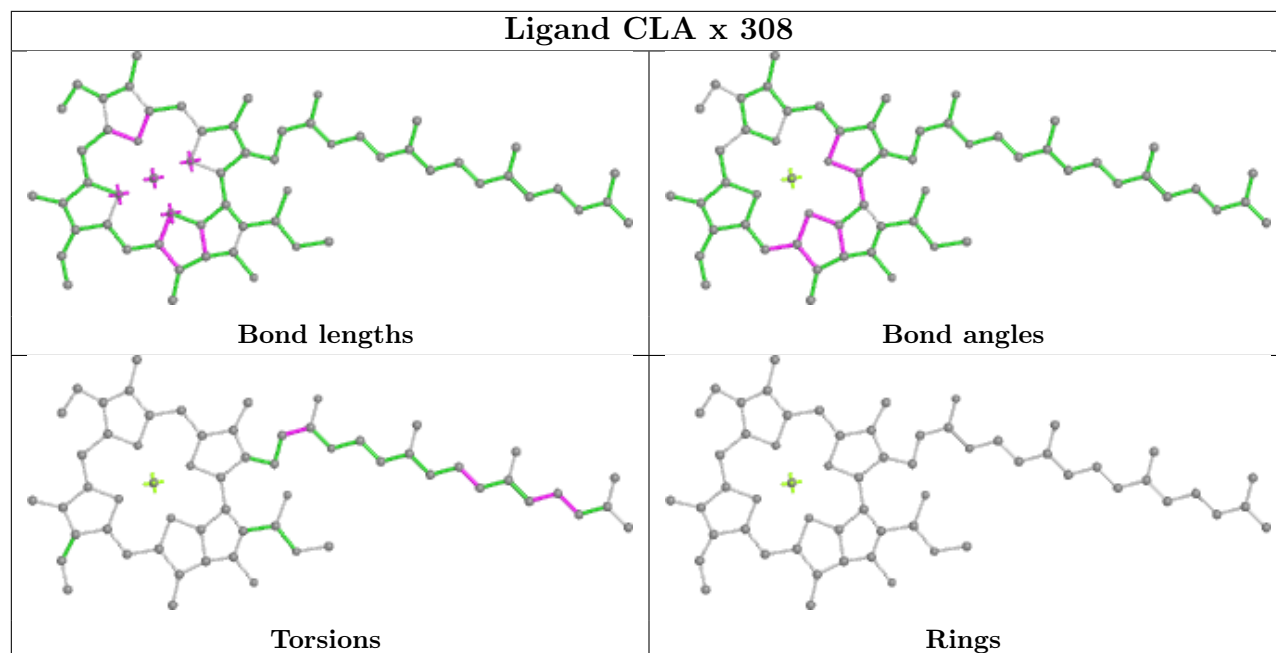
Torsions



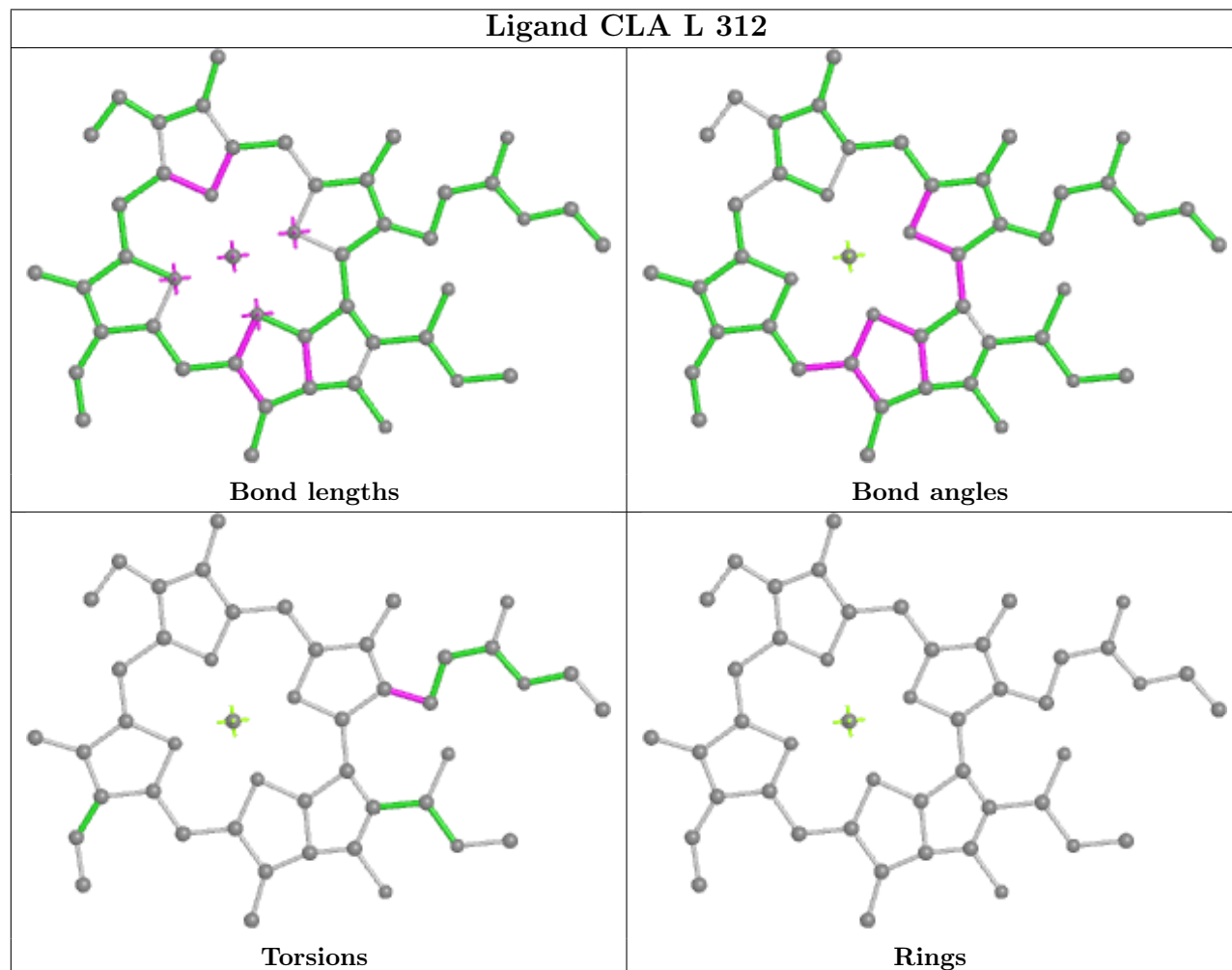
Rings

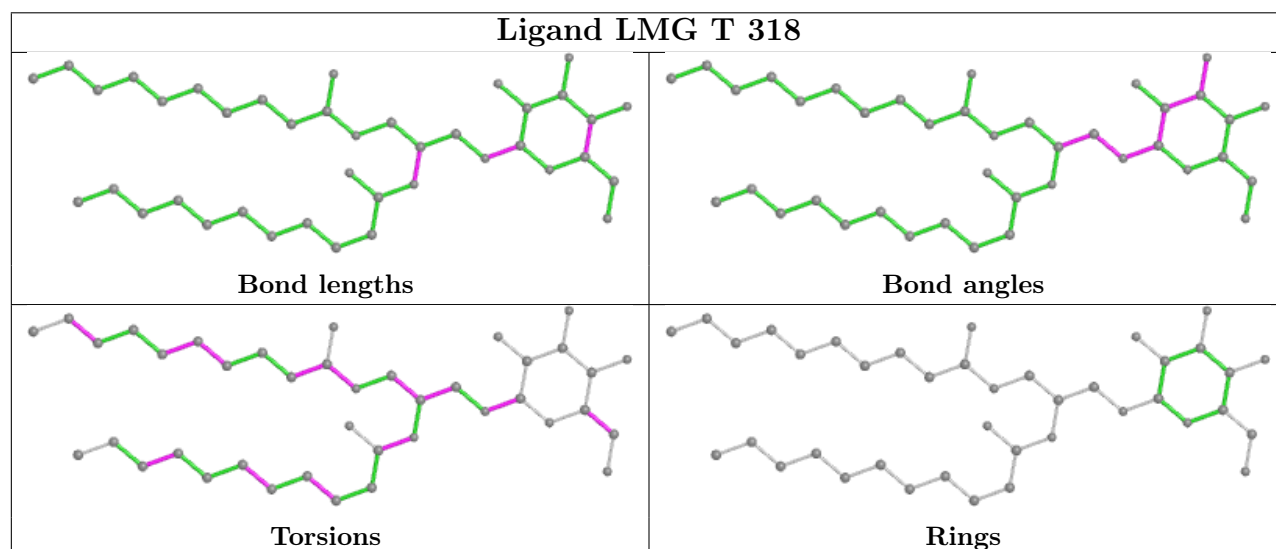
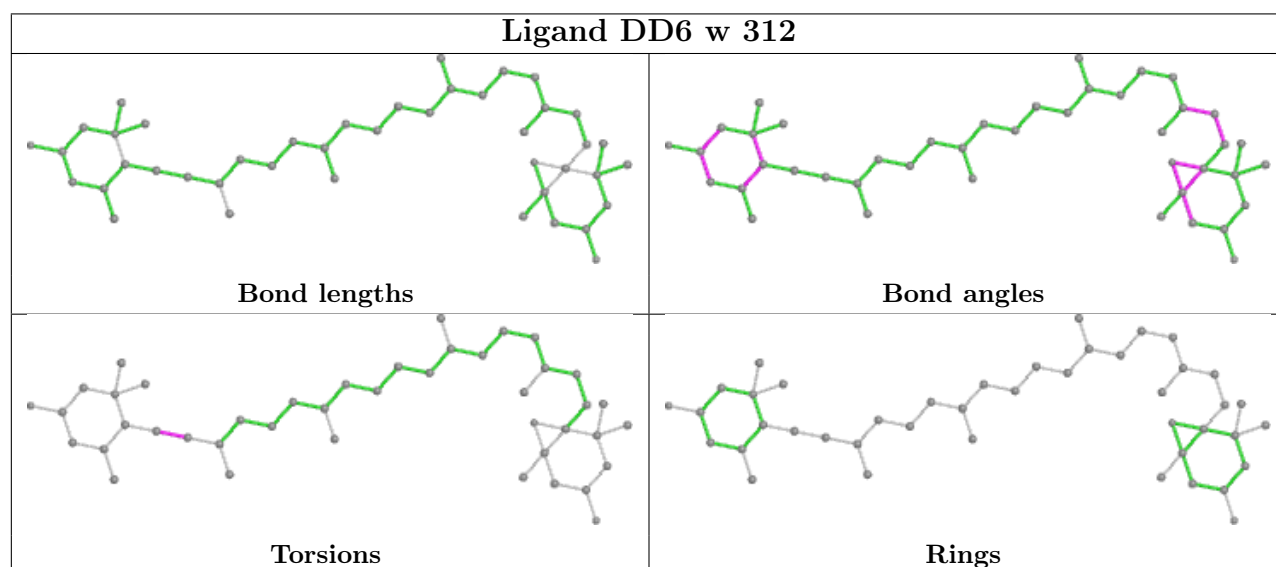
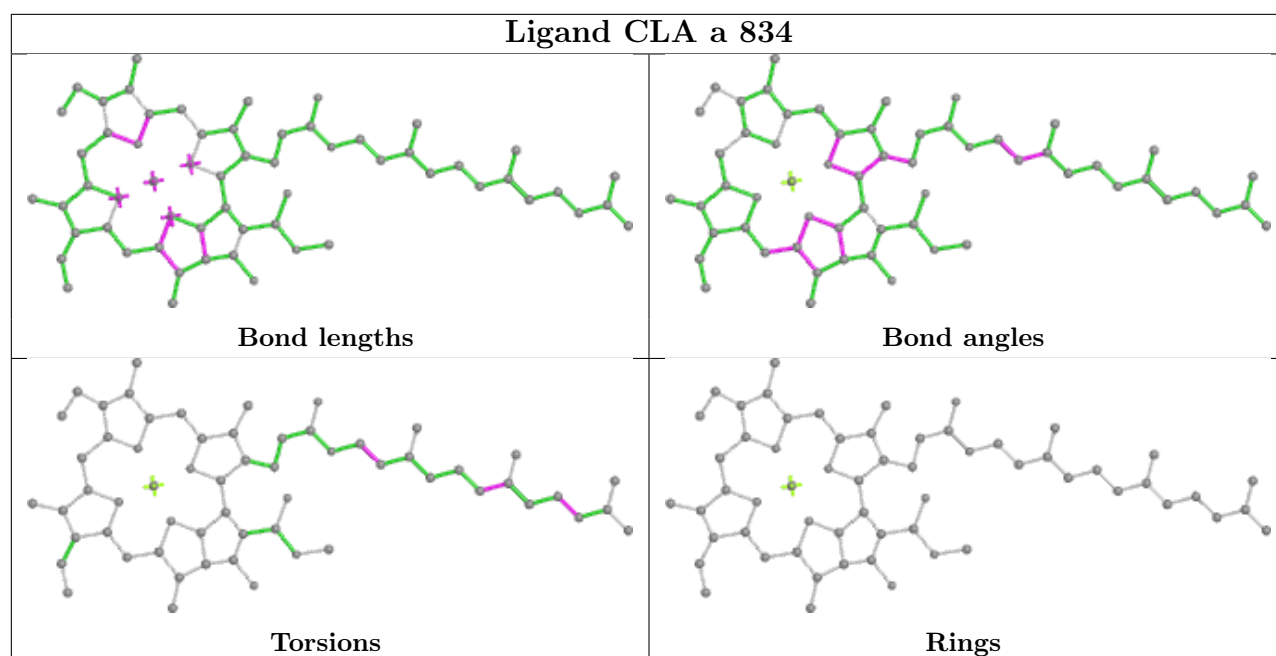


Ligand CLA x 308

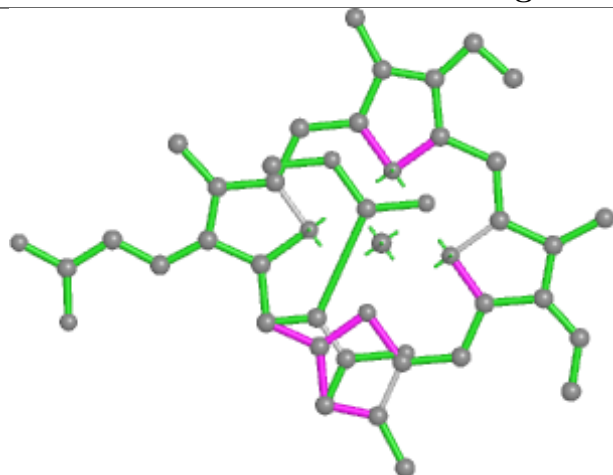


Ligand CLA L 312

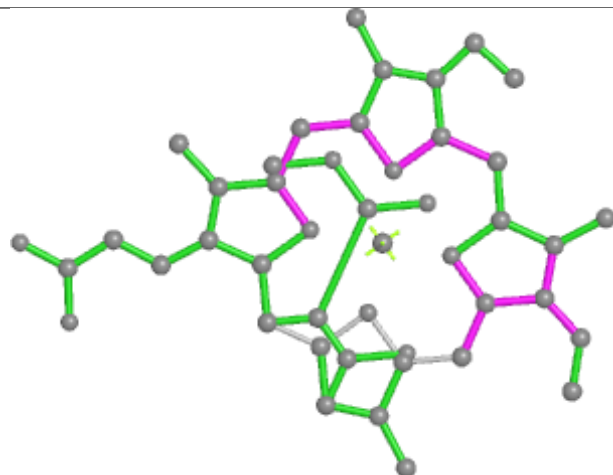




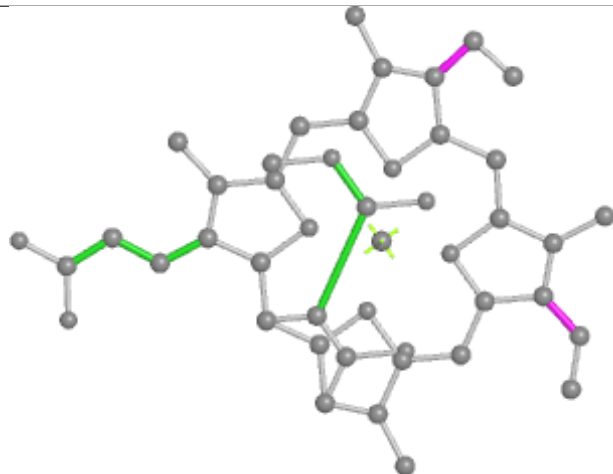
Ligand KC2 N 303



Bond lengths



Bond angles

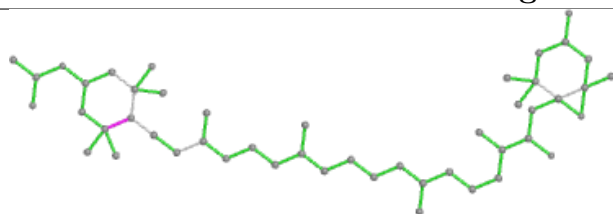


Torsions

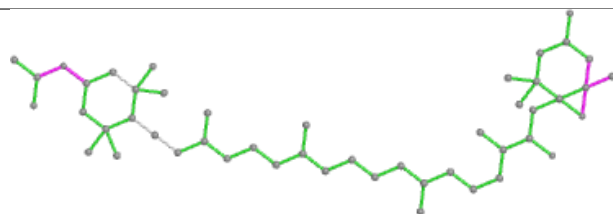


Rings

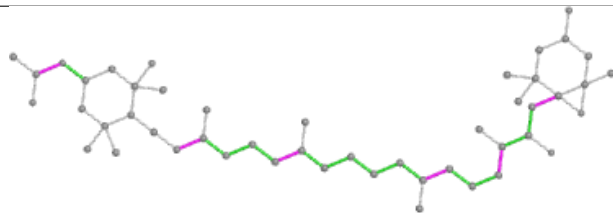
Ligand A86 Y 318



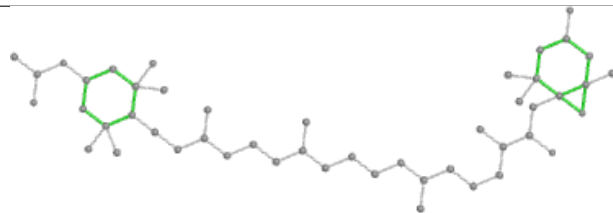
Bond lengths



Bond angles

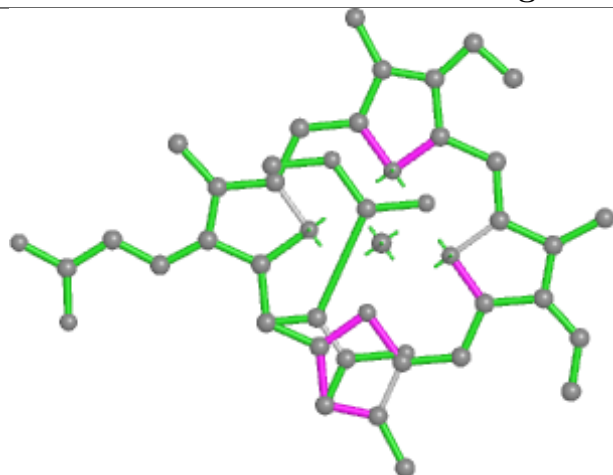


Torsions

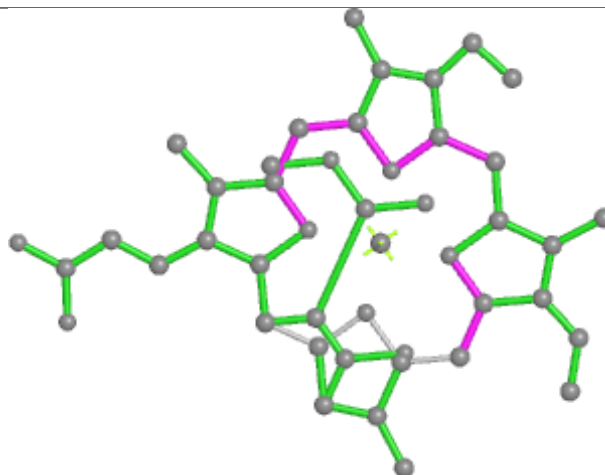


Rings

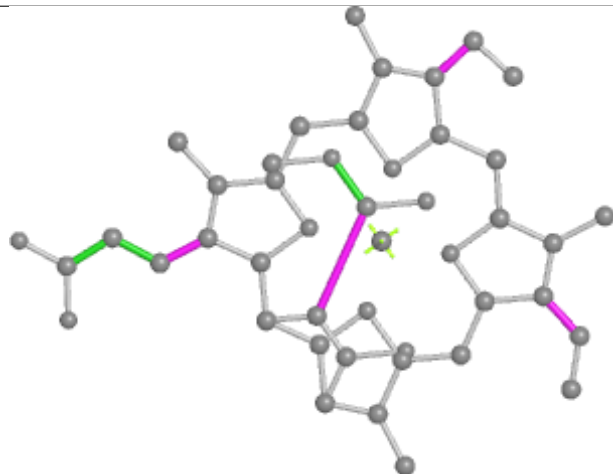
Ligand KC2 L 313



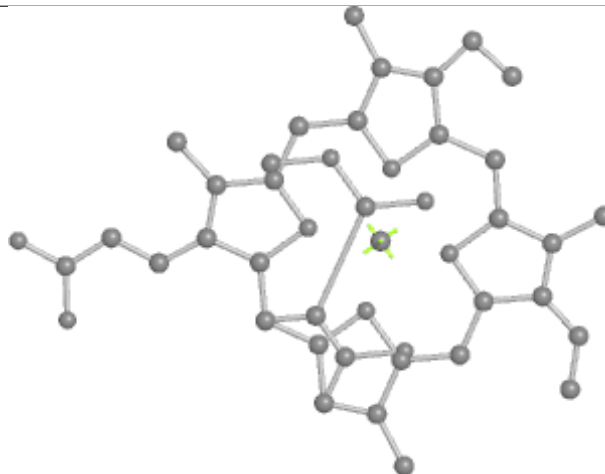
Bond lengths



Bond angles

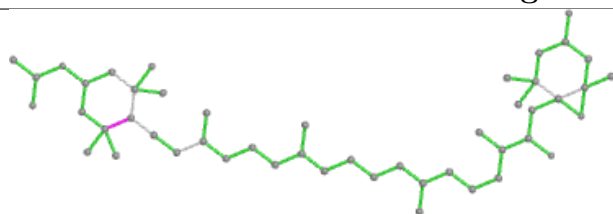


Torsions

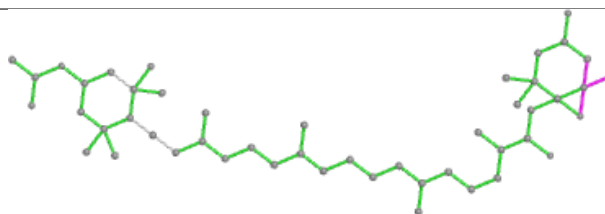


Rings

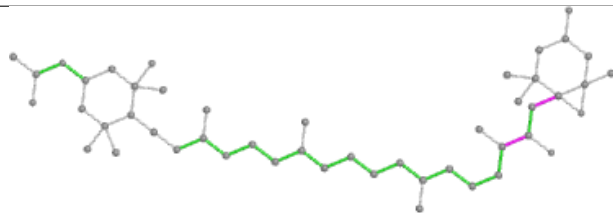
Ligand A86 P 321



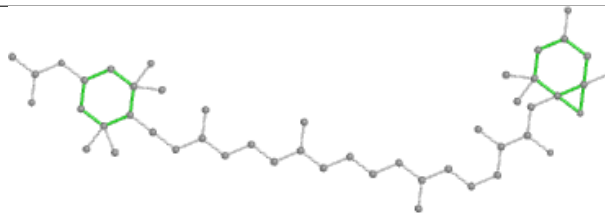
Bond lengths



Bond angles

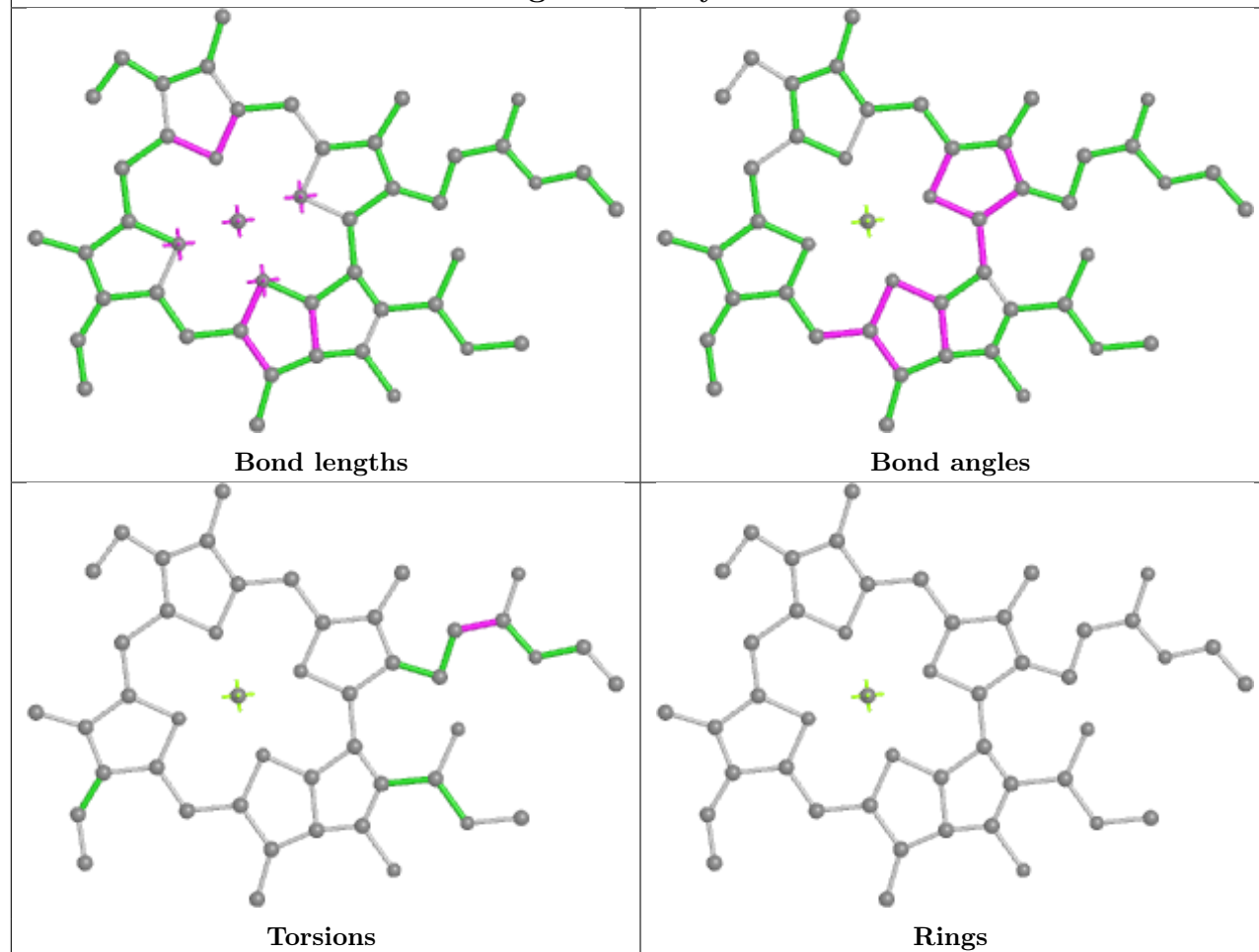


Torsions

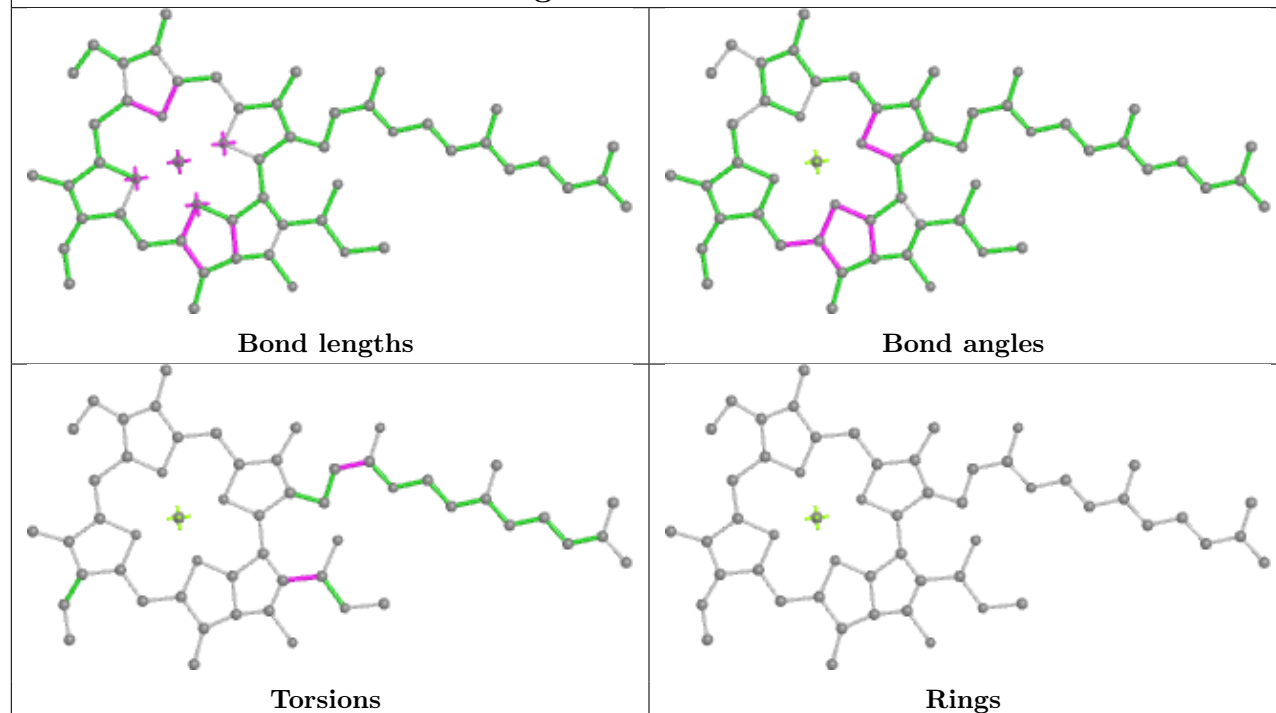


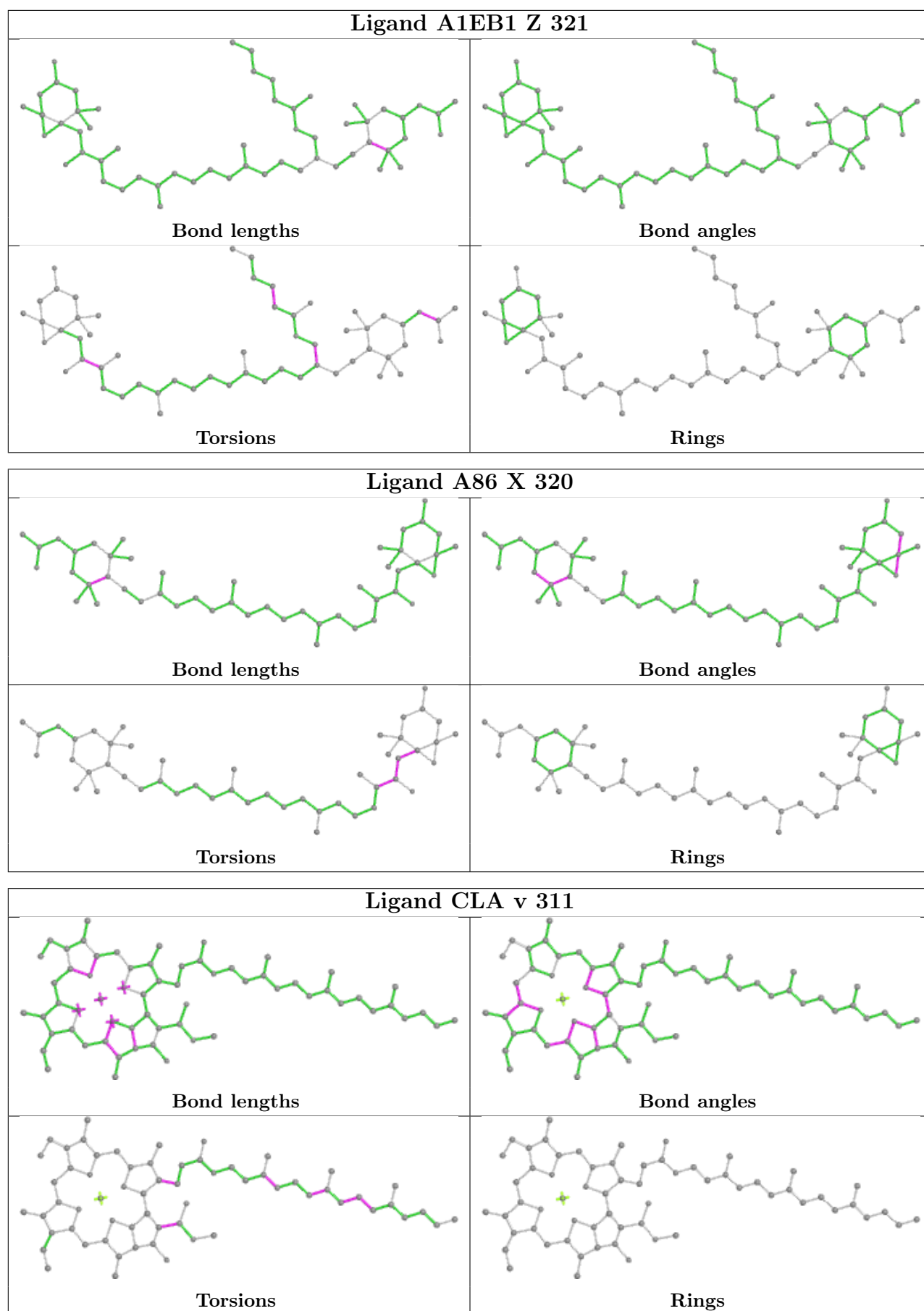
Rings

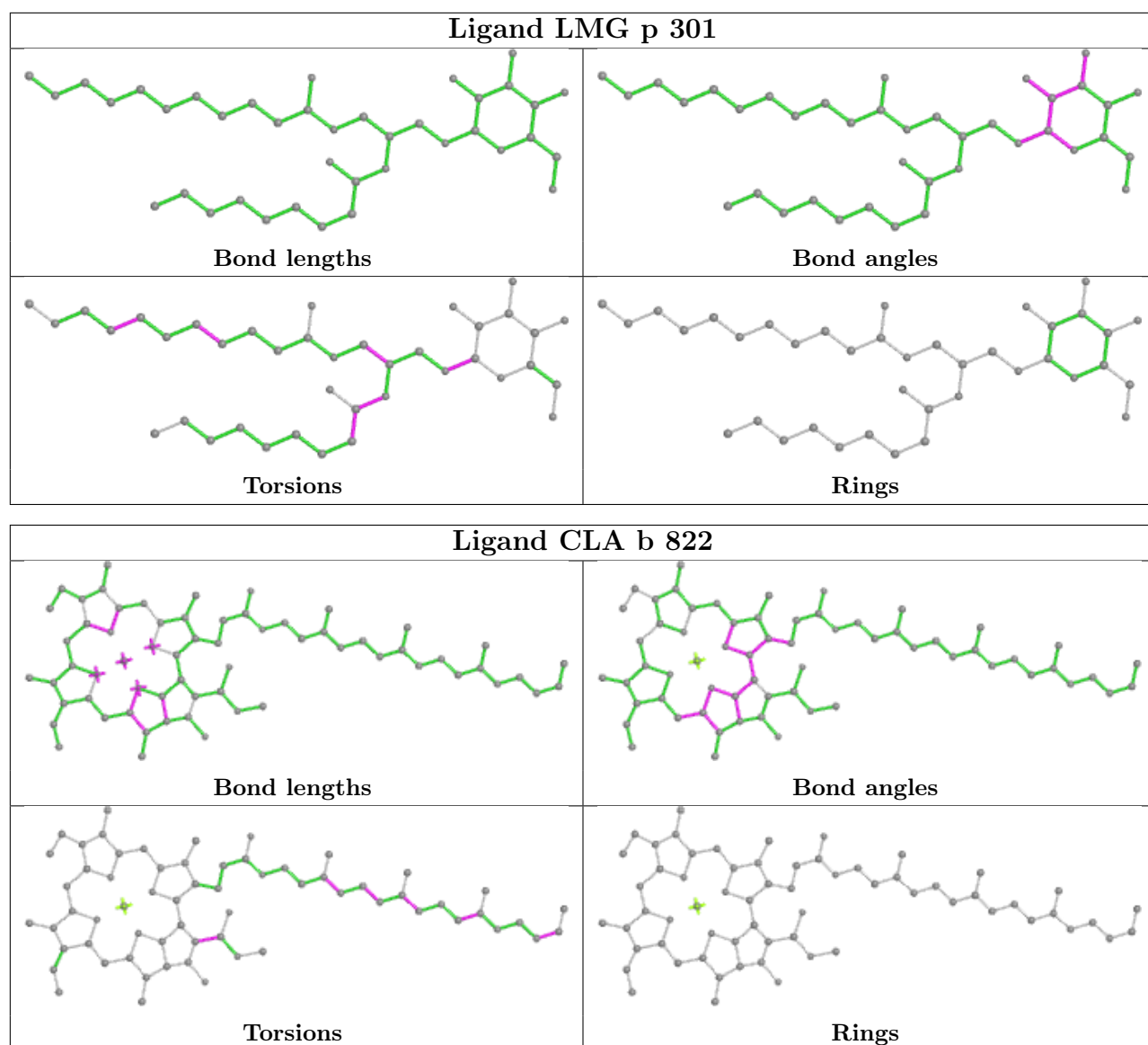
Ligand CLA y 302

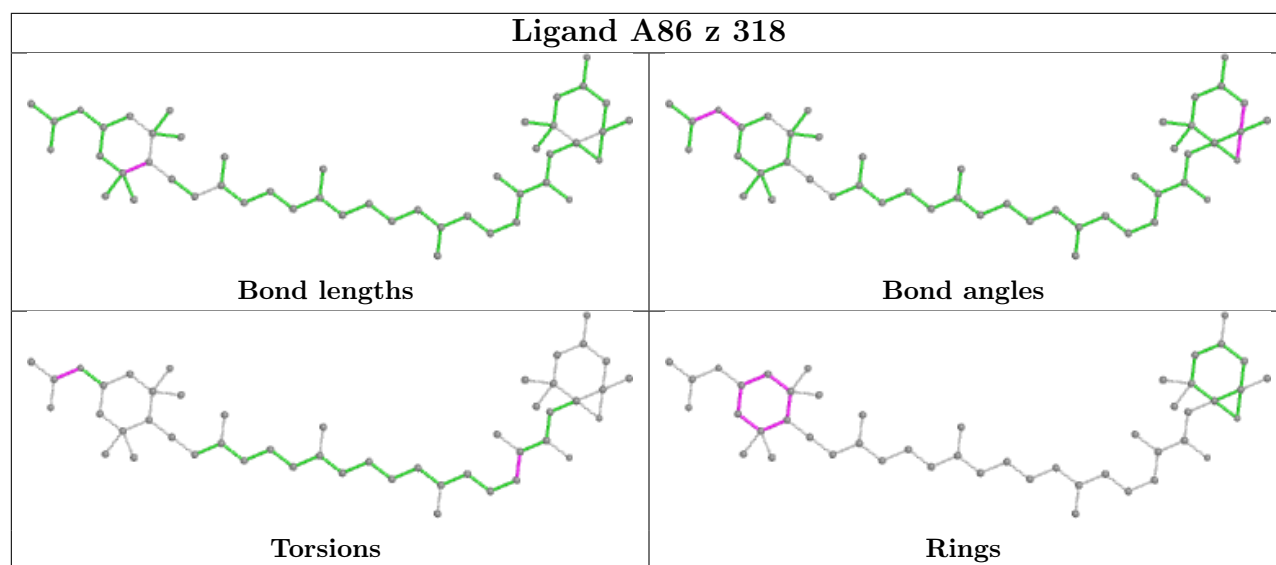
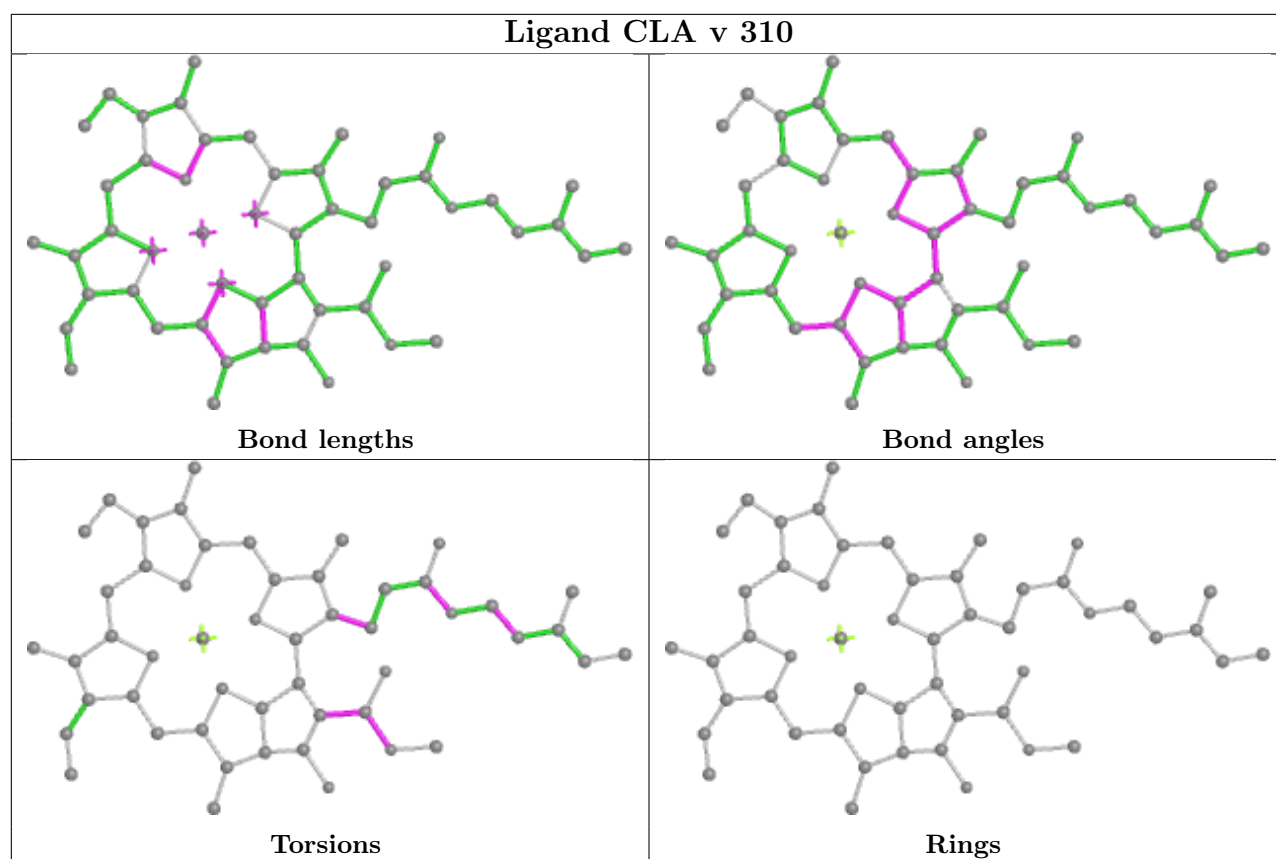


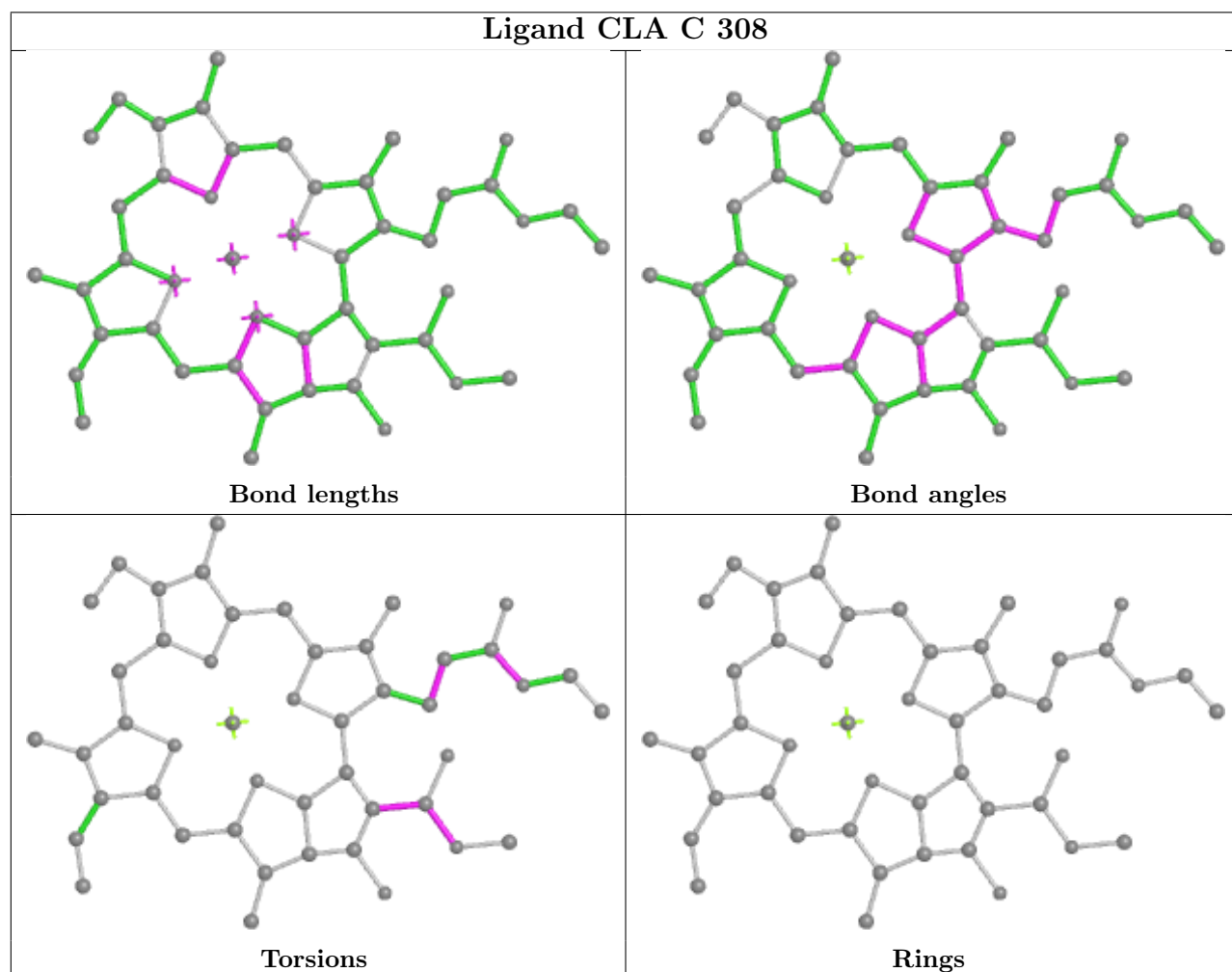
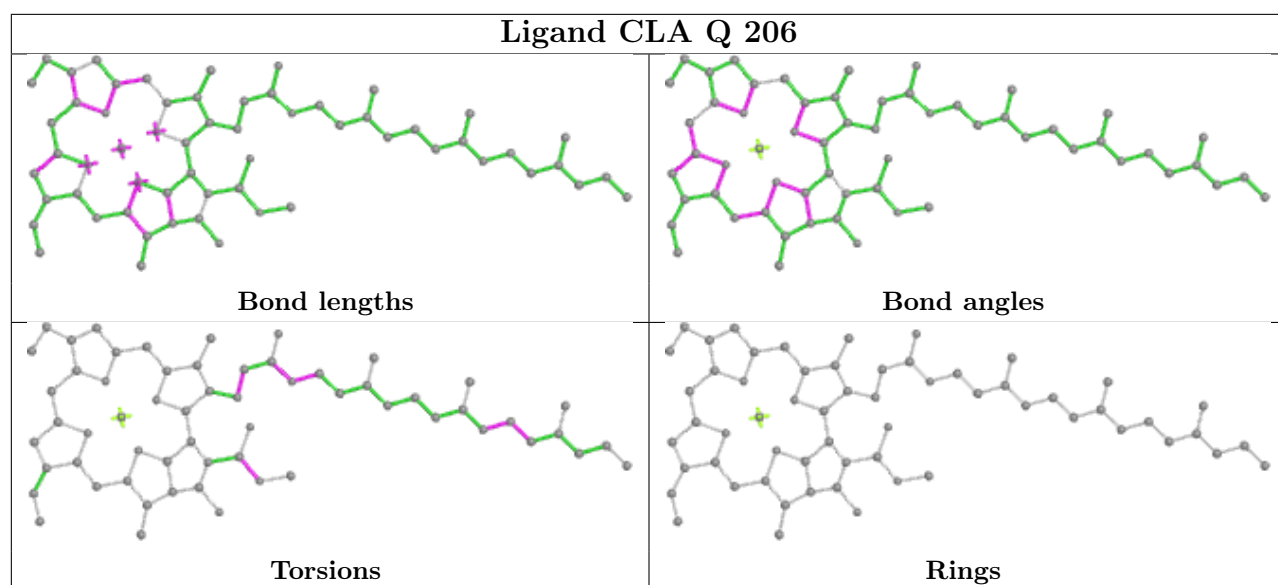
Ligand CLA L 307



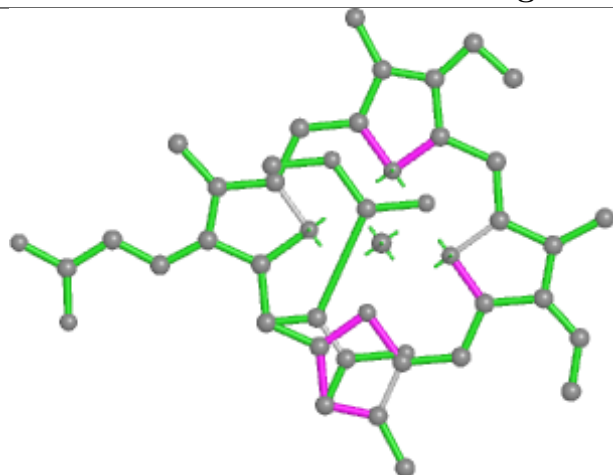




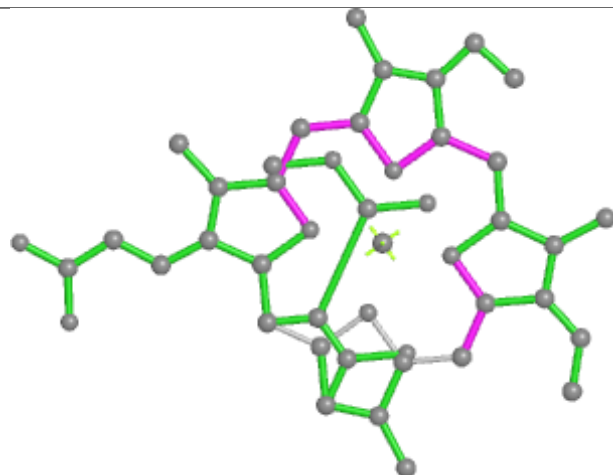




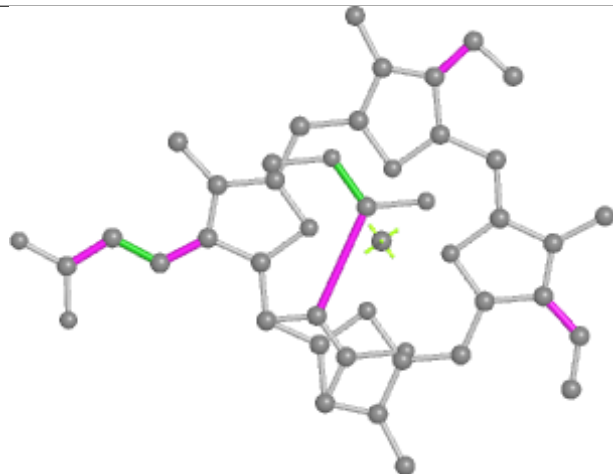
Ligand KC2 E 319



Bond lengths



Bond angles

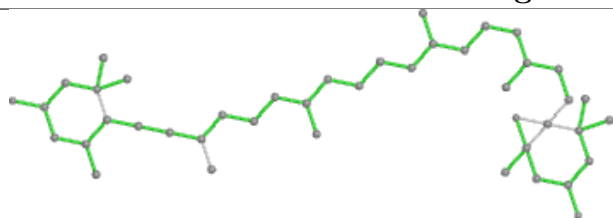


Torsions

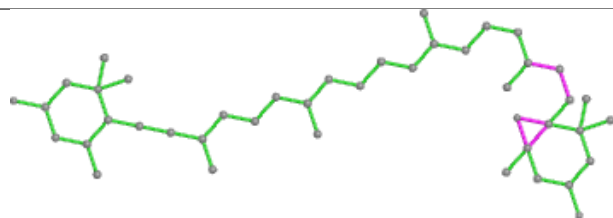


Rings

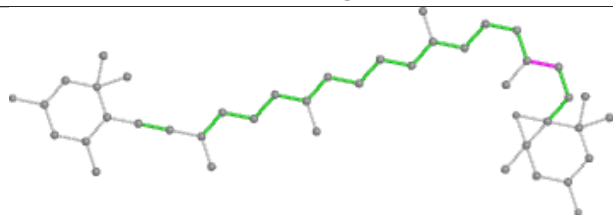
Ligand DD6 A 313



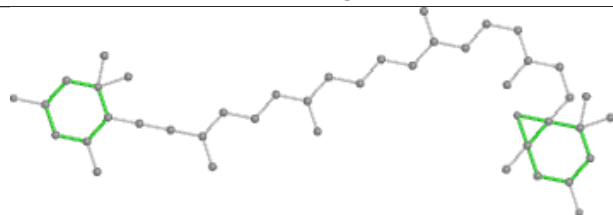
Bond lengths



Bond angles

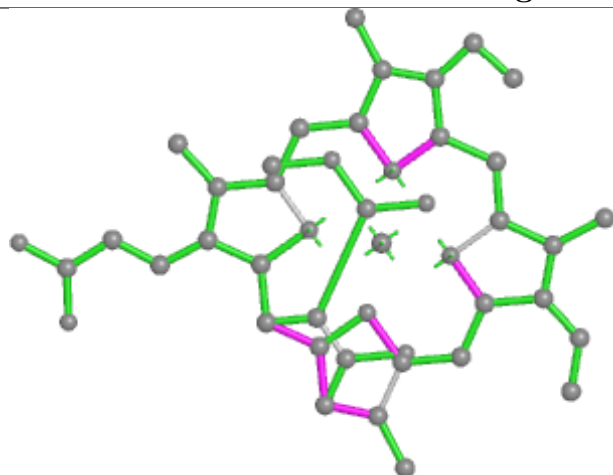


Torsions

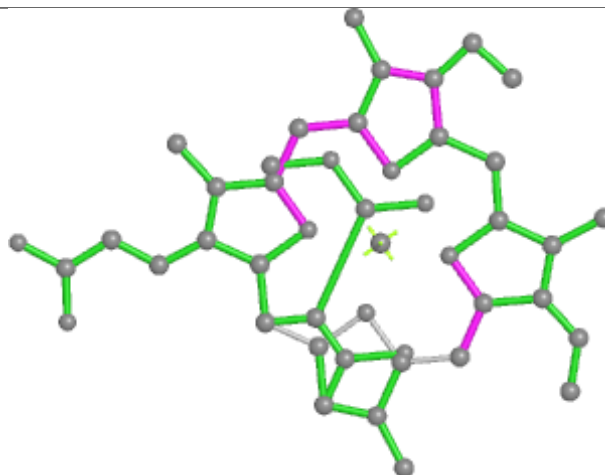


Rings

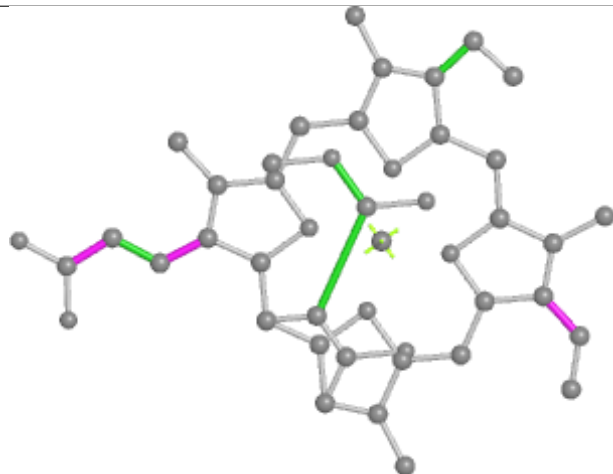
Ligand KC2 Y 302



Bond lengths



Bond angles

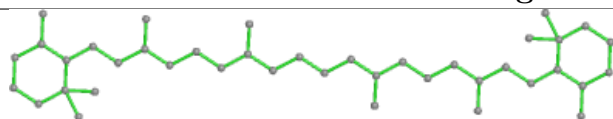


Torsions

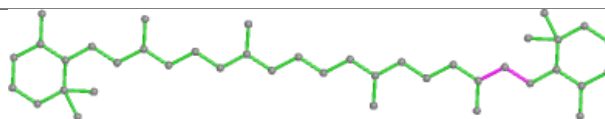


Rings

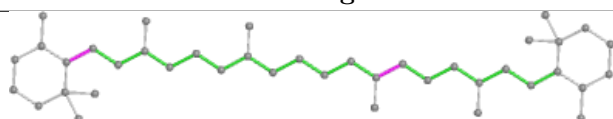
Ligand BCR k 203



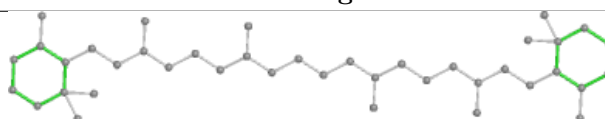
Bond lengths



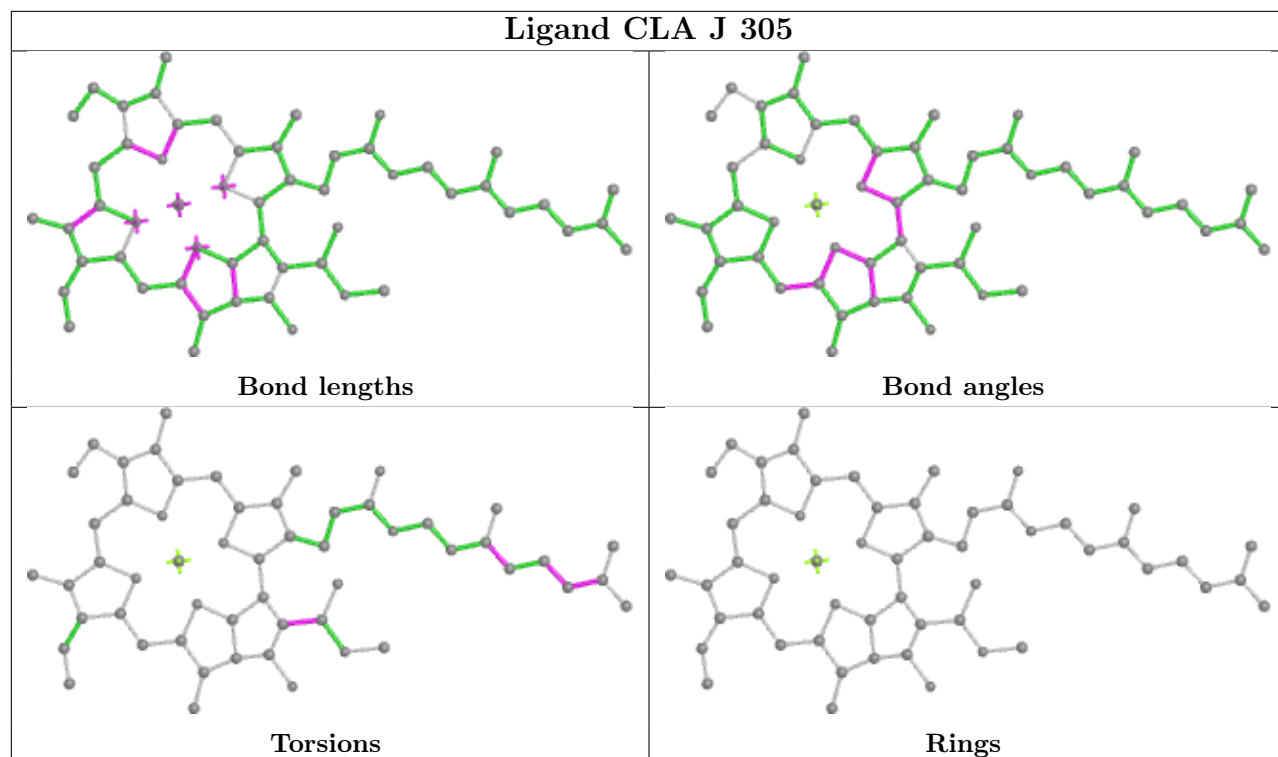
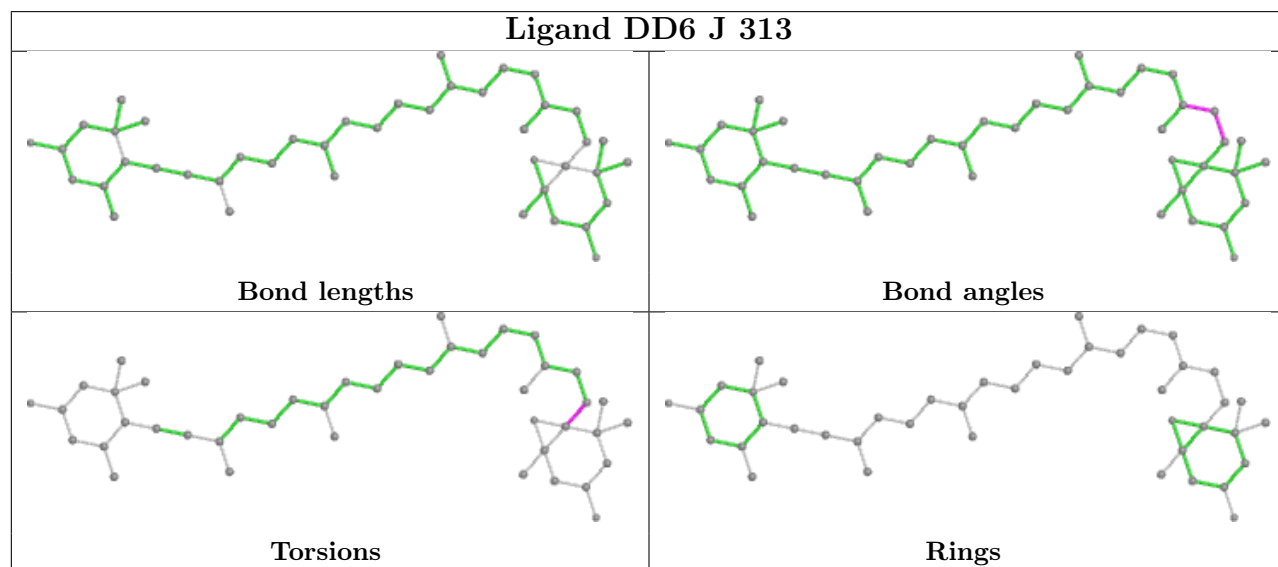
Bond angles



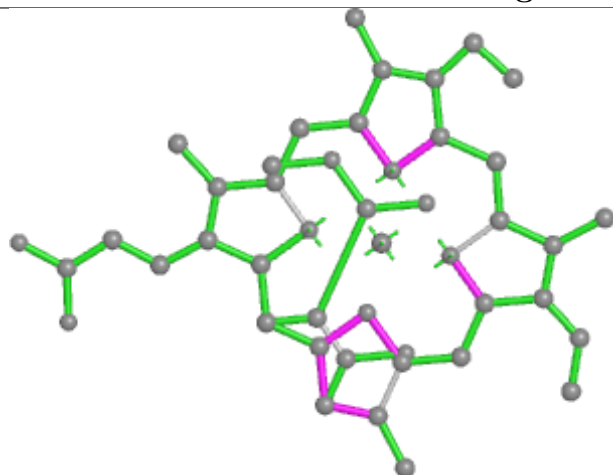
Torsions



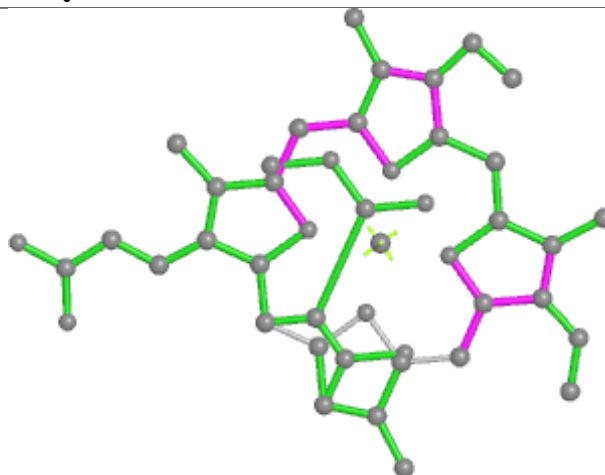
Rings

Ligand CLA J 305**Ligand DD6 J 313**

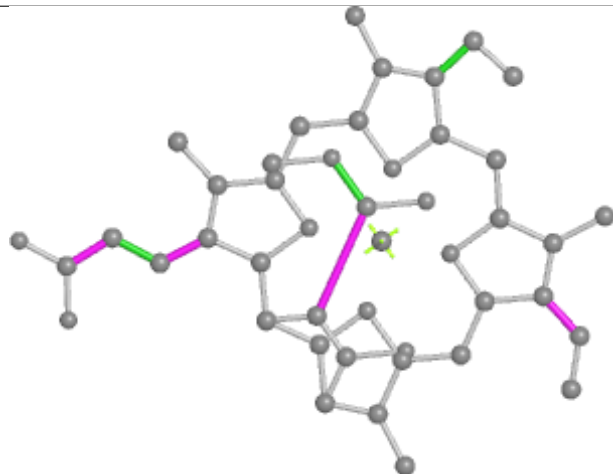
Ligand KC2 Q 216



Bond lengths



Bond angles

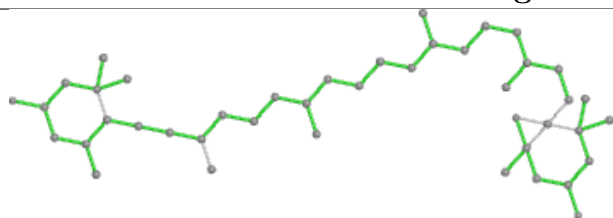


Torsions

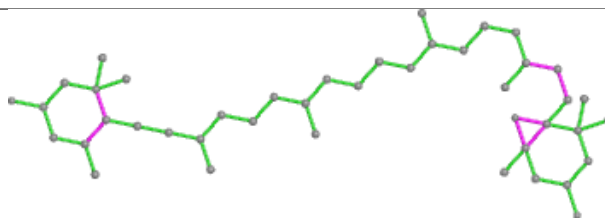


Rings

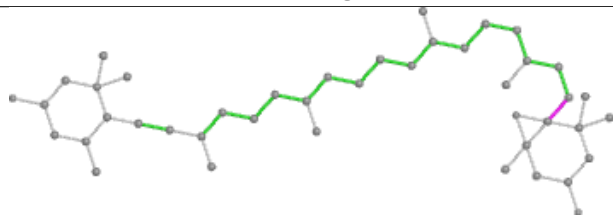
Ligand DD6 N 319



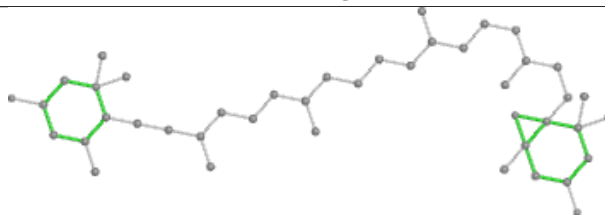
Bond lengths



Bond angles

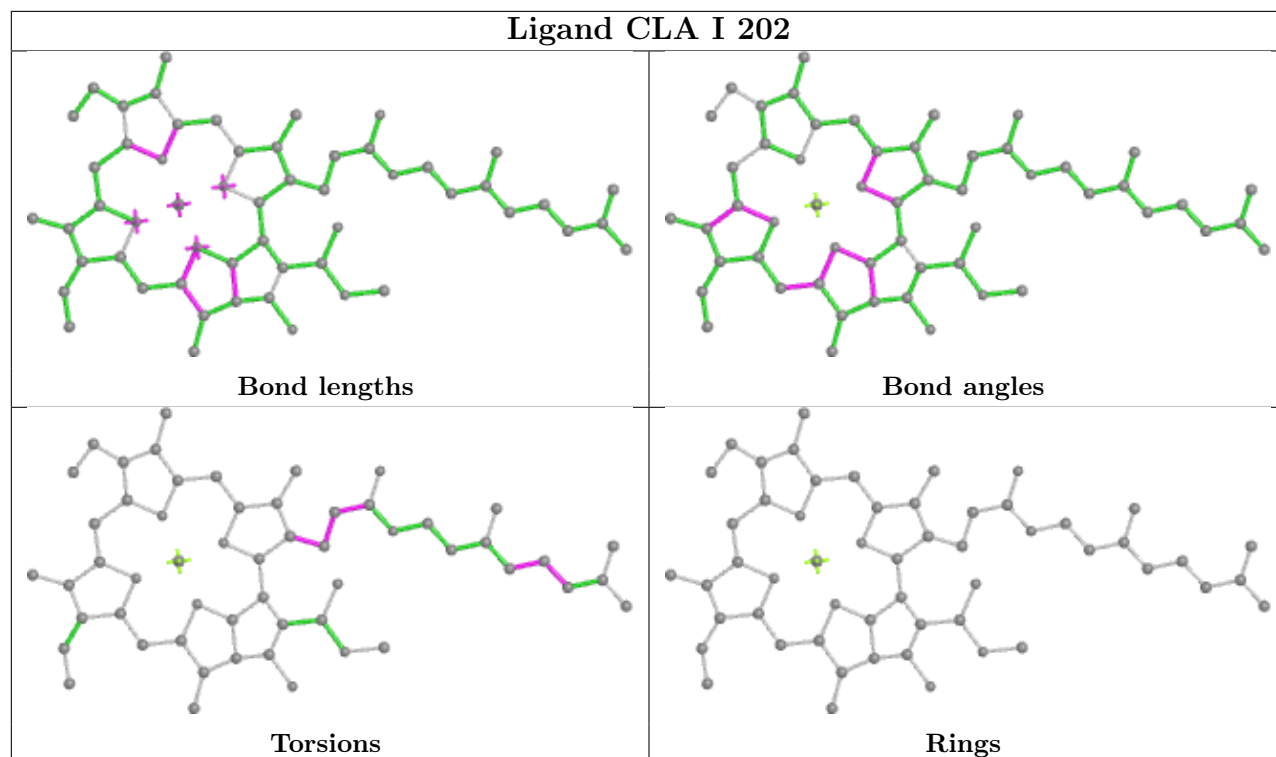


Torsions

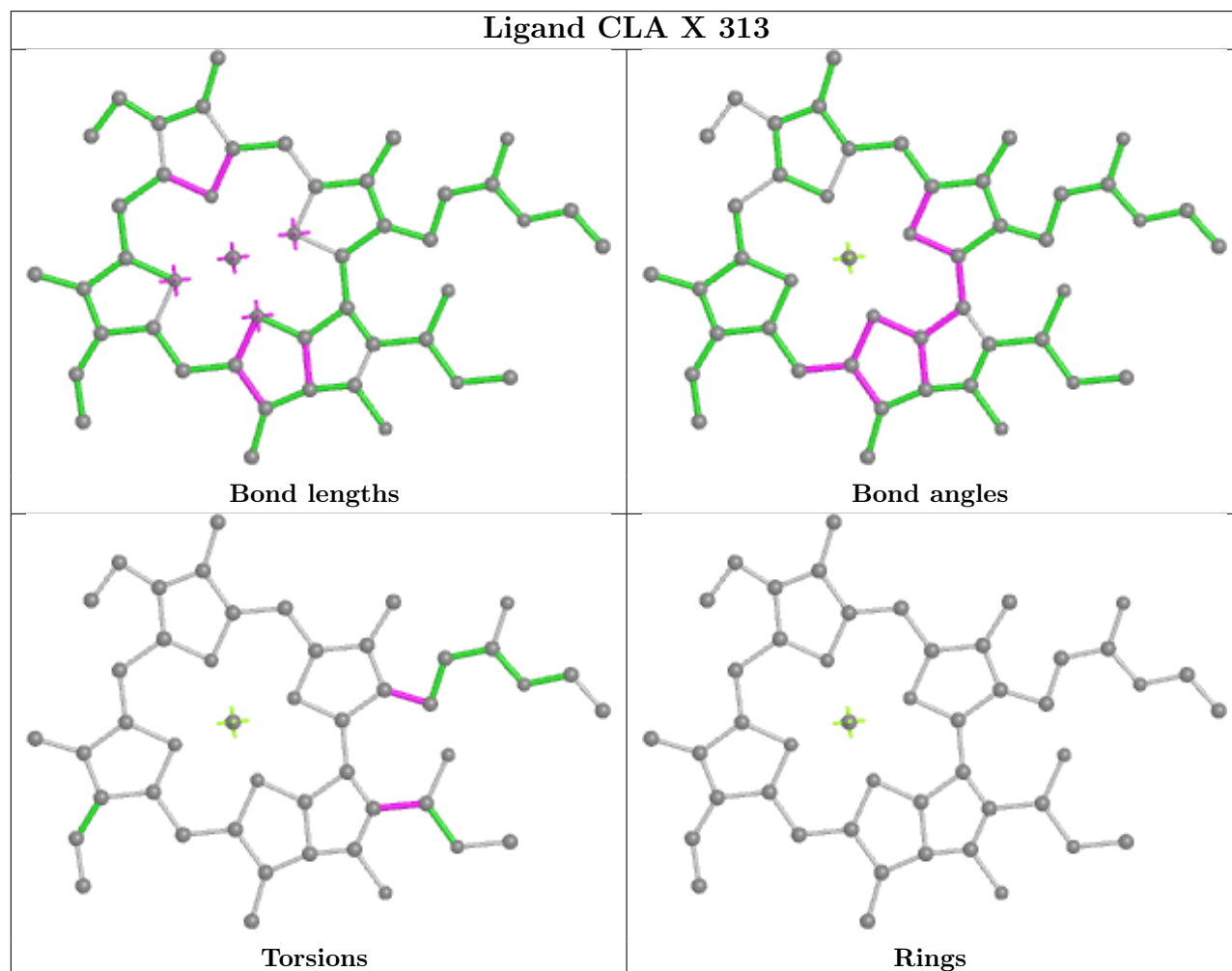


Rings

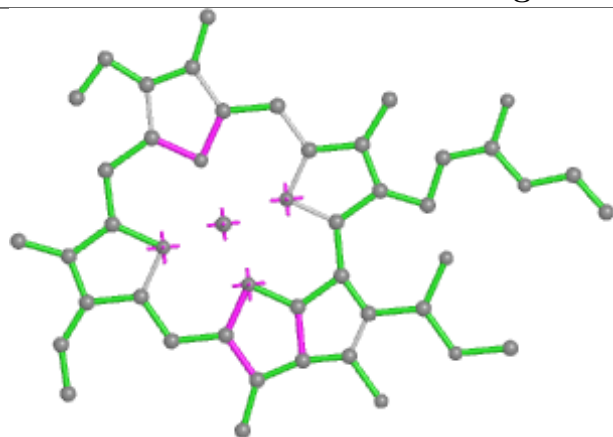
Ligand CLA I 202



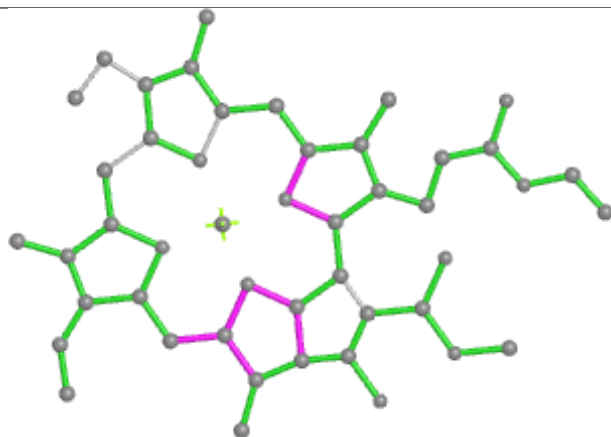
Ligand CLA X 313



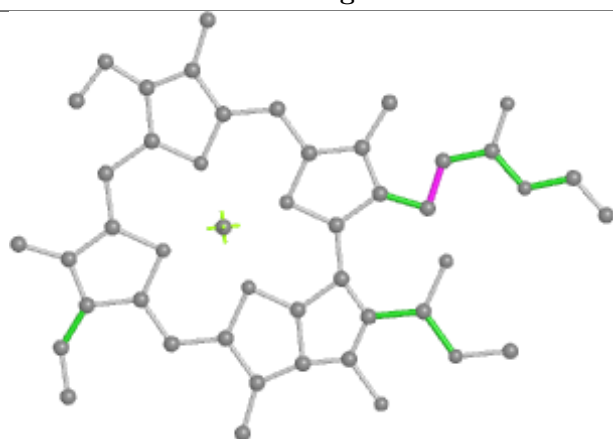
Ligand CLA H 311



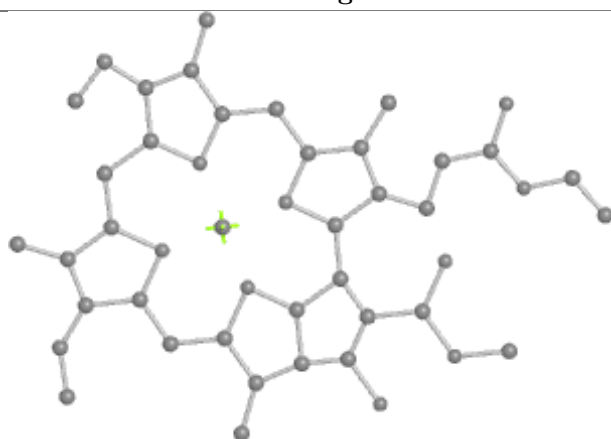
Bond lengths



Bond angles

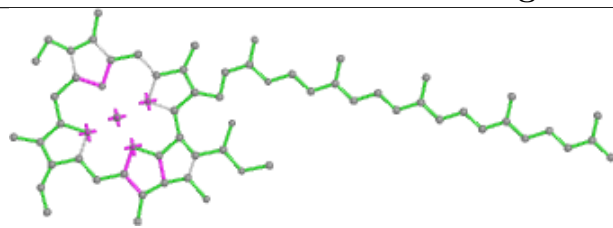


Torsions

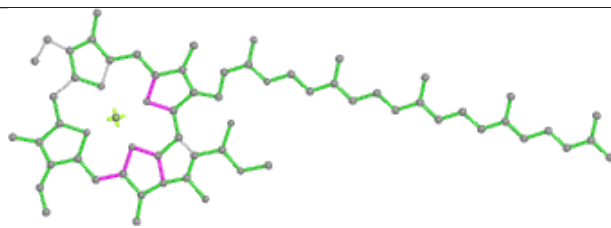


Rings

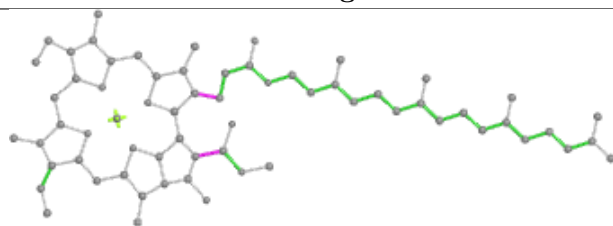
Ligand CLA a 827



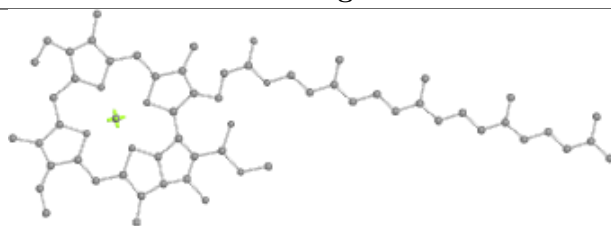
Bond lengths



Bond angles

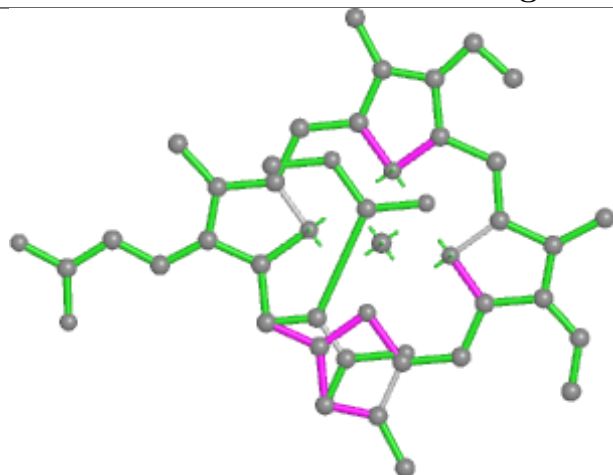


Torsions

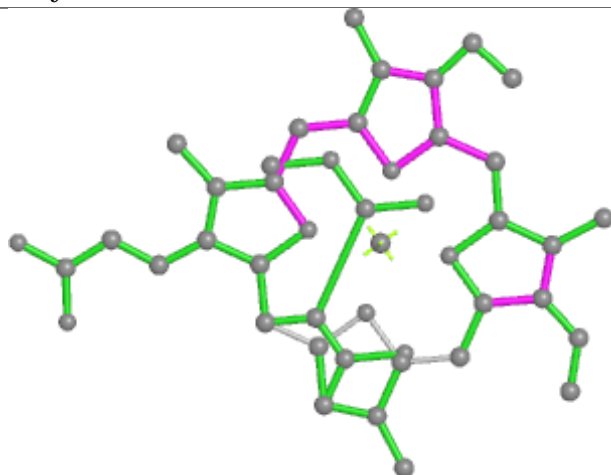


Rings

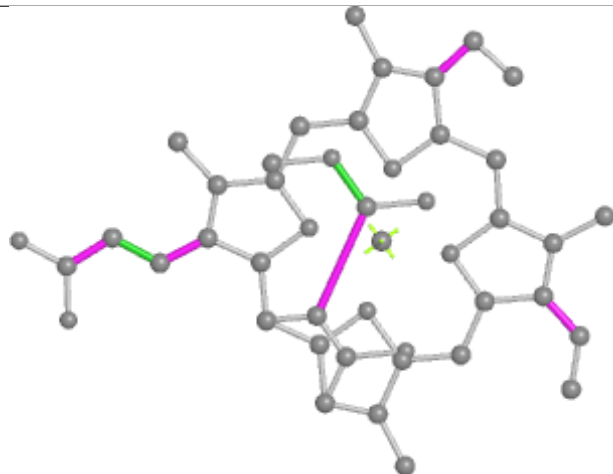
Ligand KC2 y 301



Bond lengths



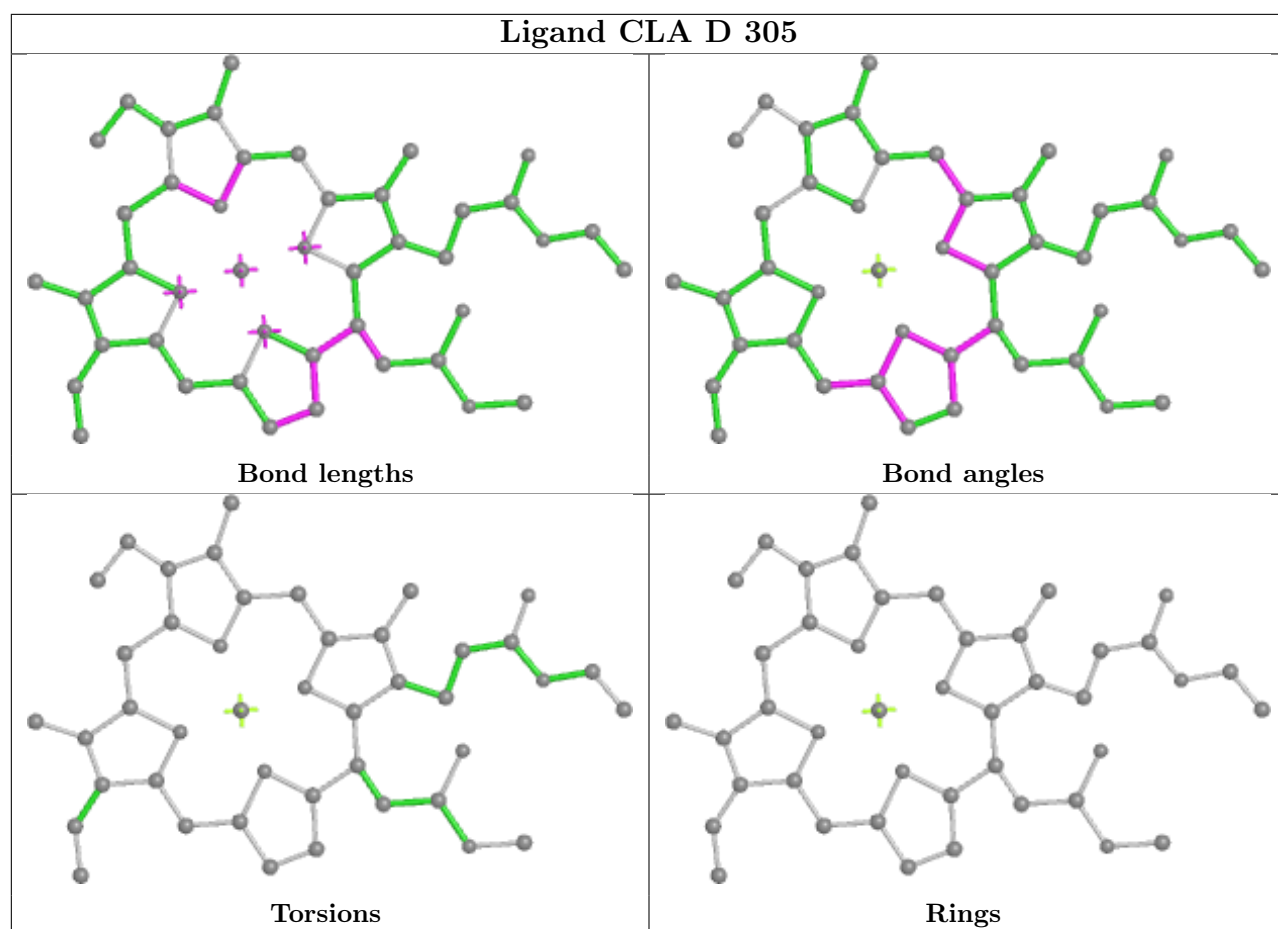
Bond angles



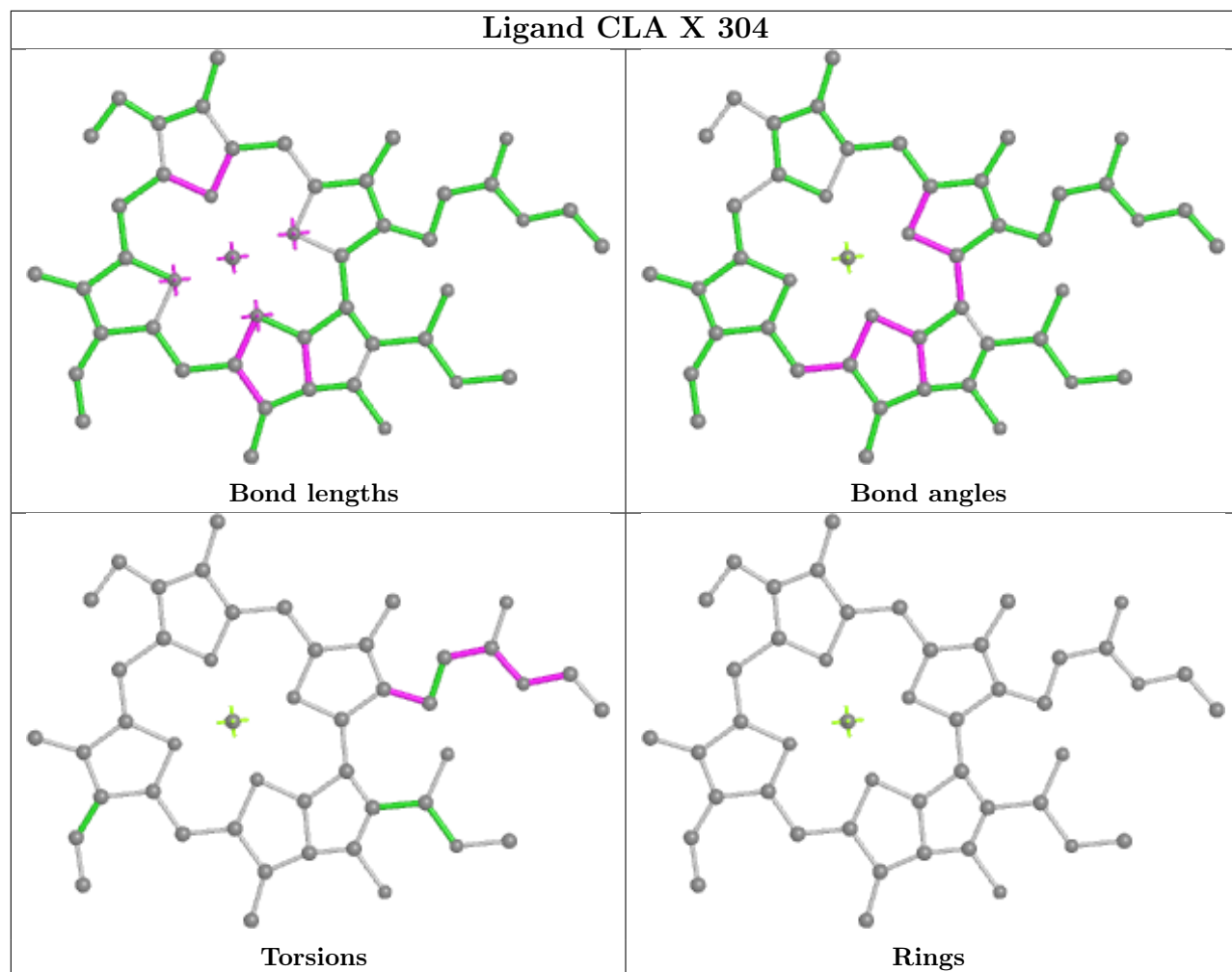
Torsions

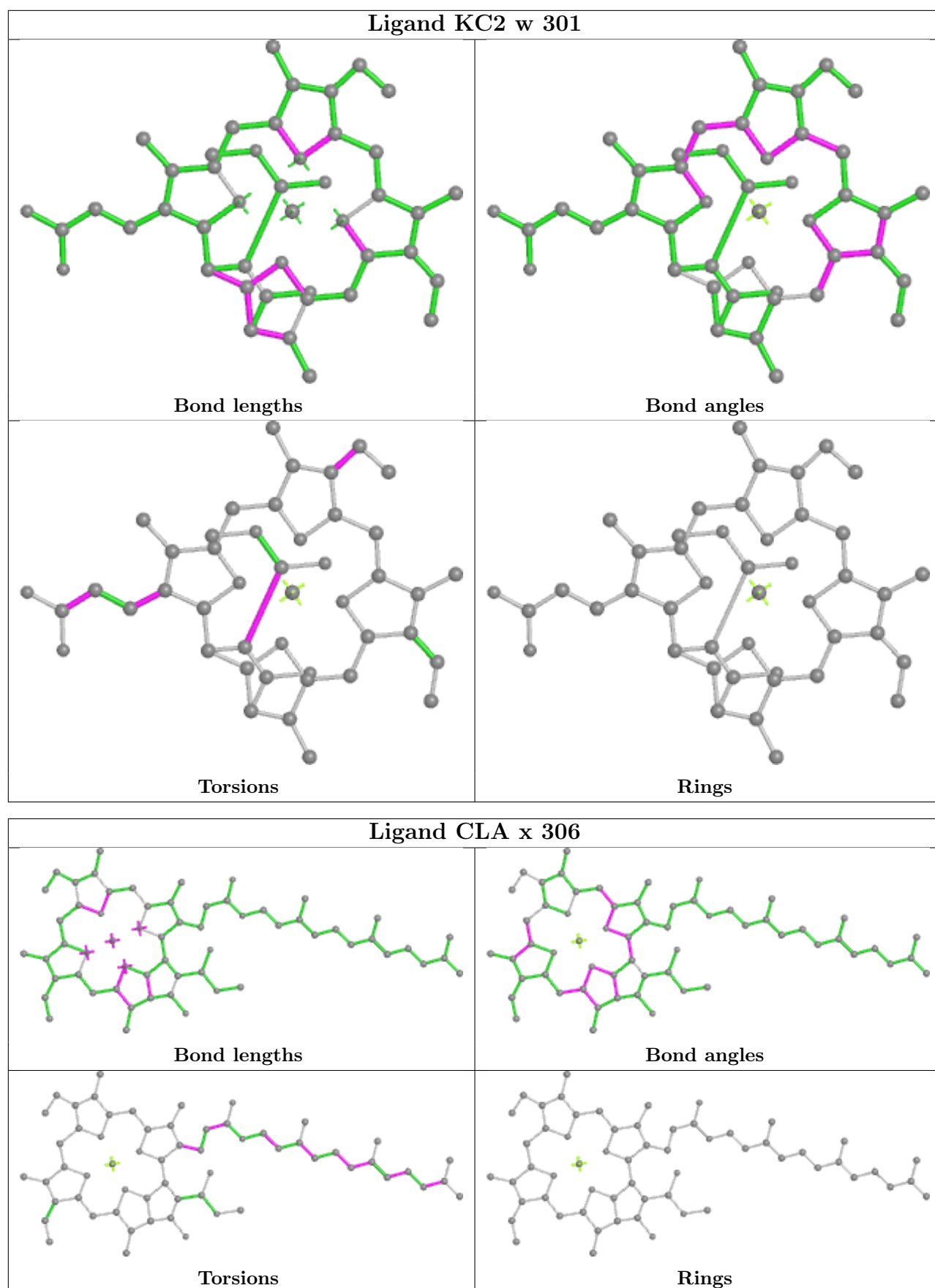


Rings

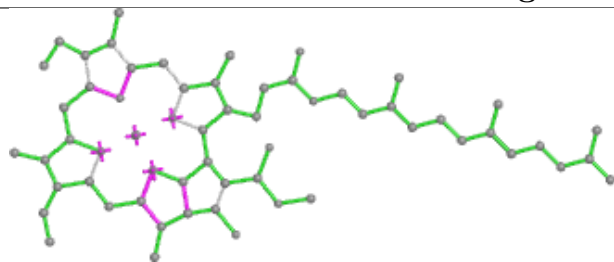


Ligand CLA X 304

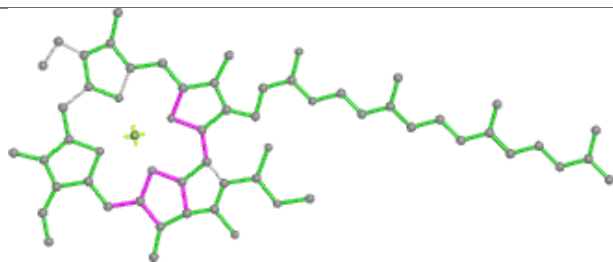




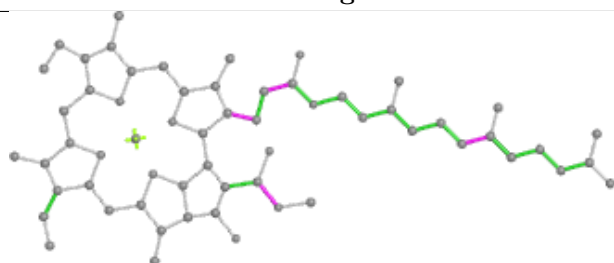
Ligand CLA a 813



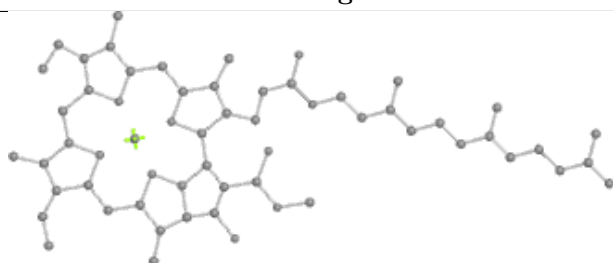
Bond lengths



Bond angles

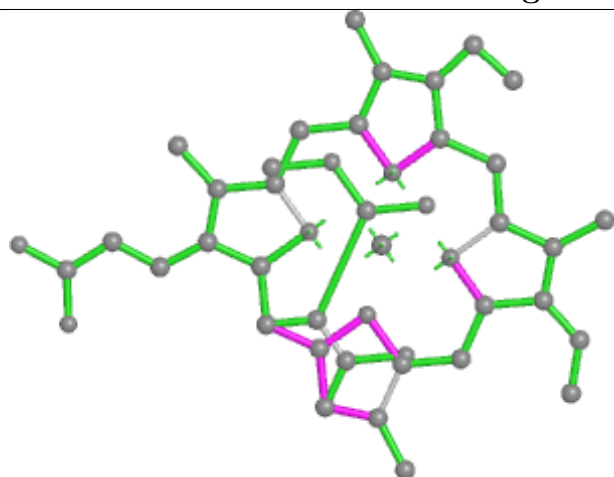


Torsions

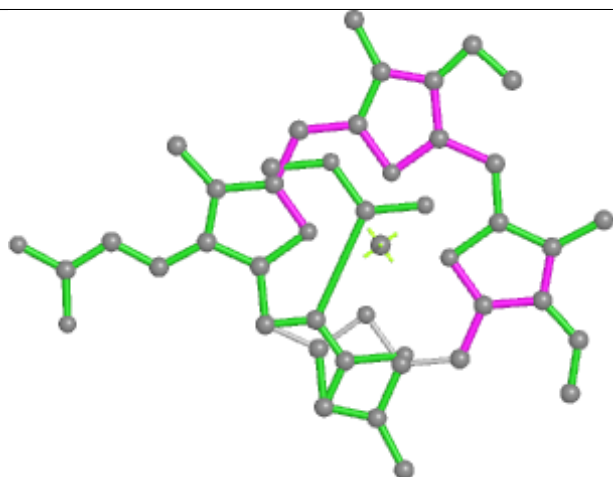


Rings

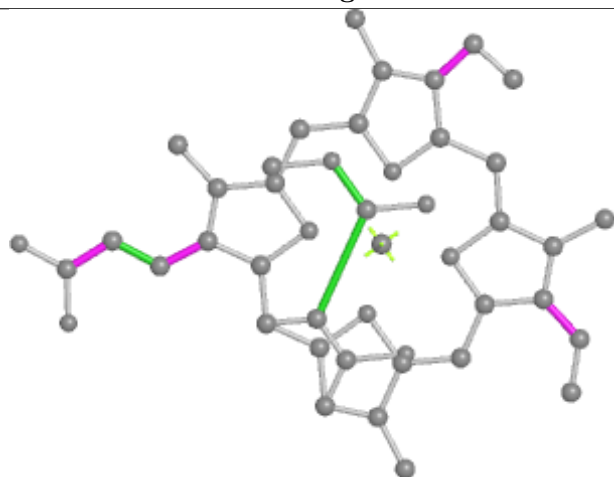
Ligand KC2 I 209



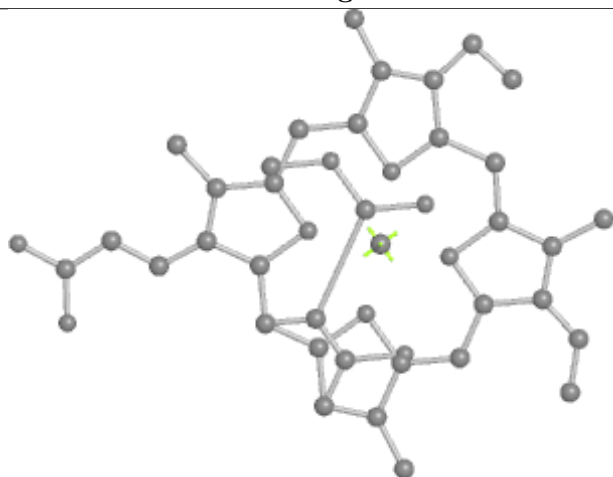
Bond lengths



Bond angles

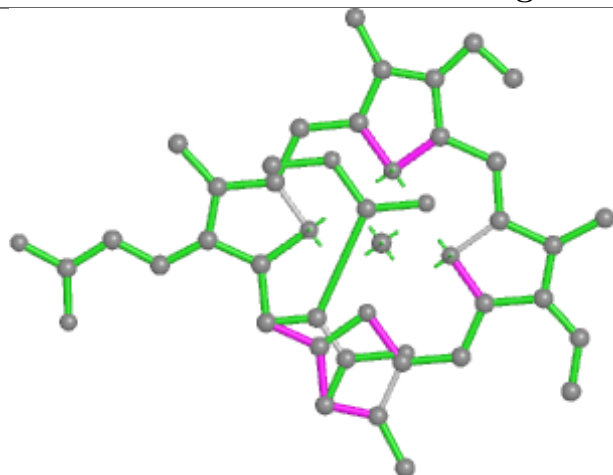


Torsions

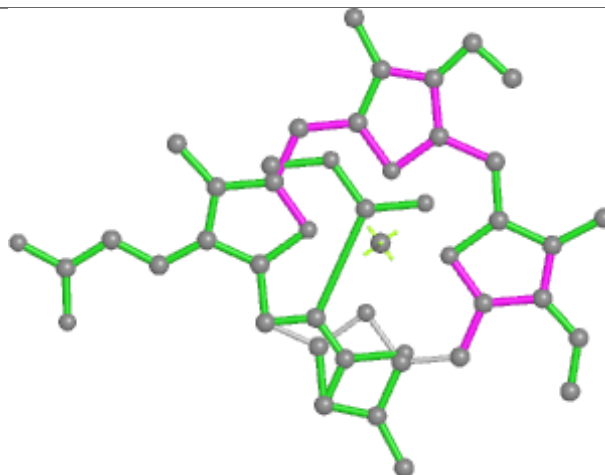


Rings

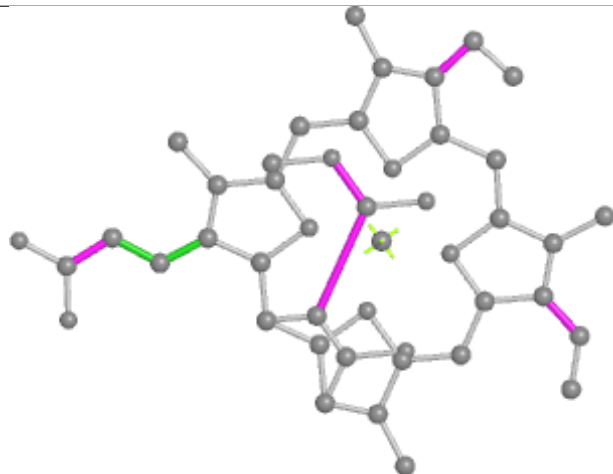
Ligand KC2 w 306



Bond lengths



Bond angles

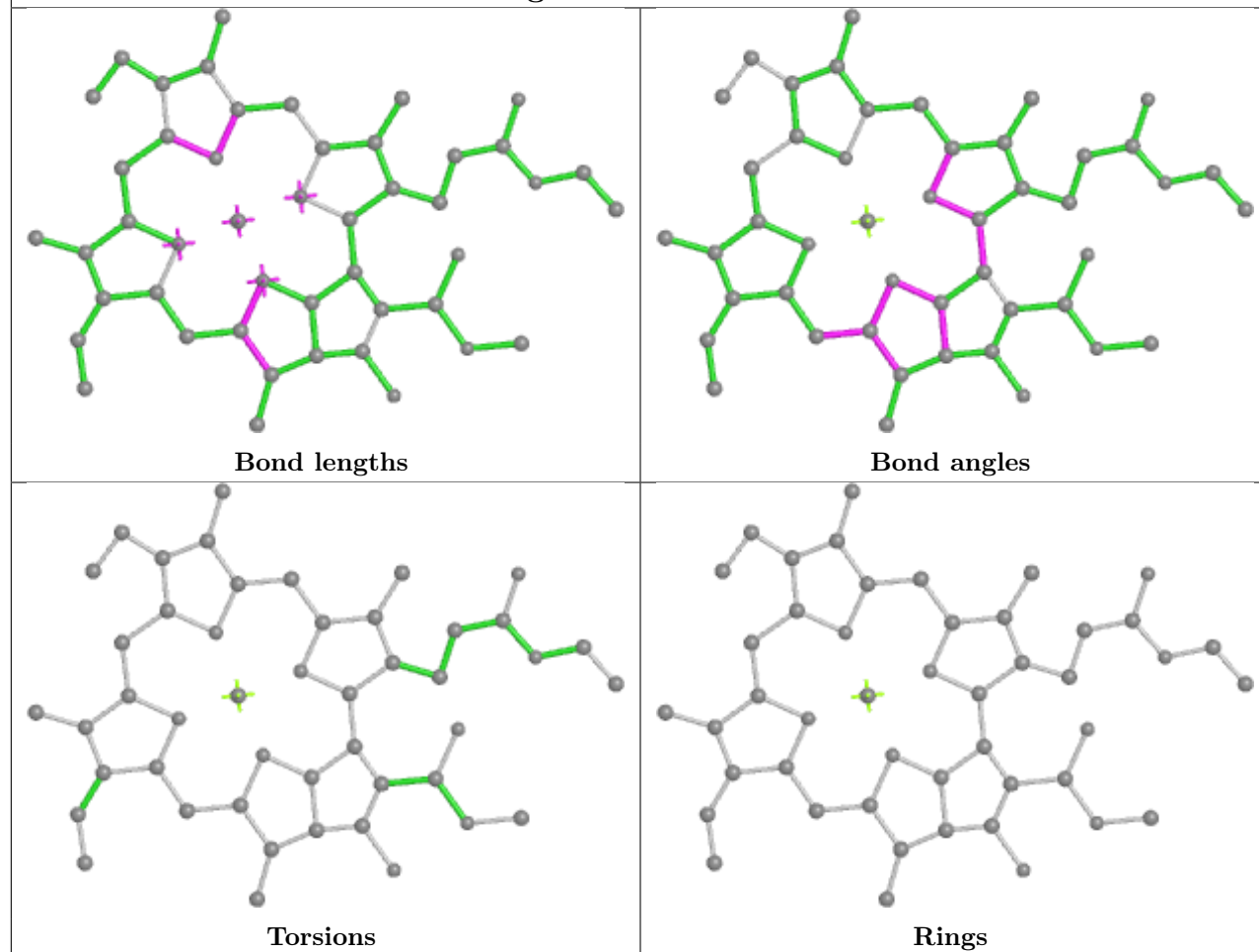


Torsions

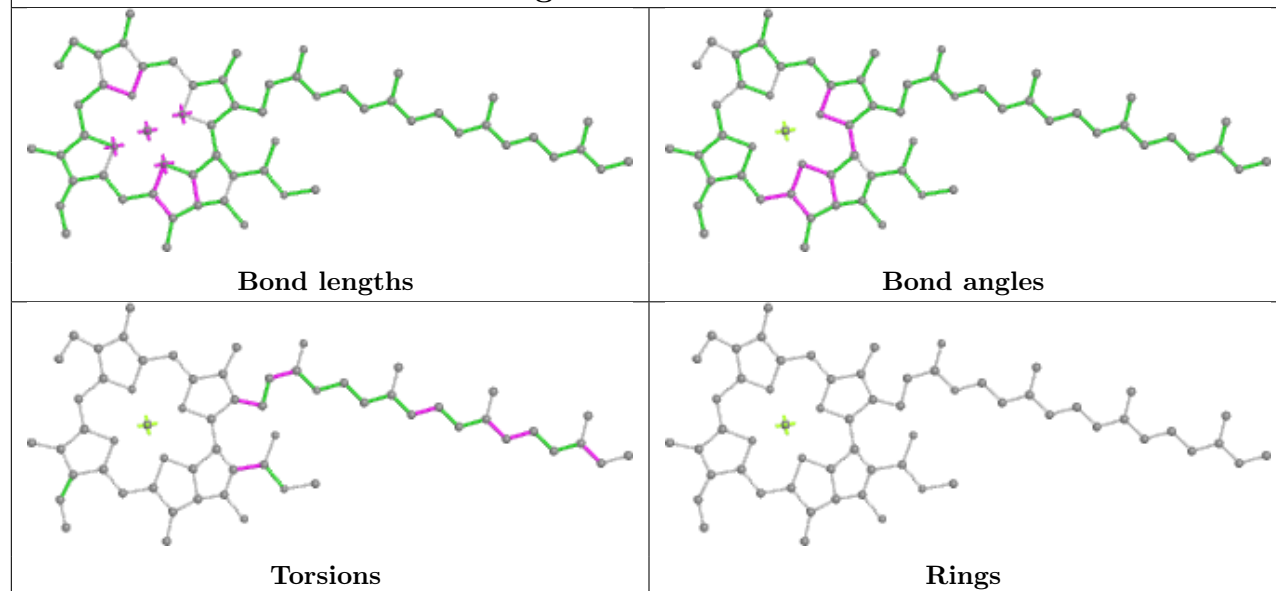


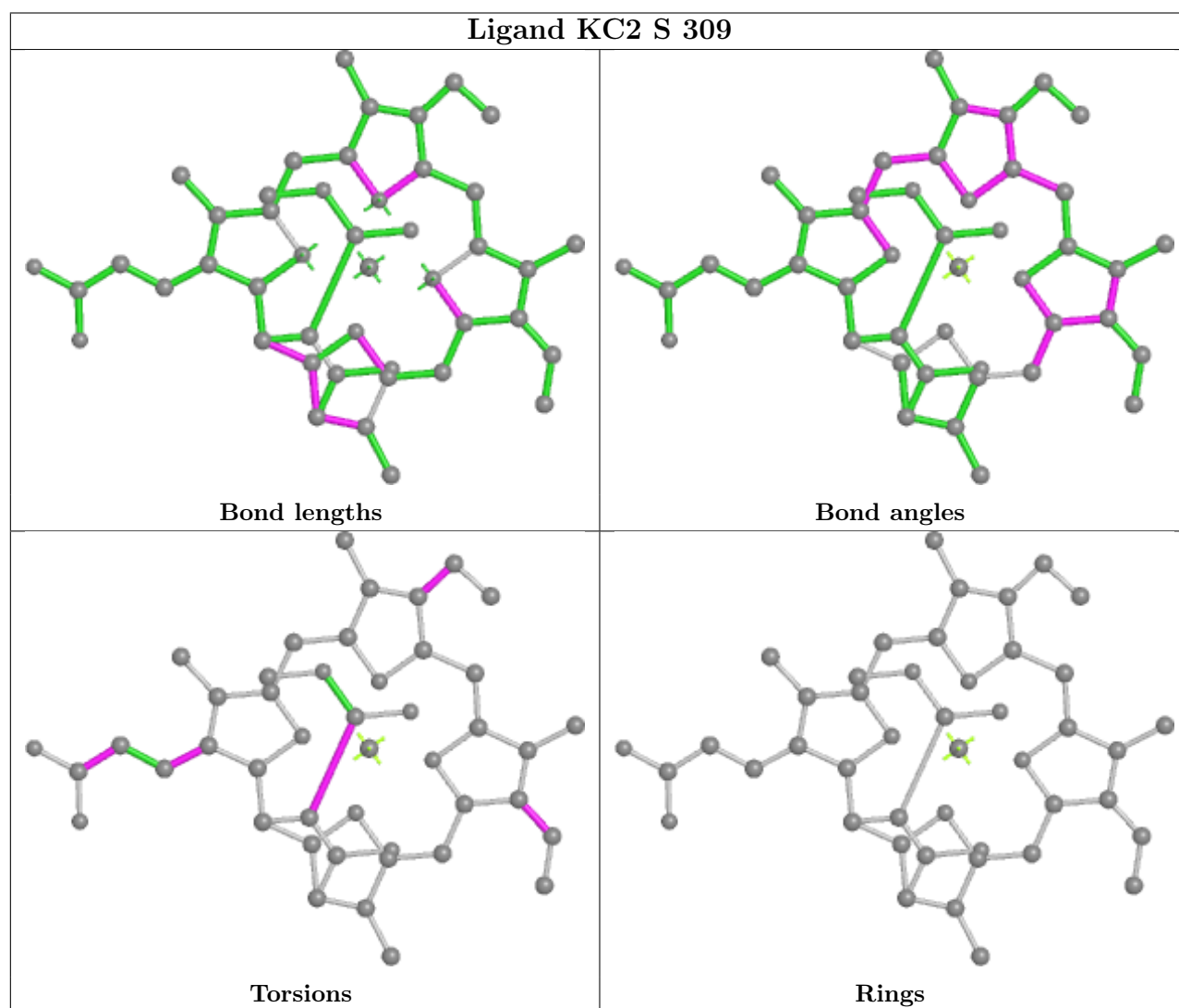
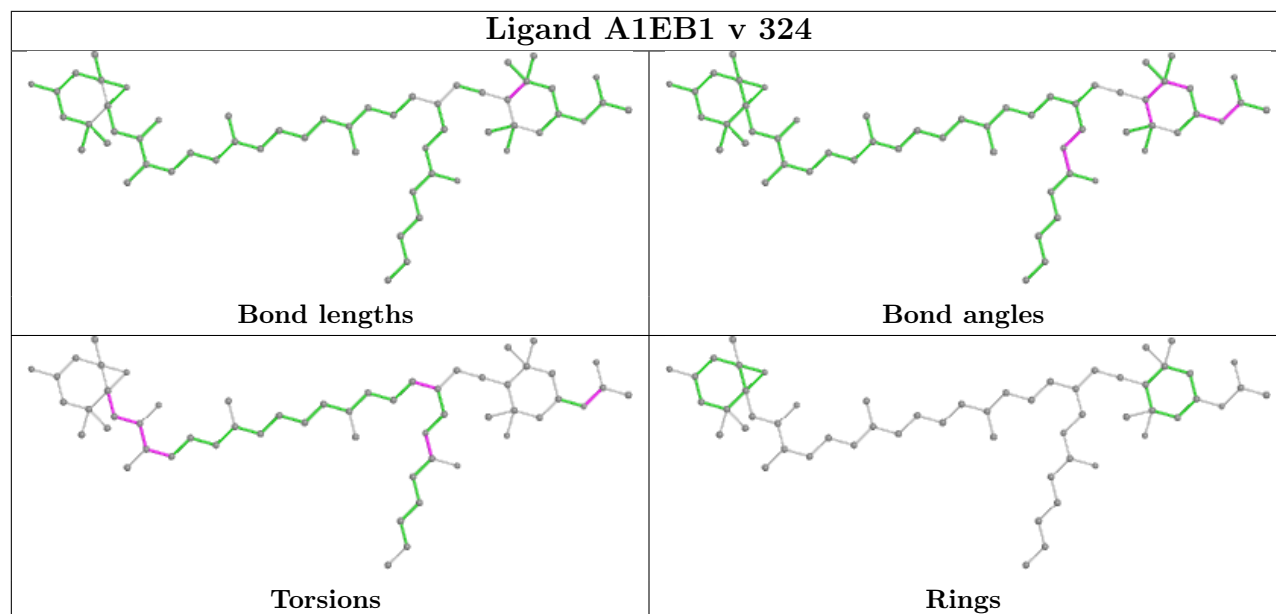
Rings

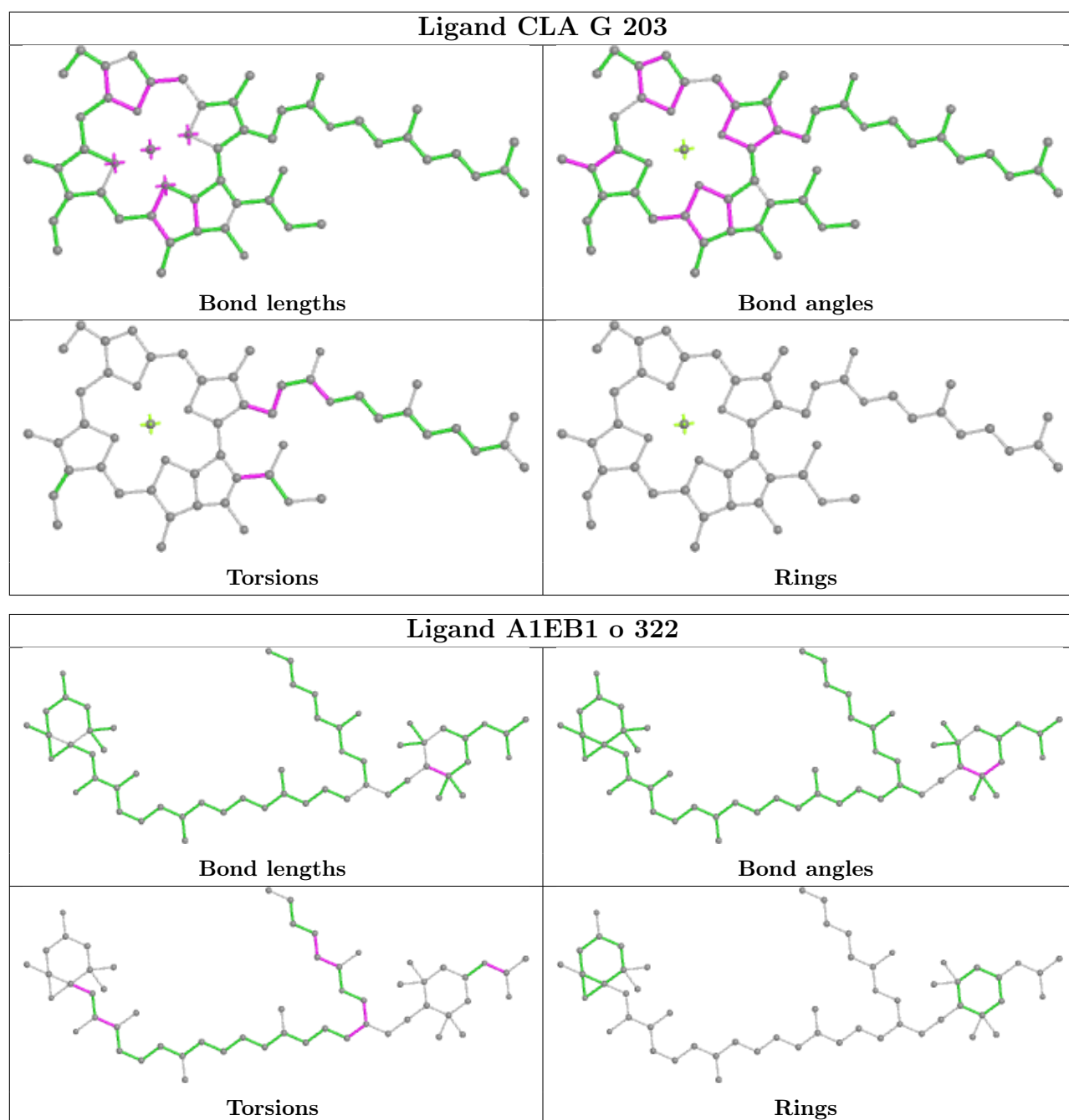
Ligand CLA L 301



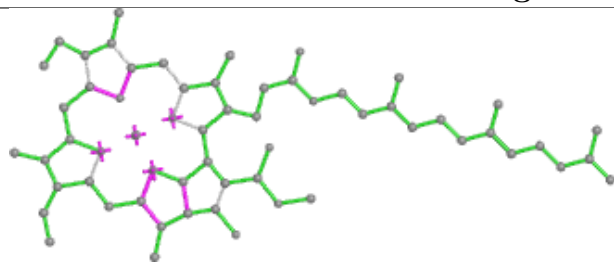
Ligand CLA b 842



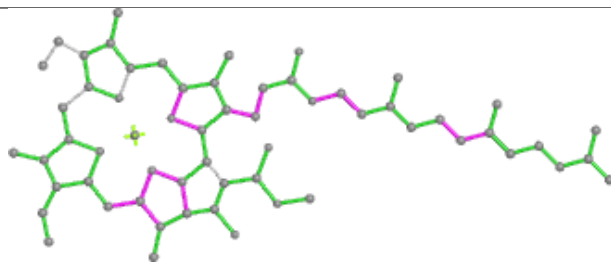




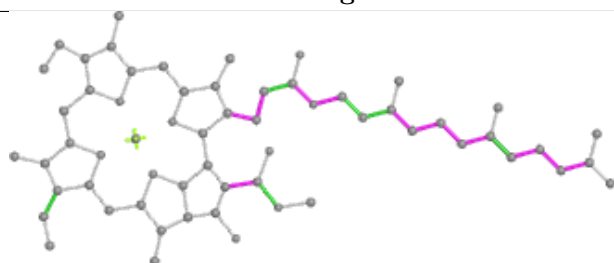
Ligand CLA H 307



Bond lengths



Bond angles

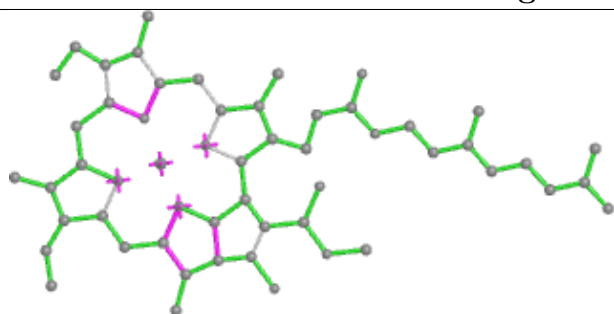


Torsions

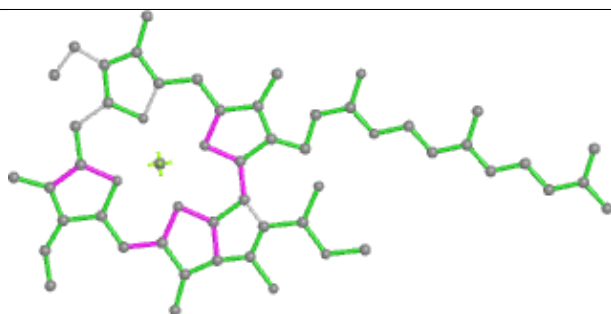


Rings

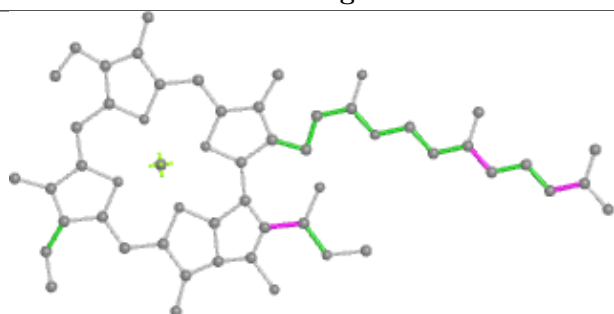
Ligand CLA a 837



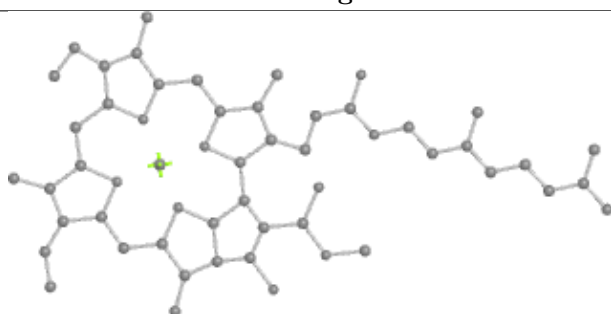
Bond lengths



Bond angles

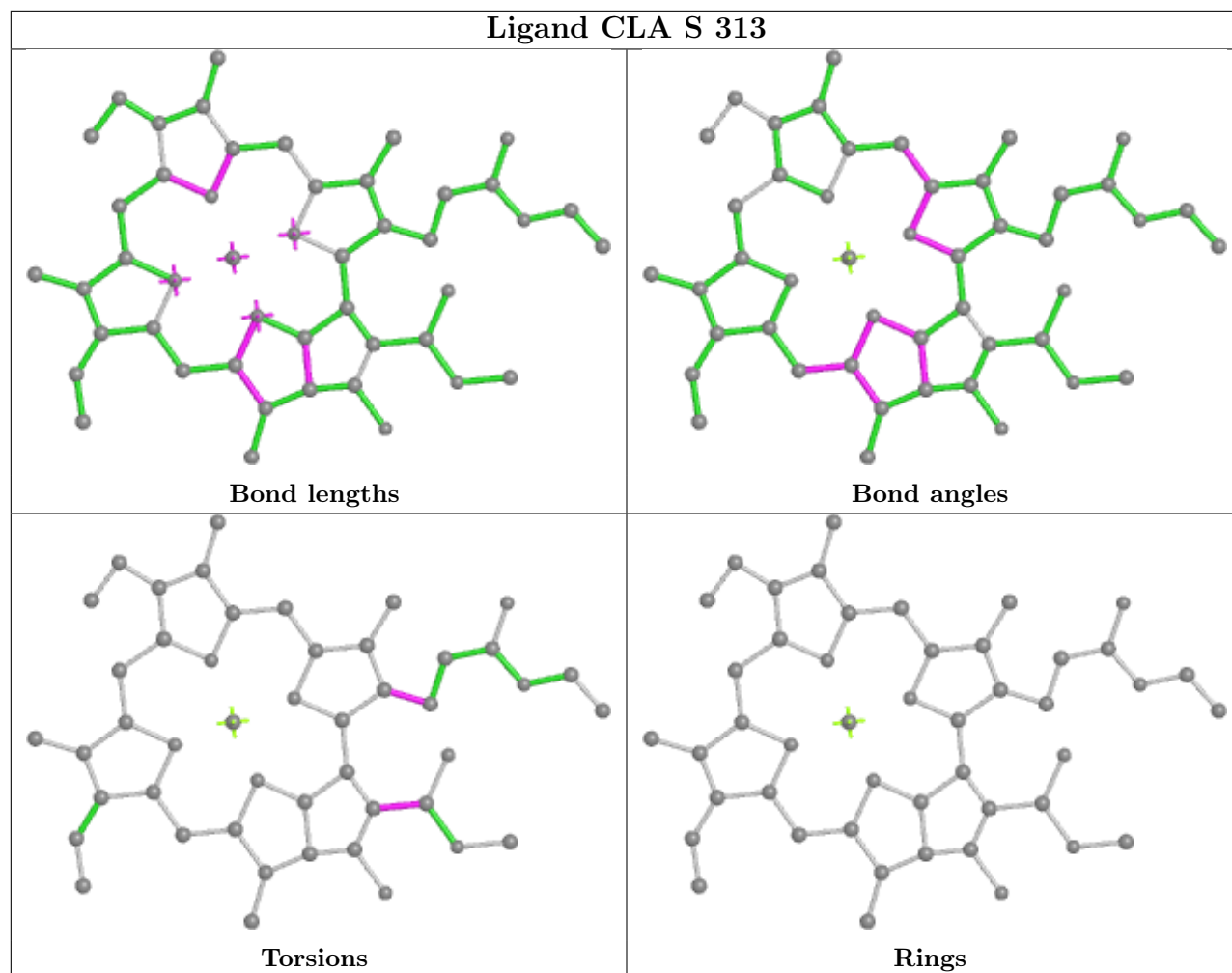


Torsions

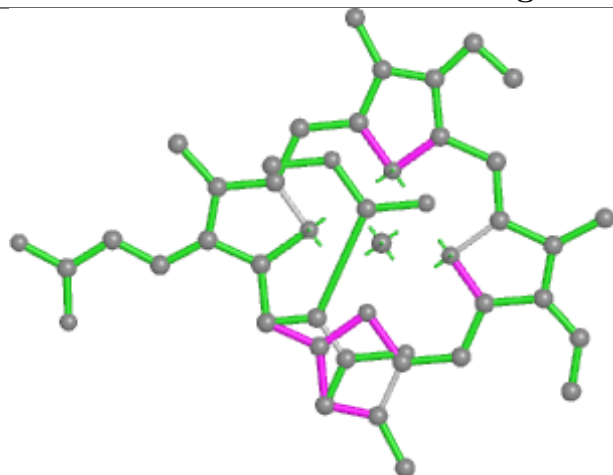


Rings

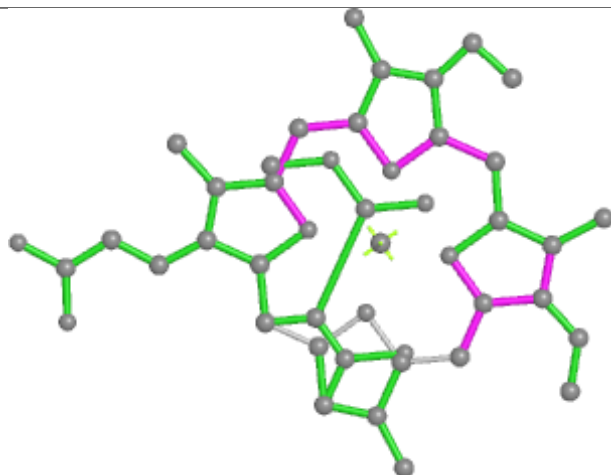
Ligand CLA S 313



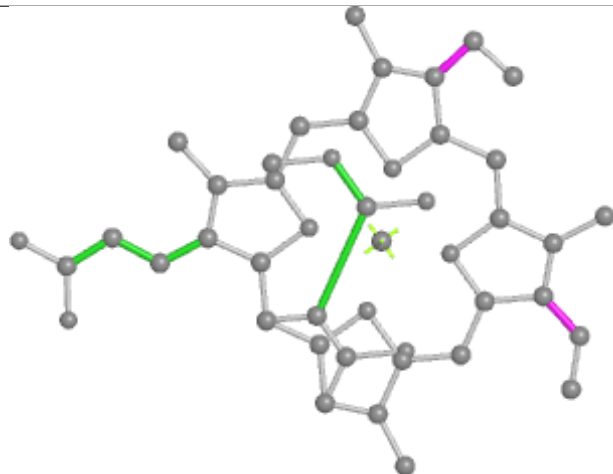
Ligand KC2 P 302



Bond lengths



Bond angles

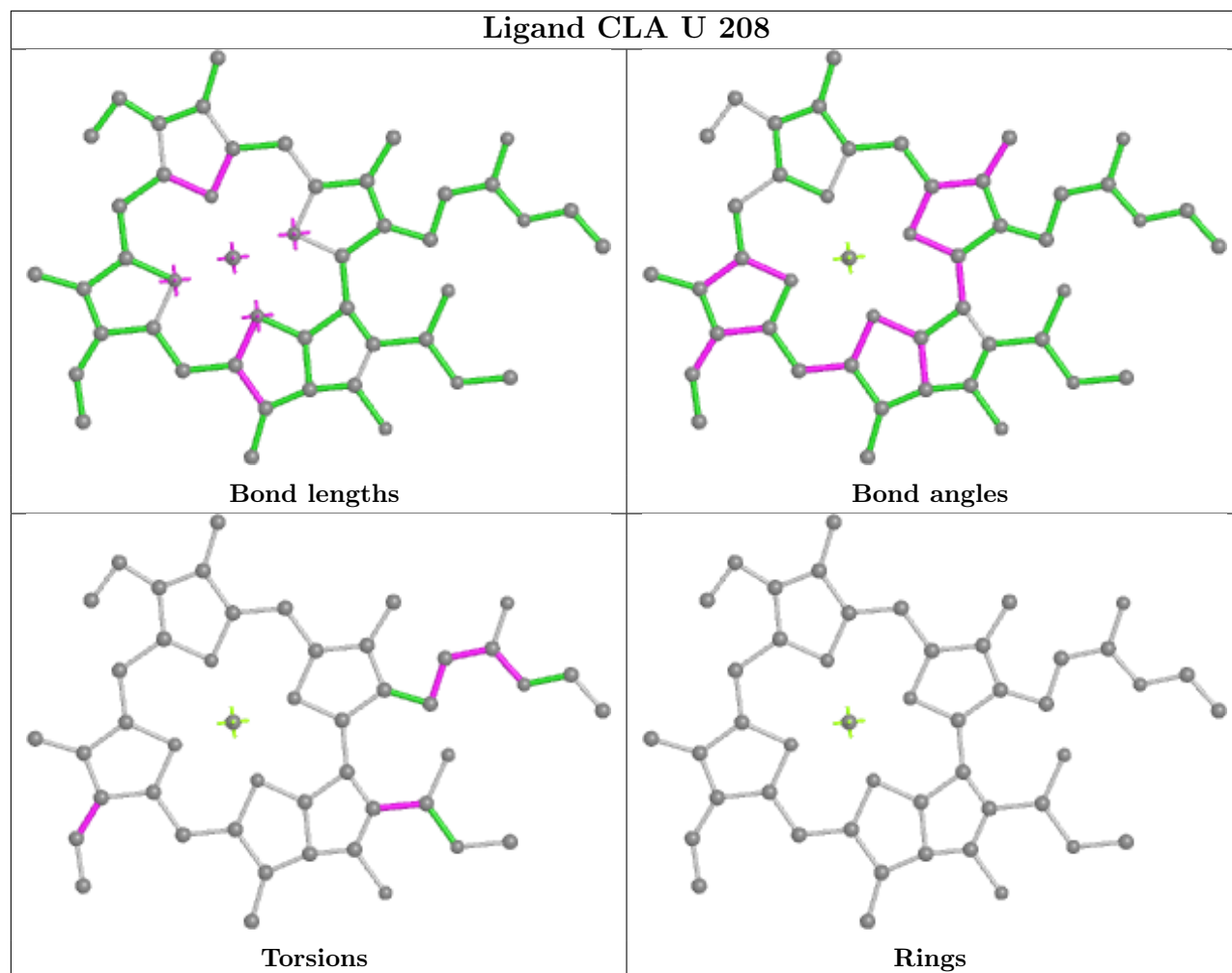


Torsions

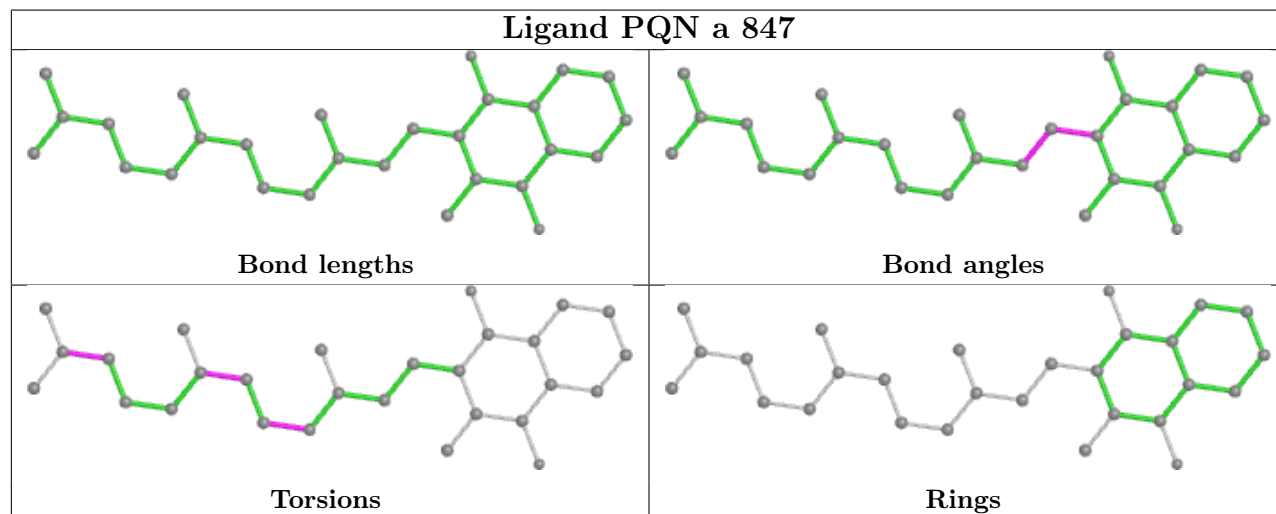


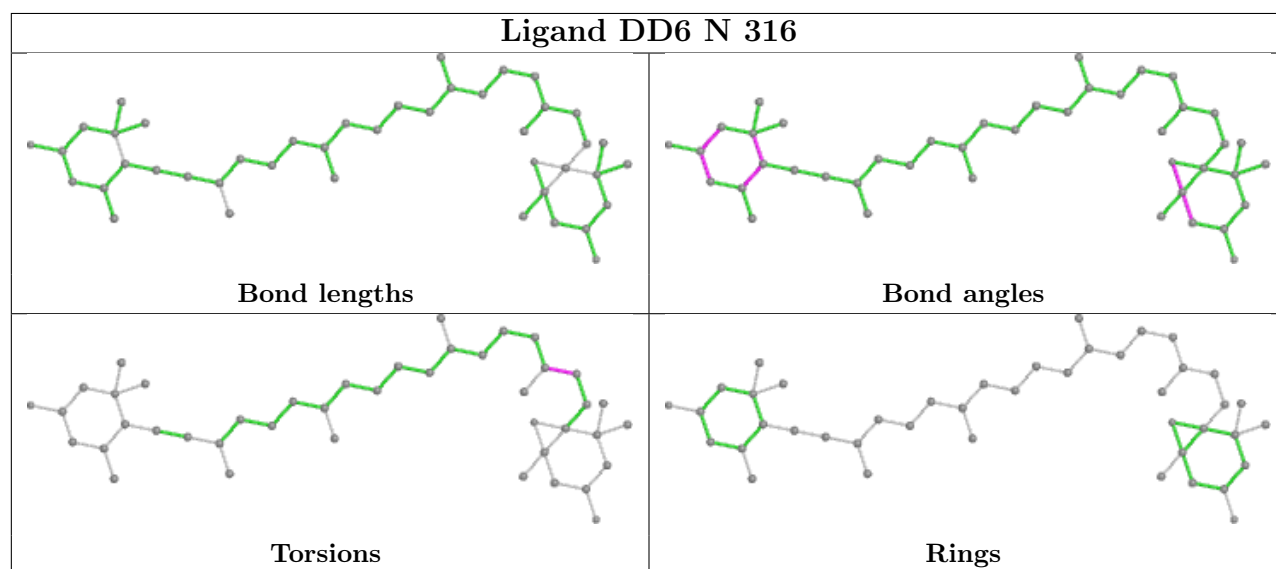
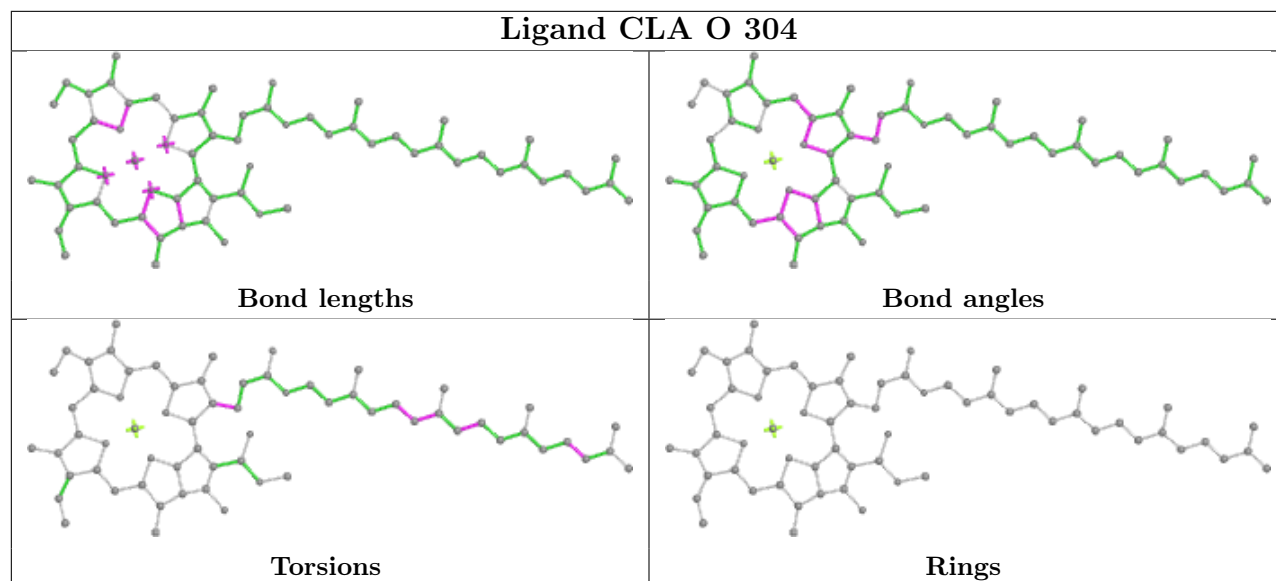
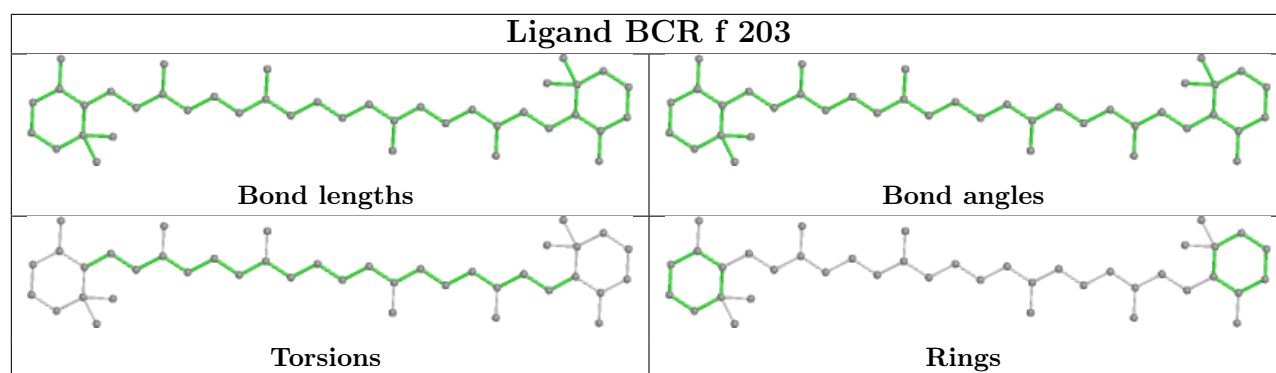
Rings

Ligand CLA U 208

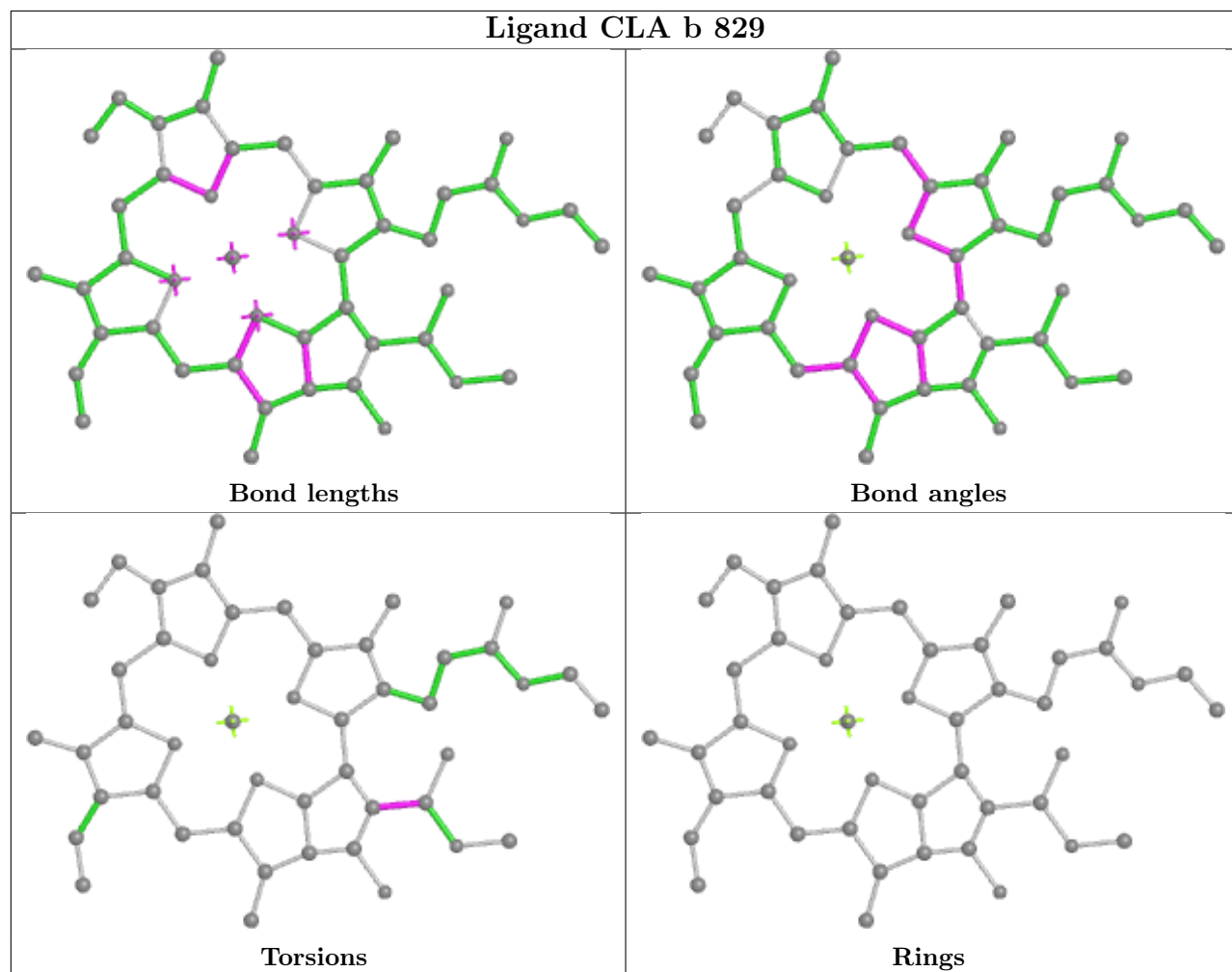


Ligand PQN a 847

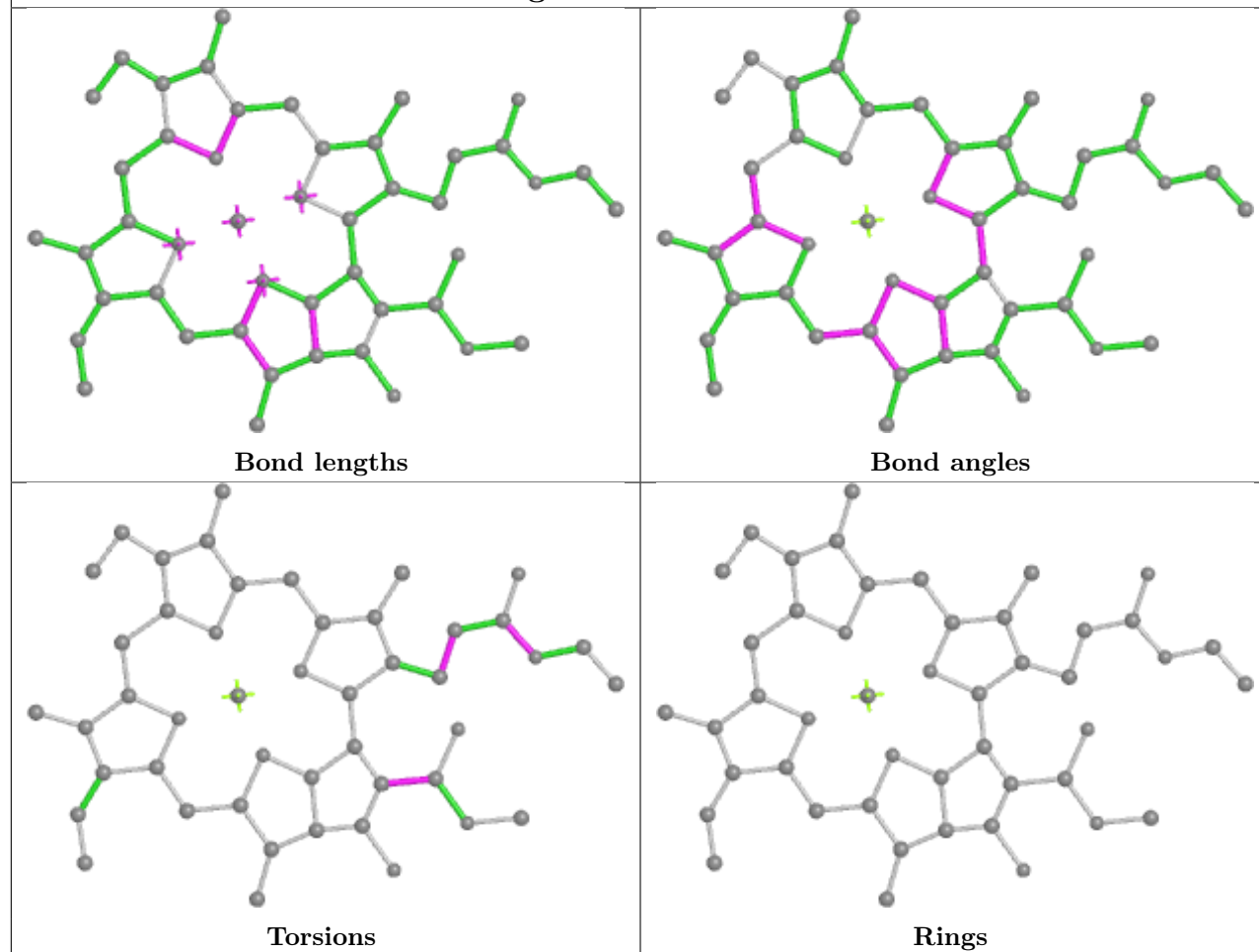




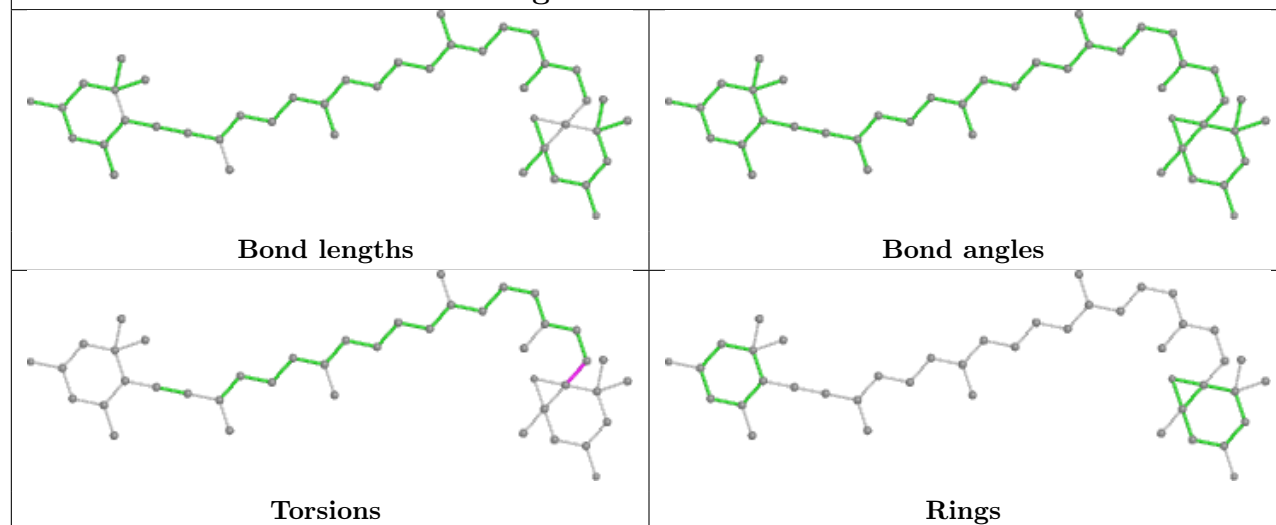
Ligand CLA b 829



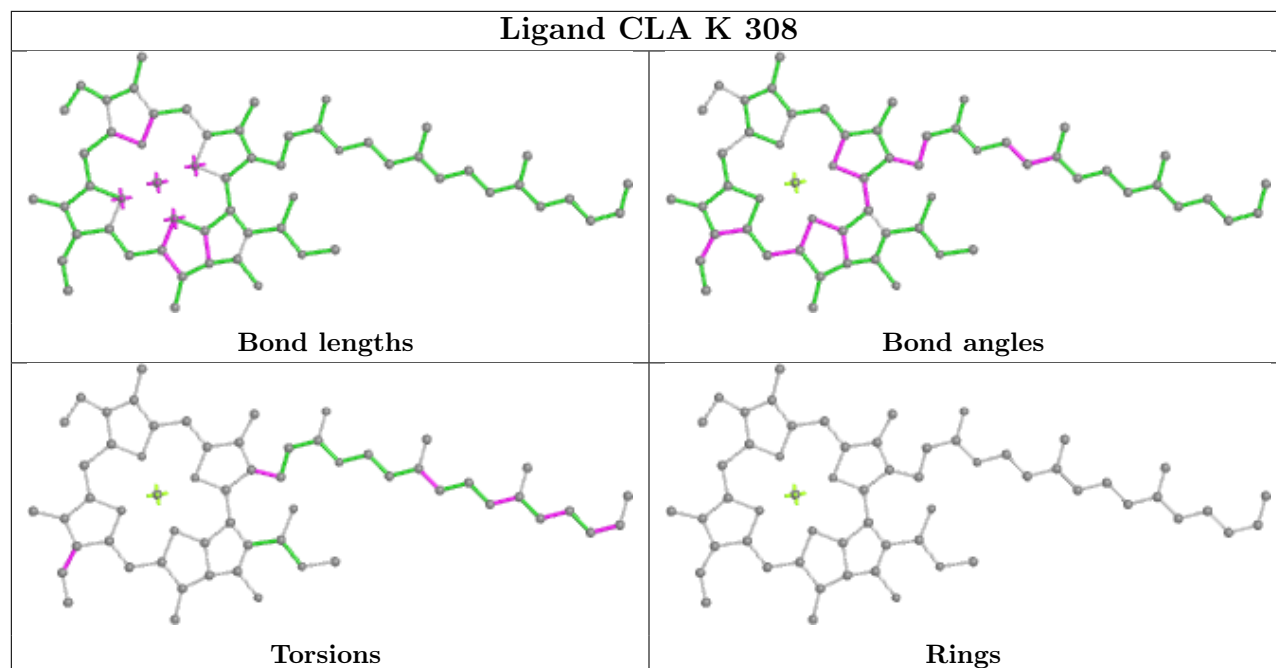
Ligand CLA b 811



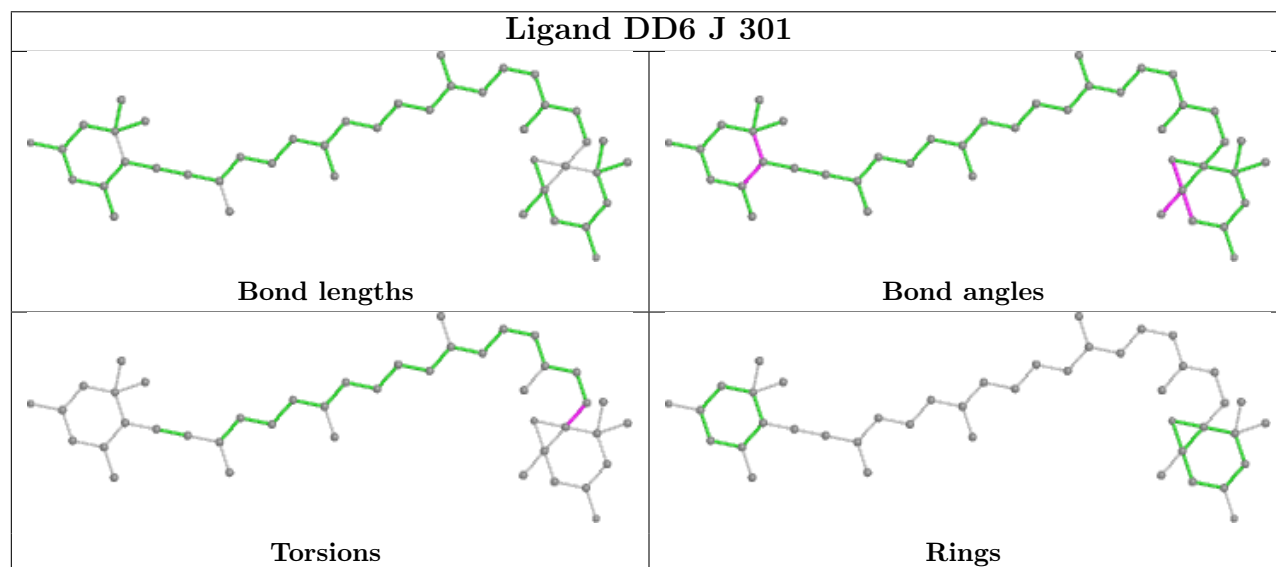
Ligand DD6 D 316

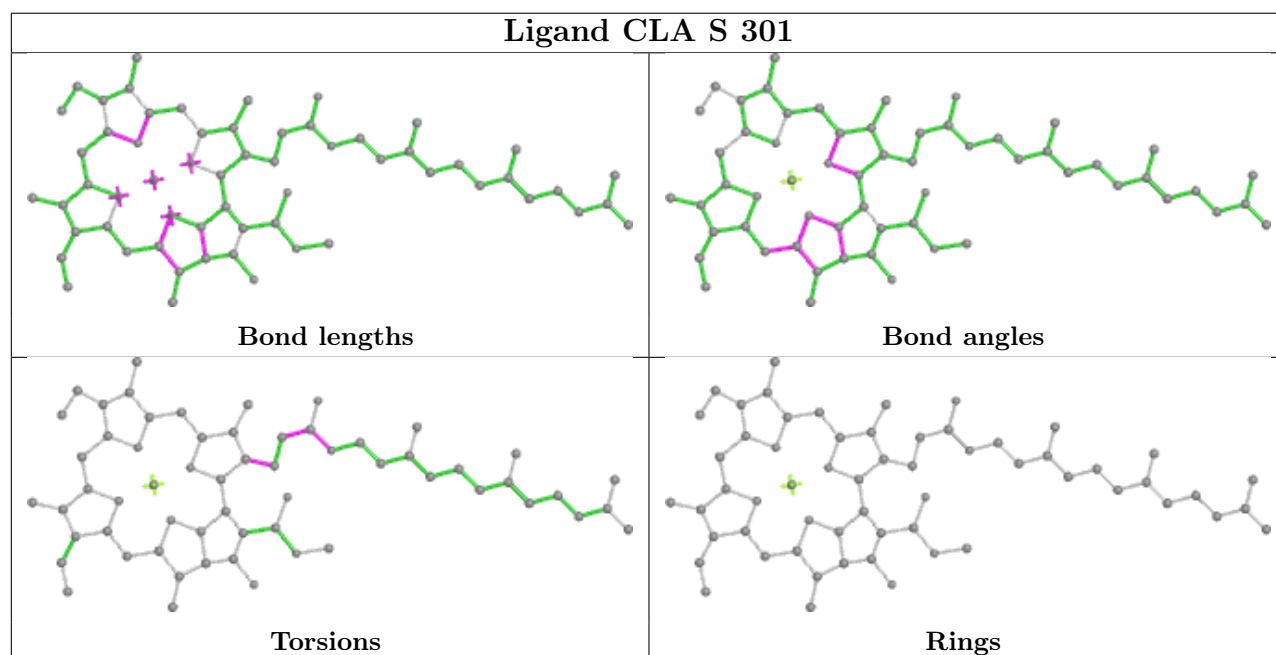
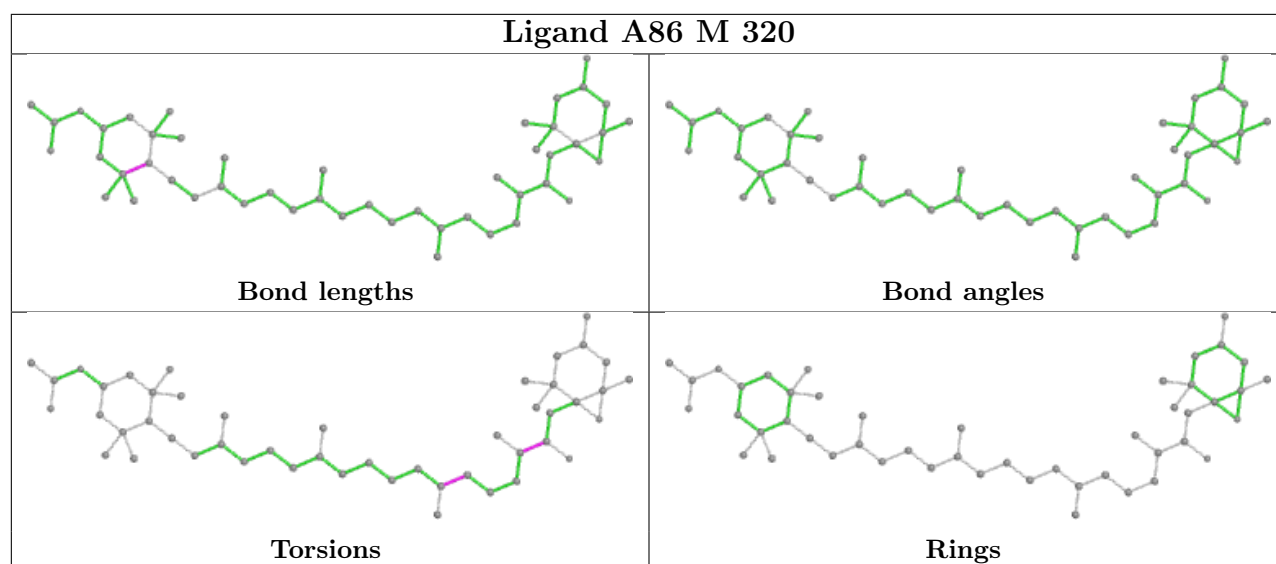


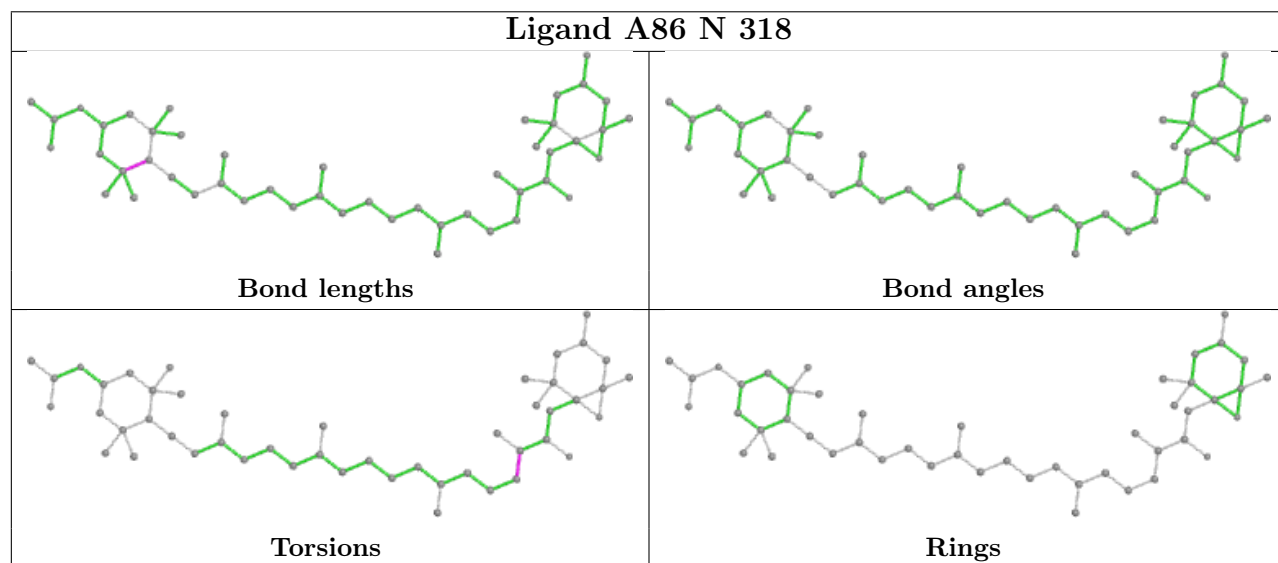
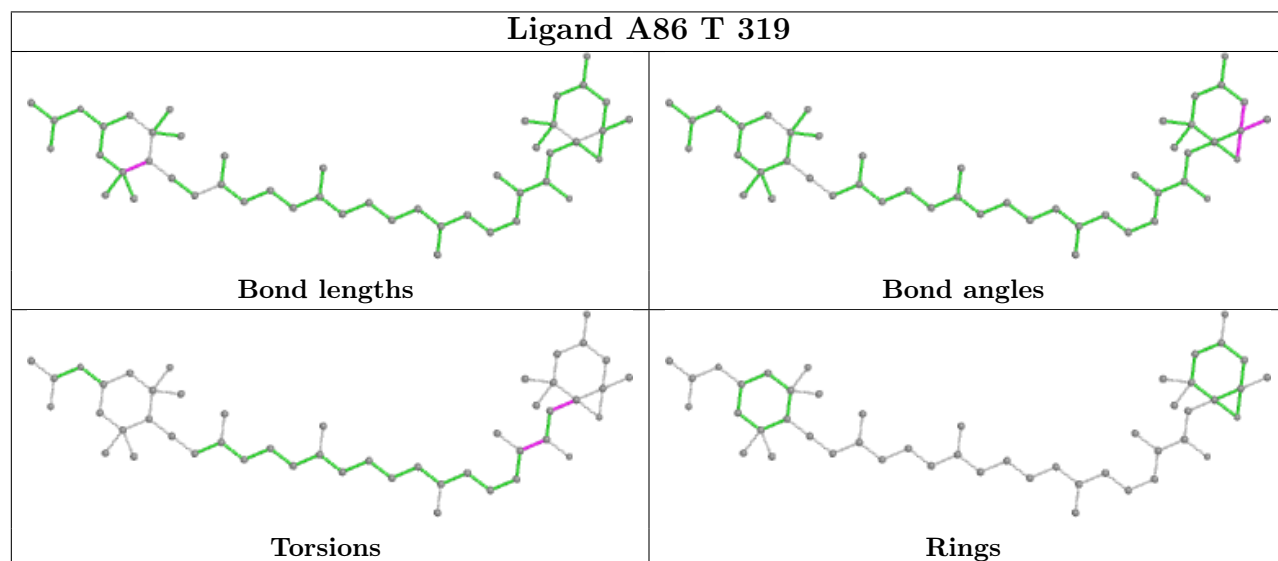
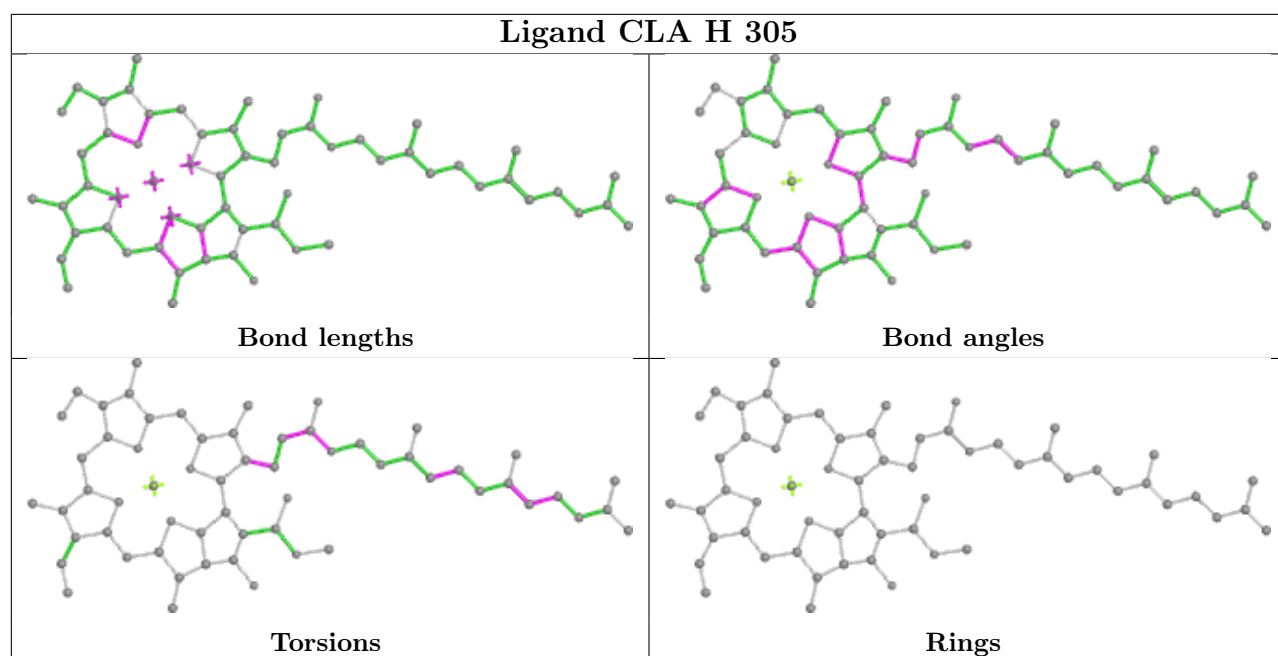
Ligand CLA K 308

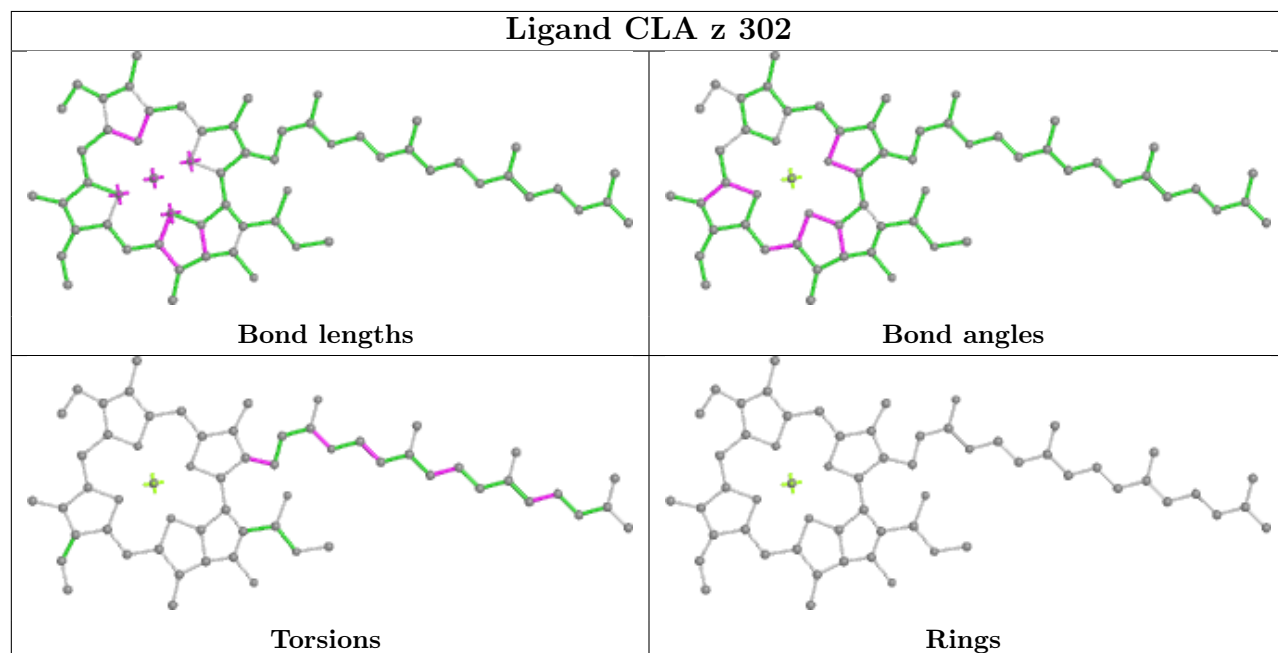
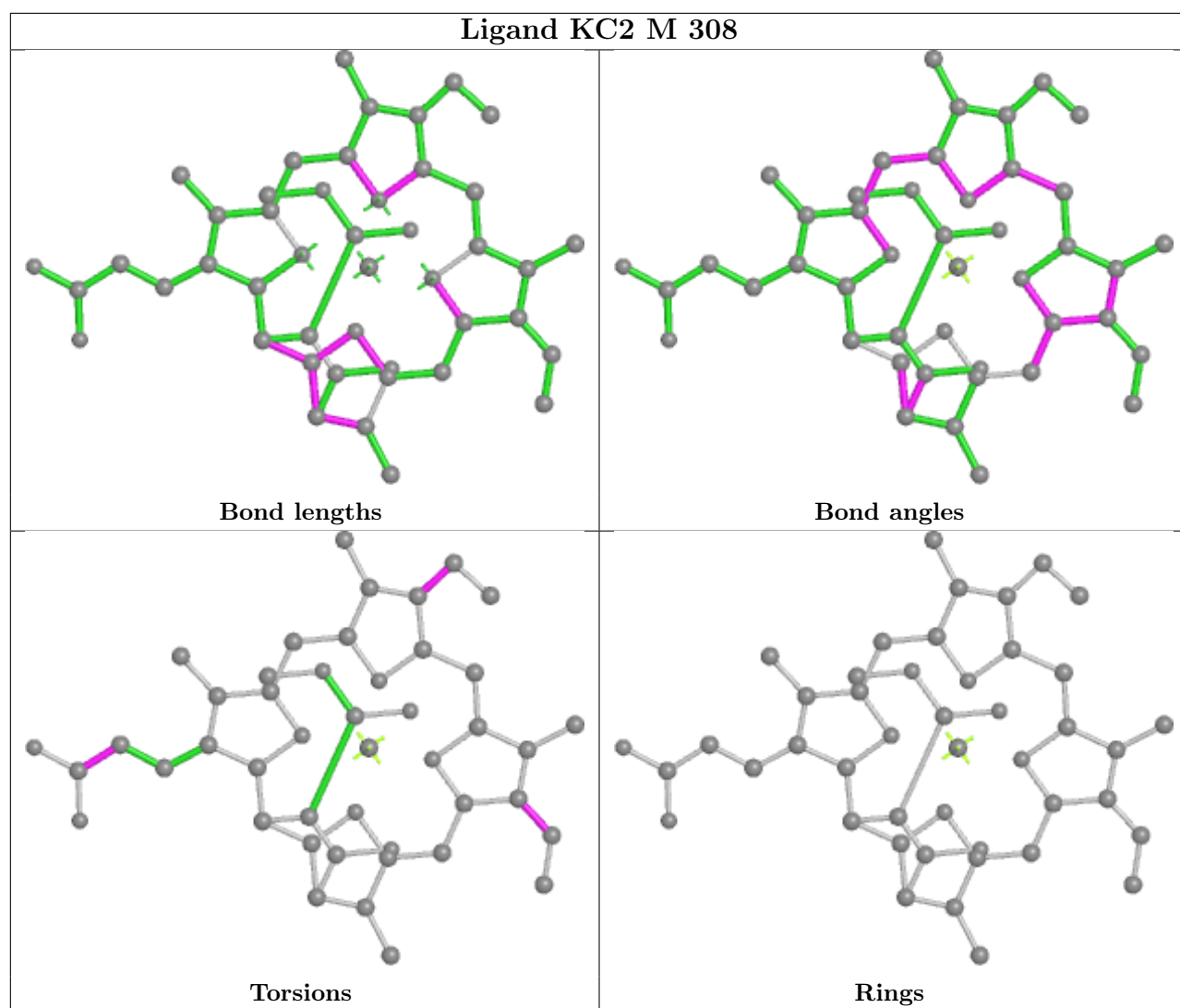


Ligand DD6 J 301

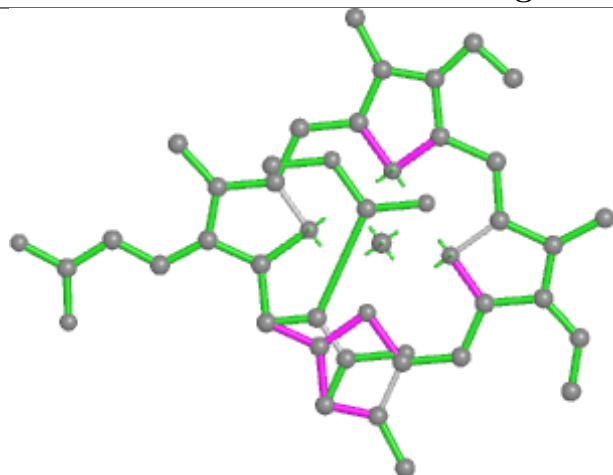




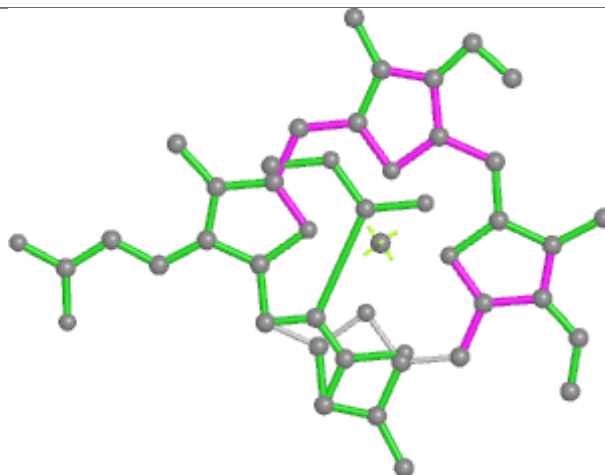




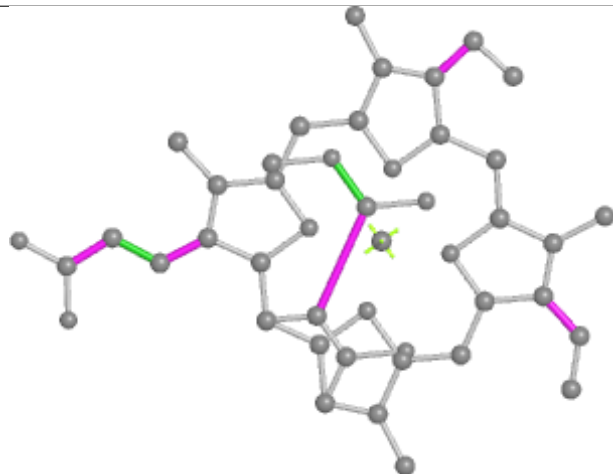
Ligand KC2 N 312



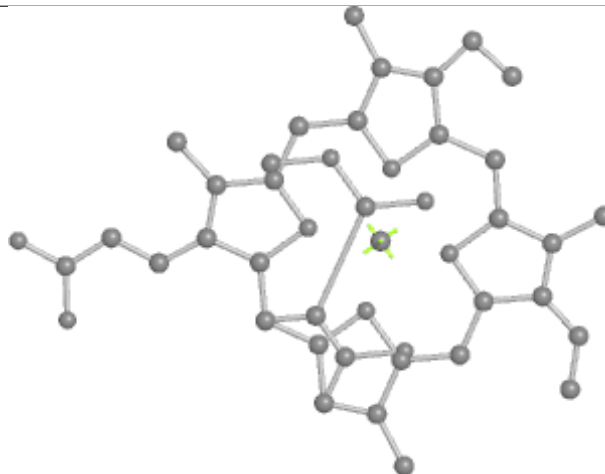
Bond lengths



Bond angles

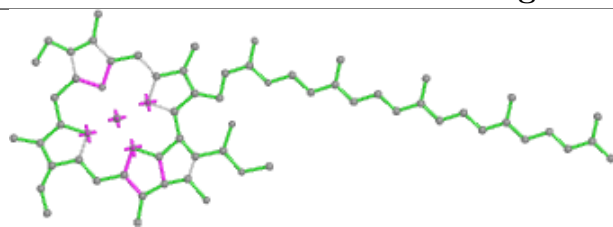


Torsions

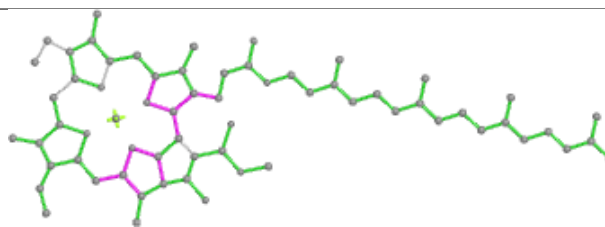


Rings

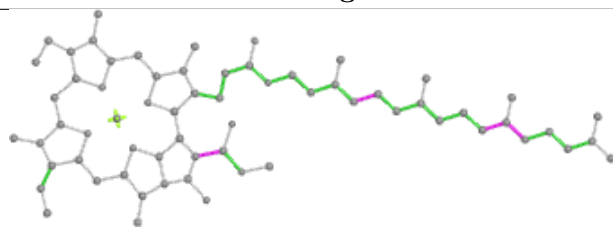
Ligand CLA a 815



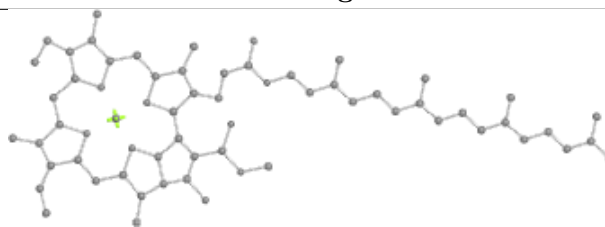
Bond lengths



Bond angles

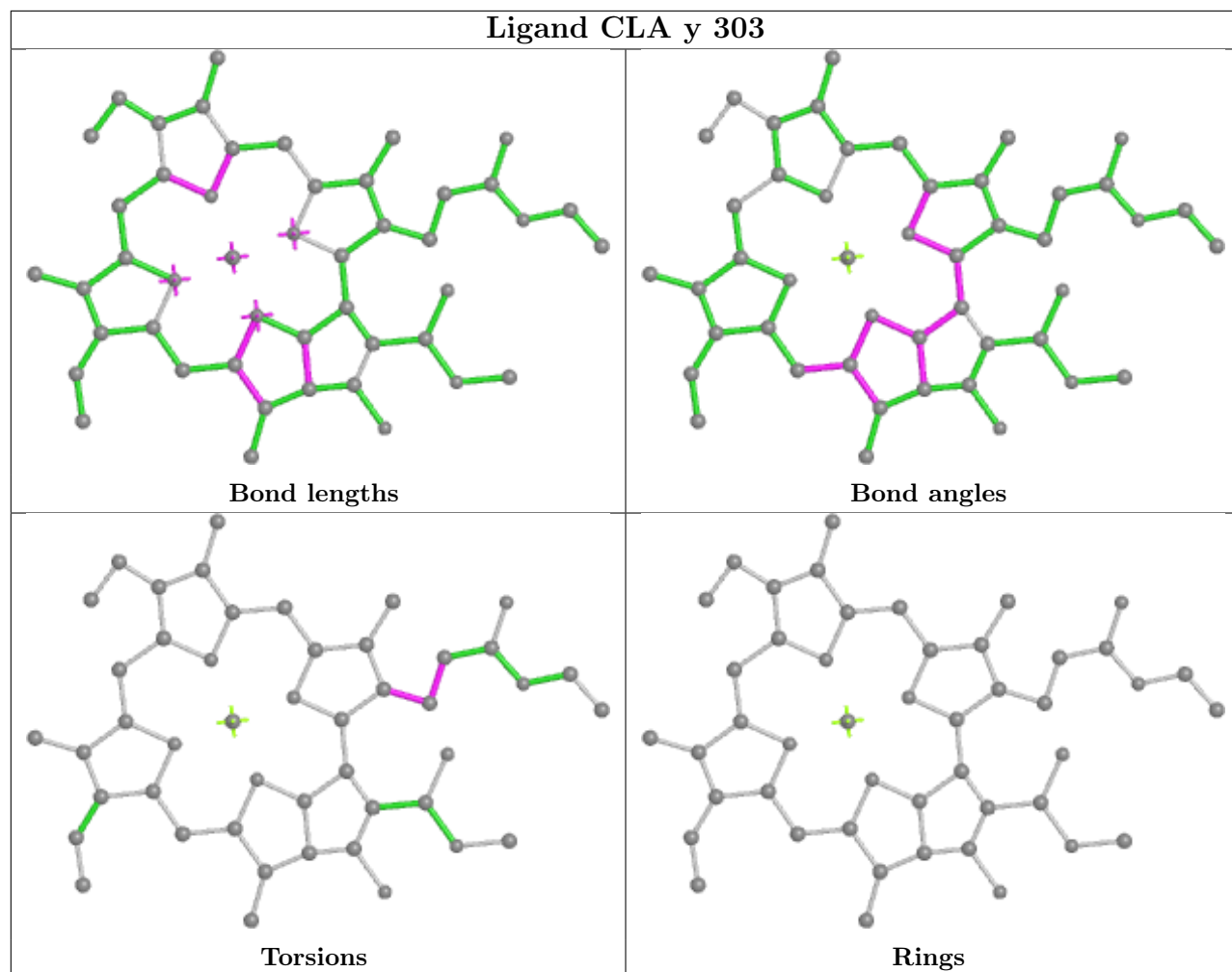


Torsions

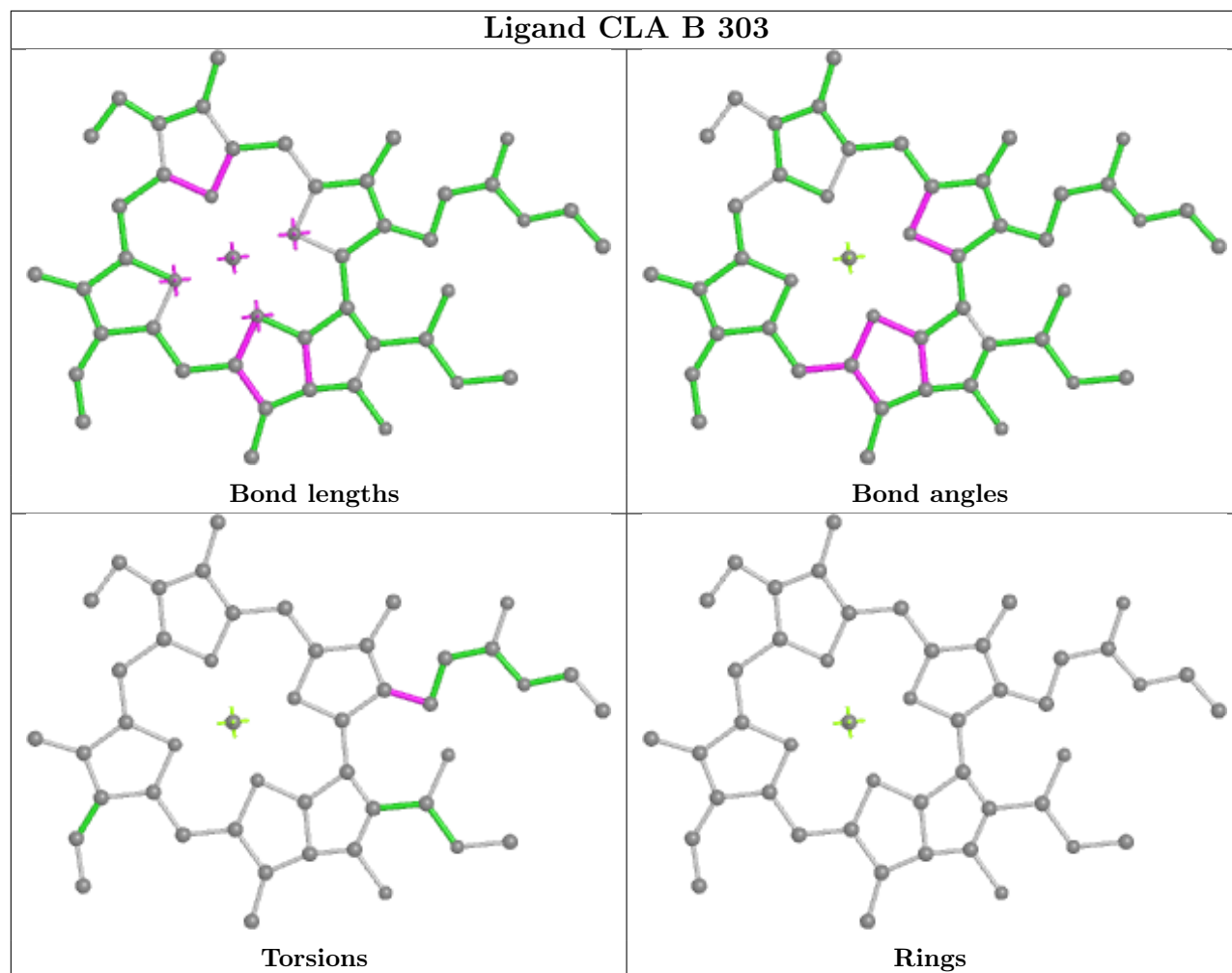


Rings

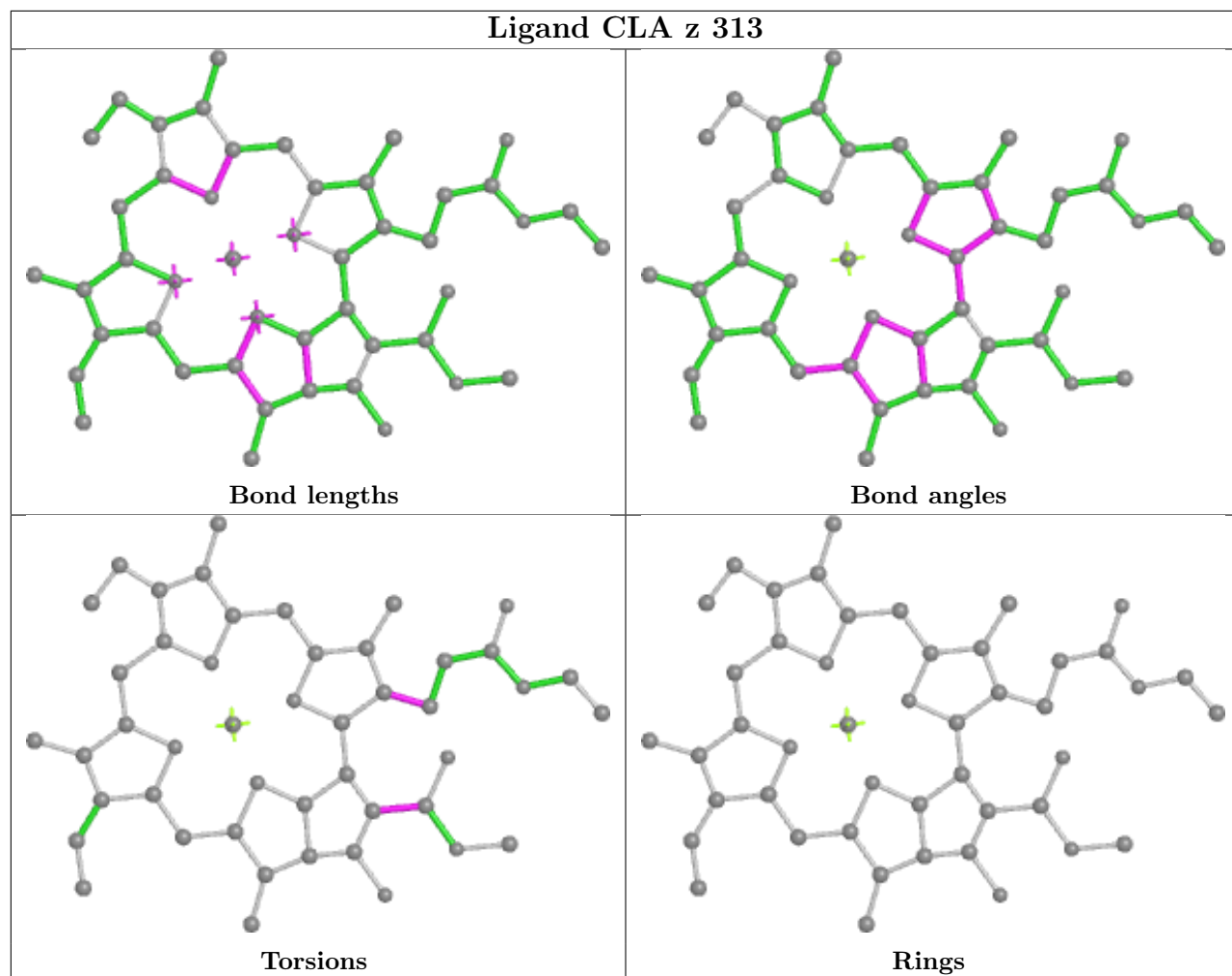
Ligand CLA y 303



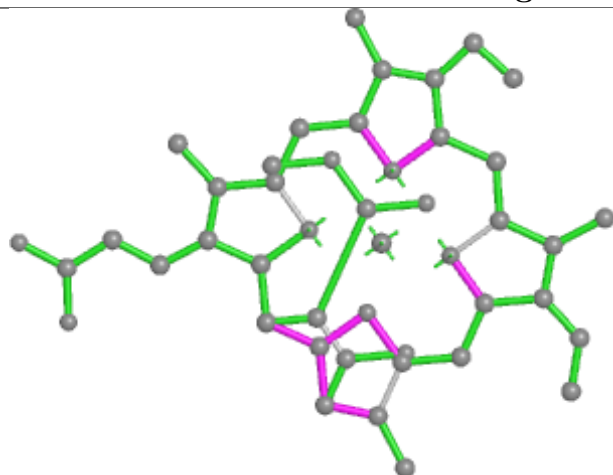
Ligand CLA B 303



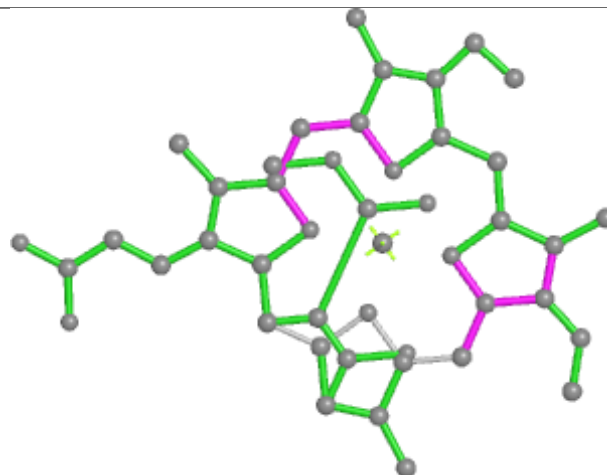
Ligand CLA z 313



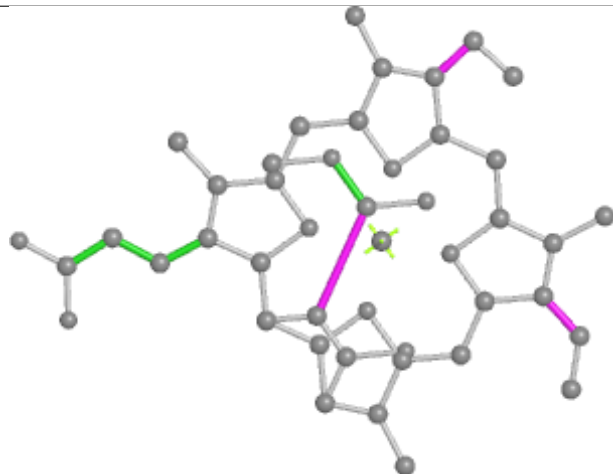
Ligand KC2 U 201



Bond lengths



Bond angles

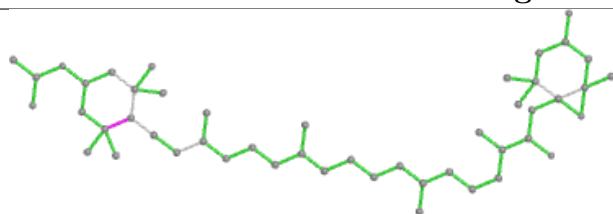


Torsions

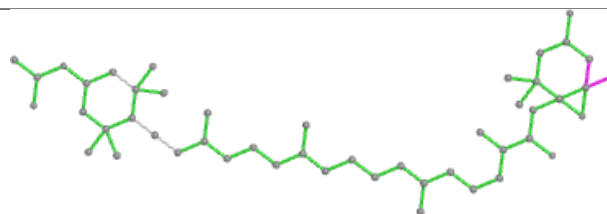


Rings

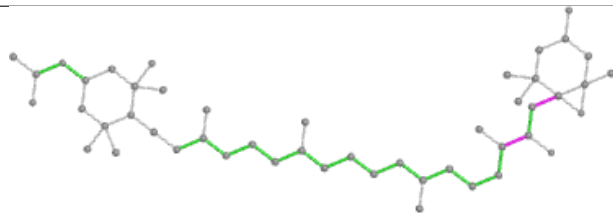
Ligand A86 W 316



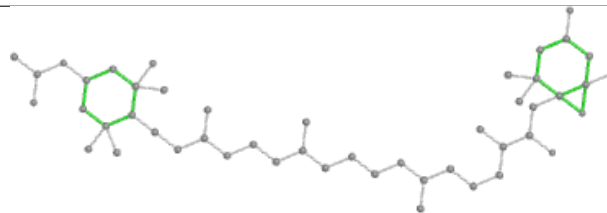
Bond lengths



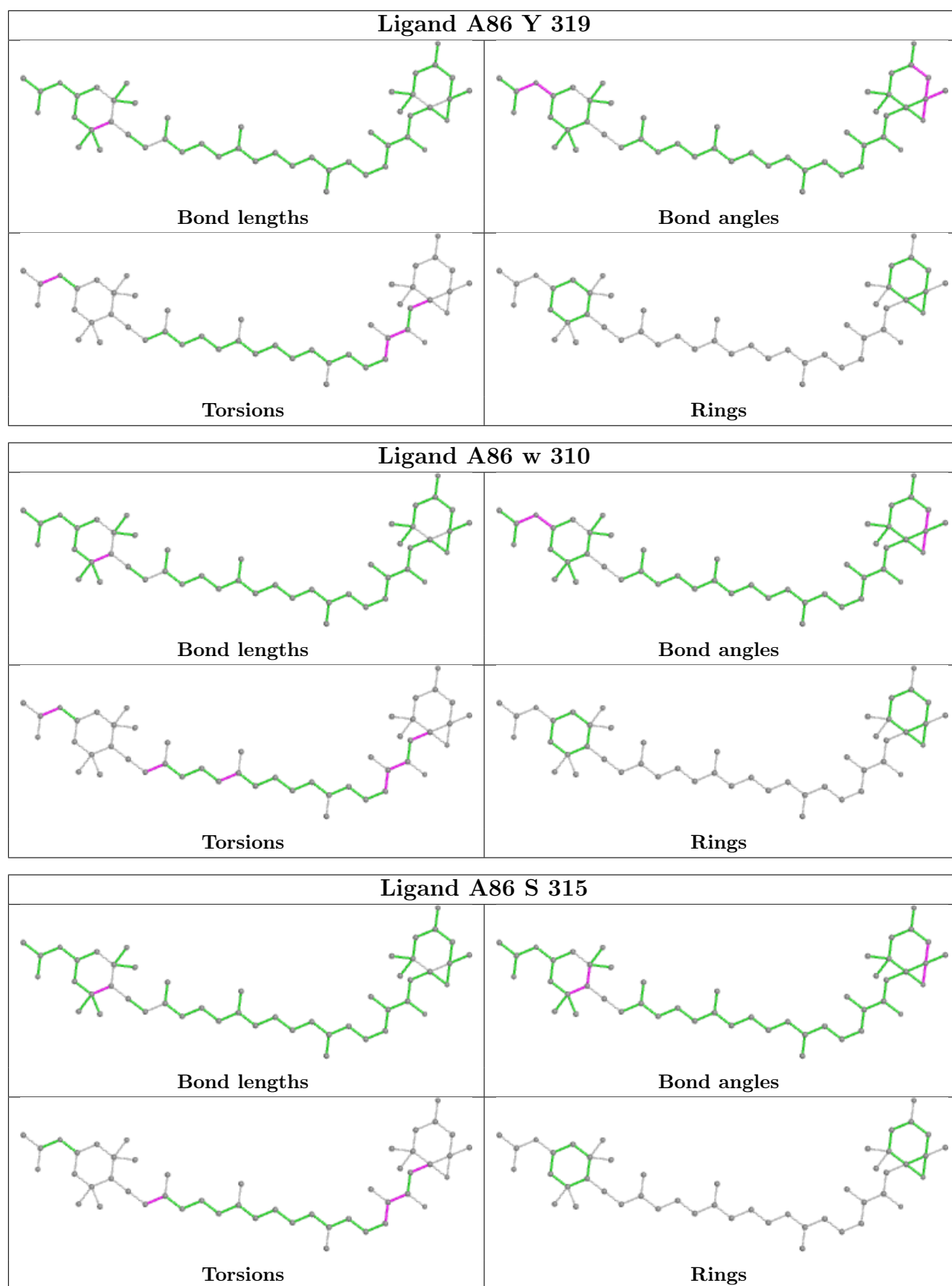
Bond angles

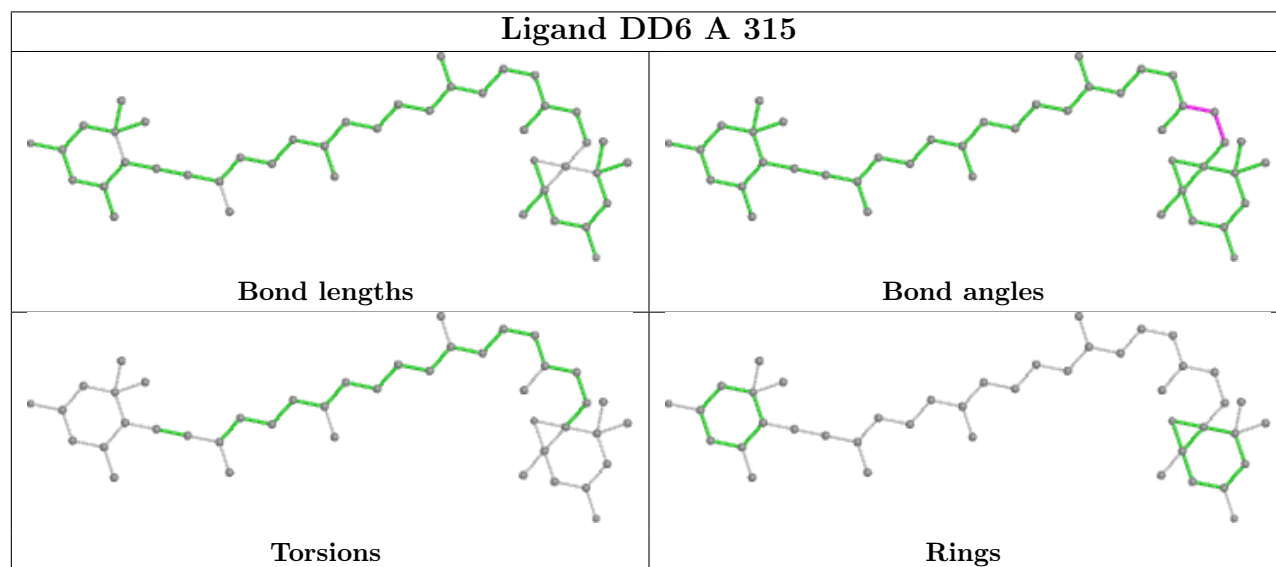
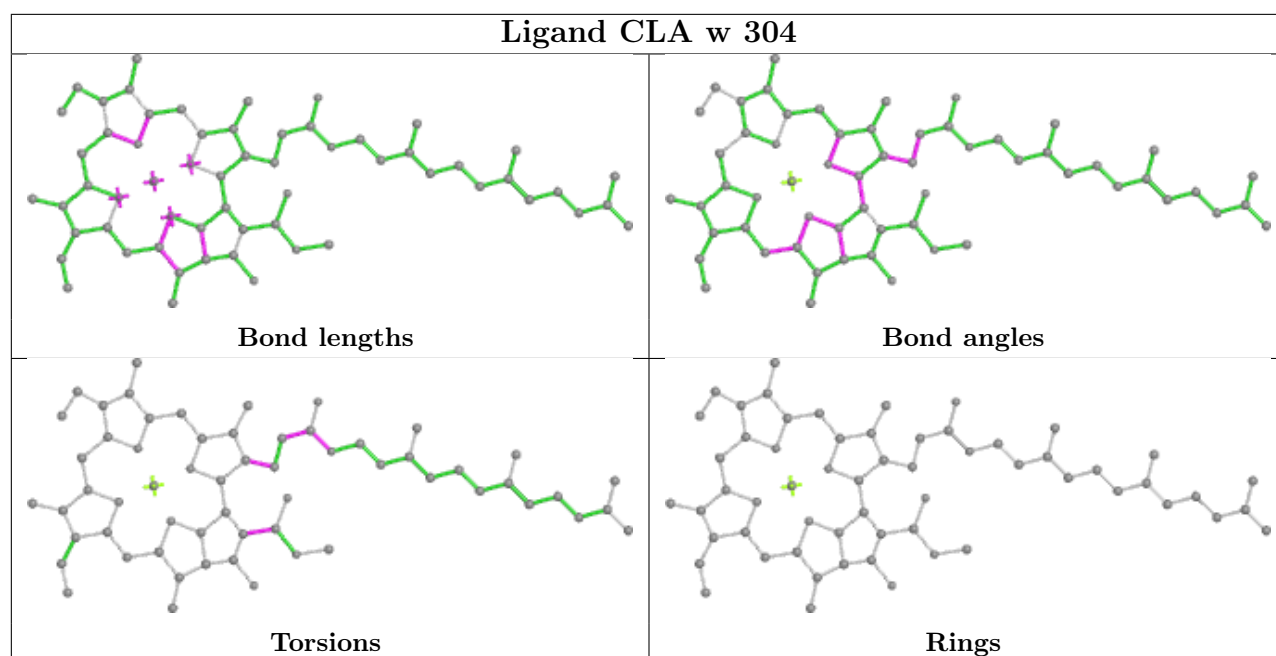


Torsions

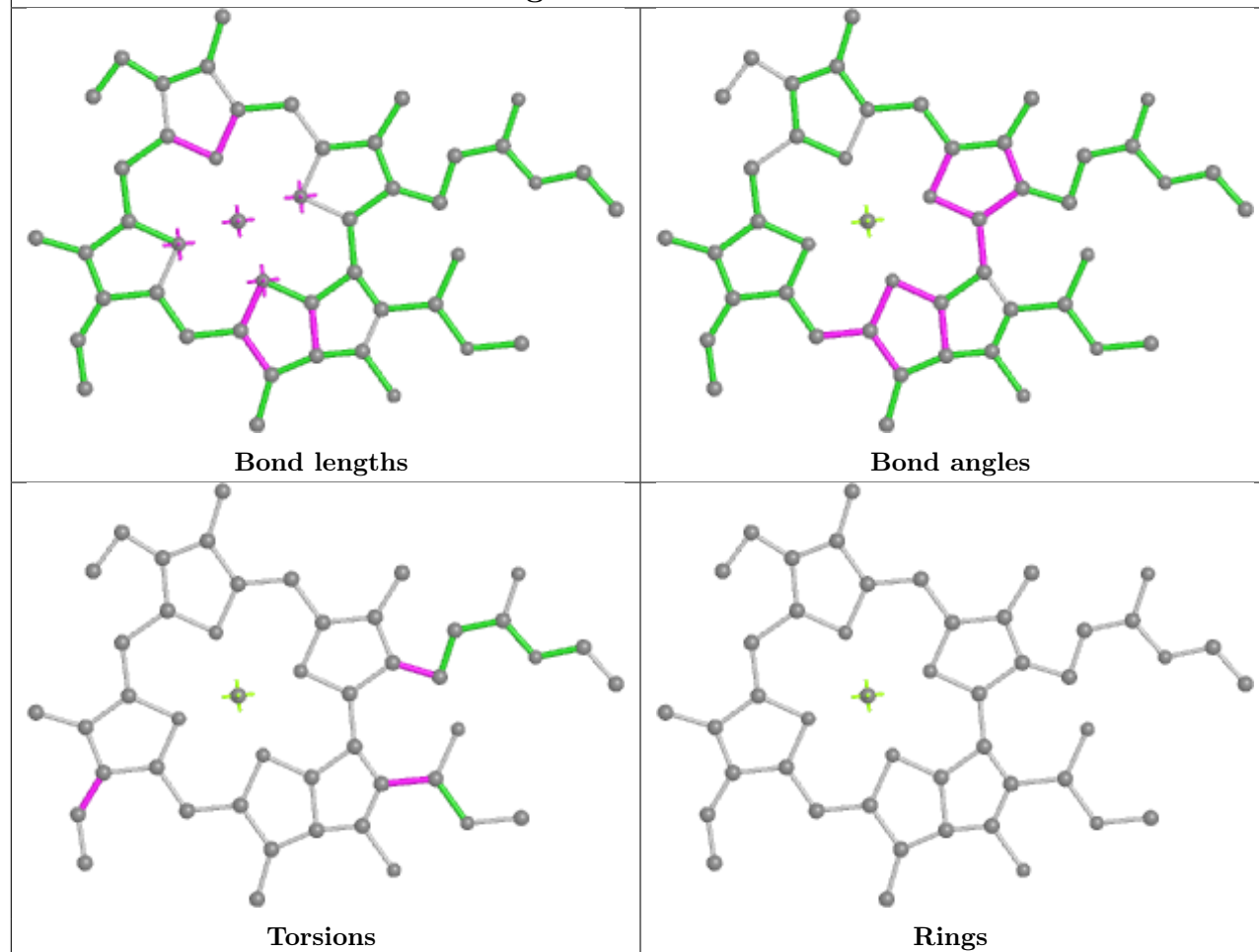


Rings

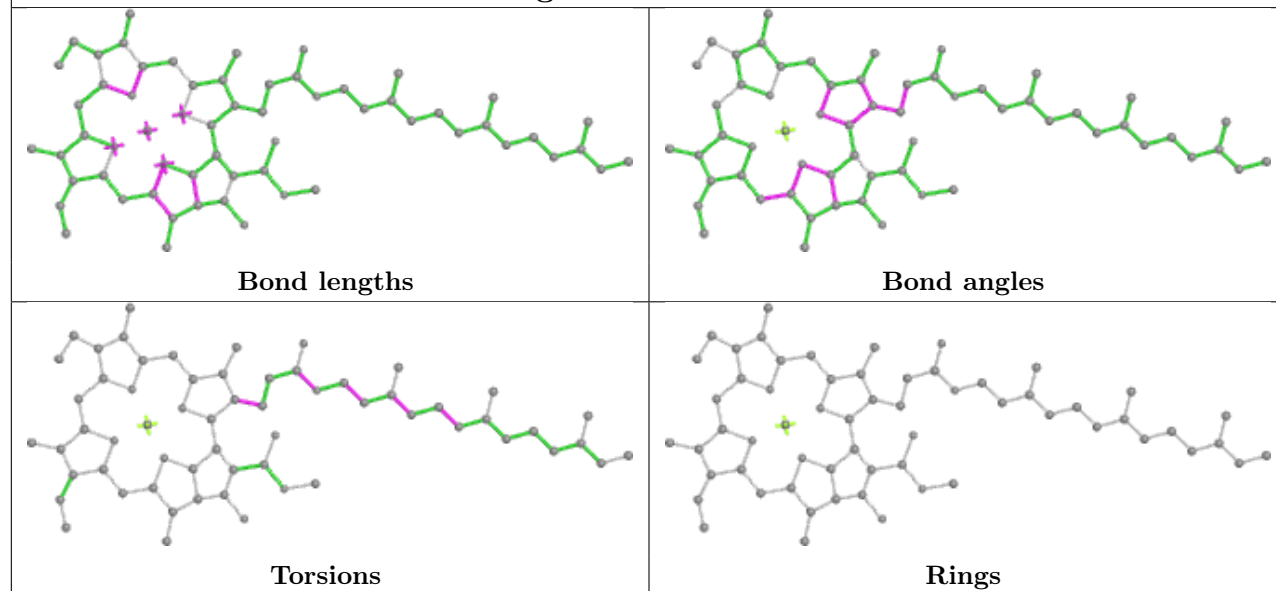


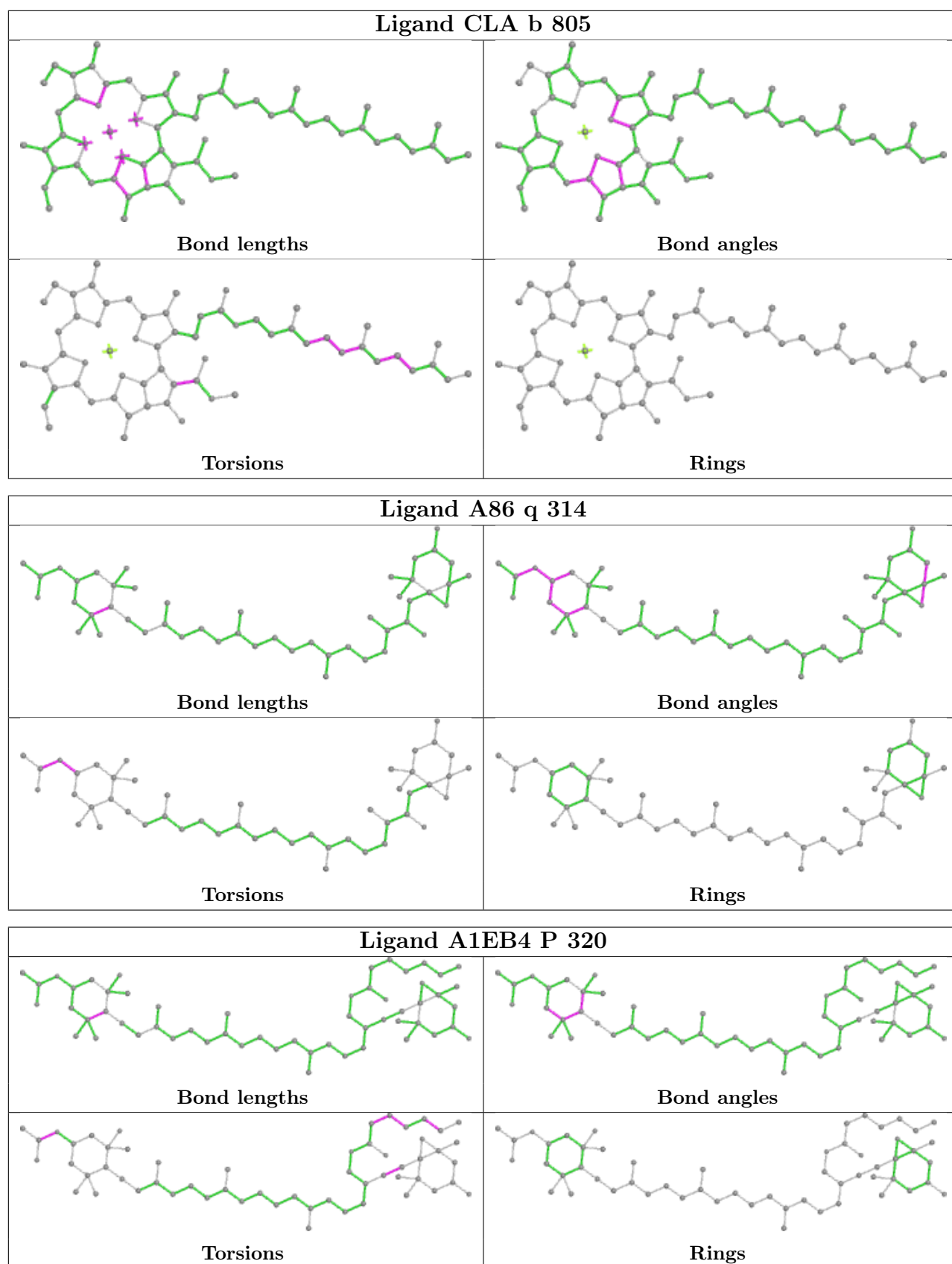


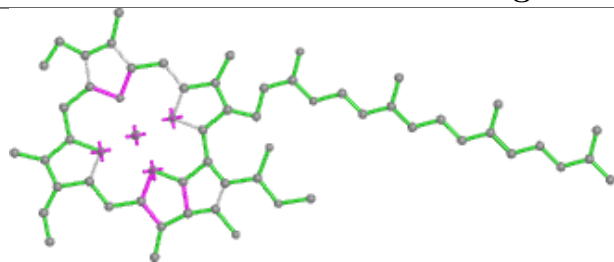
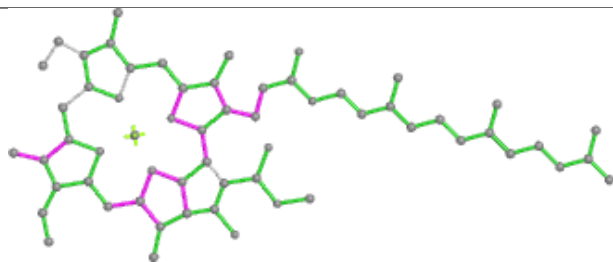
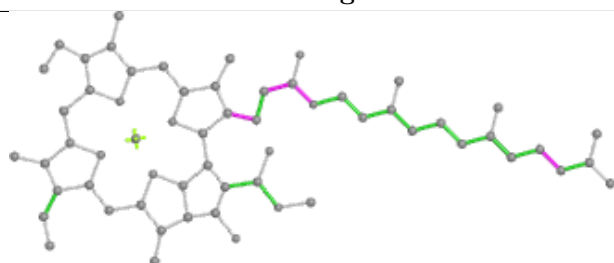
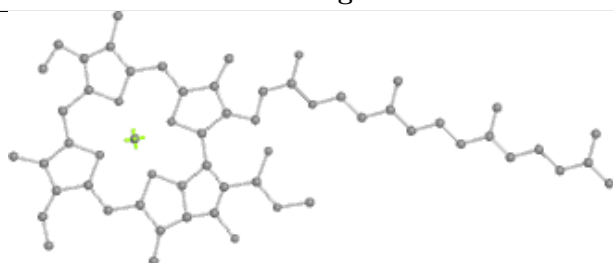
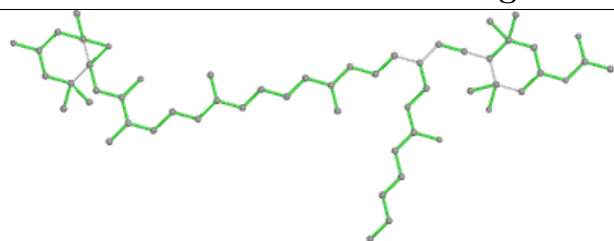
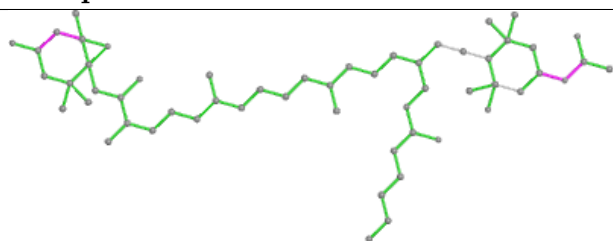
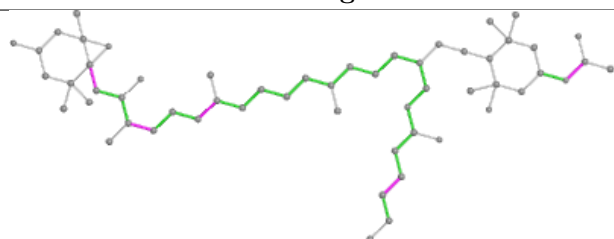
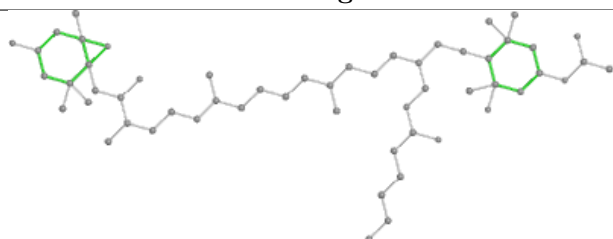
Ligand CLA E 302

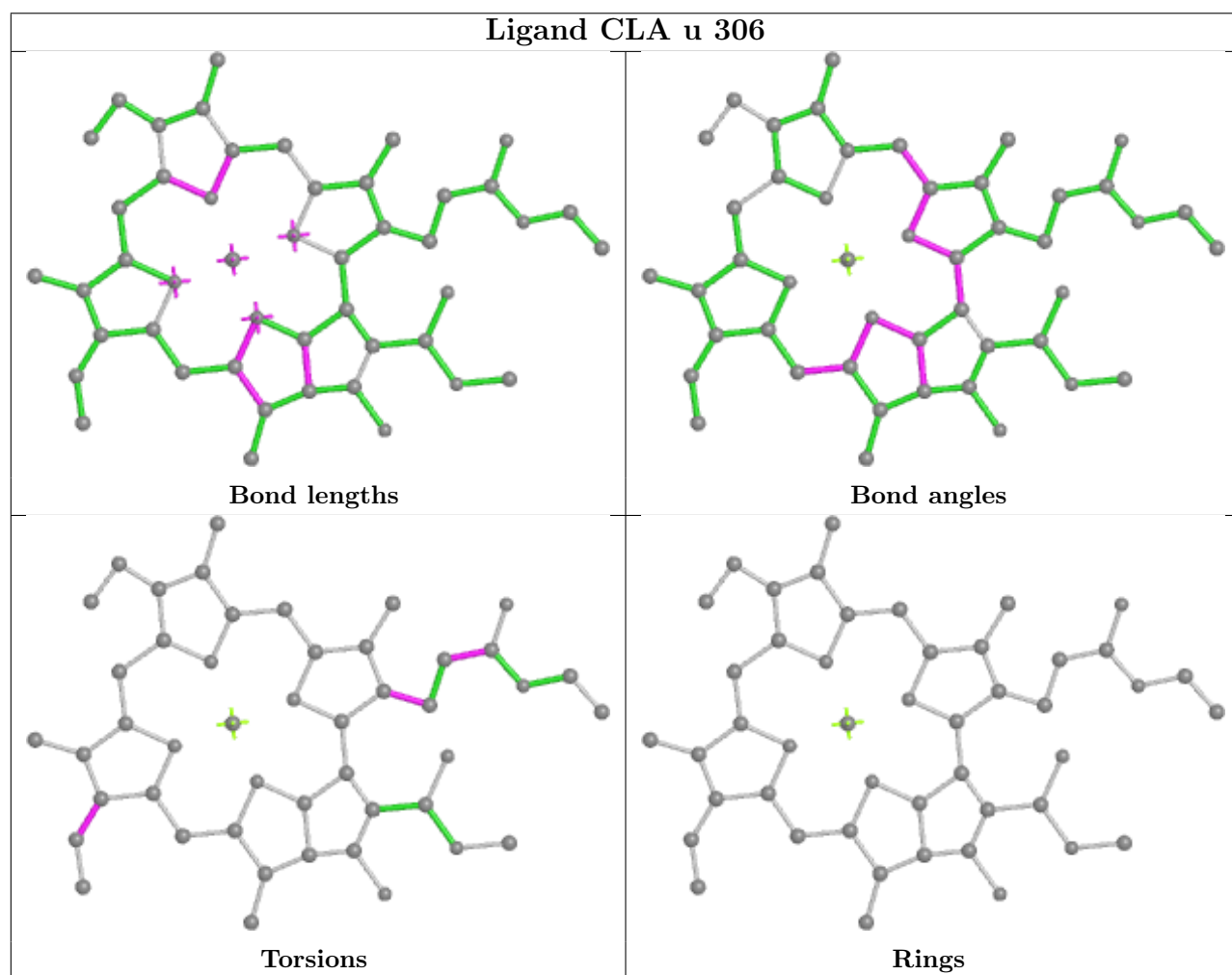
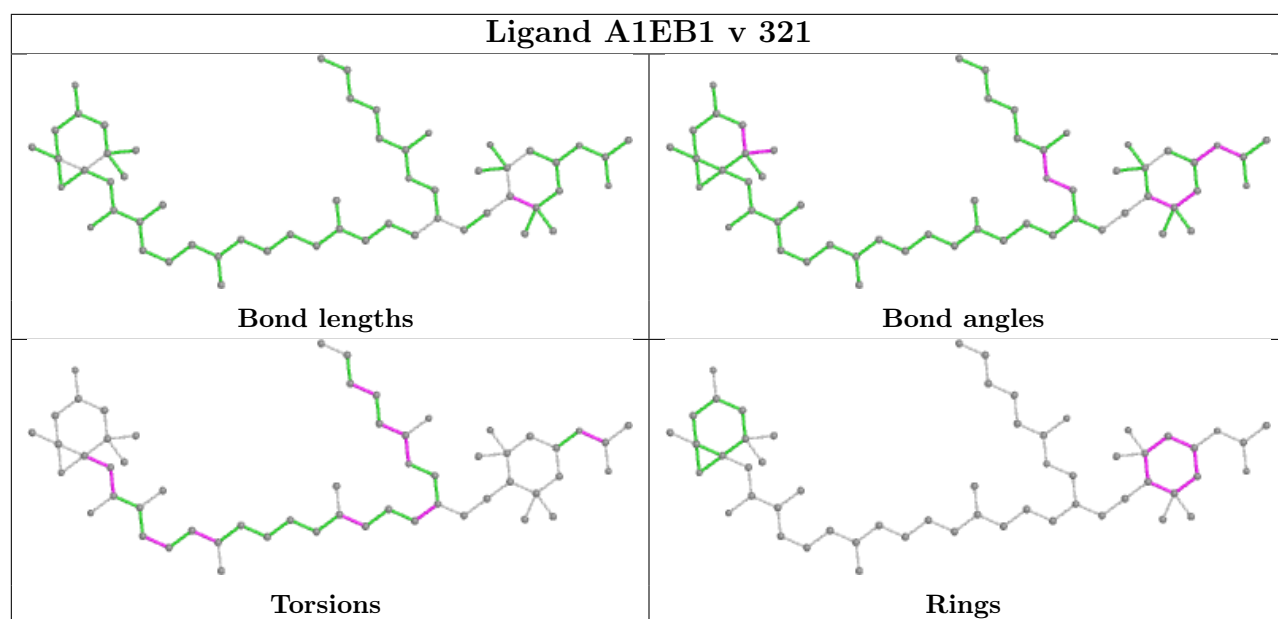


Ligand CLA a 819

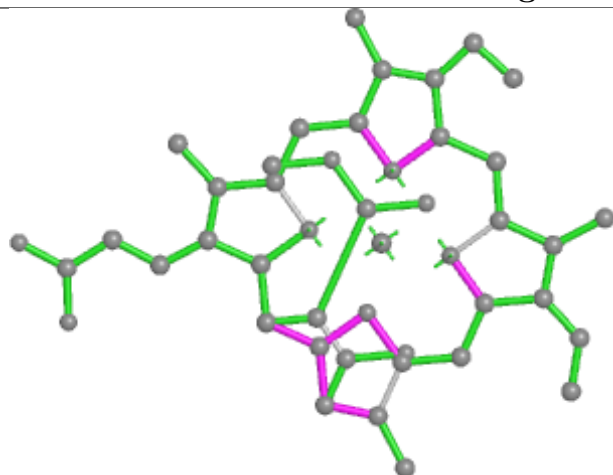




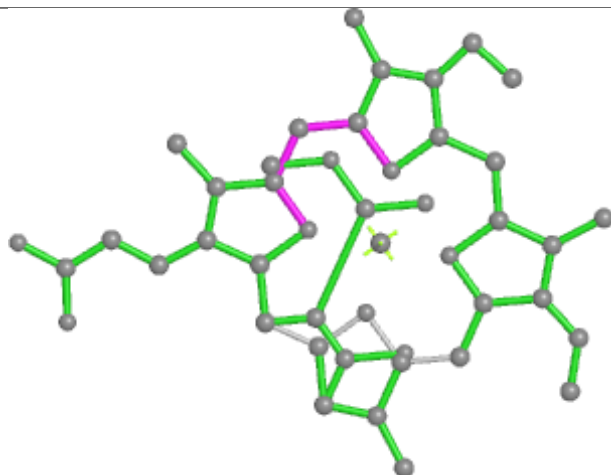
Ligand CLA K 306**Bond lengths****Bond angles****Torsions****Rings****Ligand A1EB1 q 322****Bond lengths****Bond angles****Torsions****Rings**



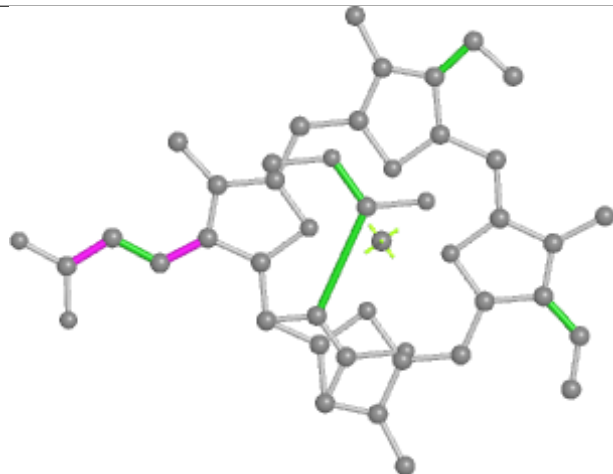
Ligand KC2 L 308



Bond lengths



Bond angles

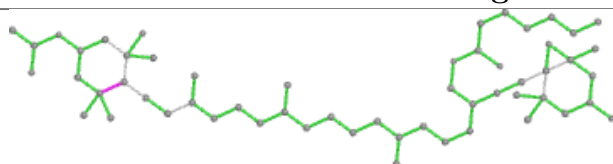


Torsions

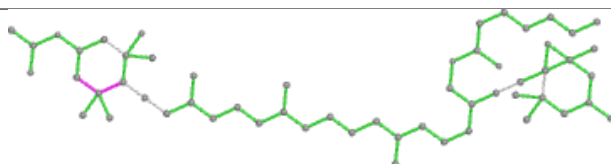


Rings

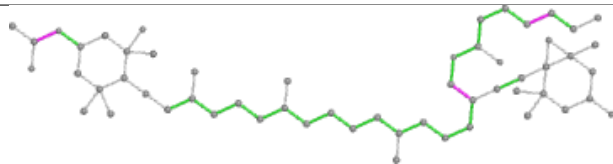
Ligand A1EB4 M 319



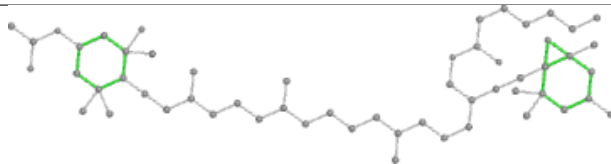
Bond lengths



Bond angles

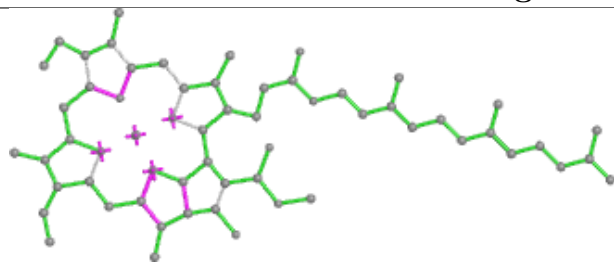


Torsions

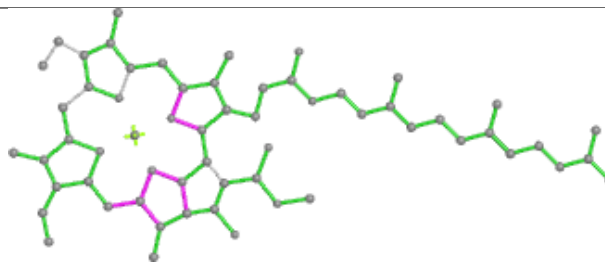


Rings

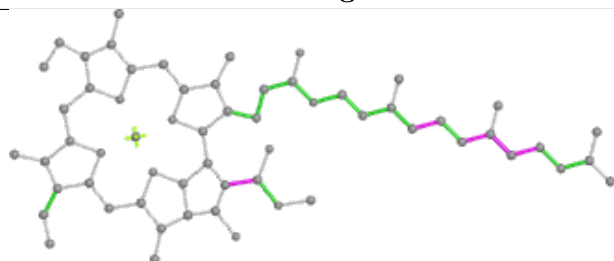
Ligand CLA T 304



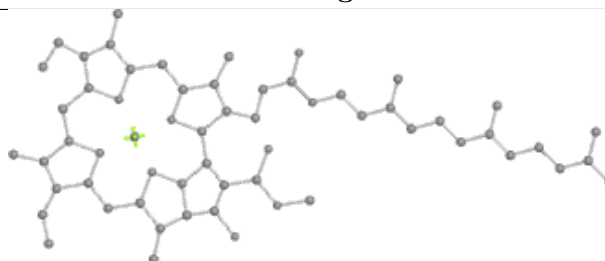
Bond lengths



Bond angles

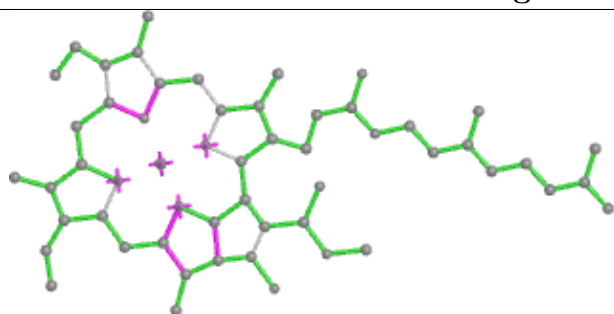


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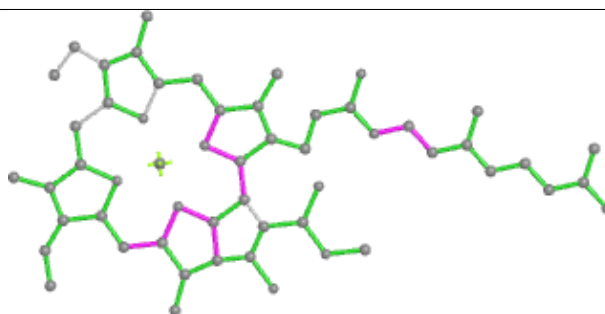


Rings

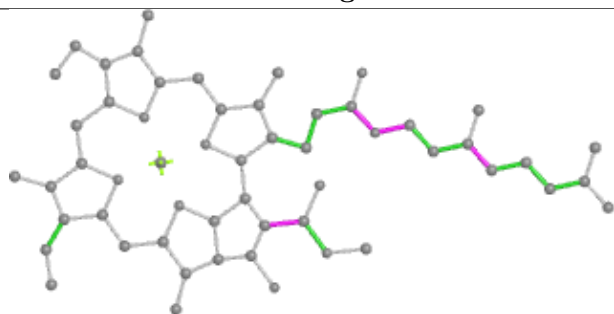
Ligand CLA D 312



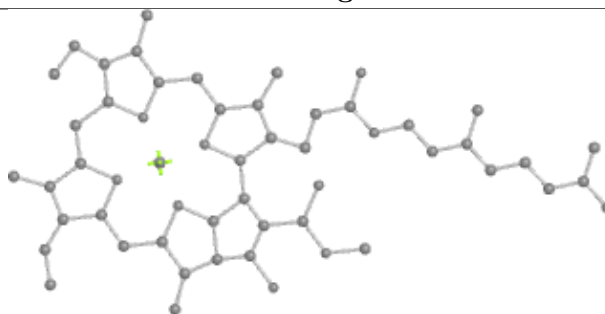
Bond lengths



Bond angles

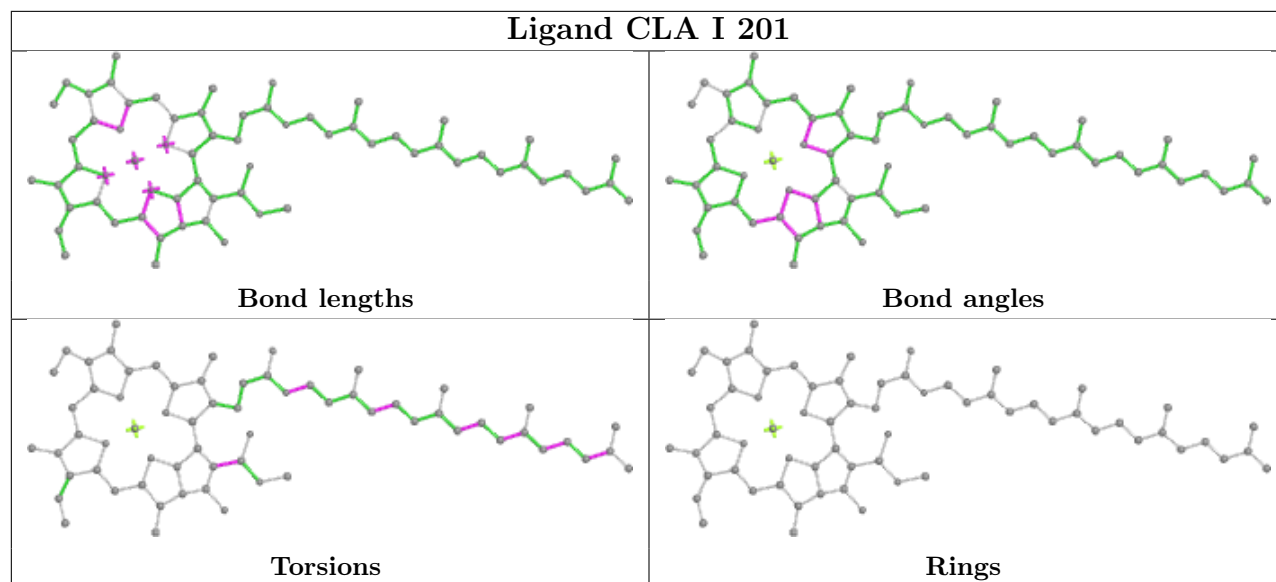


Torsions

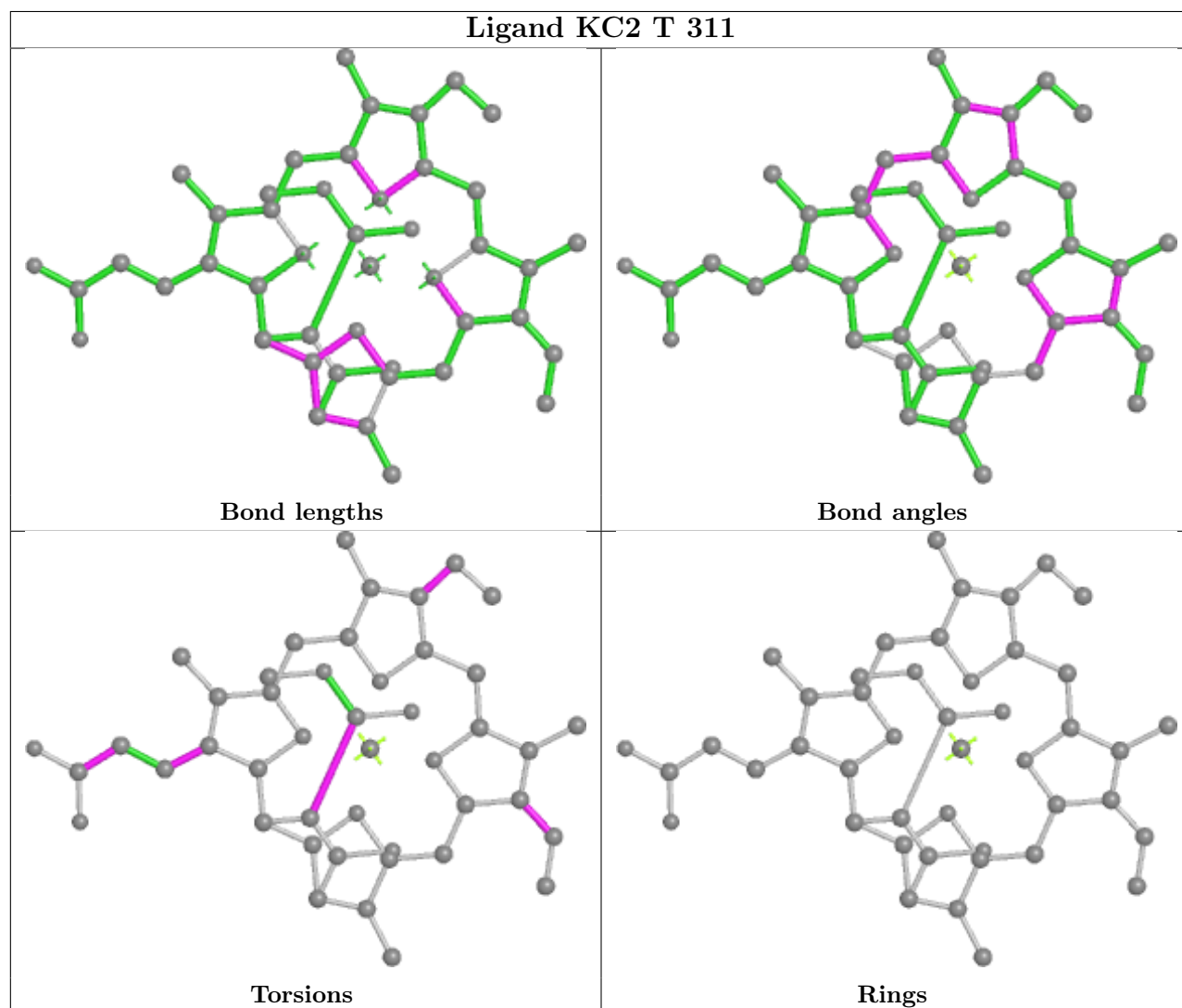


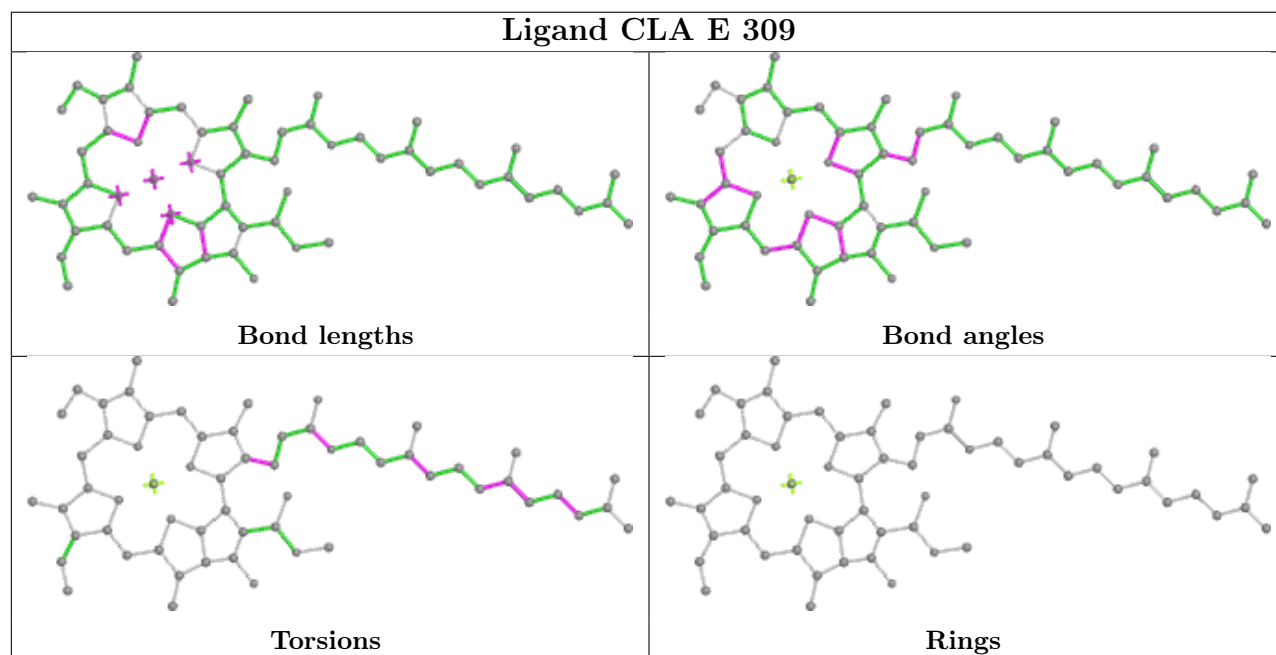
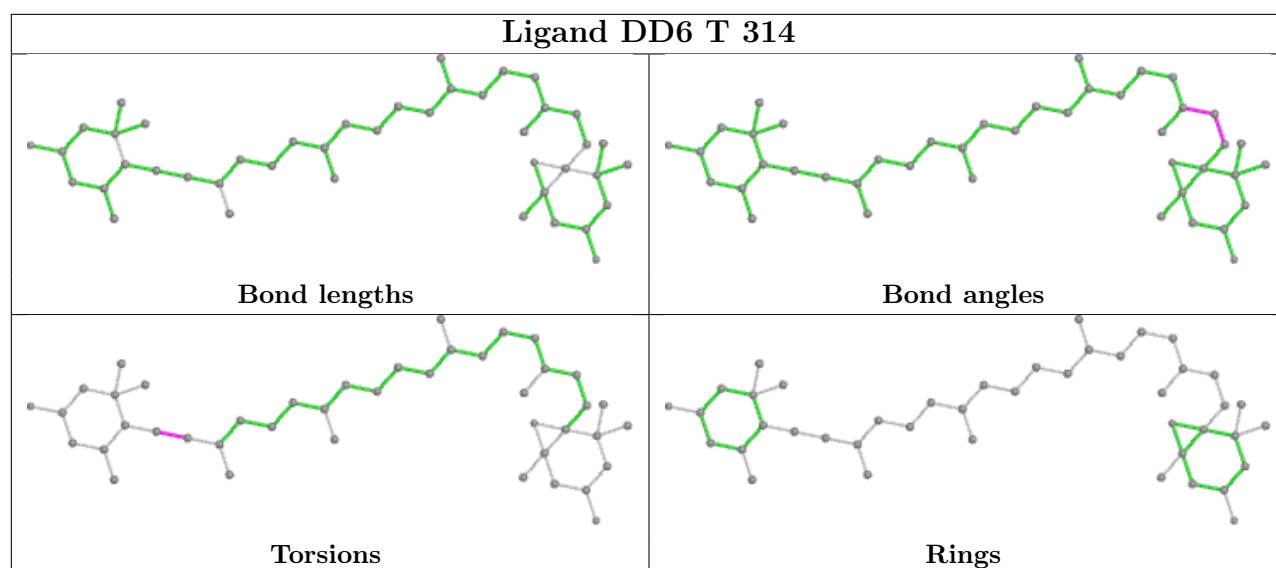
Rings

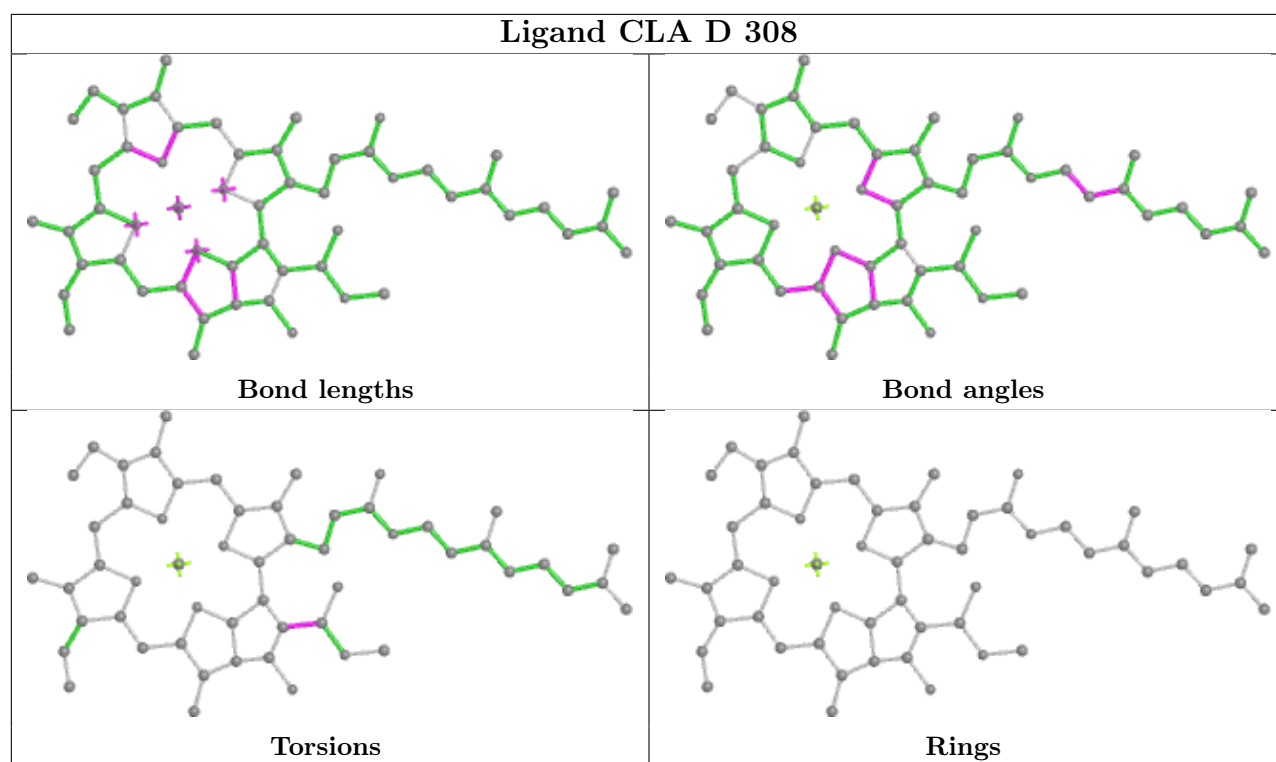
Ligand CLA I 201



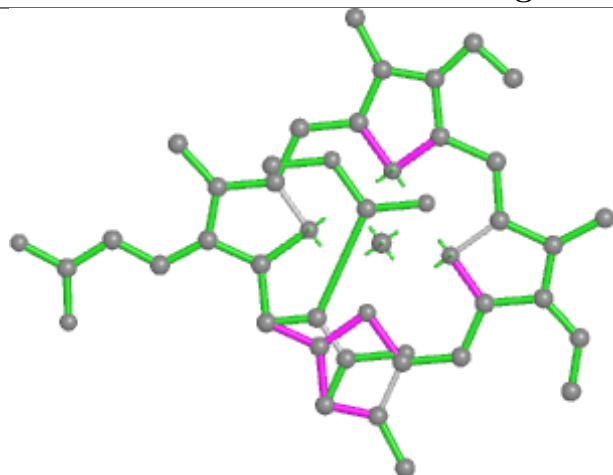
Ligand KC2 T 311



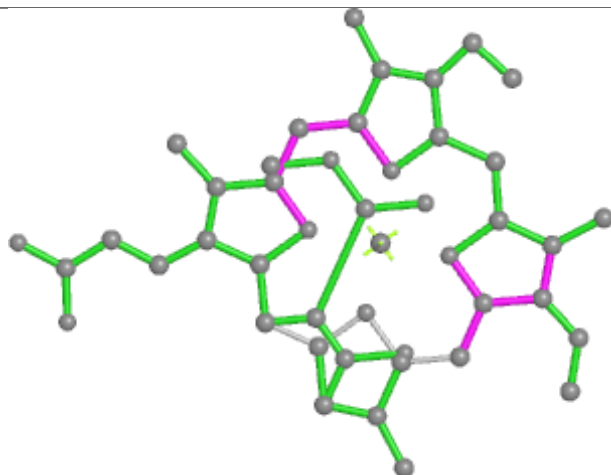




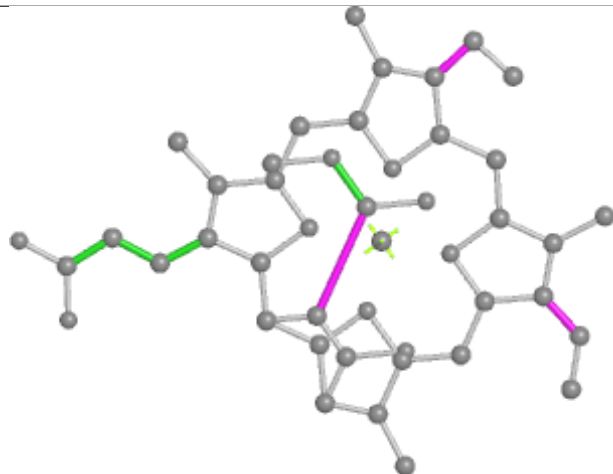
Ligand KC2 H 303



Bond lengths



Bond angles

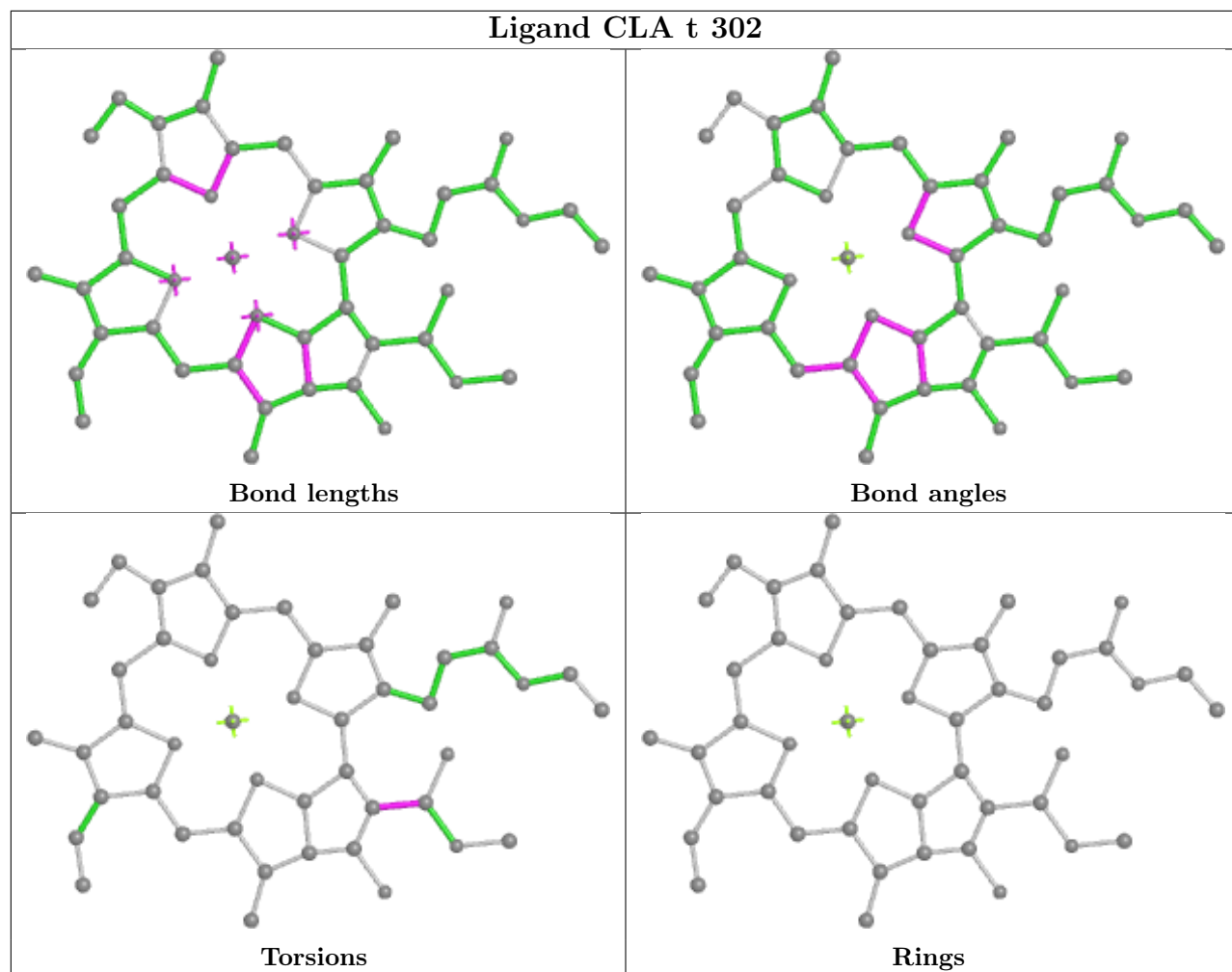


Torsions

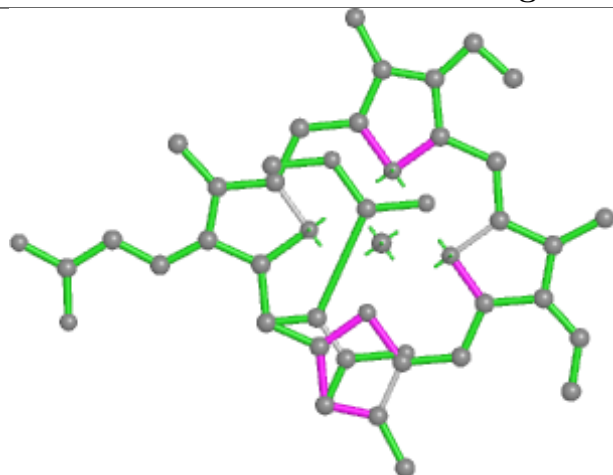


Rings

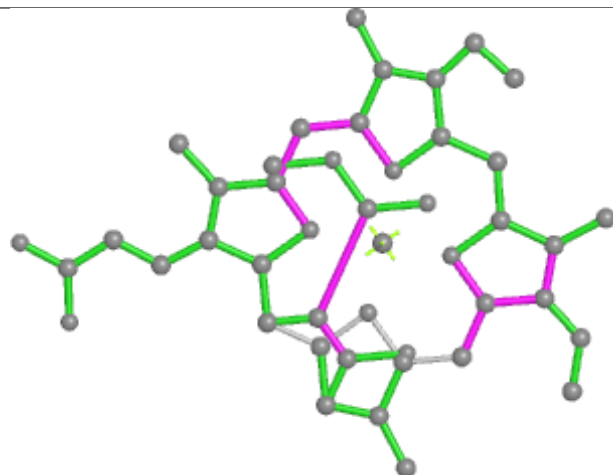
Ligand CLA t 302



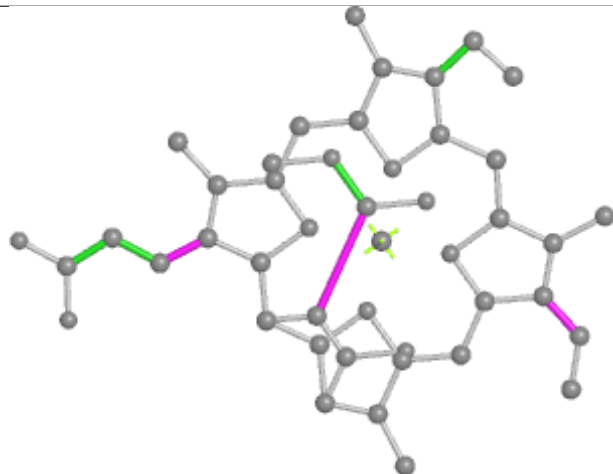
Ligand KC2 S 303



Bond lengths



Bond angles

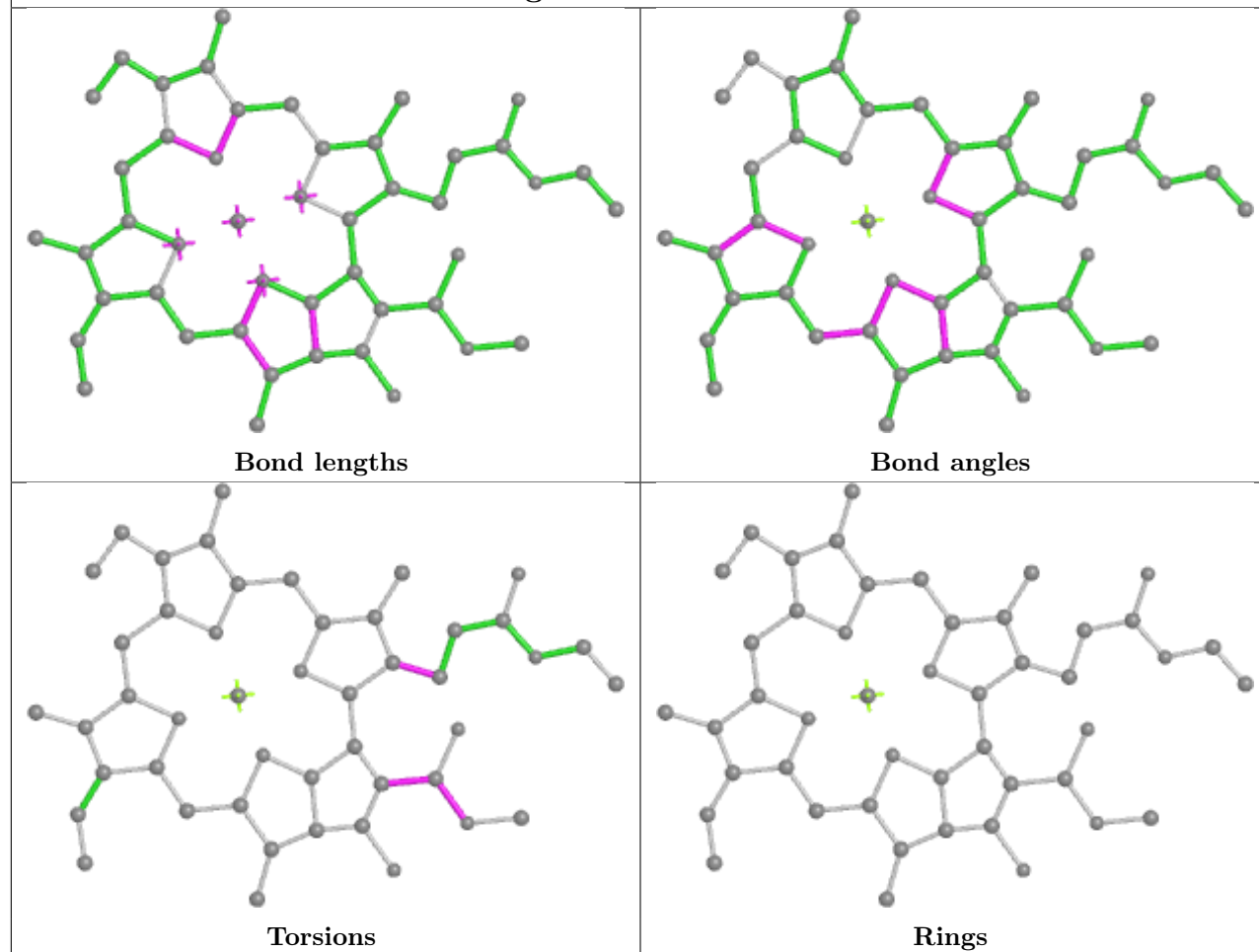


Torsions

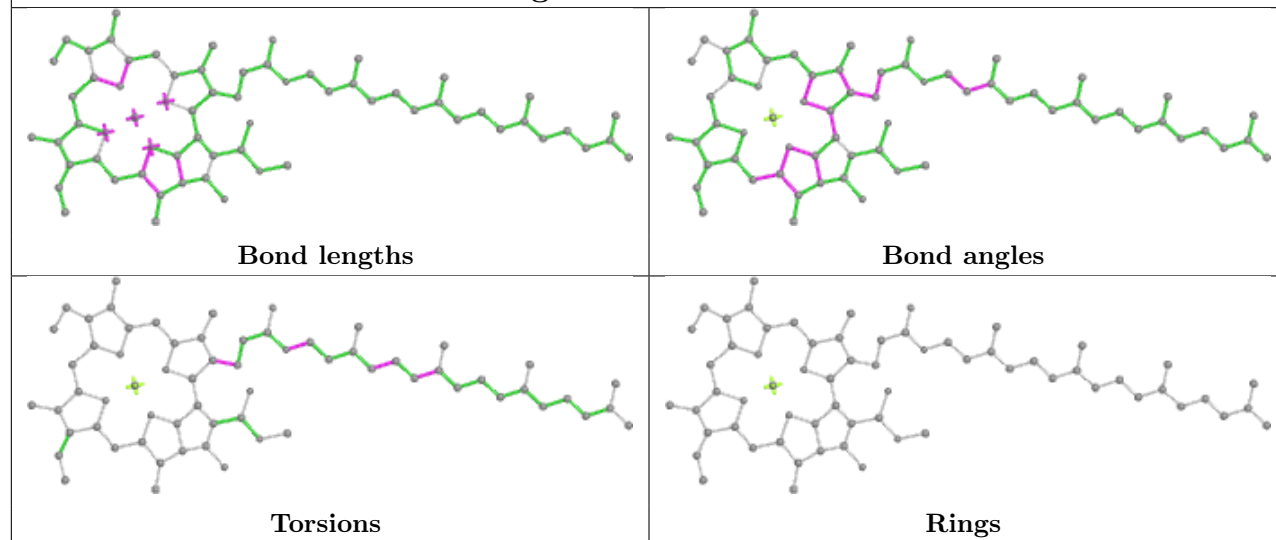


Rings

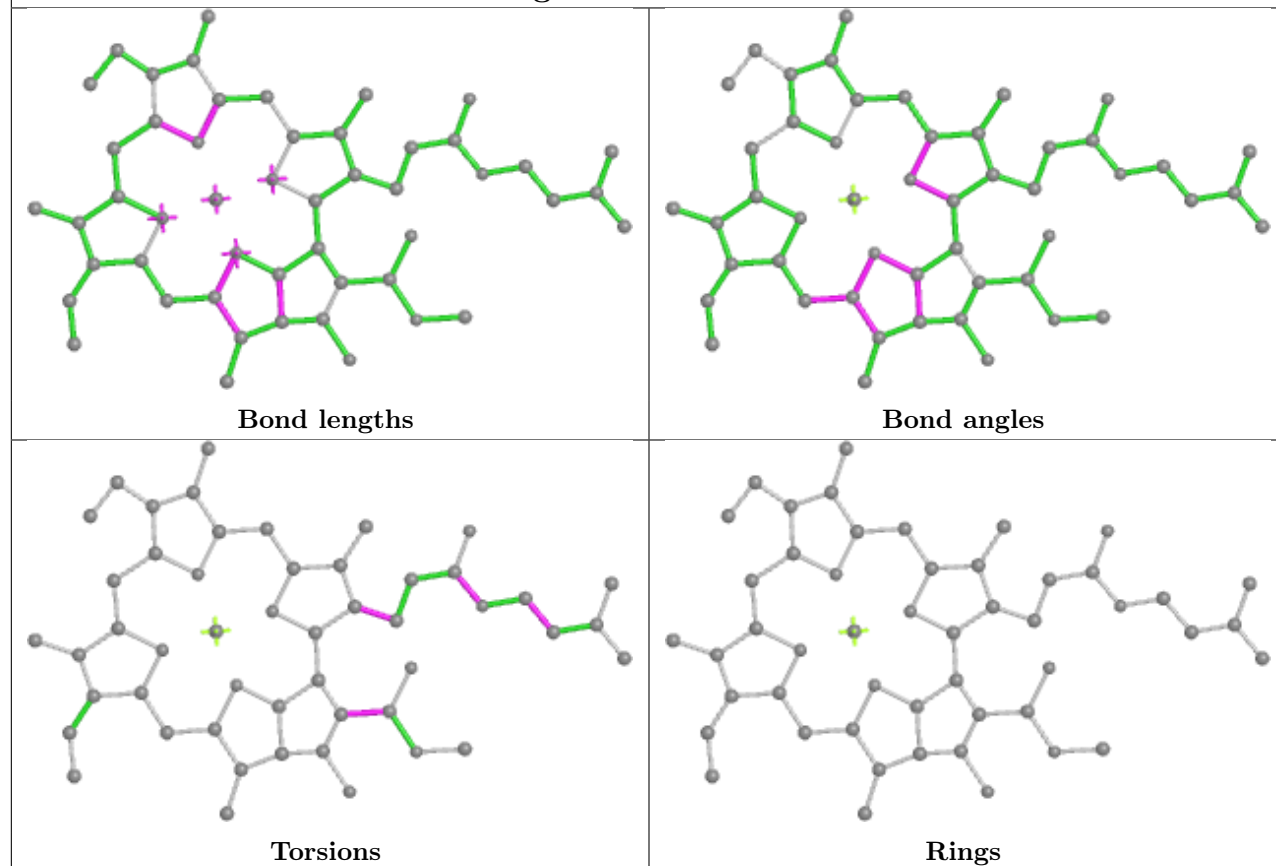
Ligand CLA w 308



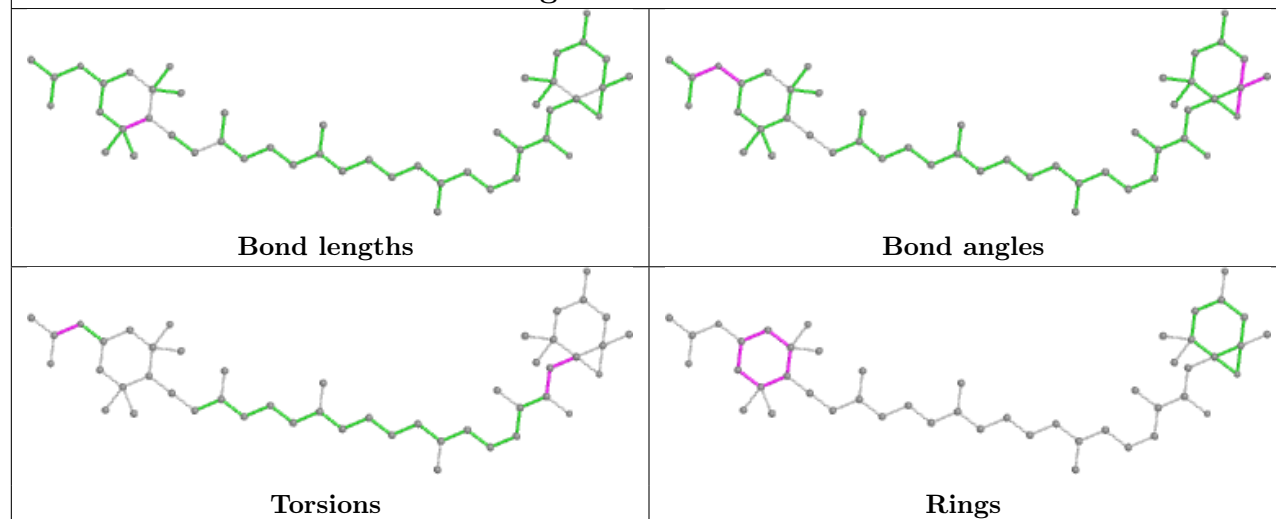
Ligand CLA D 307



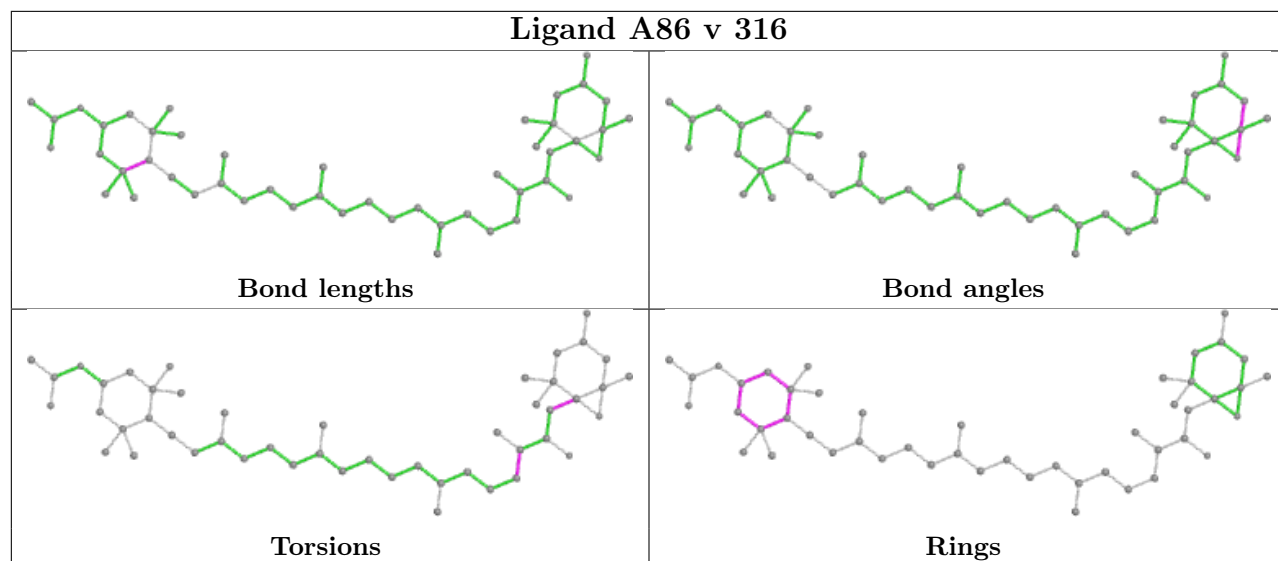
Ligand CLA E 311



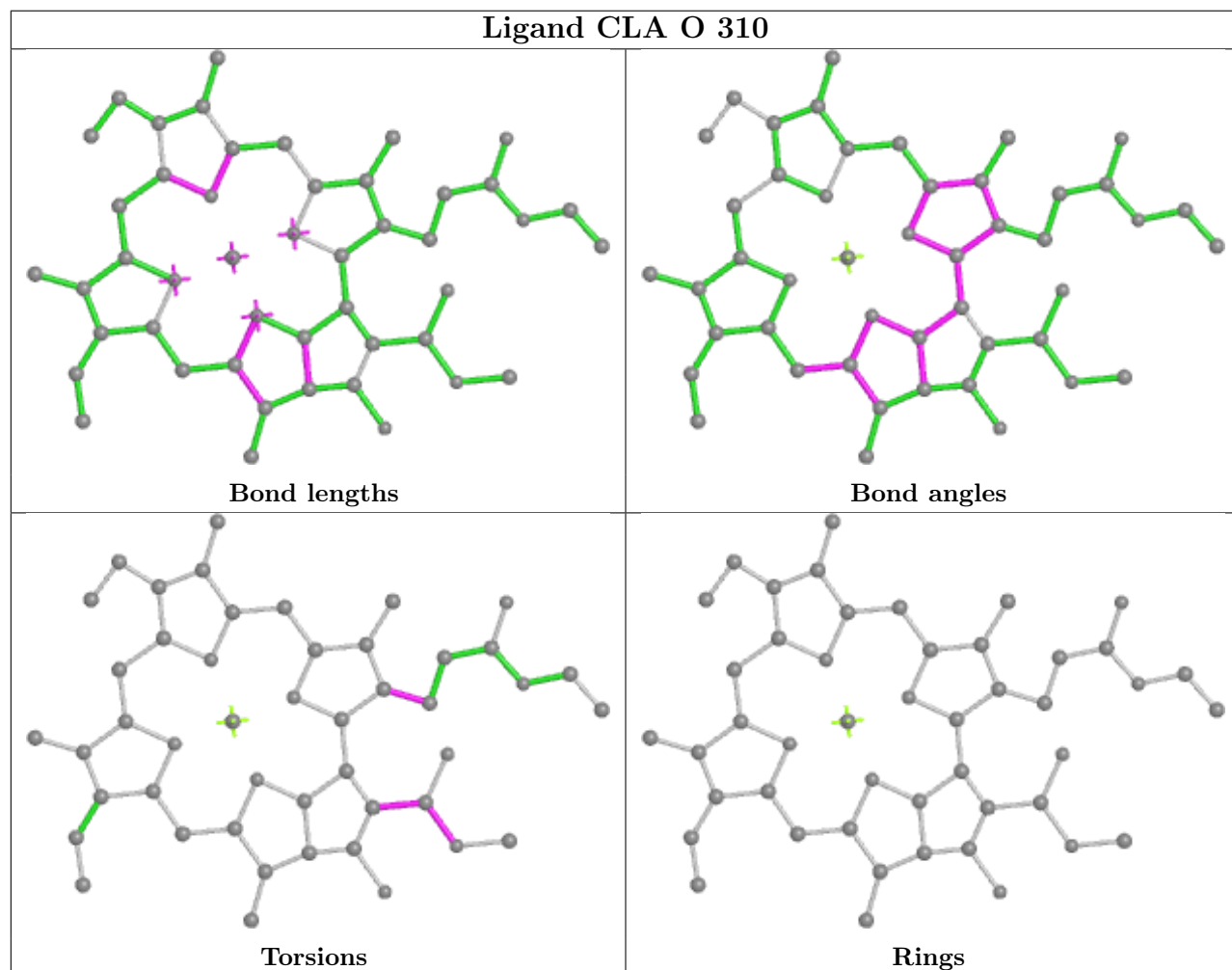
Ligand A86 Z 316

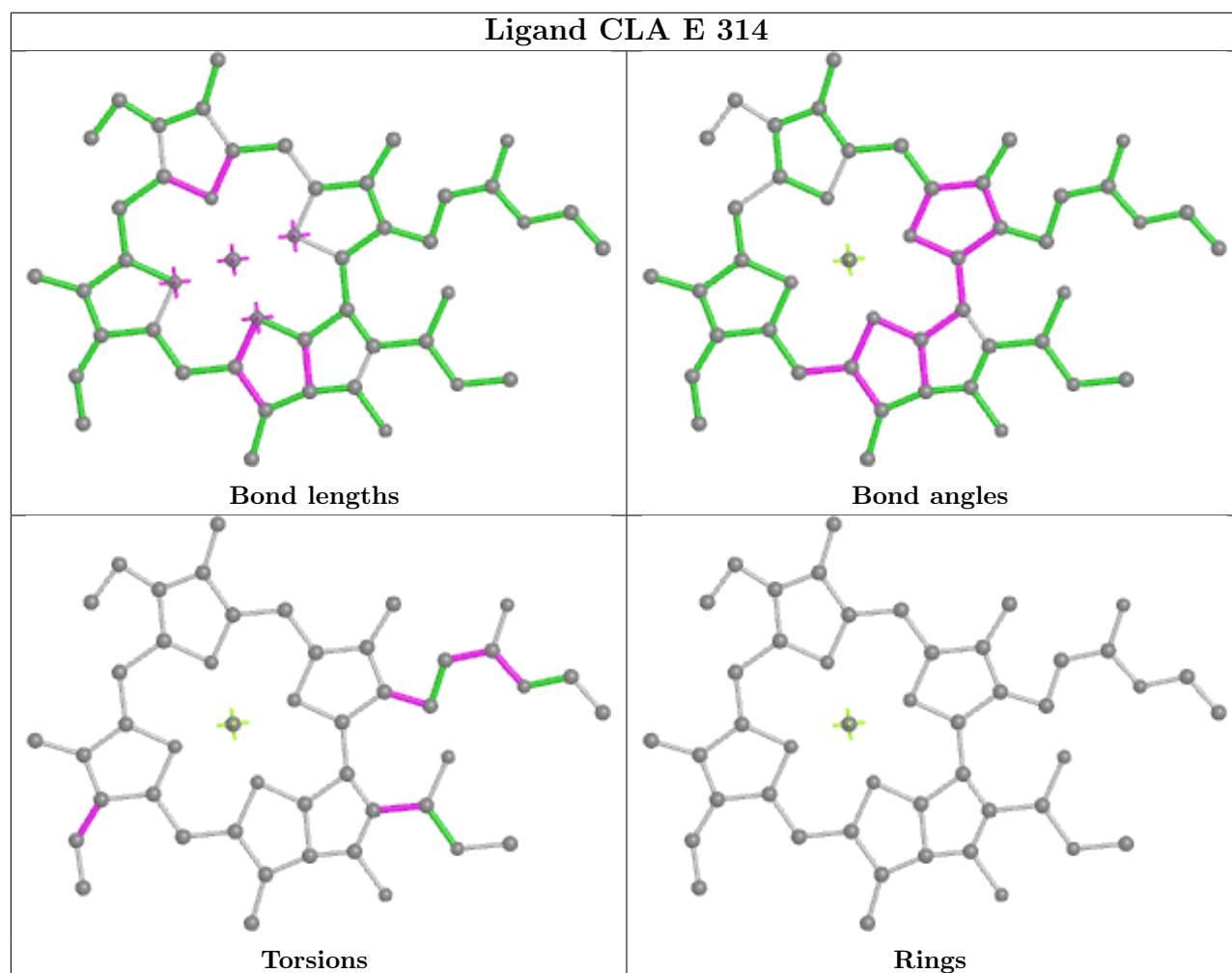
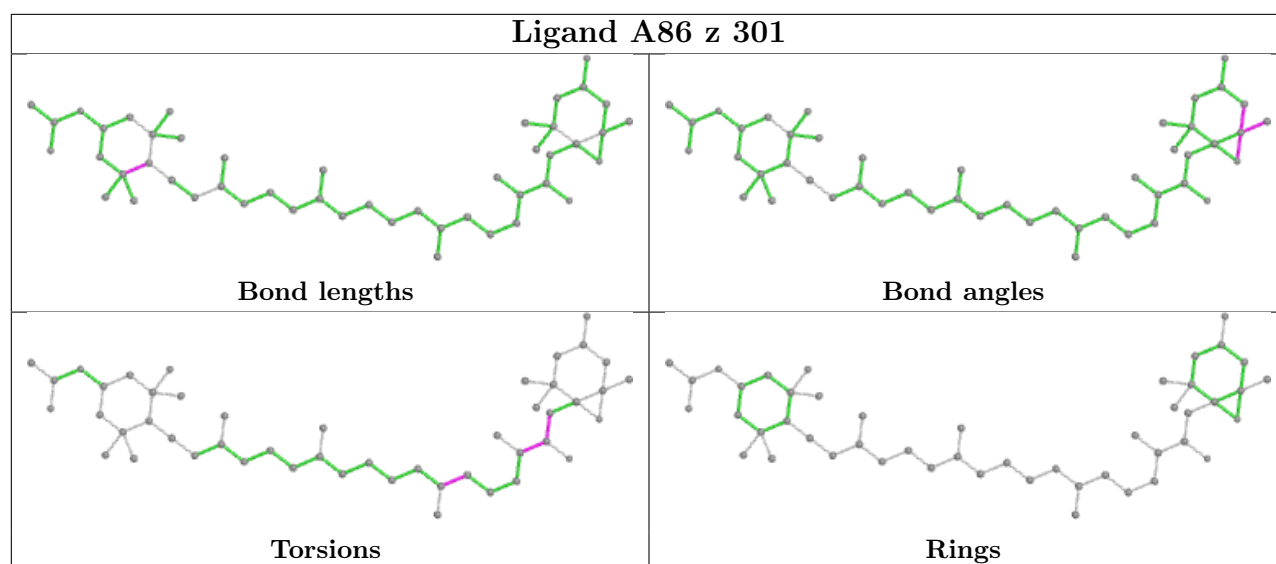


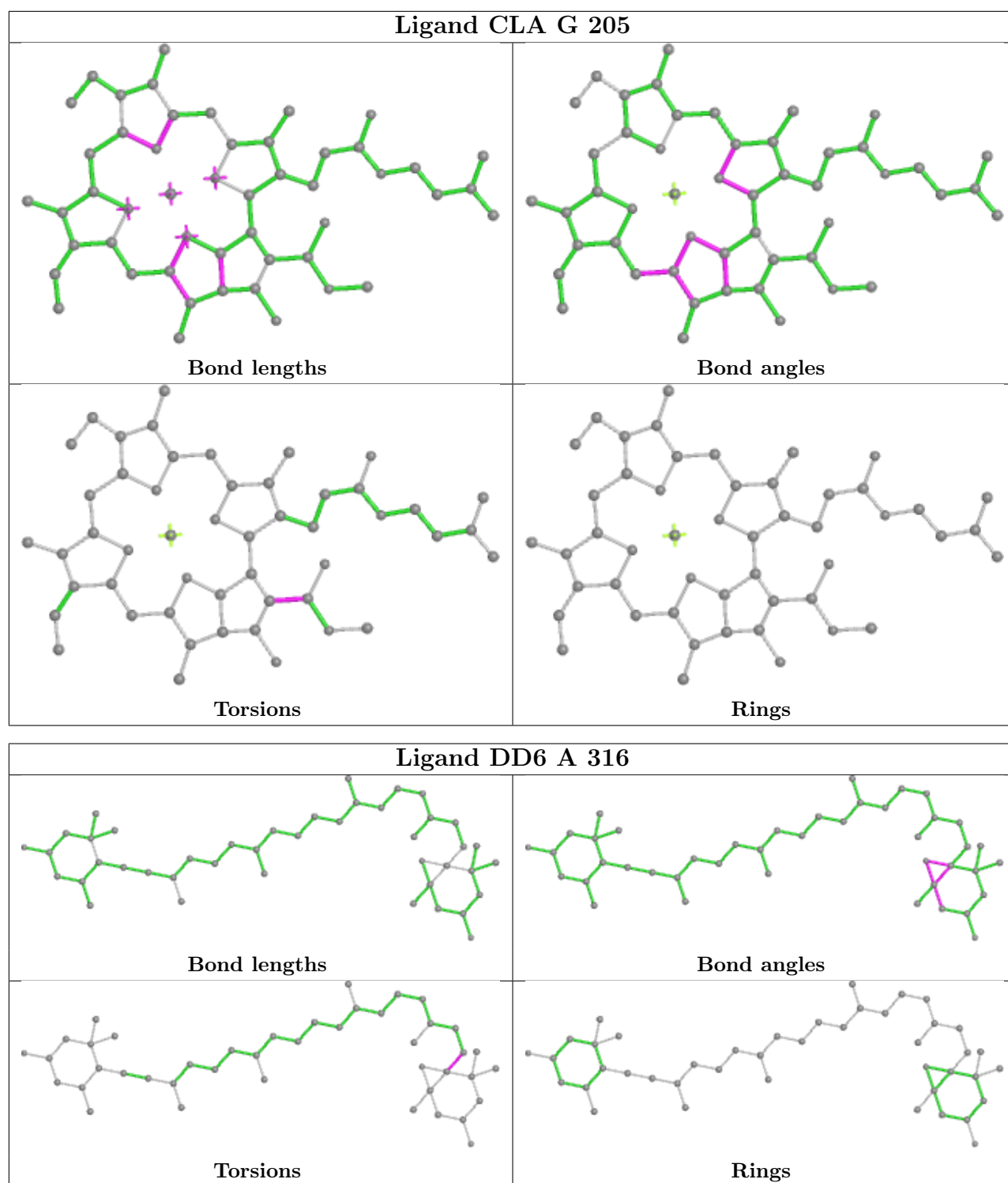
Ligand A86 v 316

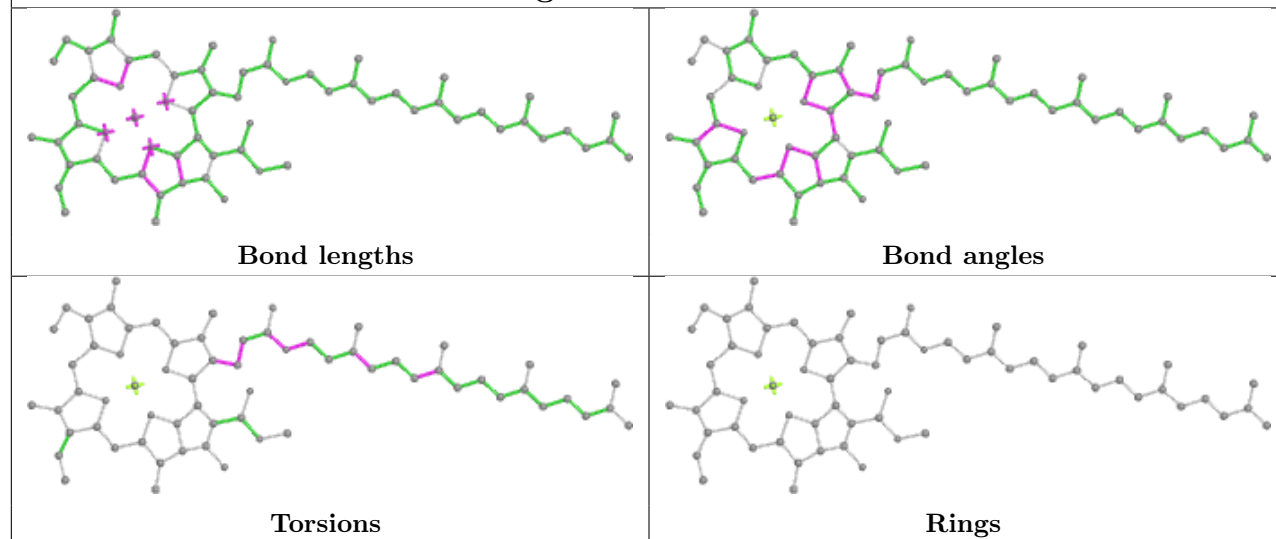
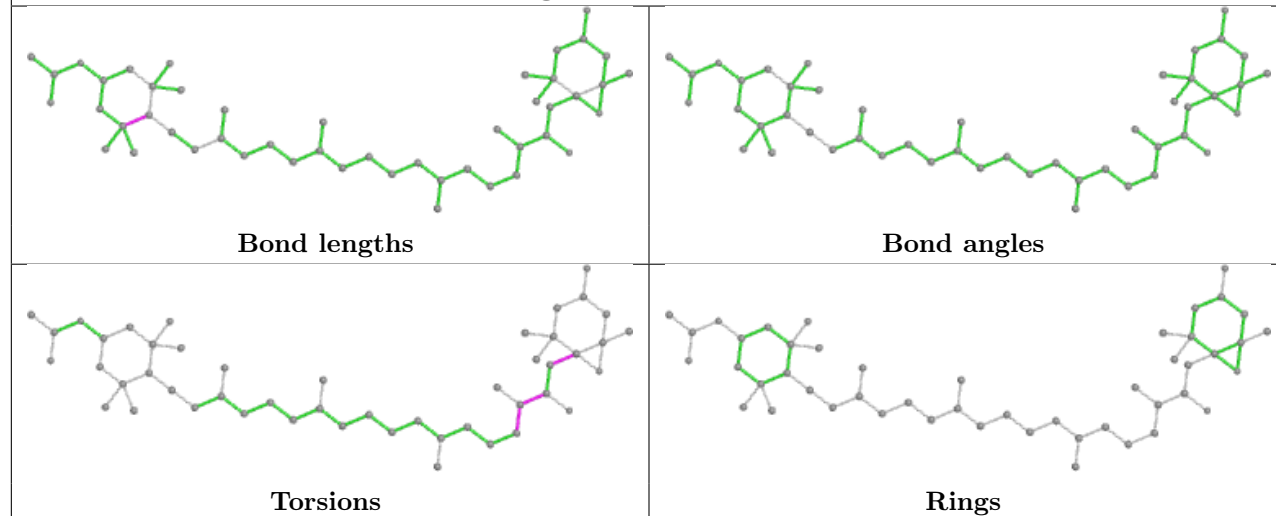
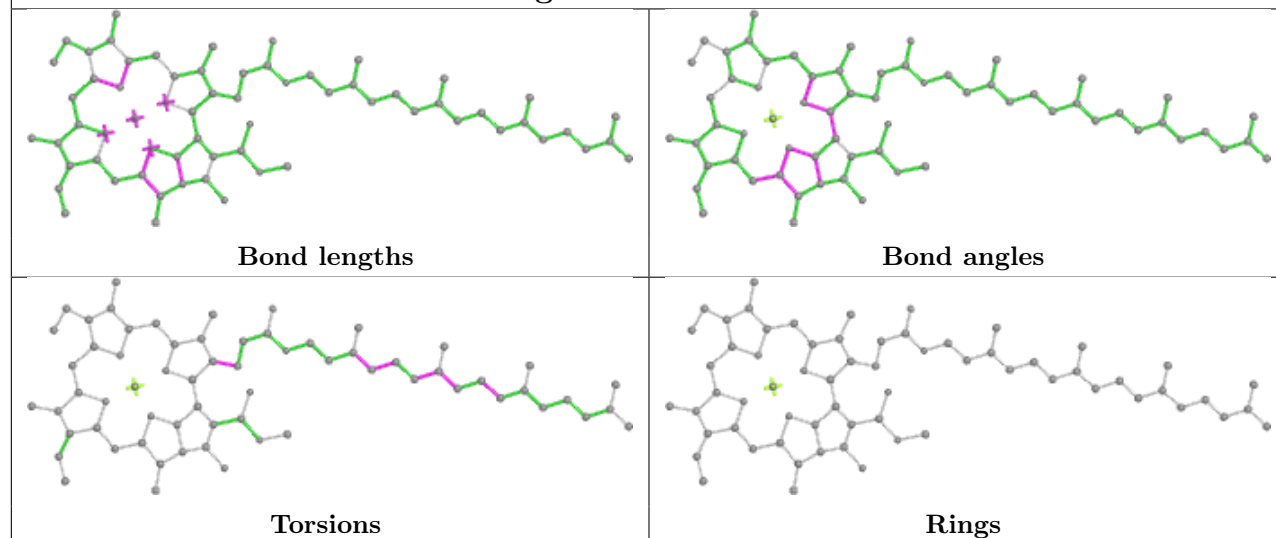


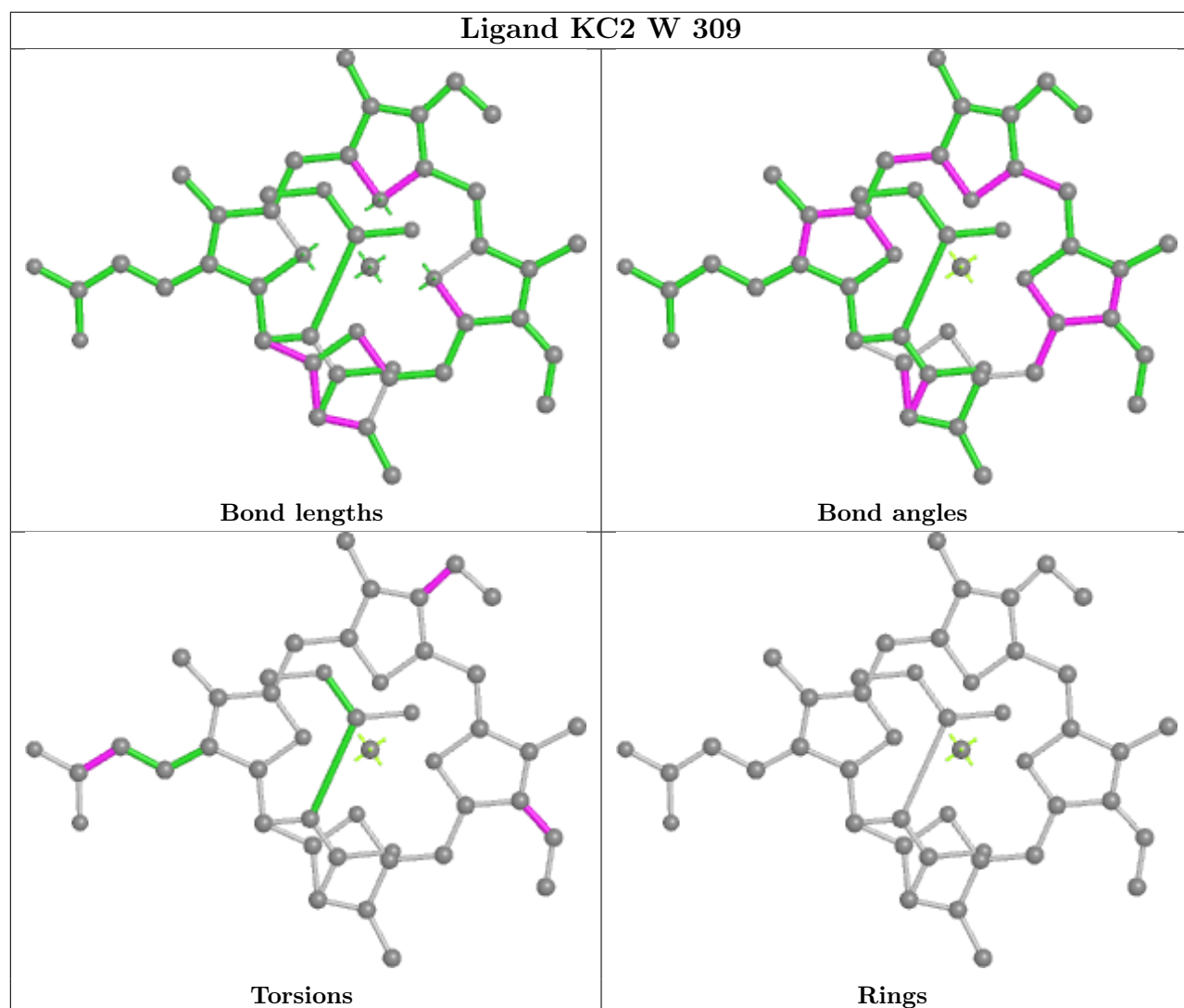
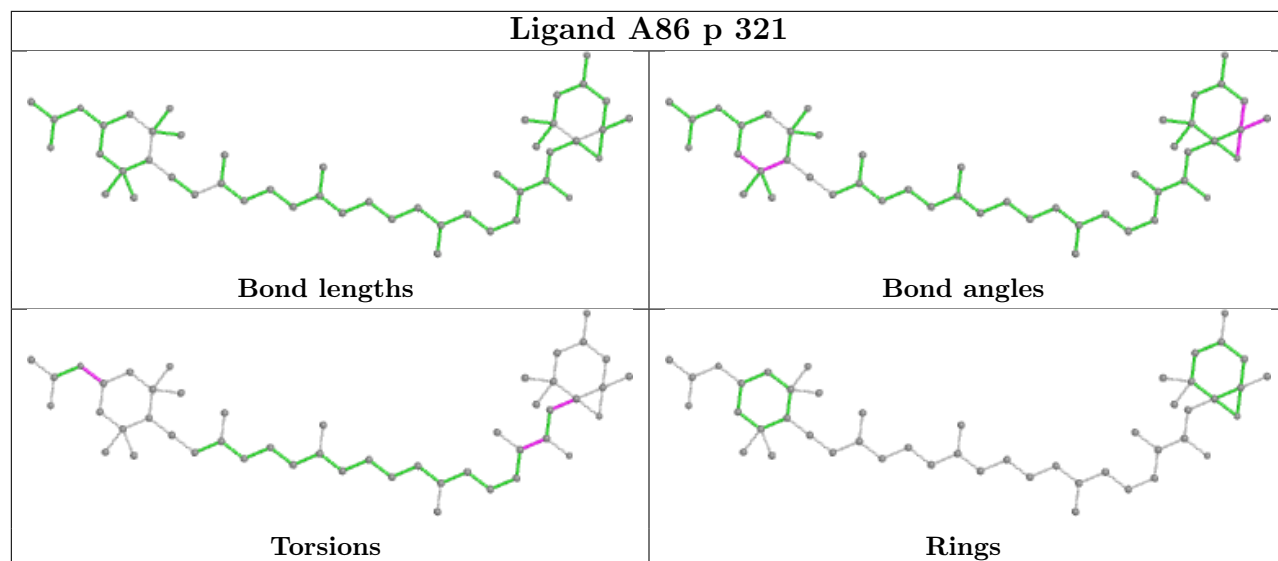
Ligand CLA O 310



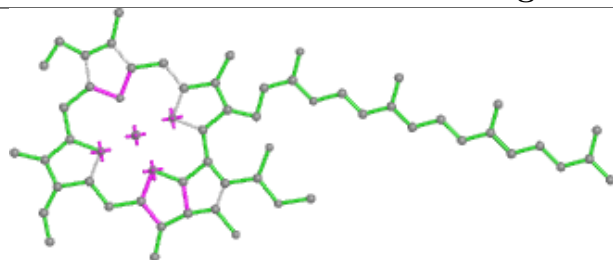




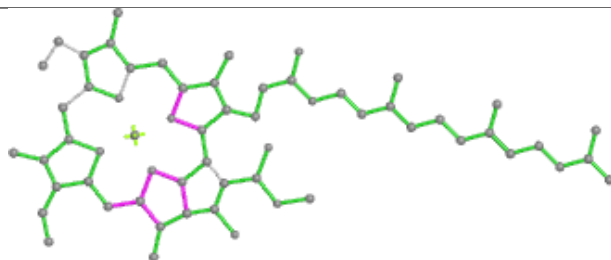
Ligand CLA a 822**Ligand A86 R 313****Ligand CLA b 838**



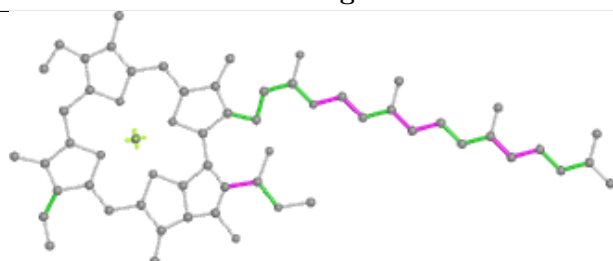
Ligand CLA b 837



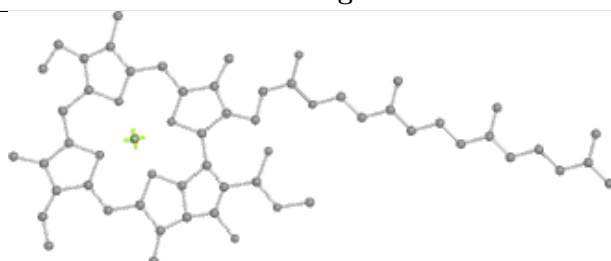
Bond lengths



Bond angles

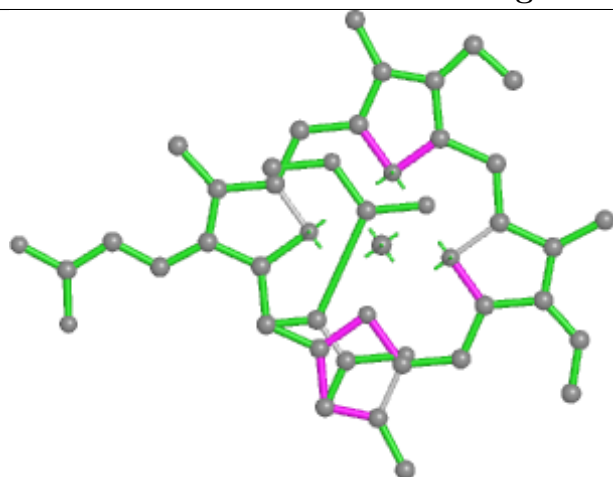


Torsions

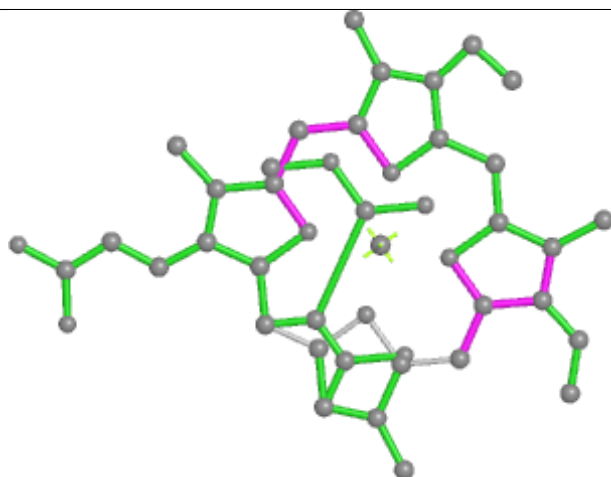


Rings

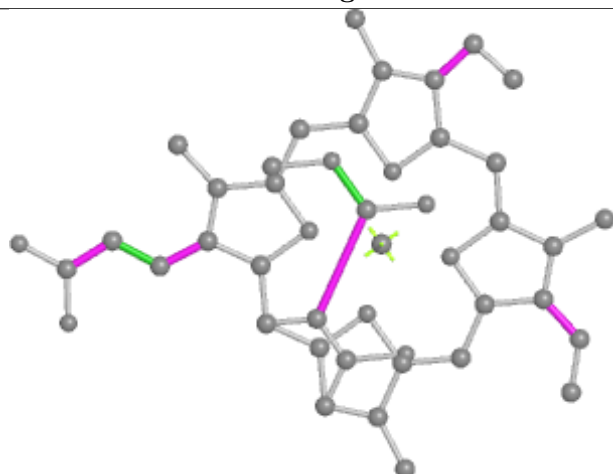
Ligand KC2 O 309



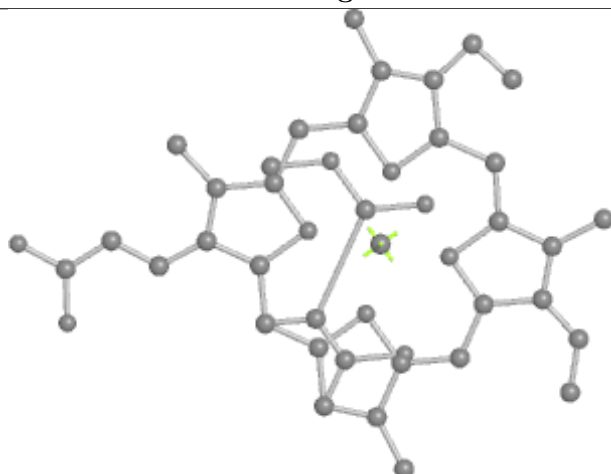
Bond lengths



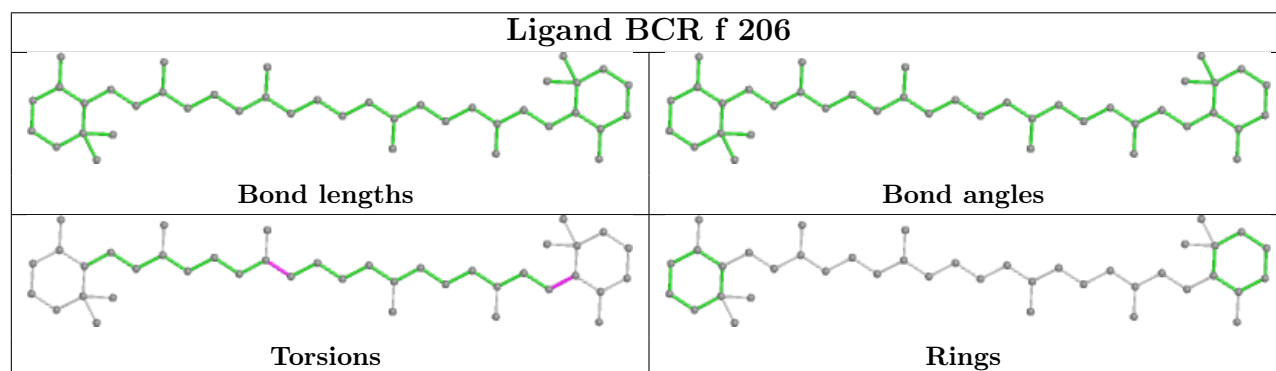
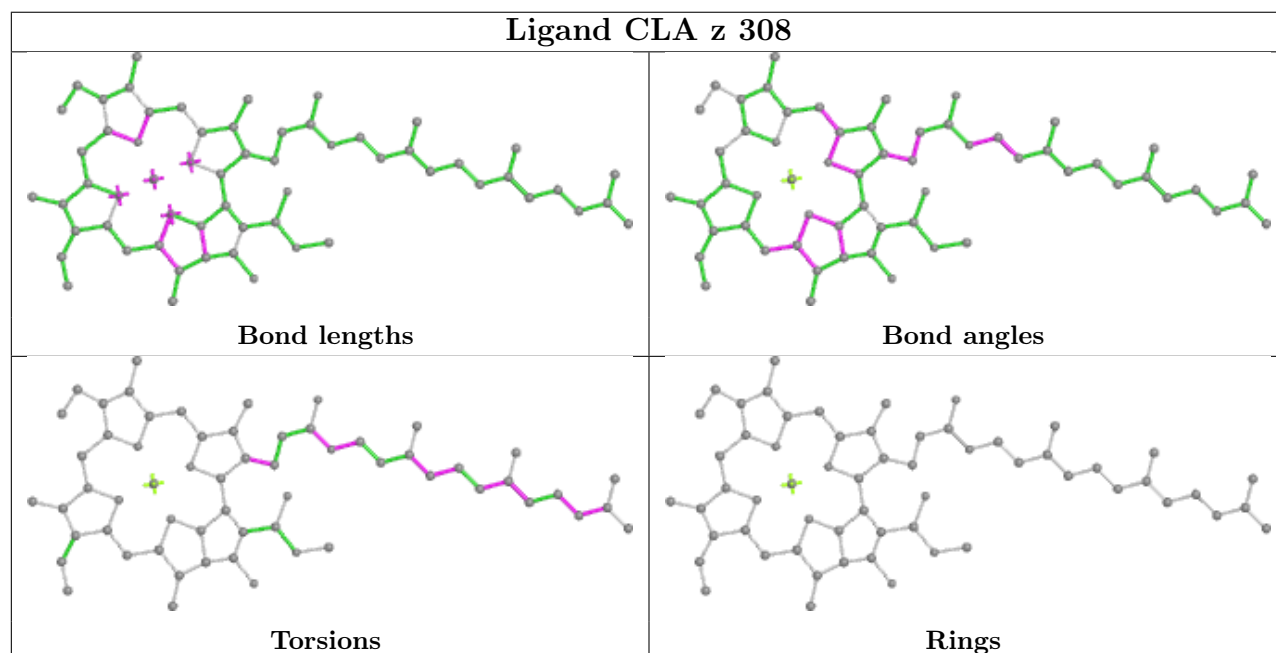
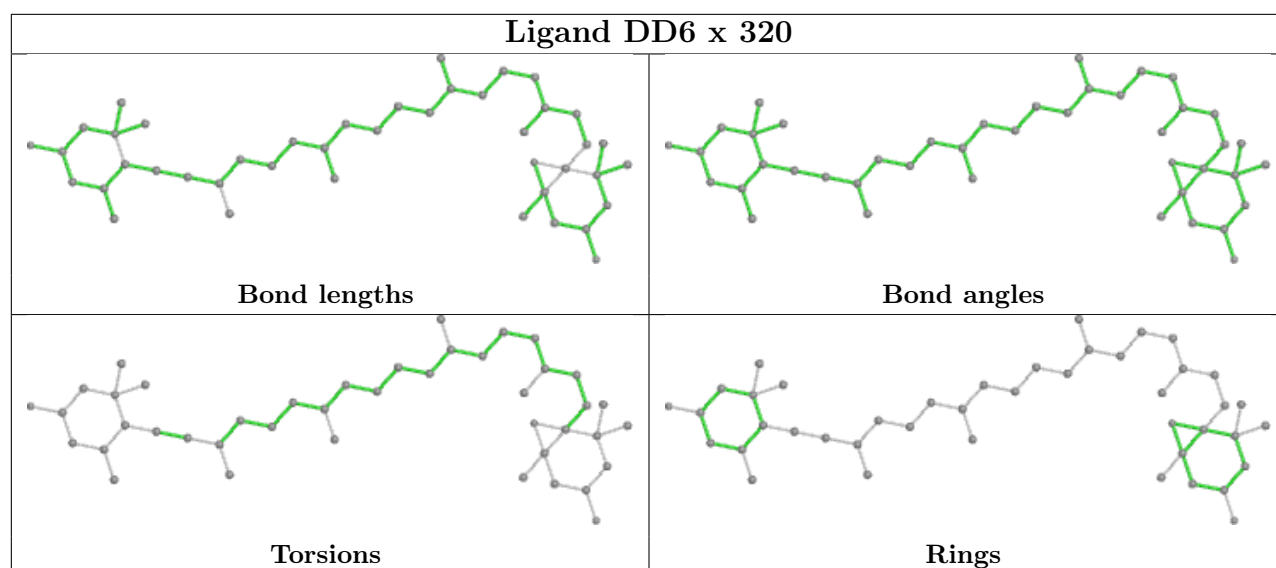
Bond angles

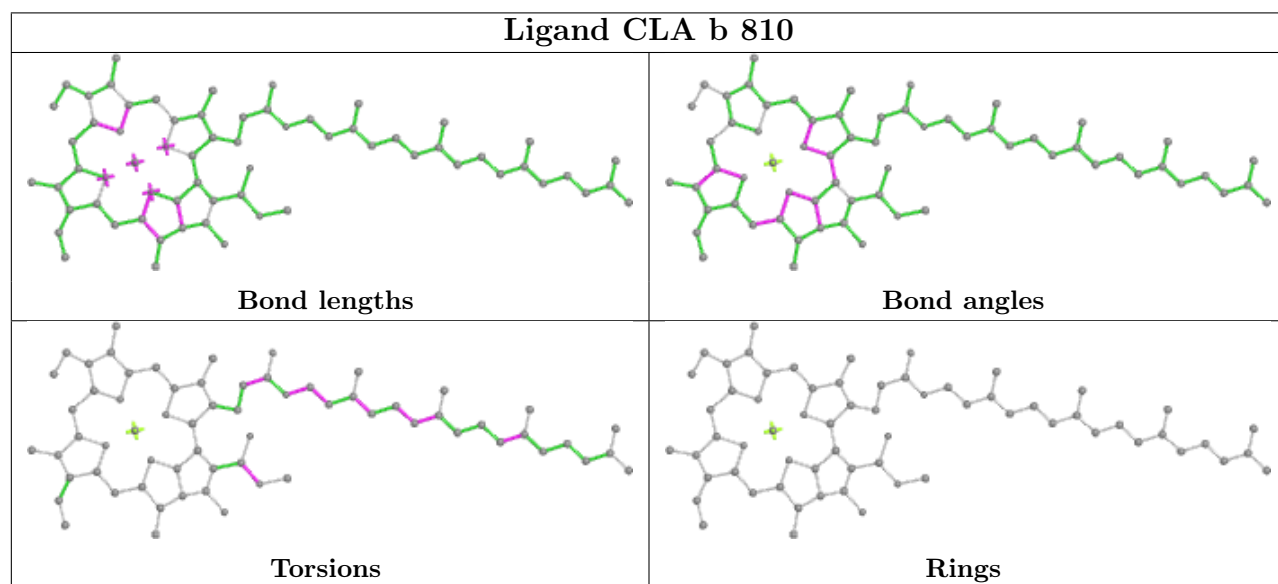
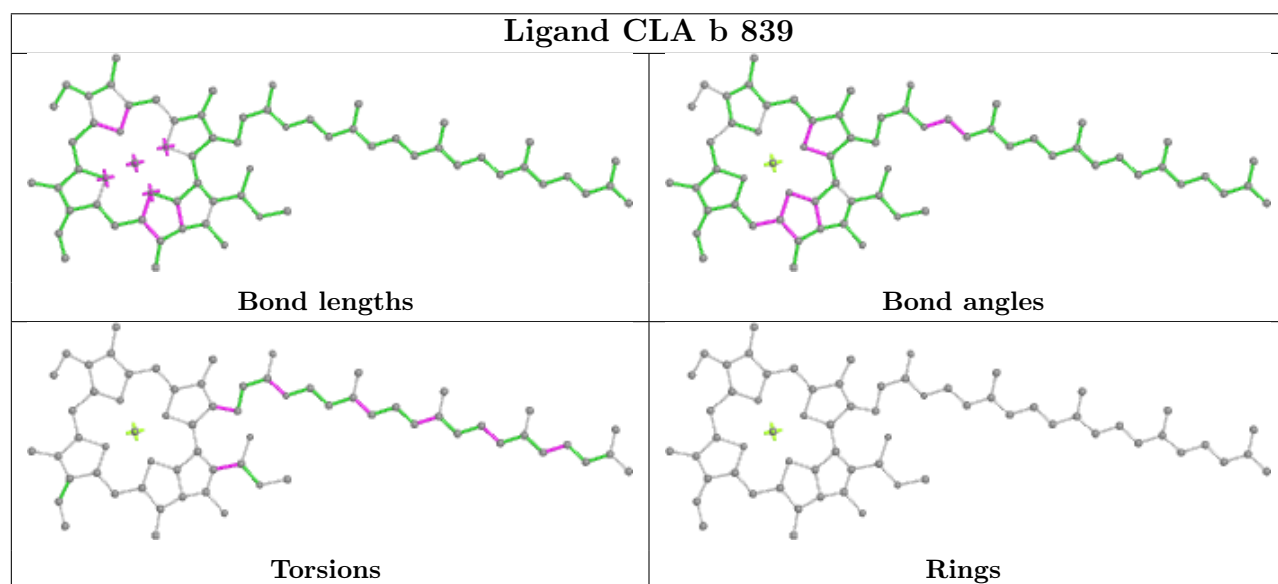
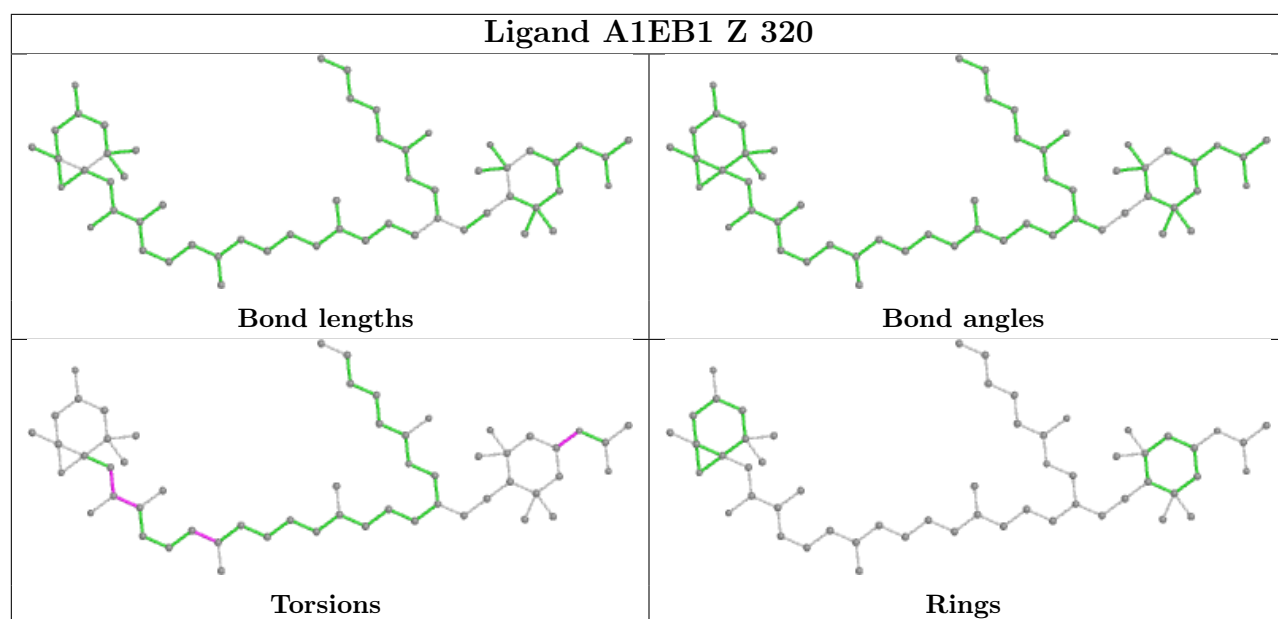


Torsions

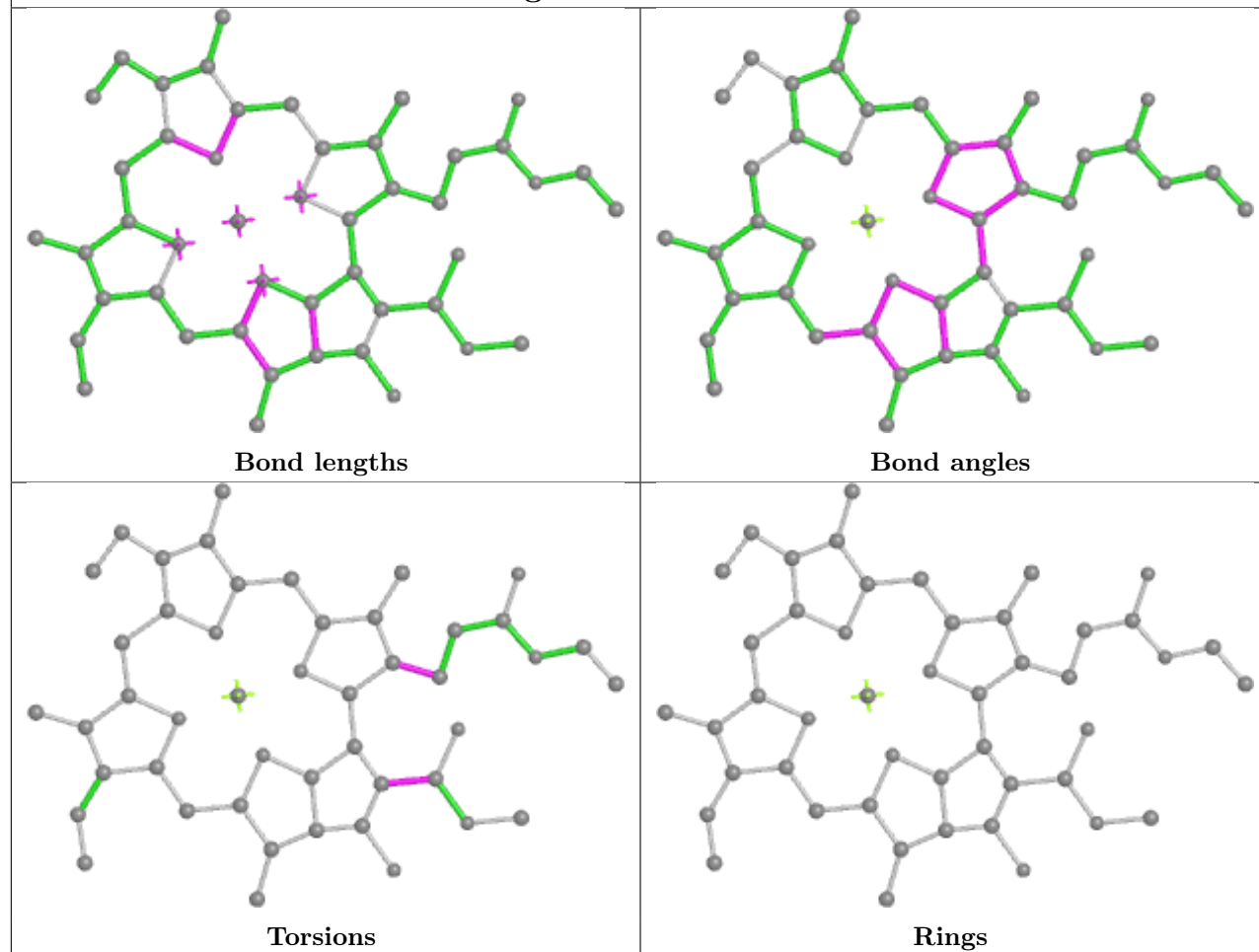


Rings

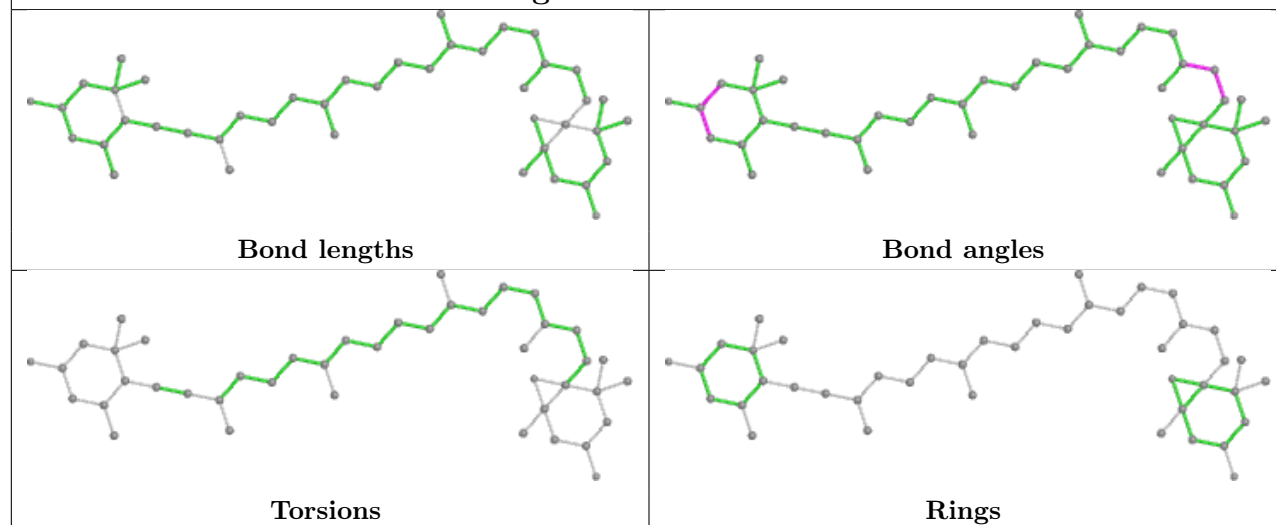


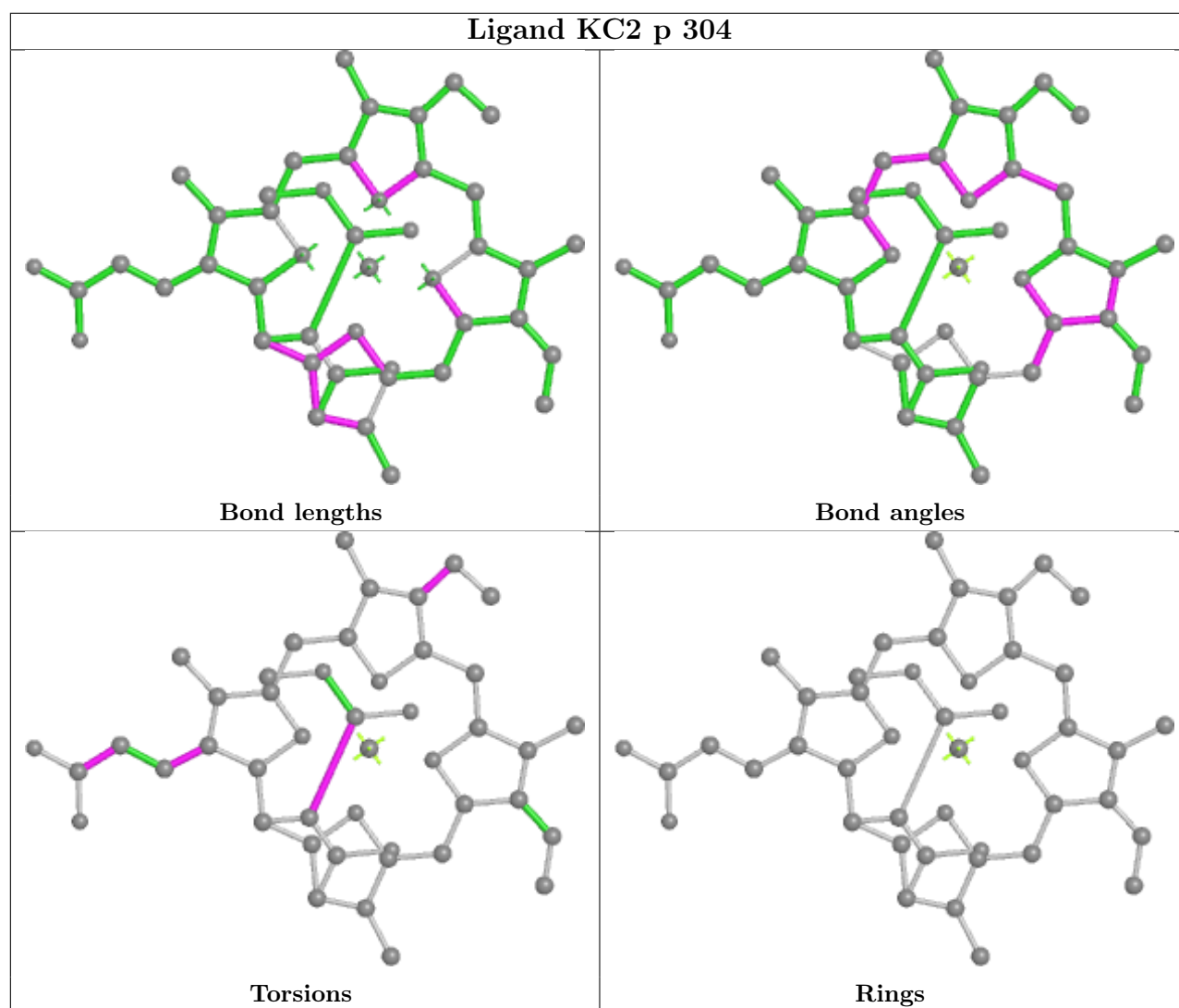
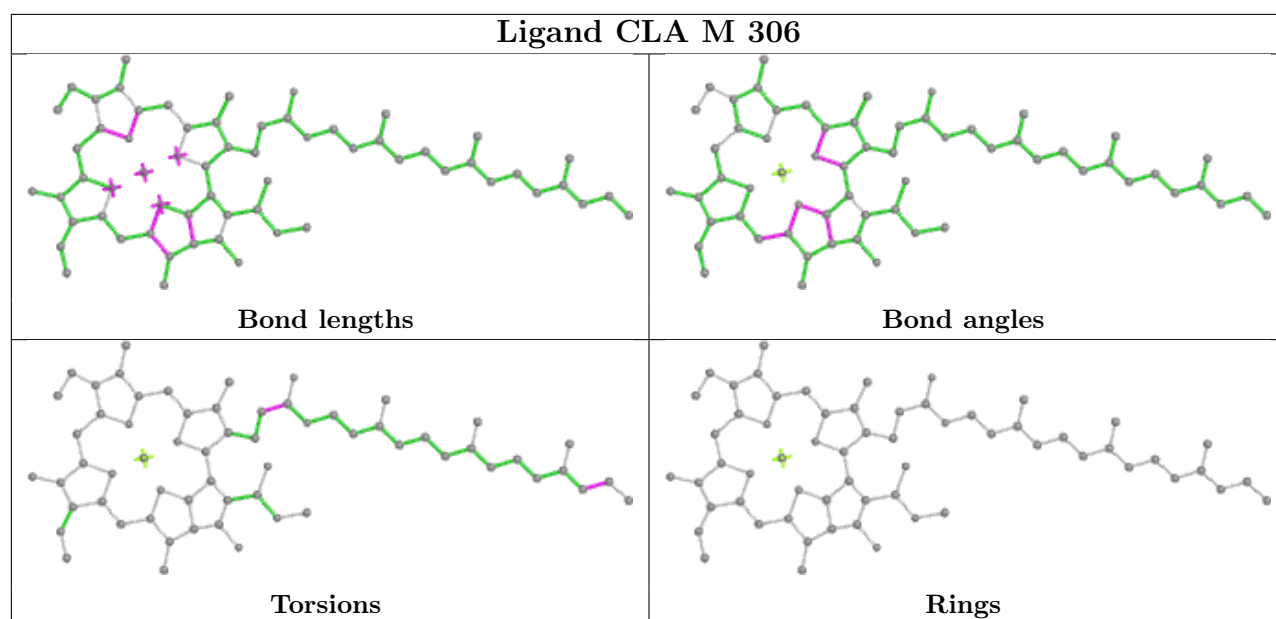


Ligand CLA Y 312

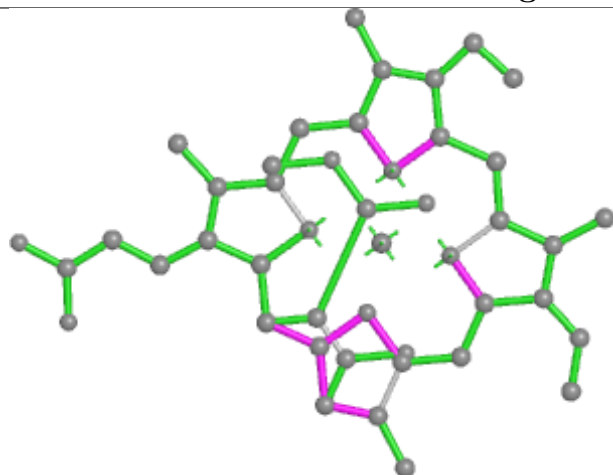


Ligand DD6 U 211

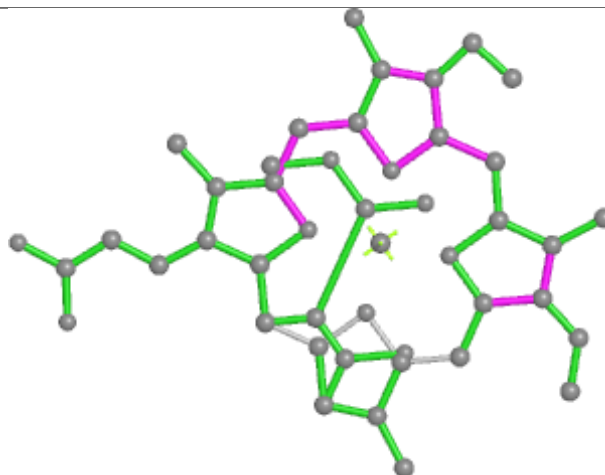




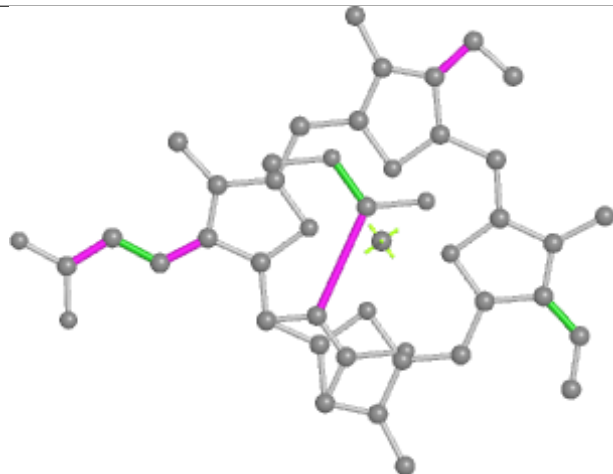
Ligand KC2 u 304



Bond lengths



Bond angles

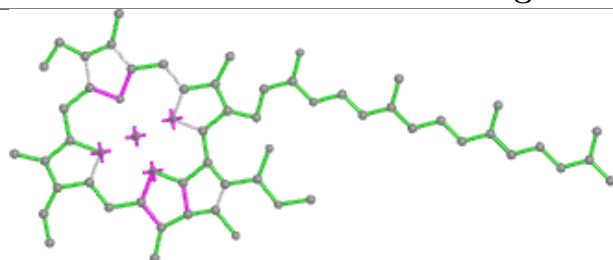


Torsions

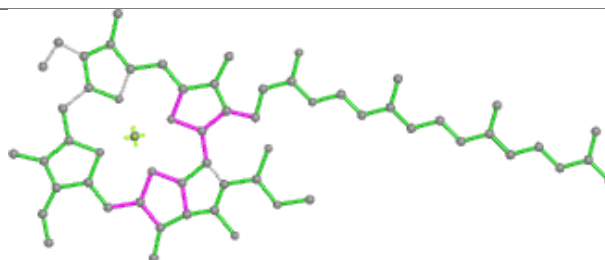


Rings

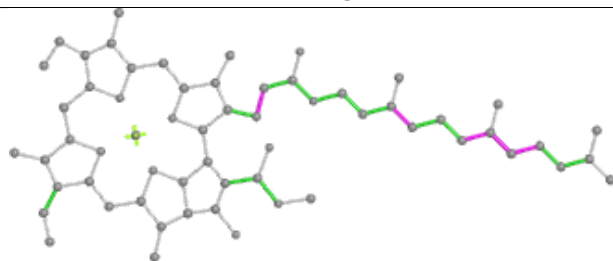
Ligand CLA C 307



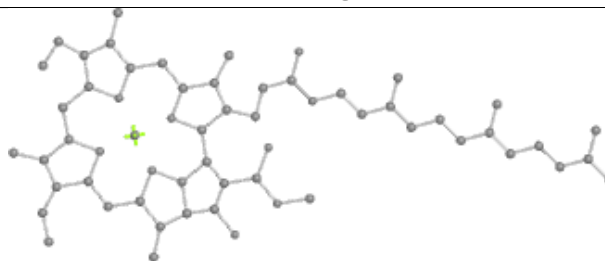
Bond lengths



Bond angles

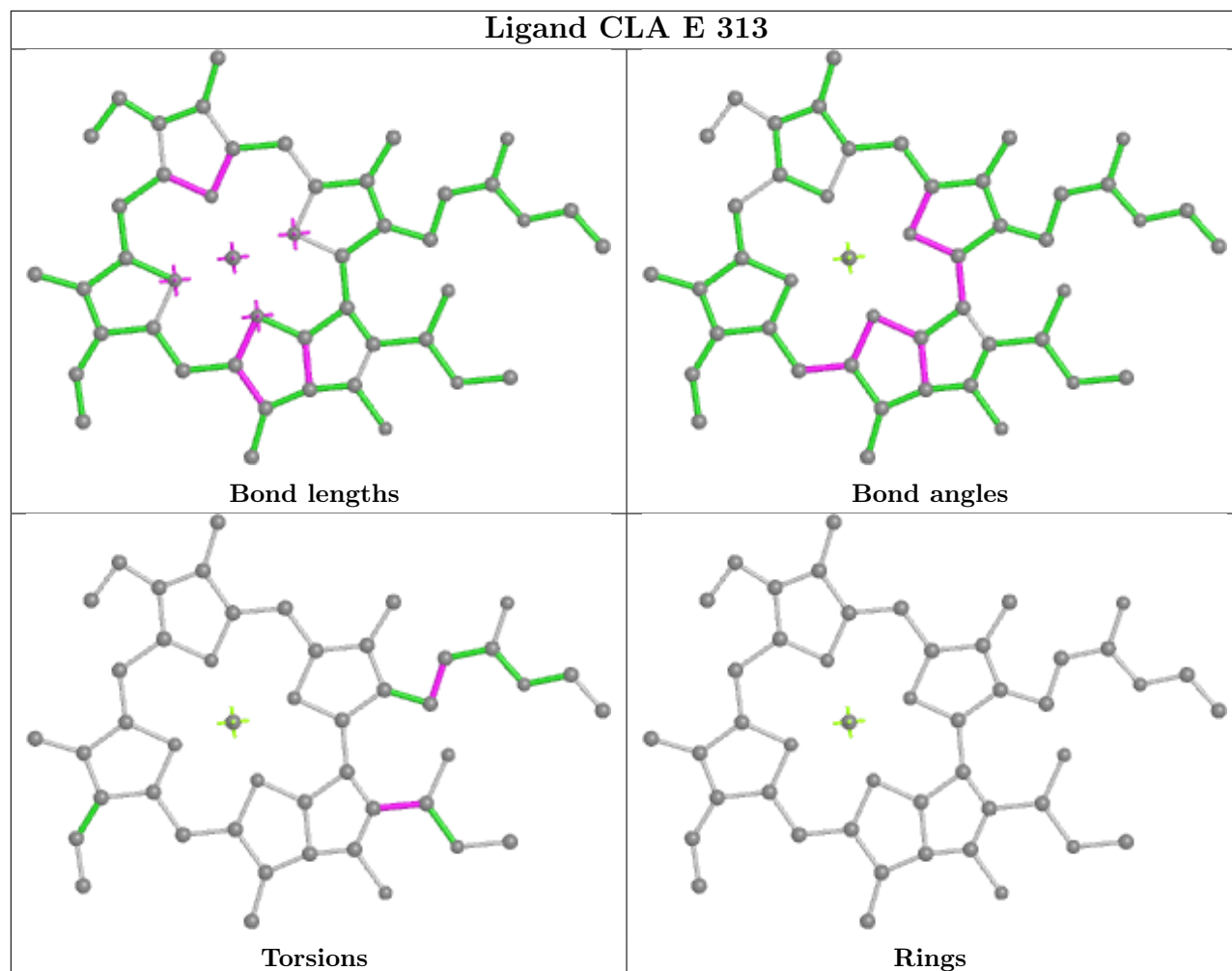


Torsions

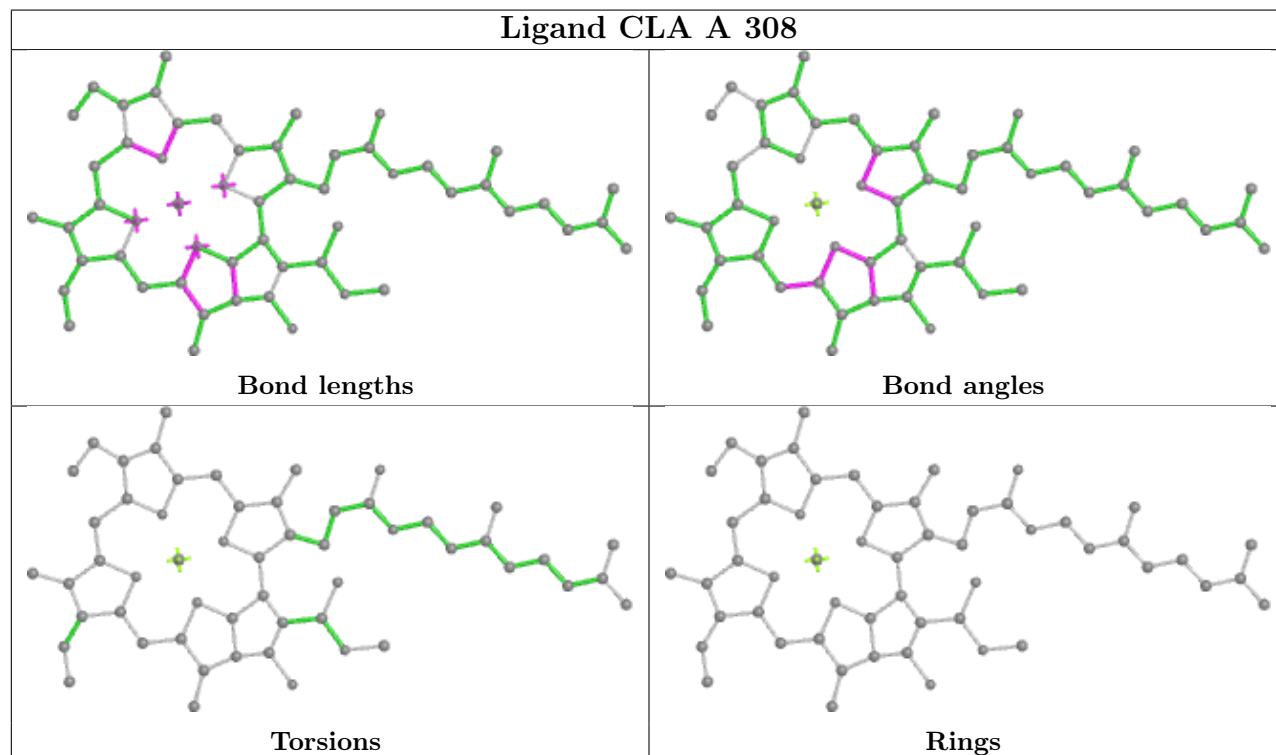


Rings

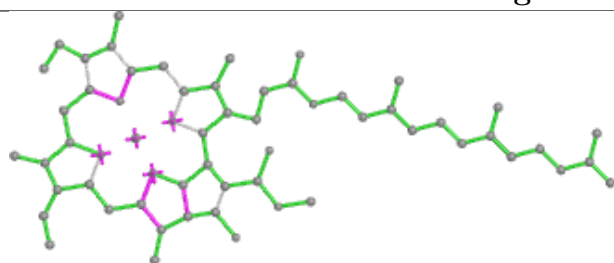
Ligand CLA E 313



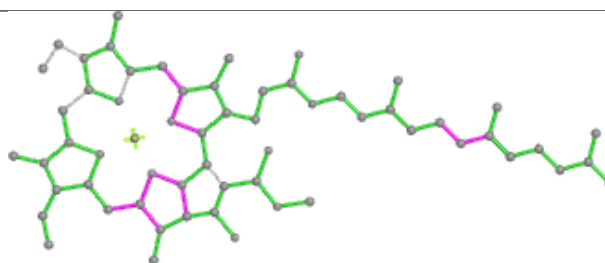
Ligand CLA A 308



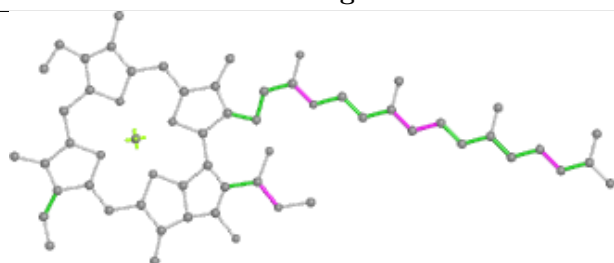
Ligand CLA Y 307



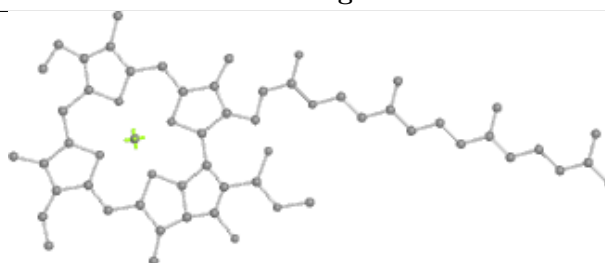
Bond lengths



Bond angles

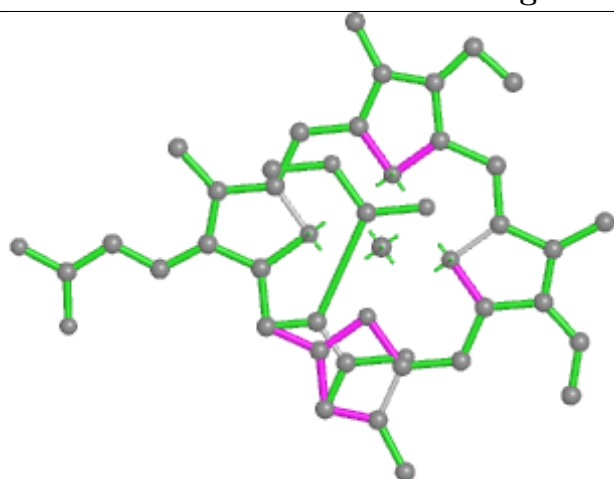


Torsions

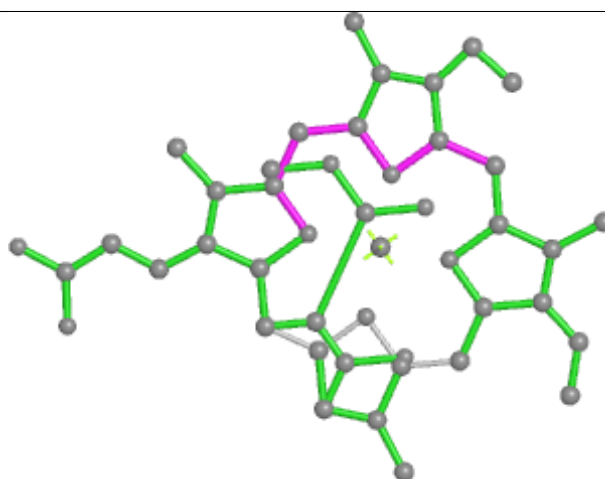


Rings

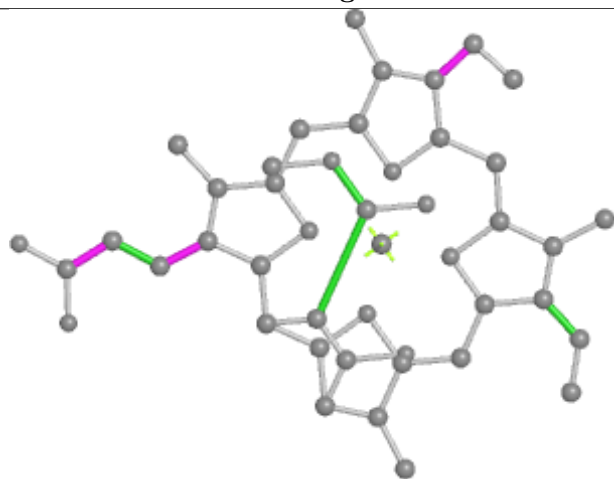
Ligand KC2 x 304



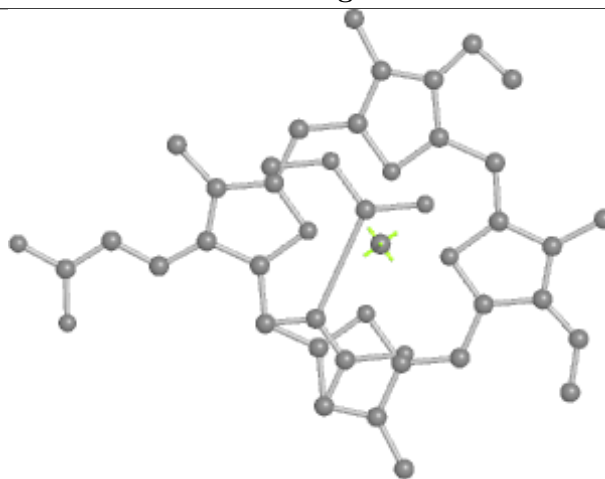
Bond lengths



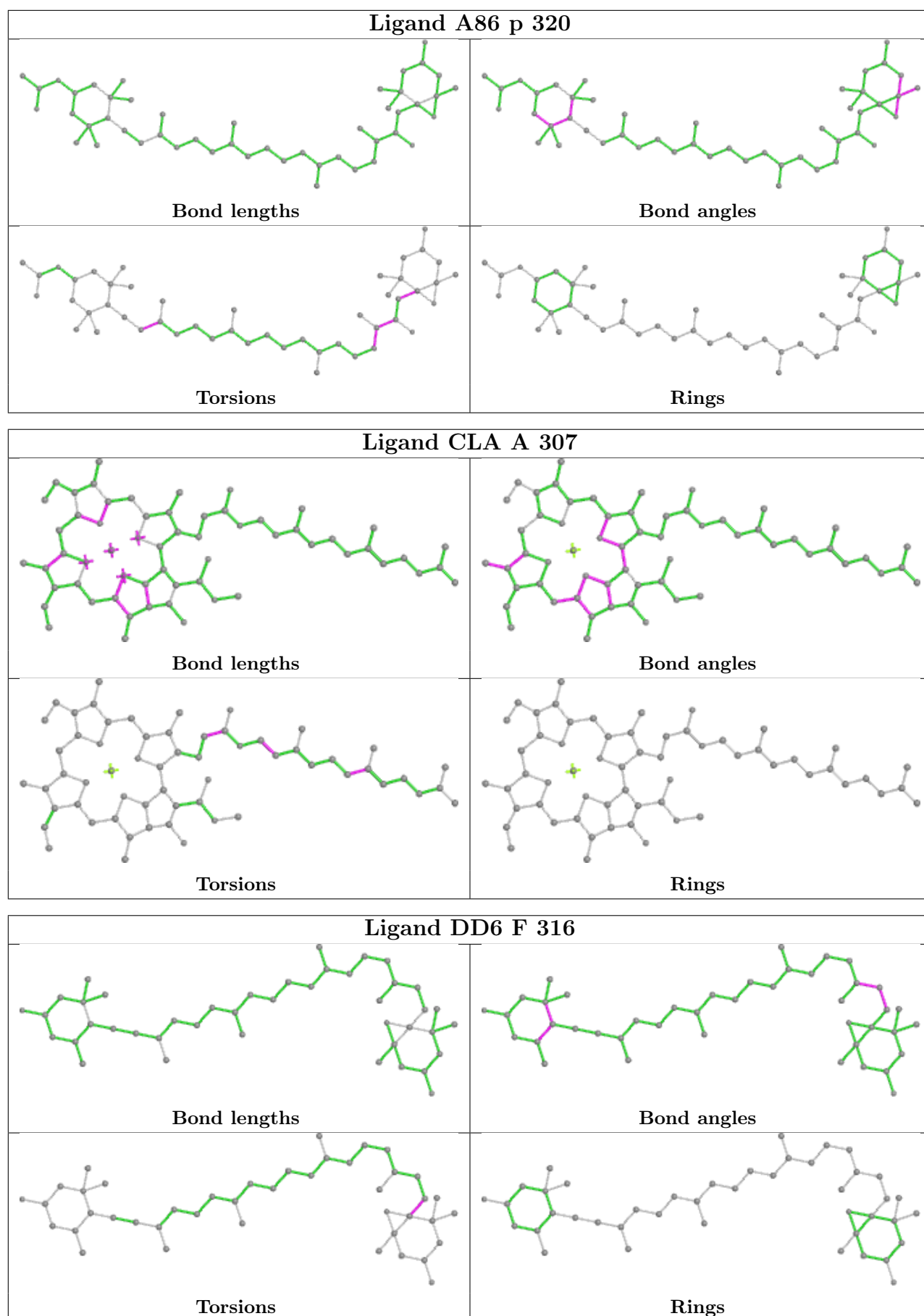
Bond angles

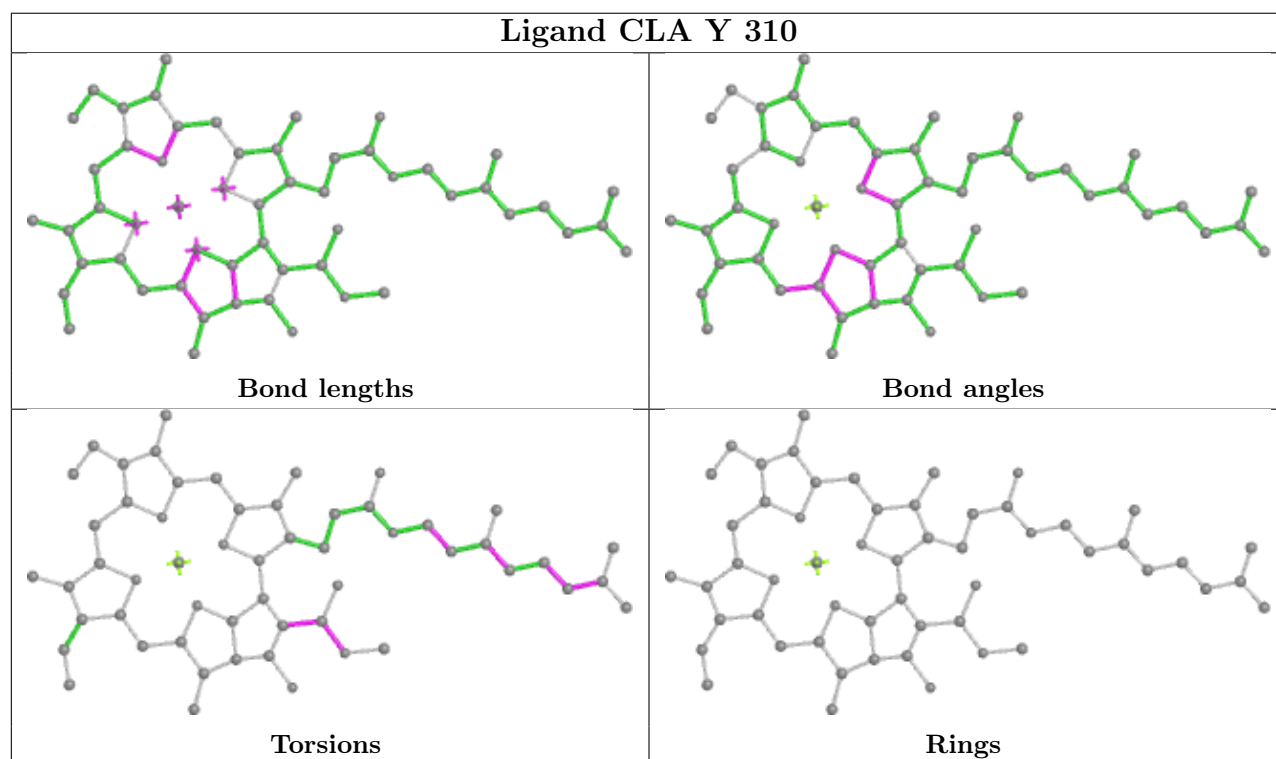
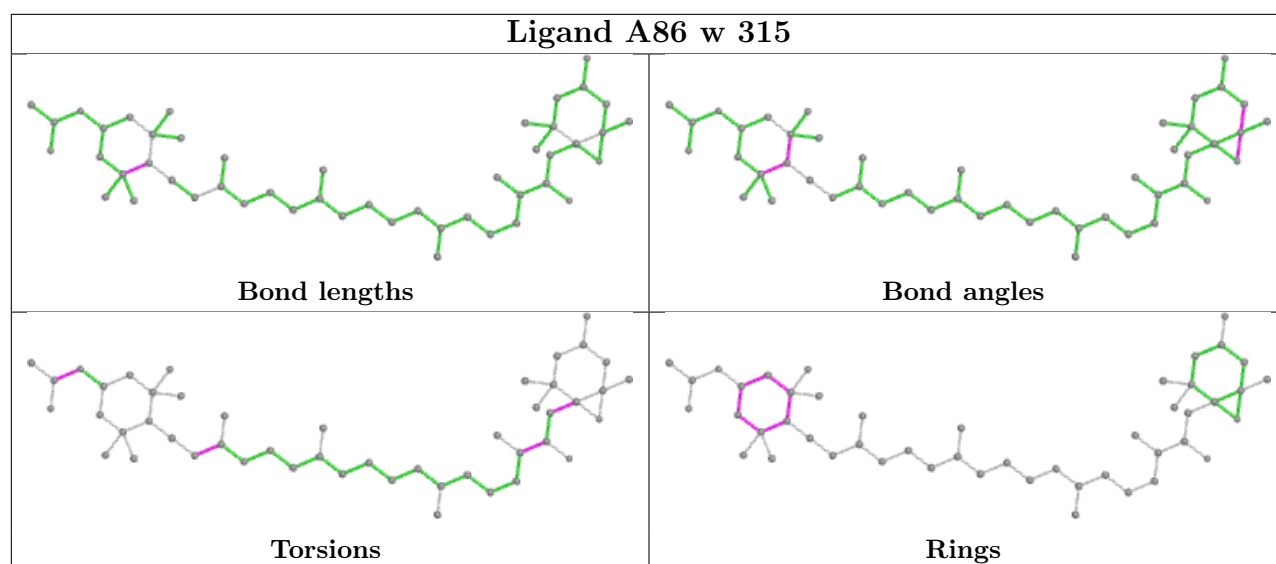


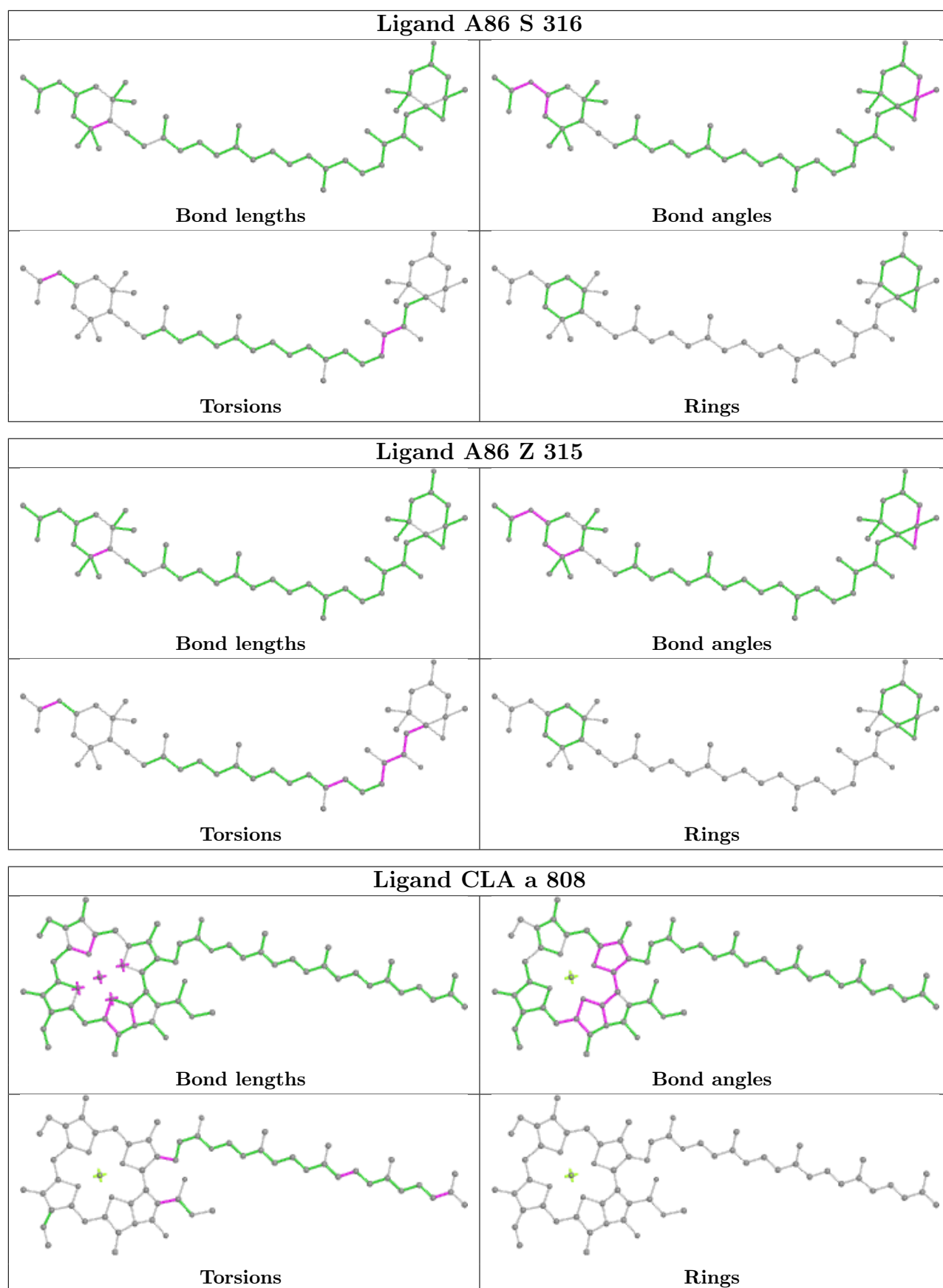
Torsions



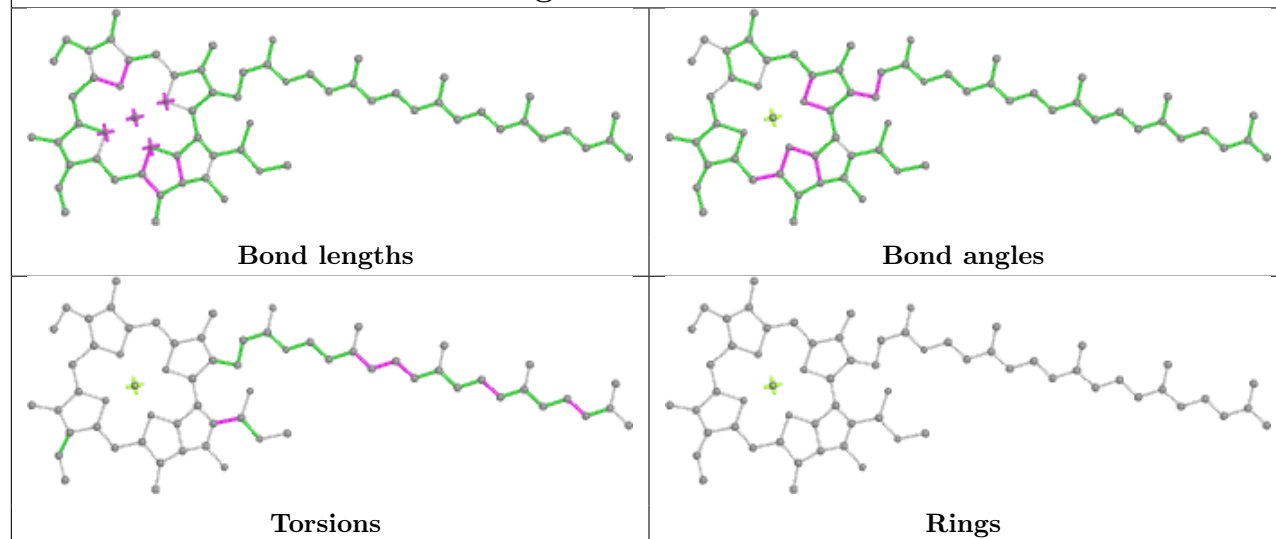
Rings



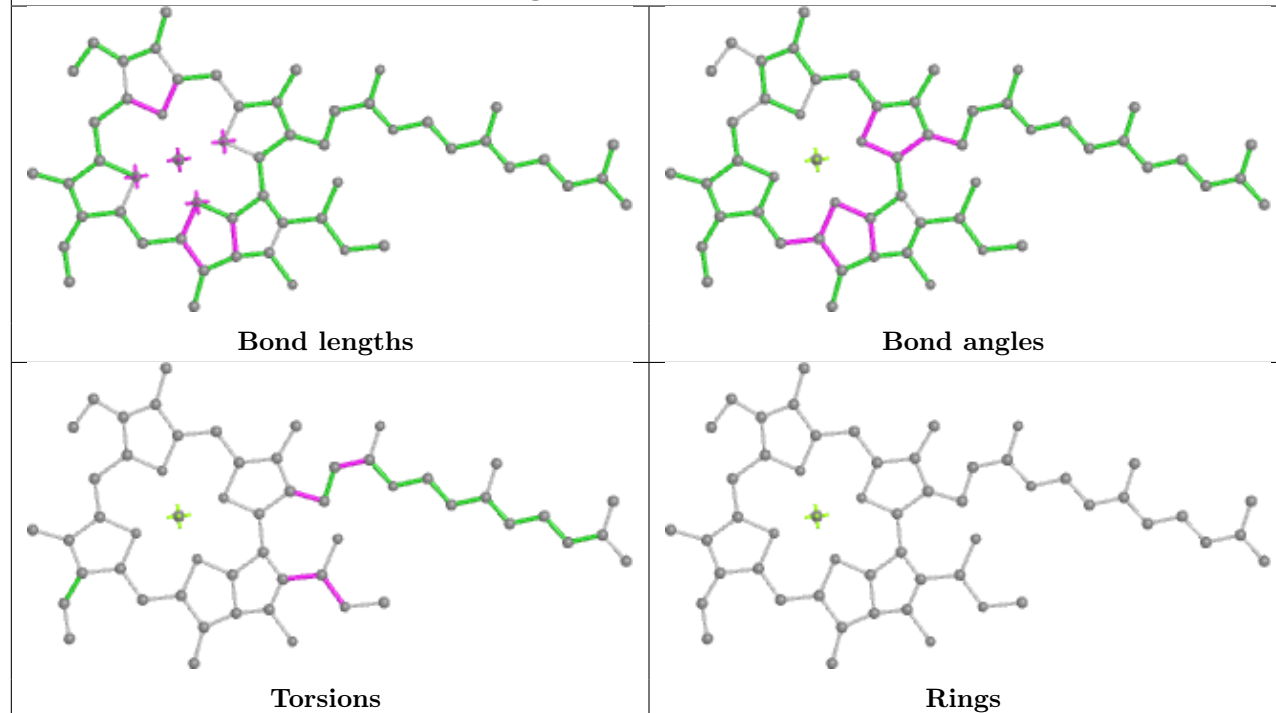




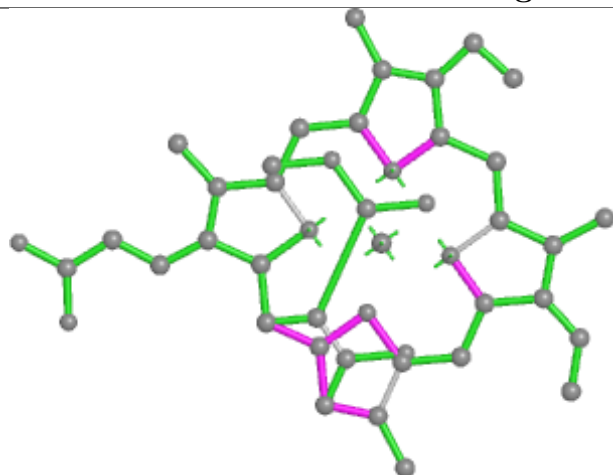
Ligand CLA b 825



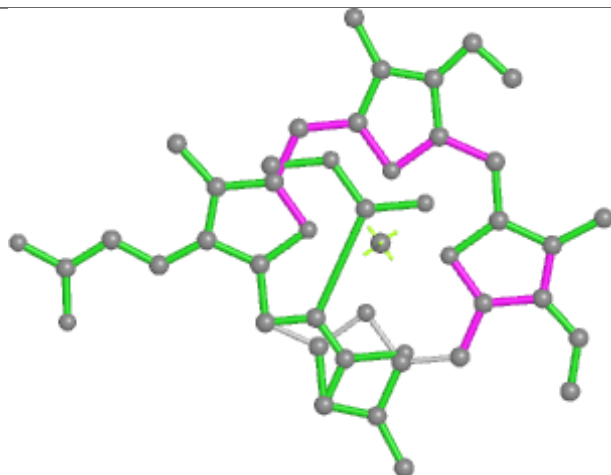
Ligand CLA W 311



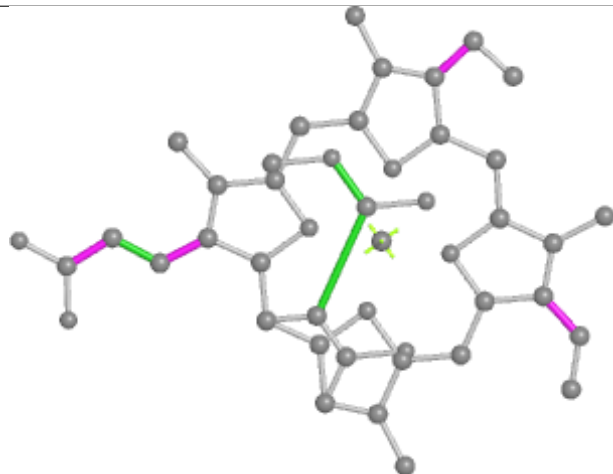
Ligand KC2 K 309



Bond lengths



Bond angles

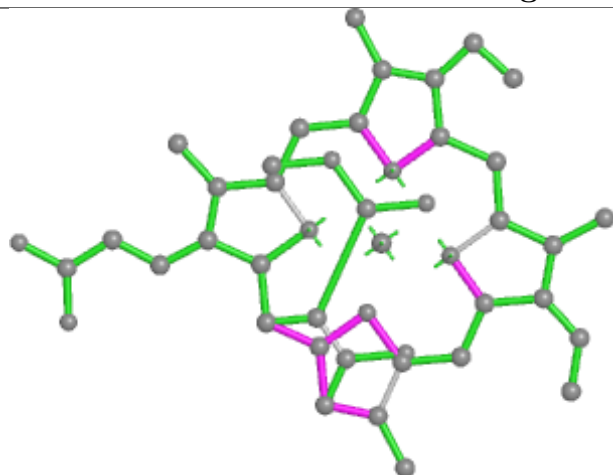


Torsions

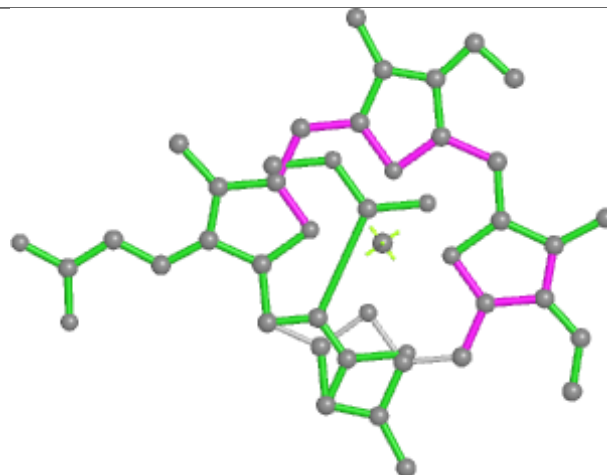


Rings

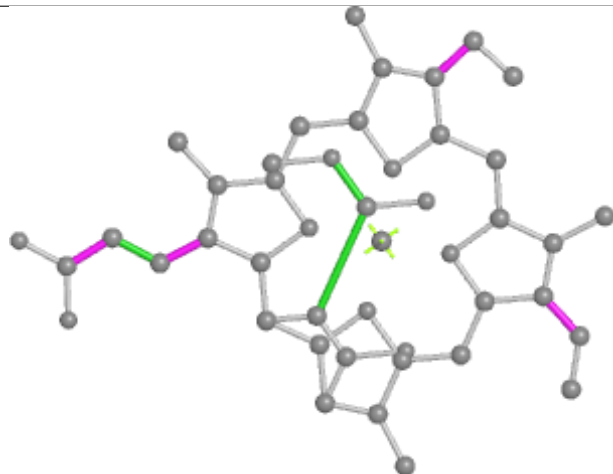
Ligand KC2 o 308



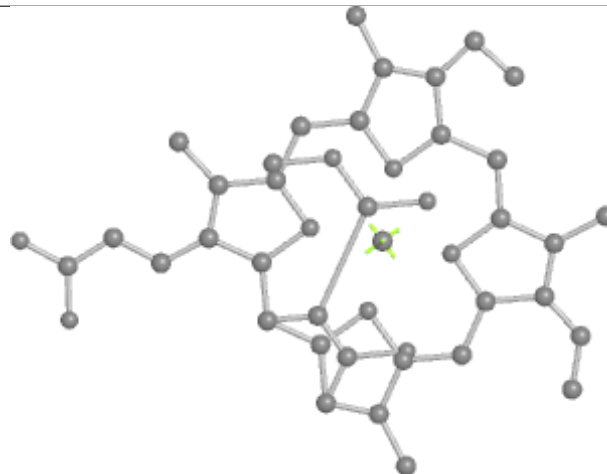
Bond lengths



Bond angles

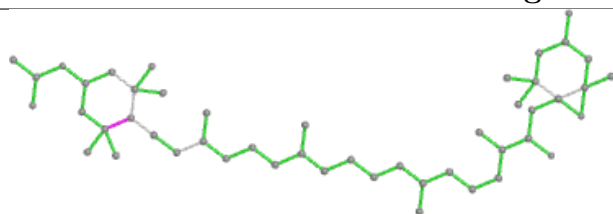


Torsions

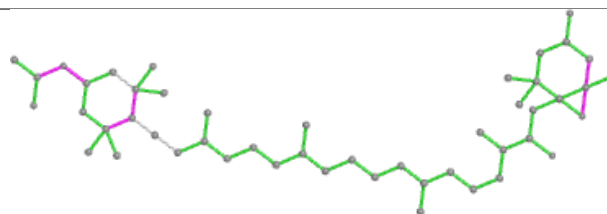


Rings

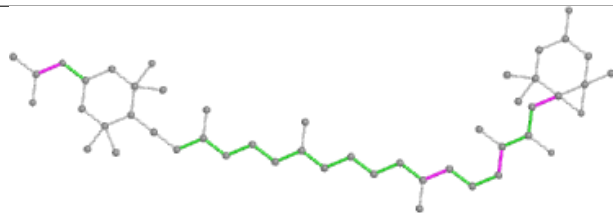
Ligand A86 o 317



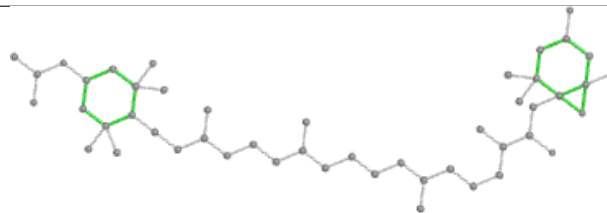
Bond lengths



Bond angles

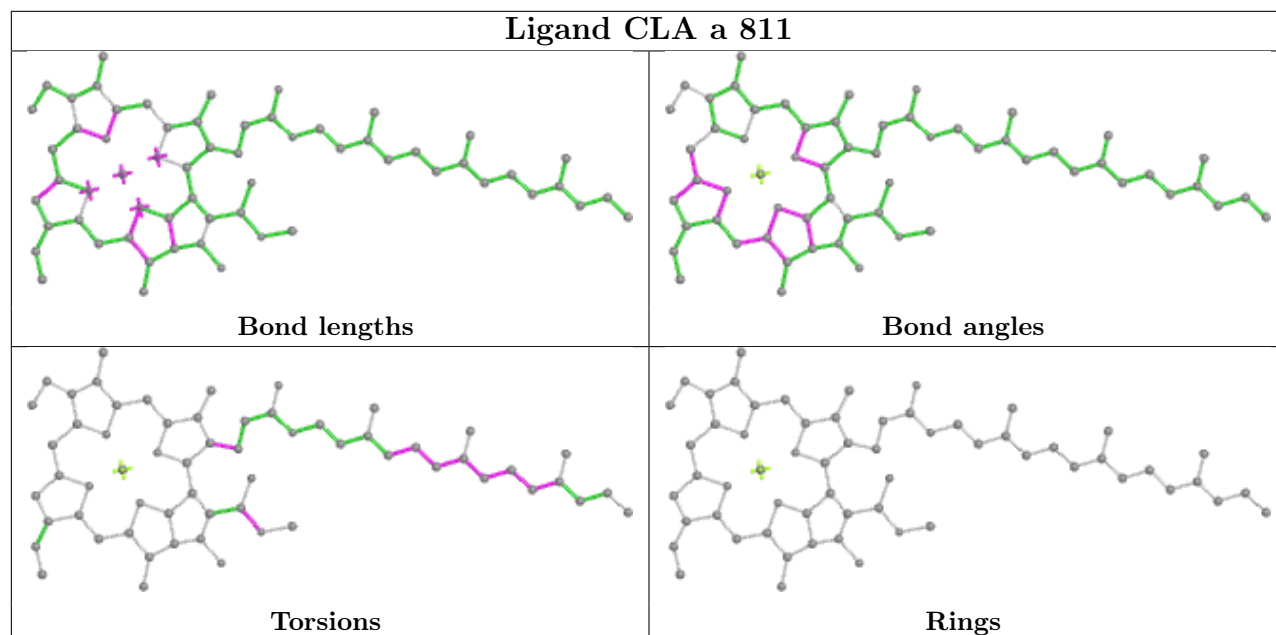


Torsions

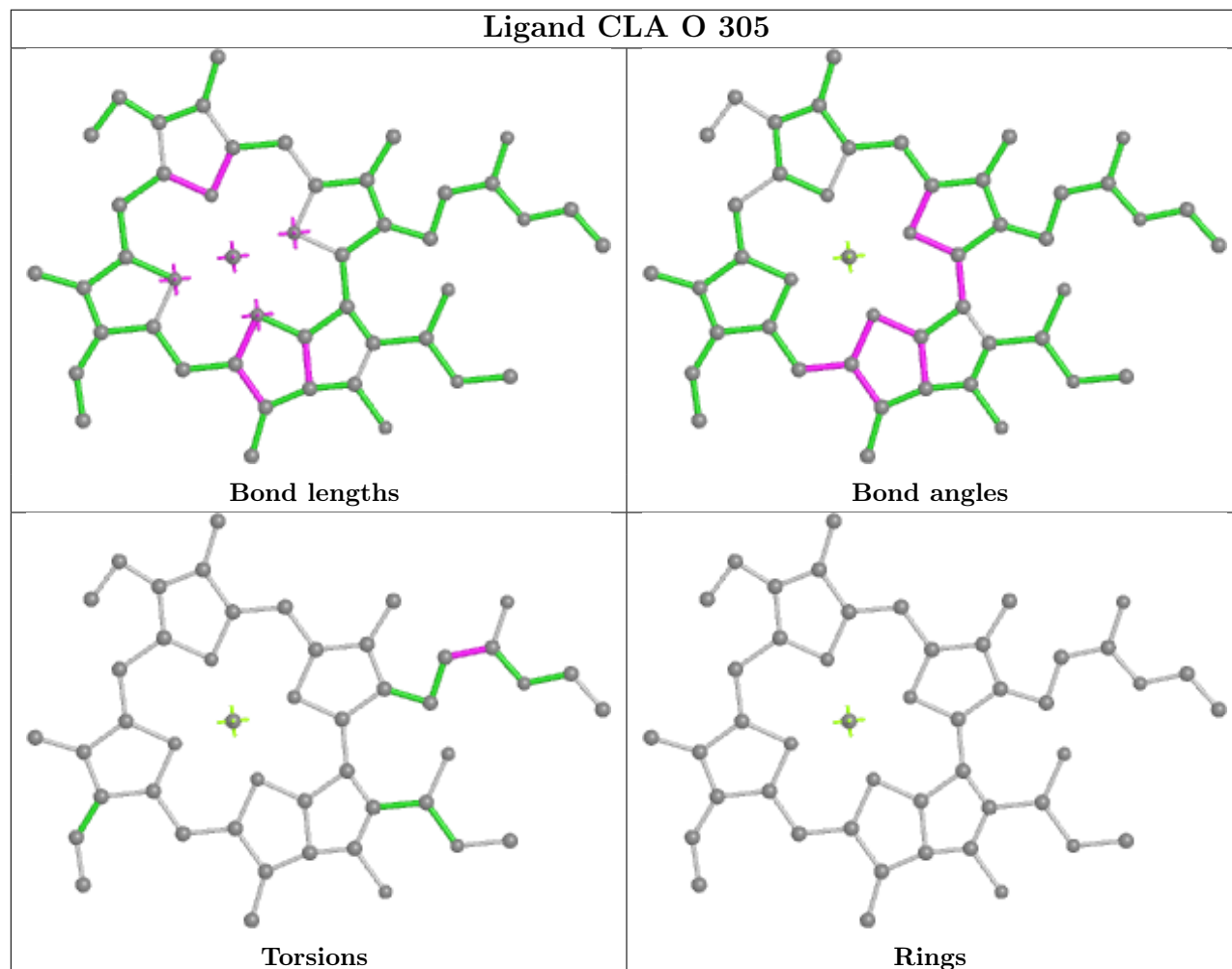


Rings

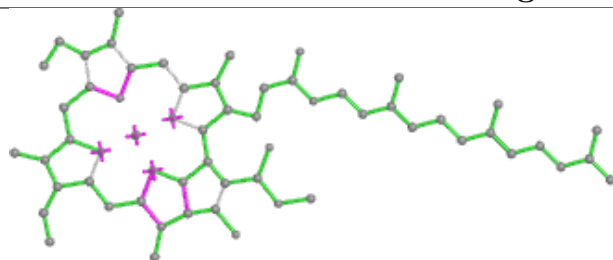
Ligand CLA a 811



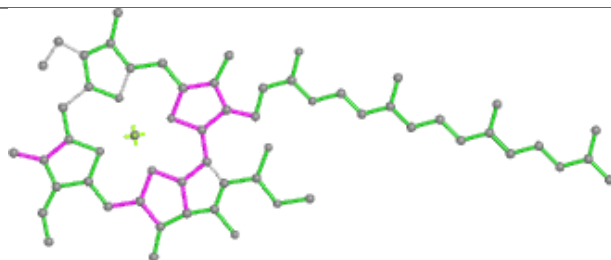
Ligand CLA O 305



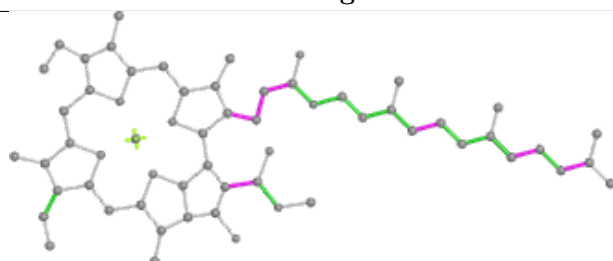
Ligand CLA b 809



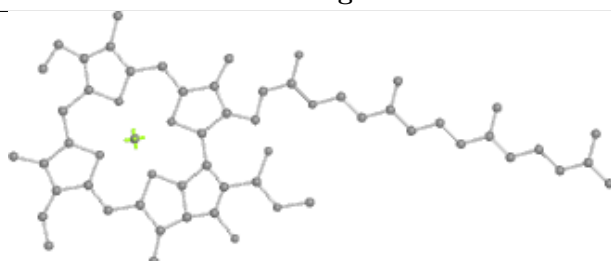
Bond lengths



Bond angles

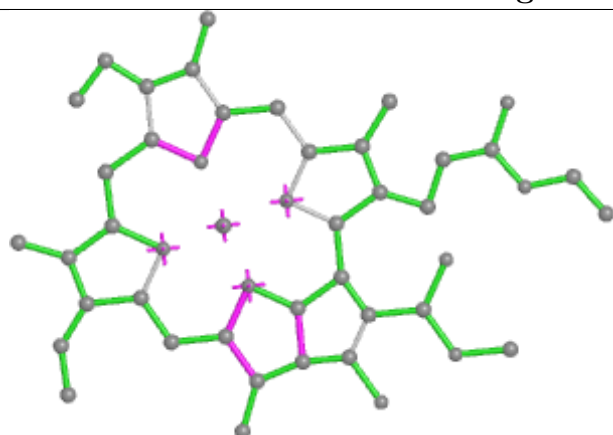


Torsions

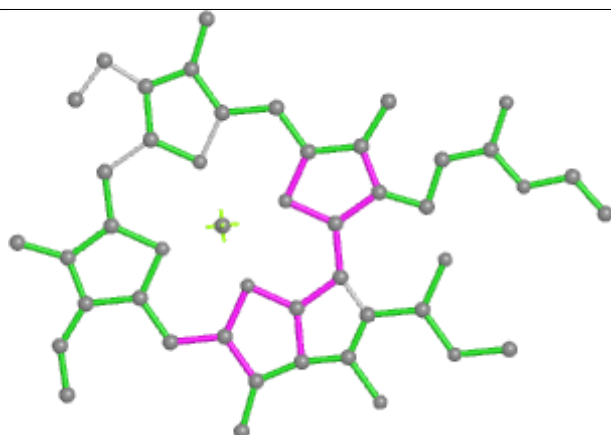


Rings

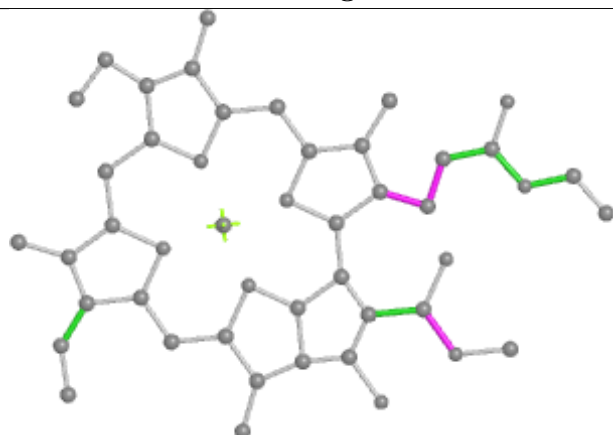
Ligand CLA L 306



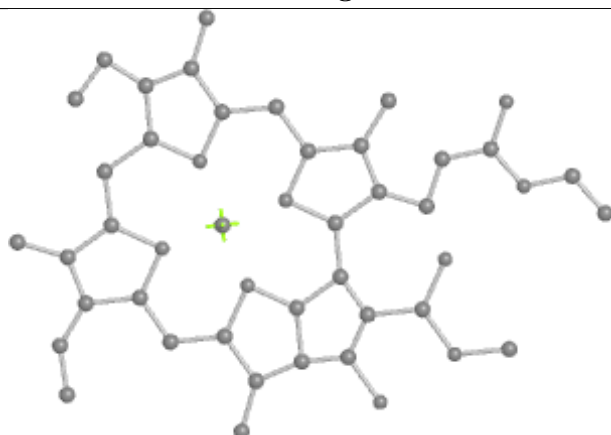
Bond lengths



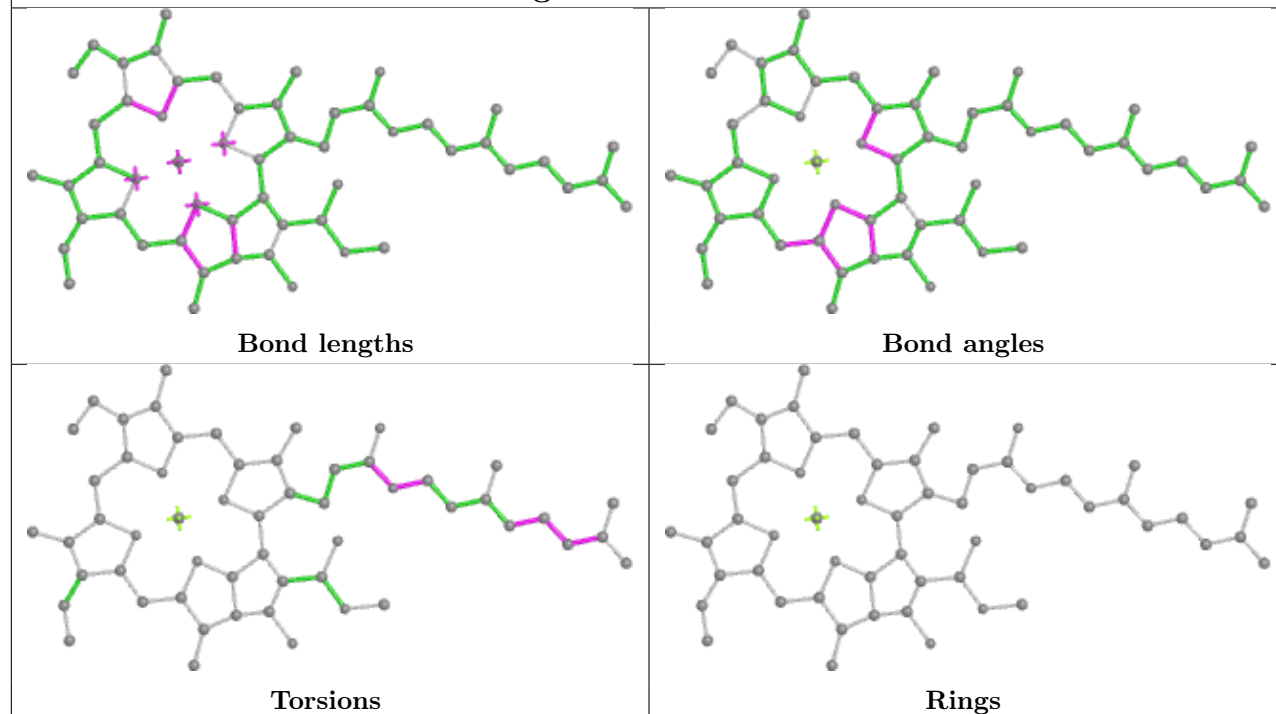
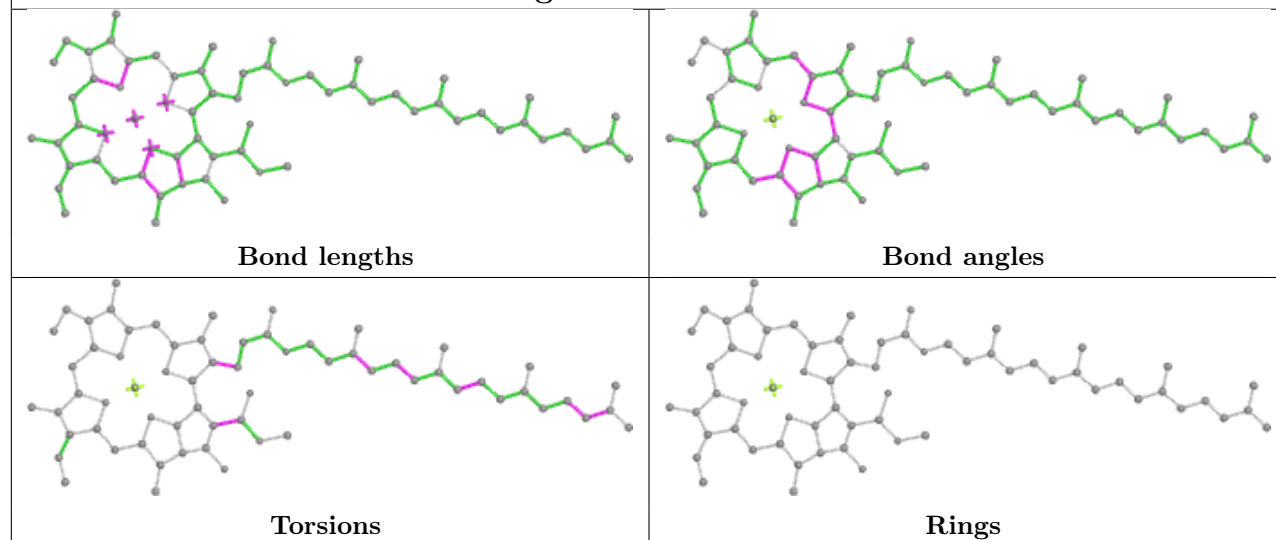
Bond angles

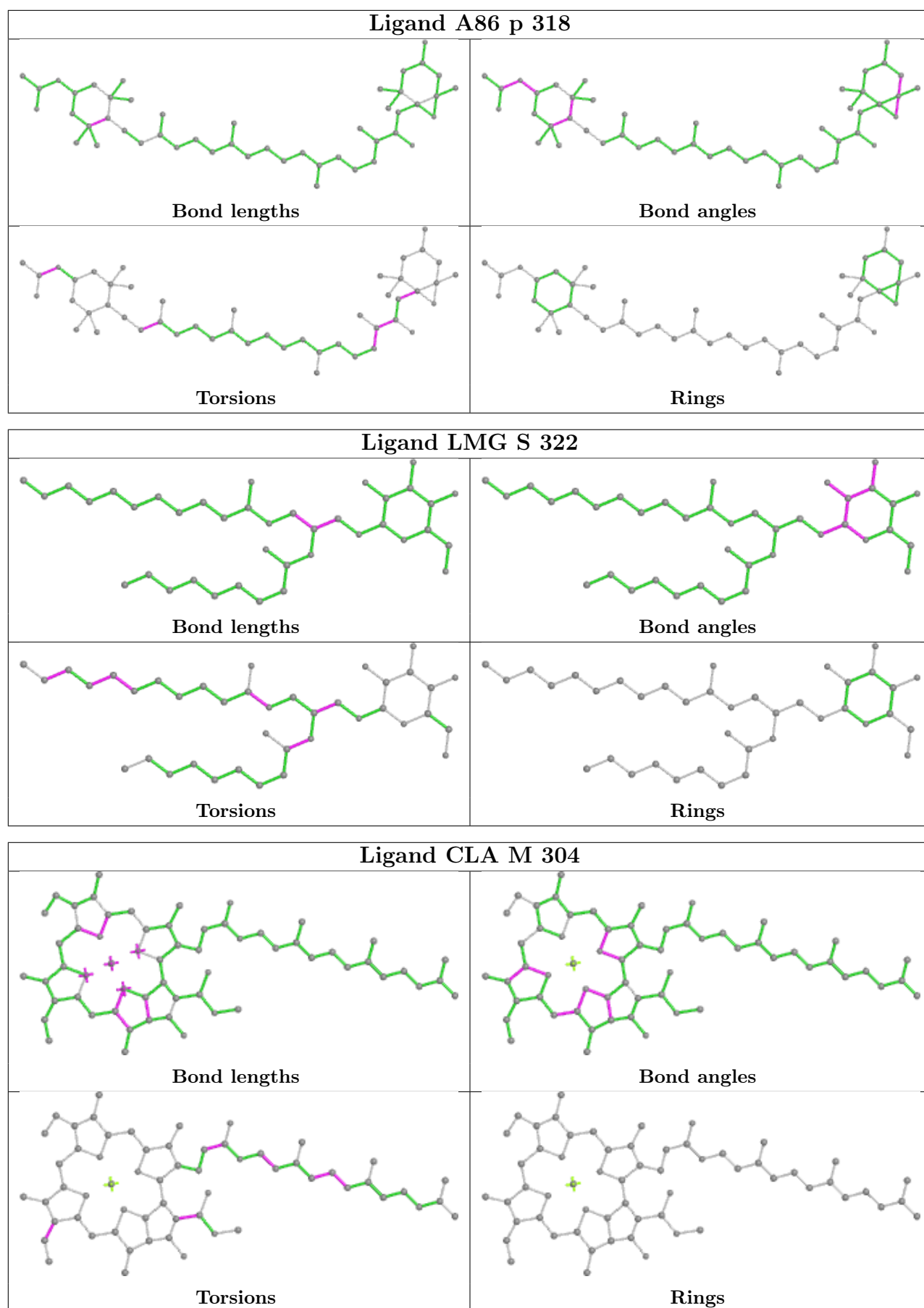


Torsions

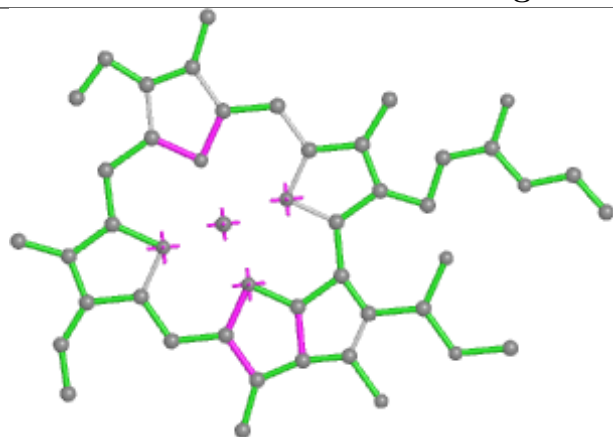


Rings

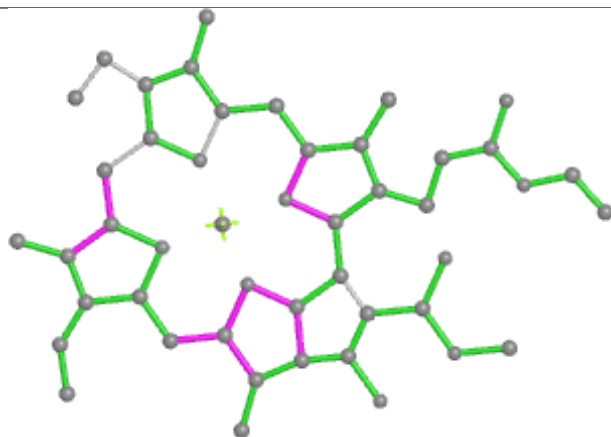
Ligand CLA E 306**Ligand CLA b 820**



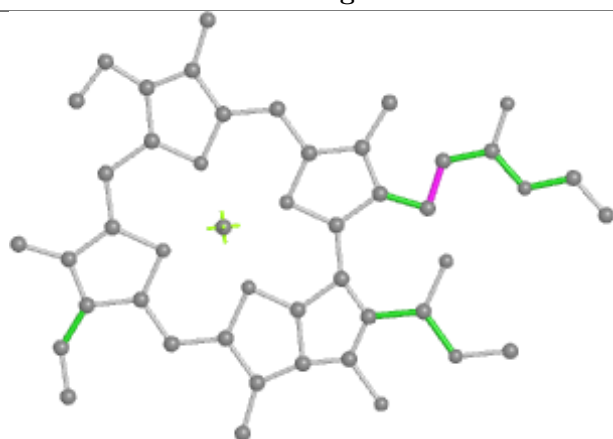
Ligand CLA U 206



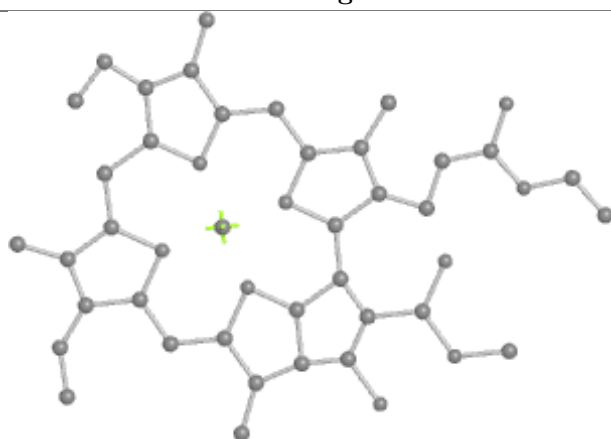
Bond lengths



Bond angles

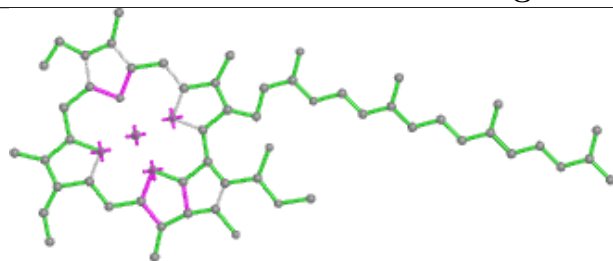


Torsions

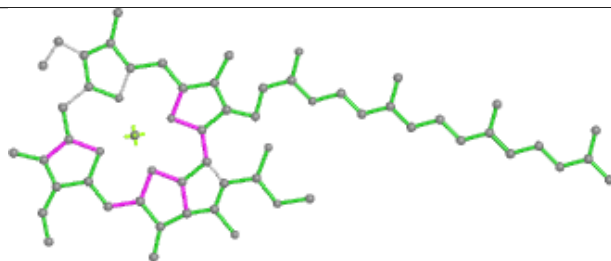


Rings

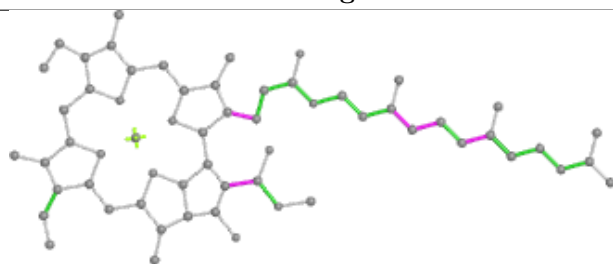
Ligand CLA A 306



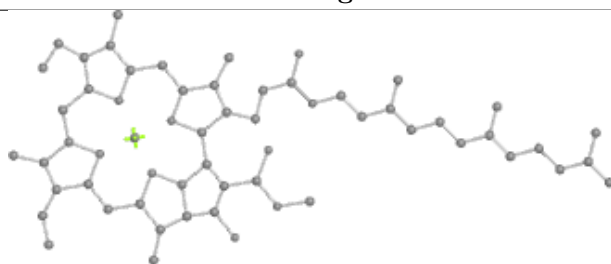
Bond lengths



Bond angles

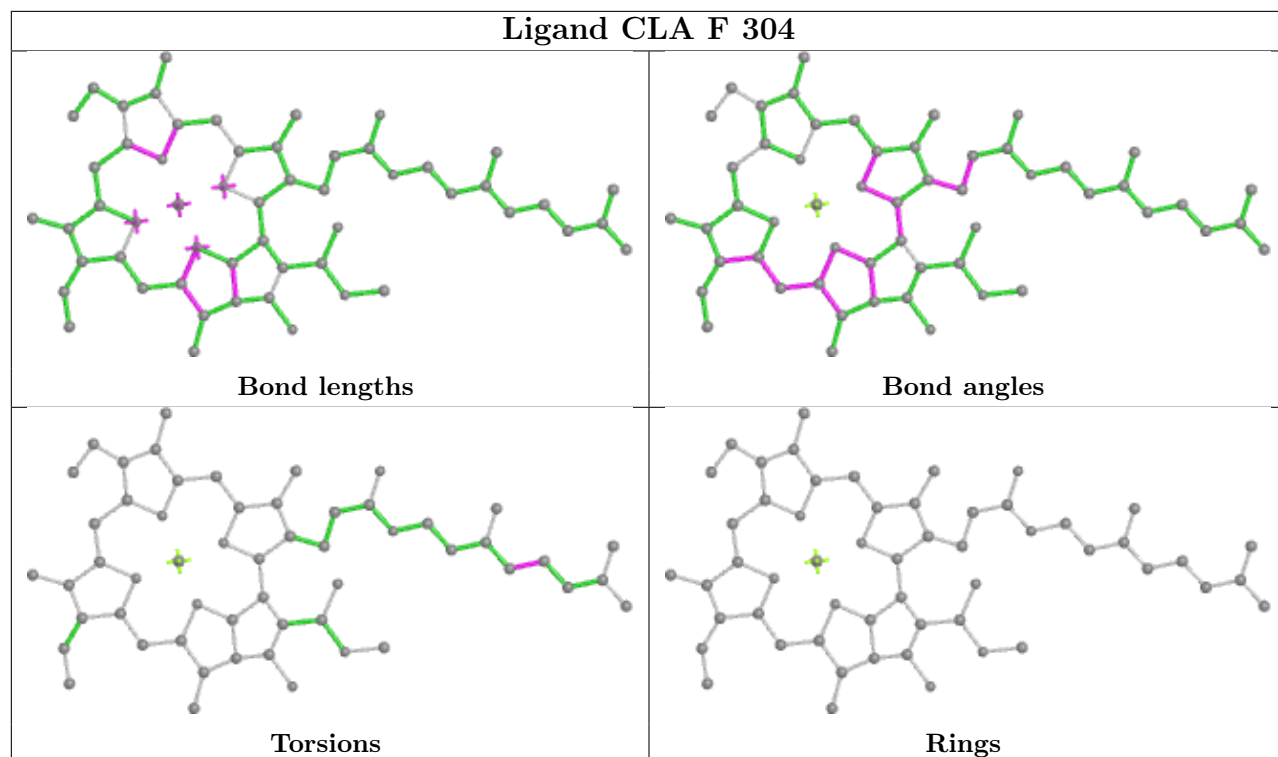


Torsions

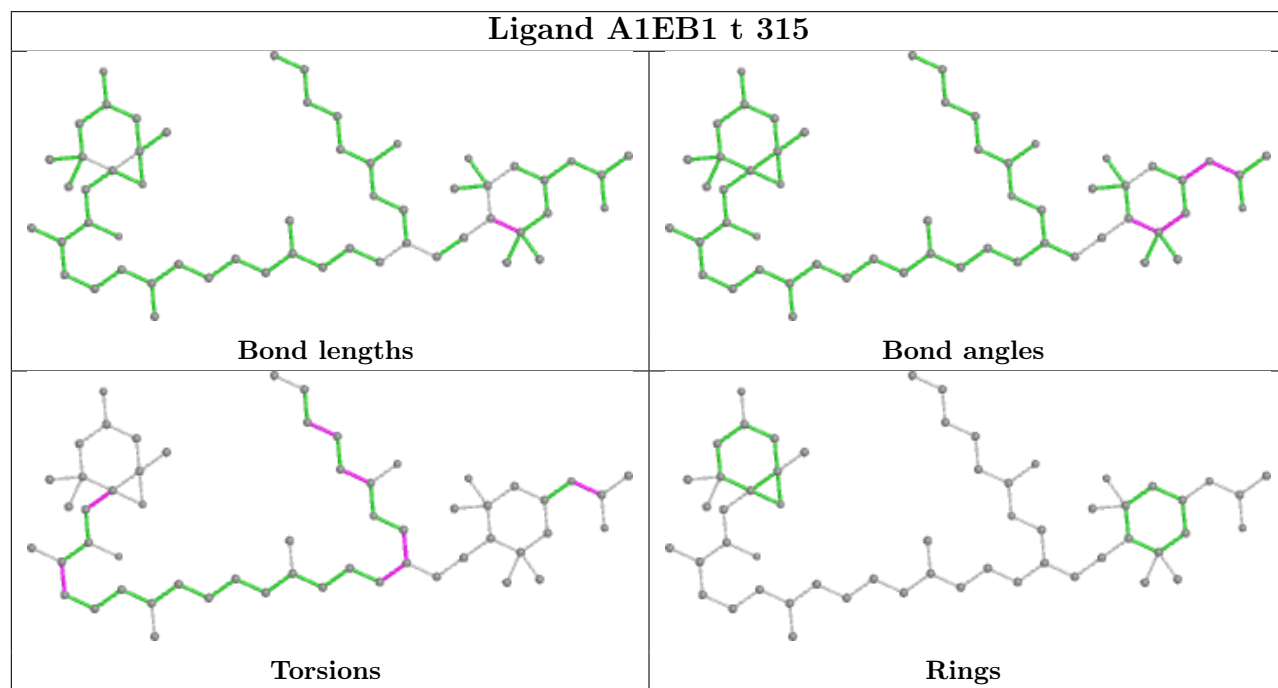


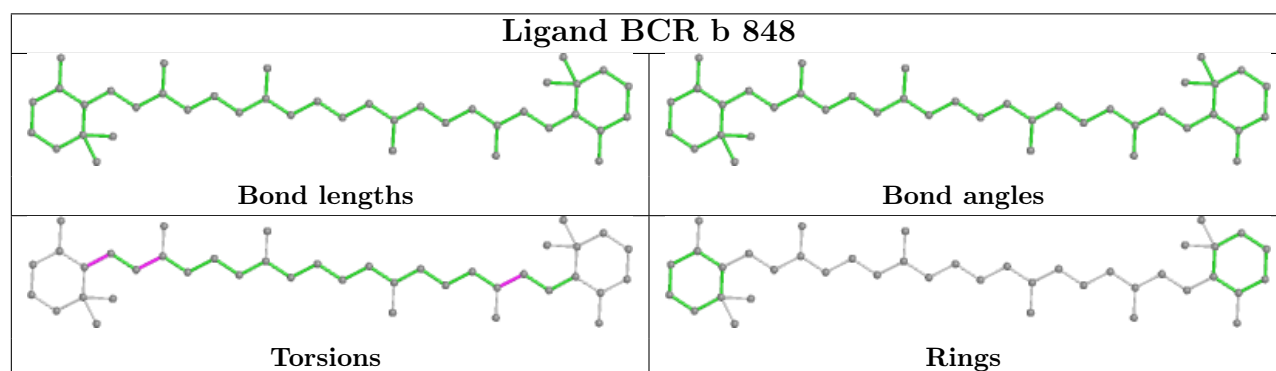
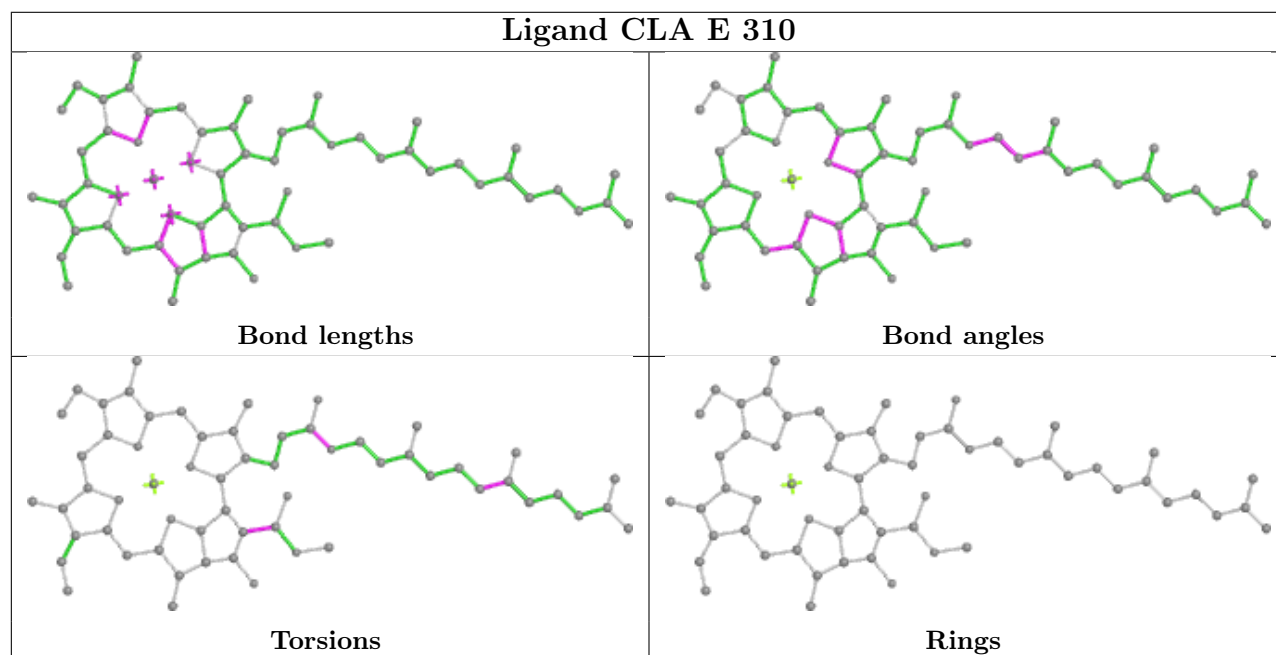
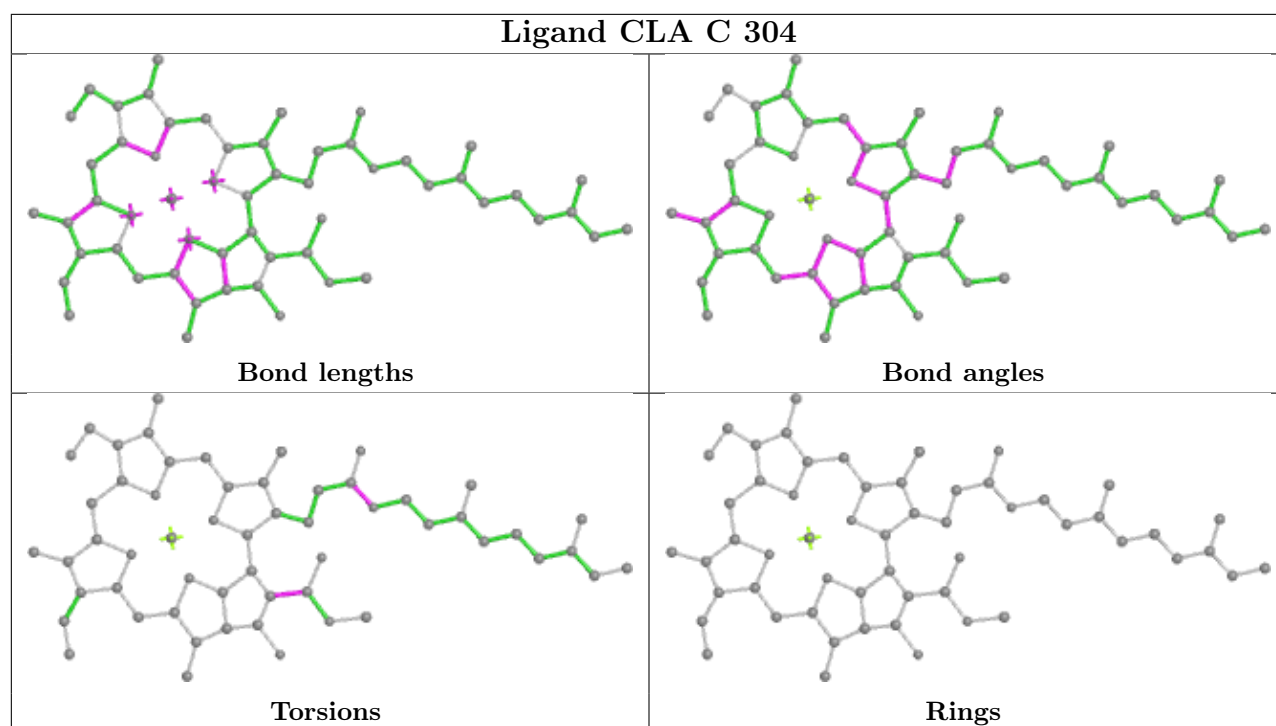
Rings

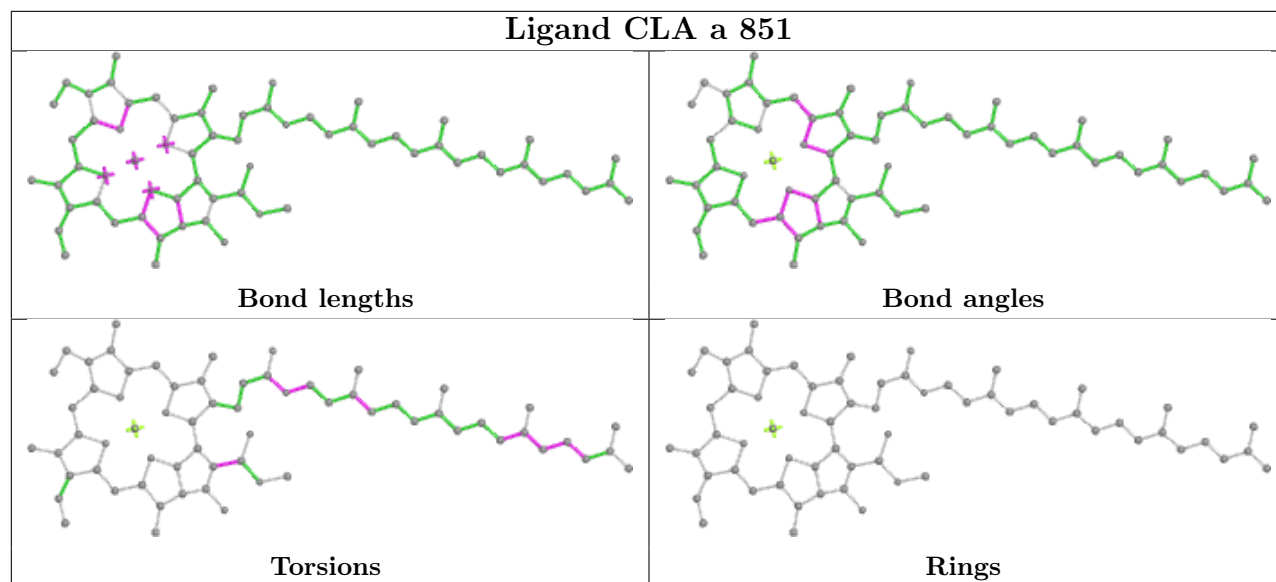
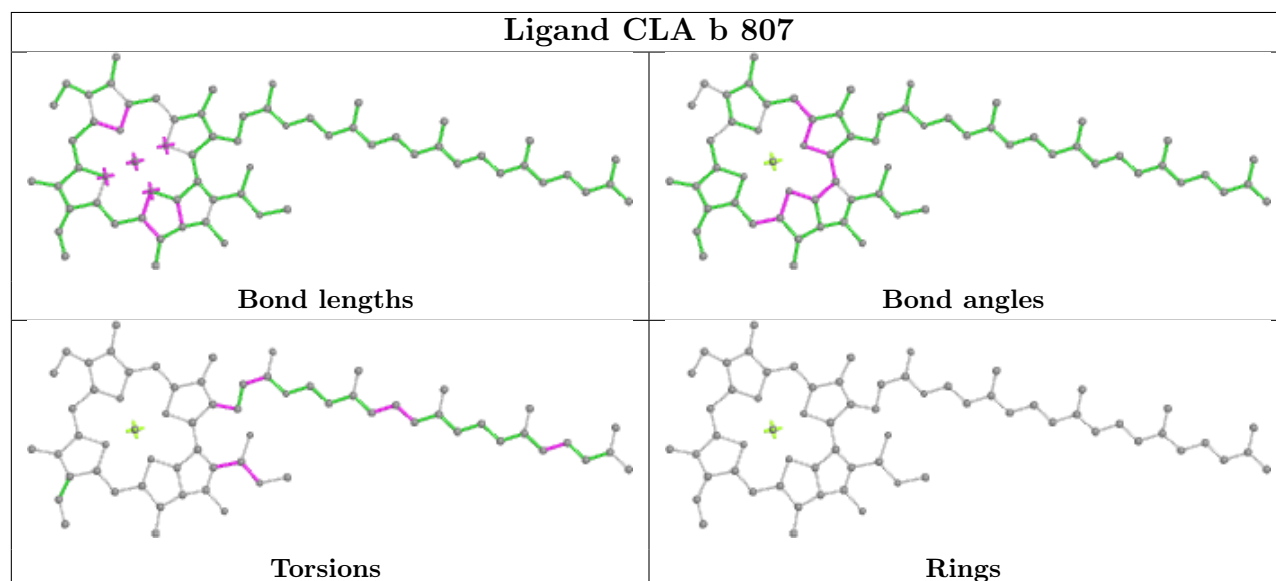
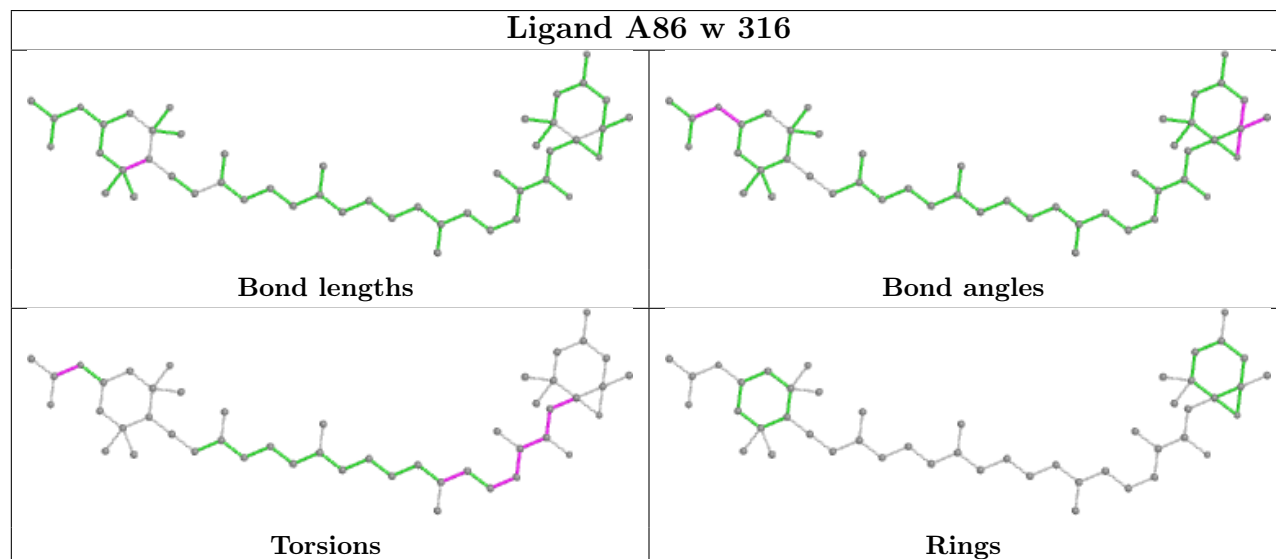
Ligand CLA F 304

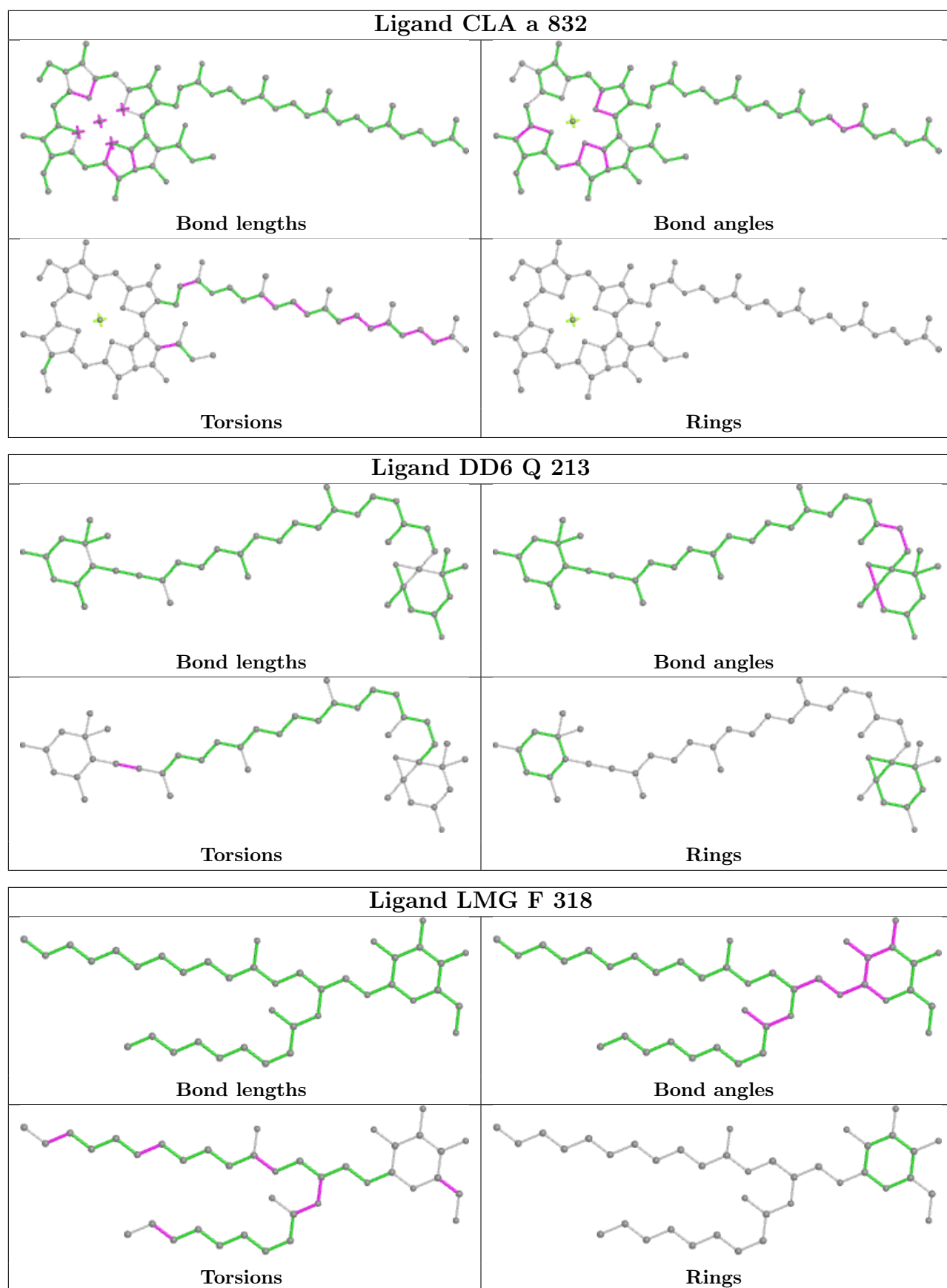


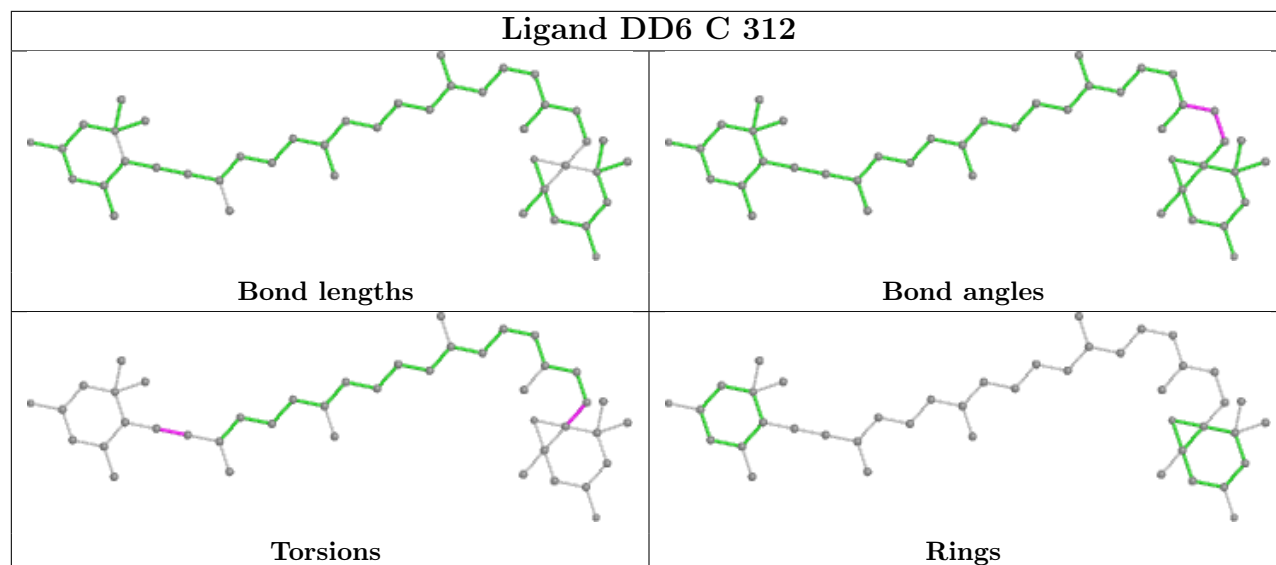
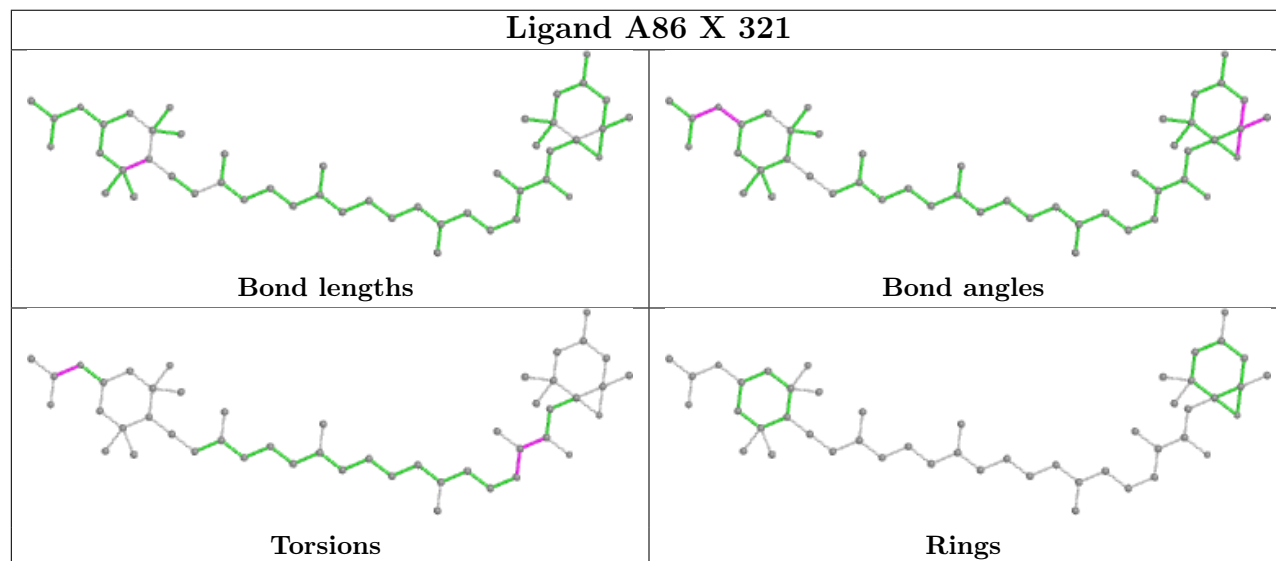
Ligand A1EB1 t 315



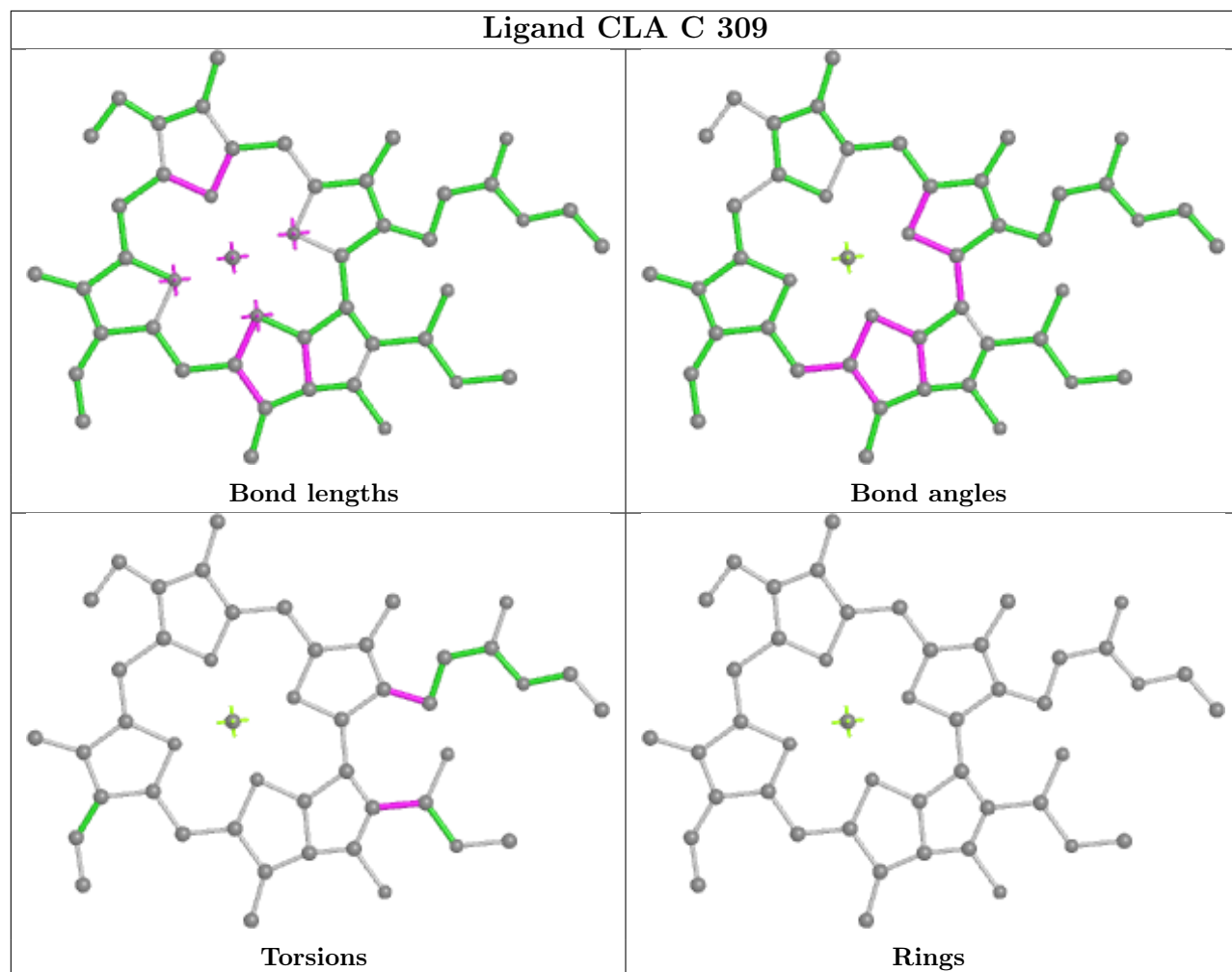


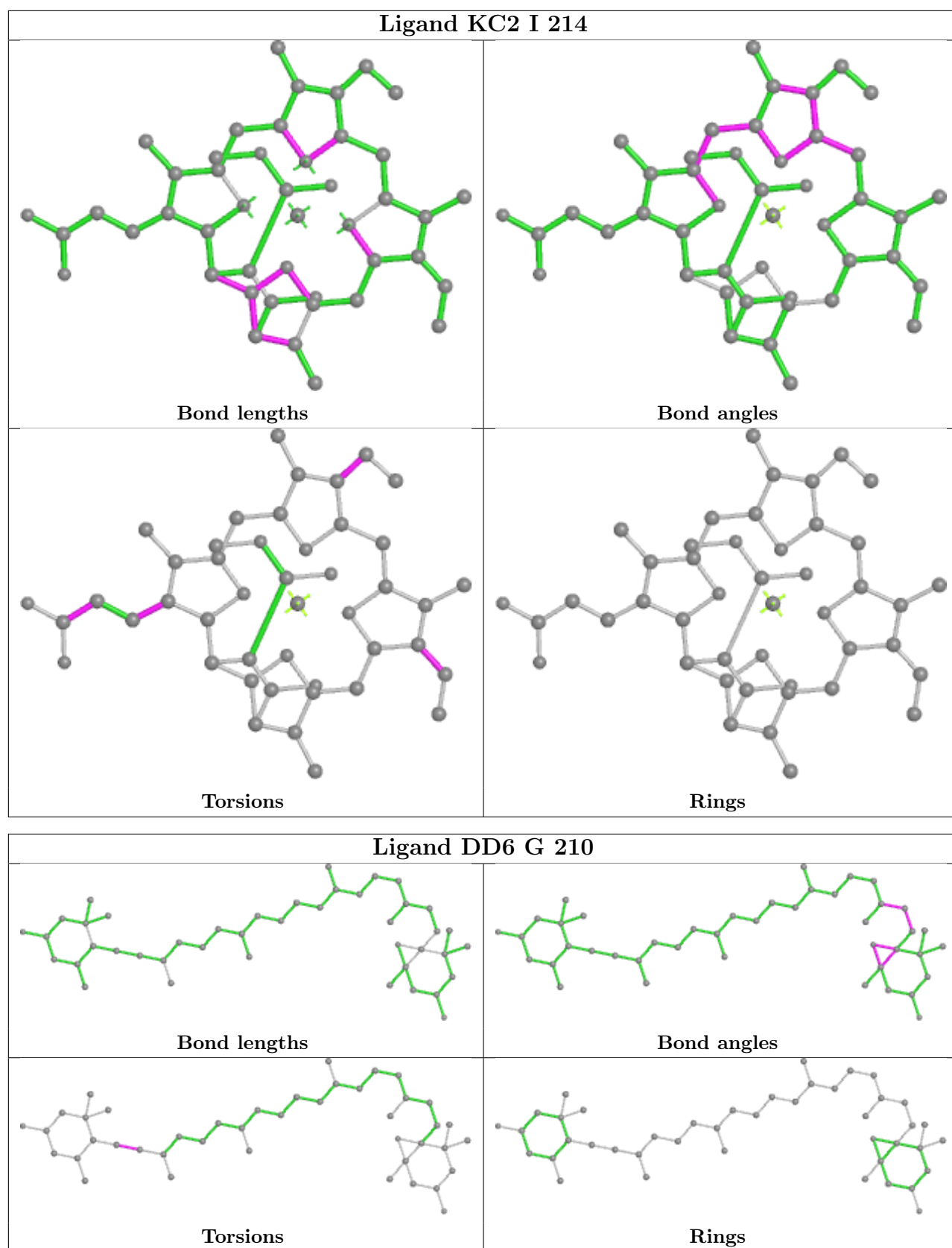
Ligand CLA a 851**Ligand CLA b 807****Ligand A86 w 316**

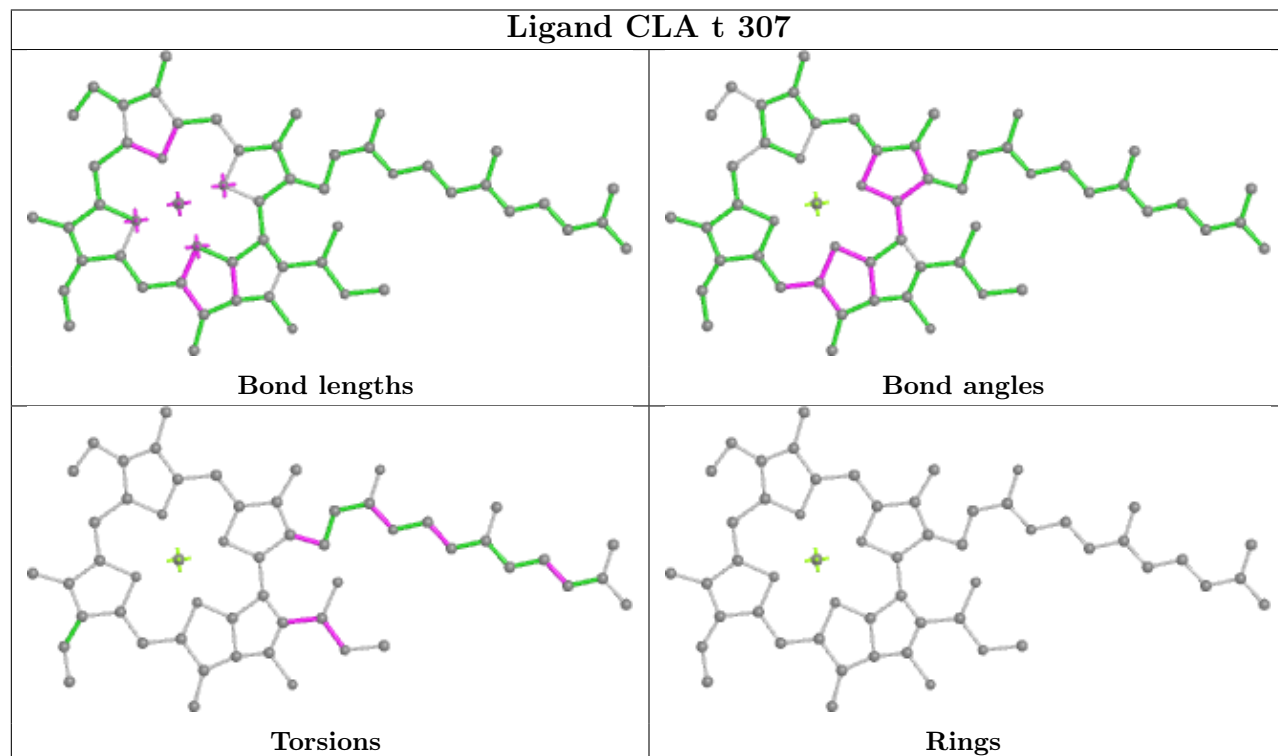
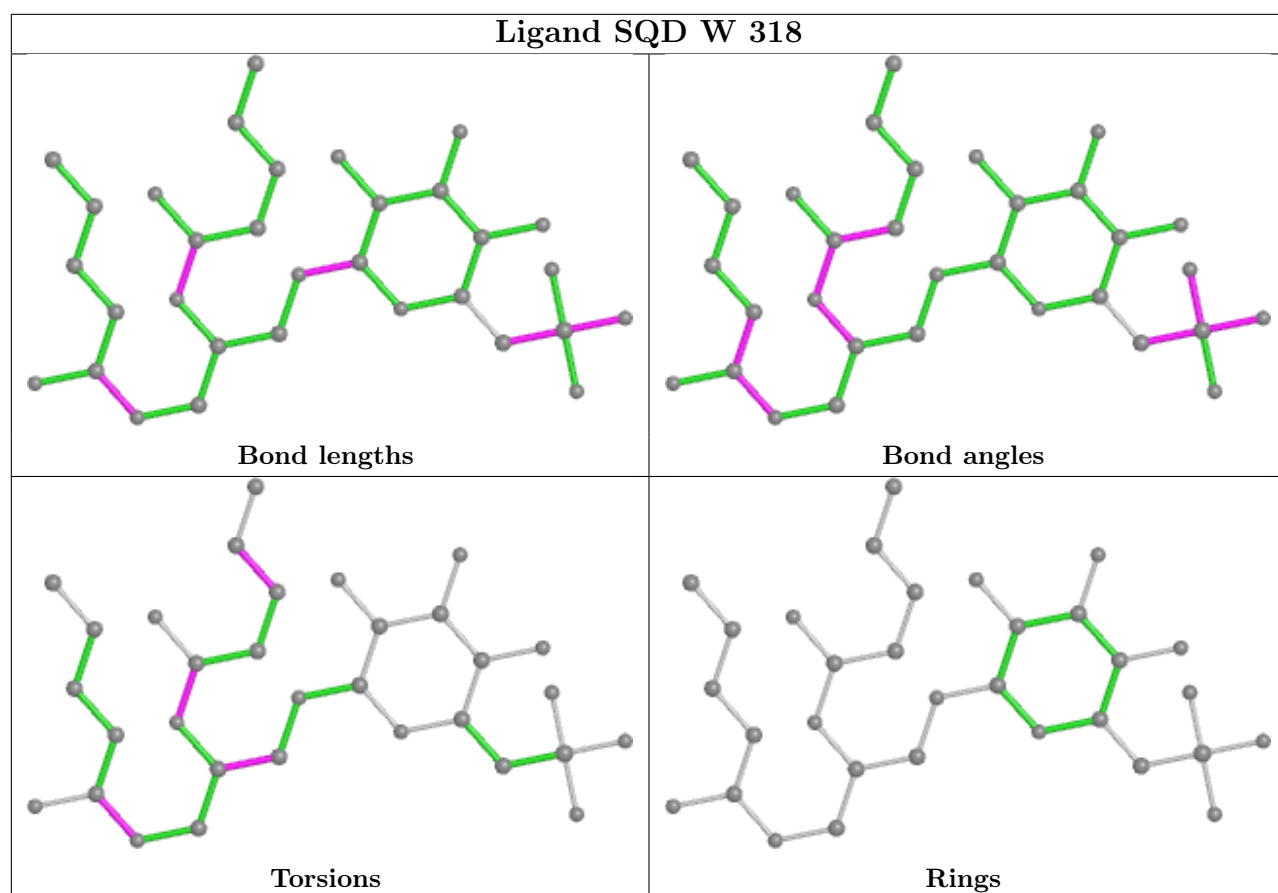


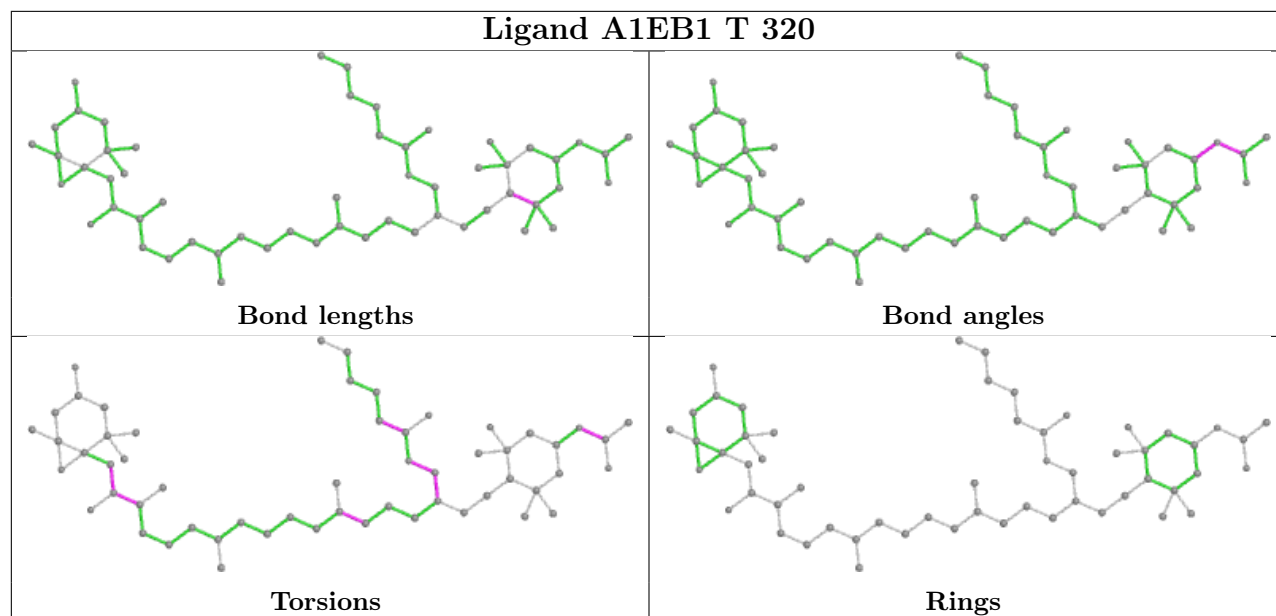
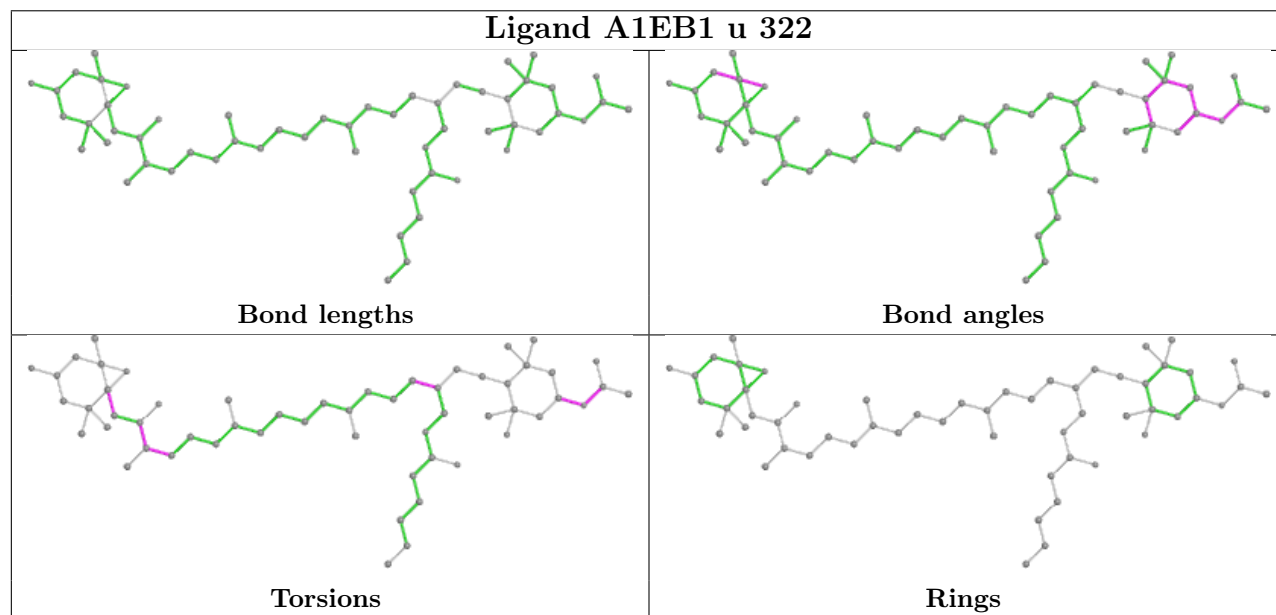
Ligand DD6 C 312**Ligand A86 X 321**

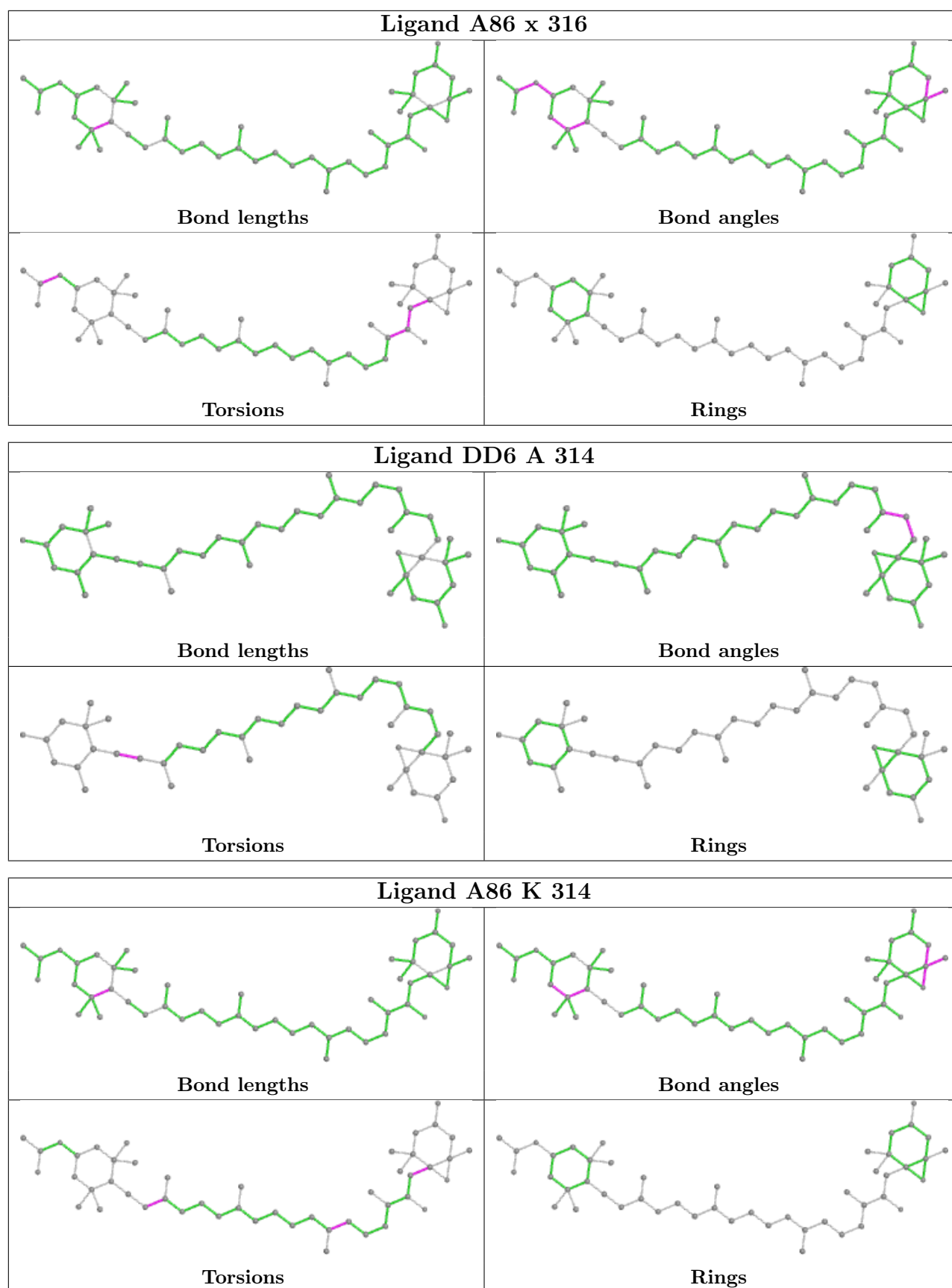
Ligand CLA C 309



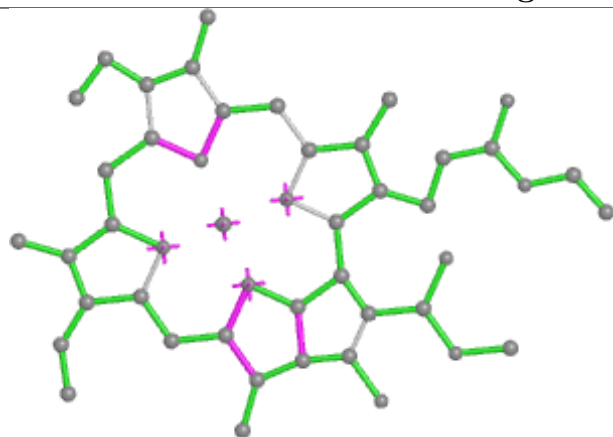




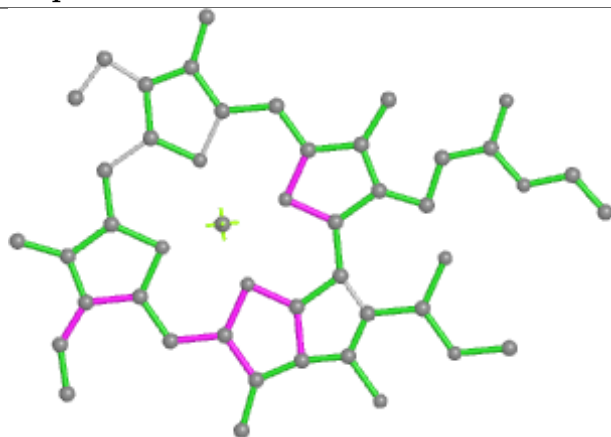
Ligand A1EB1 T 320**Ligand A1EB1 u 322**



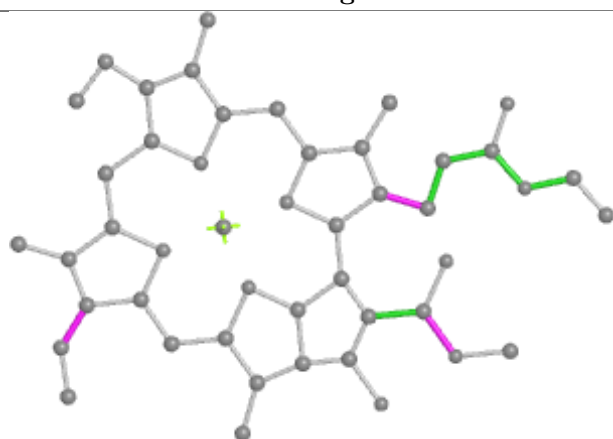
Ligand CLA p 305



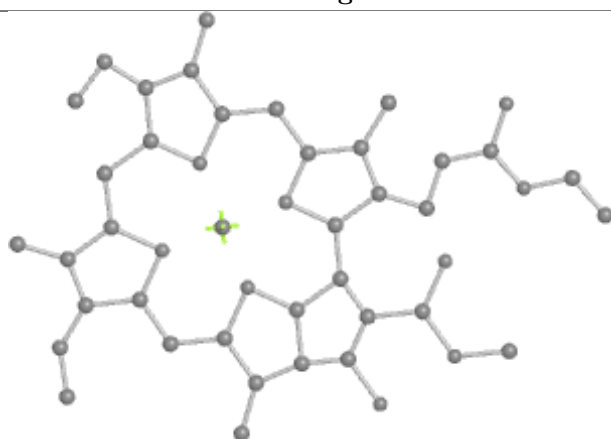
Bond lengths



Bond angles

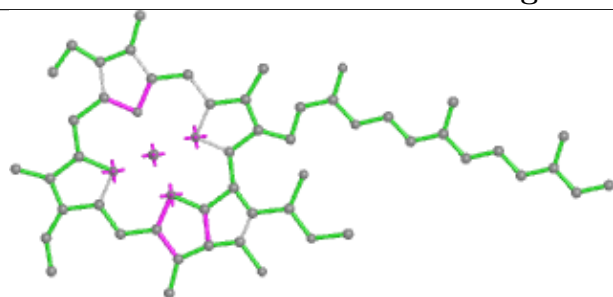


Torsions

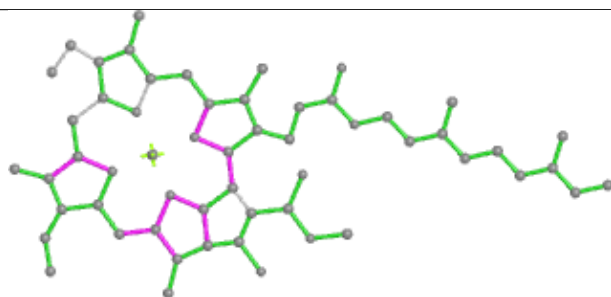


Rings

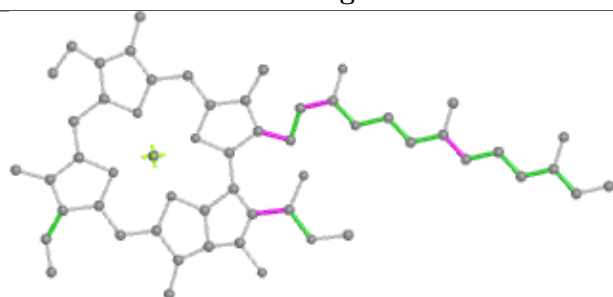
Ligand CLA I 205



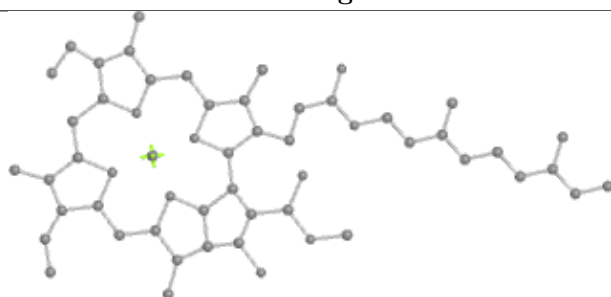
Bond lengths



Bond angles

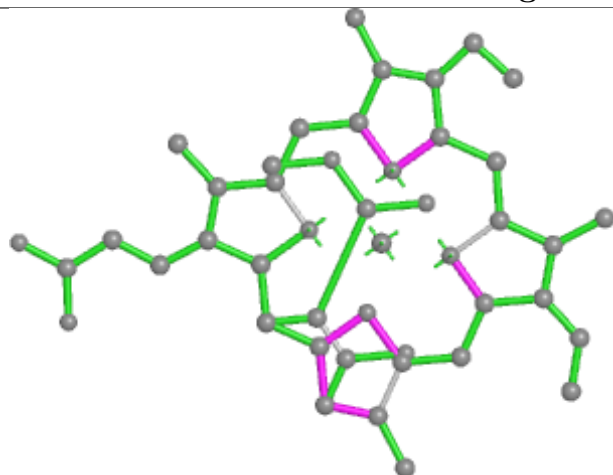


Torsions

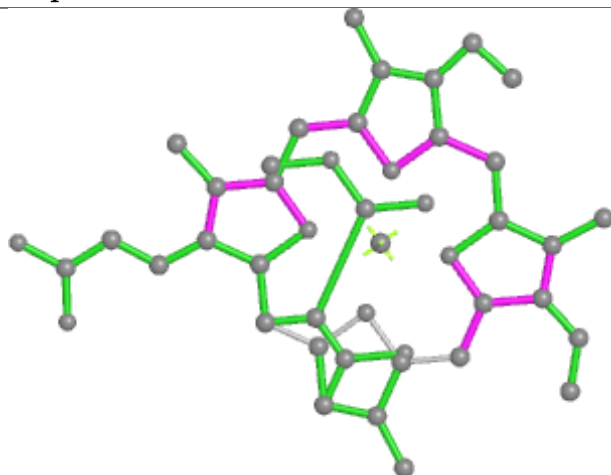


Rings

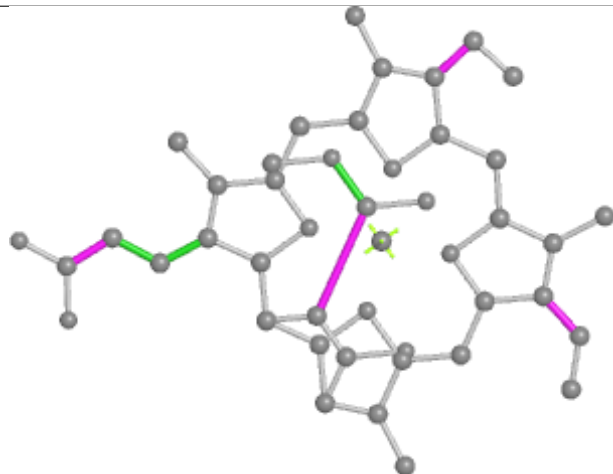
Ligand KC2 p 315



Bond lengths



Bond angles

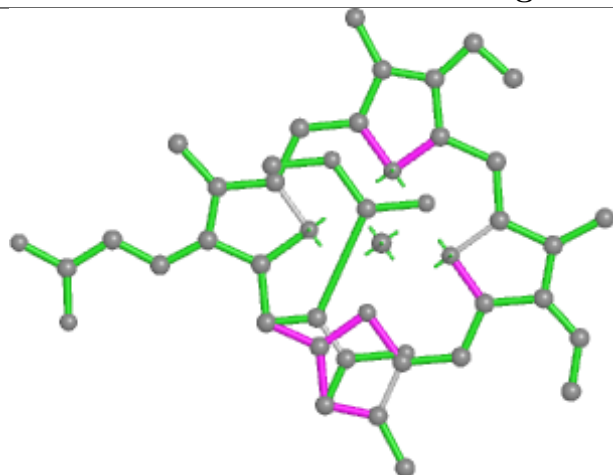


Torsions

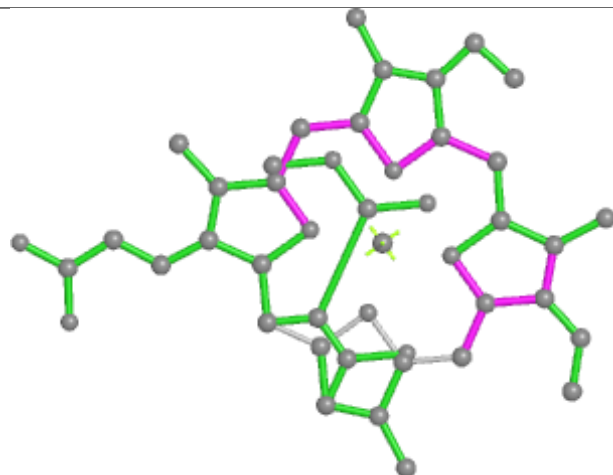


Rings

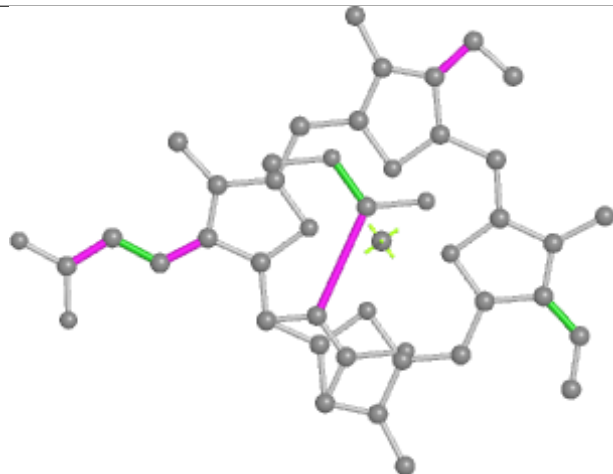
Ligand KC2 R 308



Bond lengths



Bond angles

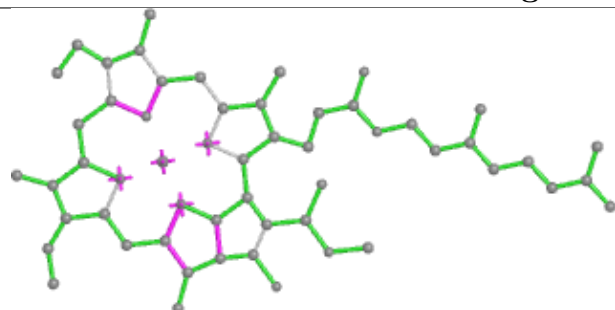


Torsions

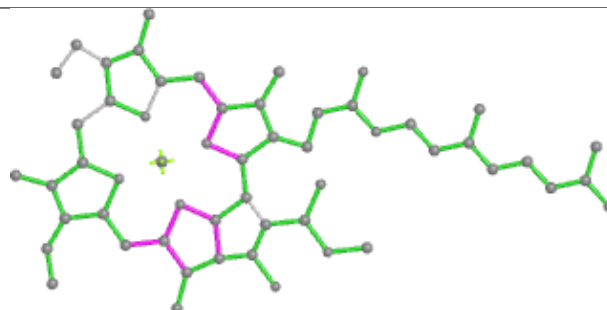


Rings

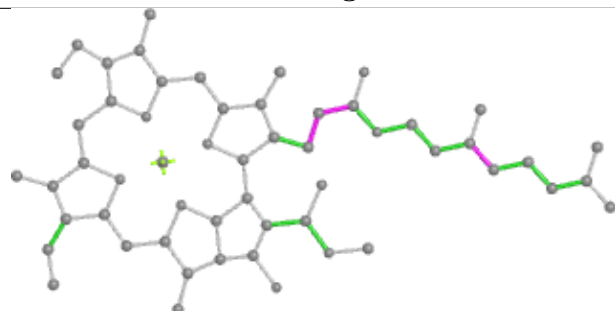
Ligand CLA z 306



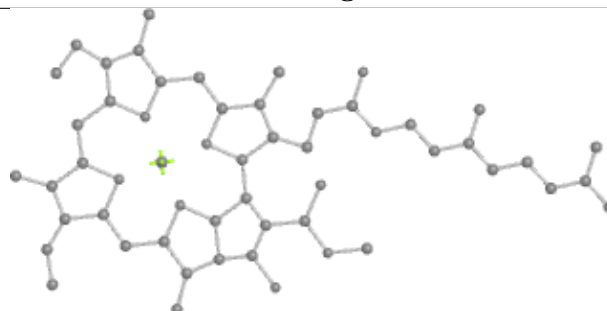
Bond lengths



Bond angles

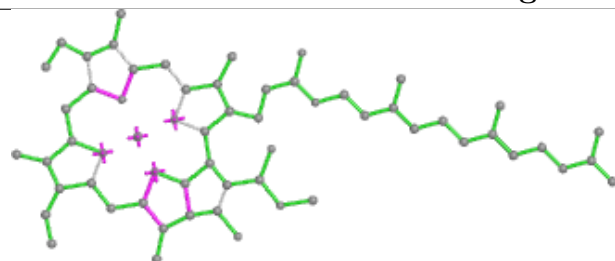


Torsions

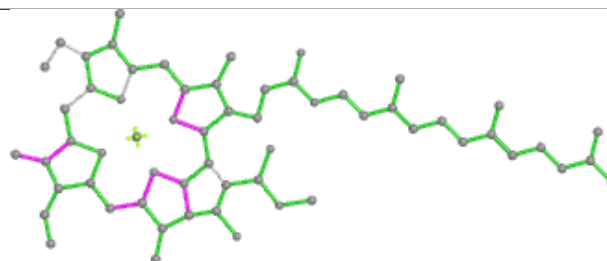


Rings

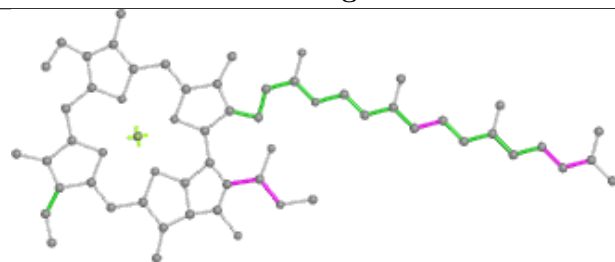
Ligand CLA u 312



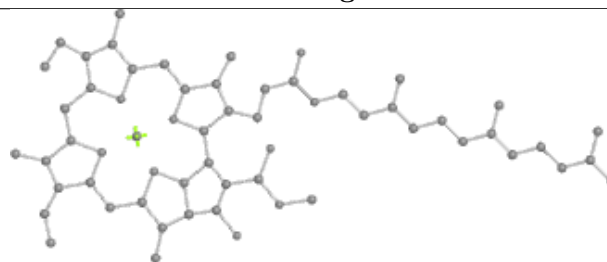
Bond lengths



Bond angles

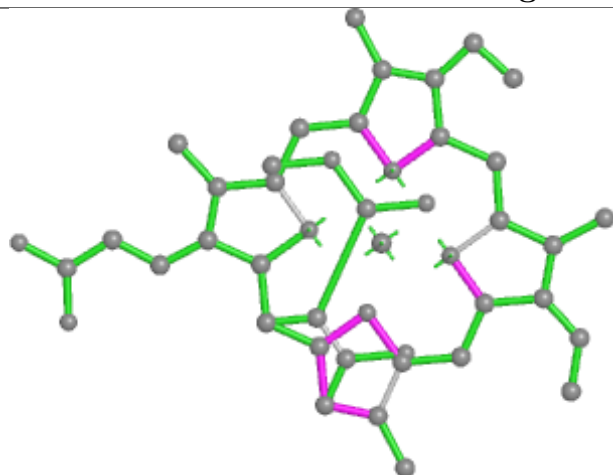


Torsions

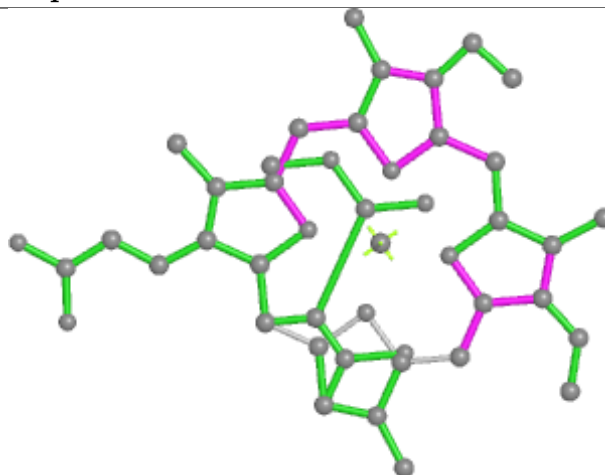


Rings

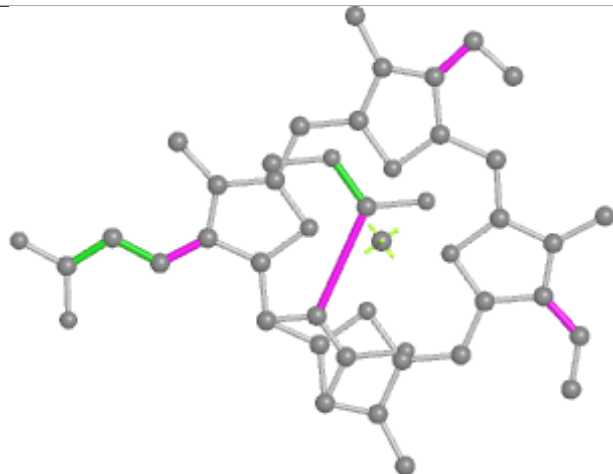
Ligand KC2 p 309



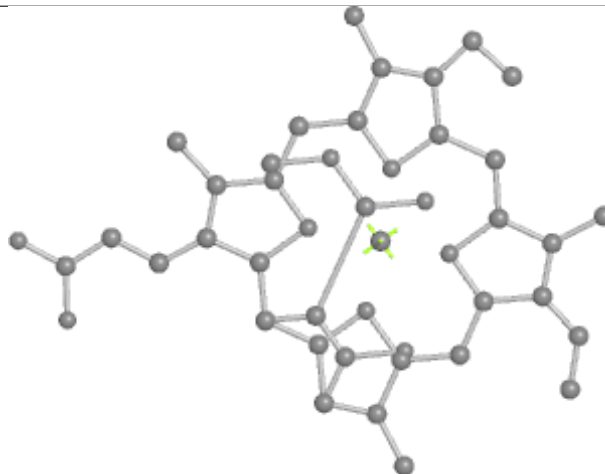
Bond lengths



Bond angles

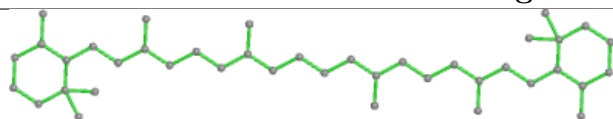


Torsions

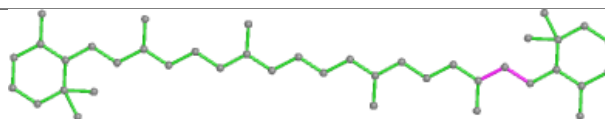


Rings

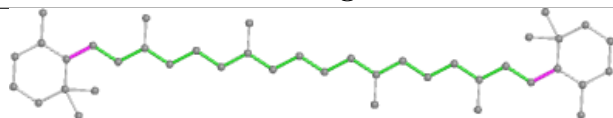
Ligand BCR b 846



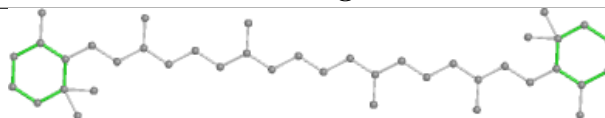
Bond lengths



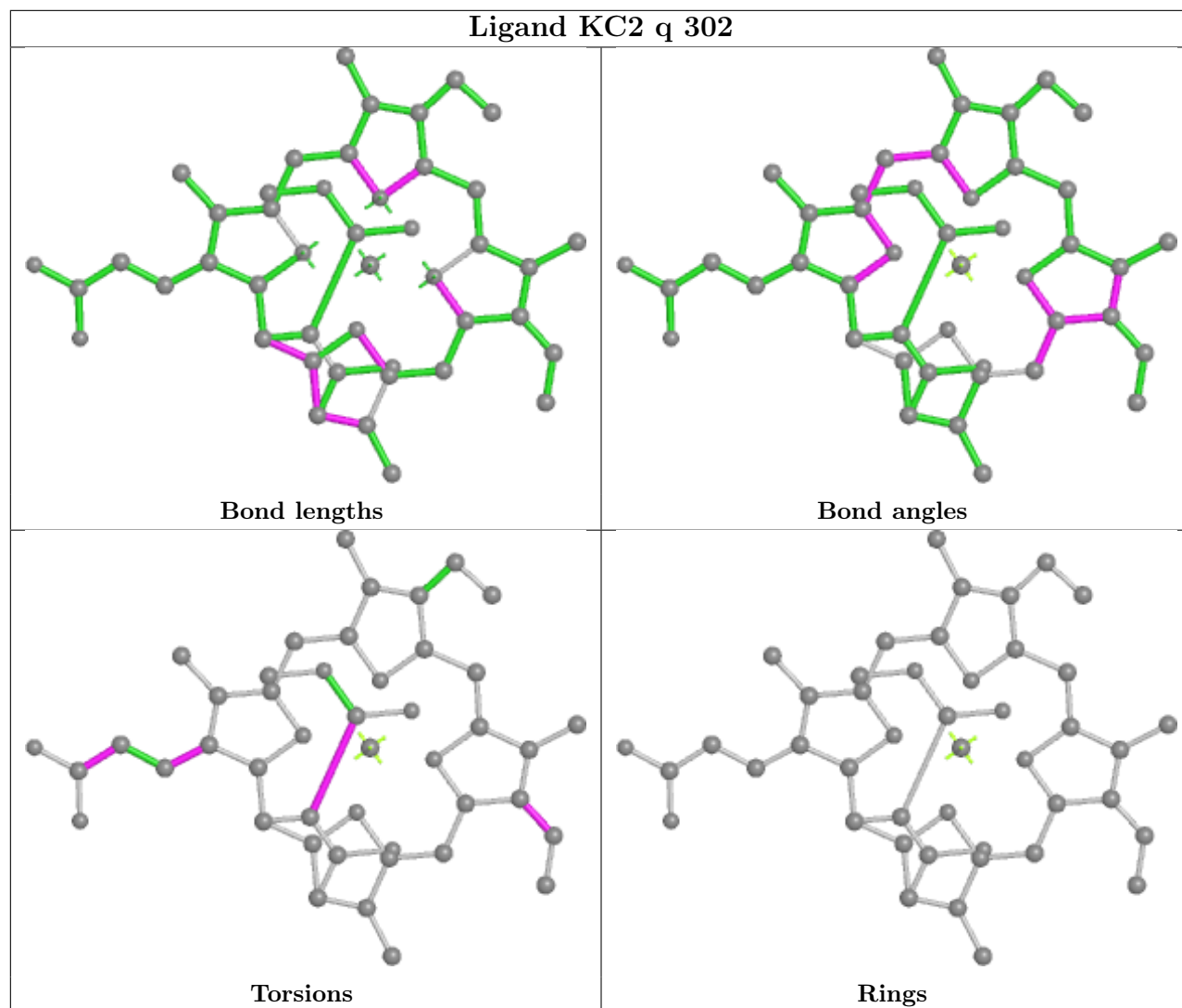
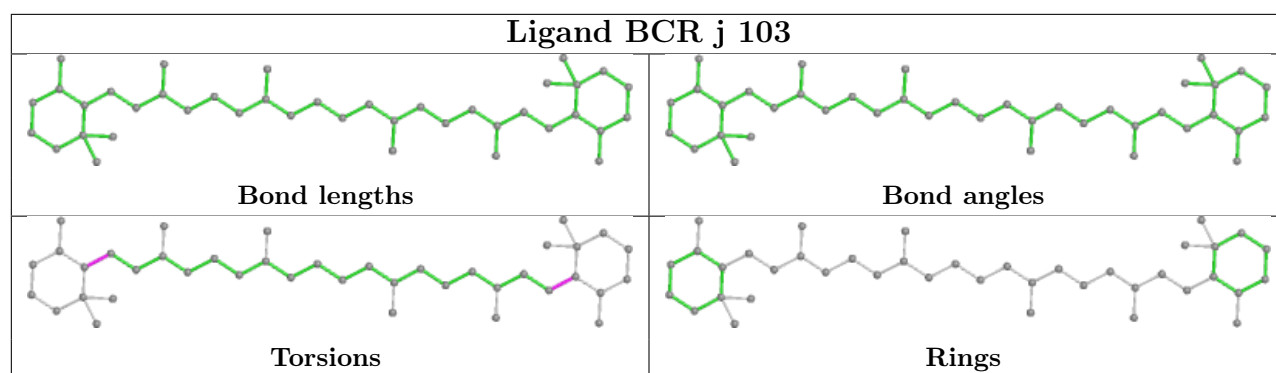
Bond angles



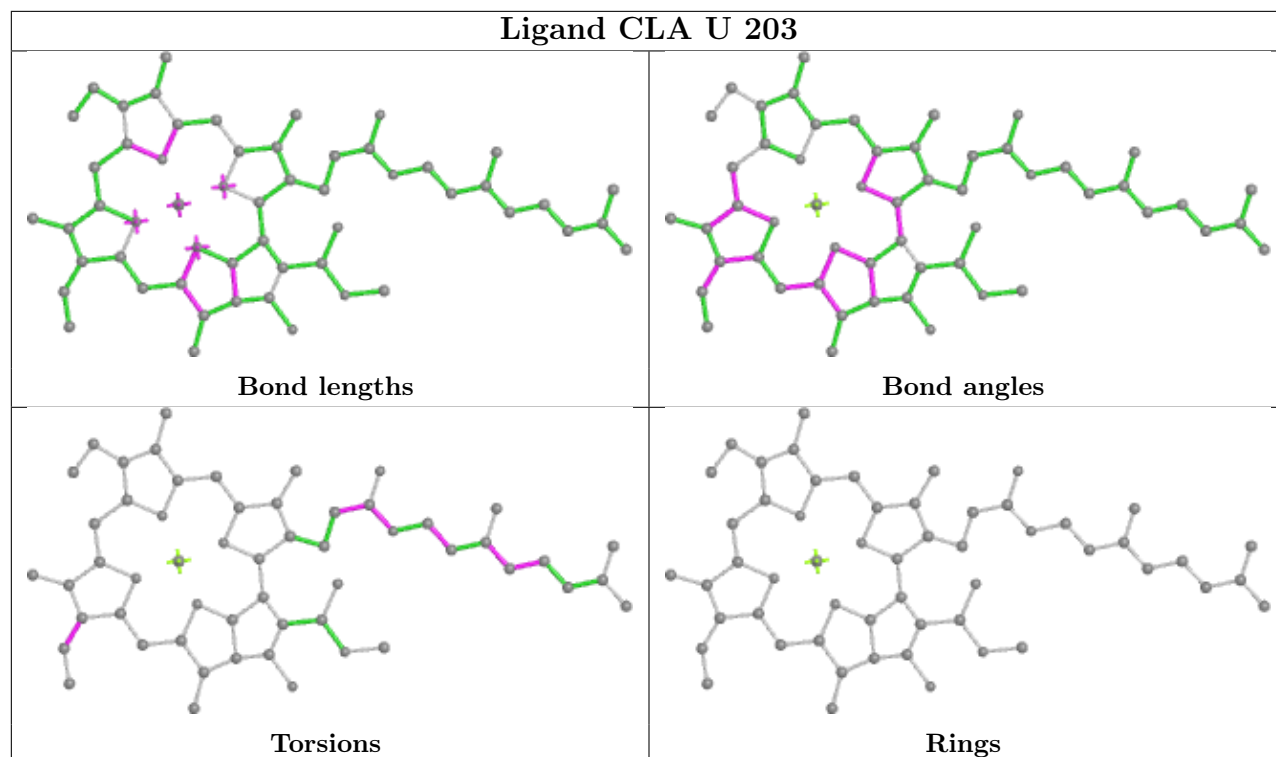
Torsions



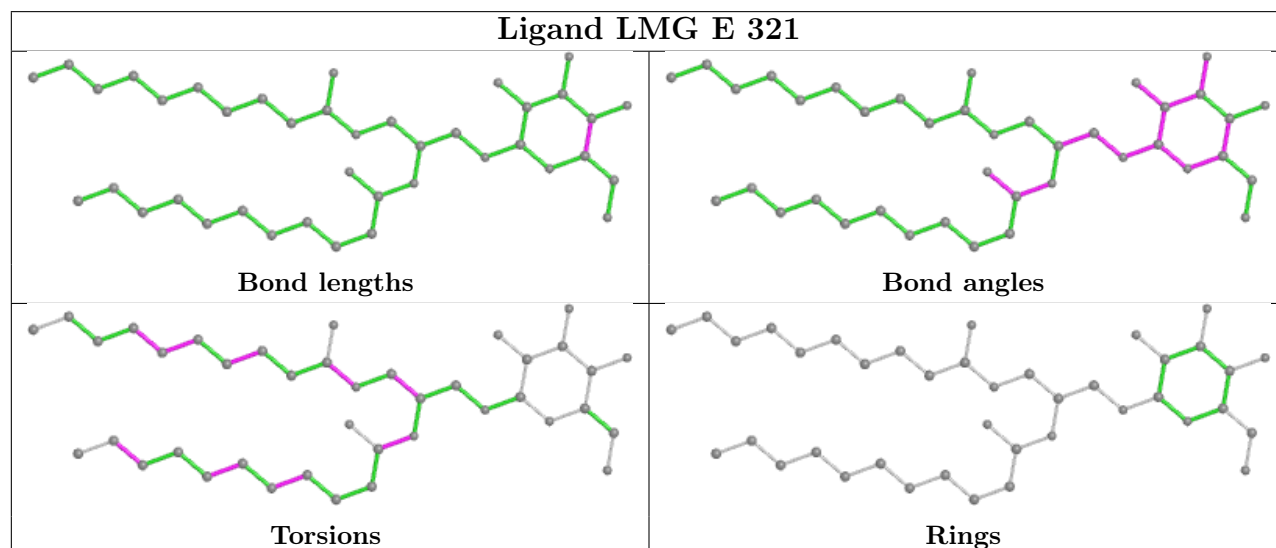
Rings

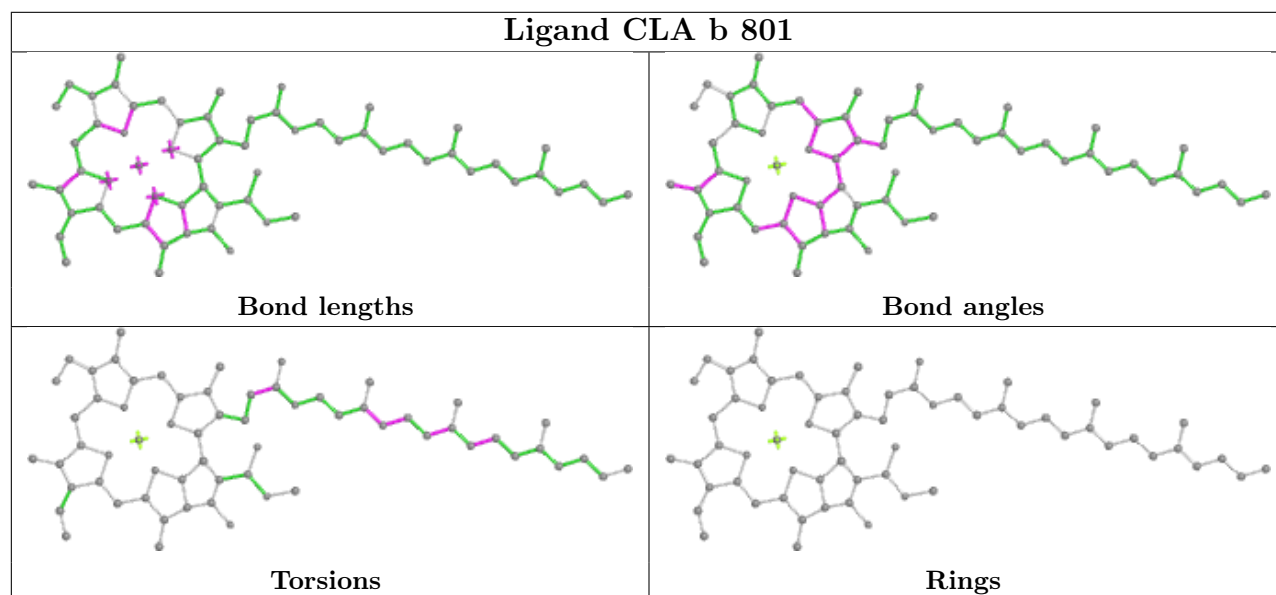
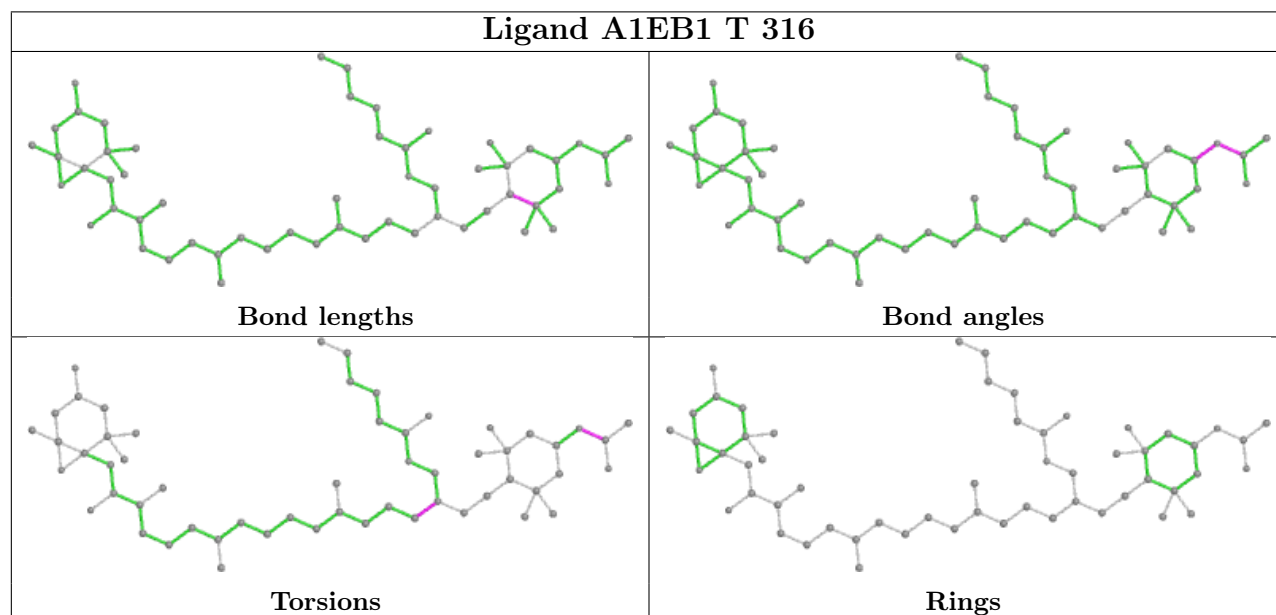
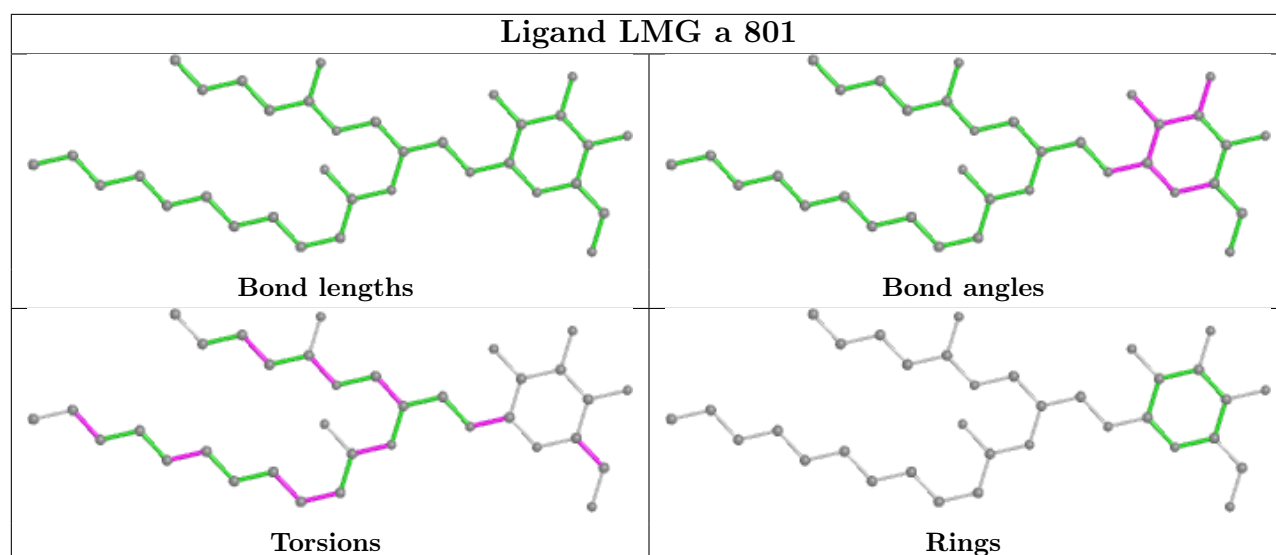


Ligand CLA U 203

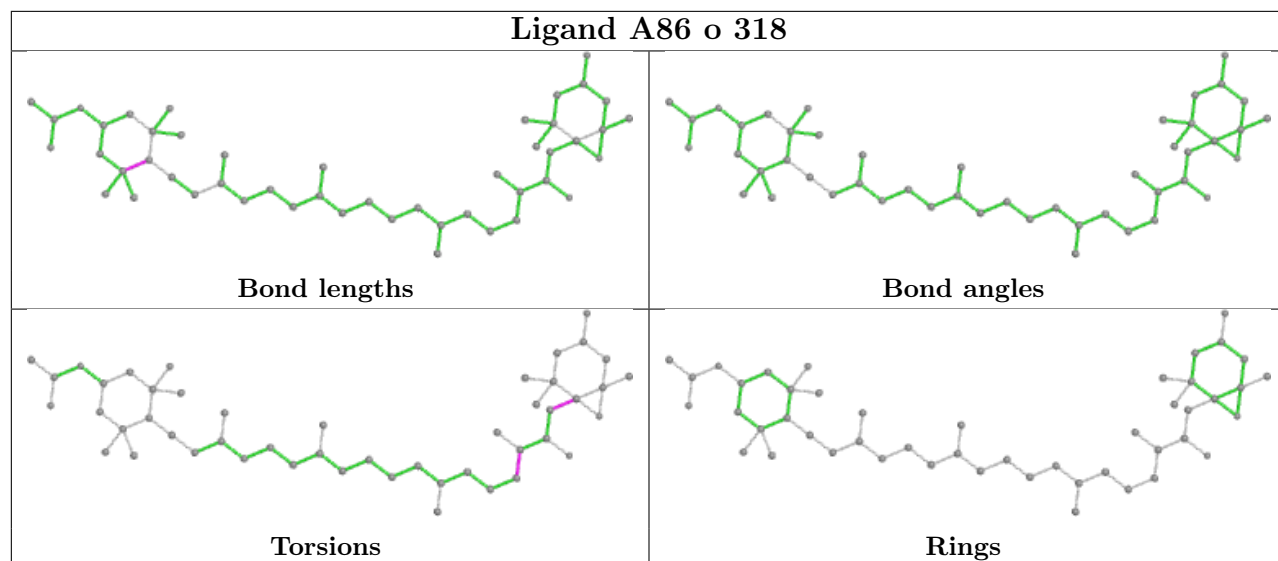


Ligand LMG E 321

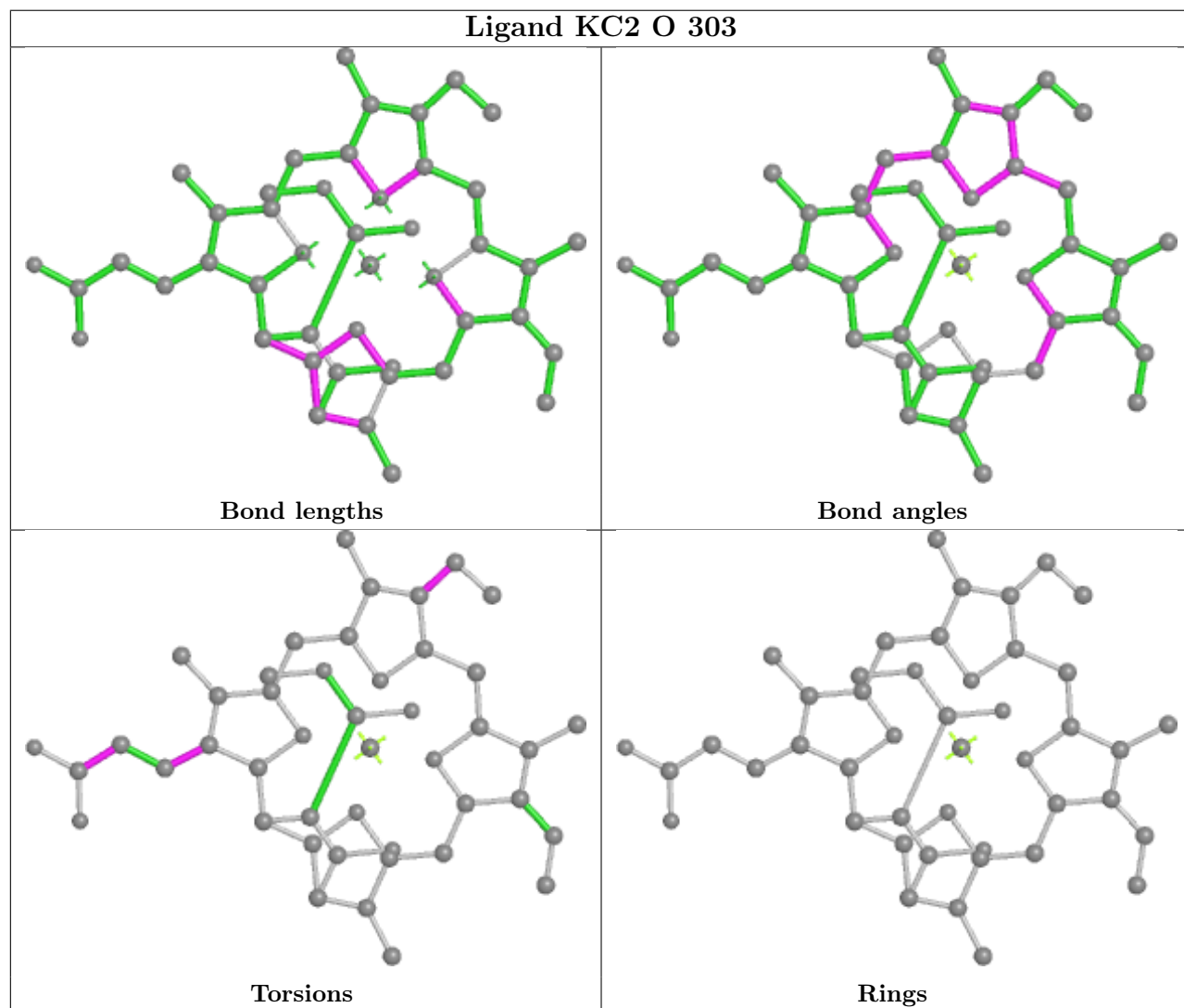




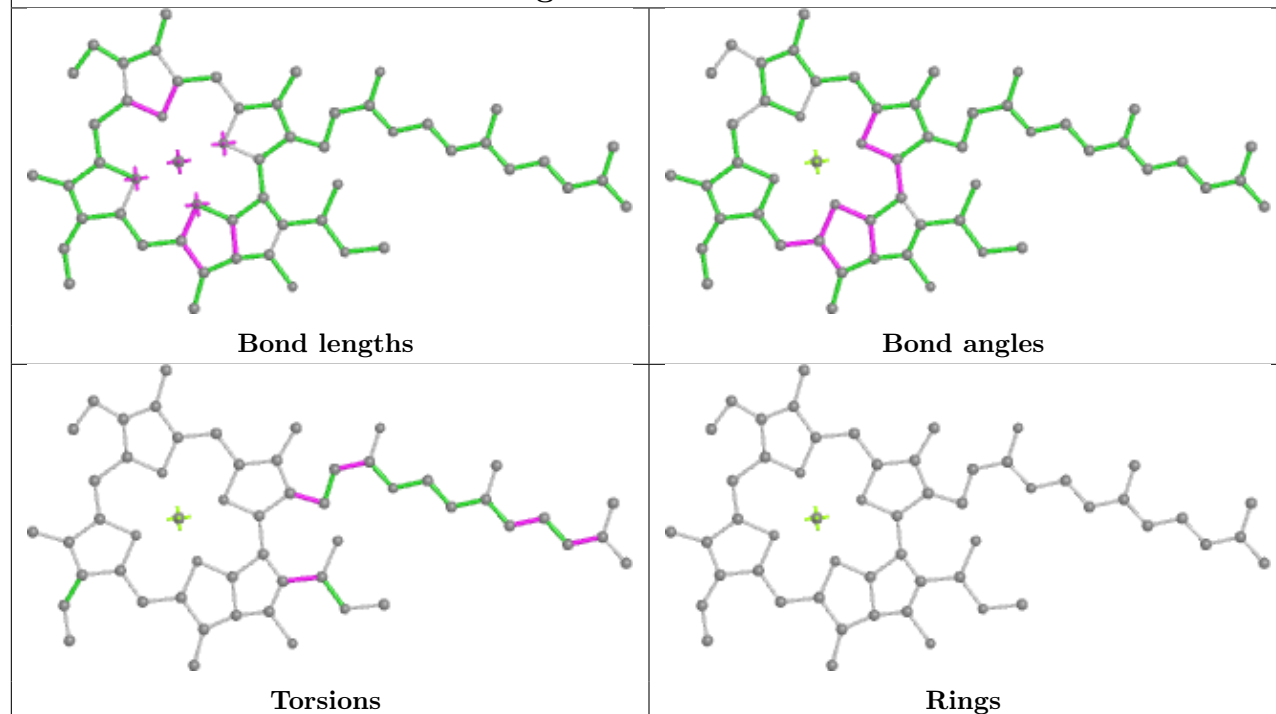
Ligand A86 o 318



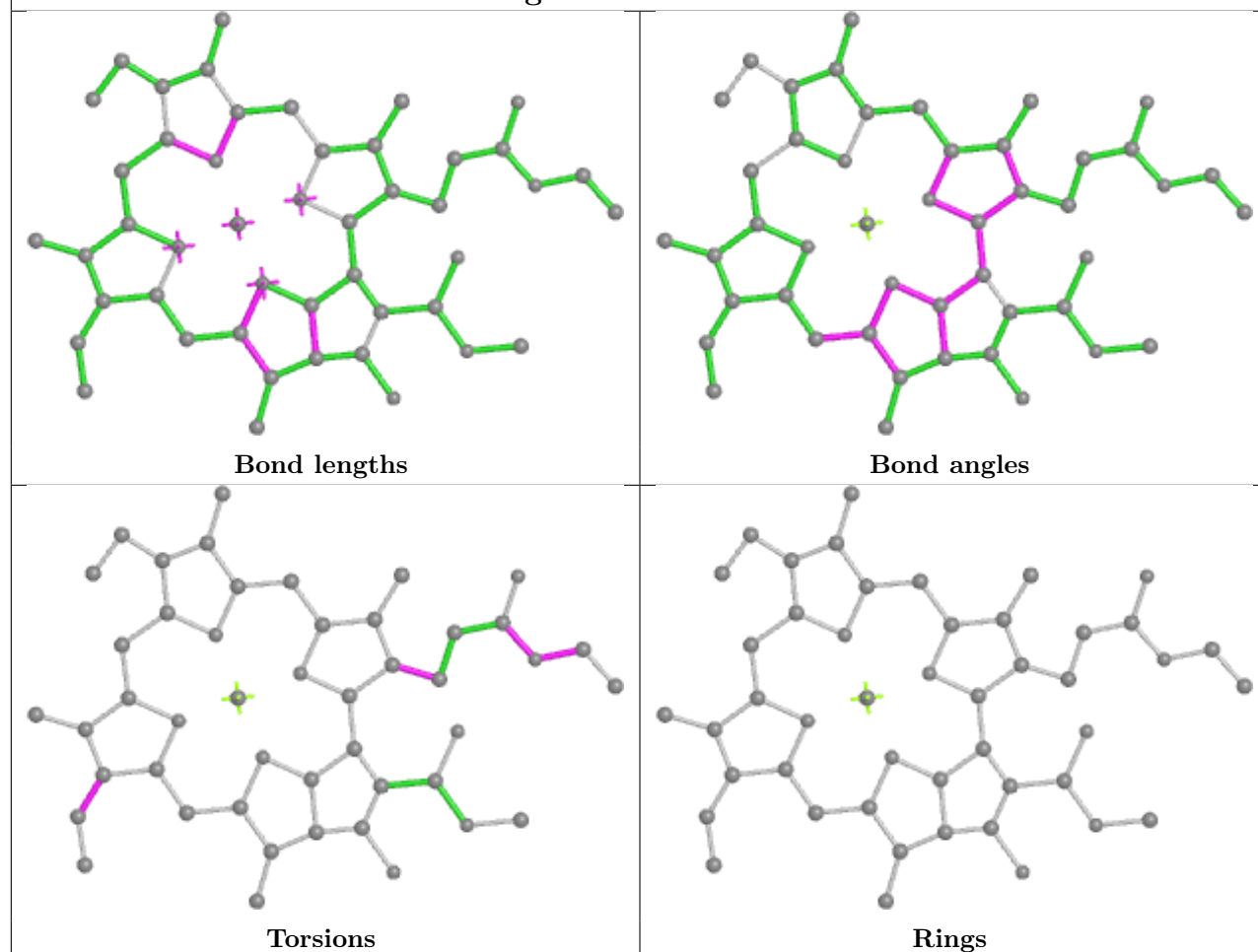
Ligand KC2 O 303

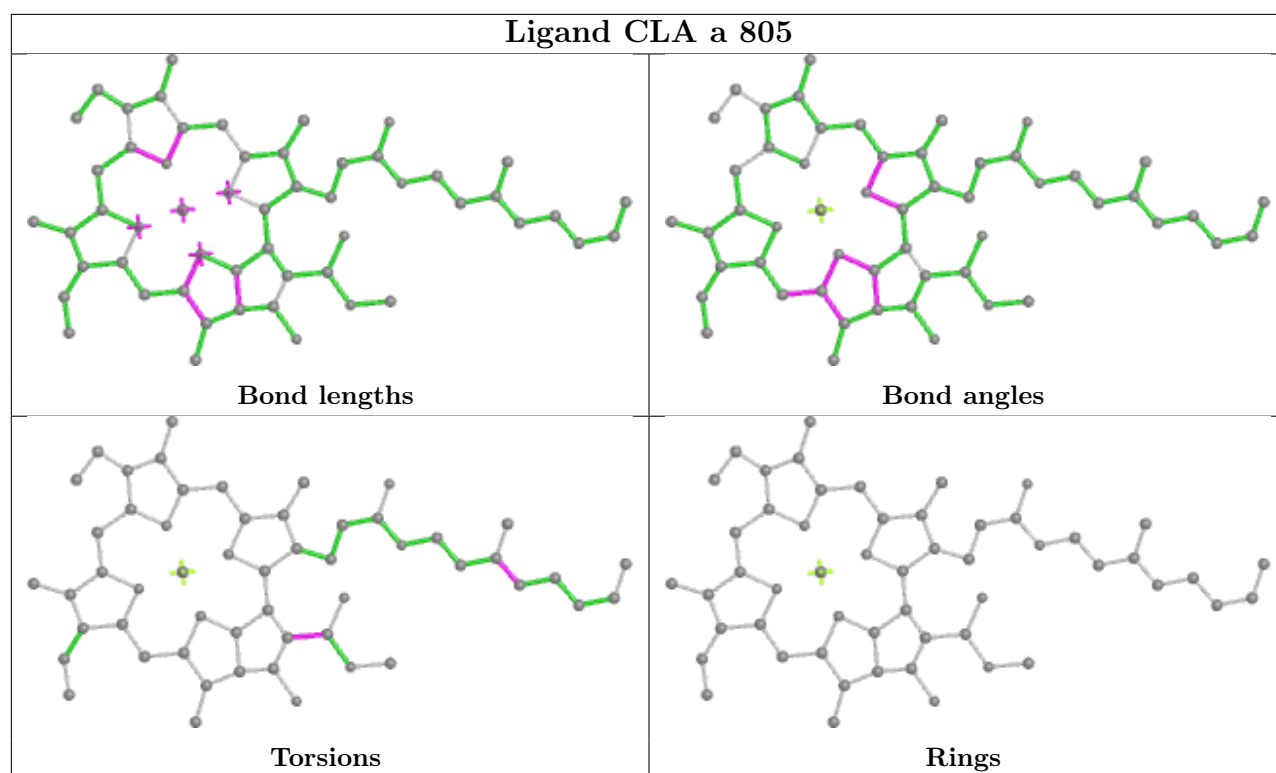


Ligand CLA a 838

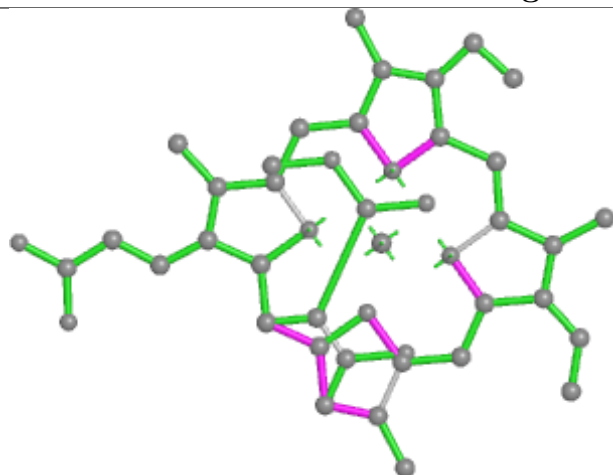


Ligand CLA B 301

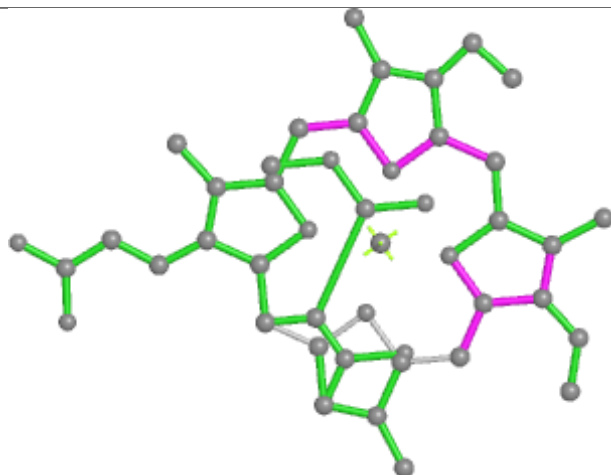




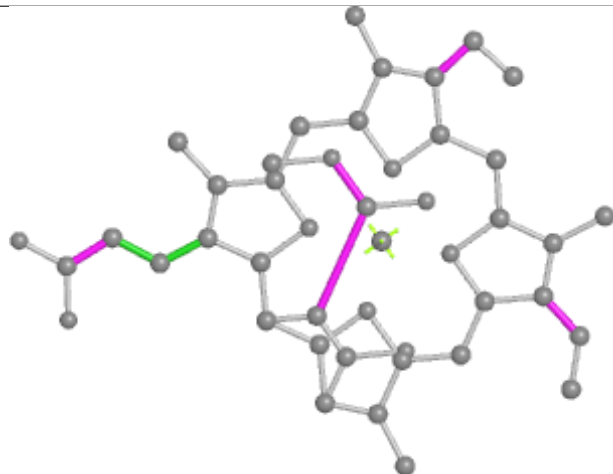
Ligand KC2 t 306



Bond lengths



Bond angles

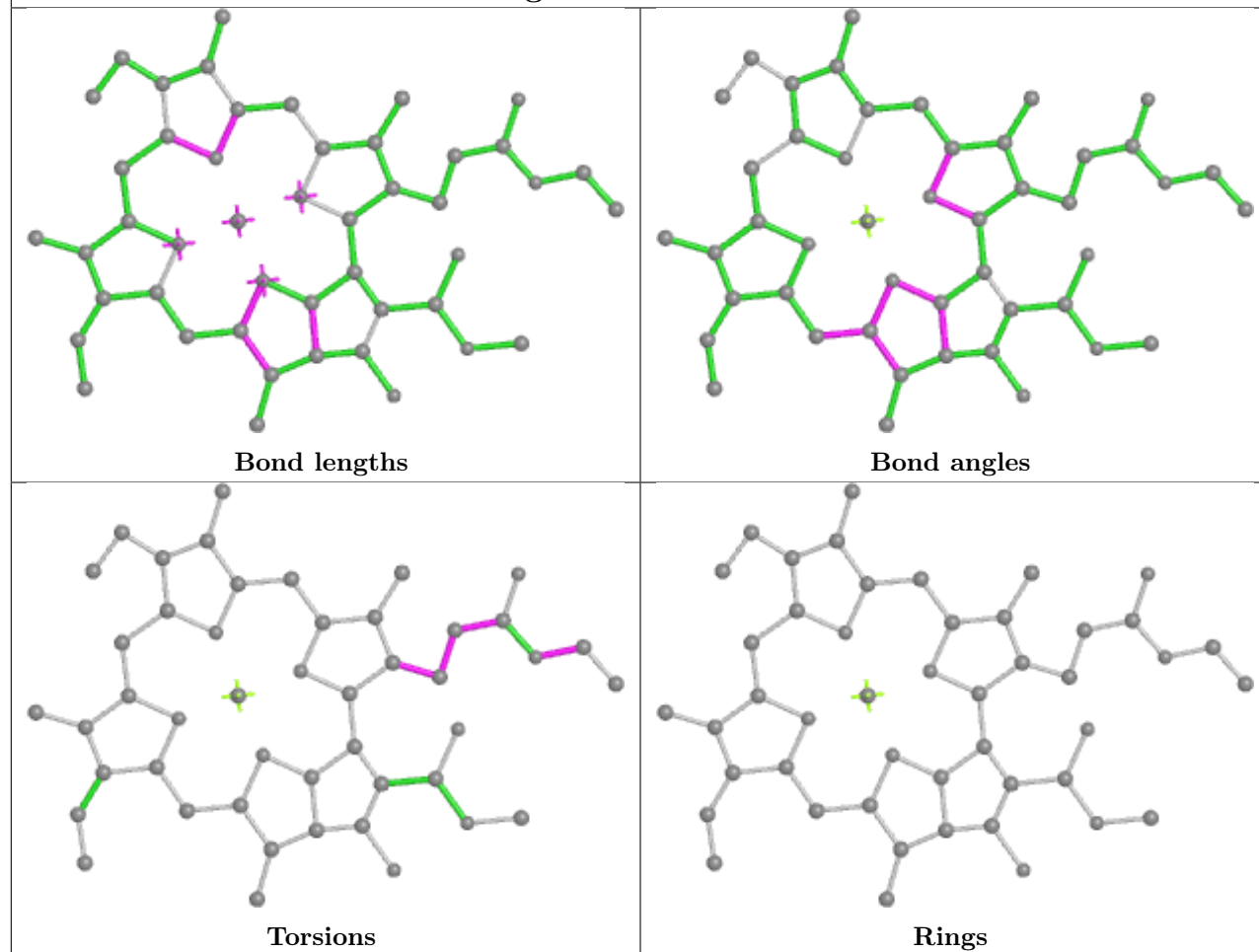


Torsions

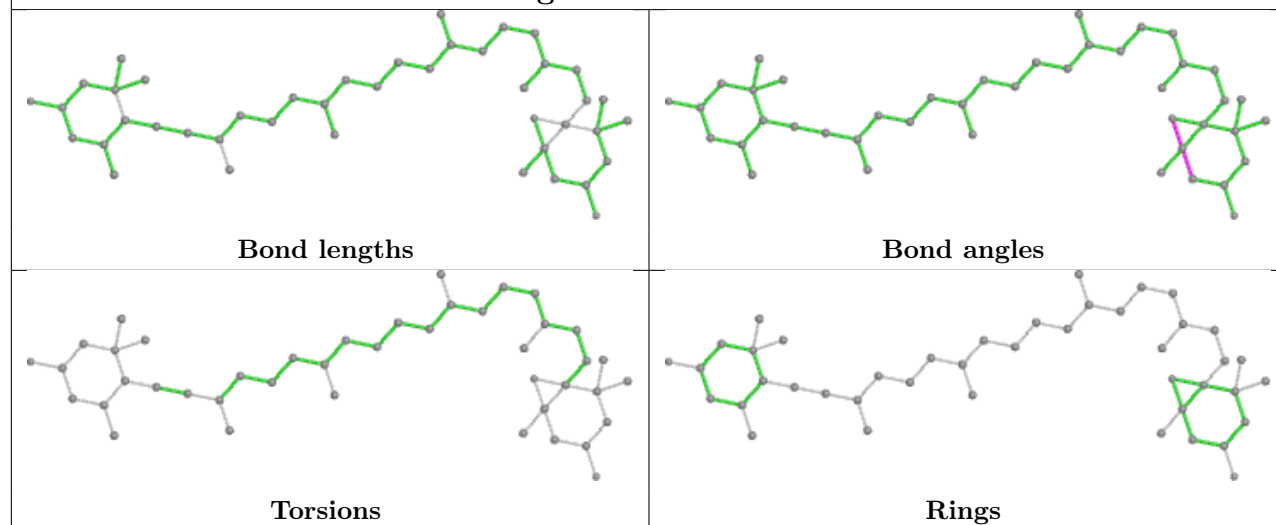


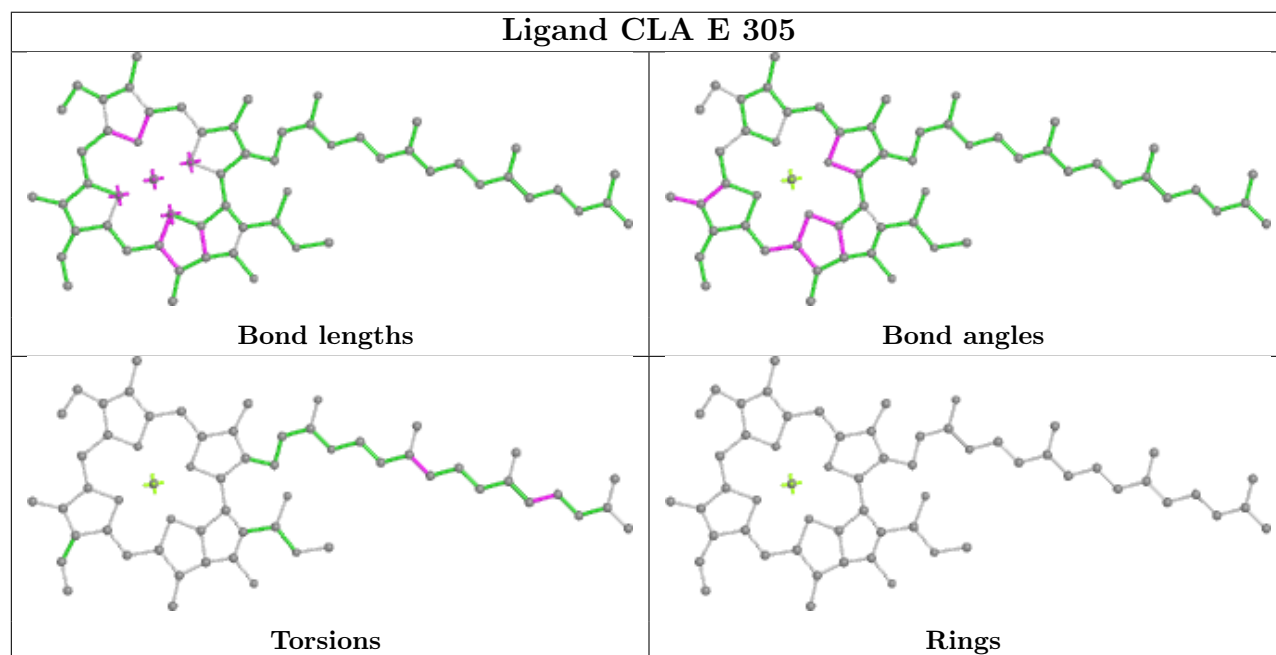
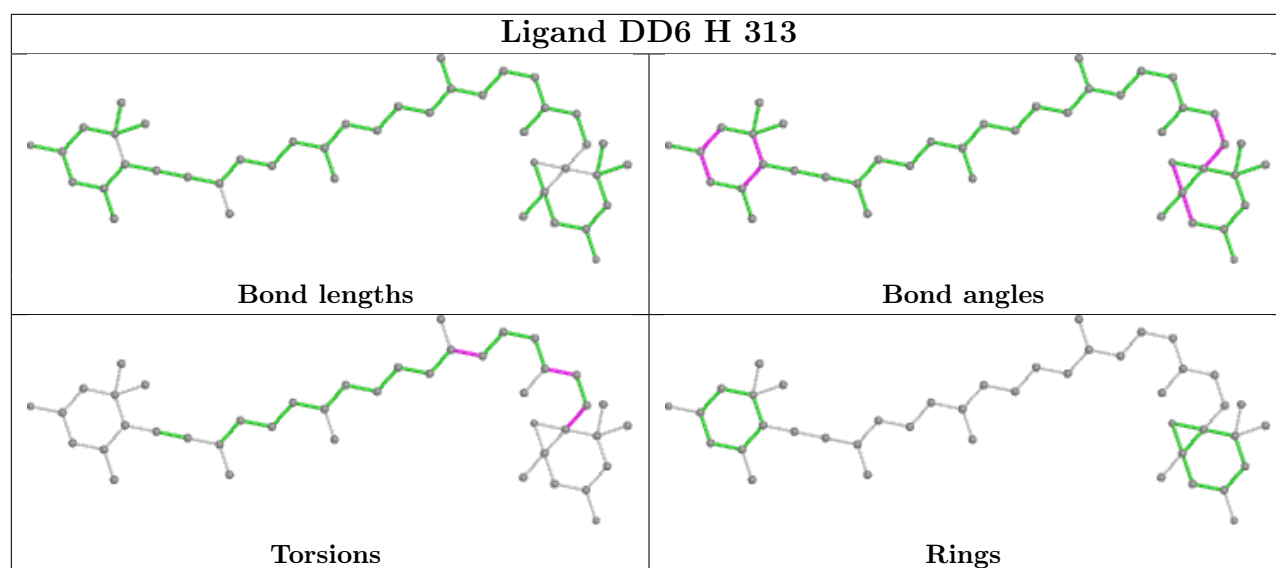
Rings

Ligand CLA w 303

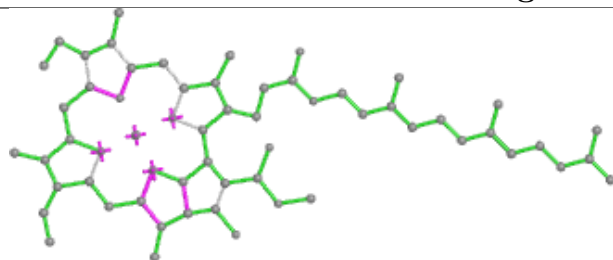


Ligand DD6 o 320

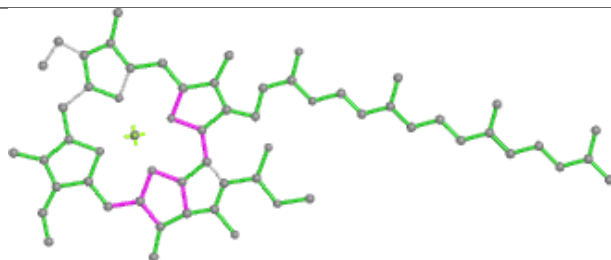




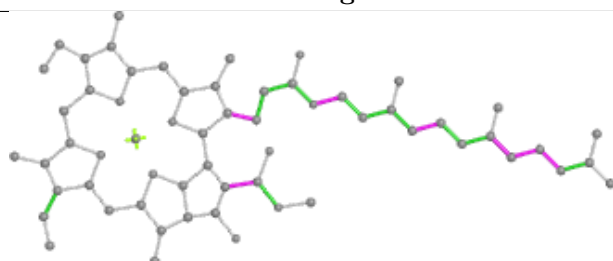
Ligand CLA b 827



Bond lengths



Bond angles

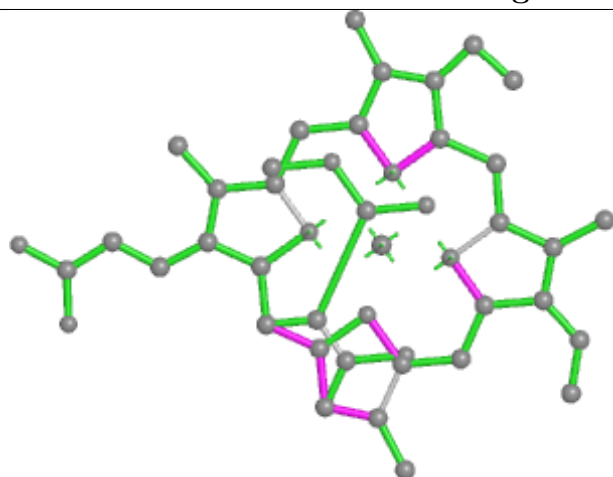


Torsions

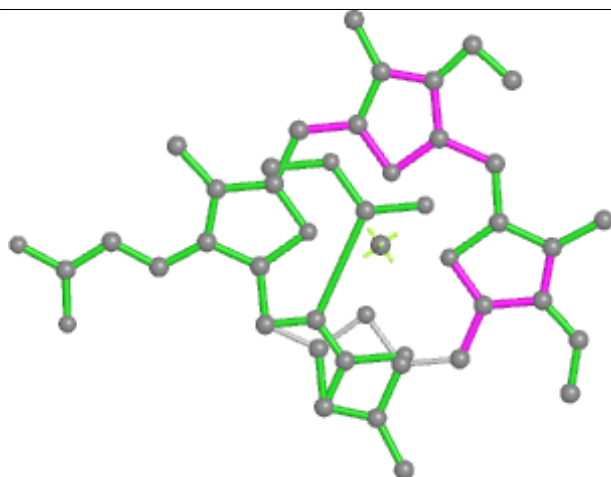


Rings

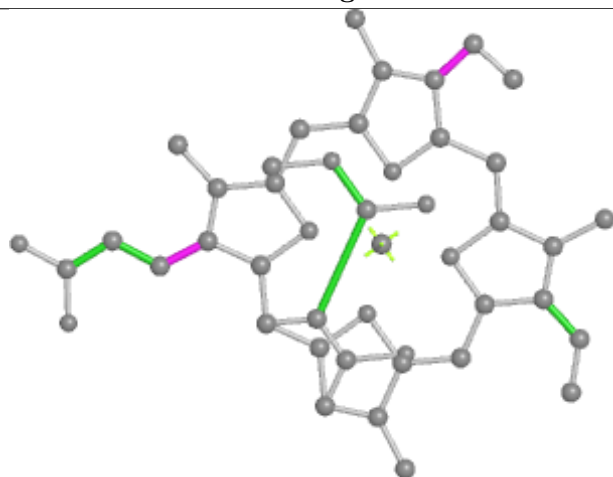
Ligand KC2 M 309



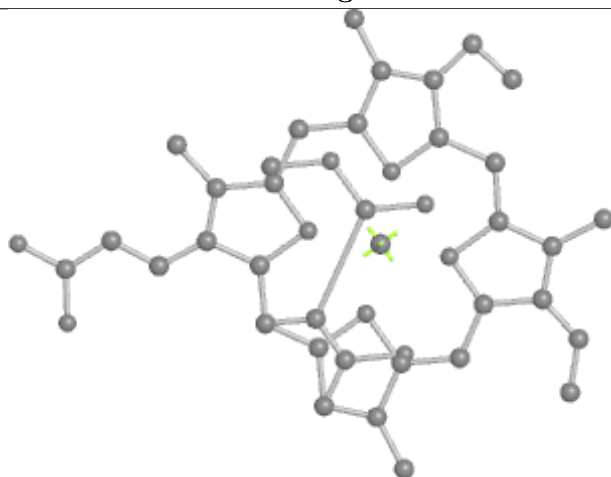
Bond lengths



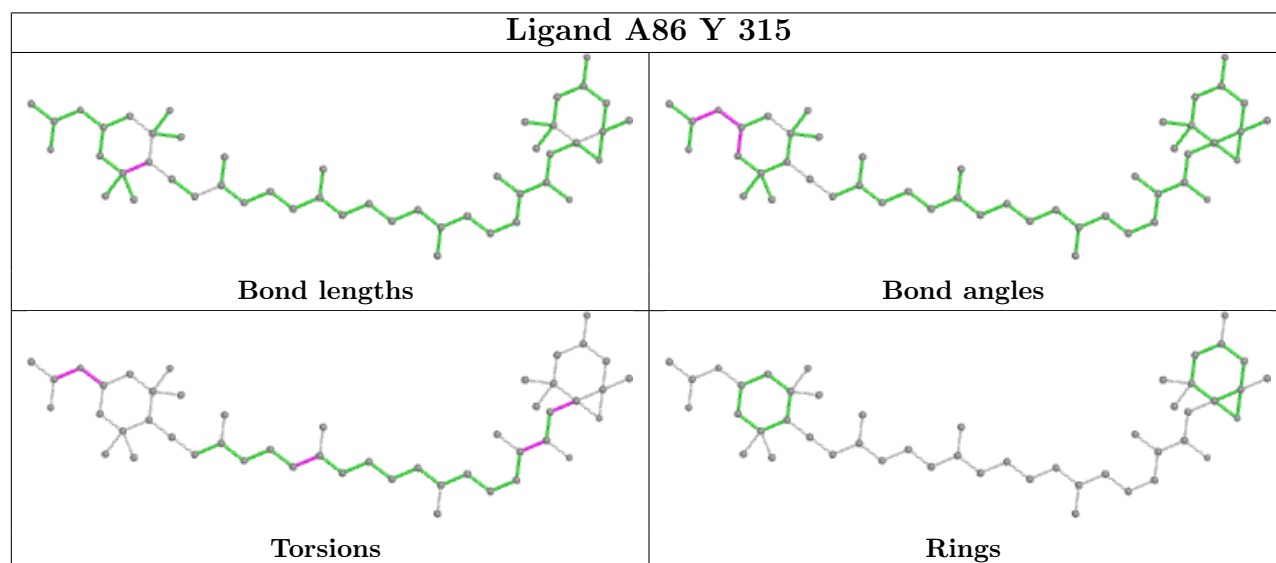
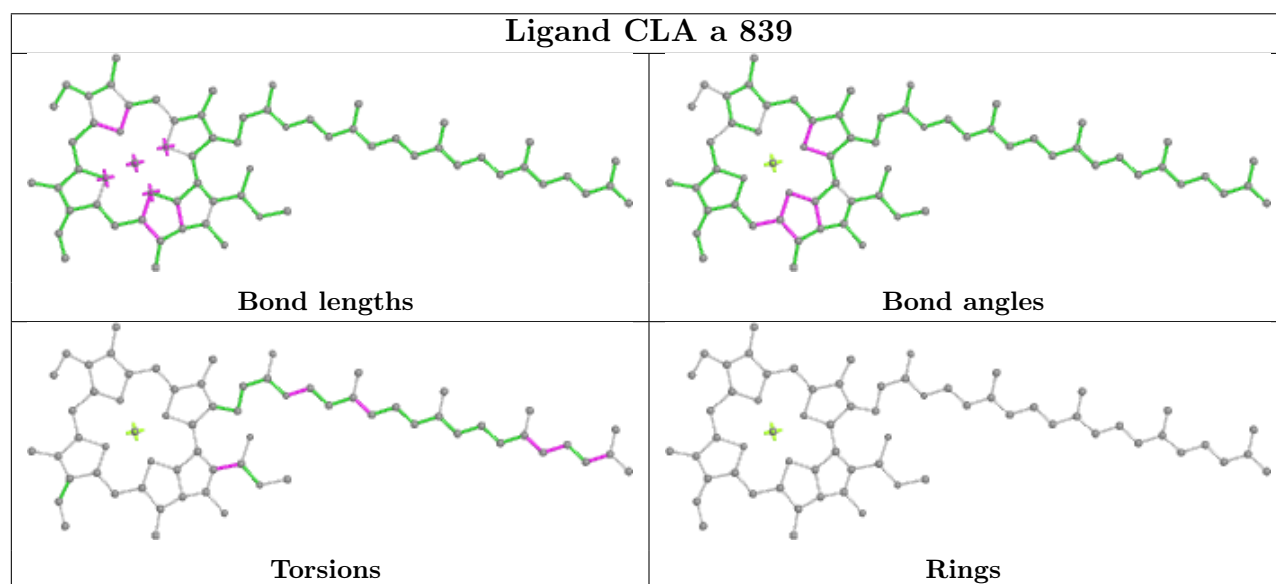
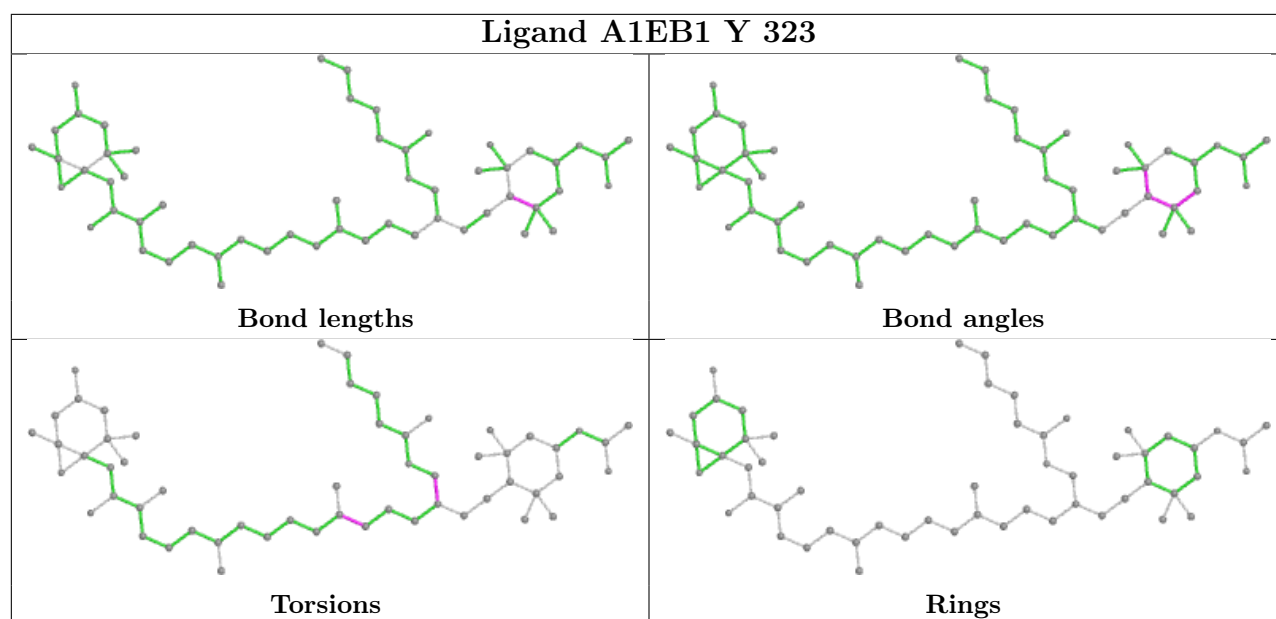
Bond angles

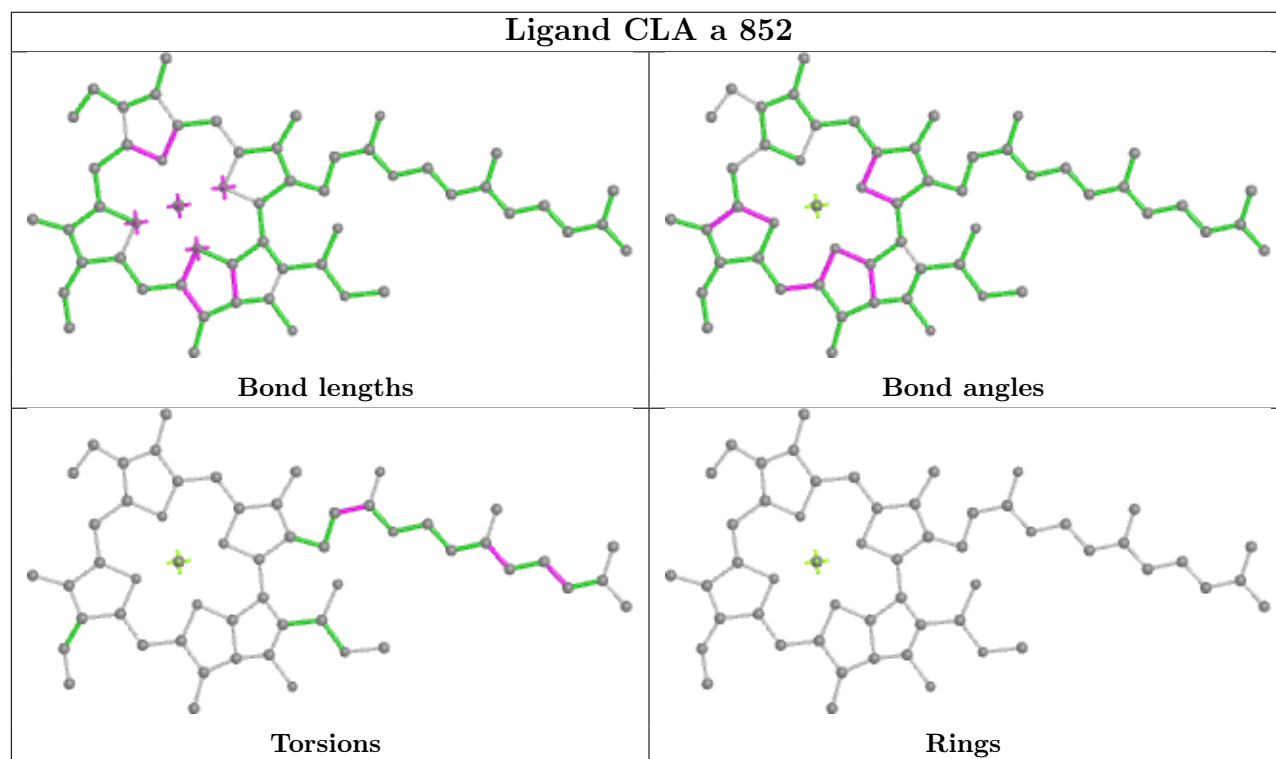
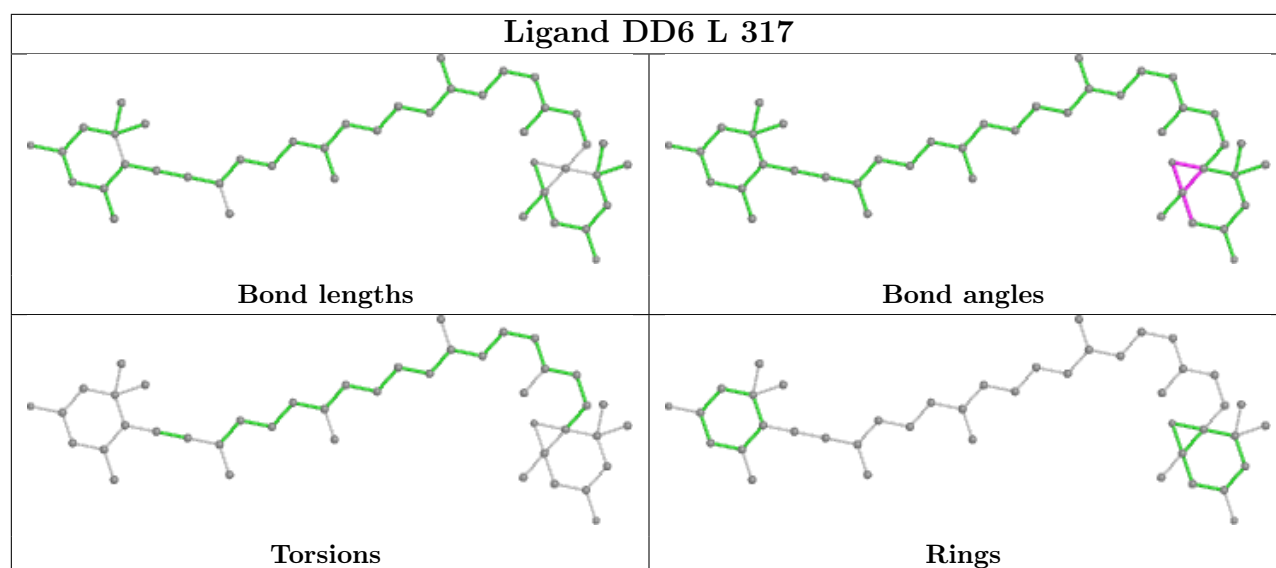


Torsions

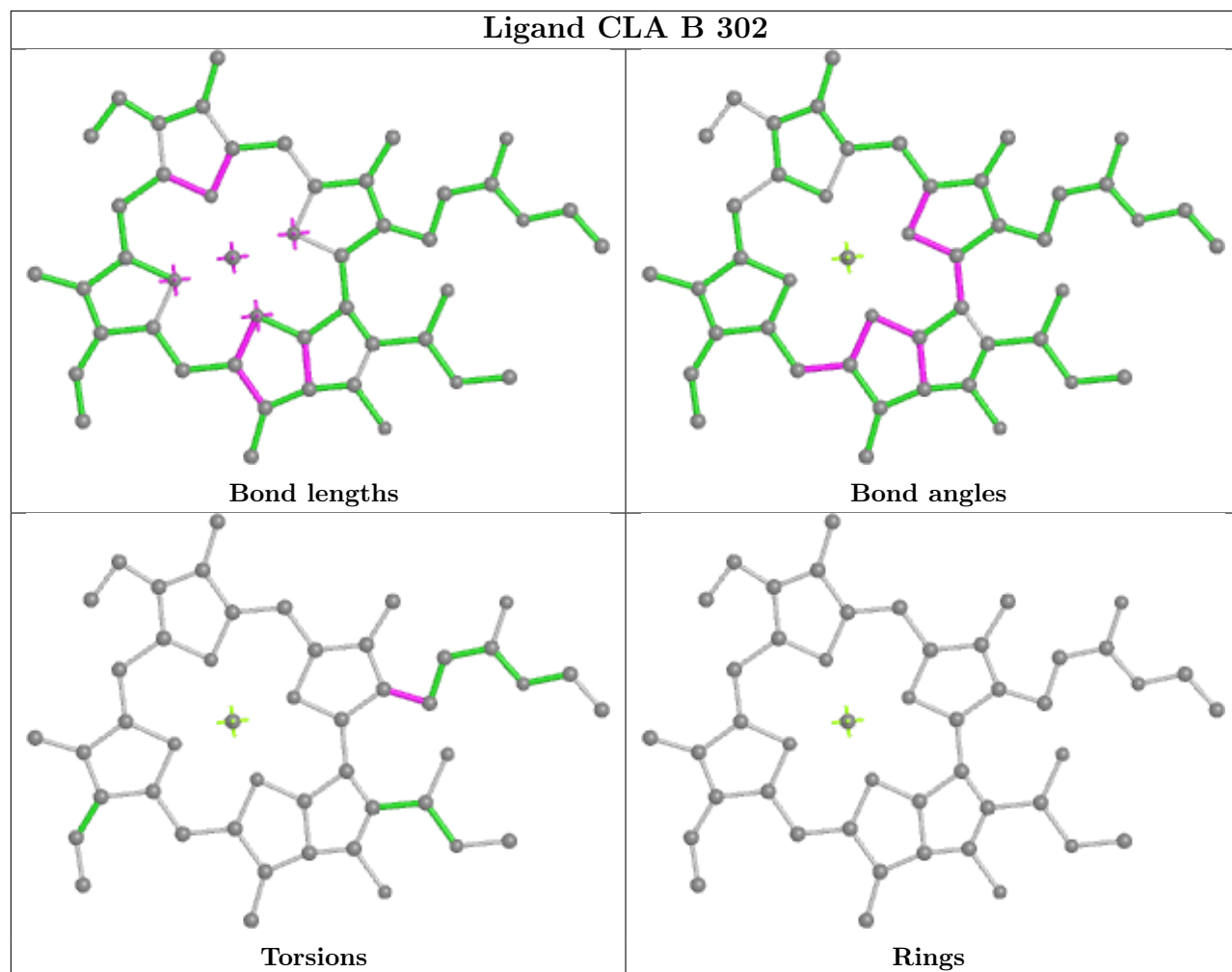


Rings

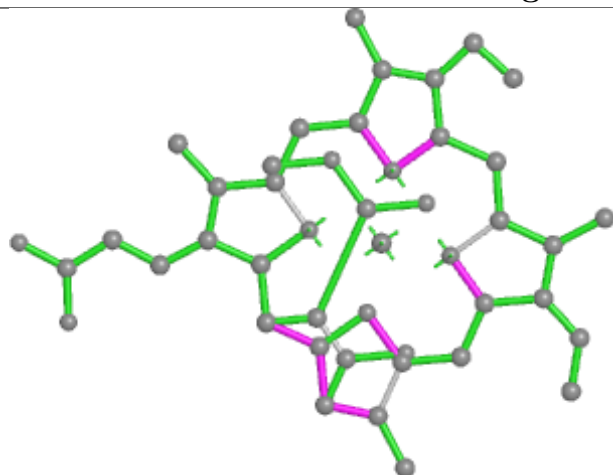




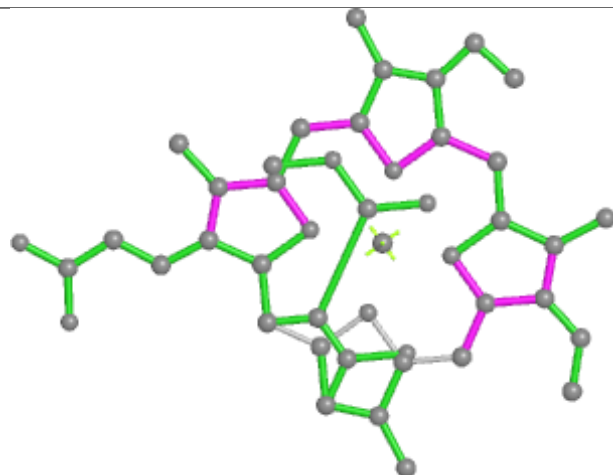
Ligand CLA B 302



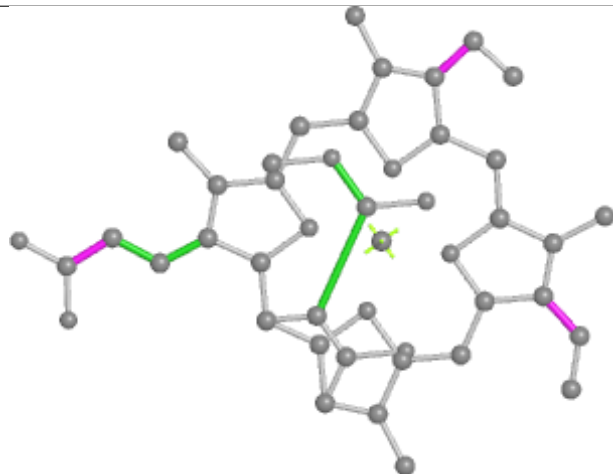
Ligand KC2 t 308



Bond lengths



Bond angles

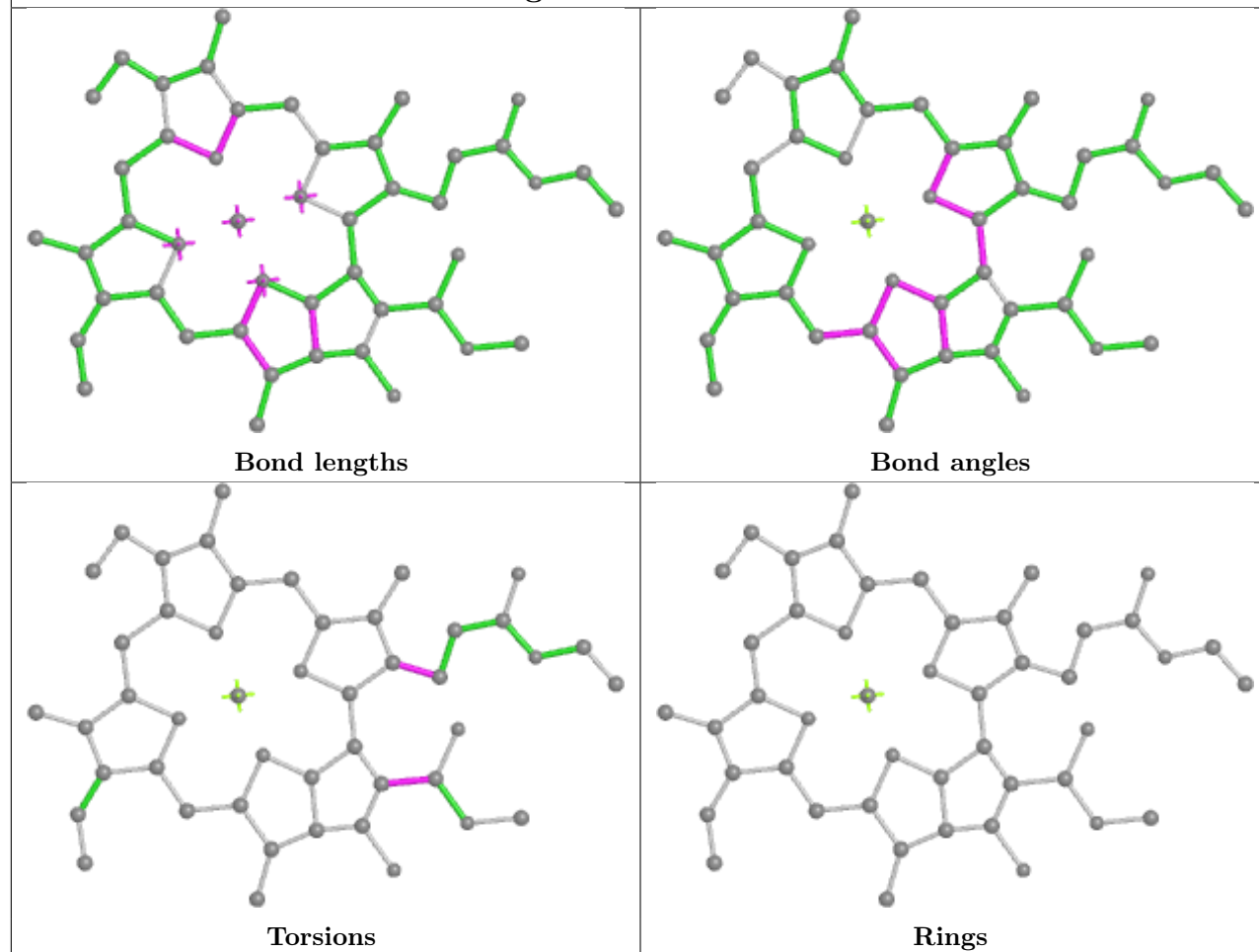


Torsions

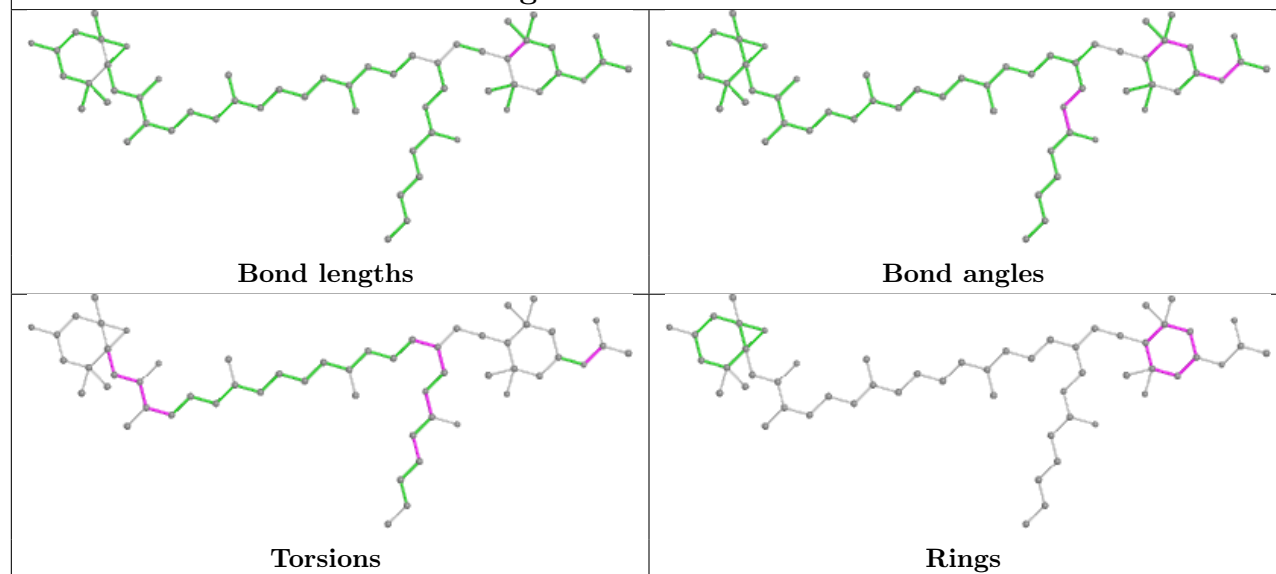


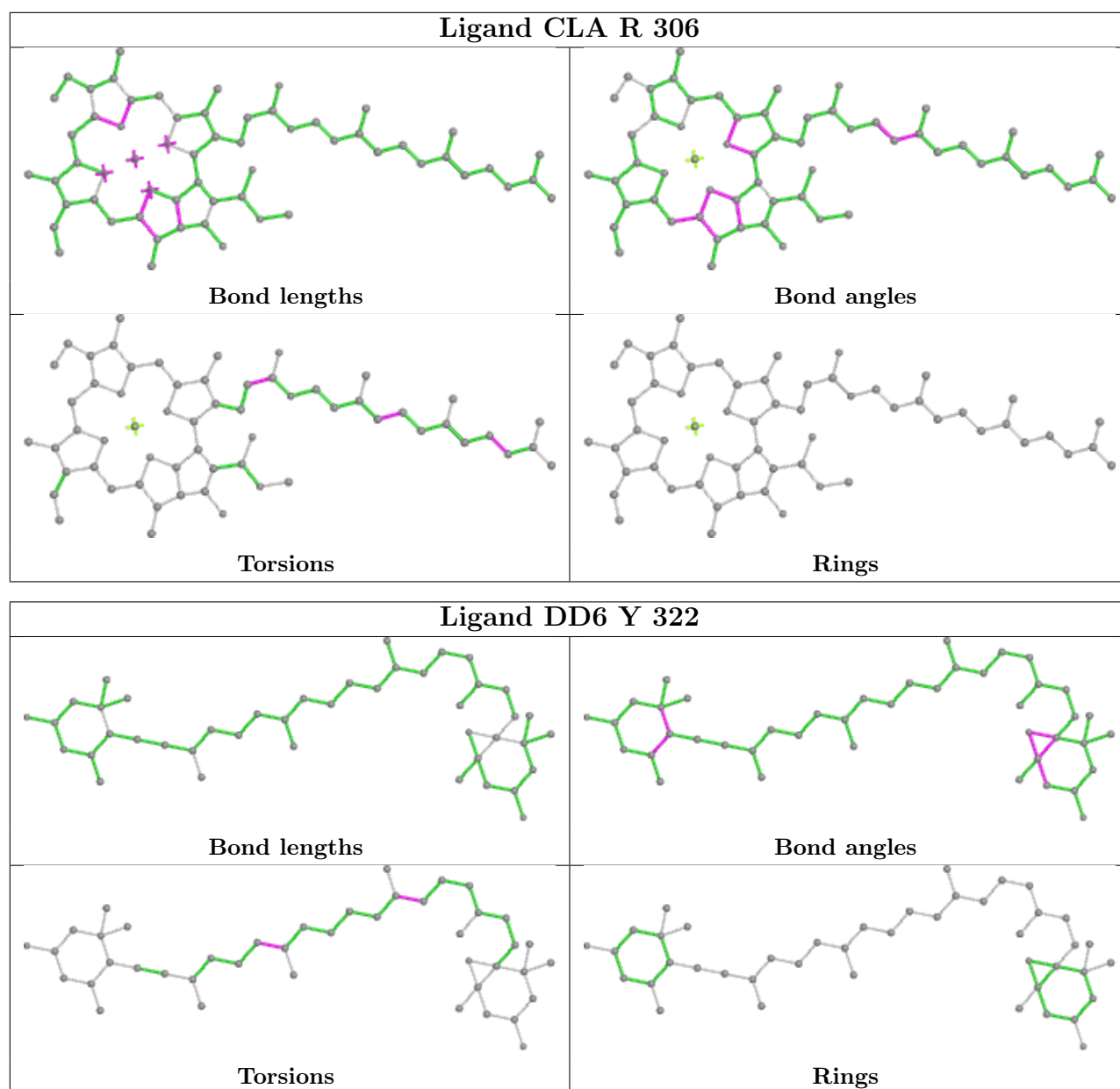
Rings

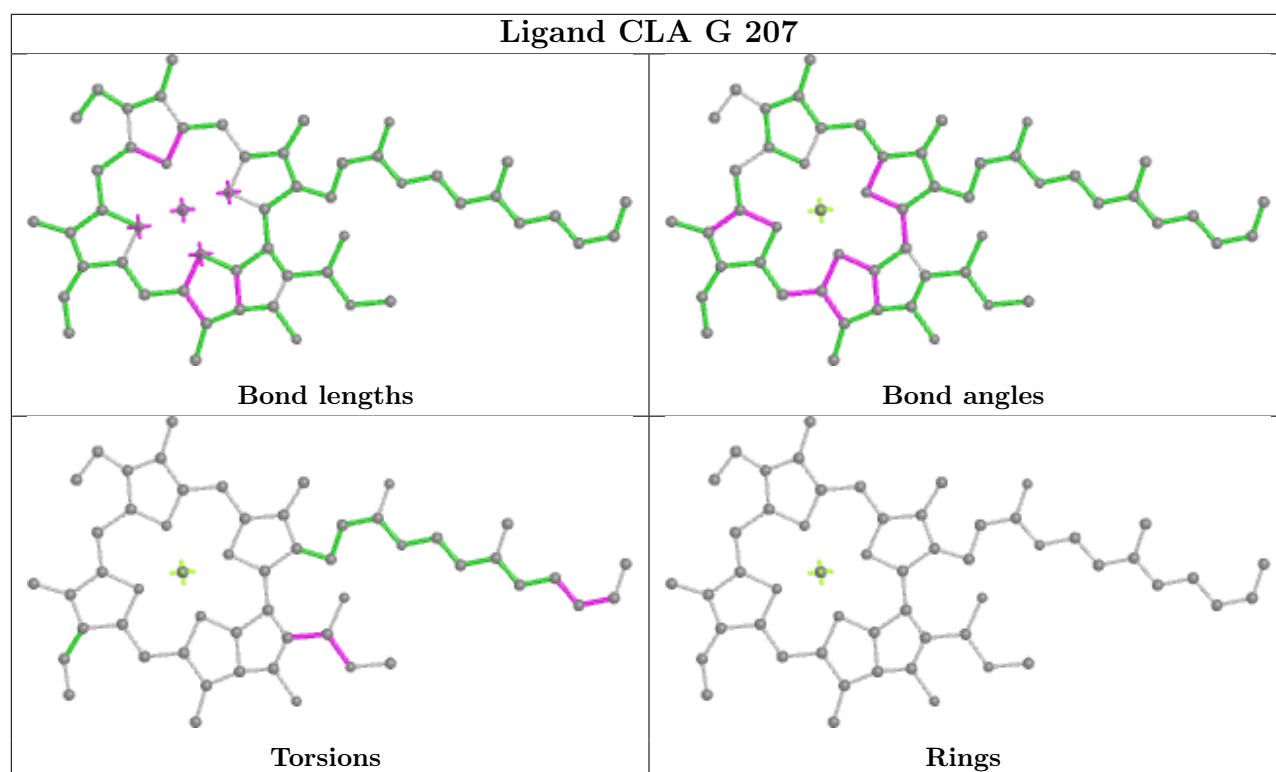
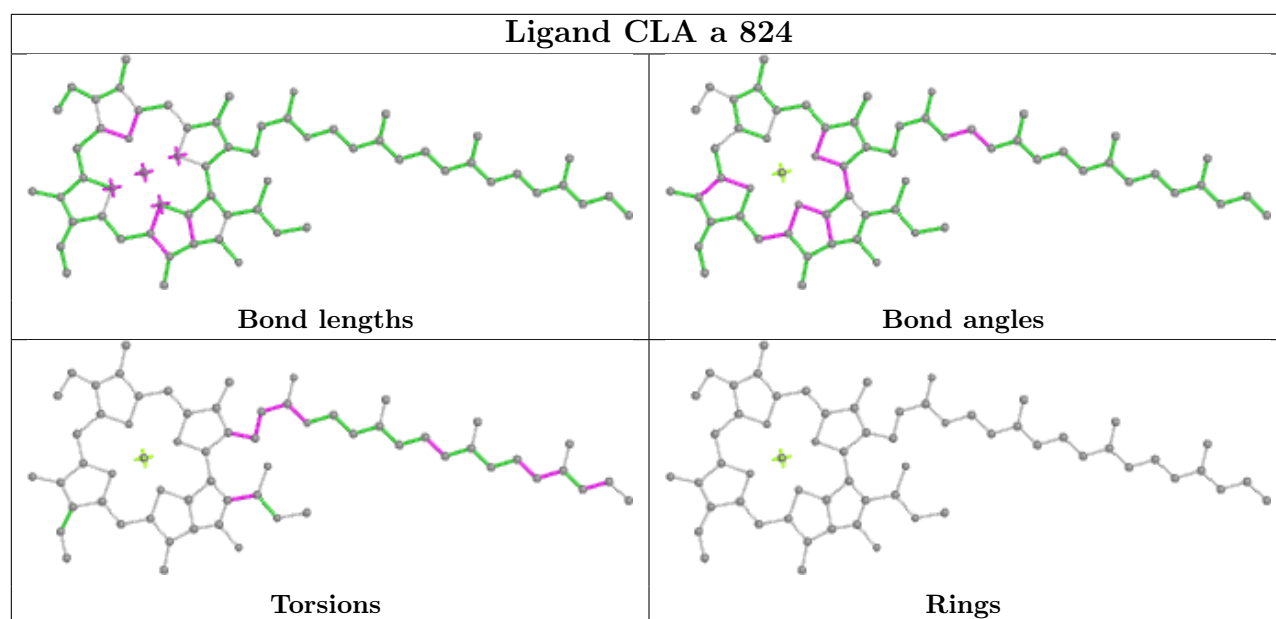
Ligand CLA C 301

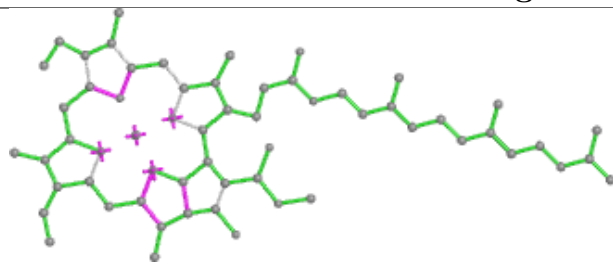


Ligand A1EB1 t 314

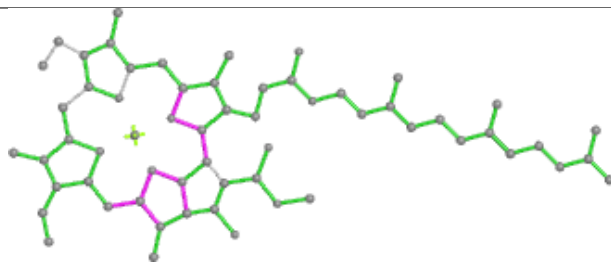




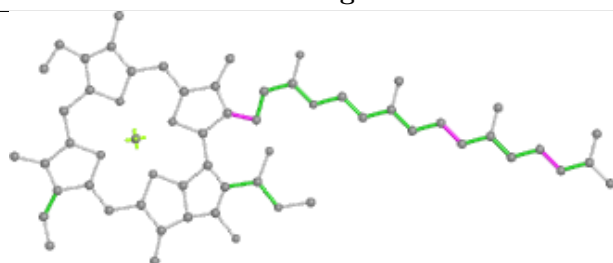


Ligand CLA E 303

Bond lengths



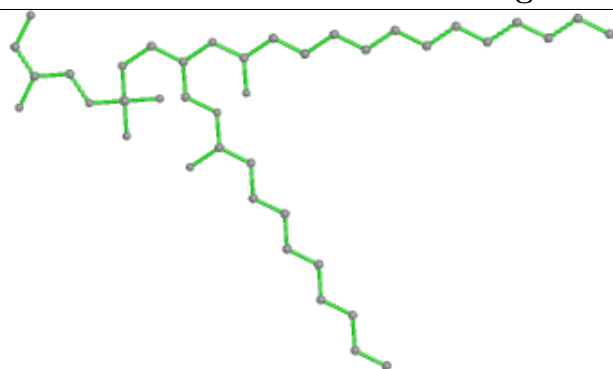
Bond angles



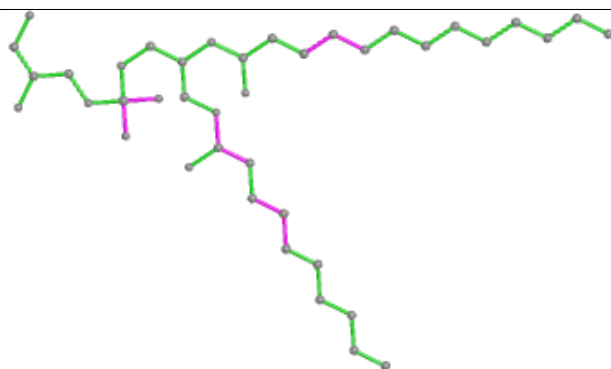
Torsions



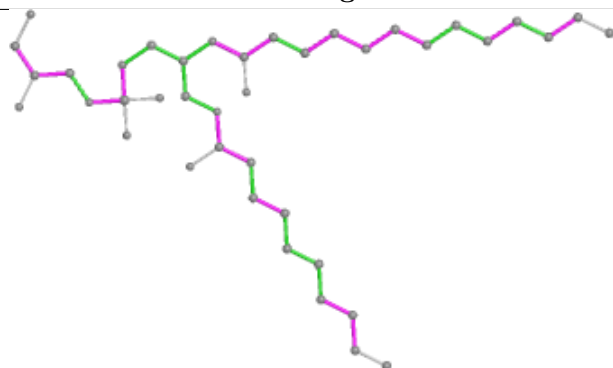
Rings

Ligand LHG S 323

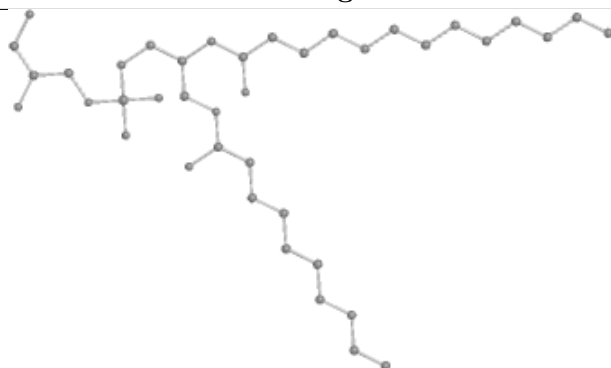
Bond lengths



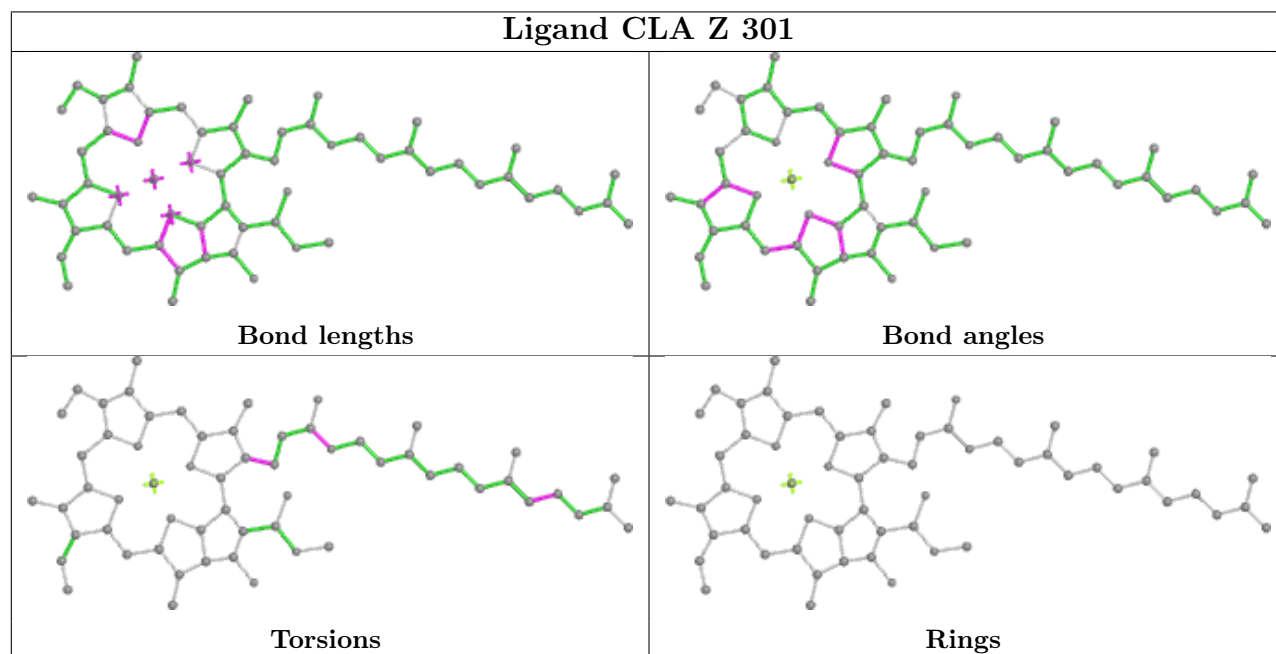
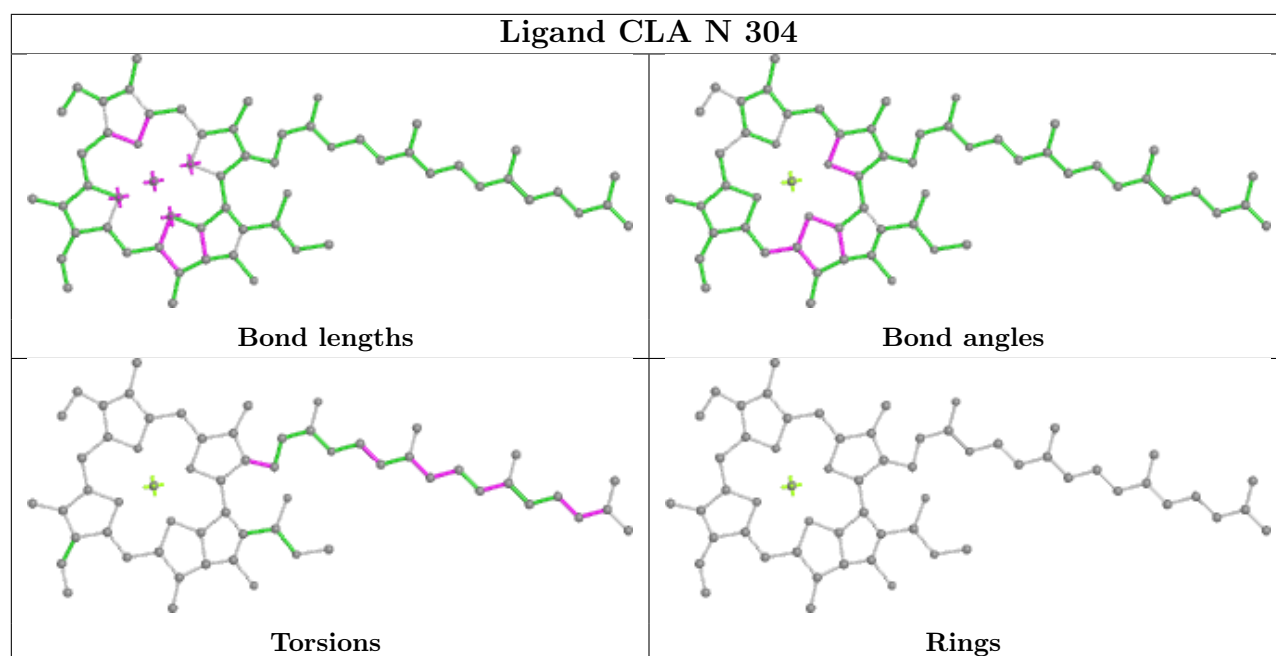
Bond angles

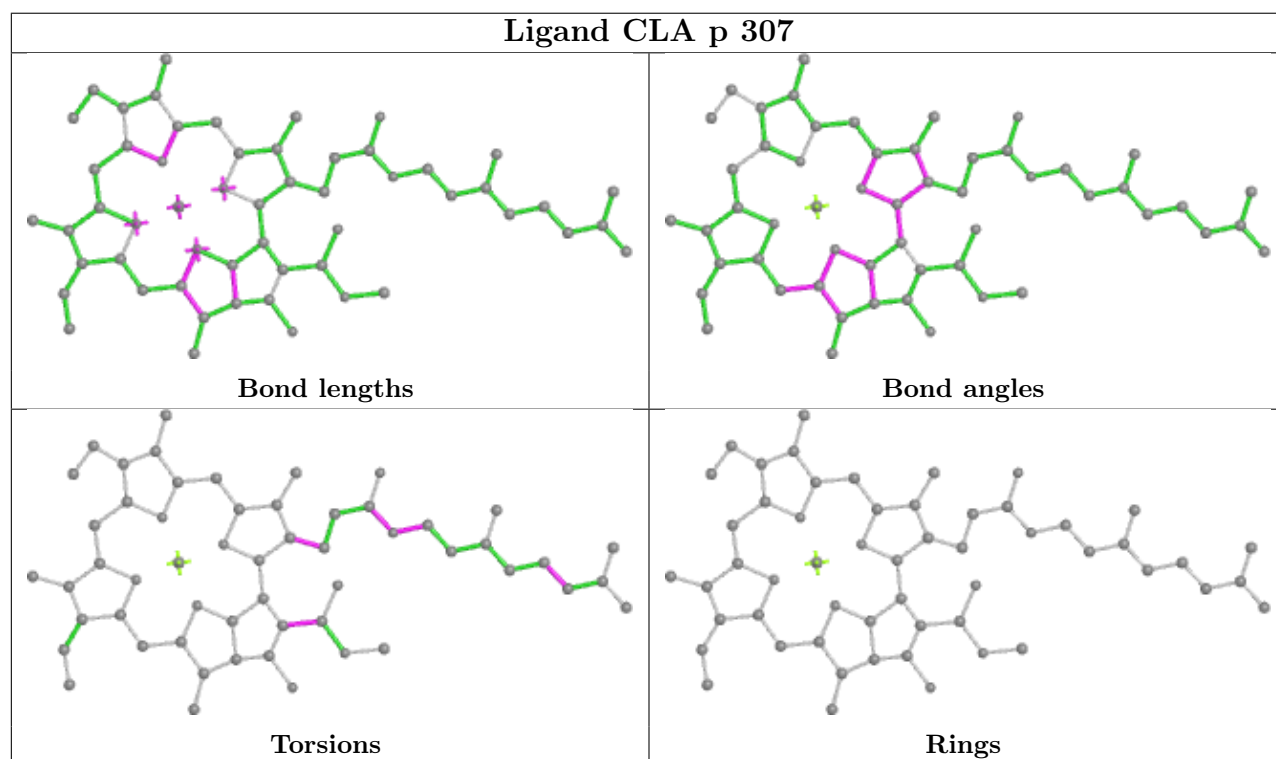
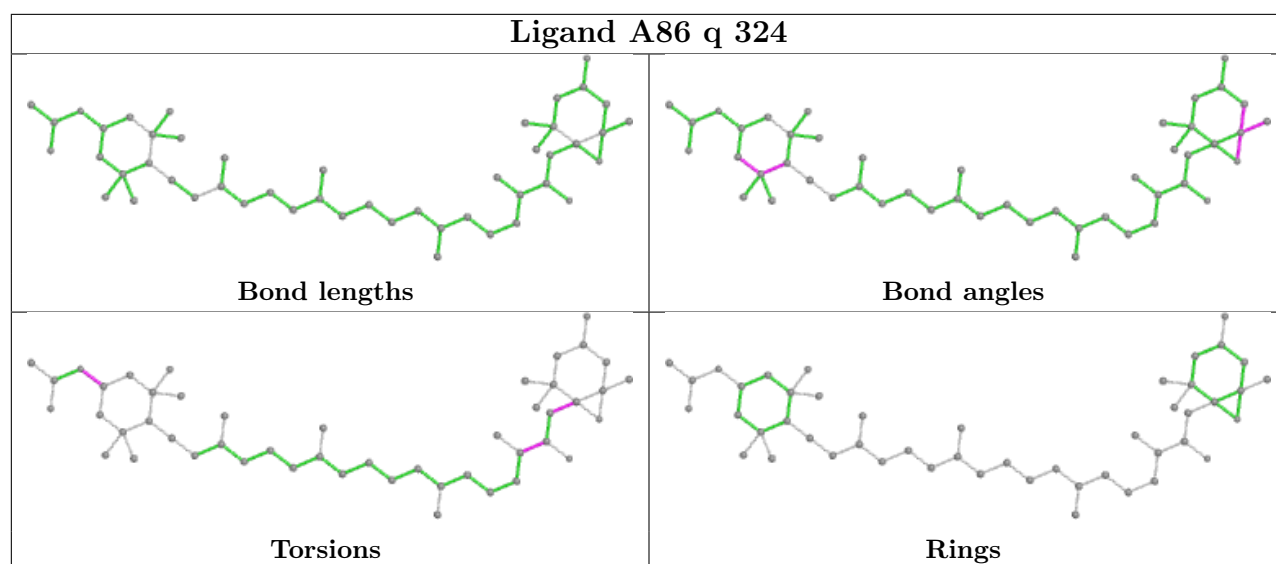


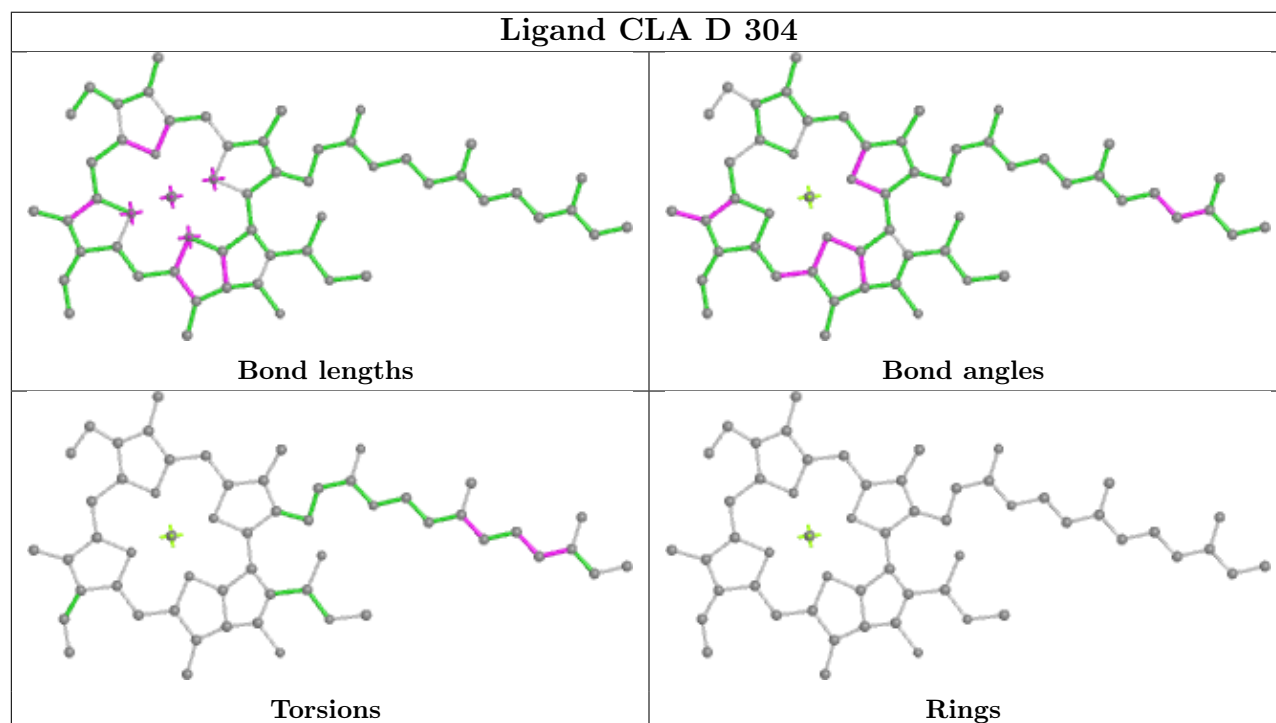
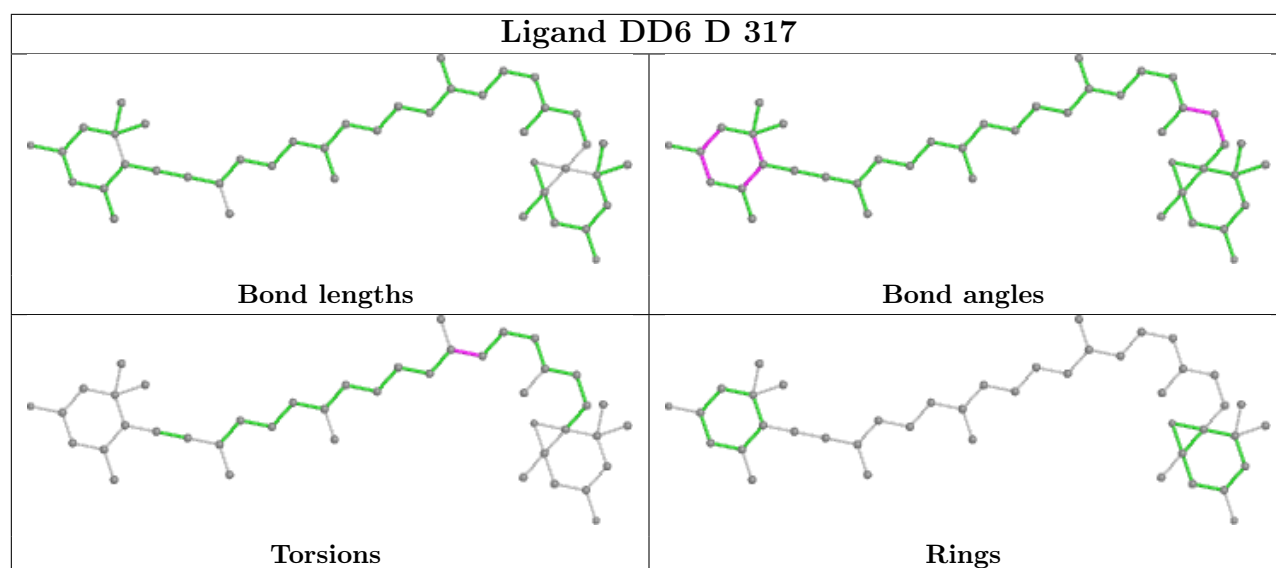
Torsions

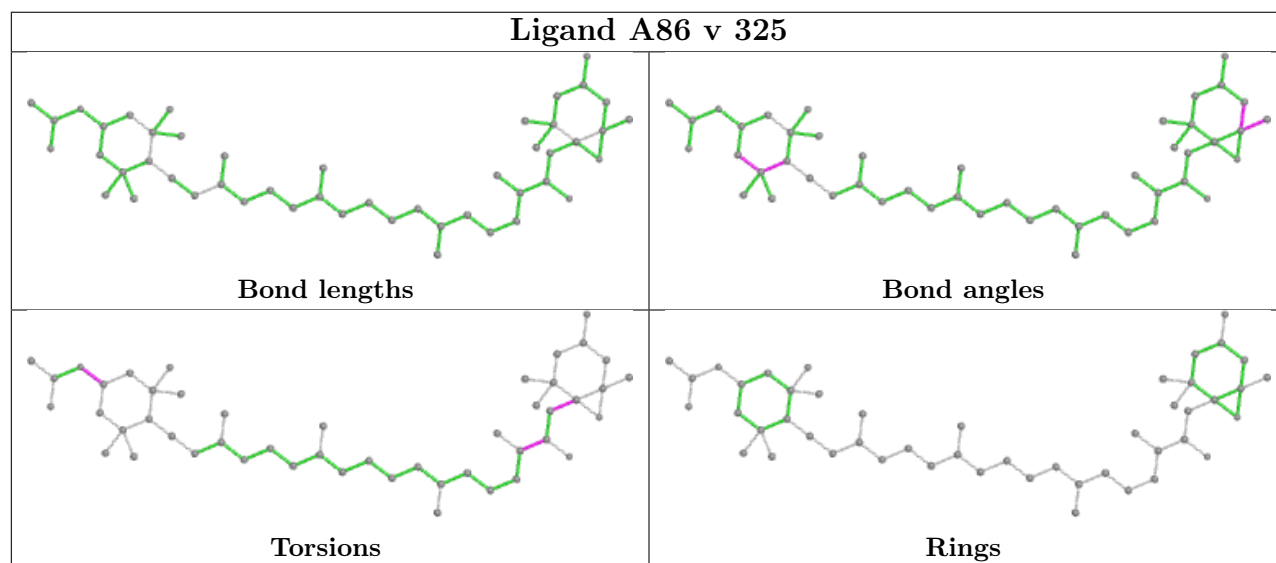
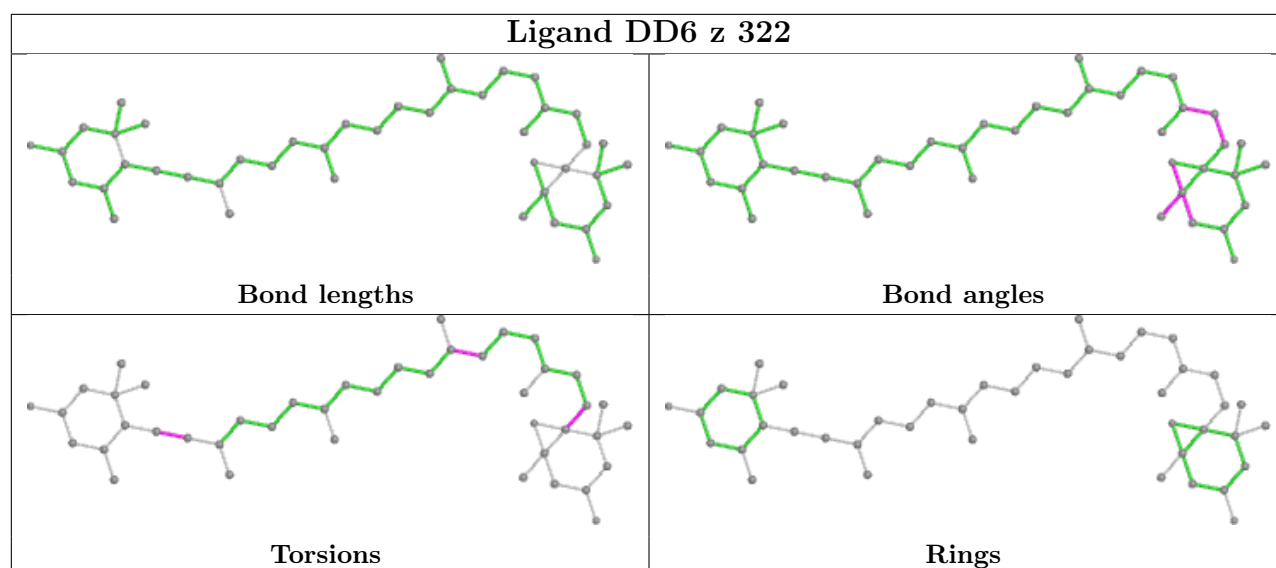


Rings

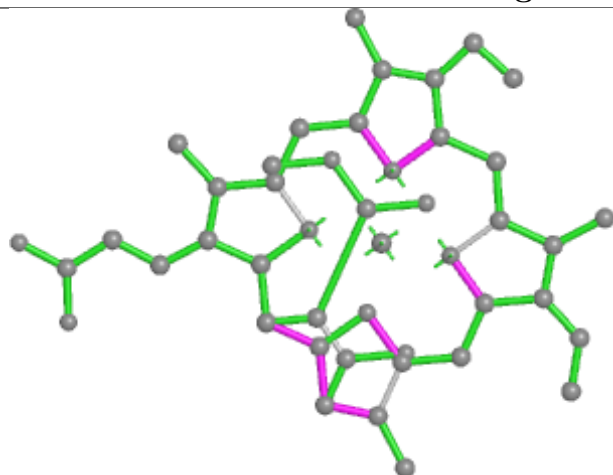




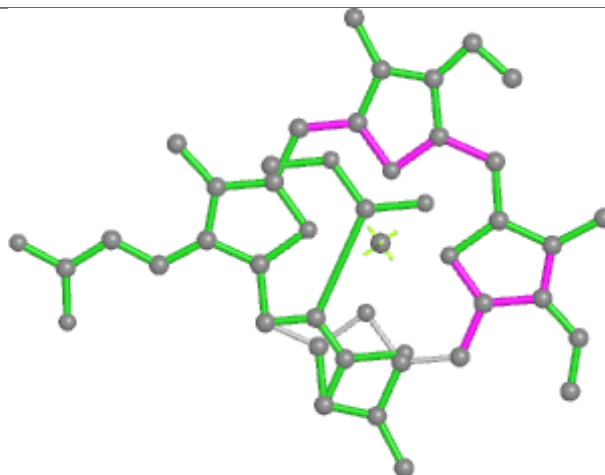




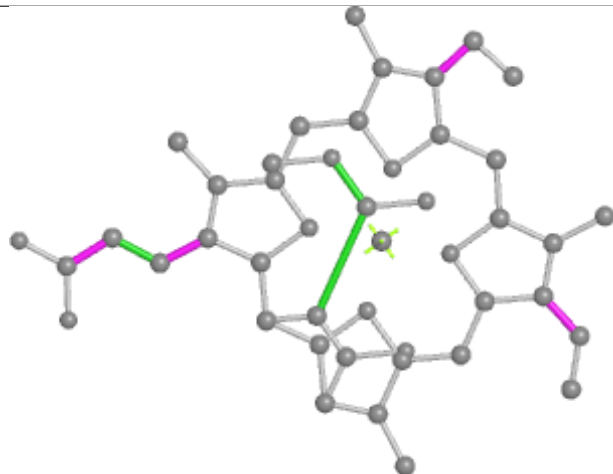
Ligand KC2 N 308



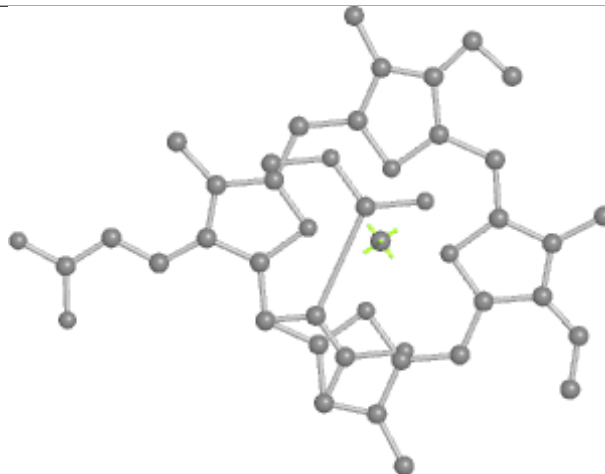
Bond lengths



Bond angles

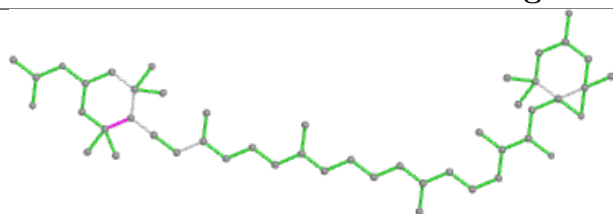


Torsions

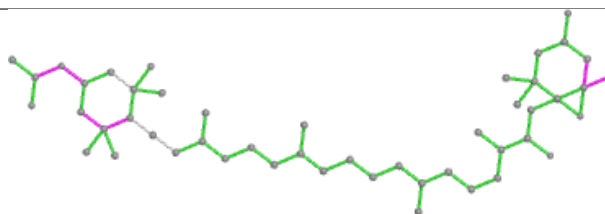


Rings

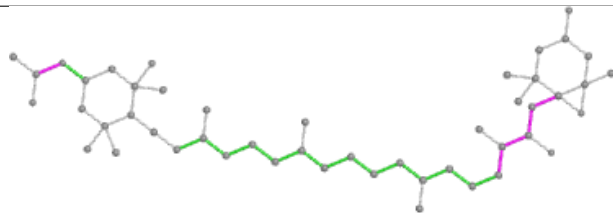
Ligand A86 o 316



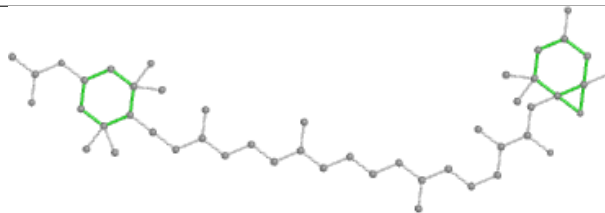
Bond lengths



Bond angles

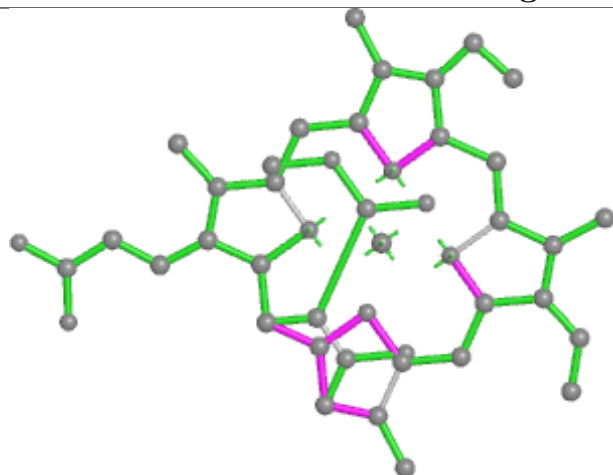


Torsions

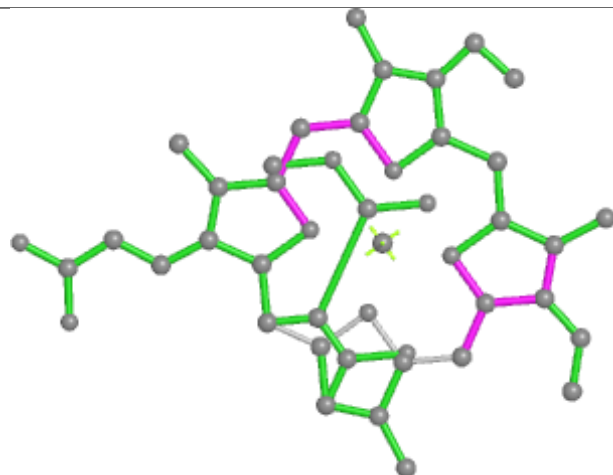


Rings

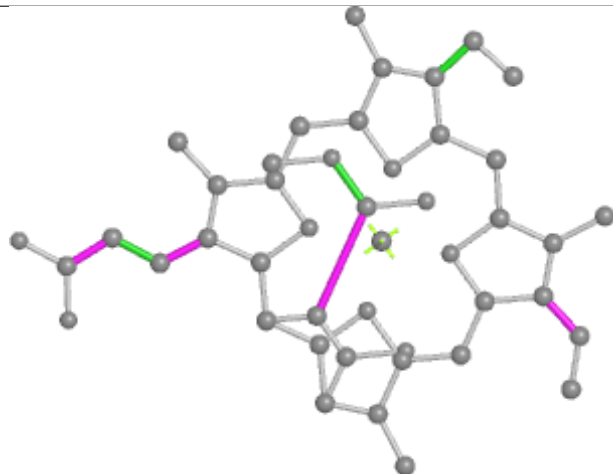
Ligand KC2 v 302



Bond lengths



Bond angles

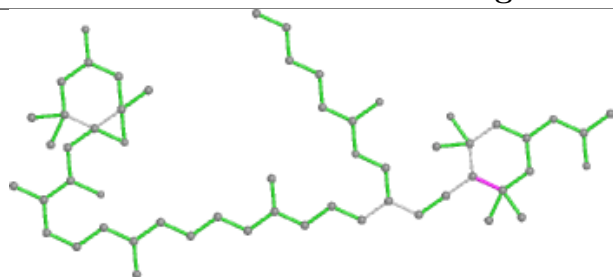


Torsions

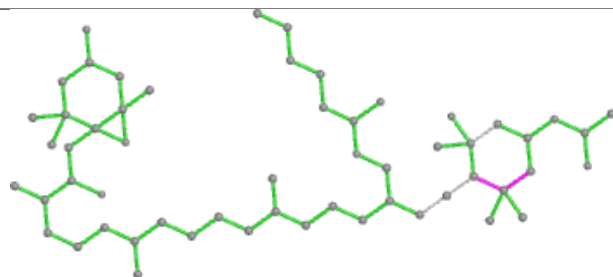


Rings

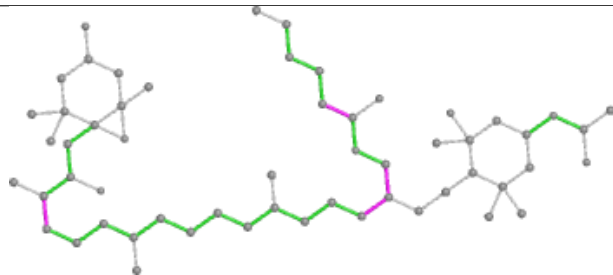
Ligand A1EB1 O 317



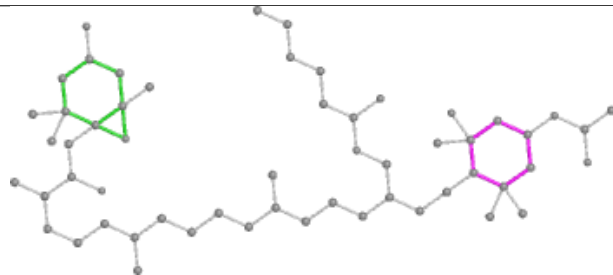
Bond lengths



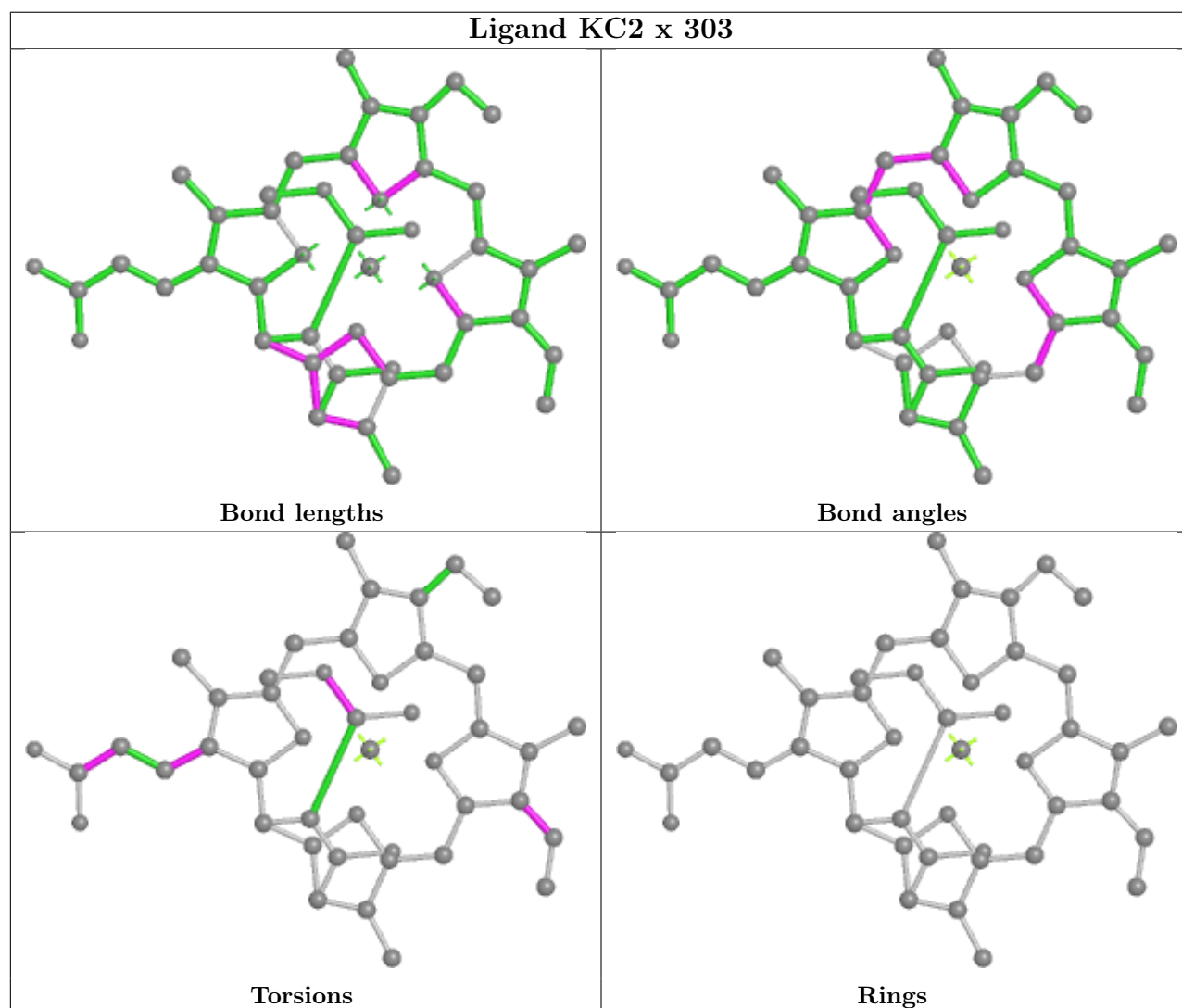
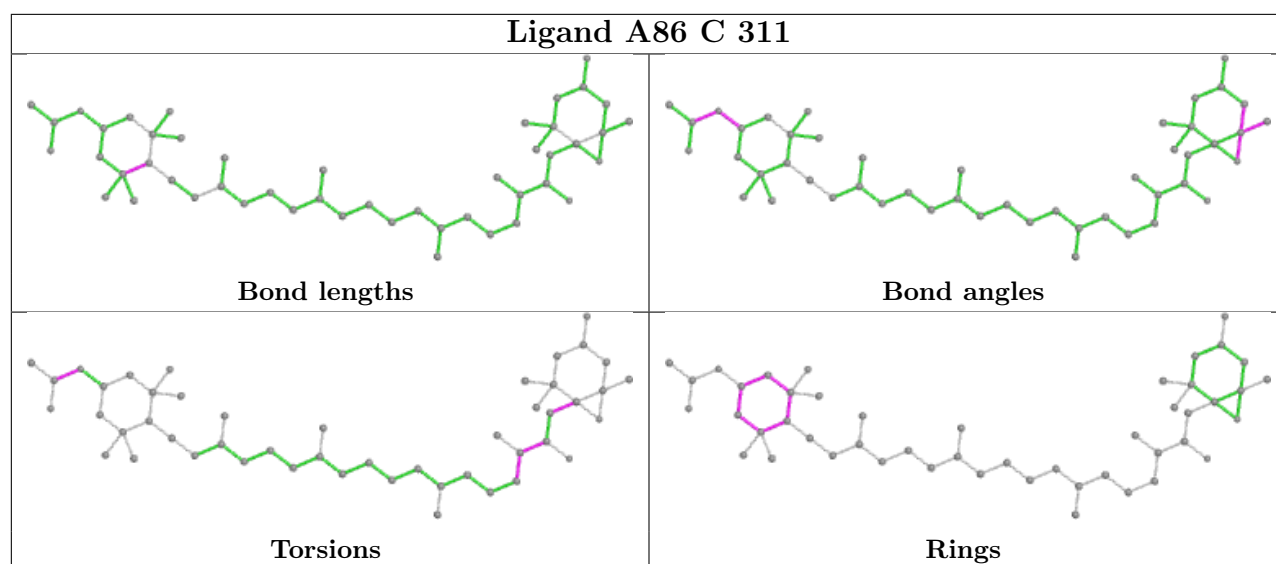
Bond angles

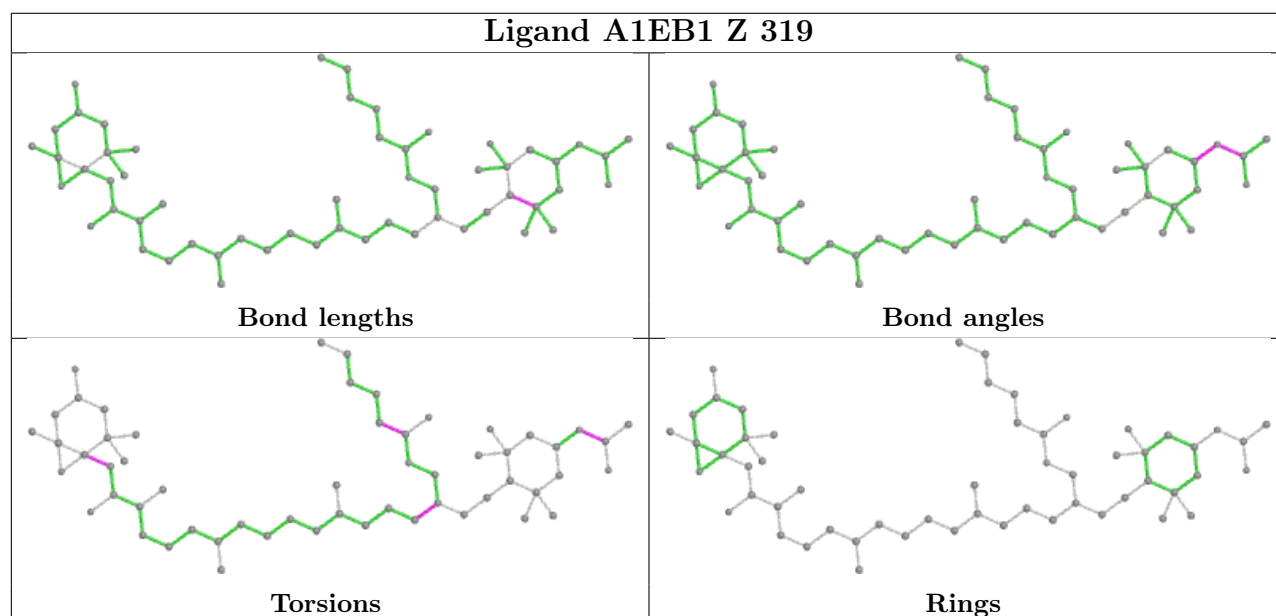
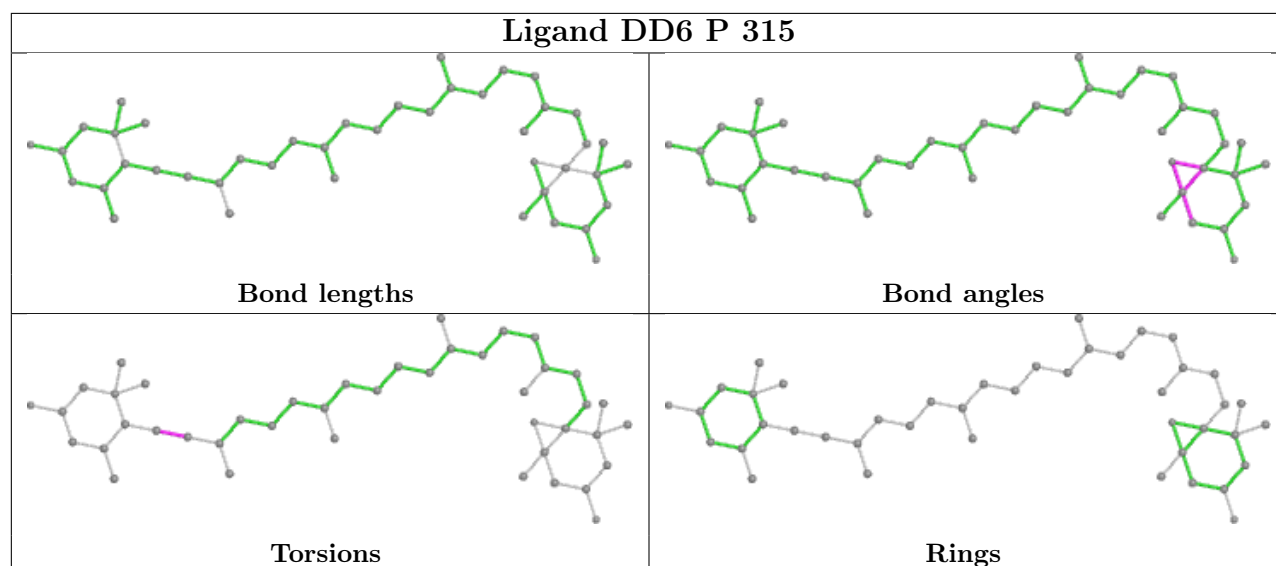
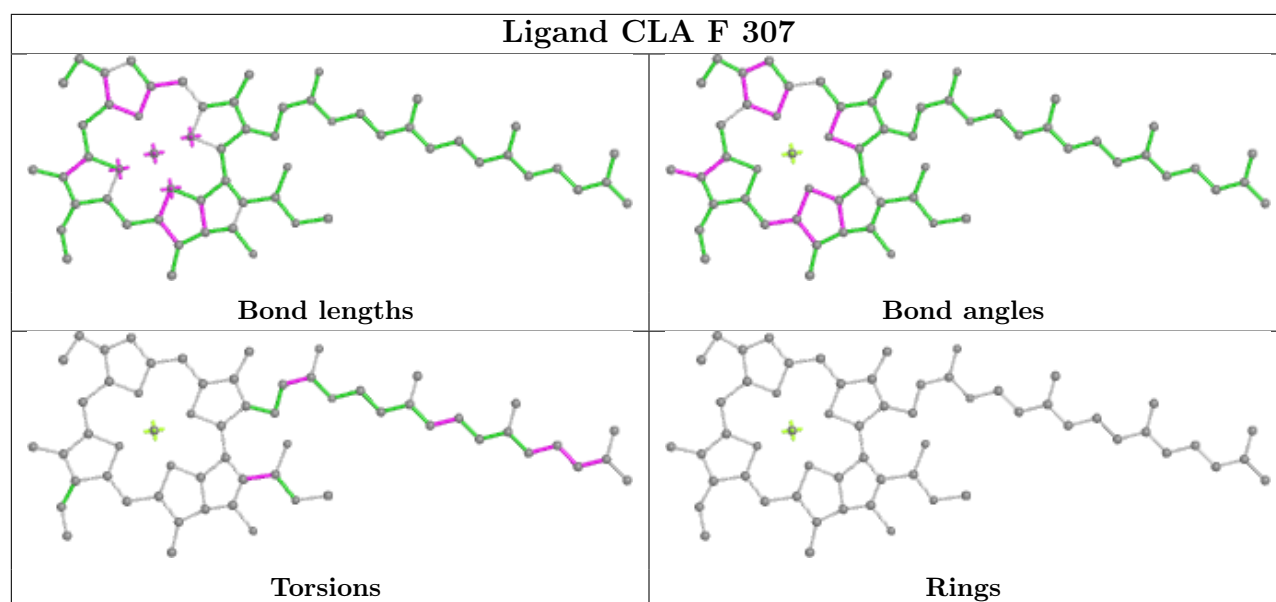


Torsions

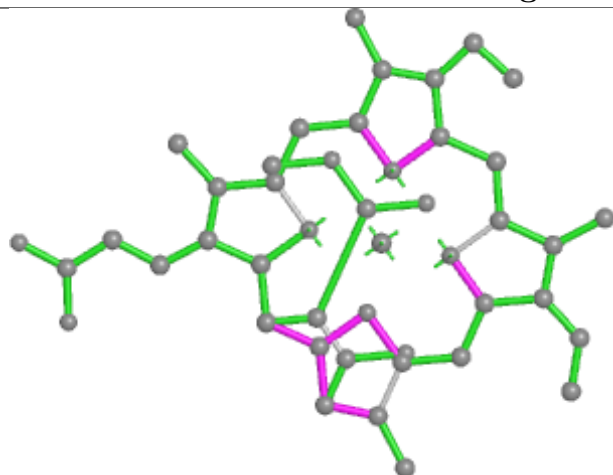


Rings

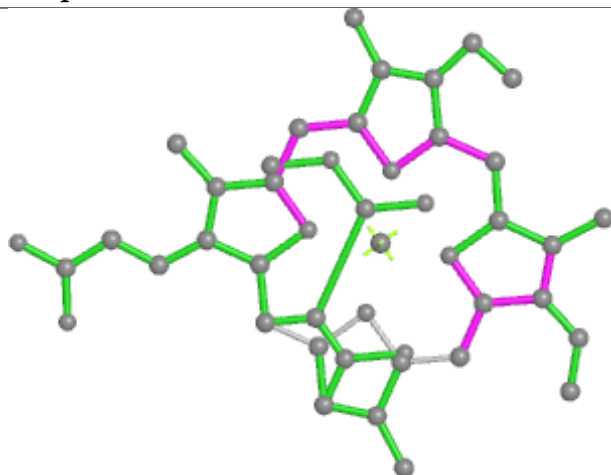




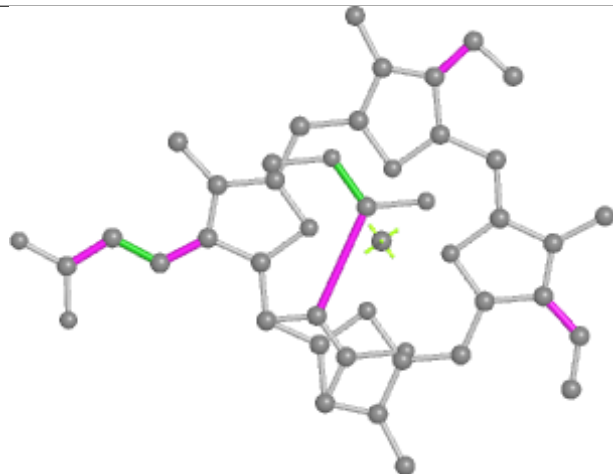
Ligand KC2 q 308



Bond lengths



Bond angles

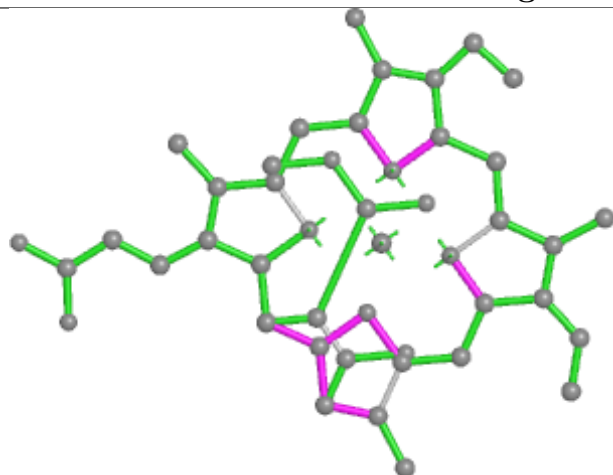


Torsions

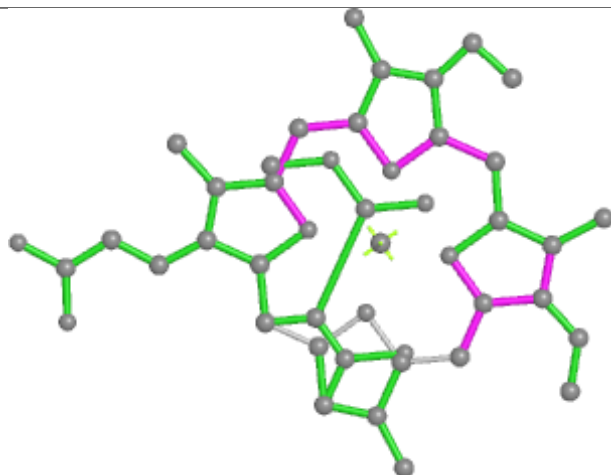


Rings

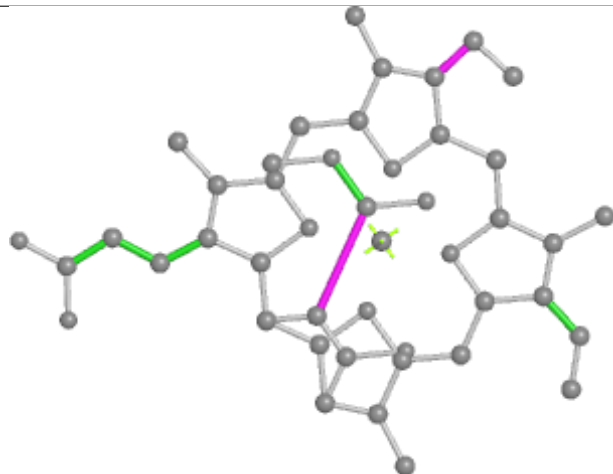
Ligand KC2 Z 303



Bond lengths



Bond angles

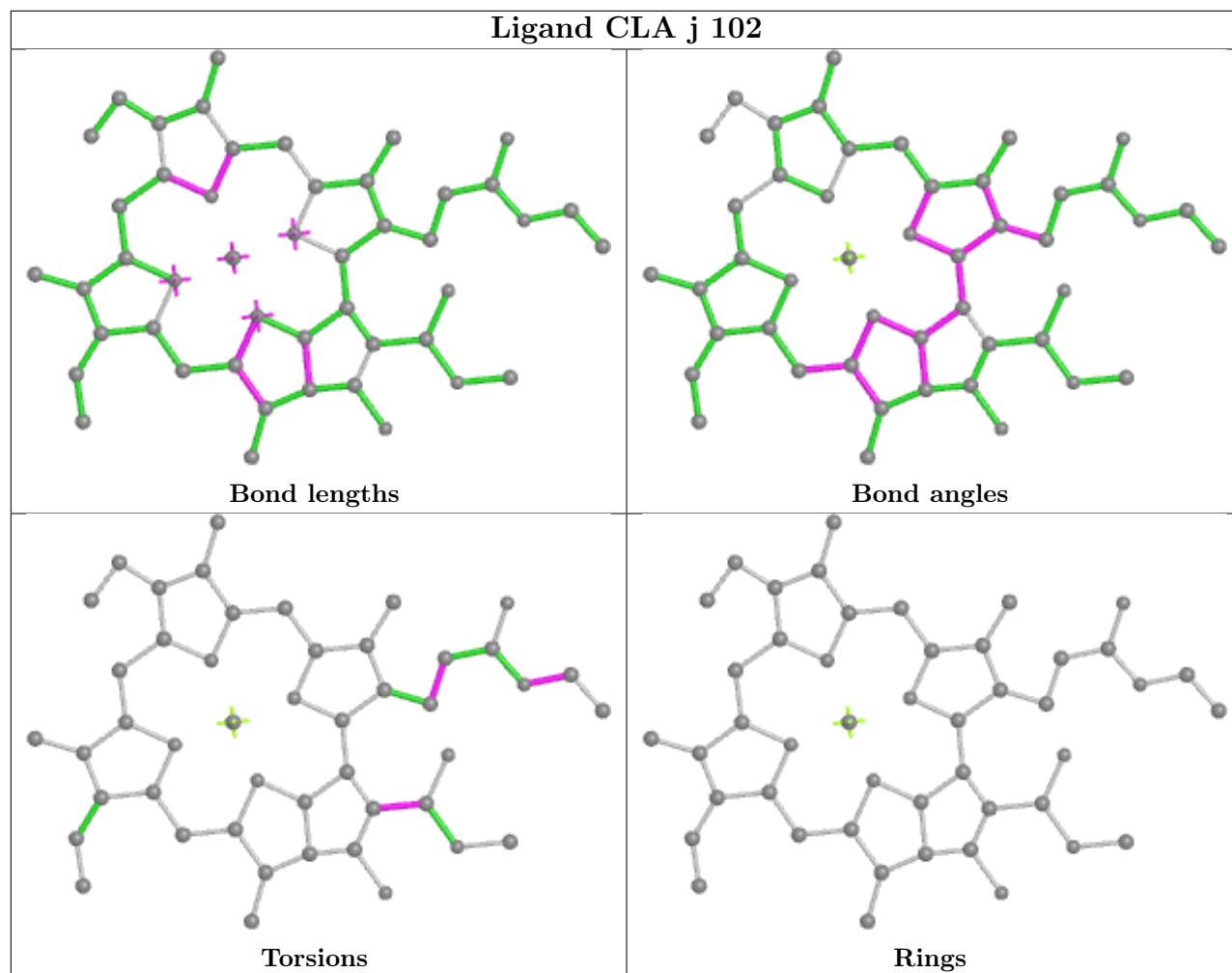


Torsions

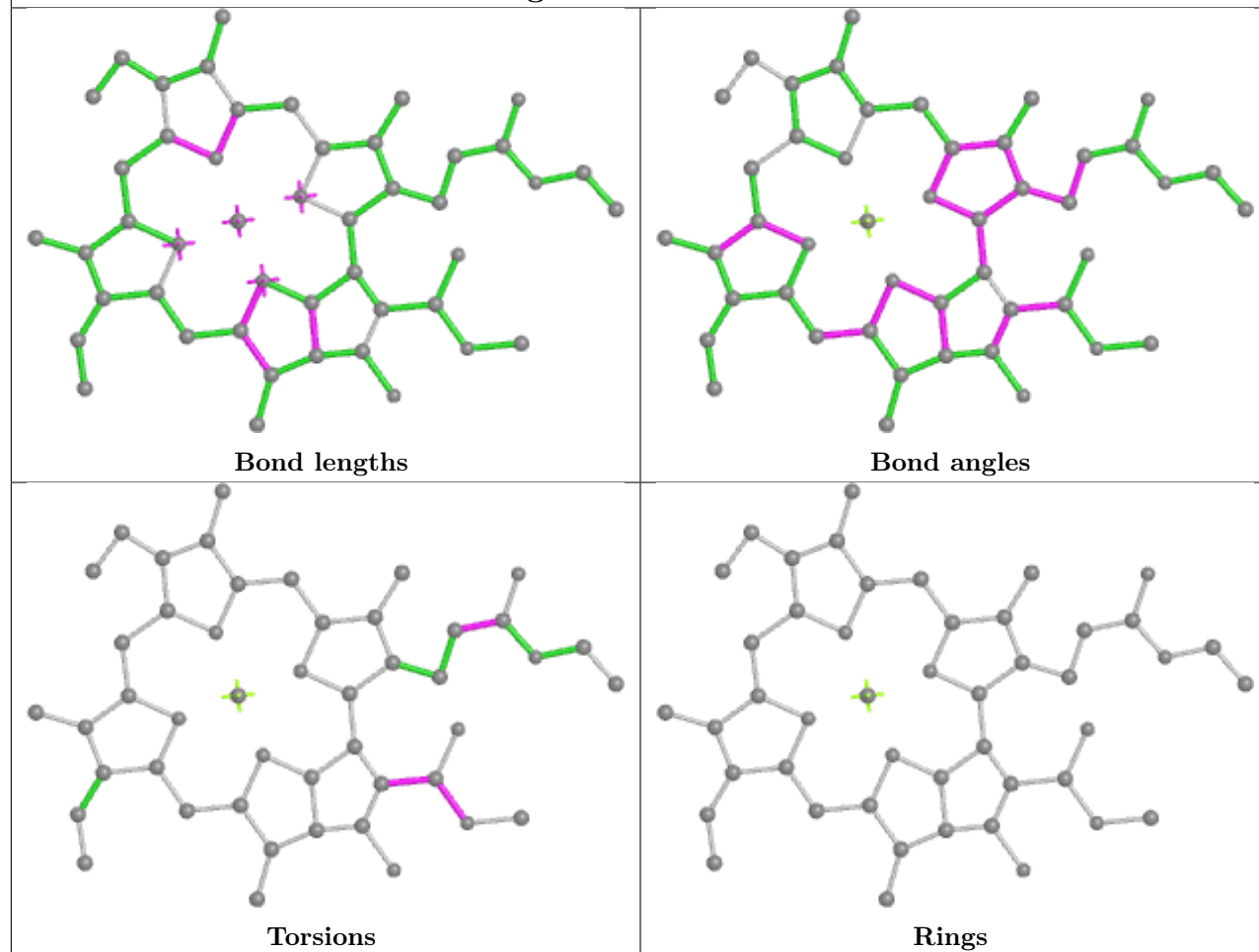


Rings

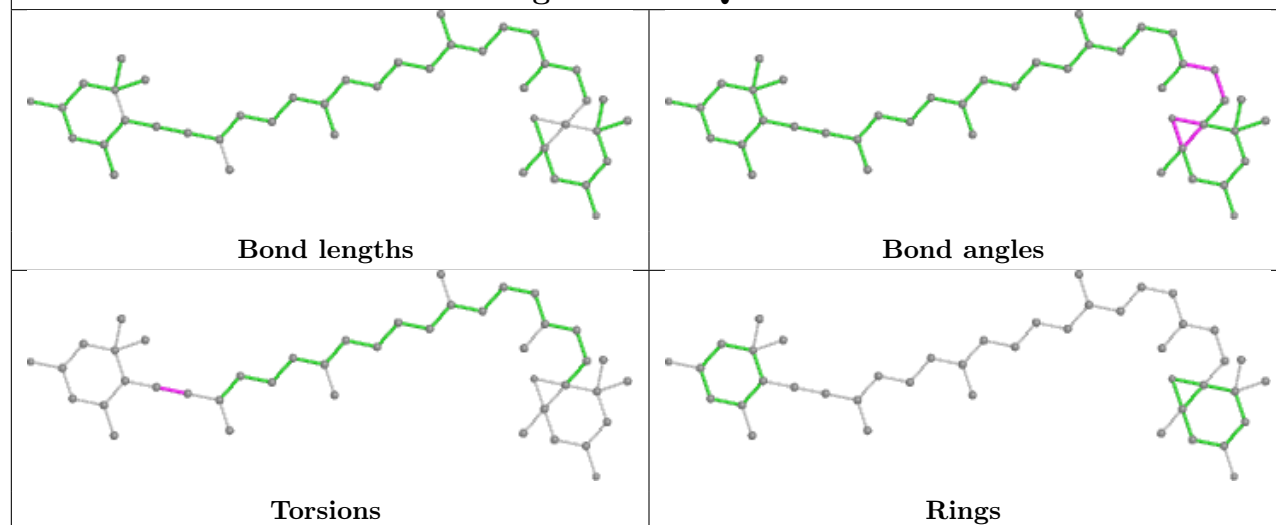
Ligand CLA j 102

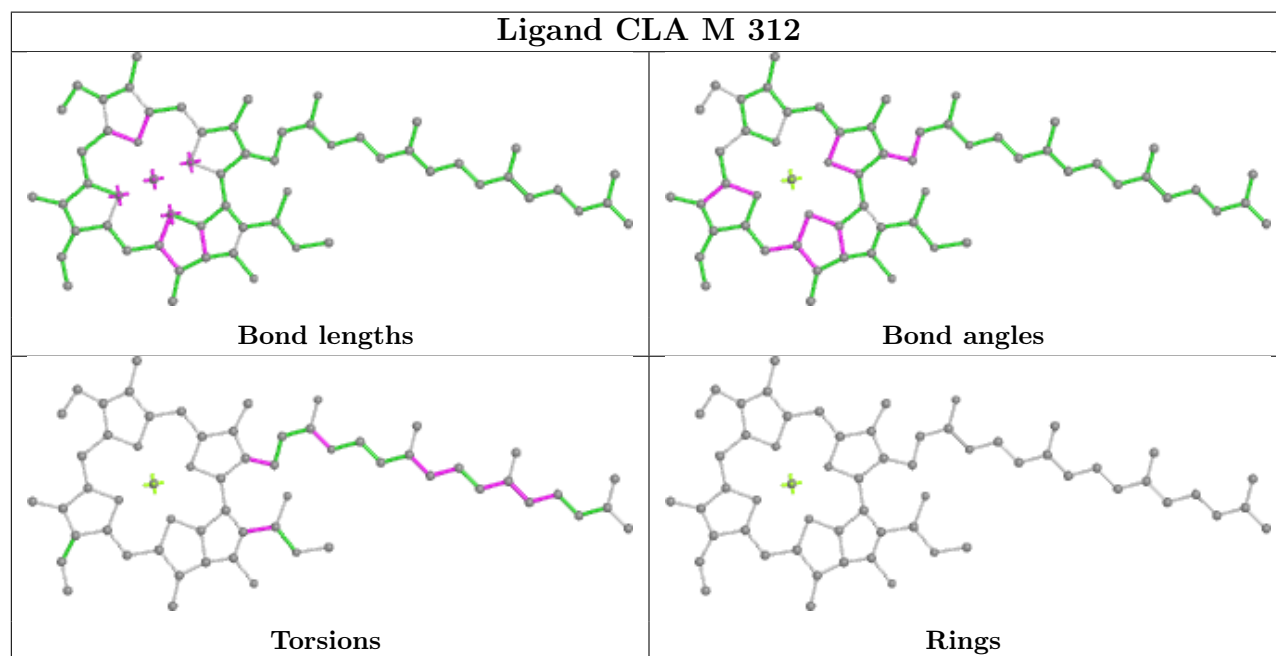
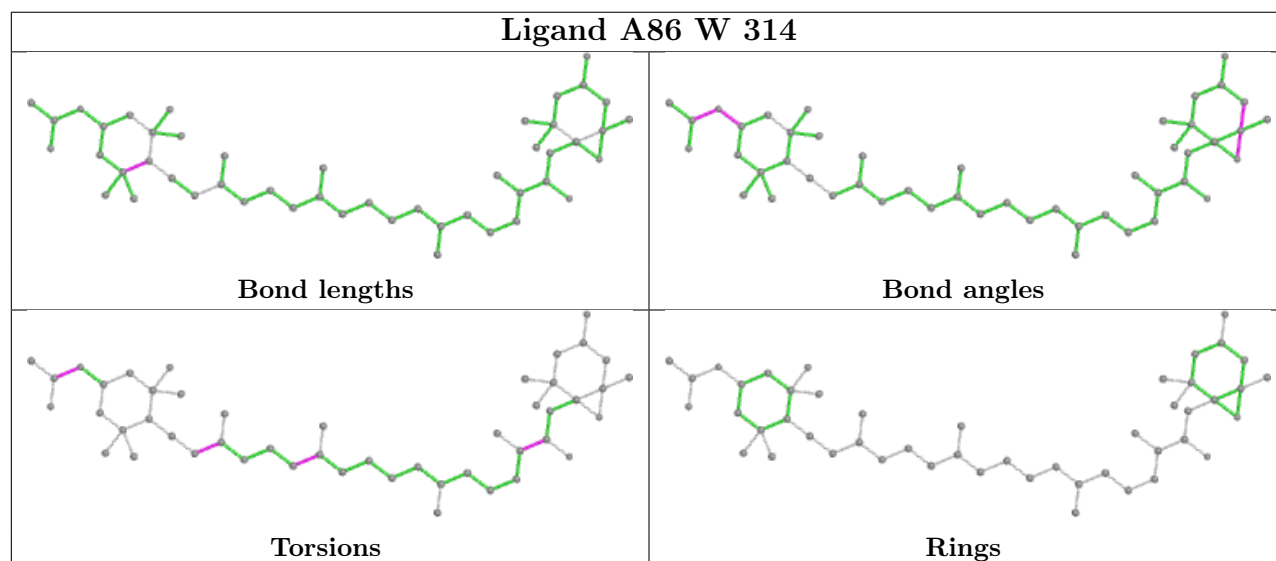
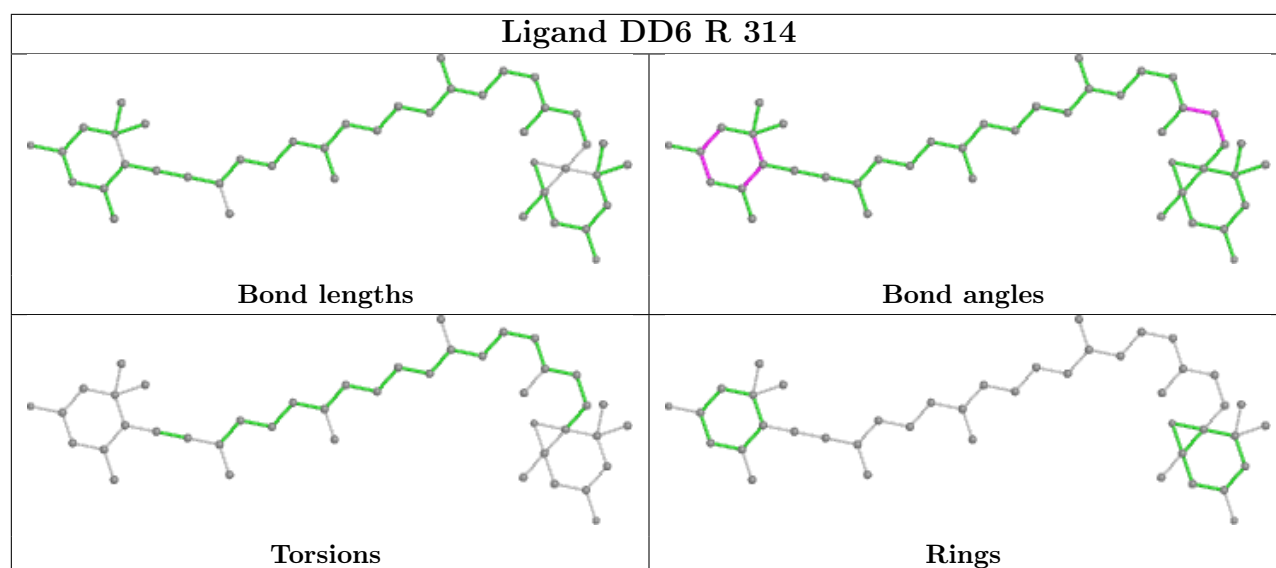


Ligand CLA F 310

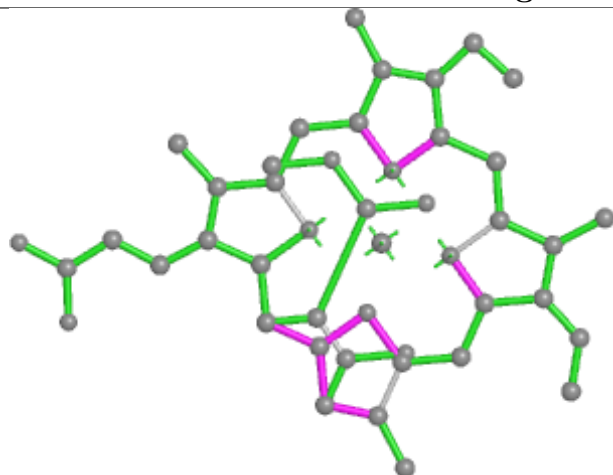


Ligand DD6 Q 212

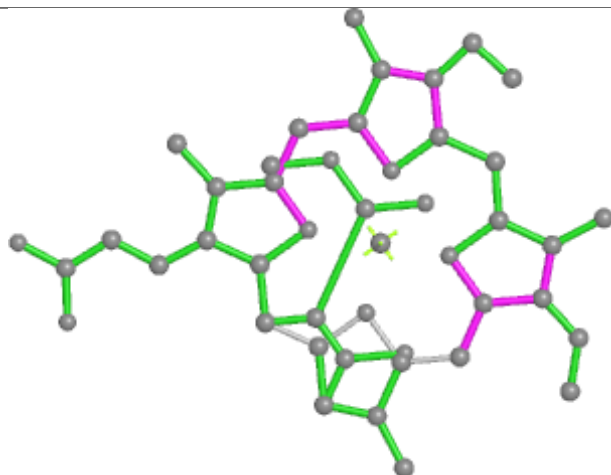




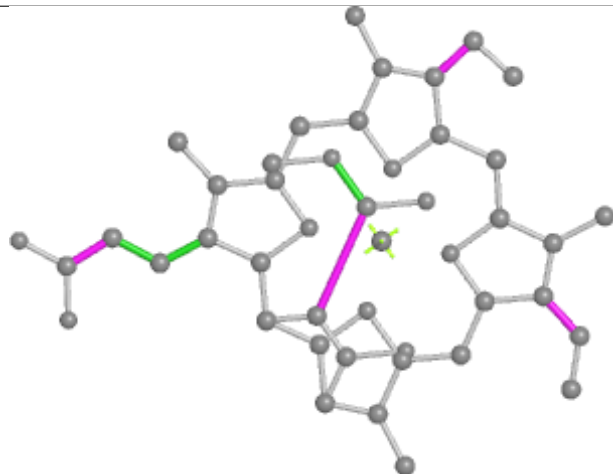
Ligand KC2 O 311



Bond lengths



Bond angles

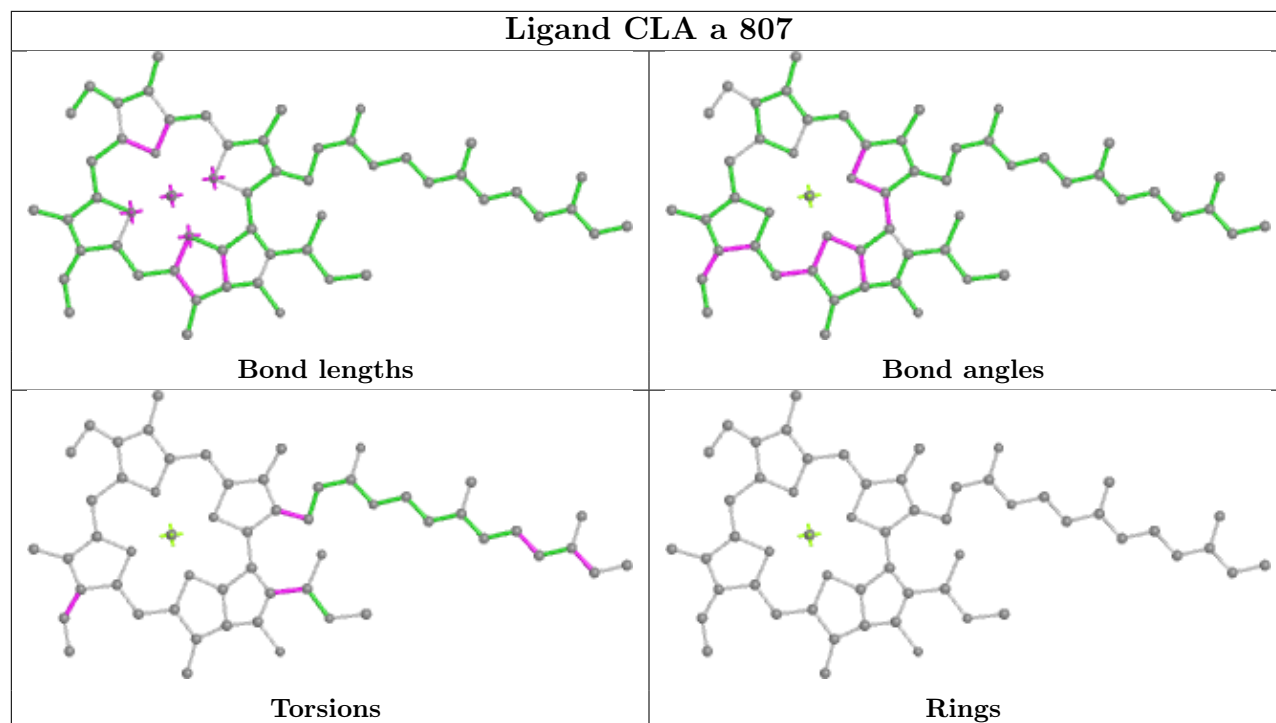


Torsions

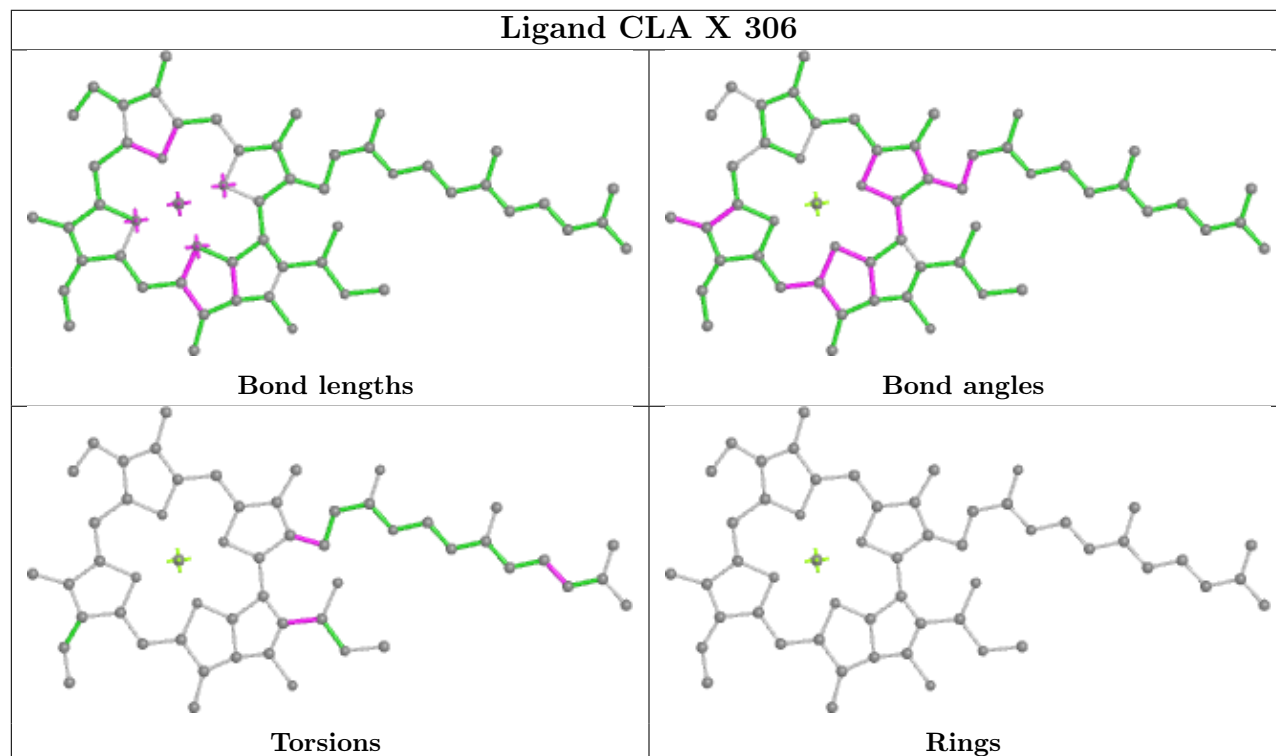


Rings

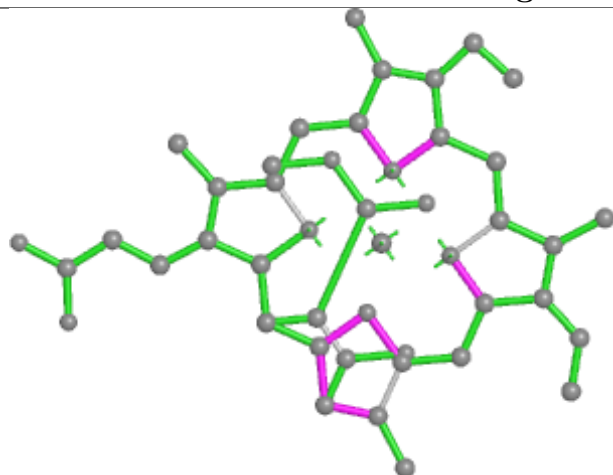
Ligand CLA a 807



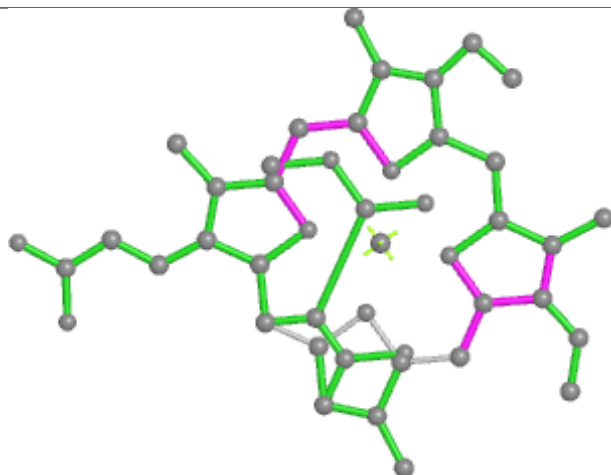
Ligand CLA X 306



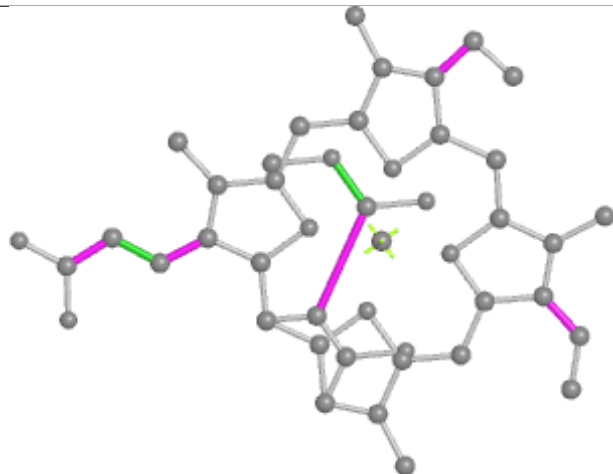
Ligand KC2 C 303



Bond lengths



Bond angles

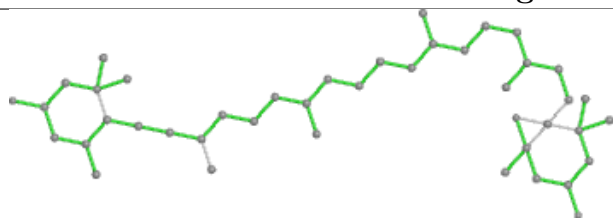


Torsions

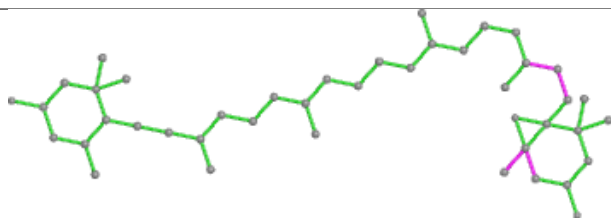


Rings

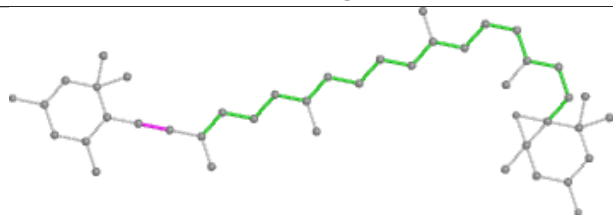
Ligand DD6 E 317



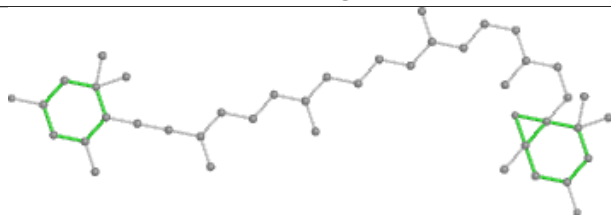
Bond lengths



Bond angles

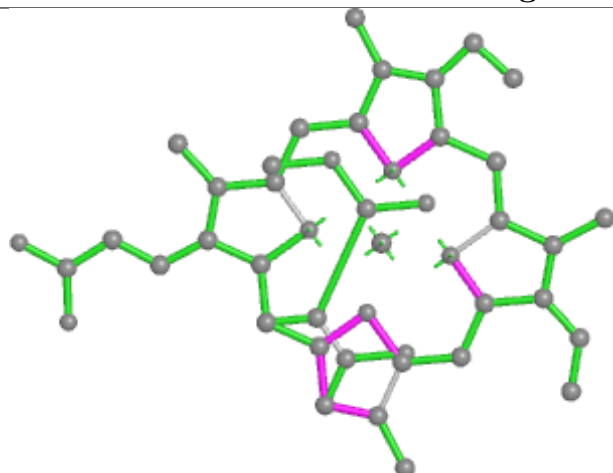


Torsions

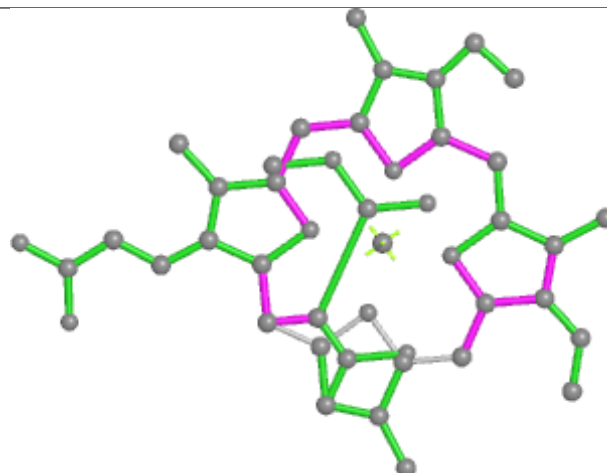


Rings

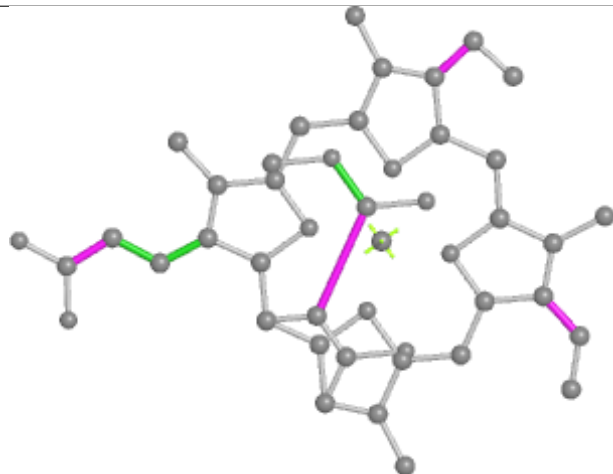
Ligand KC2 u 315



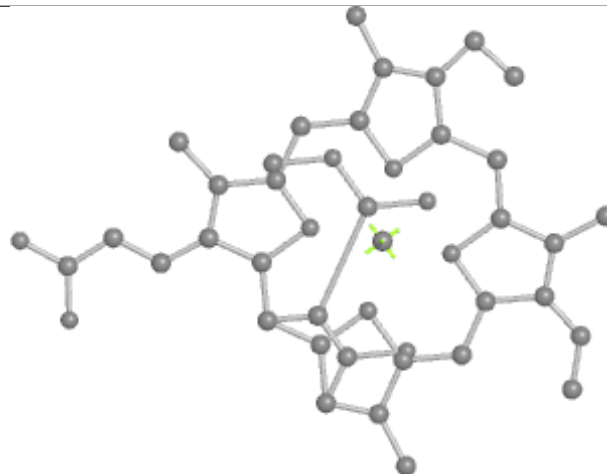
Bond lengths



Bond angles

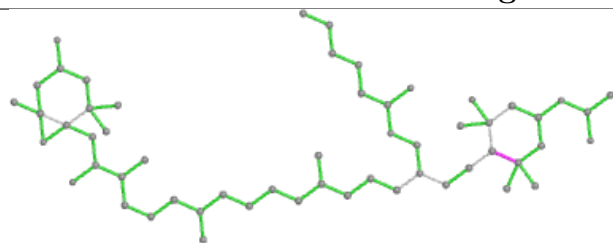


Torsions

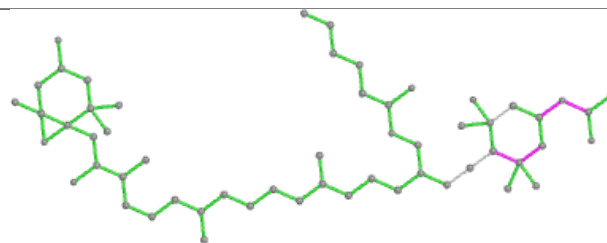


Rings

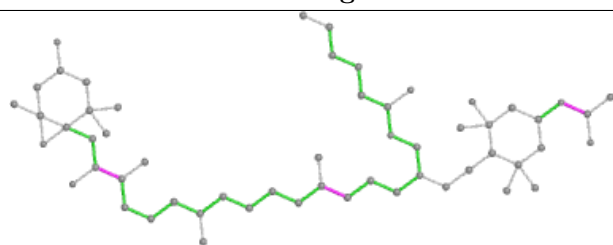
Ligand A1EB1 S 320



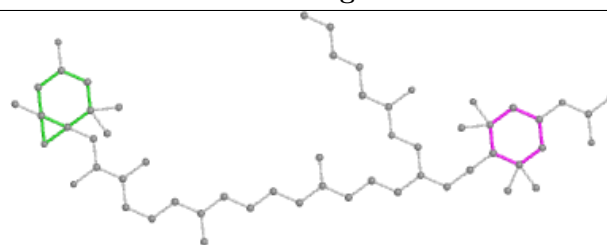
Bond lengths



Bond angles

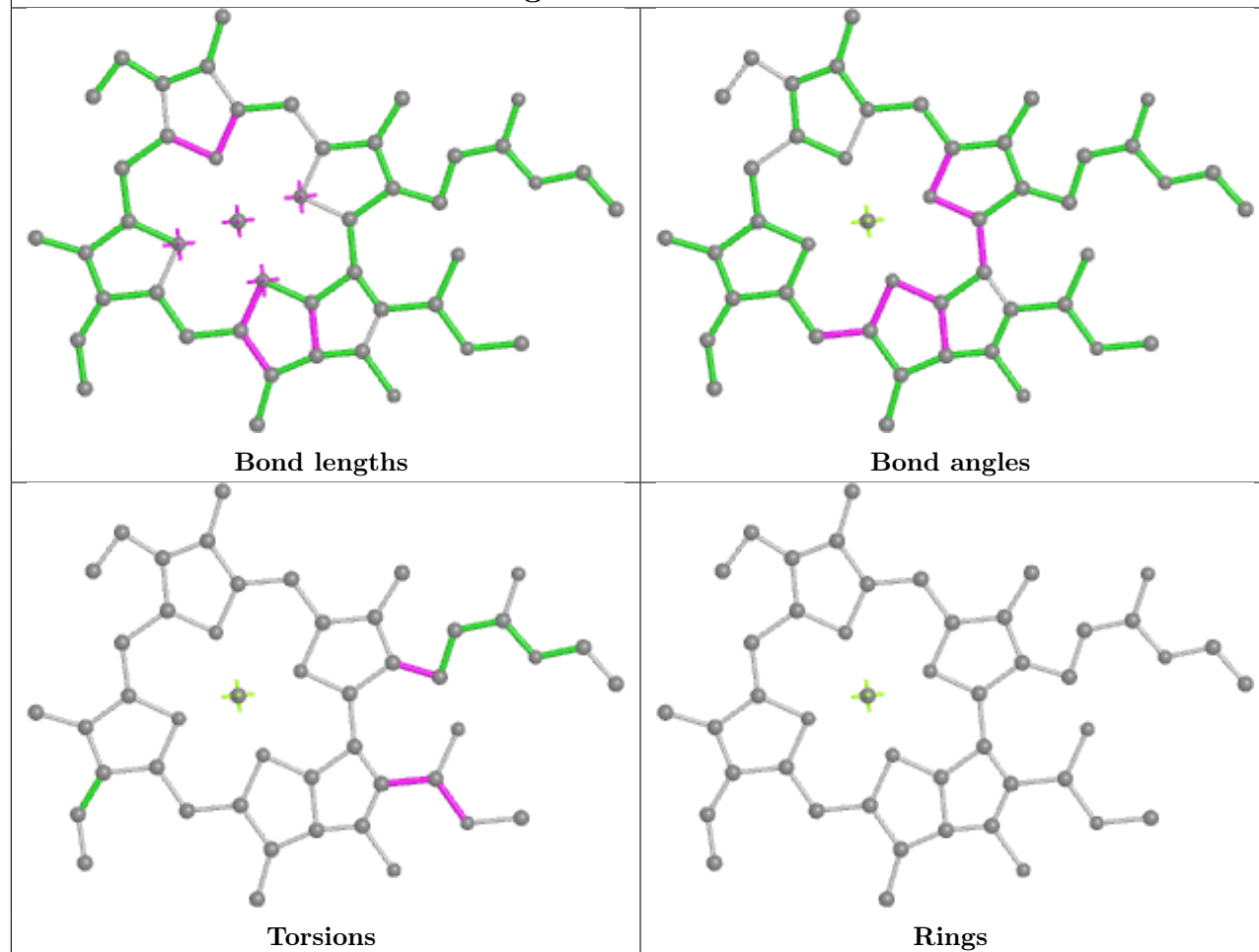


Torsions

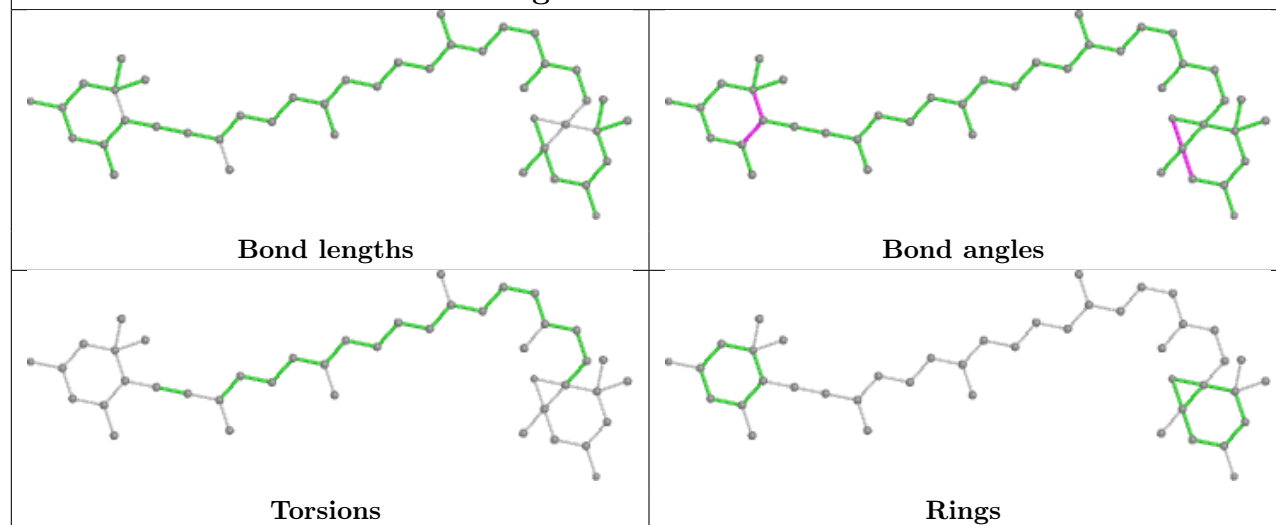


Rings

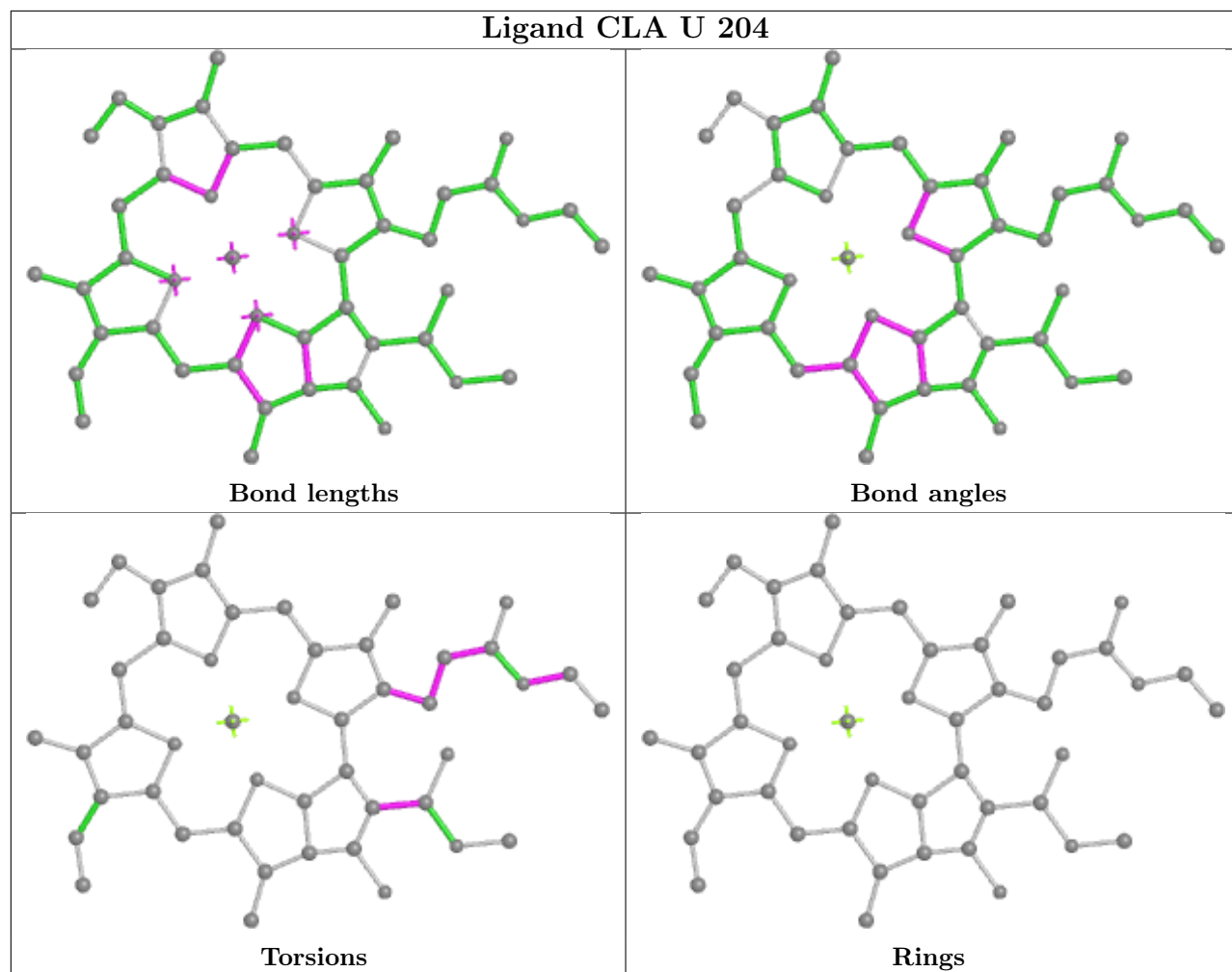
Ligand CLA U 207



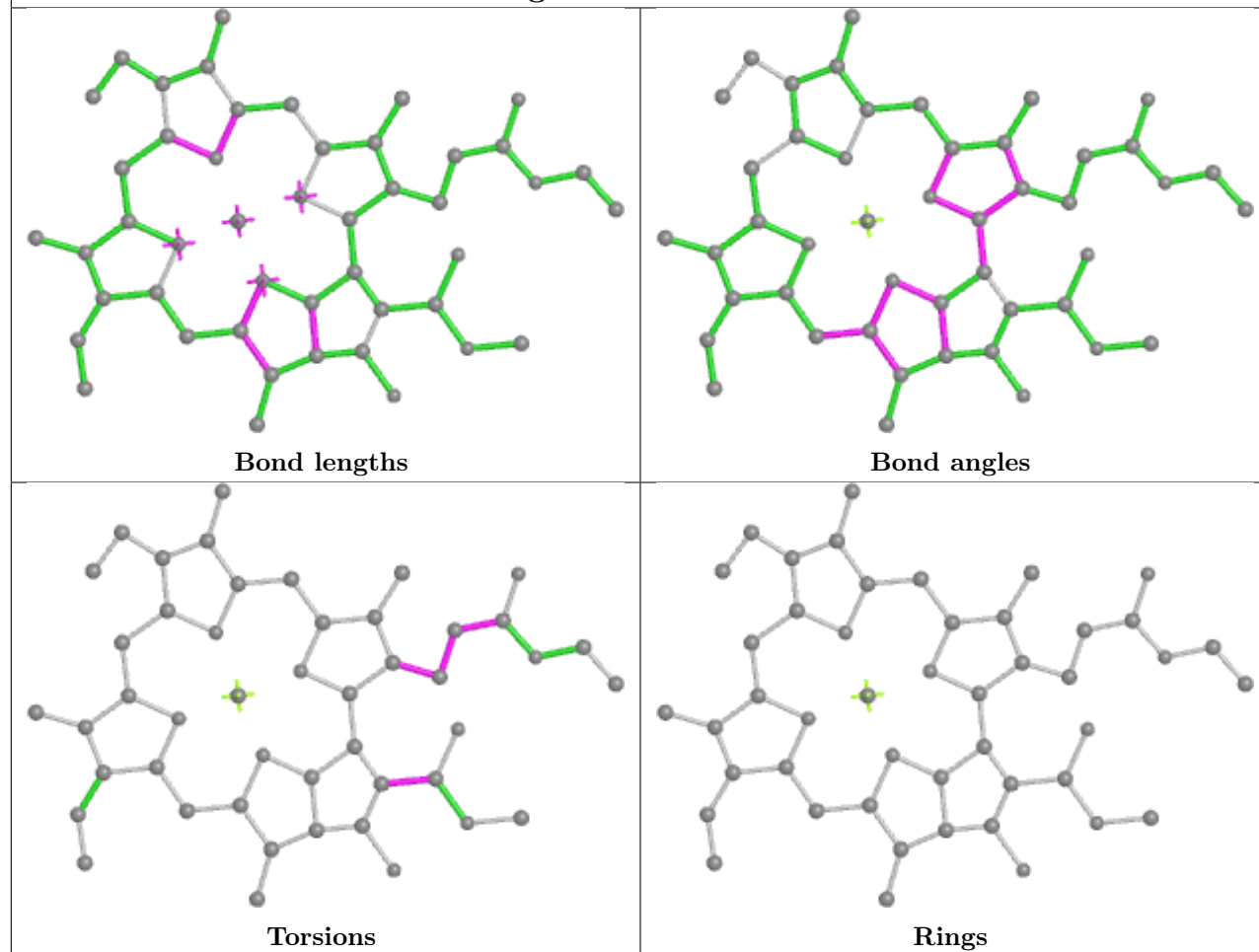
Ligand DD6 X 322



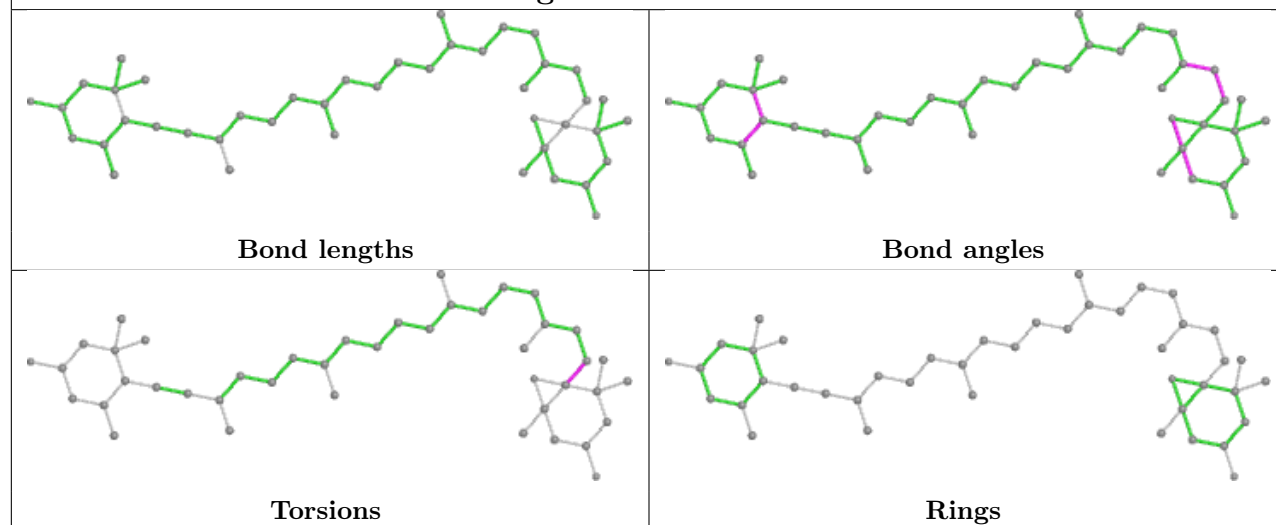
Ligand CLA U 204



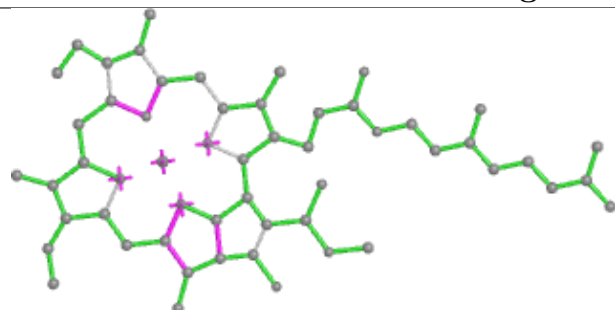
Ligand CLA u 314



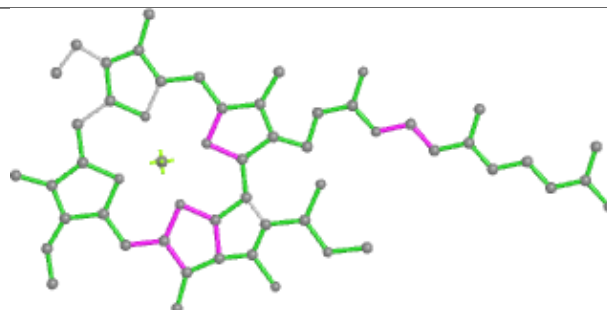
Ligand DD6 J 315



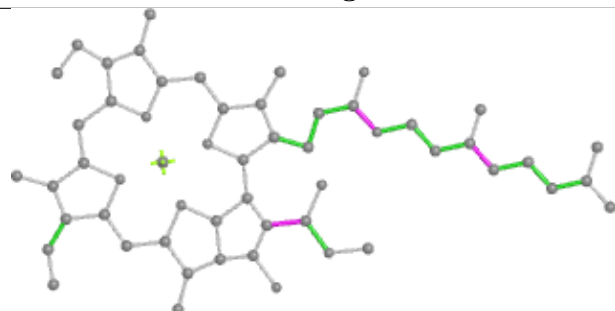
Ligand CLA k 201



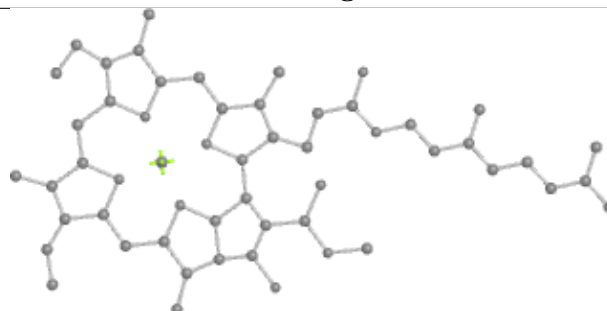
Bond lengths



Bond angles

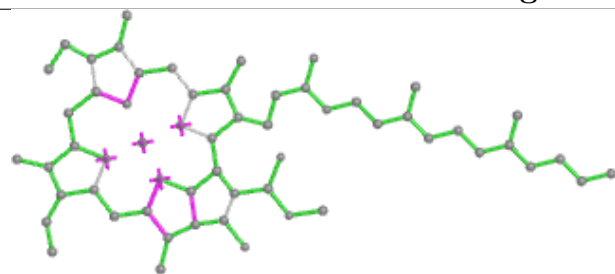


Torsions

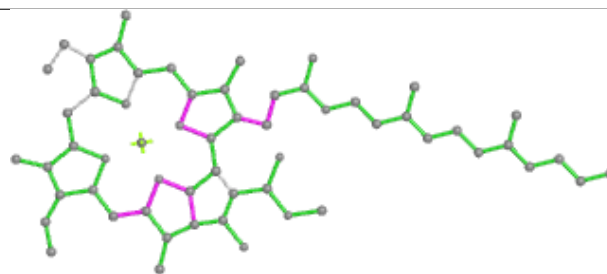


Rings

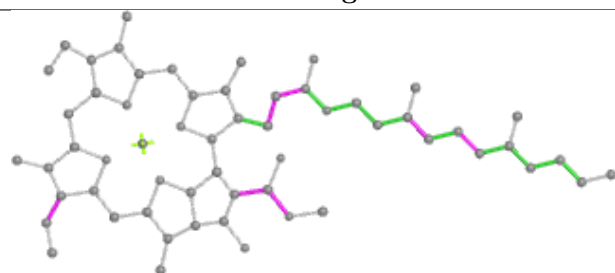
Ligand CLA J 312



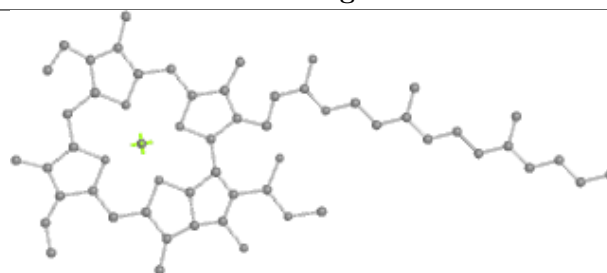
Bond lengths



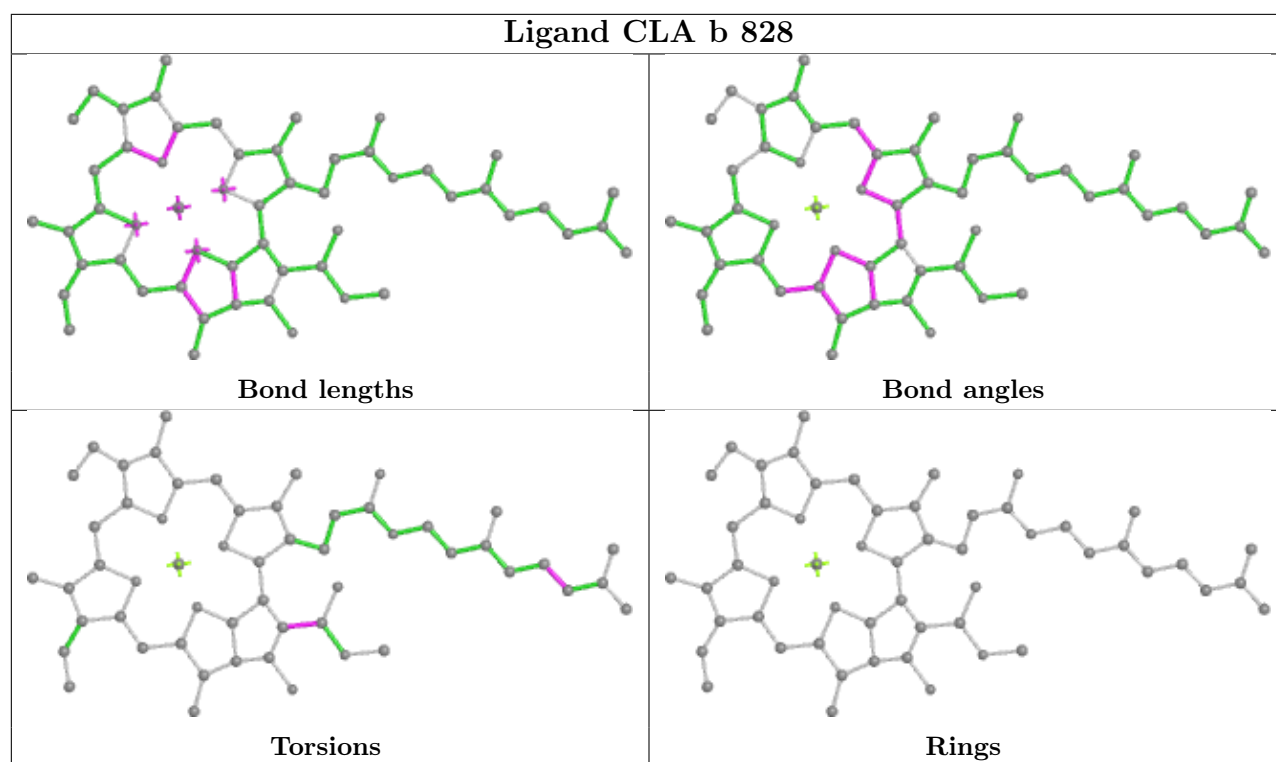
Bond angles



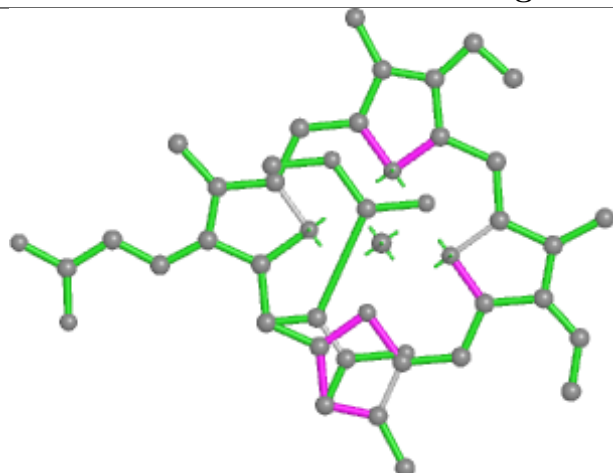
Torsions



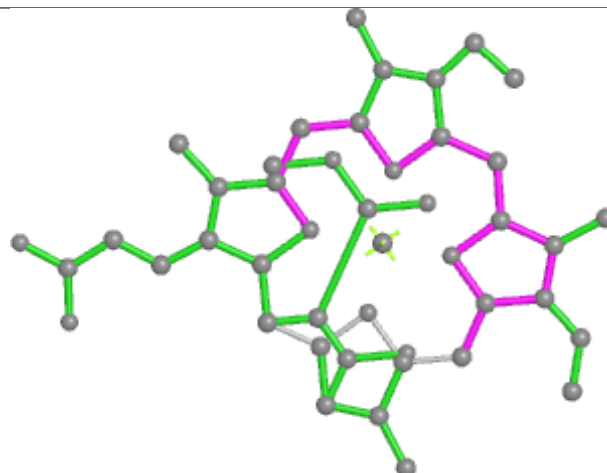
Rings



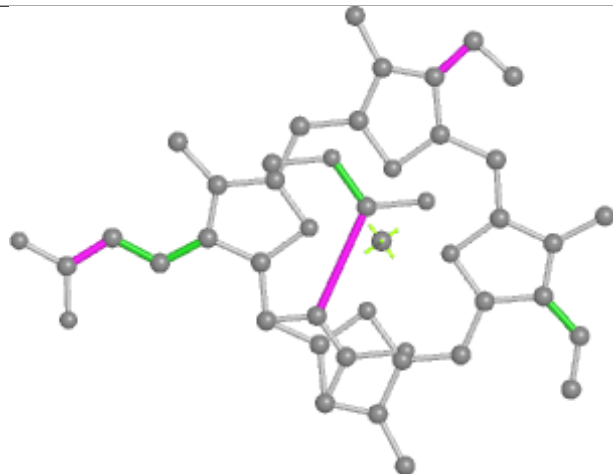
Ligand KC2 H 316



Bond lengths



Bond angles

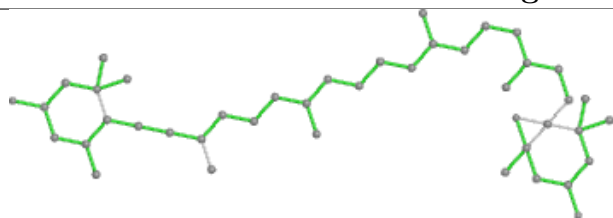


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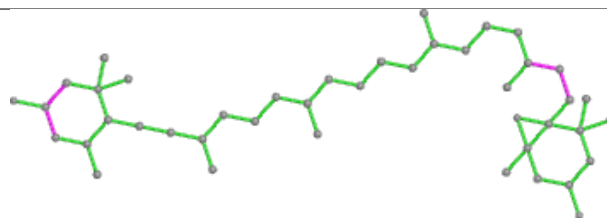


Rings

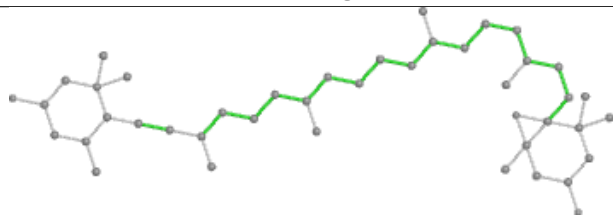
Ligand DD6 I 212



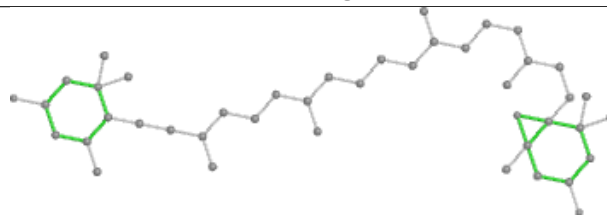
Bond lengths



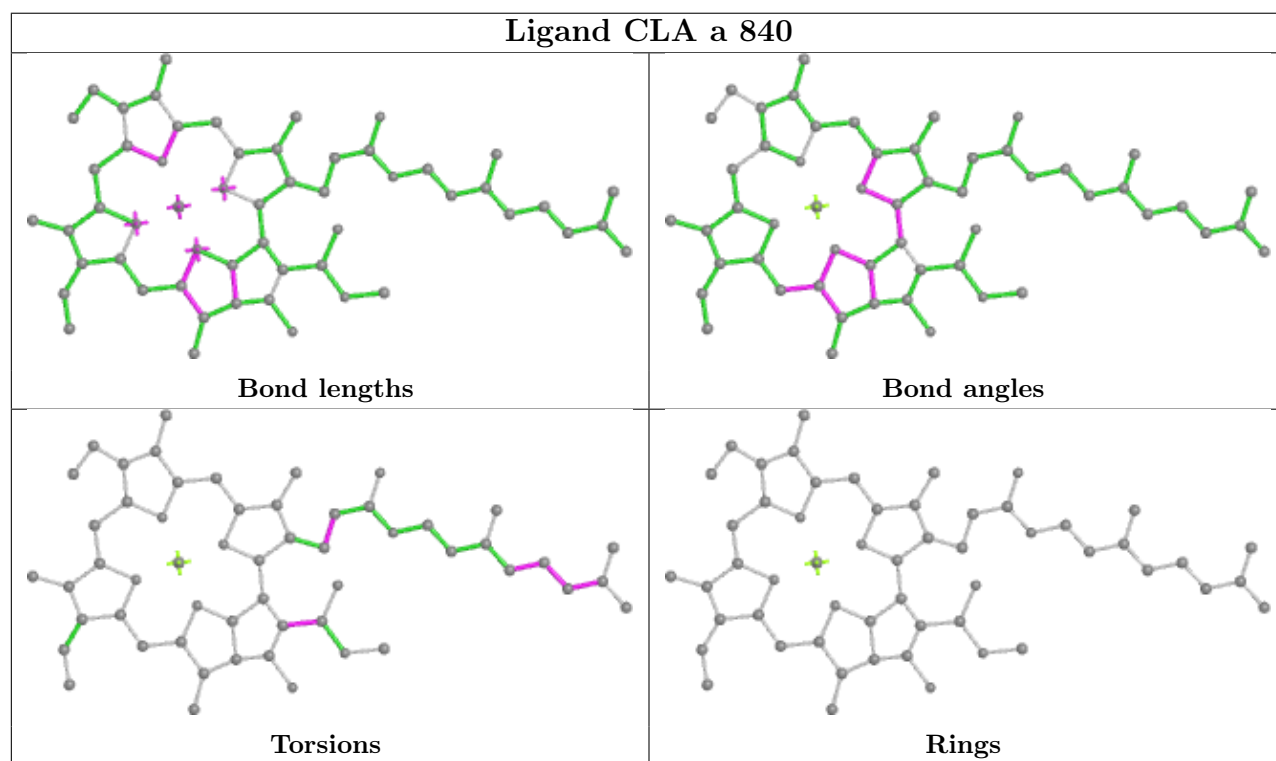
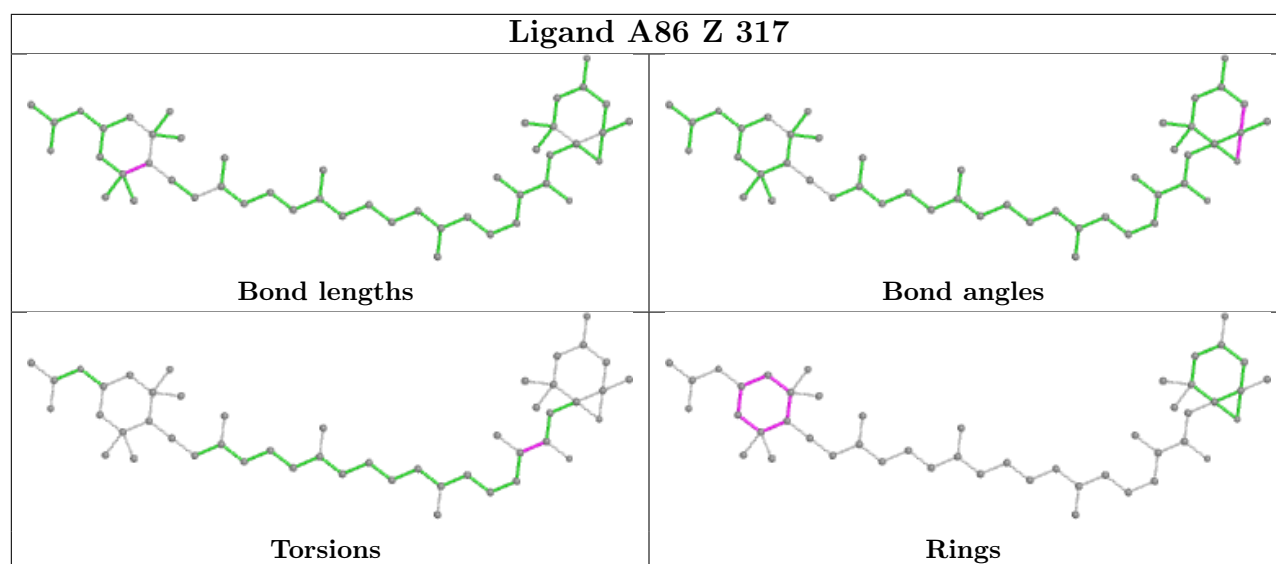
Bond angles

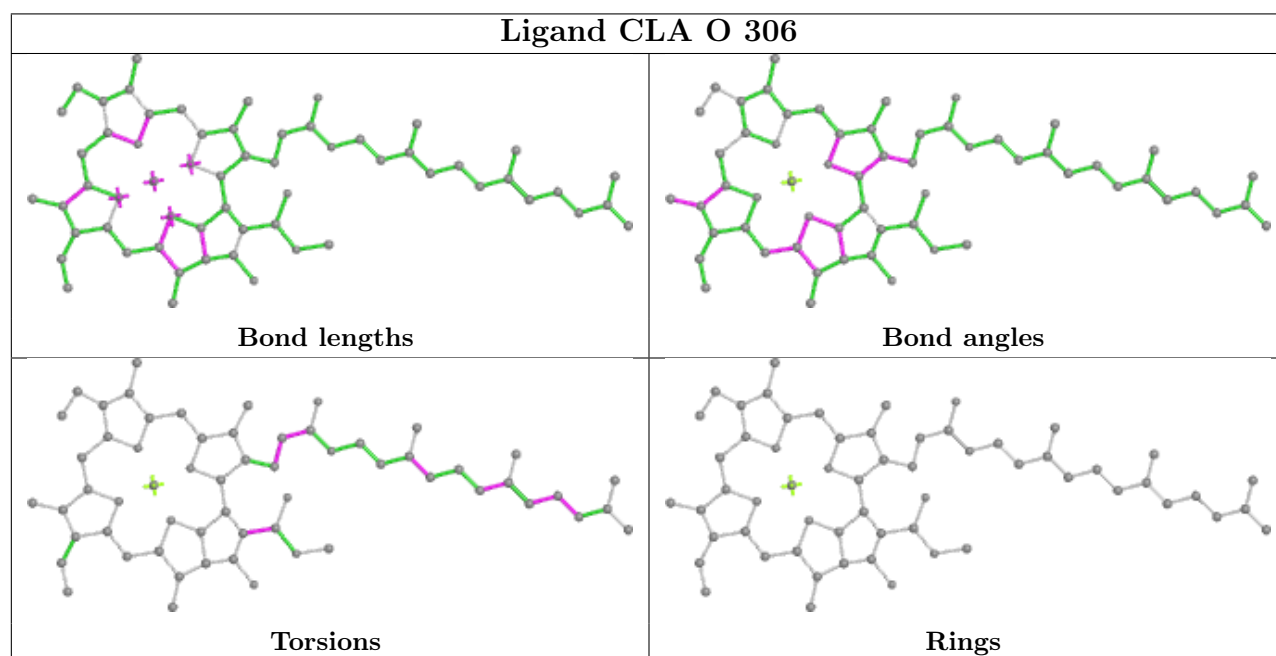
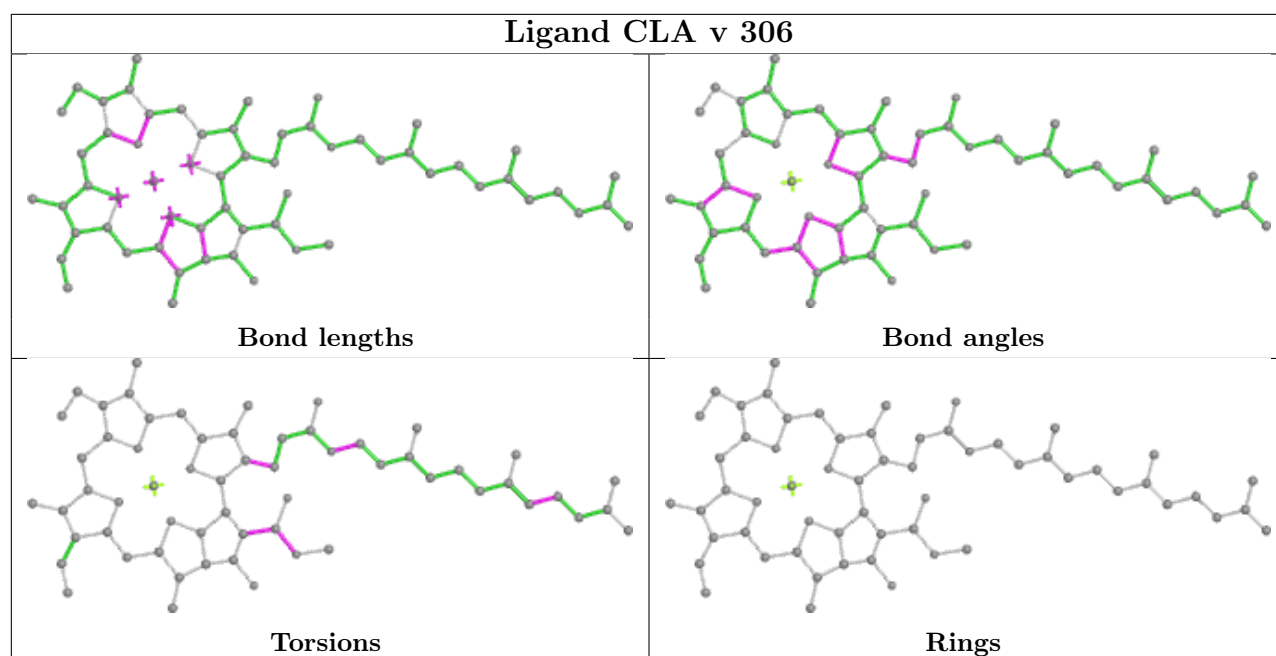


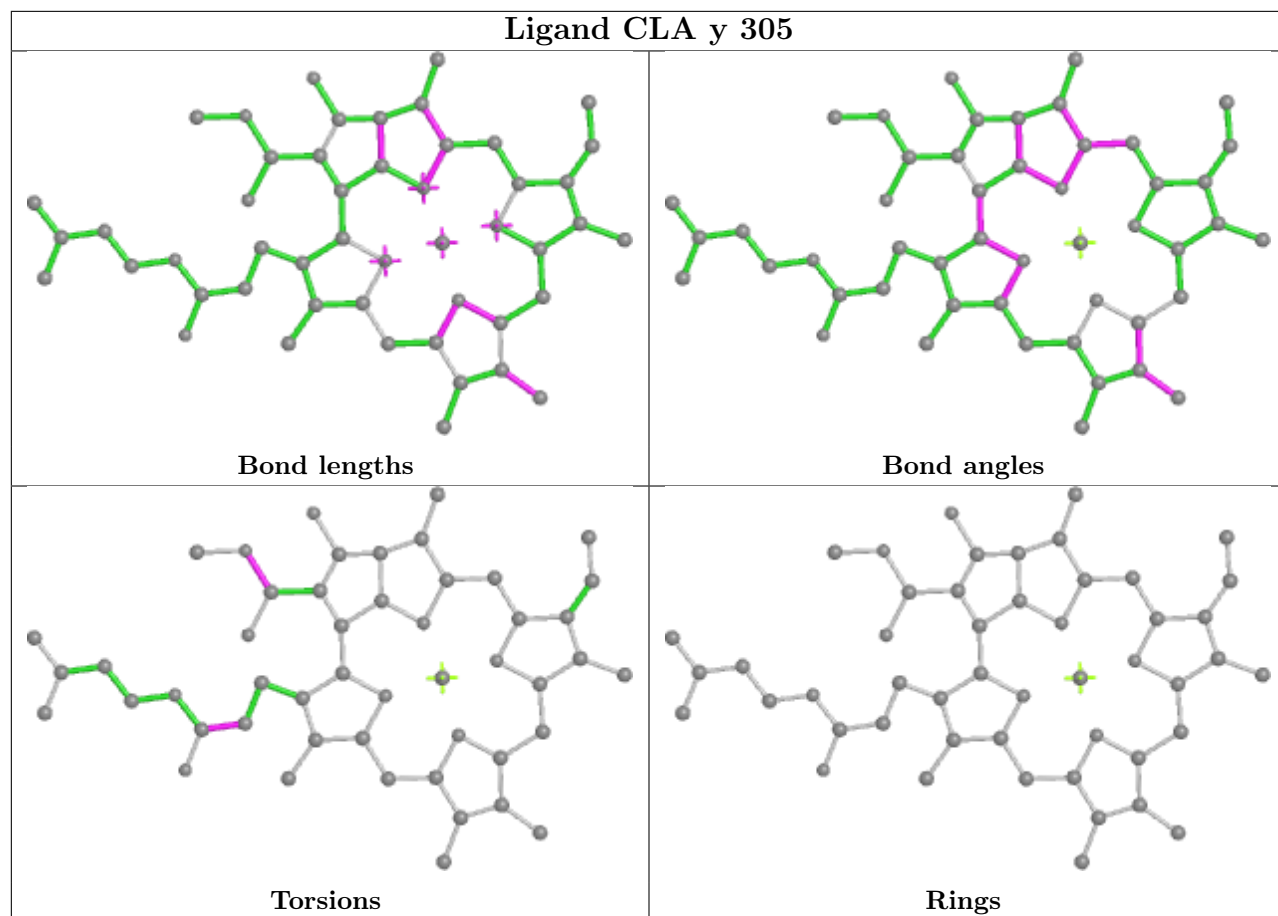
Torsions



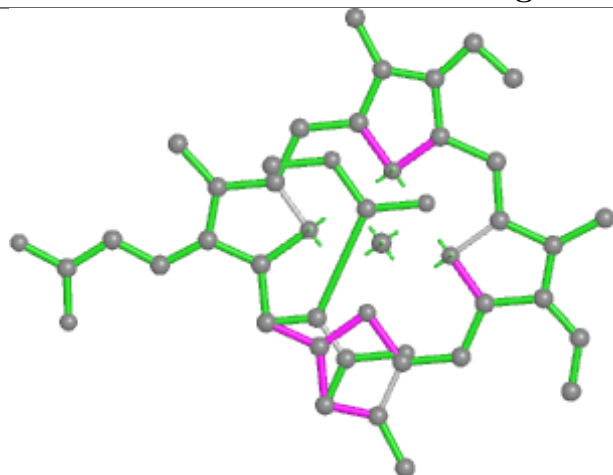
Rings



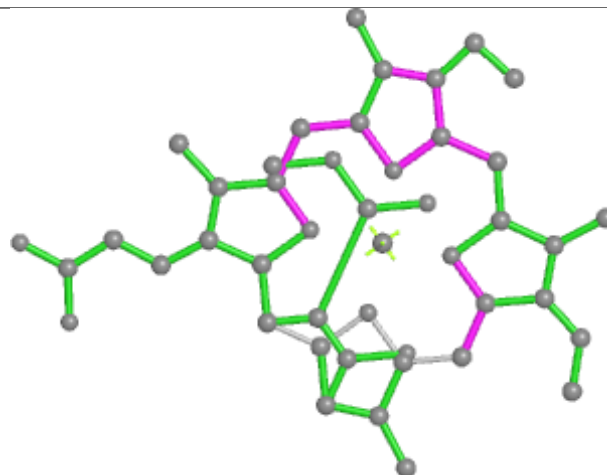




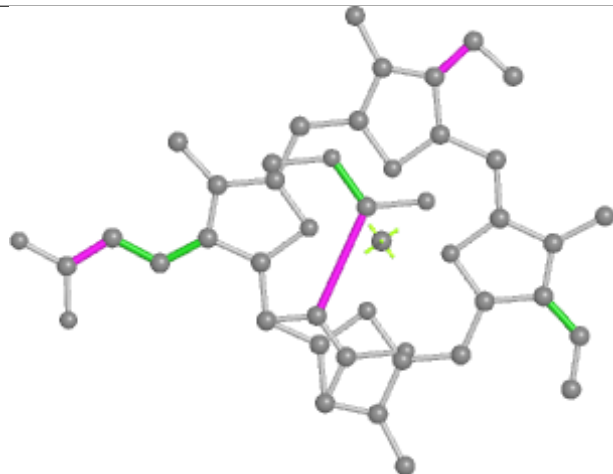
Ligand KC2 X 308



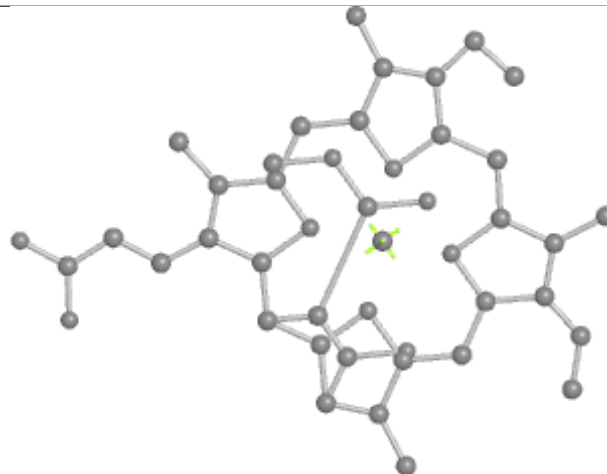
Bond lengths



Bond angles

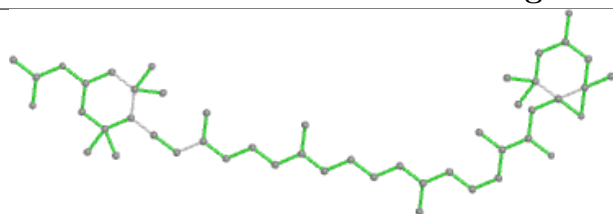


Torsions

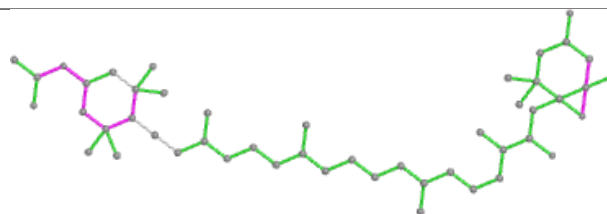


Rings

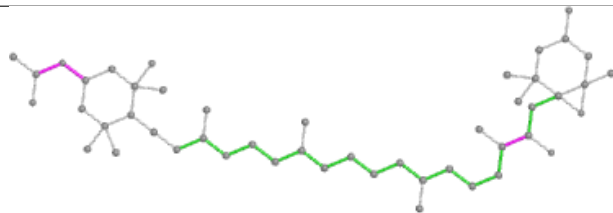
Ligand A86 z 315



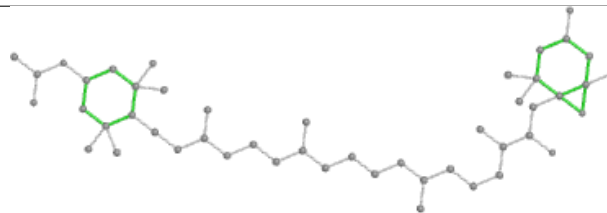
Bond lengths



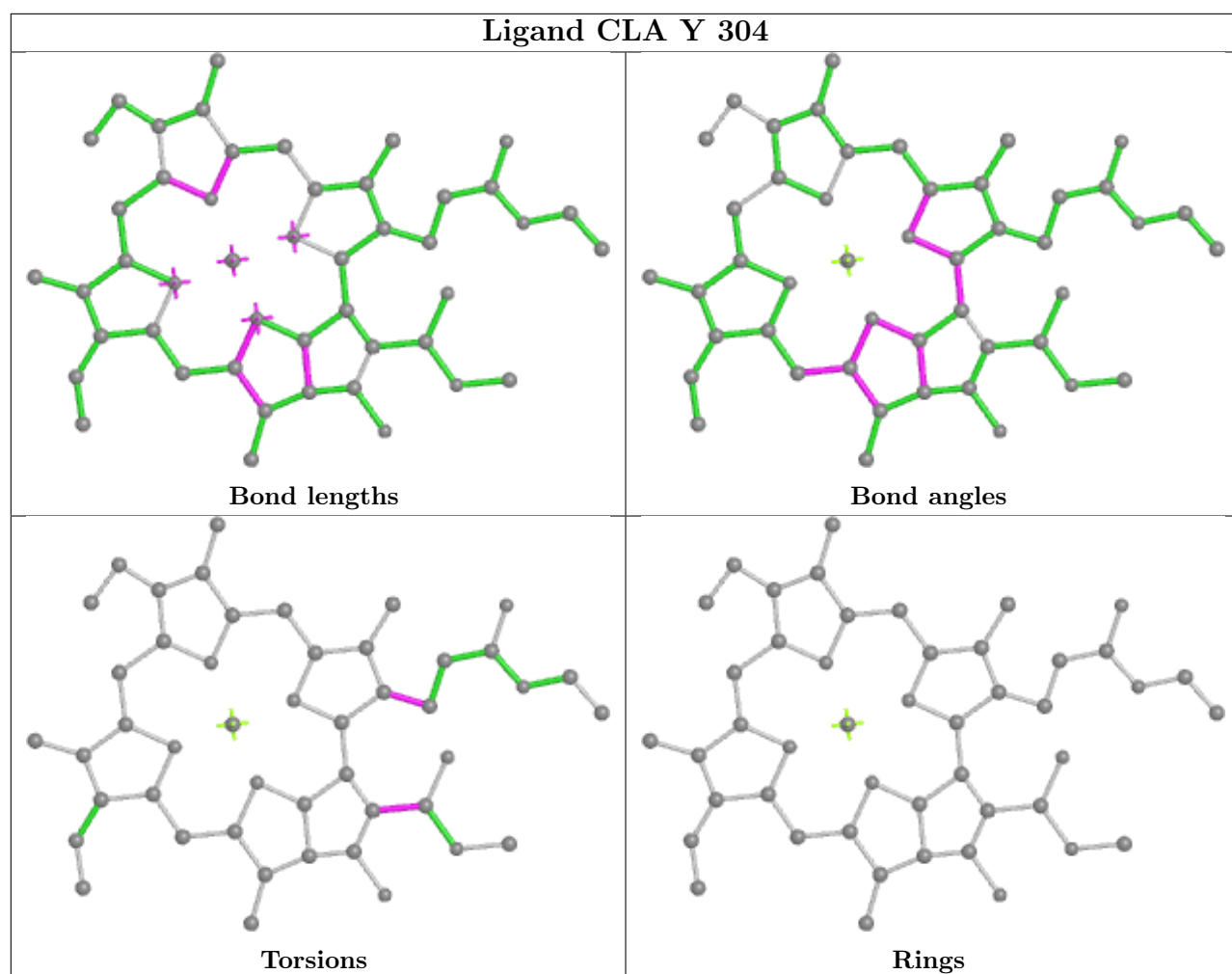
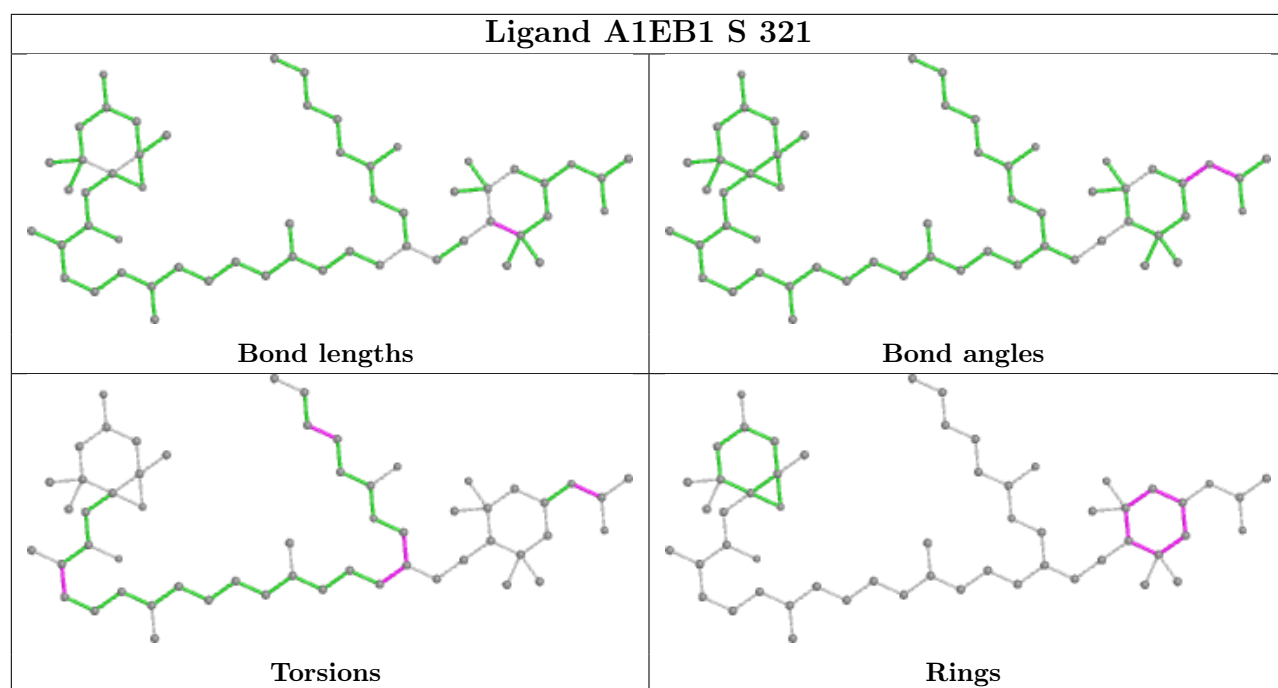
Bond angles



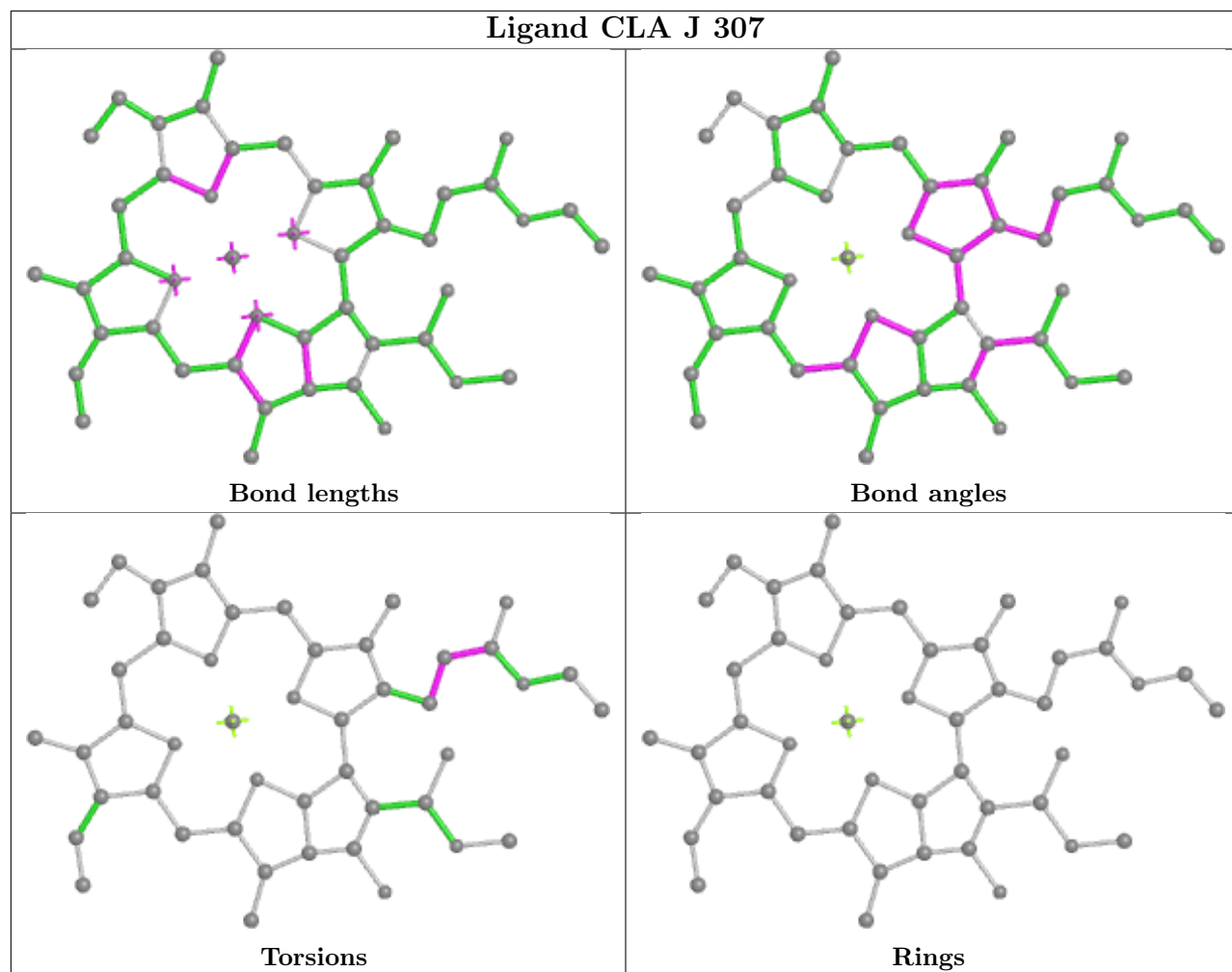
Torsions



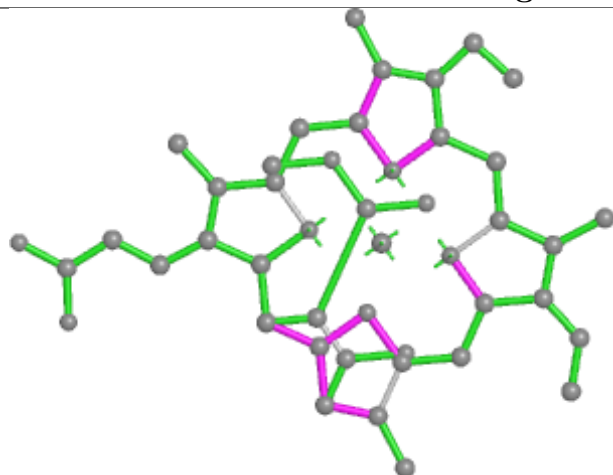
Rings



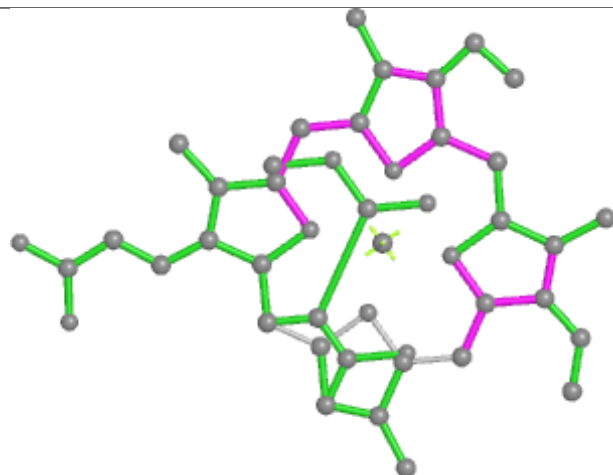
Ligand CLA J 307



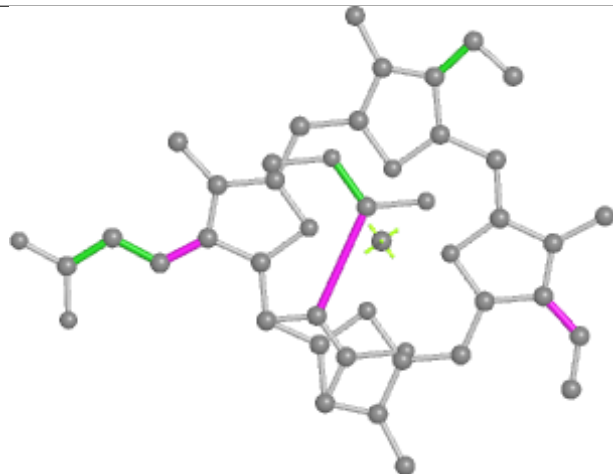
Ligand KC2 R 302



Bond lengths



Bond angles

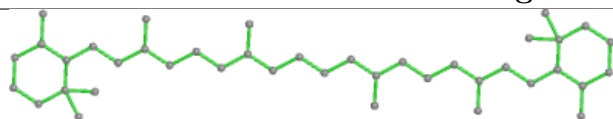


Torsions

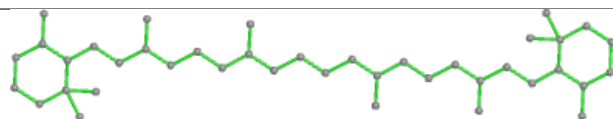


Rings

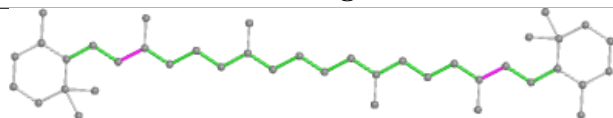
Ligand BCR b 845



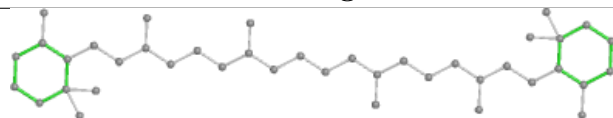
Bond lengths



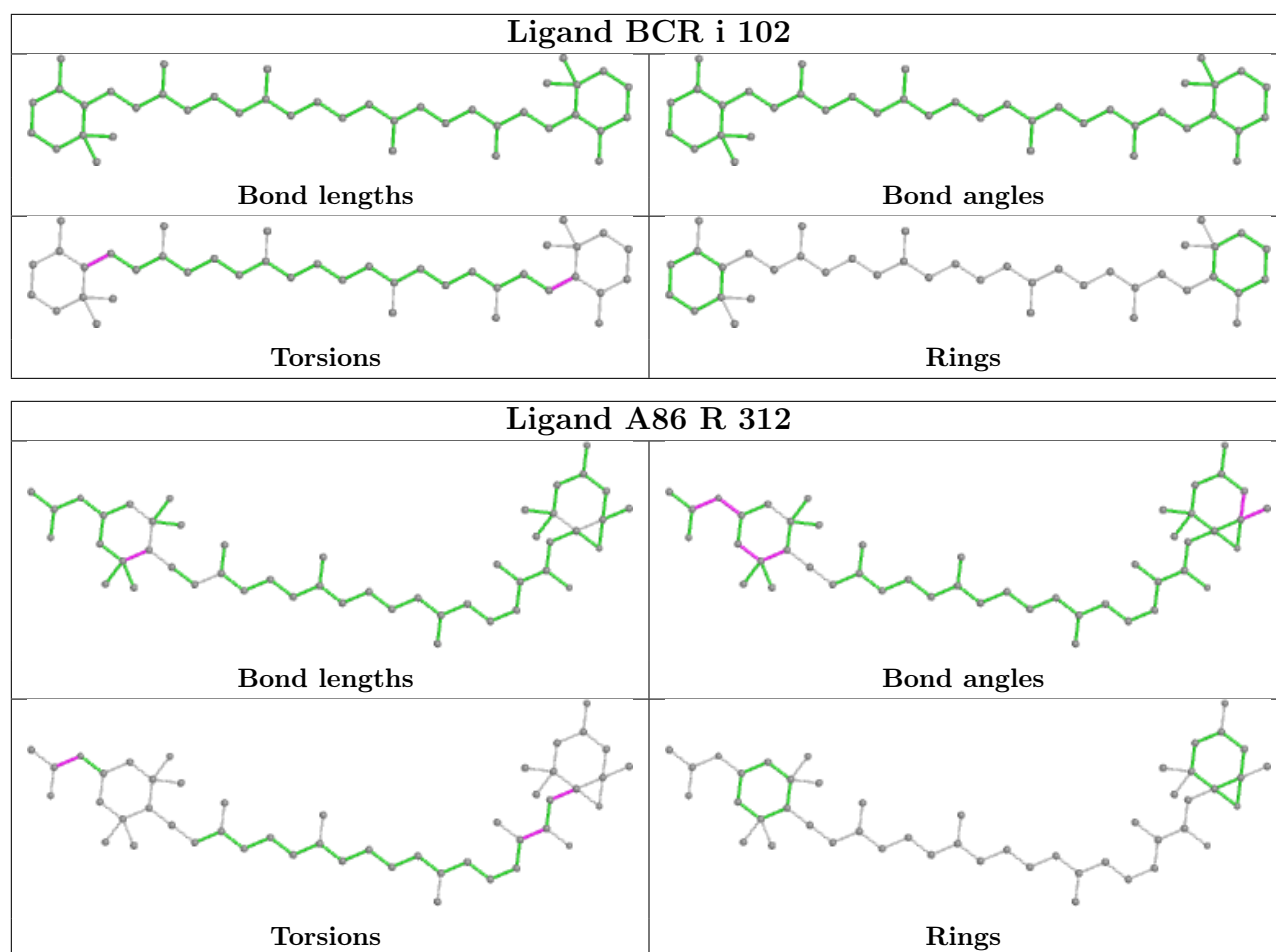
Bond angles



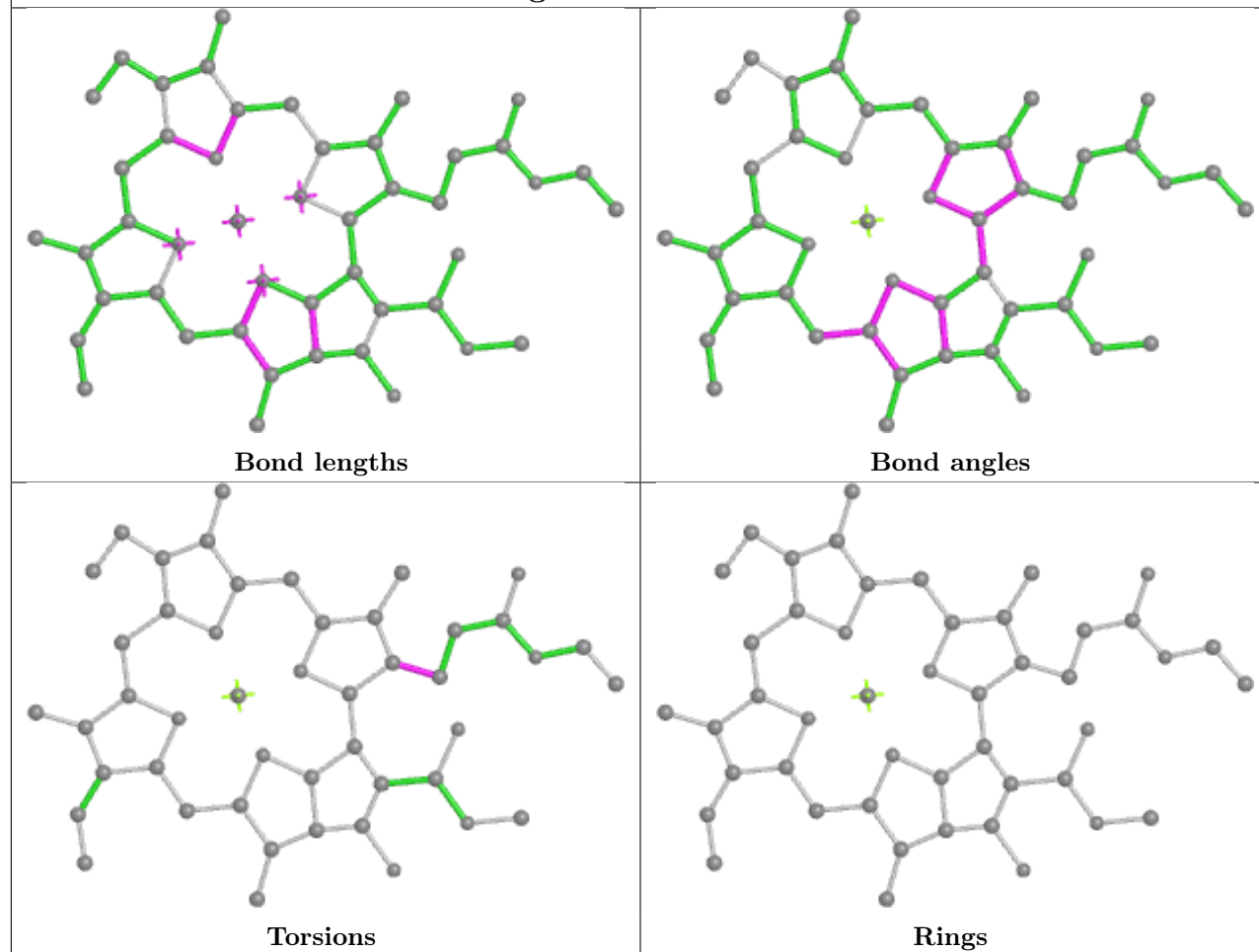
Torsions



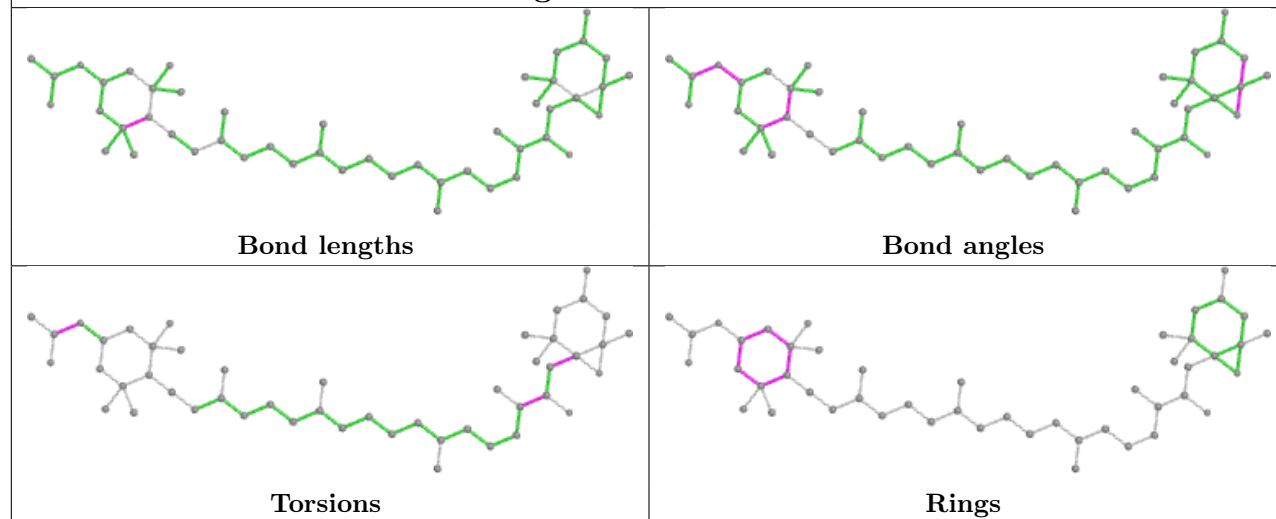
Rings



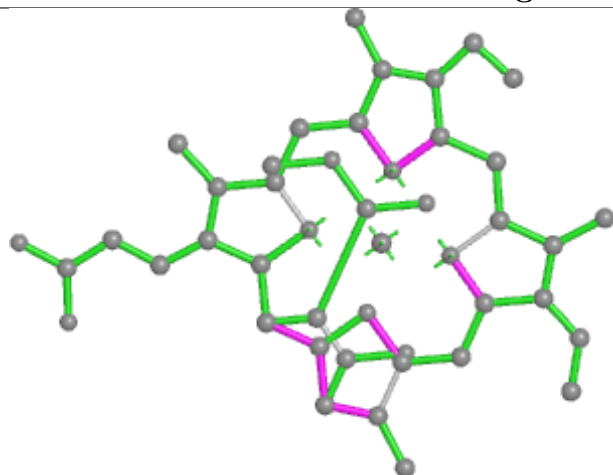
Ligand CLA J 310



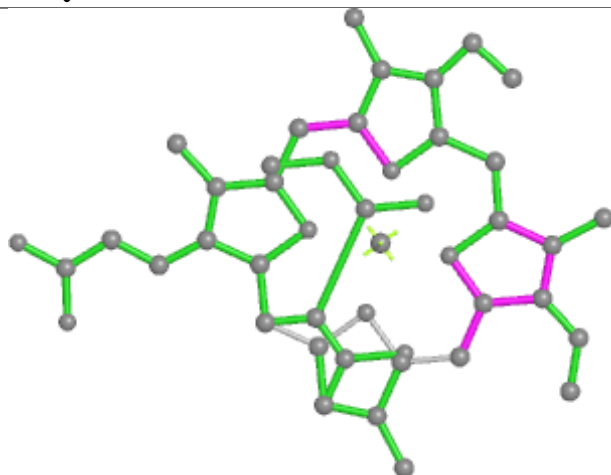
Ligand A86 M 315



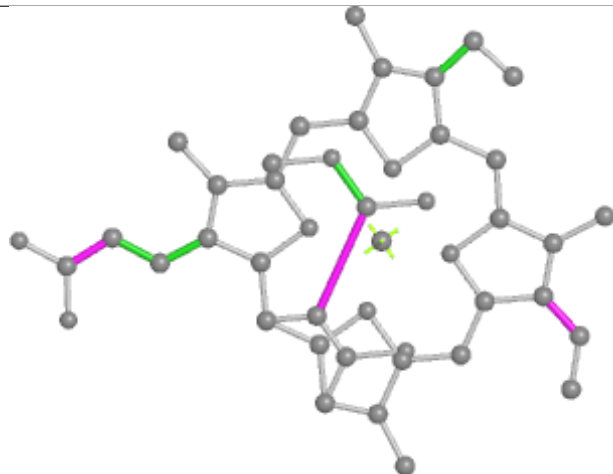
Ligand KC2 Q 201



Bond lengths



Bond angles

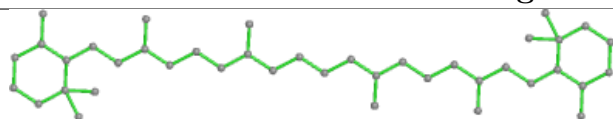


Torsions

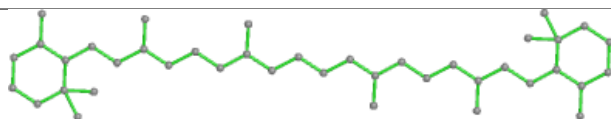


Rings

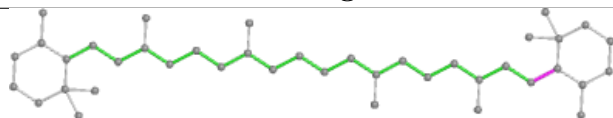
Ligand BCR a 844



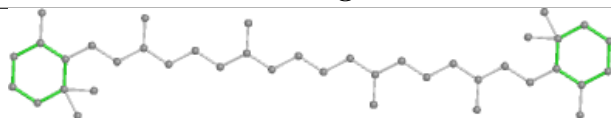
Bond lengths



Bond angles

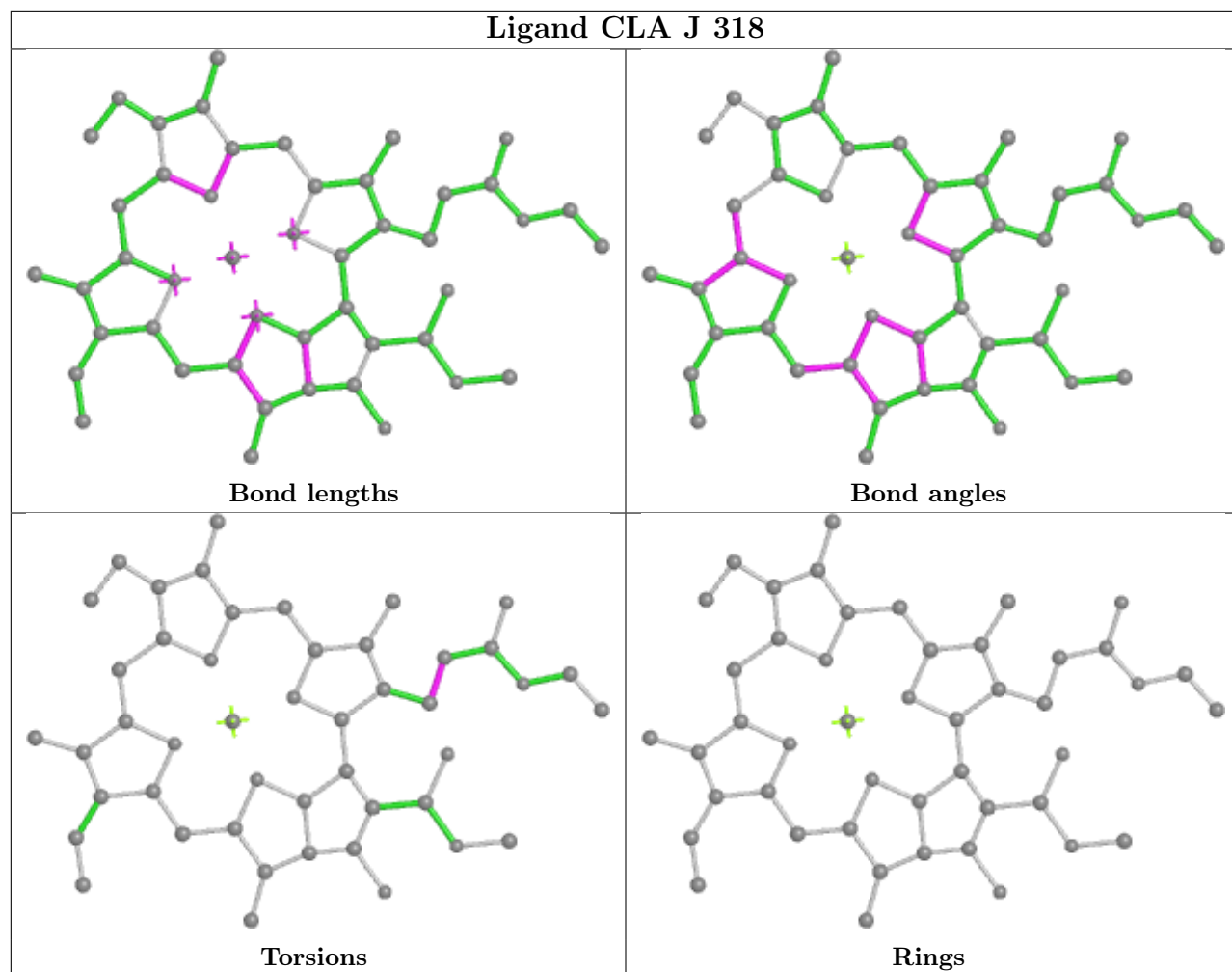


Torsions

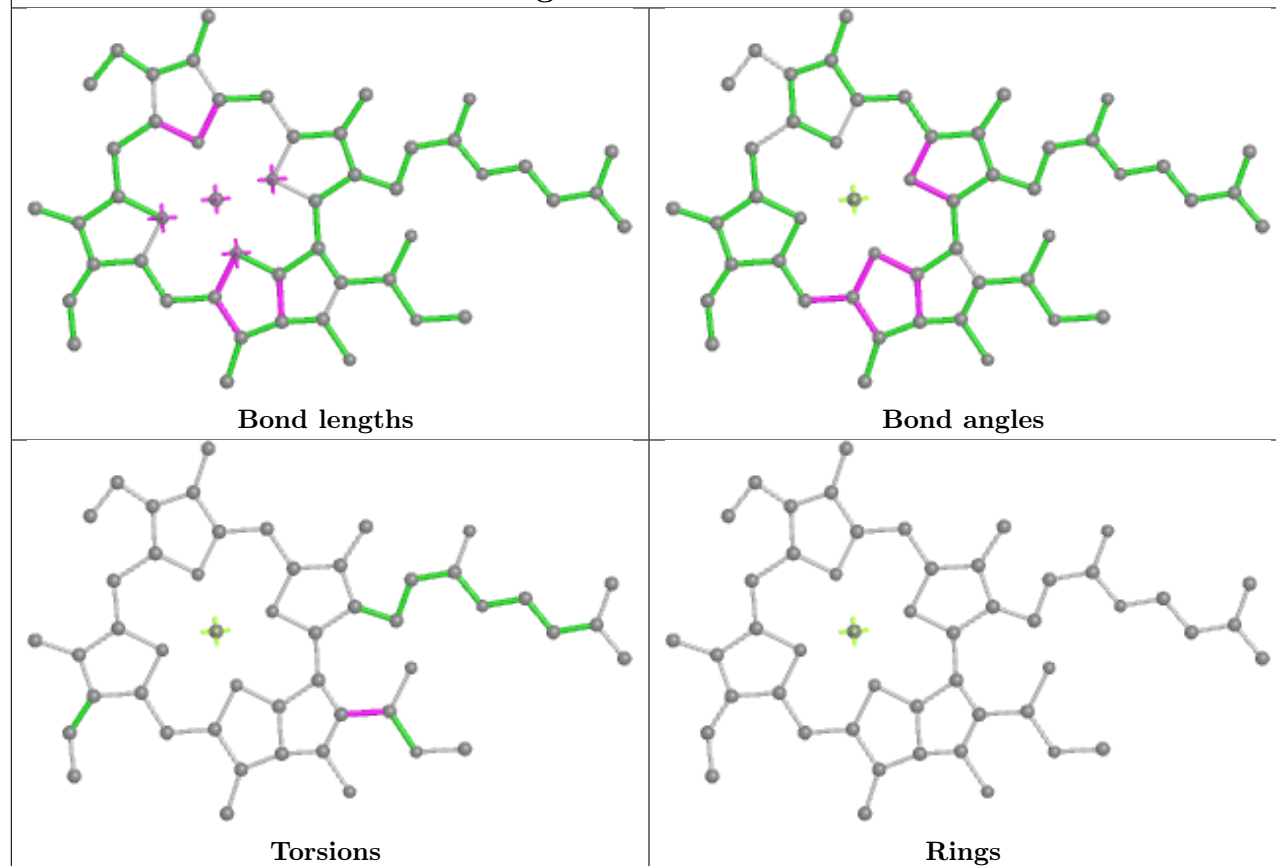


Rings

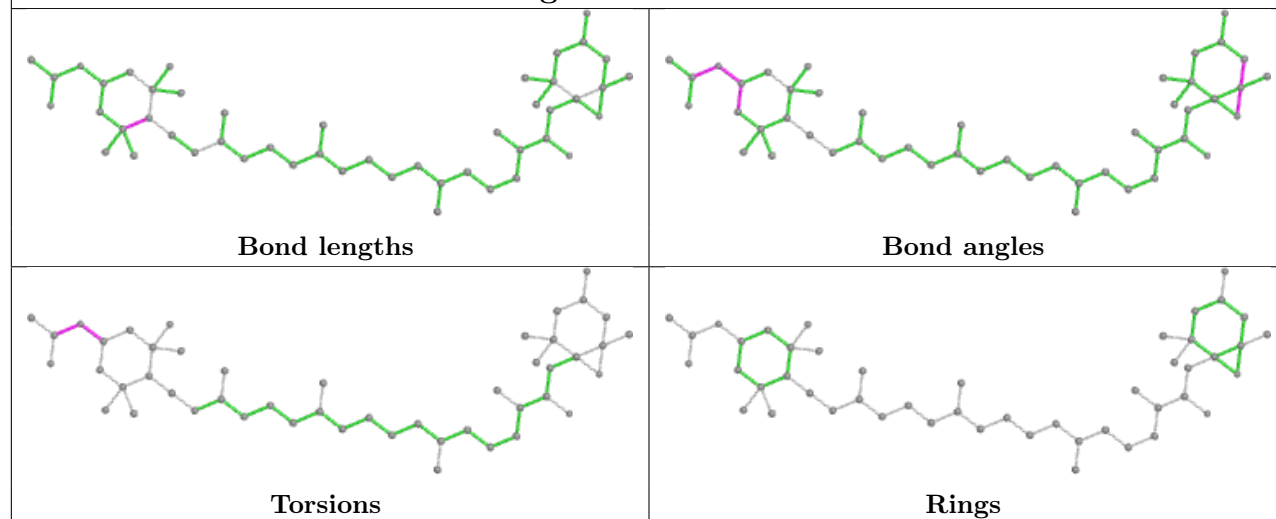
Ligand CLA J 318

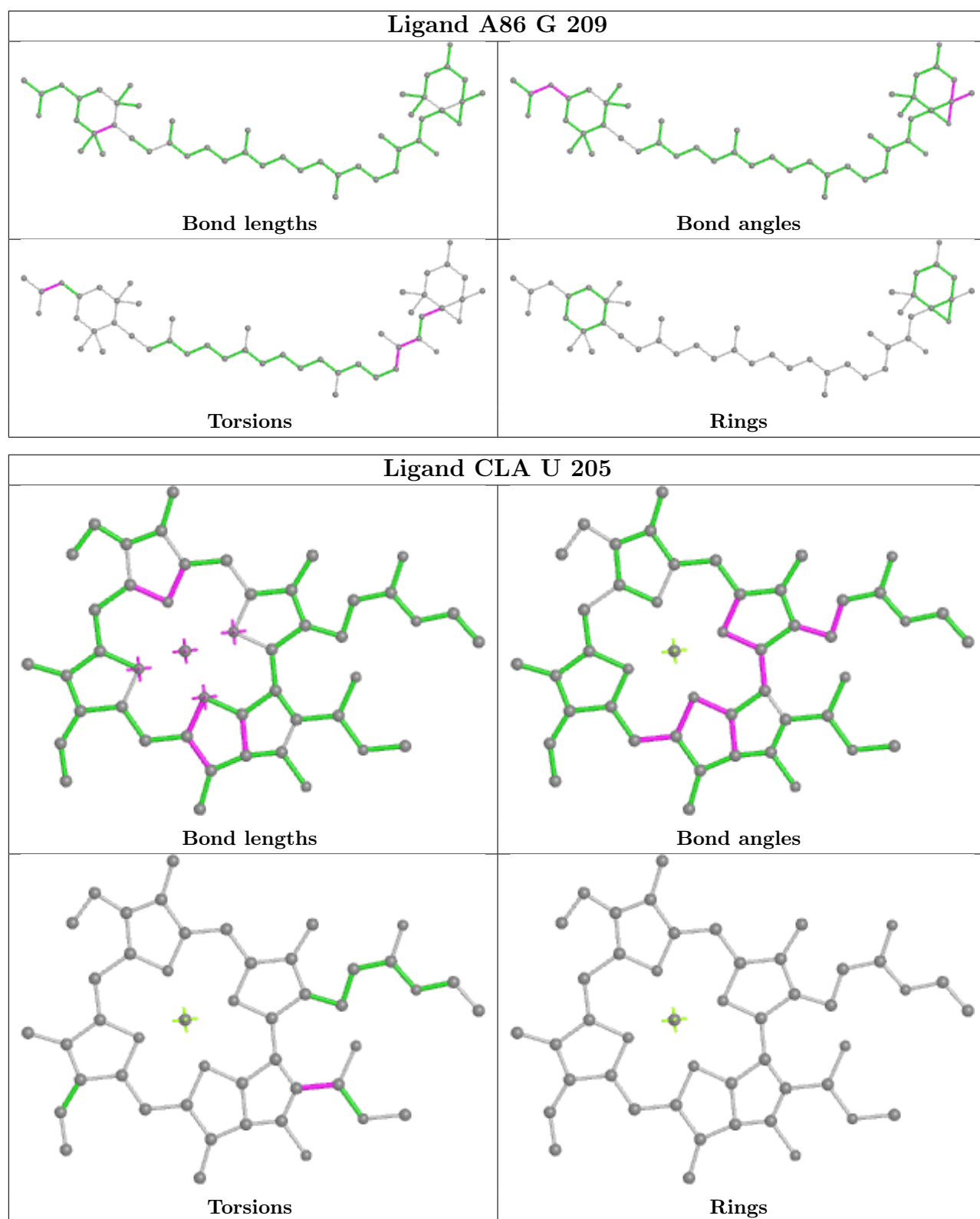


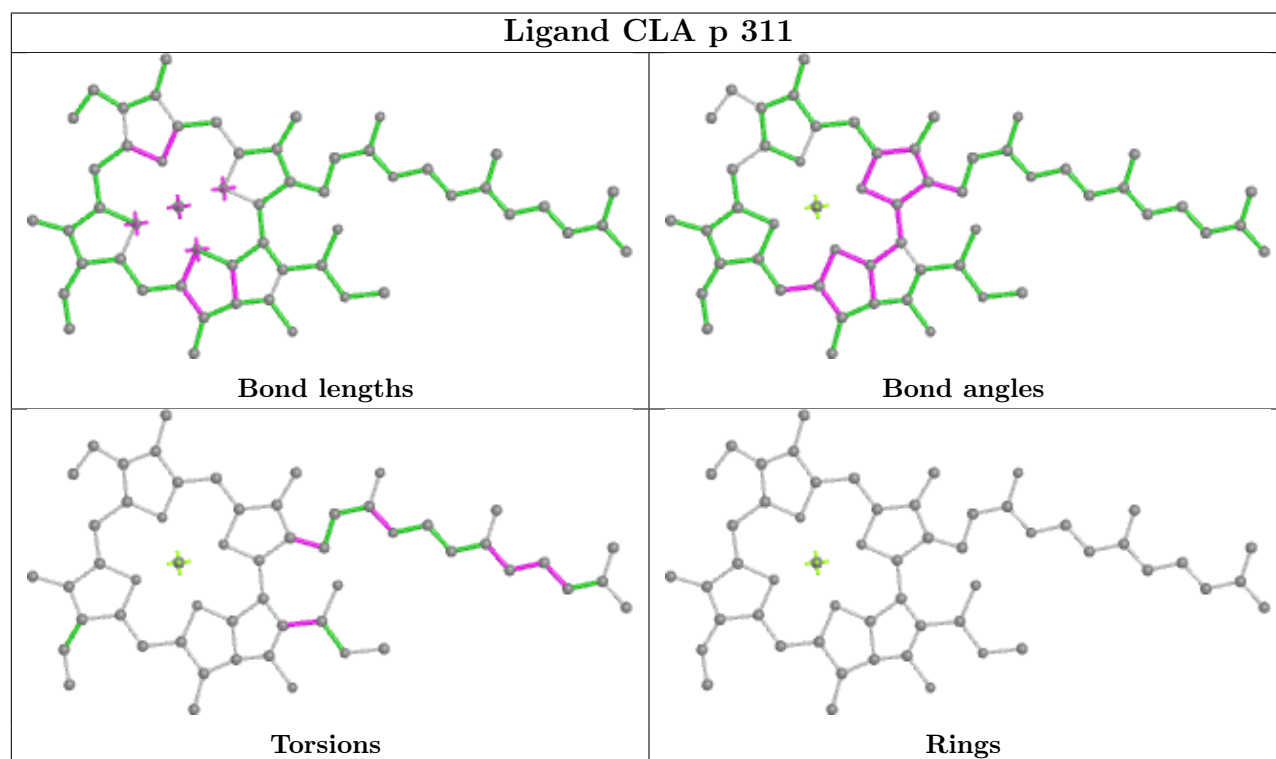
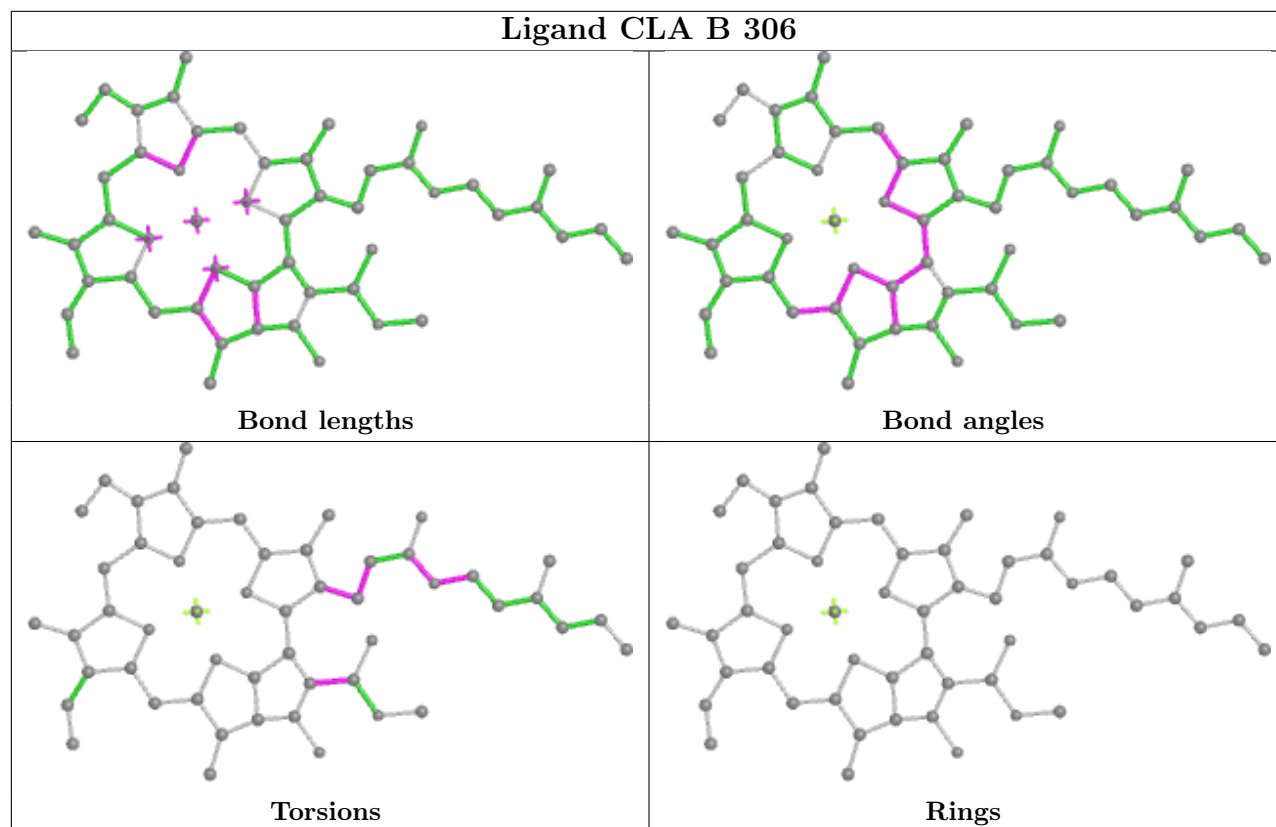
Ligand CLA a 814



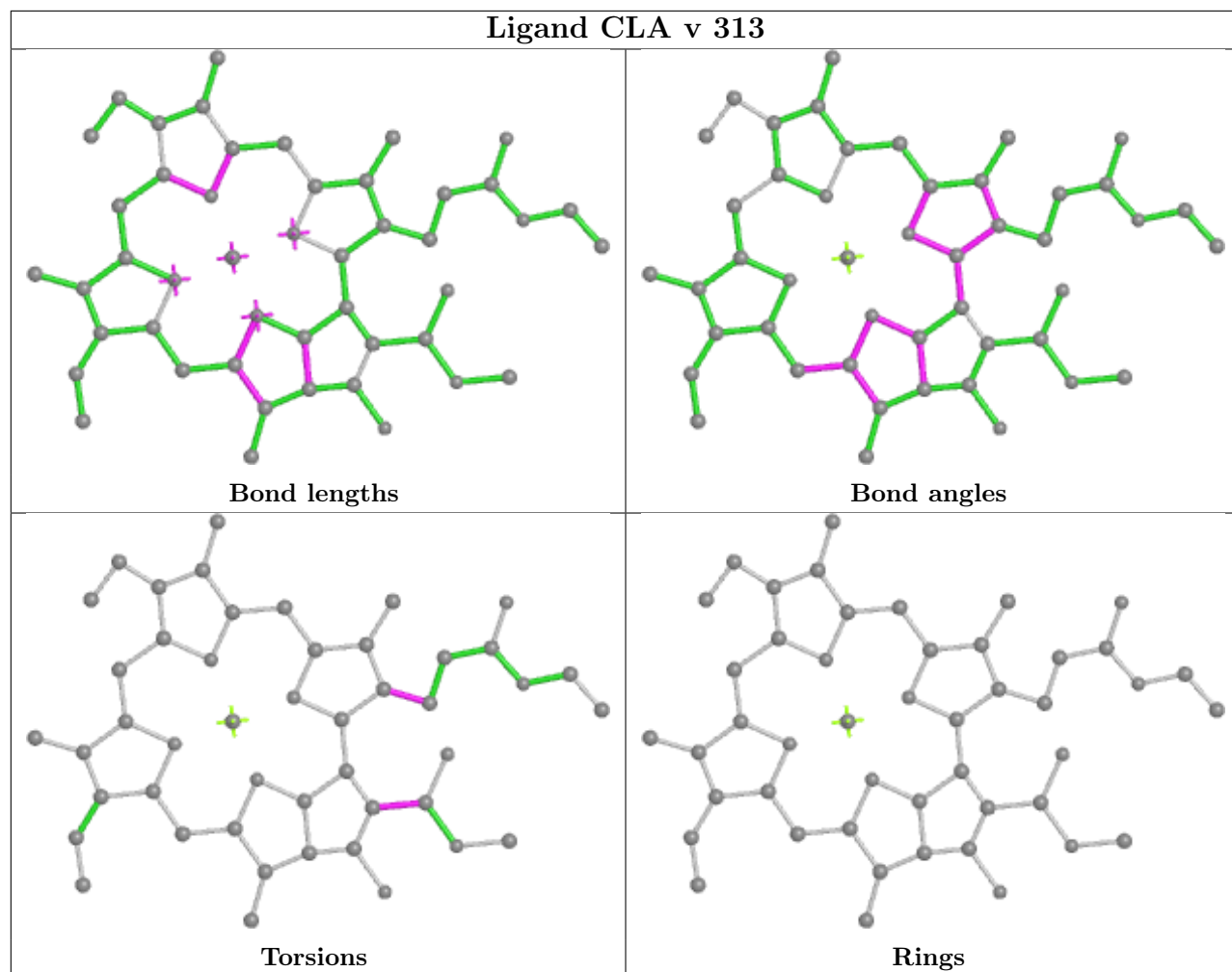
Ligand A86 Z 314



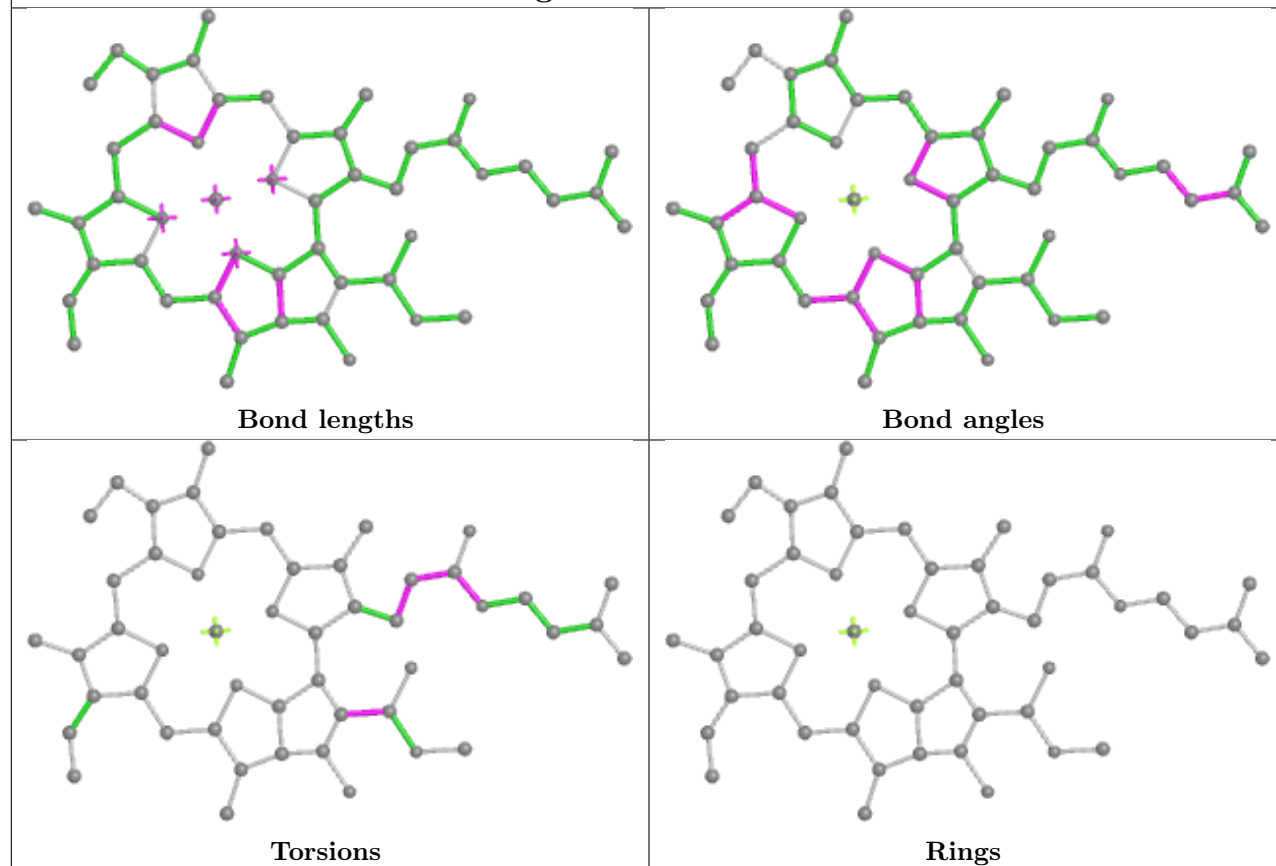




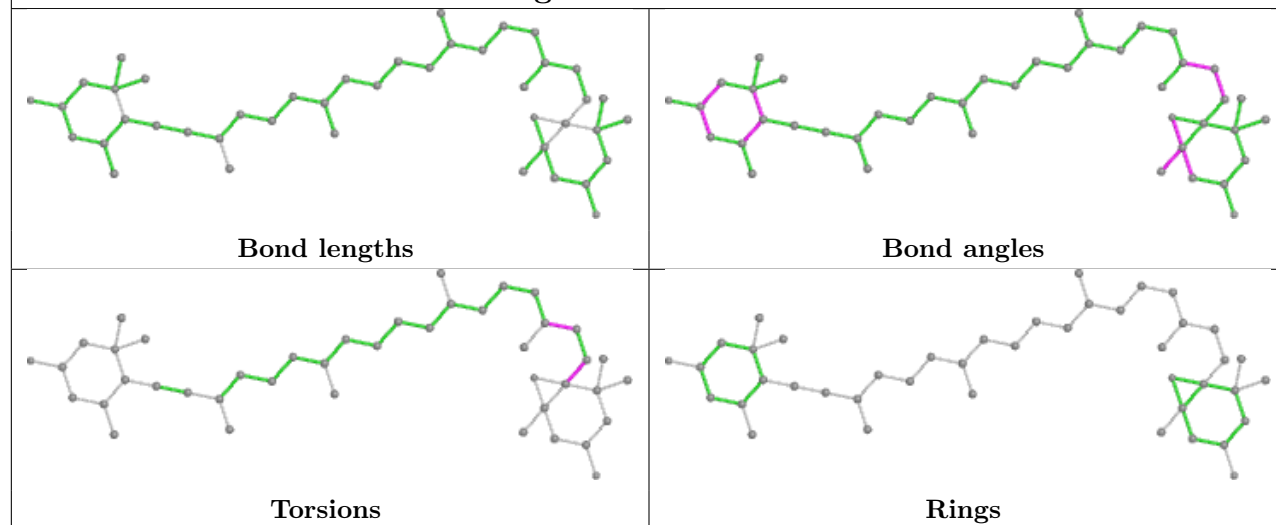
Ligand CLA v 313

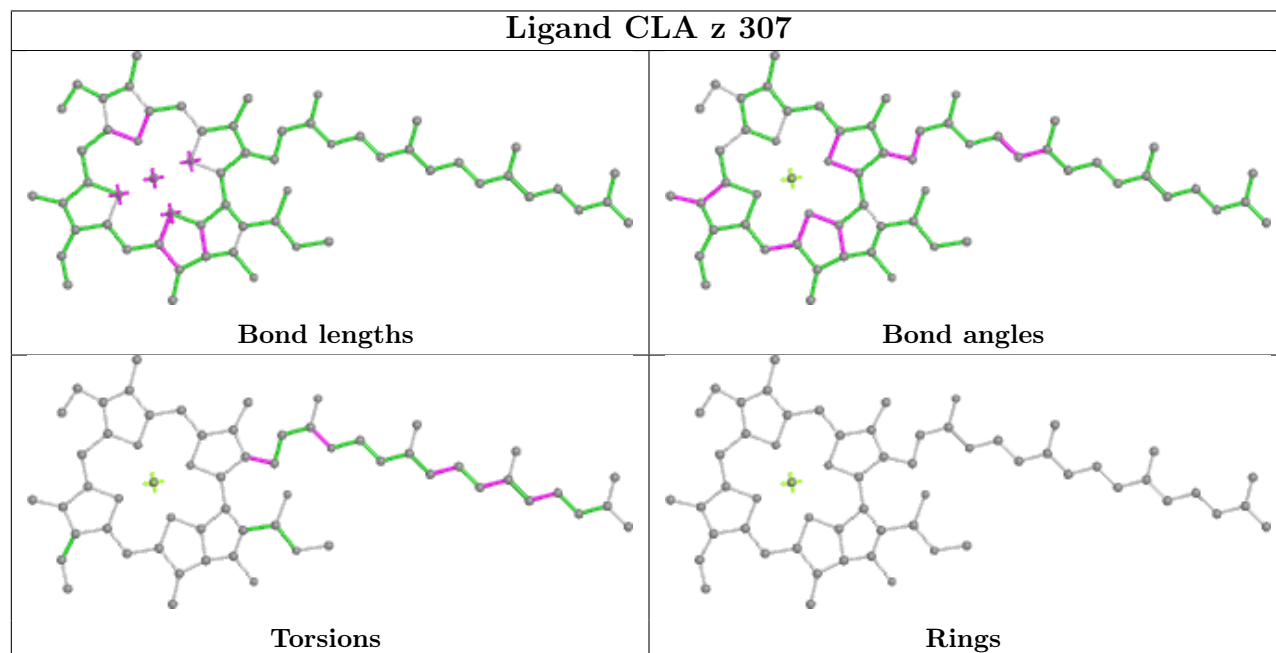
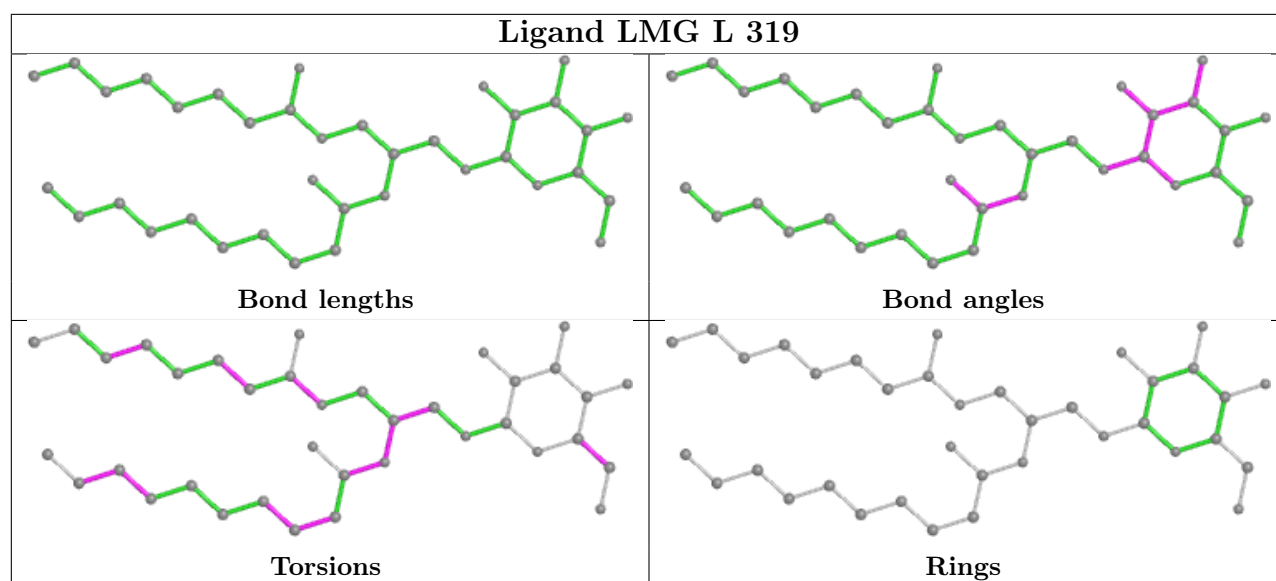


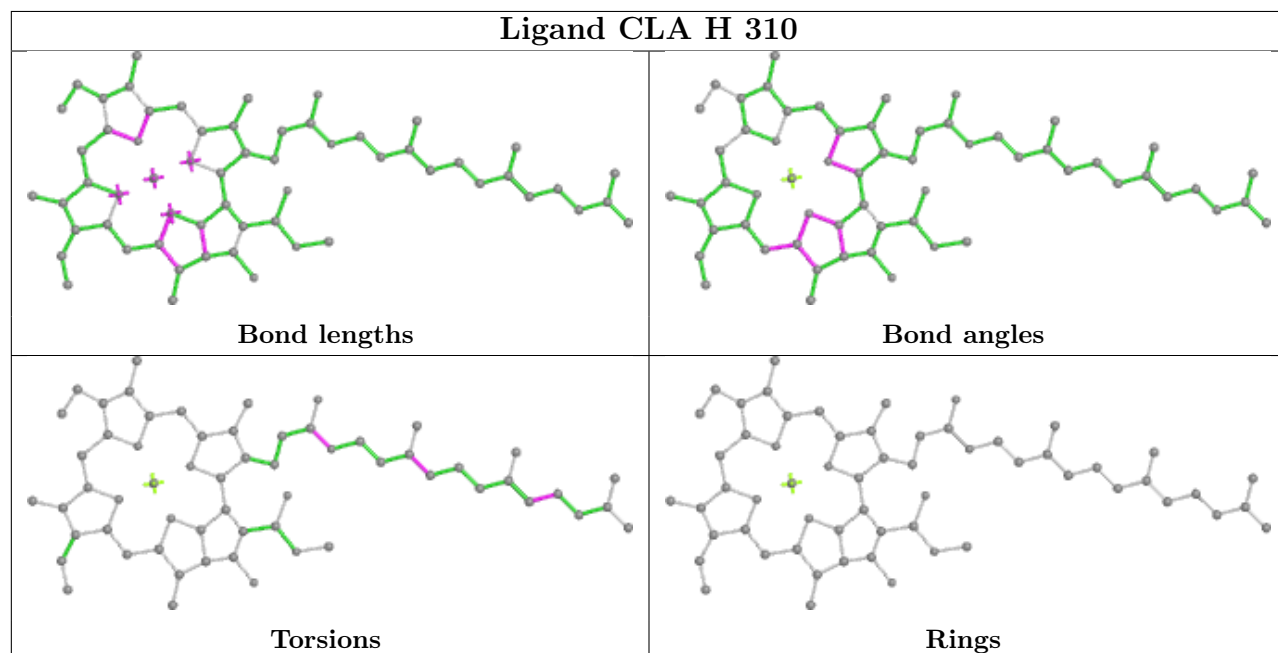
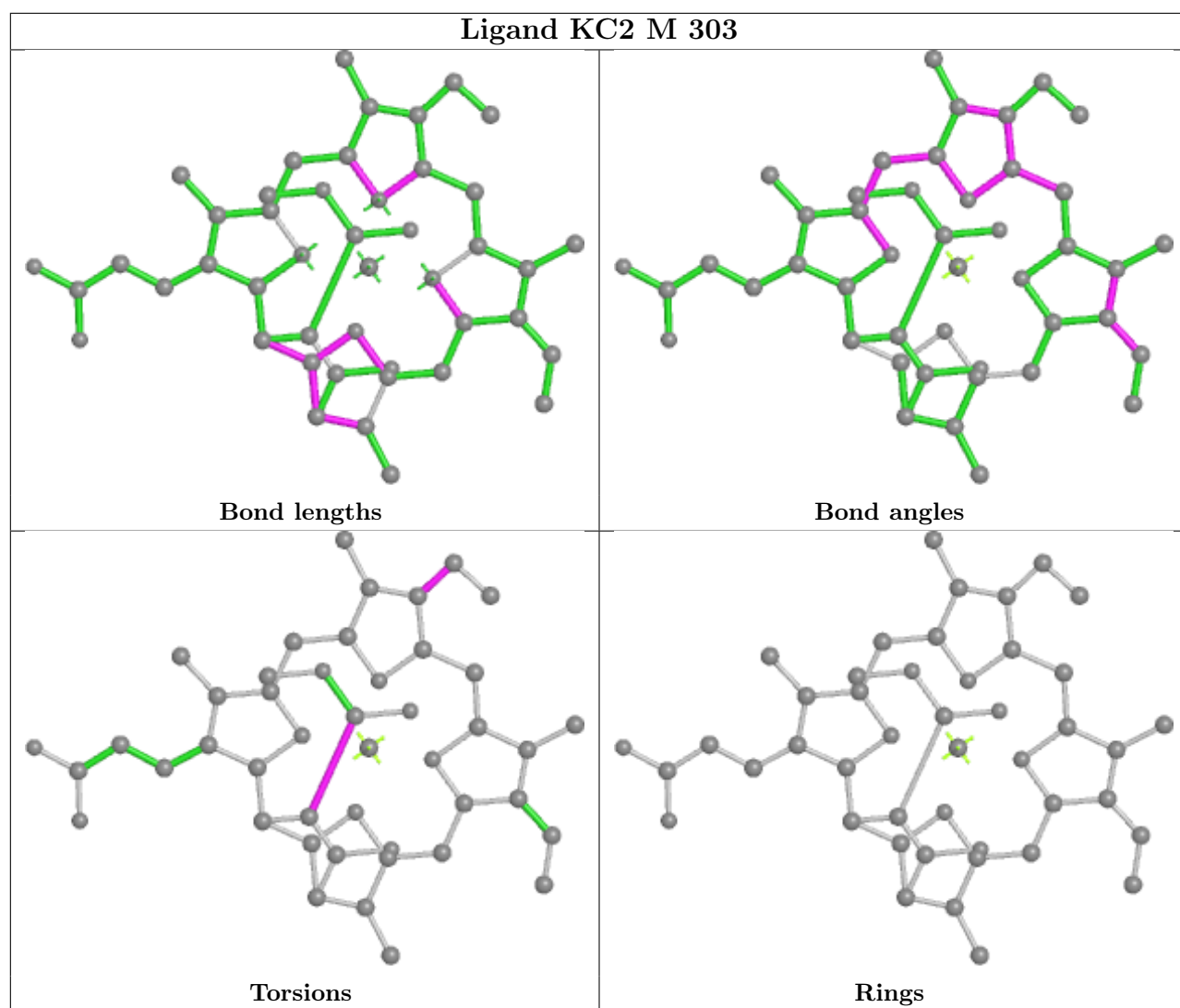
Ligand CLA b 813

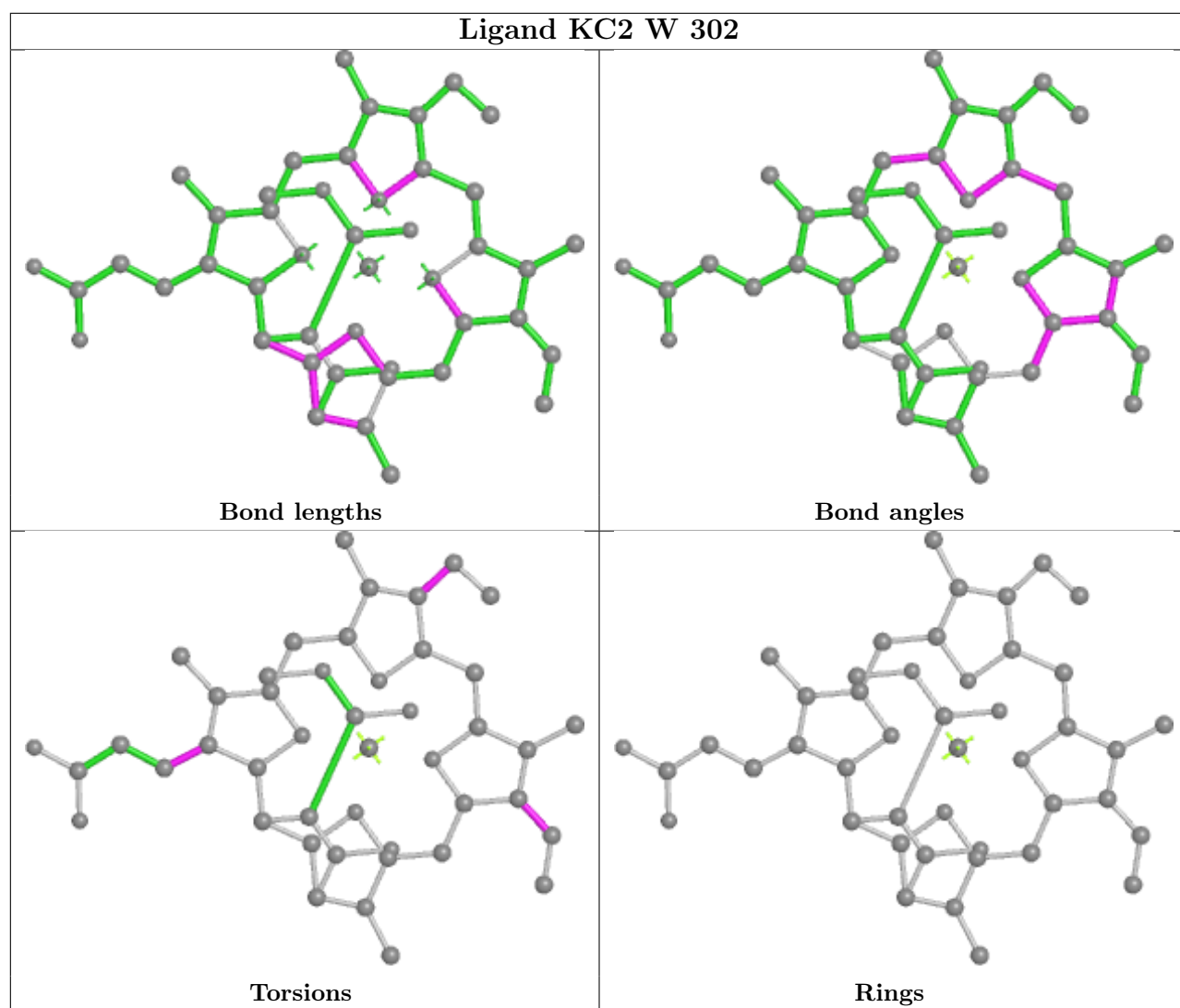


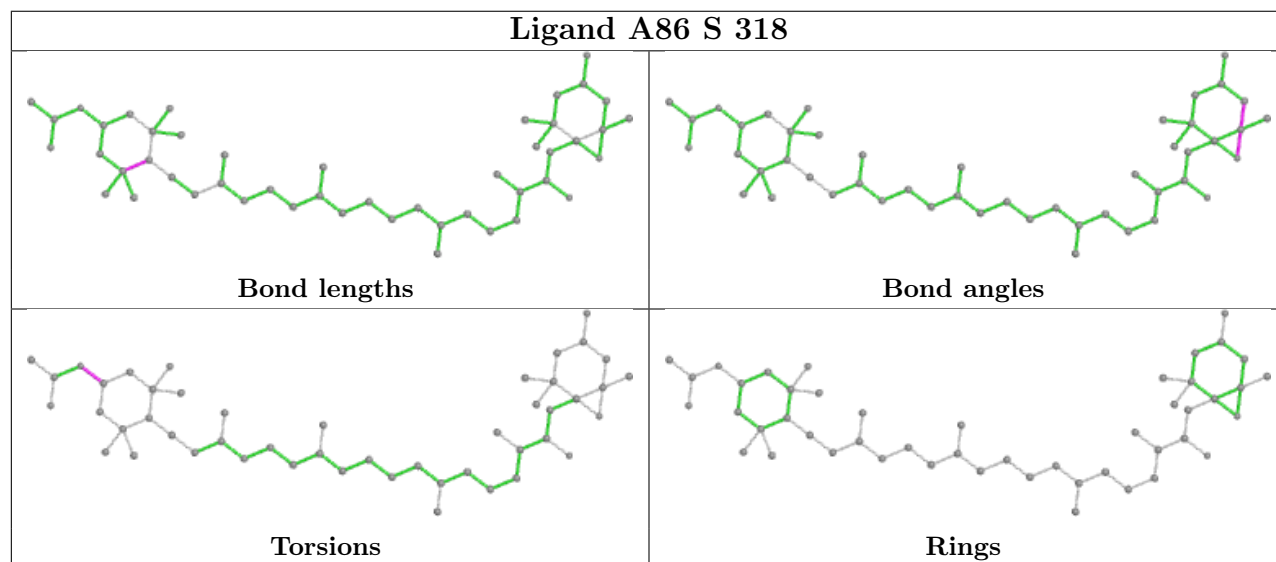
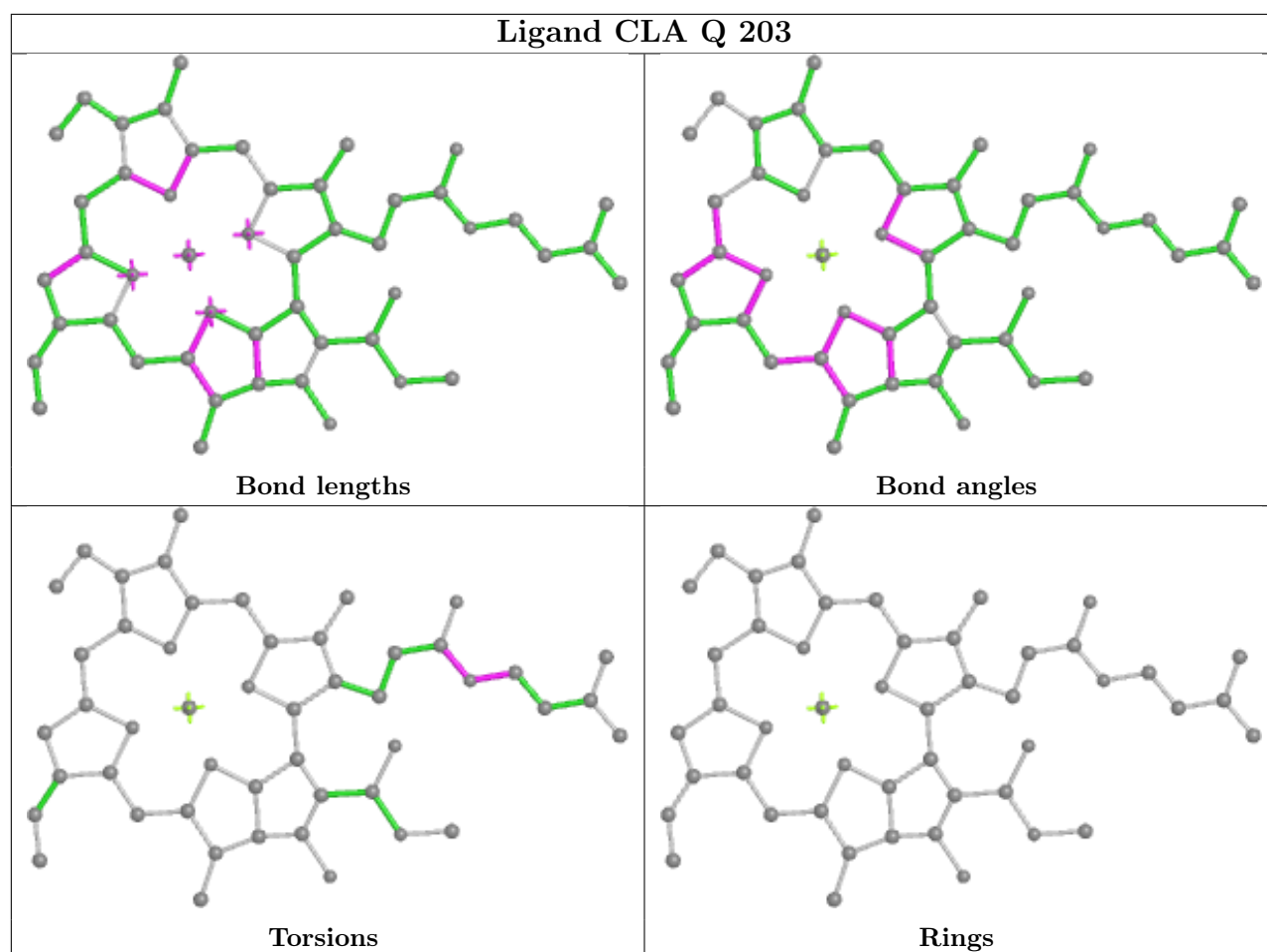
Ligand DD6 E 318

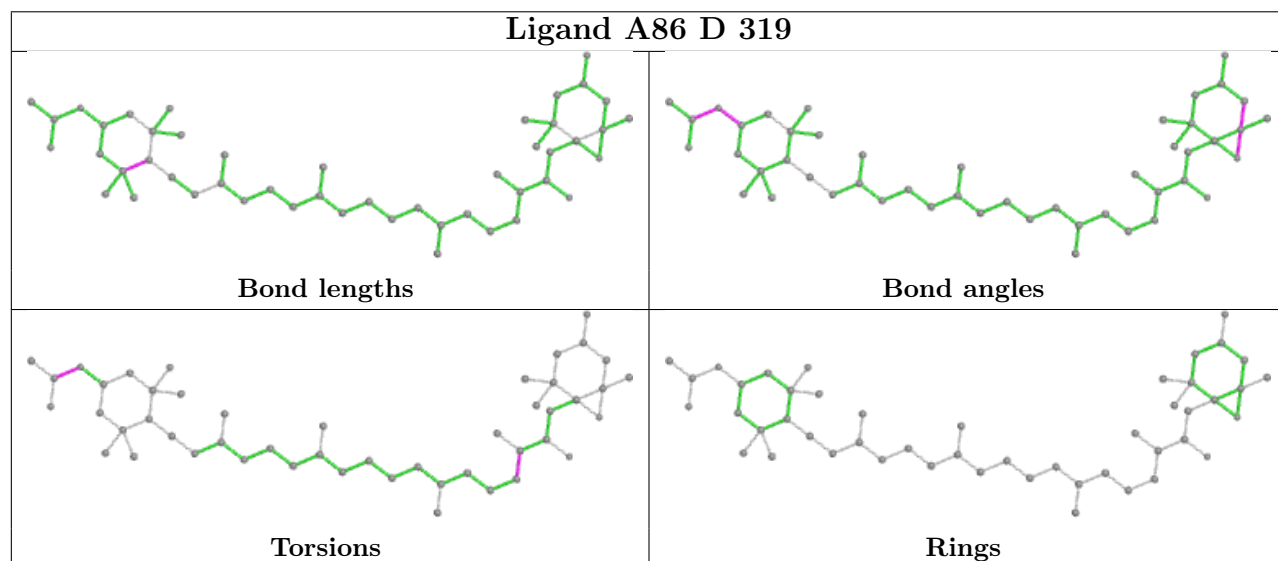
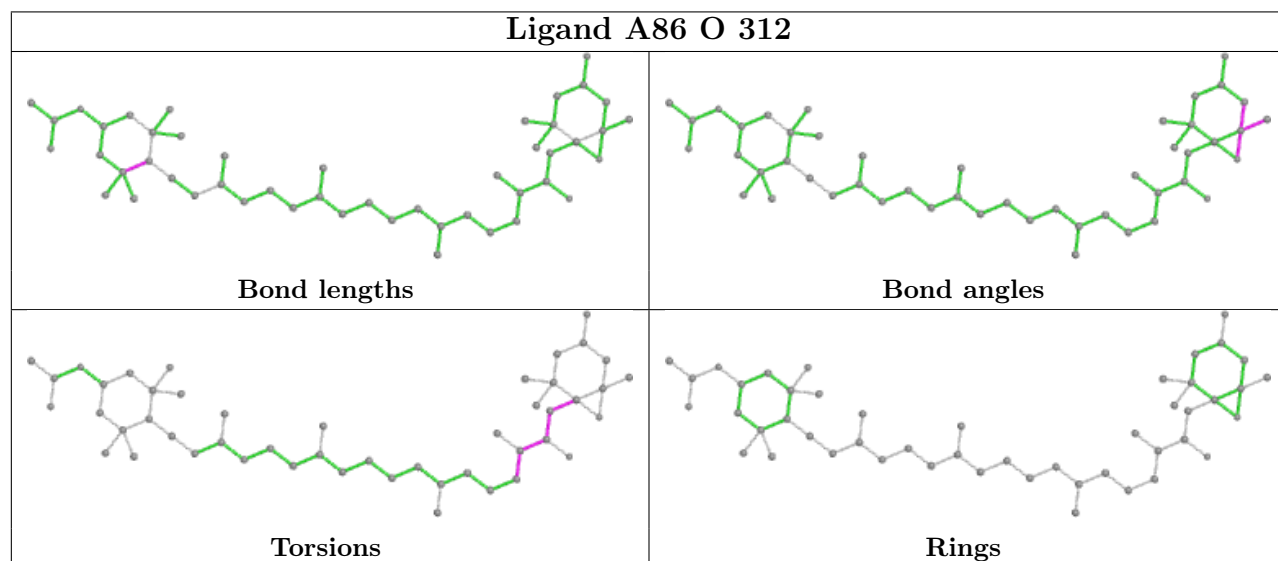
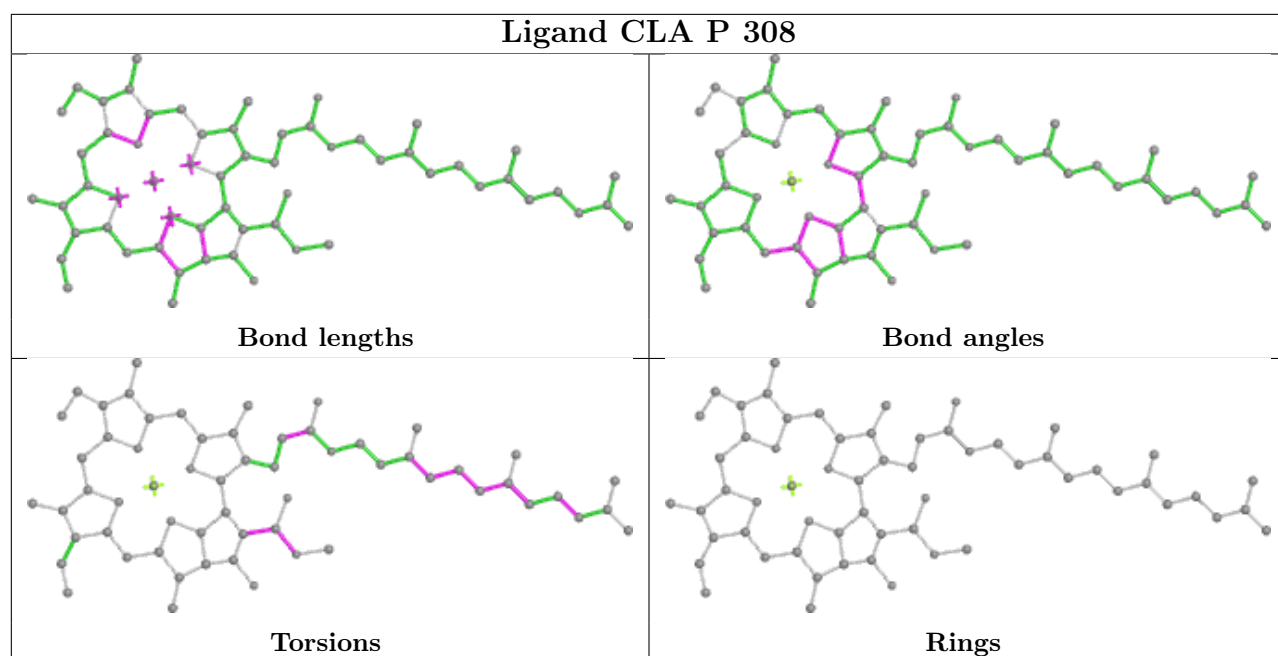




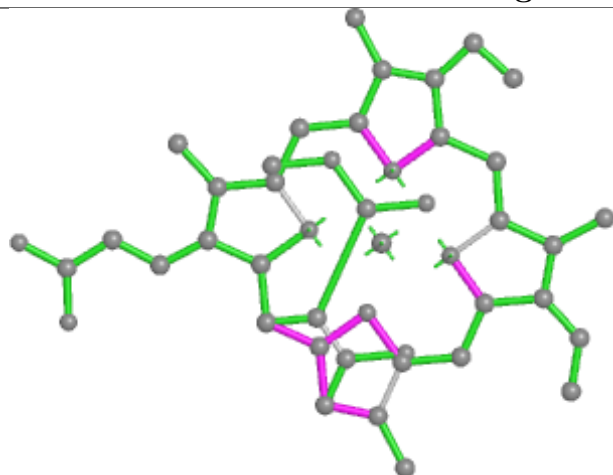




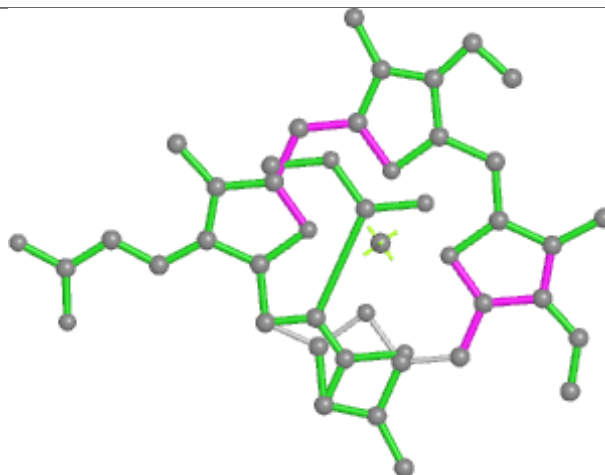




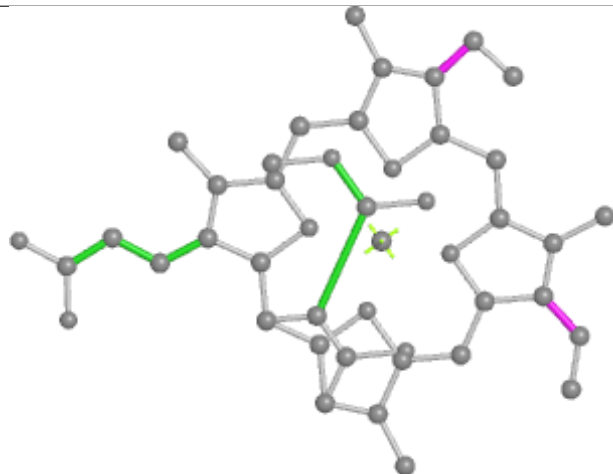
Ligand KC2 N 313



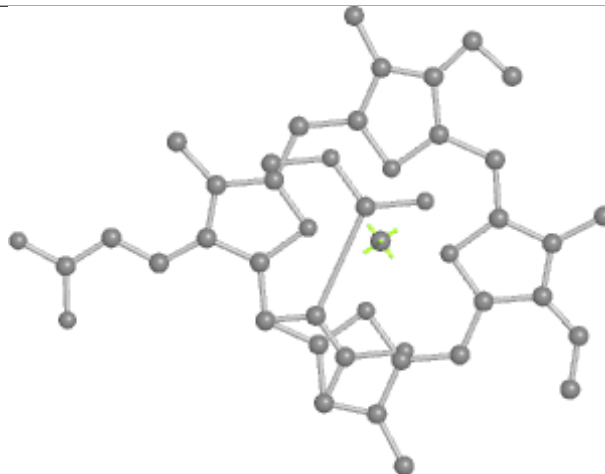
Bond lengths



Bond angles

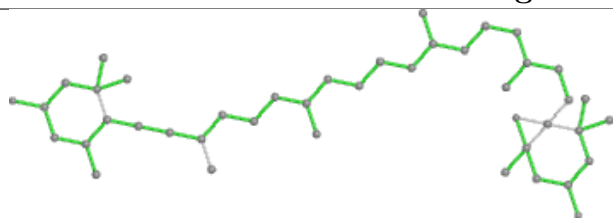


Torsions

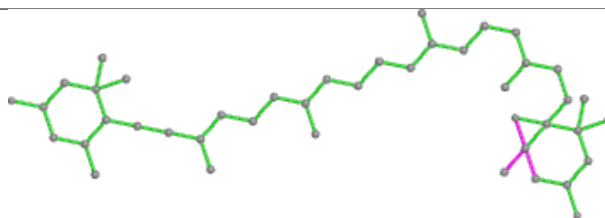


Rings

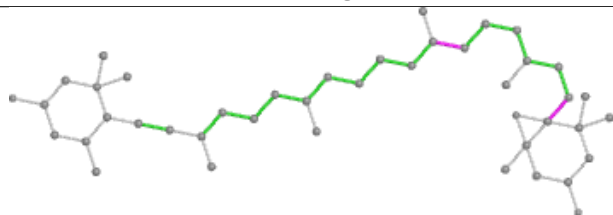
Ligand DD6 C 313



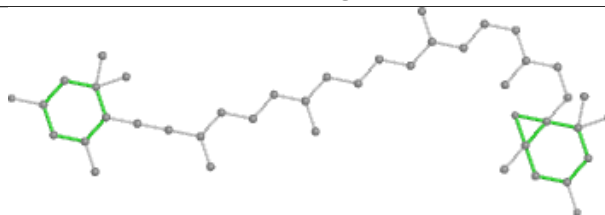
Bond lengths



Bond angles

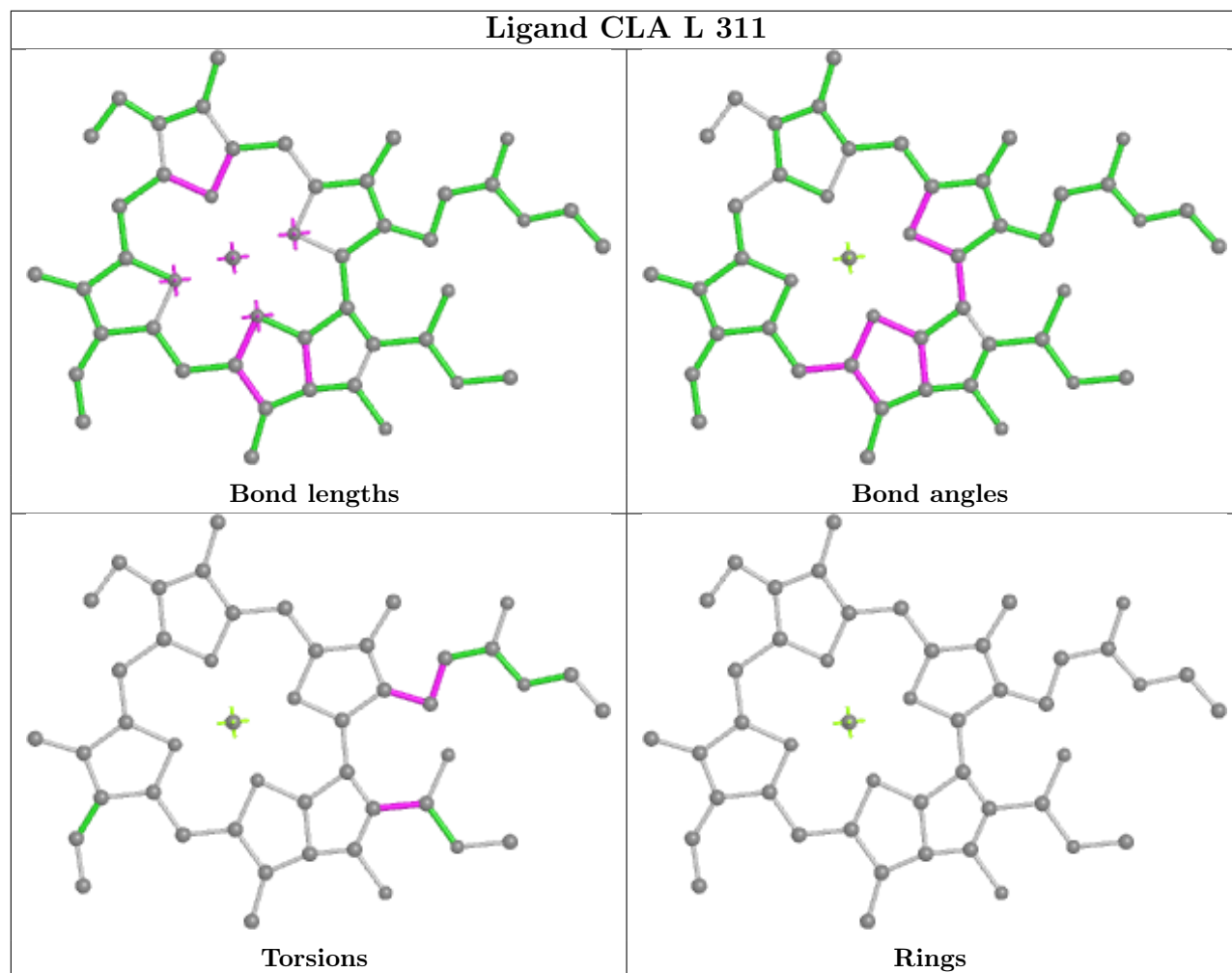


Torsions

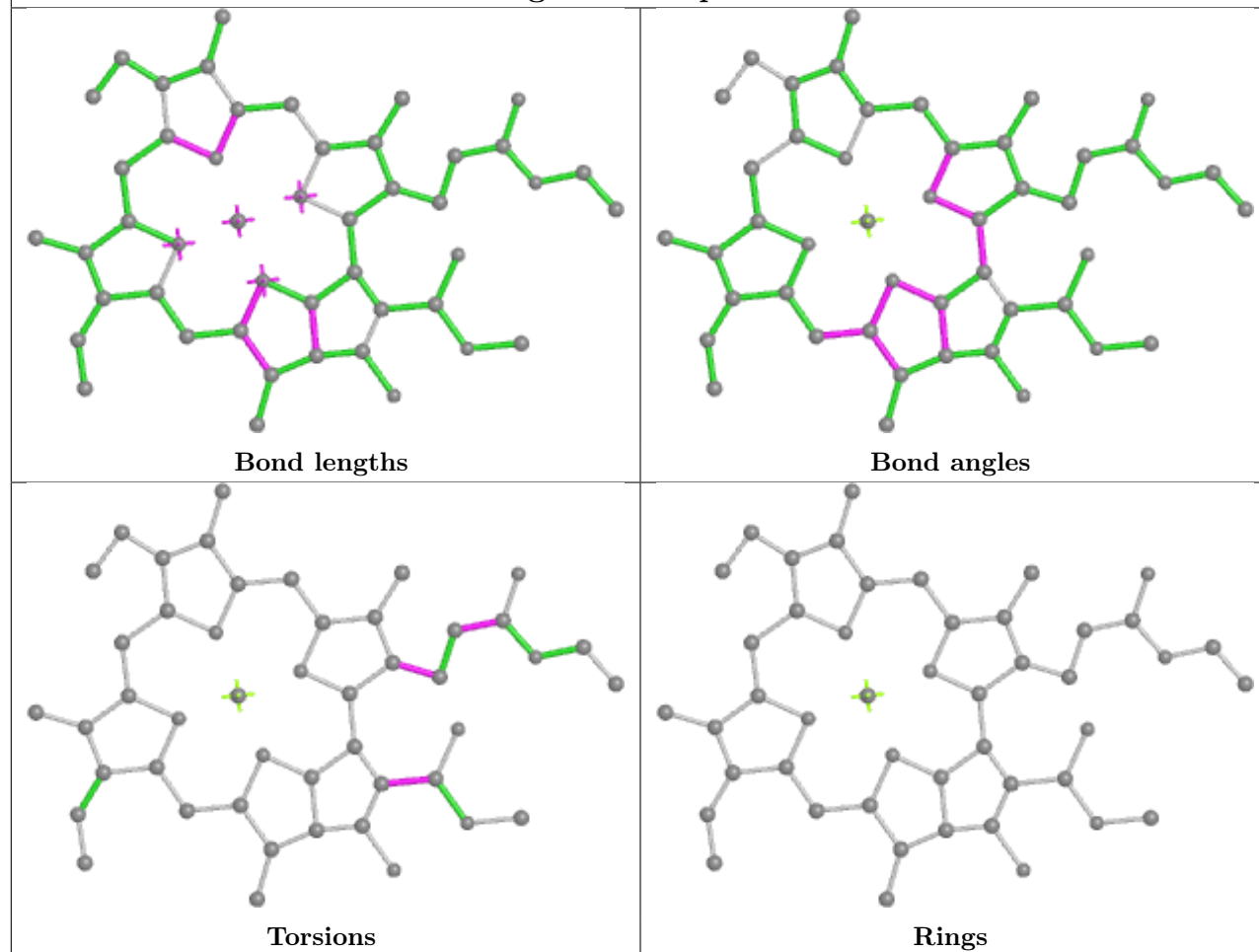


Rings

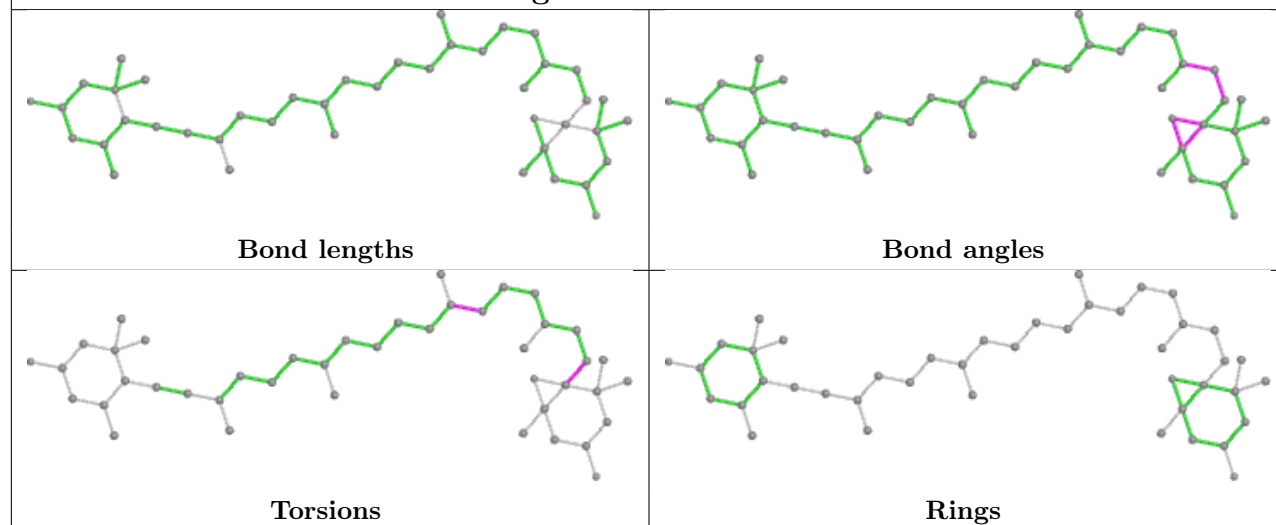
Ligand CLA L 311



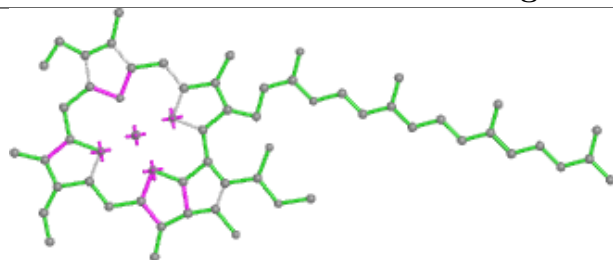
Ligand CLA p 306



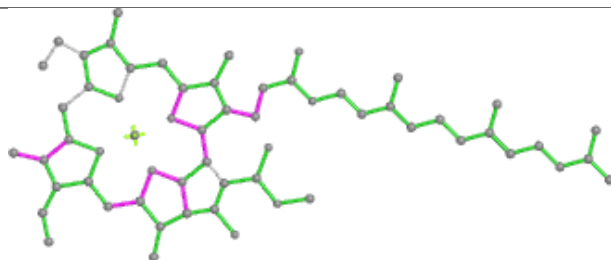
Ligand DD6 K 311



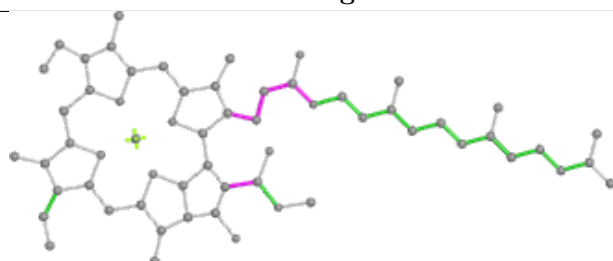
Ligand CLA t 304



Bond lengths



Bond angles

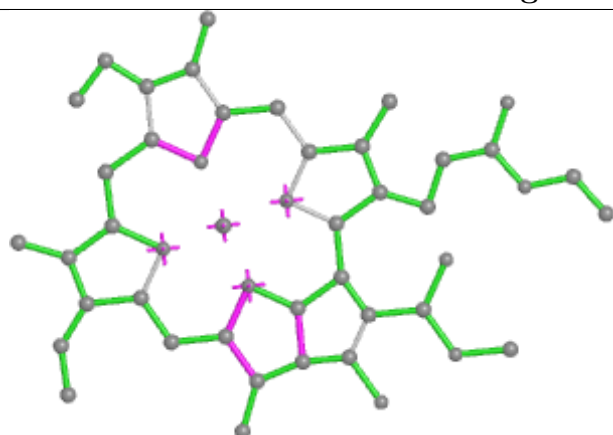


Torsions

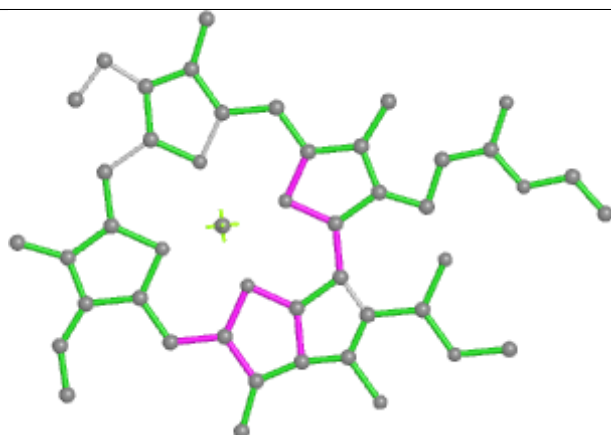


Rings

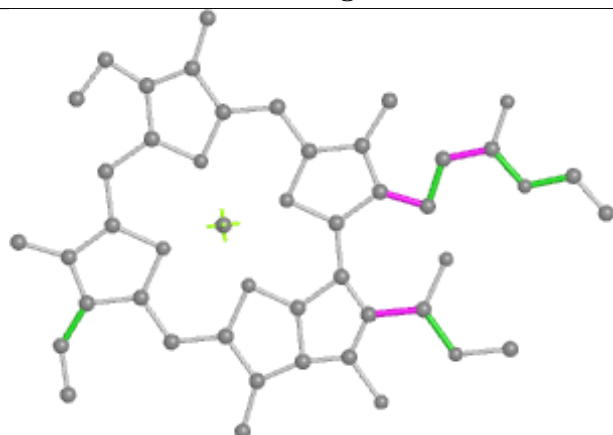
Ligand CLA I 207



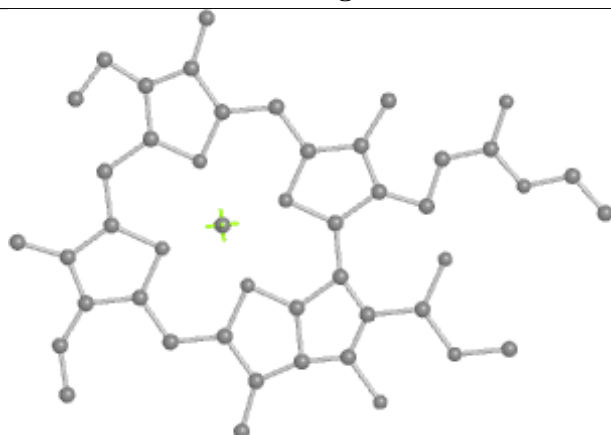
Bond lengths



Bond angles

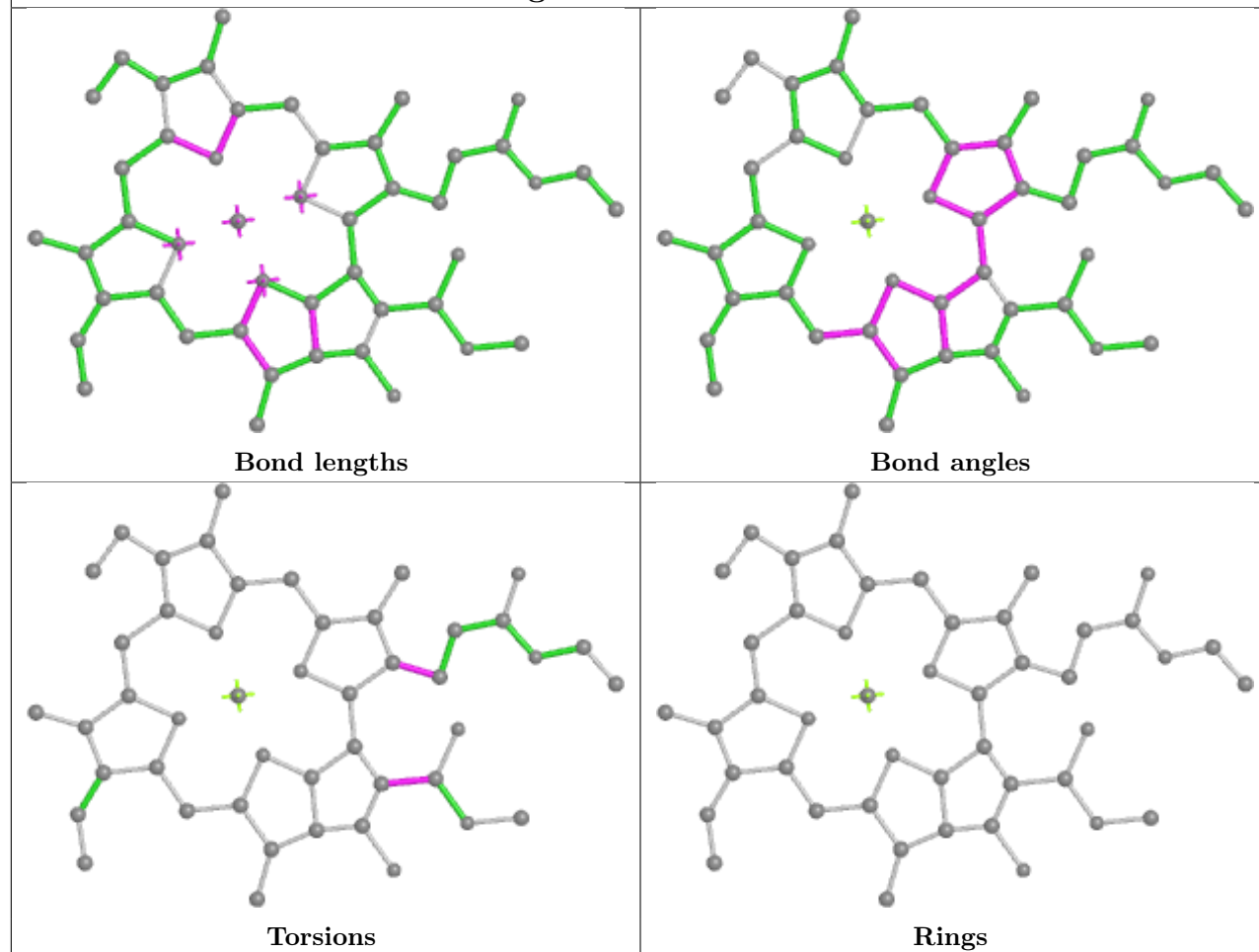


Torsions

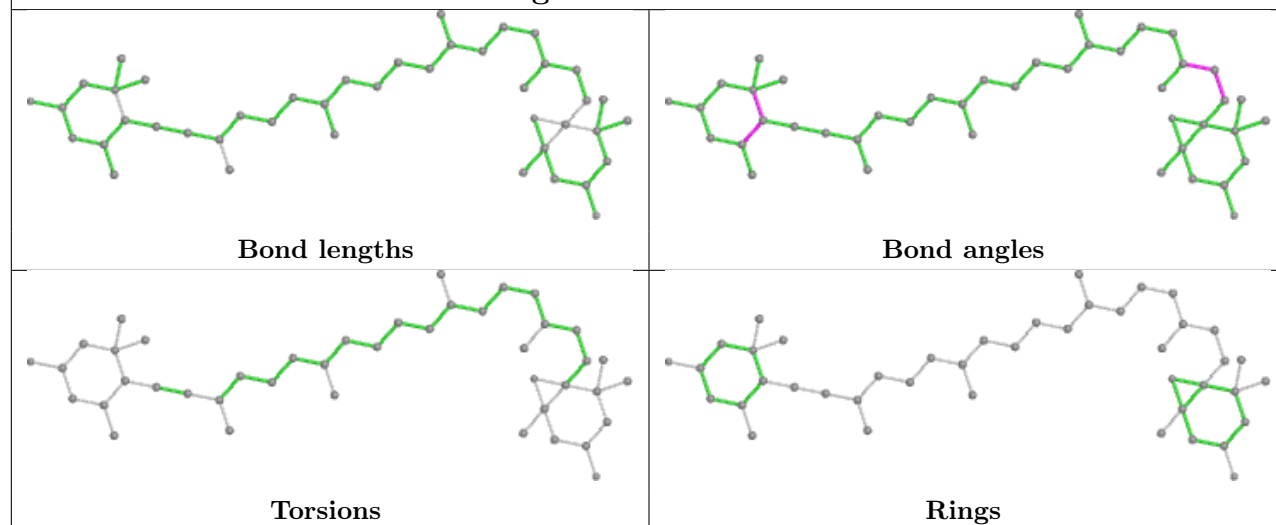


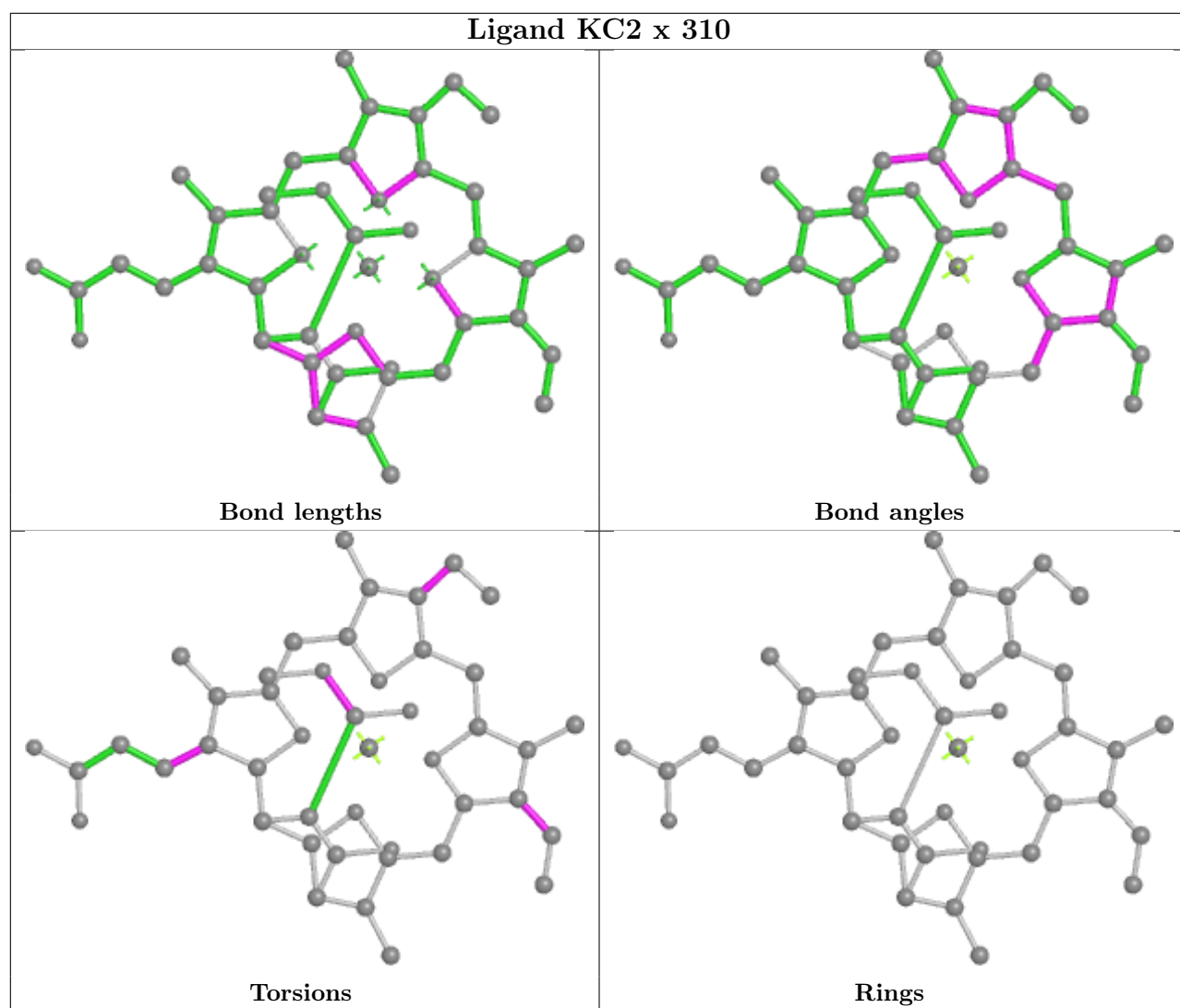
Rings

Ligand CLA S 312

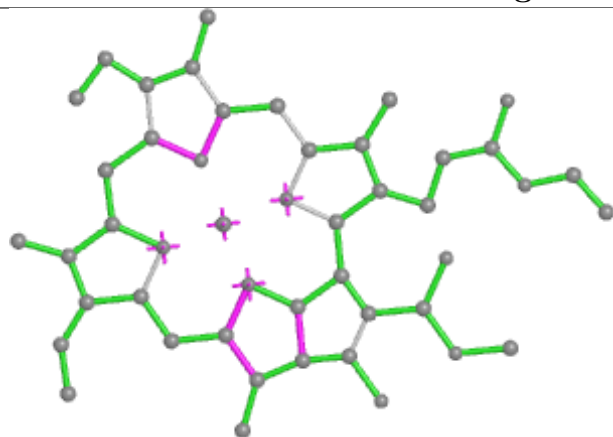


Ligand DD6 K 310

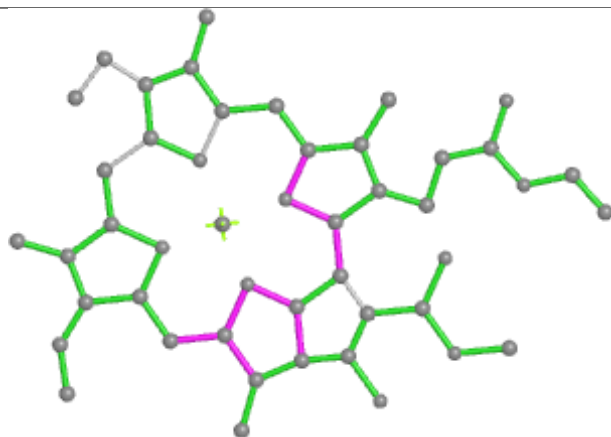




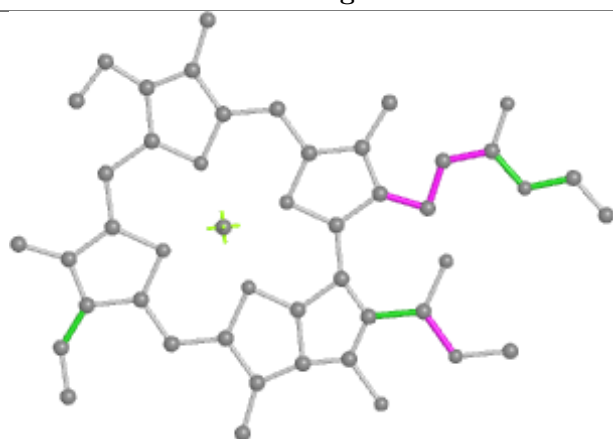
Ligand CLA B 304



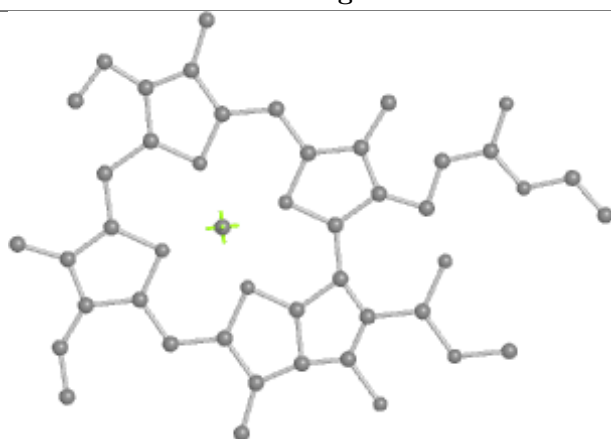
Bond lengths



Bond angles

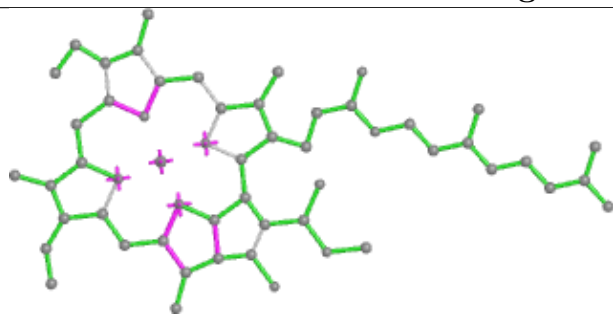


Torsions

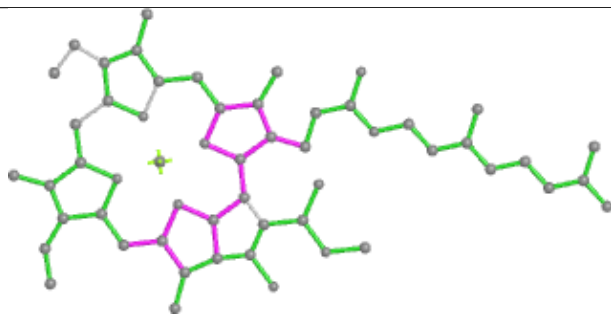


Rings

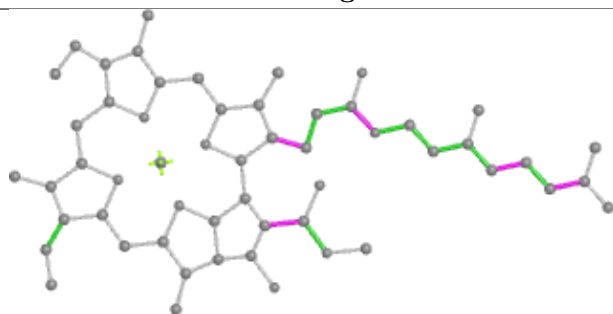
Ligand CLA o 310



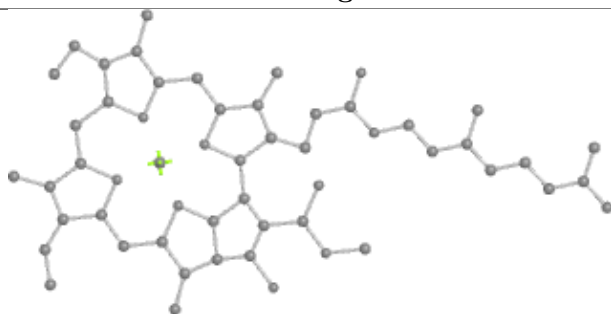
Bond lengths



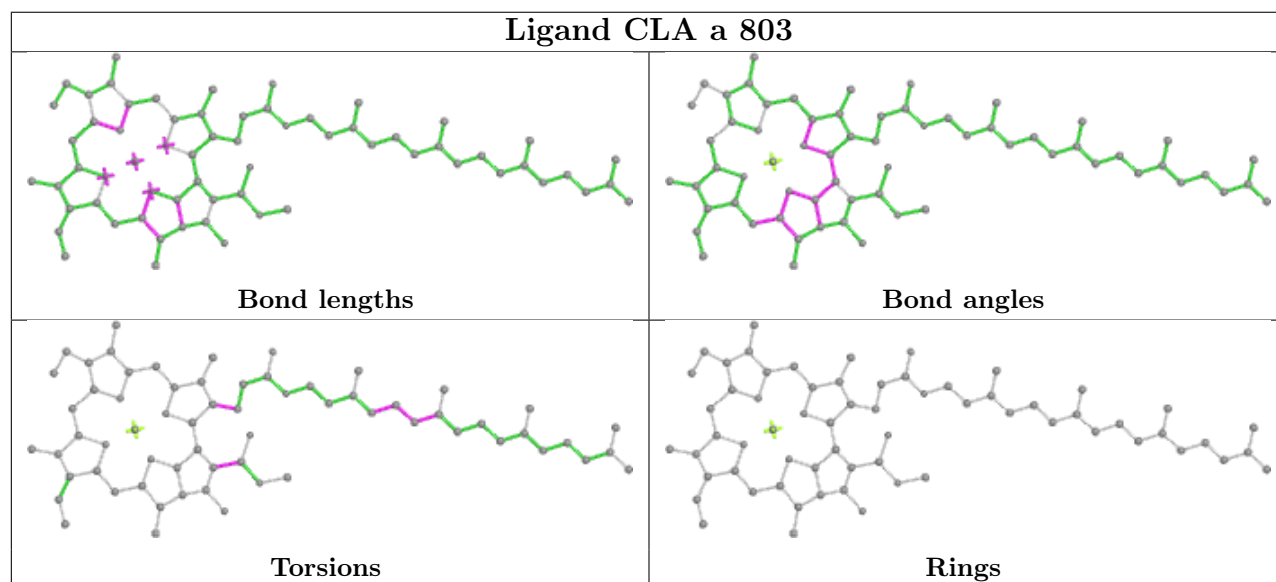
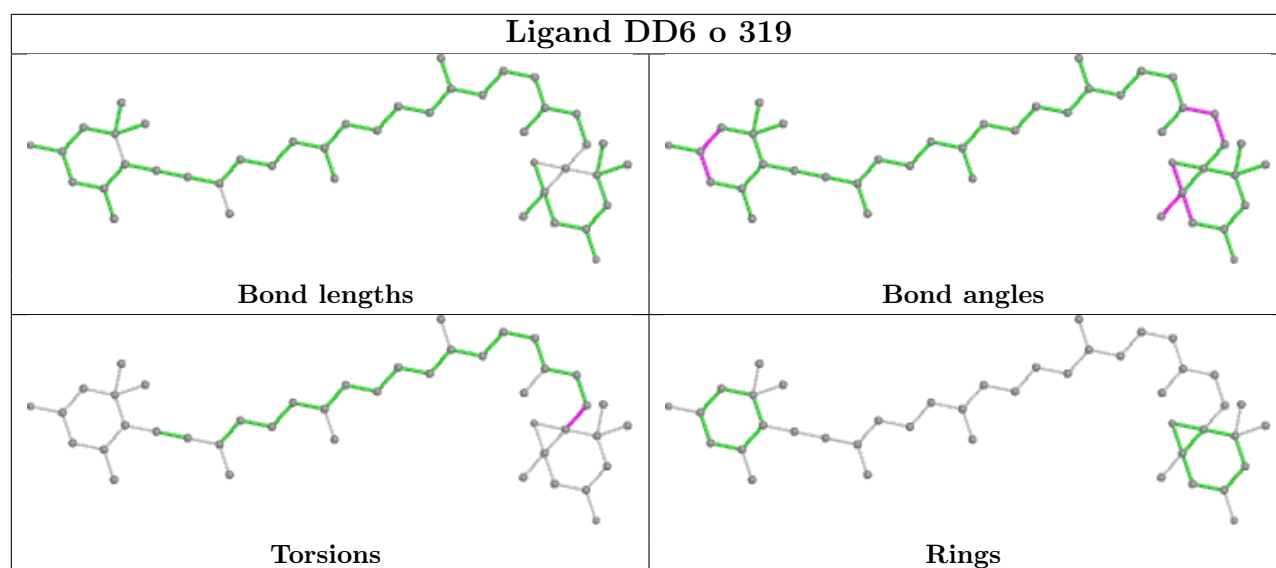
Bond angles

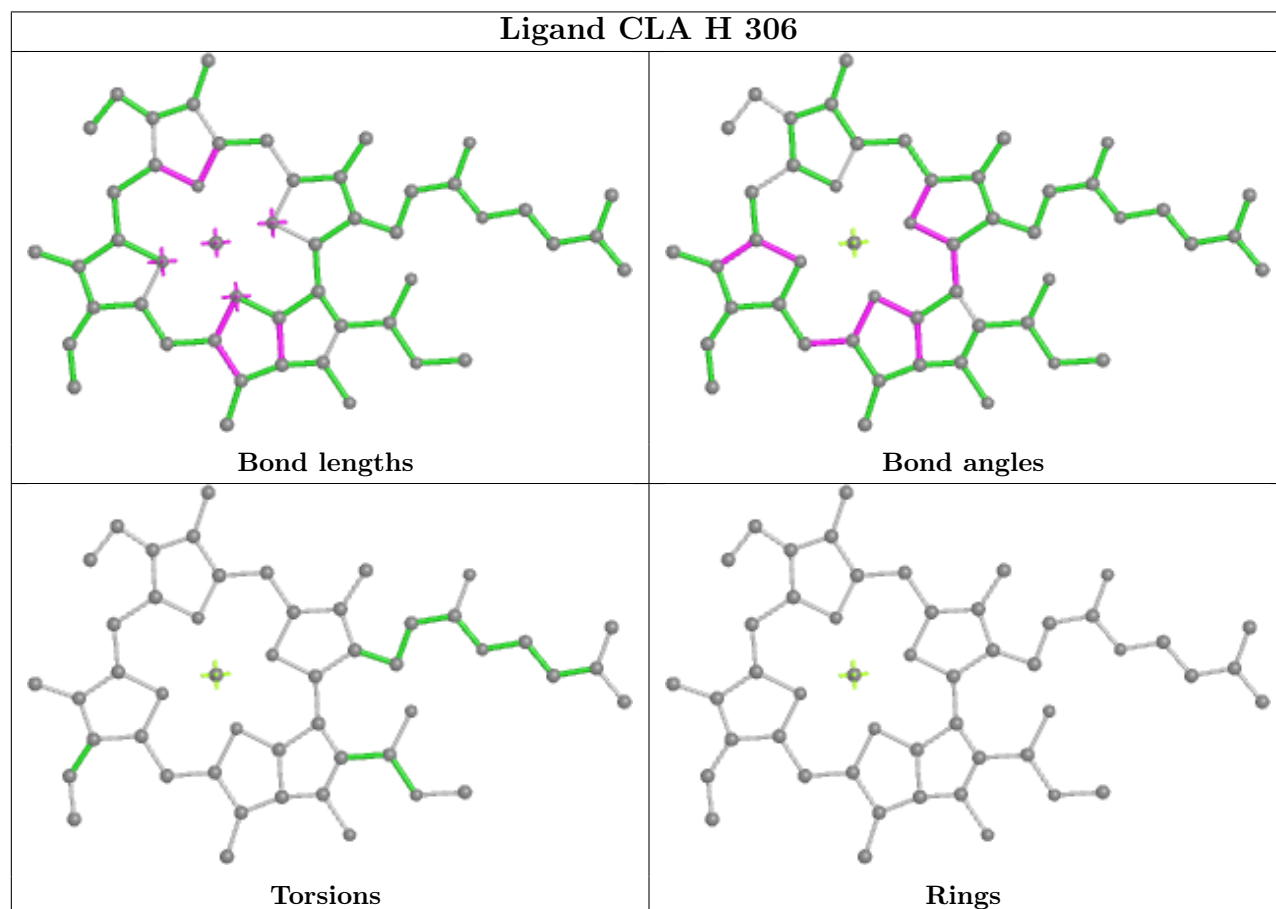
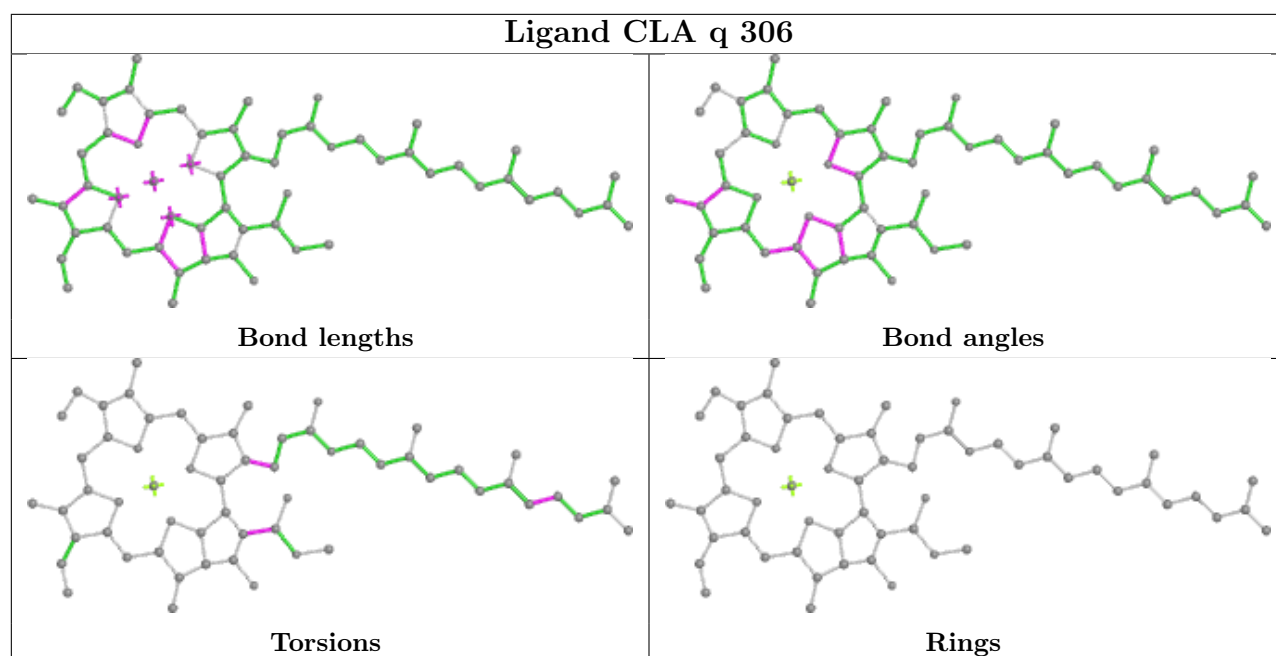


Torsions

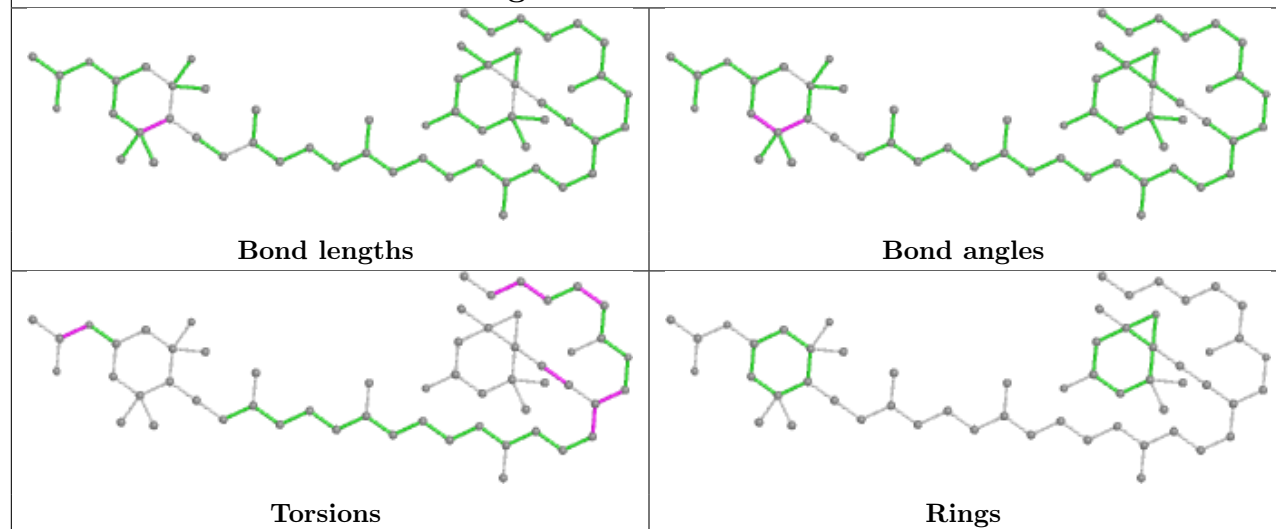


Rings

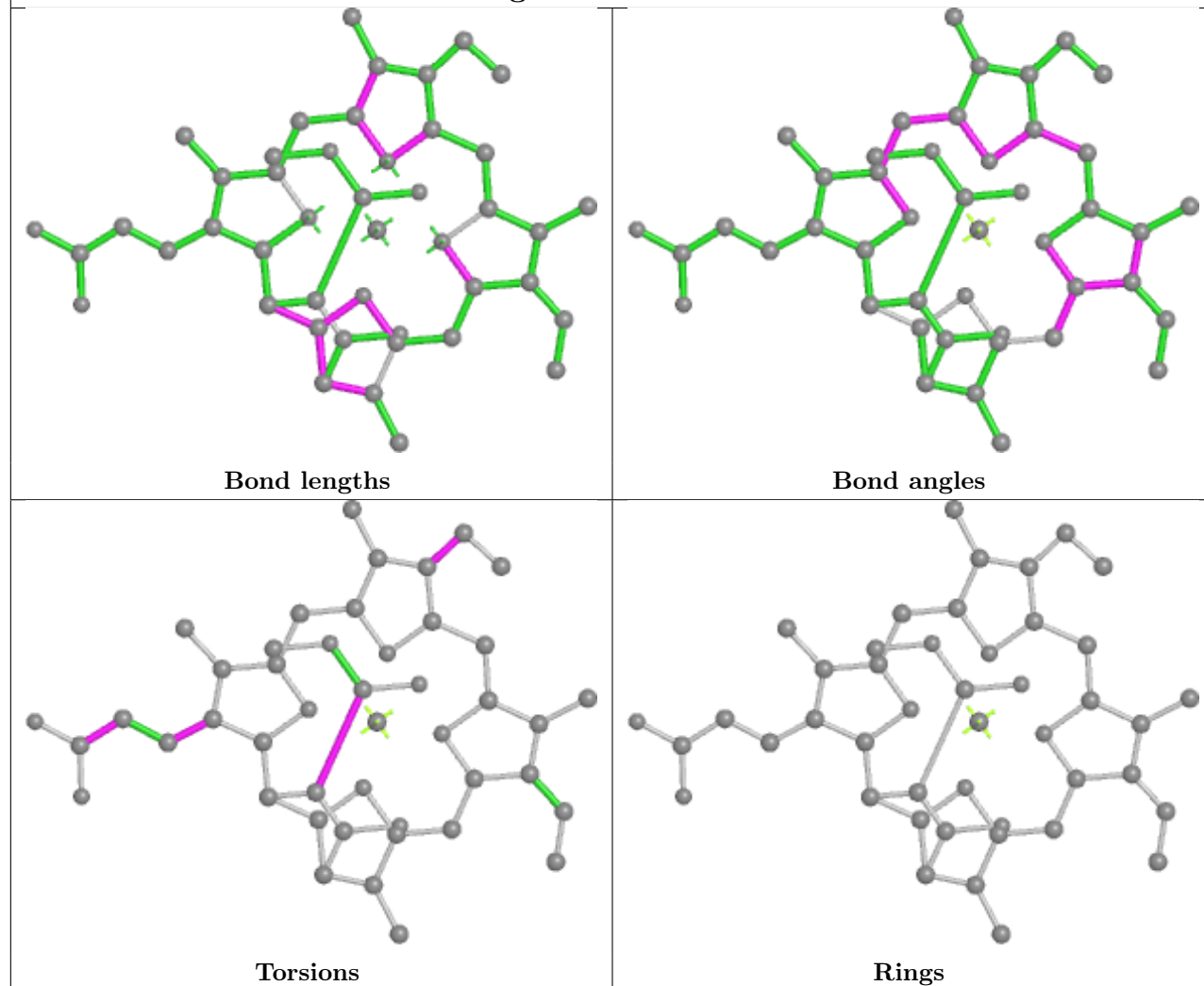


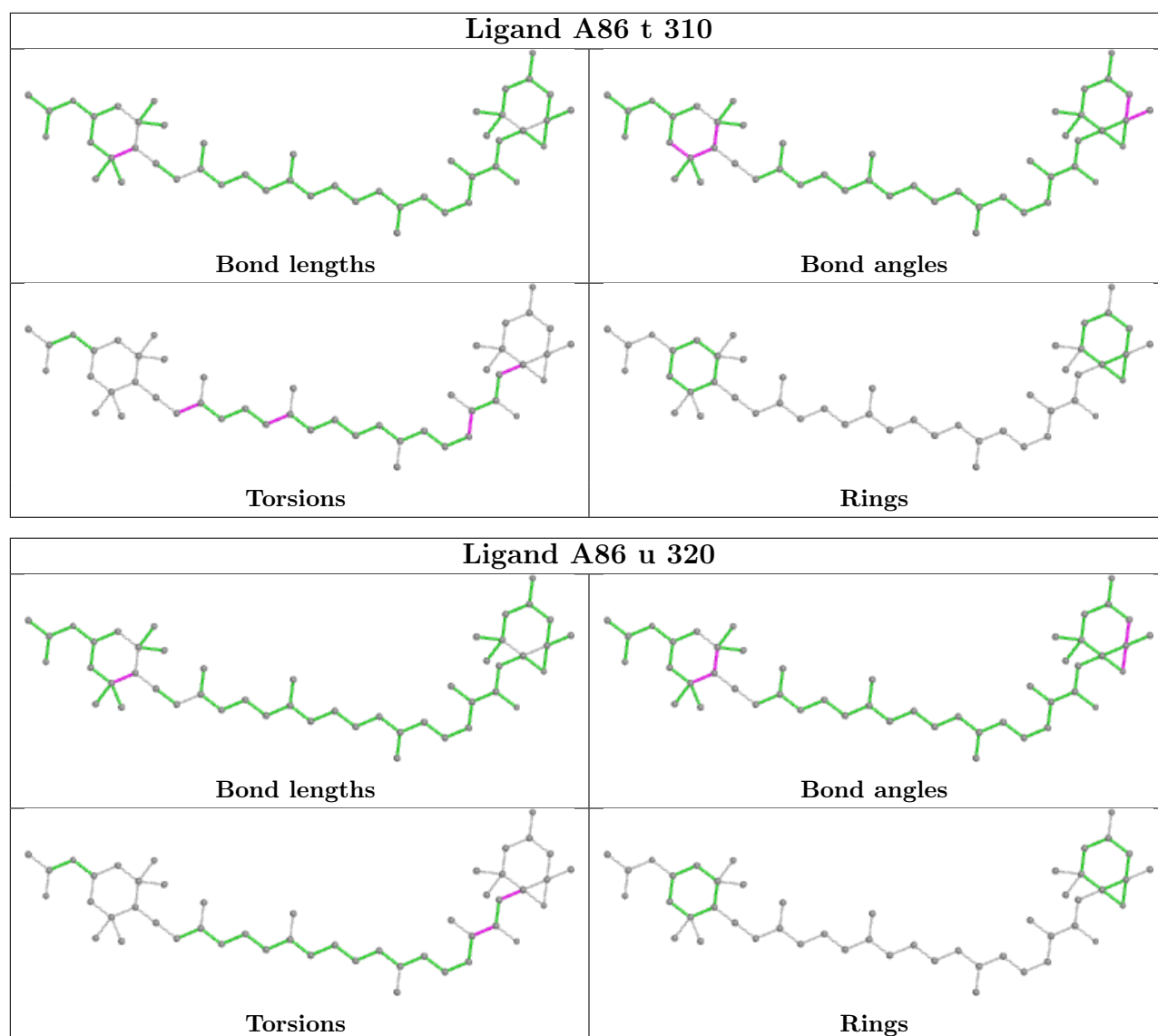


Ligand A1EB4 W 319

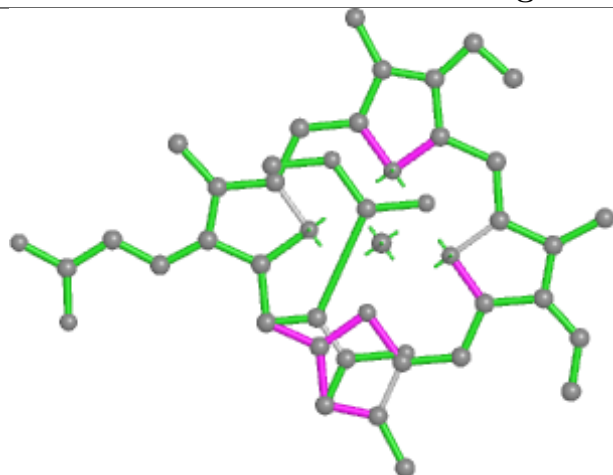


Ligand KC2 t 301

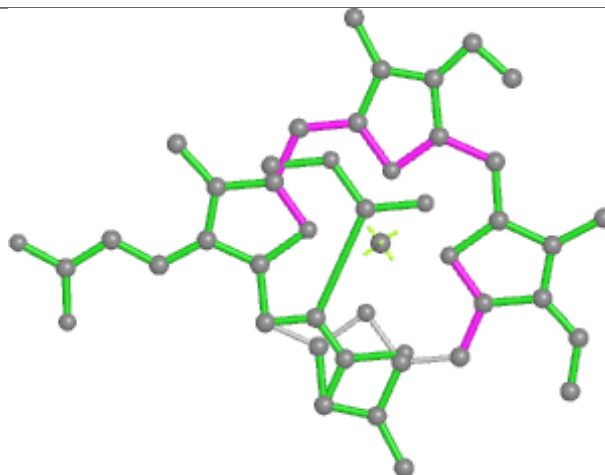




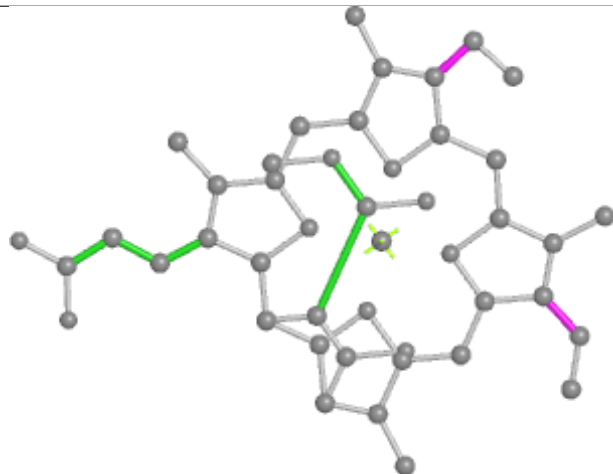
Ligand KC2 T 301



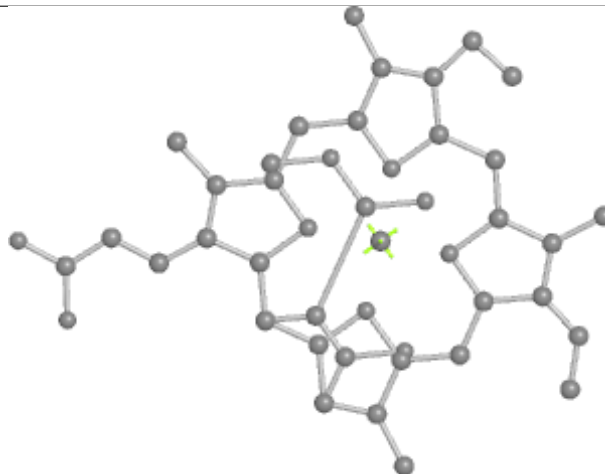
Bond lengths



Bond angles

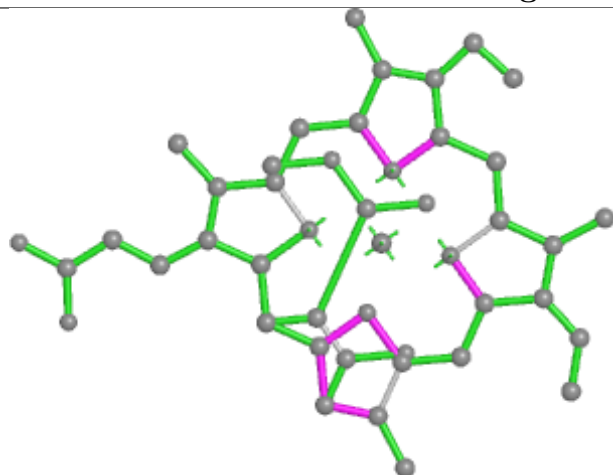


Torsions

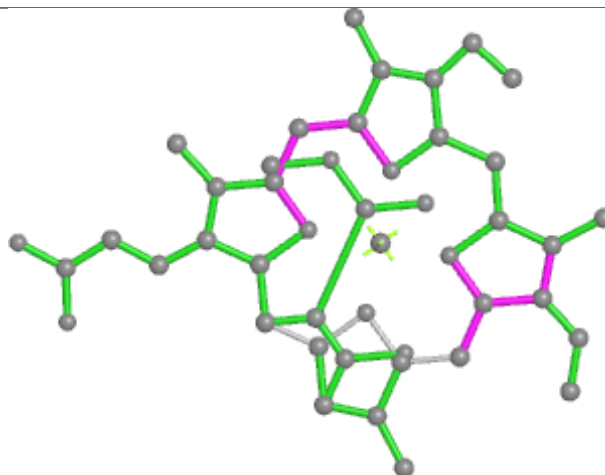


Rings

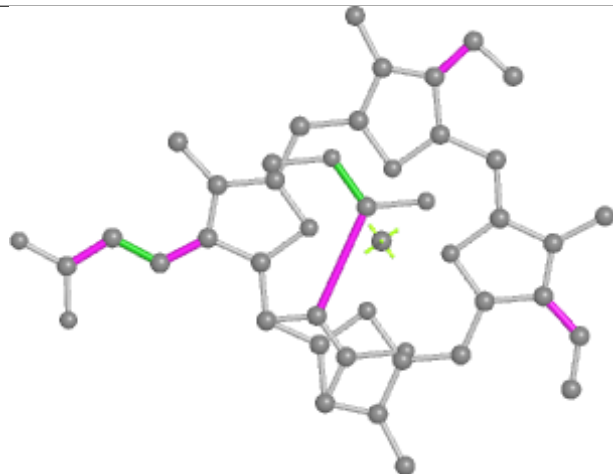
Ligand KC2 v 308



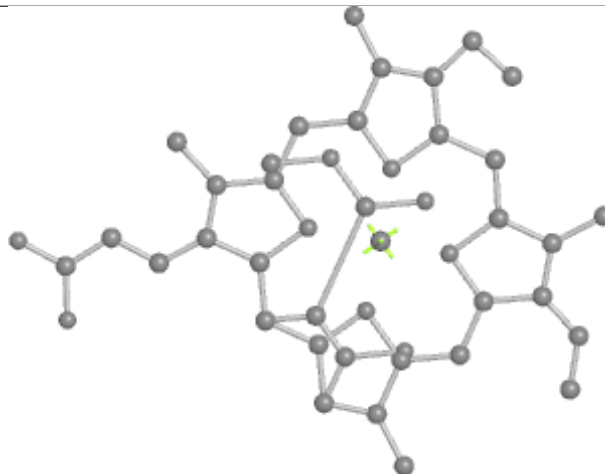
Bond lengths



Bond angles

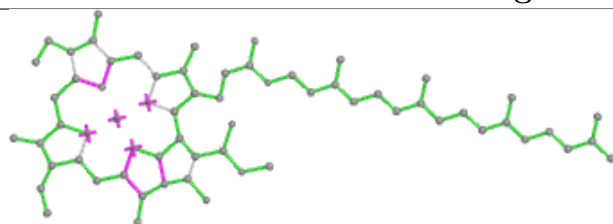


Torsions

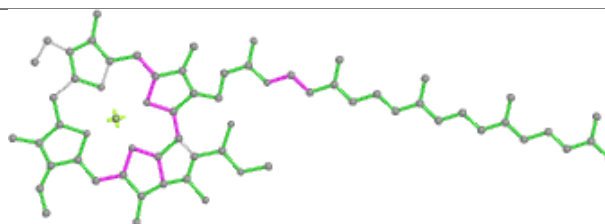


Rings

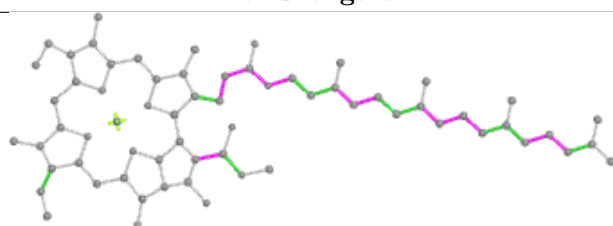
Ligand CLA C 306



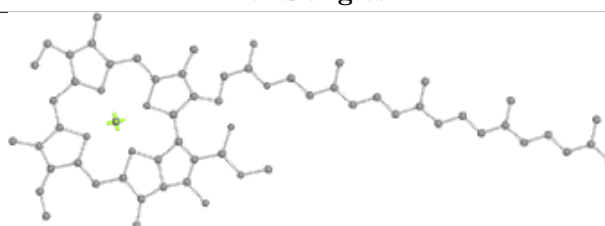
Bond lengths



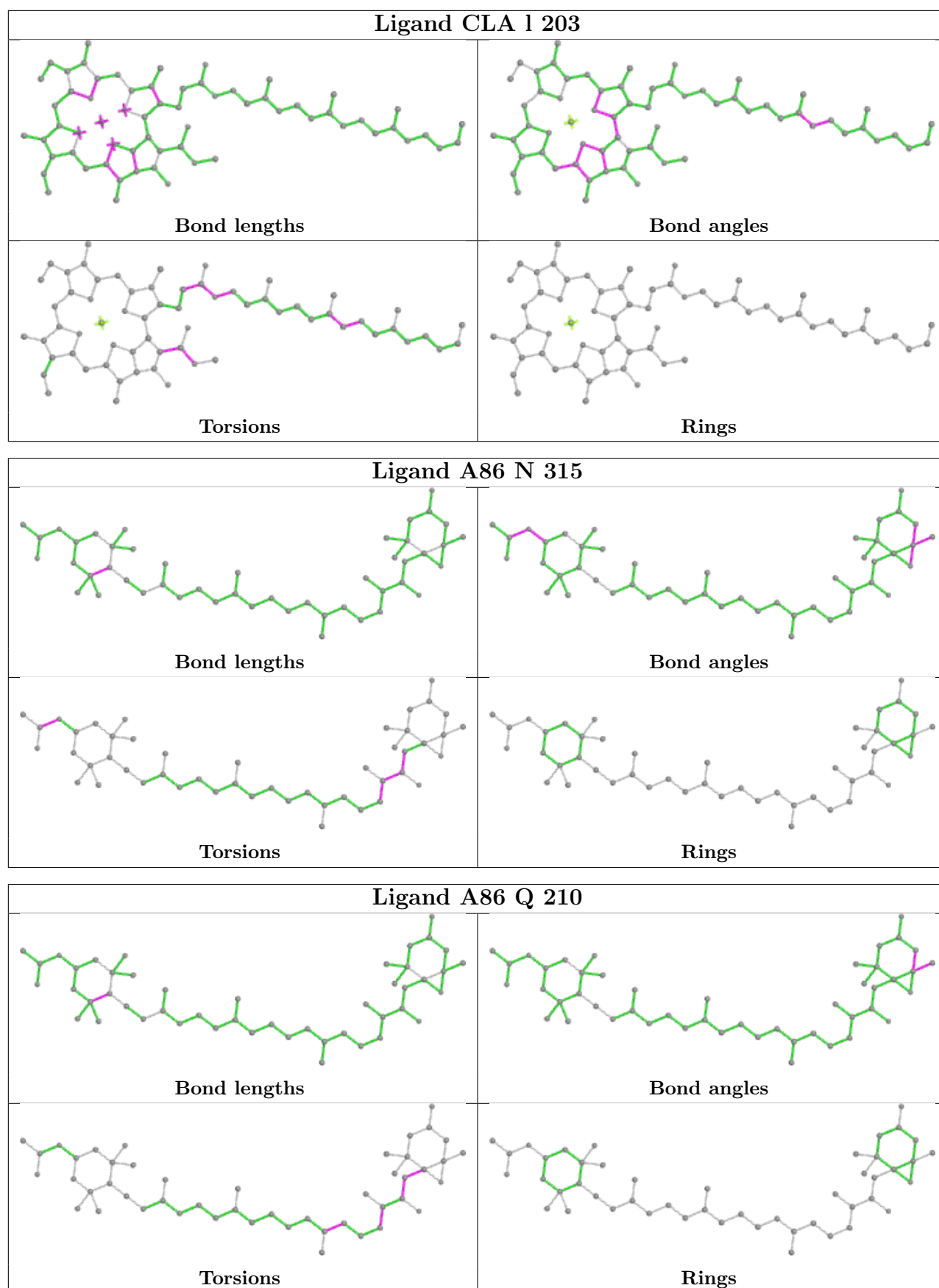
Bond angles

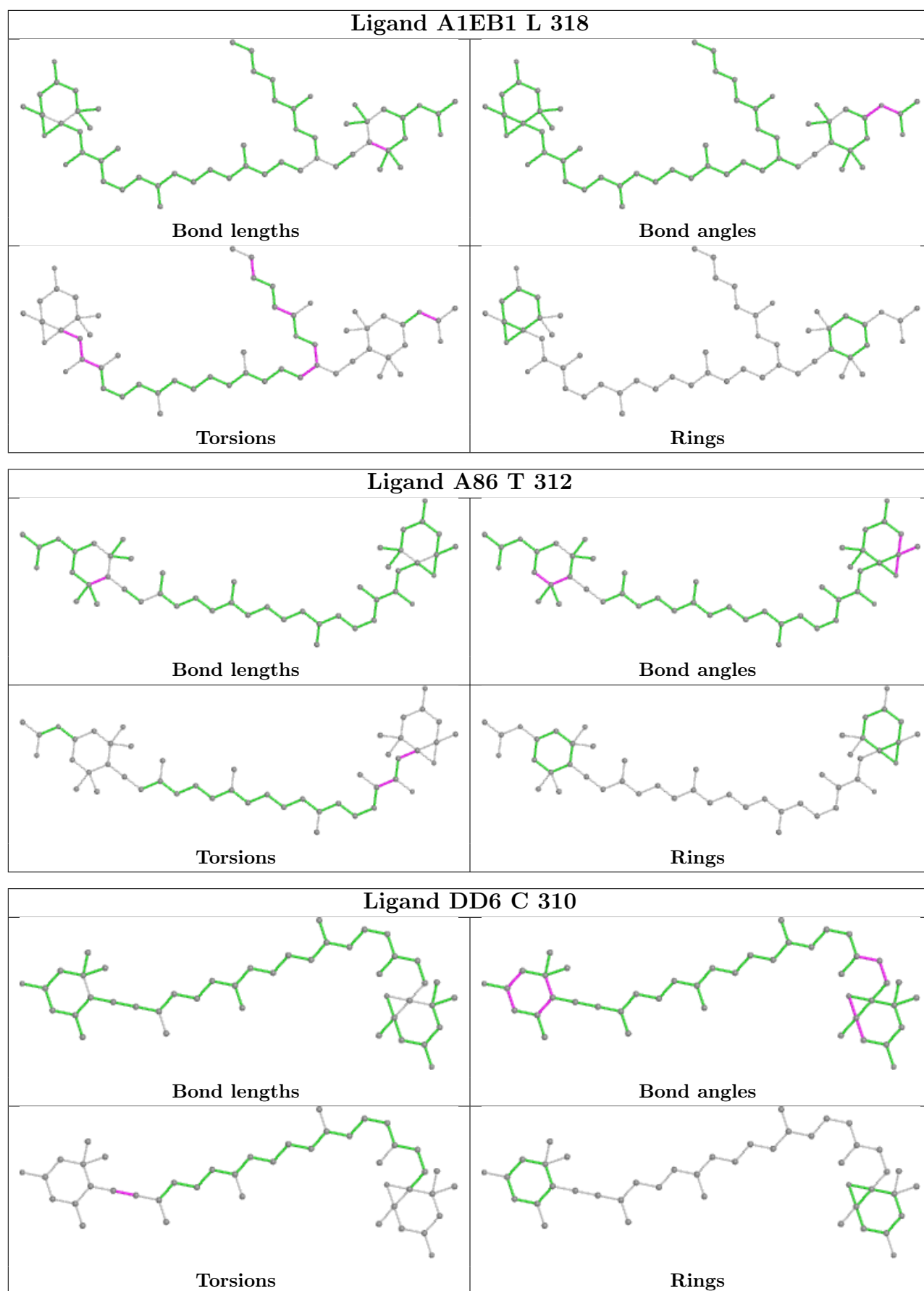


Torsions

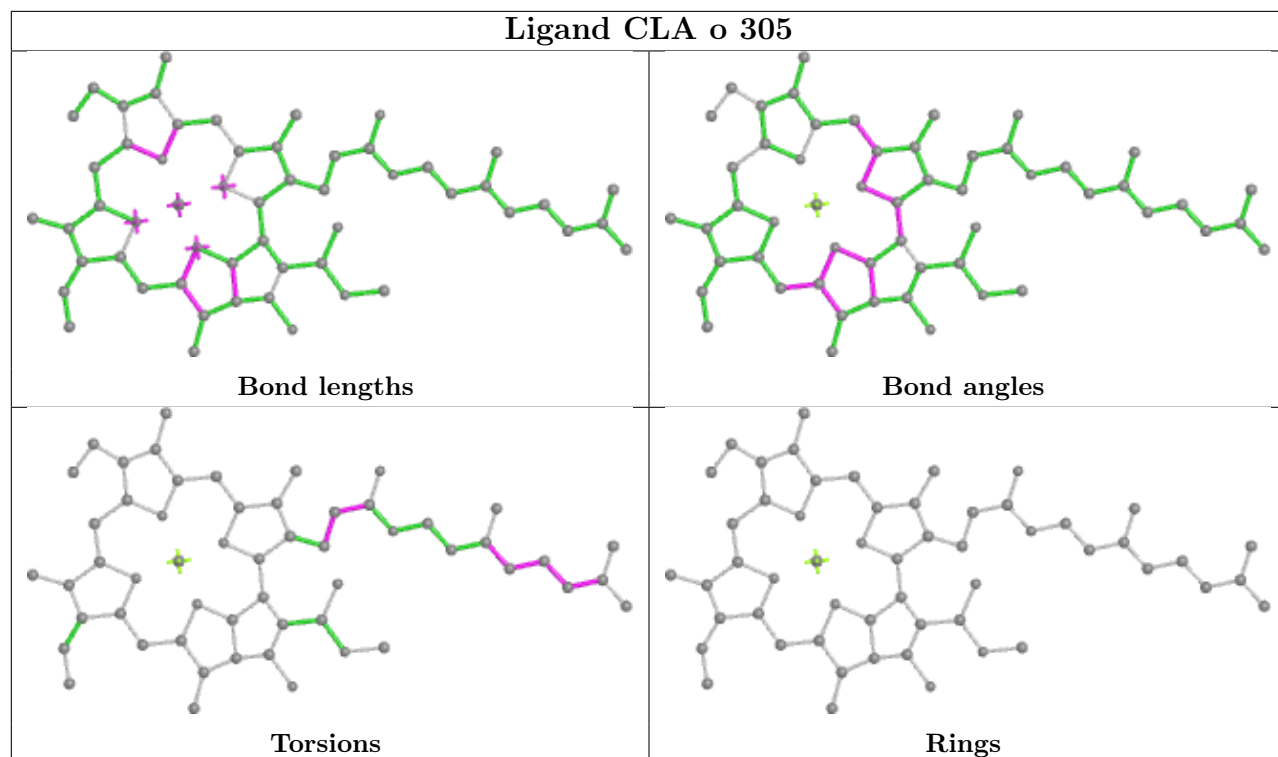


Rings

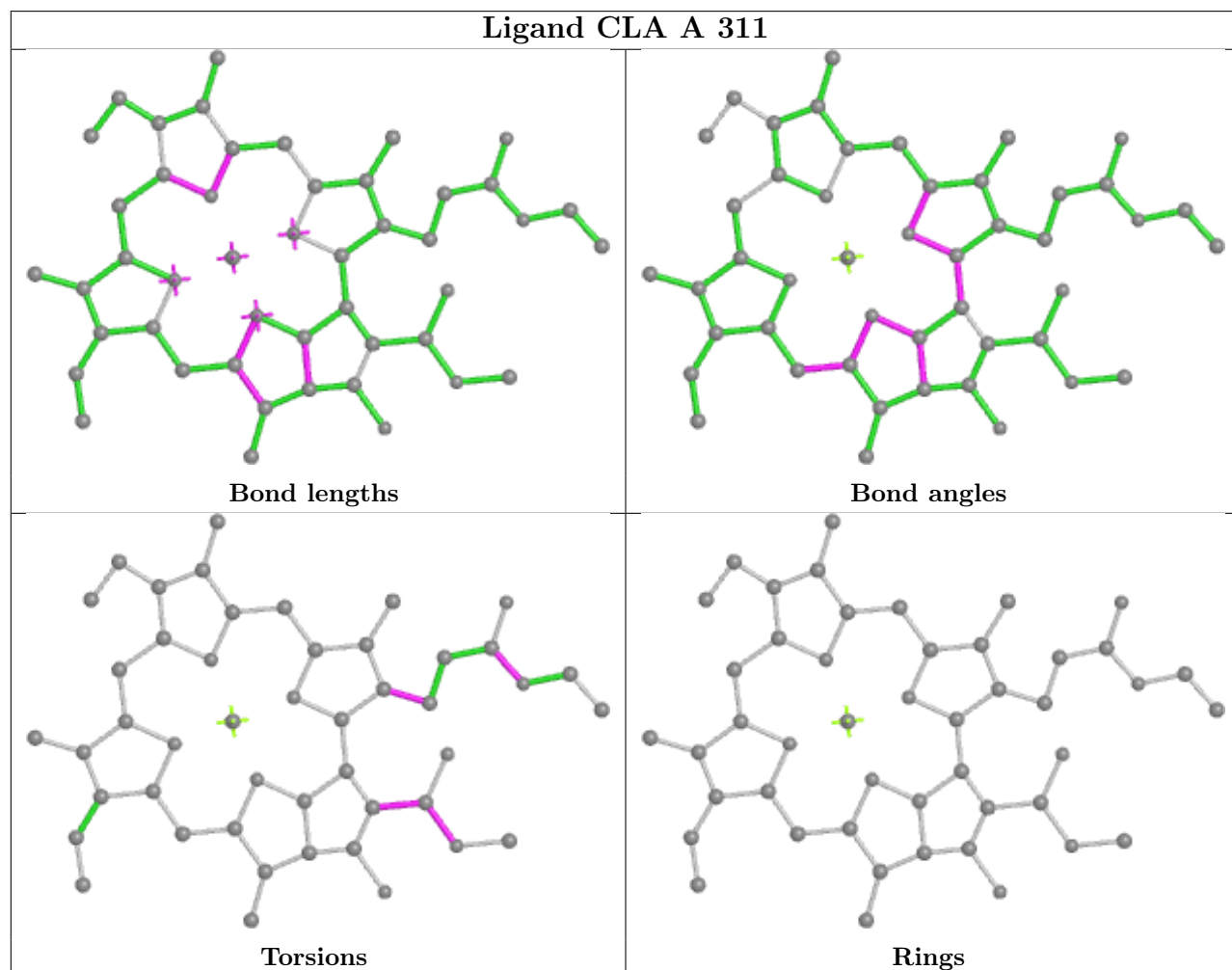


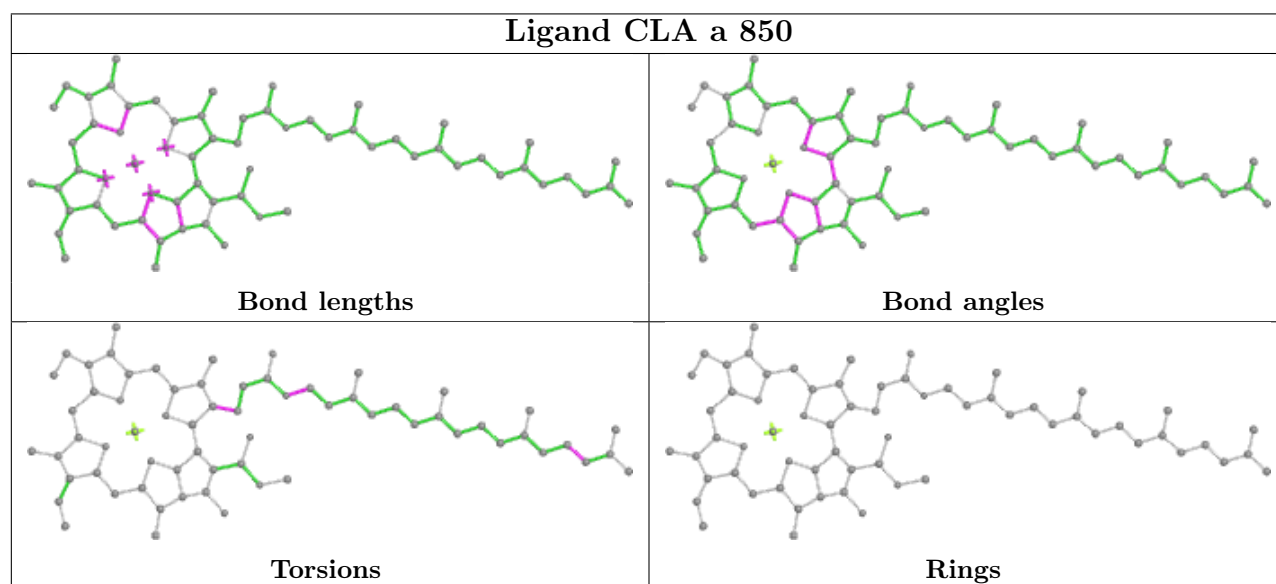
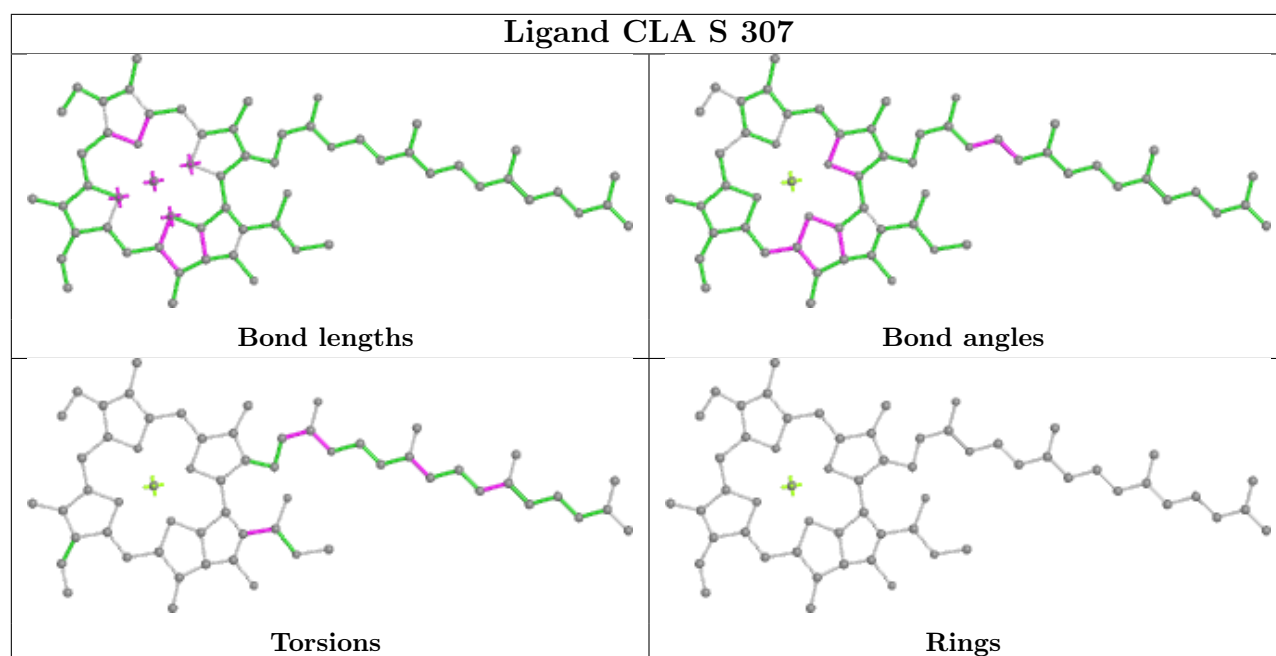


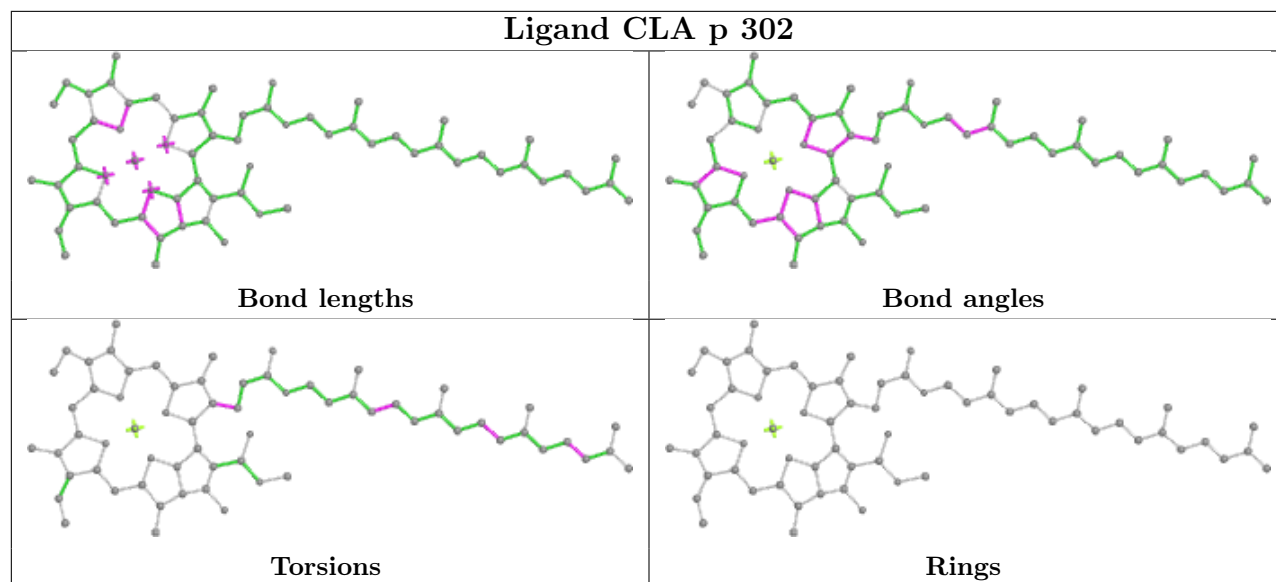
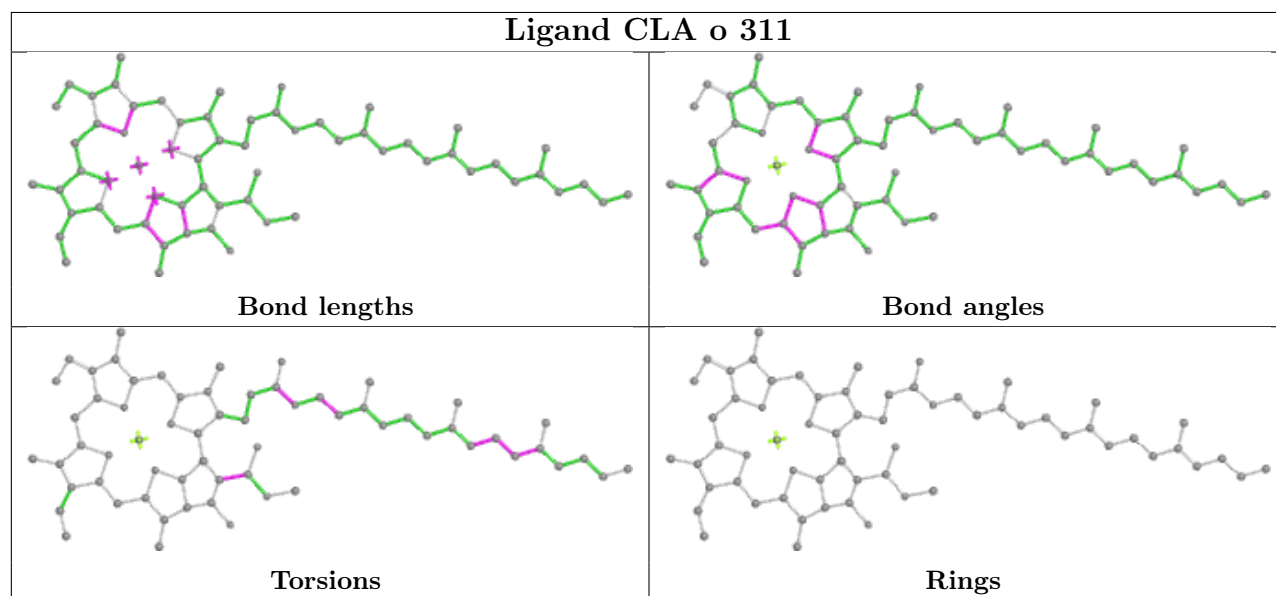
Ligand CLA o 305



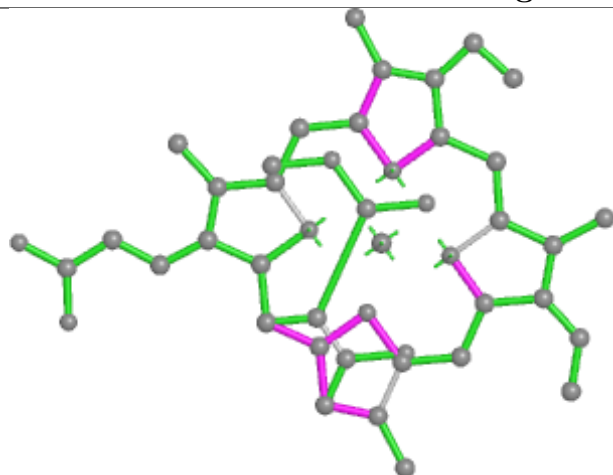
Ligand CLA A 311



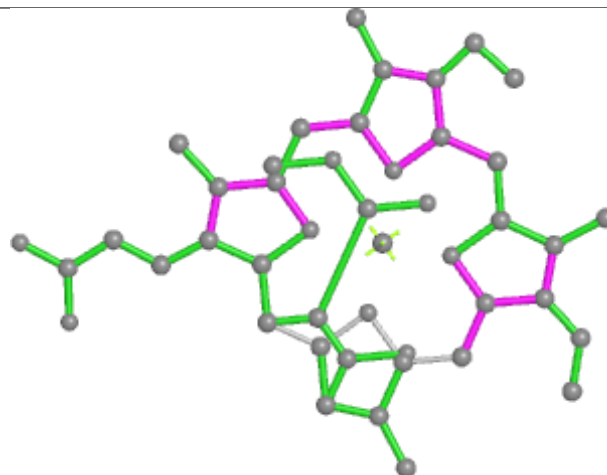


Ligand CLA p 302**Ligand CLA o 311**

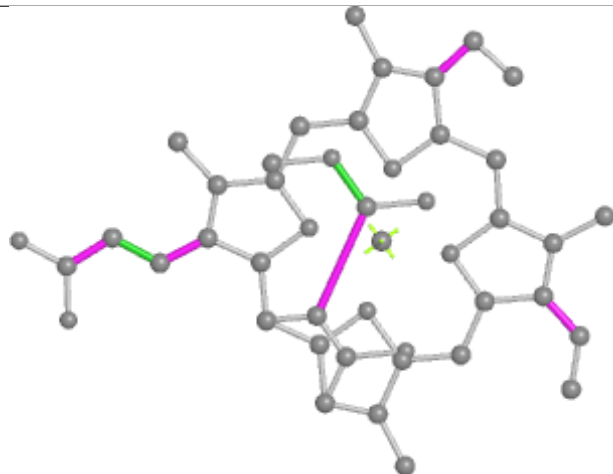
Ligand KC2 O 302



Bond lengths



Bond angles

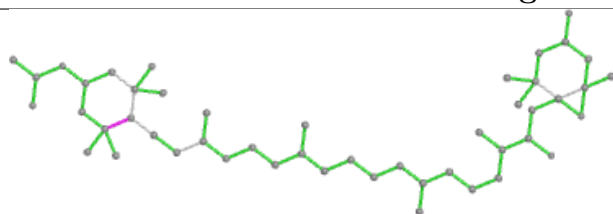


Torsions

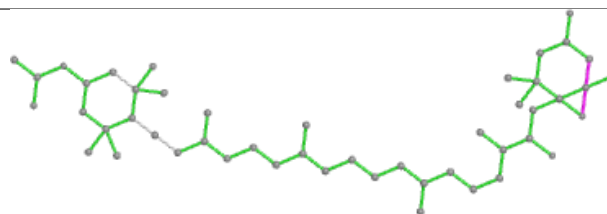


Rings

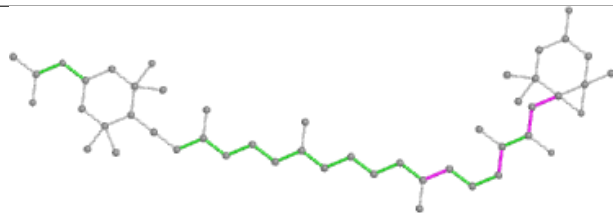
Ligand A86 Y 321



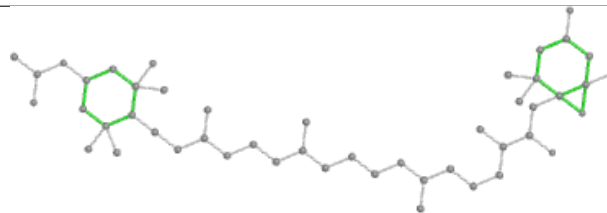
Bond lengths



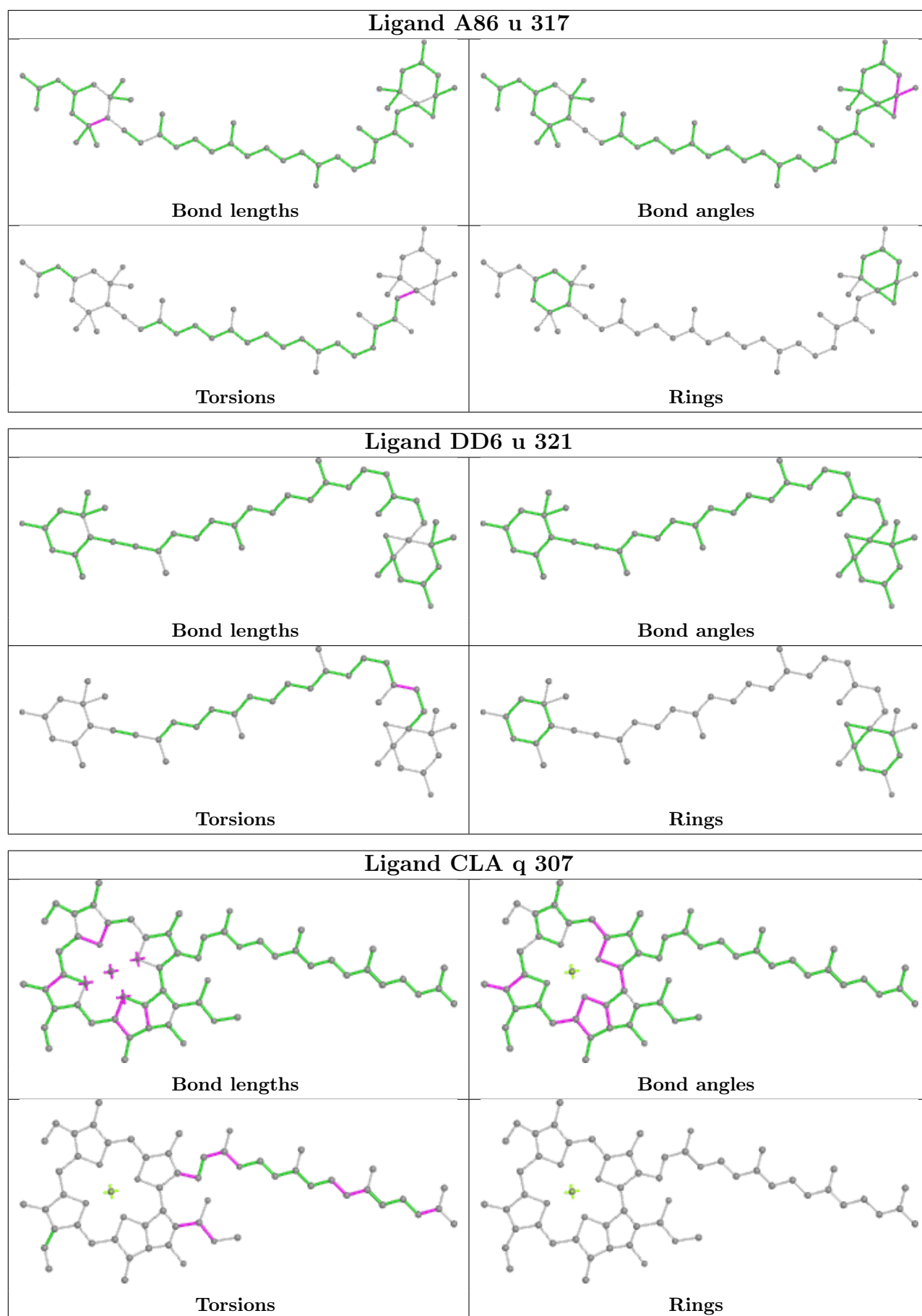
Bond angles

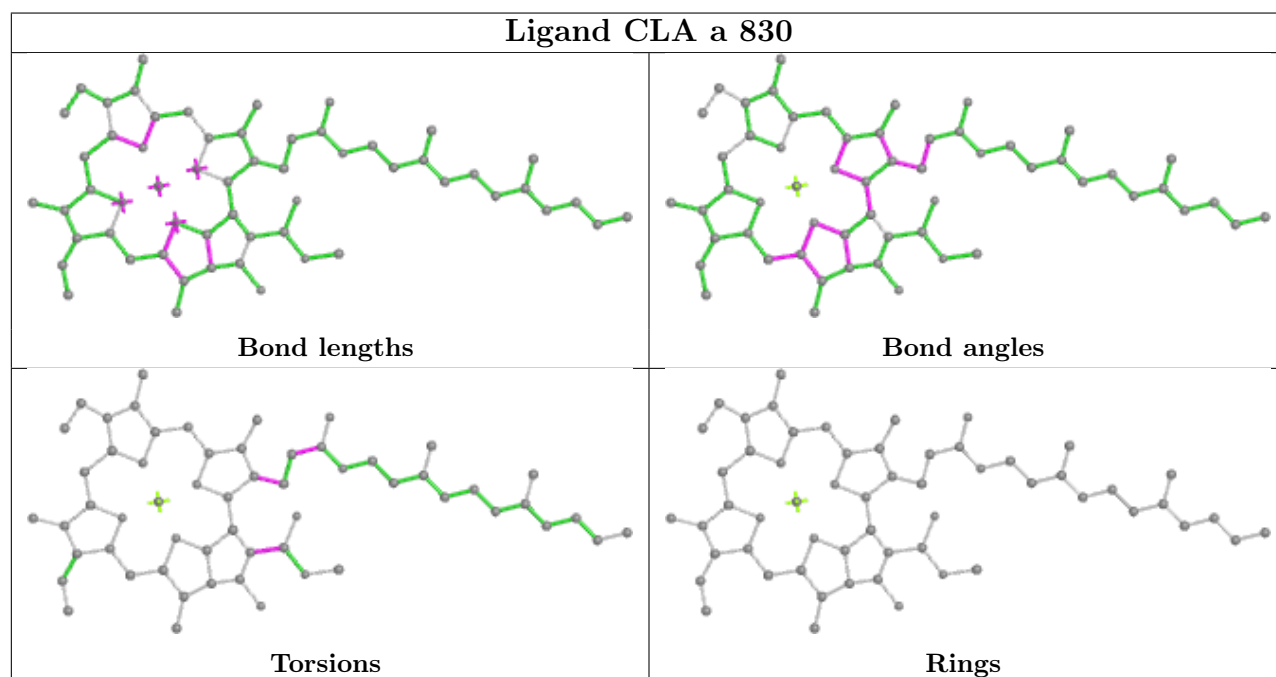
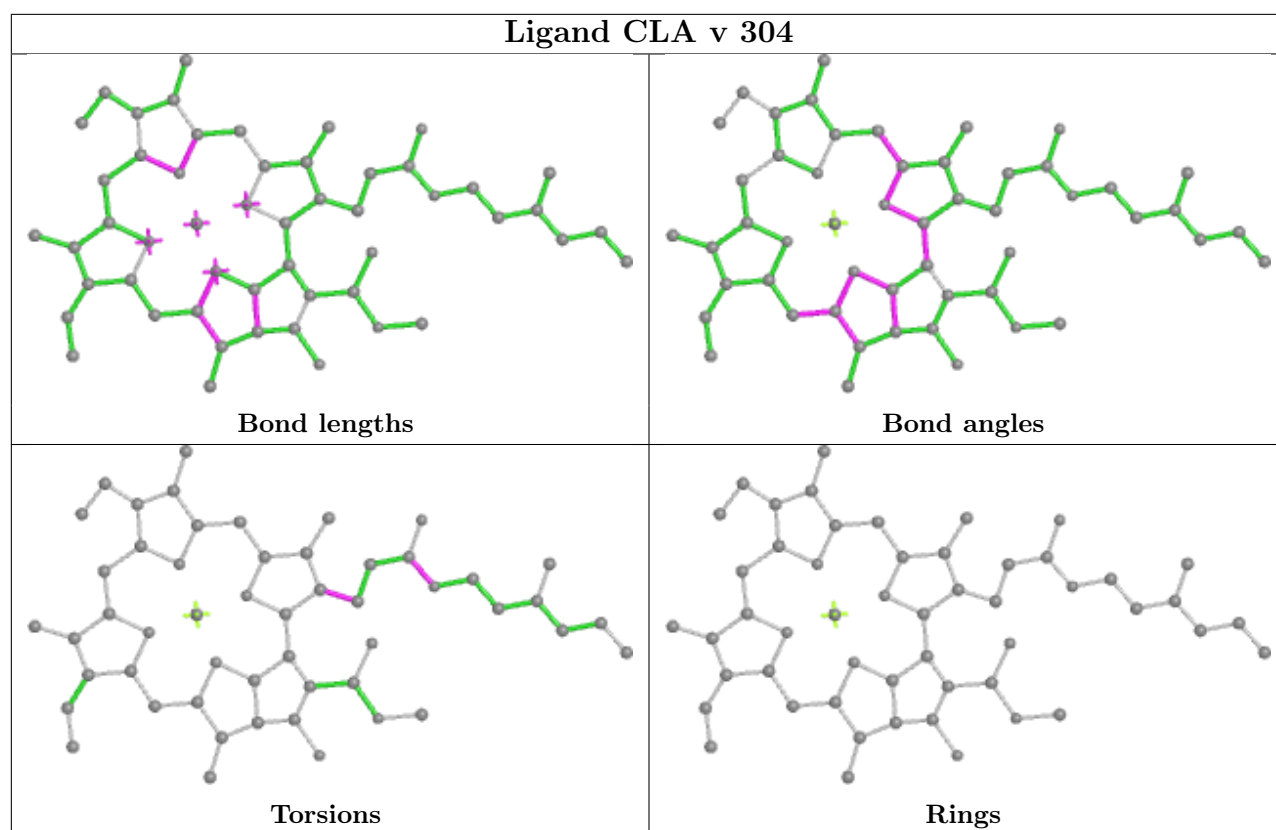


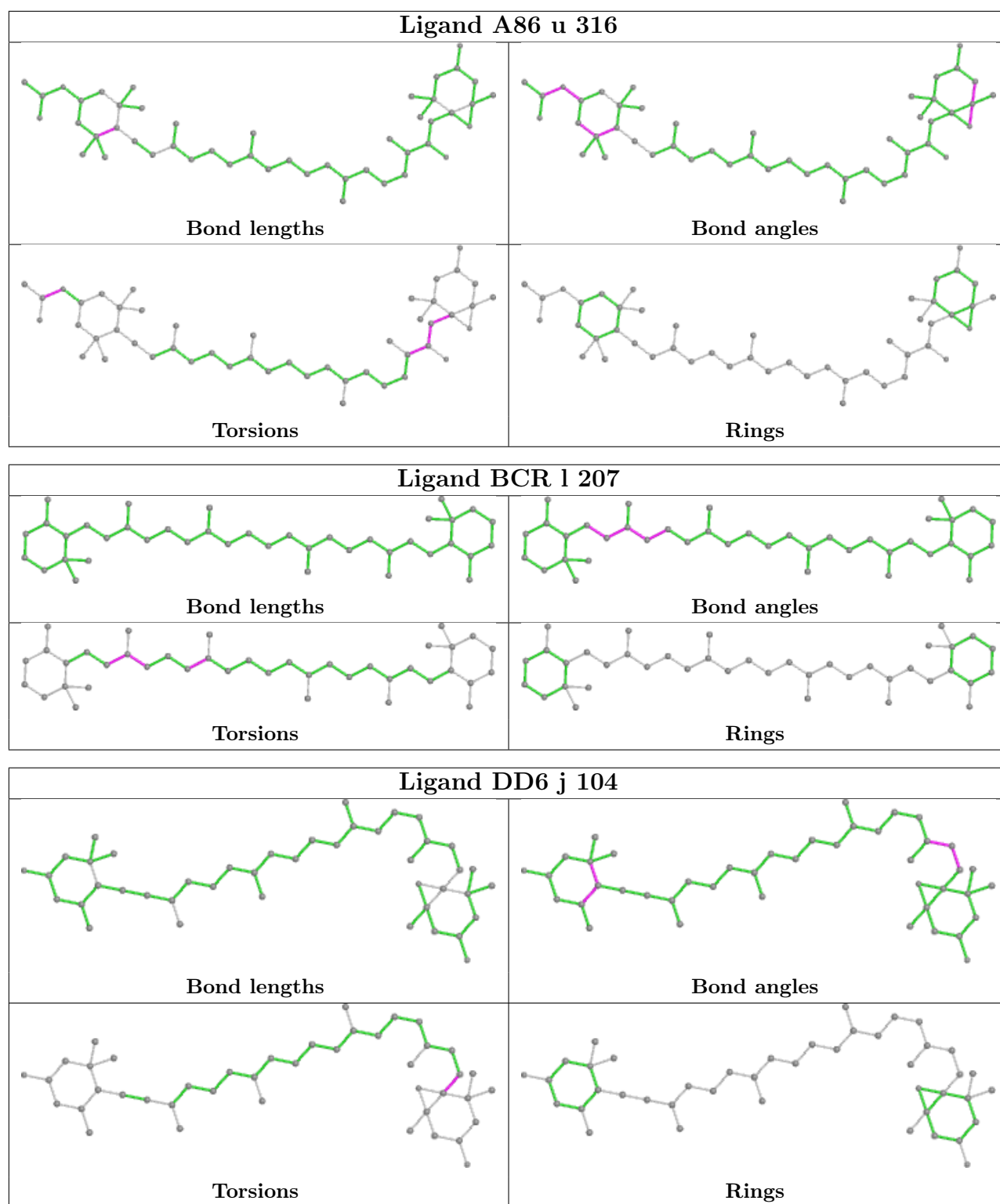
Torsions

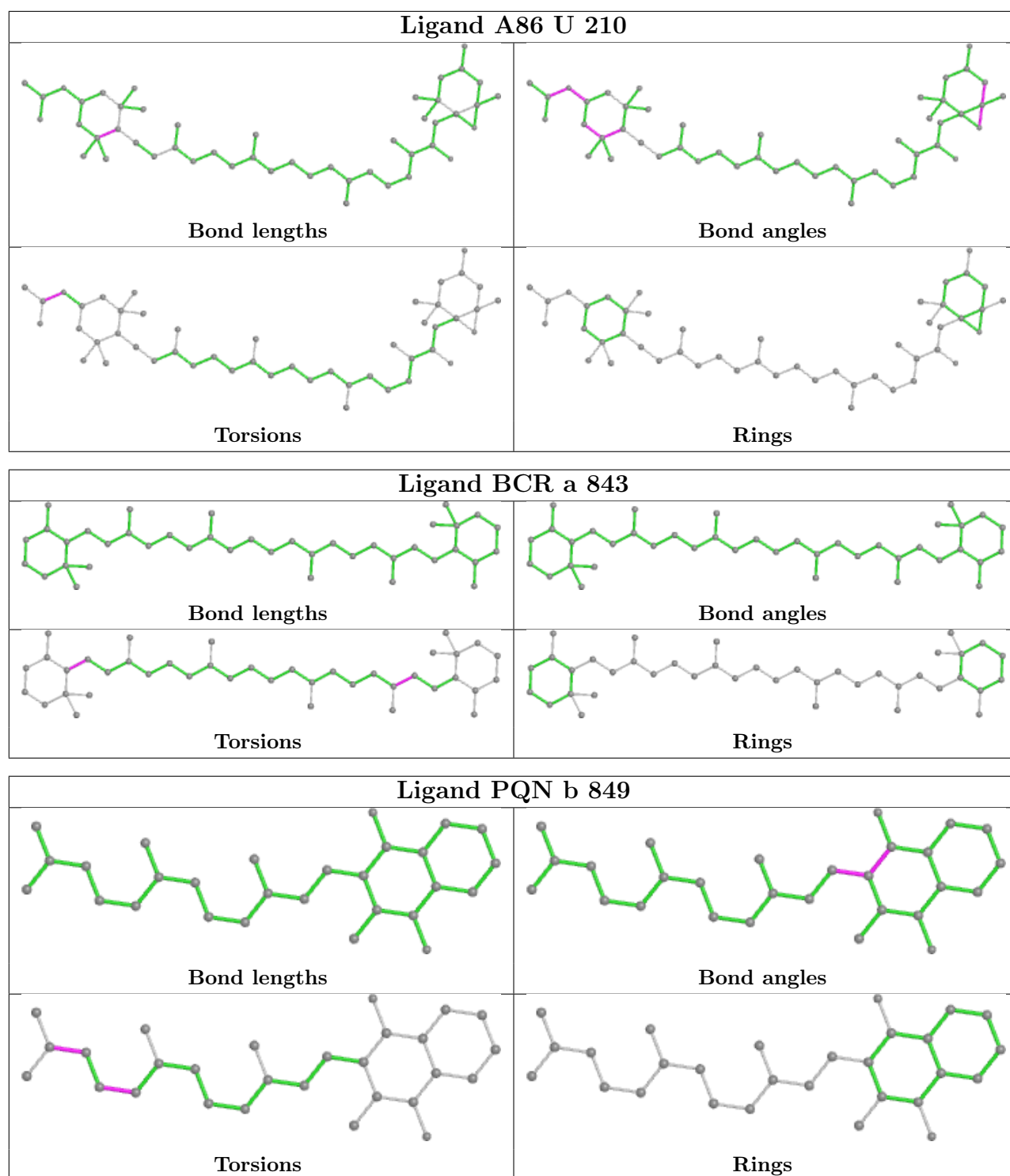


Rings

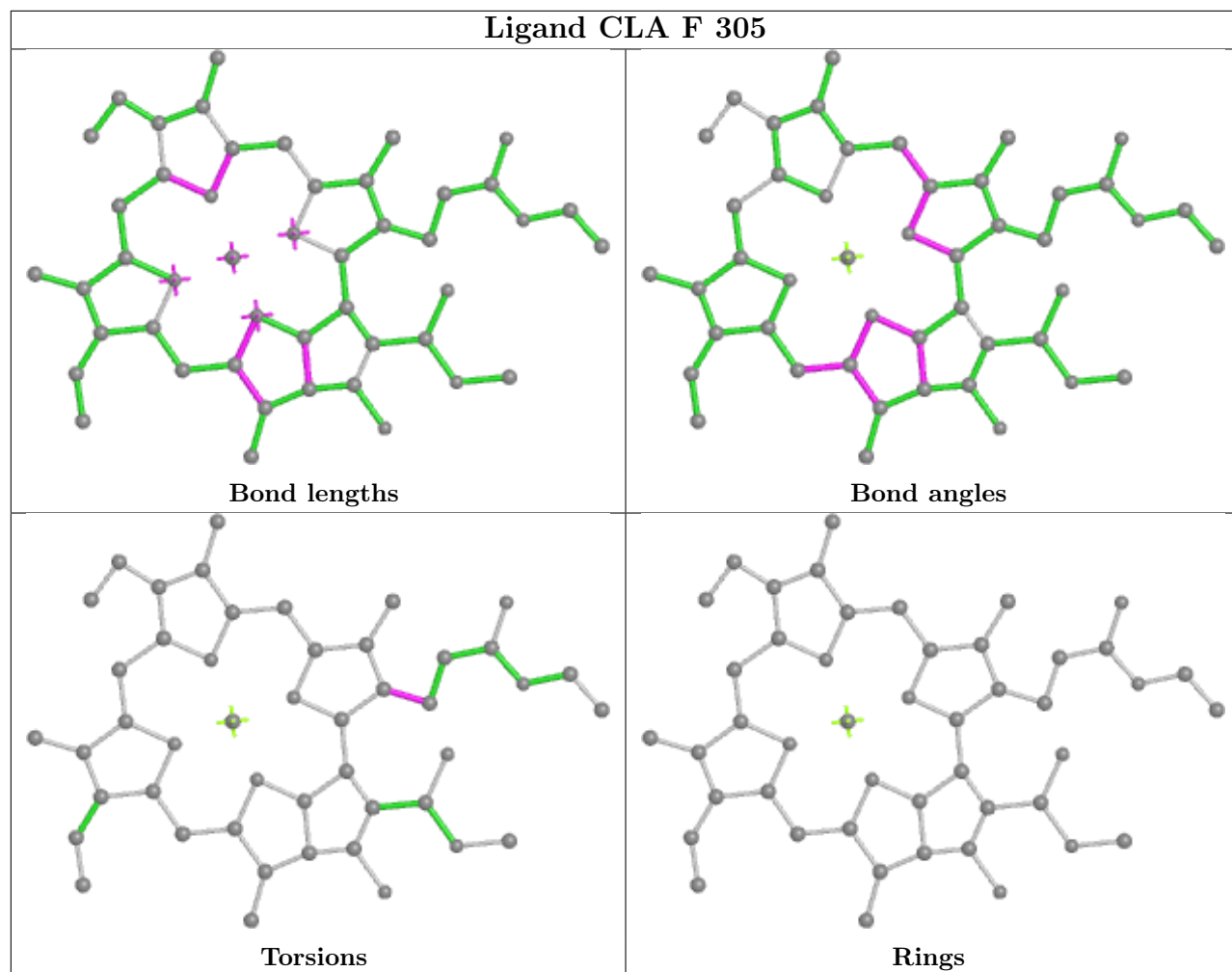


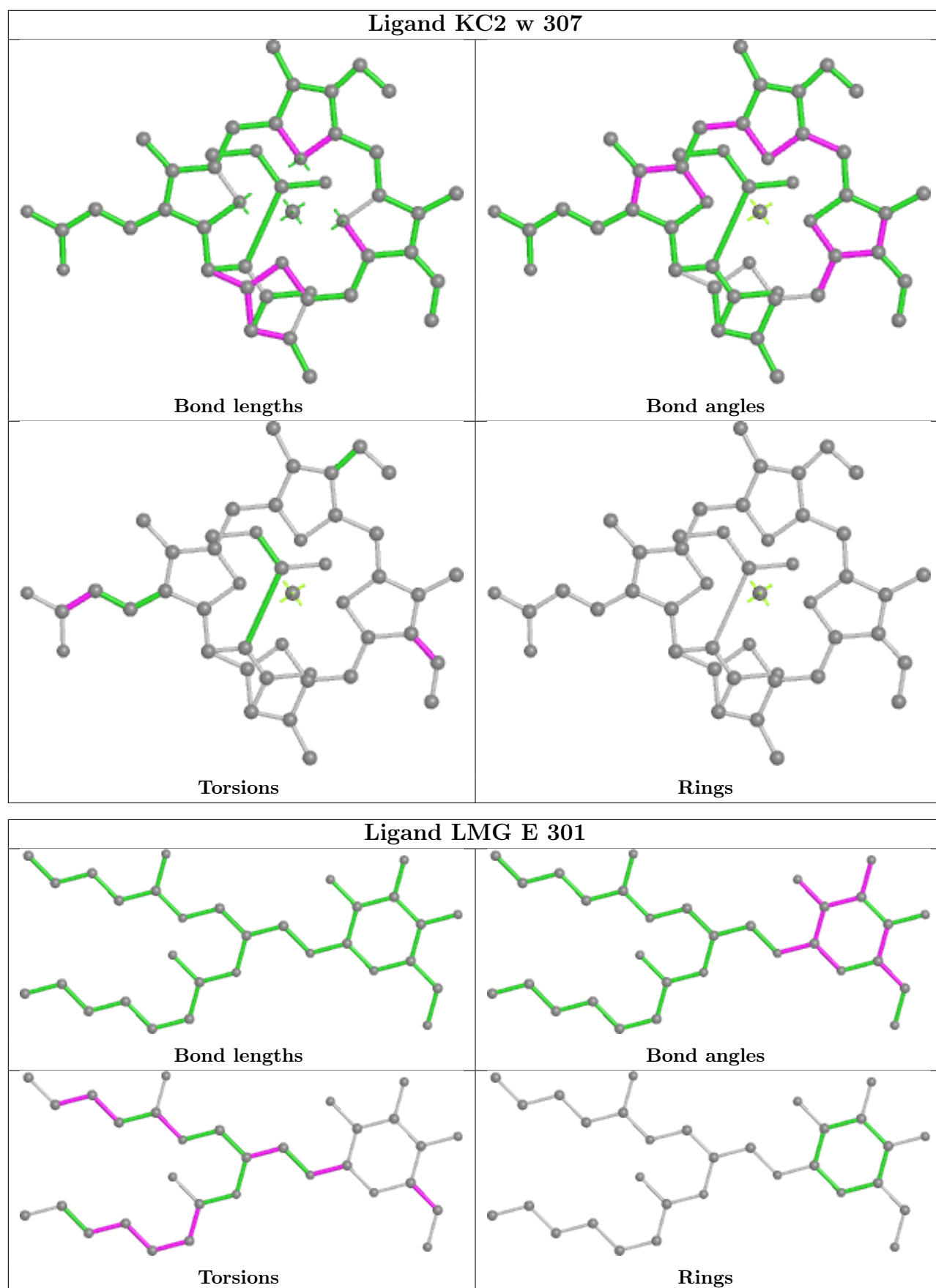




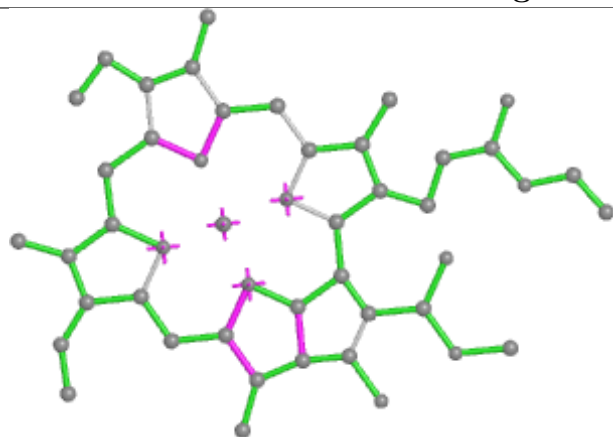


Ligand CLA F 305

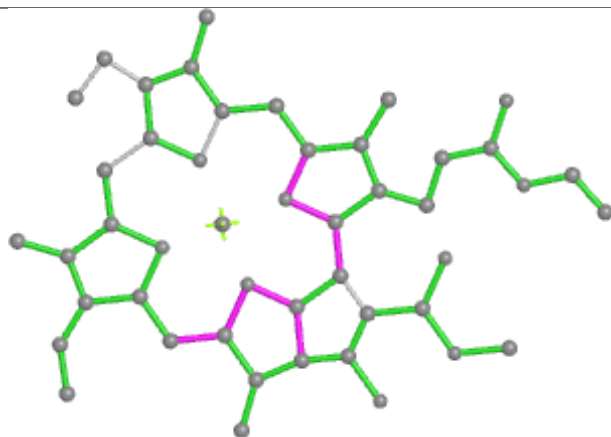




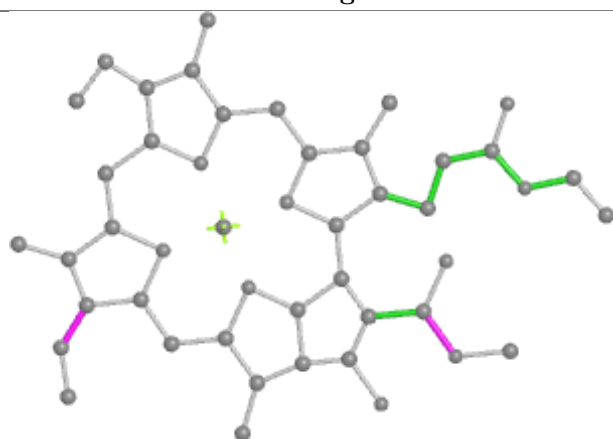
Ligand CLA K 301



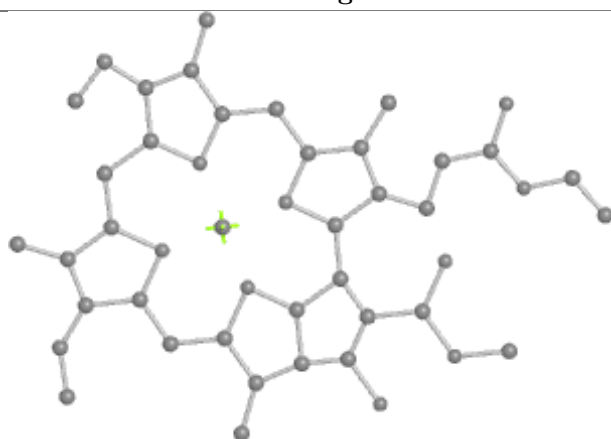
Bond lengths



Bond angles

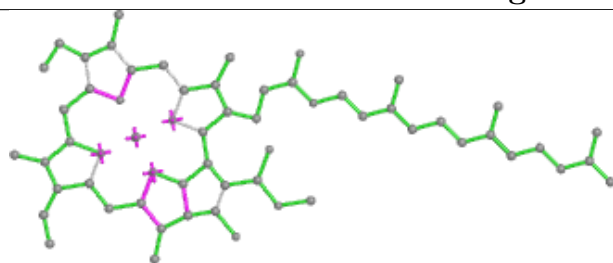


Torsions

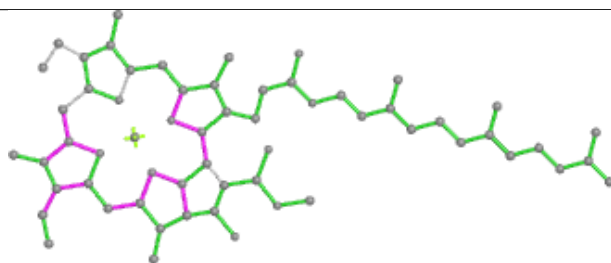


Rings

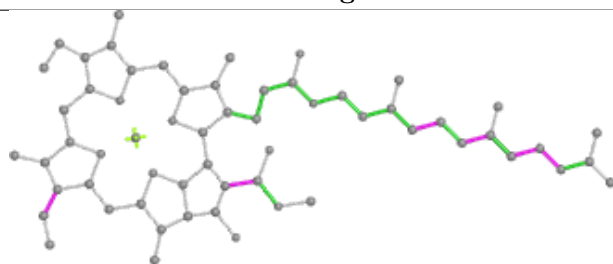
Ligand CLA W 312



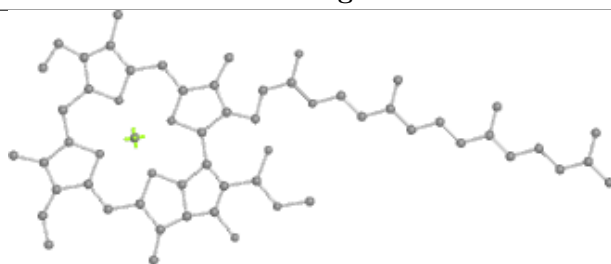
Bond lengths



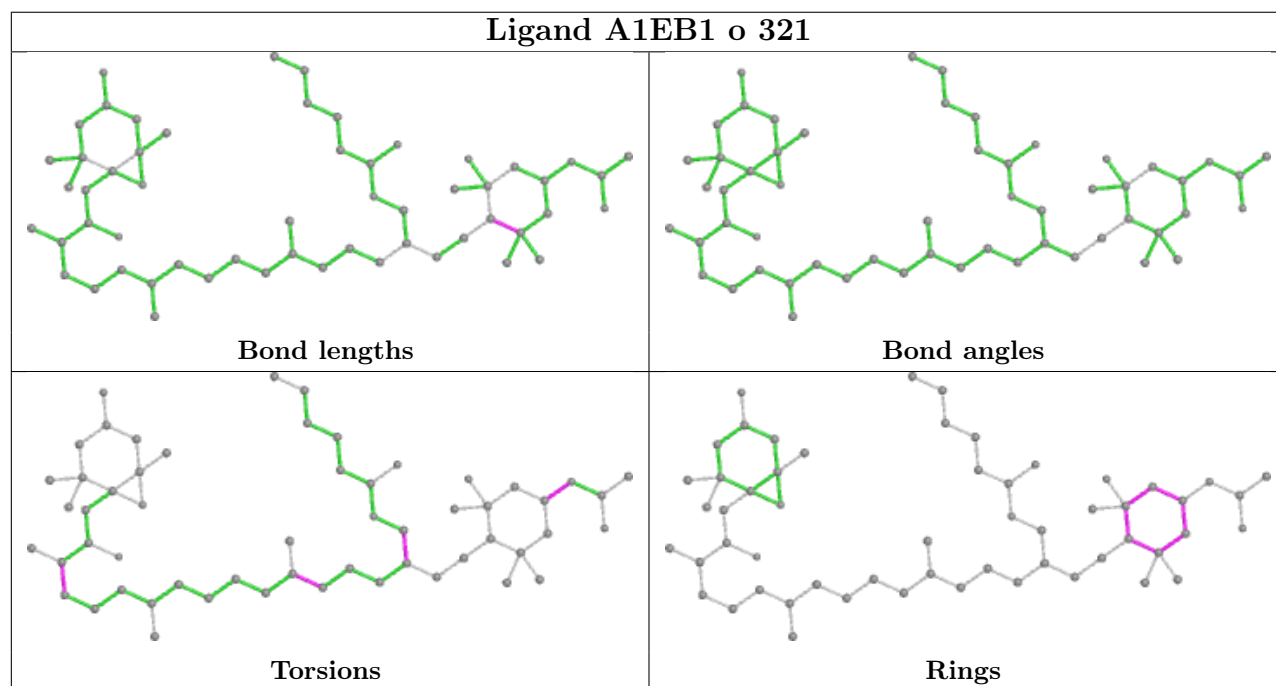
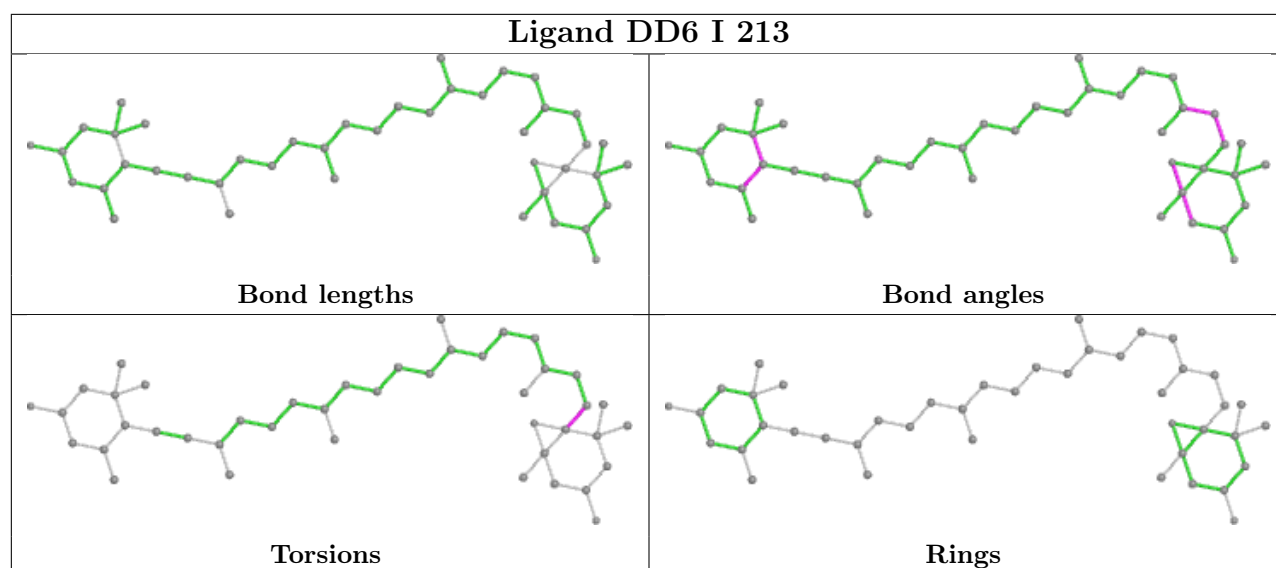
Bond angles

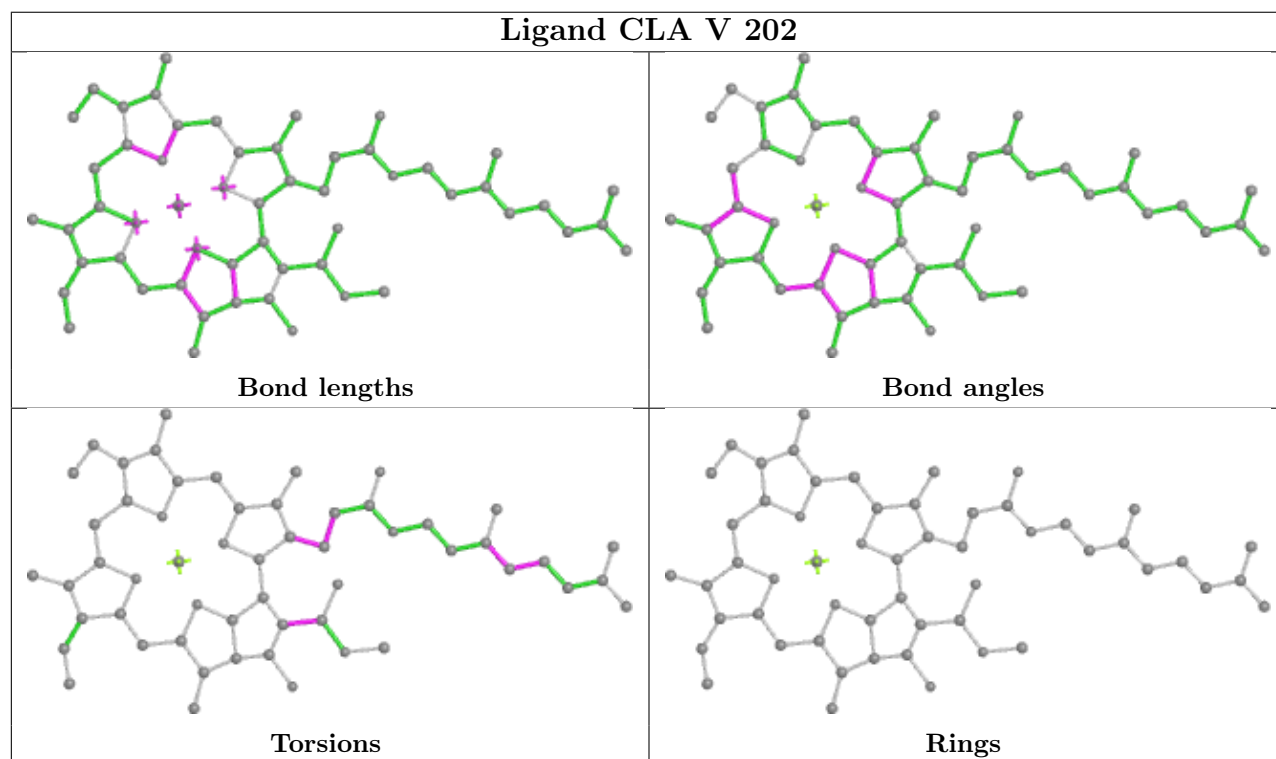
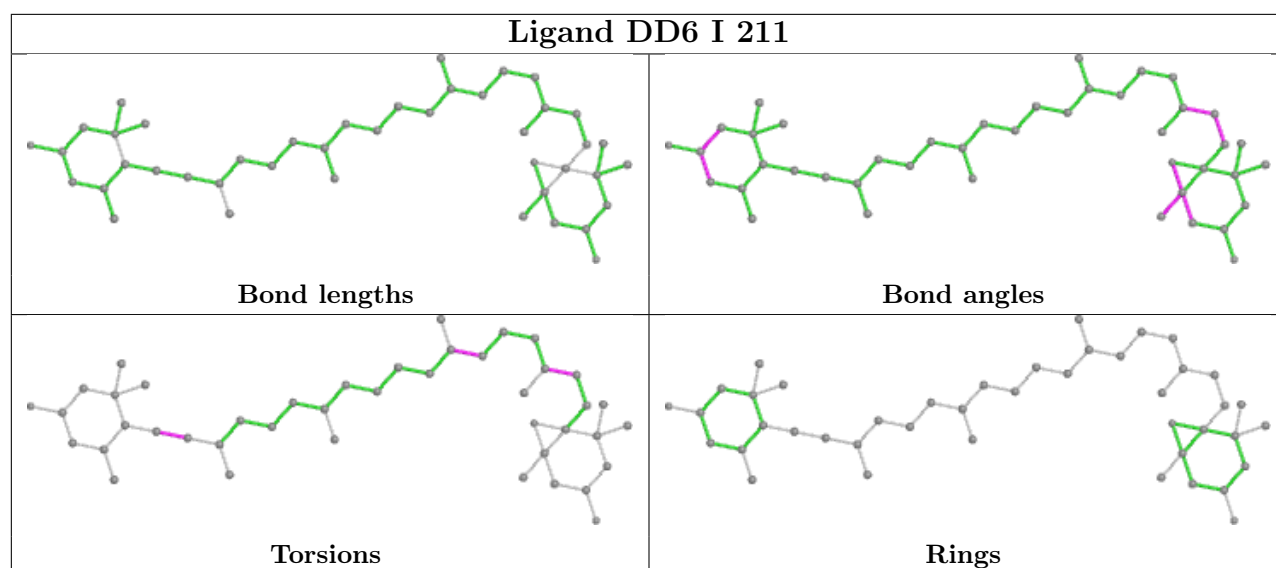


Torsions

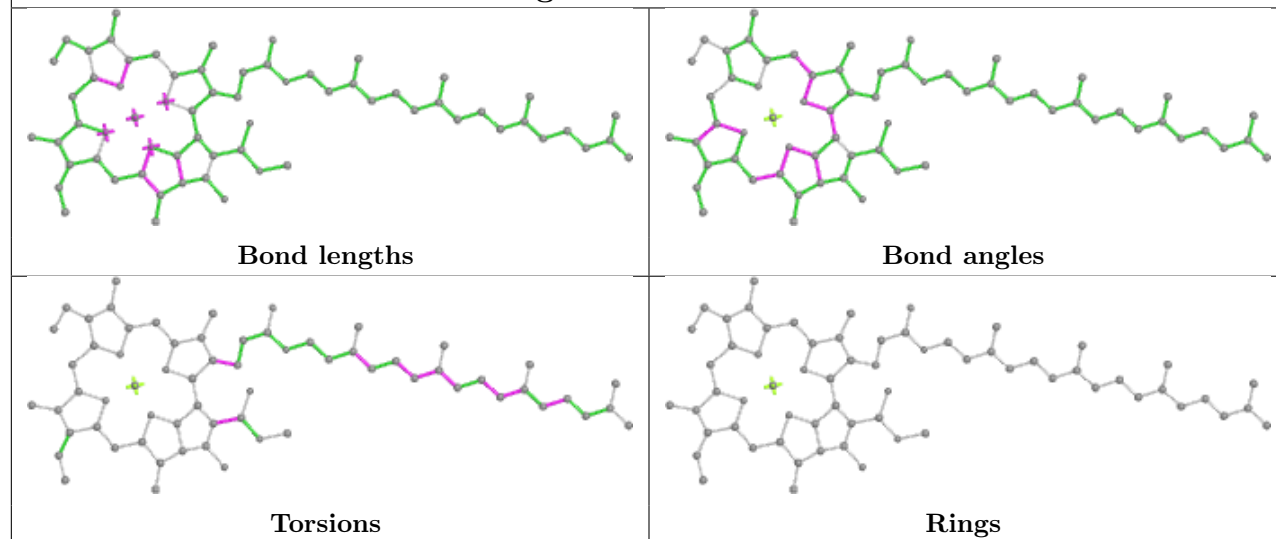


Rings

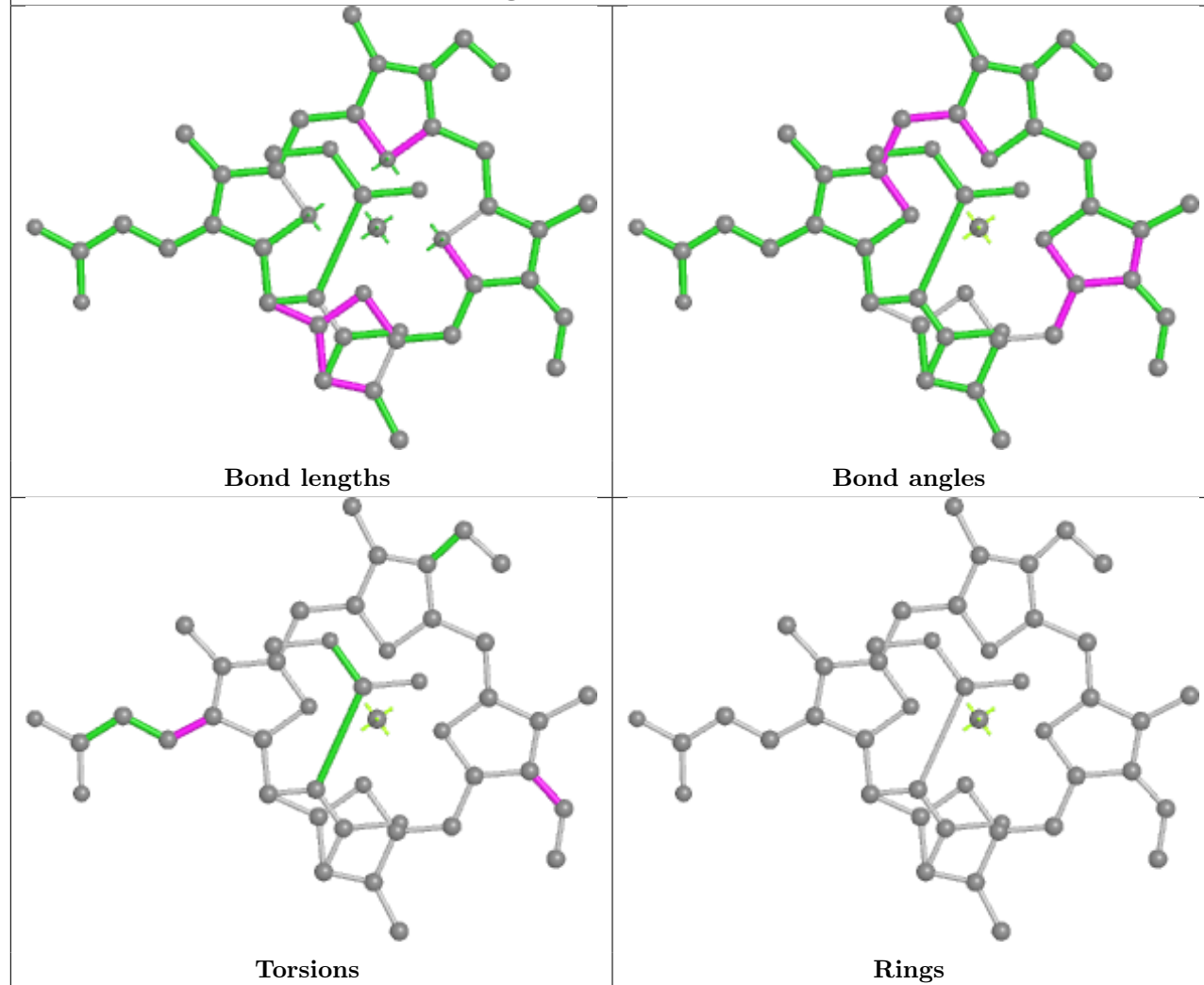


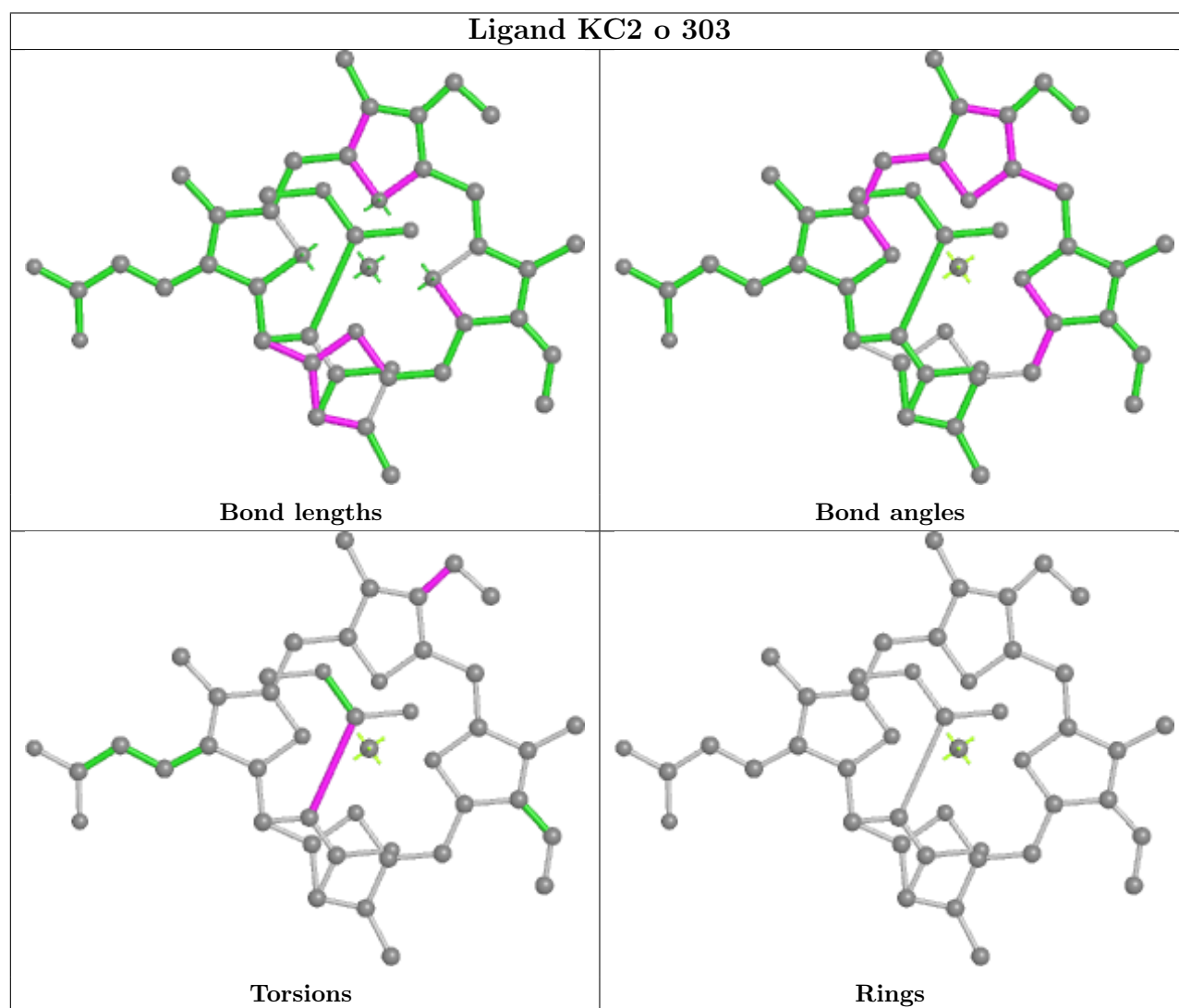
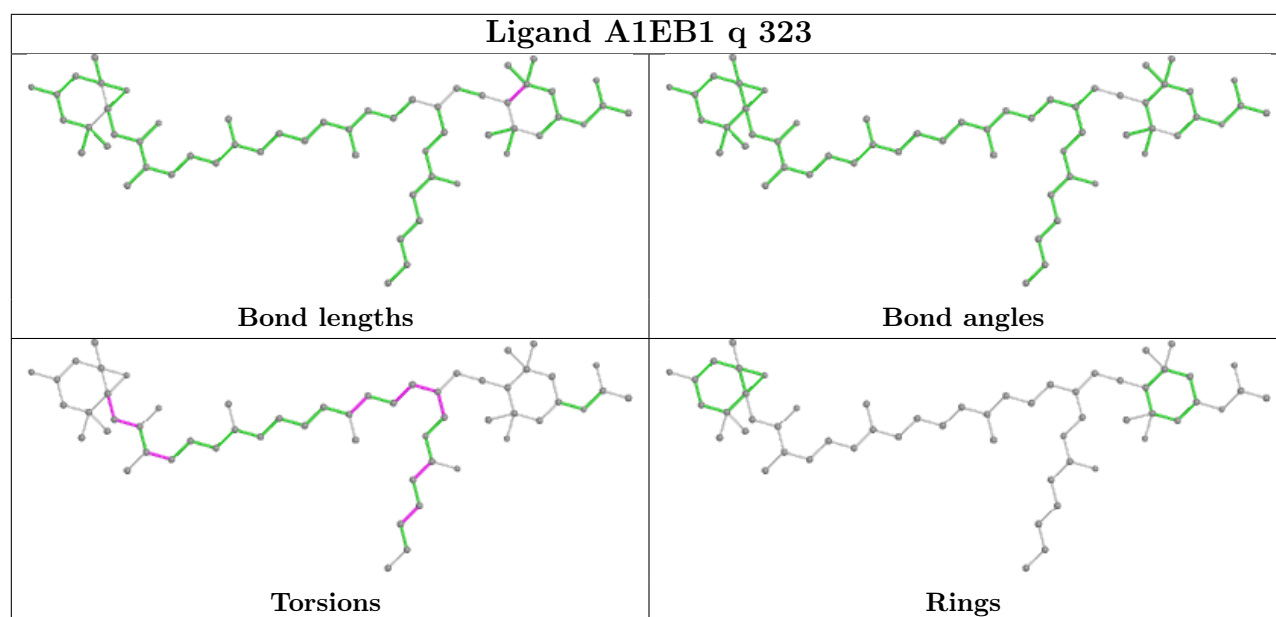


Ligand CLA a 842

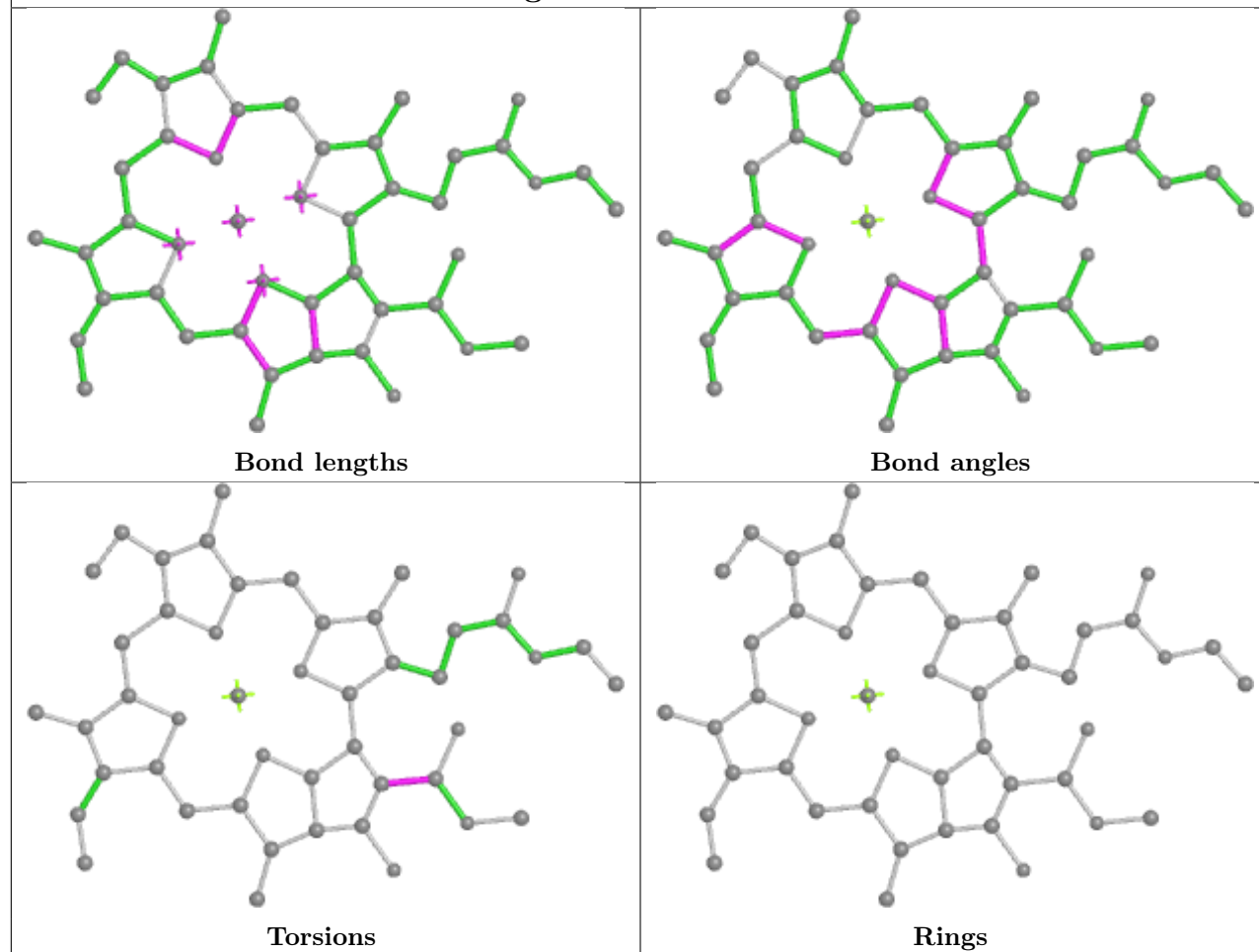


Ligand KC2 X 302

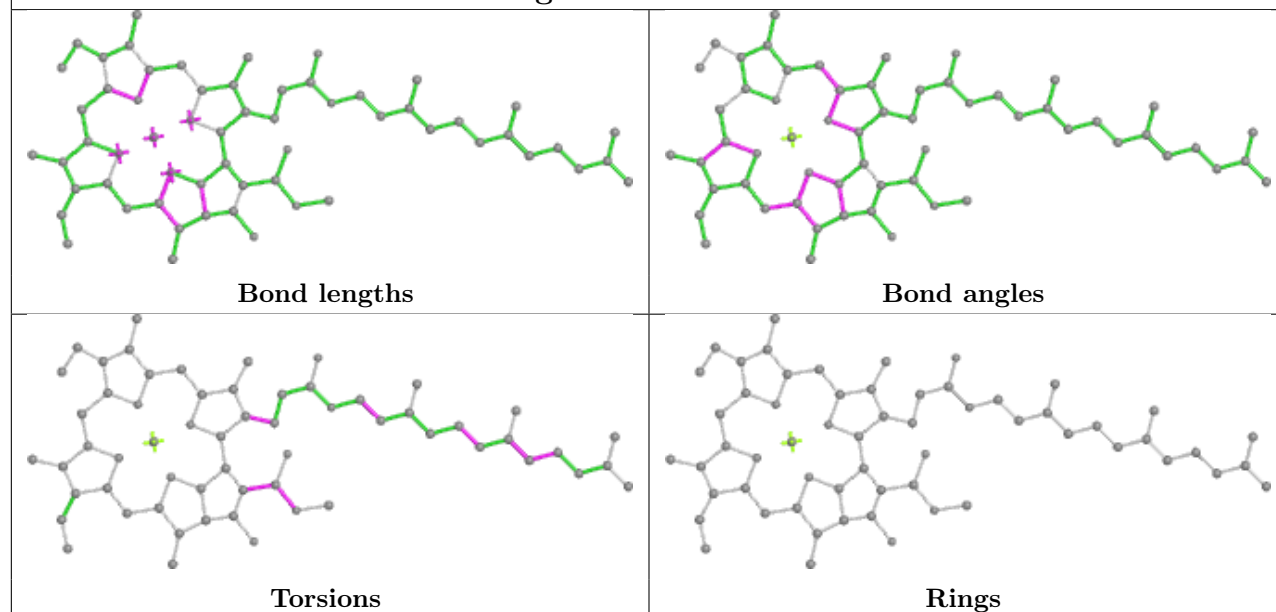


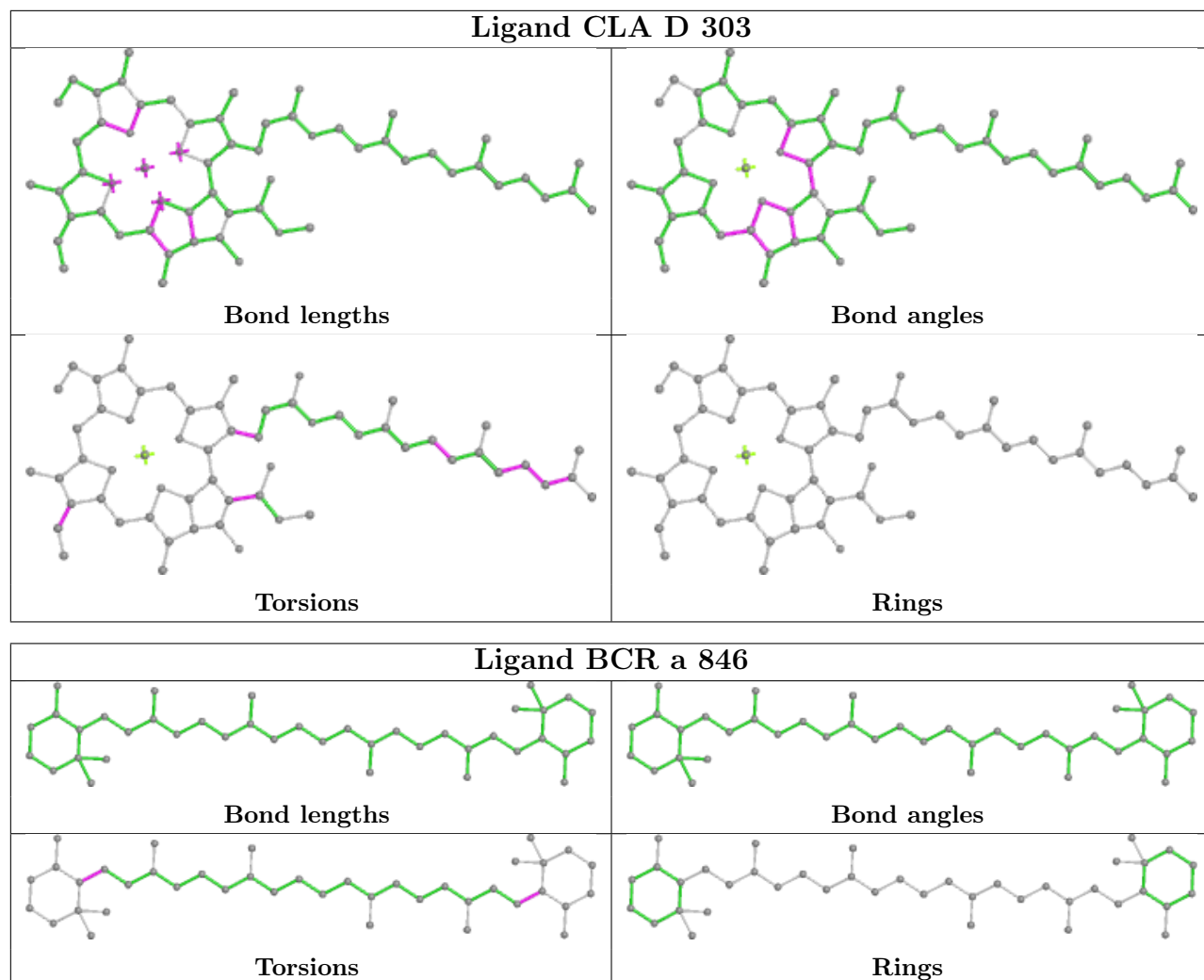


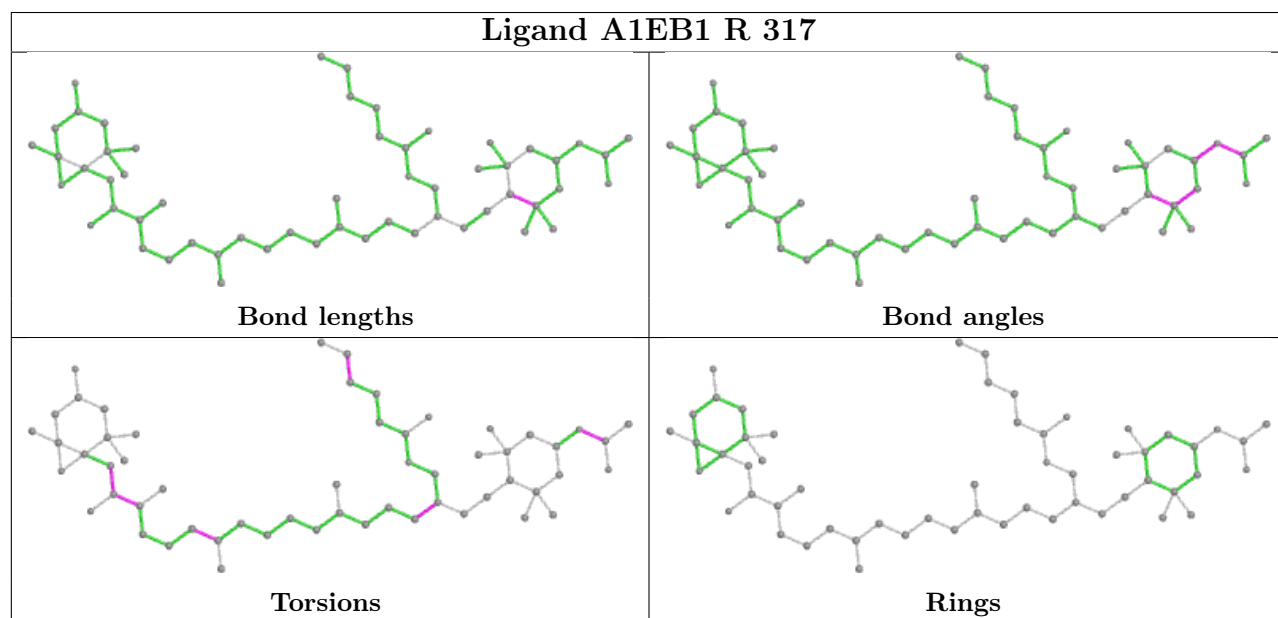
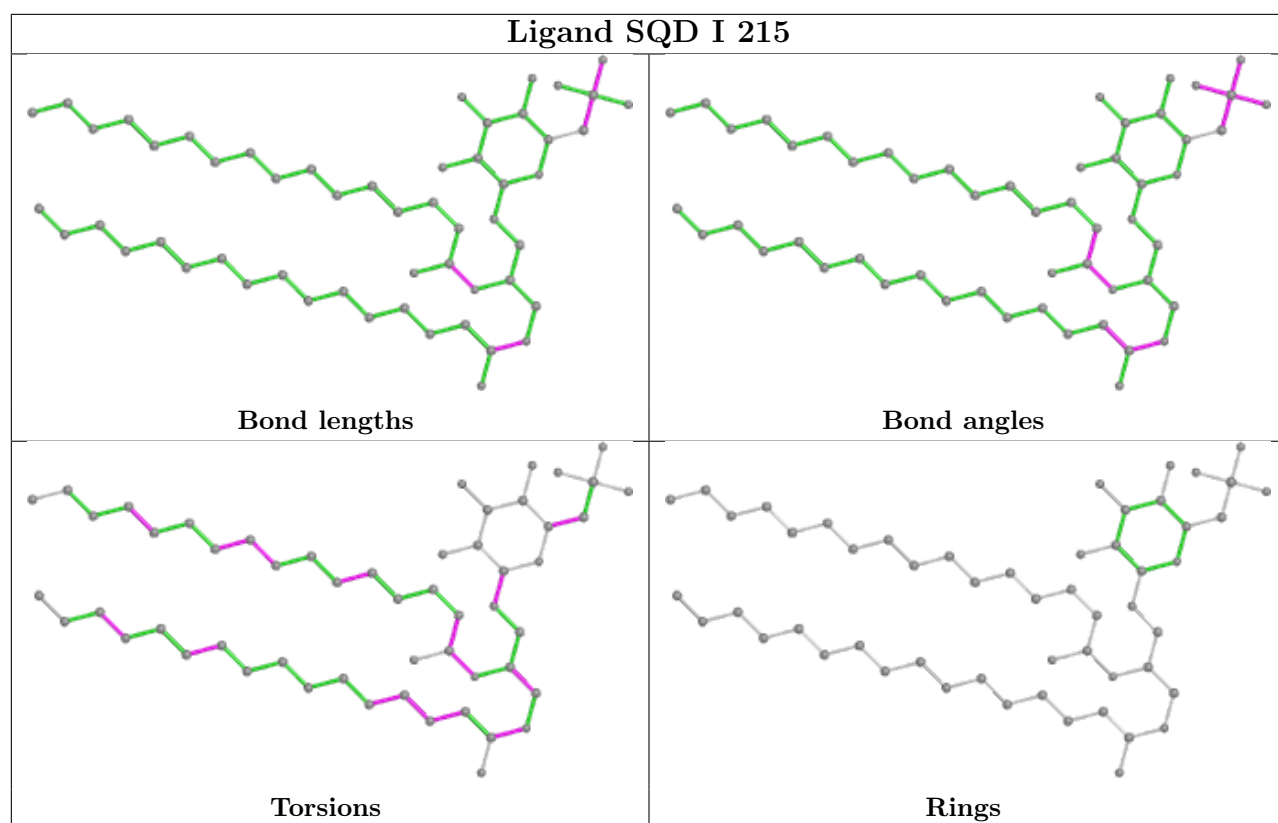
Ligand CLA O 316



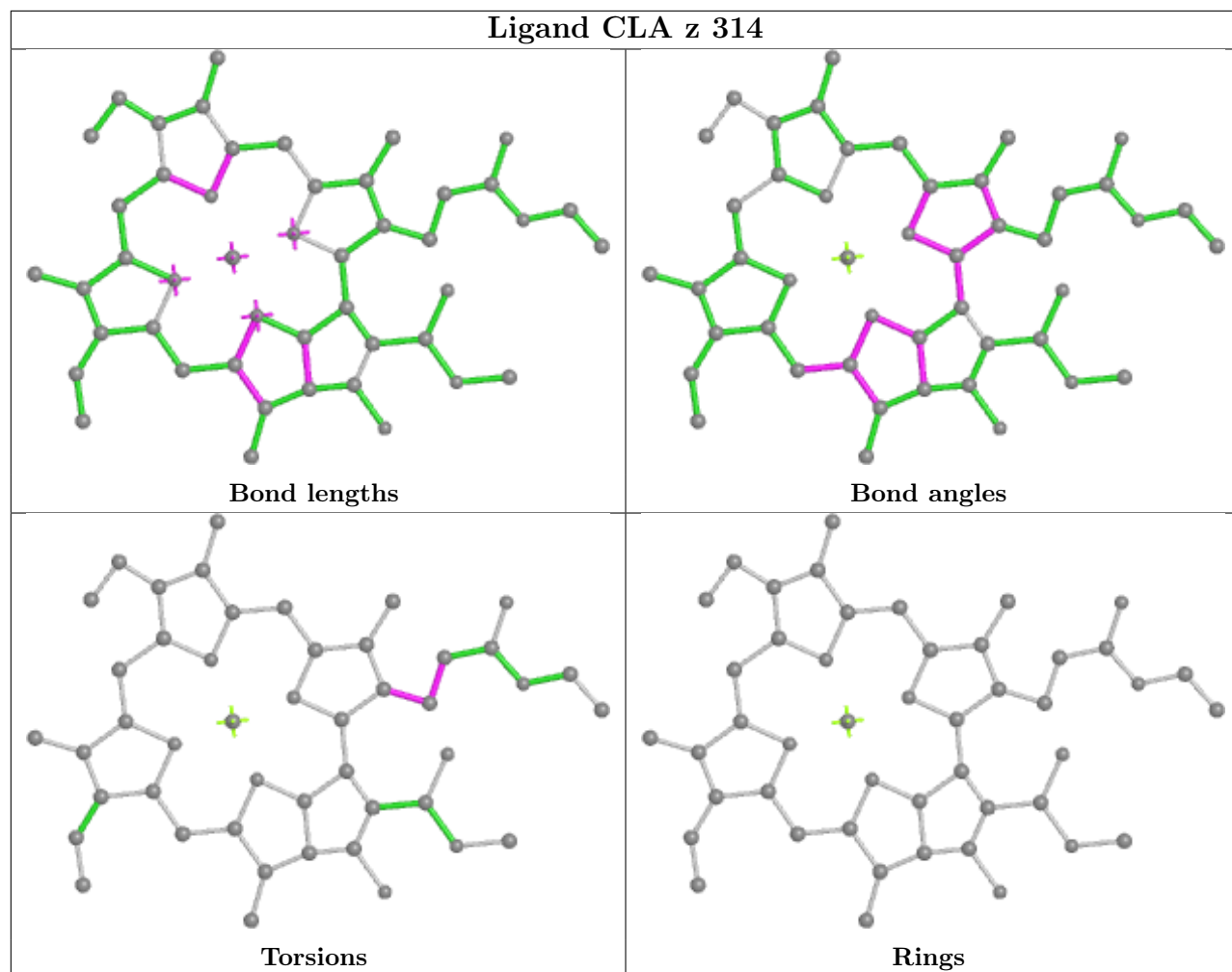
Ligand CLA b 833



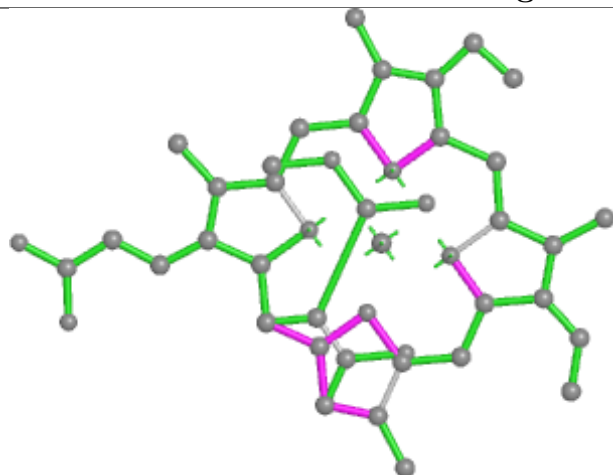




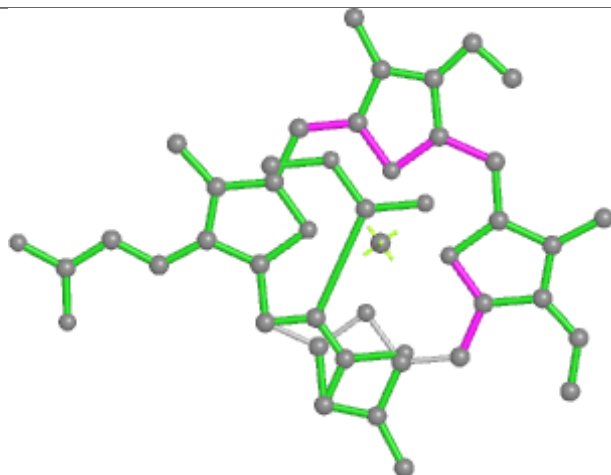
Ligand CLA z 314



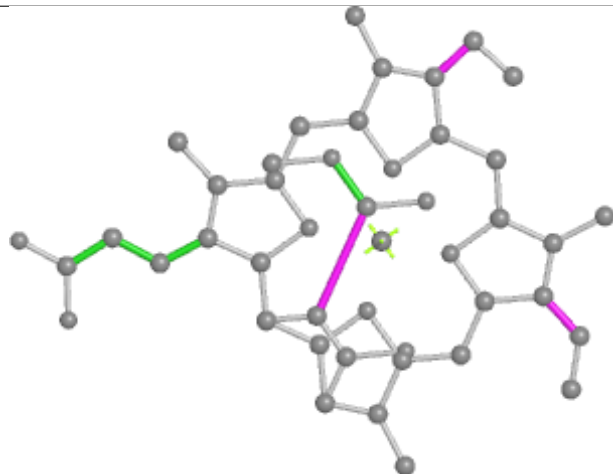
Ligand KC2 T 309



Bond lengths



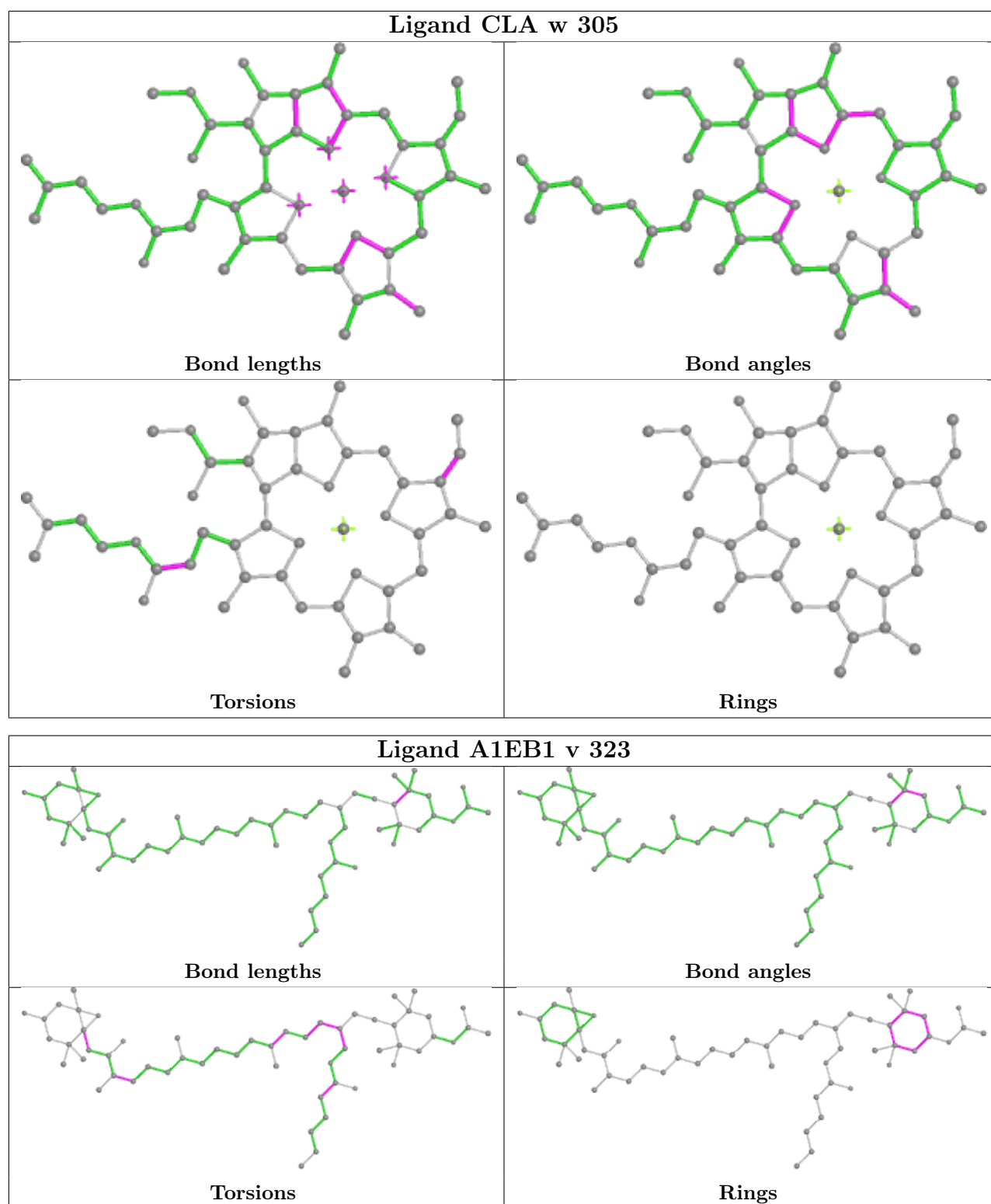
Bond angles



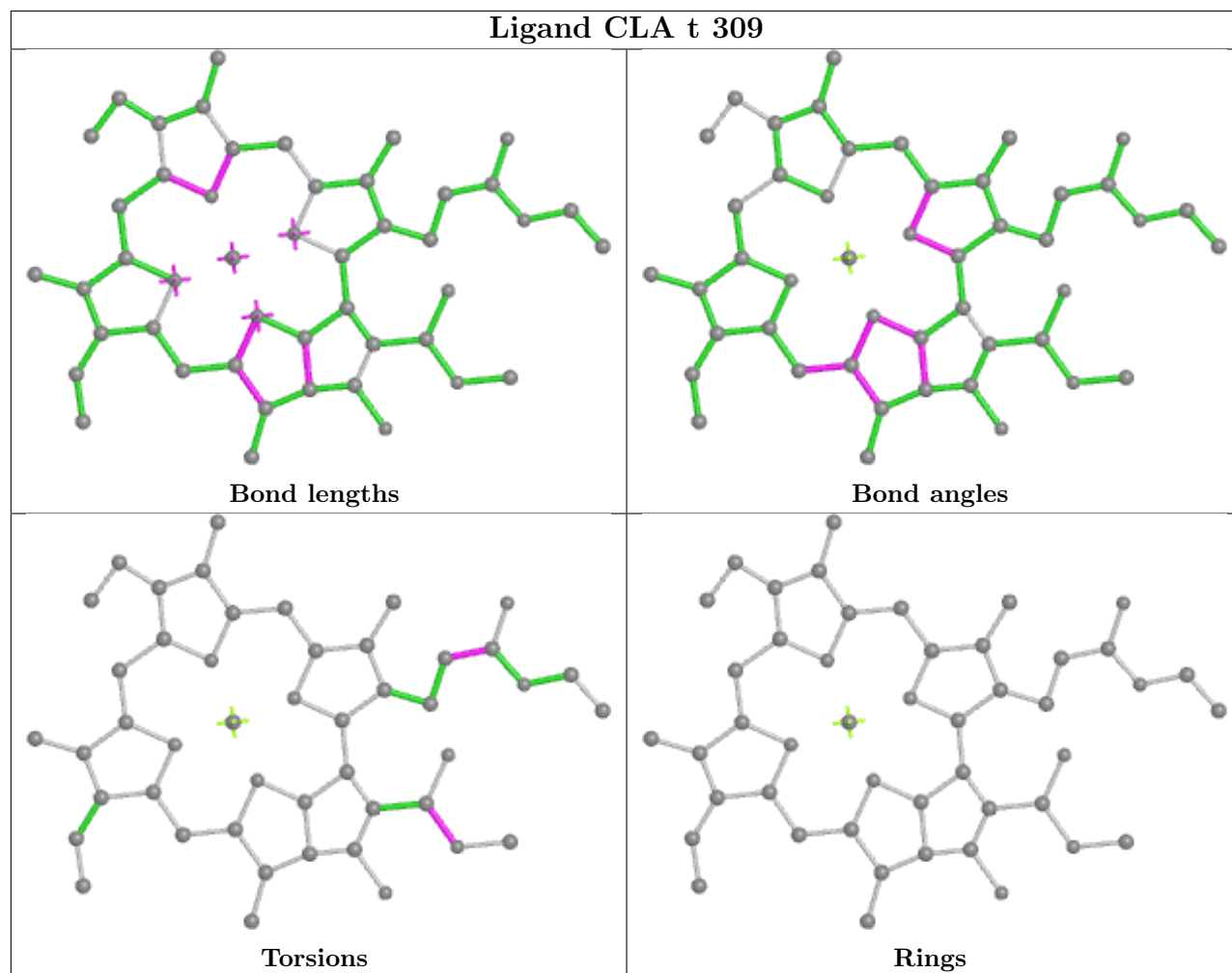
Torsions



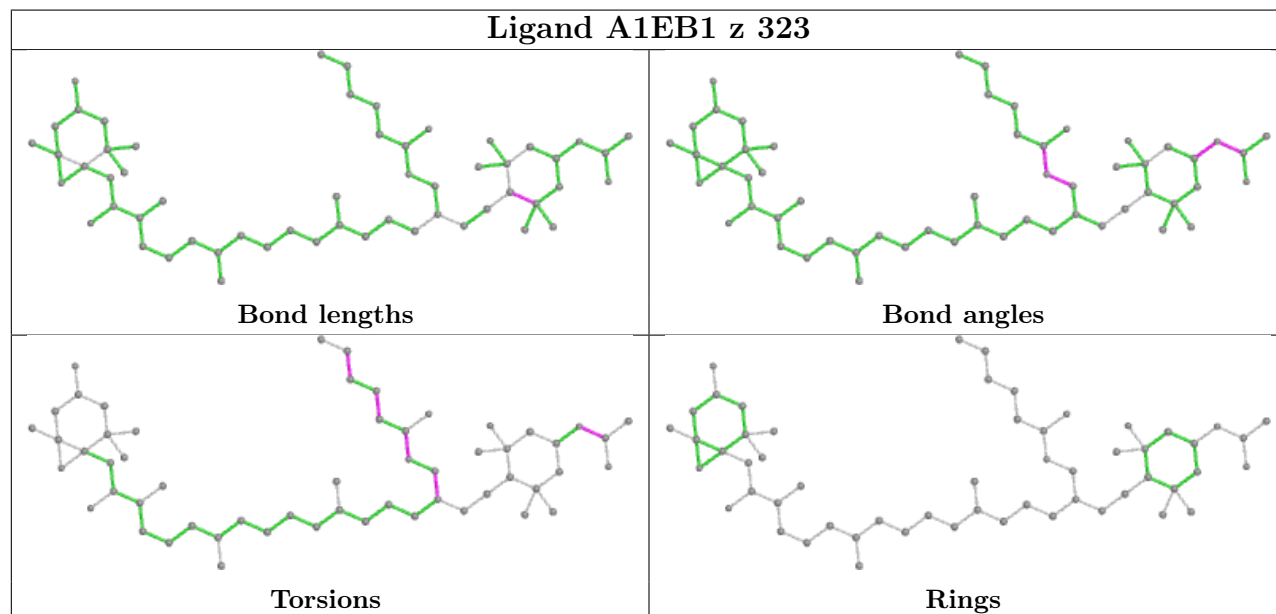
Rings

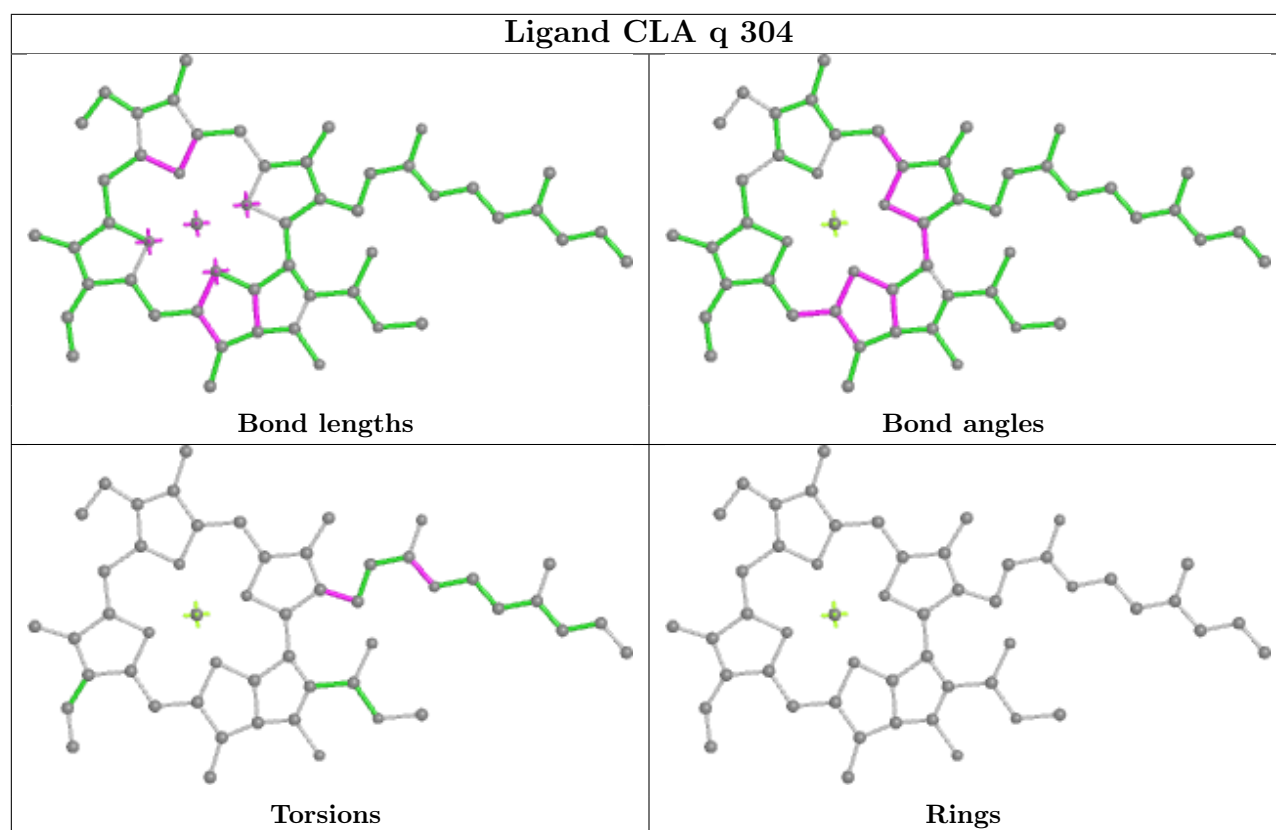


Ligand CLA t 309

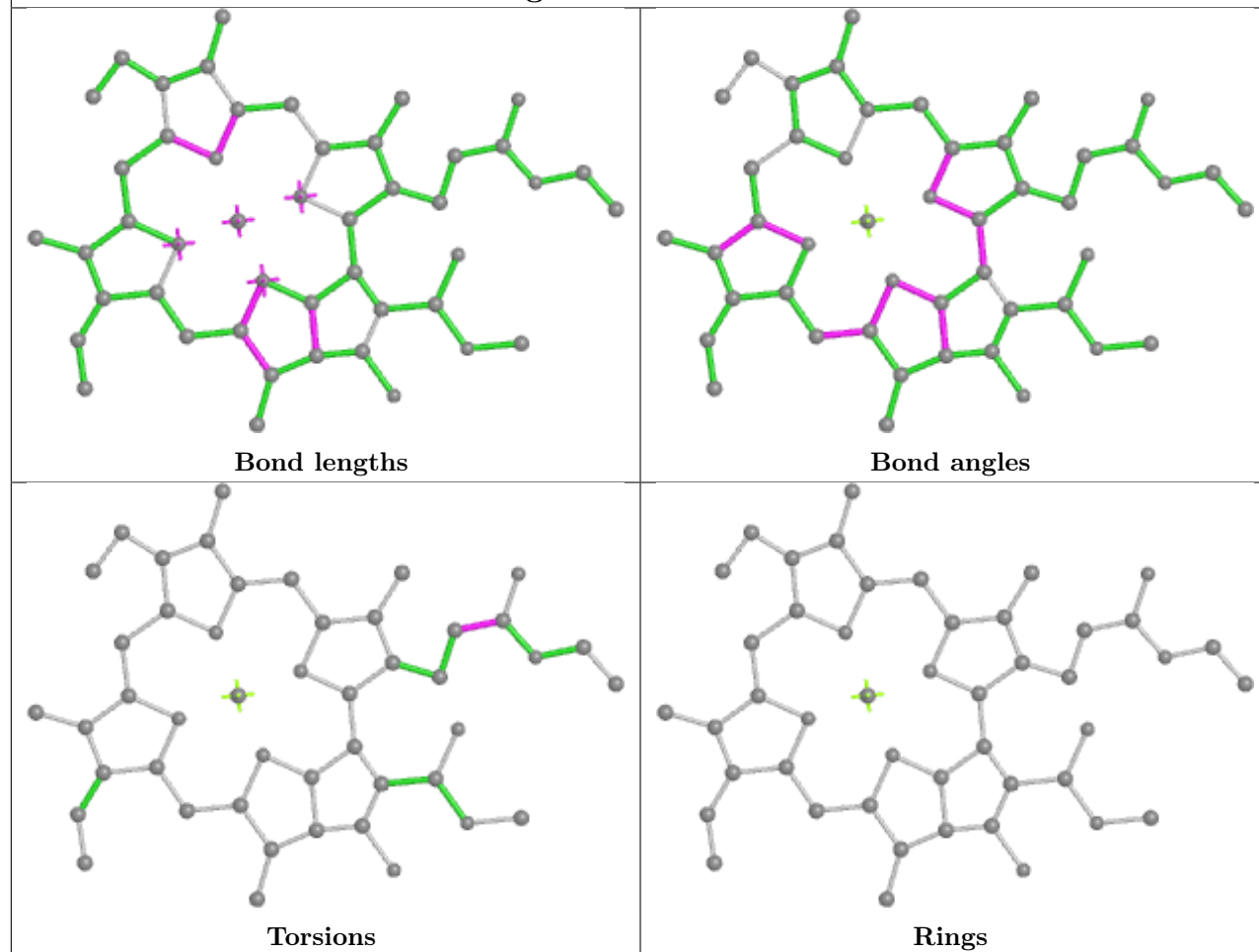


Ligand A1EB1 z 323

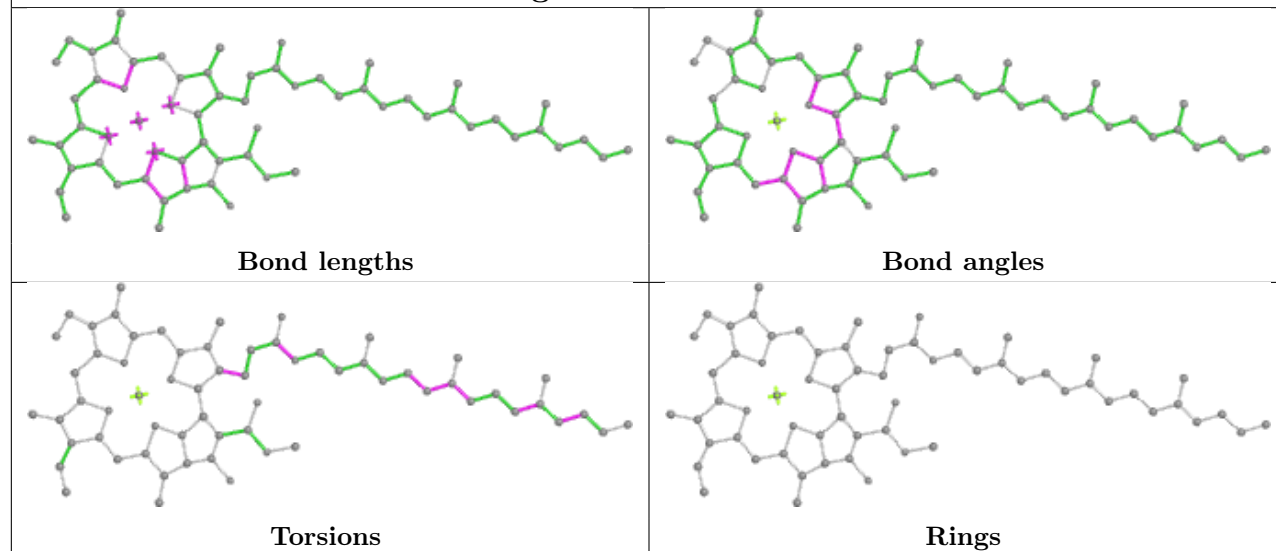


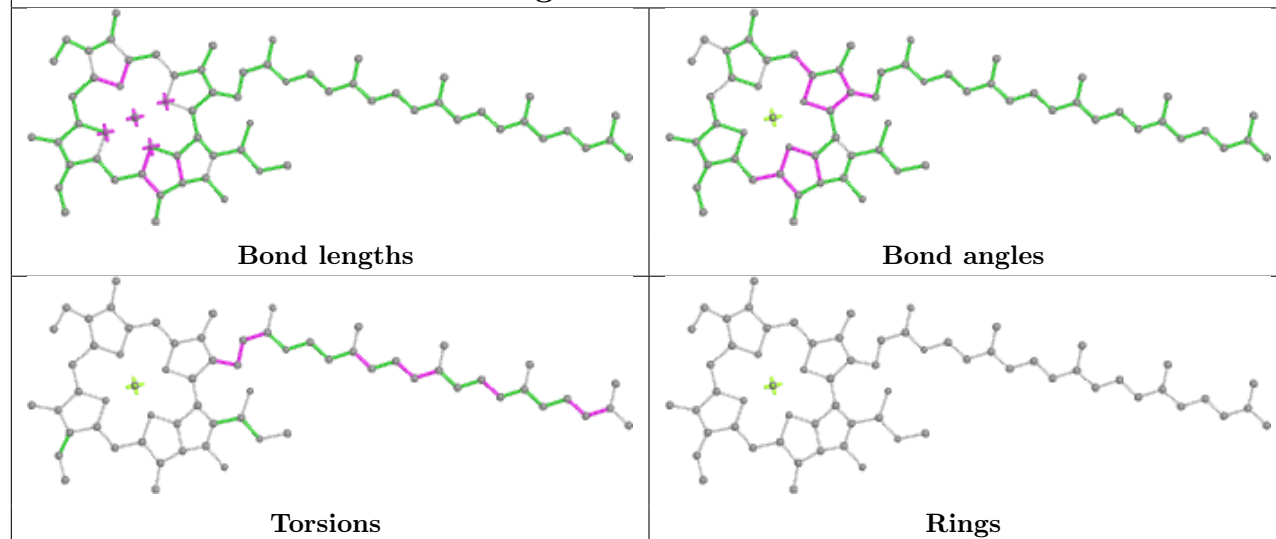
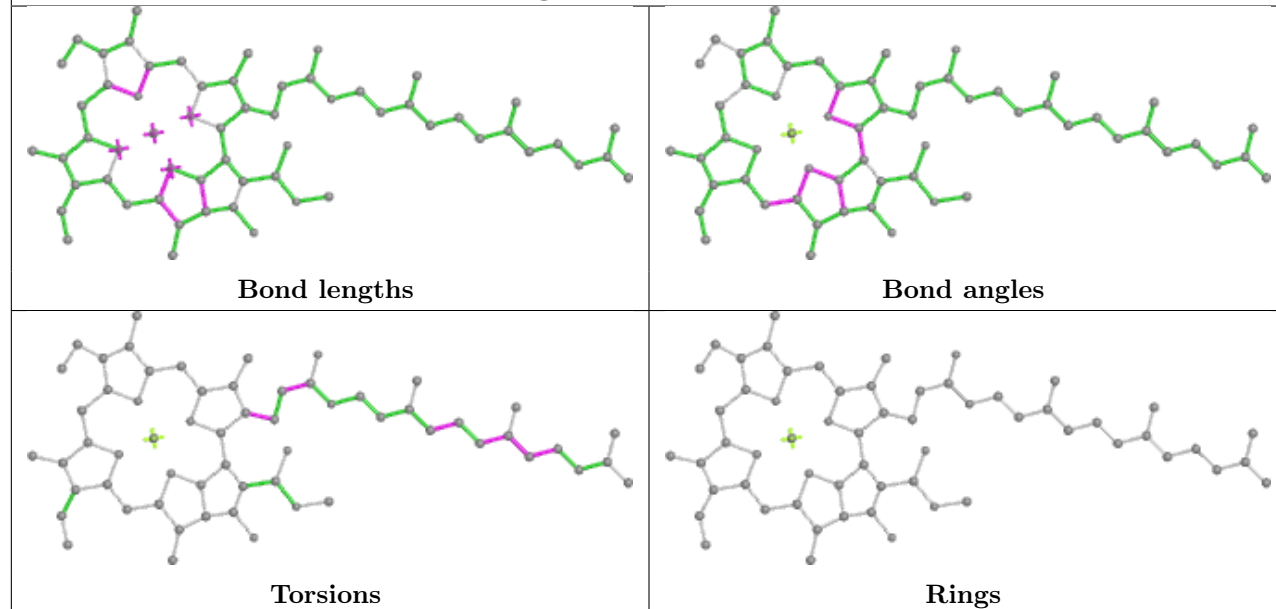


Ligand CLA P 306

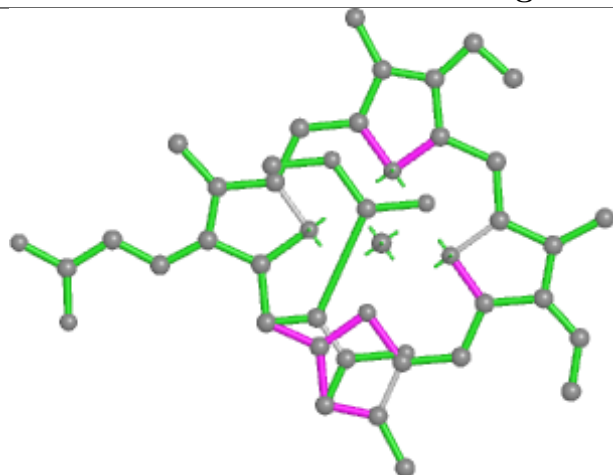


Ligand CLA X 311

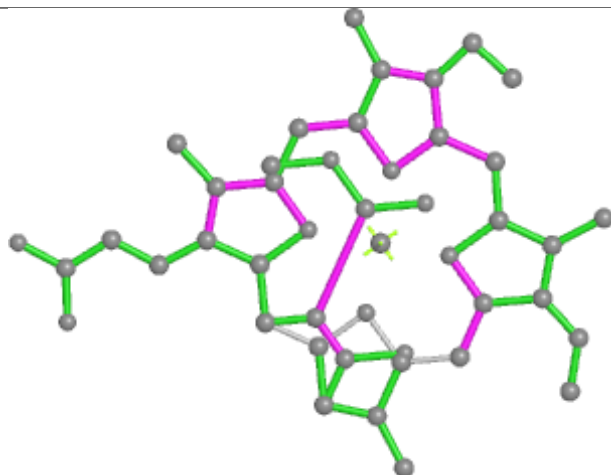


Ligand CLA b 824**Ligand CLA b 812**

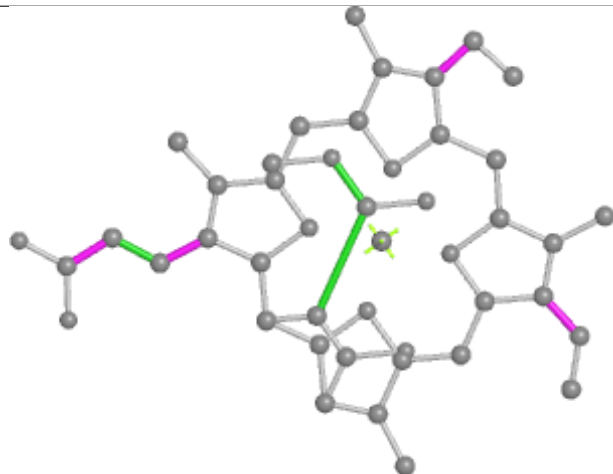
Ligand KC2 R 309



Bond lengths



Bond angles

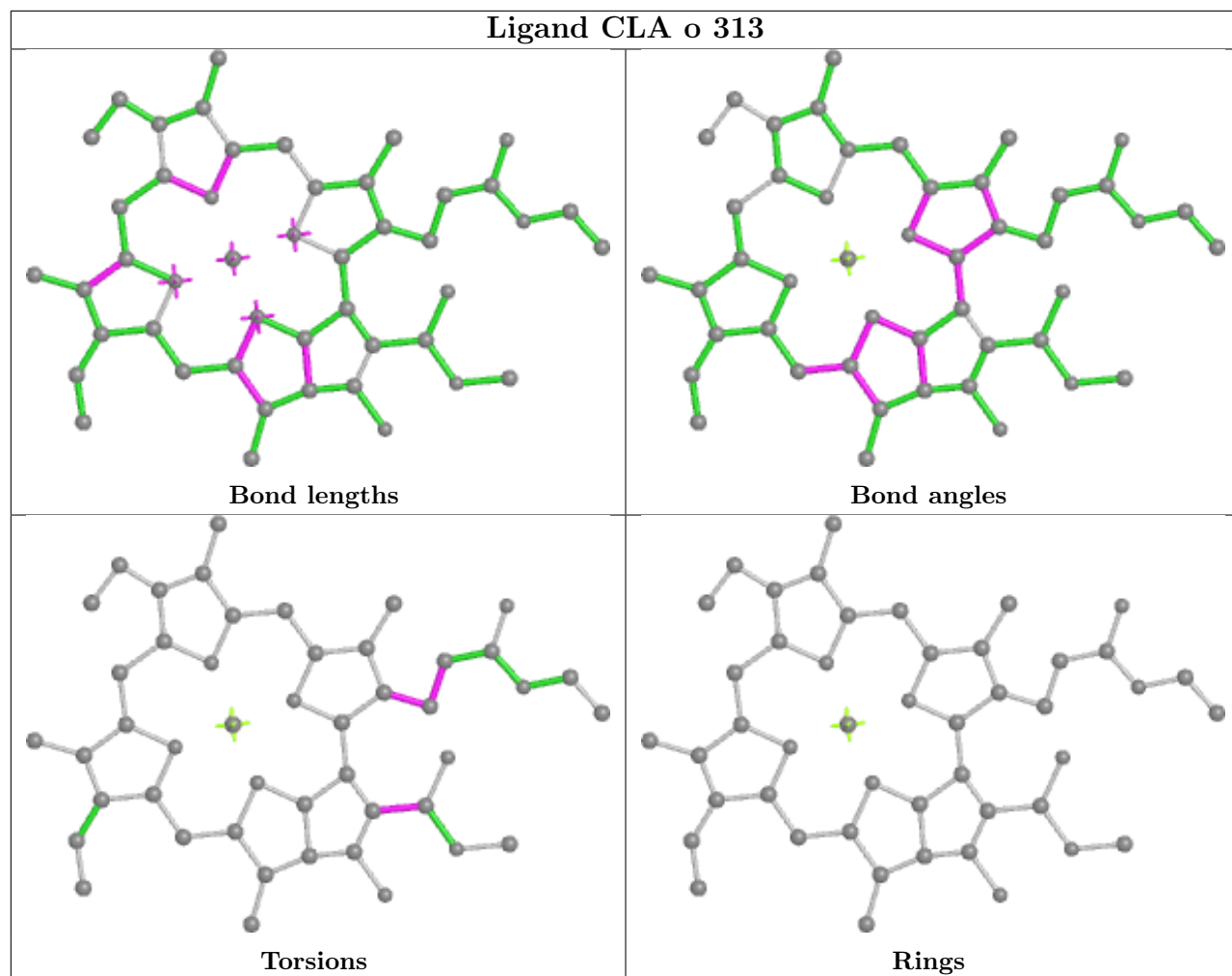


Torsions

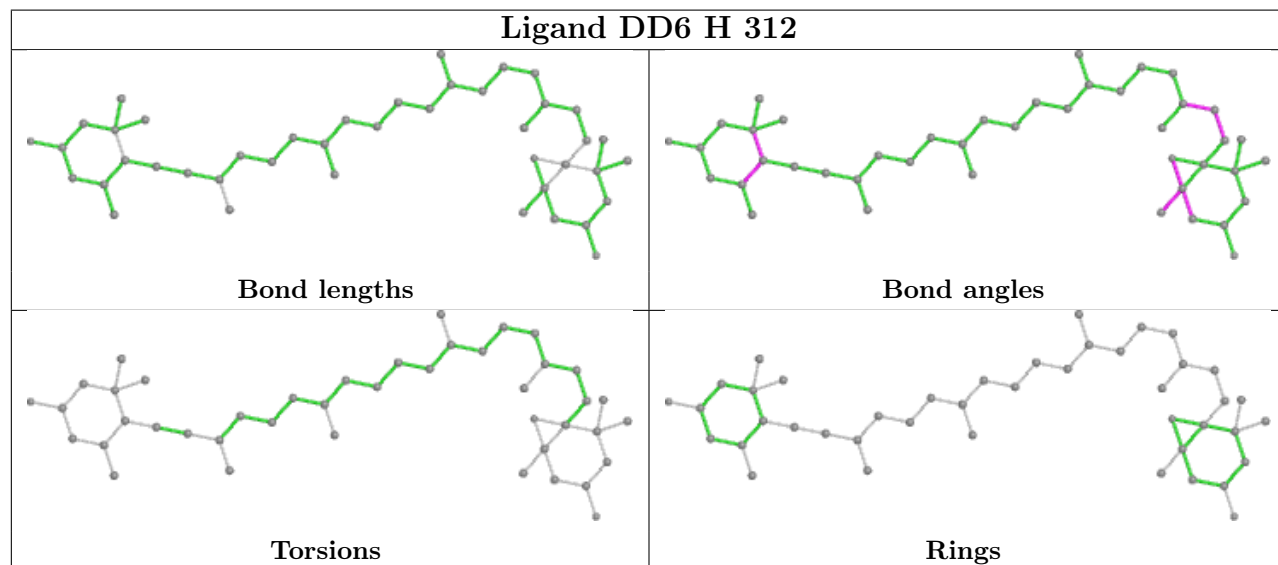


Rings

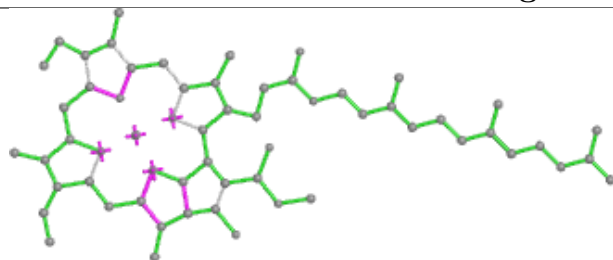
Ligand CLA o 313



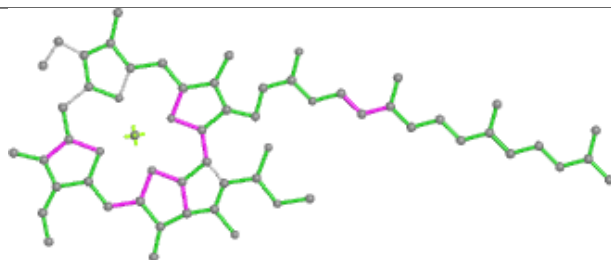
Ligand DD6 H 312



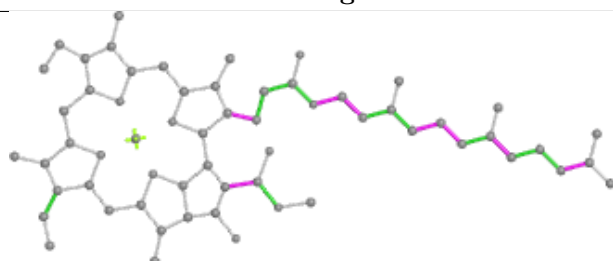
Ligand CLA z 312



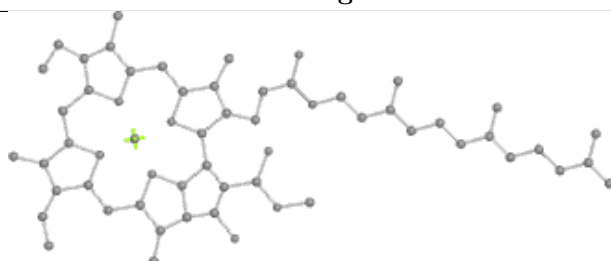
Bond lengths



Bond angles

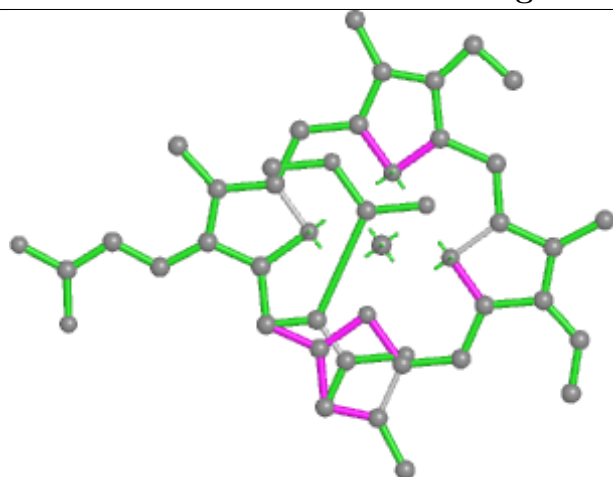


Torsions

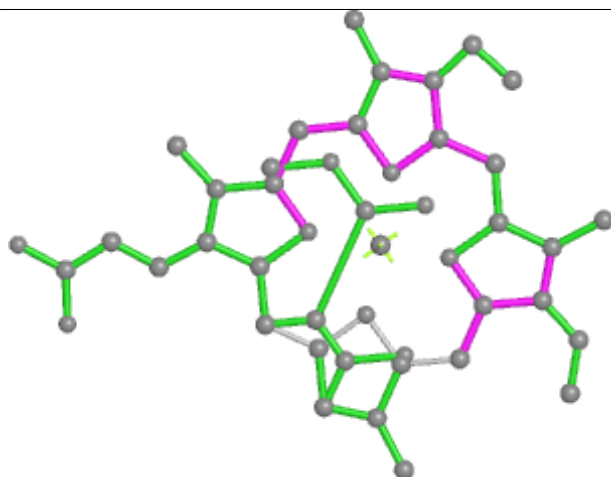


Rings

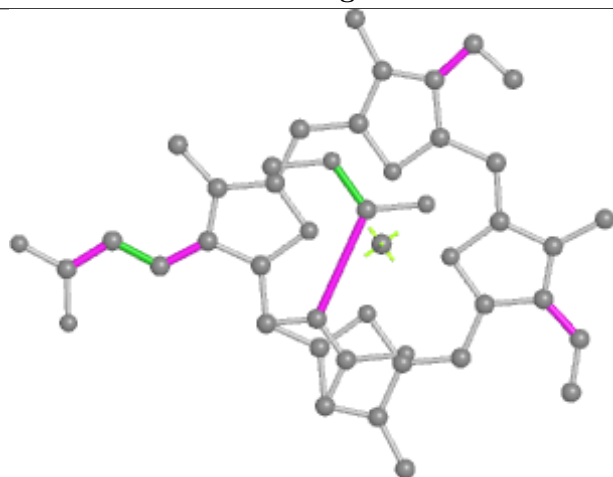
Ligand KC2 R 311



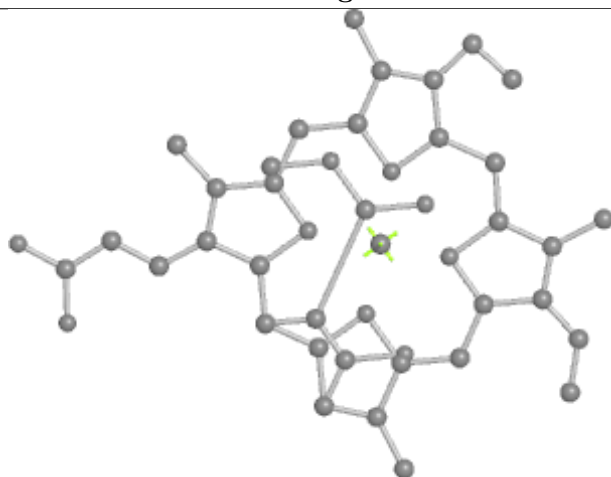
Bond lengths



Bond angles

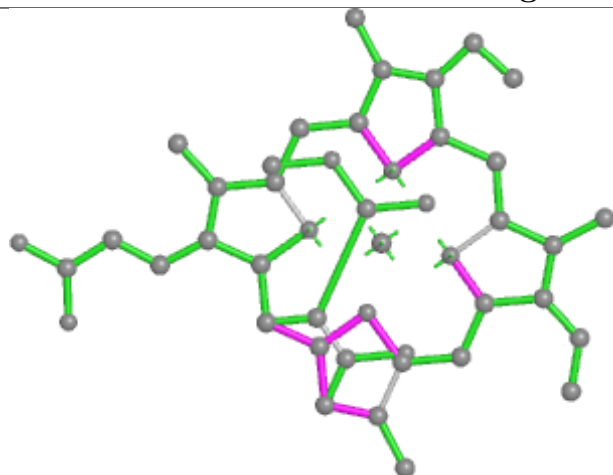


Torsions

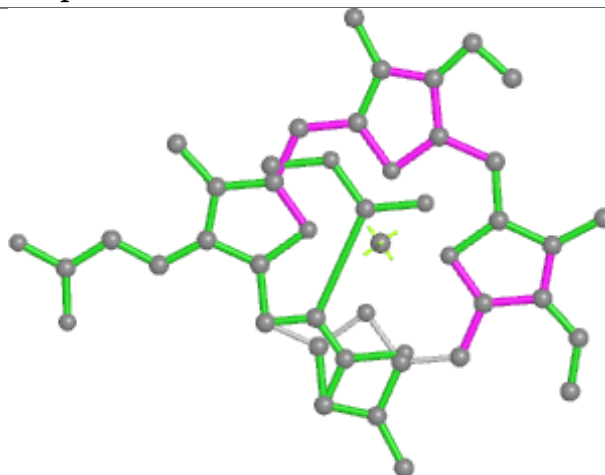


Rings

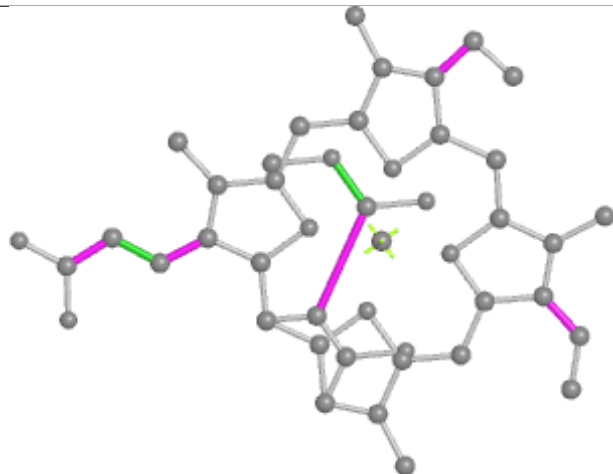
Ligand KC2 q 309



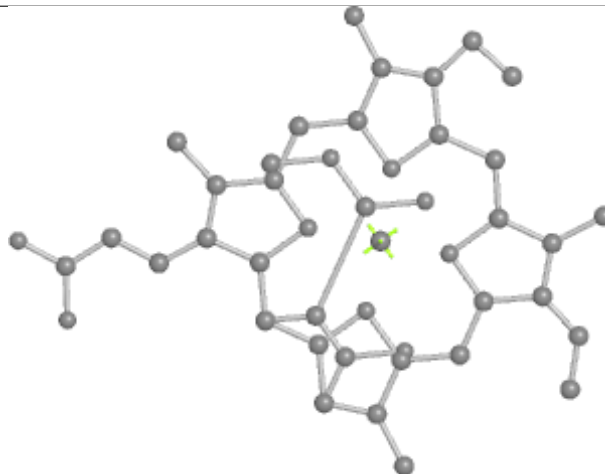
Bond lengths



Bond angles

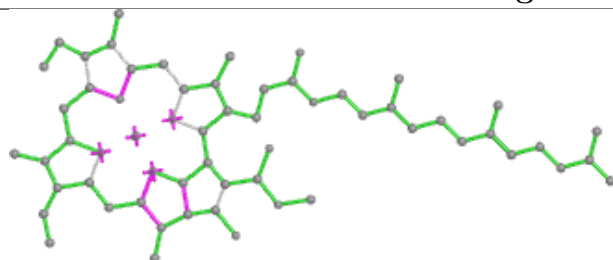


Torsions

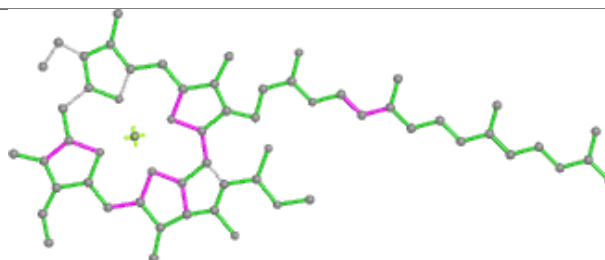


Rings

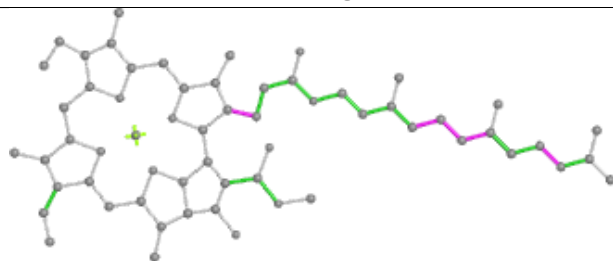
Ligand CLA F 306



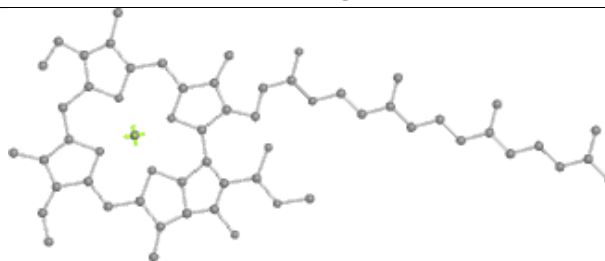
Bond lengths



Bond angles

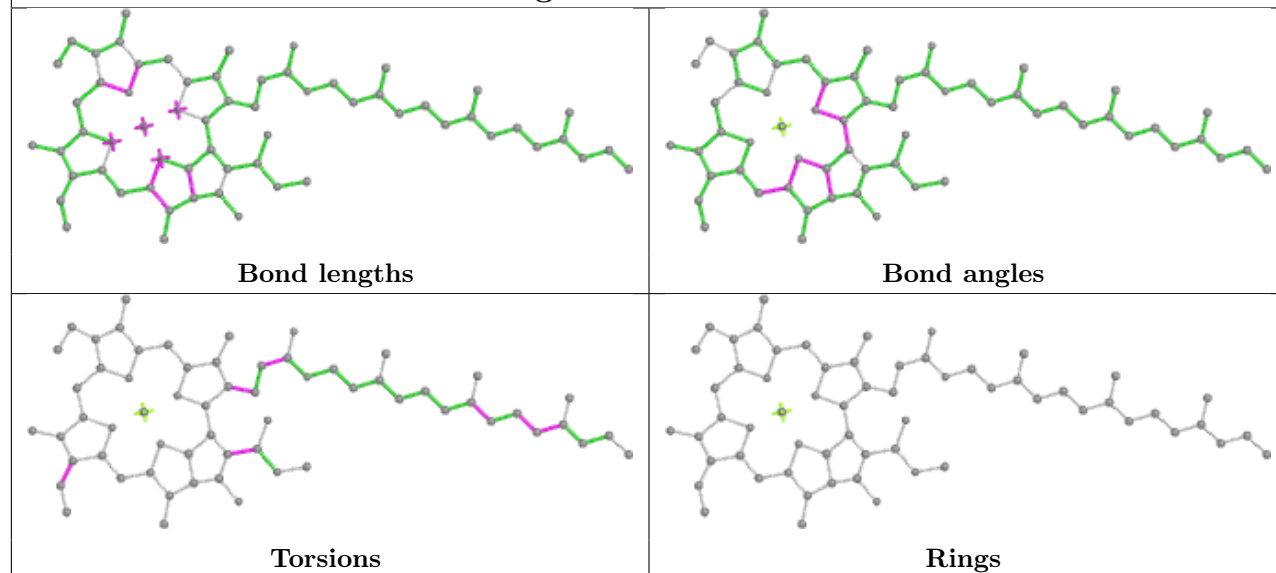


Torsions

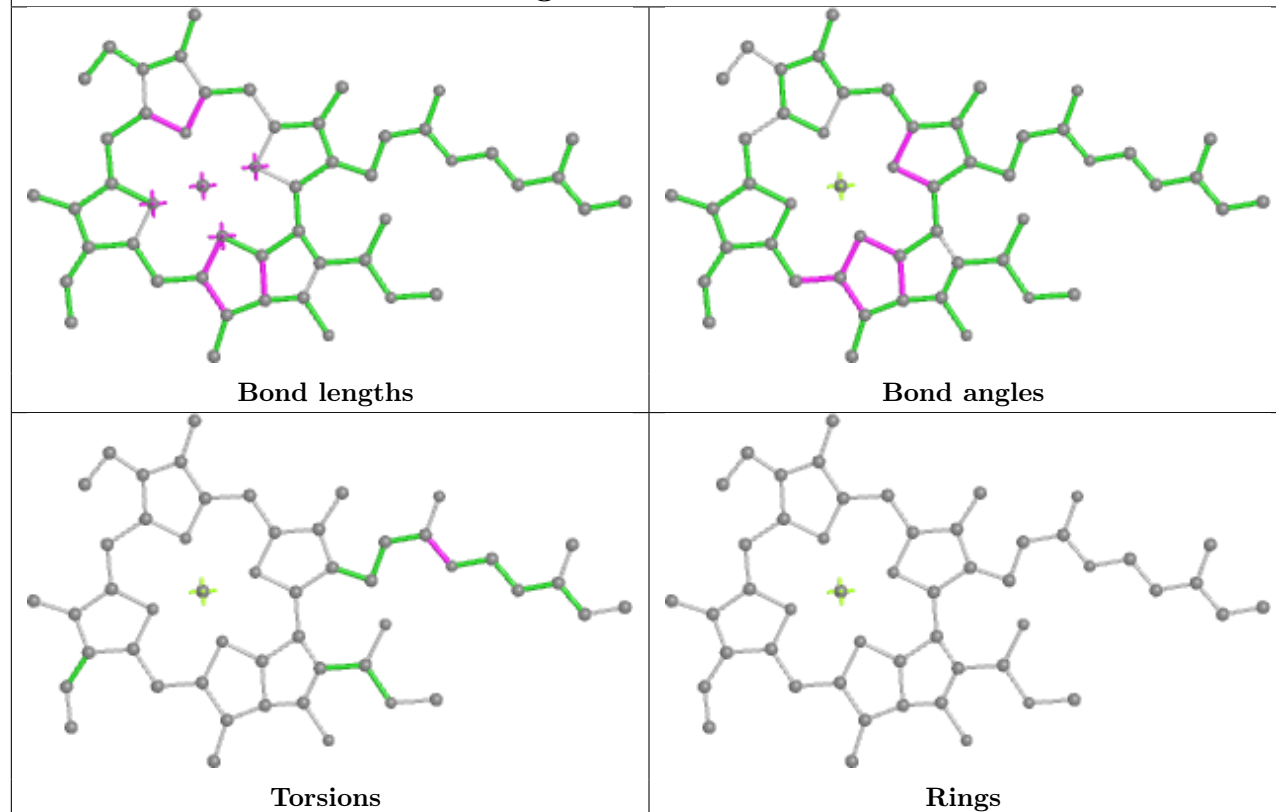


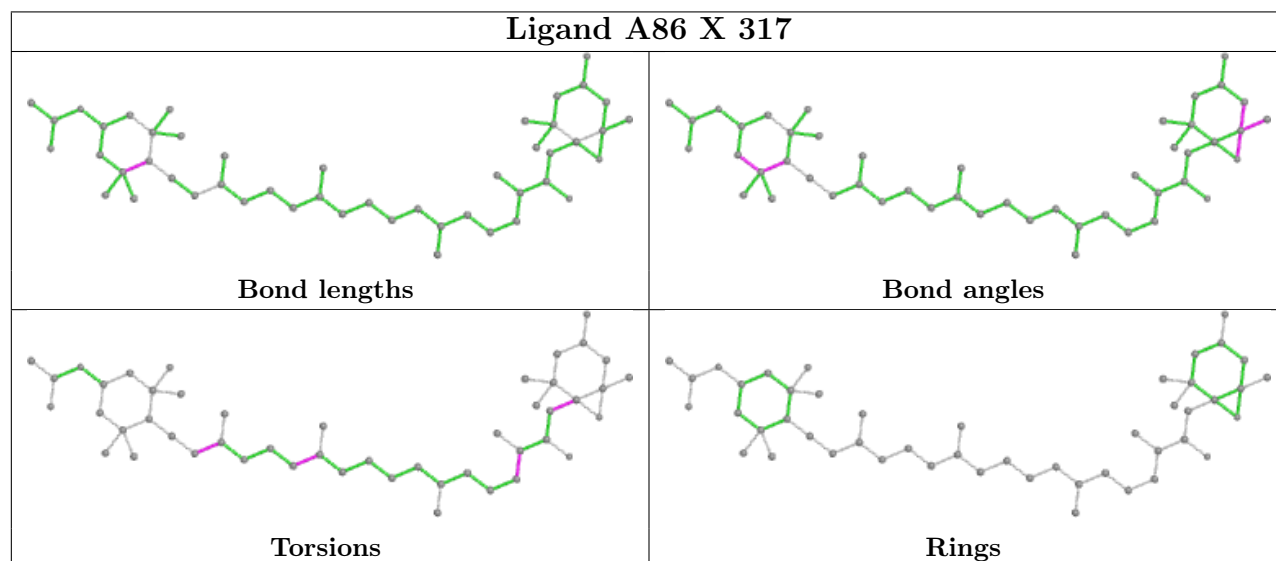
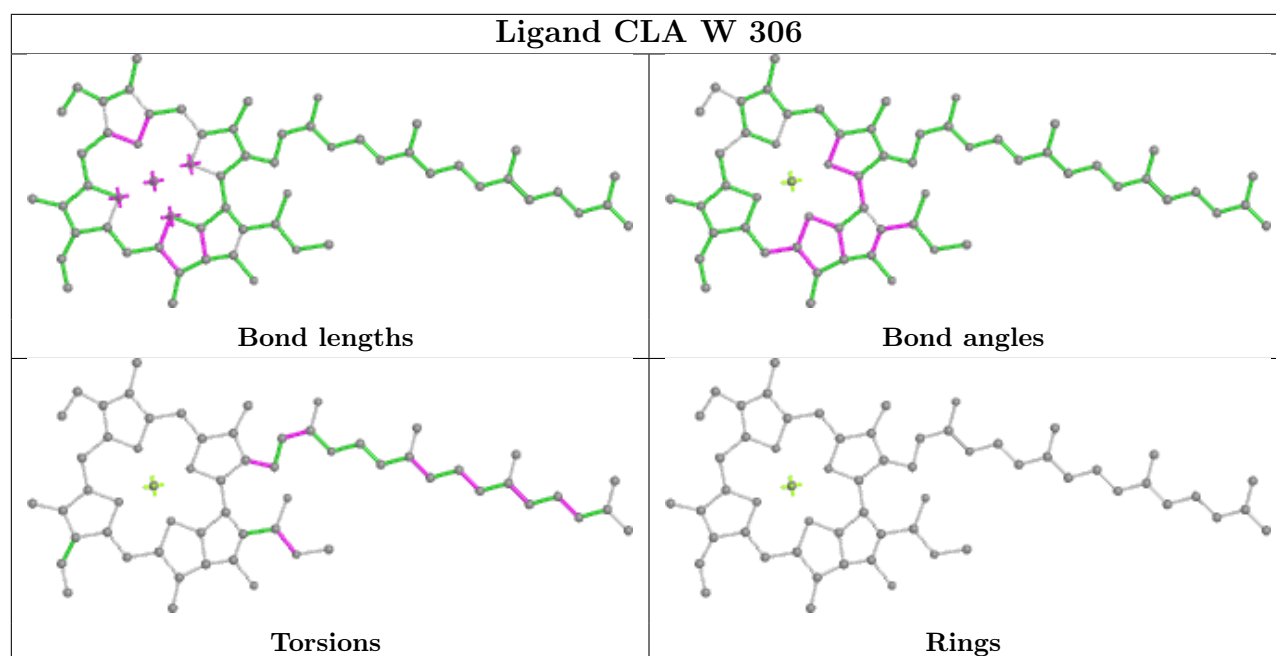
Rings

Ligand CLA b 818

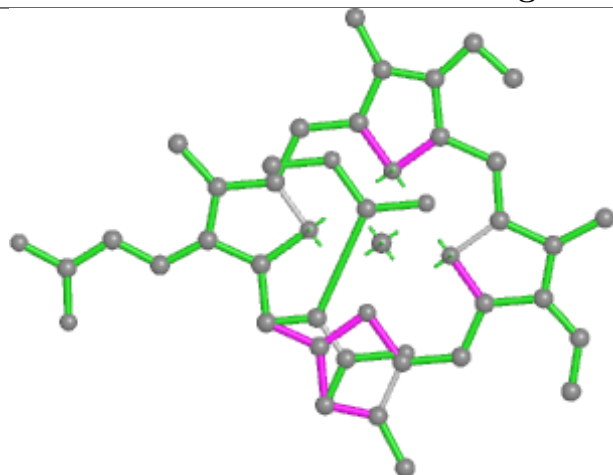


Ligand CLA x 305

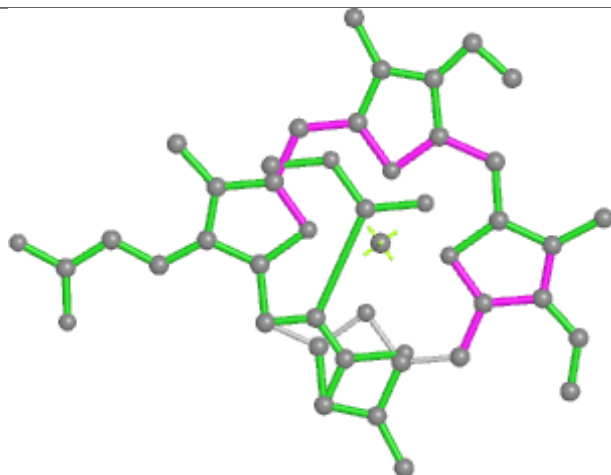




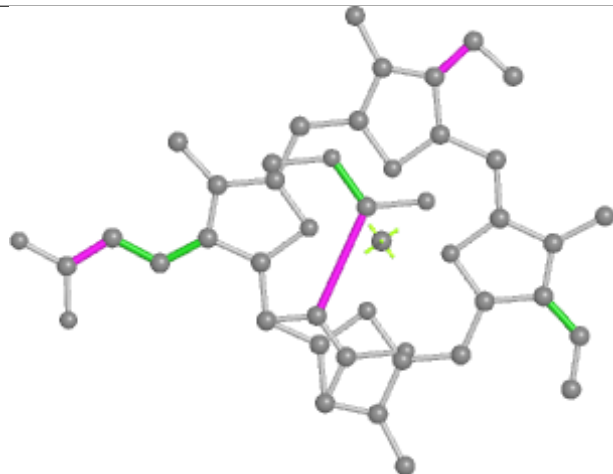
Ligand KC2 L 303



Bond lengths



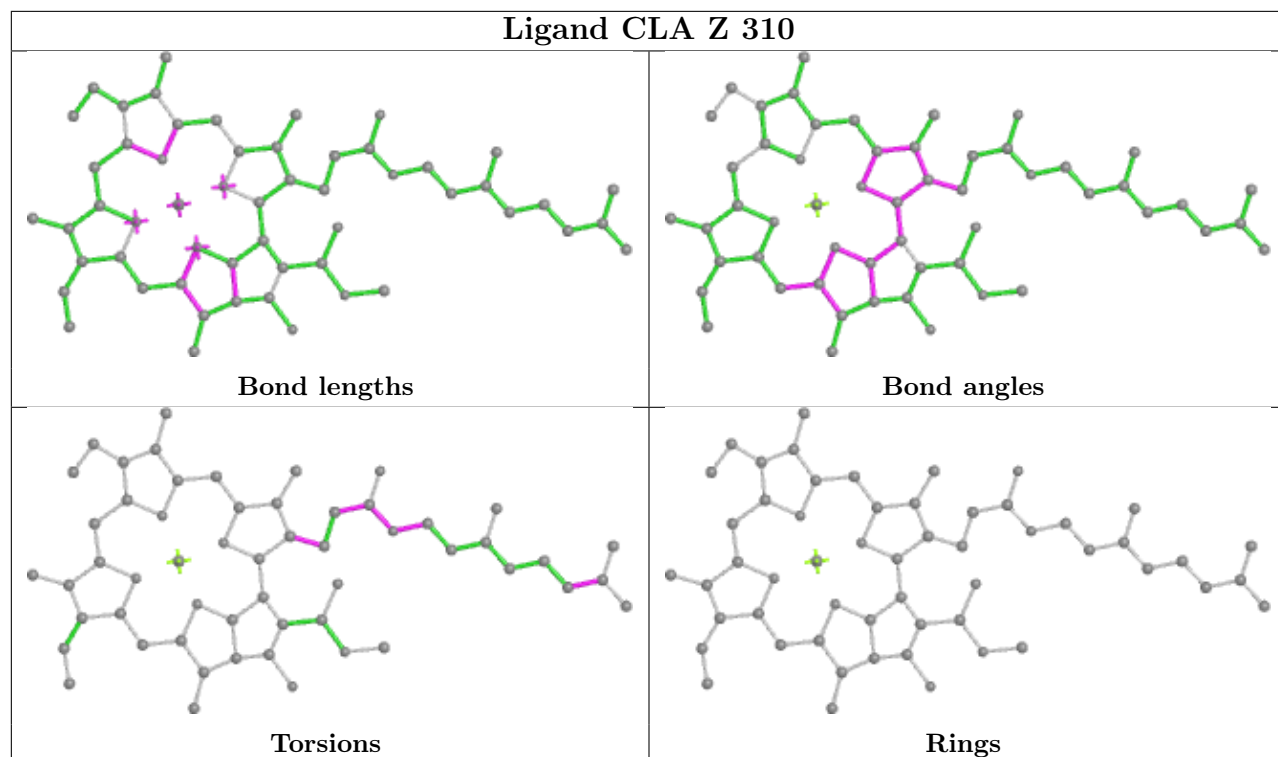
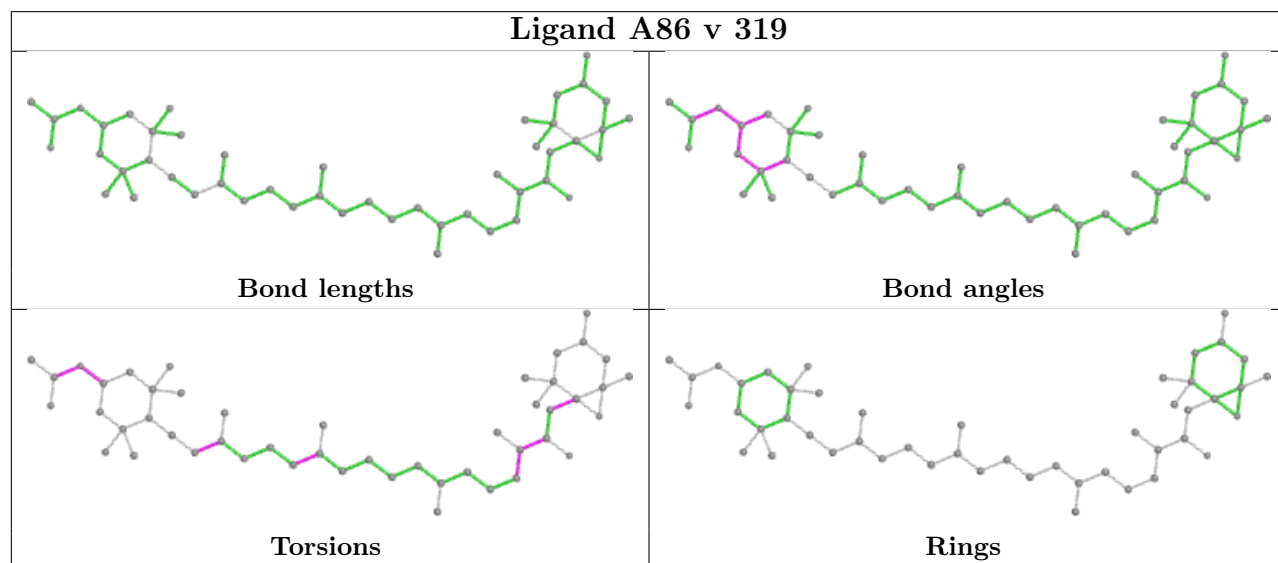
Bond angles



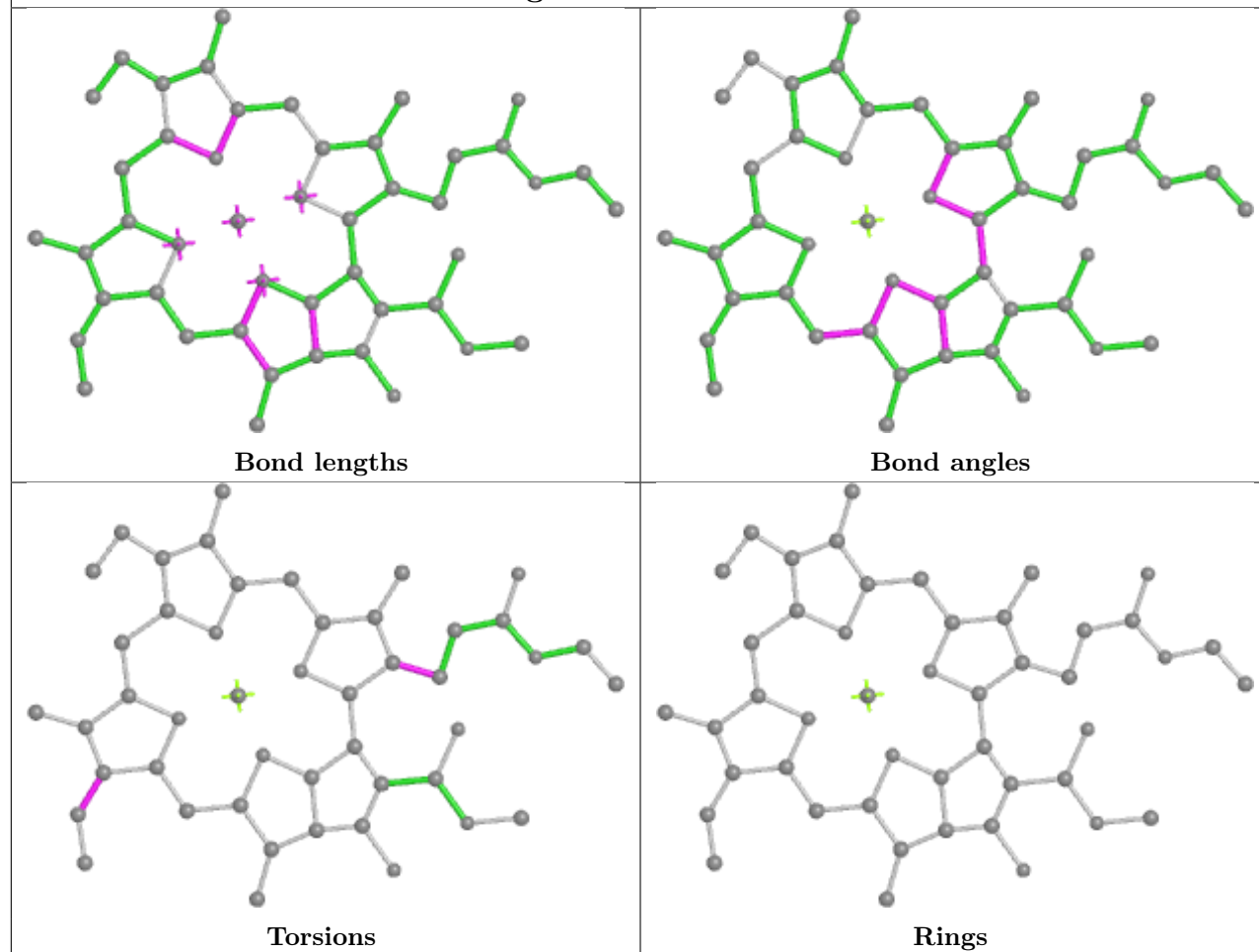
Torsions



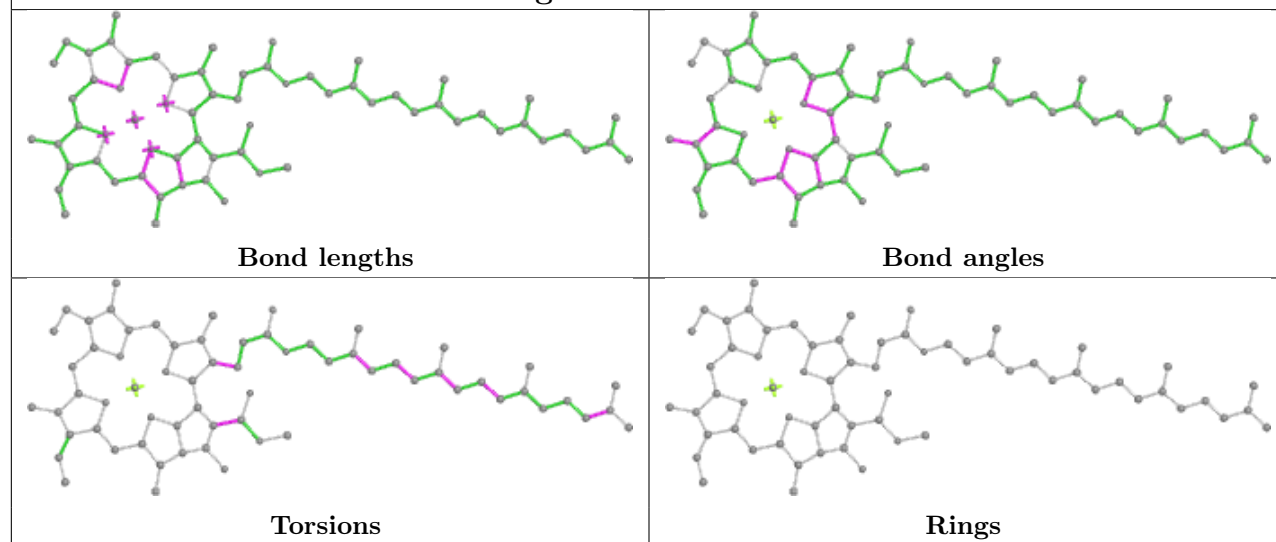
Rings

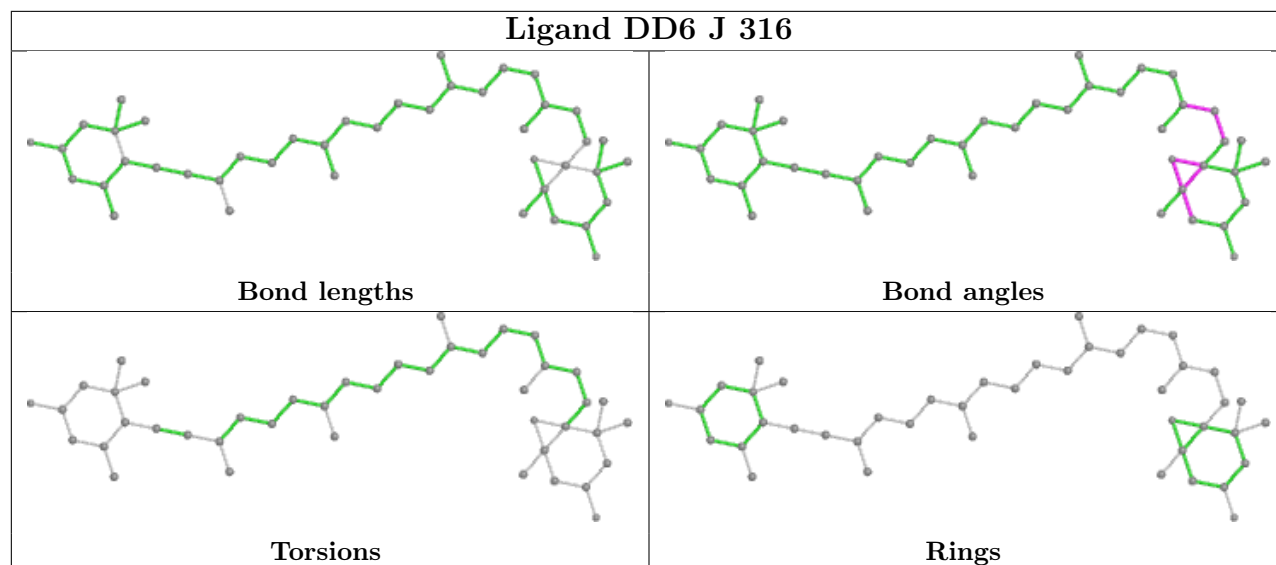
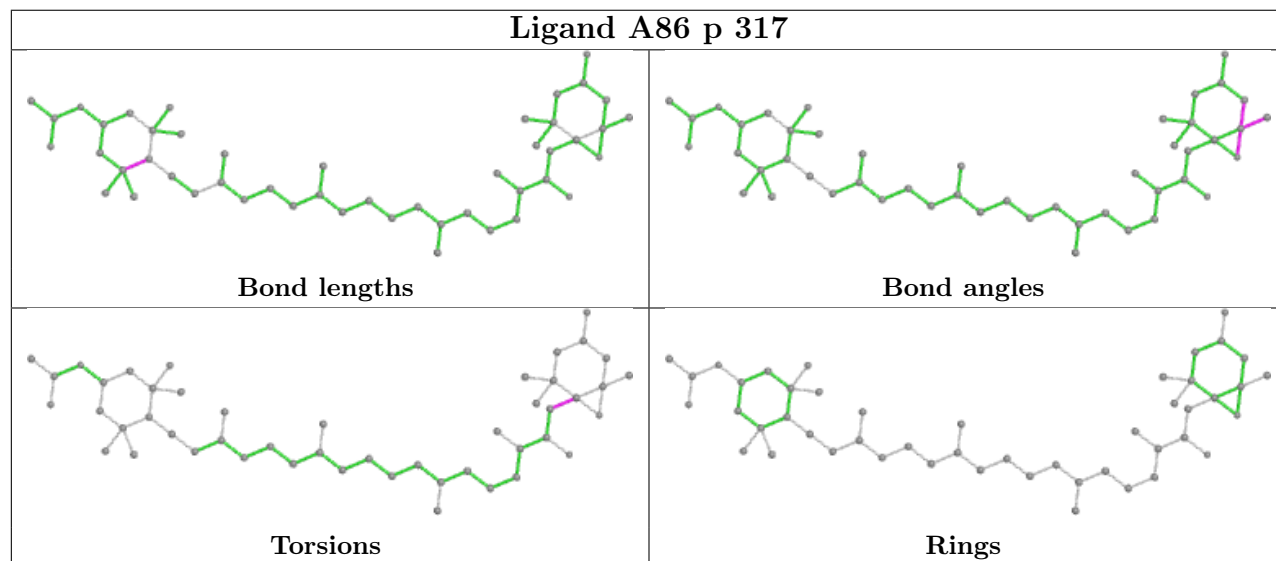
Ligand CLA Z 310**Ligand A86 v 319**

Ligand CLA E 312

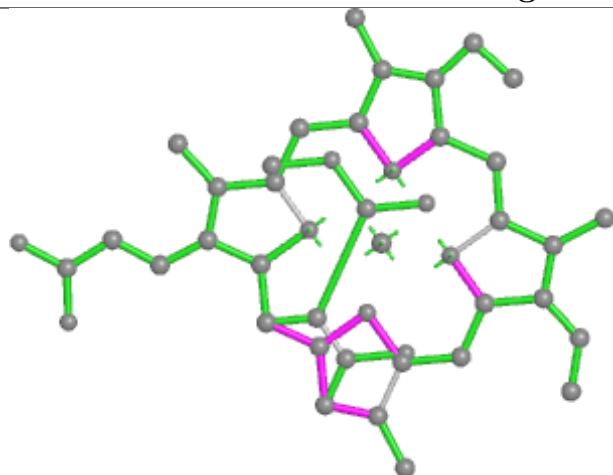


Ligand CLA b 840

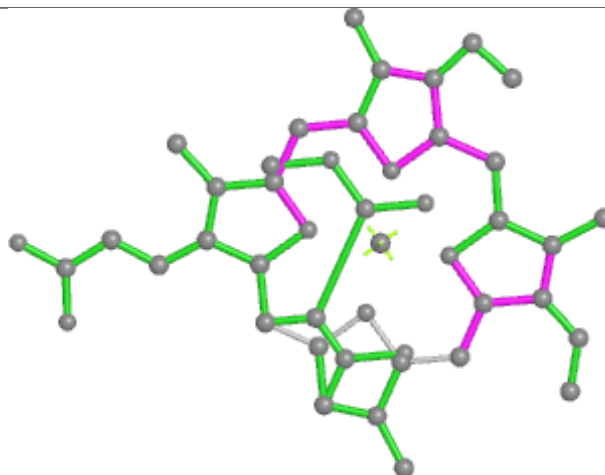


Ligand DD6 J 316**Ligand A86 p 317**

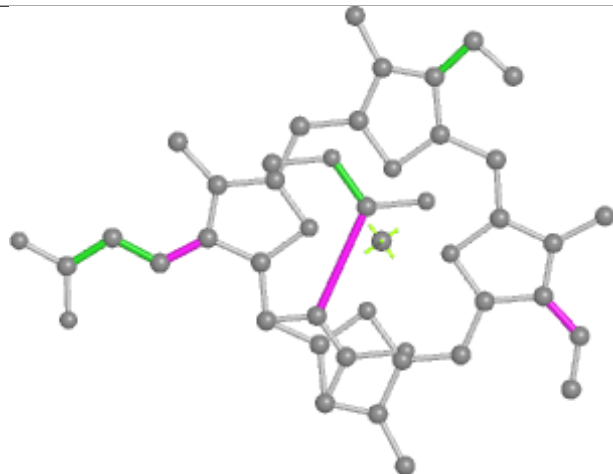
Ligand KC2 L 302



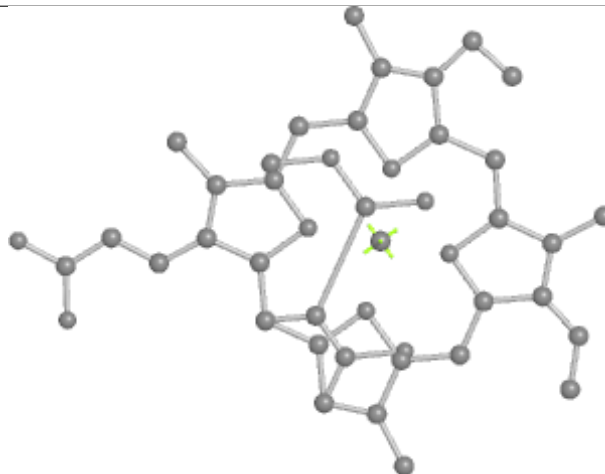
Bond lengths



Bond angles

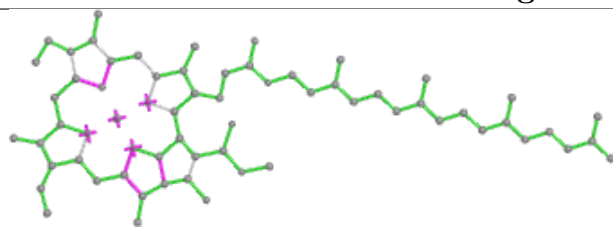


Torsions

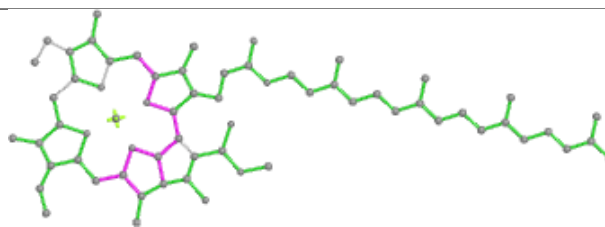


Rings

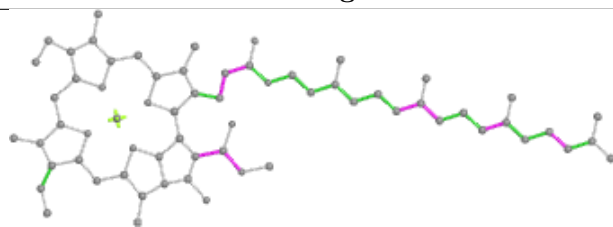
Ligand CLA b 808



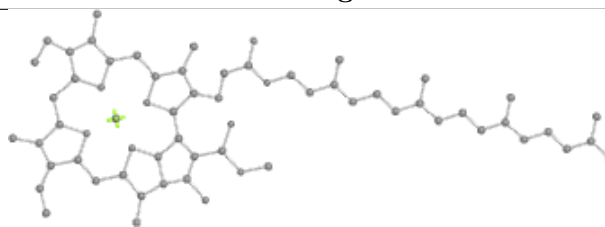
Bond lengths



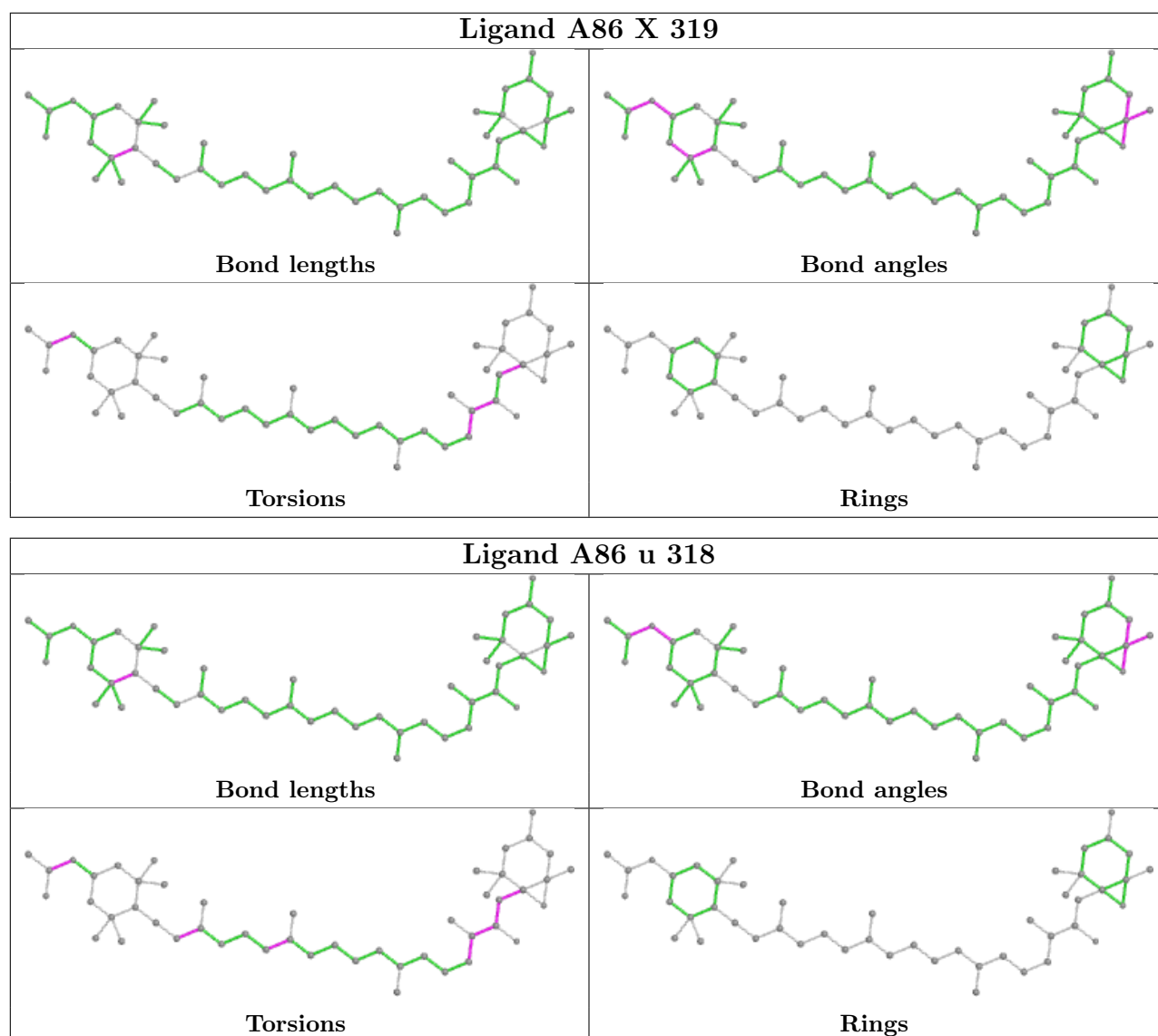
Bond angles

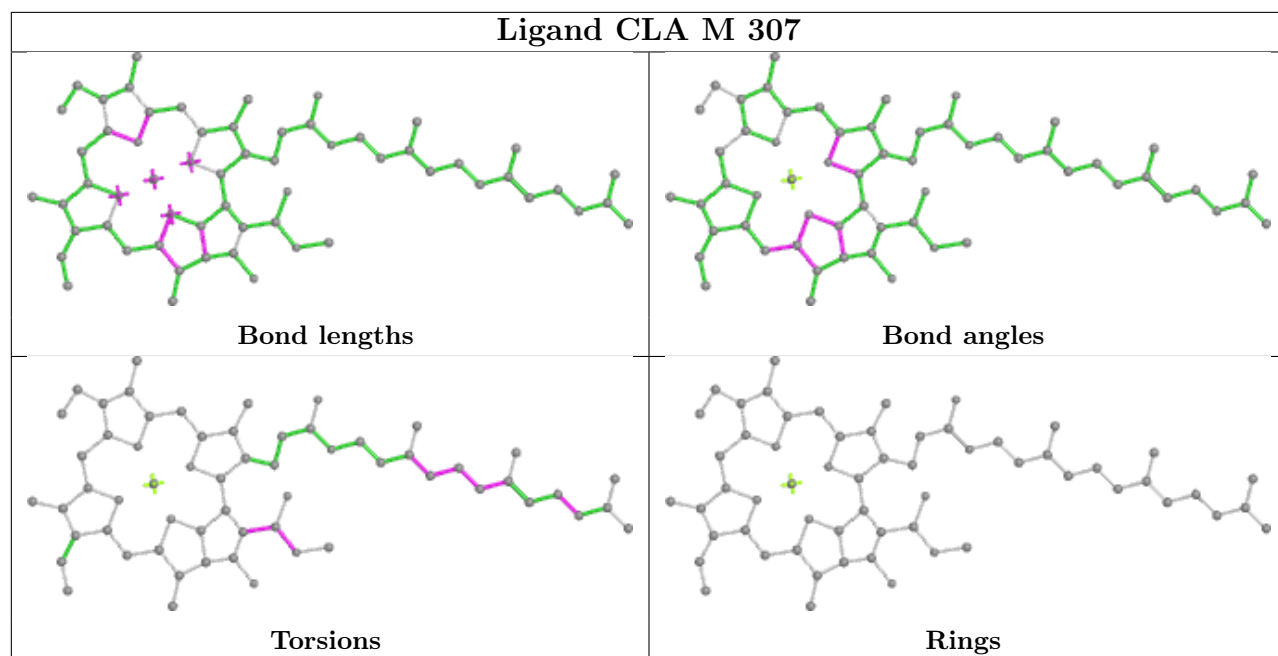
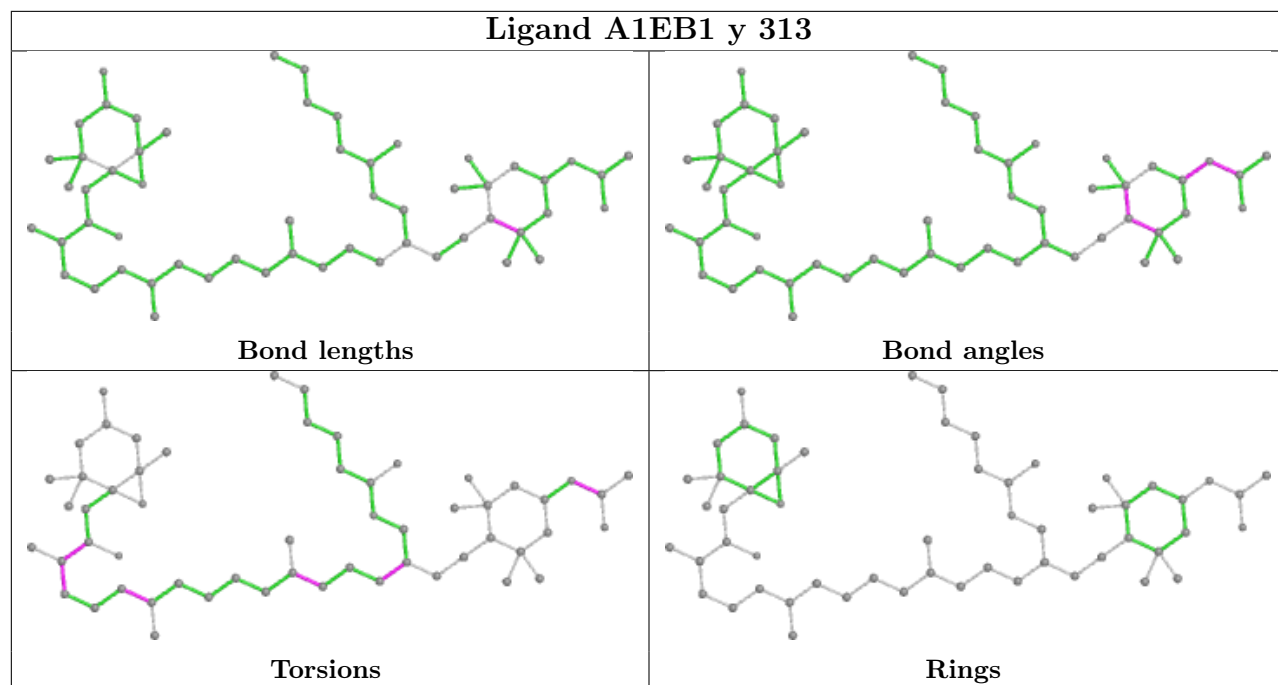


Torsions

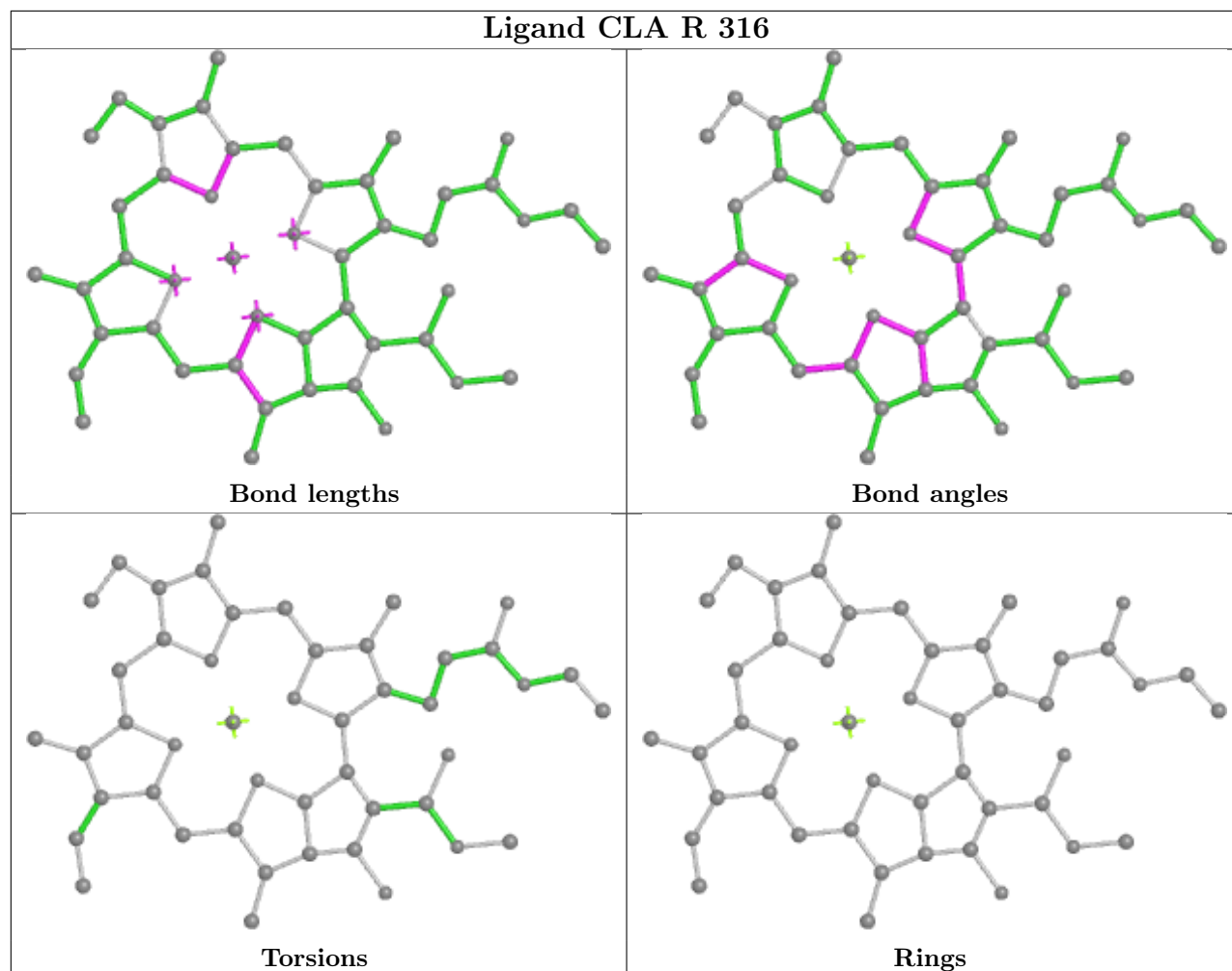


Rings

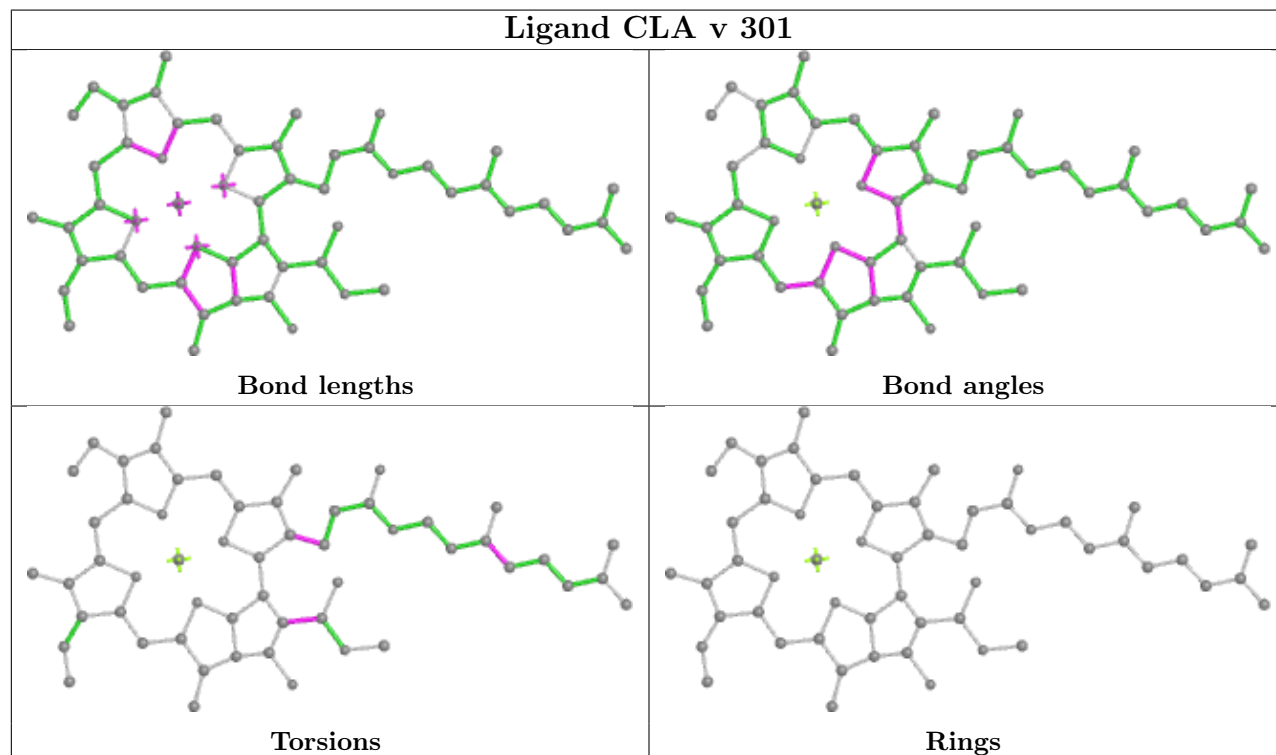


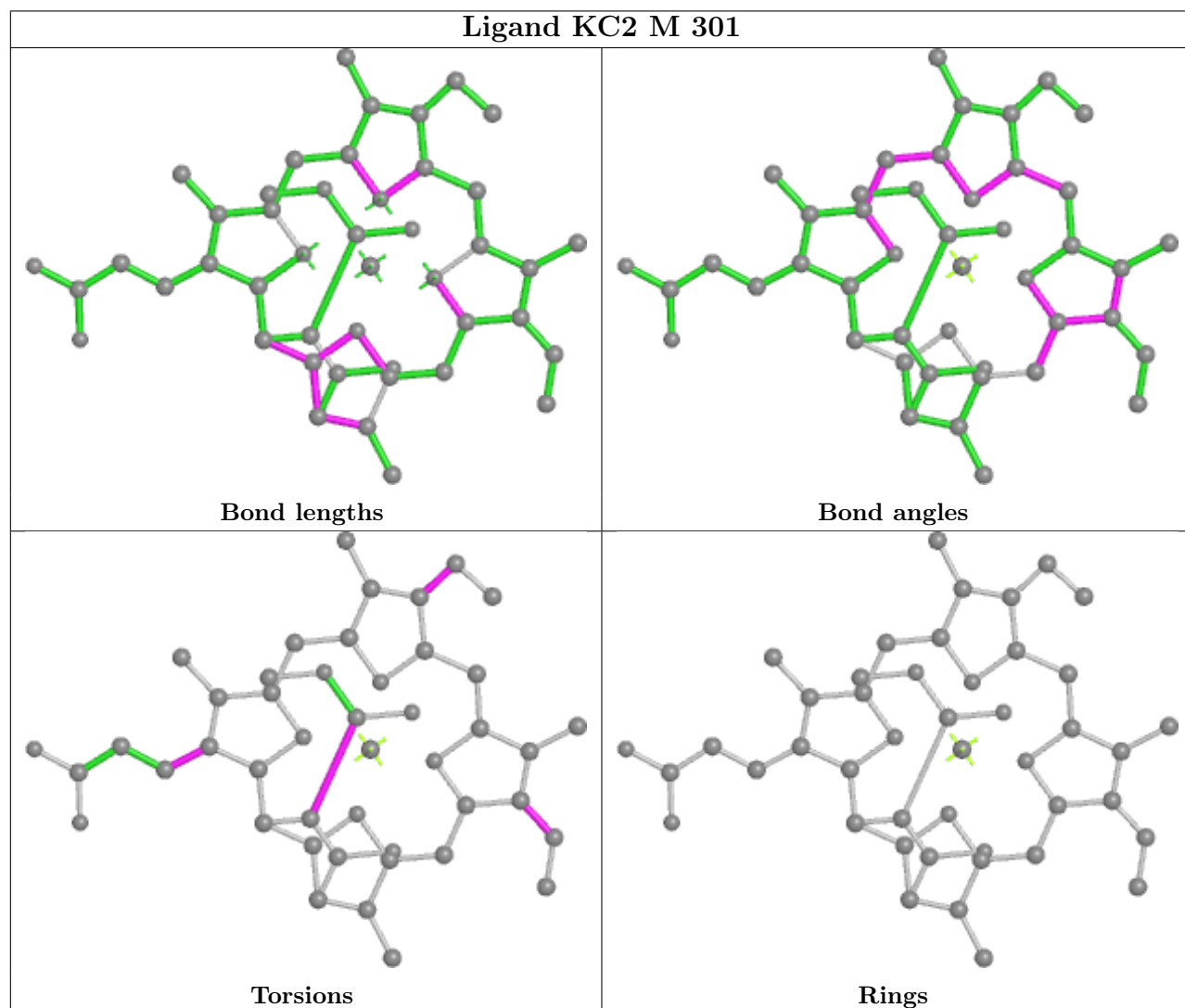
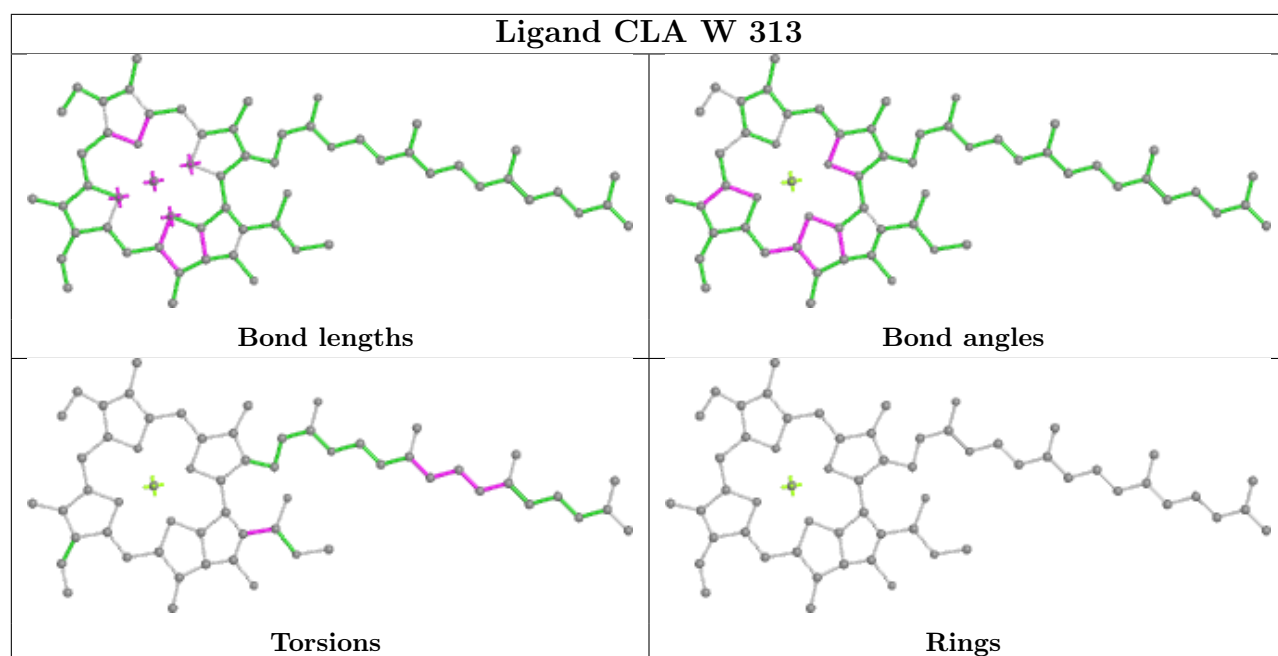


Ligand CLA R 316

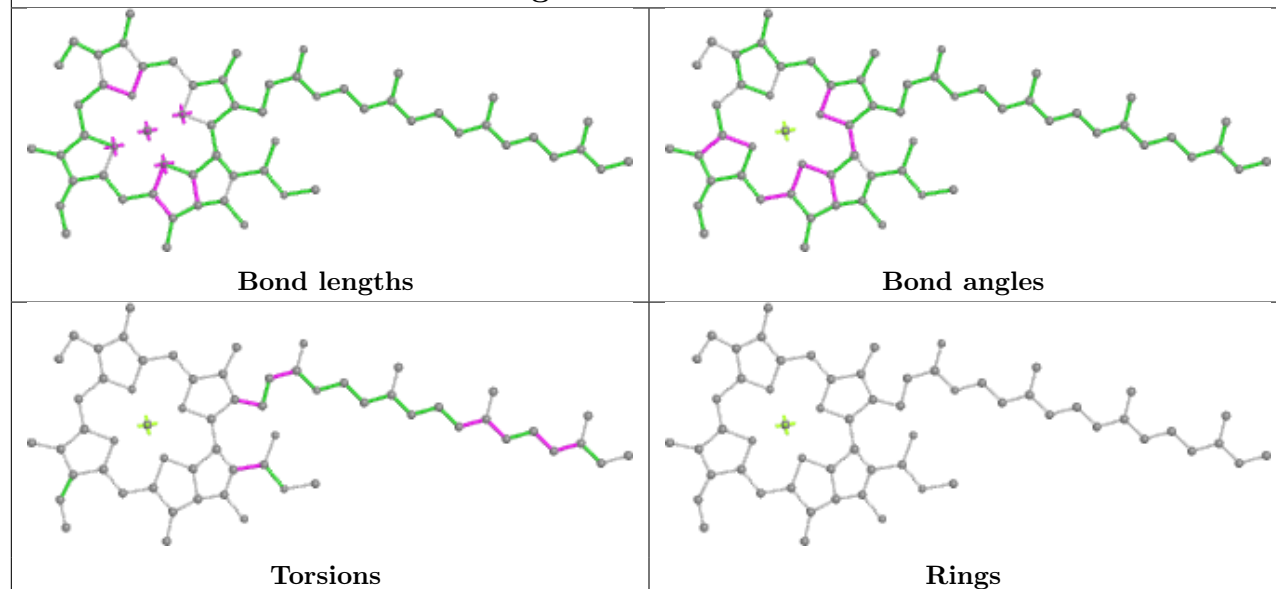


Ligand CLA v 301

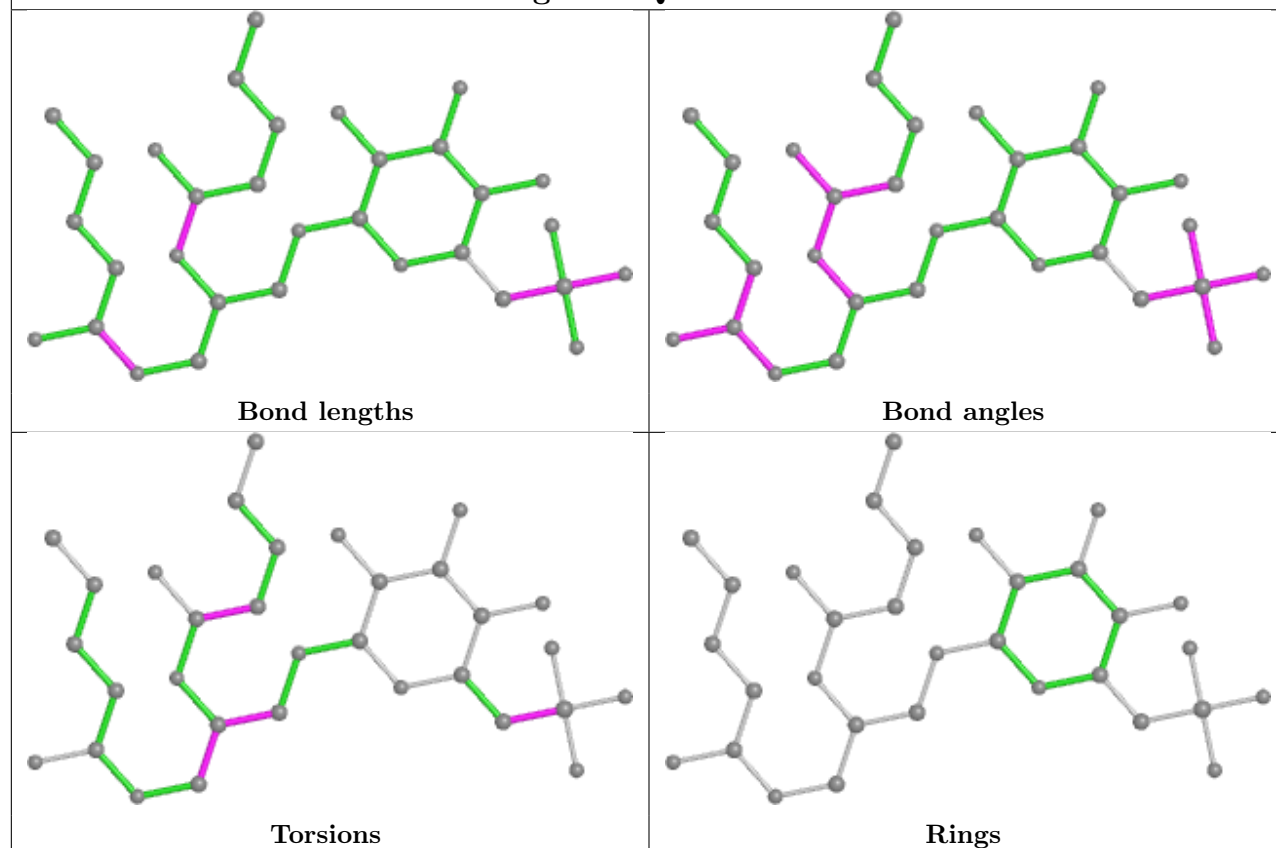




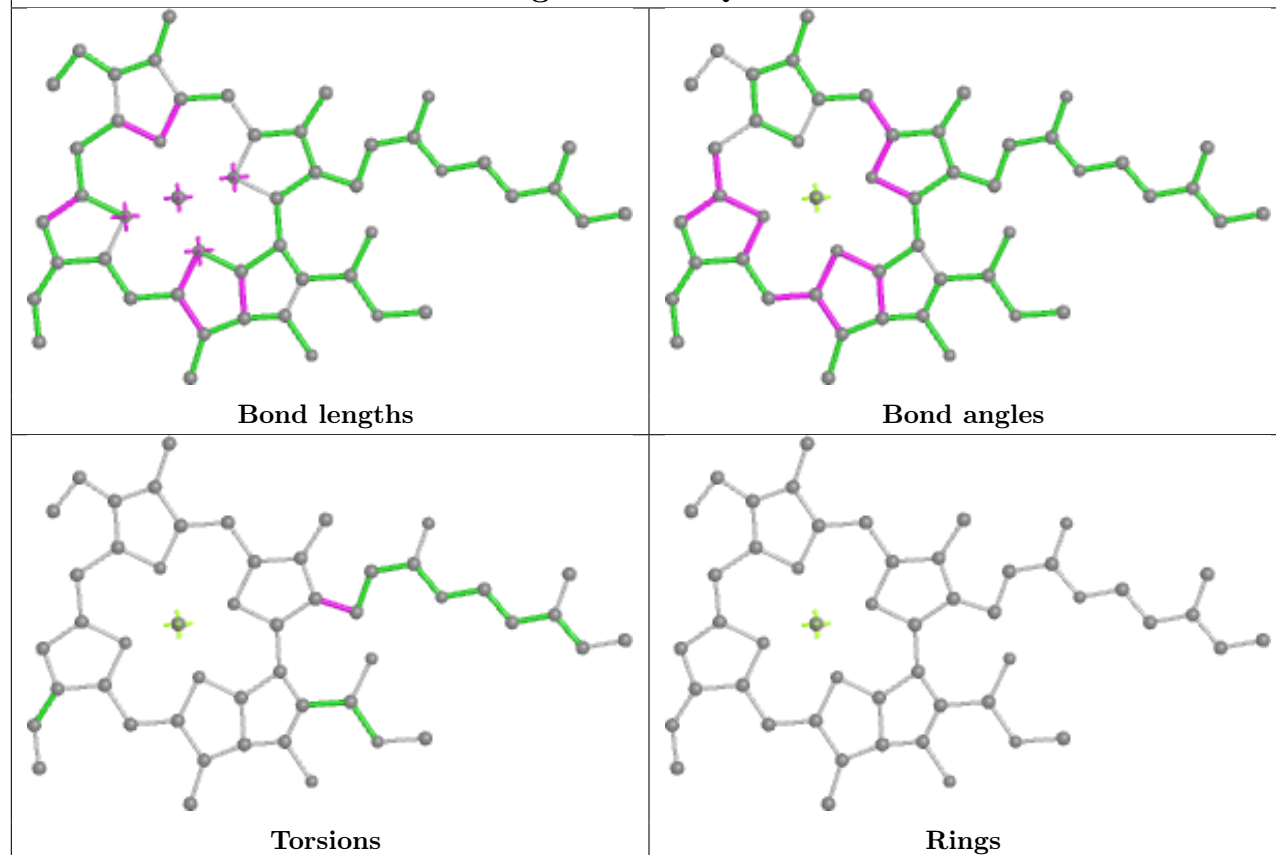
Ligand CLA A 303



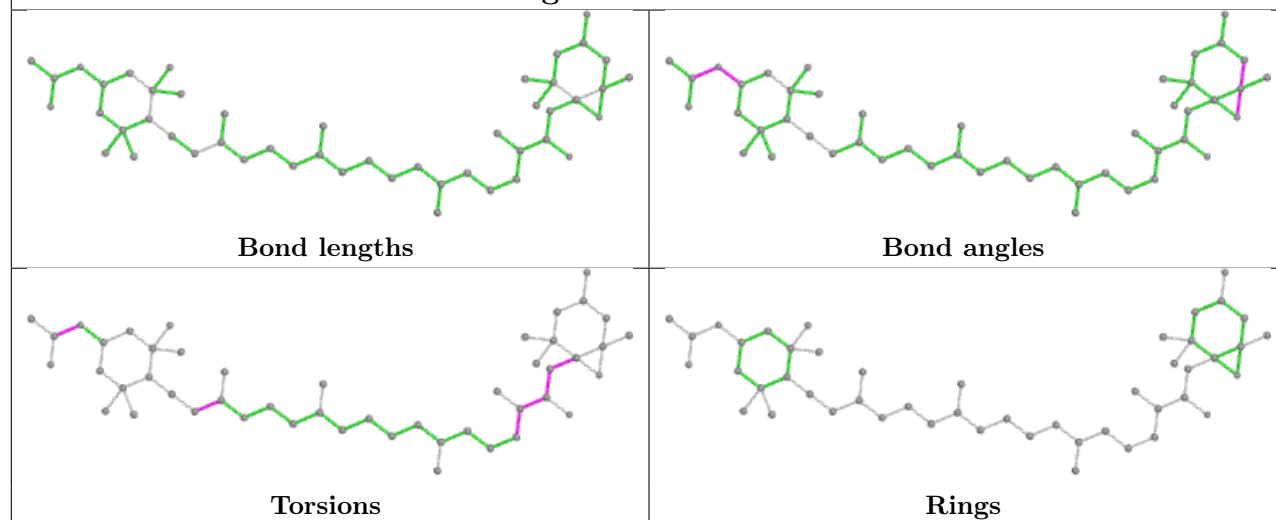
Ligand SQD P 319

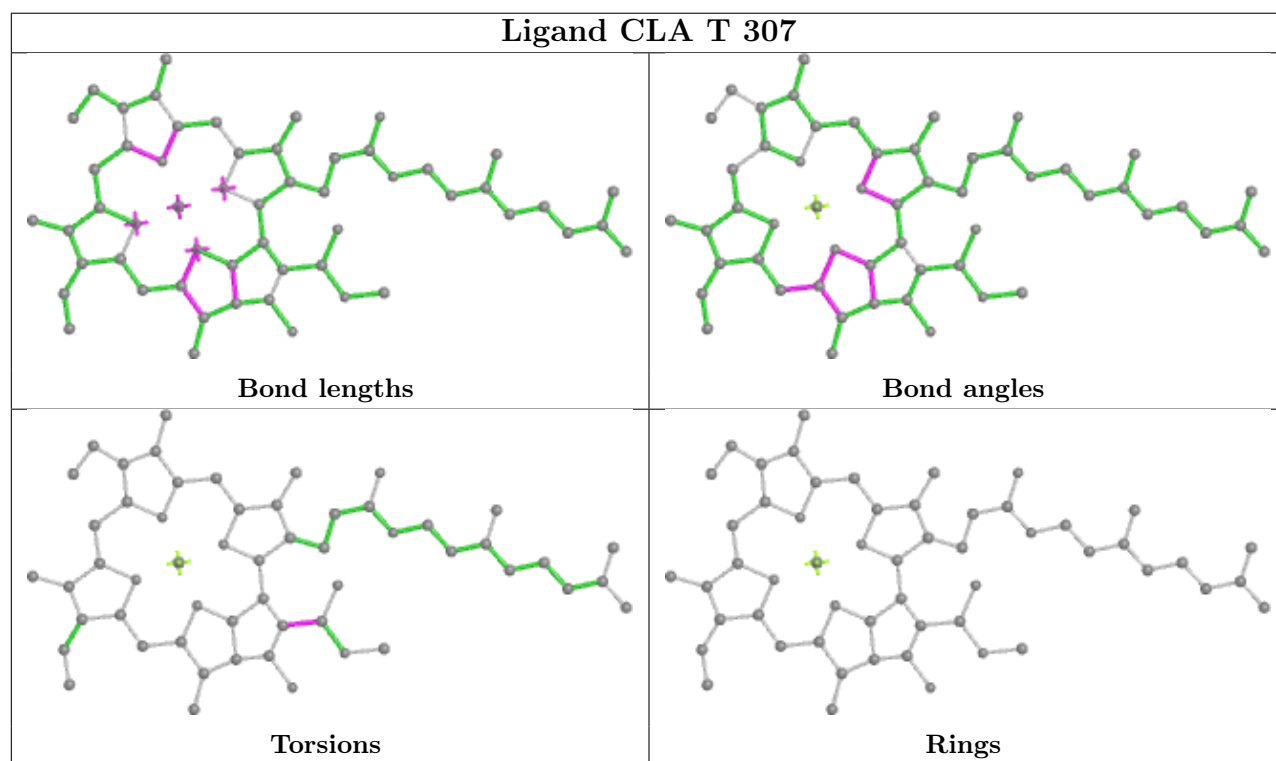
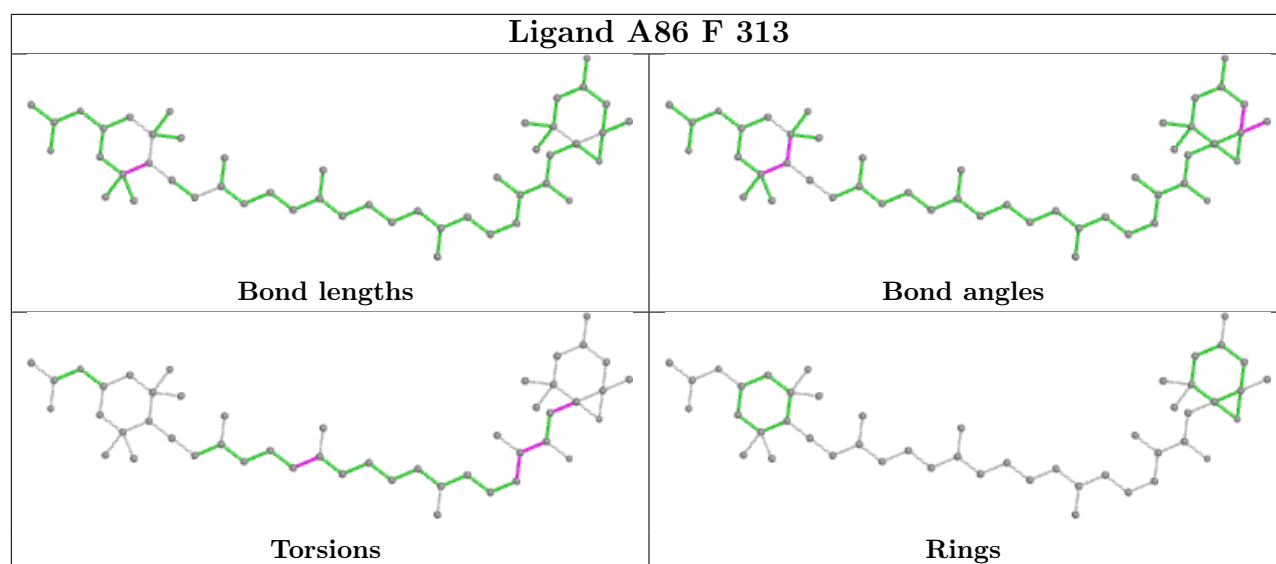


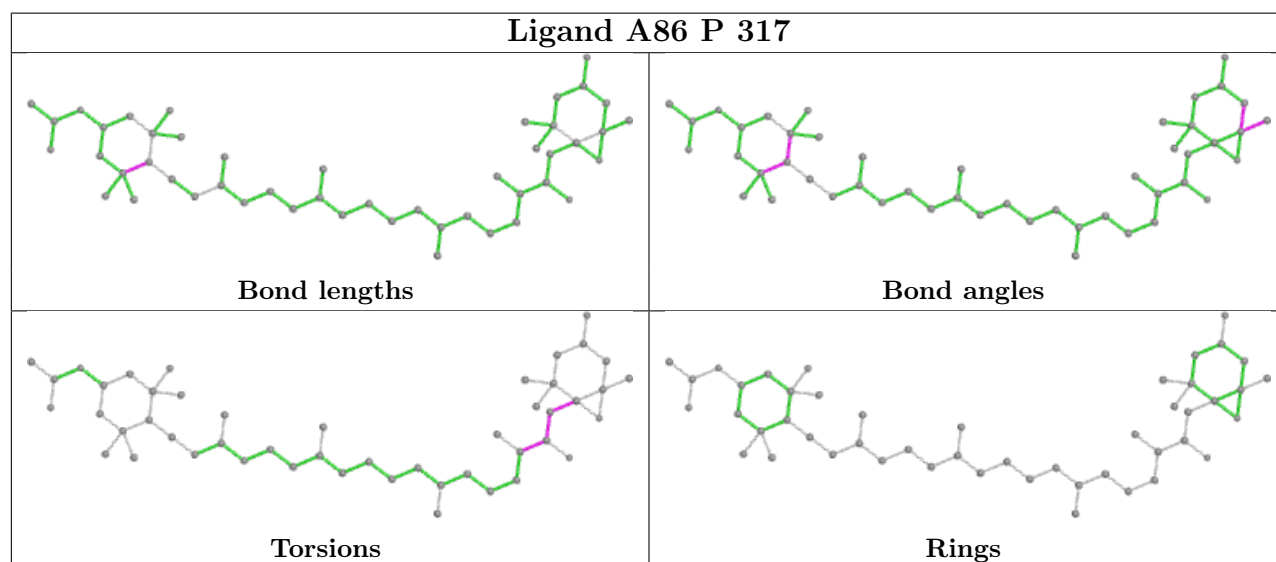
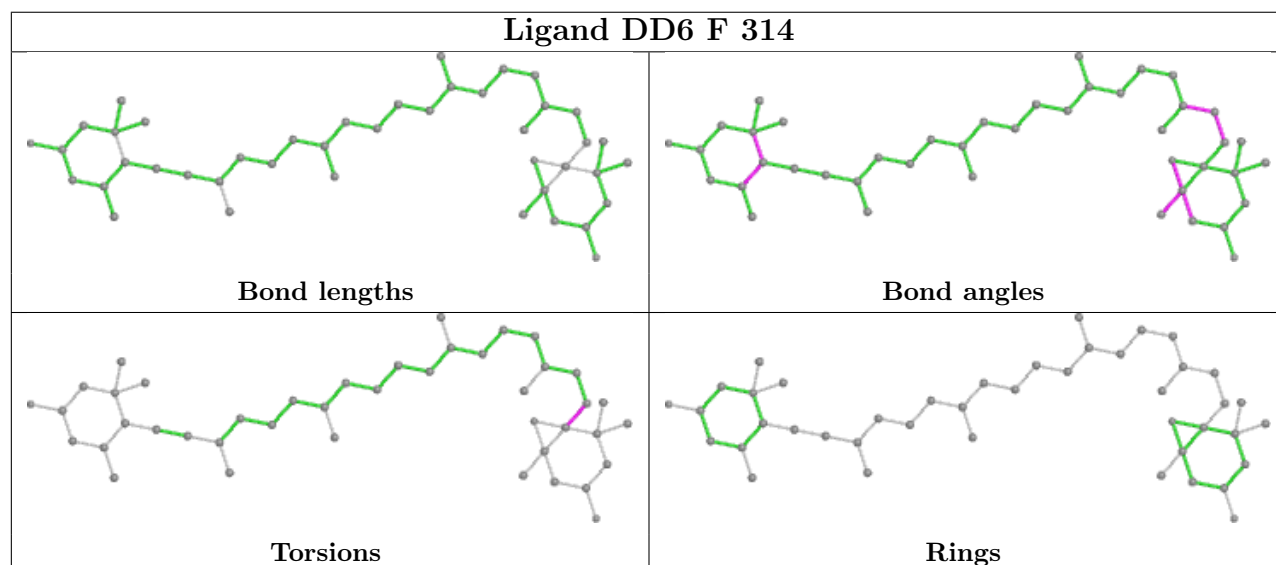
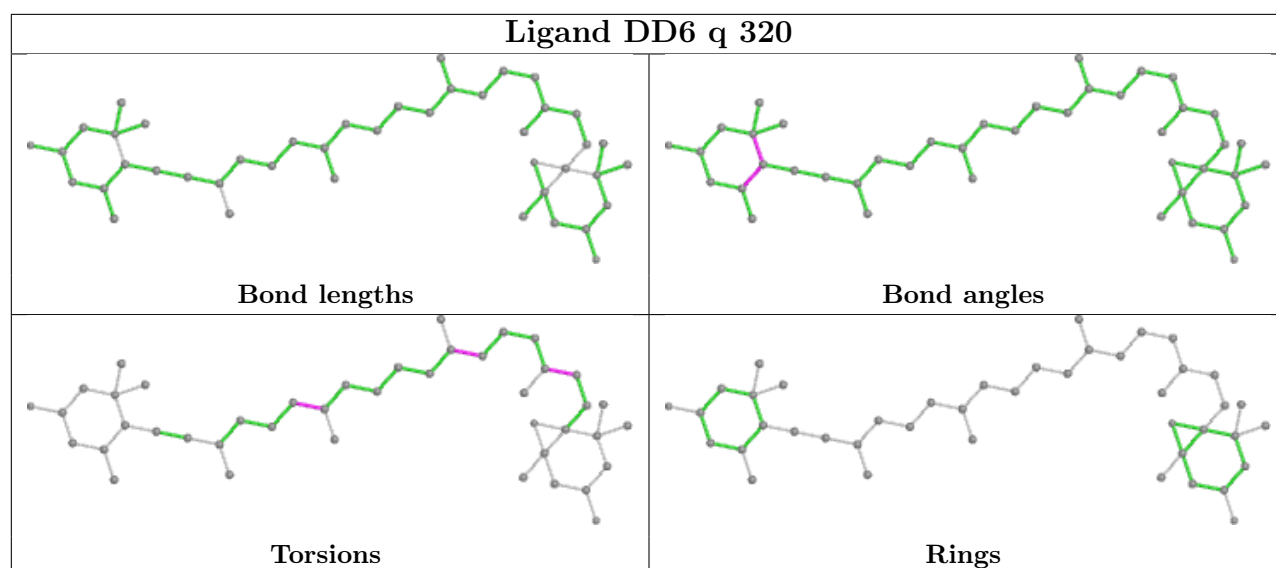
Ligand CLA Q 204



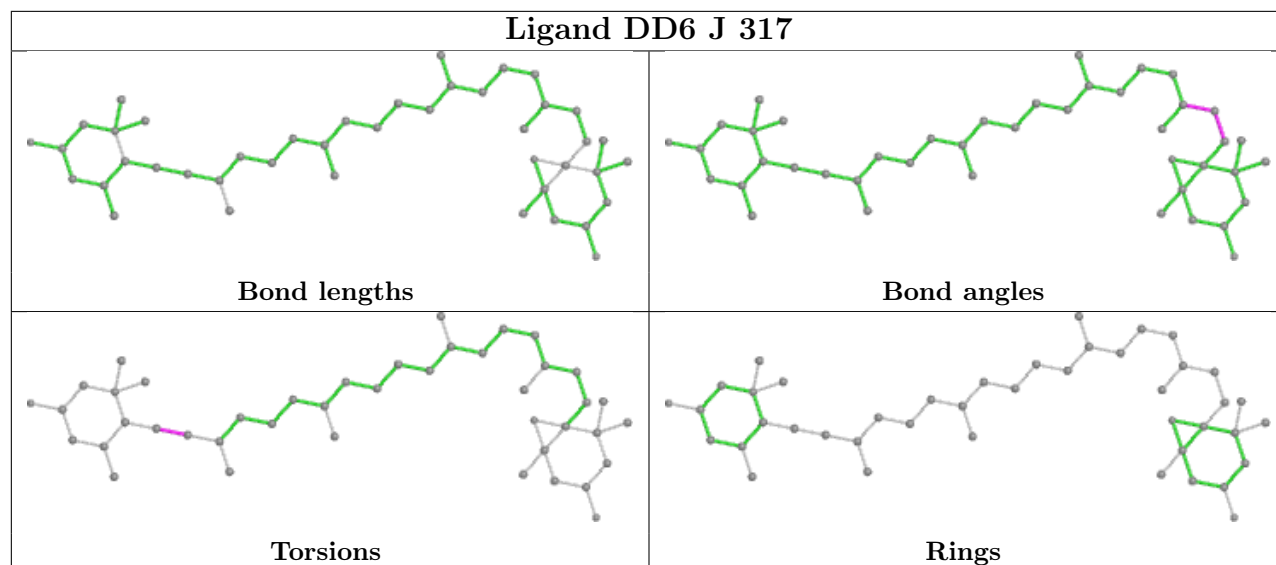
Ligand A86 x 319



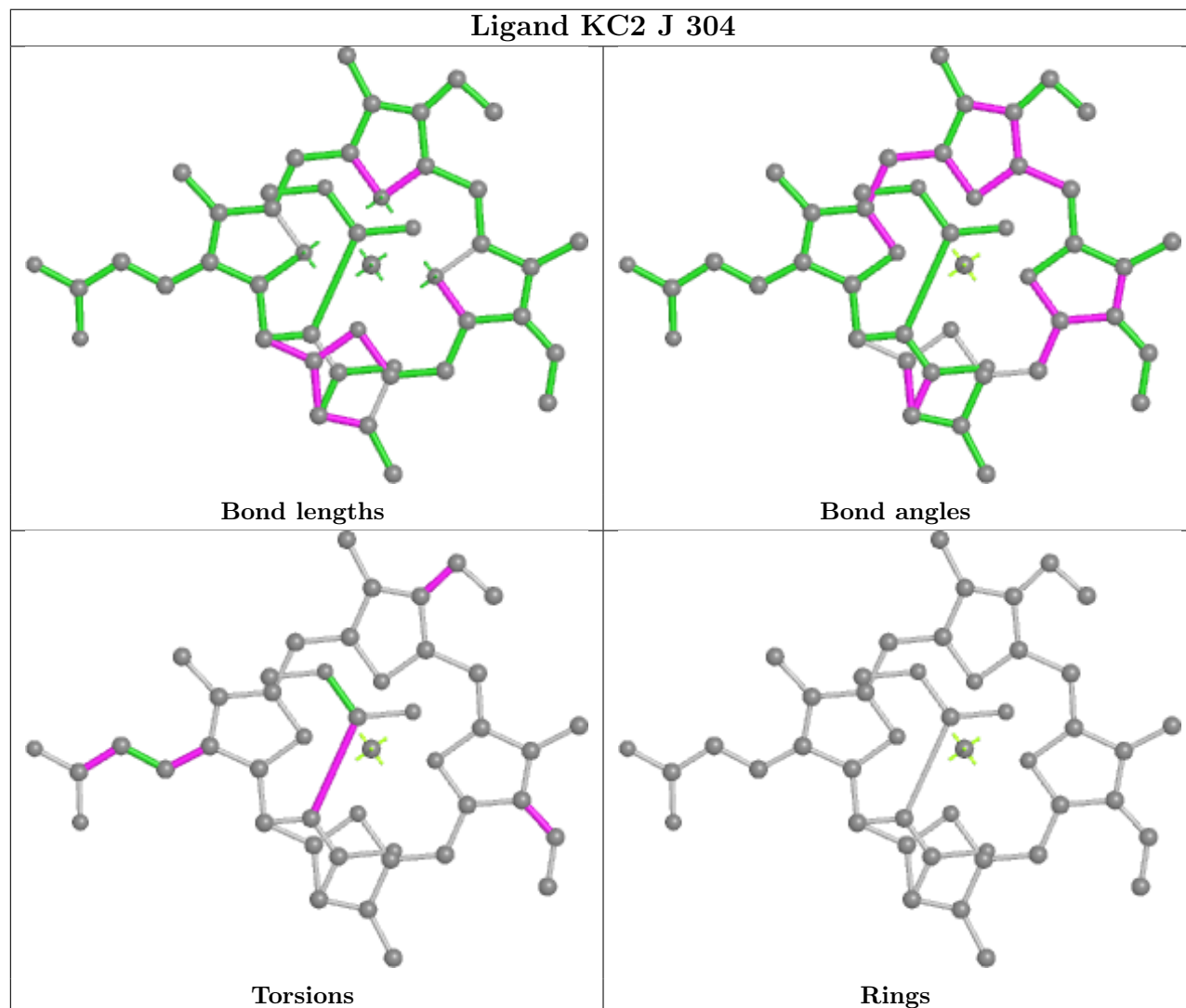


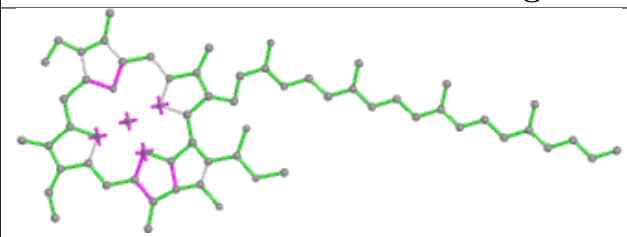
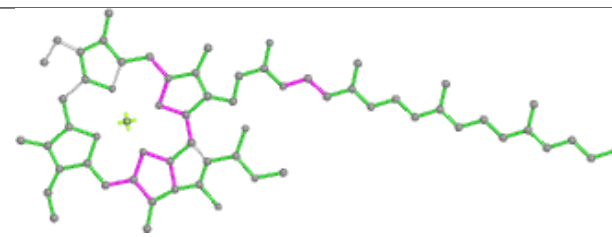
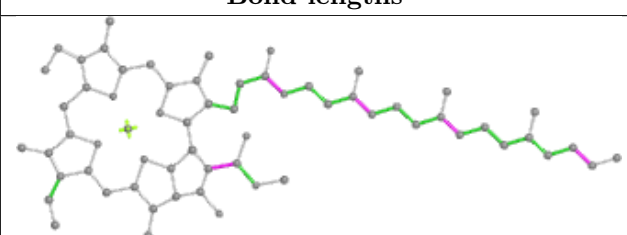
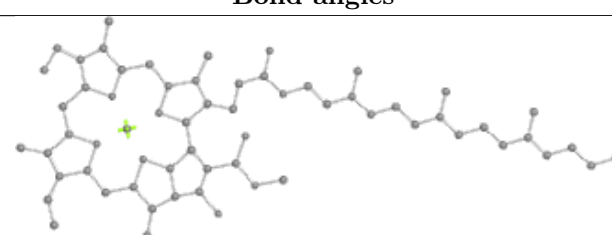


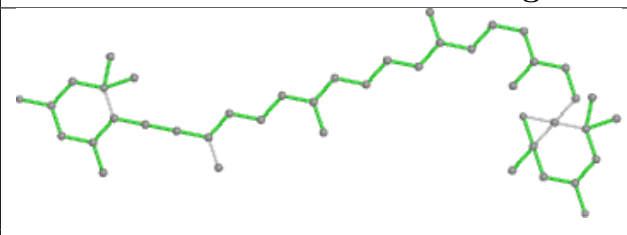
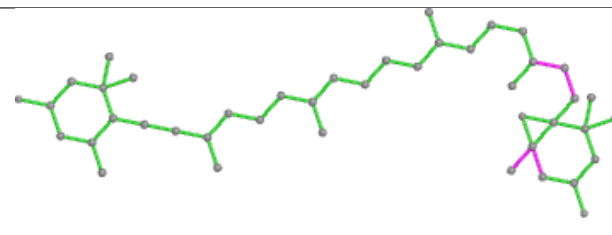
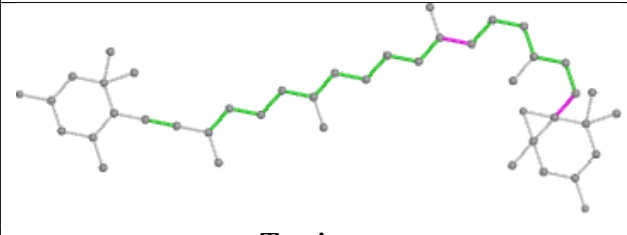
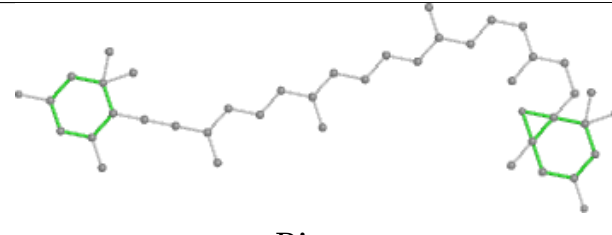
Ligand DD6 J 317

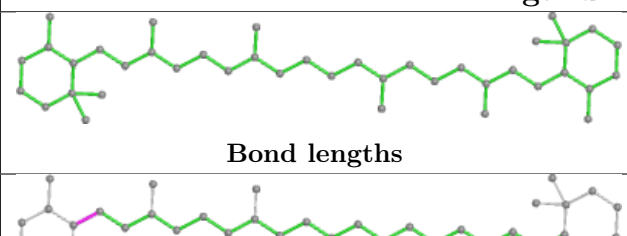
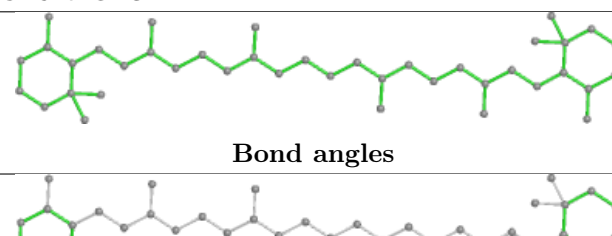
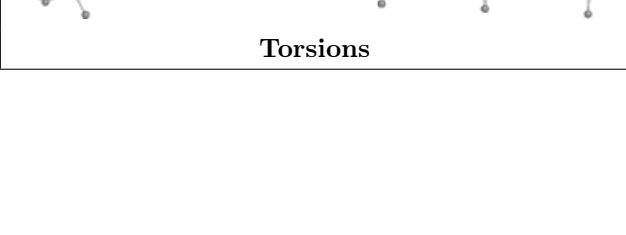
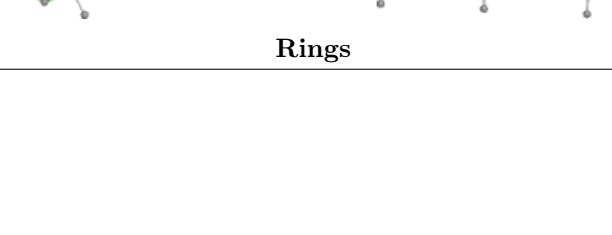


Ligand KC2 J 304

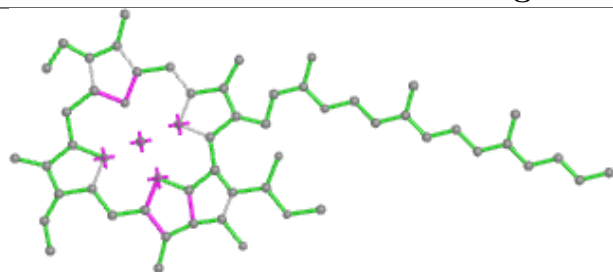


Ligand CLA Z 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

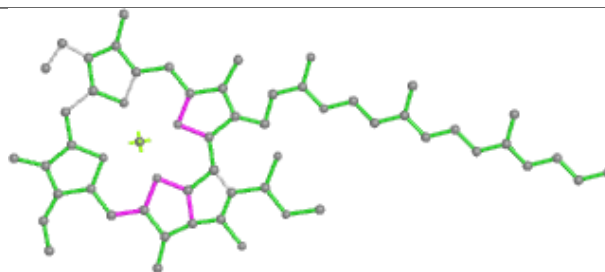
Ligand DD6 B 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

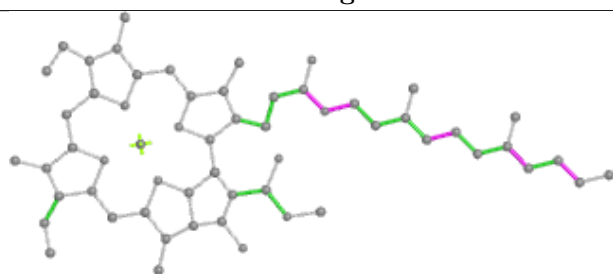
Ligand CLA V 201



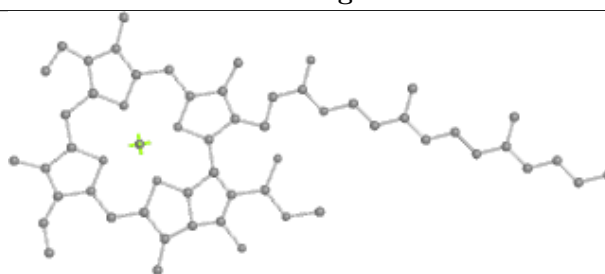
Bond lengths



Bond angles

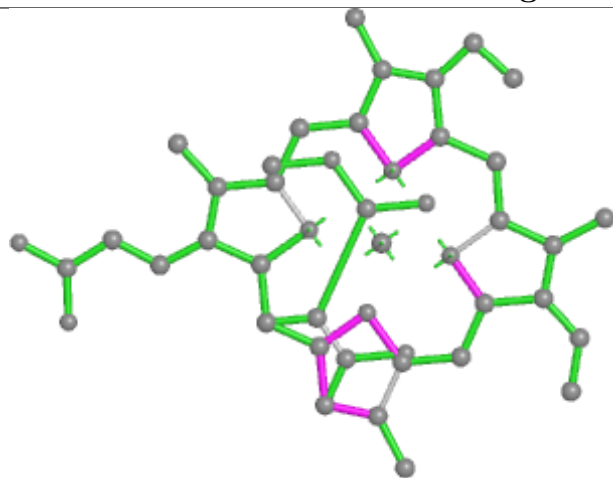


Torsions

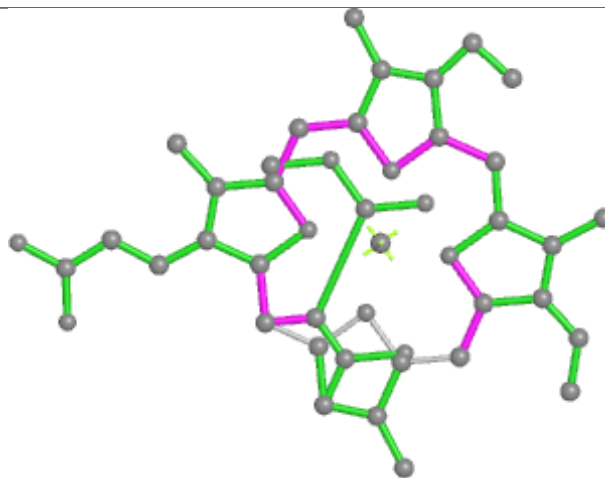


Rings

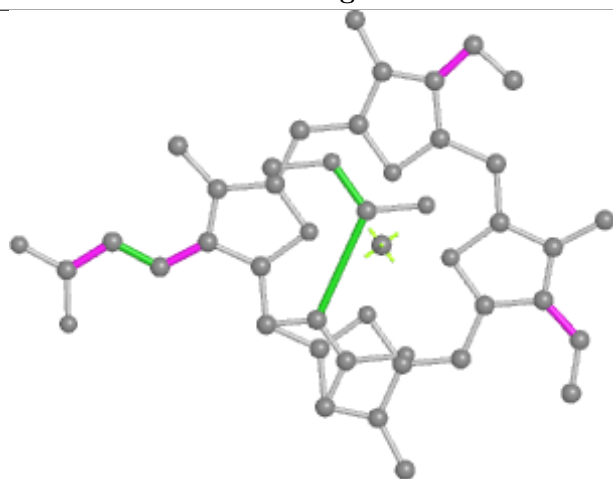
Ligand KC2 x 315



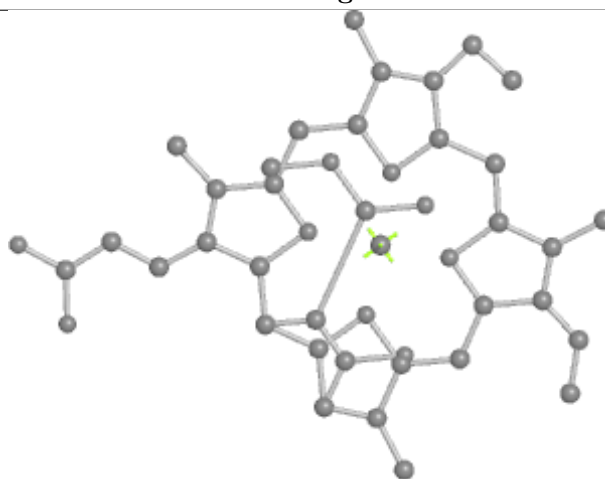
Bond lengths



Bond angles

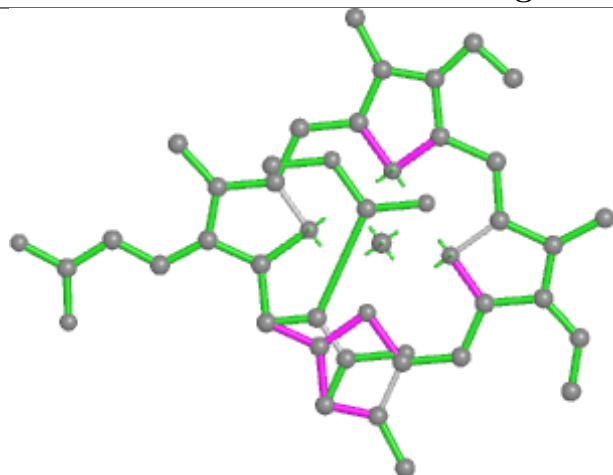


Torsions

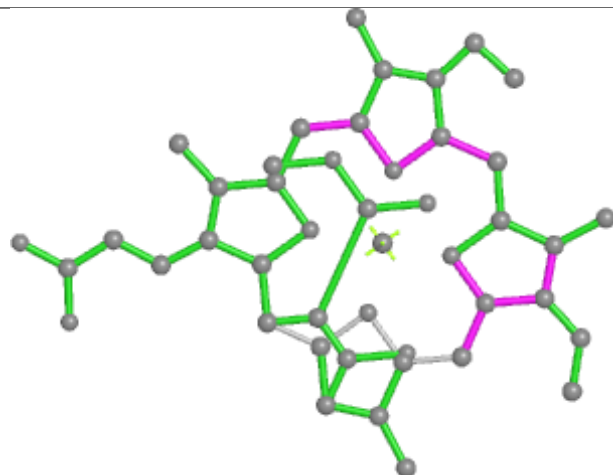


Rings

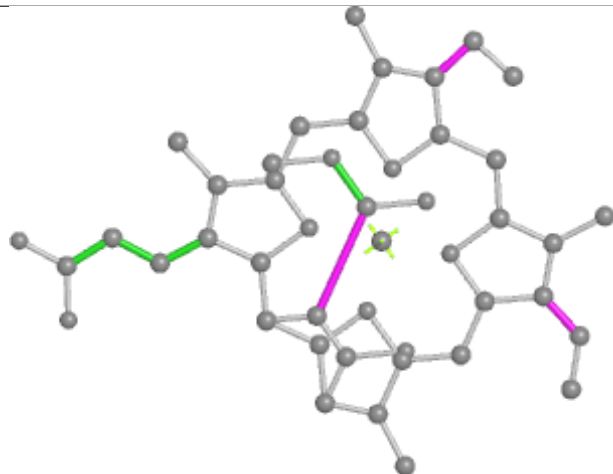
Ligand KC2 N 301



Bond lengths



Bond angles

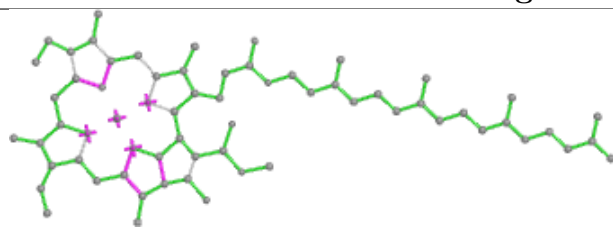


Torsions

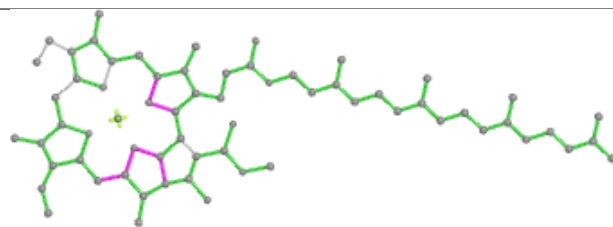


Rings

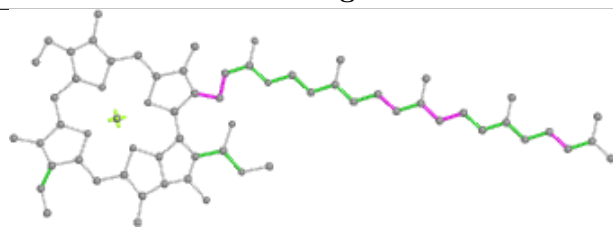
Ligand CLA E 307



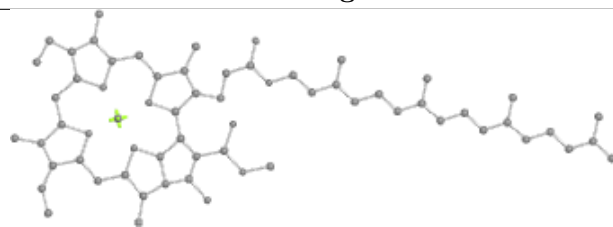
Bond lengths



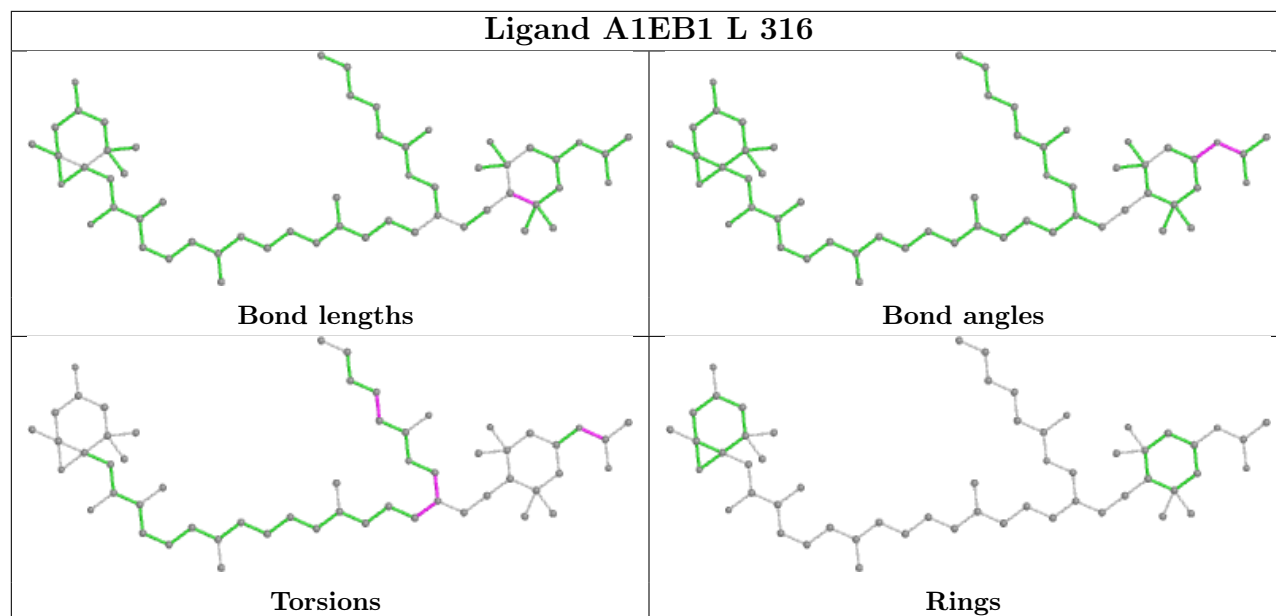
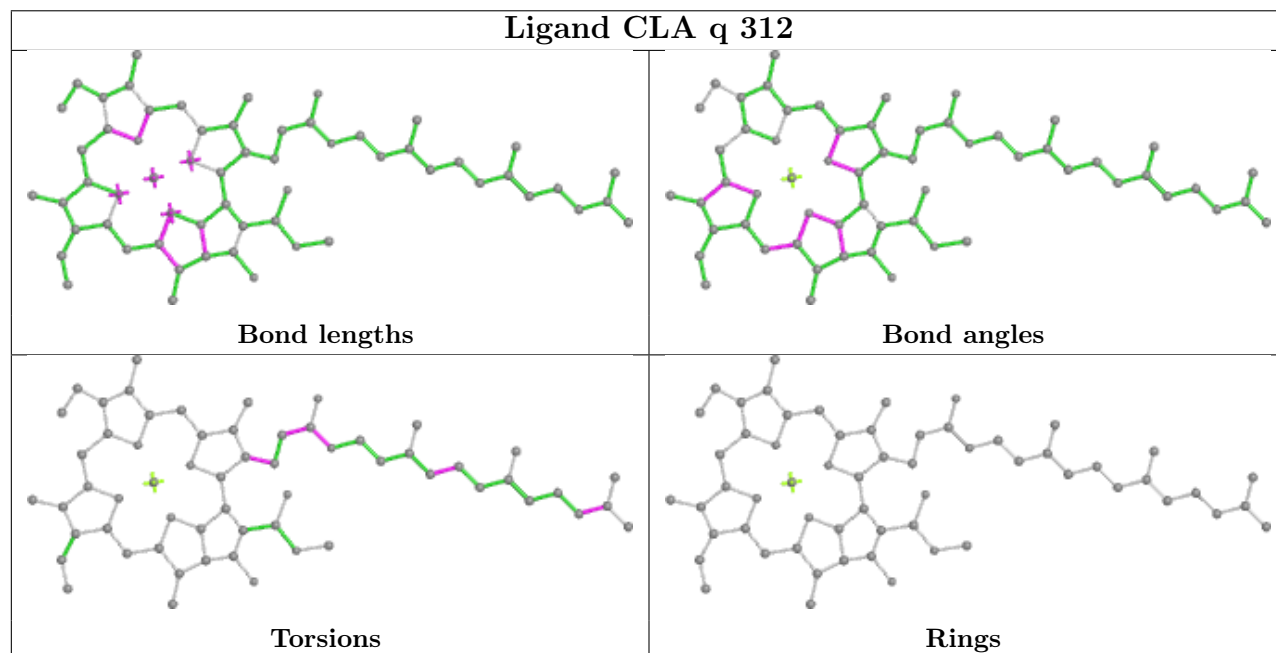
Bond angles



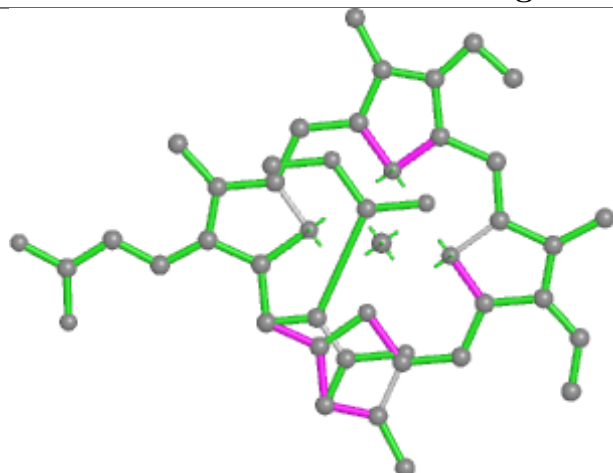
Torsions



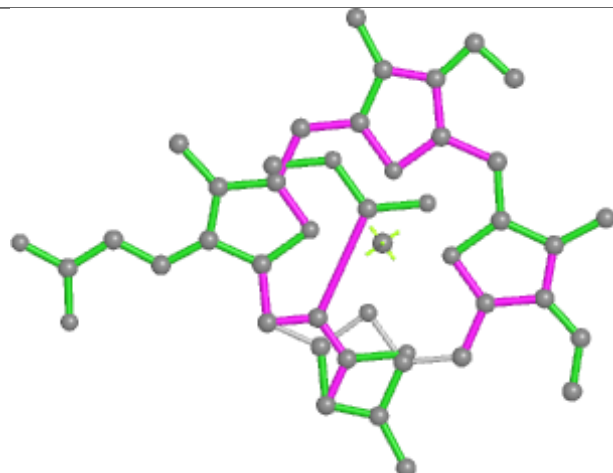
Rings

Ligand A1EB1 L 316**Ligand CLA q 312**

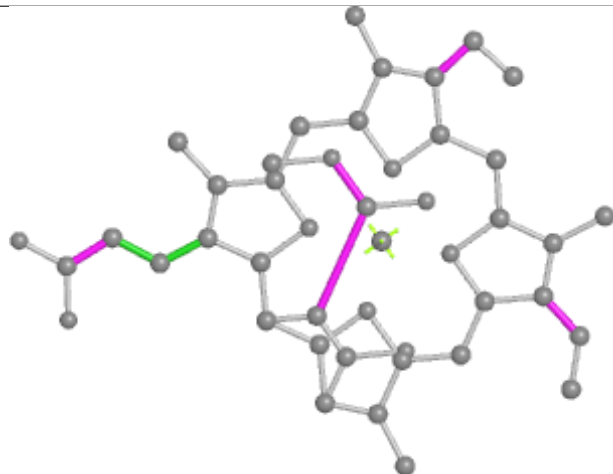
Ligand KC2 Y 314



Bond lengths



Bond angles

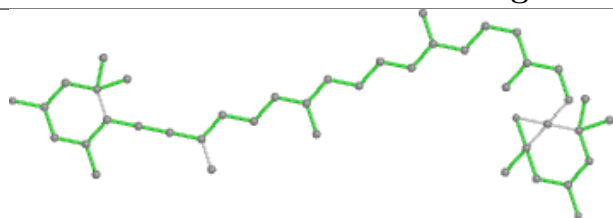


Torsions

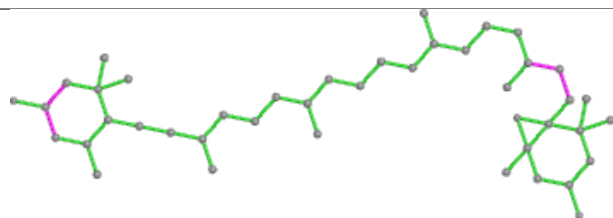


Rings

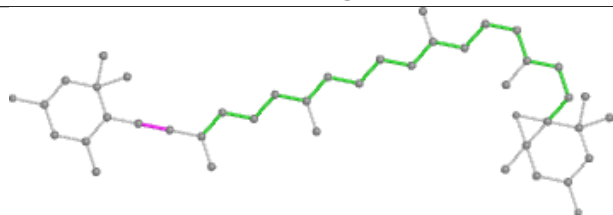
Ligand DD6 M 314



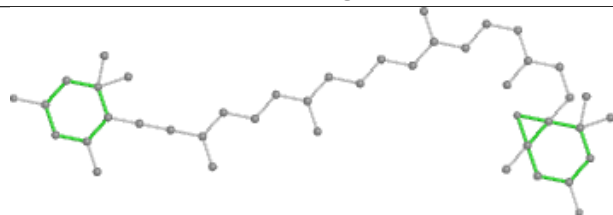
Bond lengths



Bond angles

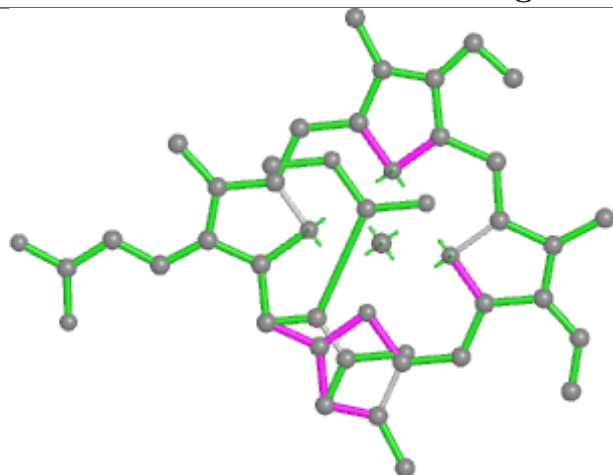


Torsions

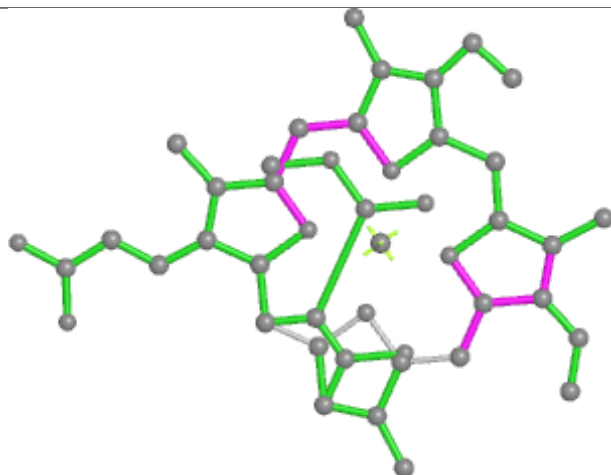


Rings

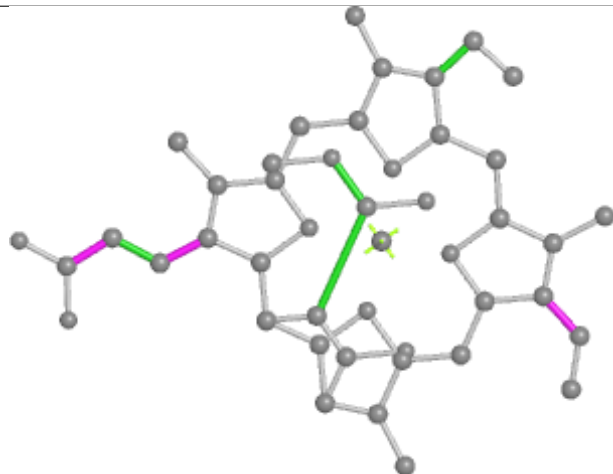
Ligand KC2 K 305



Bond lengths



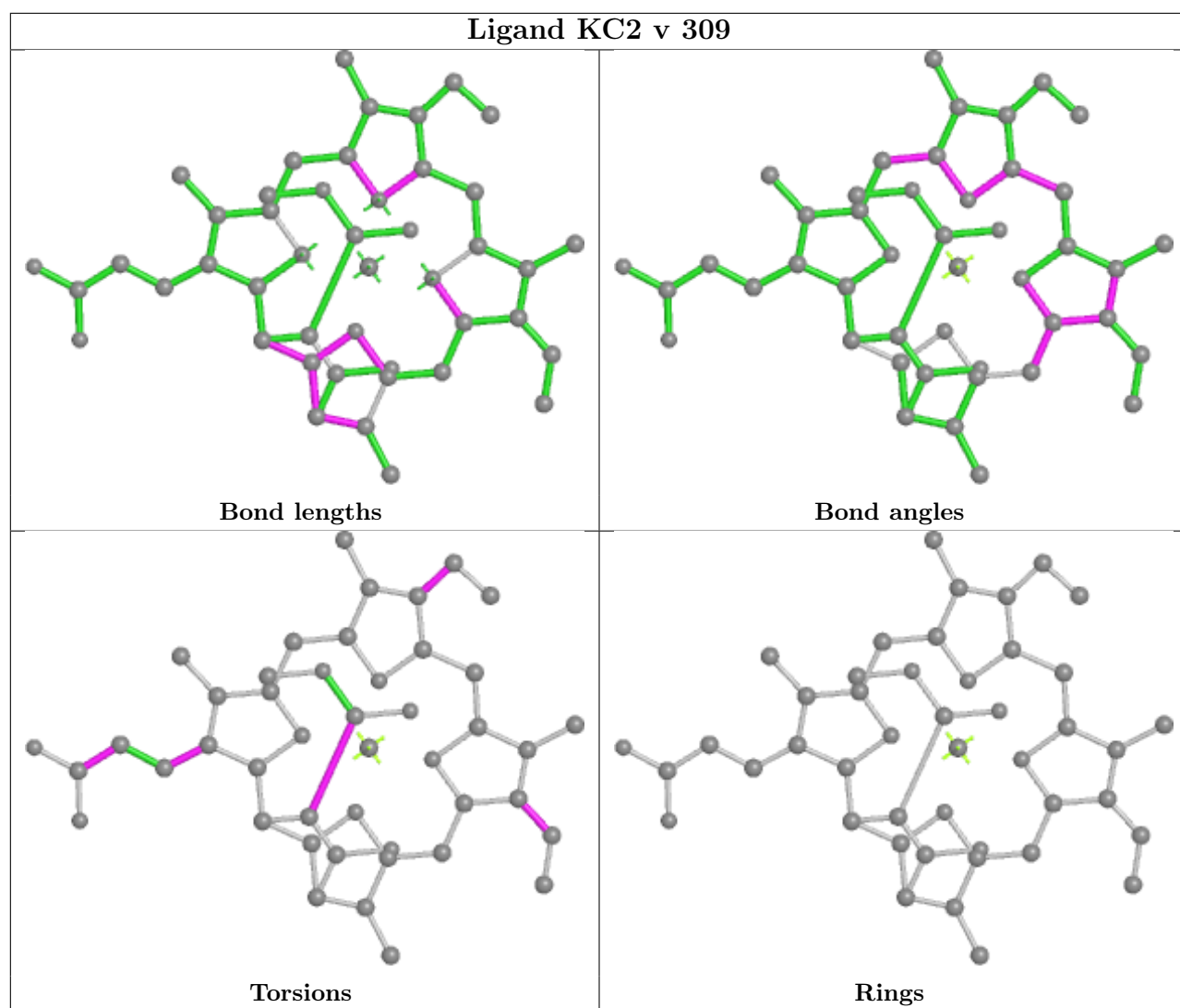
Bond angles



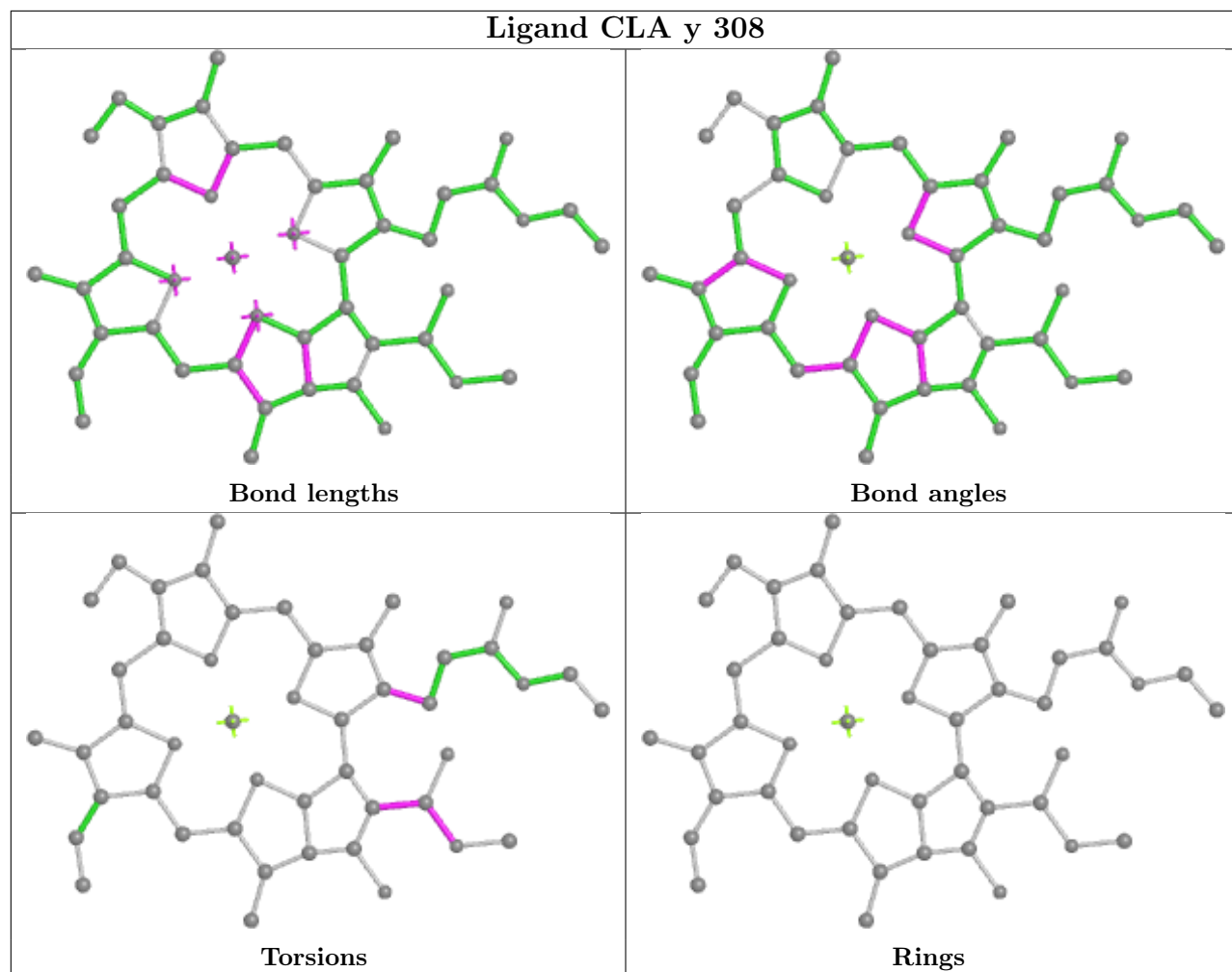
Torsions



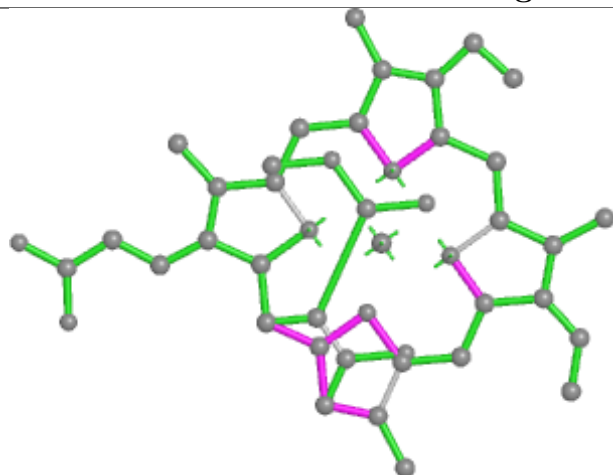
Rings



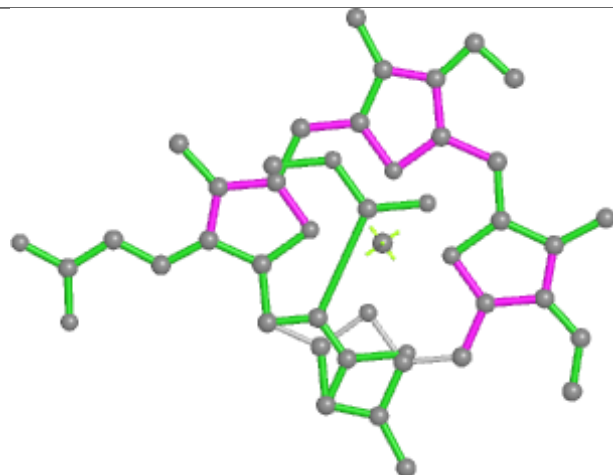
Ligand CLA y 308



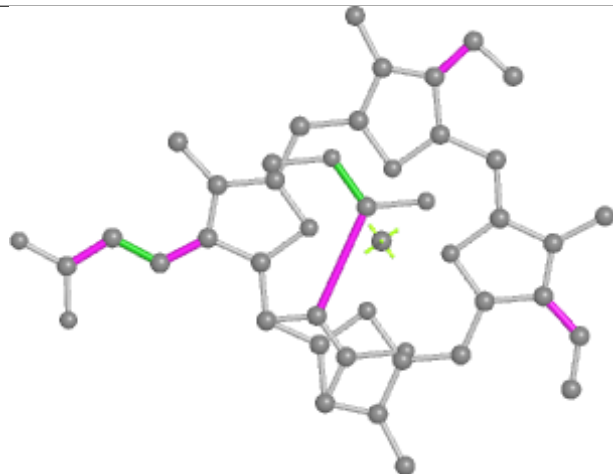
Ligand KC2 G 202



Bond lengths



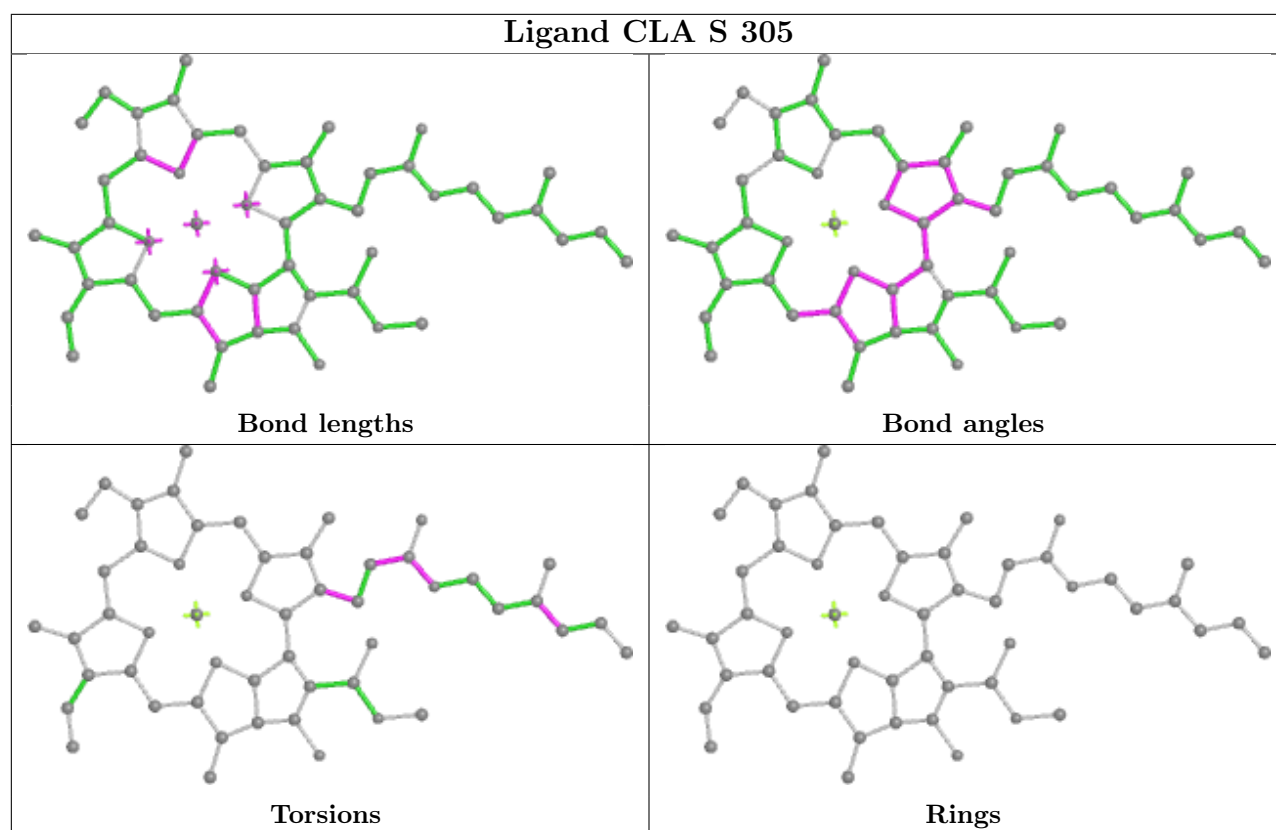
Bond angles



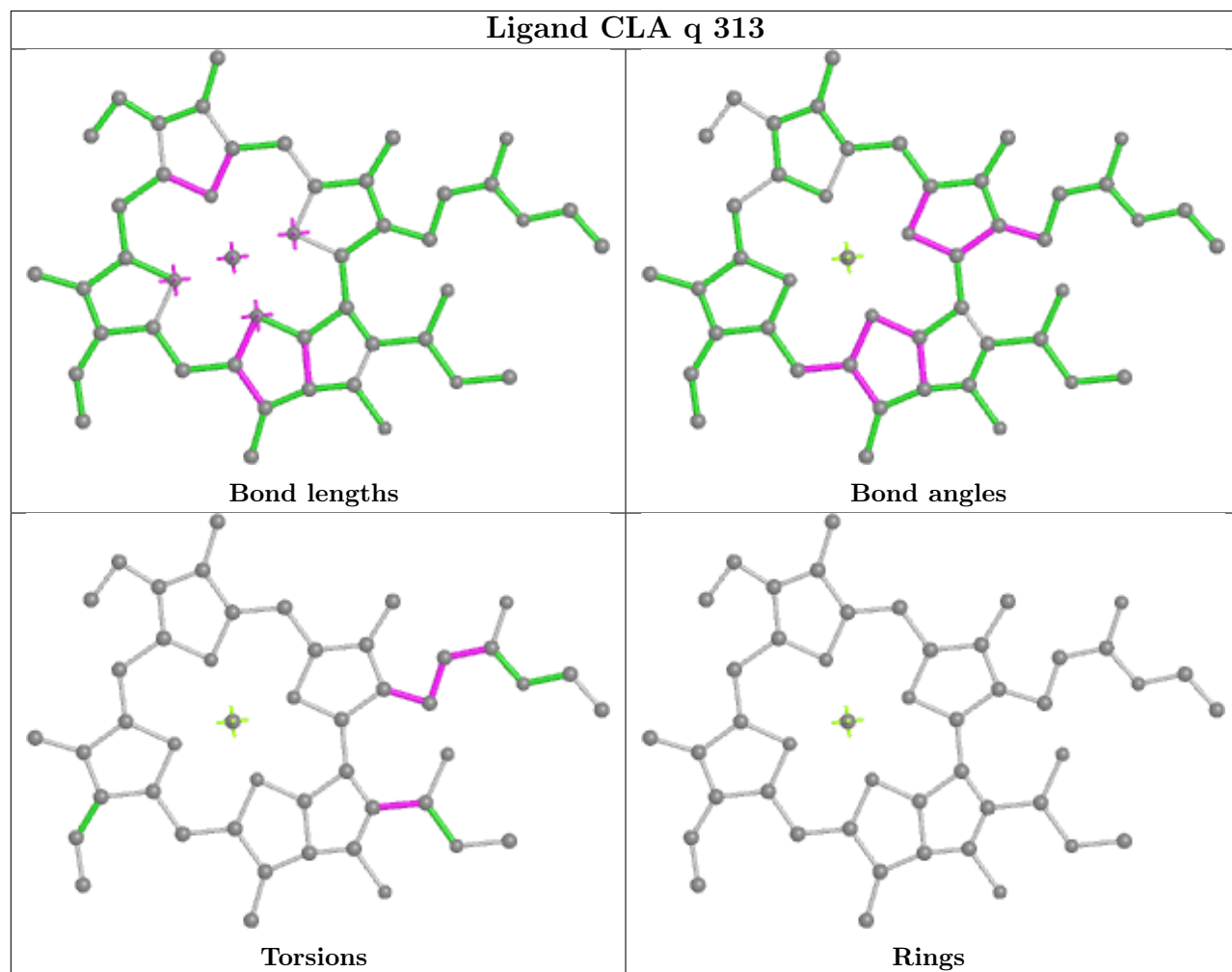
Torsions



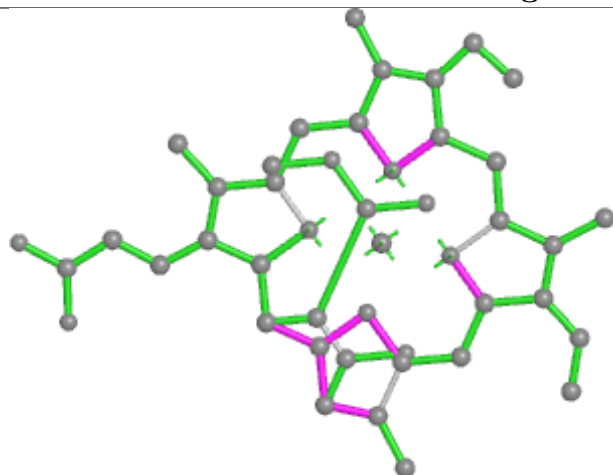
Rings



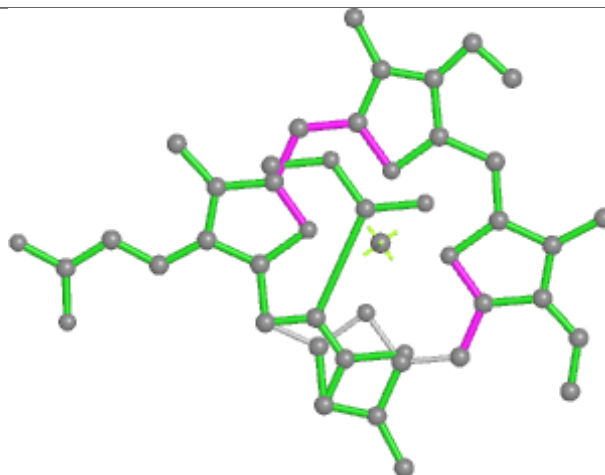
Ligand CLA q 313



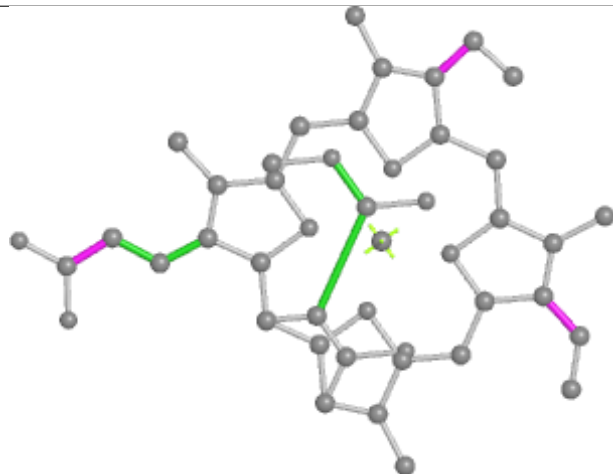
Ligand KC2 z 309



Bond lengths



Bond angles

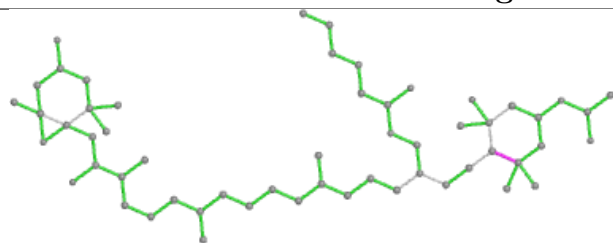


Torsions

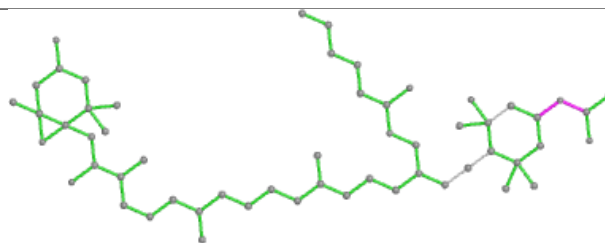


Rings

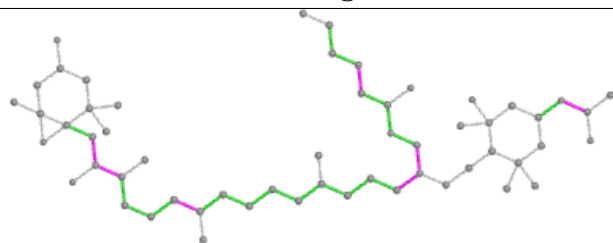
Ligand A1EB1 w 313



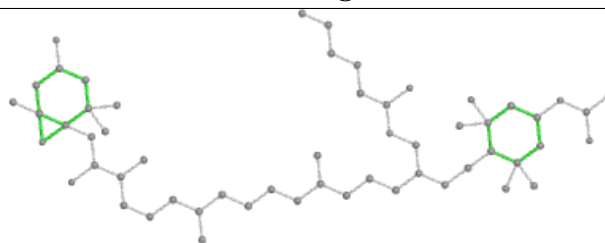
Bond lengths



Bond angles

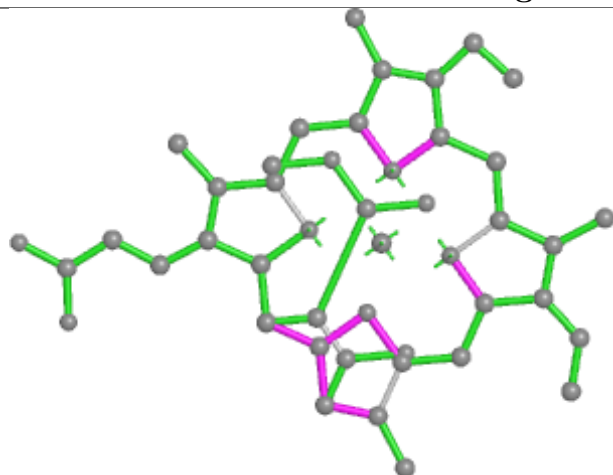


Torsions

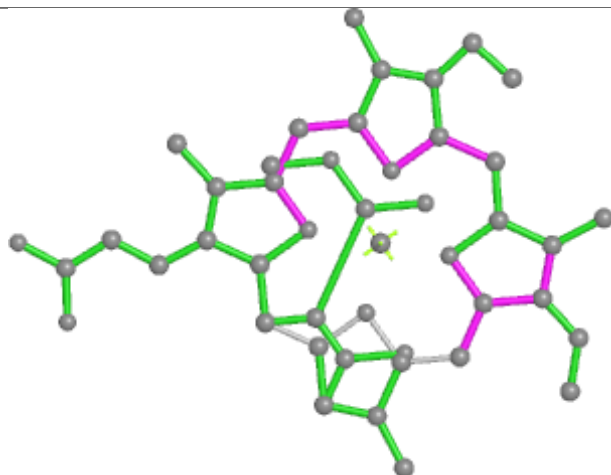


Rings

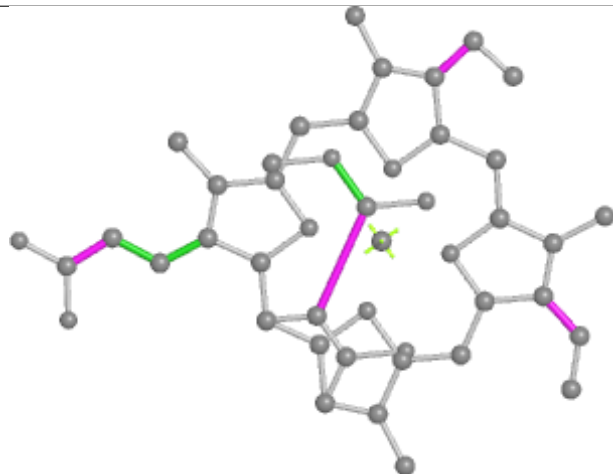
Ligand KC2 Y 308



Bond lengths



Bond angles

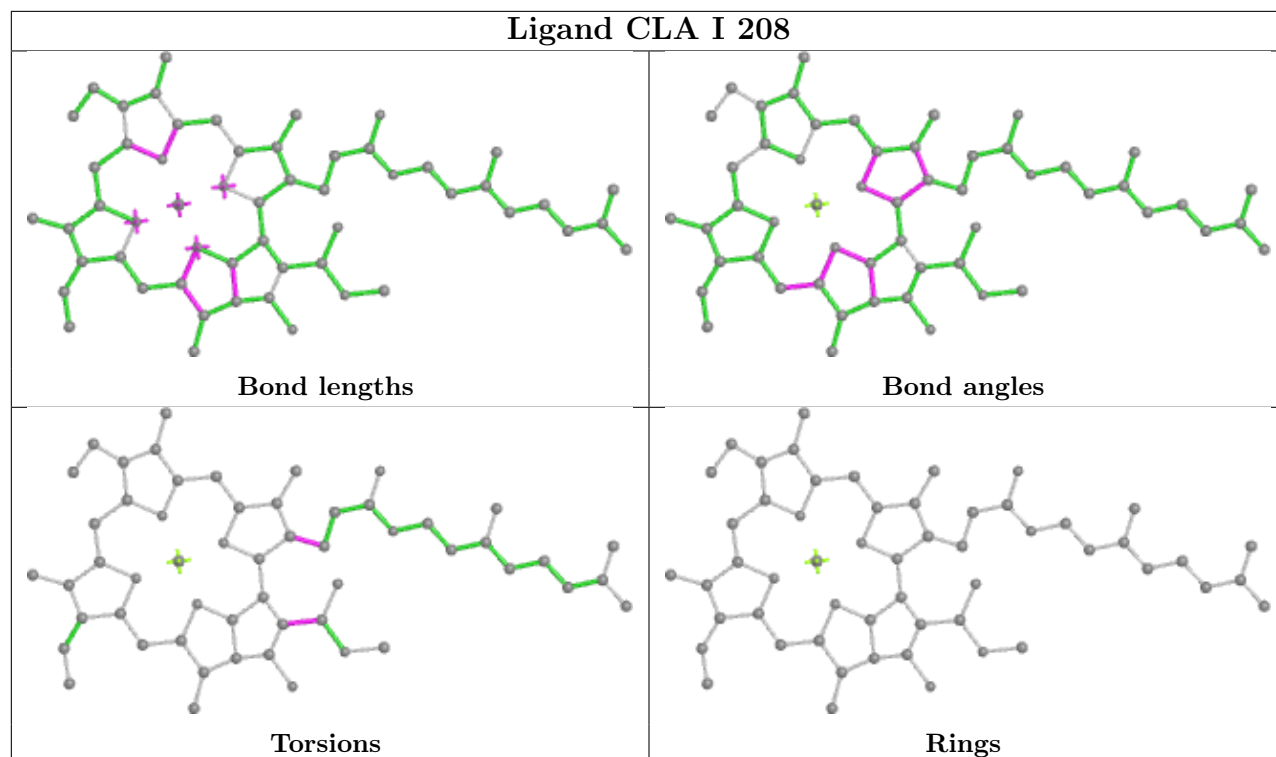


Torsions

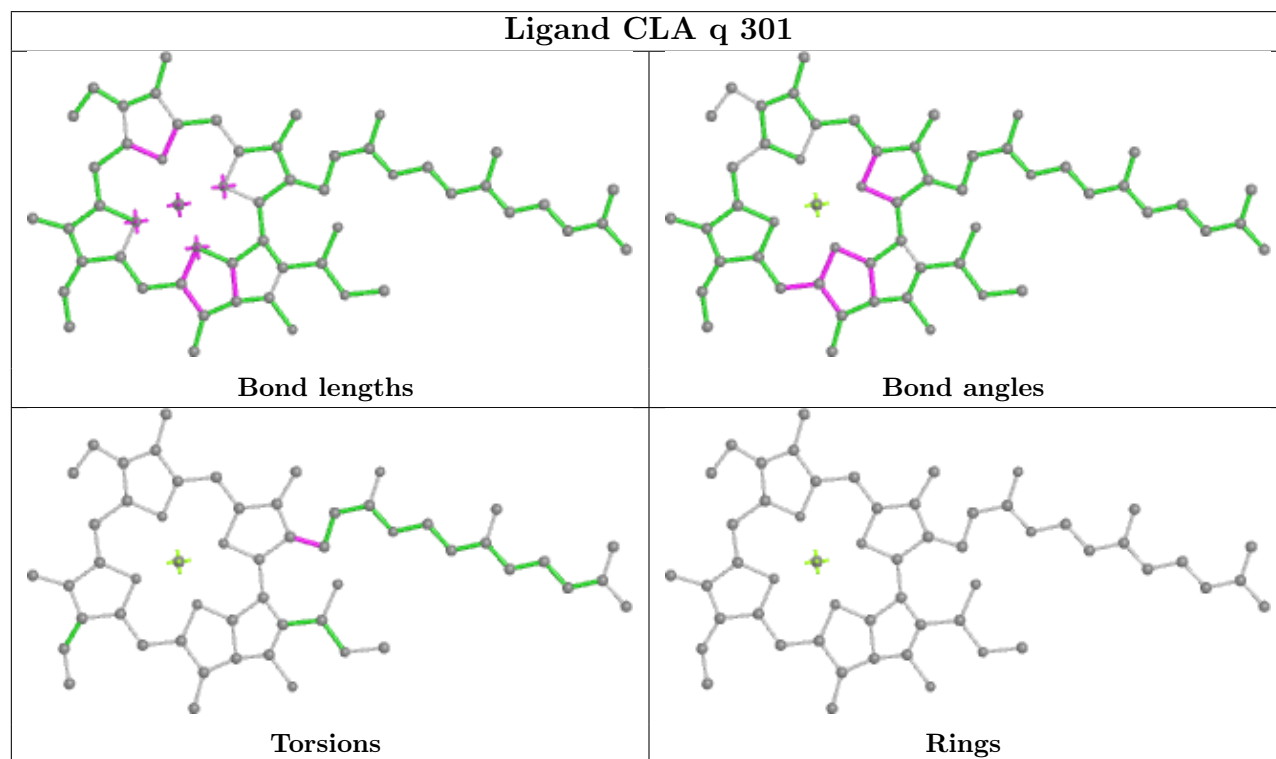


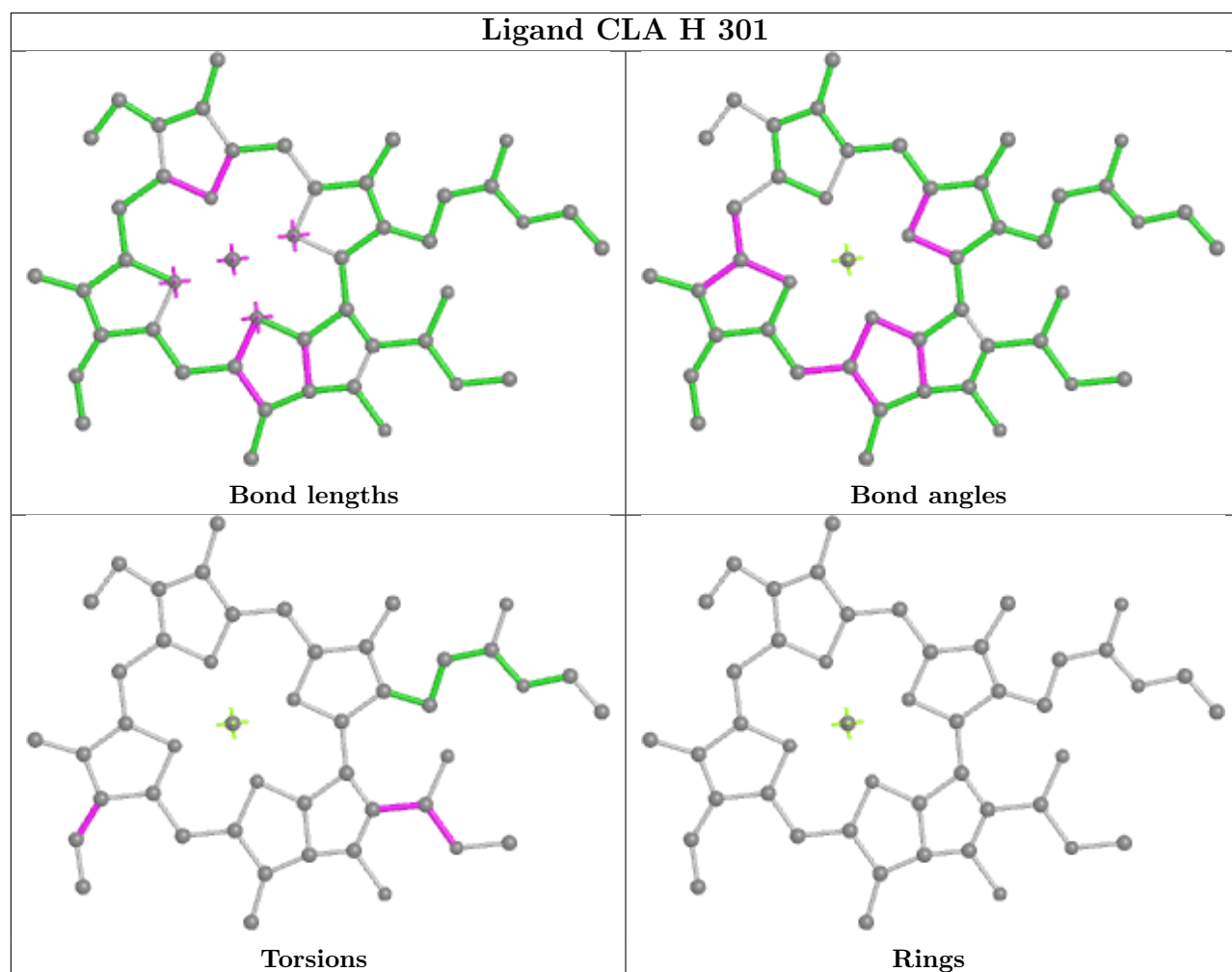
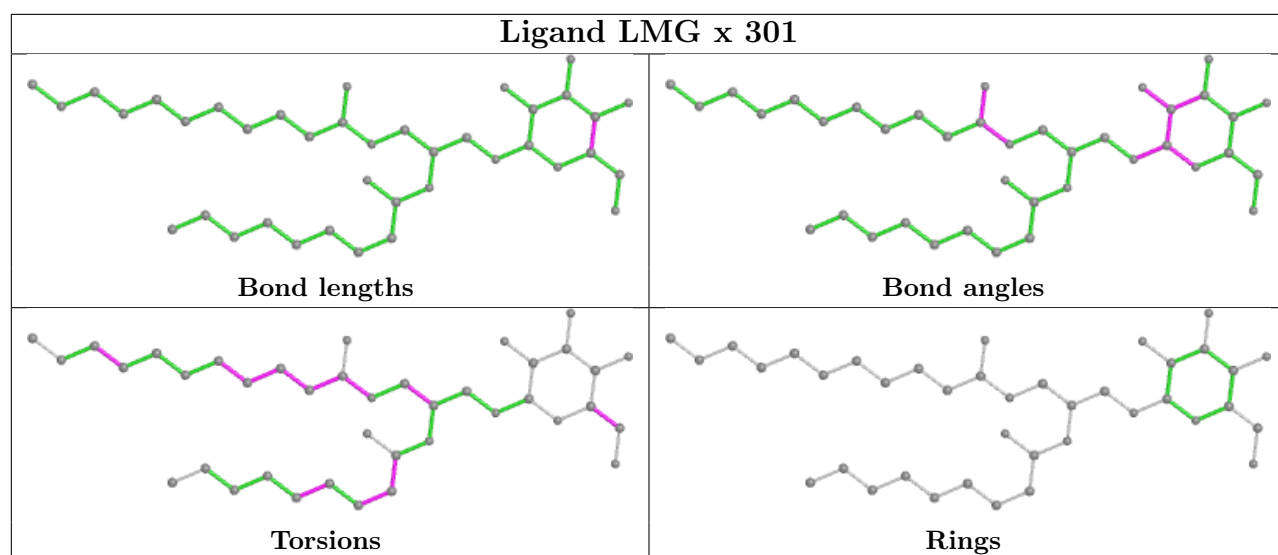
Rings

Ligand CLA I 208

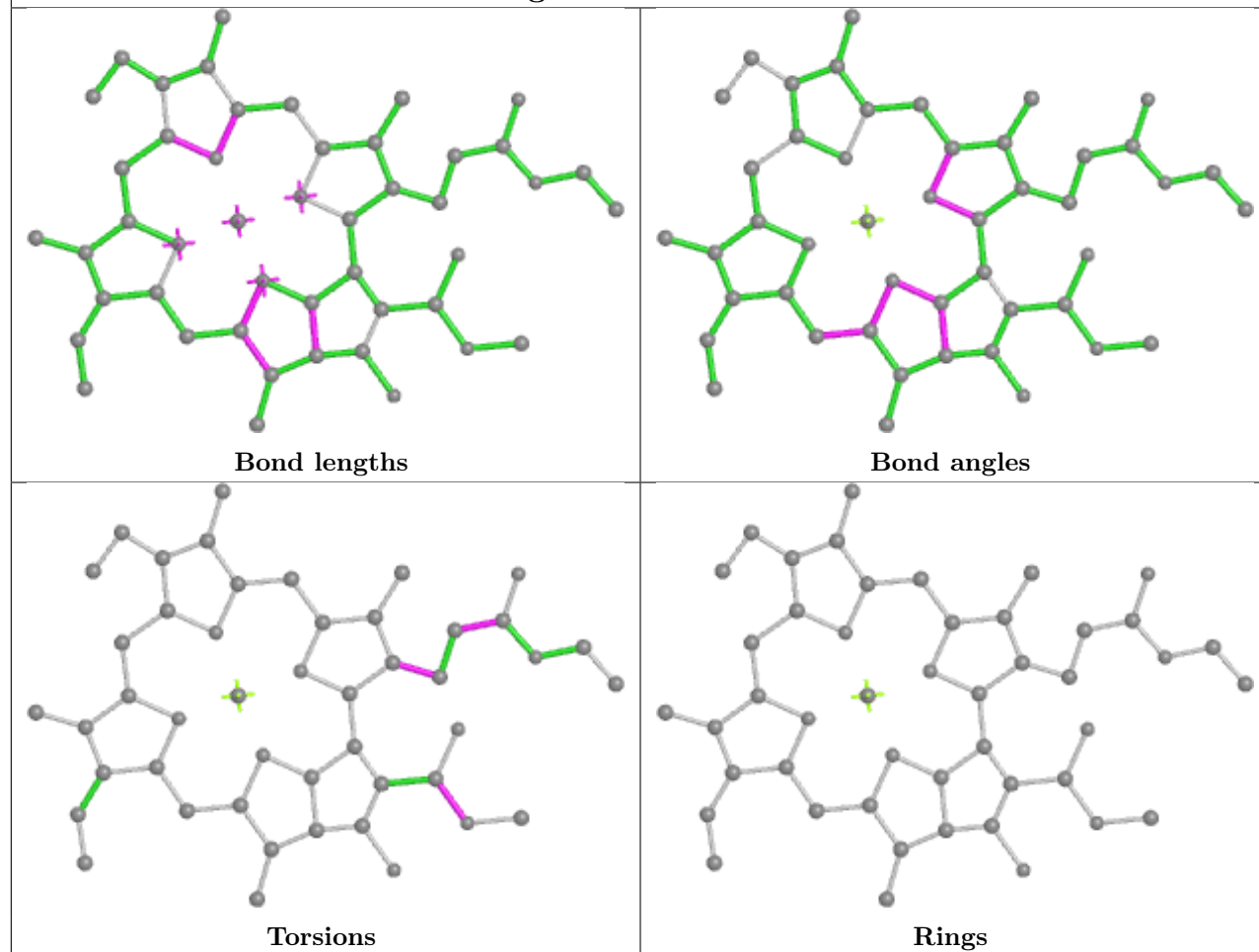


Ligand CLA q 301

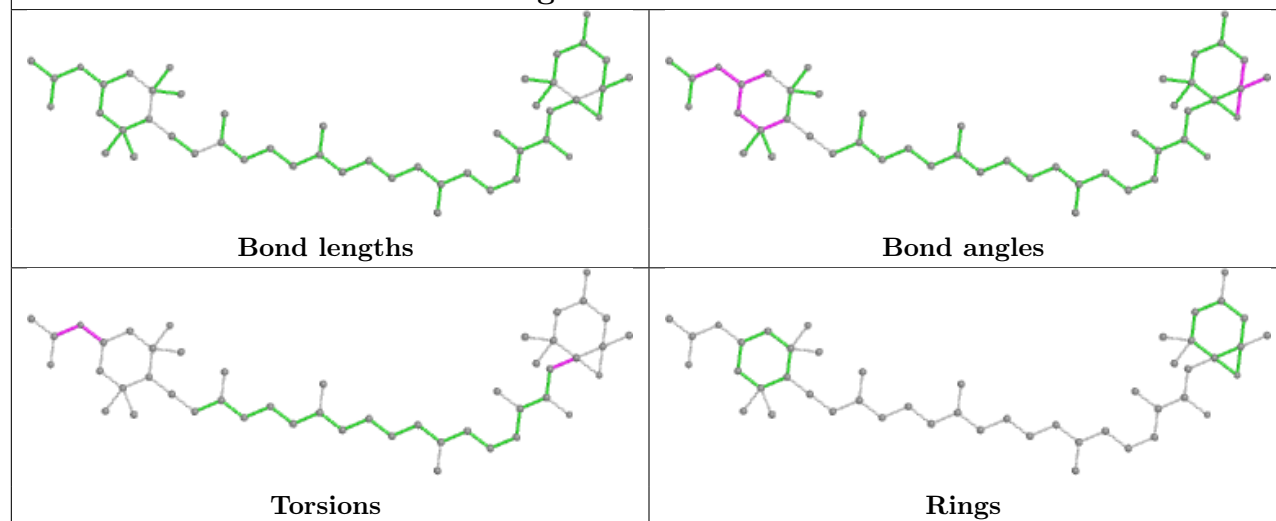




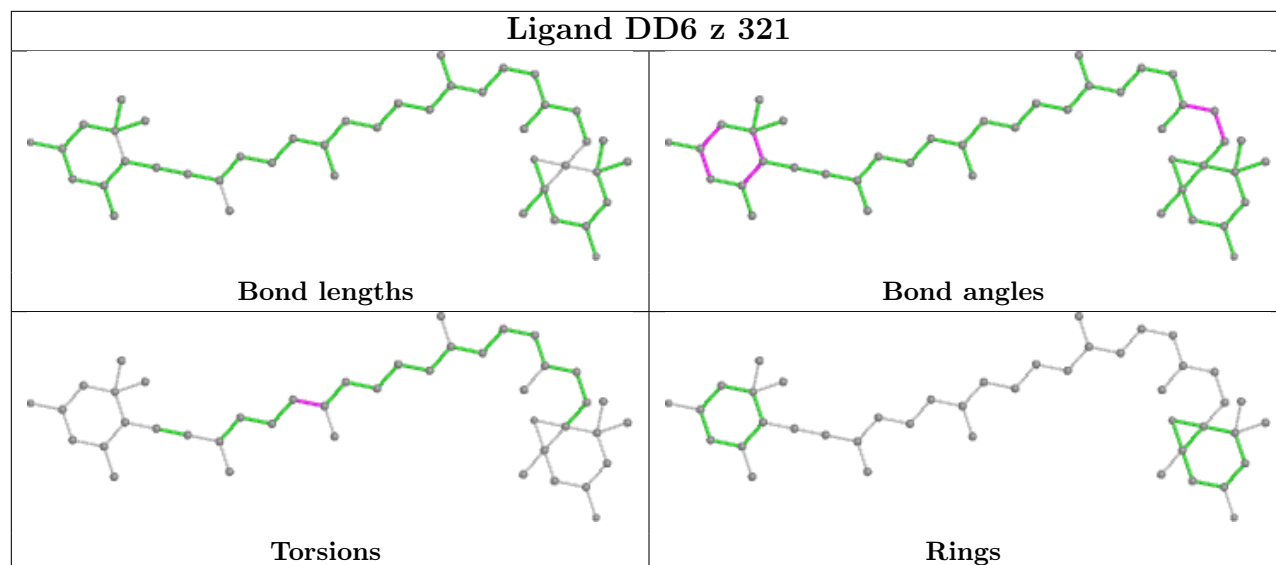
Ligand CLA S 319



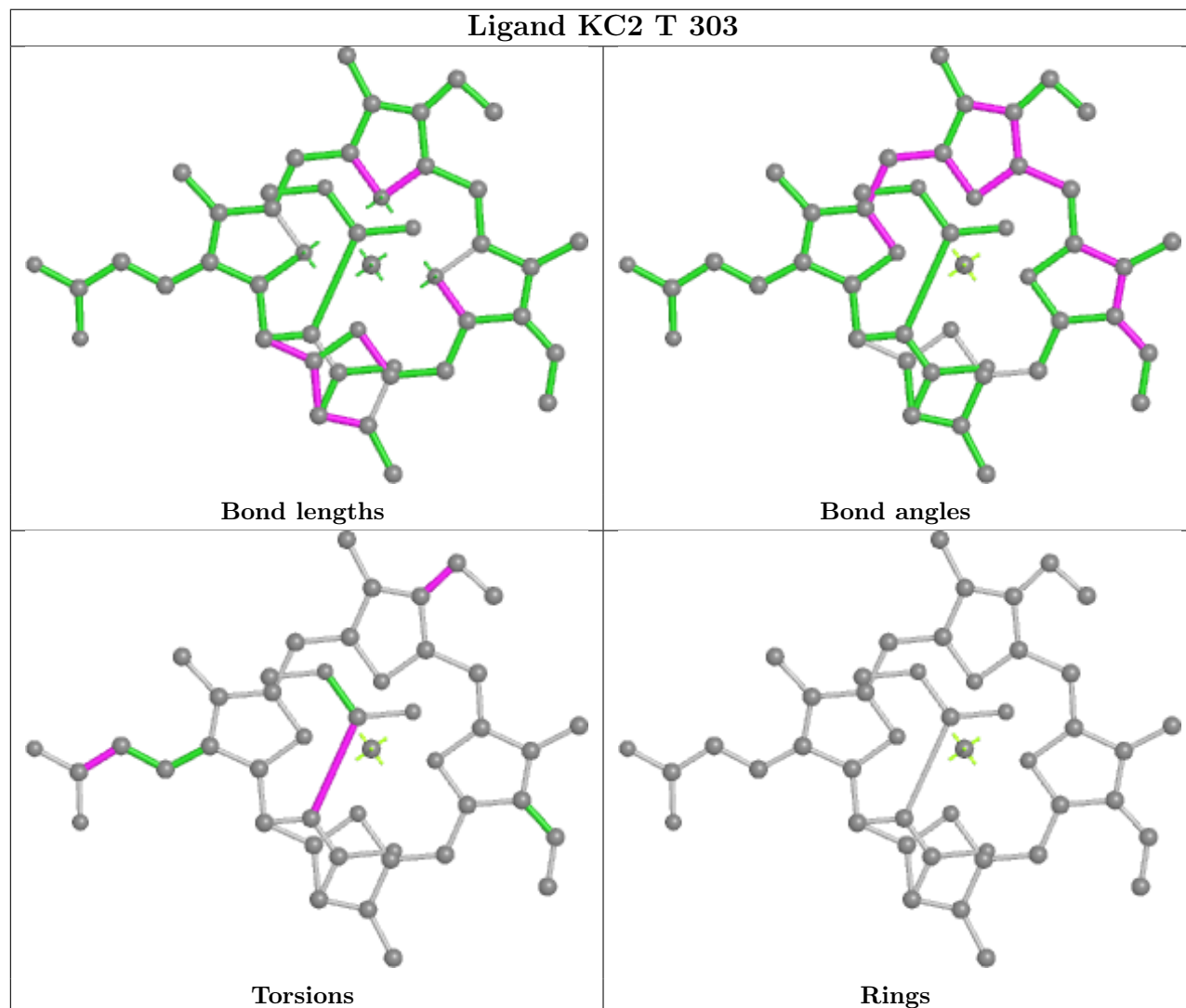
Ligand A86 X 315



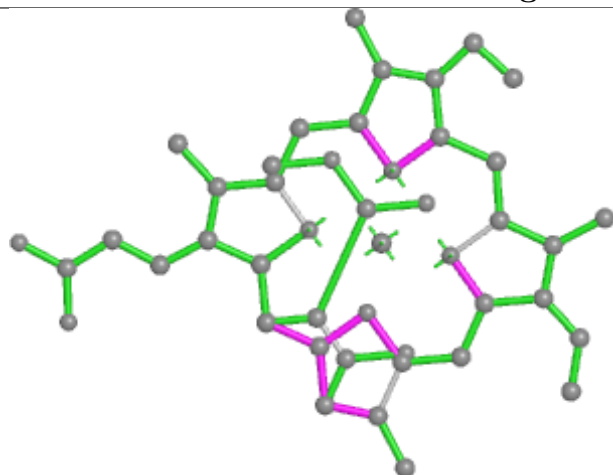
Ligand DD6 z 321



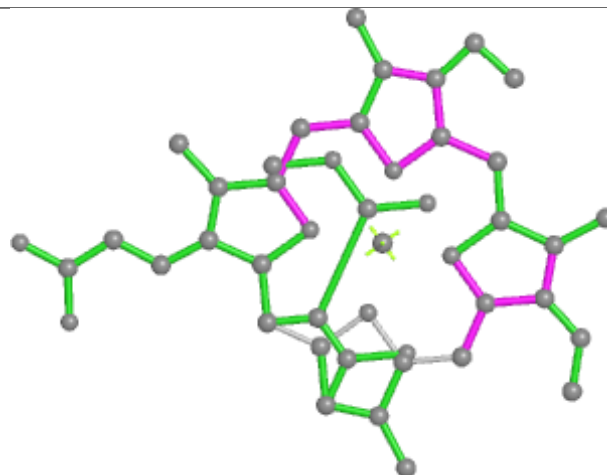
Ligand KC2 T 303



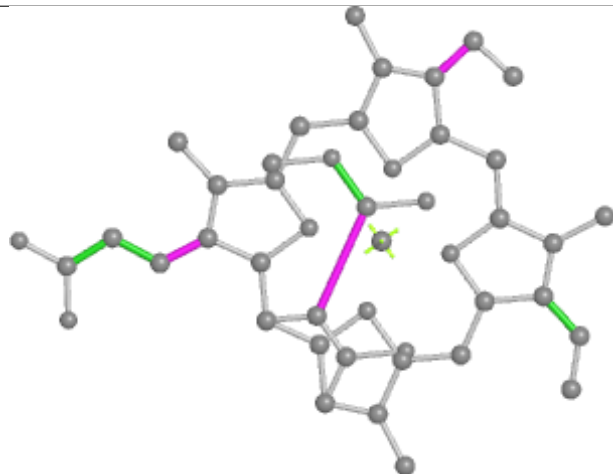
Ligand KC2 x 309



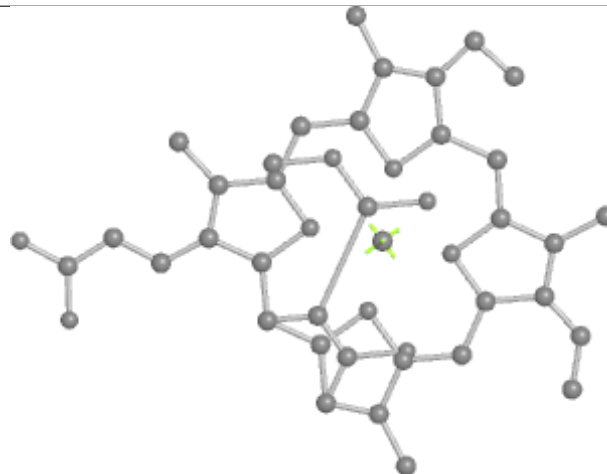
Bond lengths



Bond angles

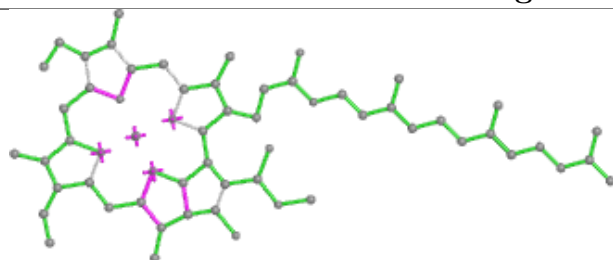


Torsions

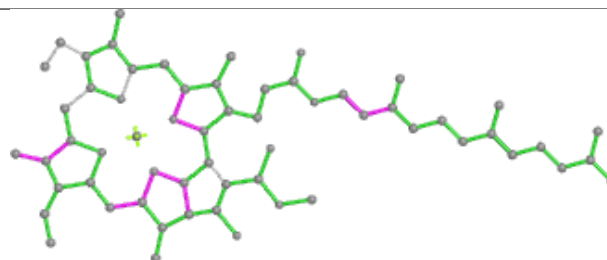


Rings

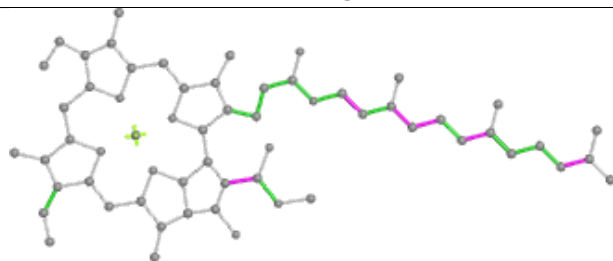
Ligand CLA P 305



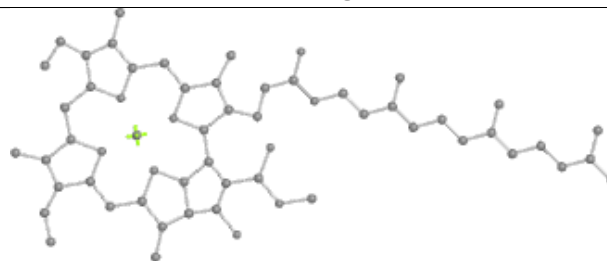
Bond lengths



Bond angles

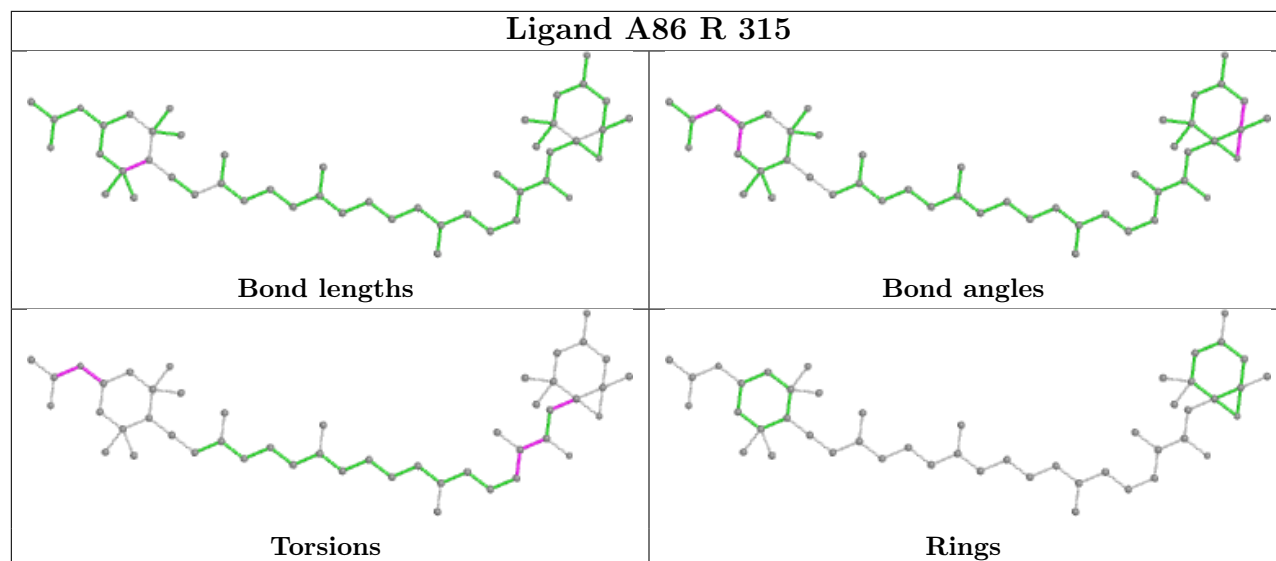


Torsions

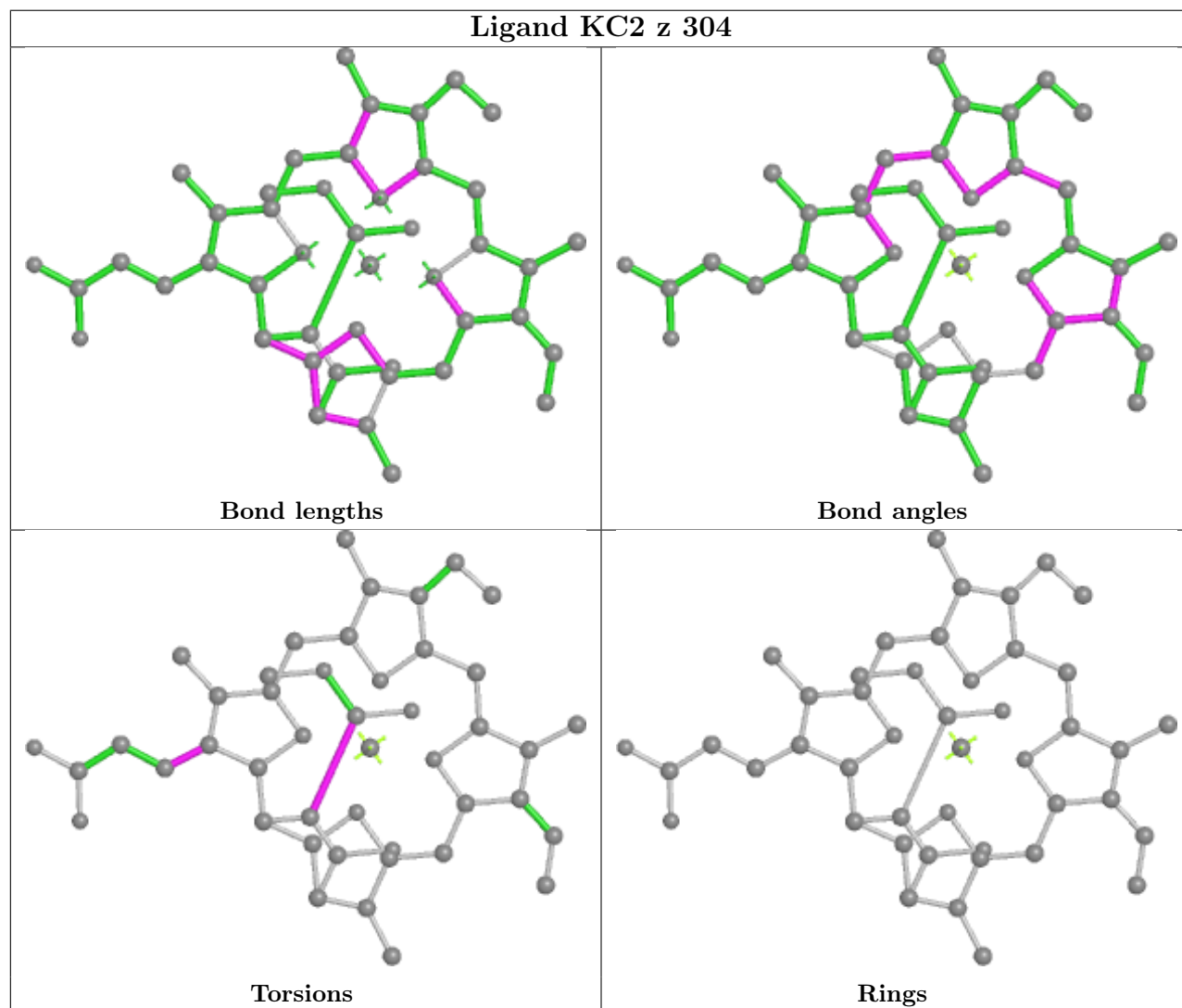


Rings

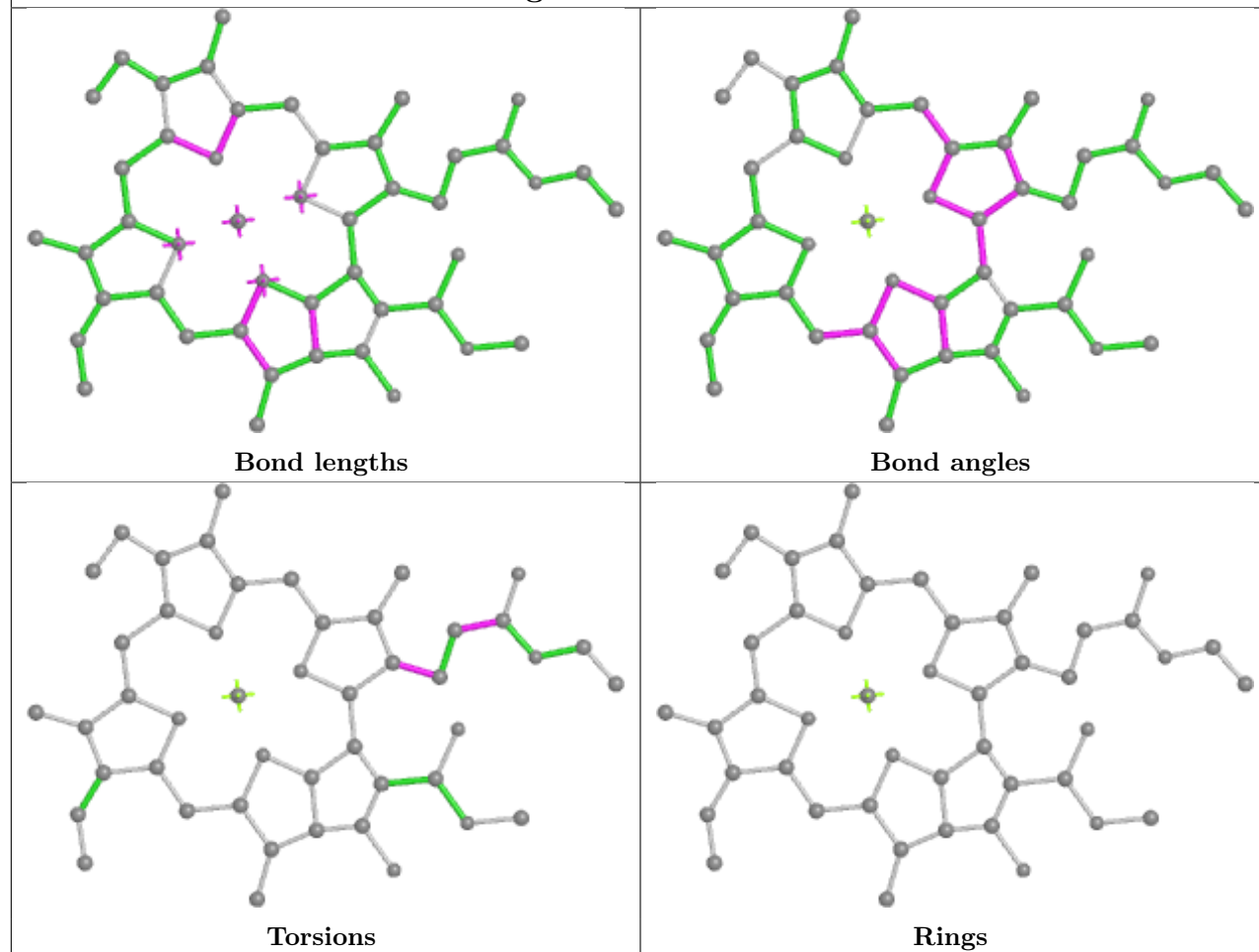
Ligand A86 R 315



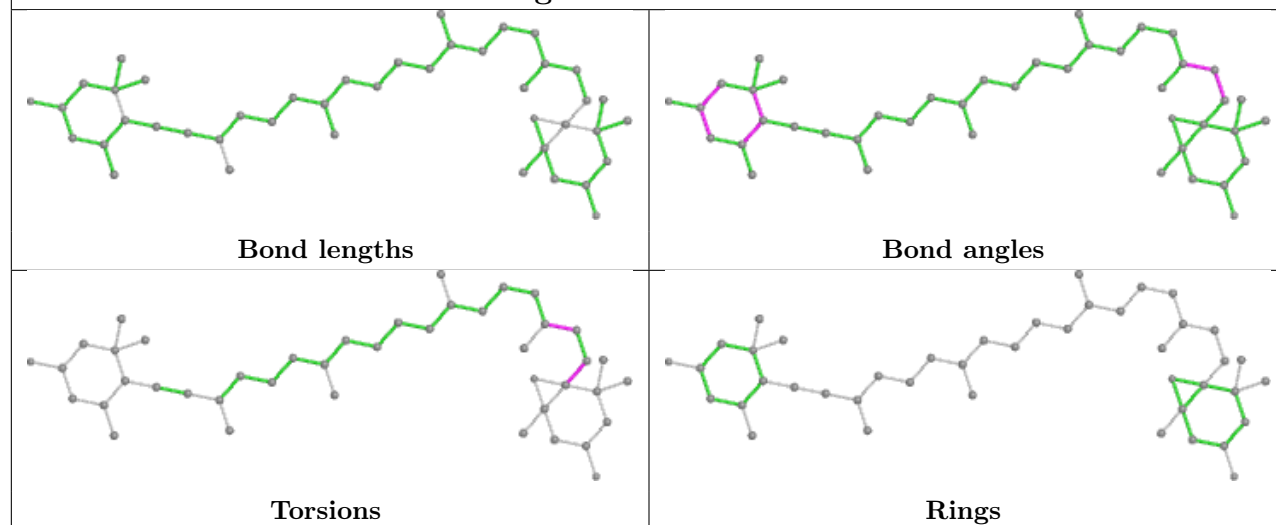
Ligand KC2 z 304

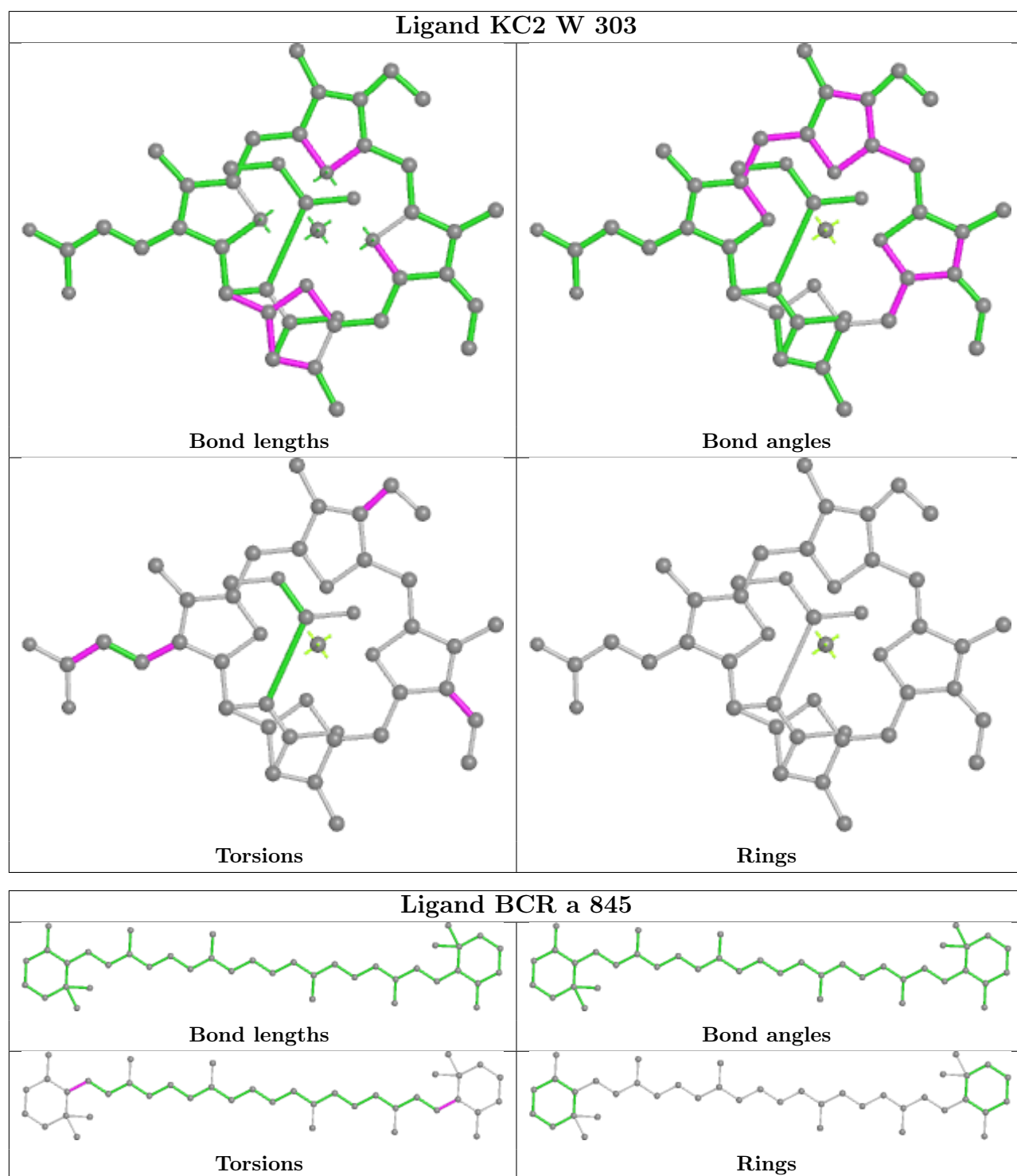


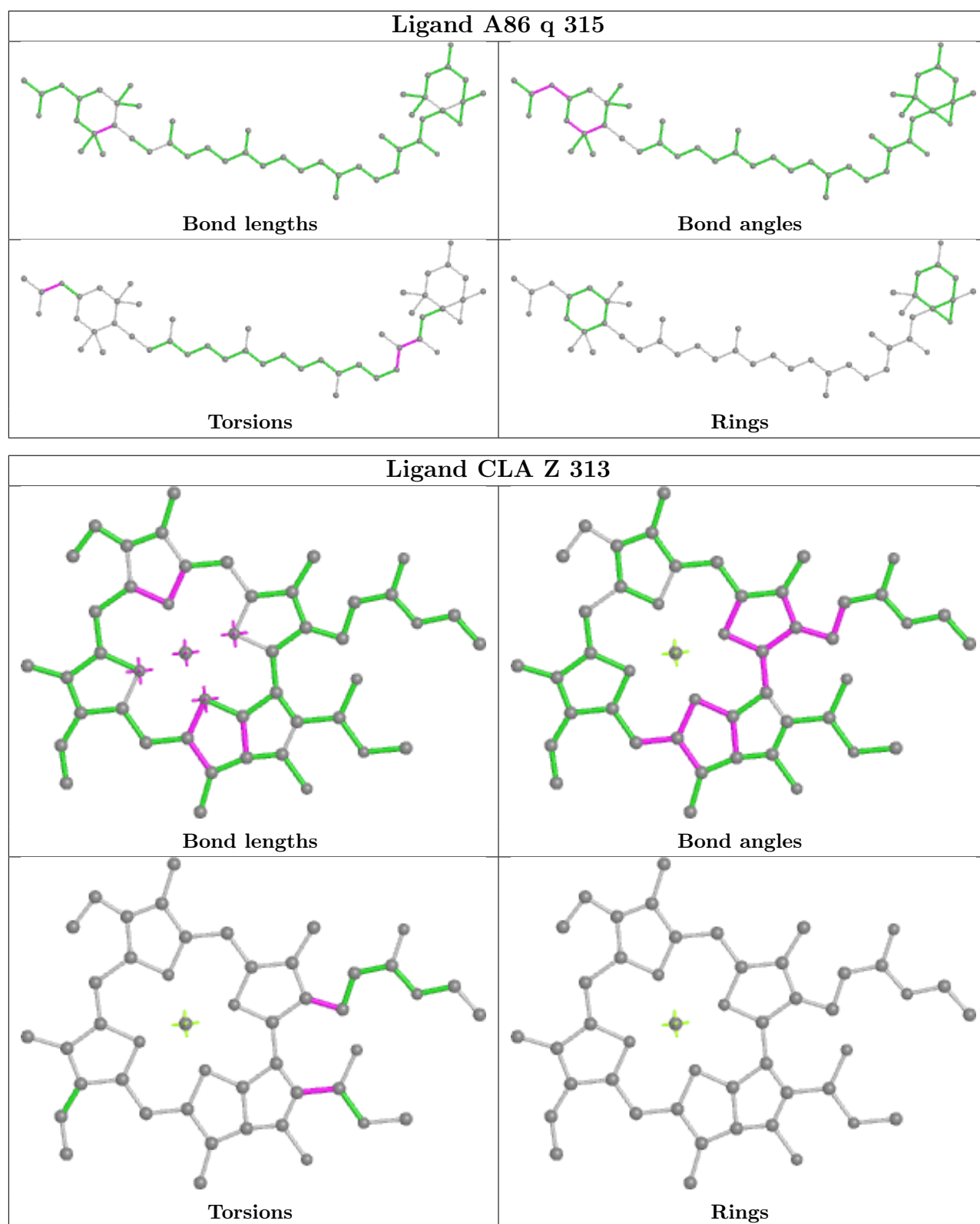
Ligand CLA P 311

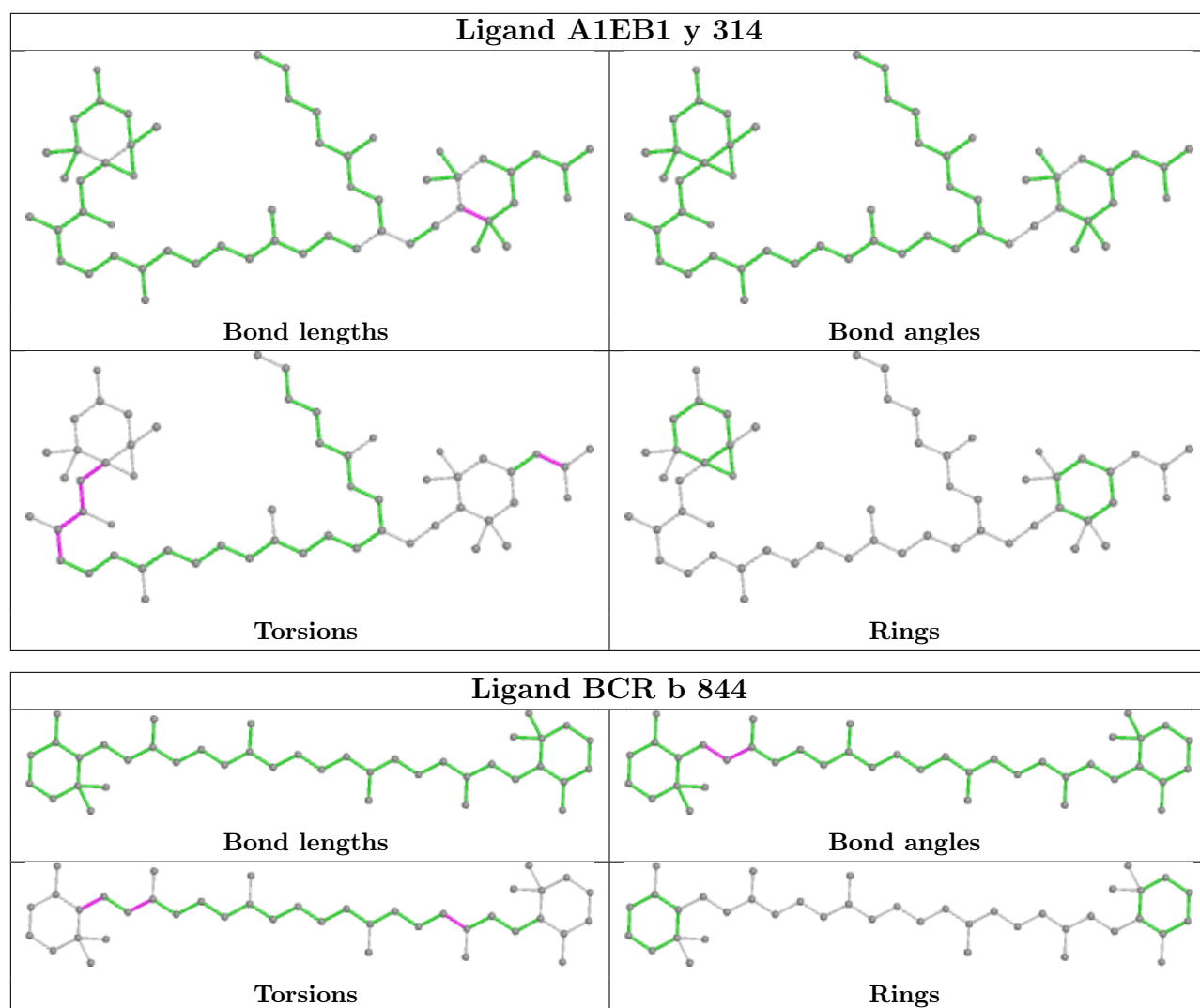


Ligand DD6 F 315

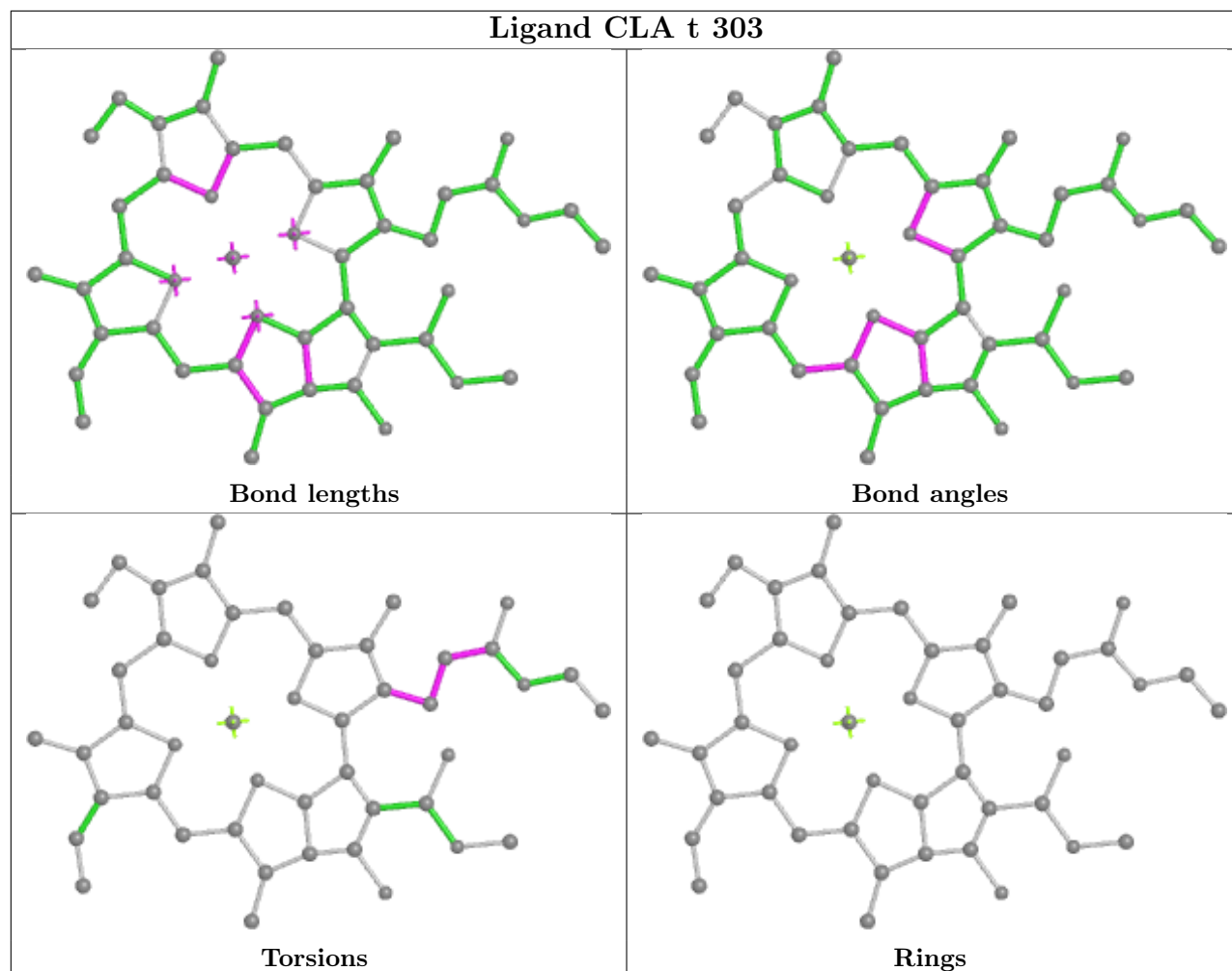




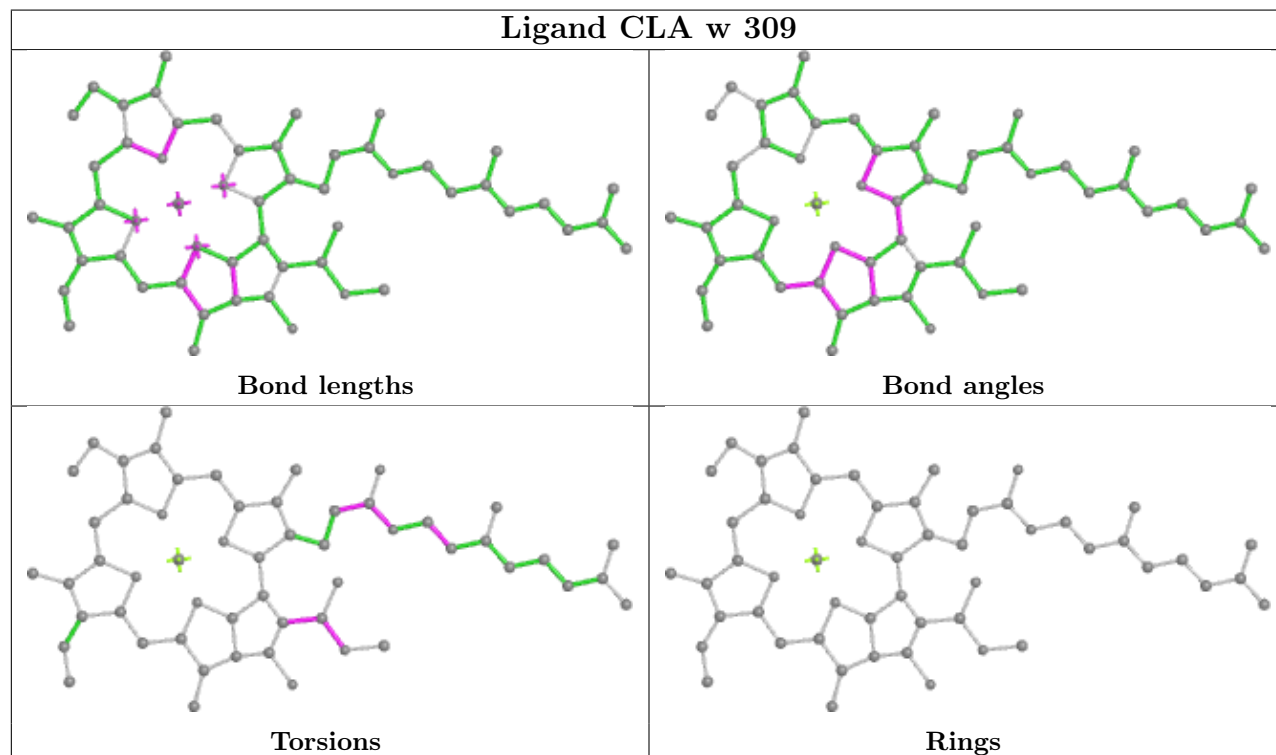


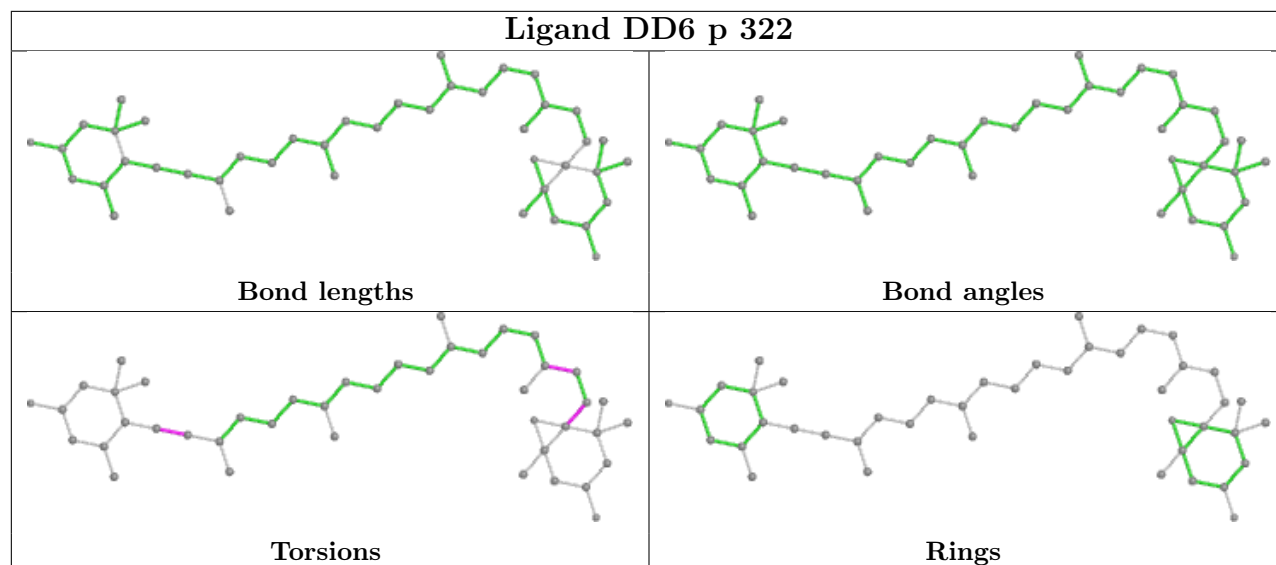
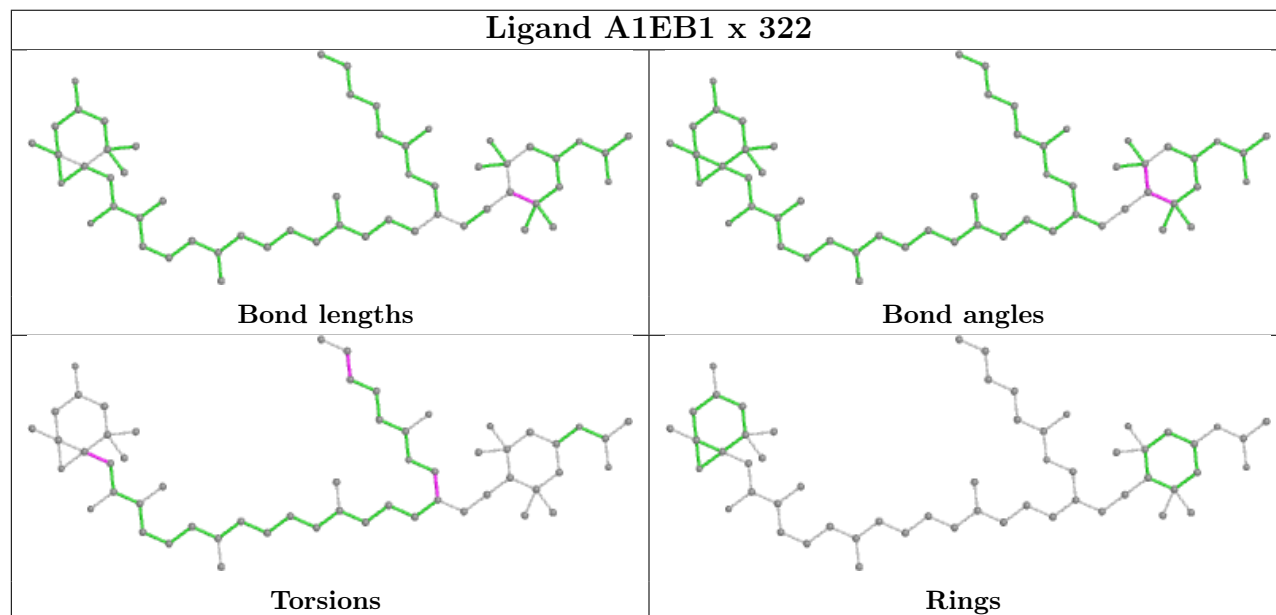


Ligand CLA t 303

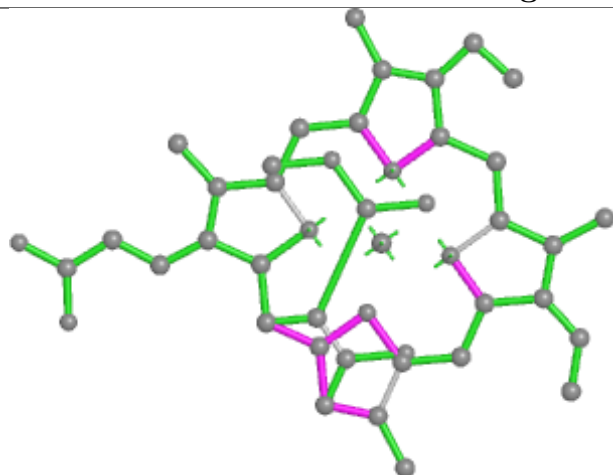


Ligand CLA w 309

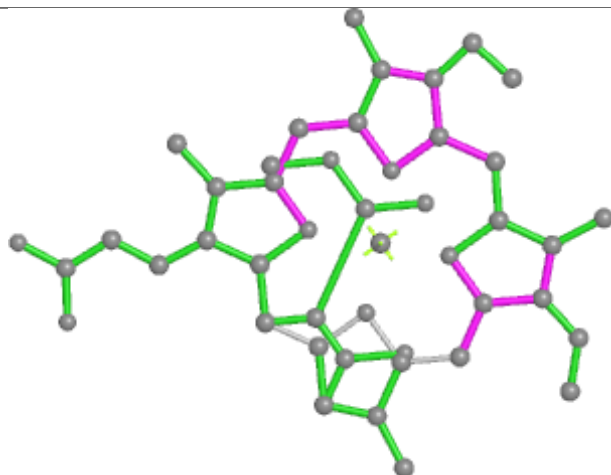


Ligand DD6 p 322**Ligand A1EB1 x 322**

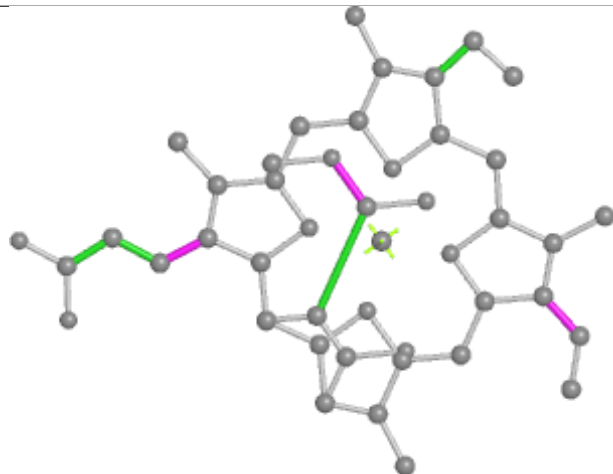
Ligand KC2 o 302



Bond lengths



Bond angles

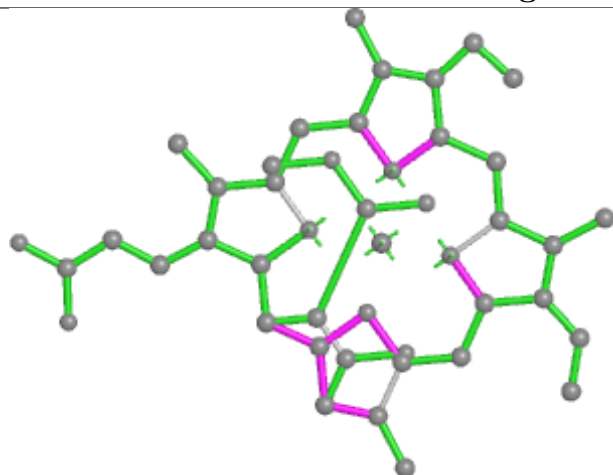


Torsions

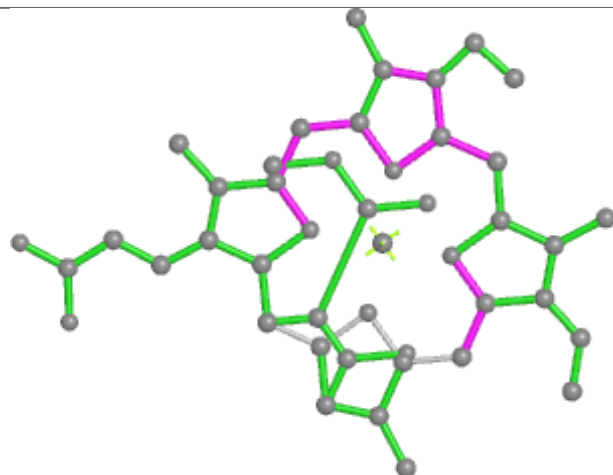


Rings

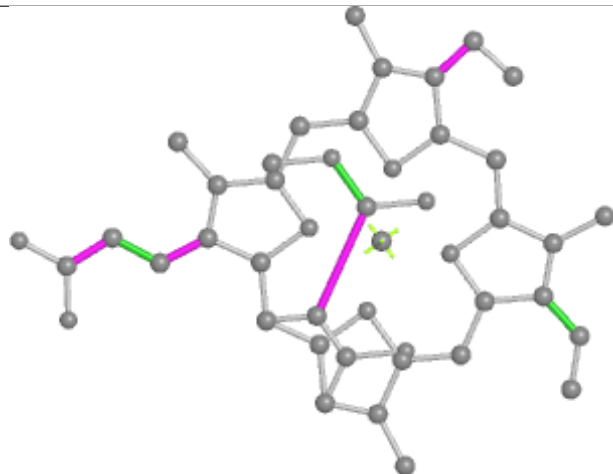
Ligand KC2 S 304



Bond lengths



Bond angles

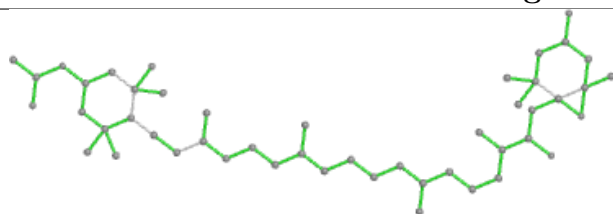


Torsions

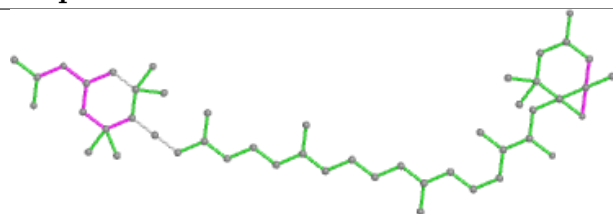


Rings

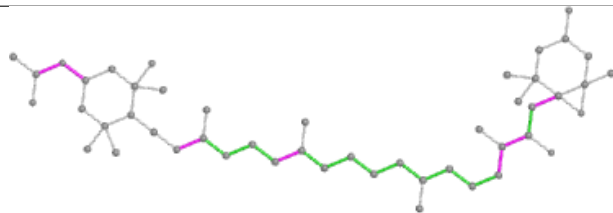
Ligand A86 q 319



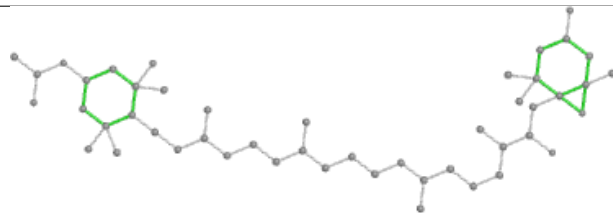
Bond lengths



Bond angles

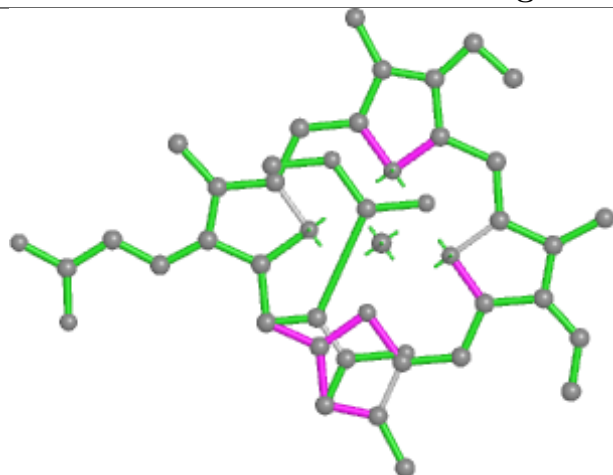


Torsions

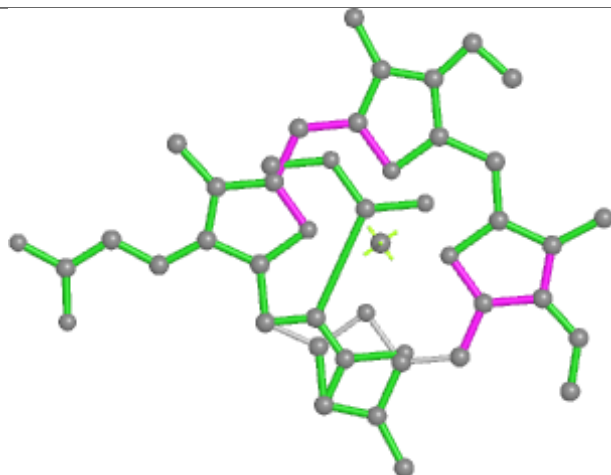


Rings

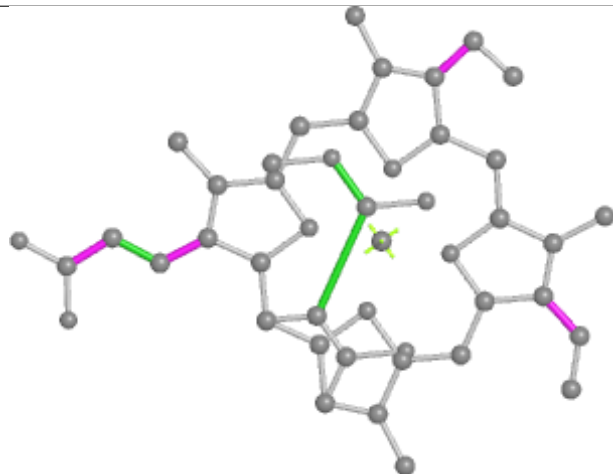
Ligand KC2 P 310



Bond lengths



Bond angles

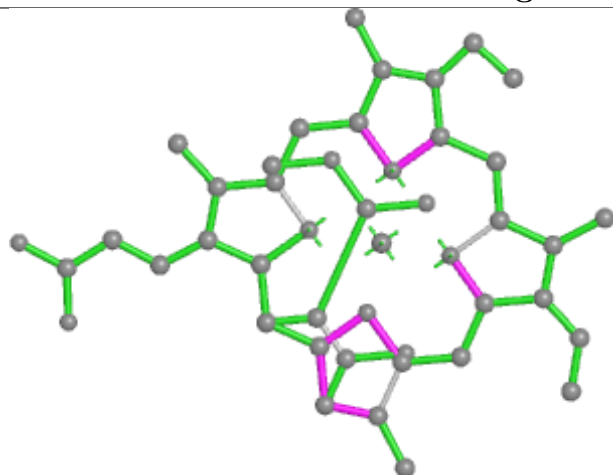


Torsions

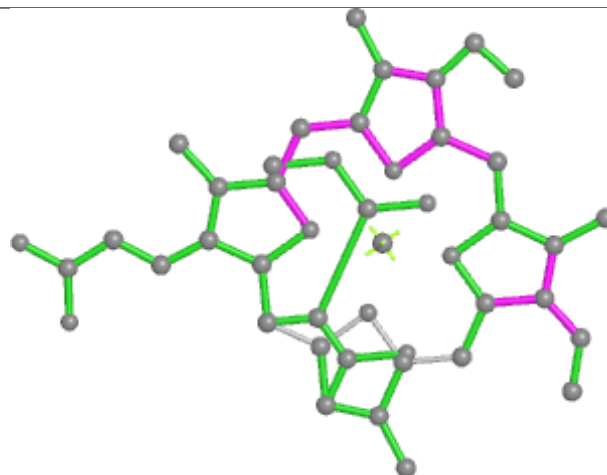


Rings

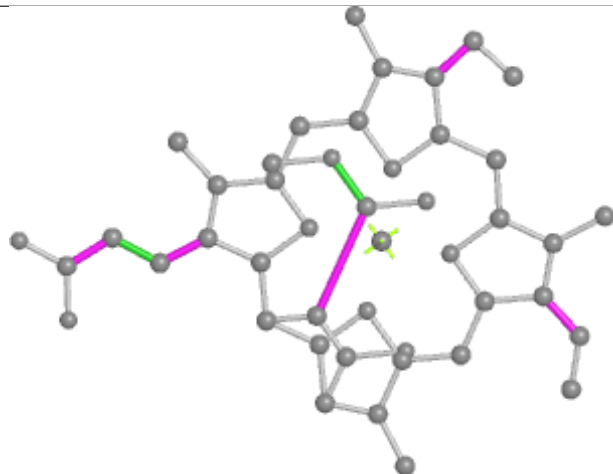
Ligand KC2 R 303



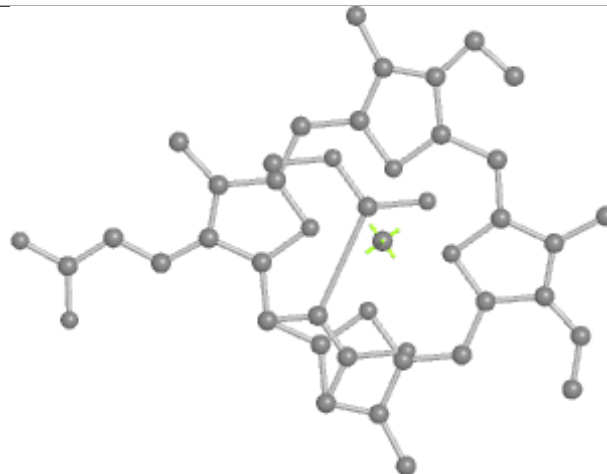
Bond lengths



Bond angles

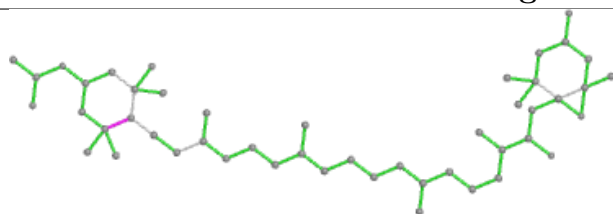


Torsions

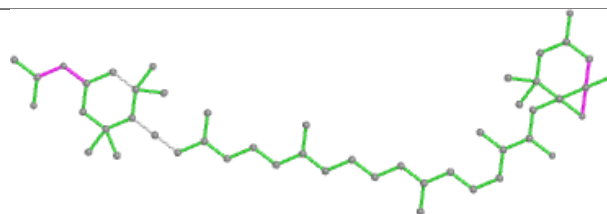


Rings

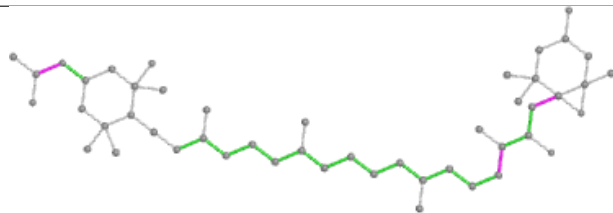
Ligand A86 D 320



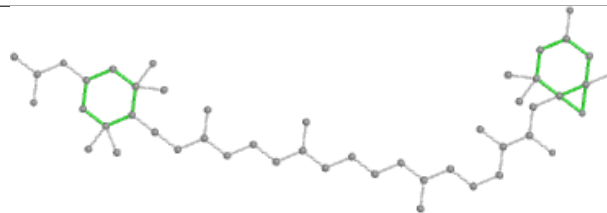
Bond lengths



Bond angles

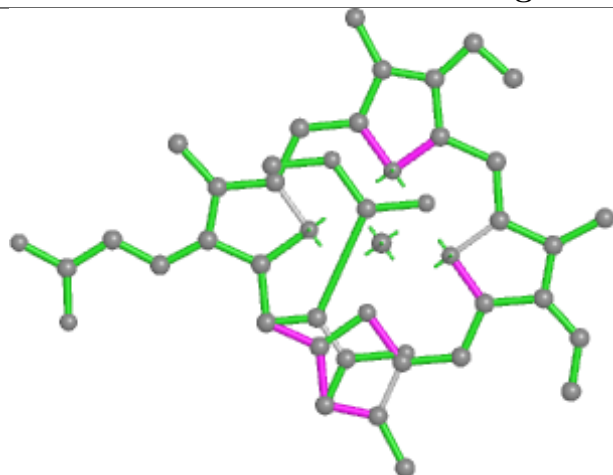


Torsions

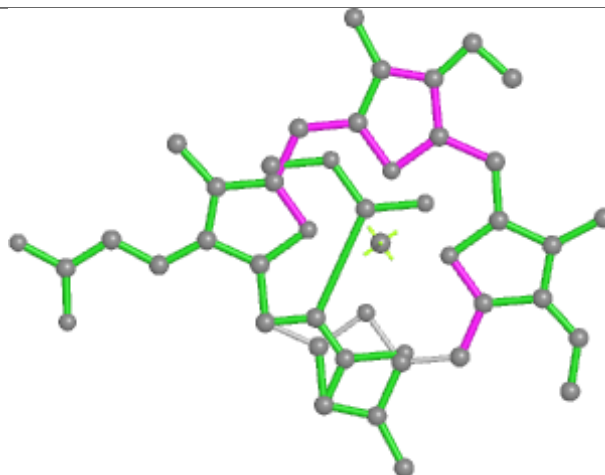


Rings

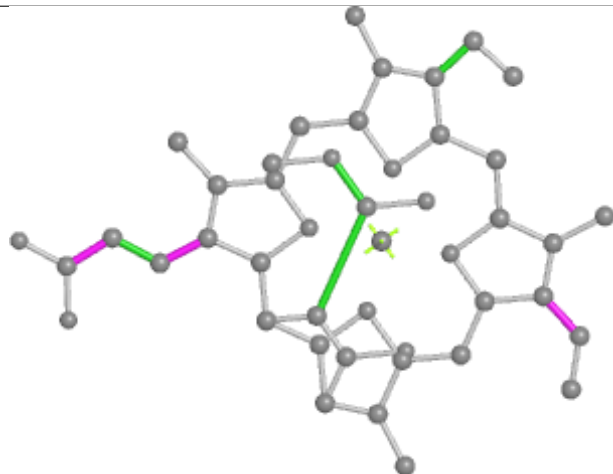
Ligand KC2 N 302



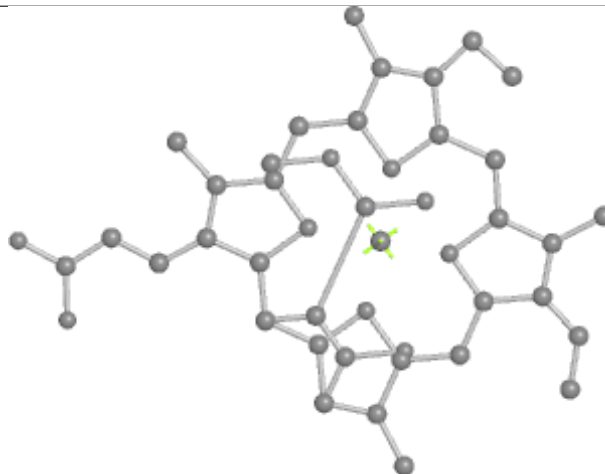
Bond lengths



Bond angles

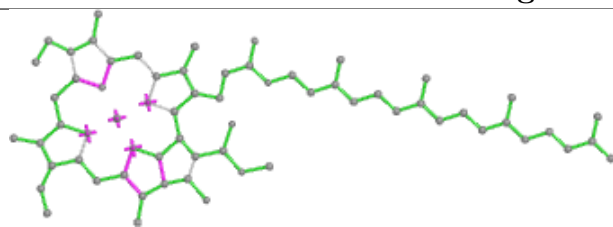


Torsions

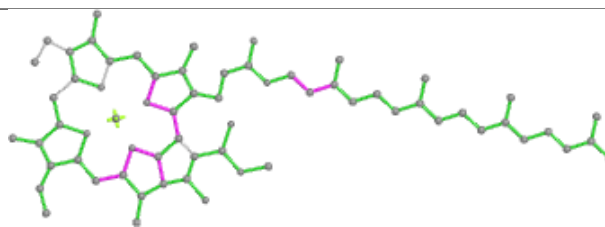


Rings

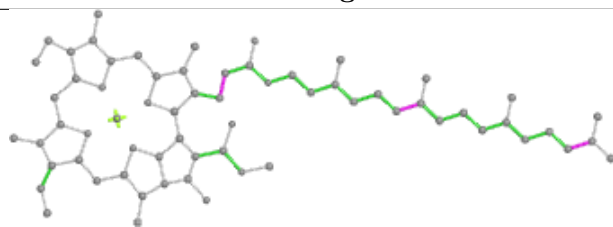
Ligand CLA b 841



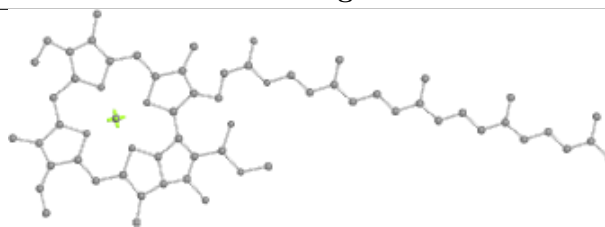
Bond lengths



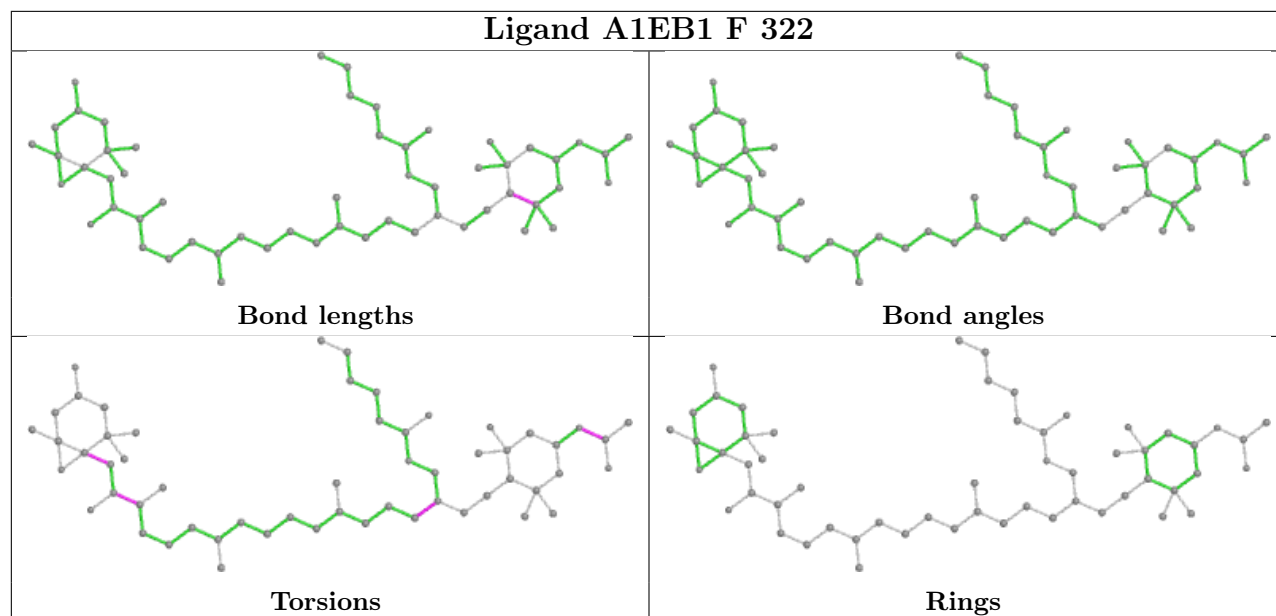
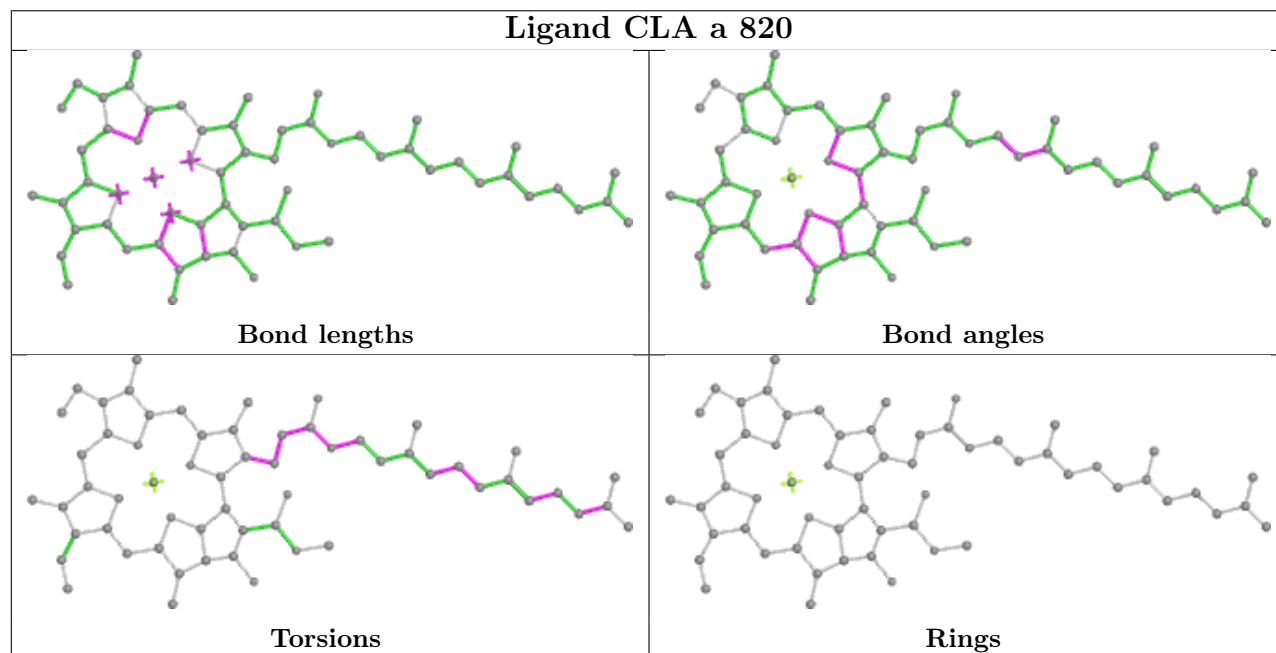
Bond angles

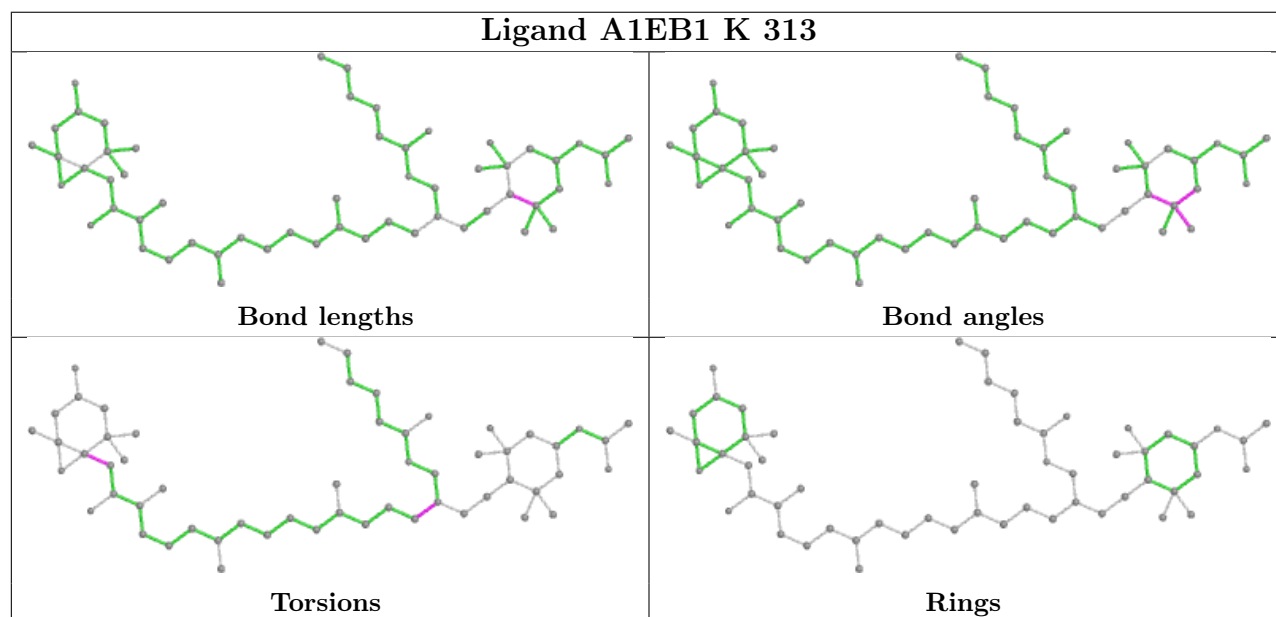
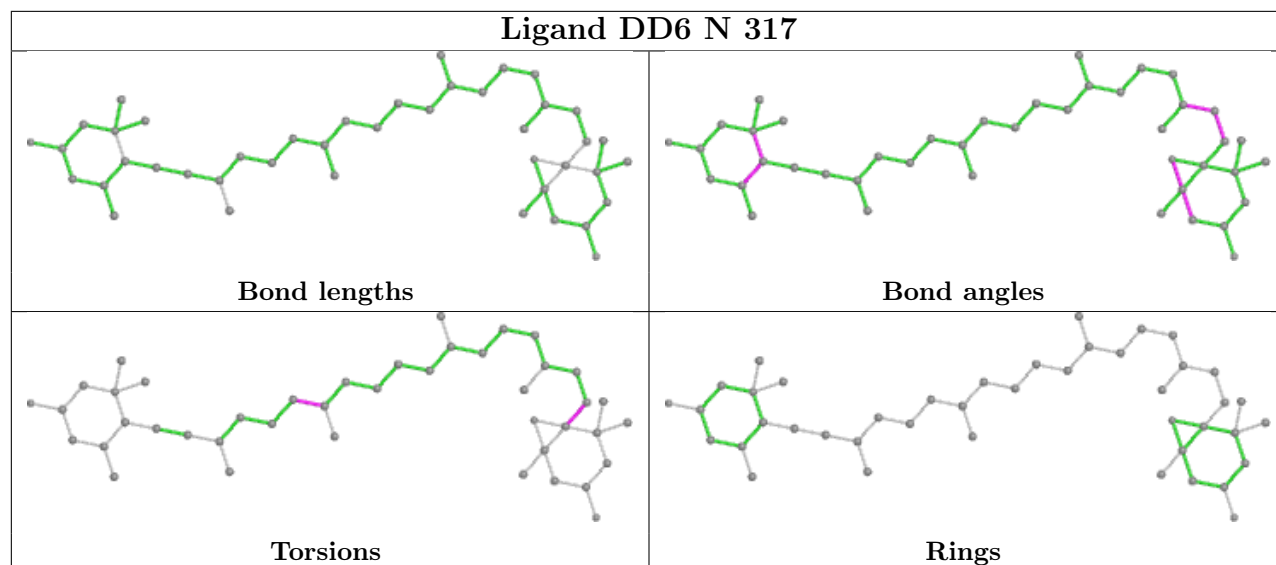


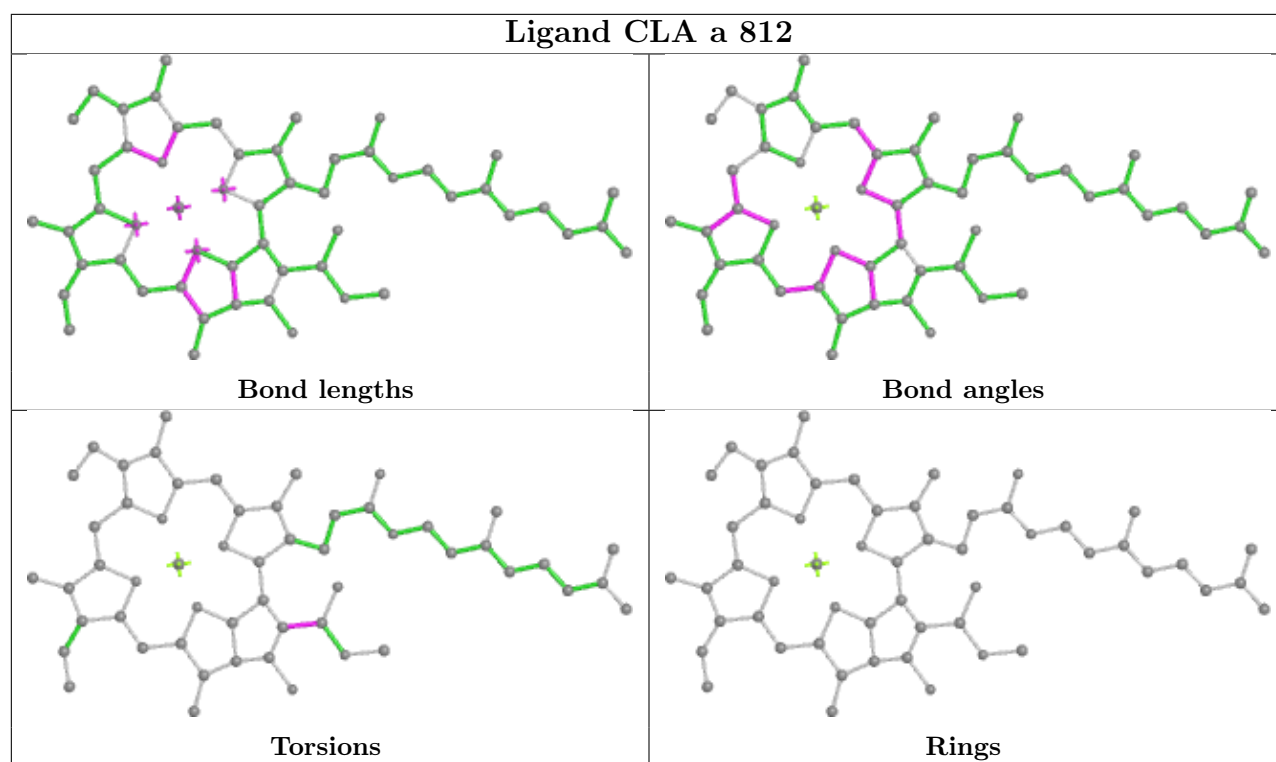
Torsions



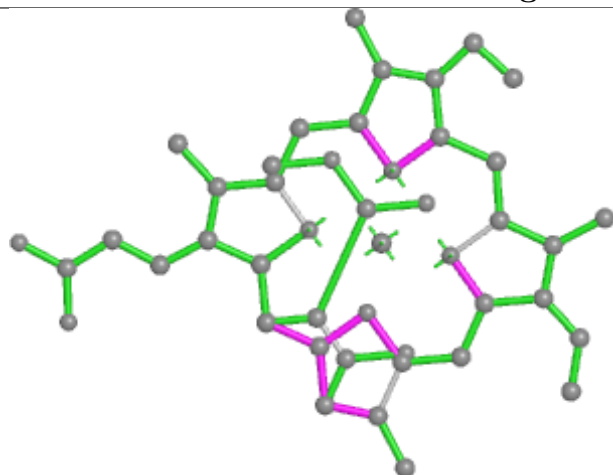
Rings

Ligand A1EB1 F 322**Ligand CLA a 820**

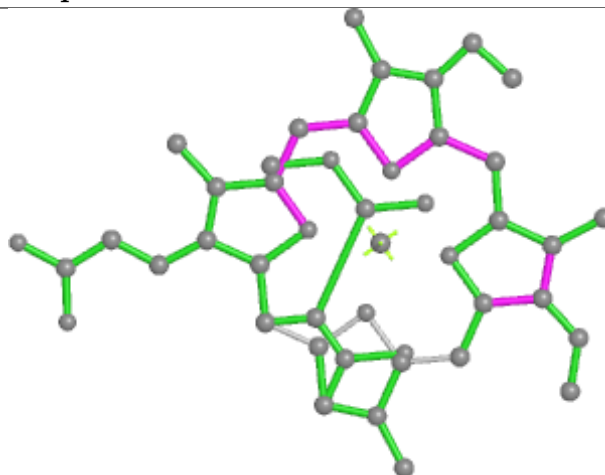




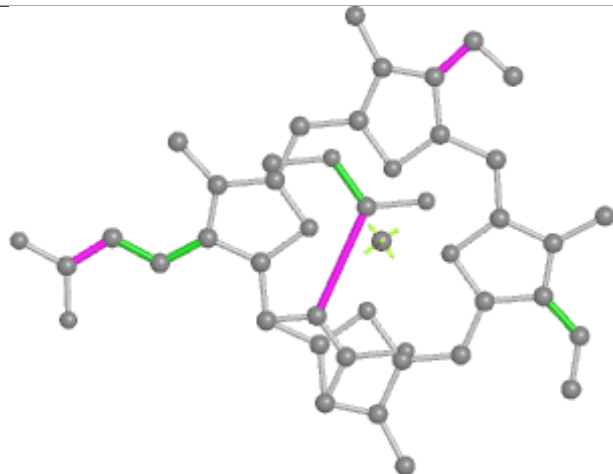
Ligand KC2 q 303



Bond lengths



Bond angles

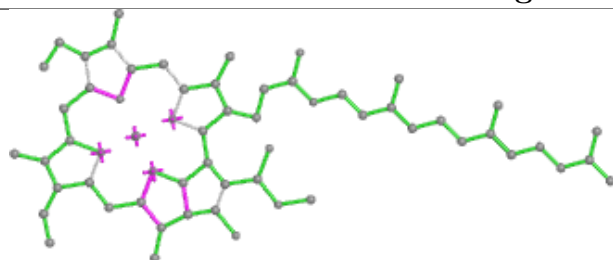


Torsions

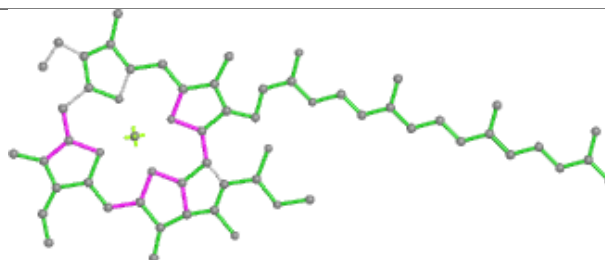


Rings

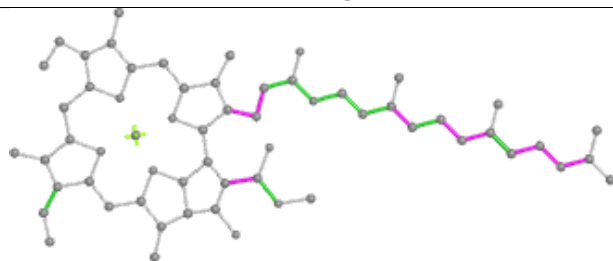
Ligand CLA P 312



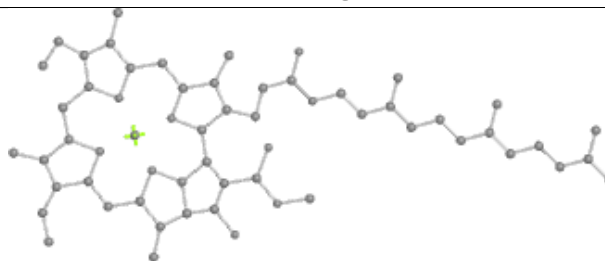
Bond lengths



Bond angles

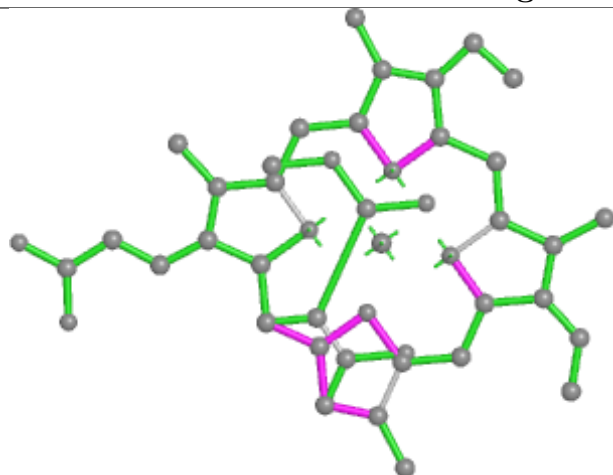


Torsions

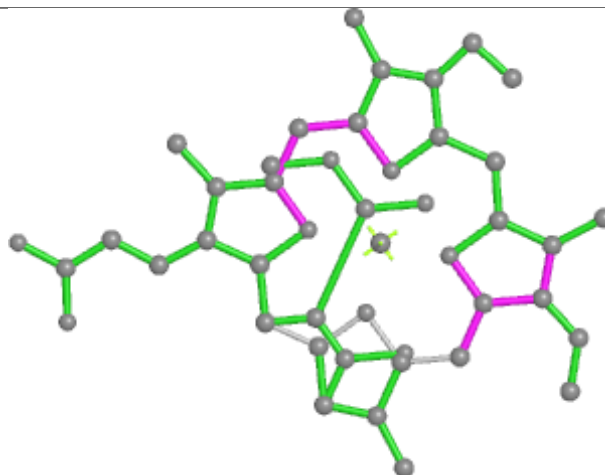


Rings

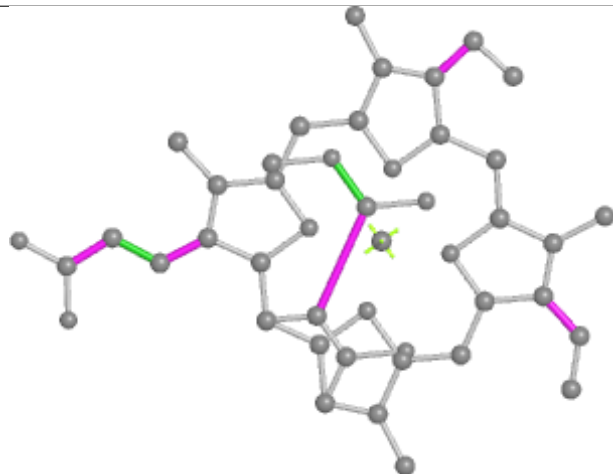
Ligand KC2 T 308



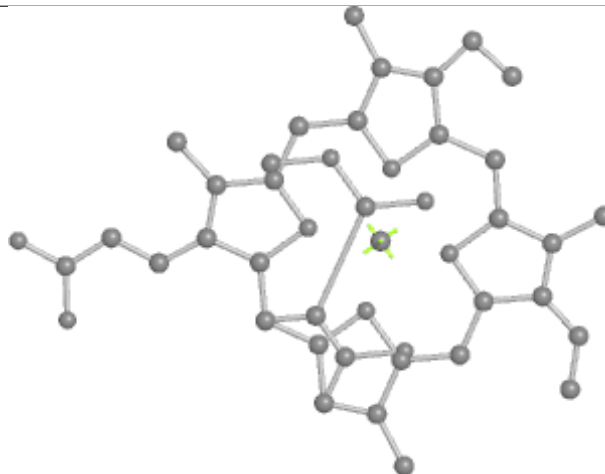
Bond lengths



Bond angles

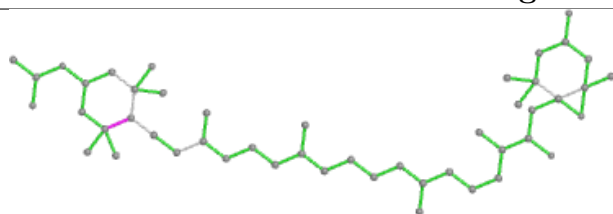


Torsions

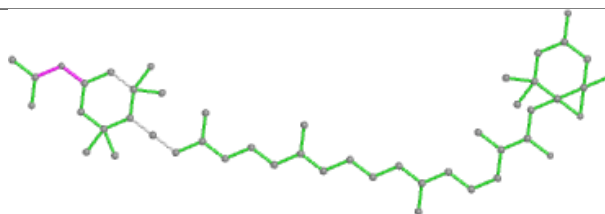


Rings

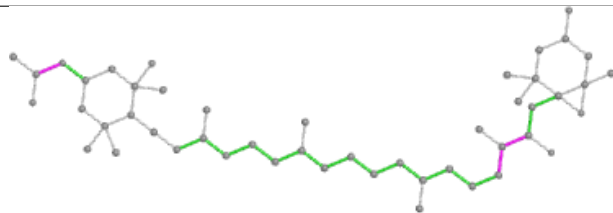
Ligand A86 G 211



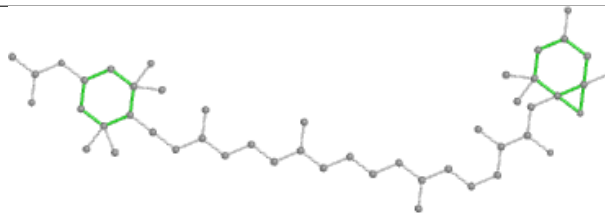
Bond lengths



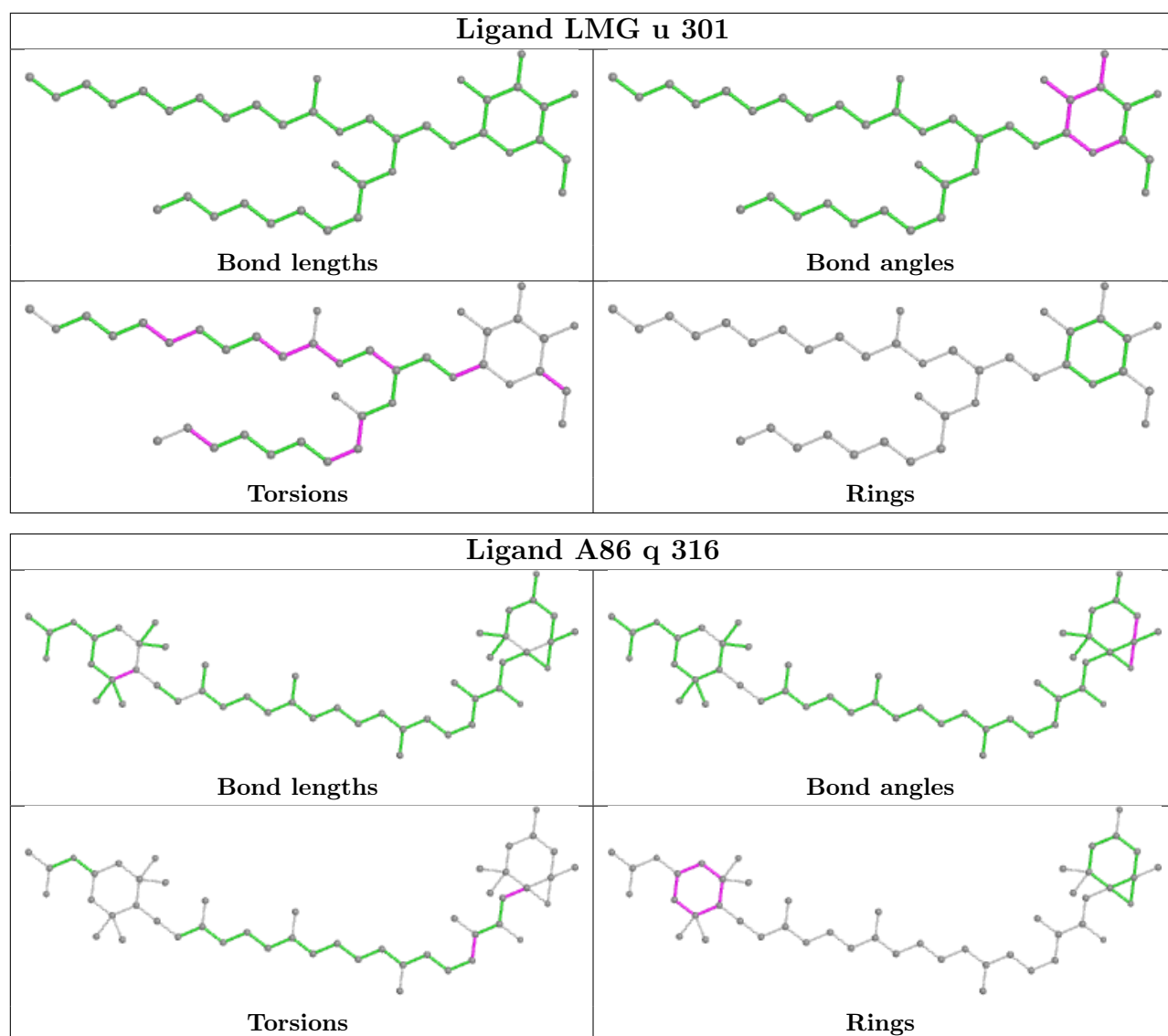
Bond angles

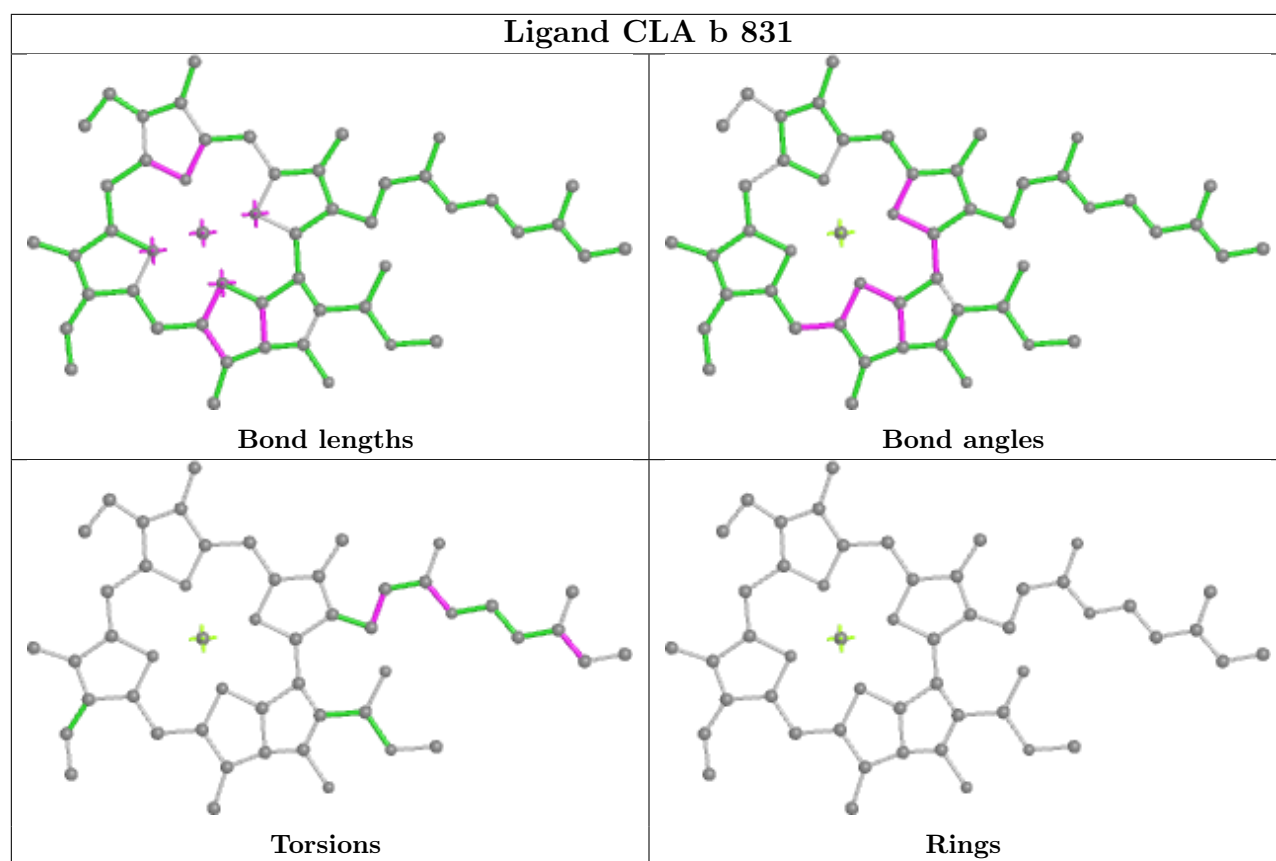


Torsions

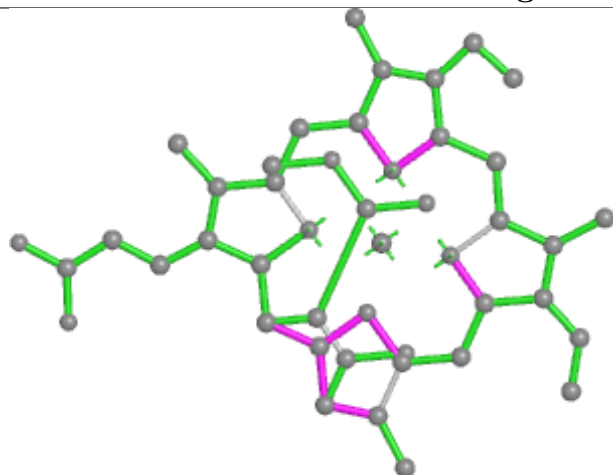


Rings

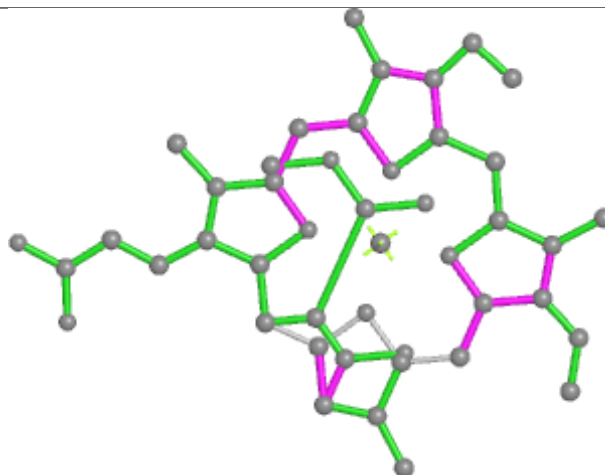




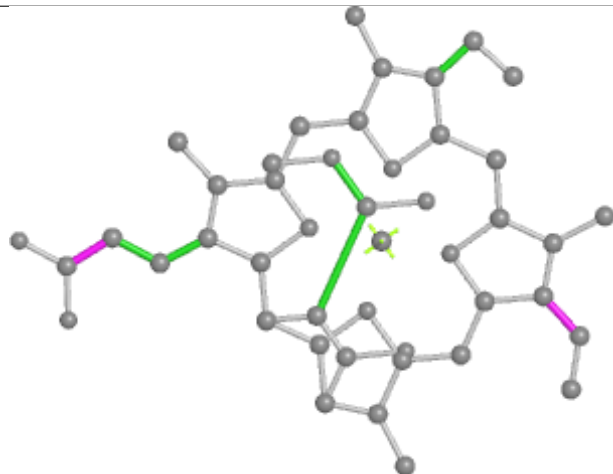
Ligand KC2 P 309



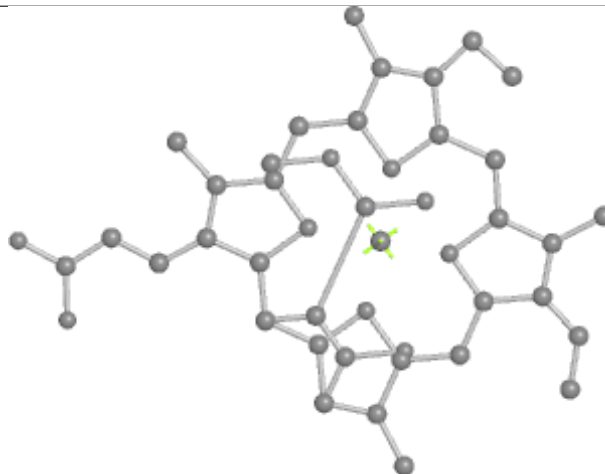
Bond lengths



Bond angles

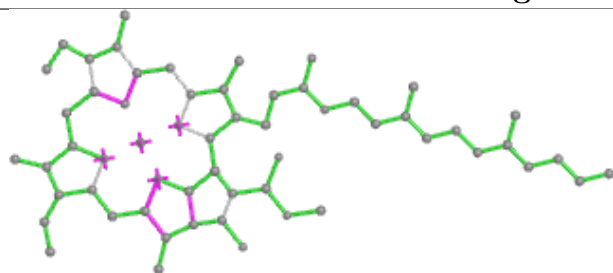


Torsions

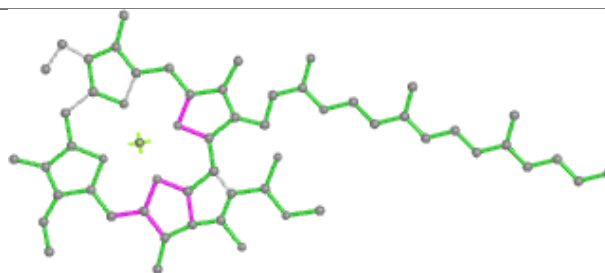


Rings

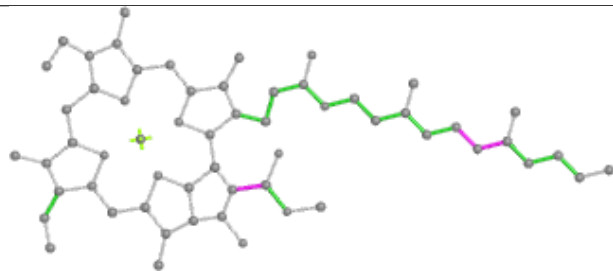
Ligand CLA D 309



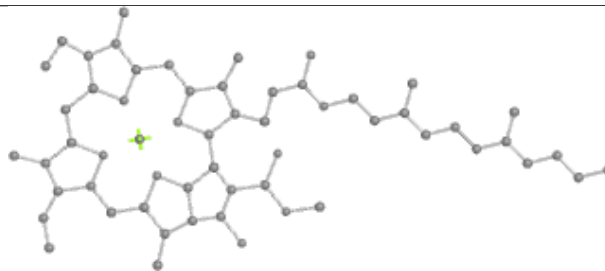
Bond lengths



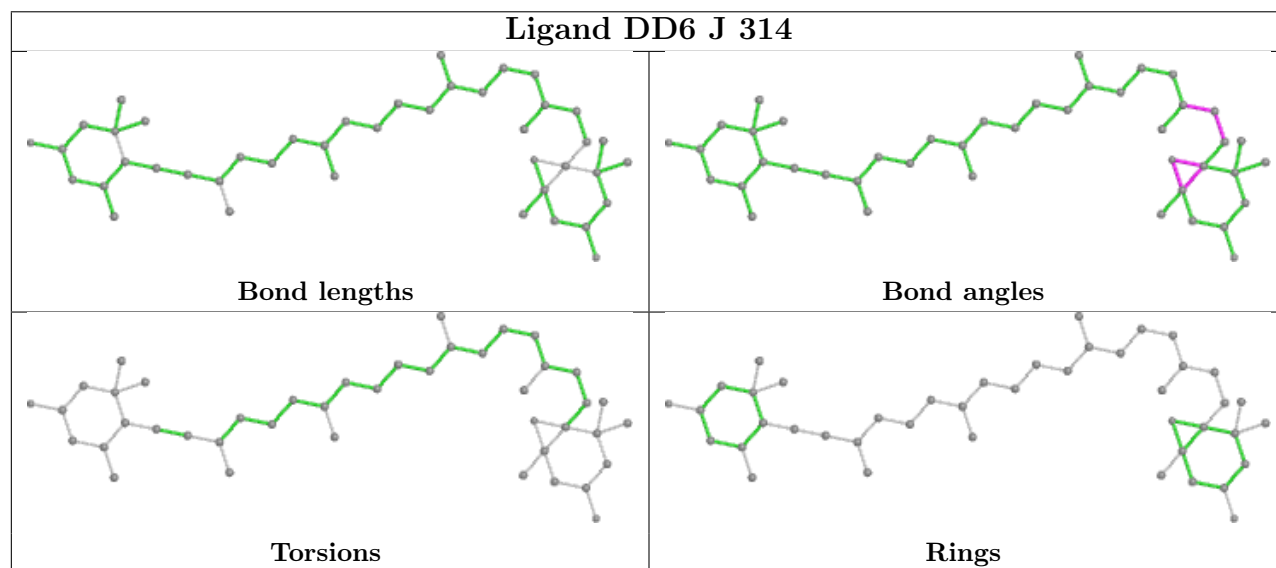
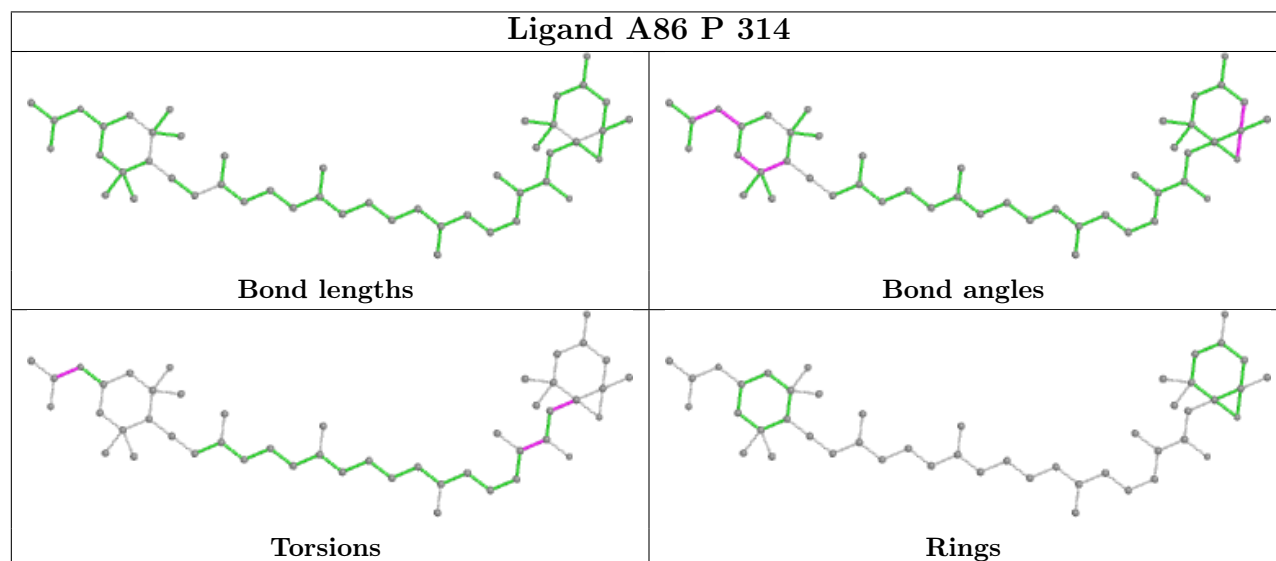
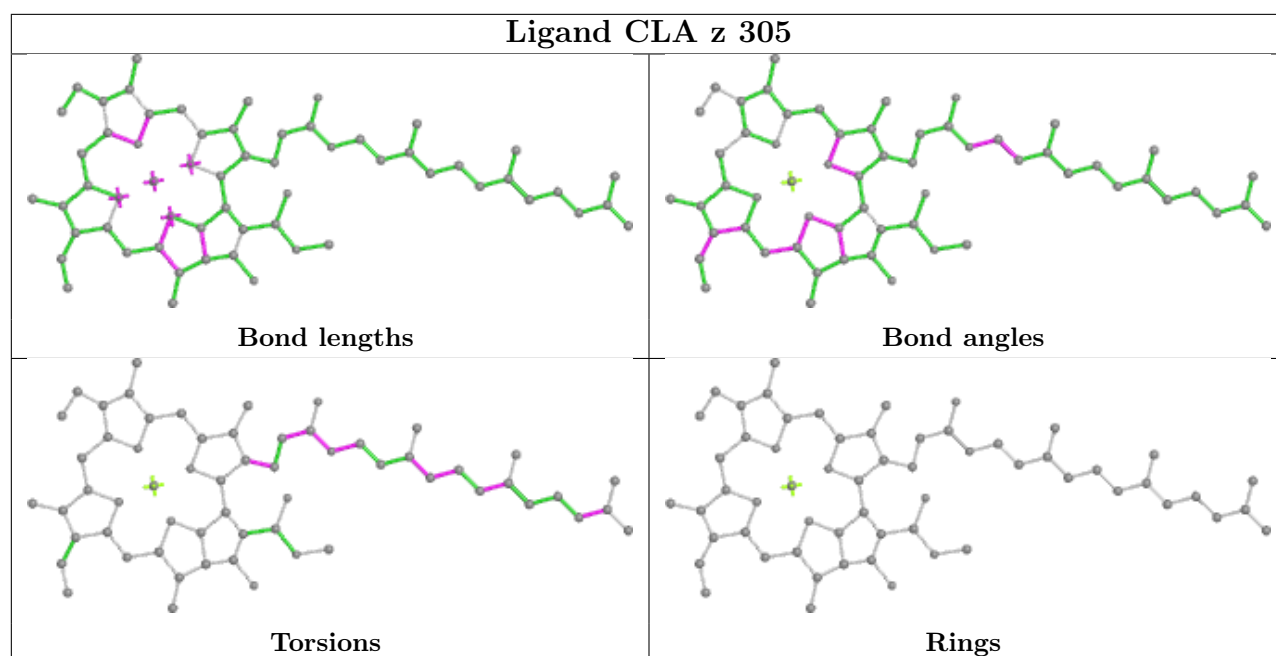
Bond angles



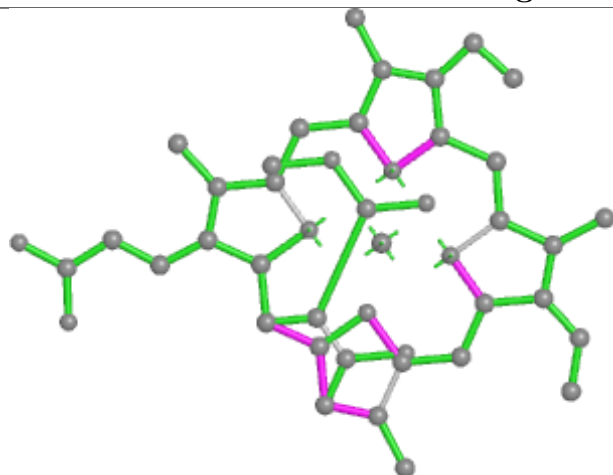
Torsions



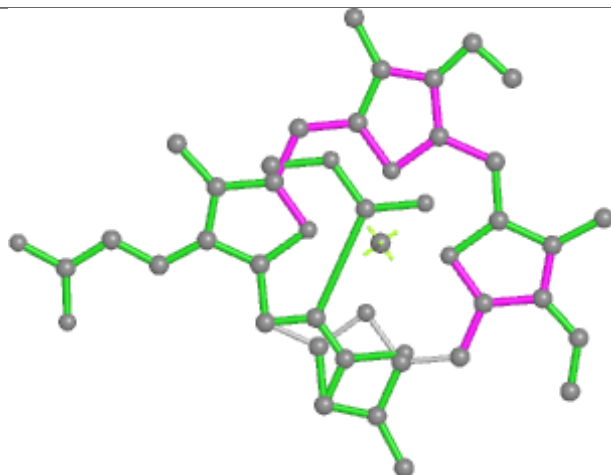
Rings



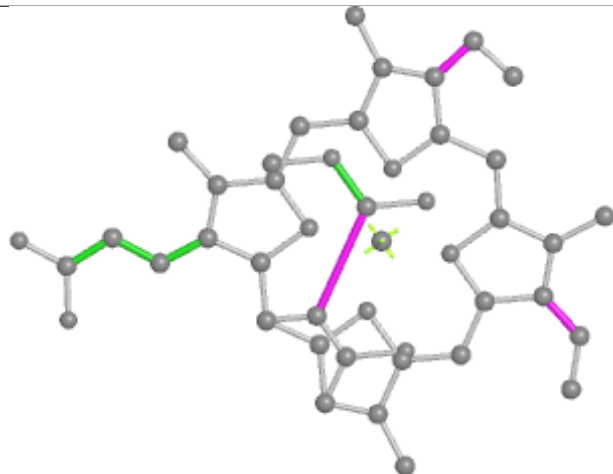
Ligand KC2 R 301



Bond lengths



Bond angles

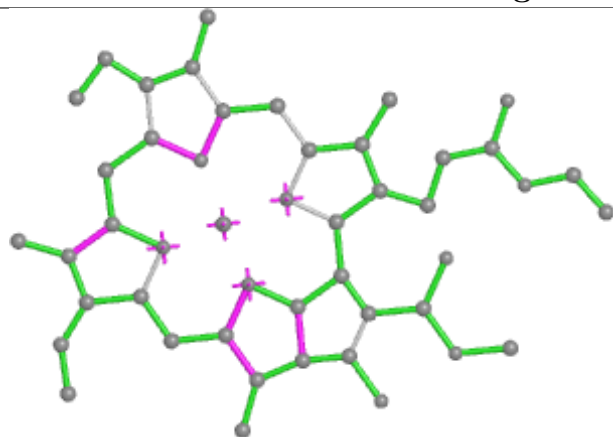


Torsions

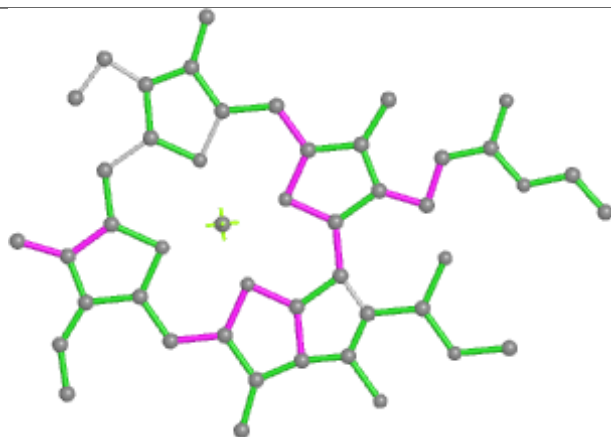


Rings

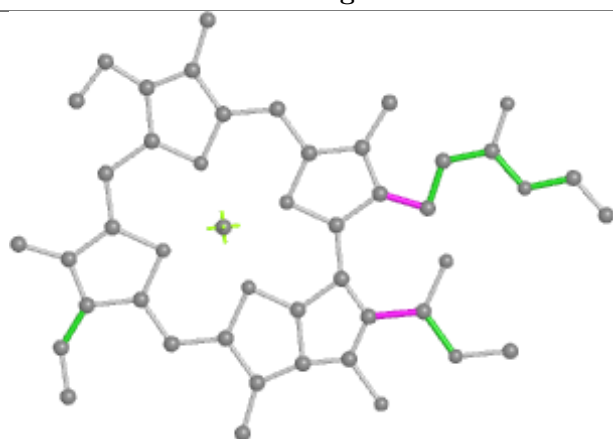
Ligand CLA H 304



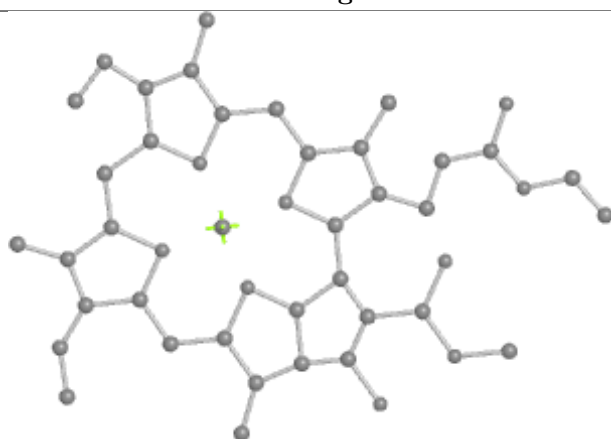
Bond lengths



Bond angles

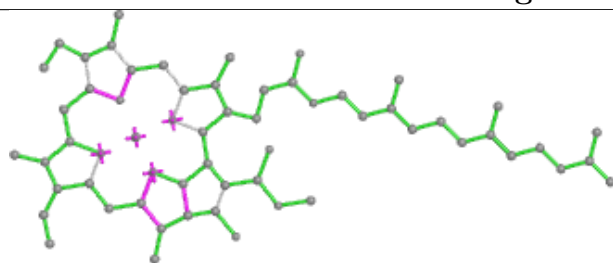


Torsions

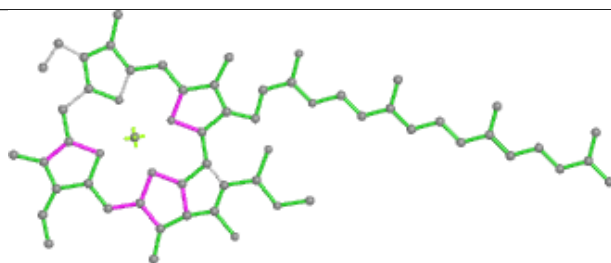


Rings

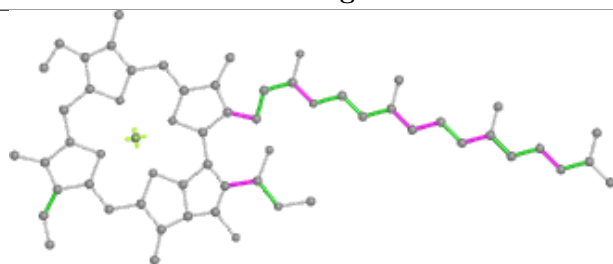
Ligand CLA P 313



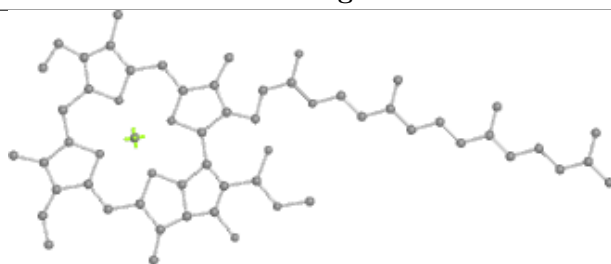
Bond lengths



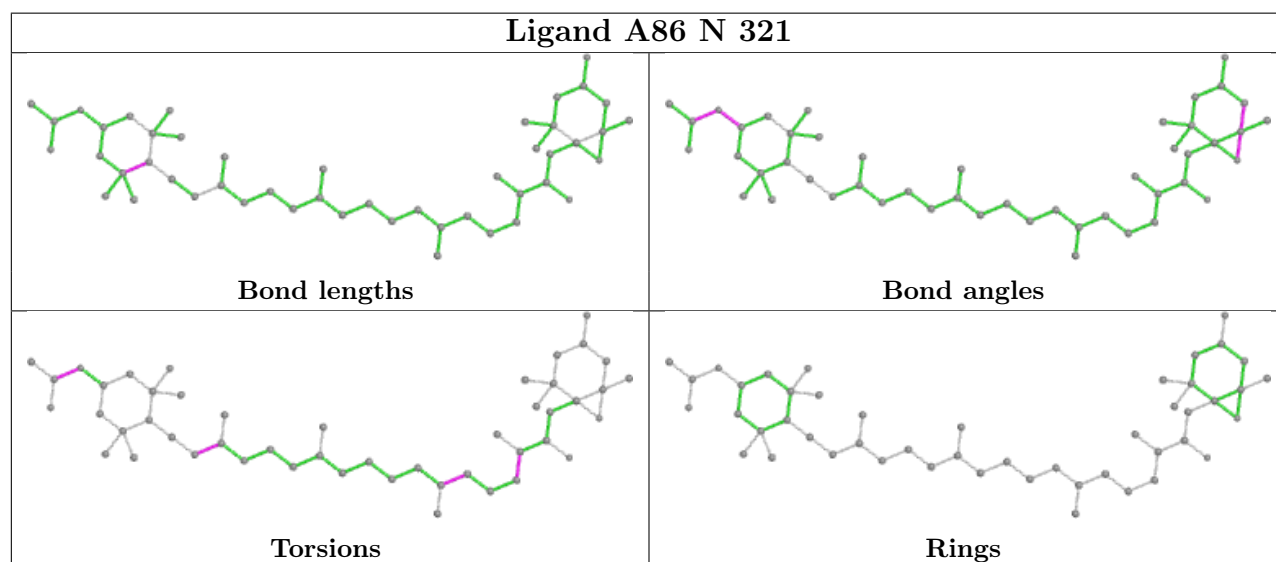
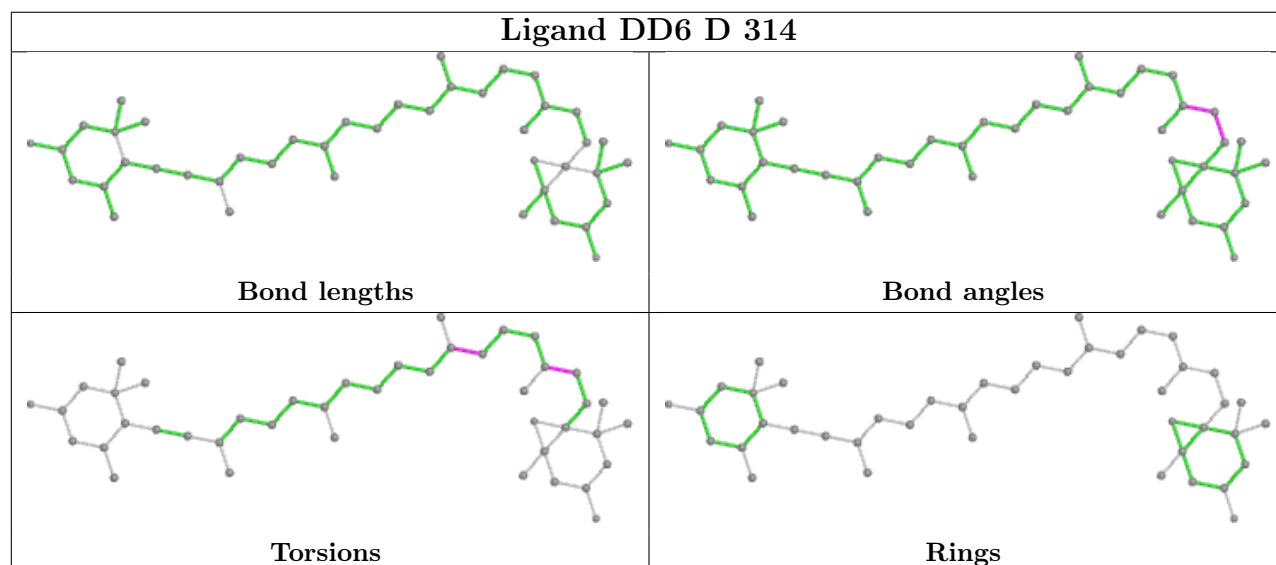
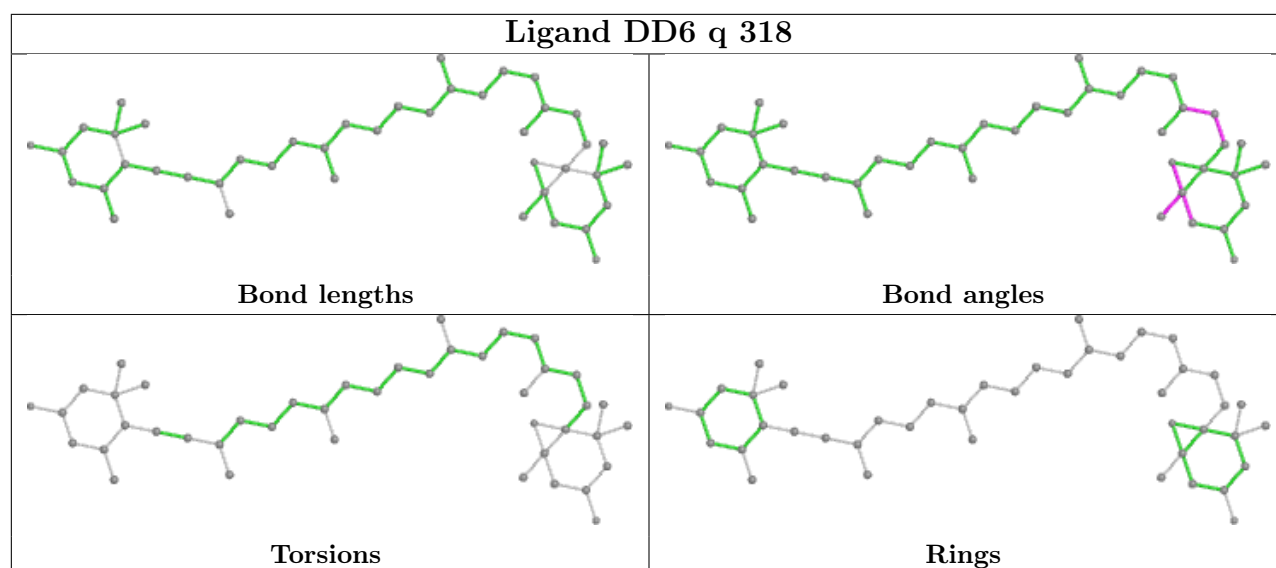
Bond angles



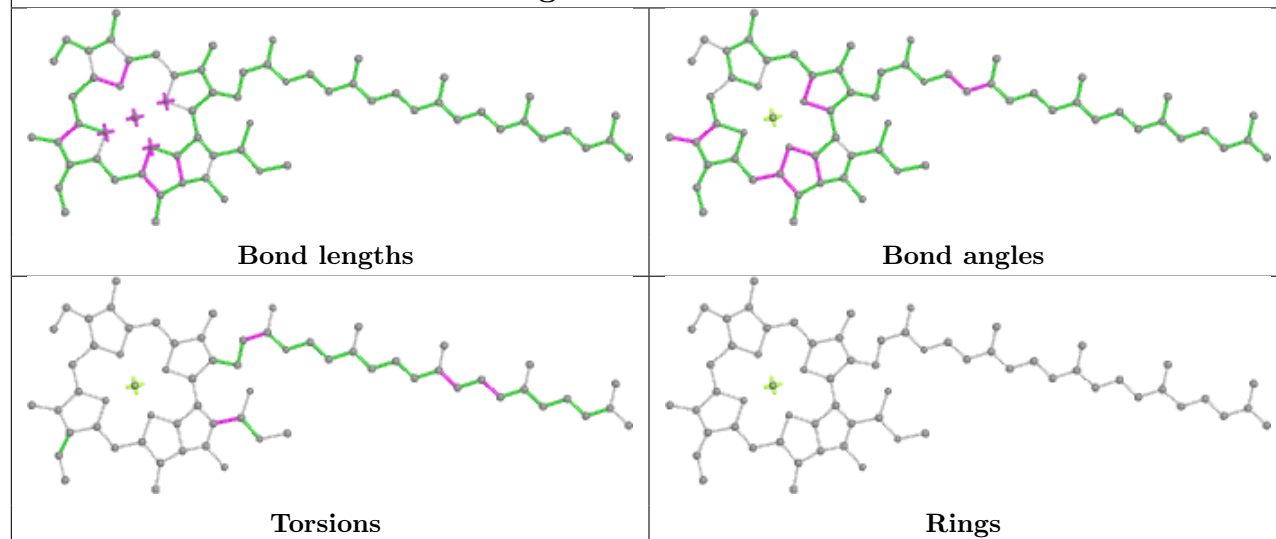
Torsions



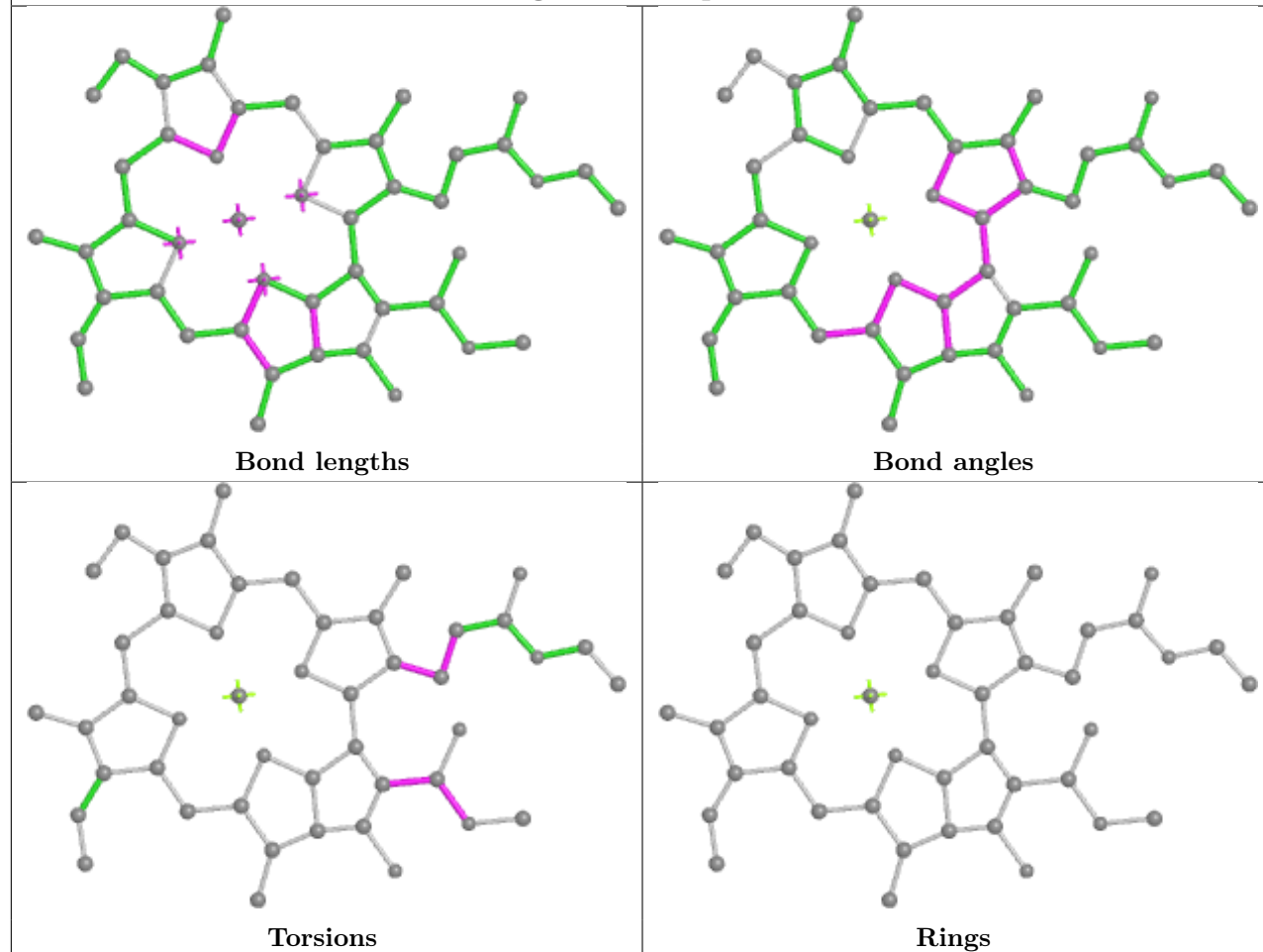
Rings

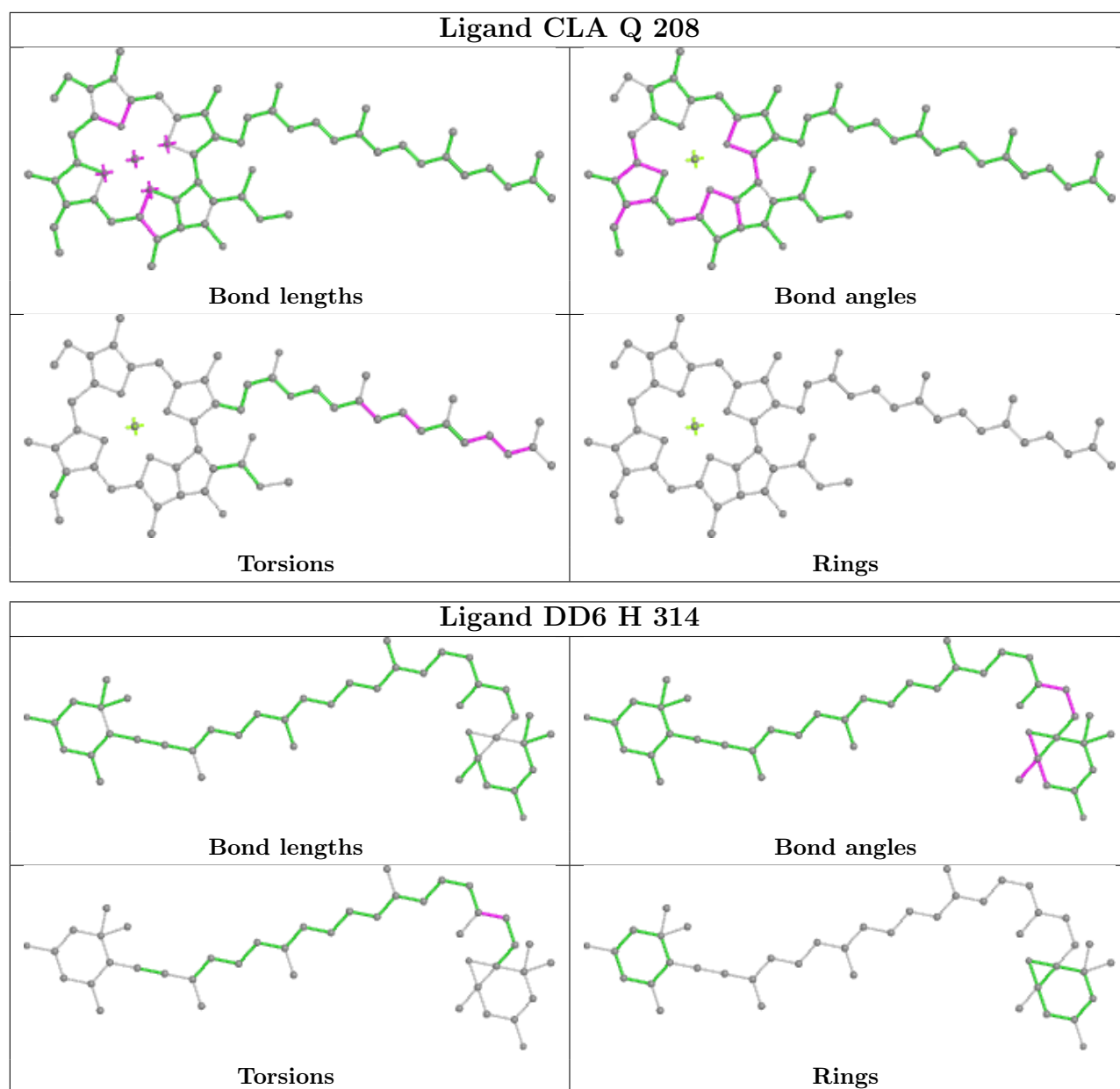


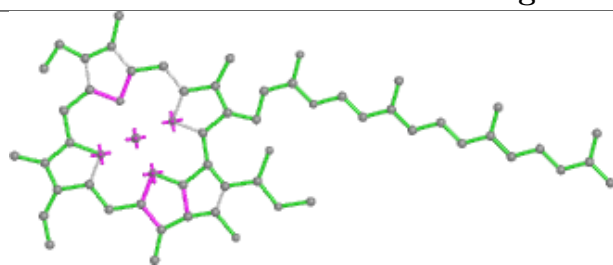
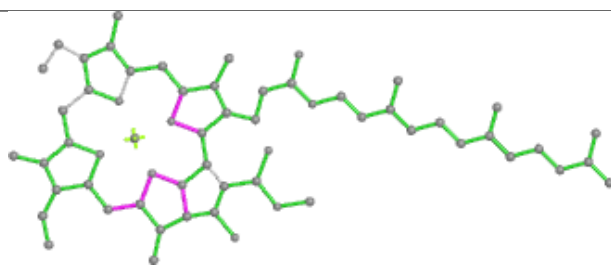
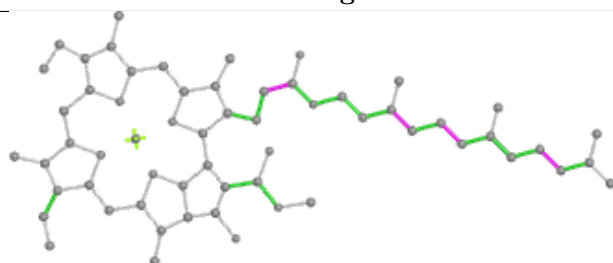
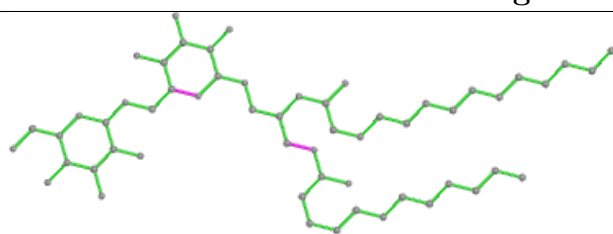
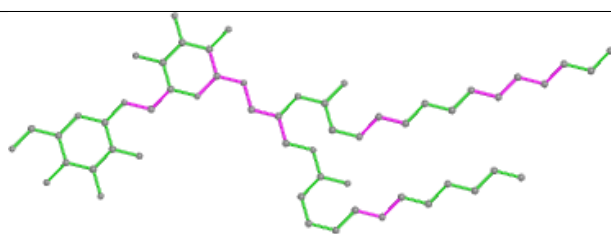
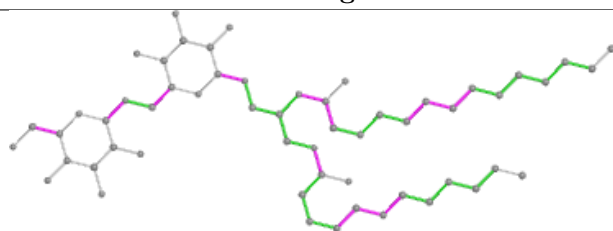
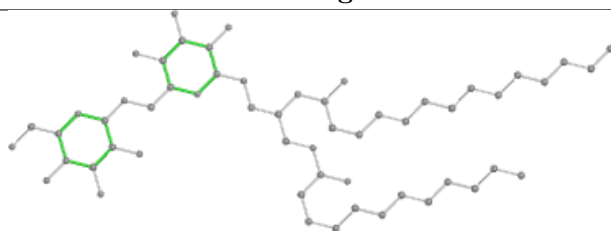
Ligand CLA I 206

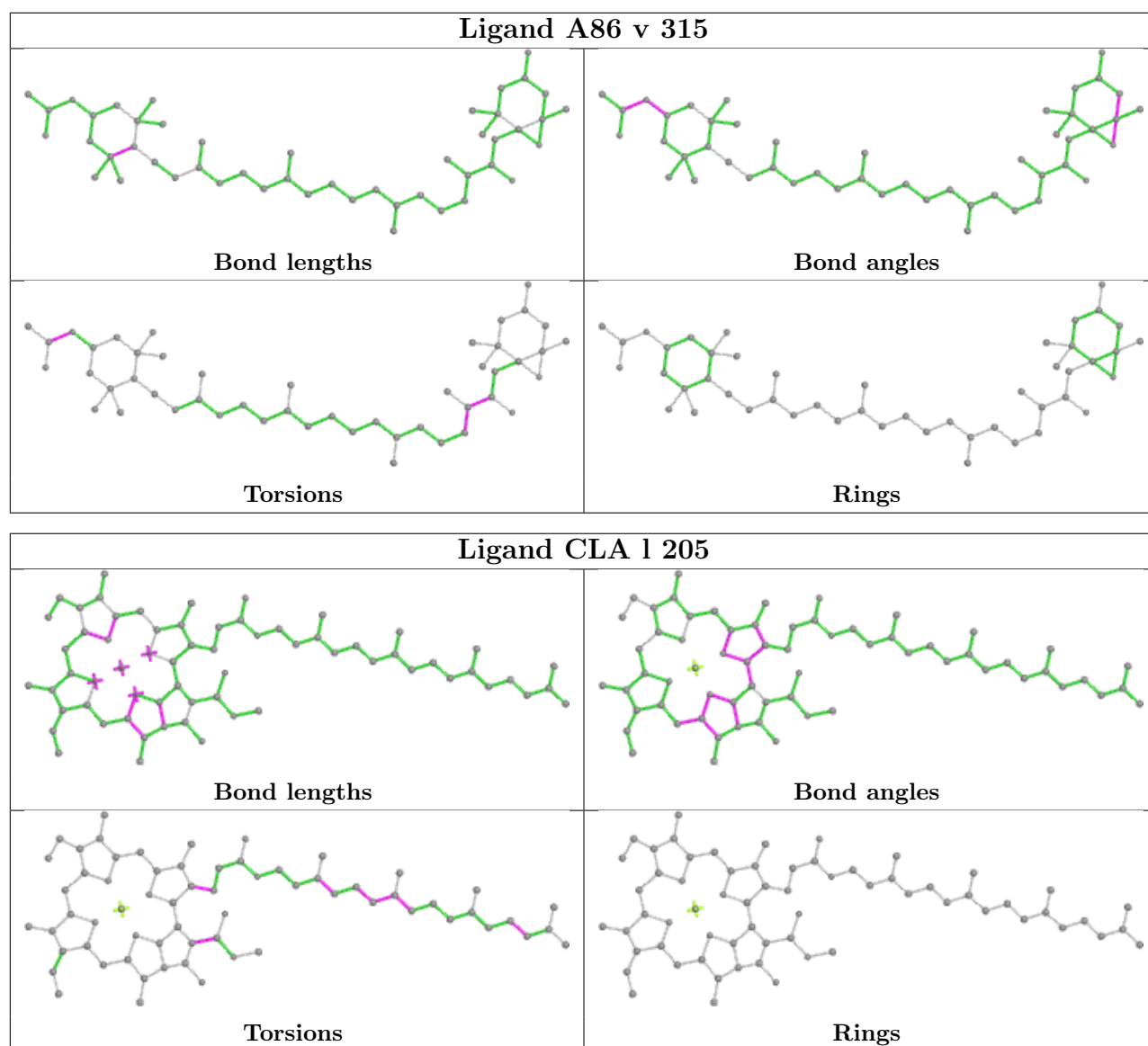


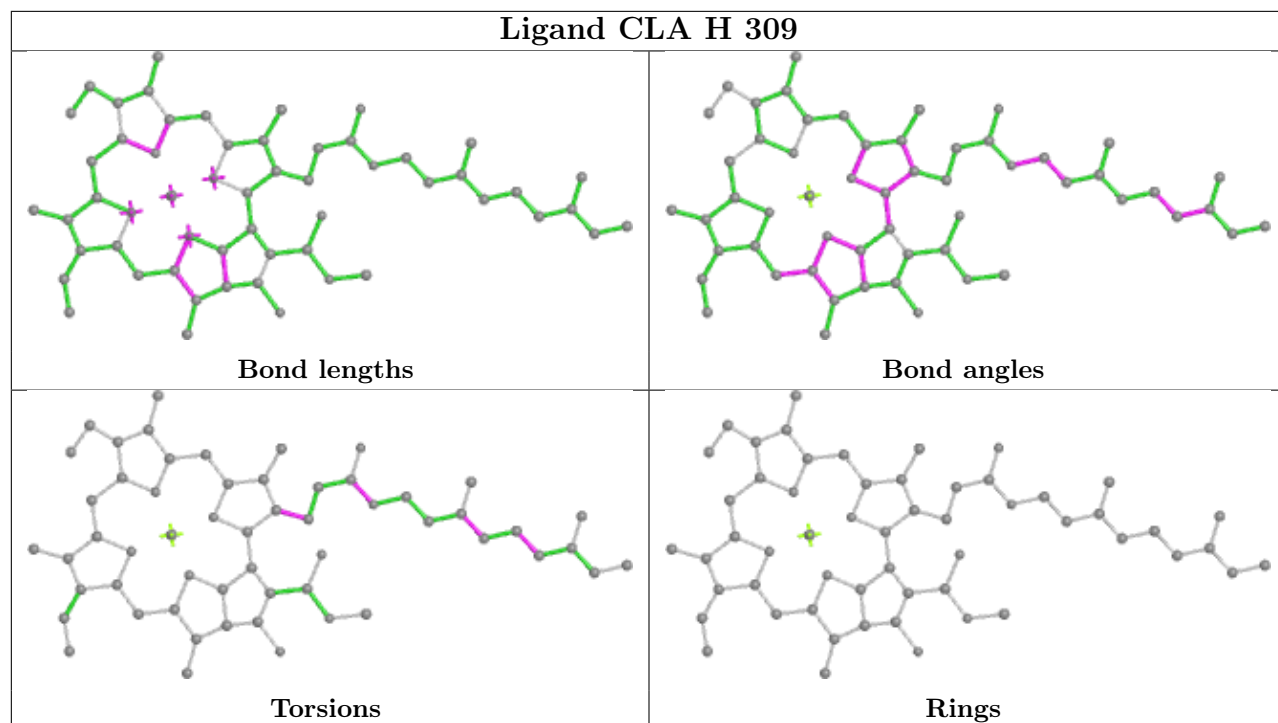
Ligand CLA p 314



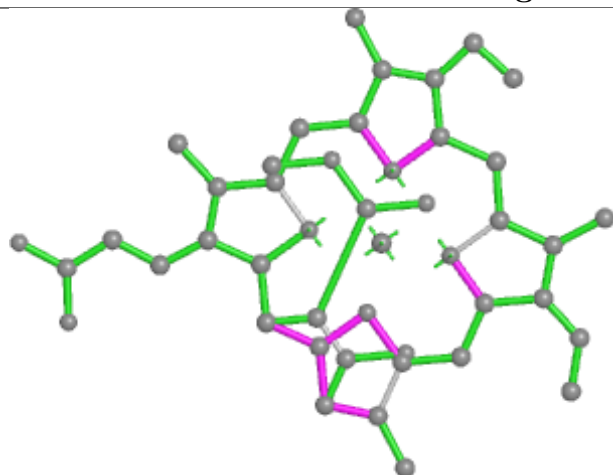


Ligand CLA o 301**Bond lengths****Bond angles****Torsions****Rings****Ligand DGD b 850****Bond lengths****Bond angles****Torsions****Rings**

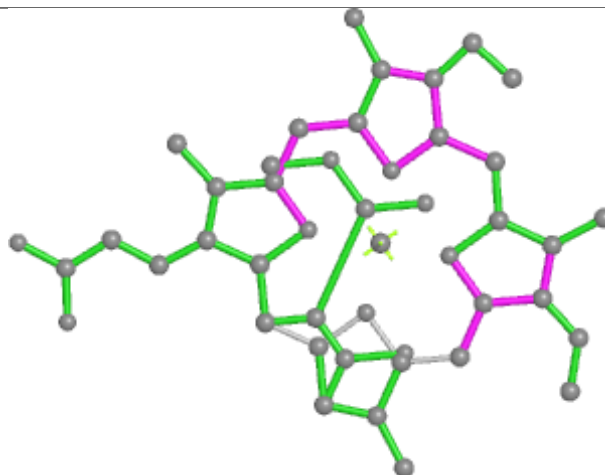




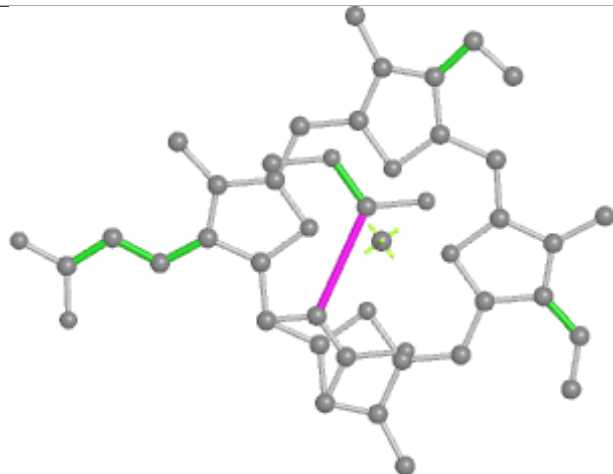
Ligand KC2 X 303



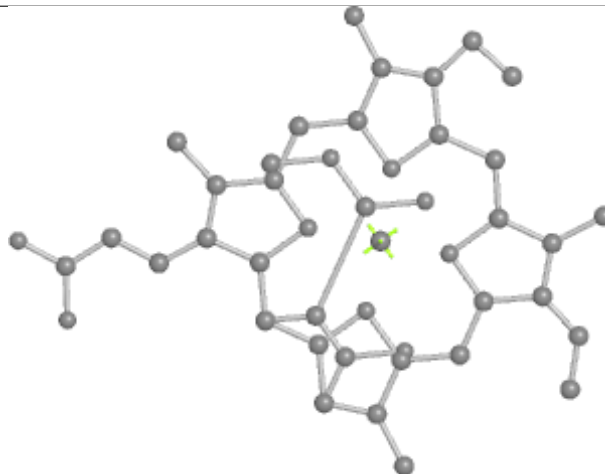
Bond lengths



Bond angles

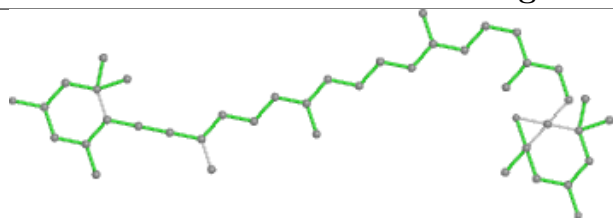


Torsions

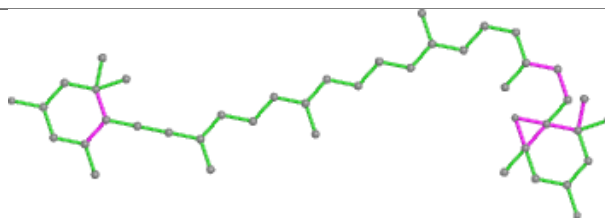


Rings

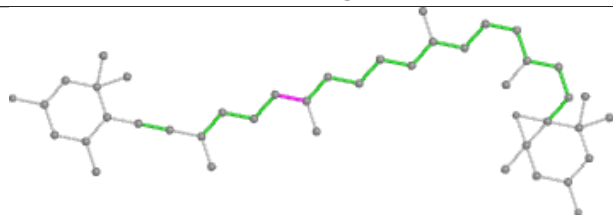
Ligand DD6 k 204



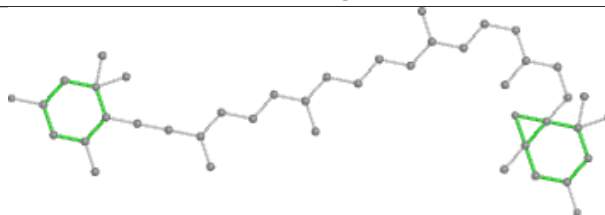
Bond lengths



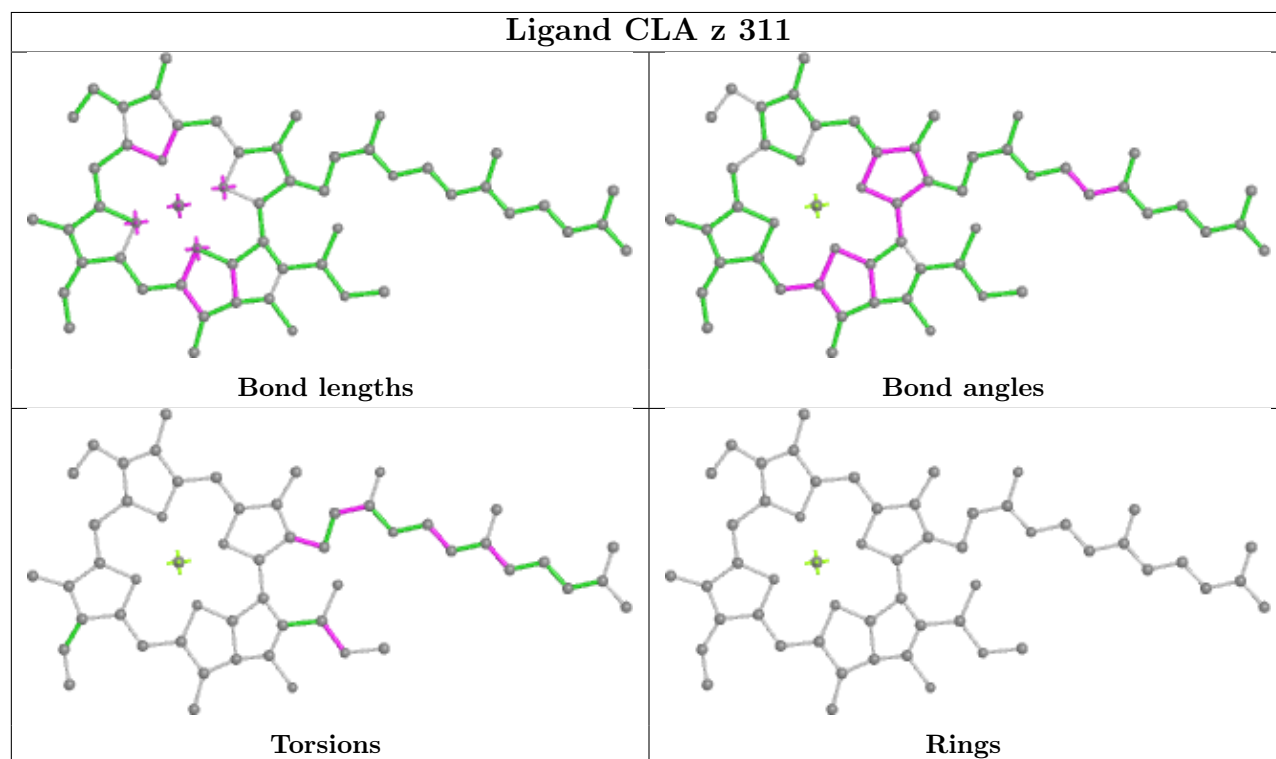
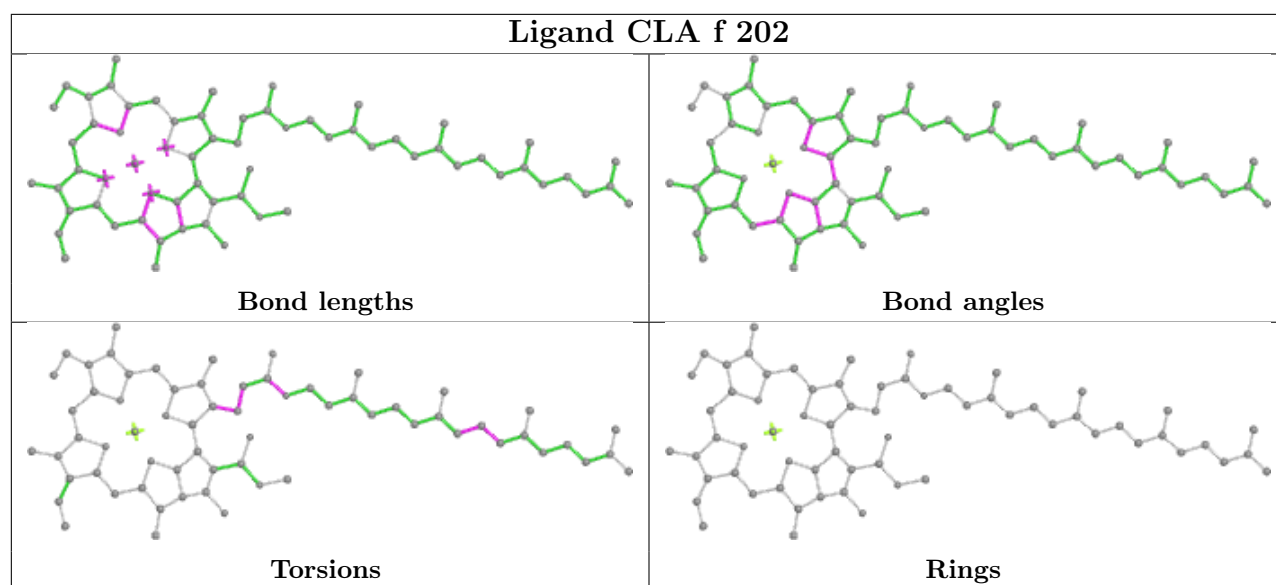
Bond angles



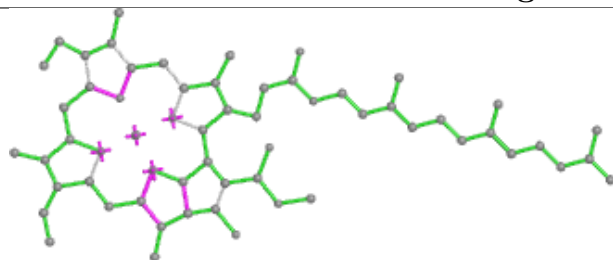
Torsions



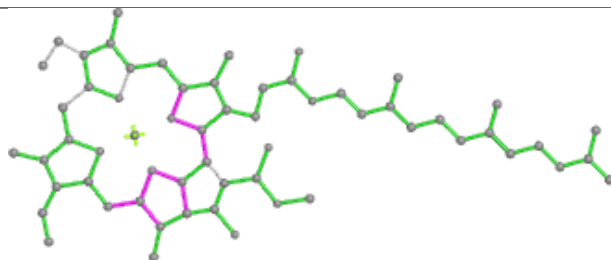
Rings



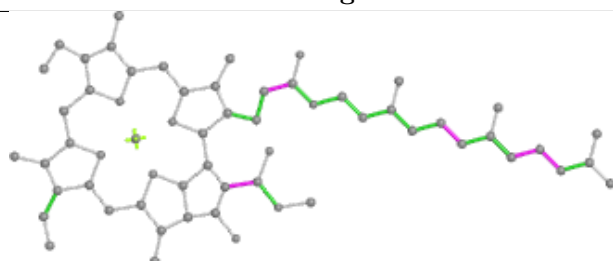
Ligand CLA u 308



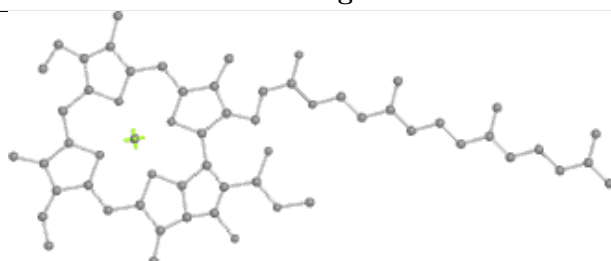
Bond lengths



Bond angles

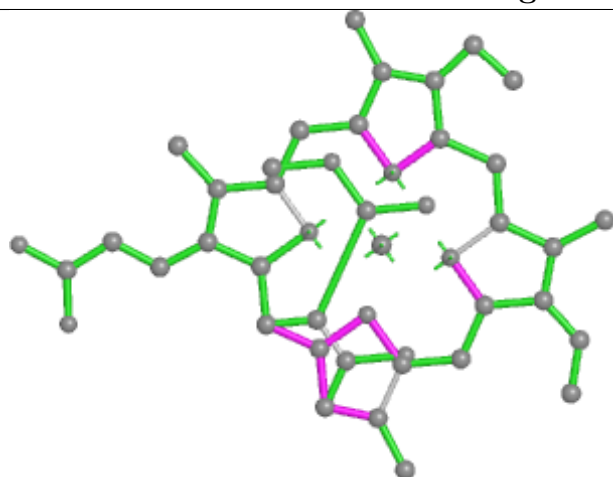


Torsions

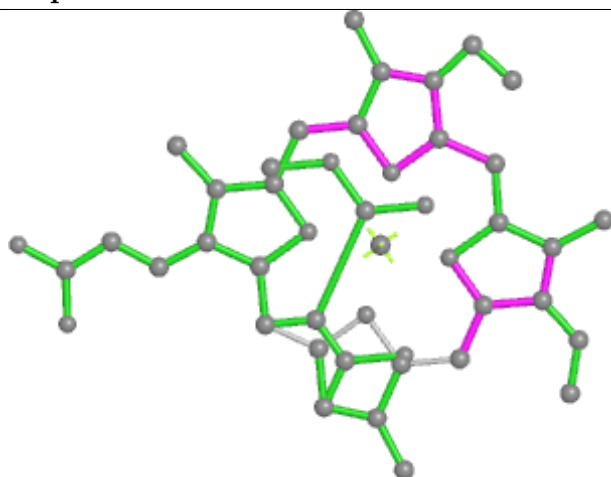


Rings

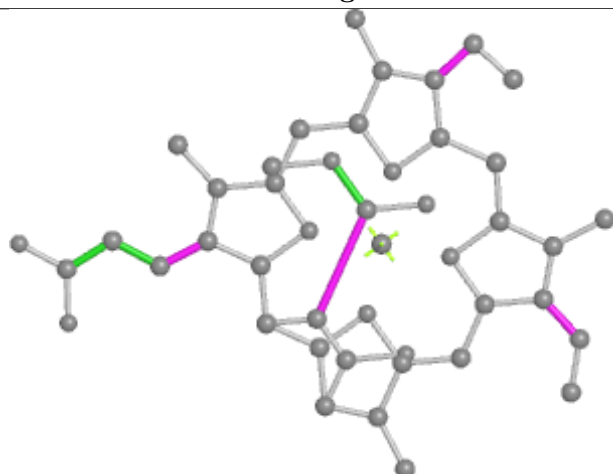
Ligand KC2 p 310



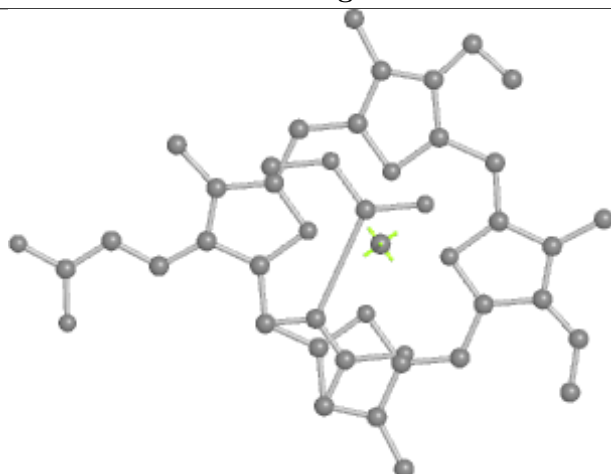
Bond lengths



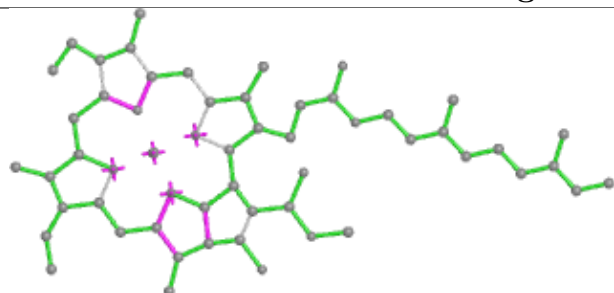
Bond angles



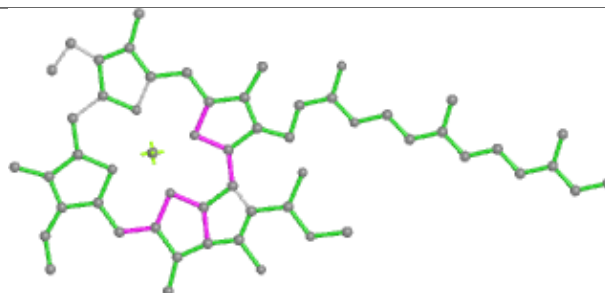
Torsions



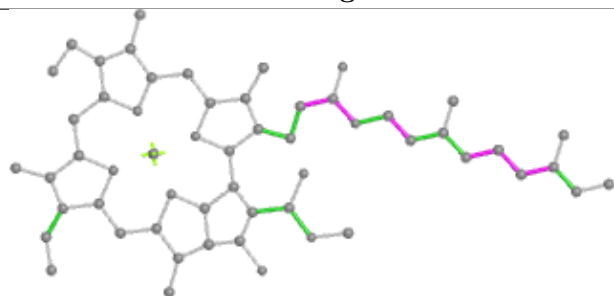
Rings

Ligand CLA S 306

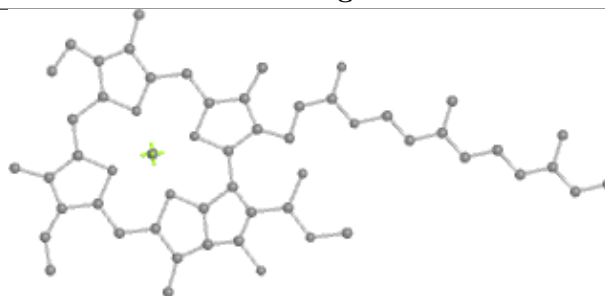
Bond lengths



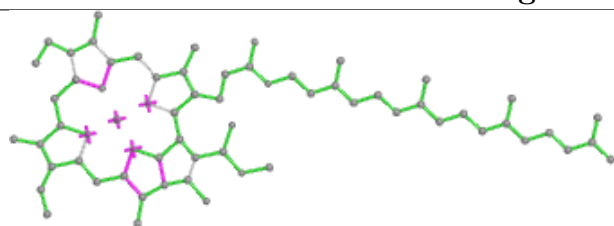
Bond angles



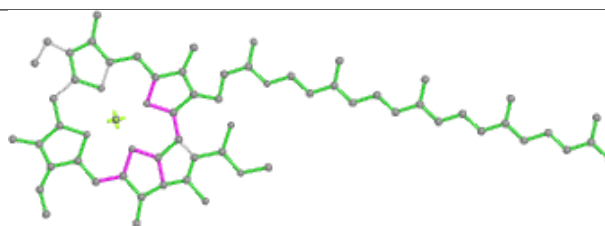
Torsions



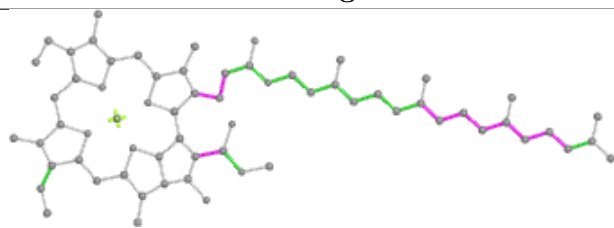
Rings

Ligand CLA a 828

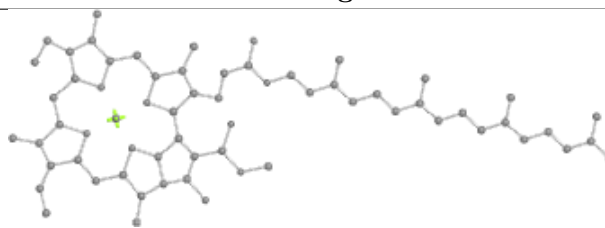
Bond lengths



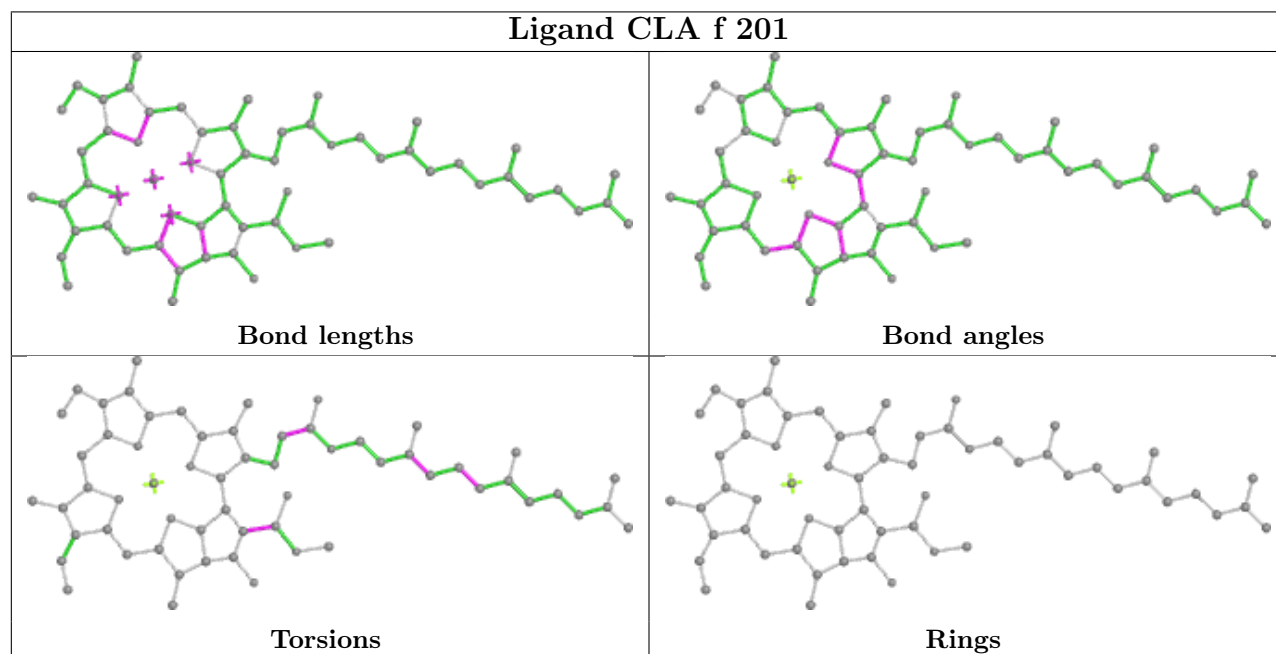
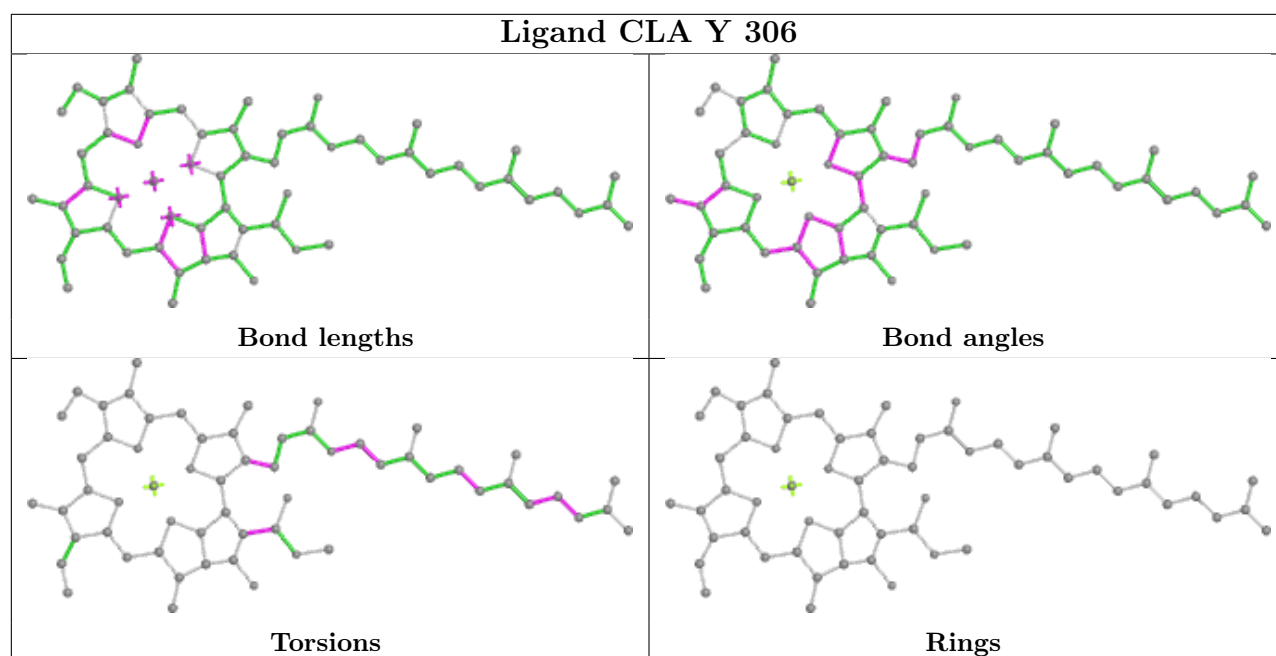
Bond angles

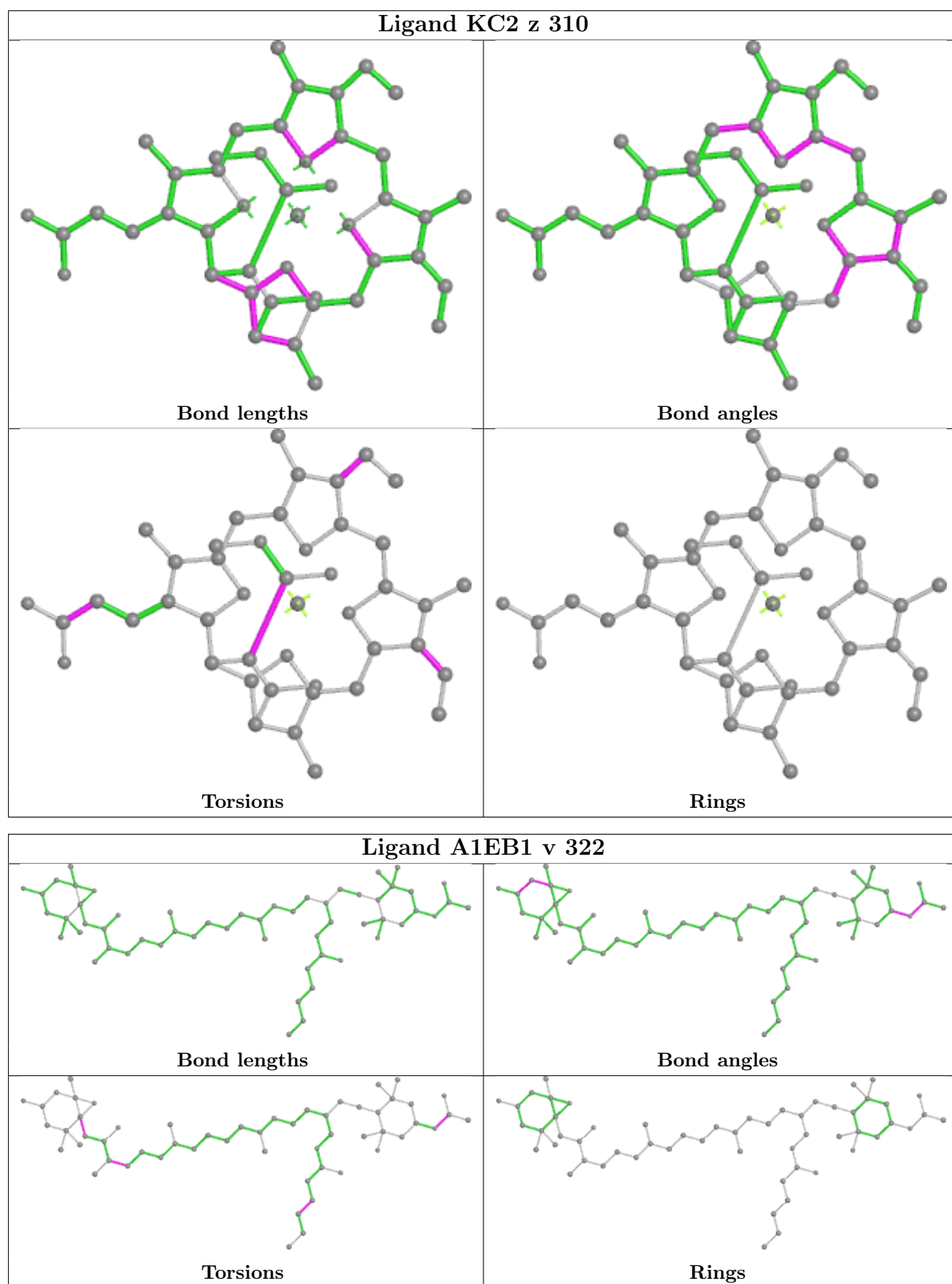


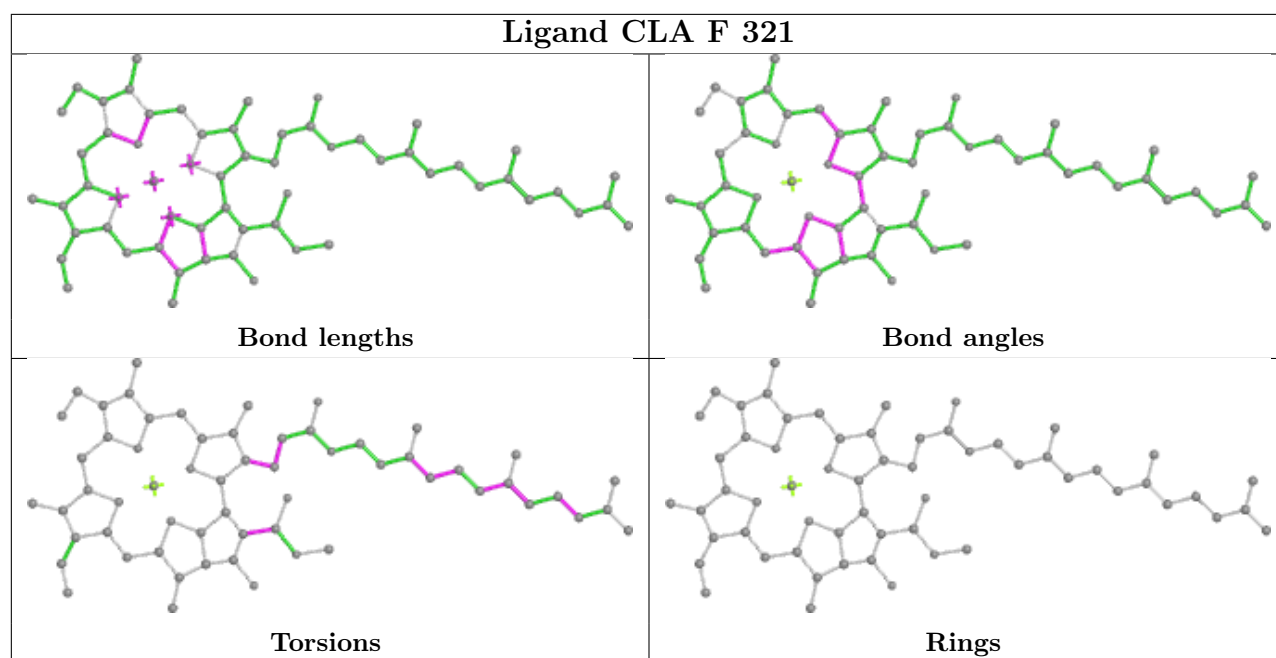
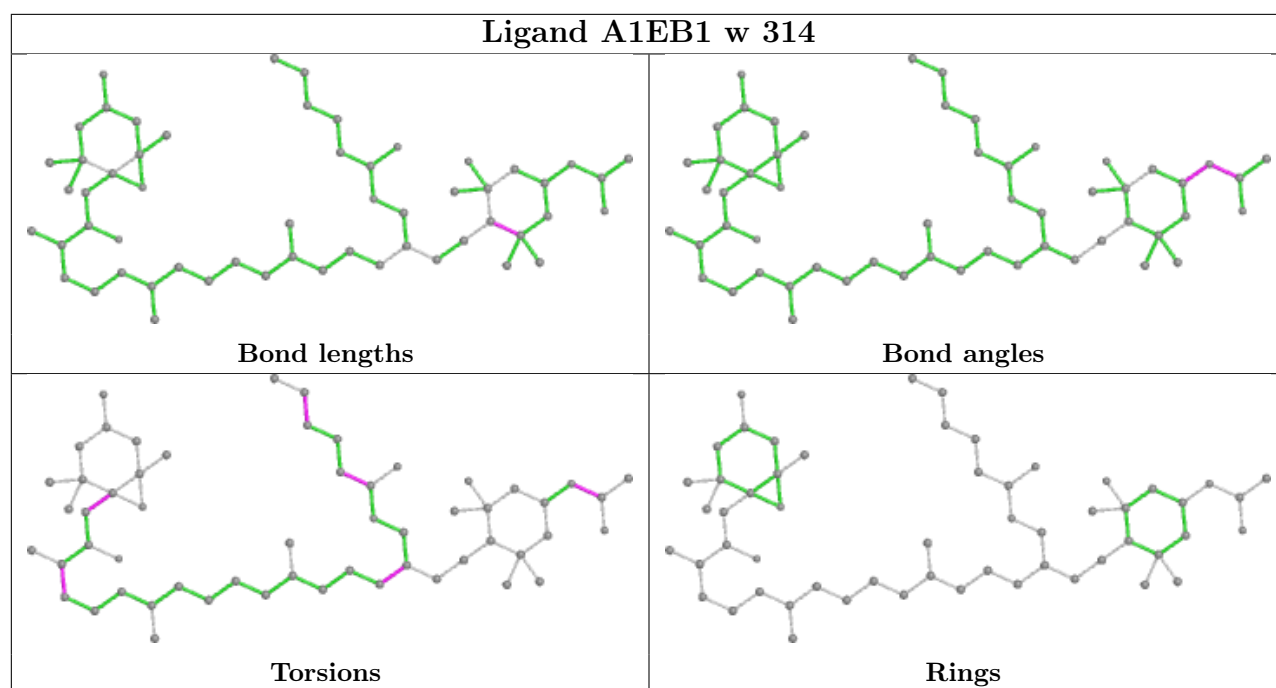
Torsions

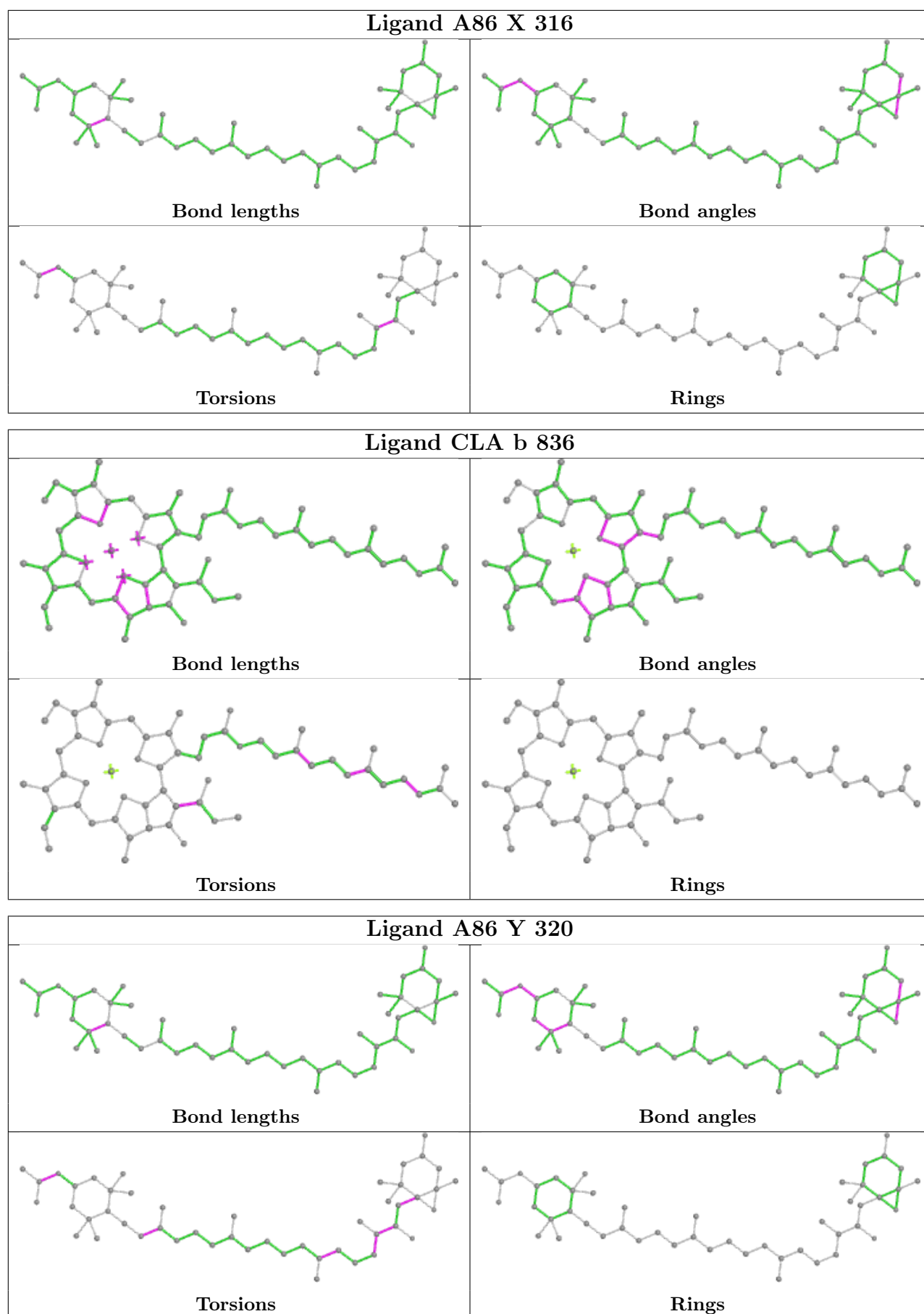


Rings

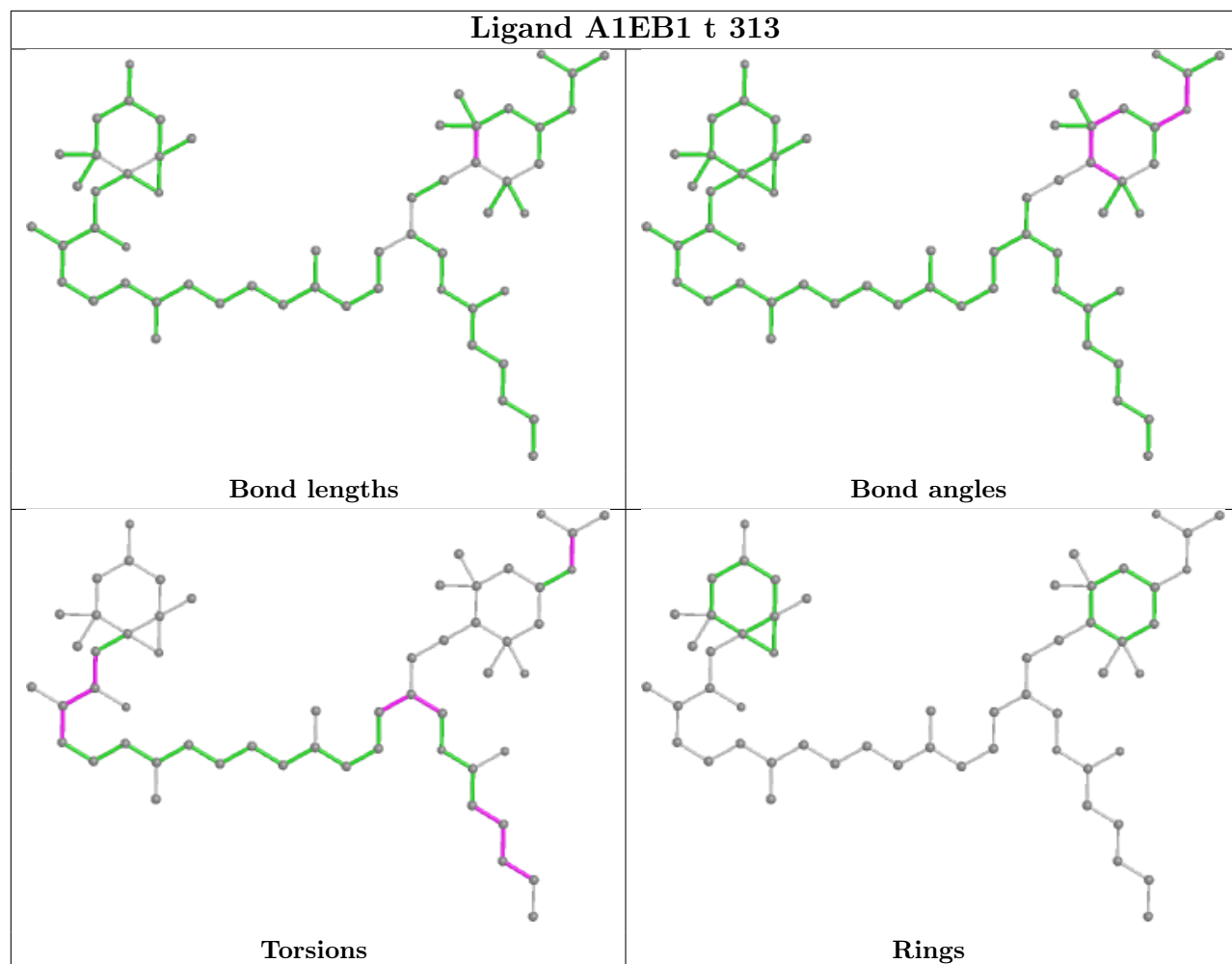




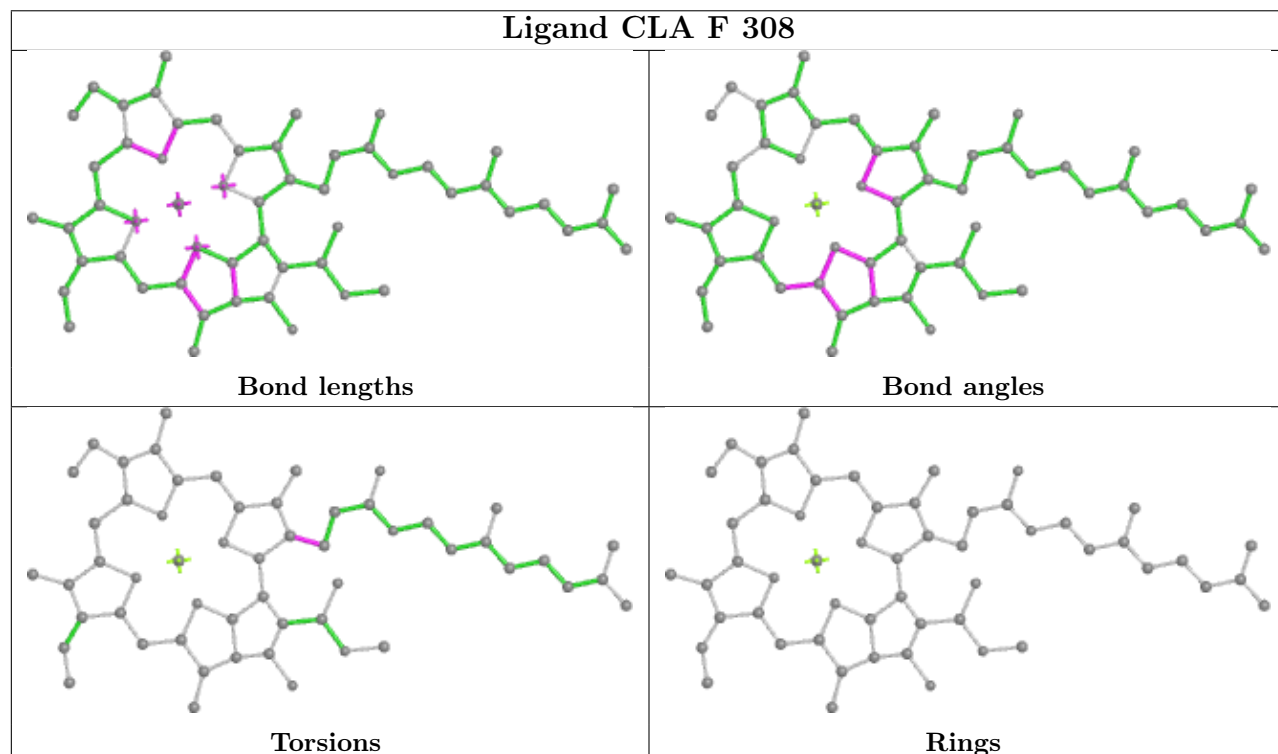


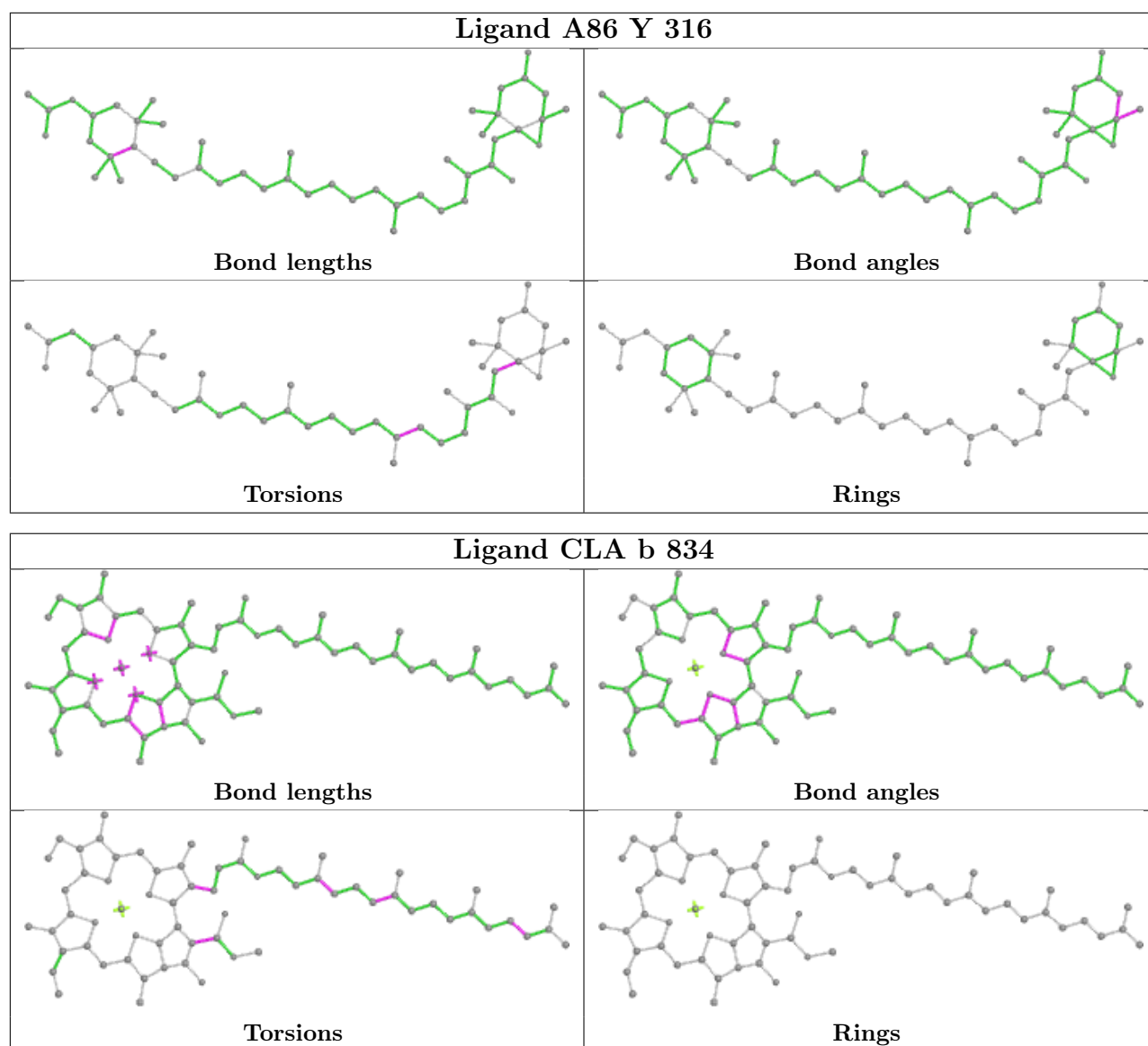


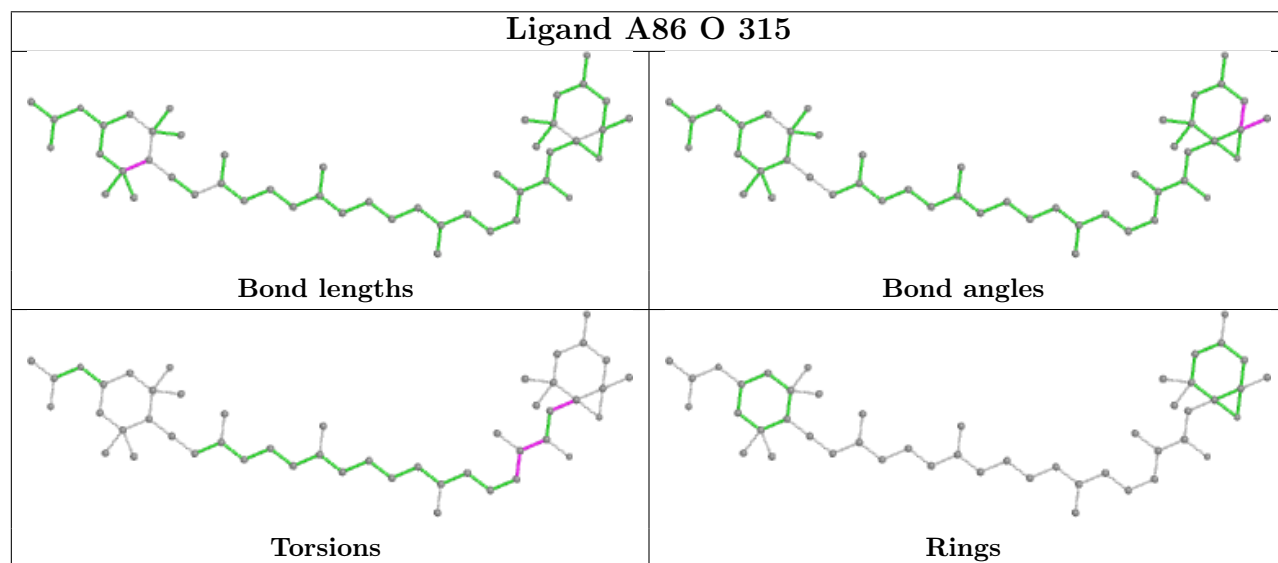
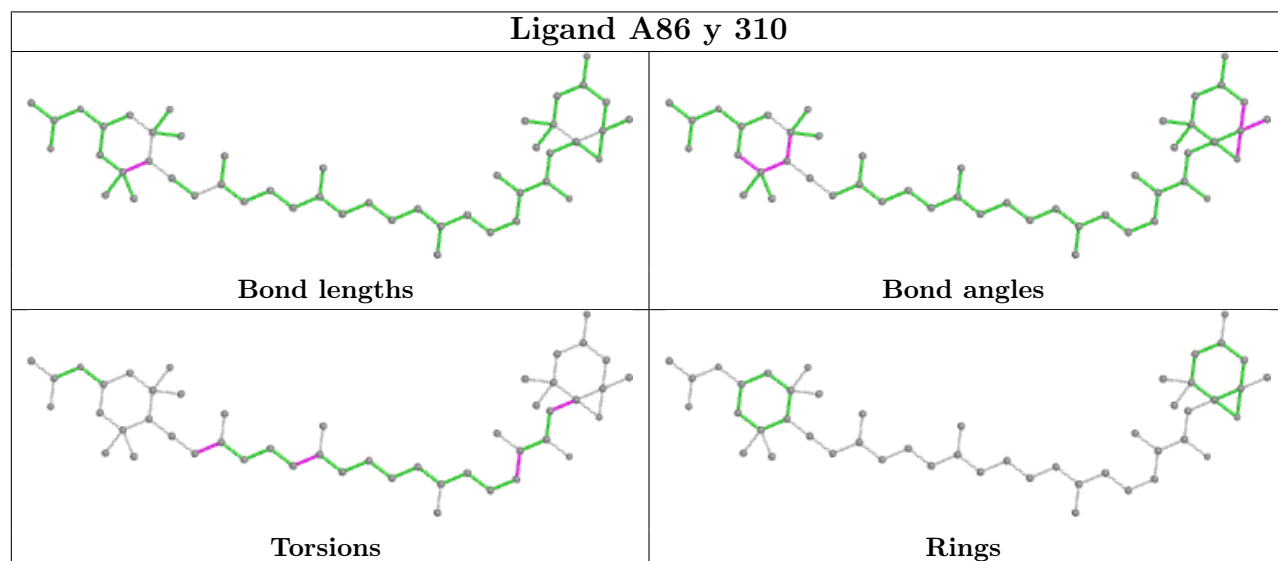
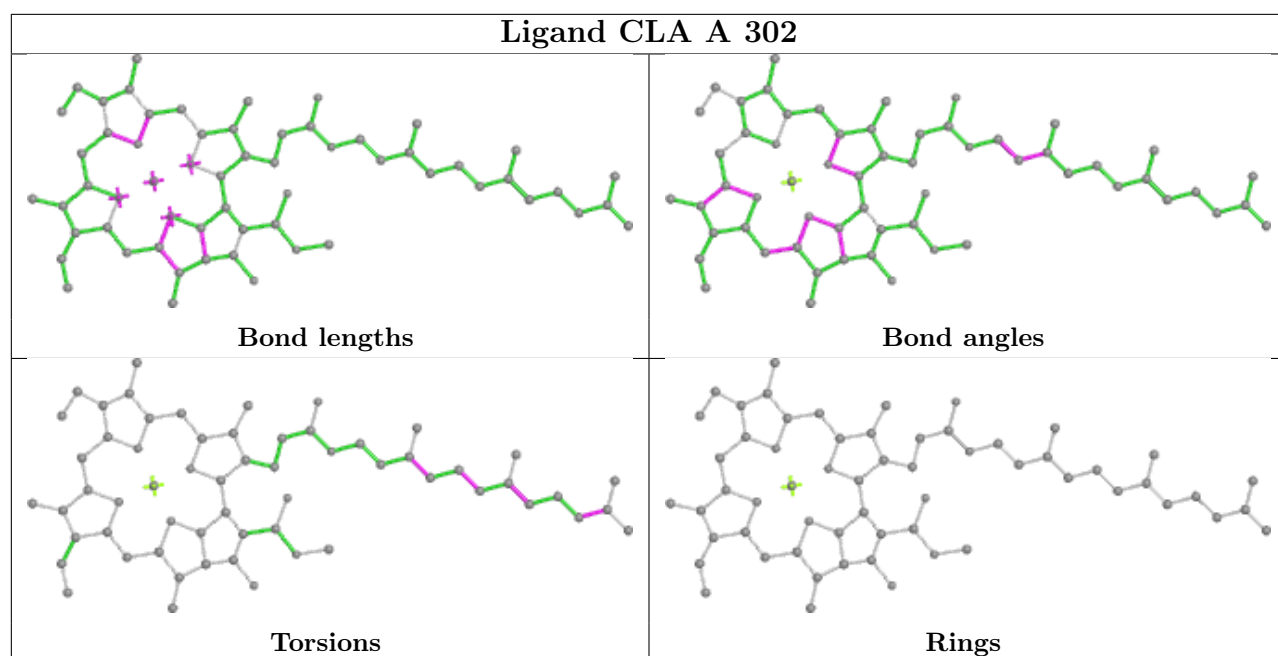
Ligand A1EB1 t 313

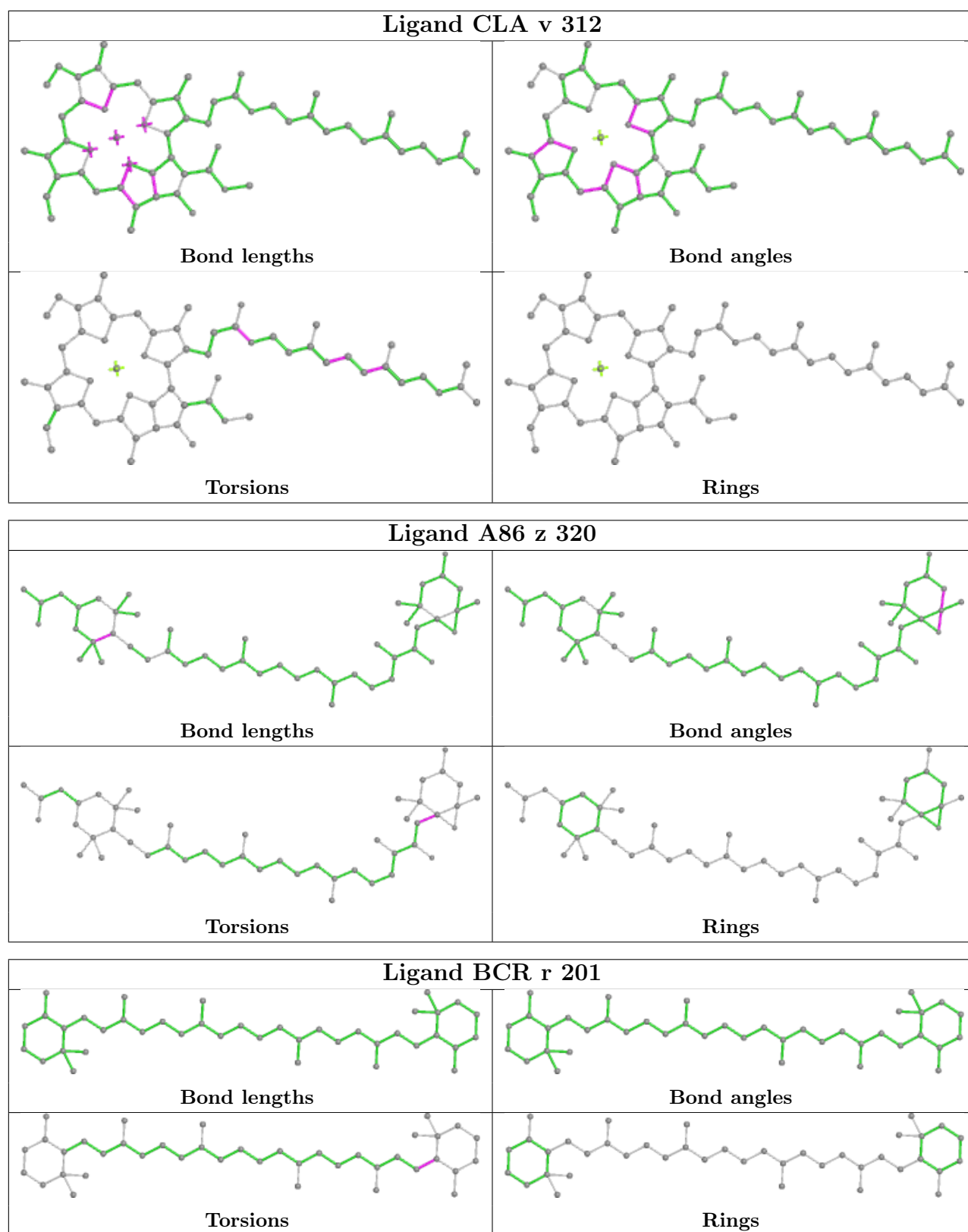


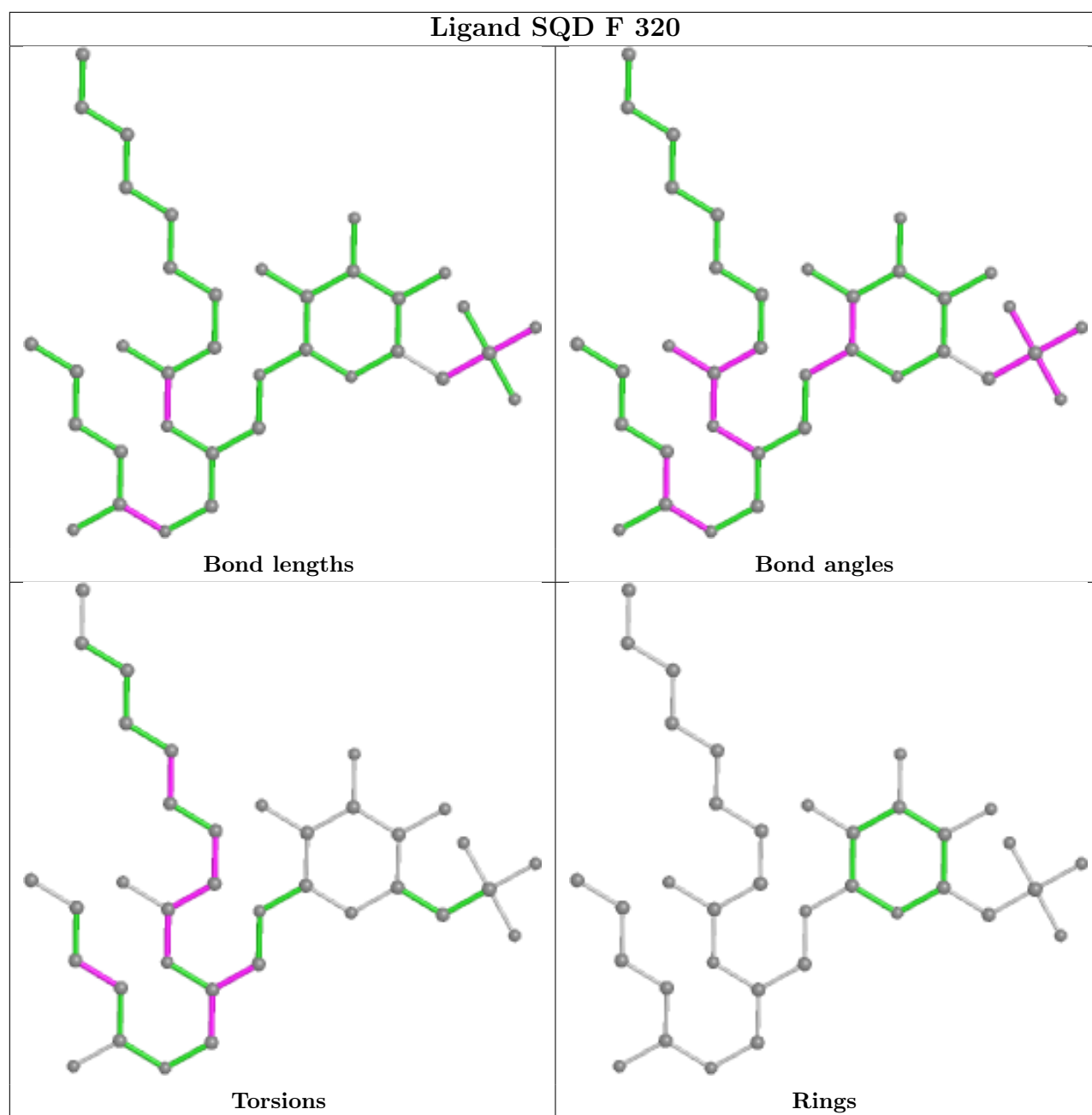
Ligand CLA F 308

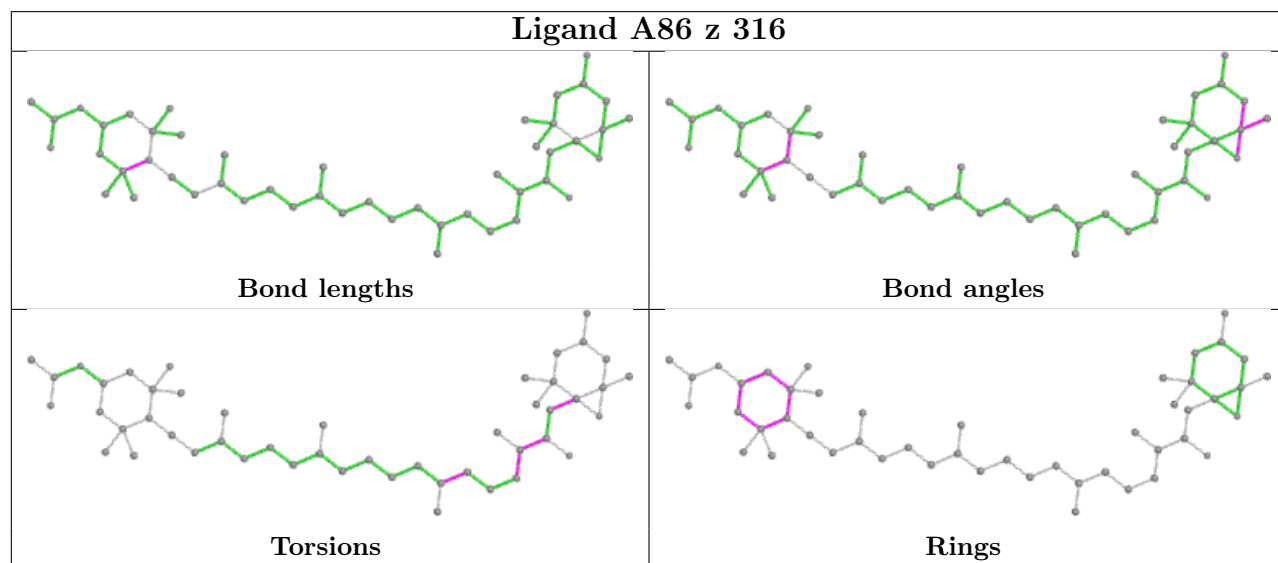
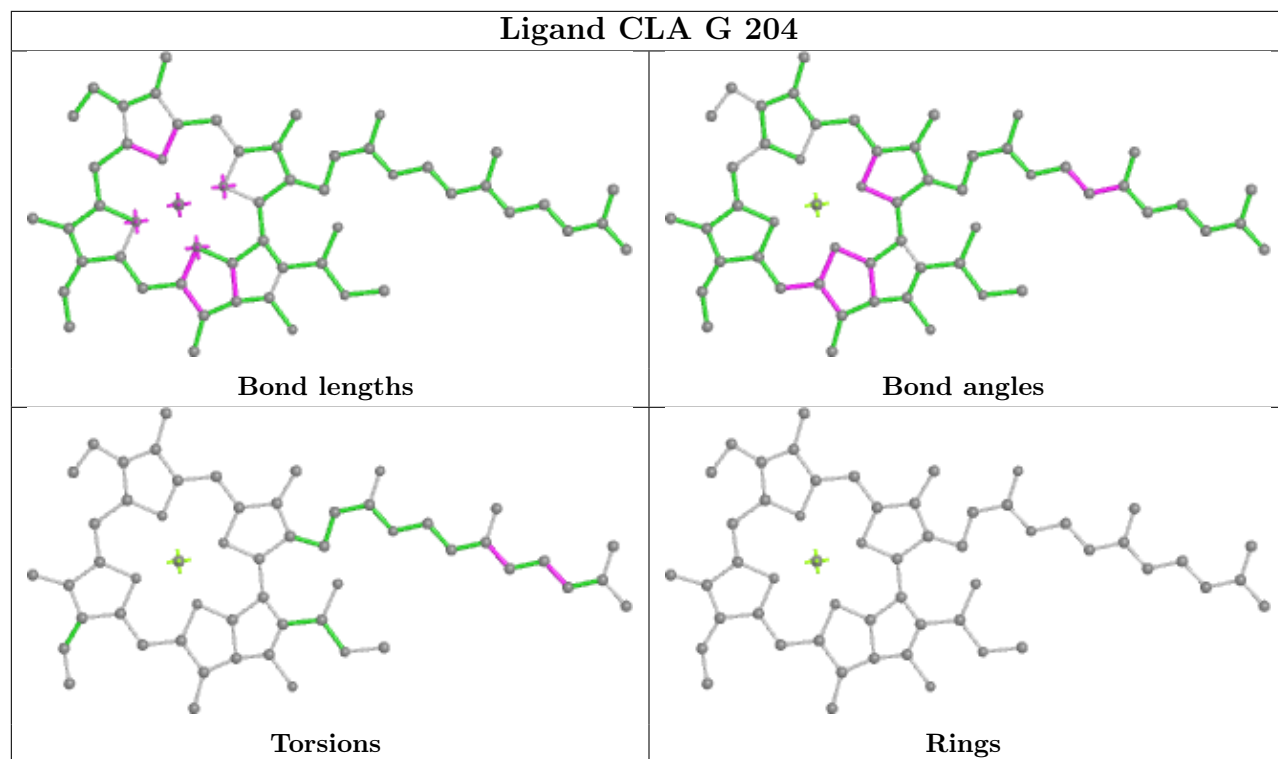


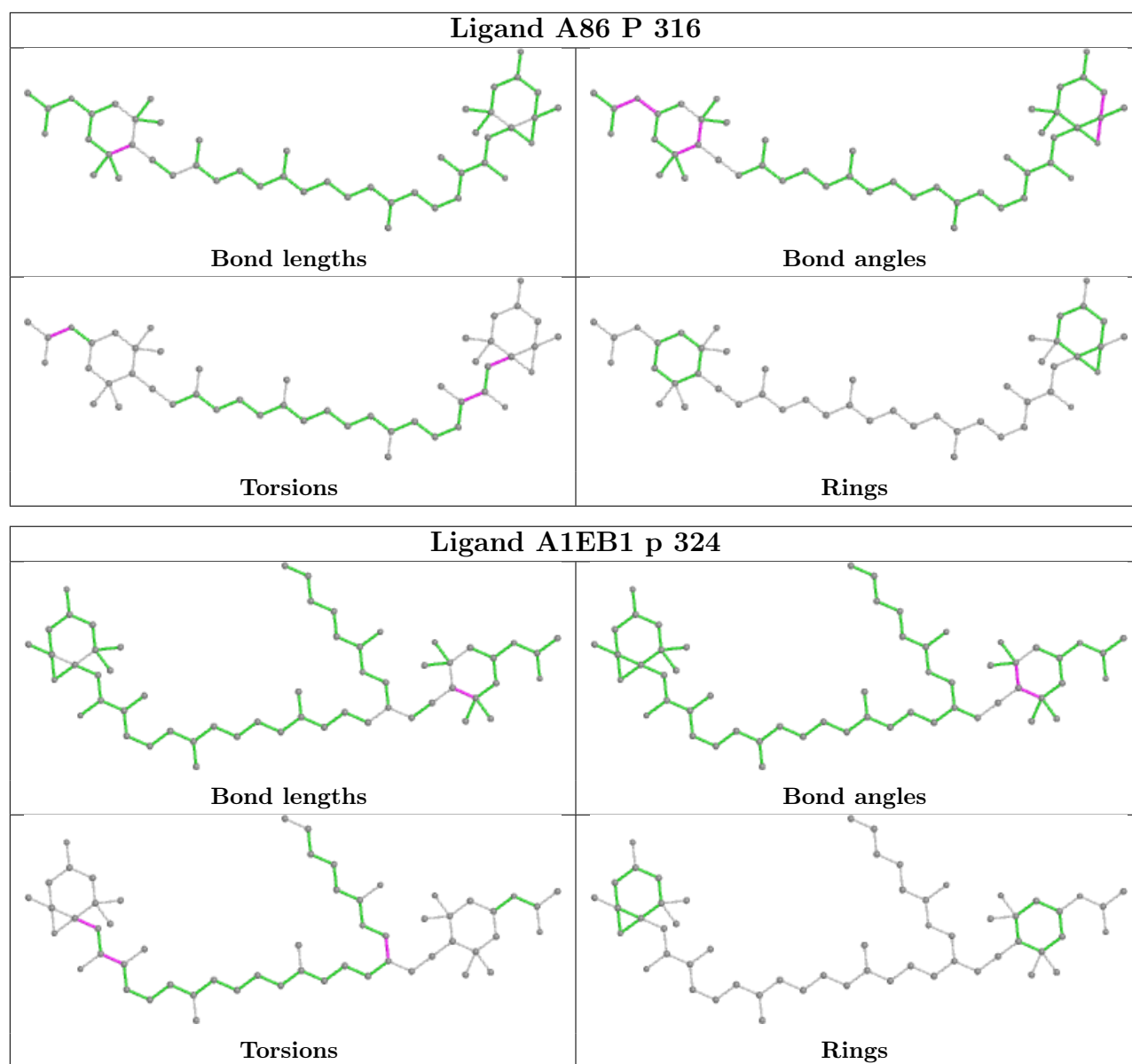




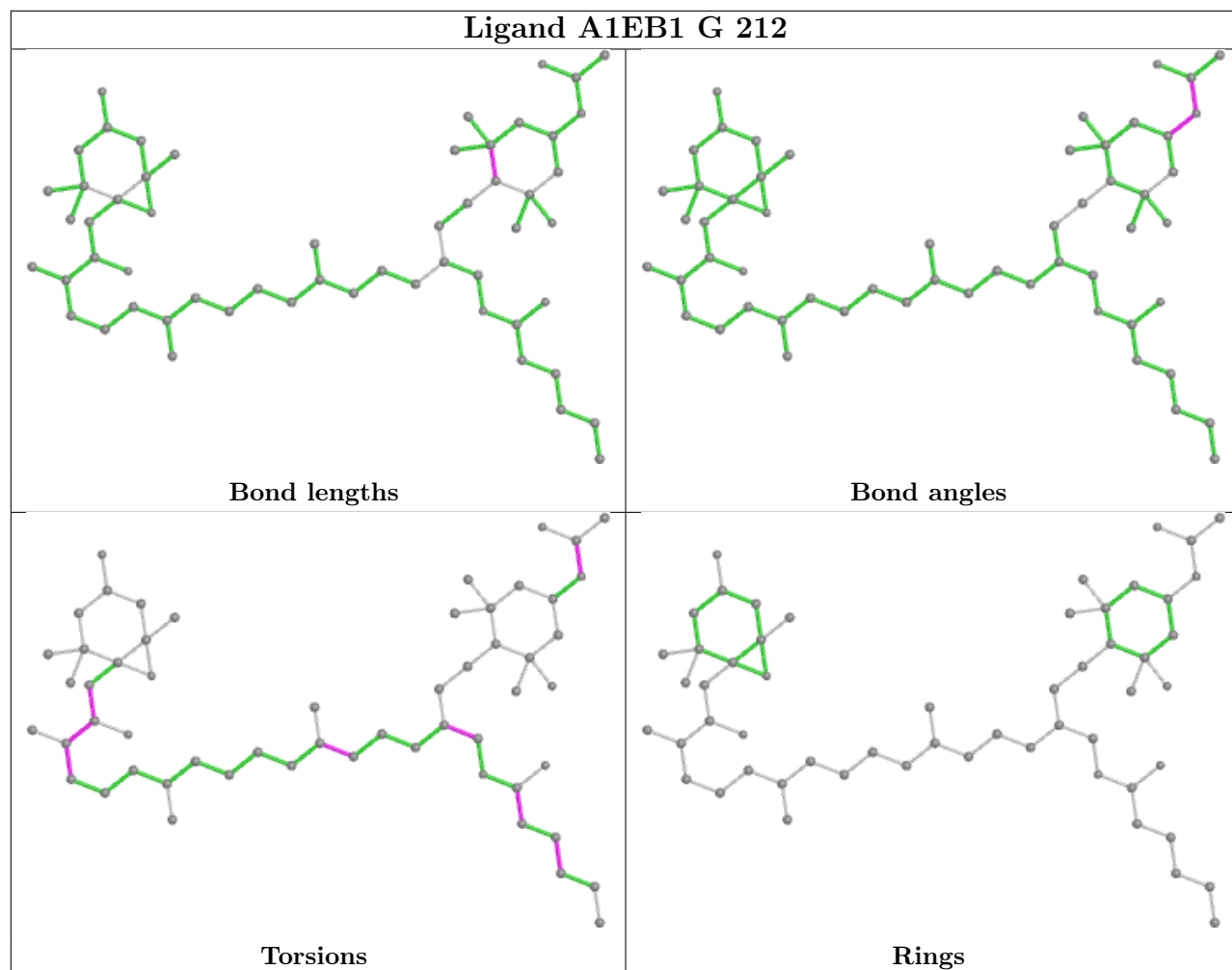




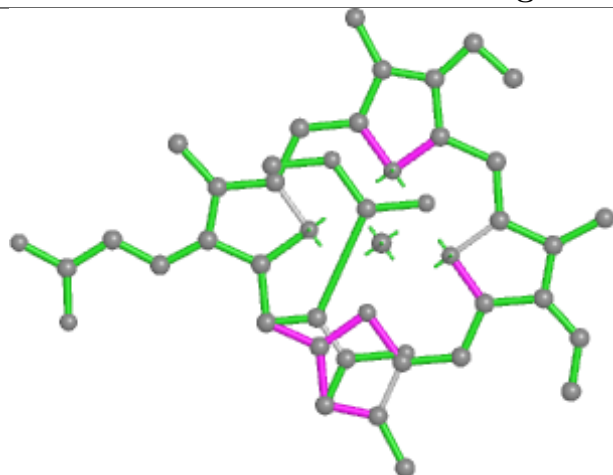




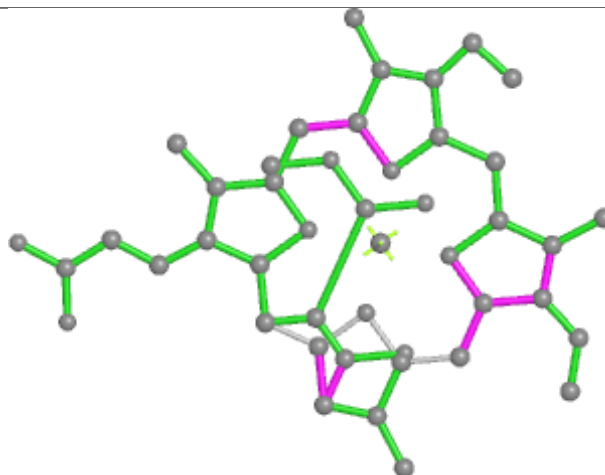
Ligand A1EB1 G 212



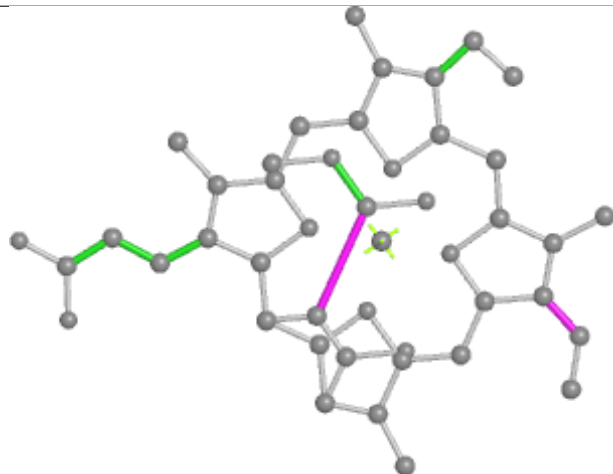
Ligand KC2 P 303



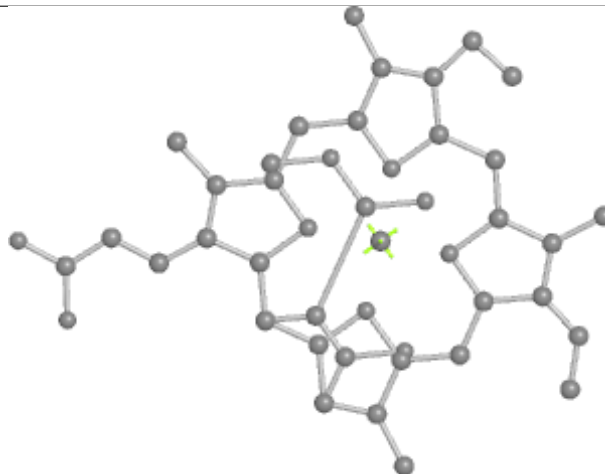
Bond lengths



Bond angles

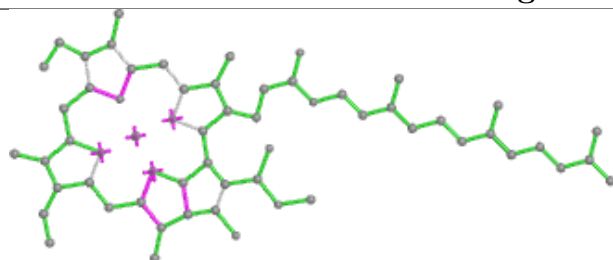


Torsions

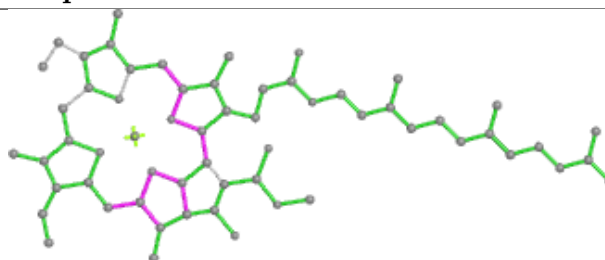


Rings

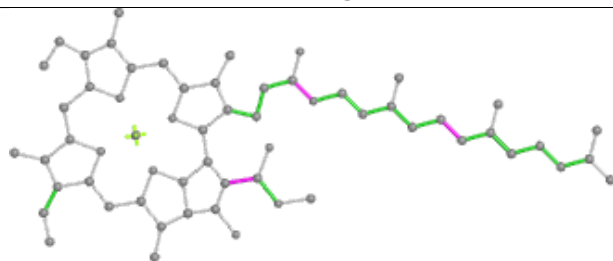
Ligand CLA q 305



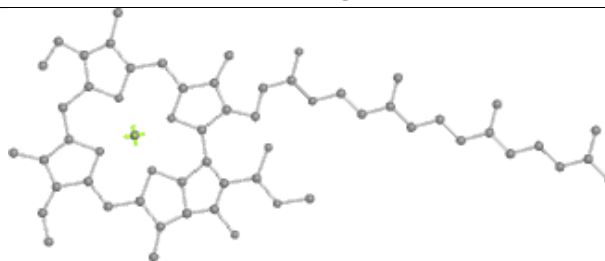
Bond lengths



Bond angles

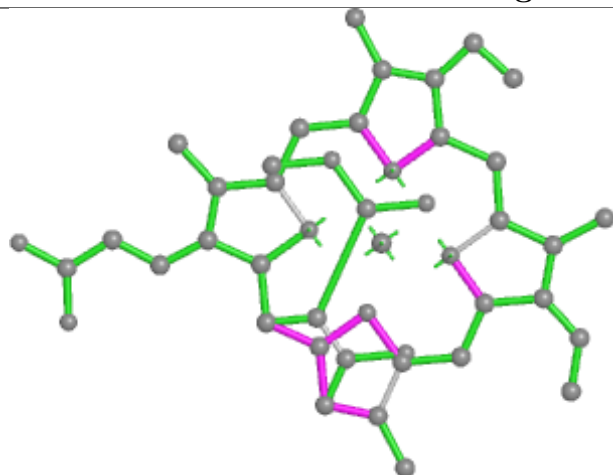


Torsions

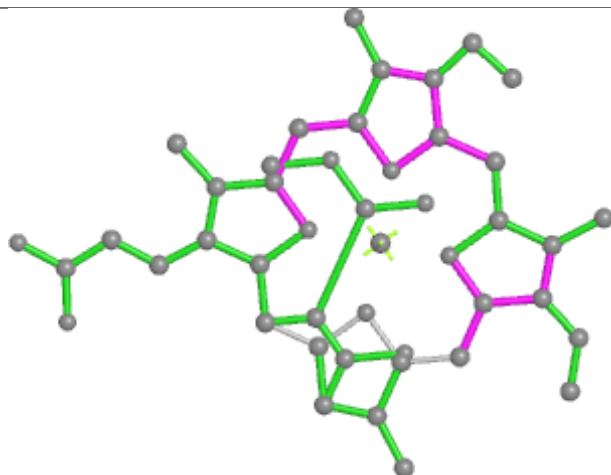


Rings

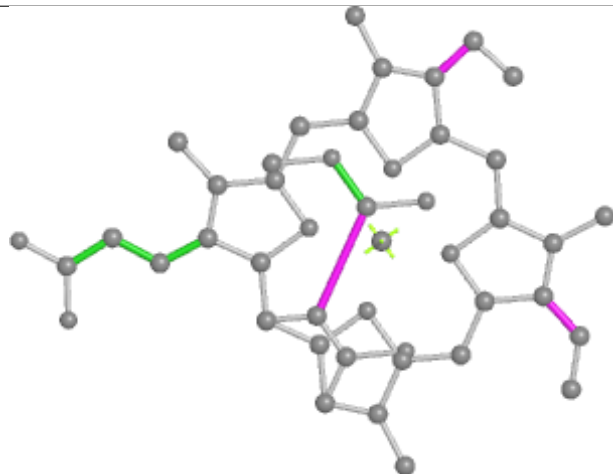
Ligand KC2 N 309



Bond lengths



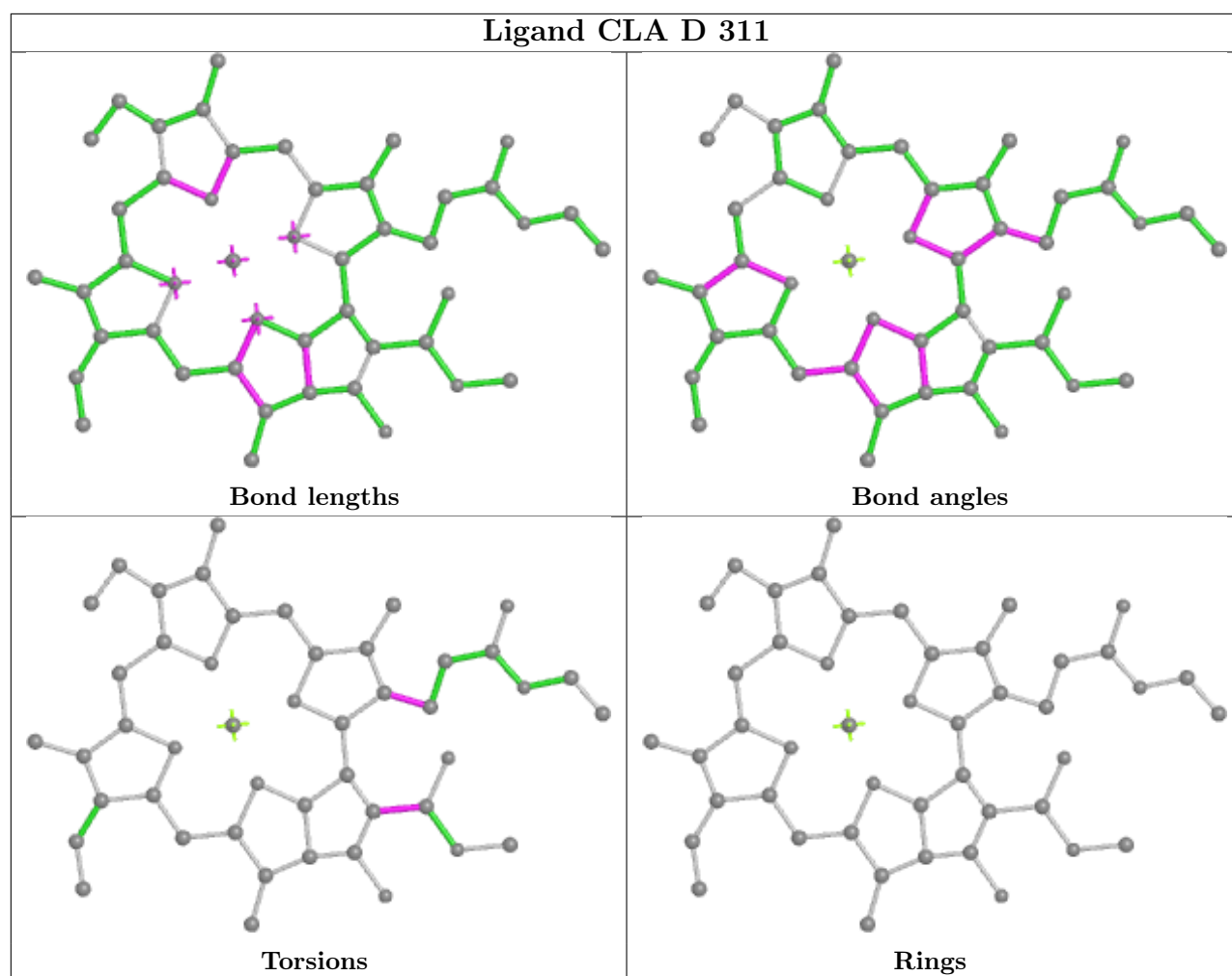
Bond angles



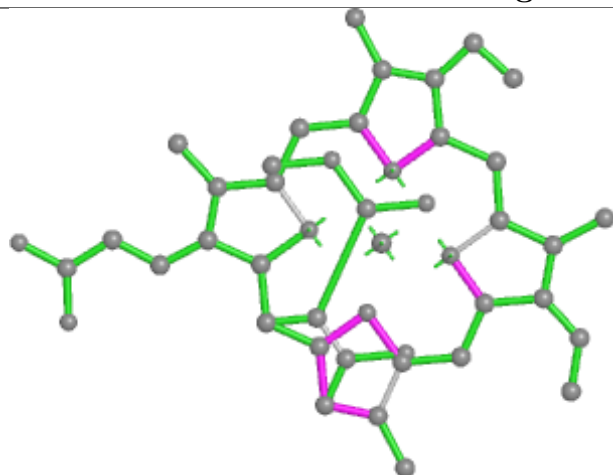
Torsions



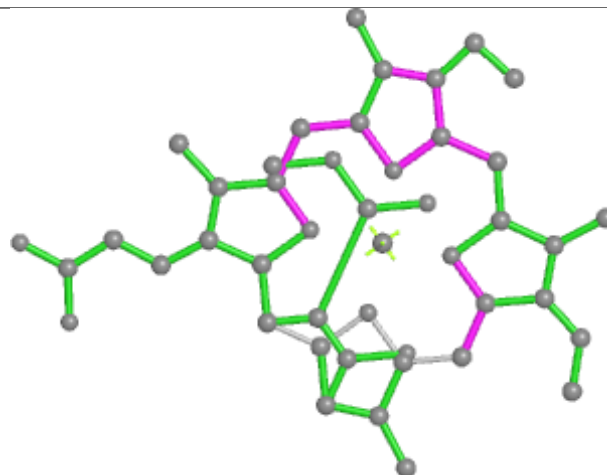
Rings



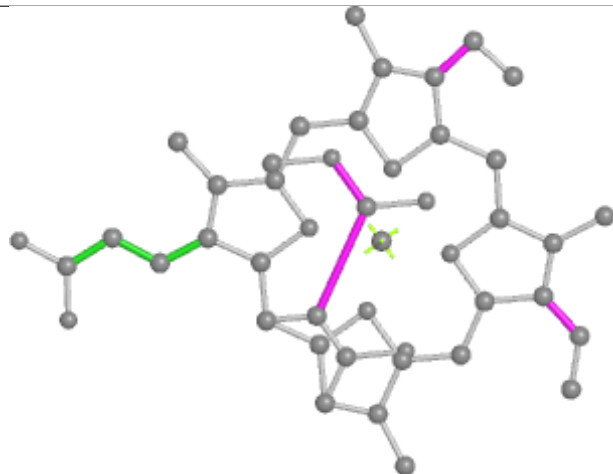
Ligand KC2 O 301



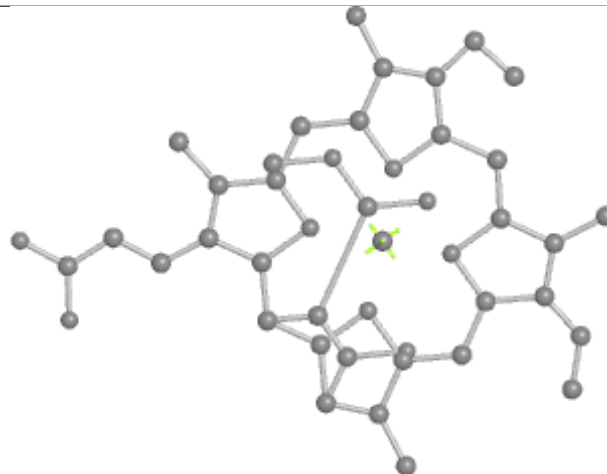
Bond lengths



Bond angles

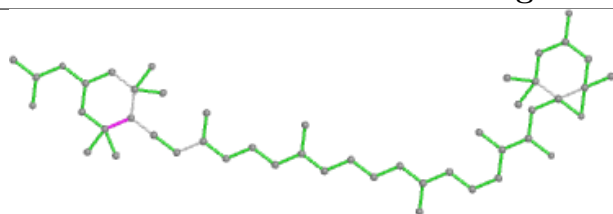


Torsions

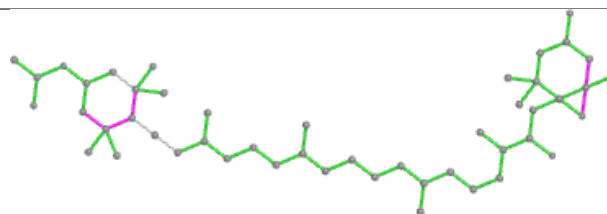


Rings

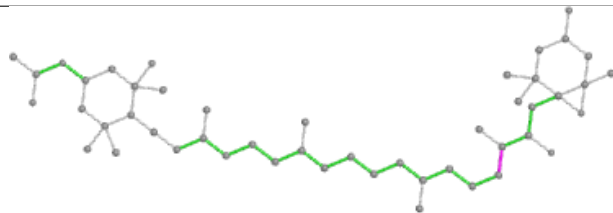
Ligand A86 M 316



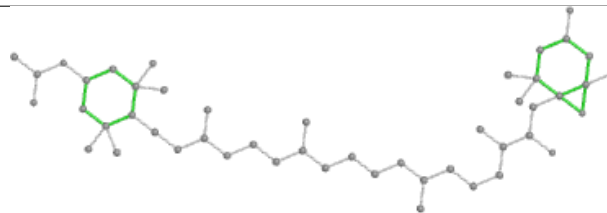
Bond lengths



Bond angles

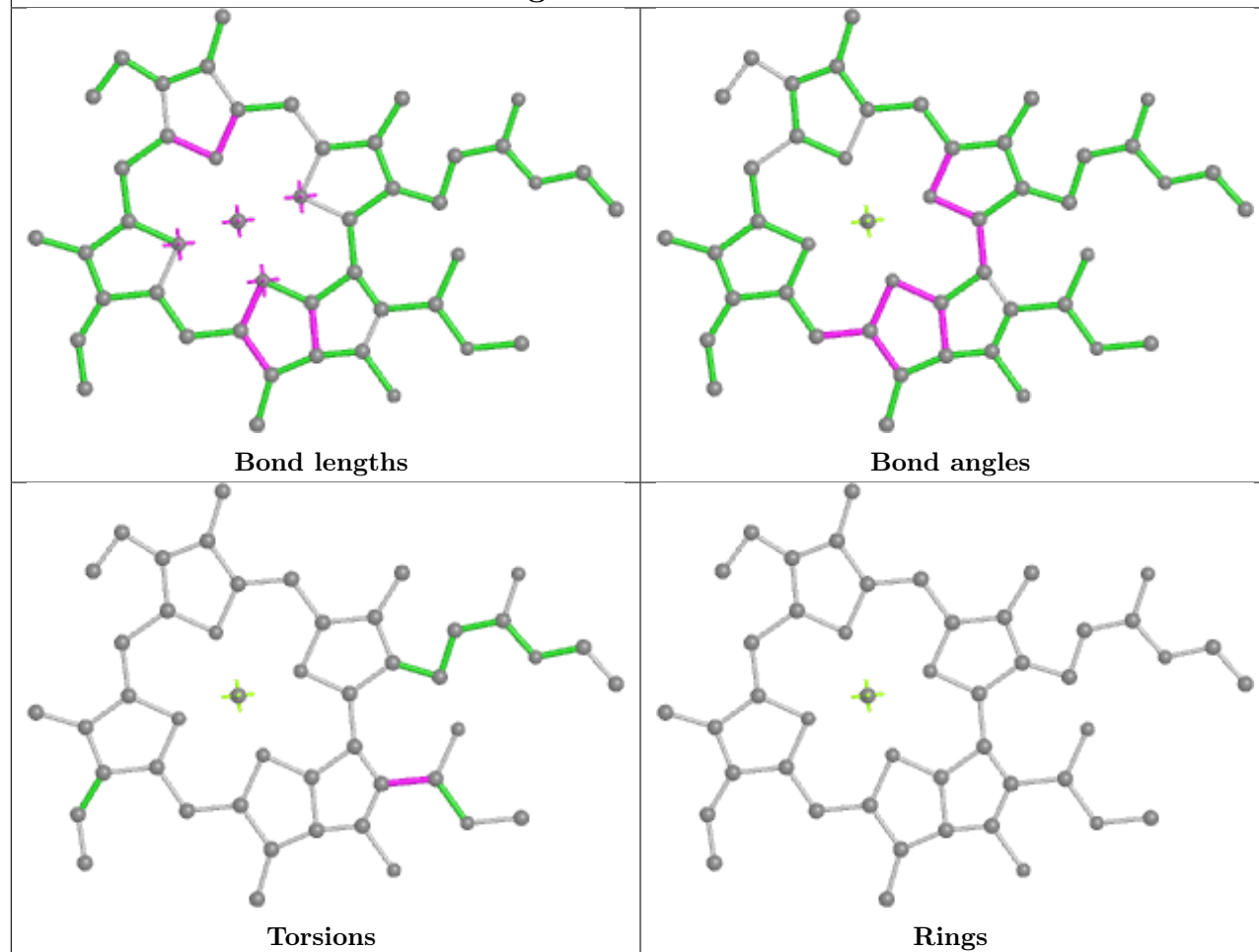


Torsions

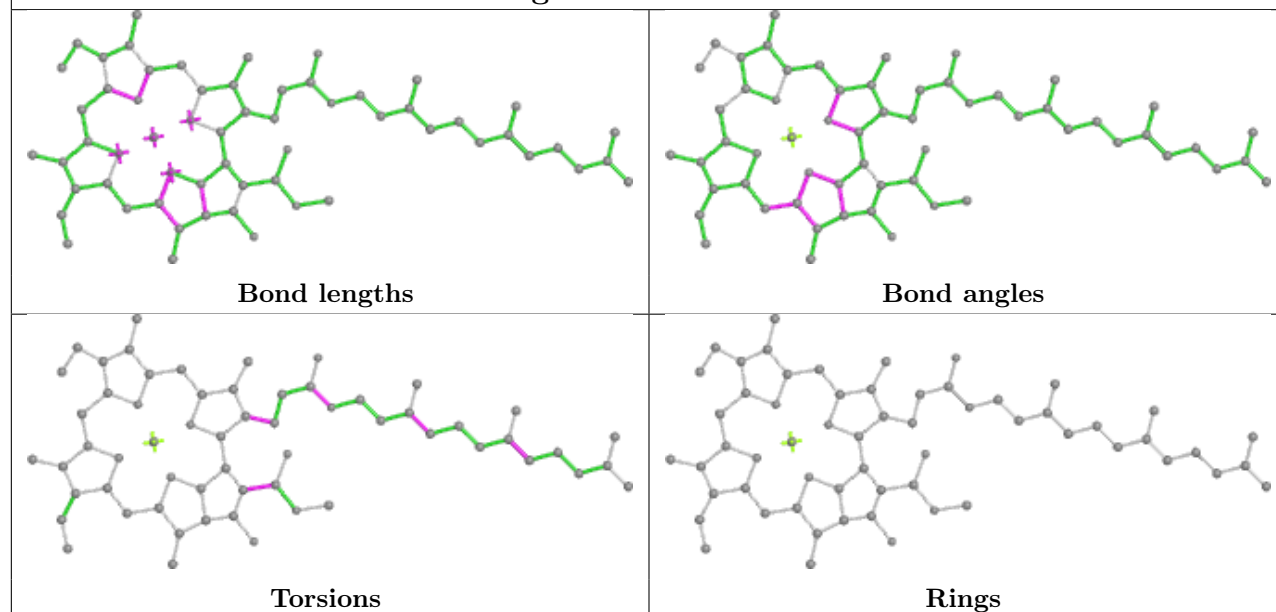


Rings

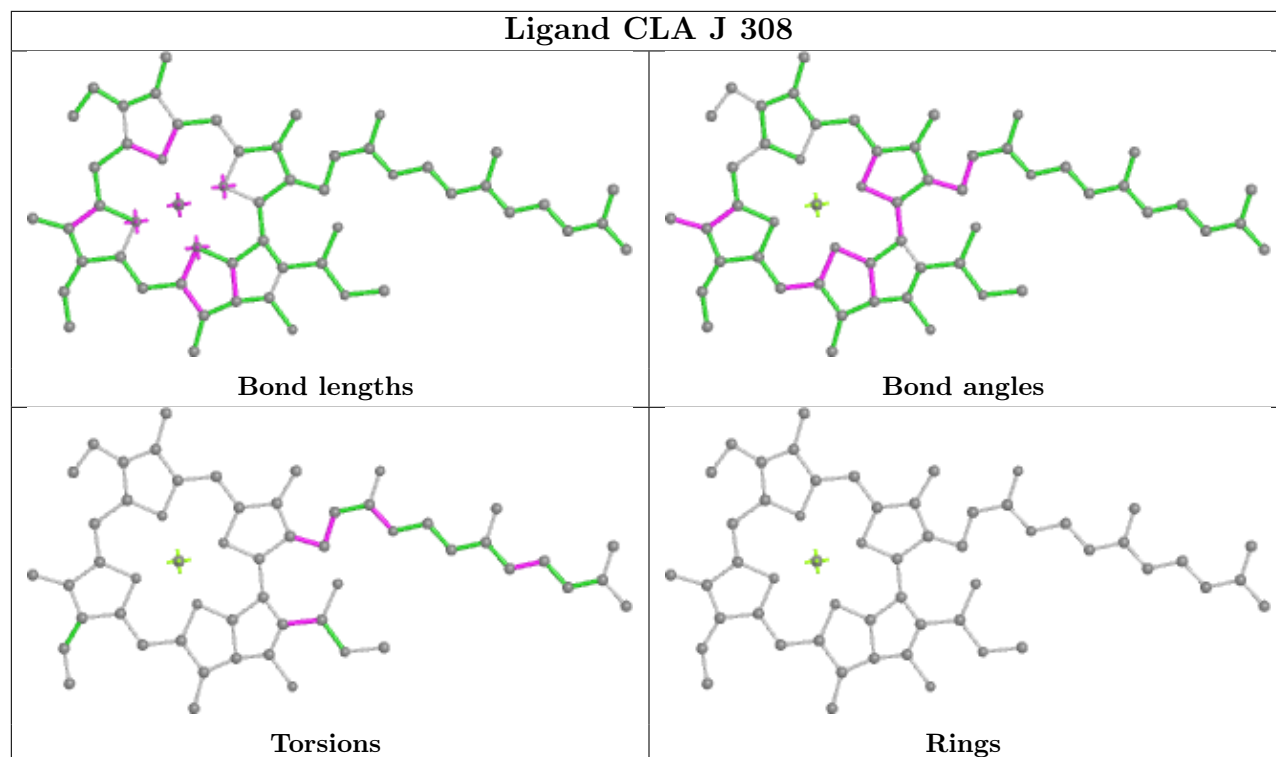
Ligand CLA u 305



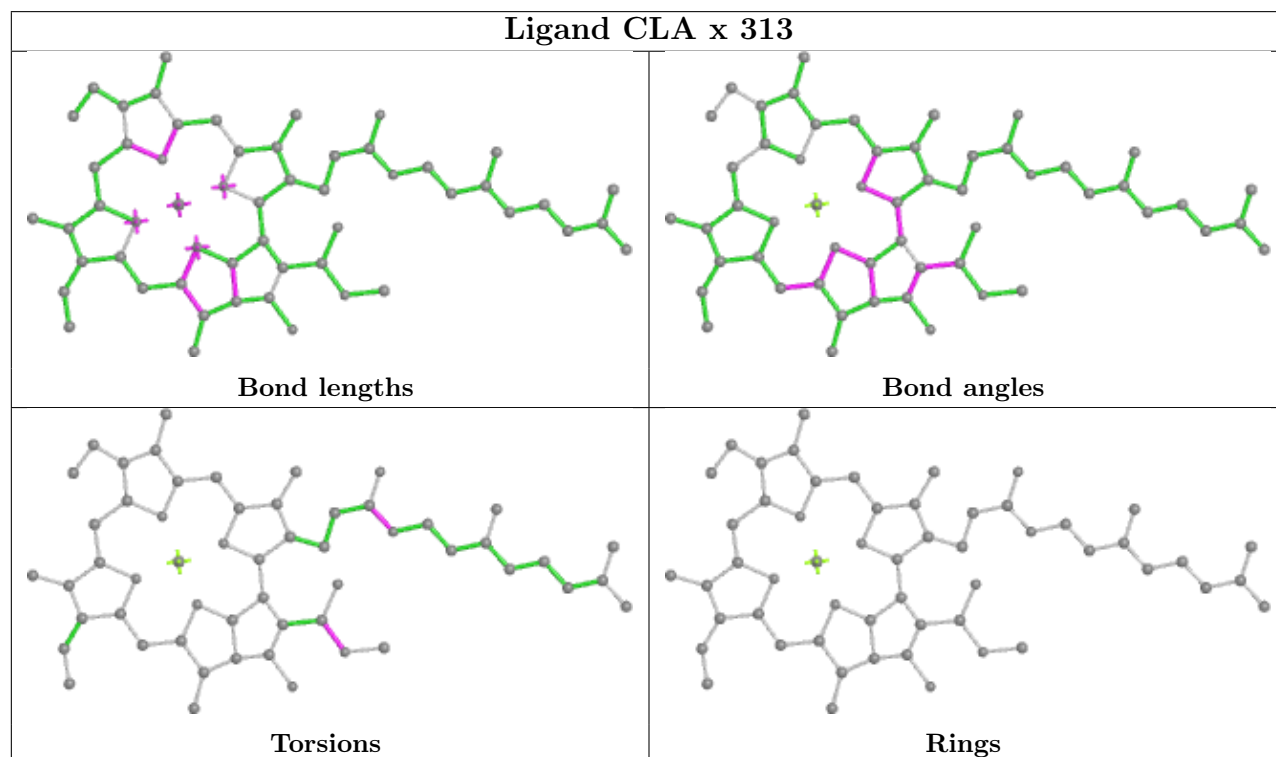
Ligand CLA Y 301

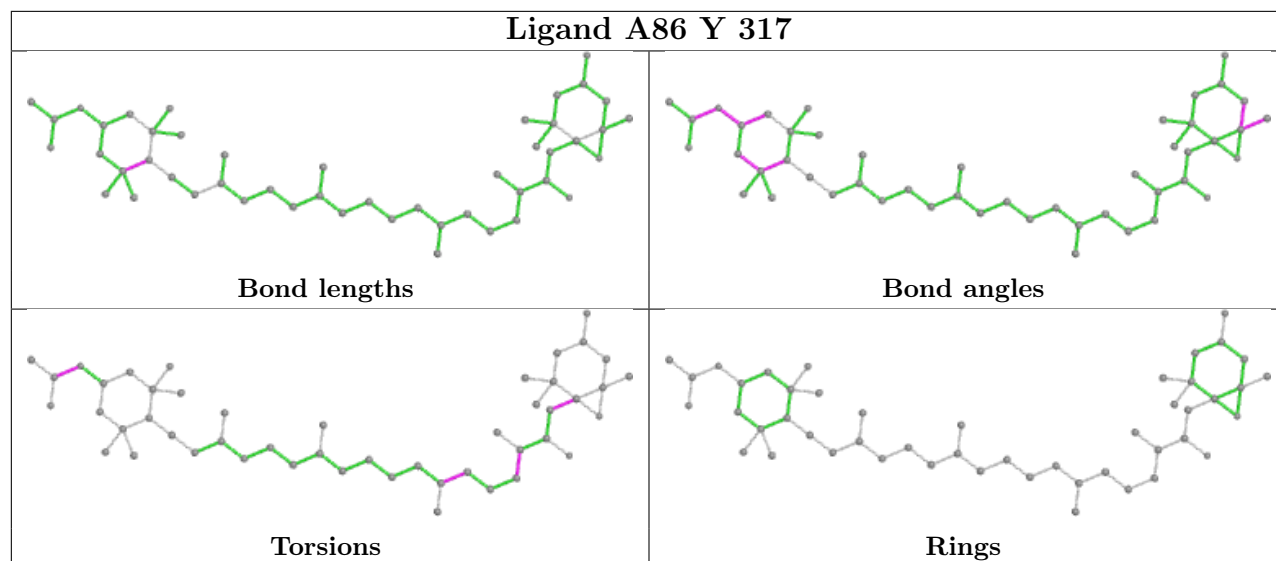
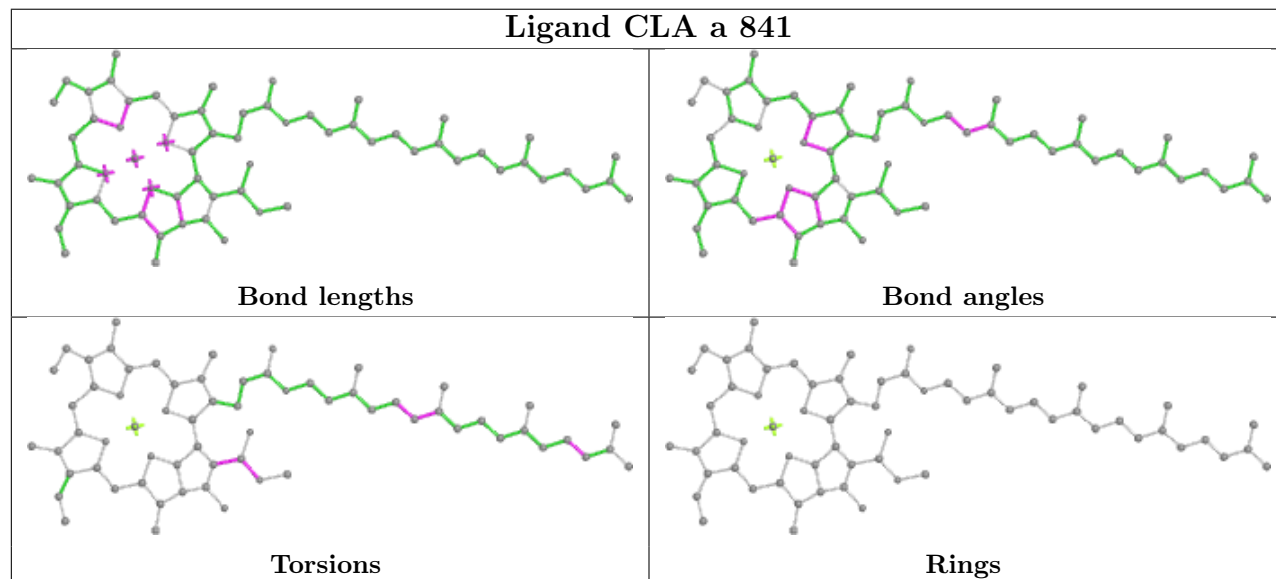


Ligand CLA J 308

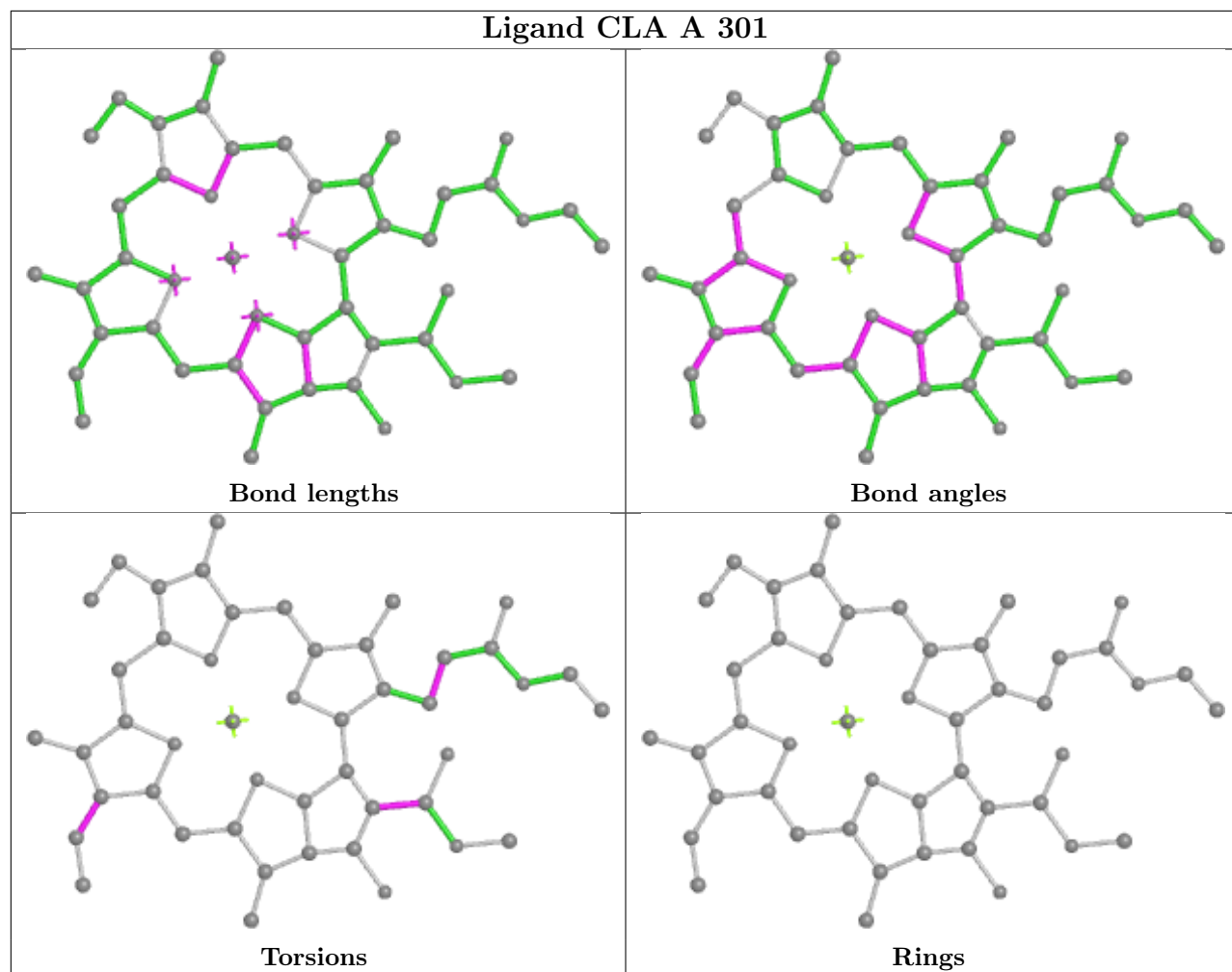


Ligand CLA x 313

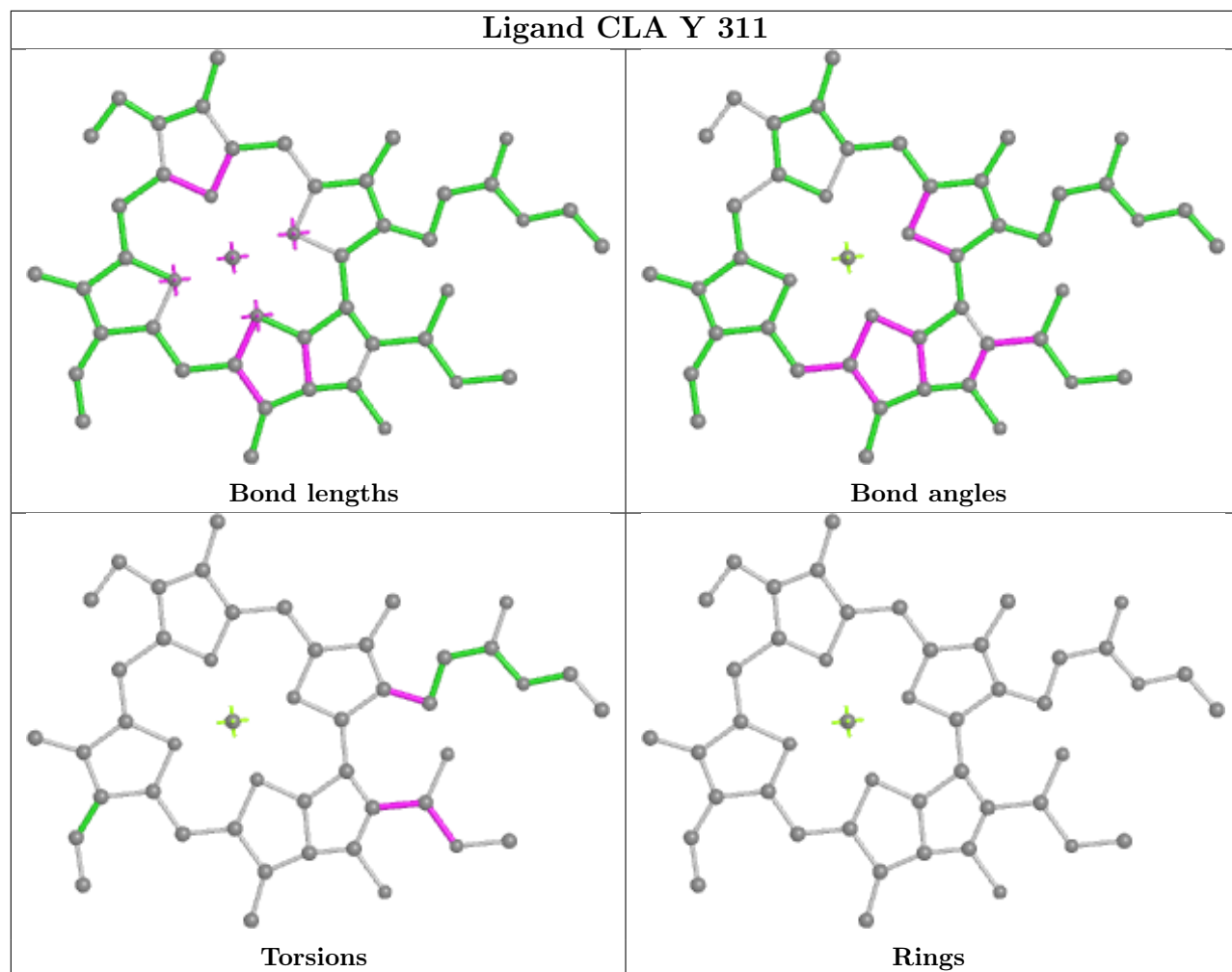


Ligand A86 Y 317**Ligand CLA a 841**

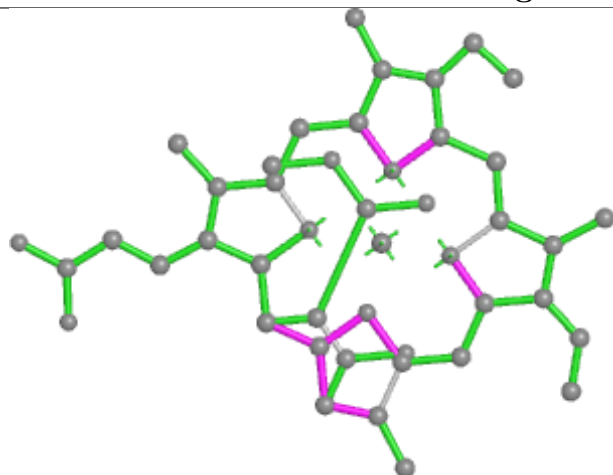
Ligand CLA A 301



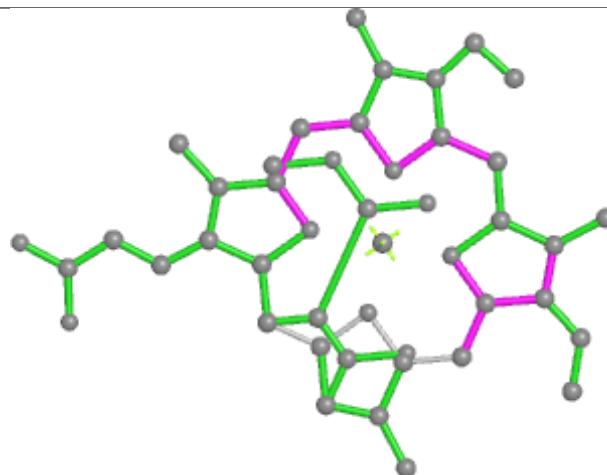
Ligand CLA Y 311



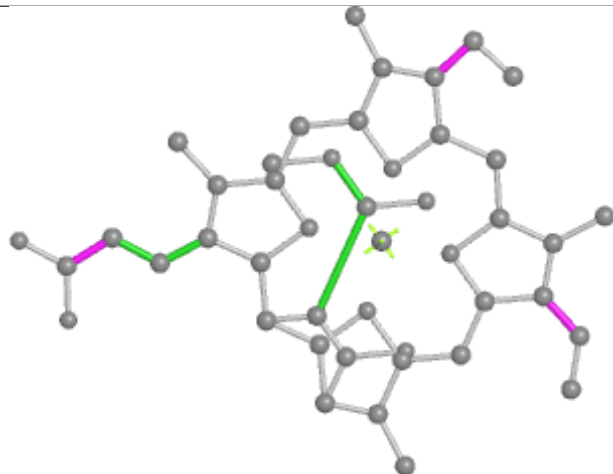
Ligand KC2 A 310



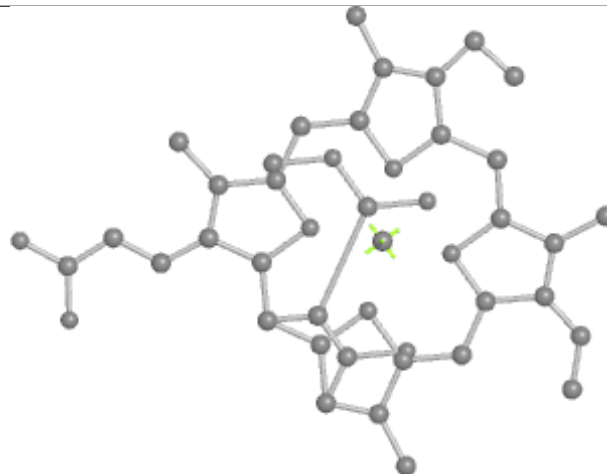
Bond lengths



Bond angles

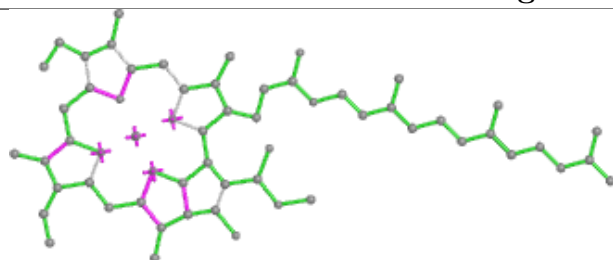


Torsions

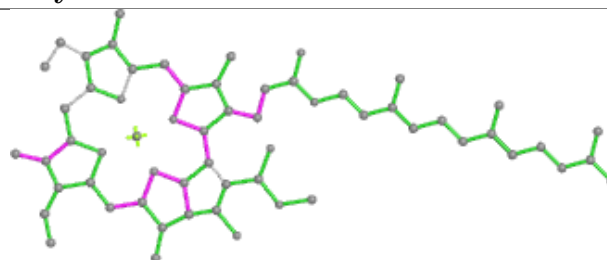


Rings

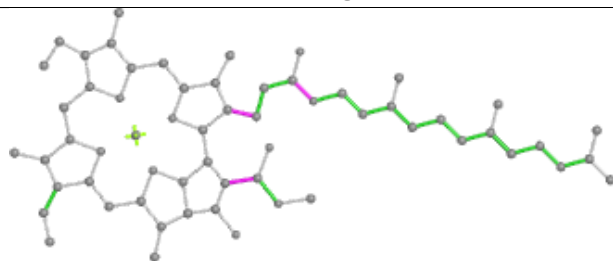
Ligand CLA y 304



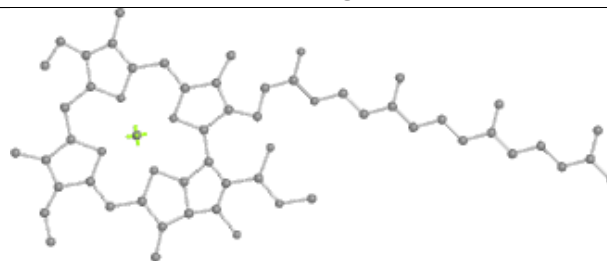
Bond lengths



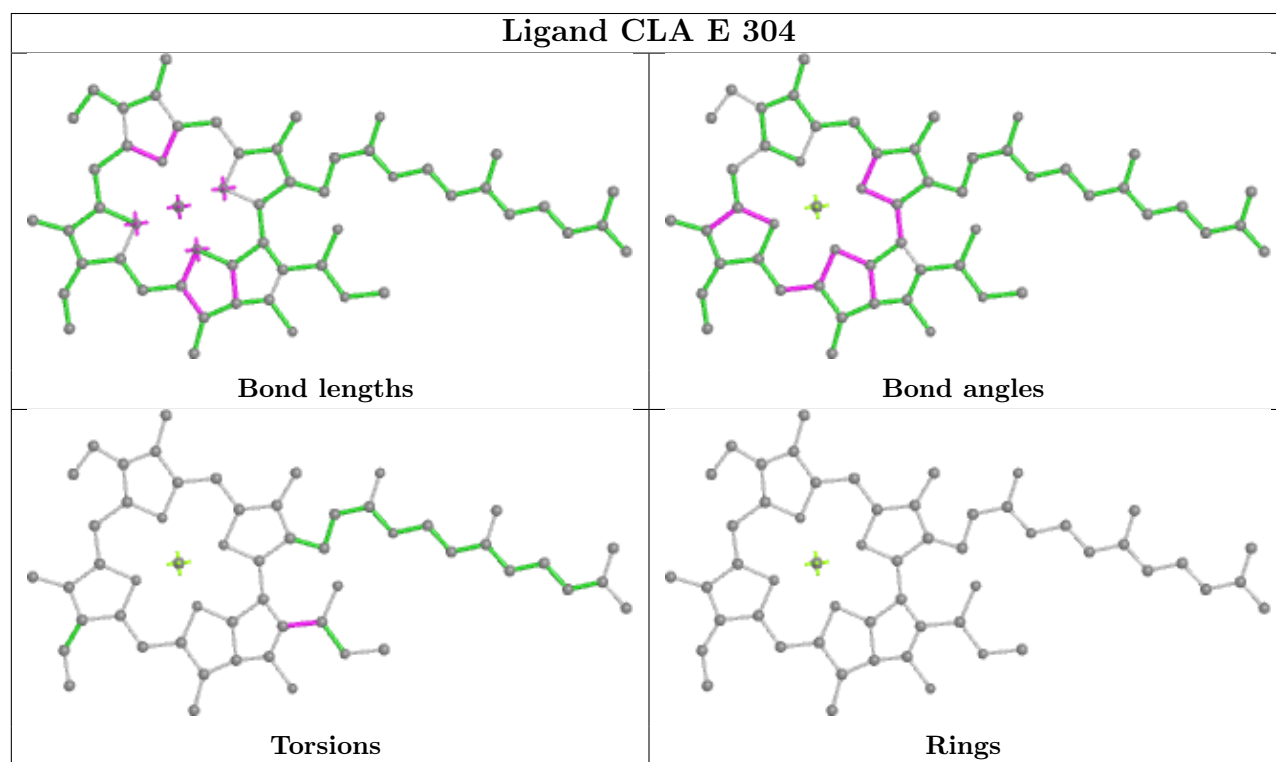
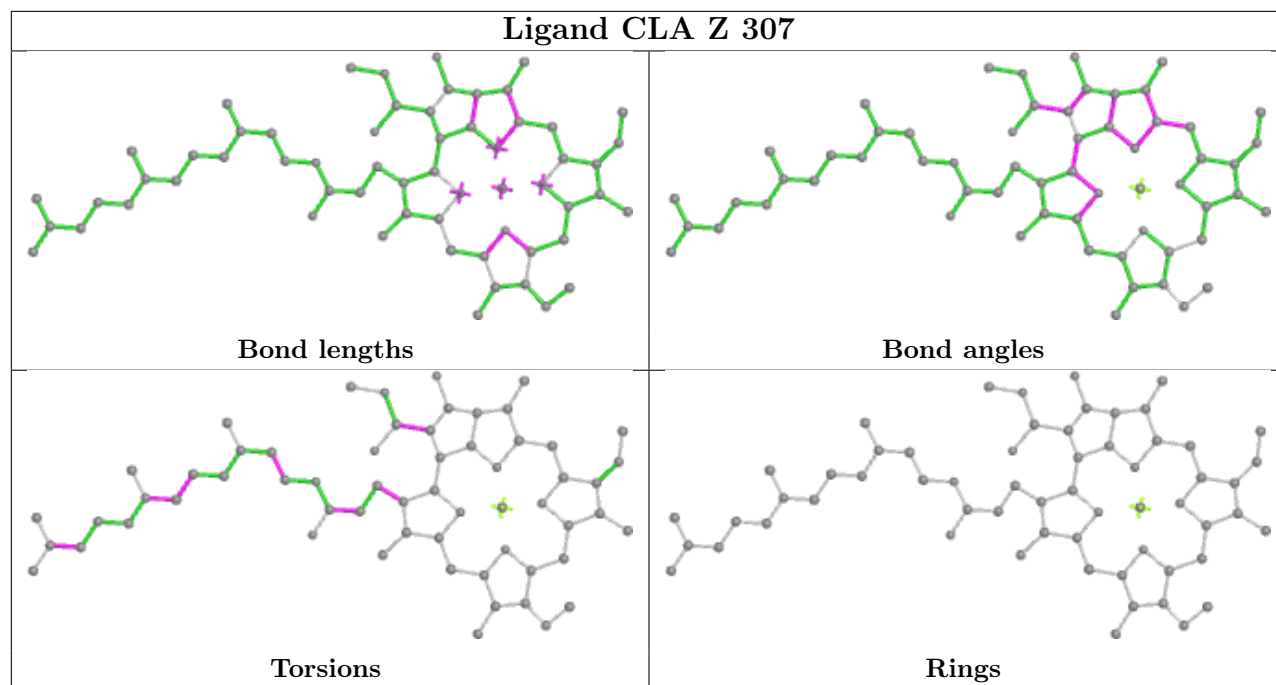
Bond angles

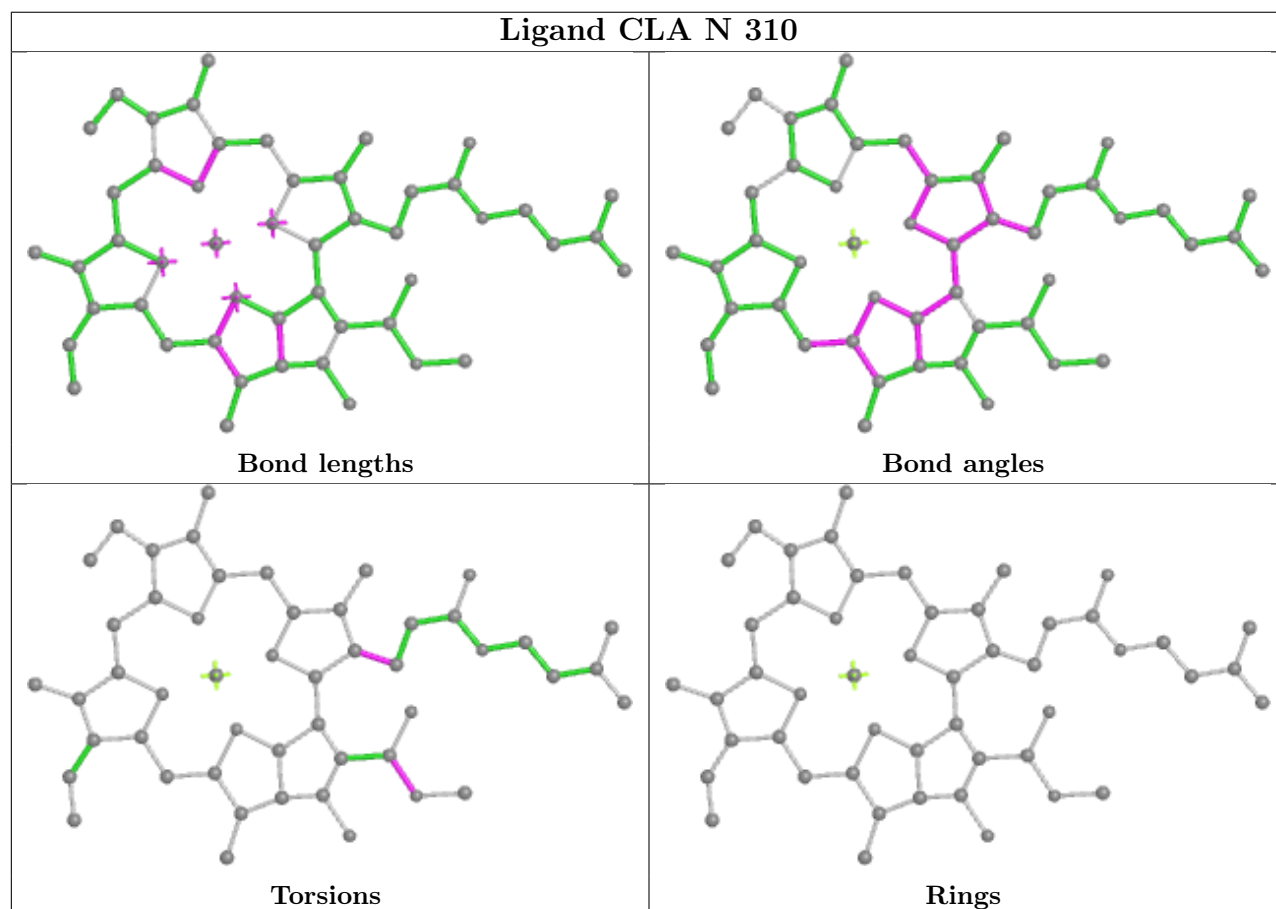
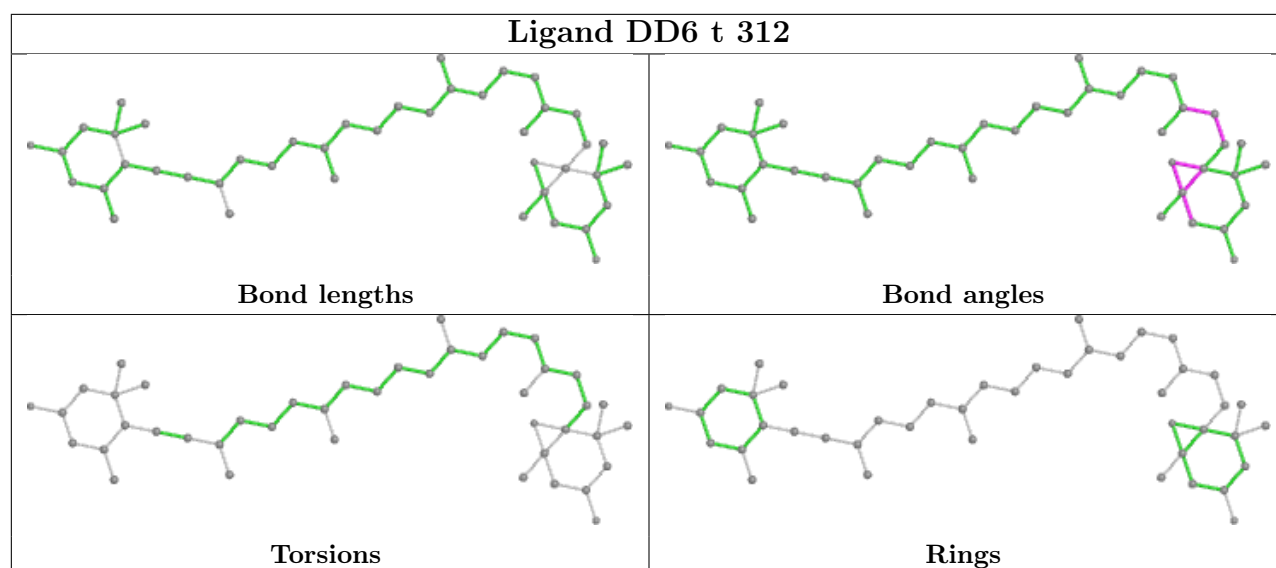


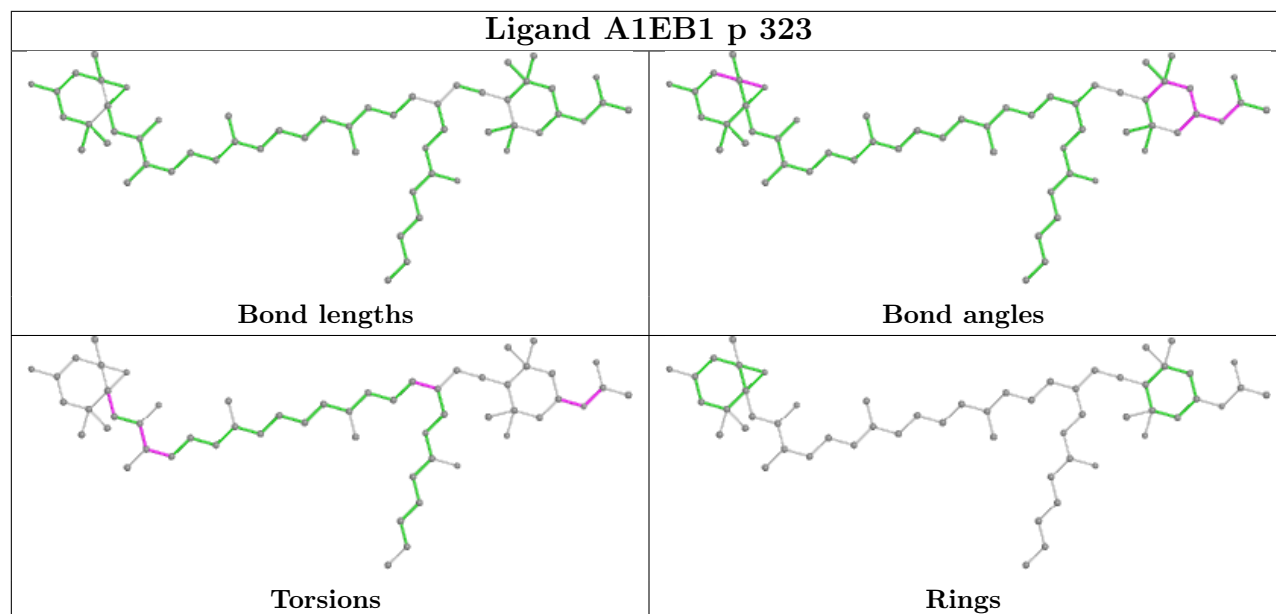
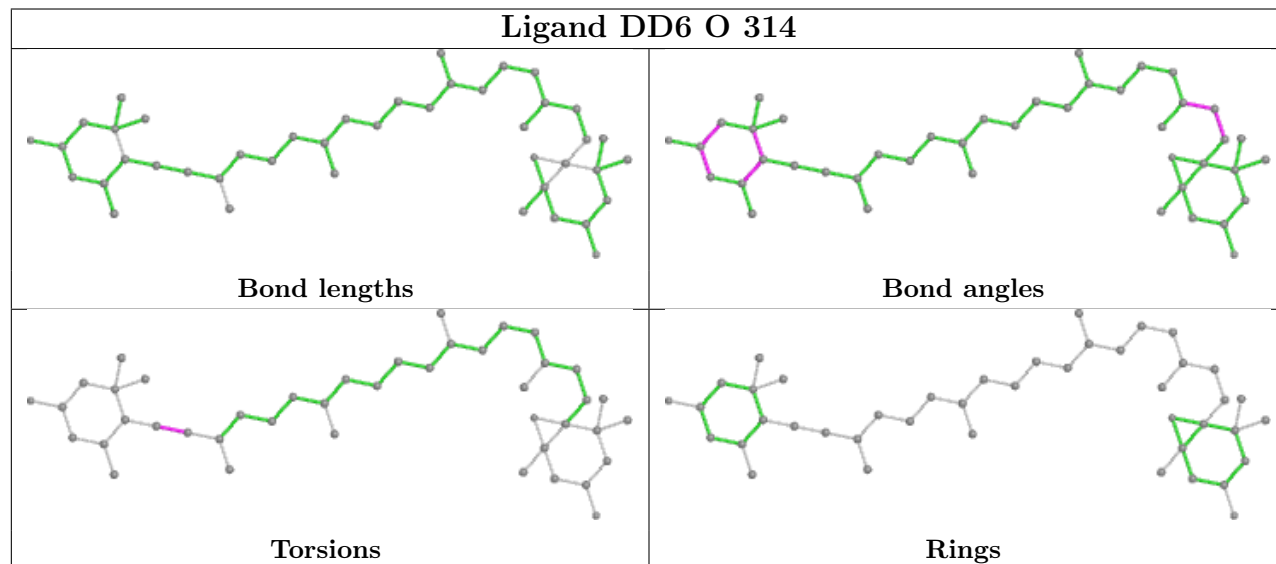
Torsions

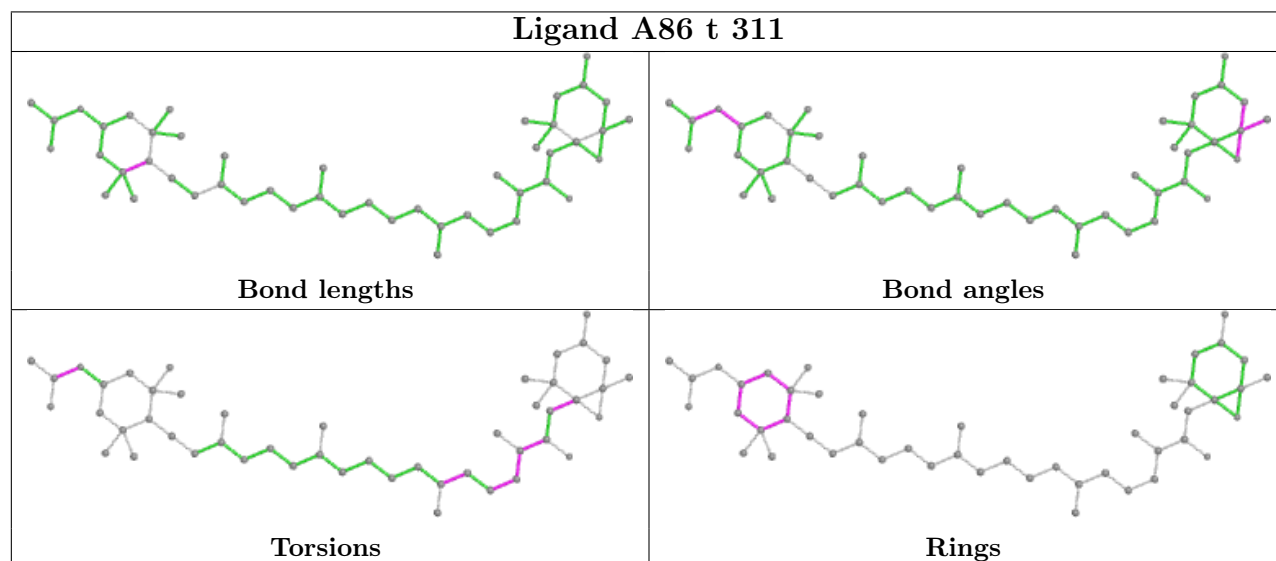
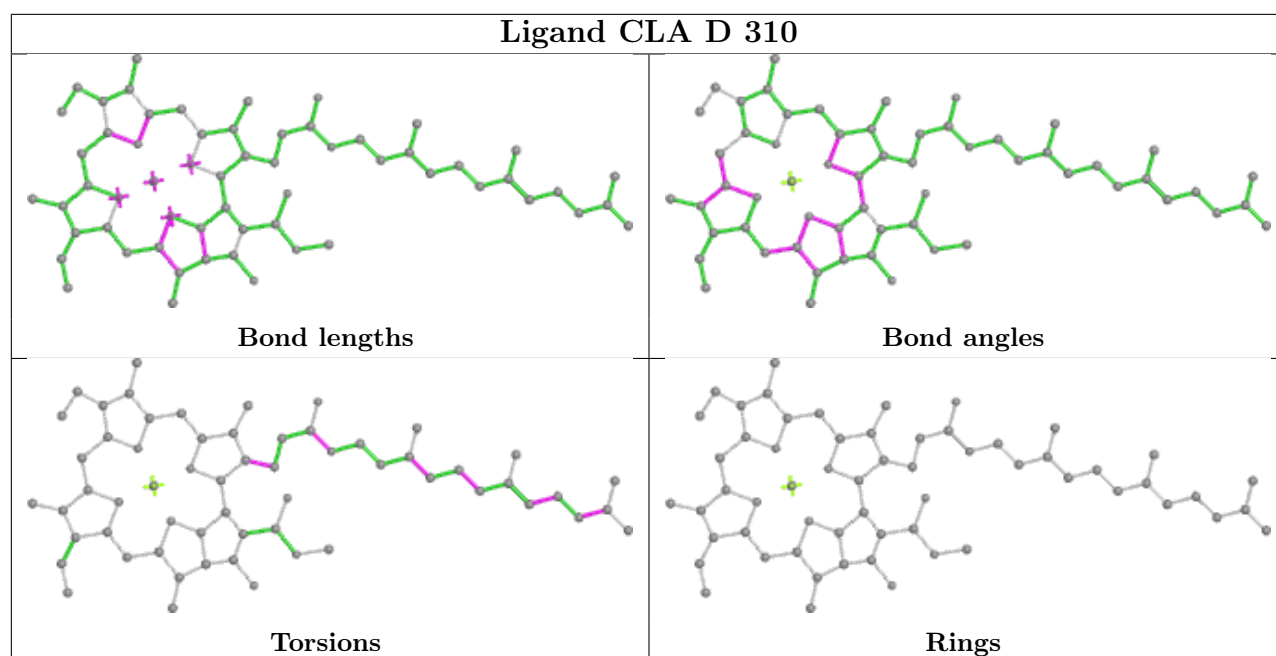


Rings

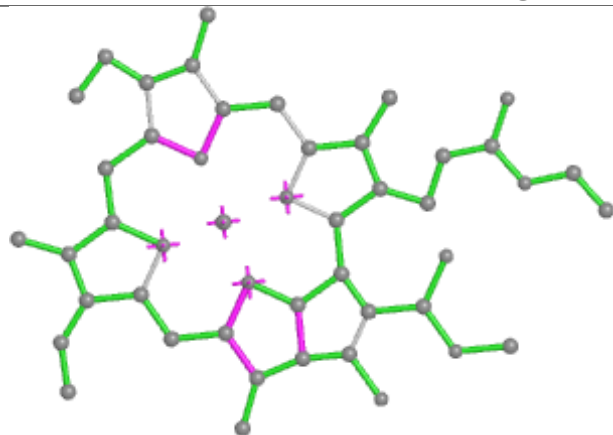




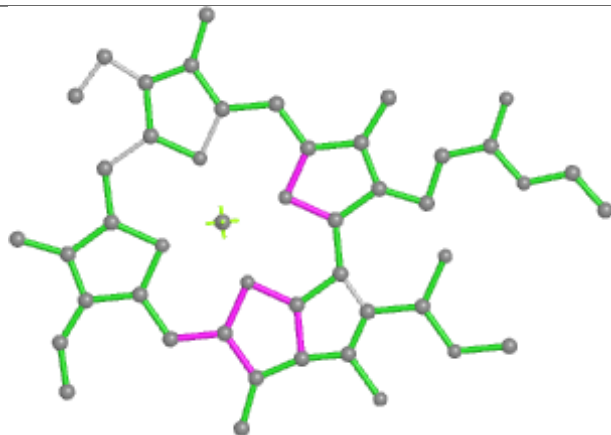
Ligand A1EB1 p 323**Ligand DD6 O 314**



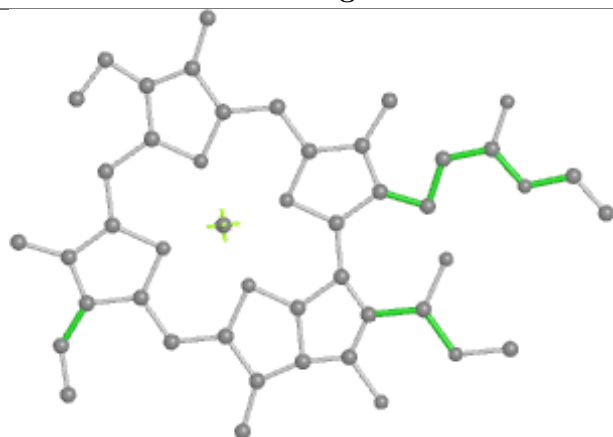
Ligand CLA w 302



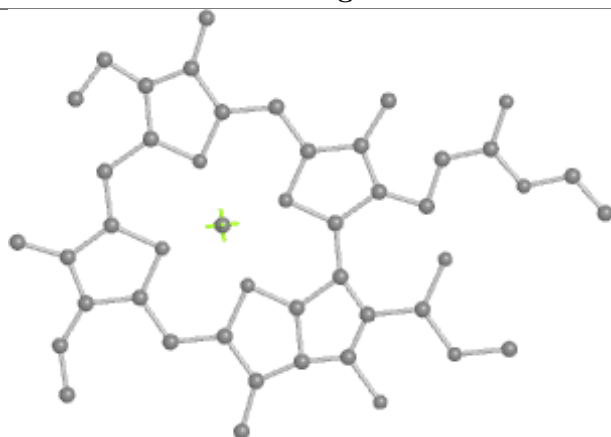
Bond lengths



Bond angles

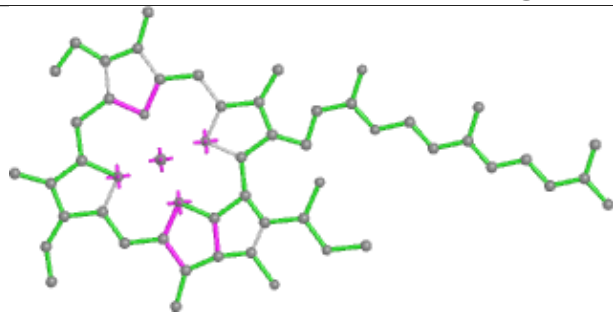


Torsions

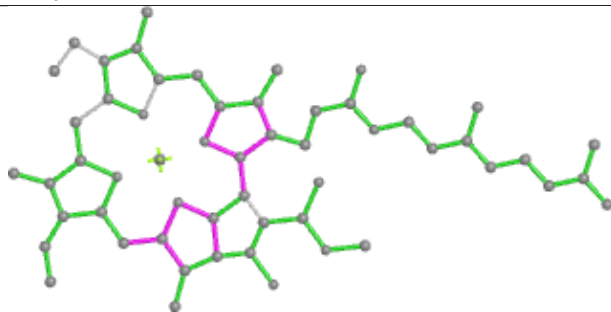


Rings

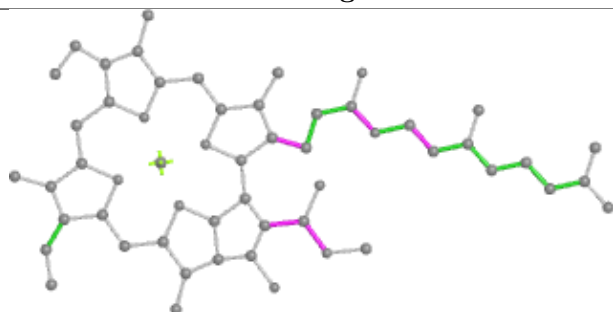
Ligand CLA y 309



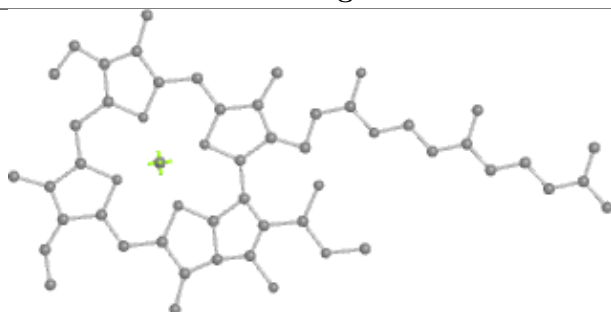
Bond lengths



Bond angles

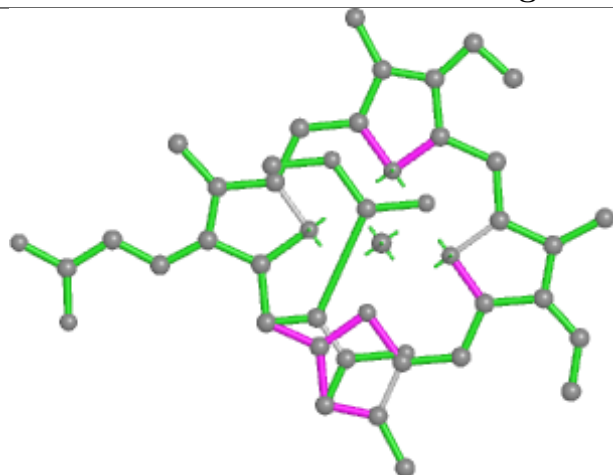


Torsions

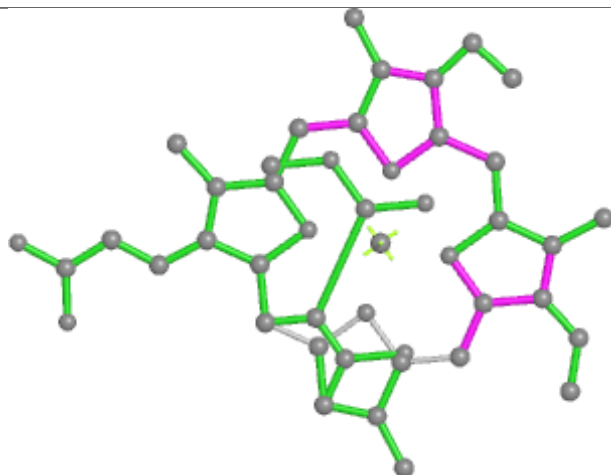


Rings

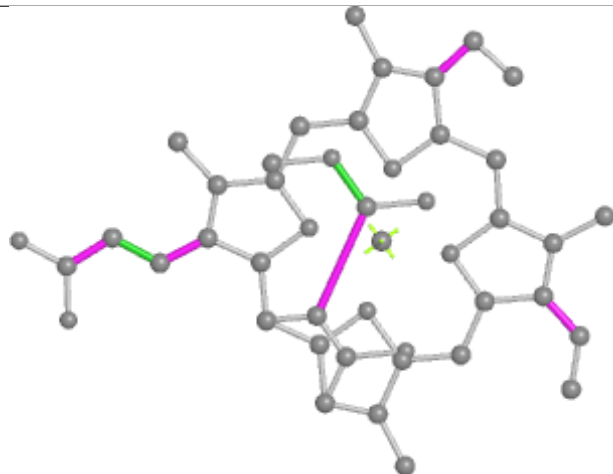
Ligand KC2 S 310



Bond lengths



Bond angles

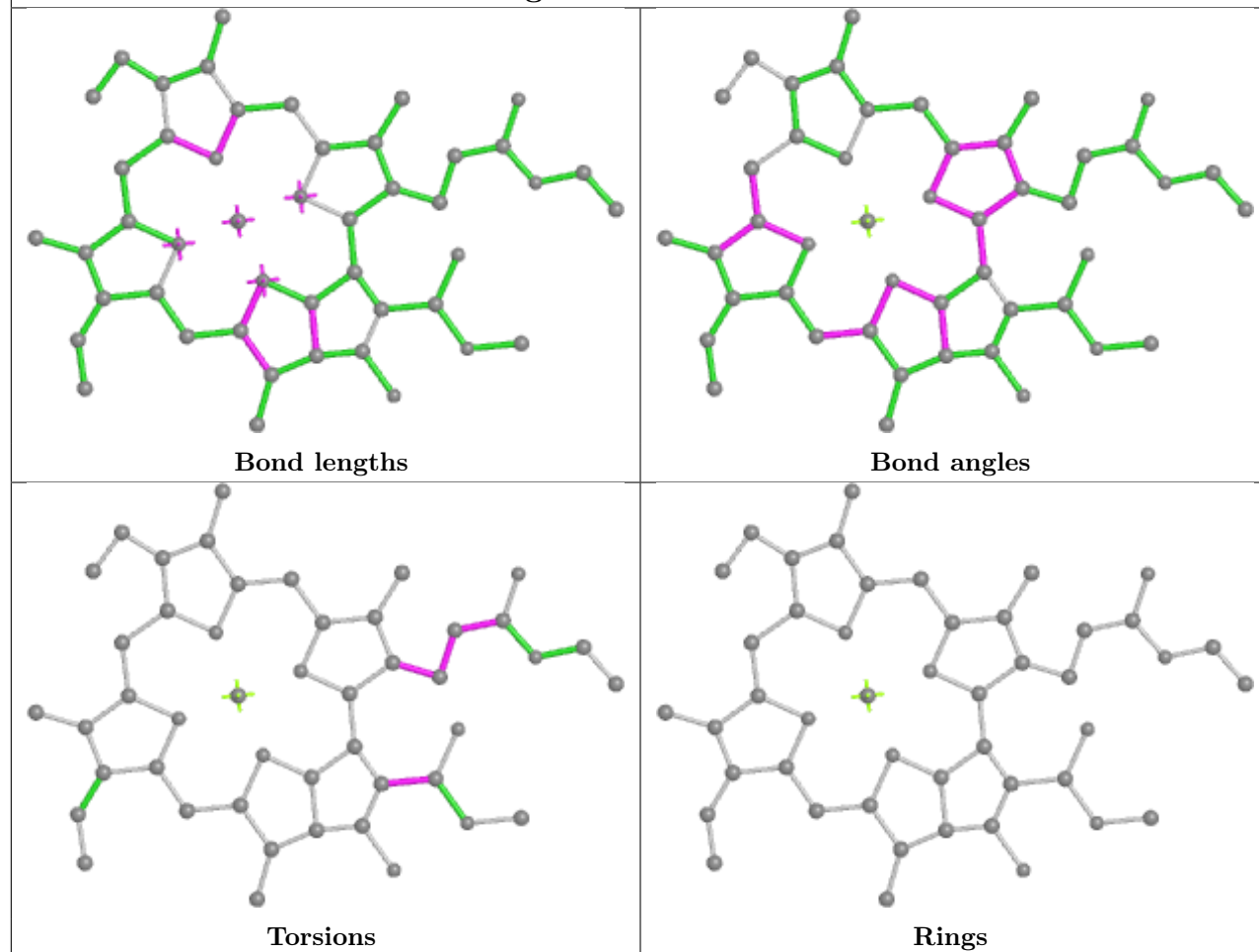


Torsions

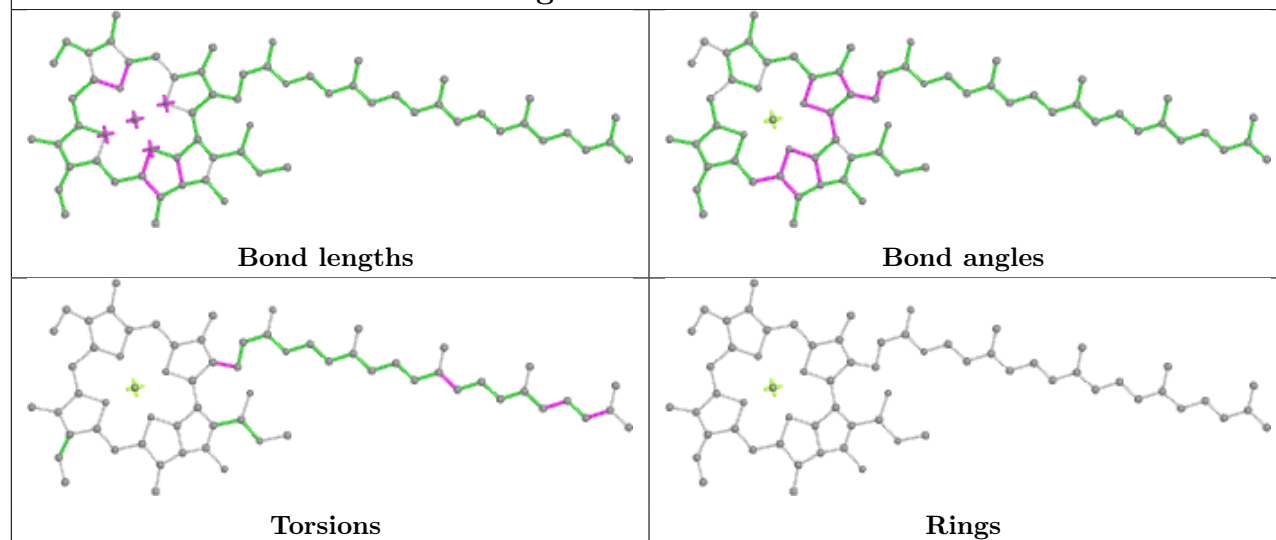


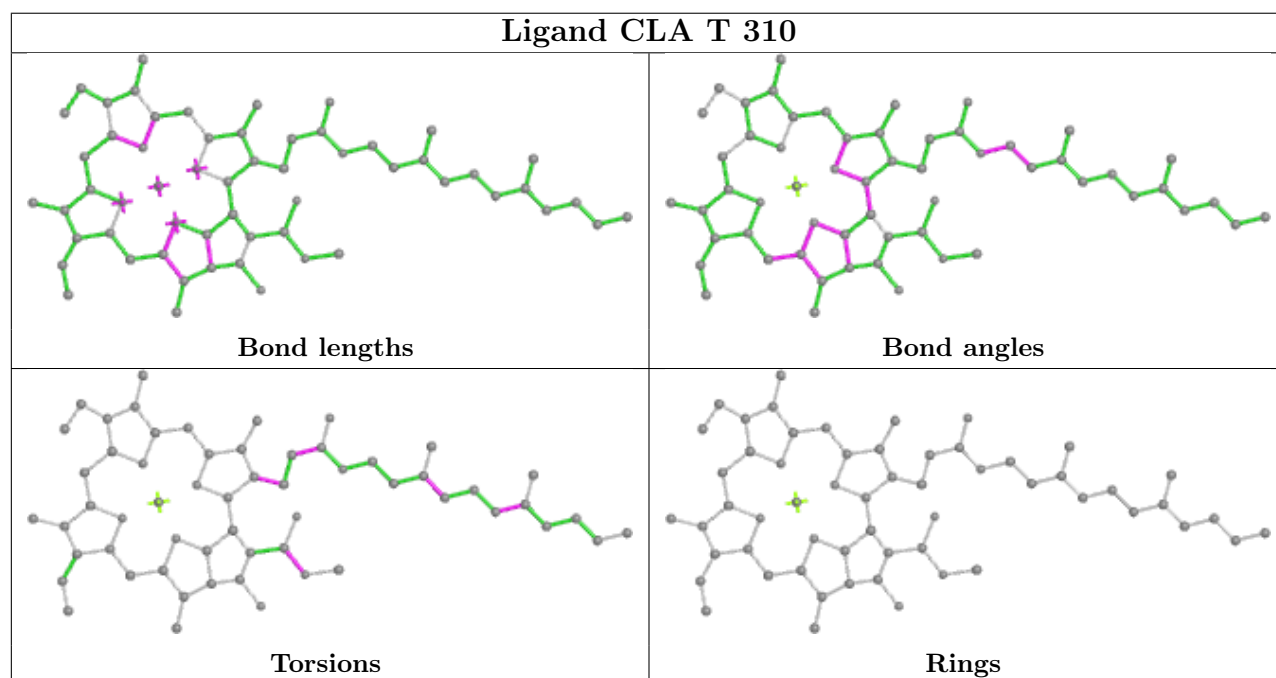
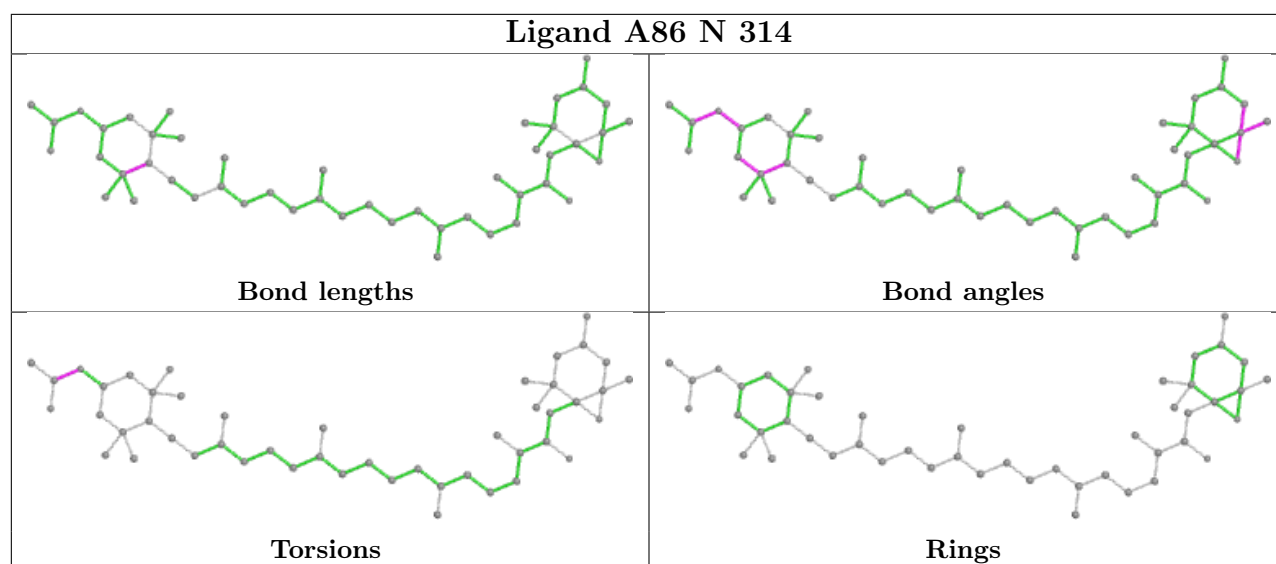
Rings

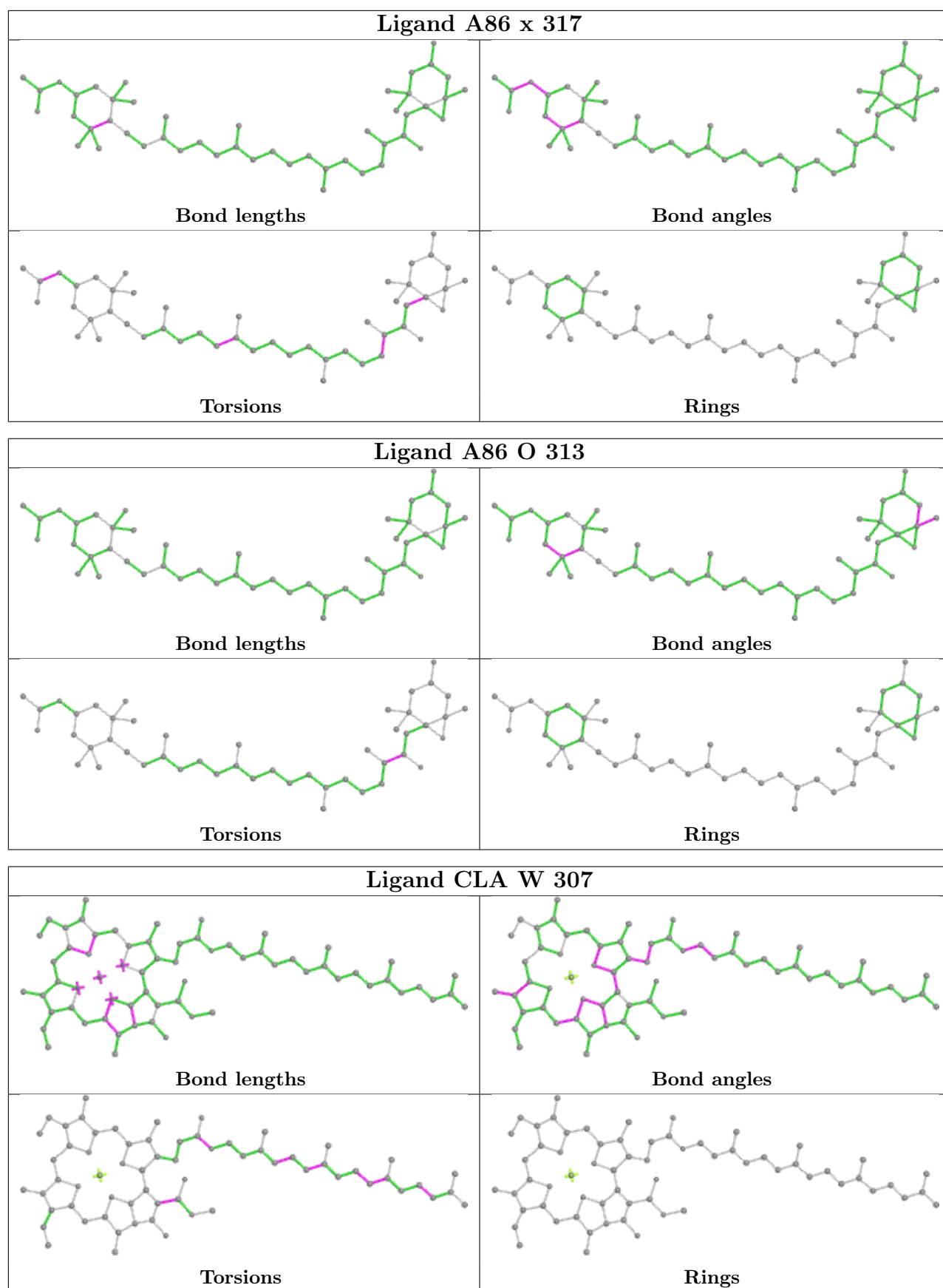
Ligand CLA B 307



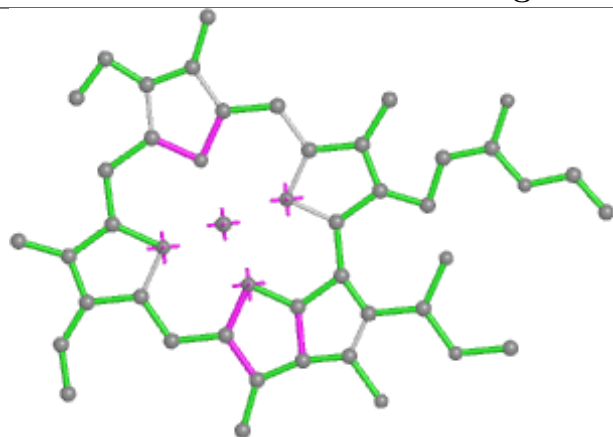
Ligand CLA a 816



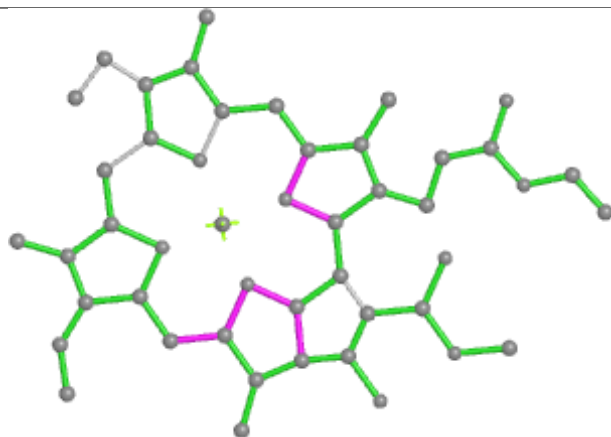




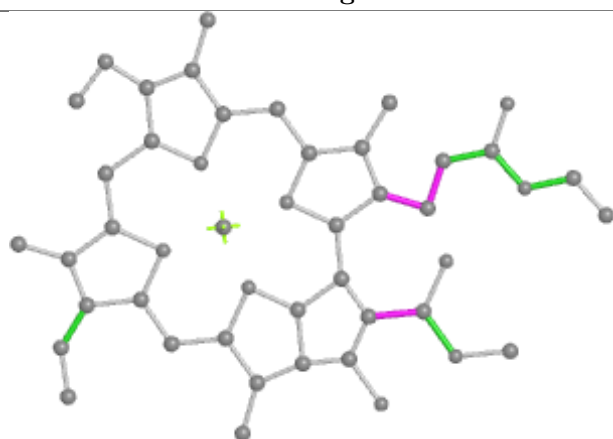
Ligand CLA H 308



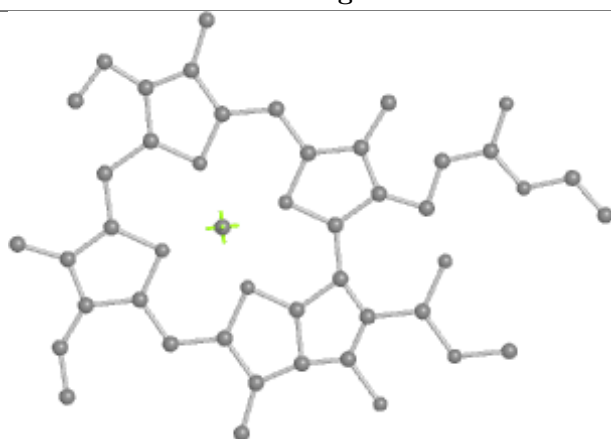
Bond lengths



Bond angles

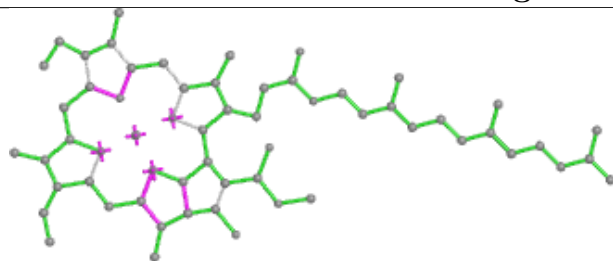


Torsions

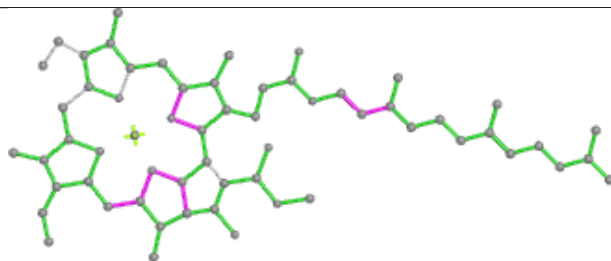


Rings

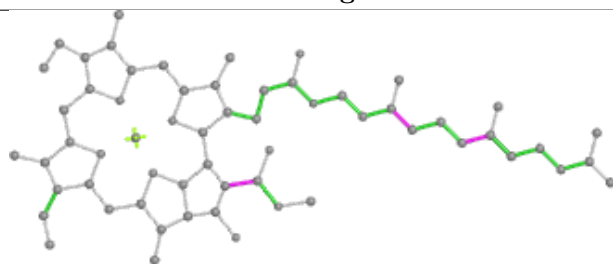
Ligand CLA N 307



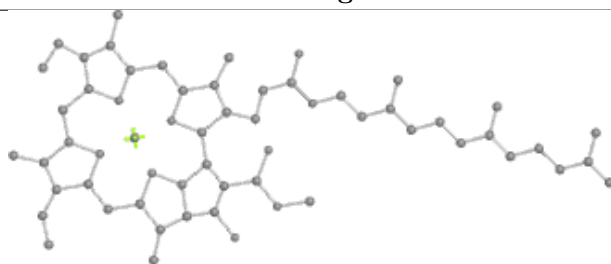
Bond lengths



Bond angles

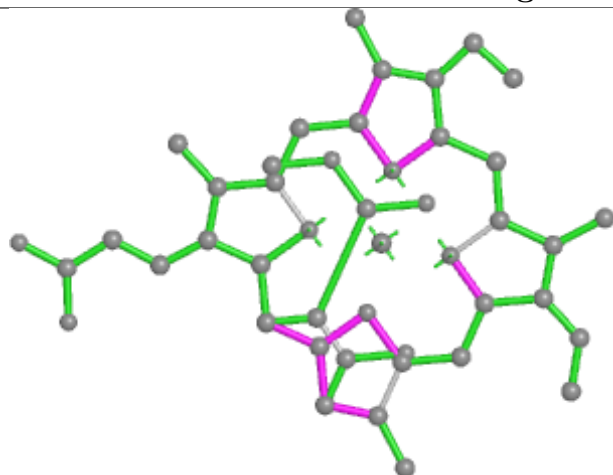


Torsions

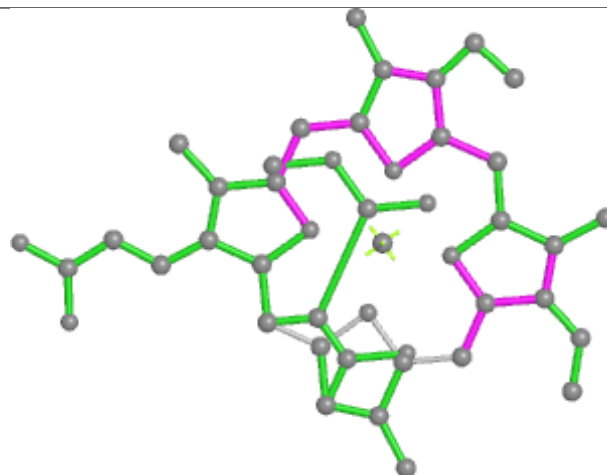


Rings

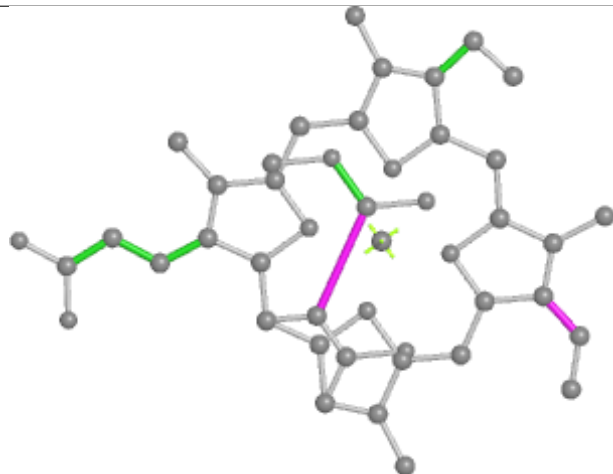
Ligand KC2 T 302



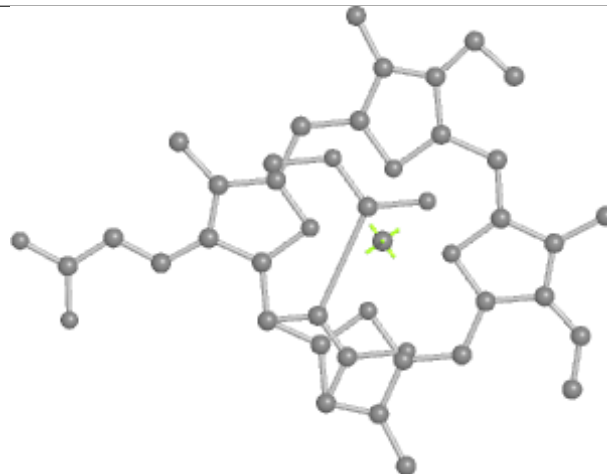
Bond lengths



Bond angles

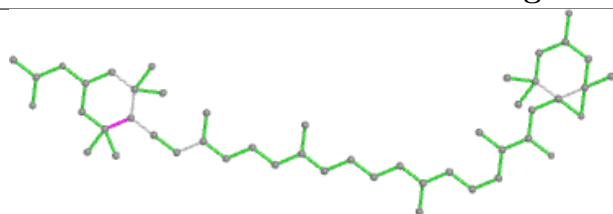


Torsions

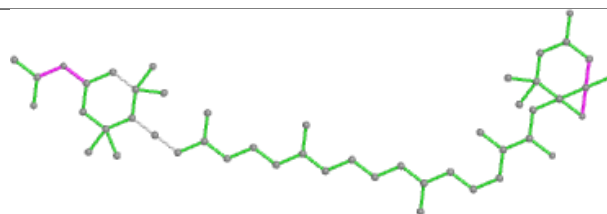


Rings

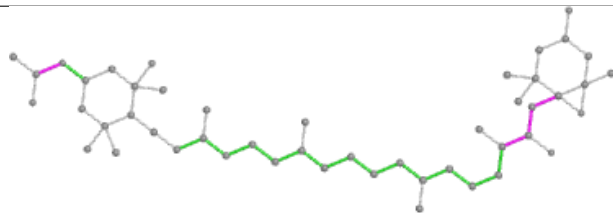
Ligand A86 x 318



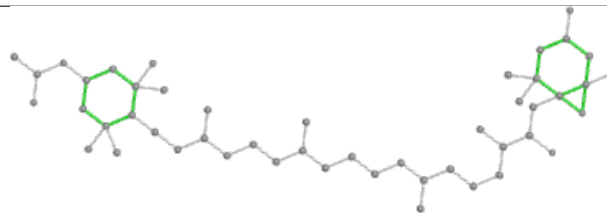
Bond lengths



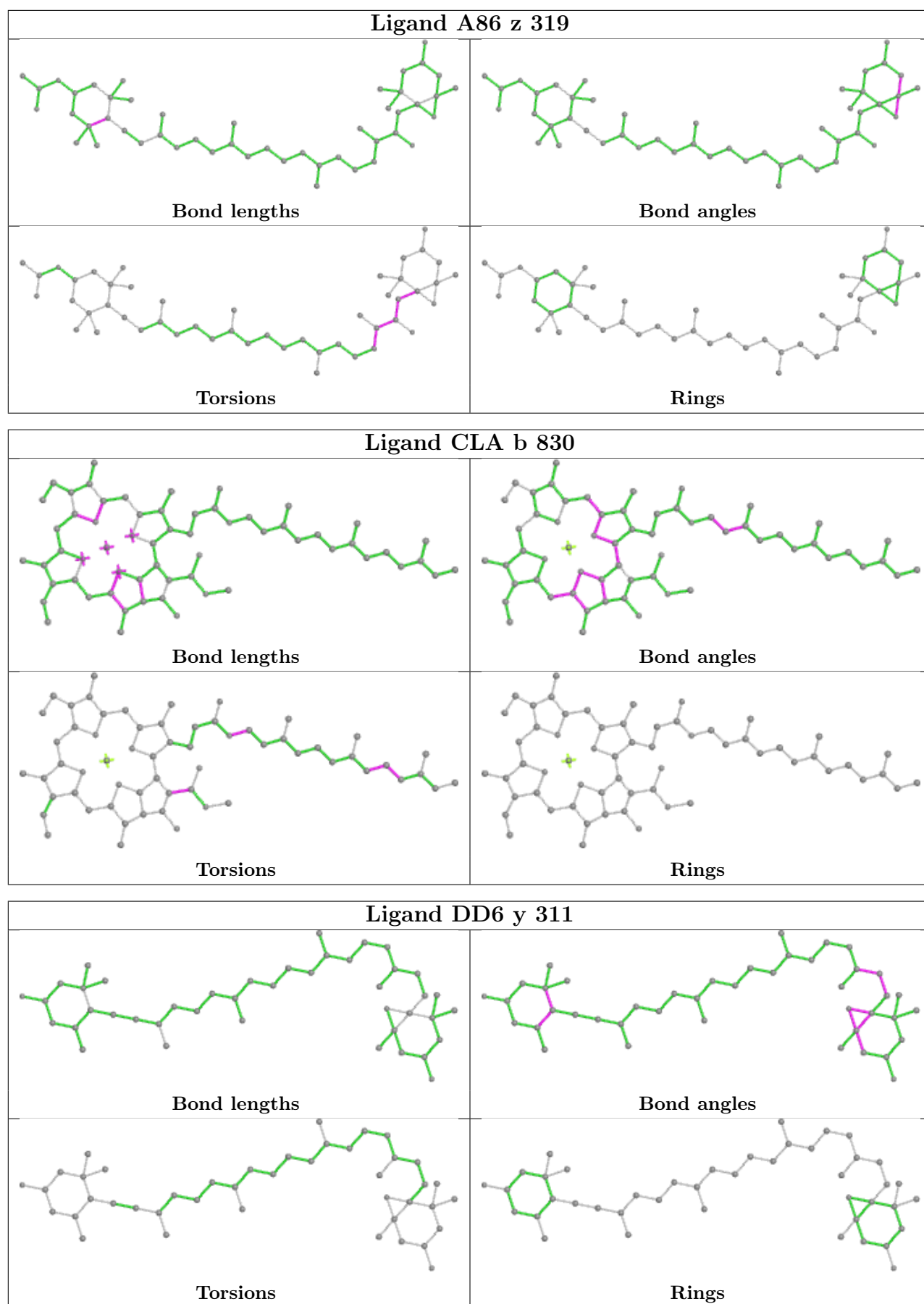
Bond angles

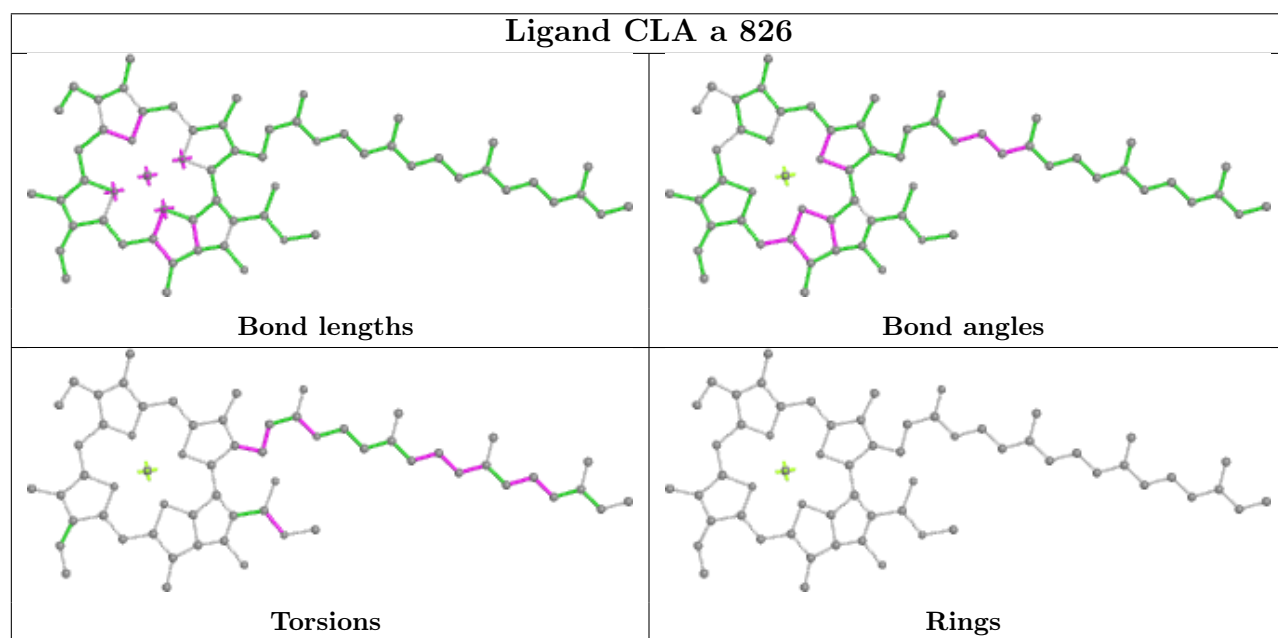
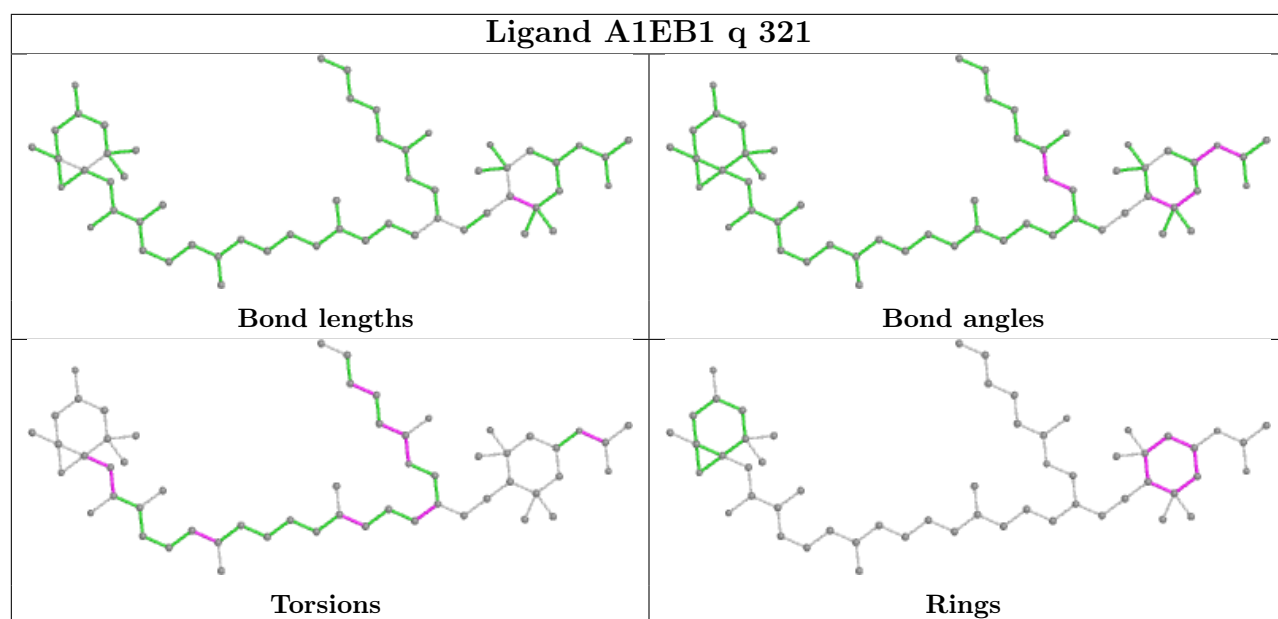


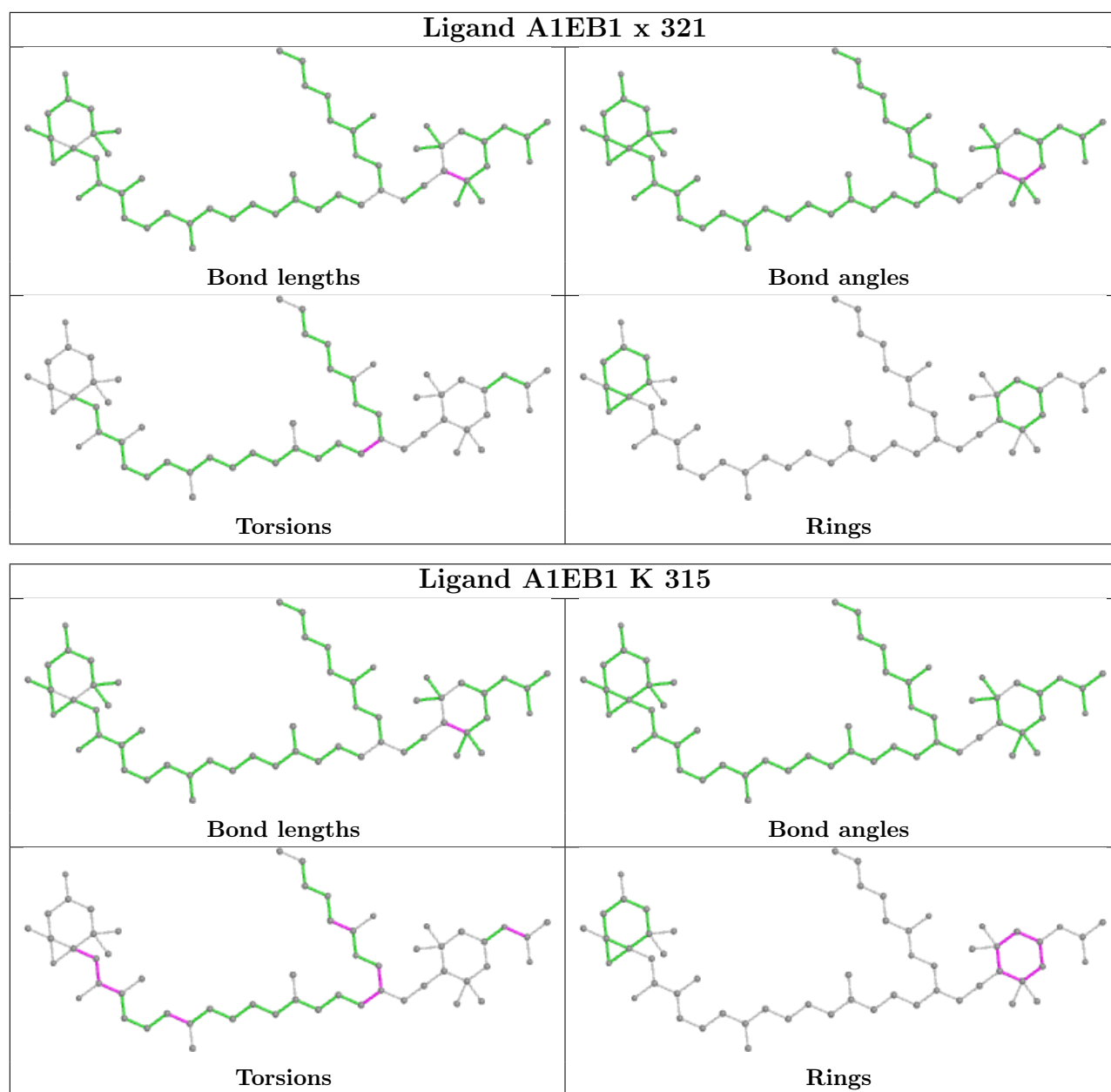
Torsions

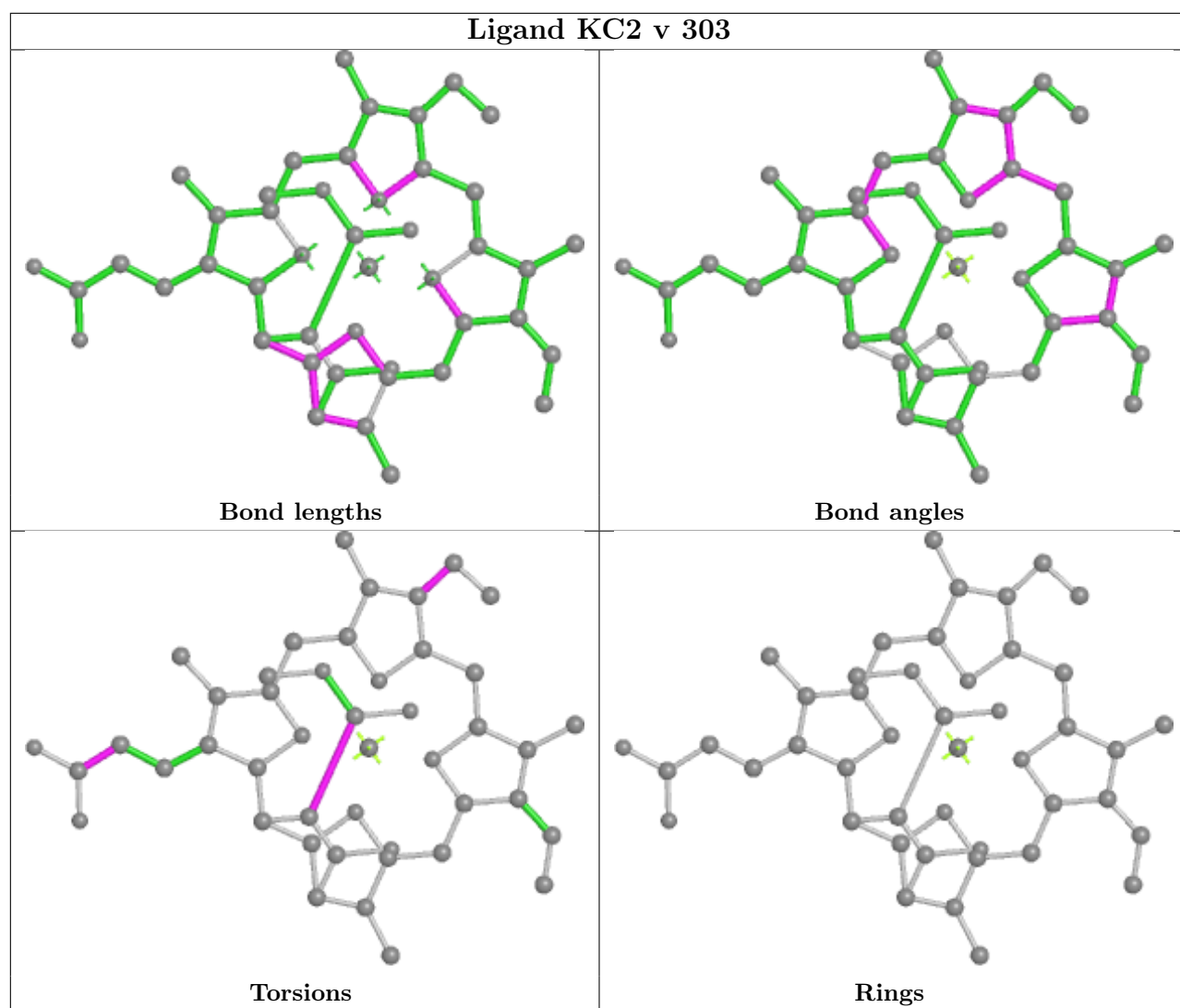


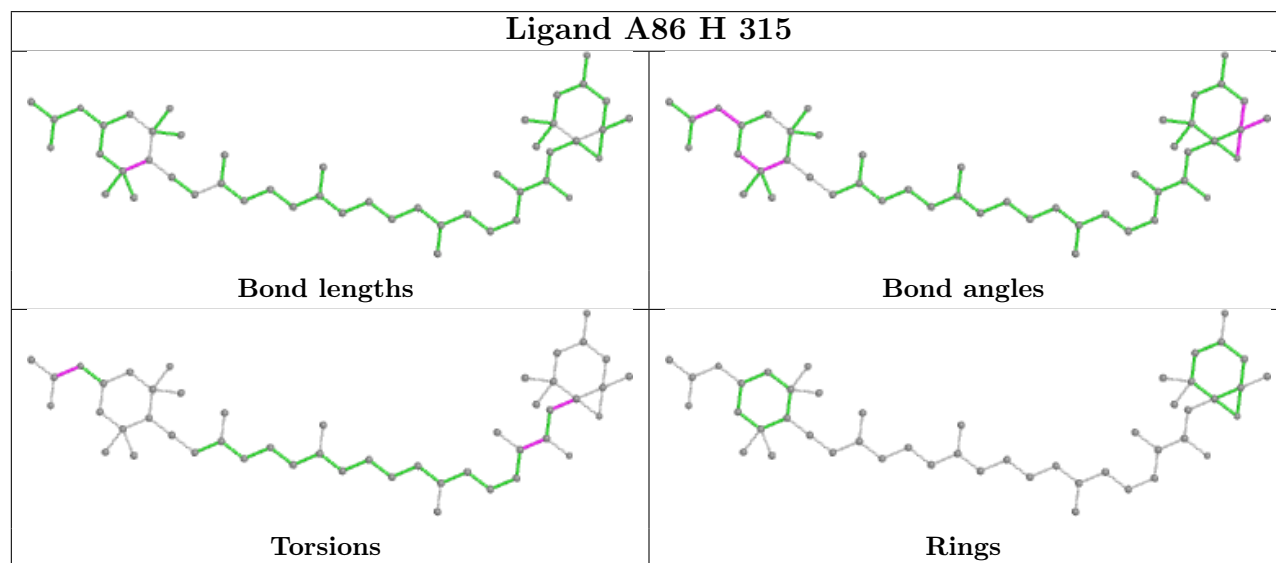
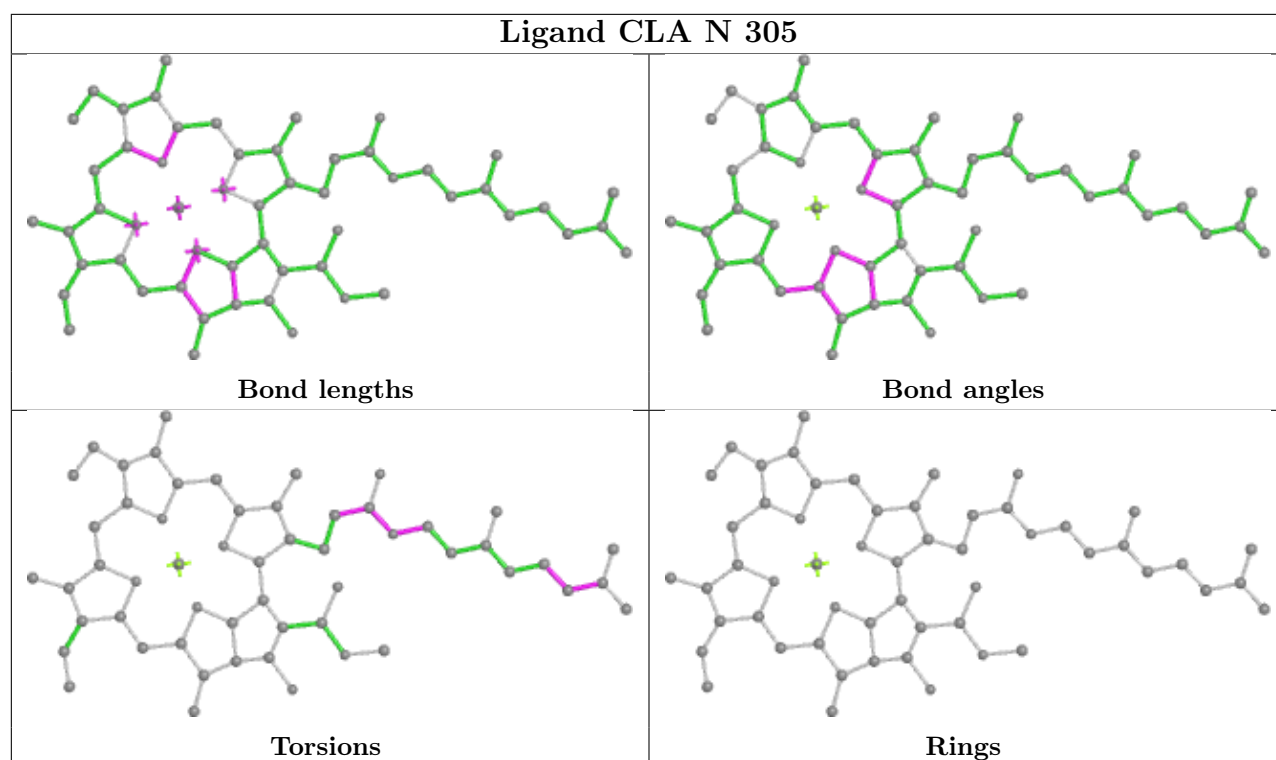
Rings

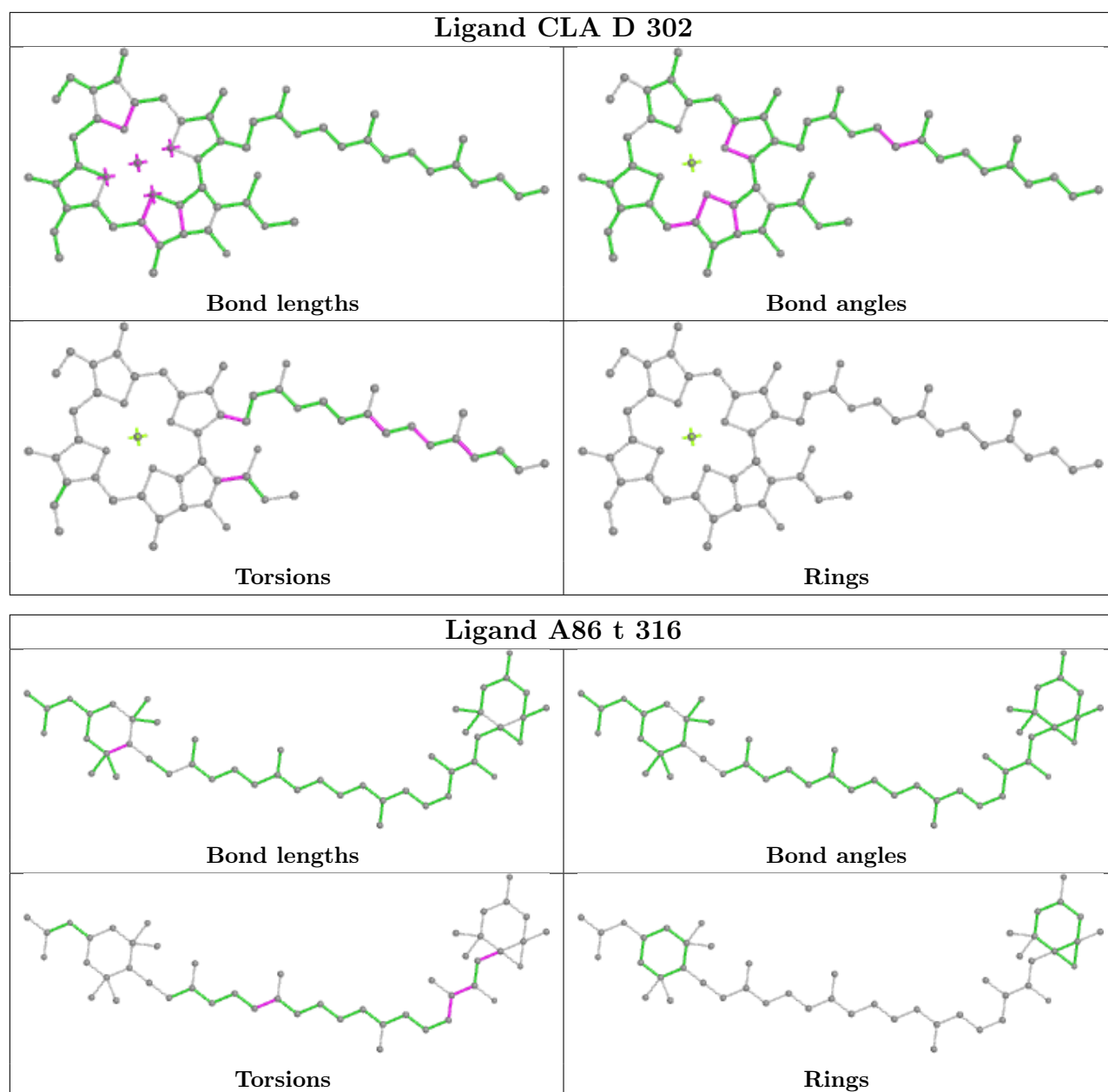


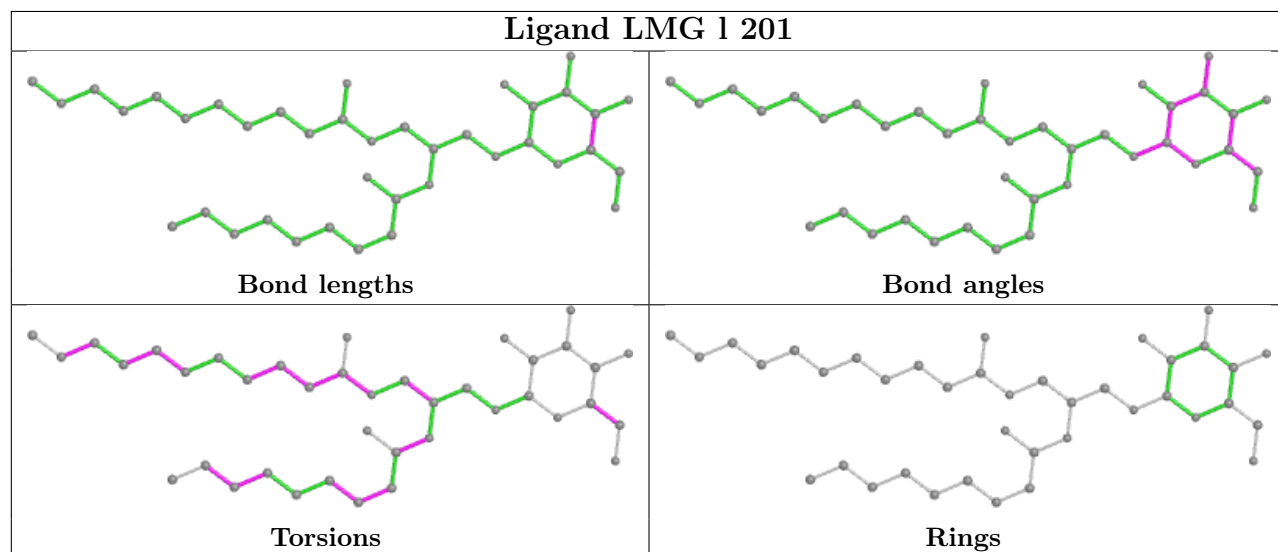
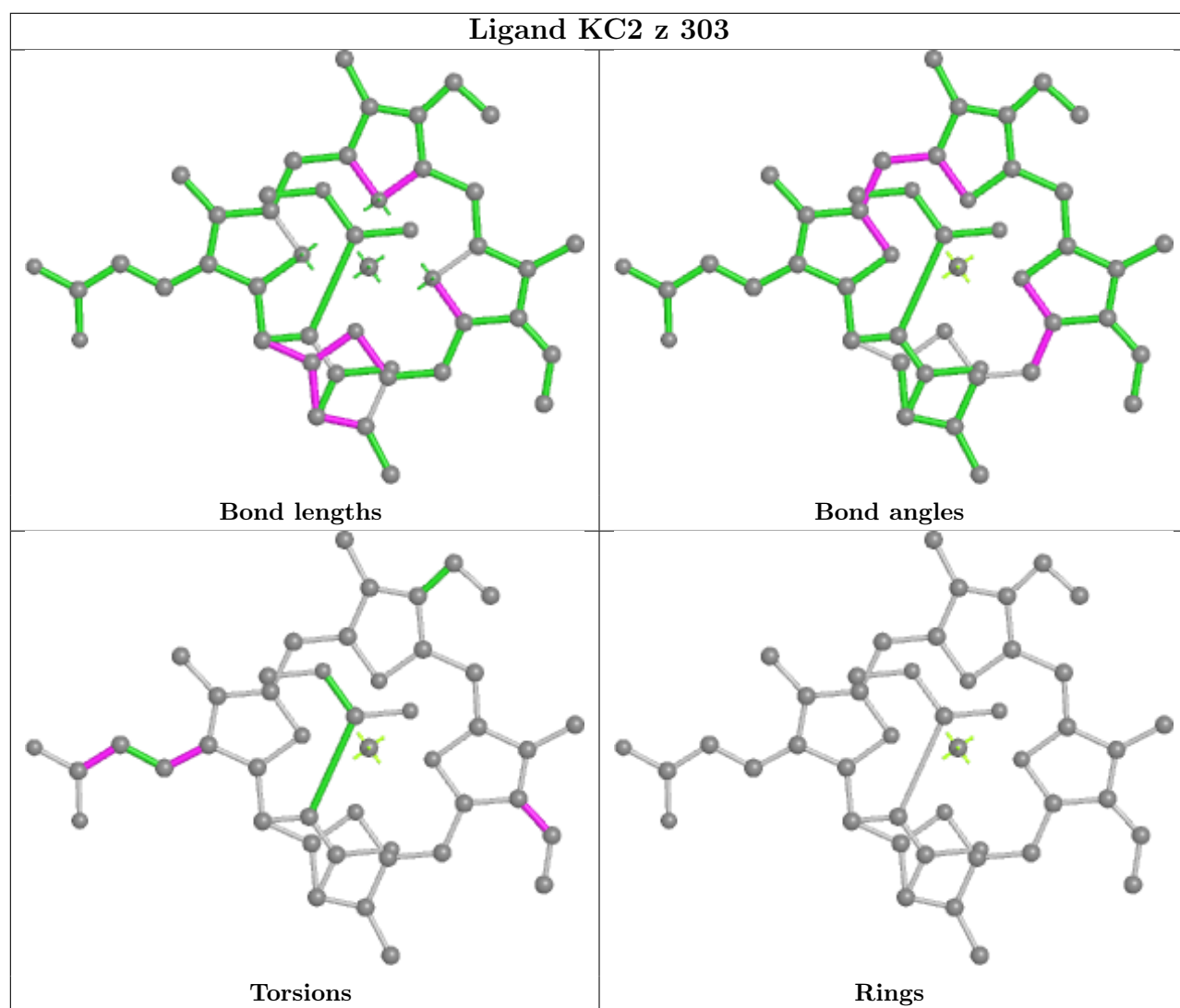


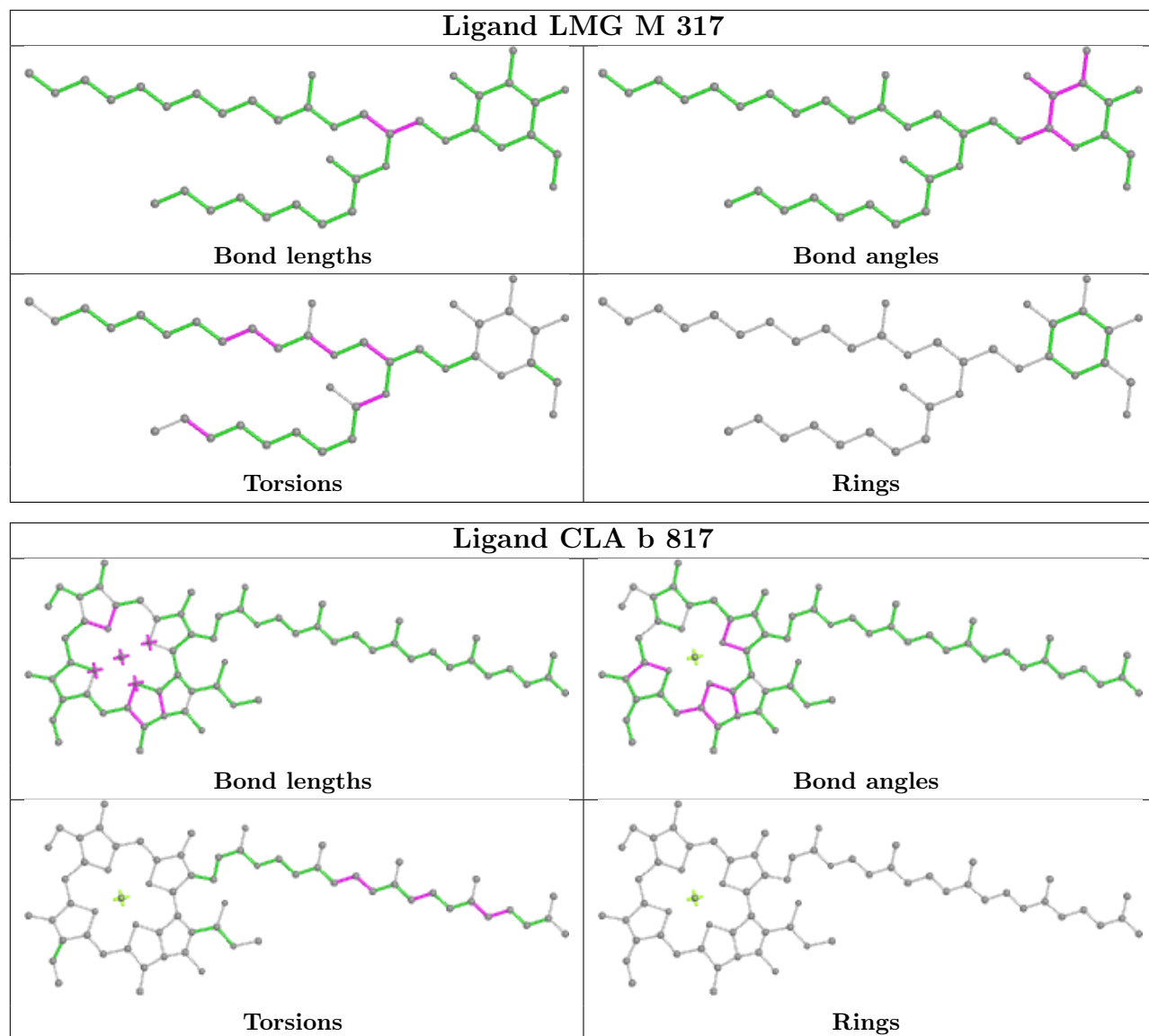




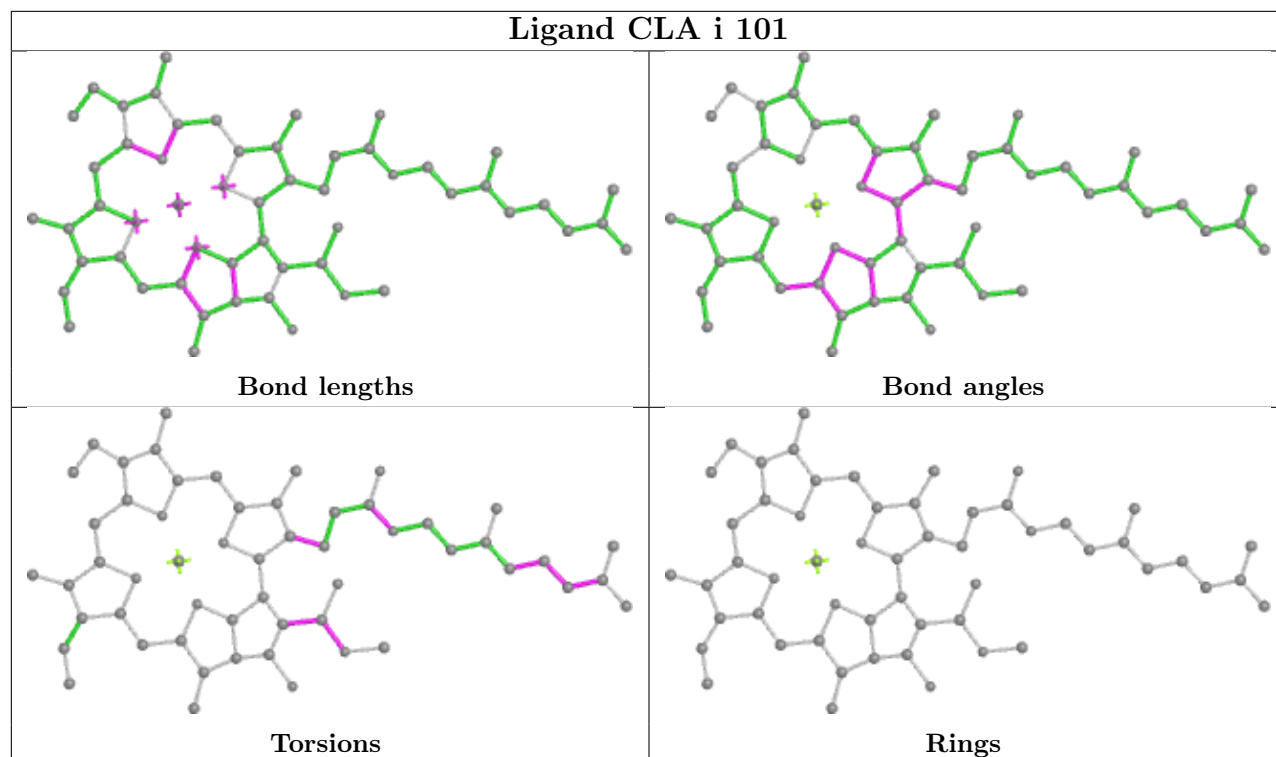




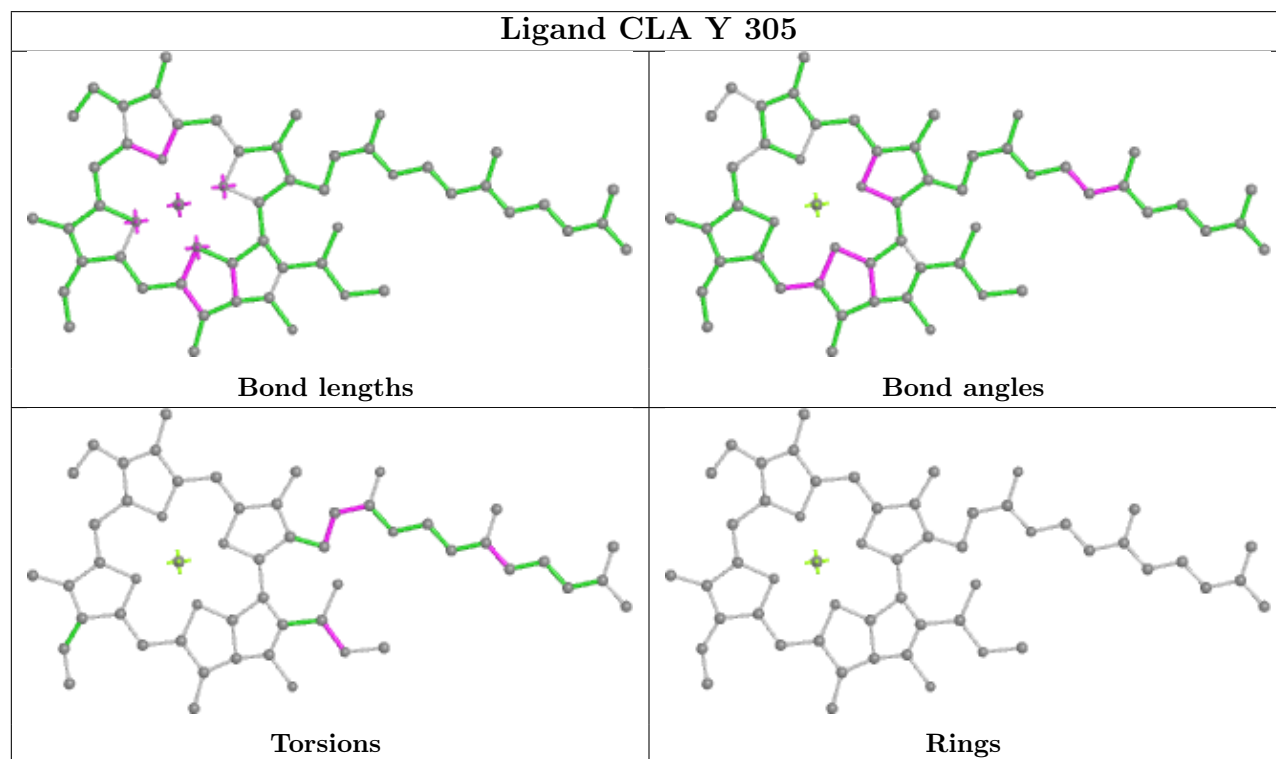


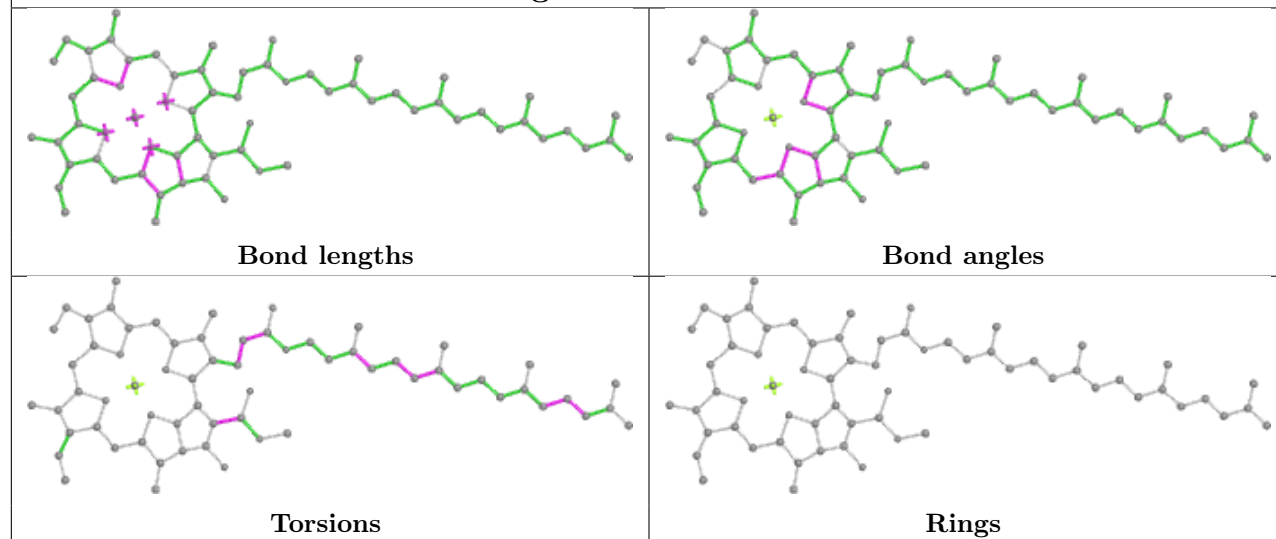
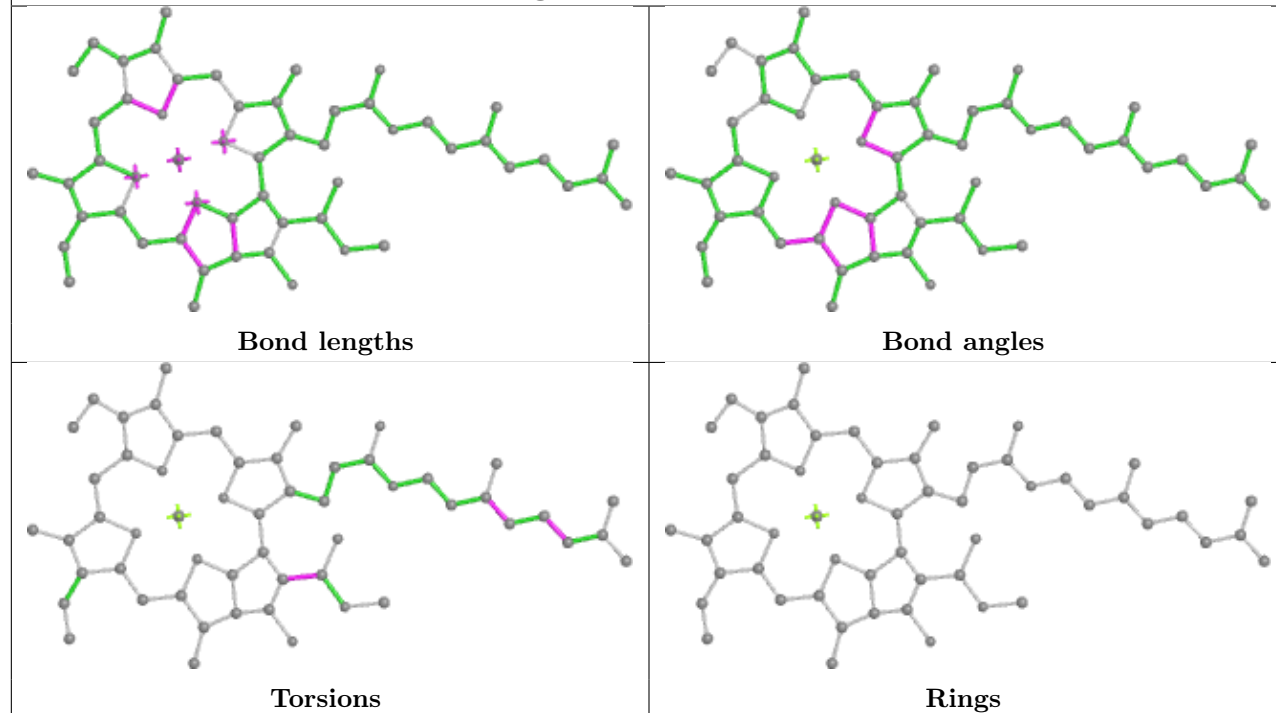


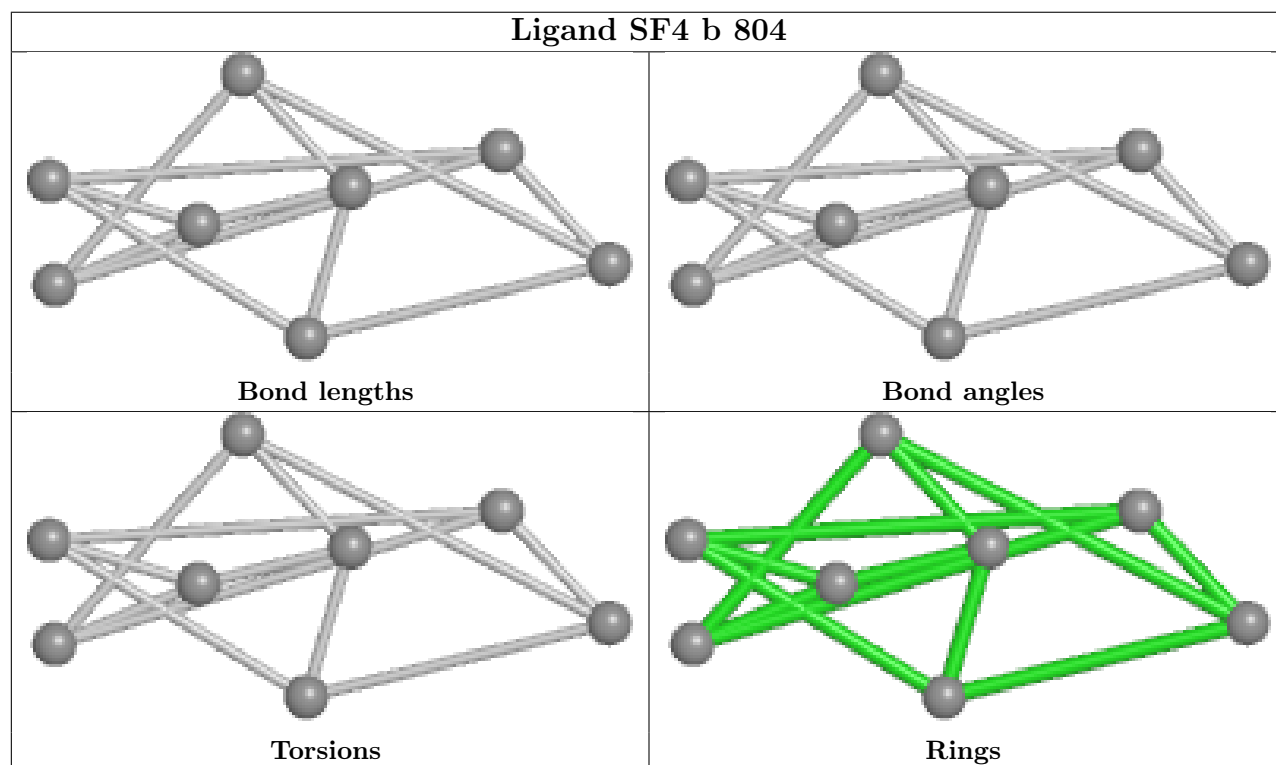
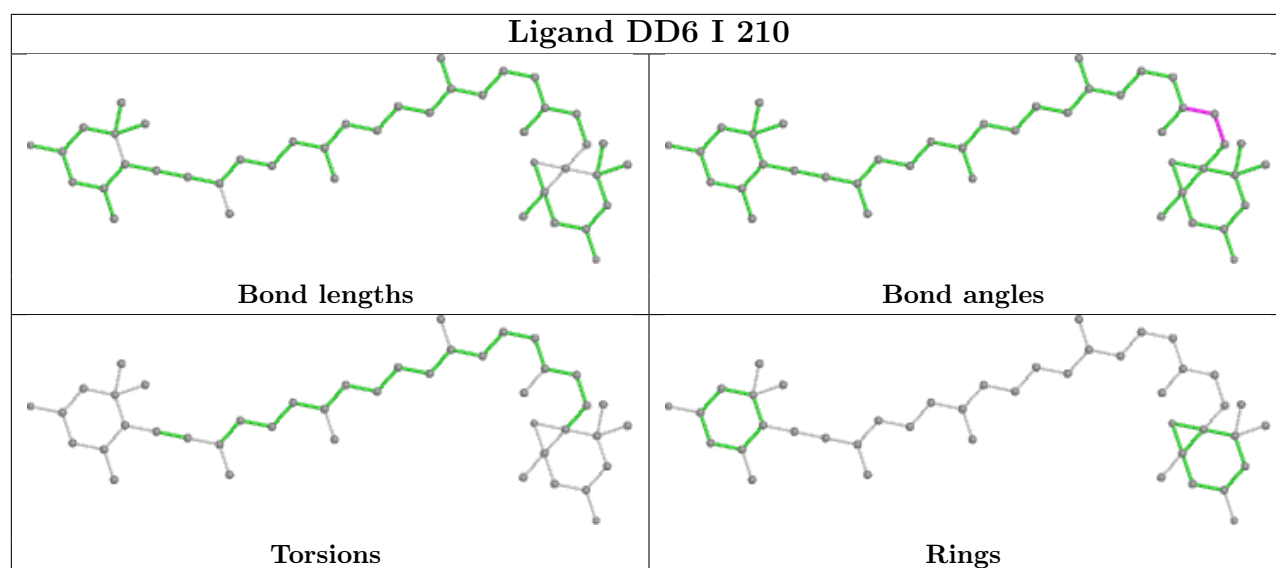
Ligand CLA i 101



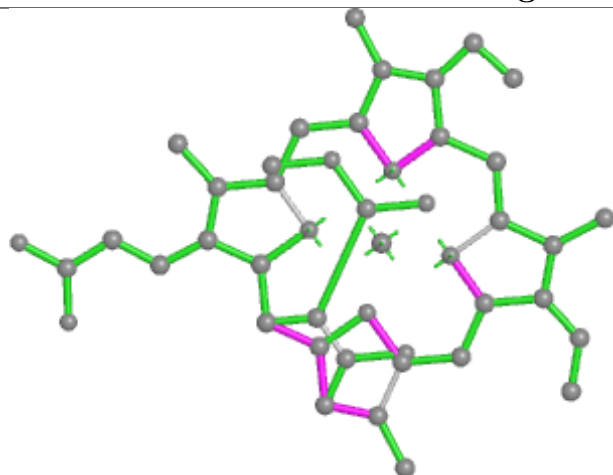
Ligand CLA Y 305



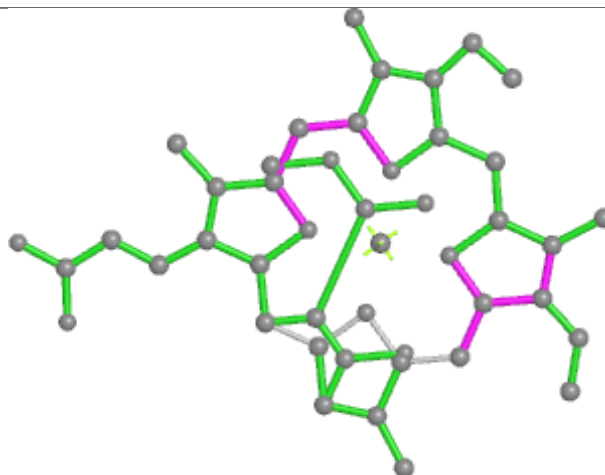
Ligand CLA A 309**Ligand CLA R 307**



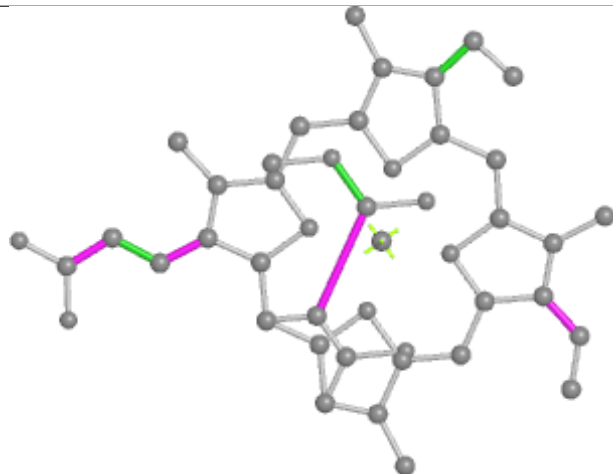
Ligand KC2 Z 302



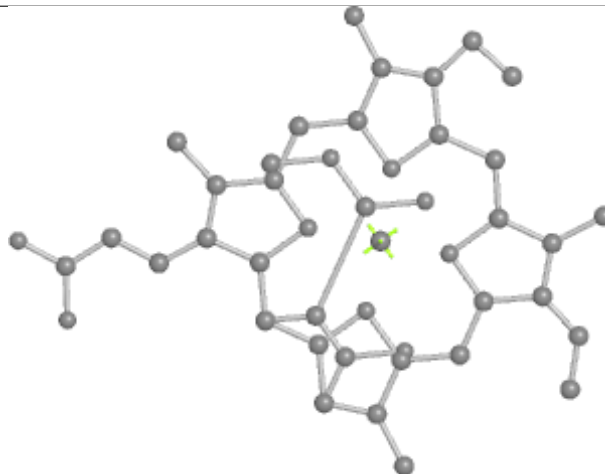
Bond lengths



Bond angles

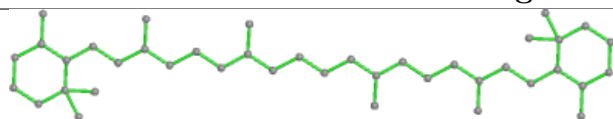


Torsions

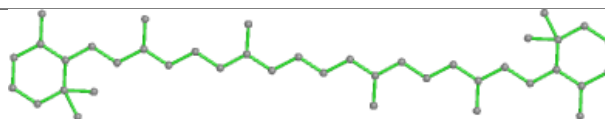


Rings

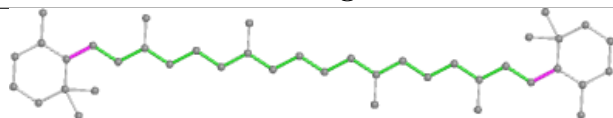
Ligand BCR b 847



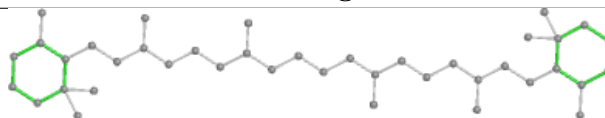
Bond lengths



Bond angles

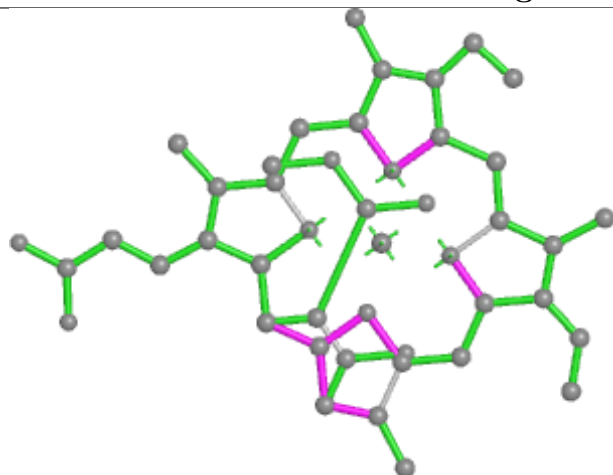


Torsions

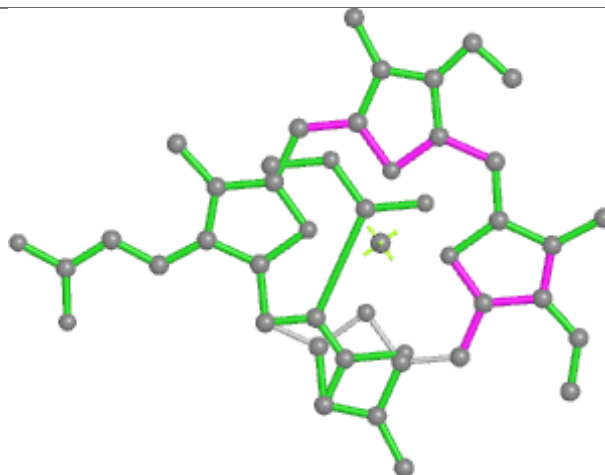


Rings

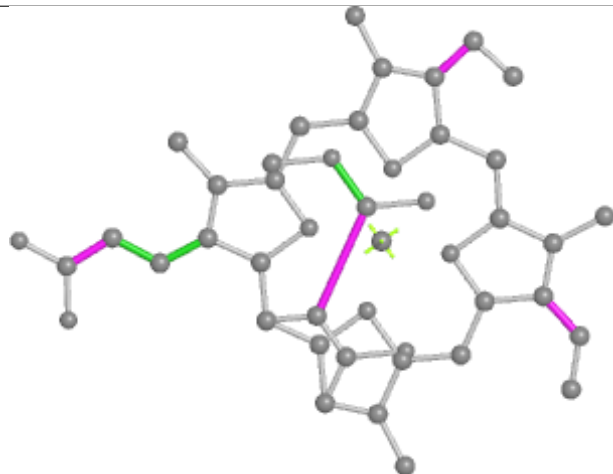
Ligand KC2 Y 309



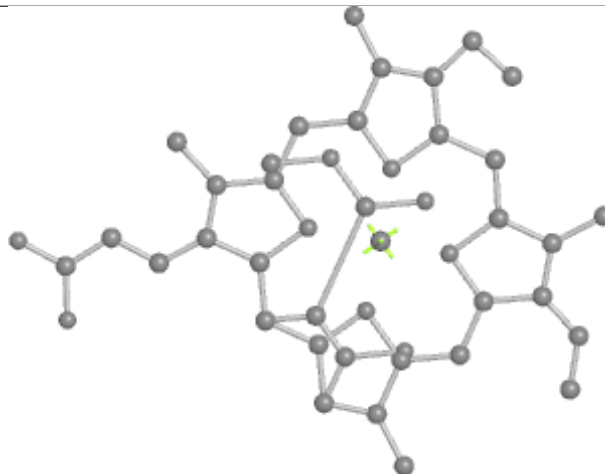
Bond lengths



Bond angles

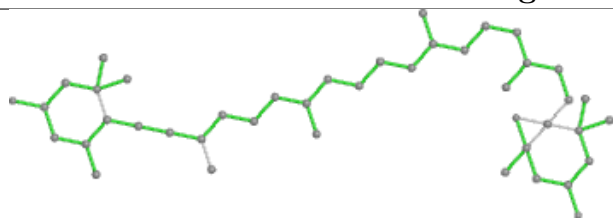


Torsions

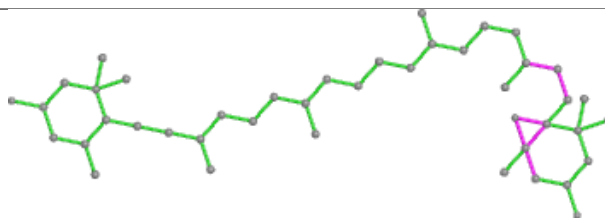


Rings

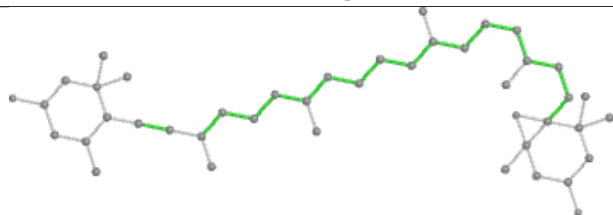
Ligand DD6 v 318



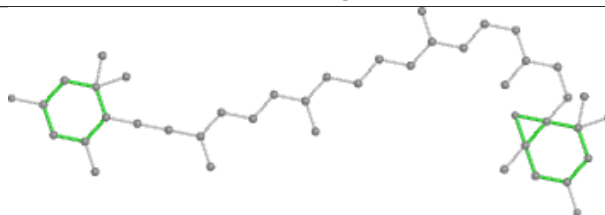
Bond lengths



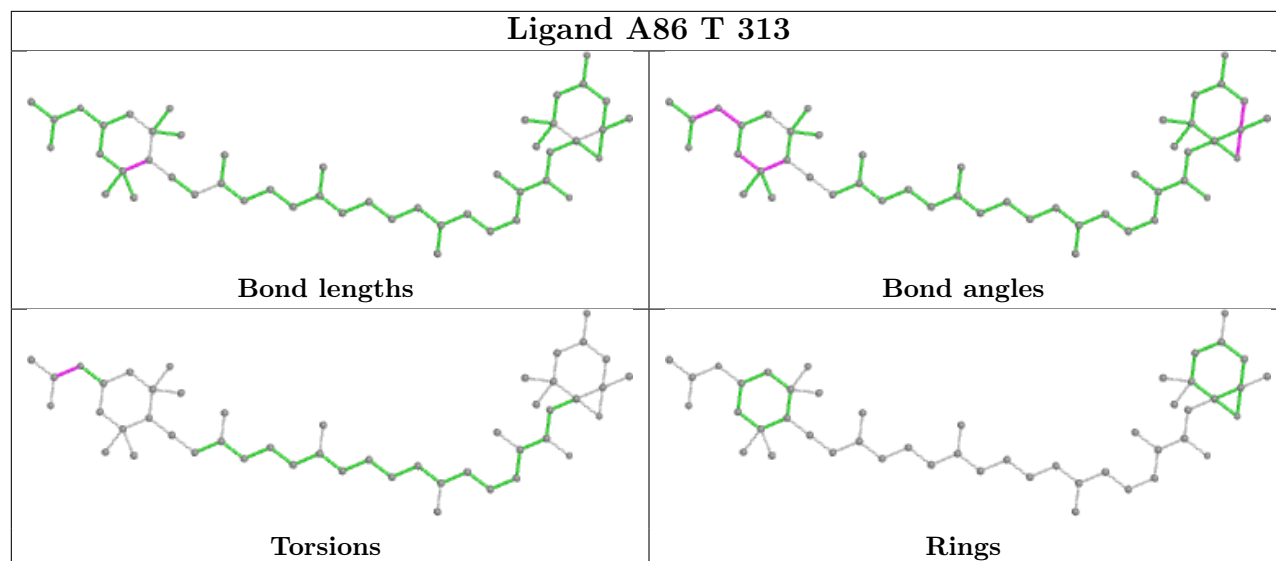
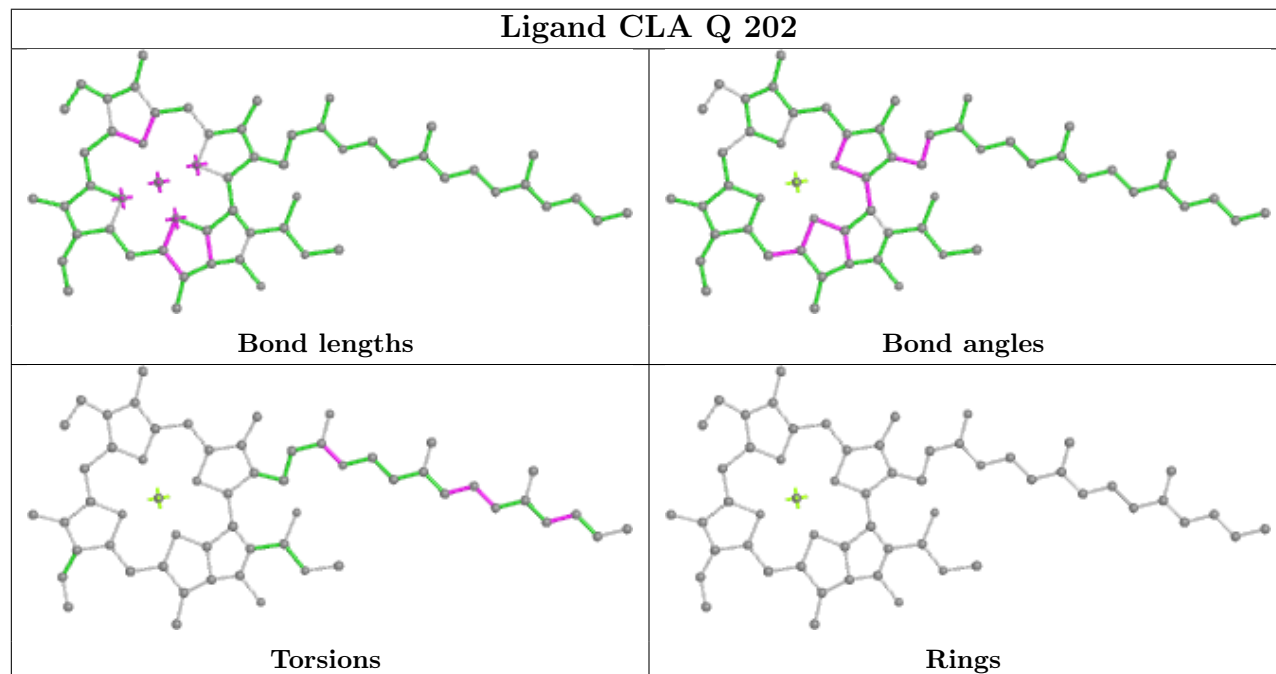
Bond angles



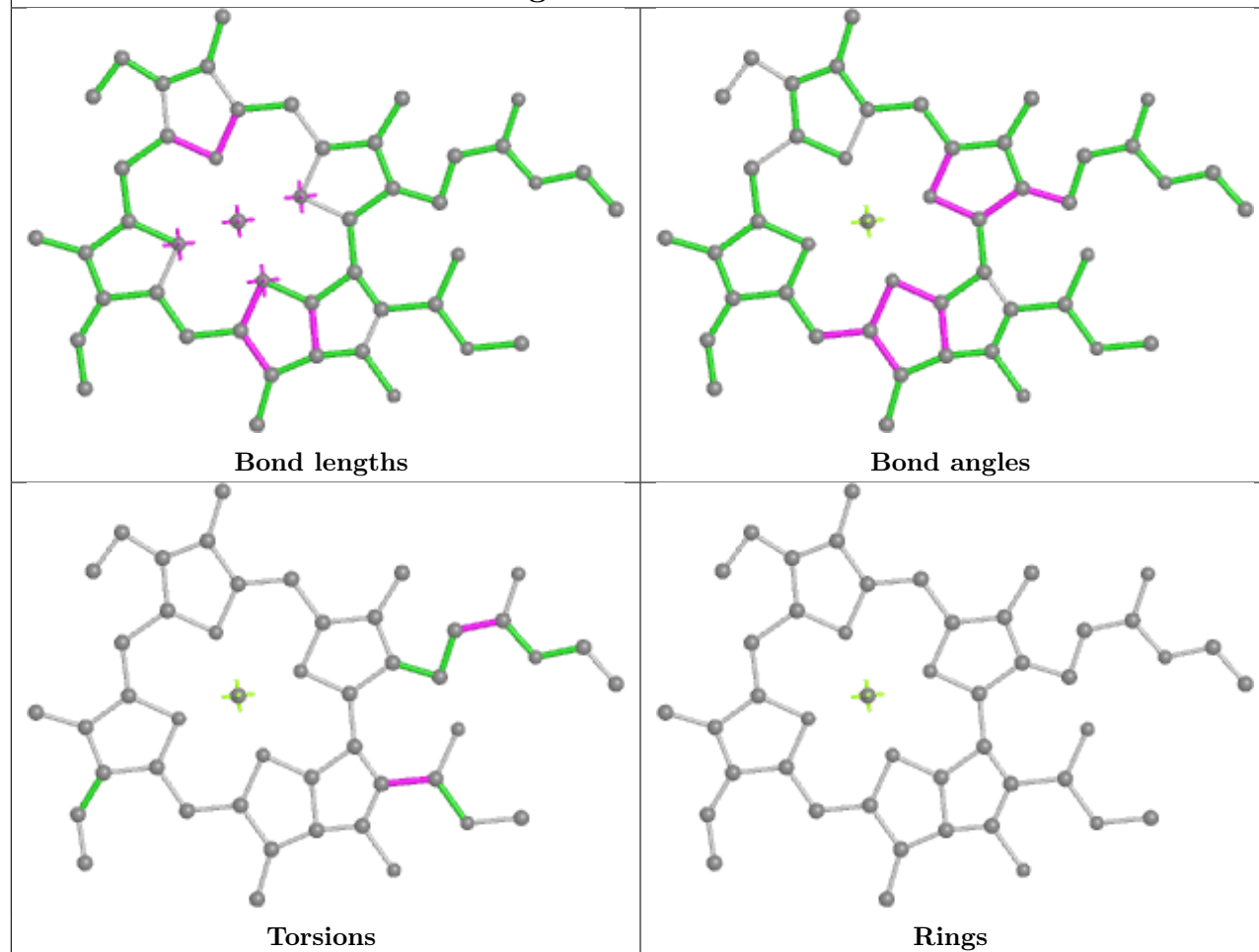
Torsions



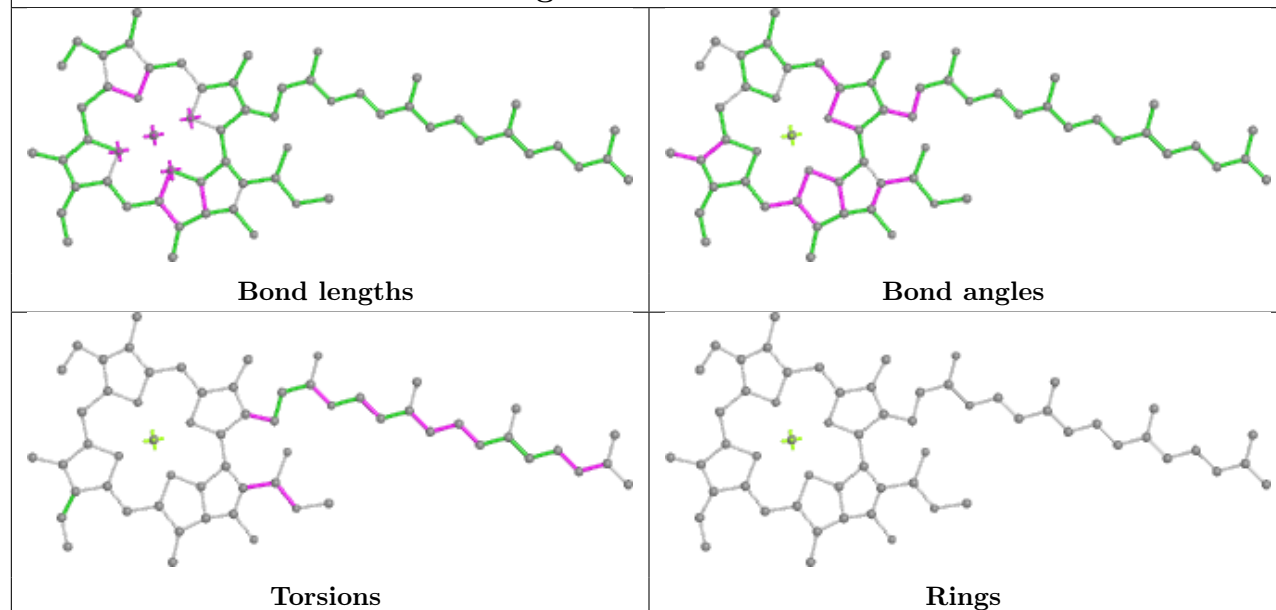
Rings

Ligand A86 T 313**Ligand CLA Q 202**

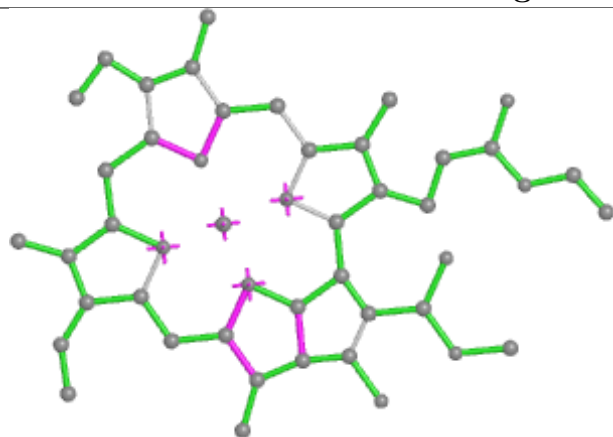
Ligand CLA J 311



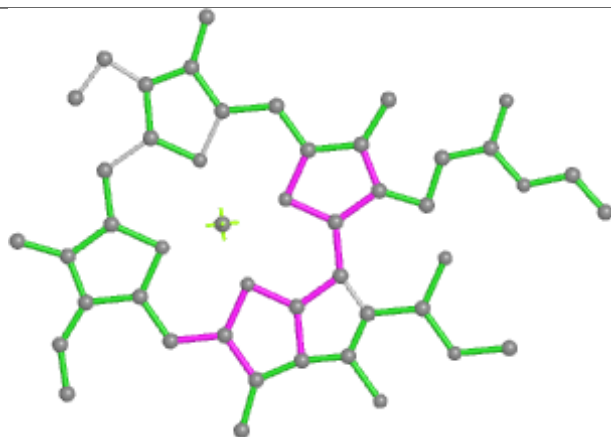
Ligand CLA o 307



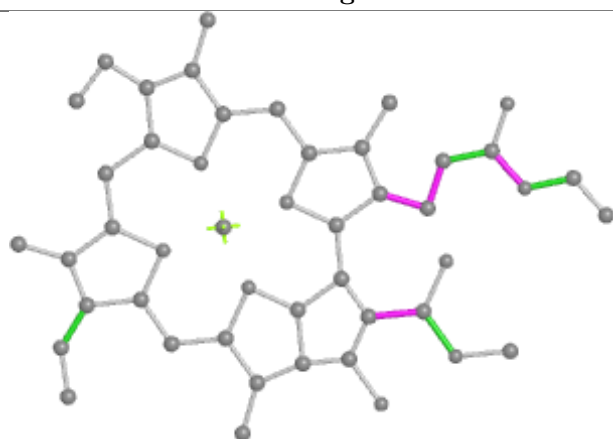
Ligand CLA Y 313



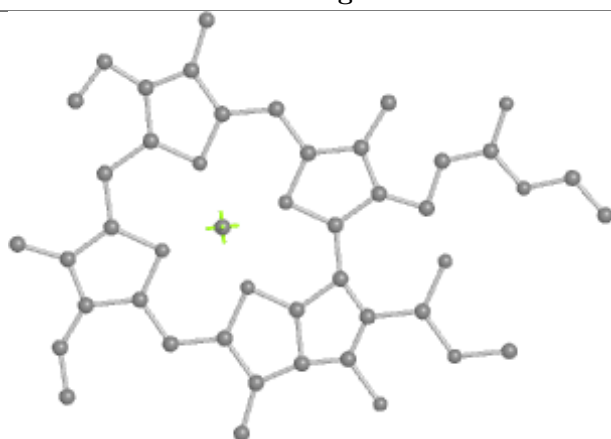
Bond lengths



Bond angles

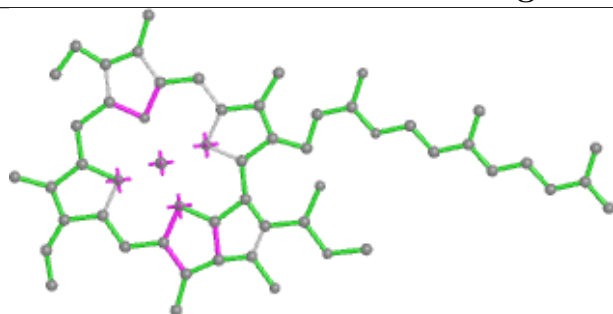


Torsions

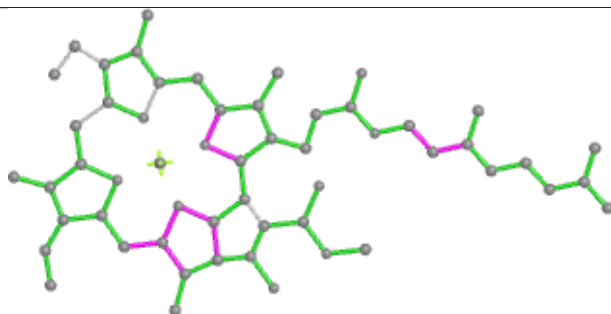


Rings

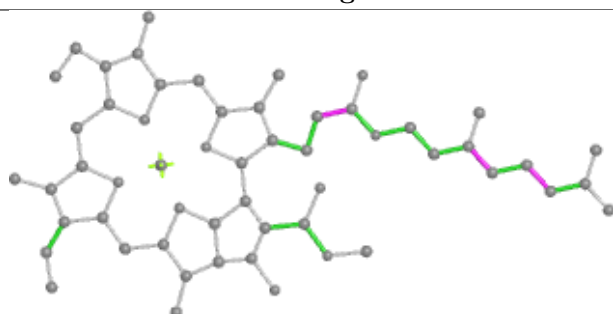
Ligand CLA b 823



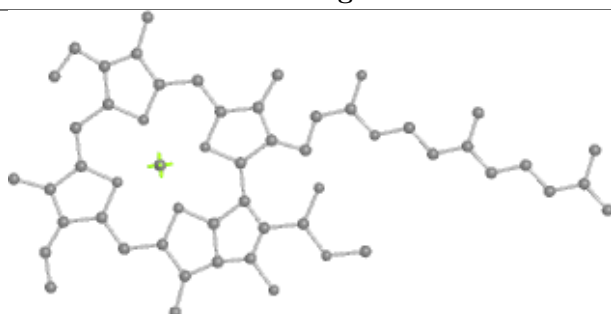
Bond lengths



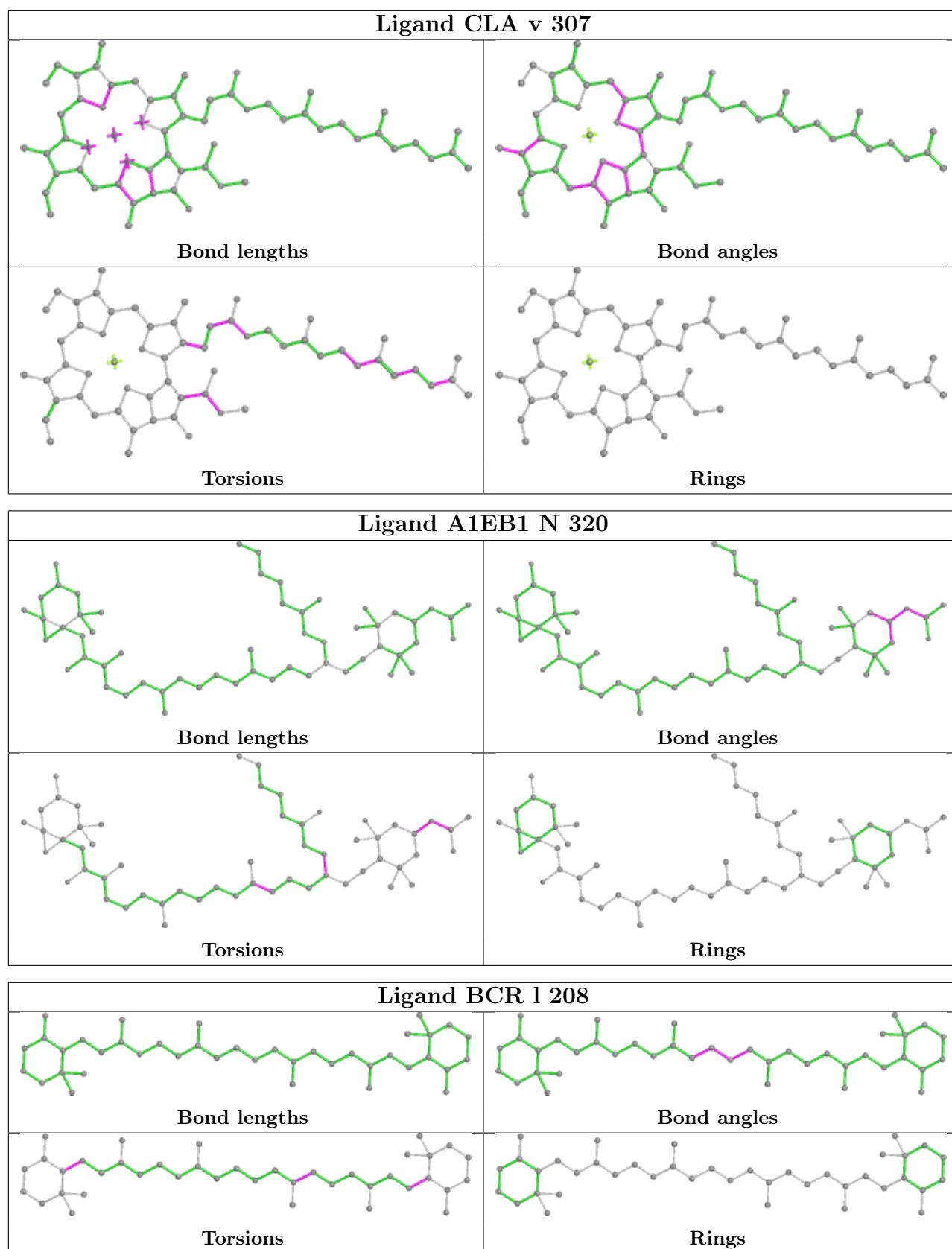
Bond angles

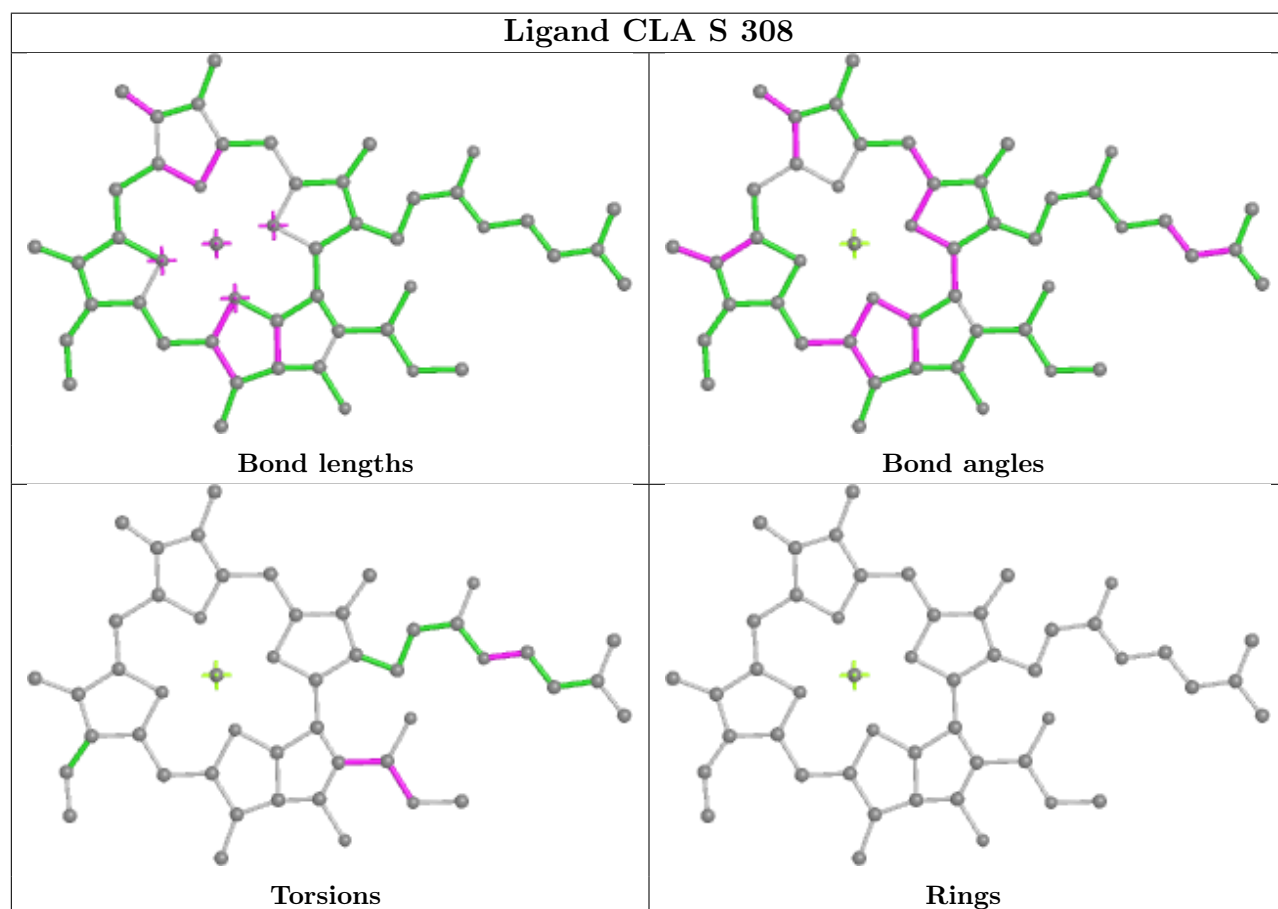
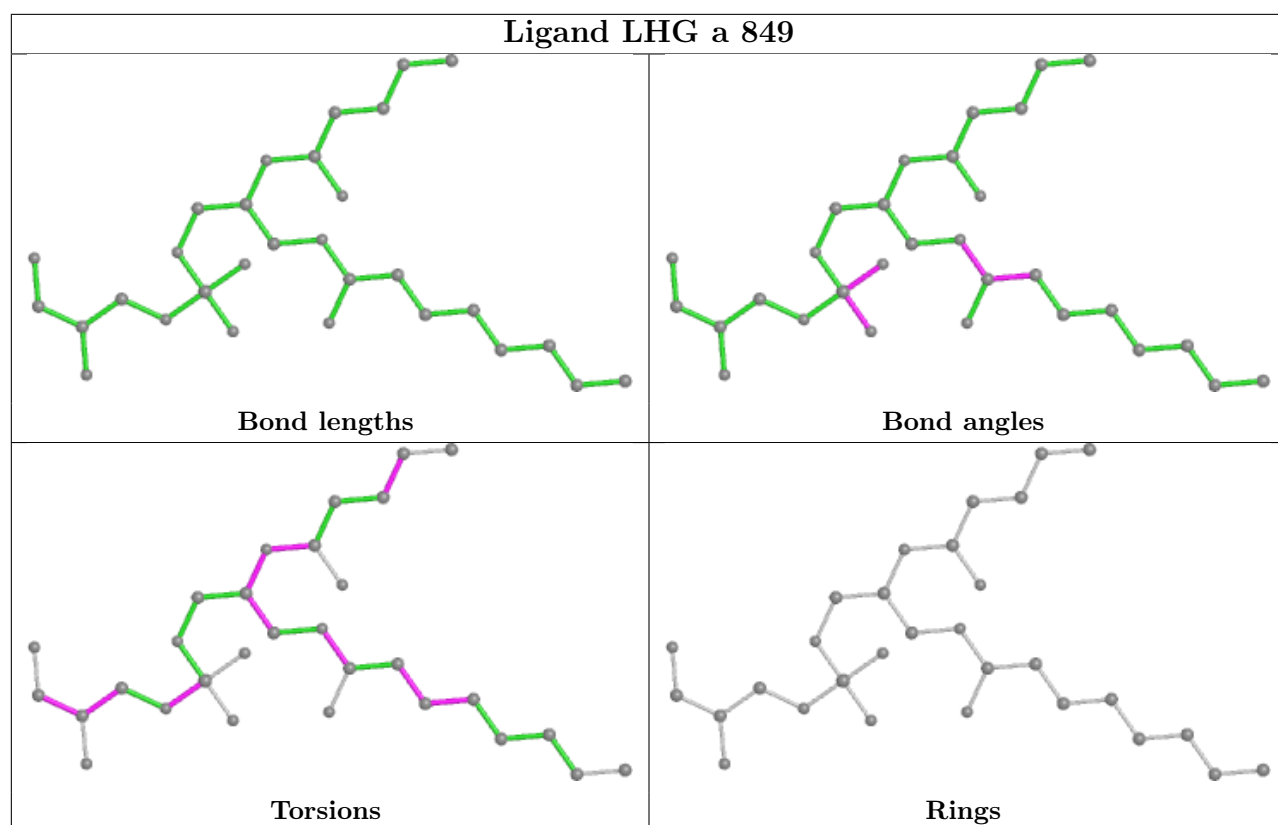


Torsions

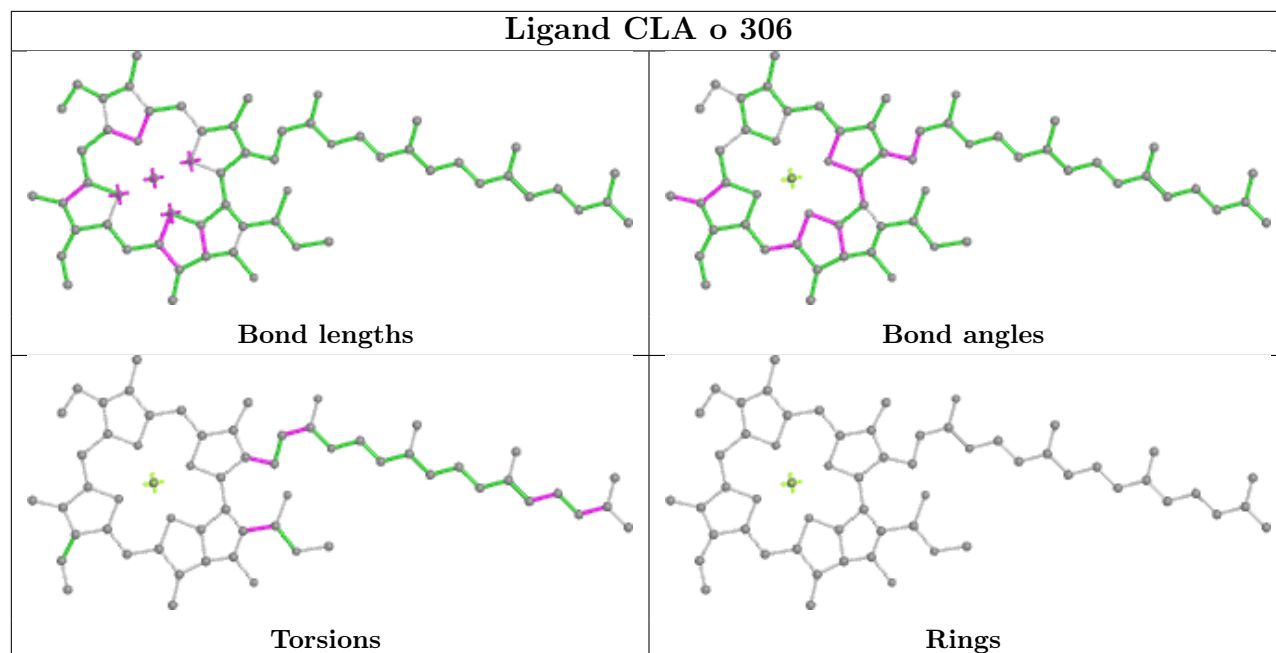


Rings

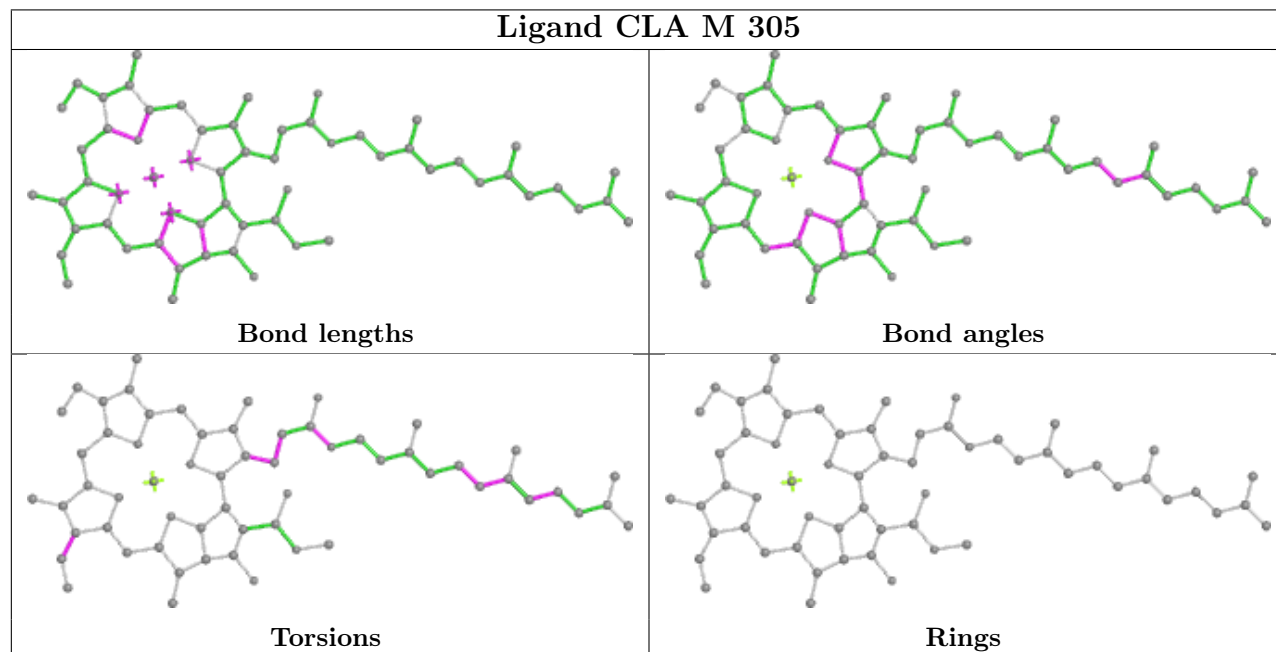




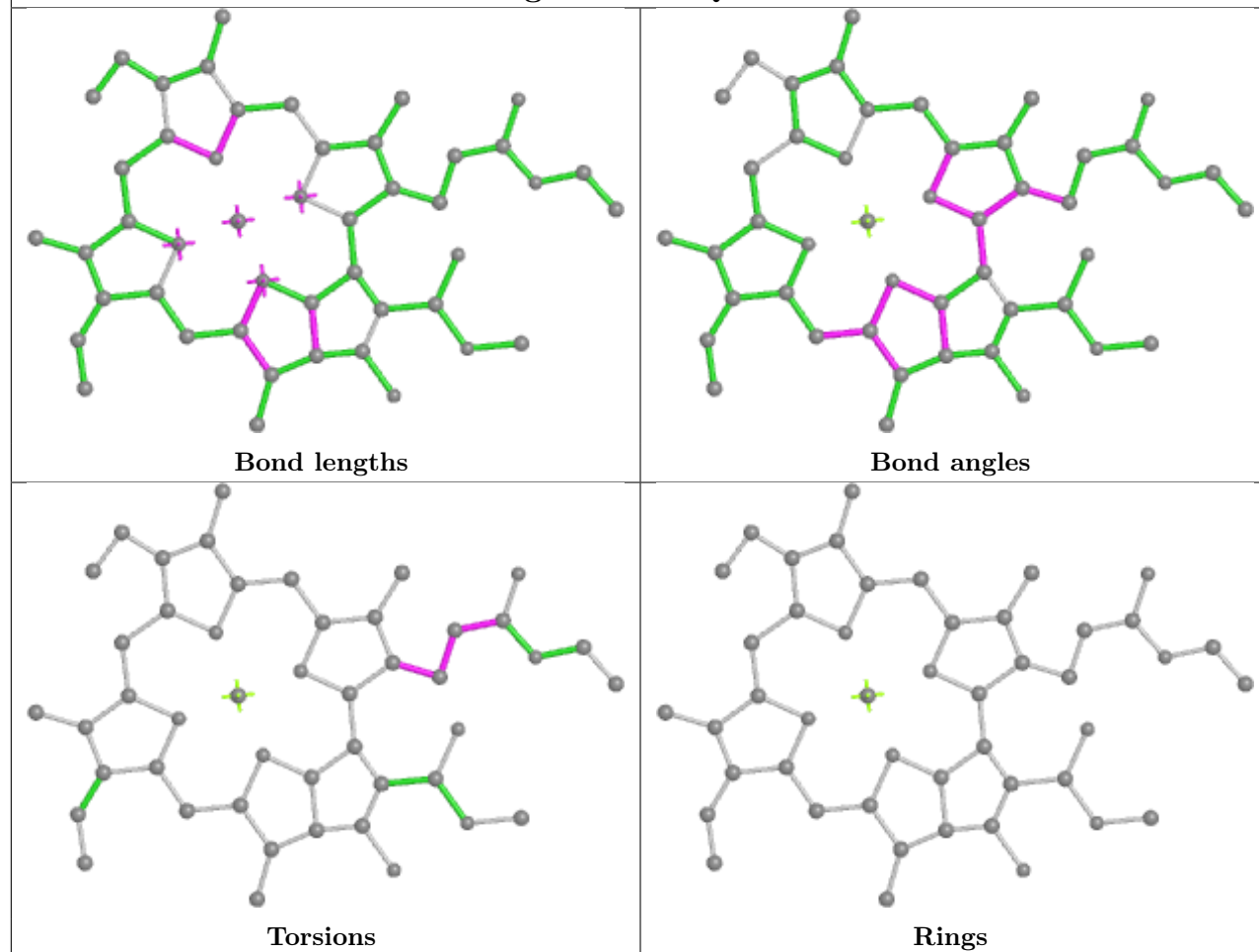
Ligand CLA o 306



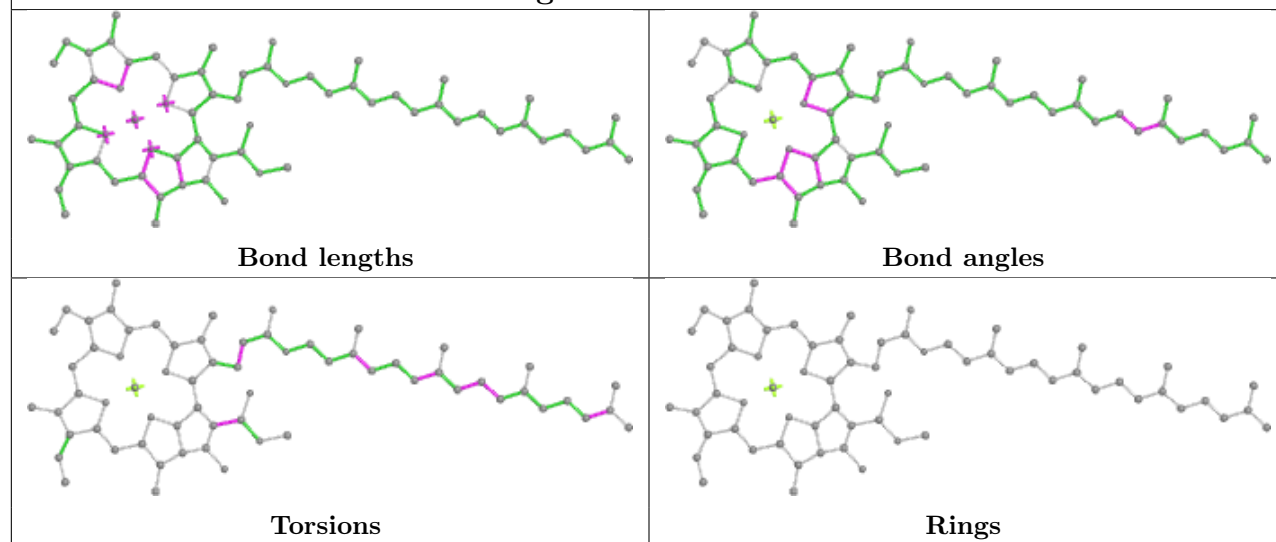
Ligand CLA M 305

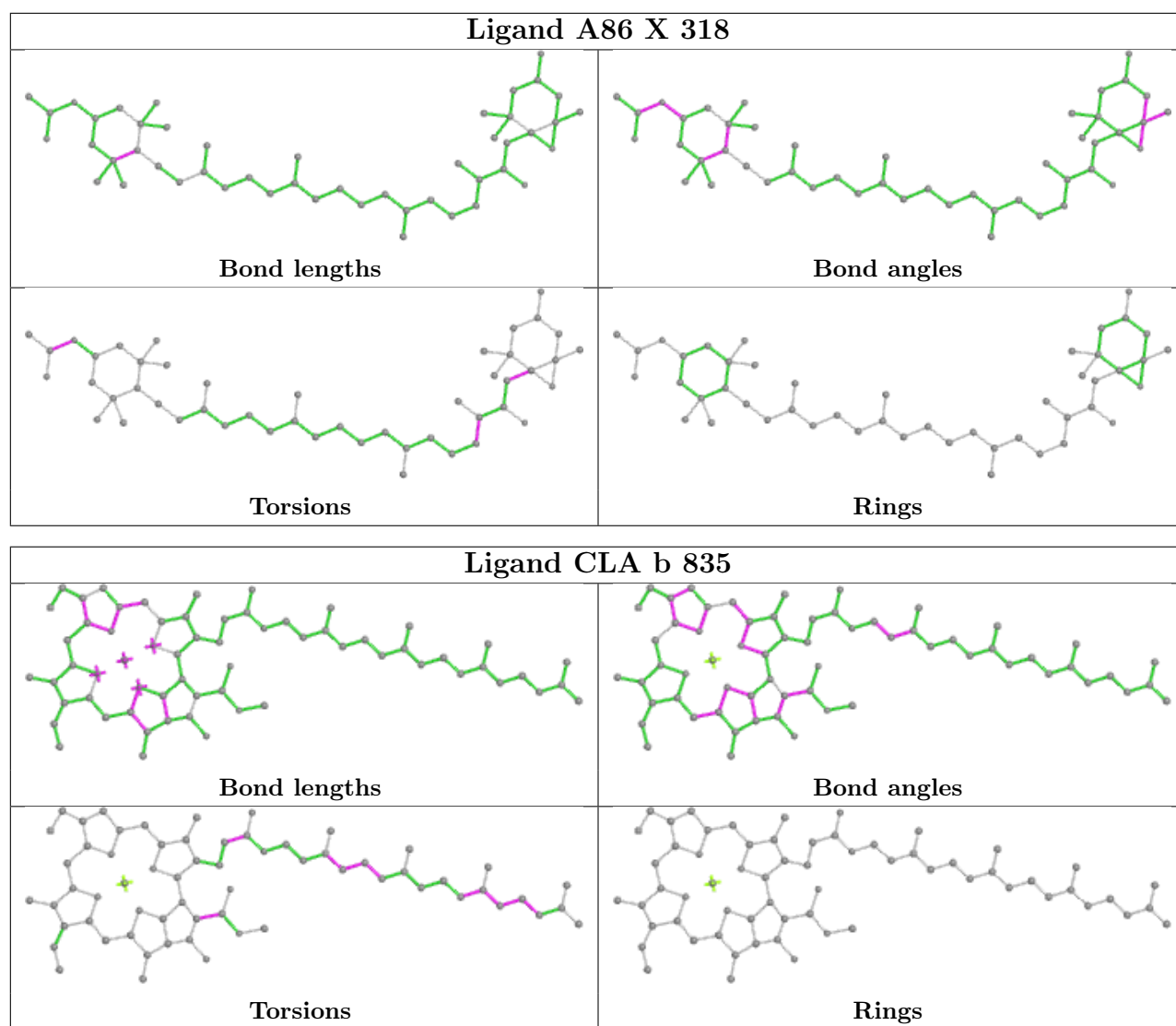


Ligand CLA Q 209

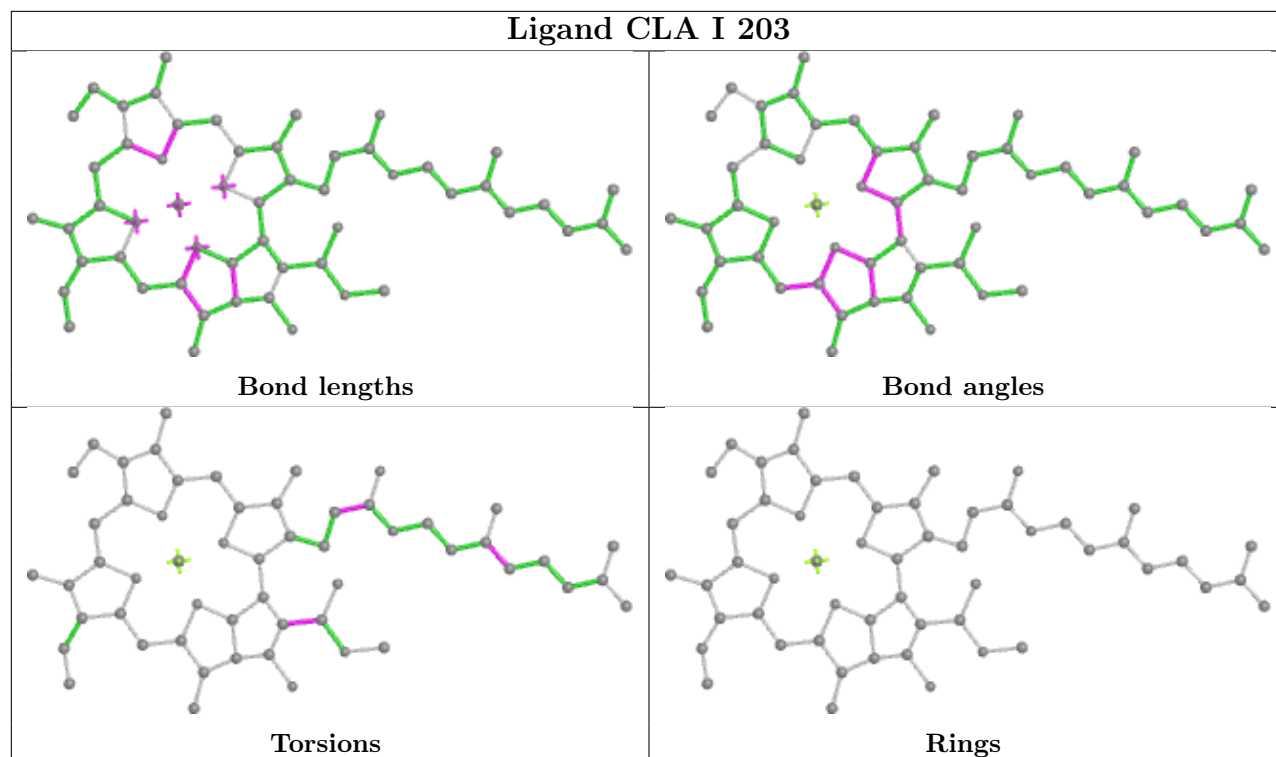


Ligand CLA a 806

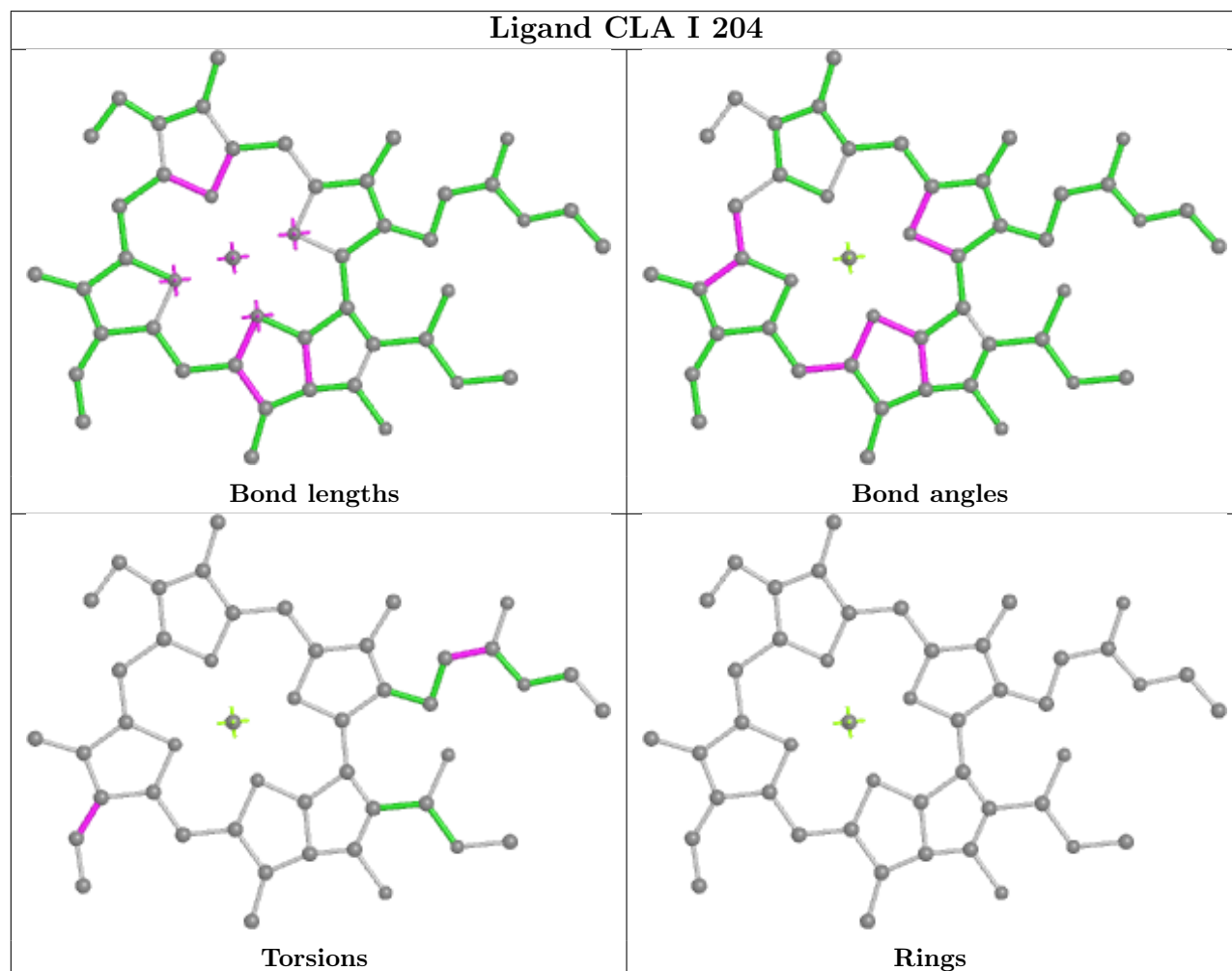


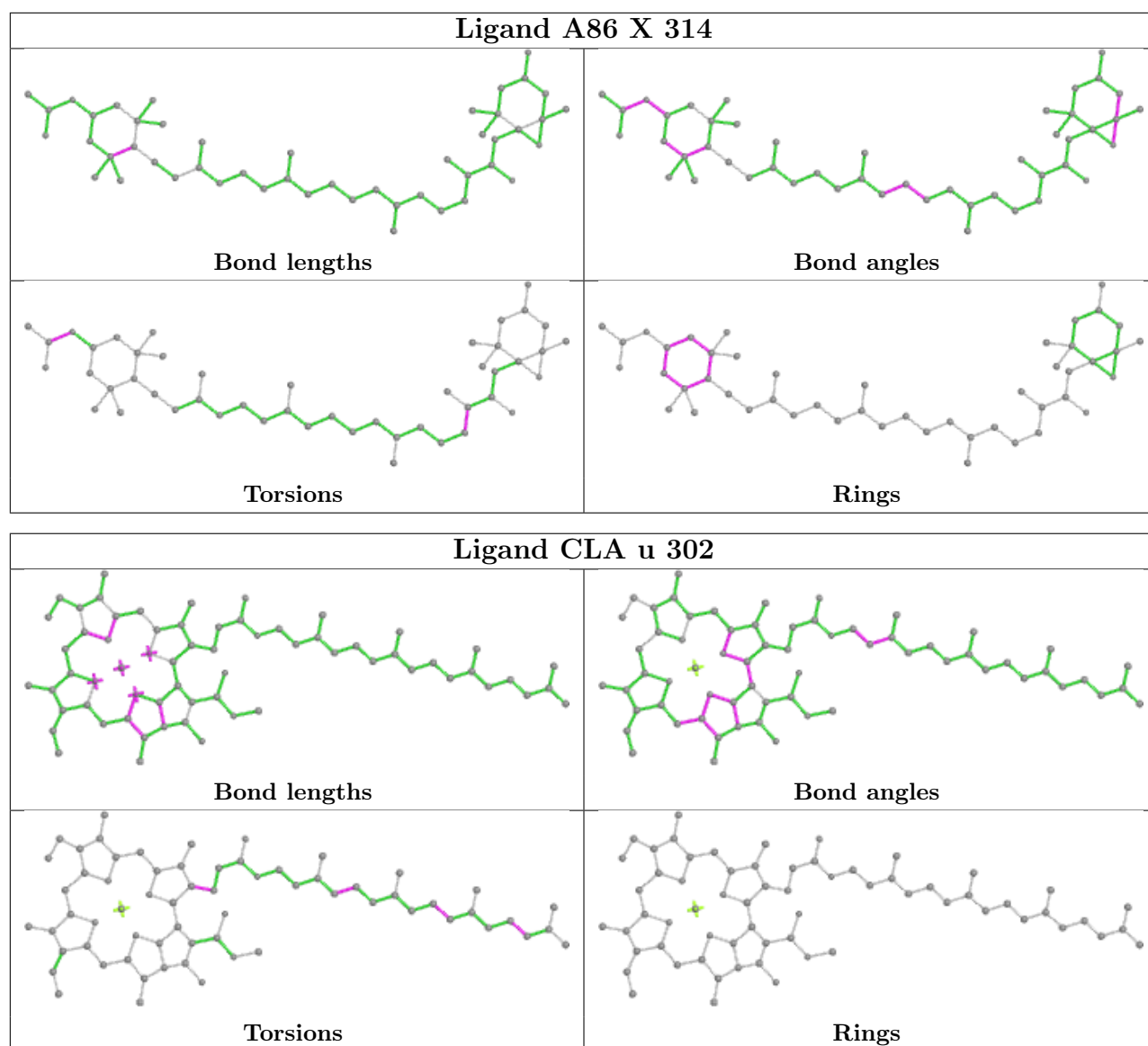


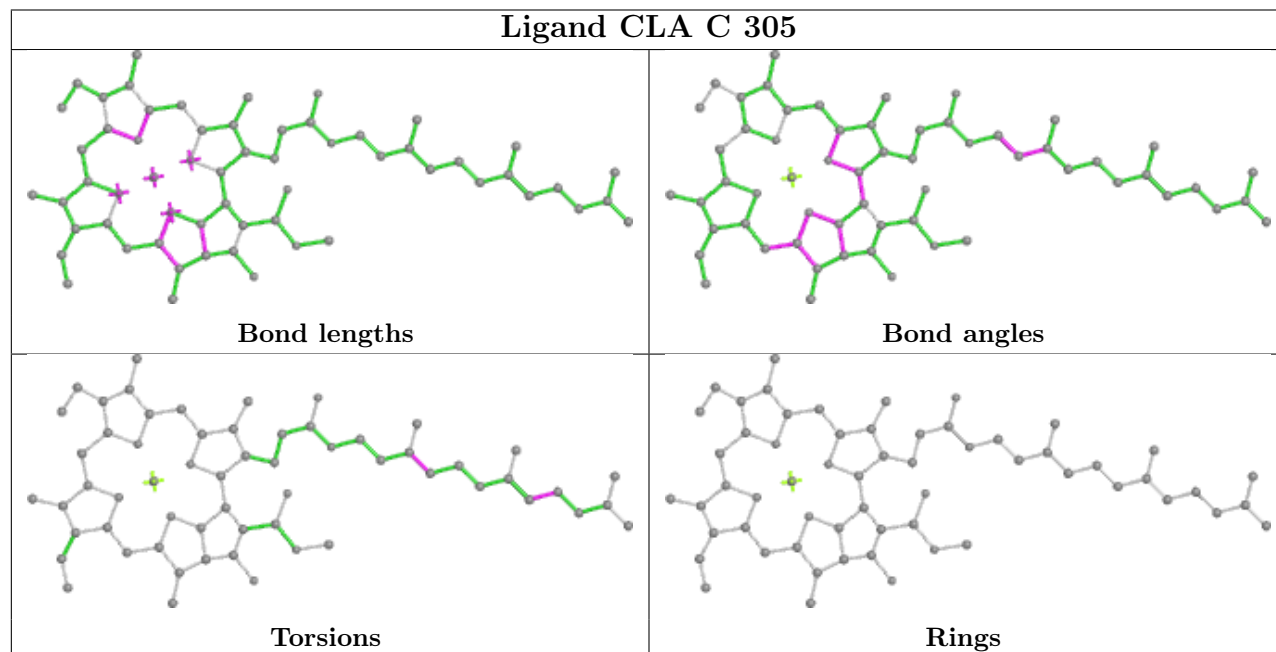
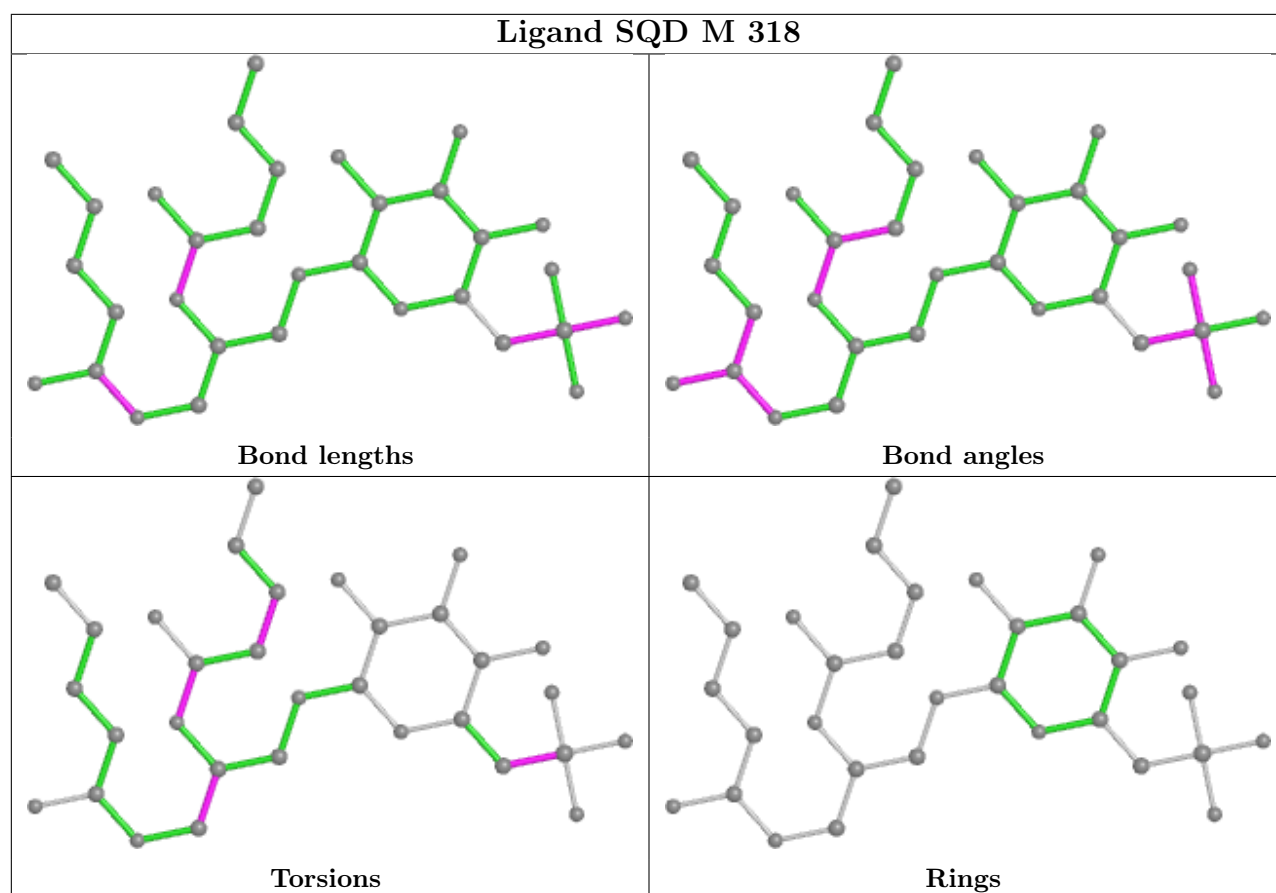
Ligand CLA I 203

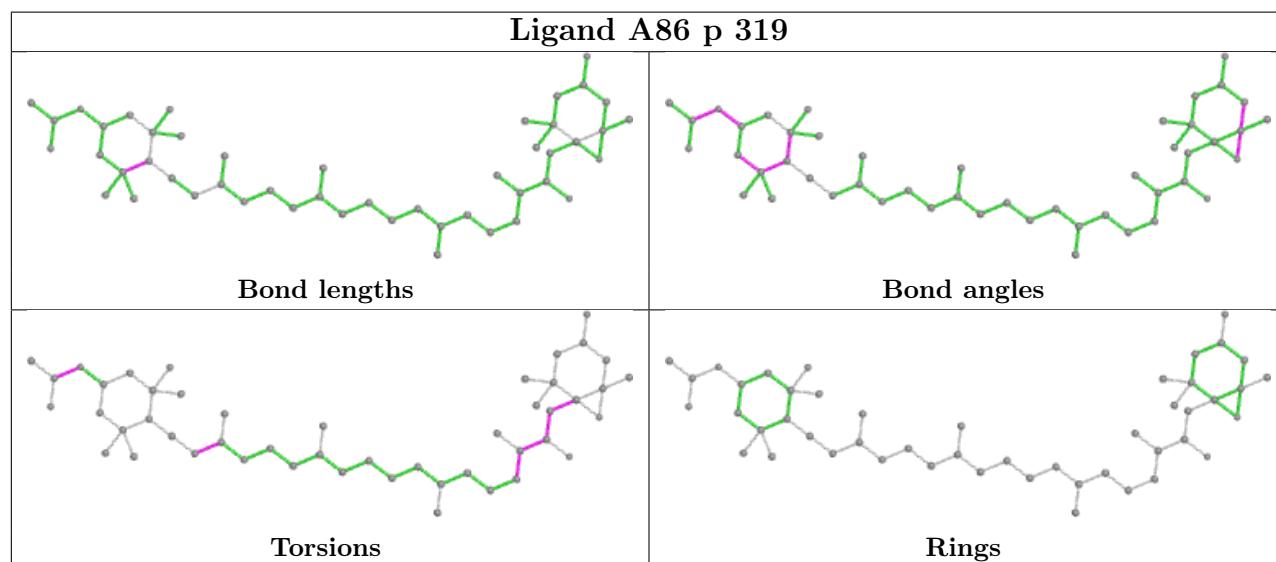
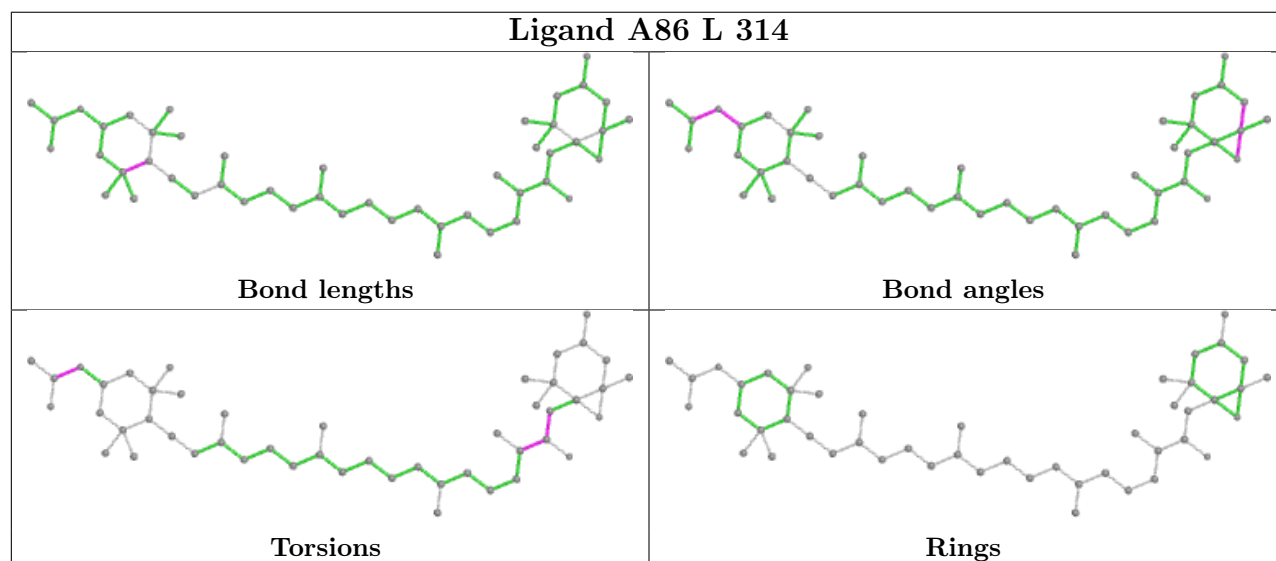
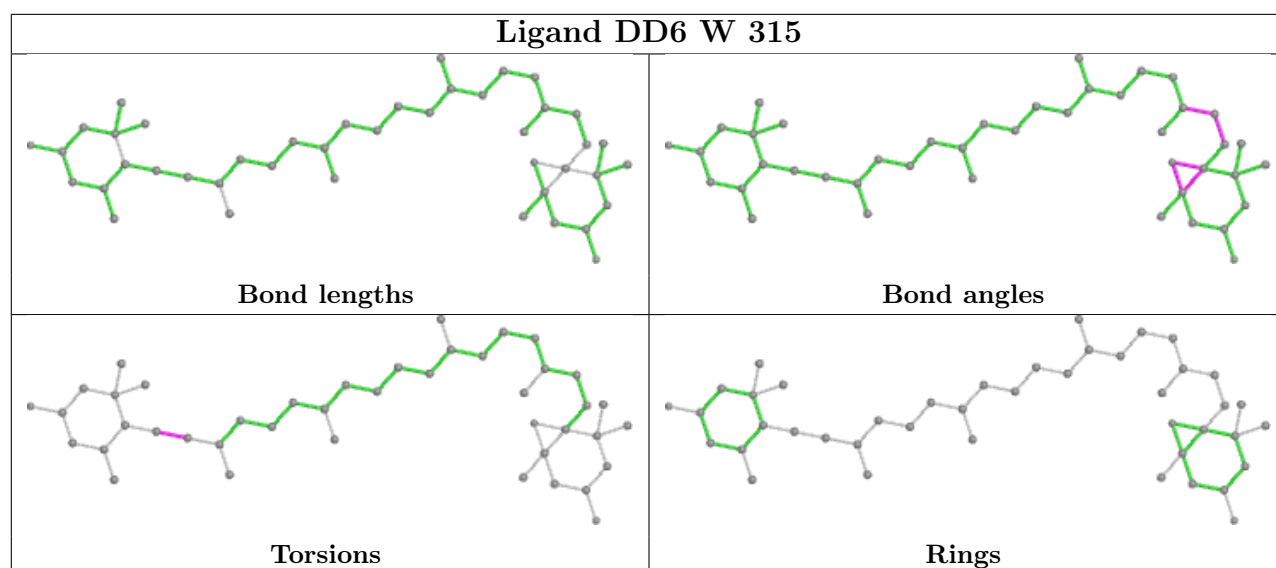


Ligand CLA I 204









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.

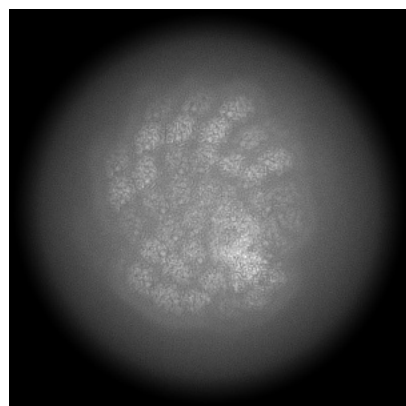
6 Map visualisation [i](#)

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.

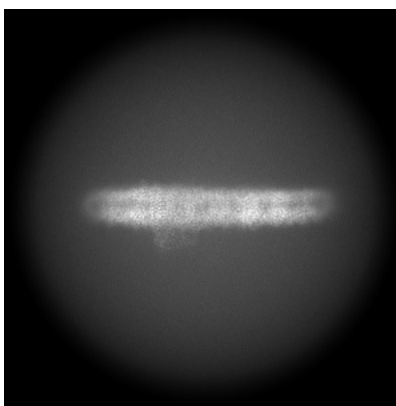
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

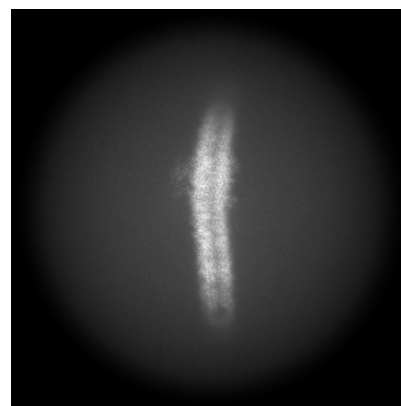
6.1.1 Primary map



X

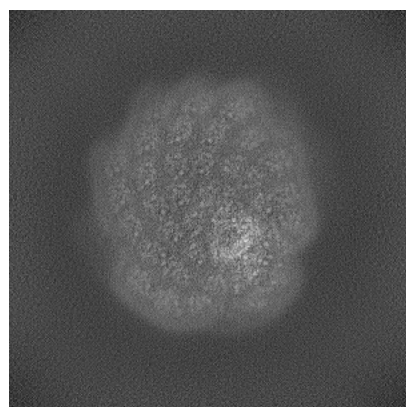


Y

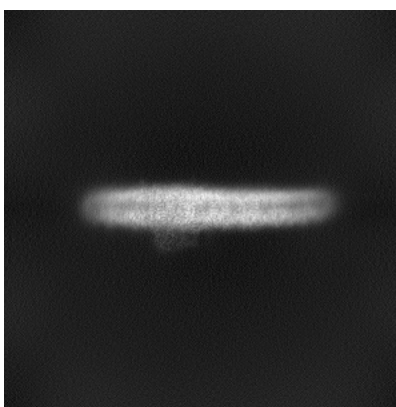


Z

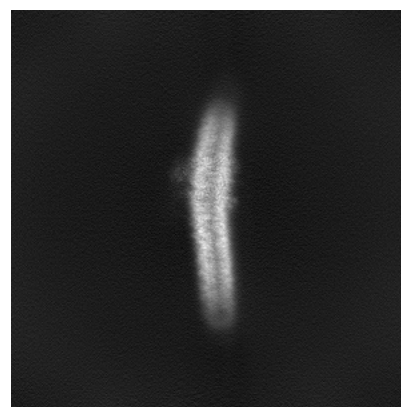
6.1.2 Raw map



X



Y

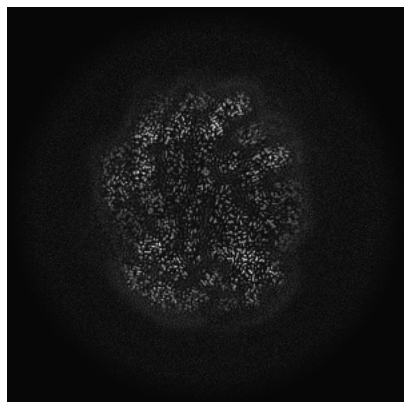


Z

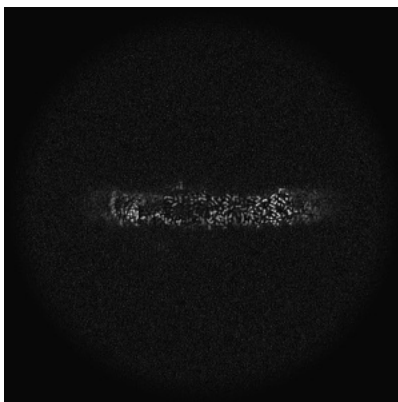
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

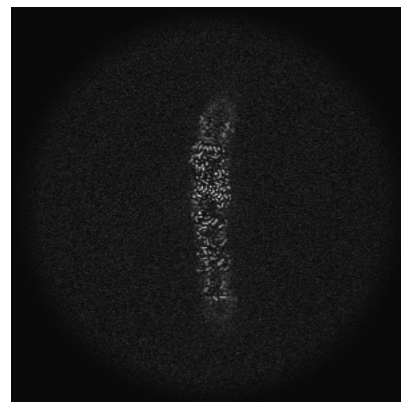
6.2.1 Primary map



X Index: 250

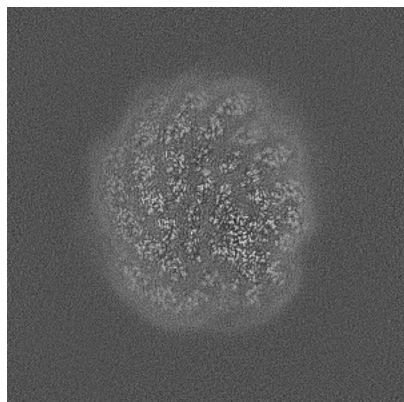


Y Index: 250

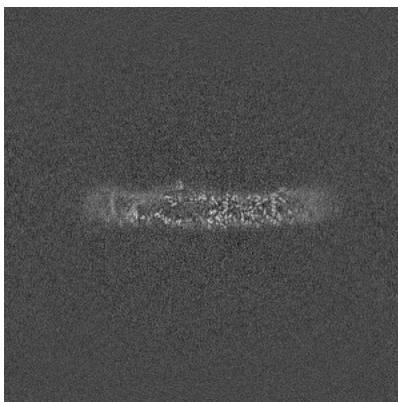


Z Index: 250

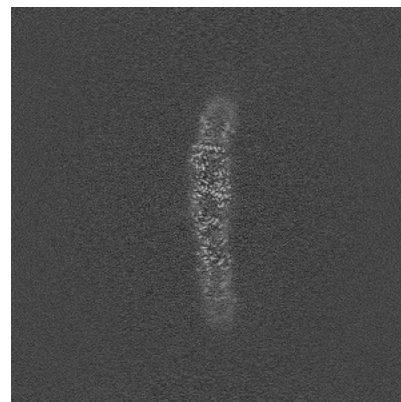
6.2.2 Raw map



X Index: 250



Y Index: 250

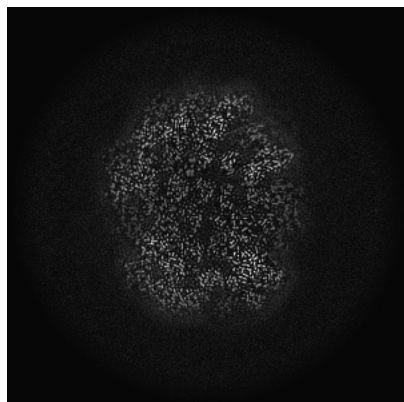


Z Index: 250

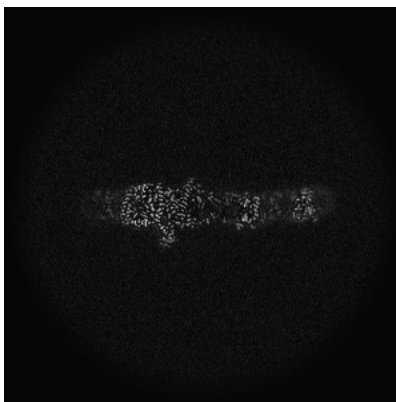
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

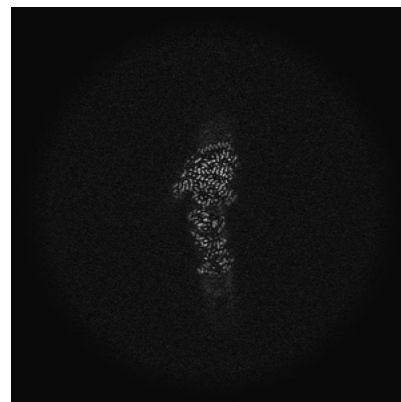
6.3.1 Primary map



X Index: 244

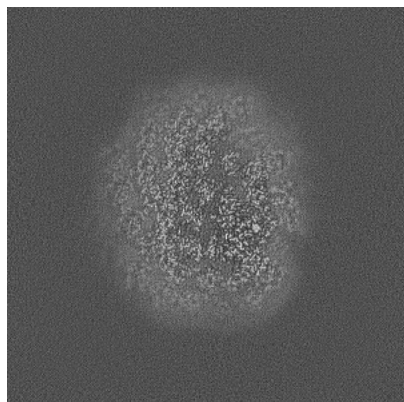


Y Index: 285



Z Index: 191

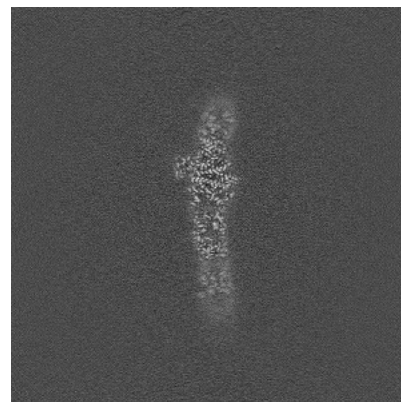
6.3.2 Raw map



X Index: 242



Y Index: 295

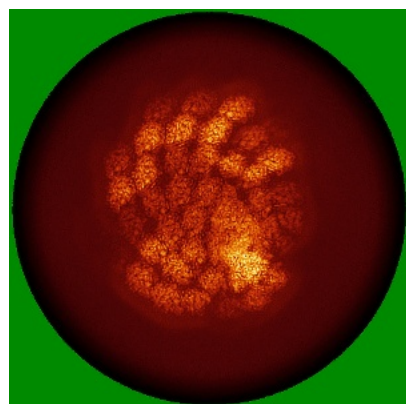


Z Index: 230

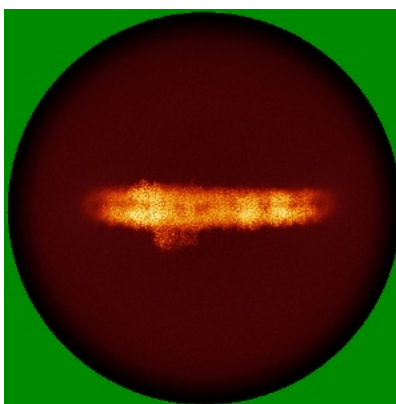
The images above show the largest variance slices of the map in three orthogonal directions.

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

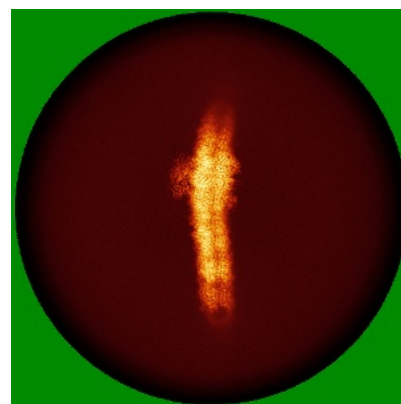
6.4.1 Primary map



X

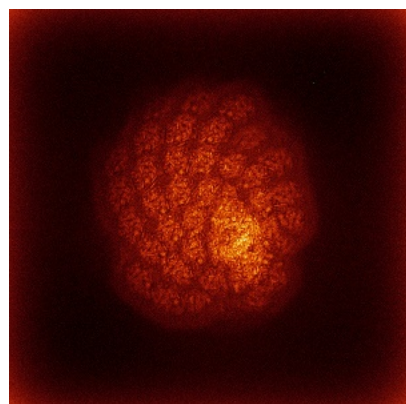


Y

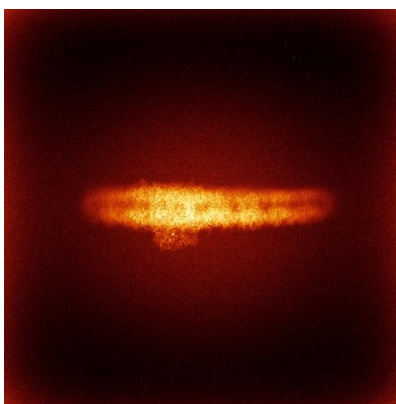


Z

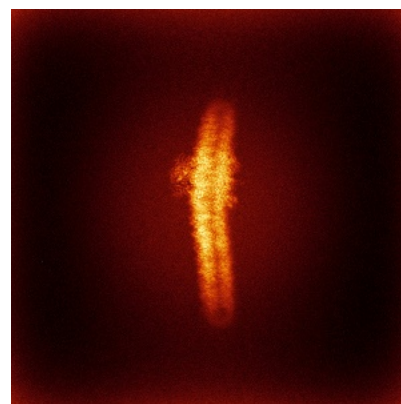
6.4.2 Raw map



X



Y

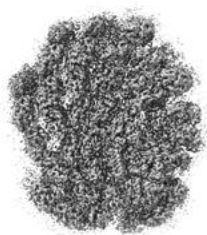


Z

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



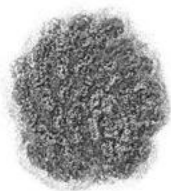
Y



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.

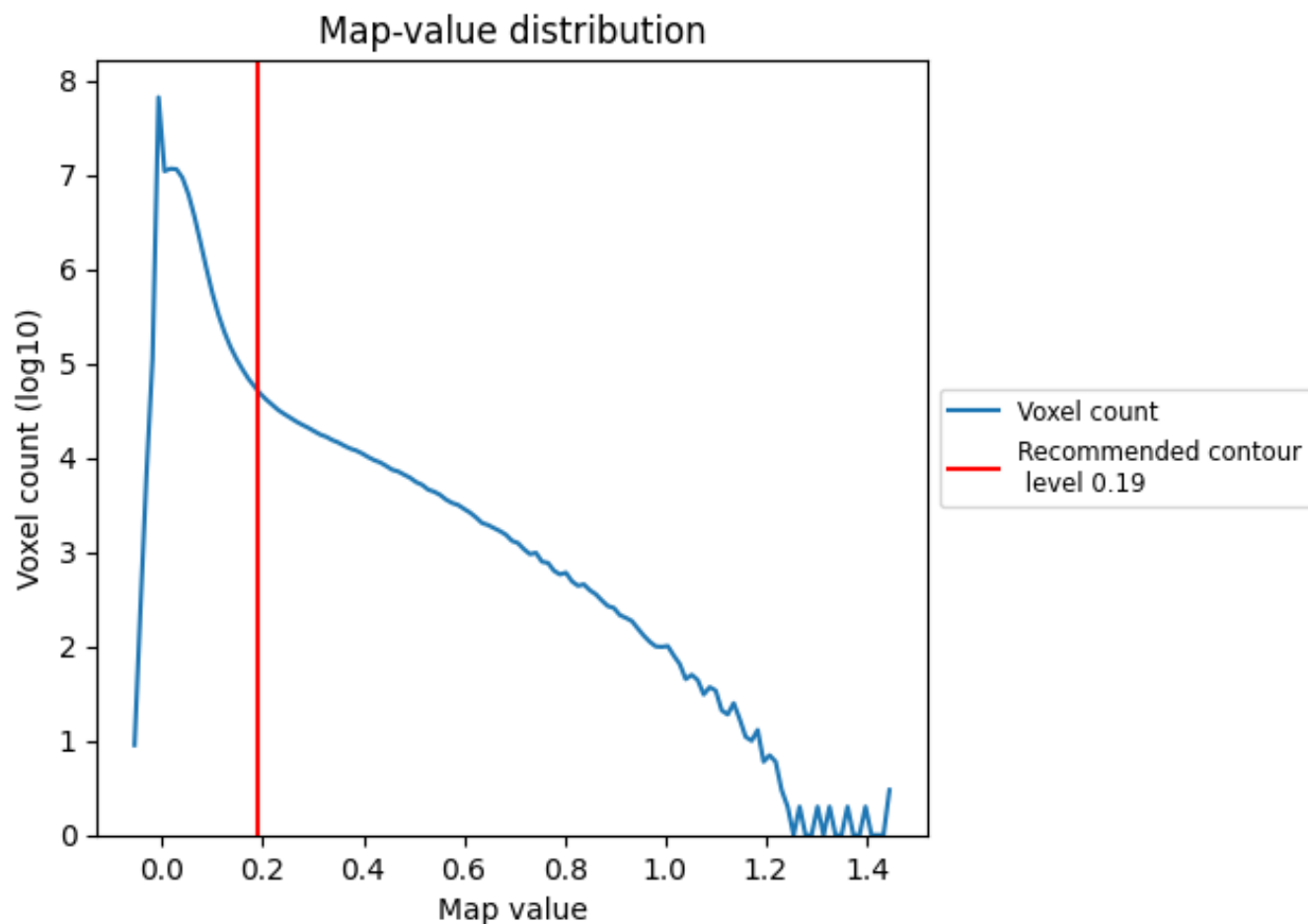
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

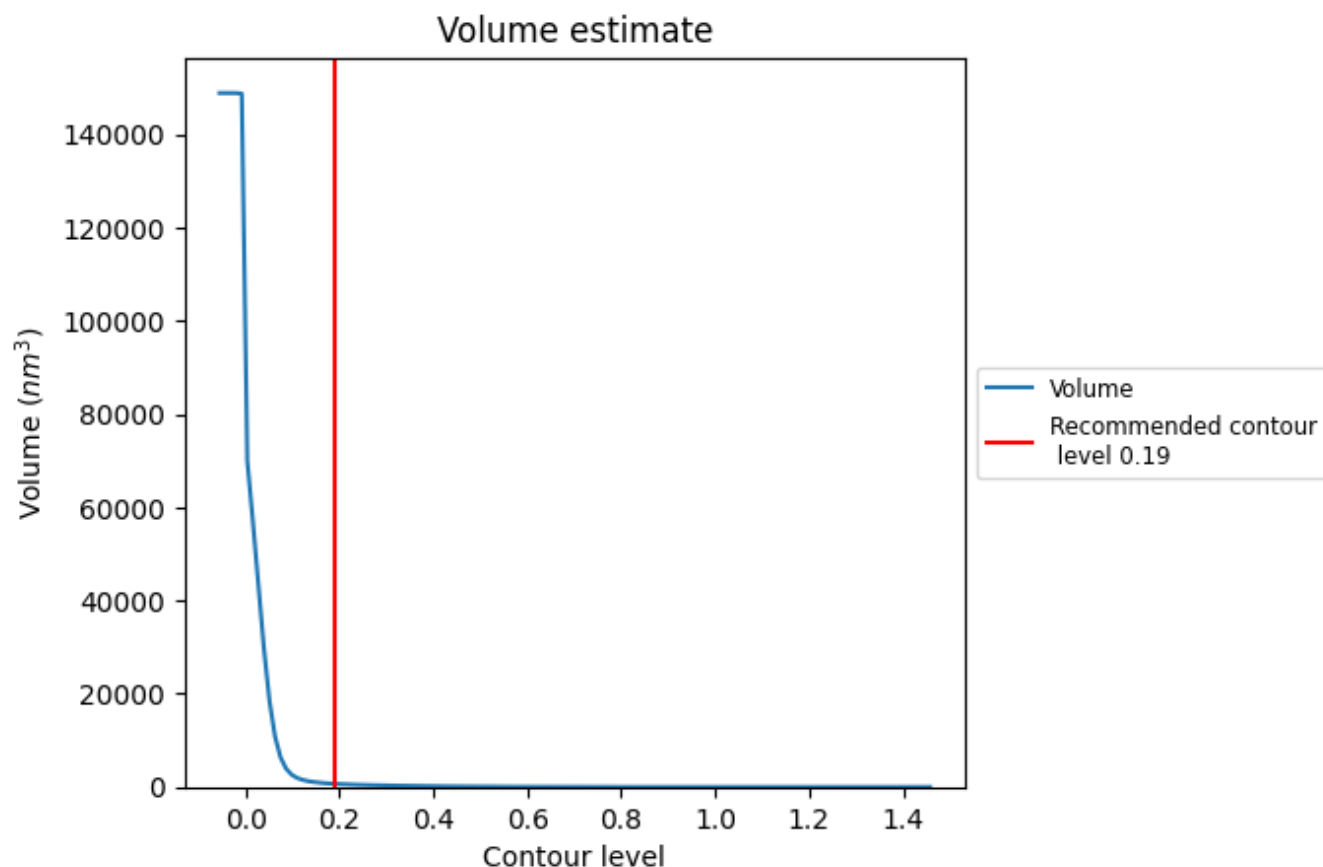
This section contains the results of statistical analysis of the map.

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.

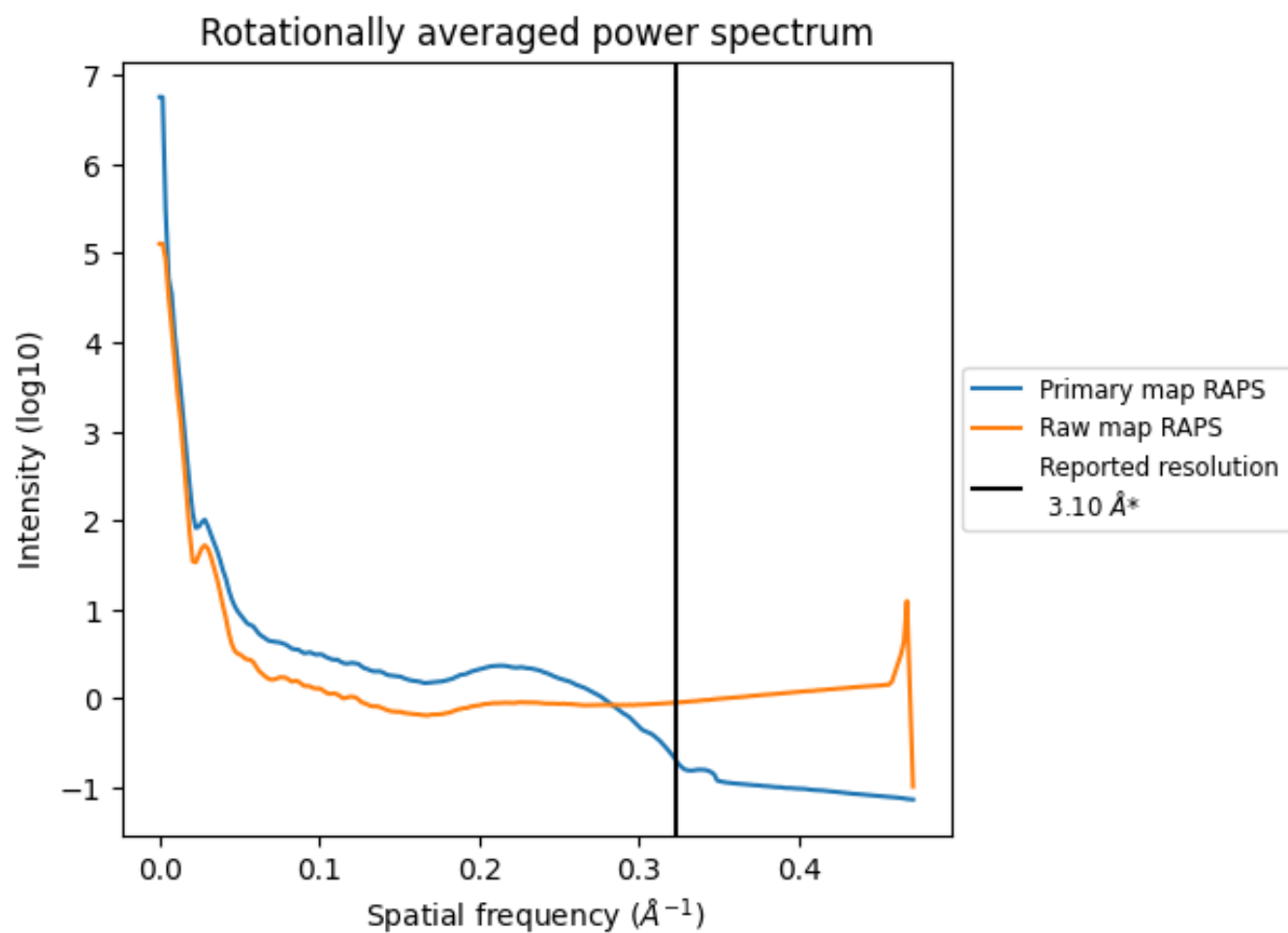
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 675 nm³; 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 ⓘ

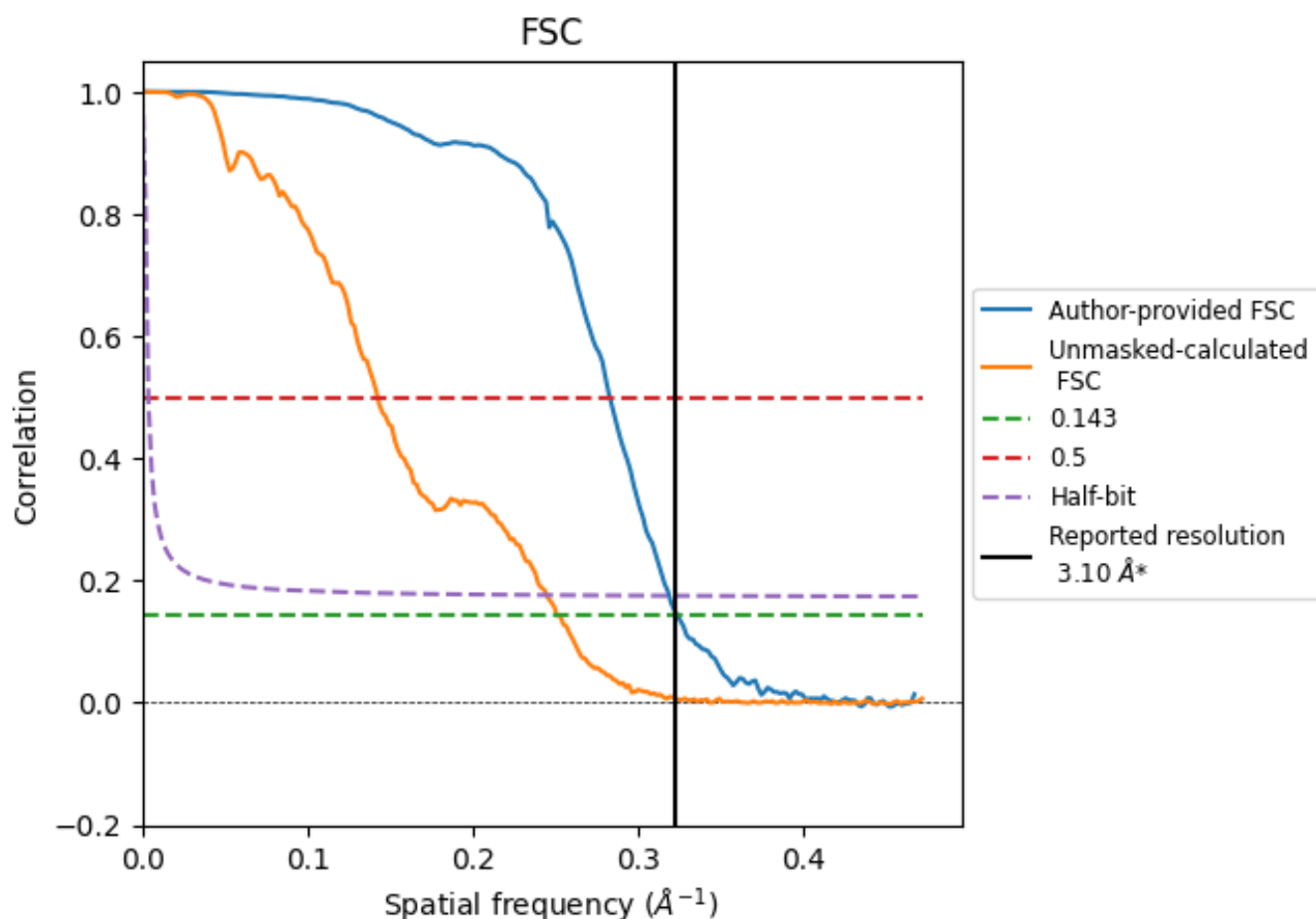


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

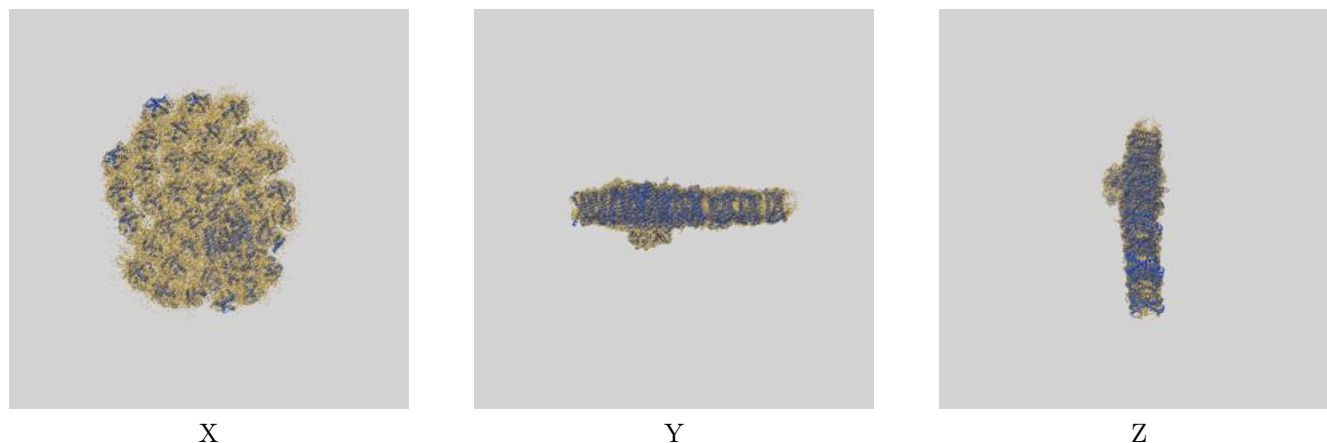
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.54	3.14
Unmasked-calculated*	3.99	7.02	4.09

*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](#)

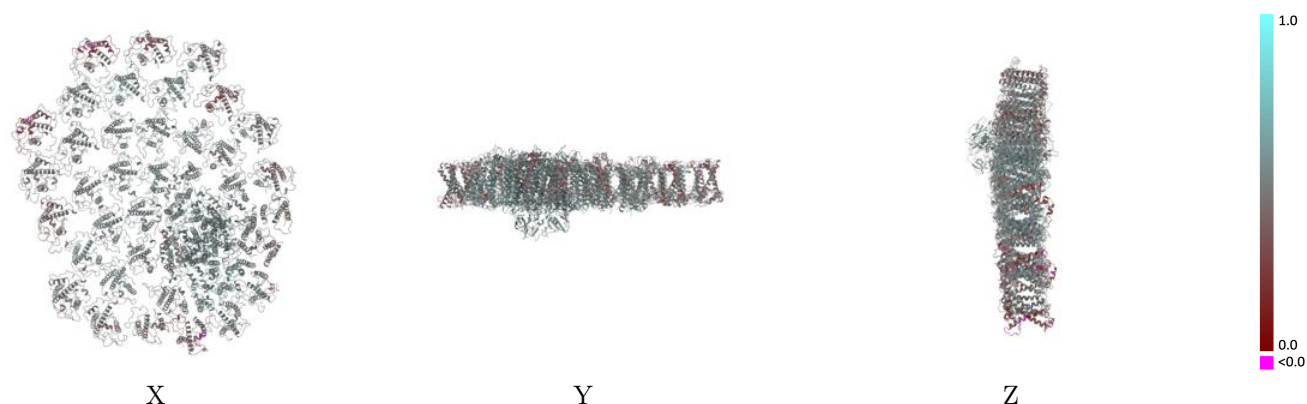
This section contains information regarding the fit between EMDB map EMD-64087 and PDB model 9UEN. Per-residue inclusion information can be found in section [3](#) on page [66](#).

9.1 Map-model overlay [i](#)



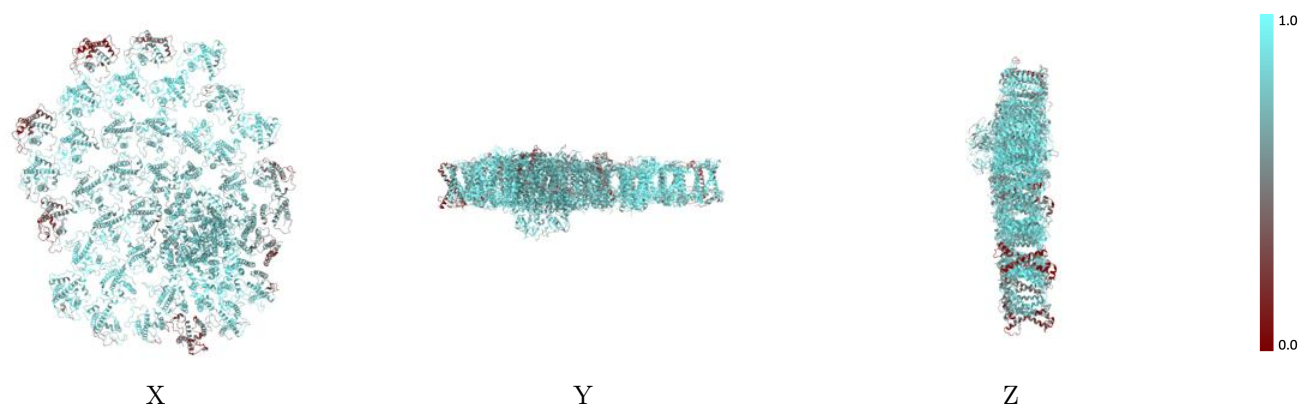
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



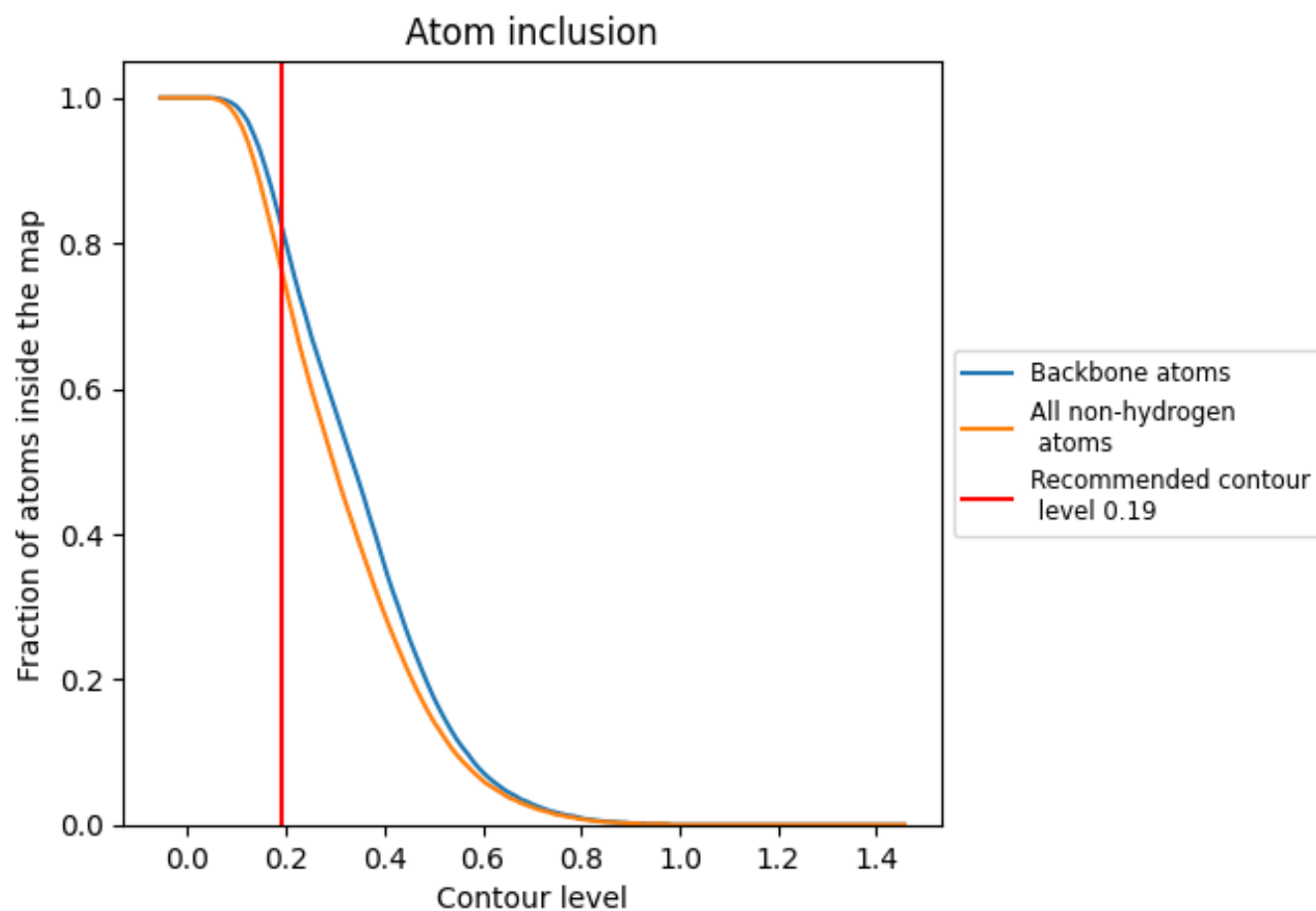
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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