wwPDB EM Validation Summary Report ⓘ

Dec 17, 2024 – 07:15 PM EST

PDB ID	:	9AU4
EMDB ID	:	EMD-43843
Title	:	Cryo-EM structure of a photosystem I variant containing an unusual plastoquinone derivative in its electron transfer chain
Authors	:	Gisriel, C.J.; Vasily, K.; Iwig, D.F.; Russell, B.P.; Vinyard, D.J.; Golbeck, J.H.; Brudvig, G.W.; Lakshmi, K.V.
Deposited on	:	2024-02-28
Resolution	:	2.03 Å(reported)

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

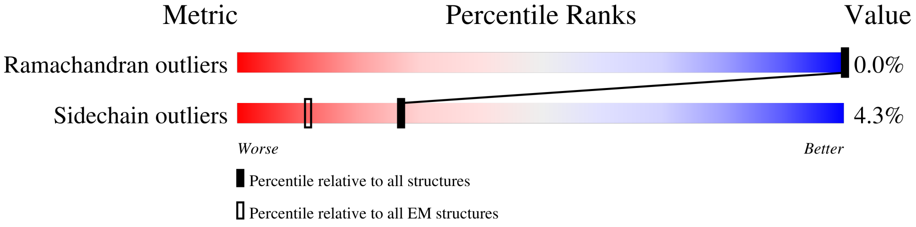
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

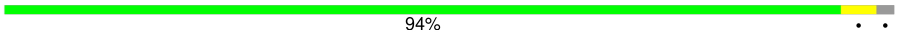
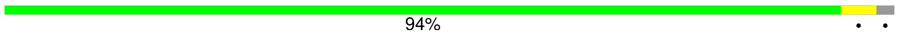
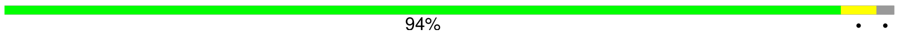
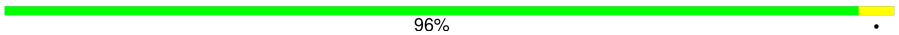
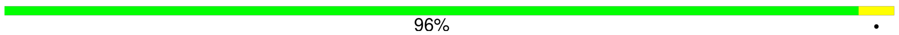
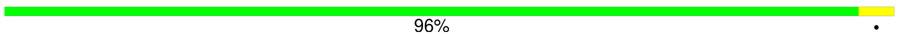
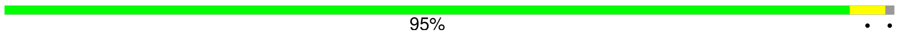
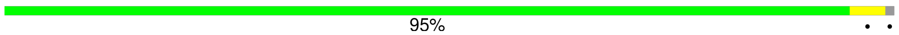
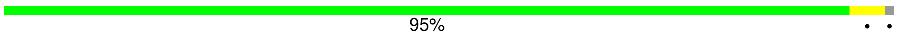
The reported resolution of this entry is 2.03 Å.

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	751	
1	G	751	
1	a	751	
2	B	730	
2	H	730	
2	b	730	
3	C	81	
3	N	81	
3	c	81	

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Mol	Chain	Length	Quality of chain
4	D	141	93% 6% •
4	O	141	93% 6% •
4	d	141	93% 6% •
5	E	74	88% 5% 7%
5	P	74	88% 5% 7%
5	e	74	88% 5% 7%
6	F	165	82% • 15%
6	Q	165	82% • 15%
6	f	165	82% • 15%
7	I	40	98% •
7	R	40	98% •
7	i	40	98% •
8	J	40	90% 8% •
8	S	40	90% 8% •
8	j	40	90% 8% •
9	K	90	68% 7% 26%
9	T	90	68% 7% 26%
9	k	90	68% 7% 26%
10	L	157	95% • •
10	U	157	95% • •
10	l	157	95% • •
11	M	31	97% •
11	V	31	97% •
11	m	31	97% •

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
12	CLA	A	801	X	-	-	-
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	806	X	-	-	-
12	CLA	A	807	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	809	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	812	X	-	-	-
12	CLA	A	813	X	-	-	-
12	CLA	A	814	X	-	-	-
12	CLA	A	815	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	817	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	819	X	-	-	-
12	CLA	A	820	X	-	-	-
12	CLA	A	821	X	-	-	-
12	CLA	A	822	X	-	-	-
12	CLA	A	823	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	825	X	-	-	-
12	CLA	A	826	X	-	-	-
12	CLA	A	827	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-
12	CLA	A	833	X	-	-	-
12	CLA	A	834	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	836	X	-	-	-
12	CLA	A	837	X	-	-	-
12	CLA	A	838	X	-	-	-
12	CLA	A	839	X	-	-	-
12	CLA	A	850	X	-	-	-
12	CLA	A	851	X	-	-	-
12	CLA	A	854	X	-	-	-
12	CLA	B	2101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	2102	X	-	-	-
12	CLA	B	2103	X	-	-	-
12	CLA	B	2104	X	-	-	-
12	CLA	B	2105	X	-	-	-
12	CLA	B	2106	X	-	-	-
12	CLA	B	2107	X	-	-	-
12	CLA	B	2108	X	-	-	-
12	CLA	B	2109	X	-	-	-
12	CLA	B	2110	X	-	-	-
12	CLA	B	2111	X	-	-	-
12	CLA	B	2112	X	-	-	-
12	CLA	B	2113	X	-	-	-
12	CLA	B	2115	X	-	-	-
12	CLA	B	2116	X	-	-	-
12	CLA	B	2117	X	-	-	-
12	CLA	B	2118	X	-	-	-
12	CLA	B	2119	X	-	-	-
12	CLA	B	2120	X	-	-	-
12	CLA	B	2121	X	-	-	-
12	CLA	B	2123	X	-	-	-
12	CLA	B	2124	X	-	-	-
12	CLA	B	2125	X	-	-	-
12	CLA	B	2126	X	-	-	-
12	CLA	B	2127	X	-	-	-
12	CLA	B	2128	X	-	-	-
12	CLA	B	2129	X	-	-	-
12	CLA	B	2130	X	-	-	-
12	CLA	B	2131	X	-	-	-
12	CLA	B	2132	X	-	-	-
12	CLA	B	2133	X	-	-	-
12	CLA	B	2134	X	-	-	-
12	CLA	B	2135	X	-	-	-
12	CLA	B	2136	X	-	-	-
12	CLA	B	2137	X	-	-	-
12	CLA	B	2138	X	-	-	-
12	CLA	B	2139	X	-	-	-
12	CLA	B	2140	X	-	-	-
12	CLA	B	2141	X	-	-	-
12	CLA	B	2142	X	-	-	-
12	CLA	F	201	X	-	-	-
12	CLA	F	203	X	-	-	-
12	CLA	F	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	G	801	X	-	-	-
12	CLA	G	802	X	-	-	-
12	CLA	G	803	X	-	-	-
12	CLA	G	804	X	-	-	-
12	CLA	G	805	X	-	-	-
12	CLA	G	806	X	-	-	-
12	CLA	G	807	X	-	-	-
12	CLA	G	808	X	-	-	-
12	CLA	G	809	X	-	-	-
12	CLA	G	810	X	-	-	-
12	CLA	G	811	X	-	-	-
12	CLA	G	812	X	-	-	-
12	CLA	G	813	X	-	-	-
12	CLA	G	814	X	-	-	-
12	CLA	G	815	X	-	-	-
12	CLA	G	816	X	-	-	-
12	CLA	G	817	X	-	-	-
12	CLA	G	818	X	-	-	-
12	CLA	G	819	X	-	-	-
12	CLA	G	820	X	-	-	-
12	CLA	G	821	X	-	-	-
12	CLA	G	822	X	-	-	-
12	CLA	G	823	X	-	-	-
12	CLA	G	824	X	-	-	-
12	CLA	G	825	X	-	-	-
12	CLA	G	826	X	-	-	-
12	CLA	G	827	X	-	-	-
12	CLA	G	828	X	-	-	-
12	CLA	G	829	X	-	-	-
12	CLA	G	831	X	-	-	-
12	CLA	G	832	X	-	-	-
12	CLA	G	833	X	-	-	-
12	CLA	G	834	X	-	-	-
12	CLA	G	835	X	-	-	-
12	CLA	G	836	X	-	-	-
12	CLA	G	837	X	-	-	-
12	CLA	G	838	X	-	-	-
12	CLA	G	839	X	-	-	-
12	CLA	G	850	X	-	-	-
12	CLA	G	851	X	-	-	-
12	CLA	G	854	X	-	-	-
12	CLA	H	2101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	H	2102	X	-	-	-
12	CLA	H	2103	X	-	-	-
12	CLA	H	2104	X	-	-	-
12	CLA	H	2105	X	-	-	-
12	CLA	H	2106	X	-	-	-
12	CLA	H	2107	X	-	-	-
12	CLA	H	2108	X	-	-	-
12	CLA	H	2109	X	-	-	-
12	CLA	H	2110	X	-	-	-
12	CLA	H	2111	X	-	-	-
12	CLA	H	2112	X	-	-	-
12	CLA	H	2114	X	-	-	-
12	CLA	H	2115	X	-	-	-
12	CLA	H	2116	X	-	-	-
12	CLA	H	2117	X	-	-	-
12	CLA	H	2118	X	-	-	-
12	CLA	H	2119	X	-	-	-
12	CLA	H	2120	X	-	-	-
12	CLA	H	2122	X	-	-	-
12	CLA	H	2123	X	-	-	-
12	CLA	H	2124	X	-	-	-
12	CLA	H	2125	X	-	-	-
12	CLA	H	2126	X	-	-	-
12	CLA	H	2127	X	-	-	-
12	CLA	H	2128	X	-	-	-
12	CLA	H	2129	X	-	-	-
12	CLA	H	2130	X	-	-	-
12	CLA	H	2131	X	-	-	-
12	CLA	H	2132	X	-	-	-
12	CLA	H	2133	X	-	-	-
12	CLA	H	2134	X	-	-	-
12	CLA	H	2135	X	-	-	-
12	CLA	H	2136	X	-	-	-
12	CLA	H	2137	X	-	-	-
12	CLA	H	2138	X	-	-	-
12	CLA	H	2139	X	-	-	-
12	CLA	H	2140	X	-	-	-
12	CLA	H	2141	X	-	-	-
12	CLA	H	2152	X	-	-	-
12	CLA	J	102	X	-	-	-
12	CLA	J	103	X	-	-	-
12	CLA	K	4002	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	L	201	X	-	-	-
12	CLA	L	203	X	-	-	-
12	CLA	L	204	X	-	-	-
12	CLA	L	205	X	-	-	-
12	CLA	Q	201	X	-	-	-
12	CLA	Q	203	X	-	-	-
12	CLA	Q	204	X	-	-	-
12	CLA	S	102	X	-	-	-
12	CLA	S	103	X	-	-	-
12	CLA	T	4002	X	-	-	-
12	CLA	U	201	X	-	-	-
12	CLA	U	203	X	-	-	-
12	CLA	U	204	X	-	-	-
12	CLA	U	205	X	-	-	-
12	CLA	a	801	X	-	-	-
12	CLA	a	802	X	-	-	-
12	CLA	a	803	X	-	-	-
12	CLA	a	804	X	-	-	-
12	CLA	a	805	X	-	-	-
12	CLA	a	806	X	-	-	-
12	CLA	a	807	X	-	-	-
12	CLA	a	808	X	-	-	-
12	CLA	a	809	X	-	-	-
12	CLA	a	810	X	-	-	-
12	CLA	a	811	X	-	-	-
12	CLA	a	812	X	-	-	-
12	CLA	a	813	X	-	-	-
12	CLA	a	814	X	-	-	-
12	CLA	a	815	X	-	-	-
12	CLA	a	816	X	-	-	-
12	CLA	a	817	X	-	-	-
12	CLA	a	818	X	-	-	-
12	CLA	a	819	X	-	-	-
12	CLA	a	820	X	-	-	-
12	CLA	a	821	X	-	-	-
12	CLA	a	822	X	-	-	-
12	CLA	a	823	X	-	-	-
12	CLA	a	824	X	-	-	-
12	CLA	a	825	X	-	-	-
12	CLA	a	826	X	-	-	-
12	CLA	a	827	X	-	-	-
12	CLA	a	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	a	829	X	-	-	-
12	CLA	a	831	X	-	-	-
12	CLA	a	832	X	-	-	-
12	CLA	a	833	X	-	-	-
12	CLA	a	834	X	-	-	-
12	CLA	a	835	X	-	-	-
12	CLA	a	836	X	-	-	-
12	CLA	a	837	X	-	-	-
12	CLA	a	838	X	-	-	-
12	CLA	a	839	X	-	-	-
12	CLA	a	850	X	-	-	-
12	CLA	a	851	X	-	-	-
12	CLA	a	854	X	-	-	-
12	CLA	b	2101	X	-	-	-
12	CLA	b	2102	X	-	-	-
12	CLA	b	2103	X	-	-	-
12	CLA	b	2104	X	-	-	-
12	CLA	b	2105	X	-	-	-
12	CLA	b	2106	X	-	-	-
12	CLA	b	2107	X	-	-	-
12	CLA	b	2108	X	-	-	-
12	CLA	b	2109	X	-	-	-
12	CLA	b	2110	X	-	-	-
12	CLA	b	2111	X	-	-	-
12	CLA	b	2112	X	-	-	-
12	CLA	b	2114	X	-	-	-
12	CLA	b	2115	X	-	-	-
12	CLA	b	2116	X	-	-	-
12	CLA	b	2117	X	-	-	-
12	CLA	b	2118	X	-	-	-
12	CLA	b	2119	X	-	-	-
12	CLA	b	2120	X	-	-	-
12	CLA	b	2122	X	-	-	-
12	CLA	b	2123	X	-	-	-
12	CLA	b	2124	X	-	-	-
12	CLA	b	2125	X	-	-	-
12	CLA	b	2126	X	-	-	-
12	CLA	b	2127	X	-	-	-
12	CLA	b	2128	X	-	-	-
12	CLA	b	2129	X	-	-	-
12	CLA	b	2130	X	-	-	-
12	CLA	b	2131	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	b	2132	X	-	-	-
12	CLA	b	2133	X	-	-	-
12	CLA	b	2134	X	-	-	-
12	CLA	b	2135	X	-	-	-
12	CLA	b	2136	X	-	-	-
12	CLA	b	2137	X	-	-	-
12	CLA	b	2138	X	-	-	-
12	CLA	b	2139	X	-	-	-
12	CLA	b	2140	X	-	-	-
12	CLA	b	2141	X	-	-	-
12	CLA	b	2152	X	-	-	-
12	CLA	f	201	X	-	-	-
12	CLA	f	203	X	-	-	-
12	CLA	f	204	X	-	-	-
12	CLA	j	102	X	-	-	-
12	CLA	j	103	X	-	-	-
12	CLA	k	4002	X	-	-	-
12	CLA	l	201	X	-	-	-
12	CLA	l	203	X	-	-	-
12	CLA	l	204	X	-	-	-
12	CLA	l	205	X	-	-	-
13	A1AGD	A	840	X	-	-	-
13	A1AGD	B	2153	X	-	-	-
13	A1AGD	G	840	X	-	-	-
13	A1AGD	H	2153	X	-	-	-
13	A1AGD	a	840	X	-	-	-
13	A1AGD	b	2153	X	-	-	-
23	ZEX	F	205	-	X	-	-
23	ZEX	Q	205	-	X	-	-
23	ZEX	f	205	-	X	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 73866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms	AltConf	Trace
1	G	737	Total C N O S 5770 3780 980 983 27	0	0
1	a	737	Total C N O S 5770 3780 980 983 27	0	0
1	A	737	Total C N O S 5770 3780 980 983 27	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
2	H	729	Total C N O S 5770 3798 967 990 15	0	0
2	b	729	Total C N O S 5770 3798 967 990 15	0	0
2	B	729	Total C N O S 5770 3798 967 990 15	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
3	N	80	Total C N O S 600 369 103 117 11	0	0
3	c	80	Total C N O S 600 369 103 117 11	0	0
3	C	80	Total C N O S 600 369 103 117 11	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
4	O	139	Total C N O S 1087 688 188 208 3	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
4	d	139	Total C N O S 1087 688 188 208 3	0	0
4	D	139	Total C N O S 1087 688 188 208 3	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
5	P	69	Total C N O 542 340 96 106	0	0
5	e	69	Total C N O 542 340 96 106	0	0
5	E	69	Total C N O 542 340 96 106	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
6	Q	141	Total C N O S 1100 711 183 201 5	0	0
6	f	141	Total C N O S 1100 711 183 201 5	0	0
6	F	141	Total C N O S 1100 711 183 201 5	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
7	R	40	Total C N O S 311 209 44 55 3	0	0
7	i	40	Total C N O S 311 209 44 55 3	0	0
7	I	40	Total C N O S 311 209 44 55 3	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
8	S	39	Total C N O S 311 210 46 53 2	0	0
8	j	39	Total C N O S 311 210 46 53 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total 311	C 210	N 46	O 53	S 2	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	67	Total 484	C 320	N 77	O 82	S 5	0	0
9	k	67	Total 484	C 320	N 77	O 82	S 5	0	0
9	K	67	Total 484	C 320	N 77	O 82	S 5	0	0

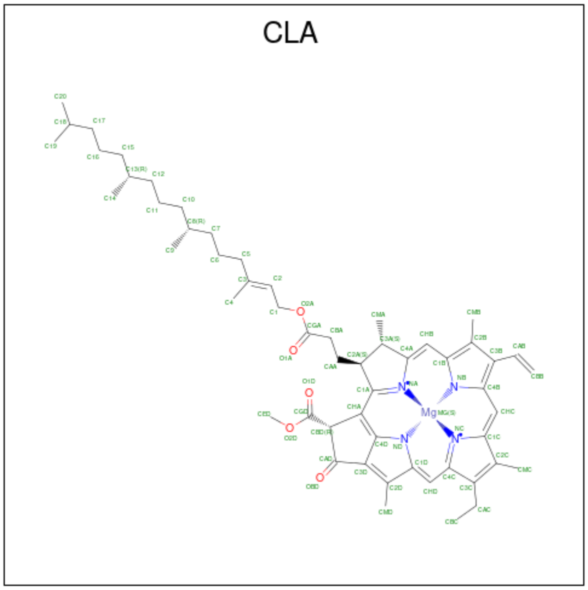
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	154	Total 1156	C 753	N 188	O 213	S 2	0	0
10	l	154	Total 1156	C 753	N 188	O 213	S 2	0	0
10	L	154	Total 1156	C 753	N 188	O 213	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	31	Total 238	C 159	N 36	O 42	S 1	0	0
11	m	31	Total 238	C 159	N 36	O 42	S 1	0	0
11	M	31	Total 238	C 159	N 36	O 42	S 1	0	0

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 55 45 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 50 40 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 51 41 1 4 5	0
12	G	1	Total C Mg N O 50 40 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 45 35 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	G	1	Total C Mg N O 45 35 1 4 5	0
12	G	1	Total C Mg N O 55 45 1 4 5	0
12	G	1	Total C Mg N O 60 50 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 60 50 1 4 5	0
12	G	1	Total C Mg N O 50 40 1 4 5	0
12	G	1	Total C Mg N O 60 50 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 60 50 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 55 45 1 4 5	0
12	G	1	Total C Mg N O 60 50 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 55 45 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 65 55 1 4 5	0
12	G	1	Total C Mg N O 55 45 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 50 40 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 55 45 1 4 5	0
12	H	1	Total C Mg N O 55 45 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 55 45 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 50 40 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 55 45 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 65 55 1 4 5	0
12	H	1	Total C Mg N O 45 35 1 4 5	0
12	H	1	Total C Mg N O 50 40 1 4 5	0
12	Q	1	Total C Mg N O 65 55 1 4 5	0
12	Q	1	Total C Mg N O 46 36 1 4 5	0
12	Q	1	Total C Mg N O 45 35 1 4 5	0
12	S	1	Total C Mg N O 45 35 1 4 5	0
12	S	1	Total C Mg N O 45 35 1 4 5	0
12	T	1	Total C Mg N O 45 35 1 4 5	0
12	U	1	Total C Mg N O 65 55 1 4 5	0
12	U	1	Total C Mg N O 65 55 1 4 5	0
12	U	1	Total C Mg N O 65 55 1 4 5	0
12	U	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 55 45 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 50 40 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 51 41 1 4 5	0
12	a	1	Total C Mg N O 50 40 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 45 35 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 45 35 1 4 5	0
12	a	1	Total C Mg N O 45 35 1 4 5	0
12	a	1	Total C Mg N O 55 45 1 4 5	0
12	a	1	Total C Mg N O 60 50 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 60 50 1 4 5	0
12	a	1	Total C Mg N O 50 40 1 4 5	0
12	a	1	Total C Mg N O 60 50 1 4 5	0
12	a	1	Total C Mg N O 65 55 1 4 5	0
12	a	1	Total C Mg N O 60 50 1 4 5	0

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

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Mol	Chain	Residues	Atoms	AltConf
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 45 35 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 45 35 1 4 5	0
12	b	1	Total C Mg N O 45 35 1 4 5	0
12	b	1	Total C Mg N O 45 35 1 4 5	0
12	b	1	Total C Mg N O 50 40 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 55 45 1 4 5	0
12	b	1	Total C Mg N O 55 45 1 4 5	0
12	b	1	Total C Mg N O 45 35 1 4 5	0
12	b	1	Total C Mg N O 55 45 1 4 5	0
12	b	1	Total C Mg N O 65 55 1 4 5	0
12	b	1	Total C Mg N O 50 40 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	b	1	65	55	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	45	35	1	4	5	0
12	b	1	55	45	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	45	35	1	4	5	0
12	b	1	45	35	1	4	5	0
12	b	1	45	35	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	45	35	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	65	55	1	4	5	0
12	b	1	45	35	1	4	5	0
12	b	1	50	40	1	4	5	0
12	f	1	65	55	1	4	5	0
12	f	1	46	36	1	4	5	0
12	f	1	45	35	1	4	5	0
12	j	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms	AltConf
12	j	1	Total C Mg N O 45 35 1 4 5	0
12	k	1	Total C Mg N O 45 35 1 4 5	0
12	l	1	Total C Mg N O 65 55 1 4 5	0
12	l	1	Total C Mg N O 65 55 1 4 5	0
12	l	1	Total C Mg N O 65 55 1 4 5	0
12	l	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 55 45 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 50 40 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 51 41 1 4 5	0
12	A	1	Total C Mg N O 50 40 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 45 35 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 45 35 1 4 5	0
12	A	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C Mg N O 55 45 1 4 5	0
12	A	1	Total C Mg N O 60 50 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 60 50 1 4 5	0
12	A	1	Total C Mg N O 50 40 1 4 5	0
12	A	1	Total C Mg N O 60 50 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 60 50 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 55 45 1 4 5	0
12	A	1	Total C Mg N O 60 50 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 55 45 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 65 55 1 4 5	0
12	A	1	Total C Mg N O 55 45 1 4 5	0
12	B	1	Total C Mg N O 50 40 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 50 40 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 55 45 1 4 5	0
12	B	1	Total C Mg N O 55 45 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 55 45 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 50 40 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 55 45 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 65 55 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0
12	B	1	Total C Mg N O 45 35 1 4 5	0

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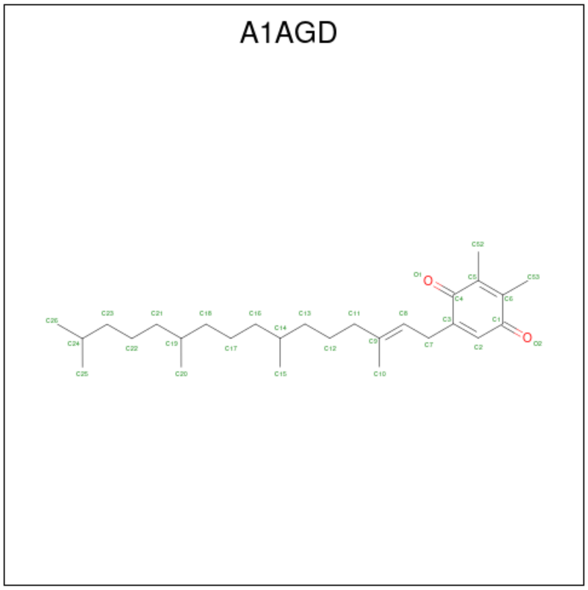
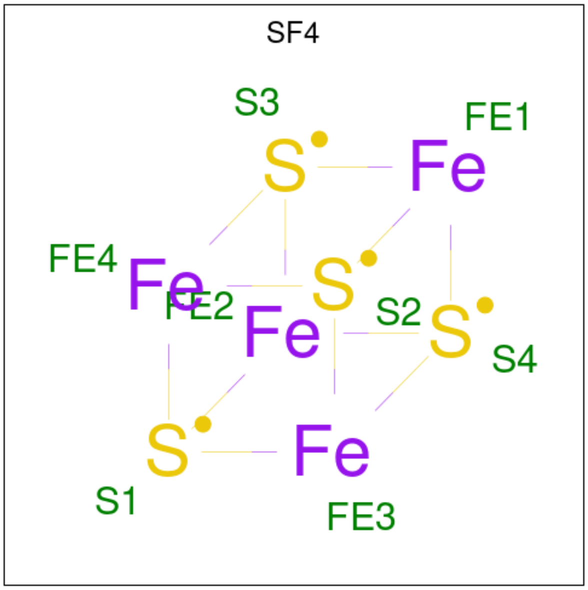
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 13 is 2,3-dimethyl-5-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (three-letter code: A1AGD) (formula: $C_{28}H_{46}O_2$).



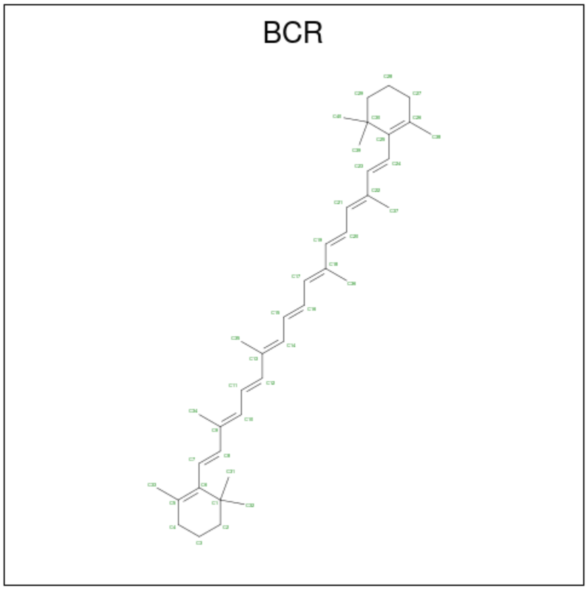
Mol	Chain	Residues	Atoms	AltConf
13	G	1	Total C O 30 28 2	0
13	H	1	Total C O 30 28 2	0
13	a	1	Total C O 30 28 2	0
13	b	1	Total C O 30 28 2	0
13	A	1	Total C O 30 28 2	0
13	B	1	Total C O 30 28 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
14	G	1	Total Fe S 8 4 4	0
14	N	1	Total Fe S 8 4 4	0
14	N	1	Total Fe S 8 4 4	0
14	a	1	Total Fe S 8 4 4	0
14	c	1	Total Fe S 8 4 4	0
14	c	1	Total Fe S 8 4 4	0
14	A	1	Total Fe S 8 4 4	0
14	C	1	Total Fe S 8 4 4	0
14	C	1	Total Fe S 8 4 4	0

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	T	1	Total C 40 40	0
15	U	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	U	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	k	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0

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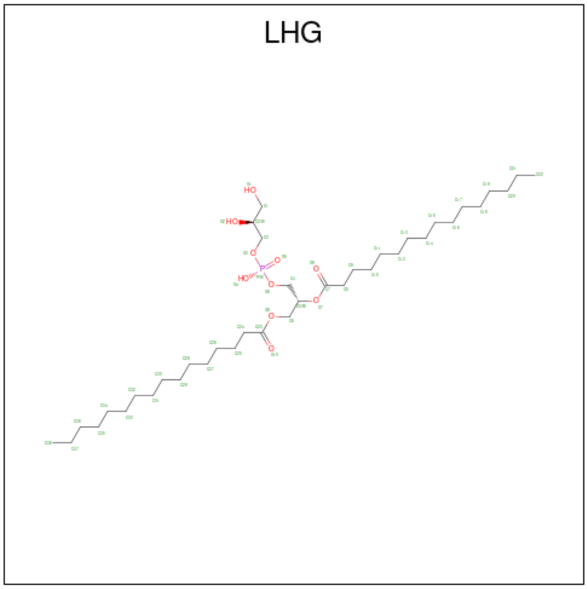
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	K	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
16	G	1	Total C O P 49 38 10 1	0

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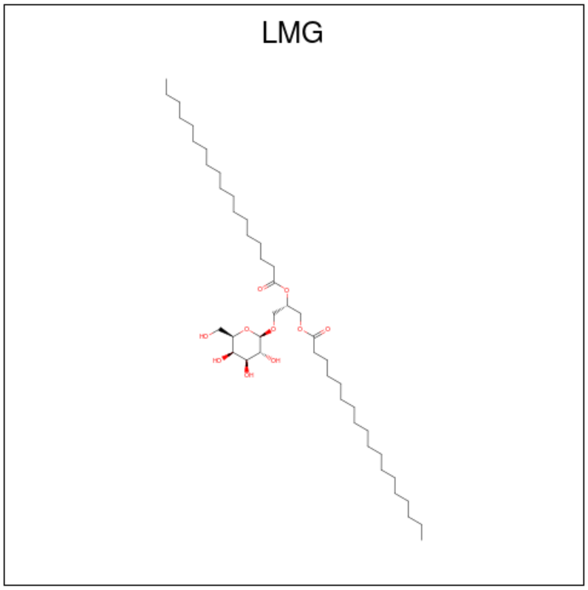
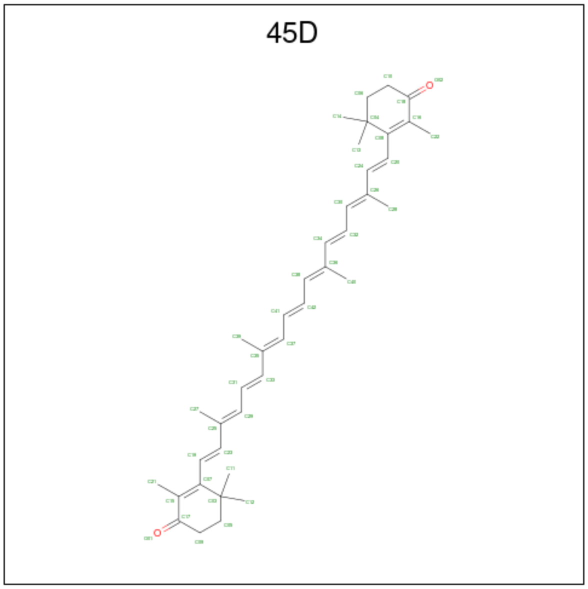
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total 49	C 38	O 10	P 1	0
16	H	1	Total 43	C 32	O 10	P 1	0
16	V	1	Total 44	C 33	O 10	P 1	0
16	a	1	Total 49	C 38	O 10	P 1	0
16	a	1	Total 49	C 38	O 10	P 1	0
16	b	1	Total 43	C 32	O 10	P 1	0
16	m	1	Total 44	C 33	O 10	P 1	0
16	A	1	Total 49	C 38	O 10	P 1	0
16	A	1	Total 49	C 38	O 10	P 1	0
16	B	1	Total 43	C 32	O 10	P 1	0
16	M	1	Total 44	C 33	O 10	P 1	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total C O 50 40 10	0
17	G	1	Total C O 32 22 10	0
17	H	1	Total C O 51 41 10	0
17	a	1	Total C O 50 40 10	0
17	a	1	Total C O 32 22 10	0
17	b	1	Total C O 51 41 10	0
17	A	1	Total C O 50 40 10	0
17	A	1	Total C O 32 22 10	0
17	B	1	Total C O 51 41 10	0

- Molecule 18 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).

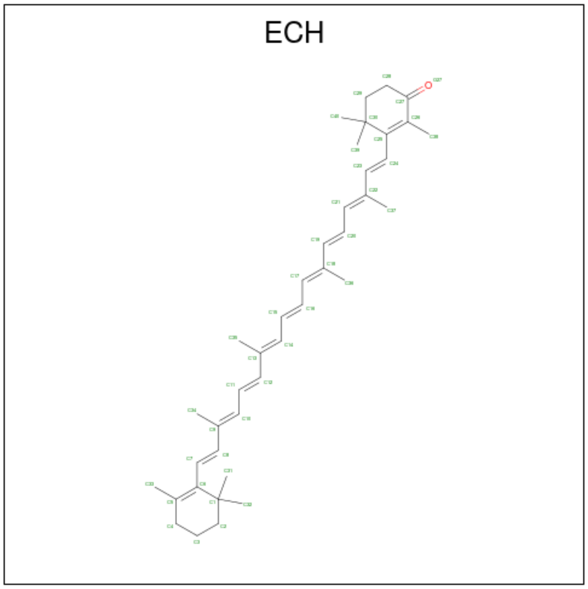


Mol	Chain	Residues	Atoms	AltConf
18	G	1	Total C O 42 40 2	0
18	a	1	Total C O 42 40 2	0
18	A	1	Total C O 42 40 2	0

- Molecule 19 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total Cl 1 1	0
19	a	1	Total Cl 1 1	0
19	A	1	Total Cl 1 1	0

- Molecule 20 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).

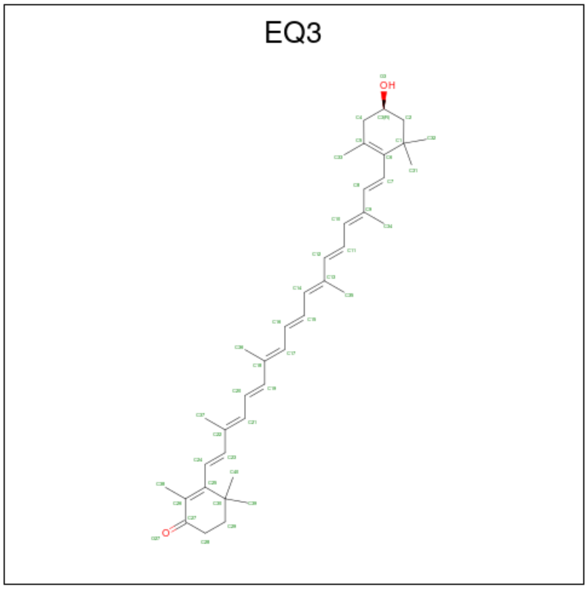


Mol	Chain	Residues	Atoms	AltConf
20	H	1	Total C O 41 40 1	0
20	V	1	Total C O 41 40 1	0
20	b	1	Total C O 41 40 1	0
20	m	1	Total C O 41 40 1	0
20	B	1	Total C O 41 40 1	0
20	M	1	Total C O 41 40 1	0

- Molecule 21 is CALCIUM ION (three-letter code: CA) (formula: Ca).

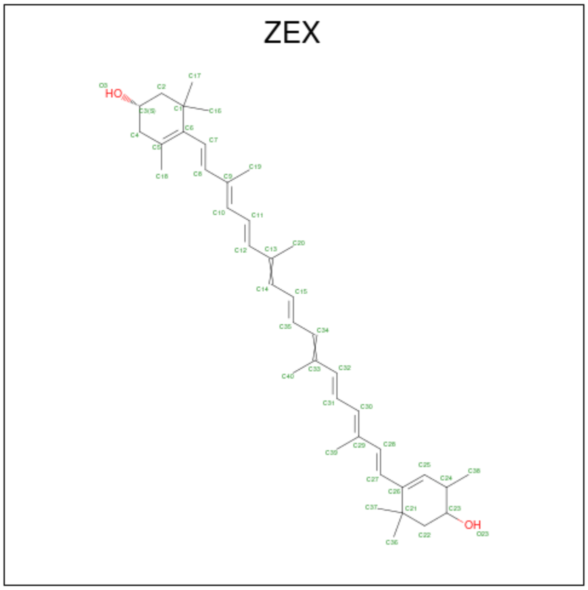
Mol	Chain	Residues	Atoms	AltConf
21	H	1	Total Ca 1 1	0
21	U	1	Total Ca 1 1	0
21	b	1	Total Ca 1 1	0
21	l	1	Total Ca 1 1	0
21	B	1	Total Ca 1 1	0
21	L	1	Total Ca 1 1	0

- Molecule 22 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: $C_{40}H_{54}O_2$).



Mol	Chain	Residues	Atoms	AltConf
22	H	1	Total C O 42 40 2	0
22	b	1	Total C O 42 40 2	0
22	B	1	Total C O 42 40 2	0

- Molecule 23 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$).



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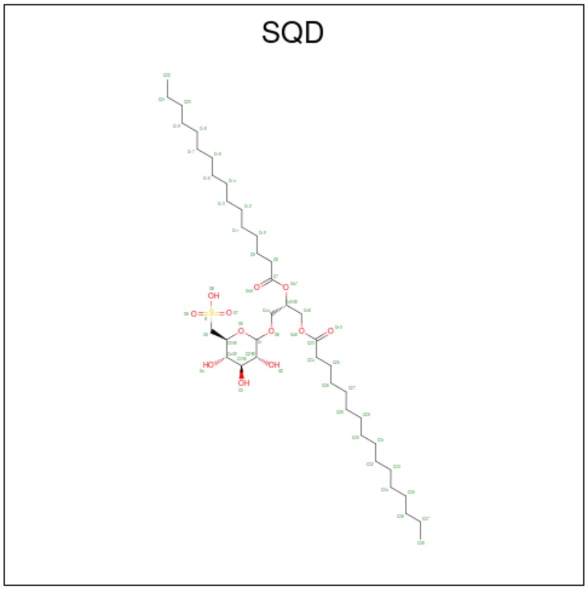
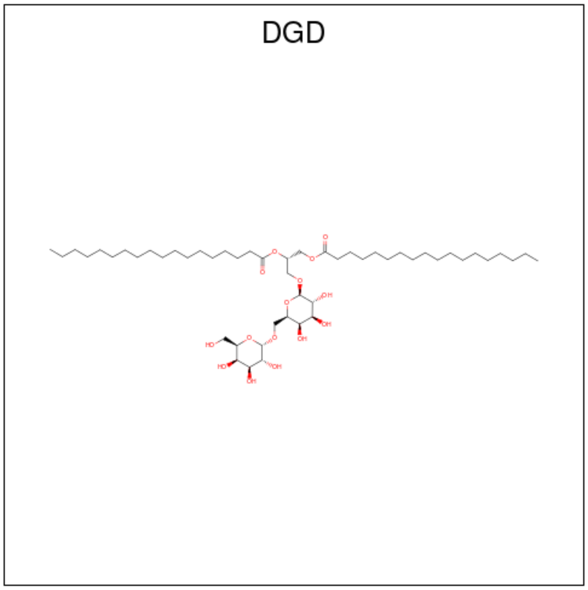
<tr><td>42</td><td>40</td><td>2</td></tr>
<tr><td rowspan="2">23</td><td rowspan="2">Q</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>O</td><td rowspan="2">0</td></tr>
<tr><td>42</td><td>40</td><td>2</td></tr>
<tr><td rowspan="2">23</td><td rowspan="2">b</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>O</td><td rowspan="2">0</td></tr>
<tr><td>42</td><td>40</td><td>2</td></tr>
<tr><td rowspan="2">23</td><td rowspan="2">f</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>O</td><td rowspan="2">0</td></tr>
<tr><td>42</td><td>40</td><td>2</td></tr>
<tr><td rowspan="2">23</td><td rowspan="2">B</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>O</td><td rowspan="2">0</td></tr>
<tr><td>42</td><td>40</td><td>2</td></tr>
<tr><td rowspan="2">23</td><td rowspan="2">F</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>O</td><td rowspan="2">0</td></tr>
<tr><td>42</td><td>40</td><td>2</td></tr>
</table>

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



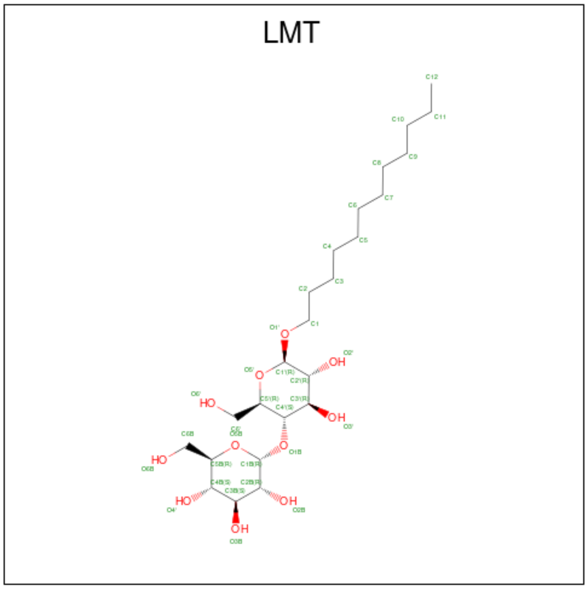
Mol	Chain	Residues	Atoms	AltConf
24	U	1	Total C O S 45 32 12 1	0
24	V	1	Total C O S 54 41 12 1	0
24	l	1	Total C O S 45 32 12 1	0
24	m	1	Total C O S 54 41 12 1	0
24	L	1	Total C O S 45 32 12 1	0
24	M	1	Total C O S 54 41 12 1	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	U	1	49	39	10	0
25	l	1	49	39	10	0
25	L	1	49	39	10	0

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
26	U	1	Total C O 35 24 11	0
26	l	1	Total C O 35 24 11	0
26	L	1	Total C O 35 24 11	0

- Molecule 27 is water.

Mol	Chain	Residues	Atoms	AltConf
27	G	90	Total O 90 90	0
27	H	112	Total O 112 112	0
27	N	36	Total O 36 36	0
27	O	28	Total O 28 28	0
27	P	7	Total O 7 7	0
27	Q	2	Total O 2 2	0
27	R	4	Total O 4 4	0
27	U	24	Total O 24 24	0
27	a	90	Total O 90 90	0
27	b	112	Total O 112 112	0
27	c	36	Total O 36 36	0
27	d	28	Total O 28 28	0
27	e	7	Total O 7 7	0
27	f	2	Total O 2 2	0
27	i	4	Total O 4 4	0
27	l	24	Total O 24 24	0
27	A	90	Total O 90 90	0

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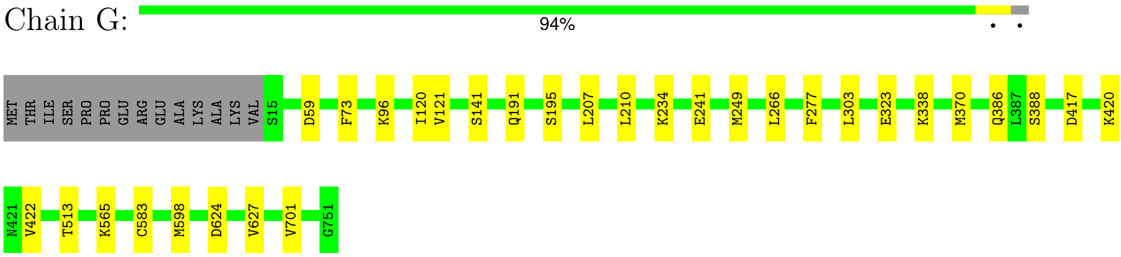
Mol	Chain	Residues	Atoms	AltConf
27	B	112	Total O 112 112	0
27	C	36	Total O 36 36	0
27	D	28	Total O 28 28	0
27	E	7	Total O 7 7	0
27	F	2	Total O 2 2	0
27	I	4	Total O 4 4	0
27	L	24	Total O 24 24	0

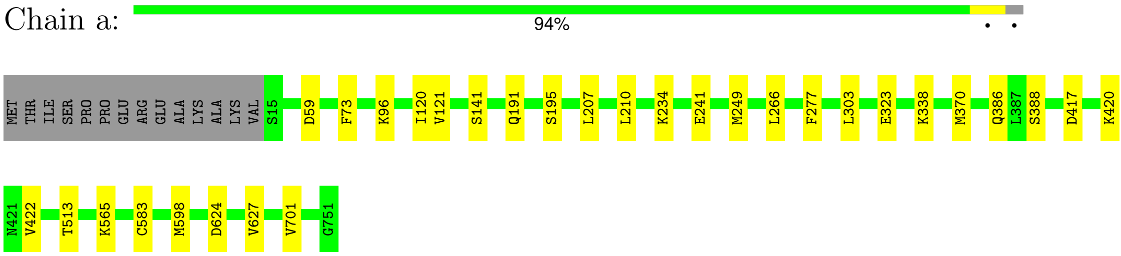
3 Residue-property plots ⓘ

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.

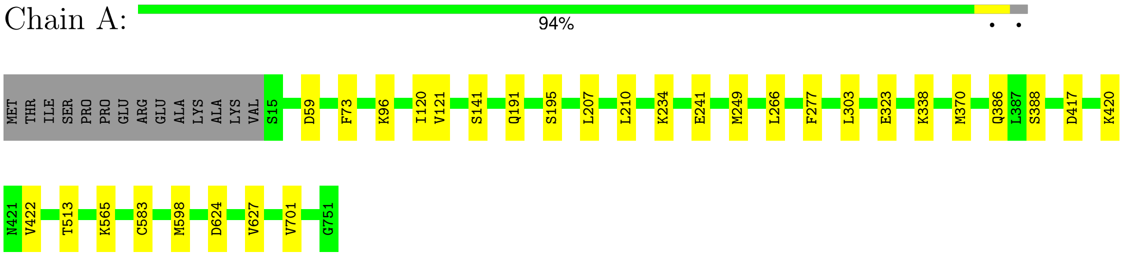
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



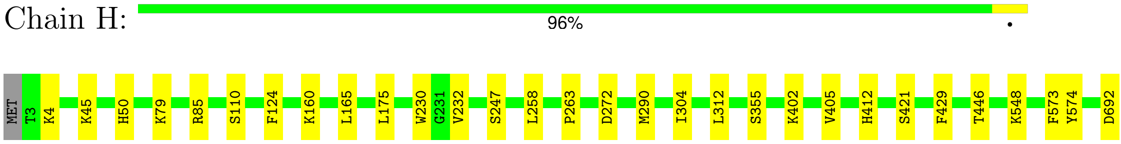
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

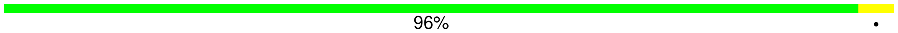


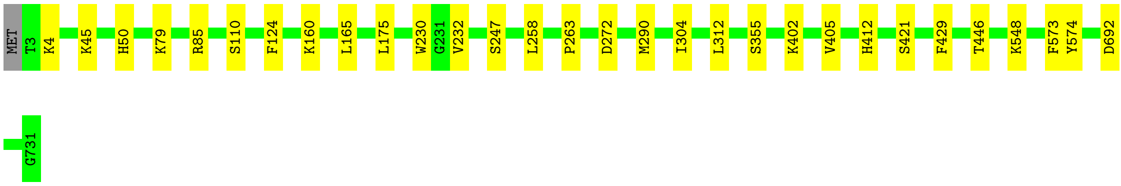
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

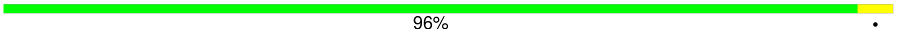
Chain b:

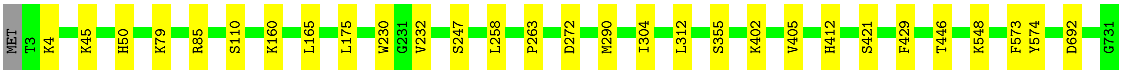




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

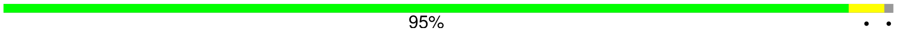
Chain B:

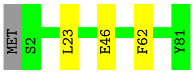




- Molecule 3: Photosystem I iron-sulfur center

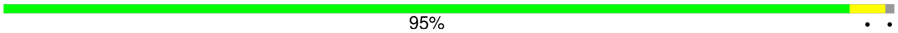
Chain N:

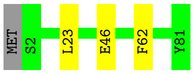




- Molecule 3: Photosystem I iron-sulfur center

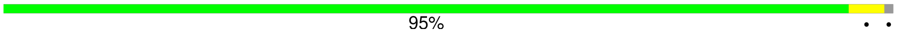
Chain c:

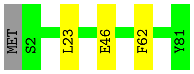




- Molecule 3: Photosystem I iron-sulfur center

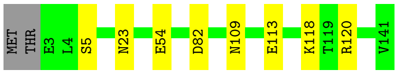
Chain C:



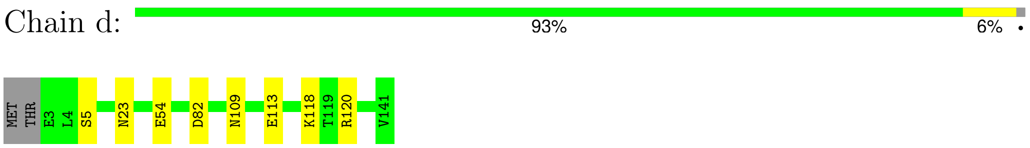


- Molecule 4: Photosystem I reaction center subunit II

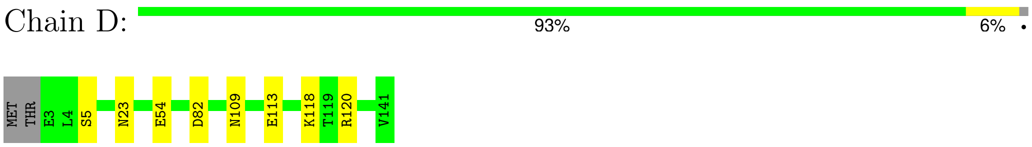
Chain O:



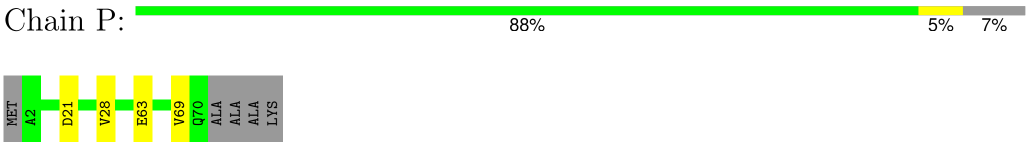
- Molecule 4: Photosystem I reaction center subunit II



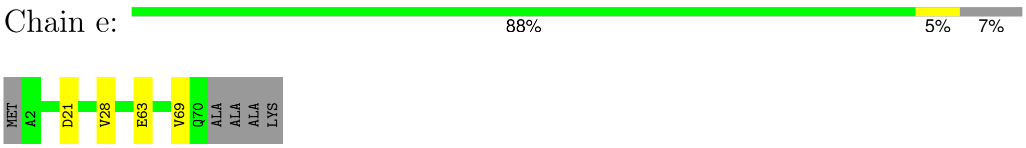
- Molecule 4: Photosystem I reaction center subunit II



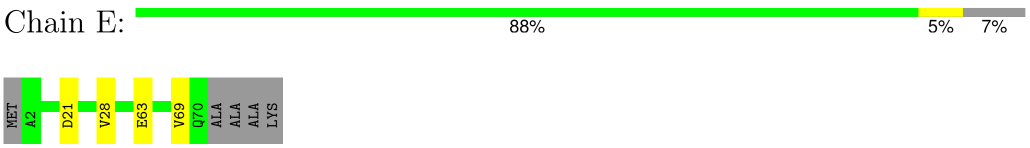
- Molecule 5: Photosystem I reaction center subunit IV



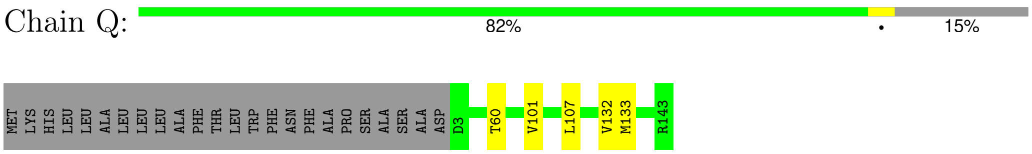
- Molecule 5: Photosystem I reaction center subunit IV



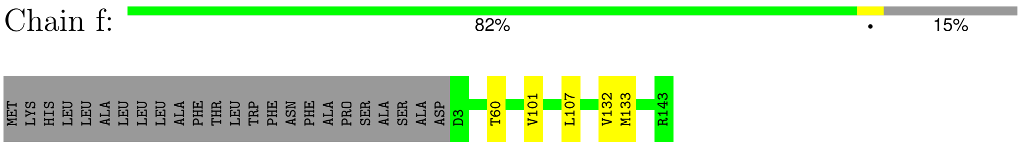
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III

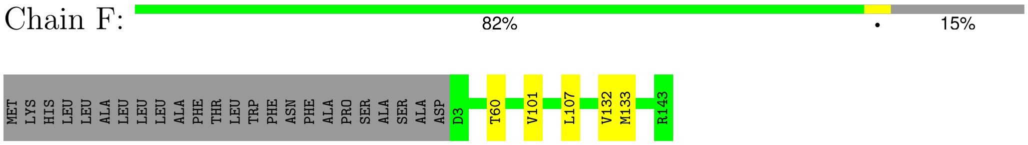


- Molecule 6: Photosystem I reaction center subunit III



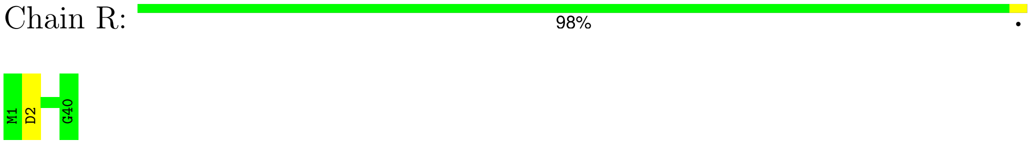
- Molecule 6: Photosystem I reaction center subunit III

Chain F:



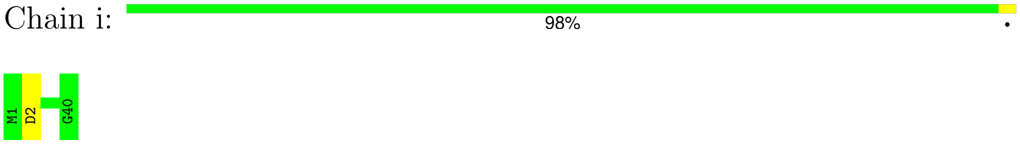
- Molecule 7: Photosystem I reaction center subunit VIII

Chain R:



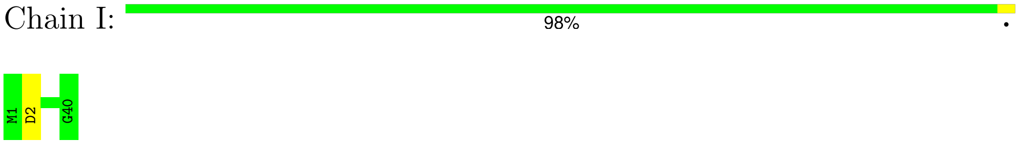
- Molecule 7: Photosystem I reaction center subunit VIII

Chain i:



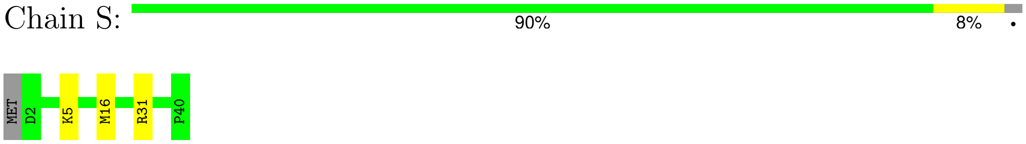
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



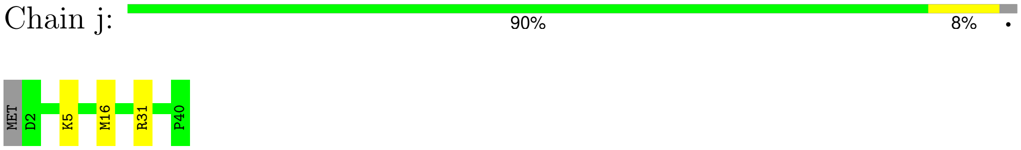
- Molecule 8: Photosystem I reaction center subunit IX

Chain S:



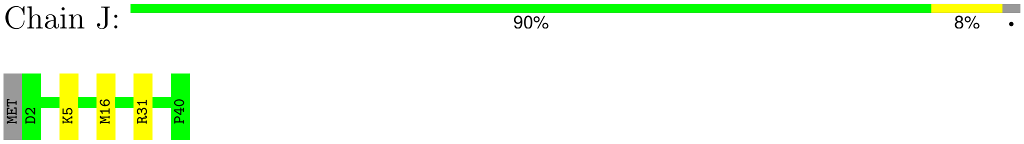
- Molecule 8: Photosystem I reaction center subunit IX

Chain j:



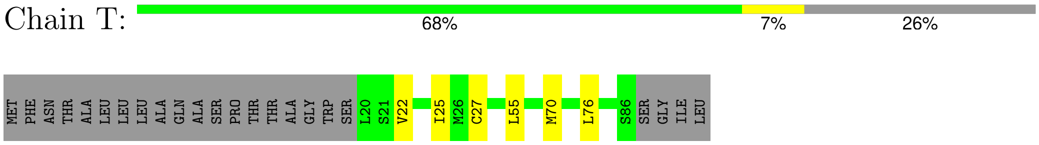
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:



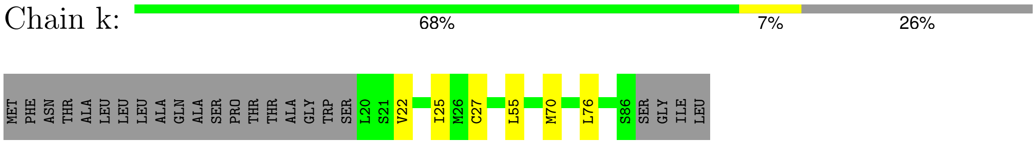
- Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain T:



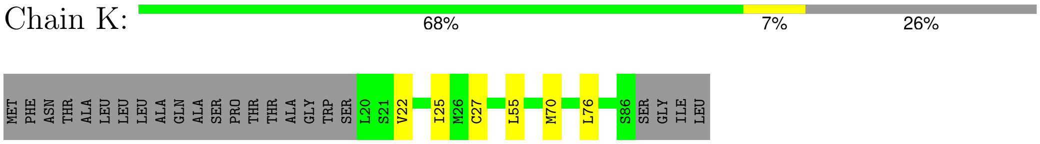
• Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain k:



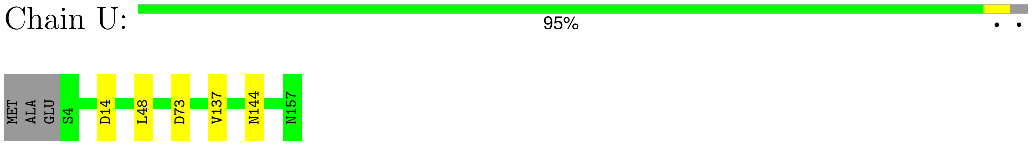
• Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain K:



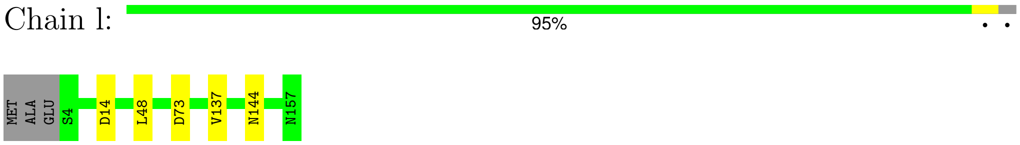
• Molecule 10: Photosystem I reaction center subunit XI

Chain U:



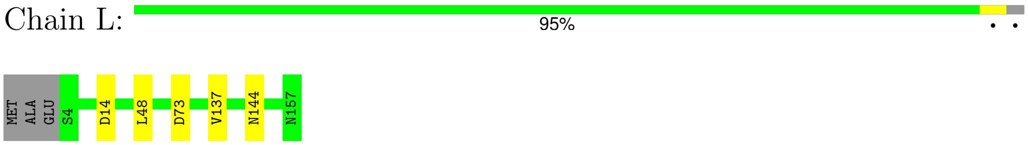
• Molecule 10: Photosystem I reaction center subunit XI

Chain l:



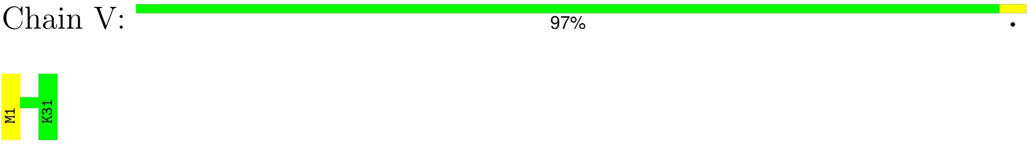
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



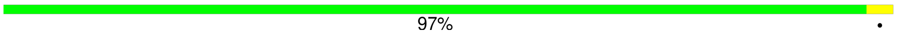
• Molecule 11: Photosystem I reaction center subunit XII

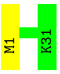
Chain V:



• Molecule 11: Photosystem I reaction center subunit XII

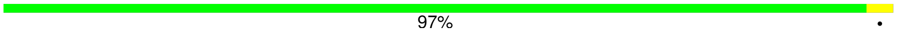
Chain m:

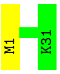




- Molecule 11: Photosystem I reaction center subunit XII

Chain M:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.972	Depositor
Minimum map value	-21.826	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.0149	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1AGD, LHG, EQ3, CL, 45D, ZEX, SF4, DGD, ECH, CA, SQD, BCR, LMG, LMT, CLA

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	0.33	0/5967	0.60	8/8133 (0.1%)
1	G	0.33	0/5967	0.60	8/8133 (0.1%)
1	a	0.33	0/5967	0.60	8/8133 (0.1%)
2	B	0.32	0/5981	0.57	5/8178 (0.1%)
2	H	0.32	0/5981	0.57	6/8178 (0.1%)
2	b	0.32	0/5981	0.57	6/8178 (0.1%)
3	C	0.31	0/610	0.65	0/826
3	N	0.31	0/610	0.65	0/826
3	c	0.31	0/610	0.65	0/826
4	D	0.29	0/1111	0.60	0/1497
4	O	0.29	0/1111	0.60	0/1497
4	d	0.29	0/1111	0.60	0/1497
5	E	0.30	0/551	0.64	0/745
5	P	0.31	0/551	0.64	0/745
5	e	0.31	0/551	0.64	0/745
6	F	0.29	0/1130	0.63	1/1535 (0.1%)
6	Q	0.29	0/1130	0.63	1/1535 (0.1%)
6	f	0.29	0/1130	0.63	1/1535 (0.1%)
7	I	0.31	0/322	0.60	0/438
7	R	0.32	0/322	0.60	0/438
7	i	0.32	0/322	0.60	0/438
8	J	0.31	0/320	0.65	1/433 (0.2%)
8	S	0.31	0/320	0.65	1/433 (0.2%)
8	j	0.31	0/320	0.65	1/433 (0.2%)
9	K	0.31	0/492	0.65	2/661 (0.3%)
9	T	0.31	0/492	0.65	2/661 (0.3%)
9	k	0.31	0/492	0.65	2/661 (0.3%)
10	L	0.32	0/1186	0.59	2/1611 (0.1%)
10	U	0.32	0/1186	0.59	2/1611 (0.1%)
10	l	0.32	0/1186	0.59	2/1611 (0.1%)
11	M	0.29	0/241	0.58	0/326
11	V	0.30	0/241	0.58	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	m	0.29	0/241	0.58	0/326
All	All	0.32	0/53733	0.60	59/73149 (0.1%)

There are no bond length outliers.

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	417	ASP	CB-CG-OD1	8.35	125.82	118.30
1	A	417	ASP	CB-CG-OD1	8.34	125.81	118.30
1	a	417	ASP	CB-CG-OD1	8.31	125.78	118.30
6	Q	107	LEU	CA-CB-CG	6.99	131.37	115.30
2	b	263	PRO	N-CD-CG	-6.99	92.72	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	46
1	G	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	46
1	a	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	46
2	B	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
2	H	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
2	b	727/730 (100%)	692 (95%)	35 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	N	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
4	O	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
4	d	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
5	E	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
5	P	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
5	e	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
6	F	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	Q	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	f	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
7	I	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
7	R	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
7	i	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
8	J	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	S	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
9	K	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
9	T	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
9	k	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
10	L	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
10	U	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
10	l	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	6612/6900 (96%)	6312 (96%)	297 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	121	VAL

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Mol	Chain	Res	Type
1	a	121	VAL
1	A	121	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/603 (98%)	569 (96%)	22 (4%)	29	28
1	G	591/603 (98%)	569 (96%)	22 (4%)	29	28
1	a	591/603 (98%)	569 (96%)	22 (4%)	29	28
2	B	582/583 (100%)	557 (96%)	25 (4%)	25	22
2	H	582/583 (100%)	557 (96%)	25 (4%)	25	22
2	b	582/583 (100%)	557 (96%)	25 (4%)	25	22
3	C	68/69 (99%)	65 (96%)	3 (4%)	24	21
3	N	68/69 (99%)	65 (96%)	3 (4%)	24	21
3	c	68/69 (99%)	65 (96%)	3 (4%)	24	21
4	D	114/116 (98%)	106 (93%)	8 (7%)	12	8
4	O	114/116 (98%)	106 (93%)	8 (7%)	12	8
4	d	114/116 (98%)	106 (93%)	8 (7%)	12	8
5	E	58/60 (97%)	54 (93%)	4 (7%)	13	9
5	P	58/60 (97%)	54 (93%)	4 (7%)	13	9
5	e	58/60 (97%)	54 (93%)	4 (7%)	13	9
6	F	118/137 (86%)	114 (97%)	4 (3%)	32	31
6	Q	118/137 (86%)	114 (97%)	4 (3%)	32	31
6	f	118/137 (86%)	114 (97%)	4 (3%)	32	31
7	I	32/32 (100%)	31 (97%)	1 (3%)	35	34
7	R	32/32 (100%)	31 (97%)	1 (3%)	35	34
7	i	32/32 (100%)	31 (97%)	1 (3%)	35	34
8	J	34/35 (97%)	32 (94%)	2 (6%)	16	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	34/35 (97%)	32 (94%)	2 (6%)	16	12
8	j	34/35 (97%)	32 (94%)	2 (6%)	16	12
9	K	50/68 (74%)	46 (92%)	4 (8%)	10	6
9	T	50/68 (74%)	46 (92%)	4 (8%)	10	6
9	k	50/68 (74%)	46 (92%)	4 (8%)	10	6
10	L	116/118 (98%)	113 (97%)	3 (3%)	41	42
10	U	116/118 (98%)	113 (97%)	3 (3%)	41	42
10	l	116/118 (98%)	113 (97%)	3 (3%)	41	42
11	M	25/25 (100%)	24 (96%)	1 (4%)	27	24
11	V	25/25 (100%)	24 (96%)	1 (4%)	27	24
11	m	25/25 (100%)	24 (96%)	1 (4%)	27	24
All	All	5364/5538 (97%)	5133 (96%)	231 (4%)	27	22

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	405	VAL
8	J	5	LYS
7	i	2	ASP
6	F	133	MET
2	B	574	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	111	ASN
2	B	276	HIS
3	C	3	HIS
1	a	138	GLN
10	U	157	ASN

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 ⓘ

Of 402 ligands modelled in this entry, 9 are monoatomic - leaving 393 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	H	2140	2	63,73,73	1.38	6 (9%)	74,113,113	1.44	6 (8%)
13	A1AGD	H	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
17	LMG	A	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.29	6 (10%)
12	CLA	B	2125	27	63,73,73	1.32	5 (7%)	74,113,113	1.46	8 (10%)
24	SQD	M	101	-	52,54,54	1.55	7 (13%)	62,65,65	1.37	8 (12%)
12	CLA	f	201	27	63,73,73	1.36	5 (7%)	74,113,113	1.36	7 (9%)
13	A1AGD	b	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
15	BCR	Q	202	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	5 (8%)
12	CLA	b	2120	-	53,63,73	1.47	6 (11%)	62,101,113	1.53	7 (11%)
12	CLA	b	2130	-	43,53,73	1.61	6 (13%)	50,89,113	1.63	6 (12%)
12	CLA	H	2123	2	53,63,73	1.43	6 (11%)	62,101,113	1.62	8 (12%)
15	BCR	b	2145	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
12	CLA	A	822	-	48,58,73	1.54	5 (10%)	56,95,113	1.59	7 (12%)
12	CLA	A	823	1	58,68,73	1.38	6 (10%)	68,107,113	1.50	8 (11%)
12	CLA	B	2140	27	63,73,73	1.26	6 (9%)	74,113,113	1.45	9 (12%)
23	ZEX	F	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
12	CLA	H	2119	2	63,73,73	1.34	5 (7%)	74,113,113	1.42	6 (8%)
15	BCR	A	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	CLA	G	829	1	63,73,73	1.33	6 (9%)	74,113,113	1.58	7 (9%)
12	CLA	G	838	1	63,73,73	1.32	6 (9%)	74,113,113	1.50	8 (10%)
12	CLA	G	820	27	63,73,73	1.28	5 (7%)	74,113,113	1.56	7 (9%)
12	CLA	G	823	1	58,68,73	1.38	6 (10%)	68,107,113	1.51	9 (13%)
12	CLA	l	201	1	63,73,73	1.29	6 (9%)	74,113,113	1.45	8 (10%)
12	CLA	A	809	1	48,58,73	1.57	6 (12%)	56,95,113	1.62	11 (19%)
12	CLA	A	806	1	48,58,73	1.52	5 (10%)	56,95,113	1.61	8 (14%)
12	CLA	A	812	1	63,73,73	1.37	5 (7%)	74,113,113	1.38	9 (12%)
15	BCR	J	104	-	41,41,41	1.06	3 (7%)	56,56,56	1.27	7 (12%)
20	ECH	M	103	-	42,42,42	0.39	0	55,58,58	0.74	0
12	CLA	b	2103	2	63,73,73	1.38	6 (9%)	74,113,113	1.40	7 (9%)
12	CLA	G	806	1	48,58,73	1.52	5 (10%)	56,95,113	1.60	8 (14%)
12	CLA	A	819	1	63,73,73	1.36	5 (7%)	74,113,113	1.44	8 (10%)
13	A1AGD	G	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.94	12 (31%)
12	CLA	H	2103	2	63,73,73	1.38	6 (9%)	74,113,113	1.39	7 (9%)
22	EQ3	b	2150	-	43,43,43	4.23	24 (55%)	55,60,60	5.22	27 (49%)
15	BCR	U	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	F	201	27	63,73,73	1.35	5 (7%)	74,113,113	1.36	7 (9%)
12	CLA	G	816	1	53,63,73	1.43	6 (11%)	62,101,113	1.66	7 (11%)
12	CLA	J	102	-	43,53,73	1.63	5 (11%)	50,89,113	1.68	8 (16%)
12	CLA	G	819	1	63,73,73	1.37	5 (7%)	74,113,113	1.44	8 (10%)
12	CLA	G	803	12,1	53,63,73	1.42	4 (7%)	62,101,113	1.57	8 (12%)
12	CLA	A	801	1	63,73,73	1.38	6 (9%)	74,113,113	1.42	9 (12%)
14	SF4	C	101	3	0,12,12	-	-	-		
15	BCR	I	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	6 (10%)
12	CLA	H	2111	2	63,73,73	1.32	6 (9%)	74,113,113	1.69	15 (20%)
12	CLA	l	205	27	63,73,73	1.31	5 (7%)	74,113,113	1.44	7 (9%)
18	45D	a	852	-	43,43,43	0.39	0	54,60,60	0.85	0
12	CLA	b	2141	16	43,53,73	1.62	5 (11%)	50,89,113	1.74	8 (16%)
12	CLA	B	2137	2	43,53,73	1.59	5 (11%)	50,89,113	1.80	6 (12%)
15	BCR	f	202	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	B	2108	2	63,73,73	1.34	6 (9%)	74,113,113	1.38	6 (8%)
12	CLA	B	2135	-	43,53,73	1.60	5 (11%)	50,89,113	1.71	6 (12%)
12	CLA	H	2125	27	48,58,73	1.50	5 (10%)	56,95,113	1.63	9 (16%)
12	CLA	B	2110	-	63,73,73	1.32	6 (9%)	74,113,113	1.56	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
12	CLA	a	851	27	63,73,73	1.33	7 (11%)	74,113,113	1.44	8 (10%)
12	CLA	a	833	1	63,73,73	1.33	5 (7%)	74,113,113	1.47	7 (9%)
12	CLA	G	805	1	63,73,73	1.31	6 (9%)	74,113,113	1.55	9 (12%)
12	CLA	H	2116	-	43,53,73	1.62	5 (11%)	50,89,113	1.68	6 (12%)
12	CLA	b	2134	-	43,53,73	1.59	5 (11%)	50,89,113	1.71	6 (12%)
20	ECH	V	101	-	42,42,42	0.39	0	55,58,58	0.74	0
15	BCR	l	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	B	2143	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	a	818	1	63,73,73	1.27	5 (7%)	74,113,113	1.48	8 (10%)
12	CLA	G	833	1	63,73,73	1.33	5 (7%)	74,113,113	1.47	7 (9%)
12	CLA	b	2139	27	63,73,73	1.26	6 (9%)	74,113,113	1.45	9 (12%)
16	LHG	V	103	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	G	807	1	63,73,73	1.29	6 (9%)	74,113,113	1.51	8 (10%)
12	CLA	K	4002	9	43,53,73	1.62	5 (11%)	50,89,113	1.66	6 (12%)
16	LHG	b	2148	12	42,42,48	0.63	0	45,48,54	1.22	4 (8%)
20	ECH	b	2143	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	U	203	10	63,73,73	1.27	6 (9%)	74,113,113	1.53	9 (12%)
12	CLA	H	2138	-	43,53,73	1.59	5 (11%)	50,89,113	1.61	7 (14%)
12	CLA	B	2101	16	48,58,73	1.48	6 (12%)	56,95,113	1.67	6 (10%)
12	CLA	G	810	12,1	63,73,73	1.32	5 (7%)	74,113,113	1.48	8 (10%)
12	CLA	a	839	1	63,73,73	1.34	5 (7%)	74,113,113	1.42	7 (9%)
12	CLA	A	815	-	43,53,73	1.65	4 (9%)	50,89,113	1.64	6 (12%)
12	CLA	H	2104	-	63,73,73	1.30	6 (9%)	74,113,113	1.66	8 (10%)
12	CLA	G	825	27	58,68,73	1.35	5 (8%)	68,107,113	1.54	10 (14%)
20	ECH	B	2144	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	b	2109	-	63,73,73	1.32	6 (9%)	74,113,113	1.57	9 (12%)
12	CLA	b	2104	-	63,73,73	1.29	6 (9%)	74,113,113	1.66	8 (10%)
12	CLA	G	828	-	63,73,73	1.29	5 (7%)	74,113,113	1.44	6 (8%)
13	A1AGD	B	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
12	CLA	G	824	27	63,73,73	1.36	5 (7%)	74,113,113	1.53	9 (12%)
12	CLA	A	802	1	63,73,73	1.35	5 (7%)	74,113,113	1.37	8 (10%)
12	CLA	S	103	8	43,53,73	1.65	5 (11%)	50,89,113	1.65	7 (14%)
17	LMG	a	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.28	6 (10%)
12	CLA	A	817	1	58,68,73	1.40	6 (10%)	68,107,113	1.44	8 (11%)
12	CLA	G	837	1	63,73,73	1.33	5 (7%)	74,113,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	LMG	B	2148	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
16	LHG	a	848	12	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
12	CLA	G	817	1	58,68,73	1.40	6 (10%)	68,107,113	1.43	8 (11%)
12	CLA	B	2119	2	48,58,73	1.57	6 (12%)	56,95,113	1.63	8 (14%)
12	CLA	H	2137	2	63,73,73	1.31	5 (7%)	74,113,113	1.44	7 (9%)
12	CLA	H	2108	2	63,73,73	1.33	5 (7%)	74,113,113	1.45	7 (9%)
15	BCR	J	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	a	836	1	63,73,73	1.32	6 (9%)	74,113,113	1.38	6 (8%)
12	CLA	a	821	1	58,68,73	1.38	5 (8%)	68,107,113	1.45	6 (8%)
12	CLA	U	201	1	63,73,73	1.28	6 (9%)	74,113,113	1.44	8 (10%)
17	LMG	A	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.27	4 (10%)
12	CLA	b	2116	-	43,53,73	1.62	5 (11%)	50,89,113	1.67	6 (12%)
12	CLA	B	2139	-	43,53,73	1.58	5 (11%)	50,89,113	1.61	7 (14%)
12	CLA	A	839	1	63,73,73	1.33	5 (7%)	74,113,113	1.42	7 (9%)
16	LHG	G	848	12	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
23	ZEX	f	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
12	CLA	G	836	1	63,73,73	1.32	6 (9%)	74,113,113	1.37	6 (8%)
12	CLA	A	816	1	53,63,73	1.43	6 (11%)	62,101,113	1.65	7 (11%)
12	CLA	B	2116	2	43,53,73	1.64	6 (13%)	50,89,113	1.67	6 (12%)
12	CLA	A	830	1	53,63,73	1.40	5 (9%)	62,101,113	1.60	9 (14%)
12	CLA	a	830	1	53,63,73	1.40	5 (9%)	62,101,113	1.61	9 (14%)
12	CLA	G	801	1	63,73,73	1.37	6 (9%)	74,113,113	1.41	9 (12%)
12	CLA	B	2114	-	43,53,73	1.64	6 (13%)	50,89,113	1.62	7 (14%)
12	CLA	G	839	1	63,73,73	1.33	5 (7%)	74,113,113	1.42	7 (9%)
12	CLA	G	813	1	63,73,73	1.34	4 (6%)	74,113,113	1.46	8 (10%)
12	CLA	A	850	27	63,73,73	1.30	6 (9%)	74,113,113	1.45	5 (6%)
15	BCR	j	104	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	7 (12%)
12	CLA	a	804	1	63,73,73	1.34	6 (9%)	74,113,113	1.60	7 (9%)
12	CLA	a	835	1	63,73,73	1.33	6 (9%)	74,113,113	1.43	8 (10%)
15	BCR	a	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
14	SF4	N	102	3	0,12,12	-	-	-		
23	ZEX	B	2152	-	43,43,43	5.84	26 (60%)	51,60,60	10.37	30 (58%)
12	CLA	G	818	1	63,73,73	1.27	6 (9%)	74,113,113	1.48	8 (10%)
12	CLA	a	811	-	43,53,73	1.61	5 (11%)	50,89,113	1.59	6 (12%)
12	CLA	U	204	10	63,73,73	1.31	5 (7%)	74,113,113	1.45	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	A	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	G	804	1	63,73,73	1.33	6 (9%)	74,113,113	1.61	7 (9%)
12	CLA	a	807	1	63,73,73	1.29	6 (9%)	74,113,113	1.52	8 (10%)
12	CLA	B	2134	2	63,73,73	1.36	5 (7%)	74,113,113	1.45	8 (10%)
12	CLA	H	2132	2	63,73,73	1.29	4 (6%)	74,113,113	1.65	8 (10%)
12	CLA	S	102	-	43,53,73	1.63	4 (9%)	50,89,113	1.67	8 (16%)
12	CLA	B	2124	2	53,63,73	1.43	6 (11%)	62,101,113	1.63	8 (12%)
12	CLA	G	834	1	53,63,73	1.42	5 (9%)	62,101,113	1.62	12 (19%)
12	CLA	b	2123	2	53,63,73	1.43	6 (11%)	62,101,113	1.63	8 (12%)
15	BCR	A	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	B	2141	2	63,73,73	1.38	6 (9%)	74,113,113	1.45	6 (8%)
15	BCR	K	4001	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	5 (8%)
12	CLA	a	802	1	63,73,73	1.35	5 (7%)	74,113,113	1.36	8 (10%)
12	CLA	H	2139	27	63,73,73	1.26	6 (9%)	74,113,113	1.46	9 (12%)
12	CLA	b	2129	2	63,73,73	1.35	7 (11%)	74,113,113	1.55	7 (9%)
12	CLA	a	834	1	53,63,73	1.43	5 (9%)	62,101,113	1.63	12 (19%)
25	DGD	L	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.37	7 (12%)
12	CLA	A	820	27	63,73,73	1.28	5 (7%)	74,113,113	1.56	7 (9%)
12	CLA	G	822	-	48,58,73	1.54	5 (10%)	56,95,113	1.60	7 (12%)
15	BCR	b	2146	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	F	204	-	43,53,73	1.63	5 (11%)	50,89,113	1.60	6 (12%)
12	CLA	j	102	-	43,53,73	1.63	5 (11%)	50,89,113	1.68	8 (16%)
12	CLA	H	2128	2	63,73,73	1.34	7 (11%)	74,113,113	1.29	7 (9%)
12	CLA	b	2126	2	63,73,73	1.38	6 (9%)	74,113,113	1.38	6 (8%)
12	CLA	L	204	10	63,73,73	1.31	5 (7%)	74,113,113	1.45	8 (10%)
24	SQD	L	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	G	802	1	63,73,73	1.35	5 (7%)	74,113,113	1.36	8 (10%)
12	CLA	B	2104	2	63,73,73	1.38	6 (9%)	74,113,113	1.40	7 (9%)
12	CLA	a	824	27	63,73,73	1.36	5 (7%)	74,113,113	1.52	9 (12%)
17	LMG	G	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.29	6 (10%)
12	CLA	B	2115	-	63,73,73	1.36	6 (9%)	74,113,113	1.44	9 (12%)
12	CLA	b	2122	-	43,53,73	1.64	5 (11%)	50,89,113	1.55	6 (12%)
15	BCR	L	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
14	SF4	G	841	2,1	0,12,12	-	-	-		
12	CLA	b	2105	2	63,73,73	1.30	6 (9%)	74,113,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	CLA	F	203	-	43,53,73	1.63	5 (11%)	50,89,113	1.60	7 (14%)
12	CLA	G	851	27	63,73,73	1.33	7 (11%)	74,113,113	1.43	8 (10%)
16	LHG	a	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.28	7 (13%)
12	CLA	H	2130	-	43,53,73	1.60	6 (13%)	50,89,113	1.63	6 (12%)
15	BCR	H	2142	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
15	BCR	H	2145	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	3 (5%)
14	SF4	C	102	3	0,12,12	-	-	-		
12	CLA	H	2131	2	53,63,73	1.43	6 (11%)	62,101,113	1.56	7 (11%)
15	BCR	b	2142	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
12	CLA	a	819	1	63,73,73	1.36	5 (7%)	74,113,113	1.44	8 (10%)
16	LHG	G	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.29	7 (13%)
12	CLA	L	203	10	63,73,73	1.27	6 (9%)	74,113,113	1.52	9 (12%)
12	CLA	H	2134	-	43,53,73	1.60	5 (11%)	50,89,113	1.70	6 (12%)
12	CLA	f	204	-	43,53,73	1.63	5 (11%)	50,89,113	1.60	6 (12%)
12	CLA	G	809	1	48,58,73	1.58	6 (12%)	56,95,113	1.61	11 (19%)
12	CLA	b	2131	2	53,63,73	1.43	6 (11%)	62,101,113	1.56	7 (11%)
12	CLA	H	2105	2	63,73,73	1.30	6 (9%)	74,113,113	1.45	7 (9%)
12	CLA	b	2132	2	63,73,73	1.29	4 (6%)	74,113,113	1.65	8 (10%)
12	CLA	b	2115	2	43,53,73	1.64	5 (11%)	50,89,113	1.67	6 (12%)
12	CLA	J	103	8	43,53,73	1.64	5 (11%)	50,89,113	1.64	7 (14%)
12	CLA	G	812	1	63,73,73	1.37	5 (7%)	74,113,113	1.38	9 (12%)
17	LMG	b	2147	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
23	ZEX	Q	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
12	CLA	A	854	-	53,63,73	1.46	5 (9%)	62,101,113	1.57	9 (14%)
12	CLA	b	2110	2	63,73,73	1.38	7 (11%)	74,113,113	1.44	6 (8%)
12	CLA	b	2140	2	63,73,73	1.38	6 (9%)	74,113,113	1.45	6 (8%)
12	CLA	b	2133	2	63,73,73	1.37	6 (9%)	74,113,113	1.45	8 (10%)
12	CLA	G	814	-	43,53,73	1.63	6 (13%)	50,89,113	1.80	6 (12%)
15	BCR	i	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.32	6 (10%)
12	CLA	l	204	10	63,73,73	1.31	6 (9%)	74,113,113	1.45	8 (10%)
25	DGD	U	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.36	7 (12%)
12	CLA	A	811	-	43,53,73	1.61	5 (11%)	50,89,113	1.60	6 (12%)
12	CLA	H	2115	2	43,53,73	1.63	5 (11%)	50,89,113	1.67	6 (12%)
15	BCR	T	4001	-	41,41,41	1.02	3 (7%)	56,56,56	1.31	6 (10%)
12	CLA	a	828	-	63,73,73	1.30	5 (7%)	74,113,113	1.45	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	CLA	G	815	-	43,53,73	1.65	4 (9%)	50,89,113	1.65	6 (12%)
12	CLA	B	2122	-	53,63,73	1.45	5 (9%)	62,101,113	1.50	7 (11%)
12	CLA	A	814	-	43,53,73	1.63	6 (13%)	50,89,113	1.80	6 (12%)
12	CLA	a	810	12,1	63,73,73	1.32	5 (7%)	74,113,113	1.48	8 (10%)
20	ECH	H	2143	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	k	4002	9	43,53,73	1.61	5 (11%)	50,89,113	1.67	6 (12%)
12	CLA	H	2136	2	43,53,73	1.60	5 (11%)	50,89,113	1.79	6 (12%)
12	CLA	Q	201	27	63,73,73	1.35	5 (7%)	74,113,113	1.35	6 (8%)
12	CLA	G	811	-	43,53,73	1.61	5 (11%)	50,89,113	1.60	6 (12%)
12	CLA	j	103	8	43,53,73	1.63	5 (11%)	50,89,113	1.64	7 (14%)
14	SF4	c	101	3	0,12,12	-	-	-		
12	CLA	a	832	1	63,73,73	1.32	5 (7%)	74,113,113	1.32	7 (9%)
12	CLA	H	2141	16	43,53,73	1.63	5 (11%)	50,89,113	1.74	8 (16%)
12	CLA	H	2101	27	63,73,73	1.27	6 (9%)	74,113,113	1.47	7 (9%)
12	CLA	B	2128	2	63,73,73	1.35	5 (7%)	74,113,113	1.42	6 (8%)
12	CLA	B	2129	2	63,73,73	1.35	7 (11%)	74,113,113	1.29	7 (9%)
12	CLA	f	203	-	43,53,73	1.63	5 (11%)	50,89,113	1.60	7 (14%)
12	CLA	a	838	1	63,73,73	1.32	6 (9%)	74,113,113	1.50	7 (9%)
16	LHG	A	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.28	7 (13%)
12	CLA	a	817	1	58,68,73	1.40	6 (10%)	68,107,113	1.43	8 (11%)
24	SQD	m	102	-	52,54,54	1.56	7 (13%)	62,65,65	1.37	8 (12%)
15	BCR	G	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	a	820	27	63,73,73	1.28	5 (7%)	74,113,113	1.57	7 (9%)
12	CLA	b	2107	2	63,73,73	1.34	6 (9%)	74,113,113	1.38	6 (8%)
15	BCR	B	2146	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	3 (5%)
12	CLA	H	2152	16	48,58,73	1.47	5 (10%)	56,95,113	1.67	6 (10%)
12	CLA	B	2120	2	63,73,73	1.33	5 (7%)	74,113,113	1.42	7 (9%)
23	ZEX	b	2151	-	43,43,43	5.85	26 (60%)	51,60,60	10.37	30 (58%)
12	CLA	a	805	1	63,73,73	1.31	6 (9%)	74,113,113	1.56	9 (12%)
12	CLA	a	831	1	58,68,73	1.37	5 (8%)	68,107,113	1.54	7 (10%)
12	CLA	A	829	1	63,73,73	1.33	6 (9%)	74,113,113	1.59	7 (9%)
15	BCR	B	2145	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	b	2138	-	43,53,73	1.58	5 (11%)	50,89,113	1.61	7 (14%)
12	CLA	B	2131	-	43,53,73	1.60	6 (13%)	50,89,113	1.63	6 (12%)
12	CLA	H	2109	-	63,73,73	1.32	6 (9%)	74,113,113	1.56	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
12	CLA	H	2122	-	43,53,73	1.64	5 (11%)	50,89,113	1.54	6 (12%)
14	SF4	N	101	3	0,12,12	-	-	-		
12	CLA	B	2130	2	63,73,73	1.35	7 (11%)	74,113,113	1.54	7 (9%)
15	BCR	U	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	a	801	1	63,73,73	1.38	7 (11%)	74,113,113	1.42	9 (12%)
12	CLA	B	2105	-	63,73,73	1.29	6 (9%)	74,113,113	1.66	8 (10%)
15	BCR	j	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	8 (14%)
15	BCR	H	2144	-	41,41,41	1.00	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	A	808	1	48,58,73	1.49	6 (12%)	56,95,113	1.78	8 (14%)
12	CLA	a	850	27	63,73,73	1.29	6 (9%)	74,113,113	1.45	5 (6%)
12	CLA	b	2112	2	63,73,73	1.34	5 (7%)	74,113,113	1.41	7 (9%)
12	CLA	b	2135	-	43,53,73	1.61	5 (11%)	50,89,113	1.64	6 (12%)
12	CLA	b	2121	-	53,63,73	1.45	5 (9%)	62,101,113	1.50	7 (11%)
12	CLA	A	804	1	63,73,73	1.33	6 (9%)	74,113,113	1.61	7 (9%)
12	CLA	a	825	27	58,68,73	1.35	5 (8%)	68,107,113	1.53	10 (14%)
12	CLA	A	821	1	58,68,73	1.39	5 (8%)	68,107,113	1.45	6 (8%)
12	CLA	Q	204	-	43,53,73	1.63	5 (11%)	50,89,113	1.60	6 (12%)
12	CLA	G	850	27	63,73,73	1.30	6 (9%)	74,113,113	1.46	5 (6%)
12	CLA	L	205	27	63,73,73	1.31	5 (7%)	74,113,113	1.44	7 (9%)
12	CLA	B	2103	-	63,73,73	1.29	6 (9%)	74,113,113	1.65	10 (13%)
12	CLA	G	827	-	63,73,73	1.30	6 (9%)	74,113,113	1.49	7 (9%)
12	CLA	b	2127	2	63,73,73	1.35	5 (7%)	74,113,113	1.42	6 (8%)
24	SQD	U	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
15	BCR	A	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	4 (7%)
16	LHG	B	2149	12	42,42,48	0.64	0	45,48,54	1.22	4 (8%)
15	BCR	l	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	a	837	1	63,73,73	1.32	5 (7%)	74,113,113	1.43	8 (10%)
13	A1AGD	A	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.94	12 (31%)
18	45D	A	852	-	43,43,43	0.38	0	54,60,60	0.86	0
15	BCR	G	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
26	LMT	l	210	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	0
12	CLA	H	2129	2	63,73,73	1.35	6 (9%)	74,113,113	1.54	7 (9%)
20	ECH	m	101	-	42,42,42	0.39	0	55,58,58	0.74	0
17	LMG	G	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.27	4 (10%)
12	CLA	H	2102	-	63,73,73	1.28	6 (9%)	74,113,113	1.65	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	CLA	B	2111	2	63,73,73	1.39	7 (11%)	74,113,113	1.43	6 (8%)
12	CLA	b	2124	27	63,73,73	1.32	5 (7%)	74,113,113	1.46	8 (10%)
12	CLA	A	838	1	63,73,73	1.32	6 (9%)	74,113,113	1.50	7 (9%)
13	A1AGD	a	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.93	12 (31%)
15	BCR	a	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)
12	CLA	b	2152	16	48,58,73	1.47	6 (12%)	56,95,113	1.67	6 (10%)
12	CLA	H	2120	-	53,63,73	1.47	6 (11%)	62,101,113	1.53	7 (11%)
24	SQD	l	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	b	2102	-	63,73,73	1.28	6 (9%)	74,113,113	1.65	10 (13%)
12	CLA	a	803	12,1	53,63,73	1.43	5 (9%)	62,101,113	1.57	8 (12%)
12	CLA	a	809	1	48,58,73	1.57	6 (12%)	56,95,113	1.62	11 (19%)
15	BCR	G	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	8 (14%)
12	CLA	A	810	12,1	63,73,73	1.32	5 (7%)	74,113,113	1.48	8 (10%)
12	CLA	l	203	10	63,73,73	1.28	6 (9%)	74,113,113	1.52	8 (10%)
12	CLA	A	825	27	58,68,73	1.35	5 (8%)	68,107,113	1.53	10 (14%)
14	SF4	a	841	2,1	0,12,12	-	-	-		
12	CLA	H	2114	-	63,73,73	1.36	6 (9%)	74,113,113	1.43	9 (12%)
12	CLA	a	813	1	63,73,73	1.33	4 (6%)	74,113,113	1.47	7 (9%)
12	CLA	A	827	-	63,73,73	1.31	6 (9%)	74,113,113	1.49	7 (9%)
15	BCR	b	2144	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
15	BCR	L	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	B	2109	2	63,73,73	1.33	5 (7%)	74,113,113	1.45	7 (9%)
12	CLA	b	2106	-	63,73,73	1.32	4 (6%)	74,113,113	1.49	8 (10%)
12	CLA	G	831	1	58,68,73	1.37	5 (8%)	68,107,113	1.53	7 (10%)
12	CLA	B	2107	-	63,73,73	1.33	4 (6%)	74,113,113	1.50	8 (10%)
12	CLA	b	2111	2	63,73,73	1.32	6 (9%)	74,113,113	1.69	15 (20%)
12	CLA	H	2117	2	43,53,73	1.60	4 (9%)	50,89,113	1.74	8 (16%)
12	CLA	a	854	-	53,63,73	1.45	5 (9%)	62,101,113	1.57	9 (14%)
22	EQ3	B	2151	-	43,43,43	4.23	23 (53%)	55,60,60	5.22	27 (49%)
12	CLA	A	831	1	58,68,73	1.37	5 (8%)	68,107,113	1.54	7 (10%)
12	CLA	A	826	1	63,73,73	1.31	7 (11%)	74,113,113	1.35	7 (9%)
12	CLA	H	2113	-	43,53,73	1.64	6 (13%)	50,89,113	1.61	7 (14%)
12	CLA	A	828	-	63,73,73	1.30	5 (7%)	74,113,113	1.45	6 (8%)
12	CLA	b	2118	2	48,58,73	1.58	6 (12%)	56,95,113	1.62	8 (14%)
12	CLA	a	812	1	63,73,73	1.37	5 (7%)	74,113,113	1.38	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	CLA	b	2117	2	43,53,73	1.60	4 (9%)	50,89,113	1.73	8 (16%)
12	CLA	H	2126	2	63,73,73	1.38	6 (9%)	74,113,113	1.38	6 (8%)
12	CLA	H	2106	-	63,73,73	1.34	4 (6%)	74,113,113	1.49	8 (10%)
12	CLA	b	2119	2	63,73,73	1.33	5 (7%)	74,113,113	1.42	7 (9%)
12	CLA	a	826	1	63,73,73	1.31	7 (11%)	74,113,113	1.35	7 (9%)
12	CLA	G	821	1	58,68,73	1.39	5 (8%)	68,107,113	1.45	6 (8%)
12	CLA	b	2113	-	43,53,73	1.64	6 (13%)	50,89,113	1.62	7 (14%)
15	BCR	a	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
14	SF4	c	102	3	0,12,12	-	-	-		
12	CLA	A	851	27	63,73,73	1.33	7 (11%)	74,113,113	1.44	8 (10%)
12	CLA	B	2121	-	53,63,73	1.48	6 (11%)	62,101,113	1.53	7 (11%)
17	LMG	H	2147	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
12	CLA	B	2102	27	63,73,73	1.27	6 (9%)	74,113,113	1.47	7 (9%)
12	CLA	H	2118	2	48,58,73	1.57	6 (12%)	56,95,113	1.63	8 (14%)
12	CLA	a	815	-	43,53,73	1.65	5 (11%)	50,89,113	1.64	6 (12%)
22	EQ3	H	2150	-	43,43,43	4.23	24 (55%)	55,60,60	5.22	27 (49%)
12	CLA	H	2121	-	53,63,73	1.45	5 (9%)	62,101,113	1.51	7 (11%)
12	CLA	H	2133	2	63,73,73	1.36	5 (7%)	74,113,113	1.45	8 (10%)
12	CLA	b	2101	27	63,73,73	1.27	6 (9%)	74,113,113	1.47	8 (10%)
12	CLA	b	2136	2	43,53,73	1.59	6 (13%)	50,89,113	1.80	6 (12%)
12	CLA	H	2110	2	63,73,73	1.38	7 (11%)	74,113,113	1.44	6 (8%)
12	CLA	T	4002	9	43,53,73	1.62	5 (11%)	50,89,113	1.66	6 (12%)
12	CLA	A	818	1	63,73,73	1.27	5 (7%)	74,113,113	1.47	8 (10%)
26	LMT	L	210	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	0
12	CLA	A	835	1	63,73,73	1.33	6 (9%)	74,113,113	1.43	8 (10%)
12	CLA	A	805	1	63,73,73	1.32	6 (9%)	74,113,113	1.55	9 (12%)
18	45D	G	852	-	43,43,43	0.38	0	54,60,60	0.86	0
12	CLA	b	2125	27	48,58,73	1.50	5 (10%)	56,95,113	1.63	10 (17%)
12	CLA	A	836	1	63,73,73	1.32	5 (7%)	74,113,113	1.37	6 (8%)
12	CLA	A	824	27	63,73,73	1.36	5 (7%)	74,113,113	1.53	9 (12%)
15	BCR	k	4001	-	41,41,41	1.01	2 (4%)	56,56,56	1.31	5 (8%)
12	CLA	B	2138	2	63,73,73	1.31	5 (7%)	74,113,113	1.44	7 (9%)
15	BCR	F	202	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	5 (8%)
12	CLA	A	837	1	63,73,73	1.33	5 (7%)	74,113,113	1.44	8 (10%)
12	CLA	H	2107	2	63,73,73	1.34	6 (9%)	74,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
26	LMT	U	210	-	36,36,36	1.16	5 (13%)	47,47,47	1.00	0
12	CLA	a	822	-	48,58,73	1.54	5 (10%)	56,95,113	1.59	7 (12%)
12	CLA	L	201	1	63,73,73	1.29	6 (9%)	74,113,113	1.44	8 (10%)
12	CLA	B	2123	-	43,53,73	1.64	5 (11%)	50,89,113	1.55	6 (12%)
15	BCR	S	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	b	2137	2	63,73,73	1.31	5 (7%)	74,113,113	1.44	7 (9%)
12	CLA	B	2112	2	63,73,73	1.31	6 (9%)	74,113,113	1.69	15 (20%)
12	CLA	a	827	-	63,73,73	1.31	6 (9%)	74,113,113	1.49	7 (9%)
12	CLA	a	816	1	53,63,73	1.43	6 (11%)	62,101,113	1.66	7 (11%)
12	CLA	G	832	1	63,73,73	1.33	5 (7%)	74,113,113	1.33	7 (9%)
16	LHG	H	2148	12	42,42,48	0.64	0	45,48,54	1.22	4 (8%)
12	CLA	G	835	1	63,73,73	1.33	6 (9%)	74,113,113	1.43	8 (10%)
12	CLA	B	2142	16	43,53,73	1.62	5 (11%)	50,89,113	1.74	8 (16%)
15	BCR	B	2147	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	A	803	12,1	53,63,73	1.43	5 (9%)	62,101,113	1.57	7 (11%)
12	CLA	B	2113	2	63,73,73	1.33	5 (7%)	74,113,113	1.40	7 (9%)
24	SQD	V	102	-	52,54,54	1.56	7 (13%)	62,65,65	1.37	8 (12%)
12	CLA	A	832	1	63,73,73	1.32	5 (7%)	74,113,113	1.33	6 (8%)
12	CLA	B	2126	27	48,58,73	1.50	5 (10%)	56,95,113	1.63	10 (17%)
12	CLA	B	2106	2	63,73,73	1.30	6 (9%)	74,113,113	1.45	7 (9%)
12	CLA	a	829	1	63,73,73	1.33	6 (9%)	74,113,113	1.60	7 (9%)
12	CLA	H	2127	2	63,73,73	1.35	5 (7%)	74,113,113	1.42	7 (9%)
12	CLA	b	2128	2	63,73,73	1.35	7 (11%)	74,113,113	1.30	8 (10%)
12	CLA	a	823	1	58,68,73	1.37	6 (10%)	68,107,113	1.50	9 (13%)
12	CLA	A	813	1	63,73,73	1.33	4 (6%)	74,113,113	1.46	7 (9%)
12	CLA	B	2136	-	43,53,73	1.61	5 (11%)	50,89,113	1.64	6 (12%)
12	CLA	G	826	1	63,73,73	1.32	7 (11%)	74,113,113	1.34	7 (9%)
25	DGD	l	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.37	7 (12%)
12	CLA	B	2118	2	43,53,73	1.60	4 (9%)	50,89,113	1.74	8 (16%)
12	CLA	B	2117	-	43,53,73	1.62	5 (11%)	50,89,113	1.67	6 (12%)
16	LHG	m	103	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
15	BCR	R	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	6 (10%)
23	ZEX	H	2151	-	43,43,43	5.84	26 (60%)	51,60,60	10.36	30 (58%)
12	CLA	b	2108	2	63,73,73	1.33	5 (7%)	74,113,113	1.46	7 (9%)
12	CLA	a	808	1	48,58,73	1.48	6 (12%)	56,95,113	1.77	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	LHG	A	848	12	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
15	BCR	G	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	4 (7%)
16	LHG	M	102	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	G	854	-	53,63,73	1.46	6 (11%)	62,101,113	1.57	9 (14%)
12	CLA	a	814	-	43,53,73	1.62	6 (13%)	50,89,113	1.80	6 (12%)
12	CLA	A	834	1	53,63,73	1.42	5 (9%)	62,101,113	1.63	12 (19%)
14	SF4	A	841	2,1	0,12,12	-	-	-		
12	CLA	B	2127	2	63,73,73	1.38	6 (9%)	74,113,113	1.38	6 (8%)
12	CLA	G	808	1	48,58,73	1.49	6 (12%)	56,95,113	1.78	8 (14%)
15	BCR	H	2146	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
15	BCR	a	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	4 (7%)
12	CLA	Q	203	-	43,53,73	1.63	5 (11%)	50,89,113	1.59	7 (14%)
12	CLA	b	2114	-	63,73,73	1.36	6 (9%)	74,113,113	1.43	9 (12%)
12	CLA	B	2132	2	53,63,73	1.43	6 (11%)	62,101,113	1.56	7 (11%)
12	CLA	a	806	1	48,58,73	1.52	5 (10%)	56,95,113	1.61	8 (14%)
12	CLA	H	2112	2	63,73,73	1.34	5 (7%)	74,113,113	1.40	6 (8%)
17	LMG	a	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.26	4 (10%)
12	CLA	A	833	1	63,73,73	1.33	5 (7%)	74,113,113	1.47	7 (9%)
12	CLA	H	2135	-	43,53,73	1.61	5 (11%)	50,89,113	1.63	6 (12%)
15	BCR	S	104	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
12	CLA	U	205	27	63,73,73	1.31	5 (7%)	74,113,113	1.43	7 (9%)
12	CLA	A	807	1	63,73,73	1.29	6 (9%)	74,113,113	1.51	8 (10%)
12	CLA	G	830	1	53,63,73	1.40	5 (9%)	62,101,113	1.60	9 (14%)
12	CLA	H	2124	27	63,73,73	1.32	6 (9%)	74,113,113	1.46	8 (10%)
12	CLA	B	2133	2	63,73,73	1.29	4 (6%)	74,113,113	1.65	9 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	2140	2	1/1/15/20	14/37/115/115	-
13	A1AGD	H	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
17	LMG	A	847	-	-	20/45/65/70	0/1/1/1
12	CLA	B	2125	27	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	SQD	M	101	-	-	28/49/69/69	0/1/1/1
12	CLA	f	201	27	1/1/15/20	20/37/115/115	-
13	A1AGD	b	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
15	BCR	Q	202	-	-	13/29/63/63	0/2/2/2
12	CLA	b	2120	-	1/1/13/20	6/25/103/115	-
12	CLA	b	2130	-	1/1/11/20	0/13/91/115	-
12	CLA	H	2123	2	1/1/13/20	12/25/103/115	-
15	BCR	b	2145	-	-	7/29/63/63	0/2/2/2
12	CLA	A	822	-	1/1/12/20	8/19/97/115	-
12	CLA	A	823	1	1/1/14/20	8/31/109/115	-
12	CLA	B	2140	27	1/1/15/20	8/37/115/115	-
23	ZEX	F	205	-	-	14/29/67/67	0/2/2/2
12	CLA	H	2119	2	1/1/15/20	16/37/115/115	-
15	BCR	A	843	-	-	15/29/63/63	0/2/2/2
12	CLA	G	829	1	1/1/15/20	12/37/115/115	-
12	CLA	G	838	1	1/1/15/20	4/37/115/115	-
12	CLA	G	820	27	1/1/15/20	7/37/115/115	-
12	CLA	G	823	1	1/1/14/20	8/31/109/115	-
12	CLA	l	201	1	1/1/15/20	13/37/115/115	-
12	CLA	A	809	1	1/1/12/20	8/19/97/115	-
12	CLA	A	806	1	1/1/12/20	5/19/97/115	-
12	CLA	A	812	1	1/1/15/20	11/37/115/115	-
15	BCR	J	104	-	-	9/29/63/63	0/2/2/2
20	ECH	M	103	-	-	10/29/66/66	0/2/2/2
12	CLA	b	2103	2	1/1/15/20	15/37/115/115	-
12	CLA	G	806	1	1/1/12/20	5/19/97/115	-
12	CLA	A	819	1	1/1/15/20	16/37/115/115	-
13	A1AGD	G	840	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	H	2103	2	1/1/15/20	15/37/115/115	-
22	EQ3	b	2150	-	-	14/29/68/68	0/2/2/2
15	BCR	U	206	-	-	10/29/63/63	0/2/2/2
12	CLA	F	201	27	1/1/15/20	20/37/115/115	-
12	CLA	G	816	1	1/1/13/20	4/25/103/115	-
12	CLA	J	102	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	819	1	1/1/15/20	16/37/115/115	-
12	CLA	G	803	12,1	1/1/13/20	2/25/103/115	-
12	CLA	A	801	1	1/1/15/20	5/37/115/115	-
14	SF4	C	101	3	-	-	0/6/5/5
15	BCR	I	101	-	-	7/29/63/63	0/2/2/2
12	CLA	H	2111	2	1/1/15/20	12/37/115/115	-
12	CLA	l	205	27	1/1/15/20	6/37/115/115	-
18	45D	a	852	-	-	8/29/69/69	0/2/2/2
12	CLA	b	2141	16	1/1/11/20	7/13/91/115	-
12	CLA	B	2137	2	1/1/11/20	6/13/91/115	-
15	BCR	f	202	-	-	13/29/63/63	0/2/2/2
12	CLA	B	2108	2	1/1/15/20	14/37/115/115	-
12	CLA	B	2135	-	1/1/11/20	4/13/91/115	-
12	CLA	H	2125	27	1/1/12/20	2/19/97/115	-
12	CLA	B	2110	-	1/1/15/20	11/37/115/115	-
12	CLA	a	851	27	1/1/15/20	11/37/115/115	-
12	CLA	a	833	1	1/1/15/20	13/37/115/115	-
12	CLA	G	805	1	1/1/15/20	14/37/115/115	-
12	CLA	H	2116	-	1/1/11/20	7/13/91/115	-
12	CLA	b	2134	-	1/1/11/20	4/13/91/115	-
20	ECH	V	101	-	-	10/29/66/66	0/2/2/2
15	BCR	l	206	-	-	10/29/63/63	0/2/2/2
15	BCR	B	2143	-	-	6/29/63/63	0/2/2/2
12	CLA	a	818	1	1/1/15/20	10/37/115/115	-
12	CLA	G	833	1	1/1/15/20	13/37/115/115	-
12	CLA	b	2139	27	1/1/15/20	8/37/115/115	-
16	LHG	V	103	-	-	24/48/48/53	-
12	CLA	G	807	1	1/1/15/20	14/37/115/115	-
12	CLA	K	4002	9	1/1/11/20	7/13/91/115	-
16	LHG	b	2148	12	-	18/47/47/53	-
20	ECH	b	2143	-	-	12/29/66/66	0/2/2/2
12	CLA	U	203	10	1/1/15/20	12/37/115/115	-
12	CLA	H	2138	-	1/1/11/20	4/13/91/115	-
12	CLA	B	2101	16	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	810	12,1	1/1/15/20	13/37/115/115	-
12	CLA	a	839	1	1/1/15/20	8/37/115/115	-
12	CLA	A	815	-	1/1/11/20	3/13/91/115	-
12	CLA	H	2104	-	1/1/15/20	8/37/115/115	-
12	CLA	G	825	27	1/1/14/20	5/31/109/115	-
20	ECH	B	2144	-	-	12/29/66/66	0/2/2/2
12	CLA	b	2109	-	1/1/15/20	11/37/115/115	-
12	CLA	b	2104	-	1/1/15/20	8/37/115/115	-
12	CLA	G	828	-	1/1/15/20	12/37/115/115	-
13	A1AGD	B	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	G	824	27	1/1/15/20	19/37/115/115	-
12	CLA	A	802	1	1/1/15/20	7/37/115/115	-
12	CLA	S	103	8	1/1/11/20	8/13/91/115	-
17	LMG	a	847	-	-	20/45/65/70	0/1/1/1
12	CLA	A	817	1	1/1/14/20	15/31/109/115	-
12	CLA	G	837	1	1/1/15/20	11/37/115/115	-
17	LMG	B	2148	-	-	14/46/66/70	0/1/1/1
16	LHG	a	848	12	-	19/53/53/53	-
12	CLA	G	817	1	1/1/14/20	15/31/109/115	-
12	CLA	B	2119	2	1/1/12/20	5/19/97/115	-
12	CLA	H	2137	2	1/1/15/20	7/37/115/115	-
12	CLA	H	2108	2	1/1/15/20	9/37/115/115	-
15	BCR	J	101	-	-	13/29/63/63	0/2/2/2
12	CLA	a	836	1	1/1/15/20	12/37/115/115	-
12	CLA	a	821	1	1/1/14/20	7/31/109/115	-
12	CLA	U	201	1	1/1/15/20	13/37/115/115	-
17	LMG	A	849	-	-	14/26/46/70	0/1/1/1
12	CLA	b	2116	-	1/1/11/20	7/13/91/115	-
12	CLA	B	2139	-	1/1/11/20	4/13/91/115	-
12	CLA	A	839	1	1/1/15/20	8/37/115/115	-
16	LHG	G	848	12	-	18/53/53/53	-
23	ZEX	f	205	-	-	14/29/67/67	0/2/2/2
12	CLA	G	836	1	1/1/15/20	12/37/115/115	-
12	CLA	A	816	1	1/1/13/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	2116	2	1/1/11/20	2/13/91/115	-
12	CLA	A	830	1	-	7/25/103/115	-
12	CLA	a	830	1	-	7/25/103/115	-
12	CLA	G	801	1	1/1/15/20	5/37/115/115	-
12	CLA	B	2114	-	-	8/13/91/115	-
12	CLA	G	839	1	1/1/15/20	8/37/115/115	-
12	CLA	G	813	1	1/1/15/20	12/37/115/115	-
12	CLA	A	850	27	1/1/15/20	6/37/115/115	-
15	BCR	j	104	-	-	9/29/63/63	0/2/2/2
12	CLA	a	804	1	1/1/15/20	16/37/115/115	-
12	CLA	a	835	1	1/1/15/20	13/37/115/115	-
15	BCR	a	842	-	-	11/29/63/63	0/2/2/2
14	SF4	N	102	3	-	-	0/6/5/5
23	ZEX	B	2152	-	-	11/29/67/67	0/2/2/2
12	CLA	G	818	1	1/1/15/20	10/37/115/115	-
12	CLA	a	811	-	1/1/11/20	6/13/91/115	-
12	CLA	U	204	10	1/1/15/20	6/37/115/115	-
15	BCR	A	844	-	-	8/29/63/63	0/2/2/2
12	CLA	G	804	1	1/1/15/20	16/37/115/115	-
12	CLA	a	807	1	1/1/15/20	14/37/115/115	-
12	CLA	B	2134	2	1/1/15/20	16/37/115/115	-
12	CLA	H	2132	2	1/1/15/20	18/37/115/115	-
12	CLA	S	102	-	1/1/11/20	7/13/91/115	-
12	CLA	B	2124	2	1/1/13/20	12/25/103/115	-
12	CLA	G	834	1	1/1/13/20	10/25/103/115	-
12	CLA	b	2123	2	1/1/13/20	12/25/103/115	-
15	BCR	A	842	-	-	12/29/63/63	0/2/2/2
12	CLA	B	2141	2	1/1/15/20	14/37/115/115	-
15	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
12	CLA	a	802	1	1/1/15/20	7/37/115/115	-
12	CLA	H	2139	27	1/1/15/20	8/37/115/115	-
12	CLA	b	2129	2	1/1/15/20	13/37/115/115	-
12	CLA	a	834	1	1/1/13/20	10/25/103/115	-
25	DGD	L	209	-	-	21/44/64/95	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	820	27	1/1/15/20	7/37/115/115	-
12	CLA	G	822	-	1/1/12/20	8/19/97/115	-
15	BCR	b	2146	-	-	17/29/63/63	0/2/2/2
12	CLA	F	204	-	1/1/11/20	3/13/91/115	-
12	CLA	j	102	-	1/1/11/20	7/13/91/115	-
12	CLA	H	2128	2	1/1/15/20	10/37/115/115	-
12	CLA	b	2126	2	1/1/15/20	9/37/115/115	-
12	CLA	L	204	10	1/1/15/20	6/37/115/115	-
24	SQD	L	208	-	-	15/40/60/69	0/1/1/1
12	CLA	G	802	1	1/1/15/20	7/37/115/115	-
12	CLA	B	2104	2	1/1/15/20	15/37/115/115	-
12	CLA	a	824	27	1/1/15/20	19/37/115/115	-
17	LMG	G	847	-	-	20/45/65/70	0/1/1/1
12	CLA	B	2115	-	1/1/15/20	16/37/115/115	-
12	CLA	b	2122	-	1/1/11/20	5/13/91/115	-
15	BCR	L	207	-	-	6/29/63/63	0/2/2/2
14	SF4	G	841	2,1	-	-	0/6/5/5
12	CLA	b	2105	2	1/1/15/20	7/37/115/115	-
12	CLA	F	203	-	1/1/11/20	4/13/91/115	-
12	CLA	G	851	27	1/1/15/20	11/37/115/115	-
16	LHG	a	846	-	-	27/53/53/53	-
12	CLA	H	2130	-	1/1/11/20	0/13/91/115	-
15	BCR	H	2142	-	-	6/29/63/63	0/2/2/2
15	BCR	H	2145	-	-	7/29/63/63	0/2/2/2
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	H	2131	2	1/1/13/20	7/25/103/115	-
15	BCR	b	2142	-	-	6/29/63/63	0/2/2/2
12	CLA	a	819	1	1/1/15/20	16/37/115/115	-
16	LHG	G	846	-	-	28/53/53/53	-
12	CLA	L	203	10	1/1/15/20	12/37/115/115	-
12	CLA	H	2134	-	1/1/11/20	4/13/91/115	-
12	CLA	f	204	-	1/1/11/20	3/13/91/115	-
12	CLA	G	809	1	1/1/12/20	8/19/97/115	-
12	CLA	b	2131	2	1/1/13/20	7/25/103/115	-
12	CLA	H	2105	2	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	2132	2	1/1/15/20	18/37/115/115	-
12	CLA	b	2115	2	1/1/11/20	2/13/91/115	-
12	CLA	J	103	8	1/1/11/20	8/13/91/115	-
12	CLA	G	812	1	1/1/15/20	11/37/115/115	-
17	LMG	b	2147	-	-	14/46/66/70	0/1/1/1
23	ZEX	Q	205	-	-	14/29/67/67	0/2/2/2
12	CLA	A	854	-	1/1/13/20	7/25/103/115	-
12	CLA	b	2110	2	1/1/15/20	12/37/115/115	-
12	CLA	b	2140	2	1/1/15/20	14/37/115/115	-
12	CLA	b	2133	2	1/1/15/20	16/37/115/115	-
12	CLA	G	814	-	1/1/11/20	4/13/91/115	-
15	BCR	i	101	-	-	7/29/63/63	0/2/2/2
12	CLA	l	204	10	1/1/15/20	6/37/115/115	-
25	DGD	U	209	-	-	21/44/64/95	0/1/1/2
12	CLA	A	811	-	1/1/11/20	6/13/91/115	-
12	CLA	H	2115	2	1/1/11/20	2/13/91/115	-
15	BCR	T	4001	-	-	8/29/63/63	0/2/2/2
12	CLA	a	828	-	1/1/15/20	12/37/115/115	-
12	CLA	G	815	-	1/1/11/20	3/13/91/115	-
12	CLA	B	2122	-	-	10/25/103/115	-
12	CLA	A	814	-	1/1/11/20	4/13/91/115	-
12	CLA	a	810	12,1	1/1/15/20	13/37/115/115	-
20	ECH	H	2143	-	-	12/29/66/66	0/2/2/2
12	CLA	k	4002	9	1/1/11/20	7/13/91/115	-
12	CLA	H	2136	2	1/1/11/20	6/13/91/115	-
12	CLA	Q	201	27	1/1/15/20	19/37/115/115	-
12	CLA	G	811	-	1/1/11/20	6/13/91/115	-
12	CLA	j	103	8	1/1/11/20	8/13/91/115	-
14	SF4	c	101	3	-	-	0/6/5/5
12	CLA	a	832	1	1/1/15/20	10/37/115/115	-
12	CLA	H	2141	16	1/1/11/20	7/13/91/115	-
12	CLA	H	2101	27	1/1/15/20	14/37/115/115	-
12	CLA	B	2128	2	1/1/15/20	16/37/115/115	-
12	CLA	B	2129	2	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	f	203	-	1/1/11/20	4/13/91/115	-
12	CLA	a	838	1	1/1/15/20	4/37/115/115	-
16	LHG	A	846	-	-	27/53/53/53	-
12	CLA	a	817	1	1/1/14/20	15/31/109/115	-
24	SQD	m	102	-	-	28/49/69/69	0/1/1/1
15	BCR	G	844	-	-	8/29/63/63	0/2/2/2
12	CLA	a	820	27	1/1/15/20	7/37/115/115	-
12	CLA	b	2107	2	1/1/15/20	14/37/115/115	-
15	BCR	B	2146	-	-	7/29/63/63	0/2/2/2
12	CLA	H	2152	16	1/1/12/20	5/19/97/115	-
12	CLA	B	2120	2	1/1/15/20	16/37/115/115	-
23	ZEX	b	2151	-	-	11/29/67/67	0/2/2/2
12	CLA	a	805	1	1/1/15/20	14/37/115/115	-
12	CLA	a	831	1	1/1/14/20	9/31/109/115	-
12	CLA	A	829	1	1/1/15/20	12/37/115/115	-
15	BCR	B	2145	-	-	8/29/63/63	0/2/2/2
12	CLA	b	2138	-	1/1/11/20	4/13/91/115	-
12	CLA	B	2131	-	1/1/11/20	0/13/91/115	-
12	CLA	H	2109	-	1/1/15/20	11/37/115/115	-
12	CLA	H	2122	-	1/1/11/20	5/13/91/115	-
14	SF4	N	101	3	-	-	0/6/5/5
12	CLA	B	2130	2	1/1/15/20	13/37/115/115	-
15	BCR	U	207	-	-	6/29/63/63	0/2/2/2
12	CLA	a	801	1	1/1/15/20	5/37/115/115	-
12	CLA	B	2105	-	1/1/15/20	8/37/115/115	-
15	BCR	j	101	-	-	13/29/63/63	0/2/2/2
15	BCR	H	2144	-	-	8/29/63/63	0/2/2/2
12	CLA	A	808	1	1/1/12/20	3/19/97/115	-
12	CLA	a	850	27	1/1/15/20	6/37/115/115	-
12	CLA	b	2112	2	1/1/15/20	6/37/115/115	-
12	CLA	b	2135	-	1/1/11/20	7/13/91/115	-
12	CLA	b	2121	-	-	10/25/103/115	-
12	CLA	A	804	1	1/1/15/20	16/37/115/115	-
12	CLA	a	825	27	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	821	1	1/1/14/20	7/31/109/115	-
12	CLA	Q	204	-	1/1/11/20	3/13/91/115	-
12	CLA	G	850	27	1/1/15/20	6/37/115/115	-
12	CLA	L	205	27	1/1/15/20	6/37/115/115	-
12	CLA	B	2103	-	1/1/15/20	12/37/115/115	-
12	CLA	G	827	-	1/1/15/20	6/37/115/115	-
12	CLA	b	2127	2	1/1/15/20	16/37/115/115	-
24	SQD	U	208	-	-	15/40/60/69	0/1/1/1
15	BCR	A	845	-	-	8/29/63/63	0/2/2/2
16	LHG	B	2149	12	-	18/47/47/53	-
15	BCR	l	207	-	-	6/29/63/63	0/2/2/2
12	CLA	a	837	1	1/1/15/20	11/37/115/115	-
13	A1AGD	A	840	-	2/2/9/11	8/23/43/43	0/1/1/1
18	45D	A	852	-	-	8/29/69/69	0/2/2/2
15	BCR	G	842	-	-	12/29/63/63	0/2/2/2
26	LMT	l	210	-	-	12/21/61/61	0/2/2/2
12	CLA	H	2129	2	1/1/15/20	13/37/115/115	-
20	ECH	m	101	-	-	10/29/66/66	0/2/2/2
17	LMG	G	849	-	-	14/26/46/70	0/1/1/1
12	CLA	H	2102	-	1/1/15/20	12/37/115/115	-
12	CLA	B	2111	2	1/1/15/20	12/37/115/115	-
12	CLA	b	2124	27	1/1/15/20	6/37/115/115	-
12	CLA	A	838	1	1/1/15/20	4/37/115/115	-
13	A1AGD	a	840	-	2/2/9/11	8/23/43/43	0/1/1/1
15	BCR	a	843	-	-	15/29/63/63	0/2/2/2
12	CLA	b	2152	16	1/1/12/20	5/19/97/115	-
12	CLA	H	2120	-	1/1/13/20	6/25/103/115	-
24	SQD	l	208	-	-	15/40/60/69	0/1/1/1
12	CLA	b	2102	-	1/1/15/20	12/37/115/115	-
12	CLA	a	803	12,1	1/1/13/20	2/25/103/115	-
12	CLA	a	809	1	1/1/12/20	8/19/97/115	-
15	BCR	G	843	-	-	15/29/63/63	0/2/2/2
12	CLA	A	810	12,1	1/1/15/20	13/37/115/115	-
12	CLA	l	203	10	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	825	27	1/1/14/20	5/31/109/115	-
14	SF4	a	841	2,1	-	-	0/6/5/5
12	CLA	H	2114	-	1/1/15/20	16/37/115/115	-
12	CLA	a	813	1	1/1/15/20	12/37/115/115	-
12	CLA	A	827	-	1/1/15/20	6/37/115/115	-
15	BCR	b	2144	-	-	8/29/63/63	0/2/2/2
15	BCR	L	206	-	-	10/29/63/63	0/2/2/2
12	CLA	B	2109	2	1/1/15/20	9/37/115/115	-
12	CLA	b	2106	-	1/1/15/20	16/37/115/115	-
12	CLA	G	831	1	1/1/14/20	9/31/109/115	-
12	CLA	B	2107	-	1/1/15/20	16/37/115/115	-
12	CLA	b	2111	2	1/1/15/20	12/37/115/115	-
12	CLA	H	2117	2	1/1/11/20	8/13/91/115	-
12	CLA	a	854	-	1/1/13/20	7/25/103/115	-
22	EQ3	B	2151	-	-	14/29/68/68	0/2/2/2
12	CLA	A	831	1	1/1/14/20	9/31/109/115	-
12	CLA	A	826	1	1/1/15/20	13/37/115/115	-
12	CLA	H	2113	-	-	8/13/91/115	-
12	CLA	A	828	-	1/1/15/20	12/37/115/115	-
12	CLA	b	2118	2	1/1/12/20	5/19/97/115	-
12	CLA	a	812	1	1/1/15/20	11/37/115/115	-
12	CLA	b	2117	2	1/1/11/20	8/13/91/115	-
12	CLA	H	2126	2	1/1/15/20	9/37/115/115	-
12	CLA	H	2106	-	1/1/15/20	16/37/115/115	-
12	CLA	b	2119	2	1/1/15/20	16/37/115/115	-
12	CLA	a	826	1	1/1/15/20	13/37/115/115	-
12	CLA	G	821	1	1/1/14/20	7/31/109/115	-
12	CLA	b	2113	-	-	8/13/91/115	-
15	BCR	a	844	-	-	8/29/63/63	0/2/2/2
14	SF4	c	102	3	-	-	0/6/5/5
12	CLA	A	851	27	1/1/15/20	11/37/115/115	-
12	CLA	B	2121	-	1/1/13/20	6/25/103/115	-
17	LMG	H	2147	-	-	14/46/66/70	0/1/1/1
12	CLA	B	2102	27	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	2118	2	1/1/12/20	5/19/97/115	-
12	CLA	a	815	-	1/1/11/20	3/13/91/115	-
22	EQ3	H	2150	-	-	14/29/68/68	0/2/2/2
12	CLA	H	2121	-	-	10/25/103/115	-
12	CLA	H	2133	2	1/1/15/20	16/37/115/115	-
12	CLA	b	2101	27	1/1/15/20	14/37/115/115	-
12	CLA	b	2136	2	1/1/11/20	6/13/91/115	-
12	CLA	H	2110	2	1/1/15/20	12/37/115/115	-
12	CLA	T	4002	9	1/1/11/20	7/13/91/115	-
12	CLA	A	818	1	1/1/15/20	10/37/115/115	-
26	LMT	L	210	-	-	12/21/61/61	0/2/2/2
12	CLA	A	835	1	1/1/15/20	13/37/115/115	-
12	CLA	A	805	1	1/1/15/20	14/37/115/115	-
18	45D	G	852	-	-	8/29/69/69	0/2/2/2
12	CLA	b	2125	27	1/1/12/20	2/19/97/115	-
12	CLA	A	836	1	1/1/15/20	12/37/115/115	-
12	CLA	A	824	27	1/1/15/20	19/37/115/115	-
15	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
12	CLA	B	2138	2	1/1/15/20	7/37/115/115	-
15	BCR	F	202	-	-	13/29/63/63	0/2/2/2
12	CLA	A	837	1	1/1/15/20	11/37/115/115	-
12	CLA	H	2107	2	1/1/15/20	14/37/115/115	-
26	LMT	U	210	-	-	12/21/61/61	0/2/2/2
12	CLA	a	822	-	1/1/12/20	8/19/97/115	-
12	CLA	L	201	1	1/1/15/20	13/37/115/115	-
12	CLA	B	2123	-	1/1/11/20	5/13/91/115	-
15	BCR	S	101	-	-	13/29/63/63	0/2/2/2
12	CLA	b	2137	2	1/1/15/20	7/37/115/115	-
12	CLA	B	2112	2	1/1/15/20	12/37/115/115	-
12	CLA	a	827	-	1/1/15/20	6/37/115/115	-
12	CLA	a	816	1	1/1/13/20	4/25/103/115	-
12	CLA	G	832	1	1/1/15/20	10/37/115/115	-
16	LHG	H	2148	12	-	18/47/47/53	-
12	CLA	G	835	1	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	2142	16	1/1/11/20	7/13/91/115	-
15	BCR	B	2147	-	-	17/29/63/63	0/2/2/2
12	CLA	A	803	12,1	1/1/13/20	2/25/103/115	-
12	CLA	B	2113	2	1/1/15/20	6/37/115/115	-
24	SQD	V	102	-	-	28/49/69/69	0/1/1/1
12	CLA	A	832	1	1/1/15/20	10/37/115/115	-
12	CLA	B	2126	27	1/1/12/20	2/19/97/115	-
12	CLA	B	2106	2	1/1/15/20	7/37/115/115	-
12	CLA	a	829	1	1/1/15/20	12/37/115/115	-
12	CLA	H	2127	2	1/1/15/20	16/37/115/115	-
12	CLA	b	2128	2	1/1/15/20	10/37/115/115	-
12	CLA	a	823	1	1/1/14/20	8/31/109/115	-
12	CLA	A	813	1	1/1/15/20	12/37/115/115	-
12	CLA	B	2136	-	1/1/11/20	7/13/91/115	-
12	CLA	G	826	1	1/1/15/20	13/37/115/115	-
25	DGD	l	209	-	-	21/44/64/95	0/1/1/2
12	CLA	B	2118	2	1/1/11/20	8/13/91/115	-
12	CLA	B	2117	-	1/1/11/20	7/13/91/115	-
16	LHG	m	103	-	-	24/48/48/53	-
15	BCR	R	101	-	-	7/29/63/63	0/2/2/2
23	ZEX	H	2151	-	-	11/29/67/67	0/2/2/2
12	CLA	b	2108	2	1/1/15/20	9/37/115/115	-
12	CLA	a	808	1	1/1/12/20	3/19/97/115	-
16	LHG	A	848	12	-	19/53/53/53	-
15	BCR	G	845	-	-	8/29/63/63	0/2/2/2
16	LHG	M	102	-	-	24/48/48/53	-
12	CLA	G	854	-	1/1/13/20	7/25/103/115	-
12	CLA	a	814	-	1/1/11/20	4/13/91/115	-
12	CLA	A	834	1	1/1/13/20	10/25/103/115	-
14	SF4	A	841	2,1	-	-	0/6/5/5
12	CLA	B	2127	2	1/1/15/20	9/37/115/115	-
12	CLA	G	808	1	1/1/12/20	3/19/97/115	-
15	BCR	H	2146	-	-	17/29/63/63	0/2/2/2
15	BCR	a	845	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	Q	203	-	1/1/11/20	4/13/91/115	-
12	CLA	b	2114	-	1/1/15/20	16/37/115/115	-
12	CLA	B	2132	2	1/1/13/20	7/25/103/115	-
12	CLA	a	806	1	1/1/12/20	5/19/97/115	-
12	CLA	H	2112	2	1/1/15/20	6/37/115/115	-
17	LMG	a	849	-	-	14/26/46/70	0/1/1/1
12	CLA	A	833	1	1/1/15/20	13/37/115/115	-
12	CLA	H	2135	-	1/1/11/20	7/13/91/115	-
15	BCR	S	104	-	-	9/29/63/63	0/2/2/2
12	CLA	U	205	27	1/1/15/20	6/37/115/115	-
12	CLA	A	807	1	1/1/15/20	14/37/115/115	-
12	CLA	G	830	1	-	7/25/103/115	-
12	CLA	H	2124	27	1/1/15/20	6/37/115/115	-
12	CLA	B	2133	2	1/1/15/20	18/37/115/115	-

The worst 5 of 2010 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	205	ZEX	C25-C26	17.19	1.60	1.34
23	Q	205	ZEX	C25-C26	17.19	1.60	1.34
23	f	205	ZEX	C25-C26	17.17	1.60	1.34
23	b	2151	ZEX	C25-C26	17.17	1.60	1.34
23	B	2152	ZEX	C25-C26	17.12	1.60	1.34

The worst 5 of 2930 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Q	205	ZEX	C39-C29-C28	-32.45	68.51	118.09
23	F	205	ZEX	C39-C29-C28	-32.45	68.52	118.09
23	f	205	ZEX	C39-C29-C28	-32.44	68.54	118.09
23	b	2151	ZEX	C39-C29-C28	-32.08	69.09	118.09
23	B	2152	ZEX	C39-C29-C28	-32.07	69.10	118.09

5 of 285 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	G	801	CLA	ND
12	G	802	CLA	ND
12	G	803	CLA	ND

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Mol	Chain	Res	Type	Atom
12	G	804	CLA	ND
12	G	805	CLA	ND

5 of 3916 torsion outliers are listed below:

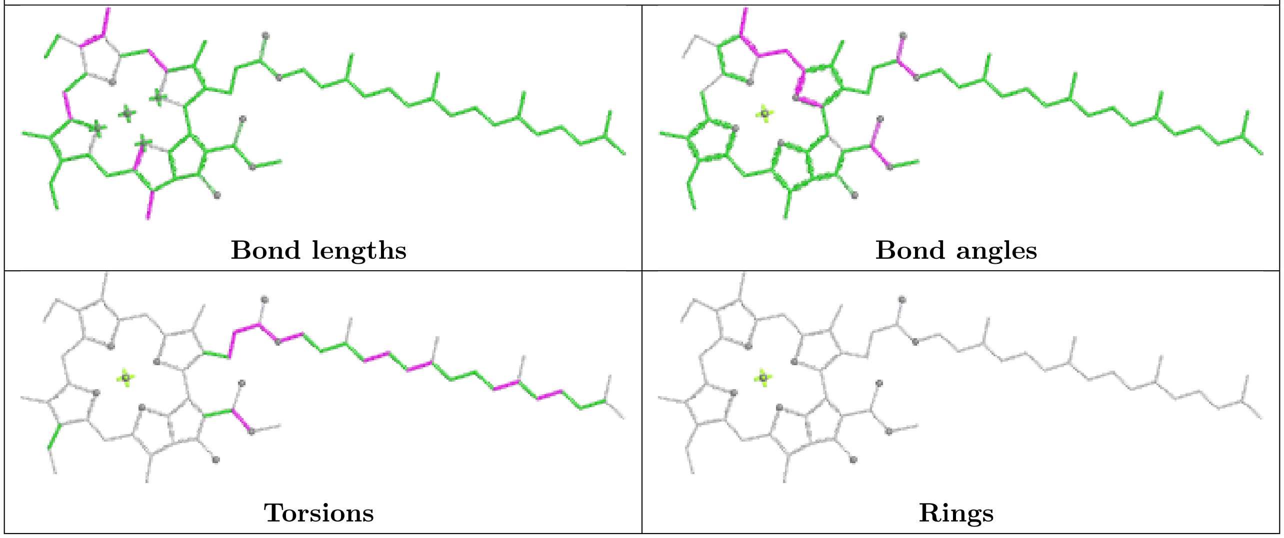
Mol	Chain	Res	Type	Atoms
12	G	802	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C3A-C2A-CAA-CBA
12	G	804	CLA	CAD-CBD-CGD-O1D
12	G	804	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand CLA H 2140



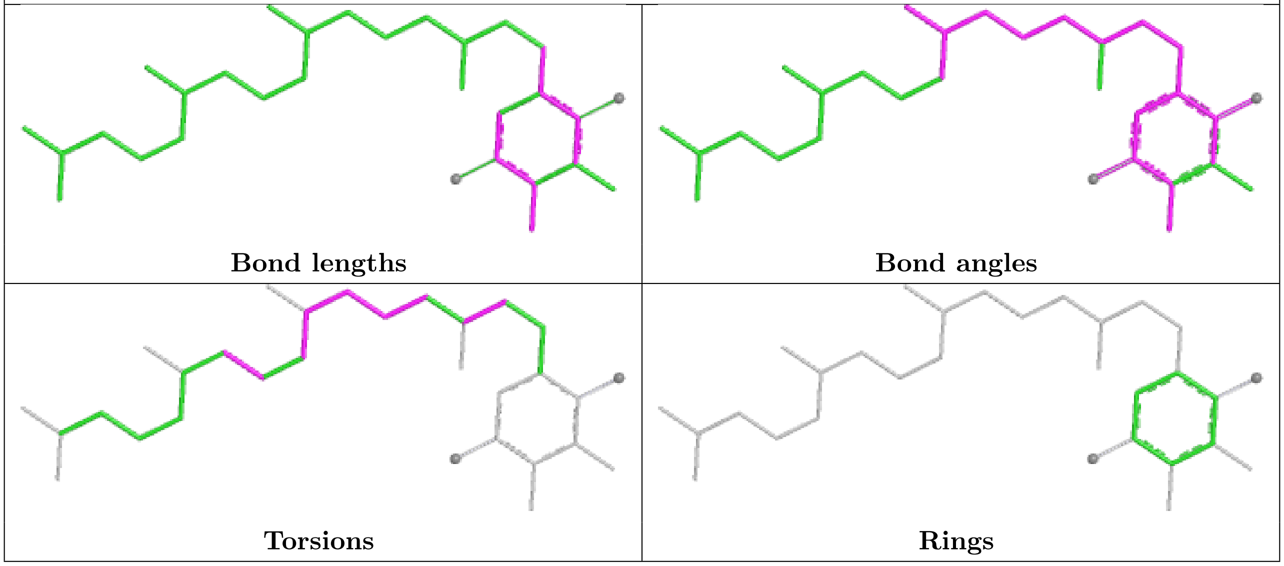
Bond lengths

Bond angles

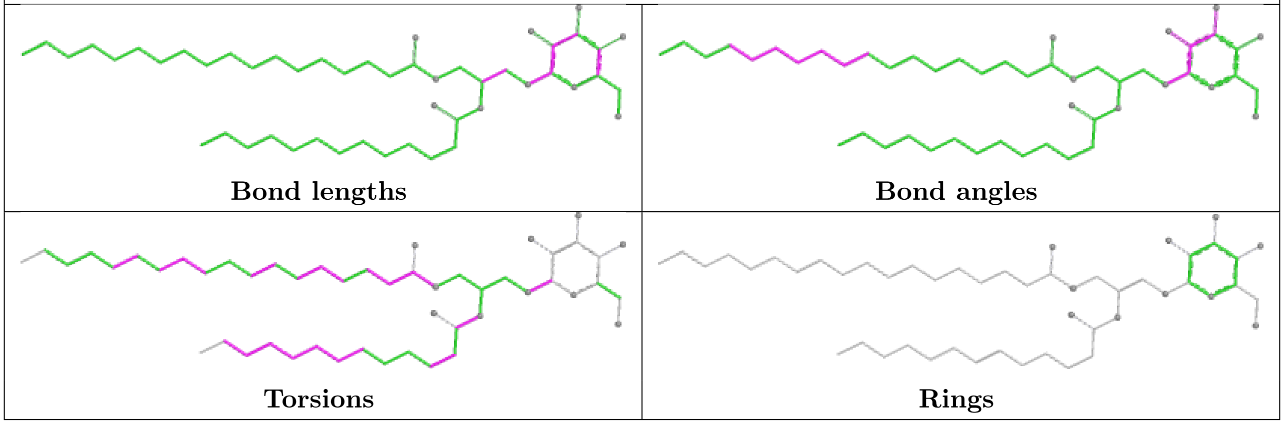
Torsions

Rings

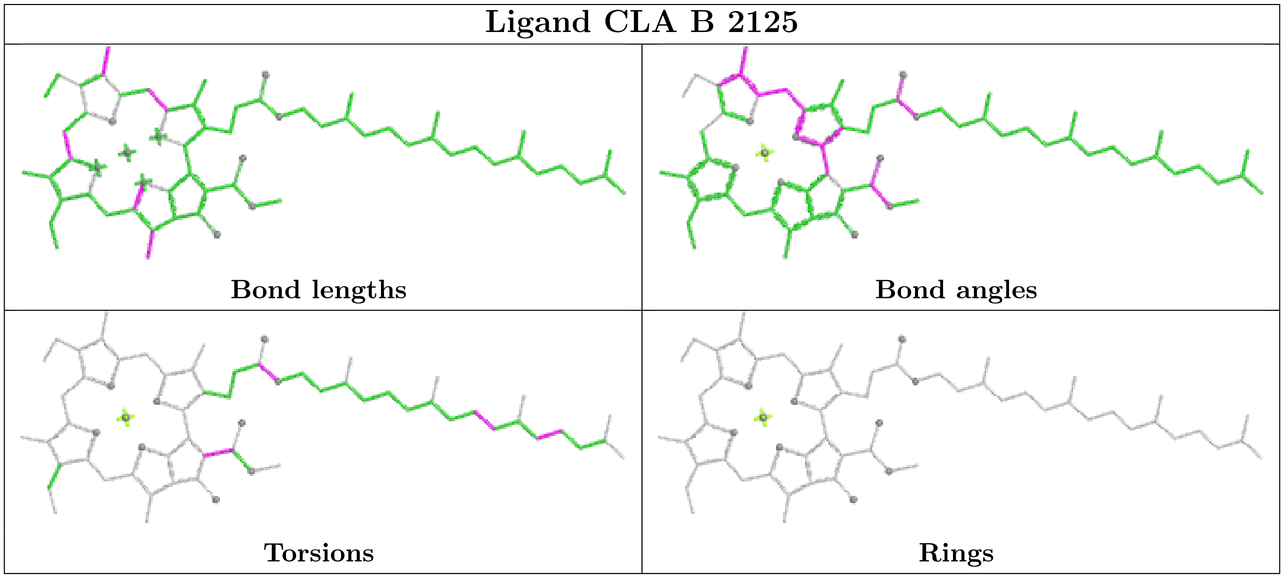
Ligand A1AGD H 2153



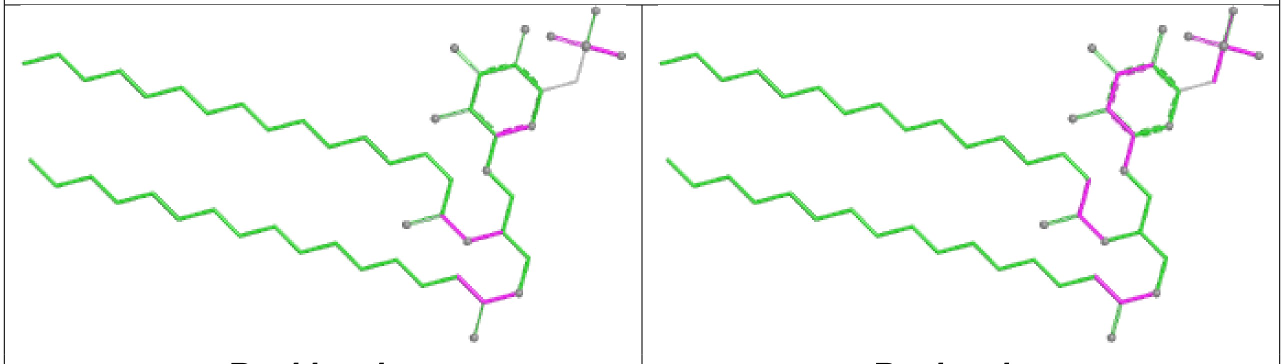
Ligand LMG A 847



Ligand CLA B 2125

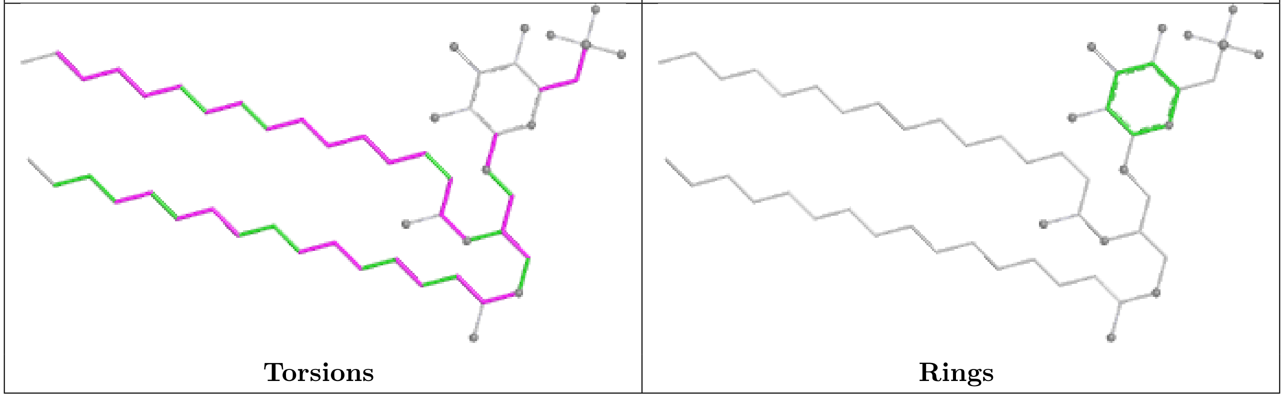


Ligand SQD M 101



Bond lengths

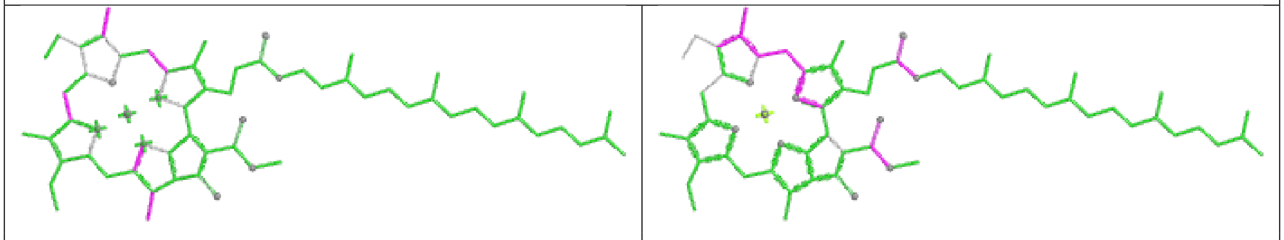
Bond angles



Torsions

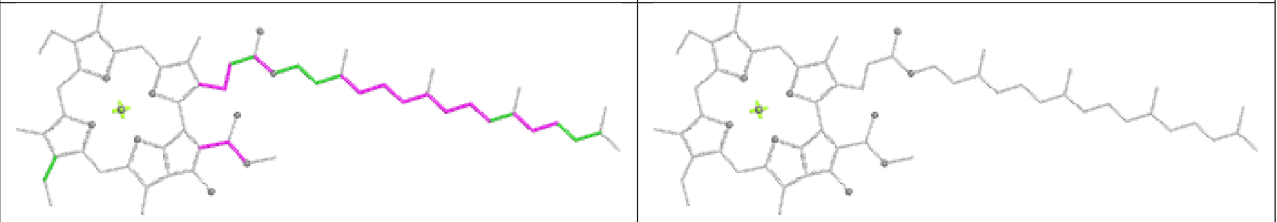
Rings

Ligand CLA f 201



Bond lengths

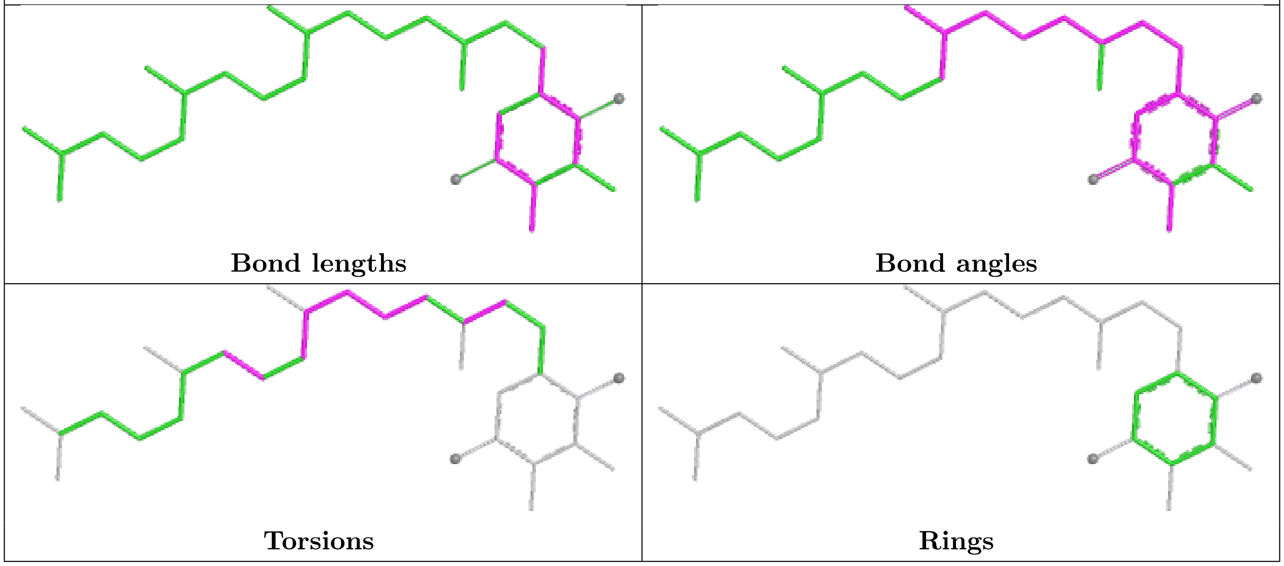
Bond angles



Torsions

Rings

Ligand A1AGD b 2153



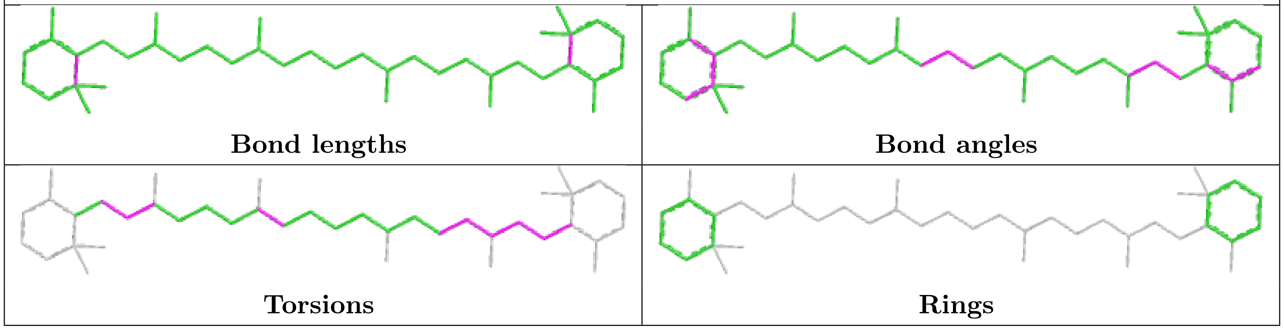
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR Q 202



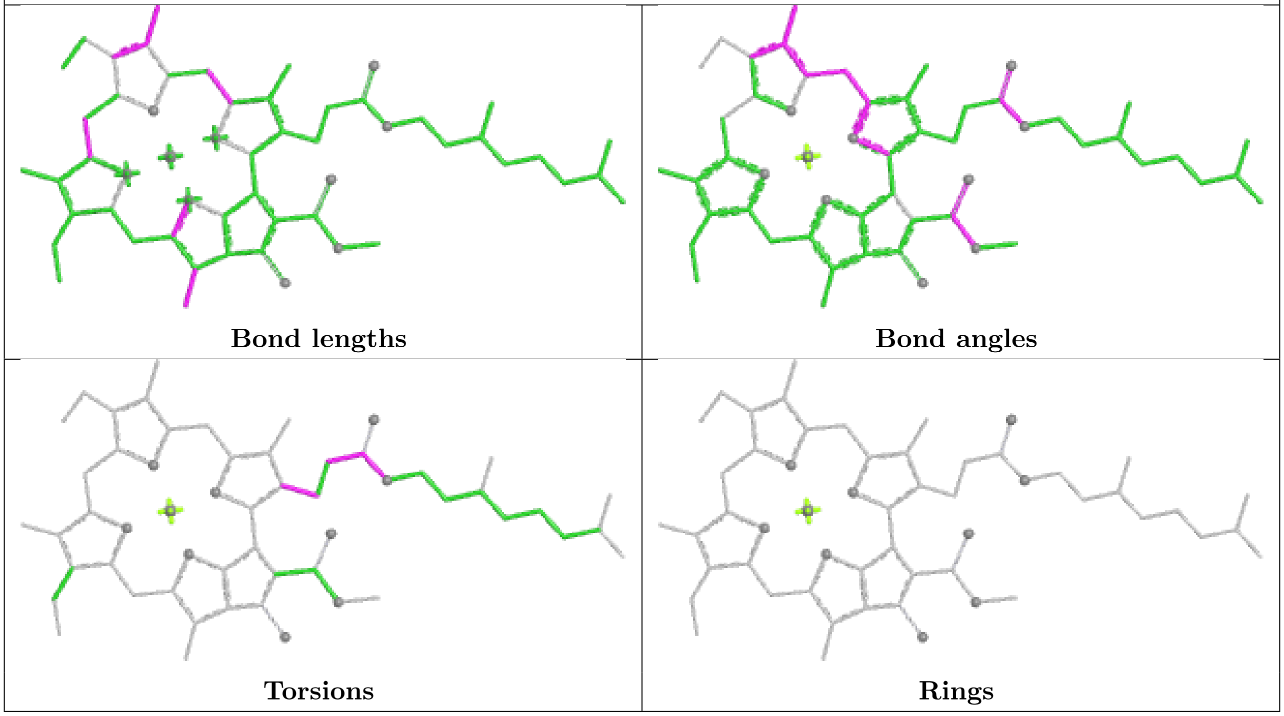
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 2120



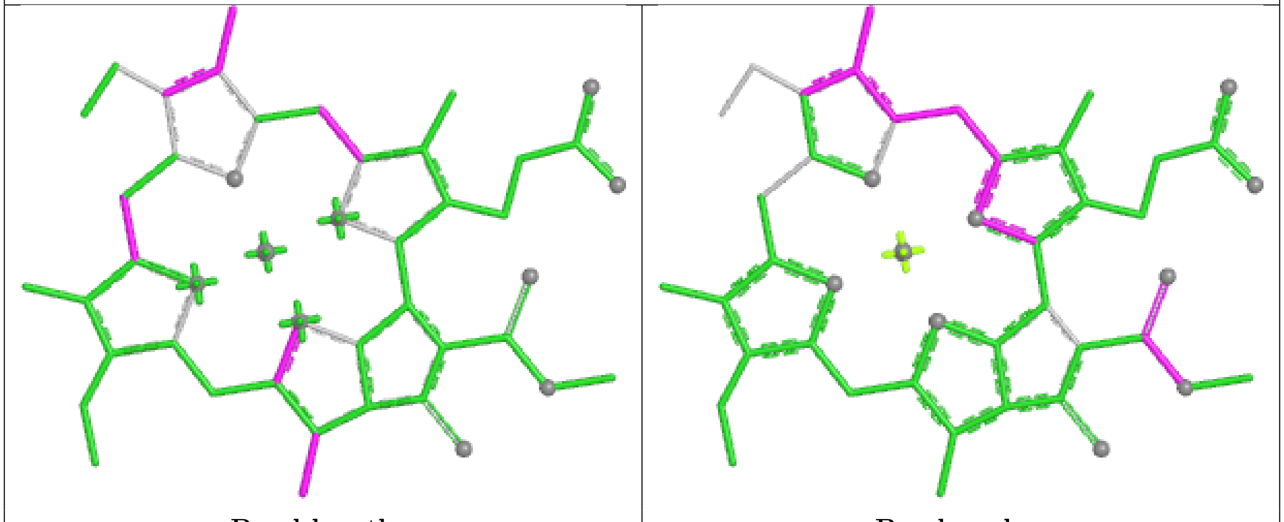
Bond lengths

Bond angles

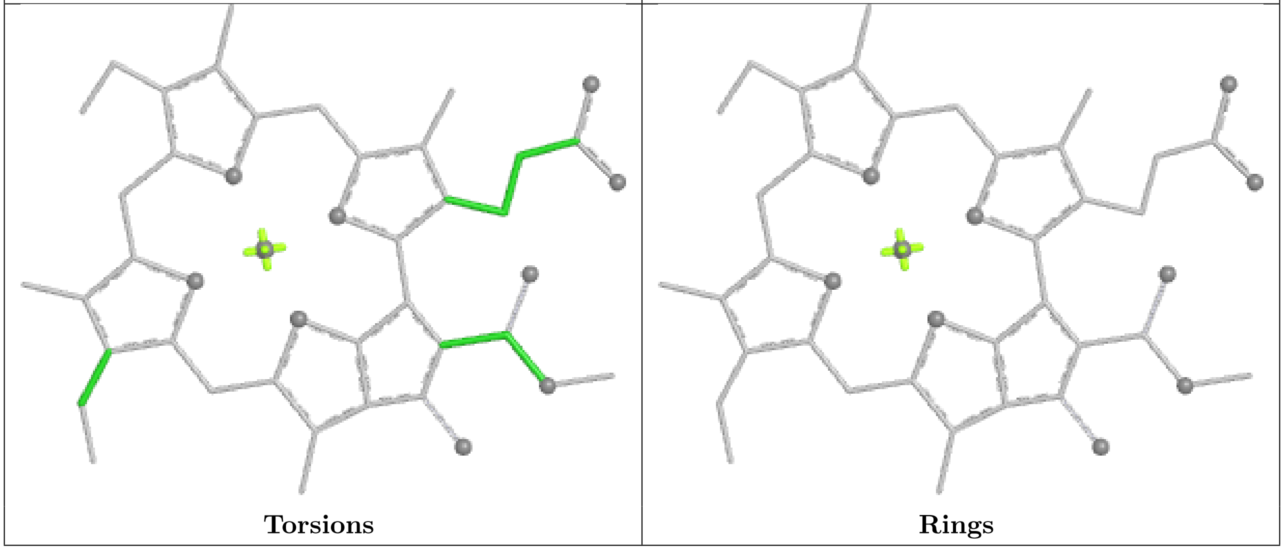
Torsions

Rings

Ligand CLA b 2130

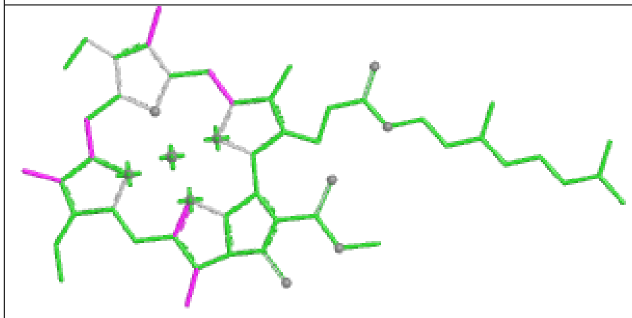


Bond lengths **Bond angles**

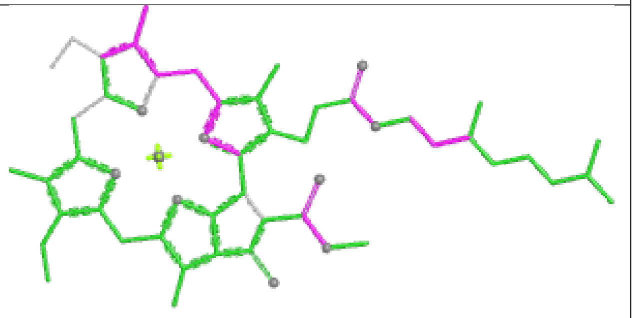


Torsions **Rings**

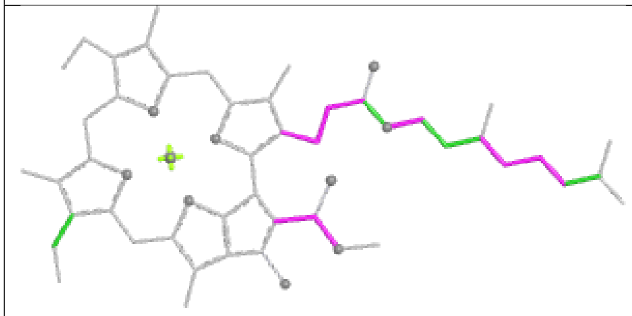
Ligand CLA H 2123



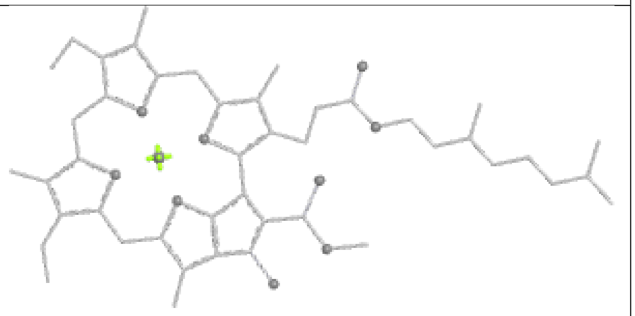
Bond lengths



Bond angles

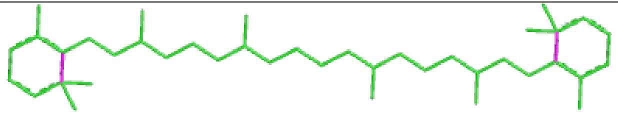


Torsions

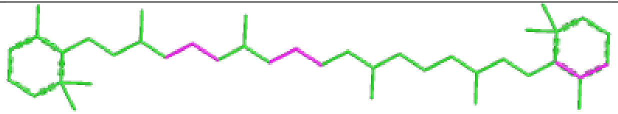


Rings

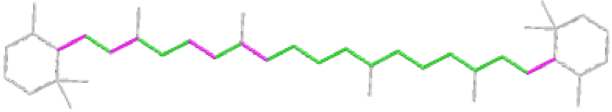
Ligand BCR b 2145



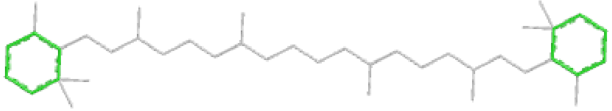
Bond lengths



Bond angles

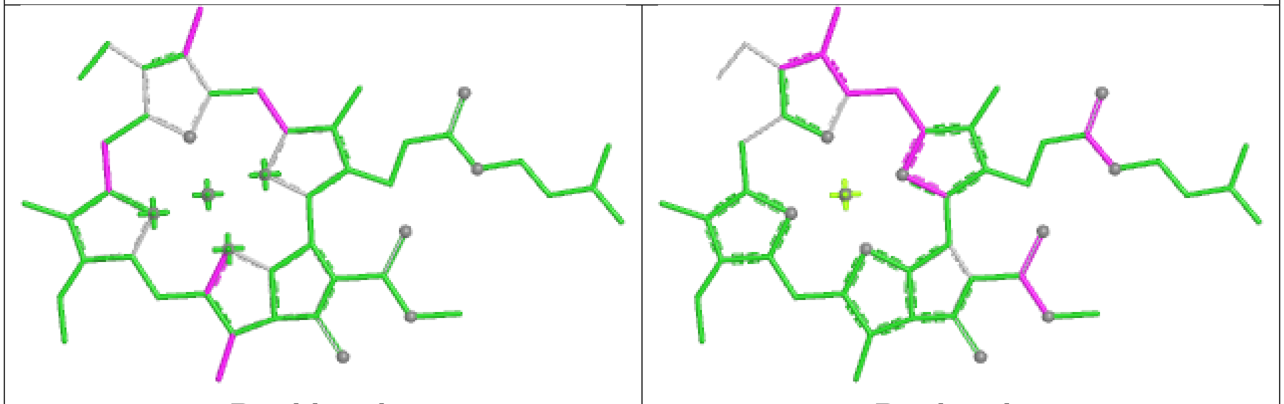


Torsions



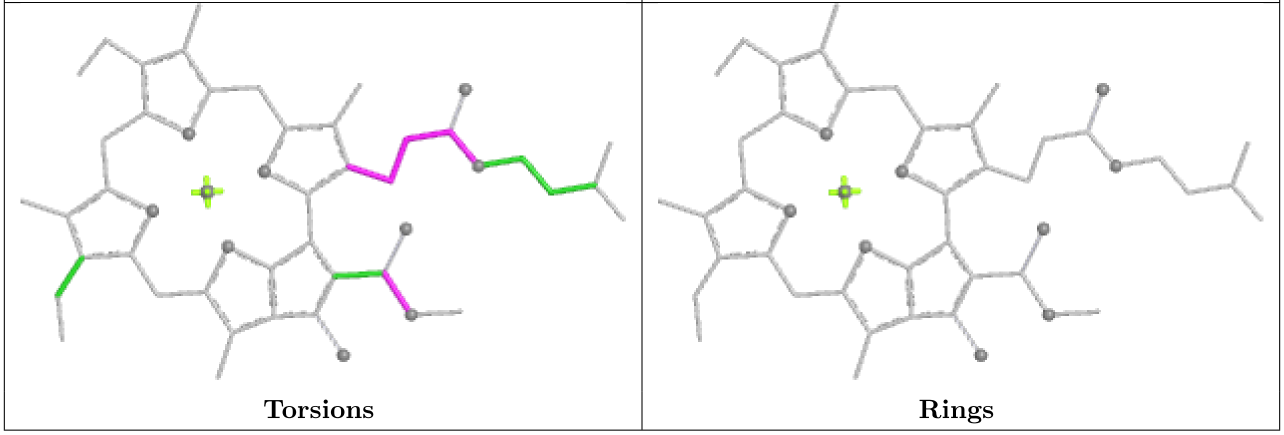
Rings

Ligand CLA A 822



Bond lengths

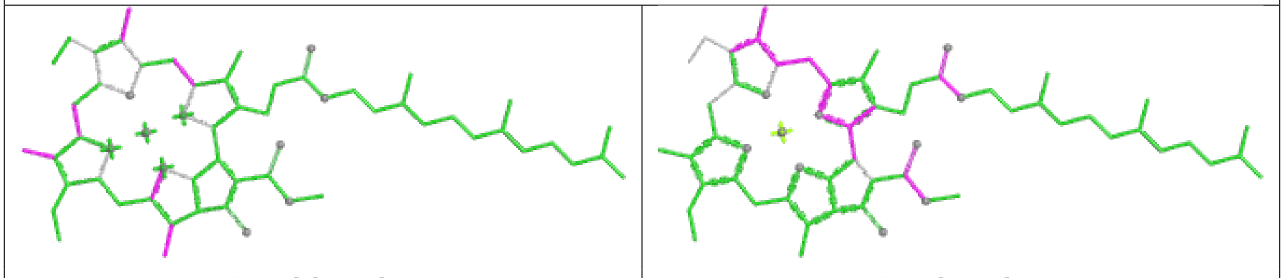
Bond angles



Torsions

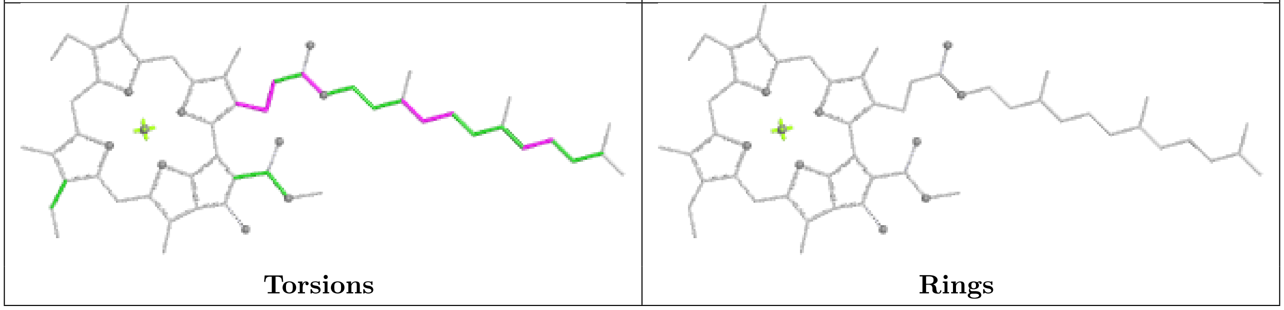
Rings

Ligand CLA A 823



Bond lengths

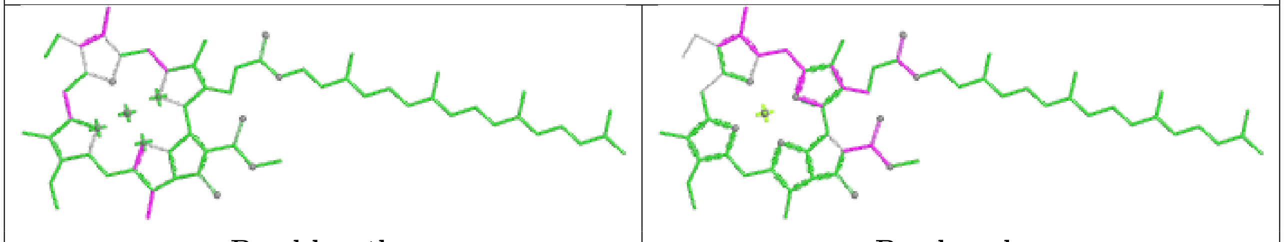
Bond angles



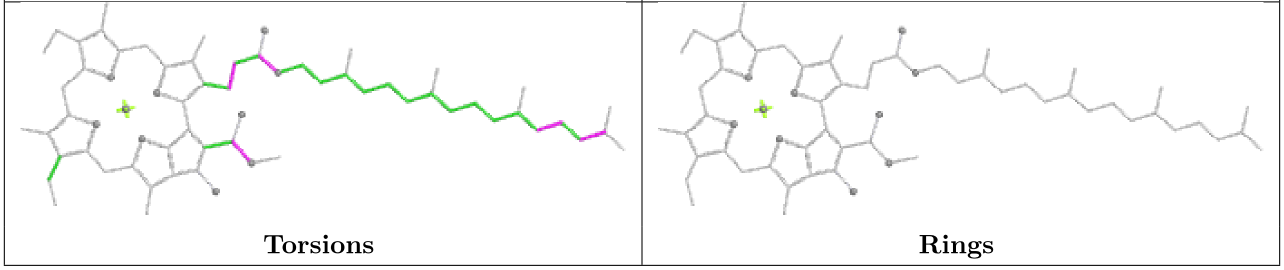
Torsions

Rings

Ligand CLA B 2140

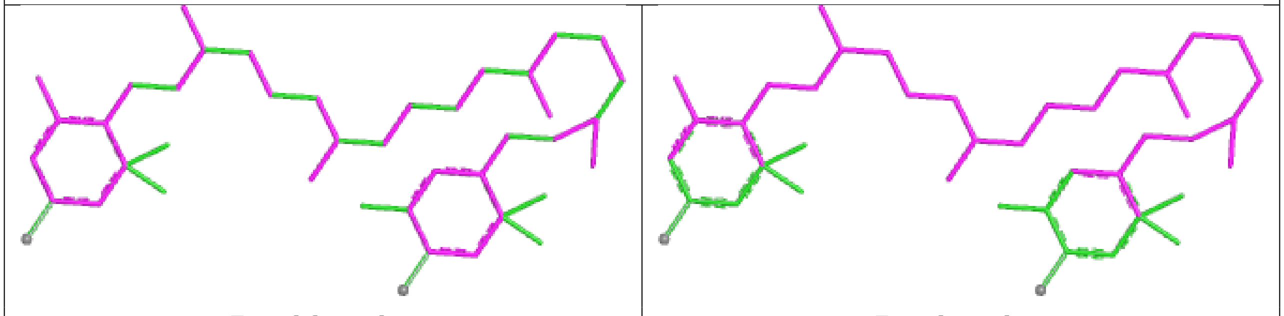


Bond lengths Bond angles

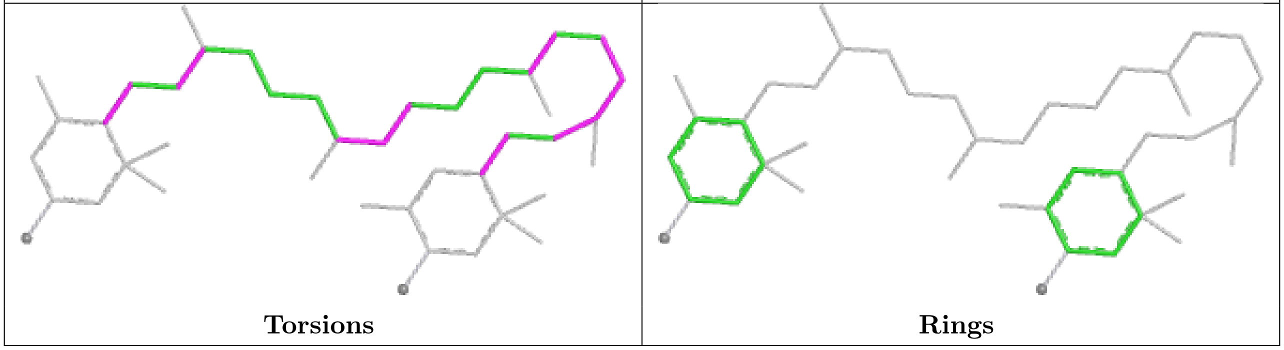


Torsions Rings

Ligand ZEX F 205

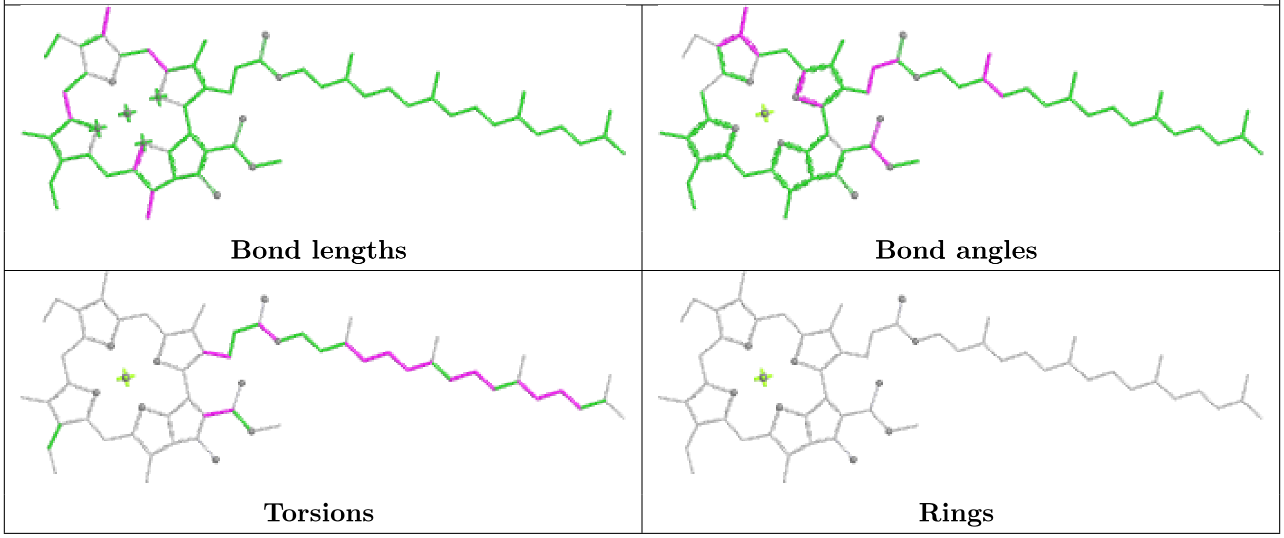


Bond lengths Bond angles



Torsions Rings

Ligand CLA H 2119



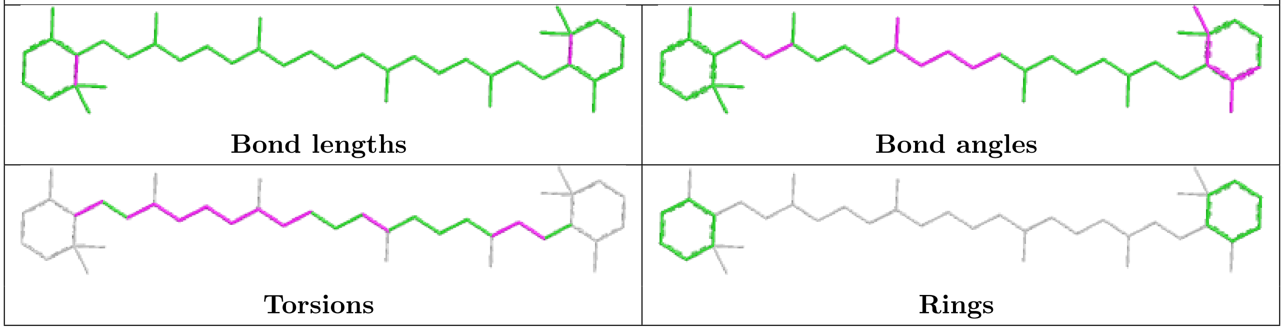
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 843



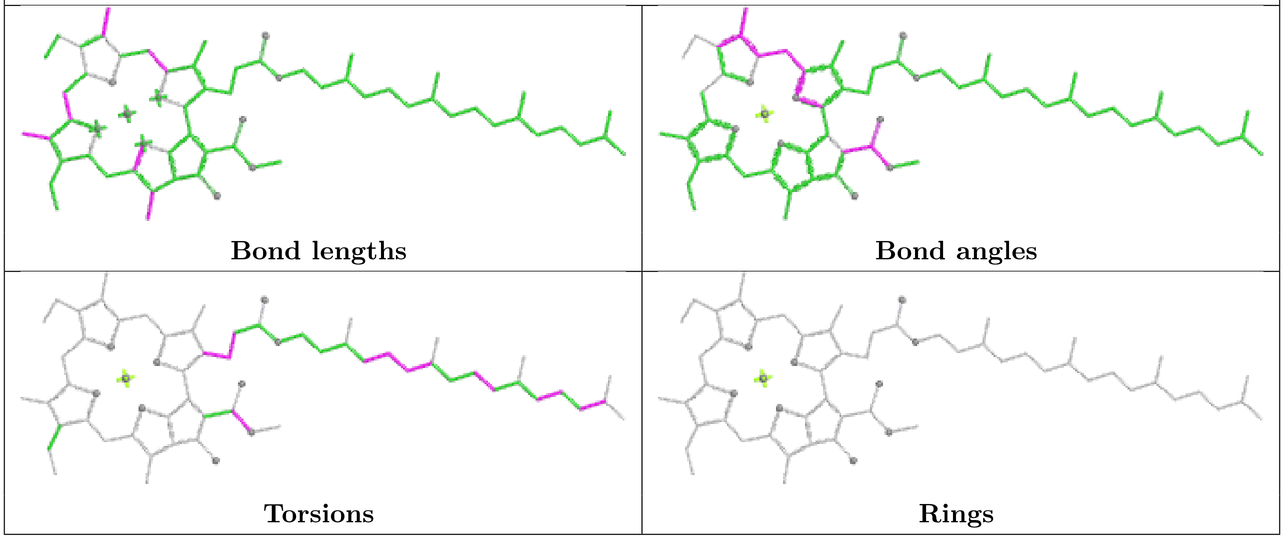
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 829



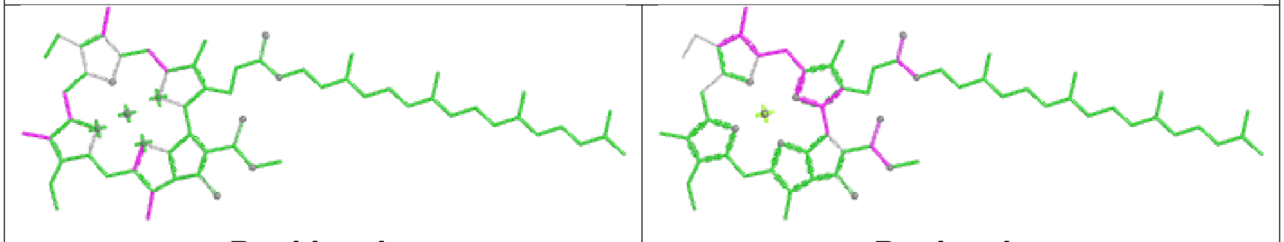
Bond lengths

Bond angles

Torsions

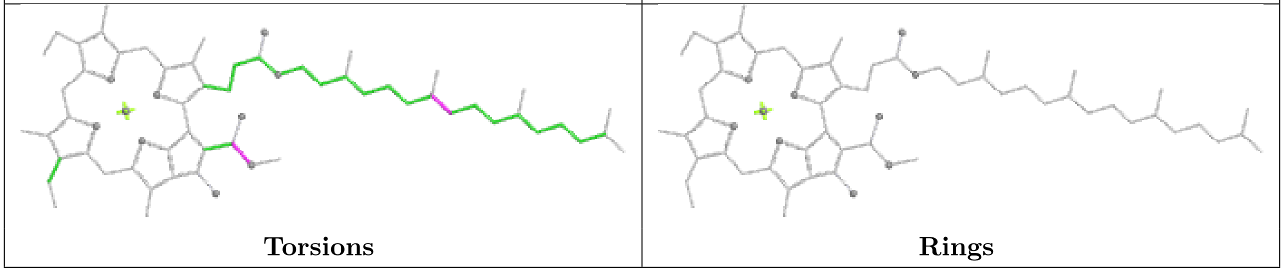
Rings

Ligand CLA G 838



Bond lengths

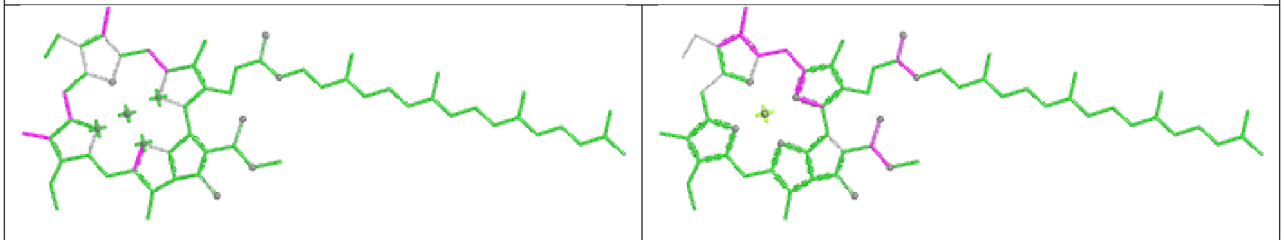
Bond angles



Torsions

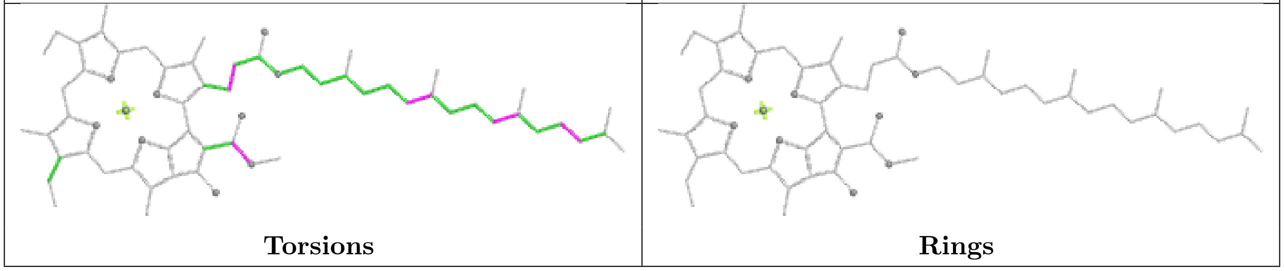
Rings

Ligand CLA G 820



Bond lengths

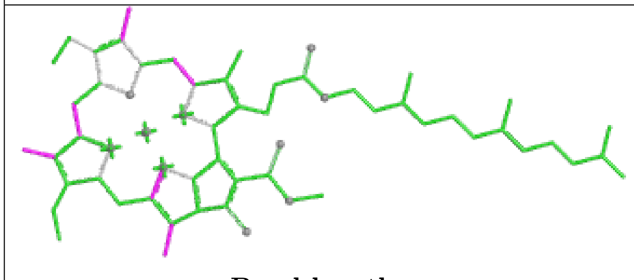
Bond angles



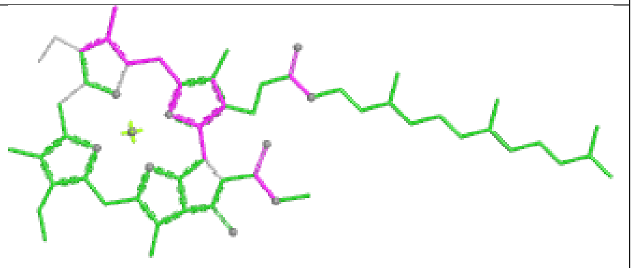
Torsions

Rings

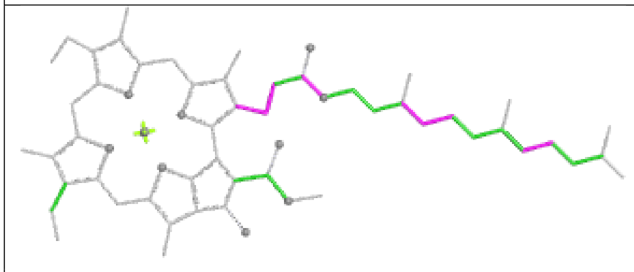
Ligand CLA G 823



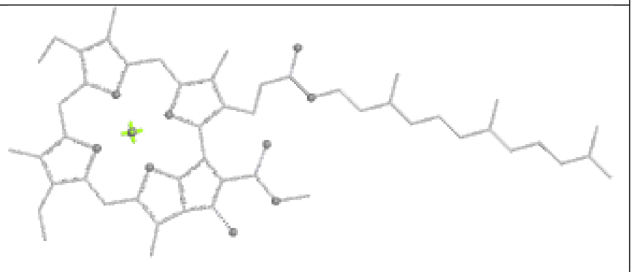
Bond lengths



Bond angles

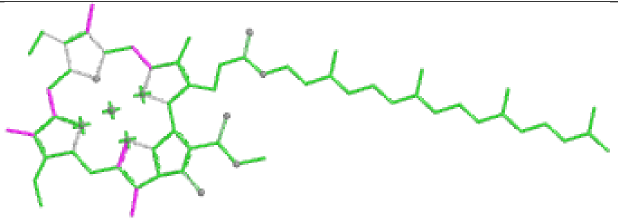


Torsions

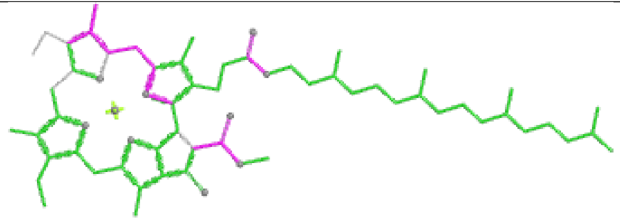


Rings

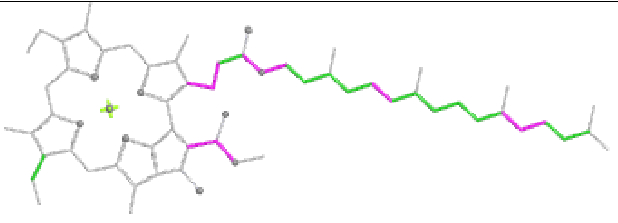
Ligand CLA l 201



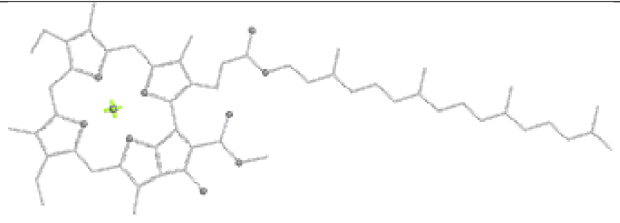
Bond lengths



Bond angles

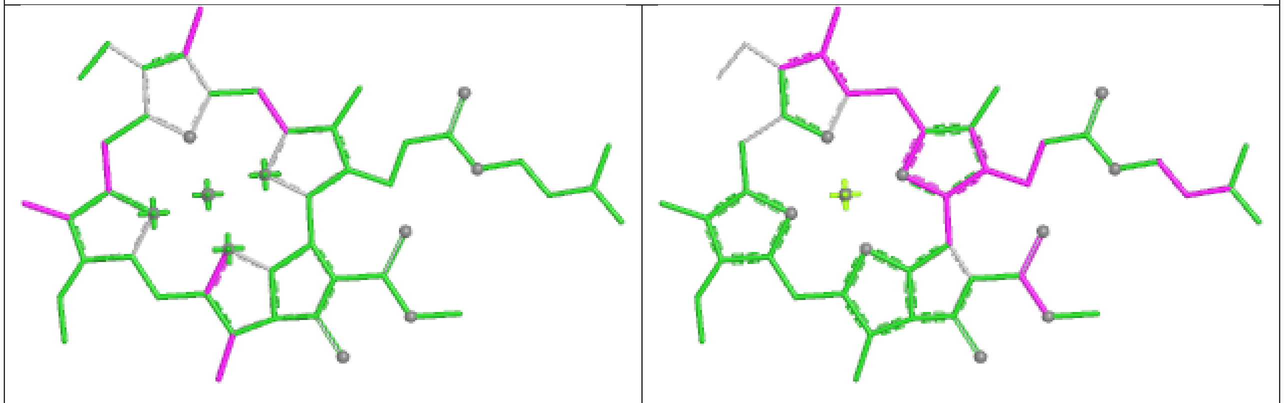


Torsions



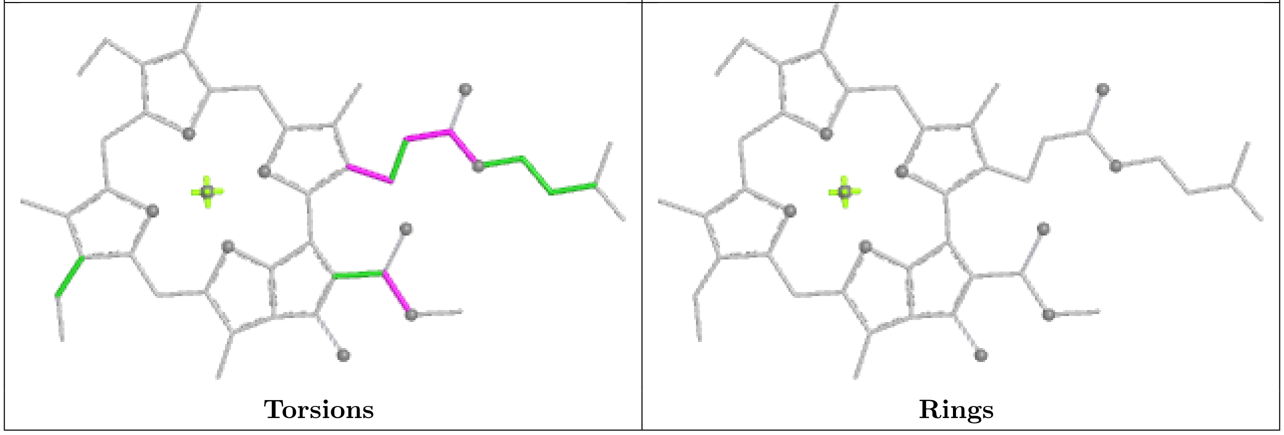
Rings

Ligand CLA A 809



Bond lengths

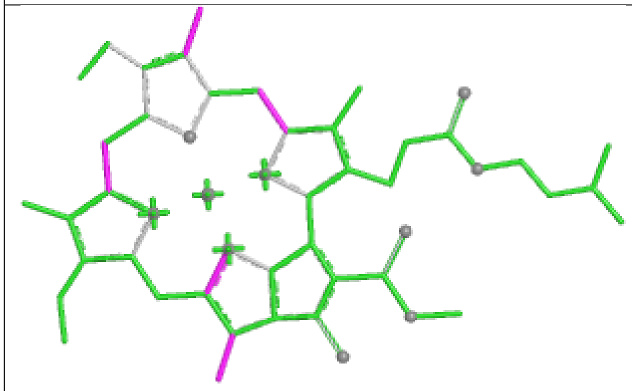
Bond angles



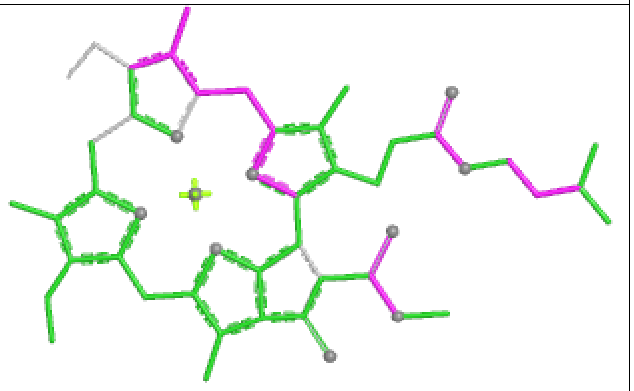
Torsions

Rings

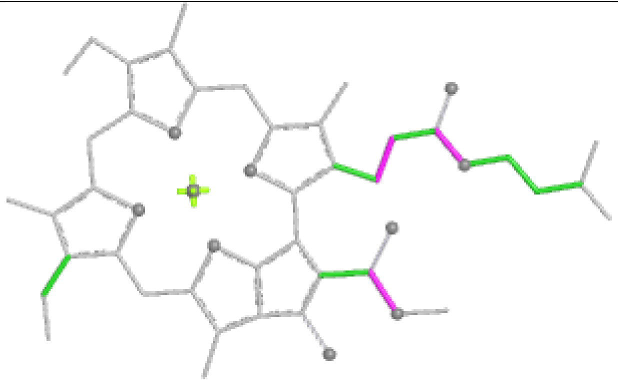
Ligand CLA A 806



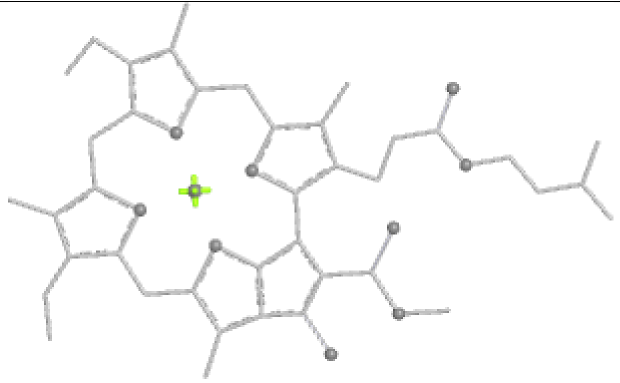
Bond lengths



Bond angles

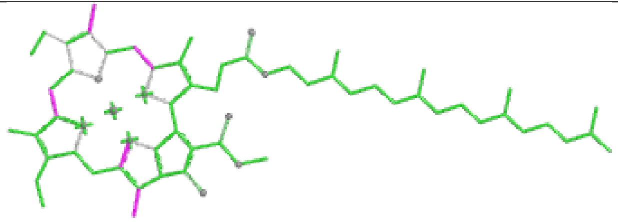


Torsions

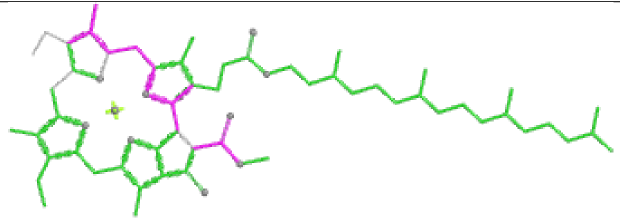


Rings

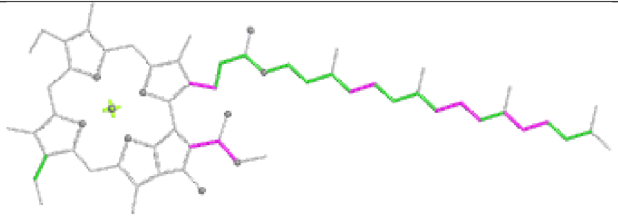
Ligand CLA A 812



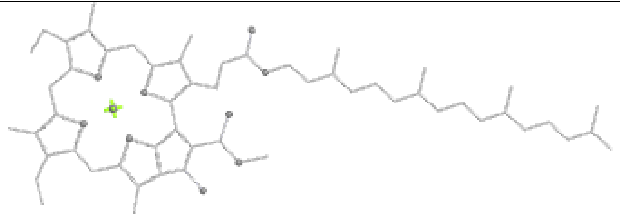
Bond lengths



Bond angles

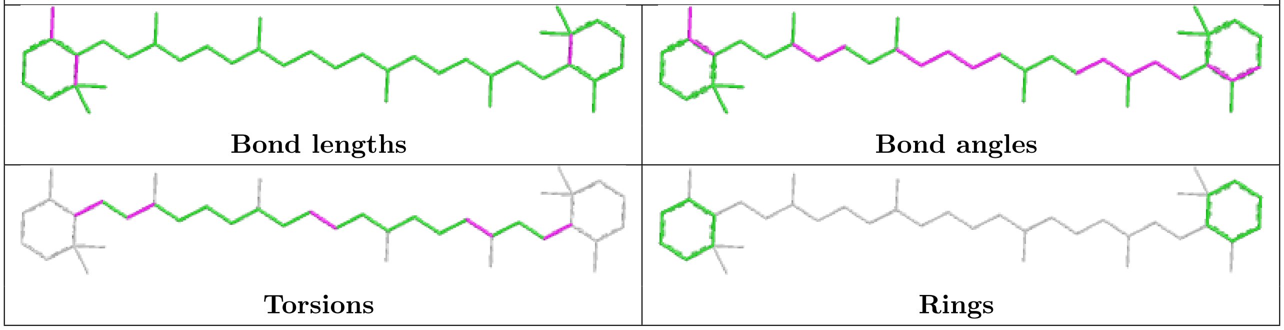


Torsions



Rings

Ligand BCR J 104



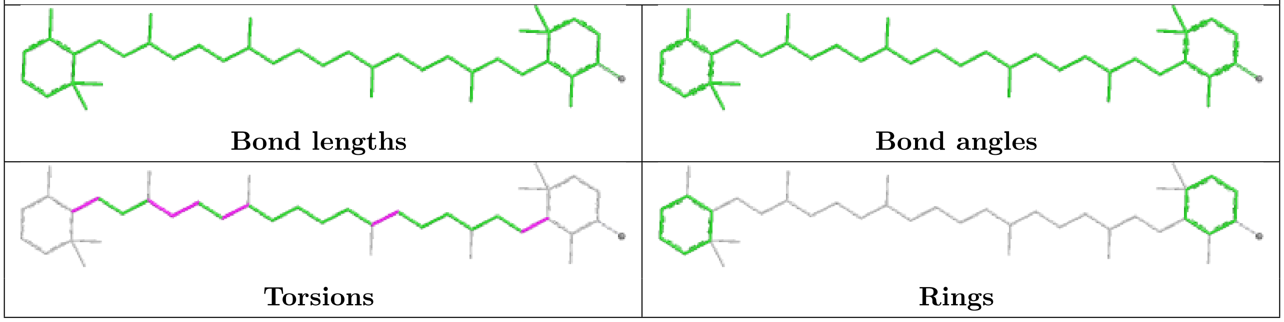
Bond lengths

Bond angles

Torsions

Rings

Ligand ECH M 103



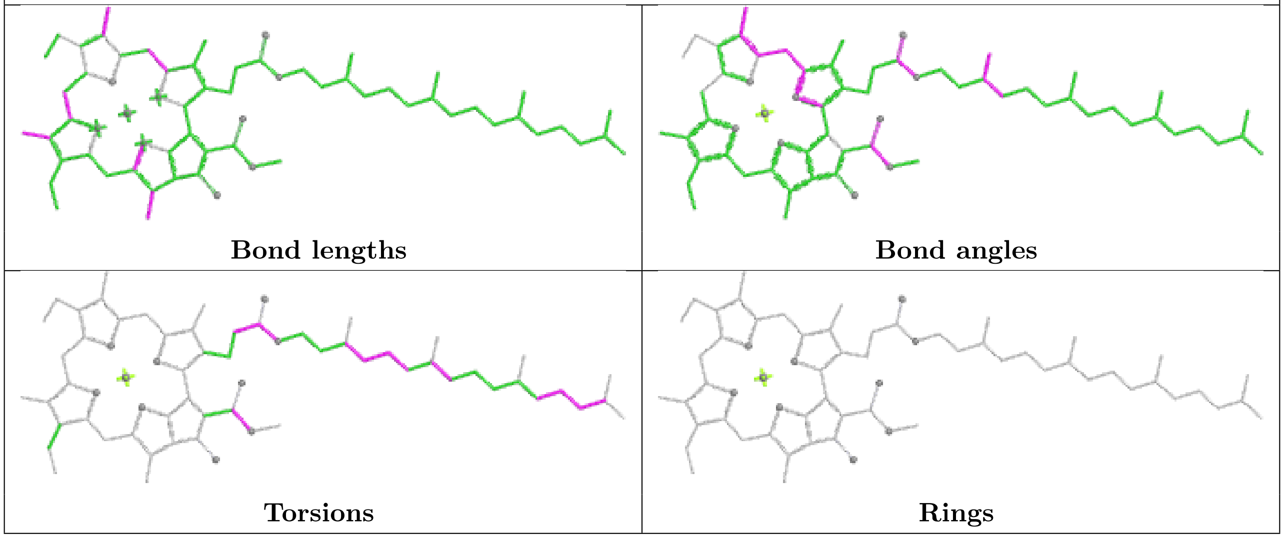
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 2103



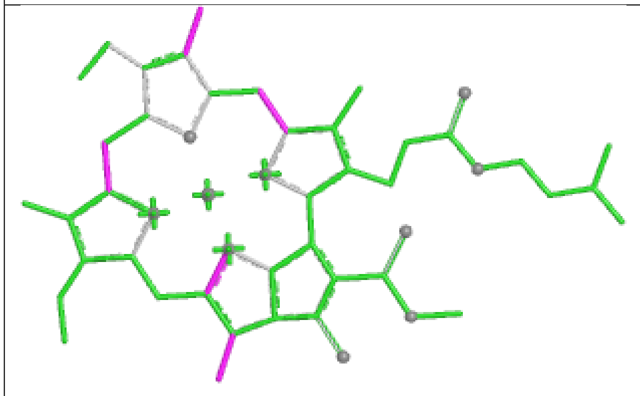
Bond lengths

Bond angles

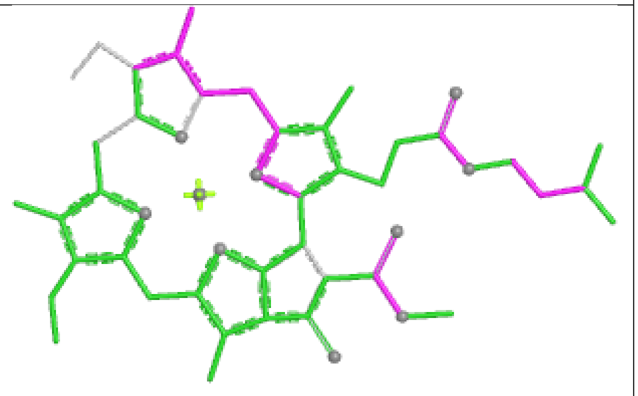
Torsions

Rings

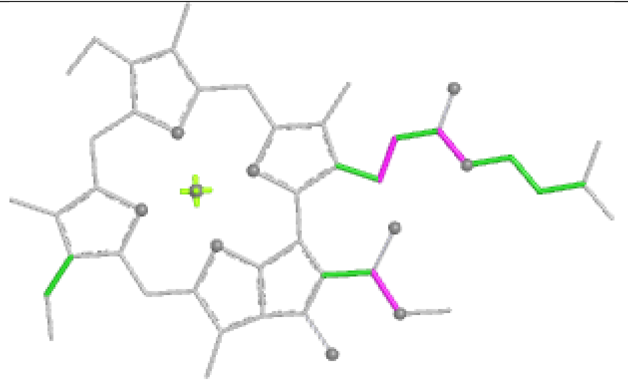
Ligand CLA G 806



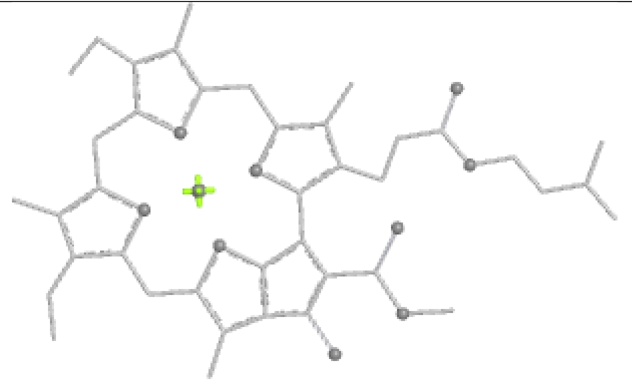
Bond lengths



Bond angles

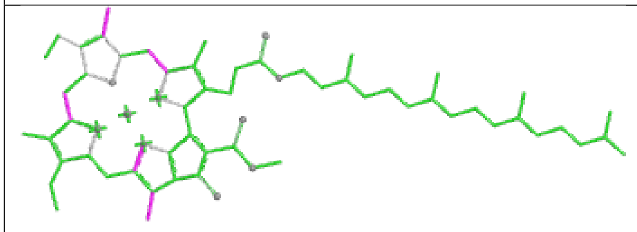


Torsions

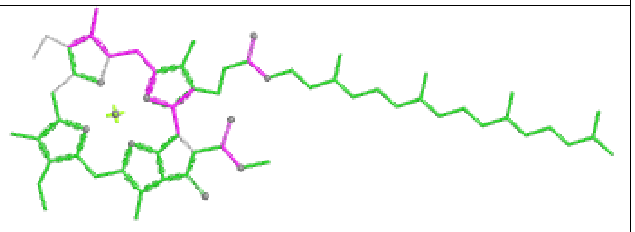


Rings

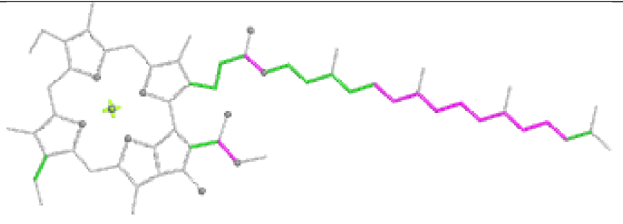
Ligand CLA A 819



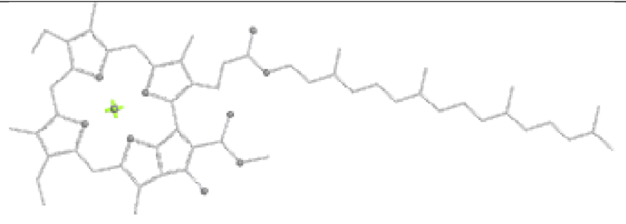
Bond lengths



Bond angles

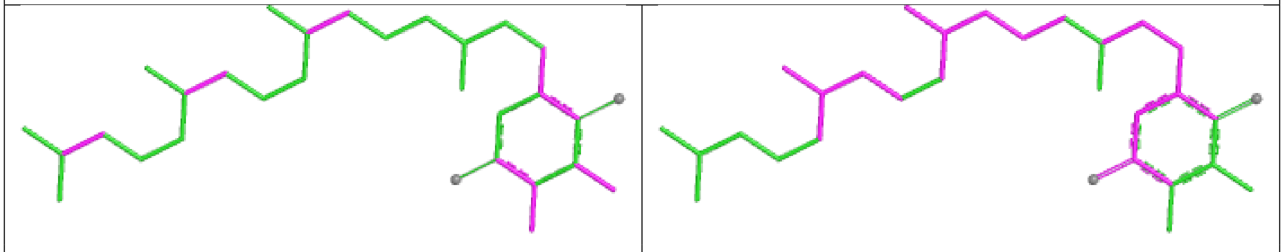


Torsions

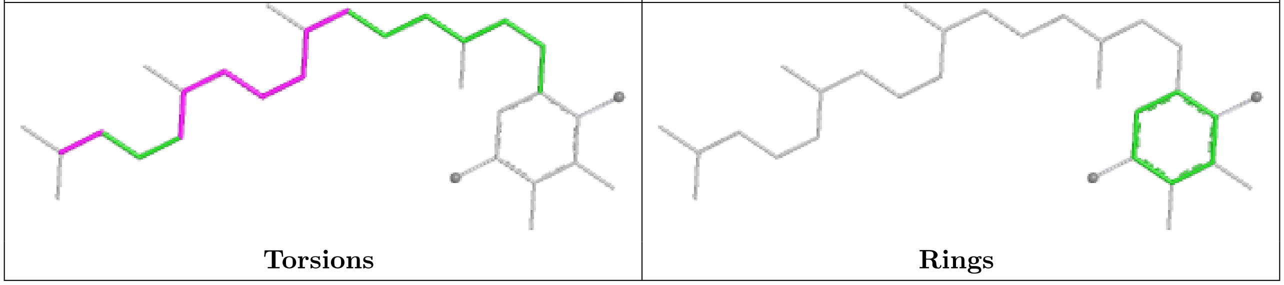


Rings

Ligand A1AGD G 840

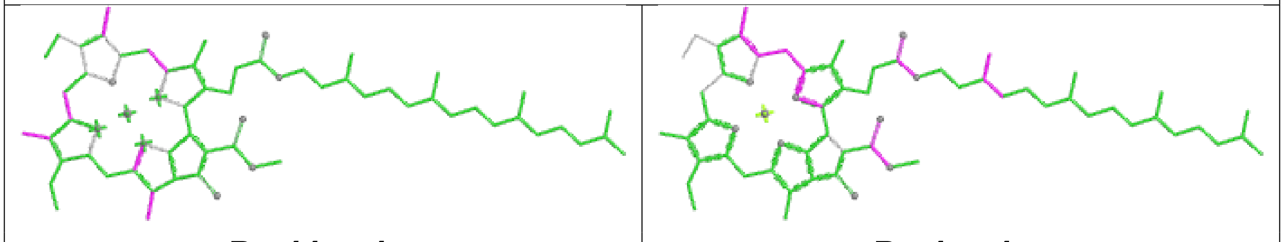


Bond lengths Bond angles

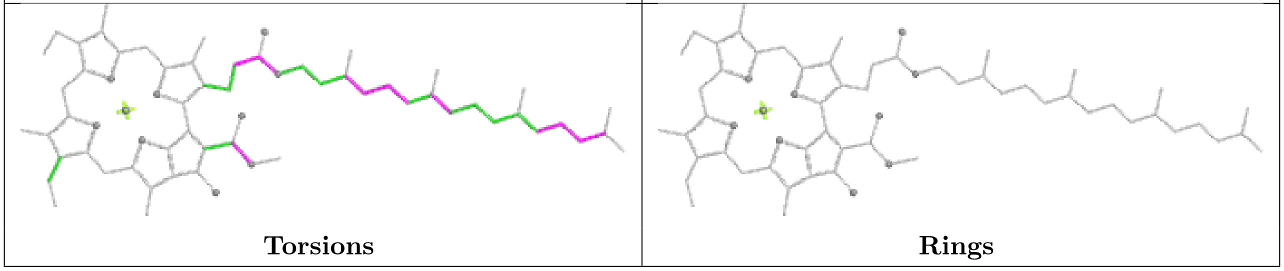


Torsions Rings

Ligand CLA H 2103

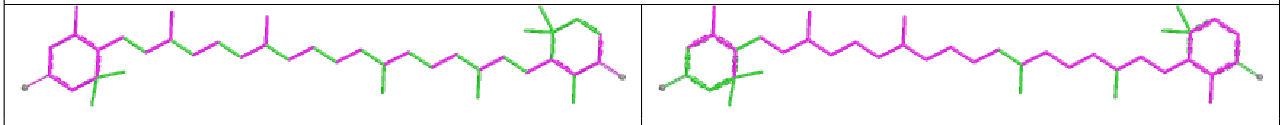


Bond lengths Bond angles

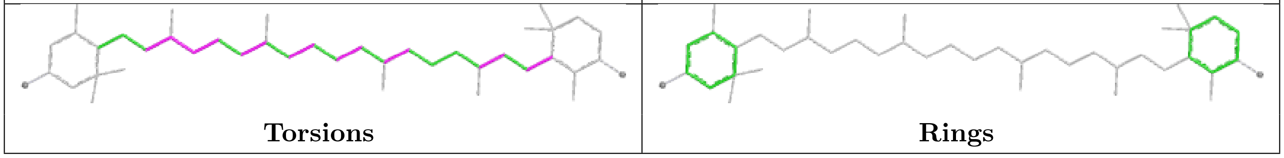


Torsions Rings

Ligand EQ3 b 2150

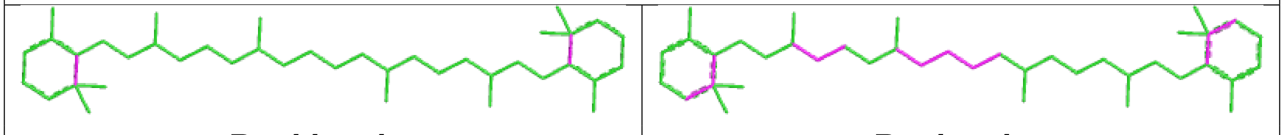


Bond lengths Bond angles



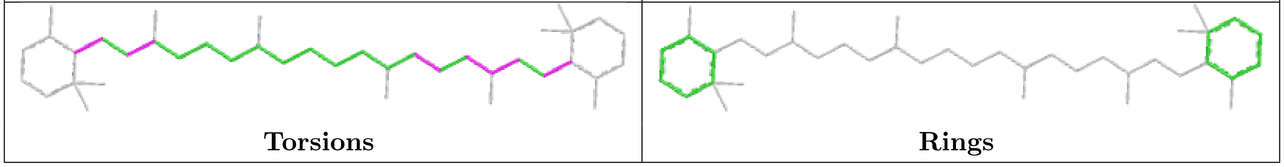
Torsions Rings

Ligand BCR U 206



Bond lengths

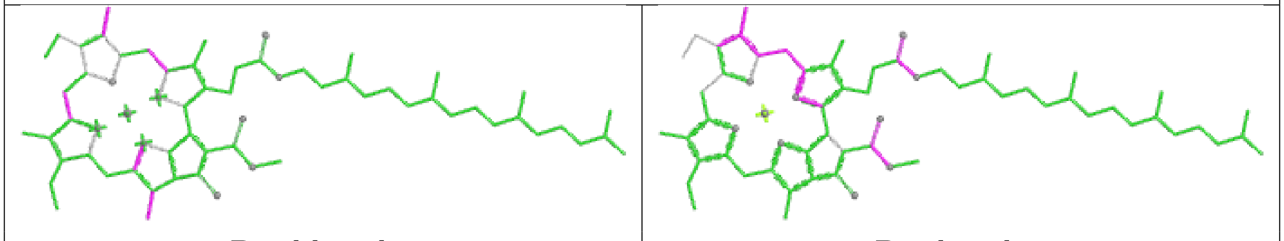
Bond angles



Torsions

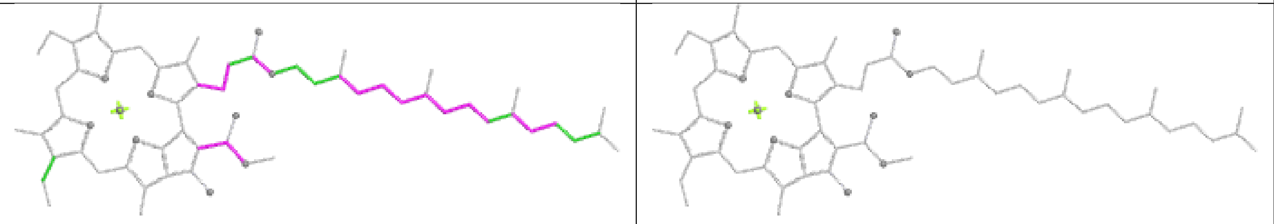
Rings

Ligand CLA F 201



Bond lengths

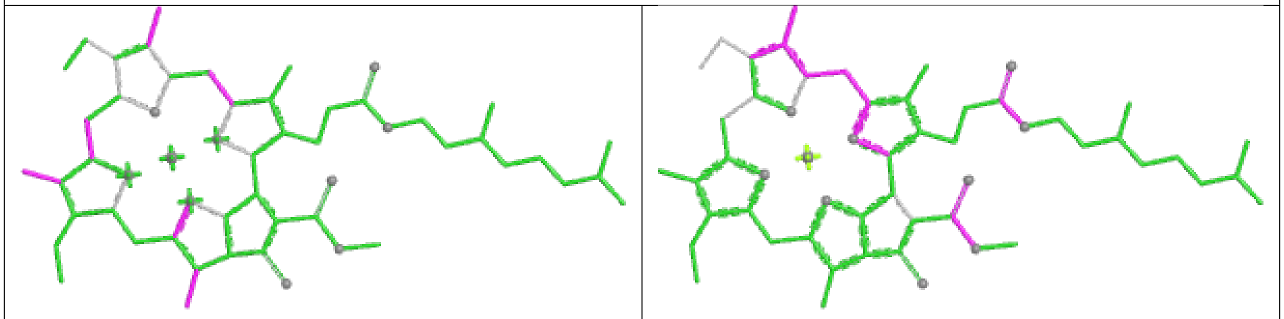
Bond angles



Torsions

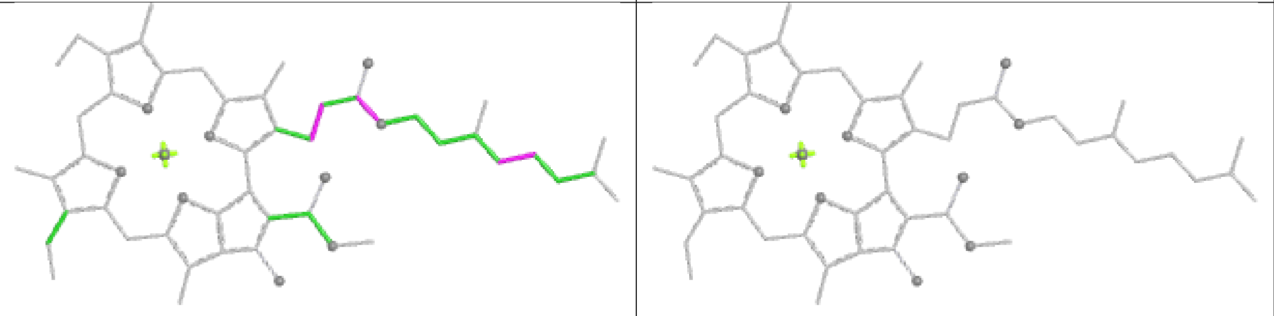
Rings

Ligand CLA G 816



Bond lengths

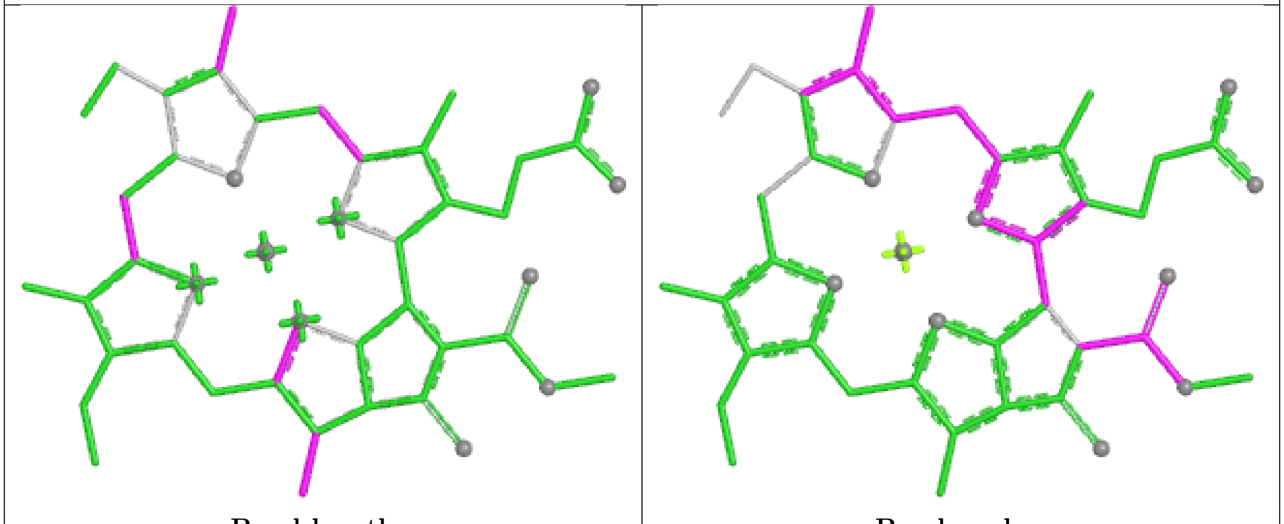
Bond angles



Torsions

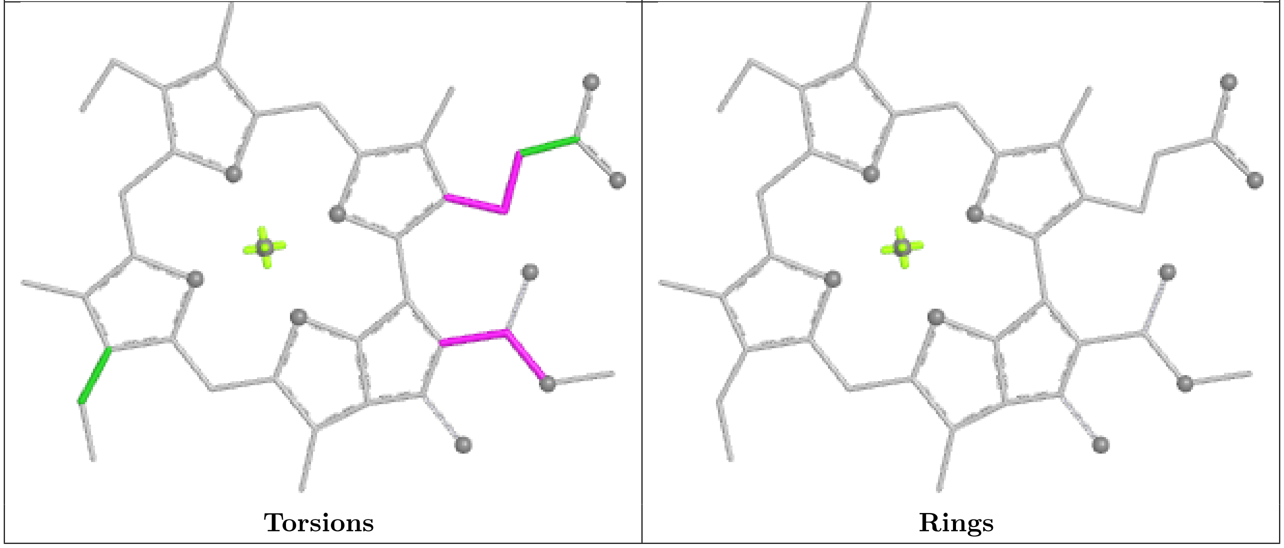
Rings

Ligand CLA J 102



Bond lengths

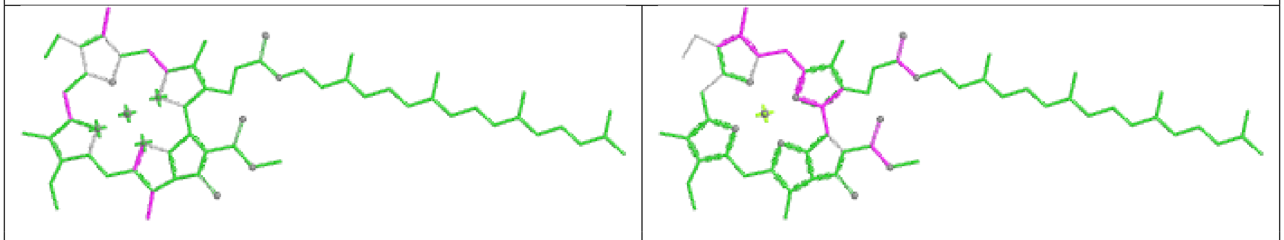
Bond angles



Torsions

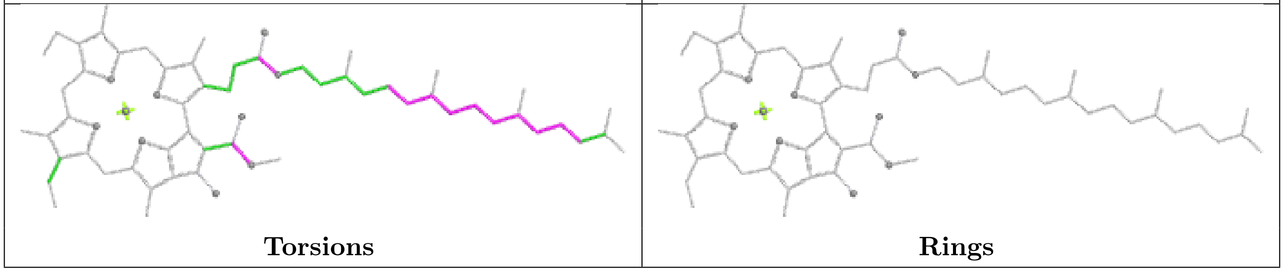
Rings

Ligand CLA G 819



Bond lengths

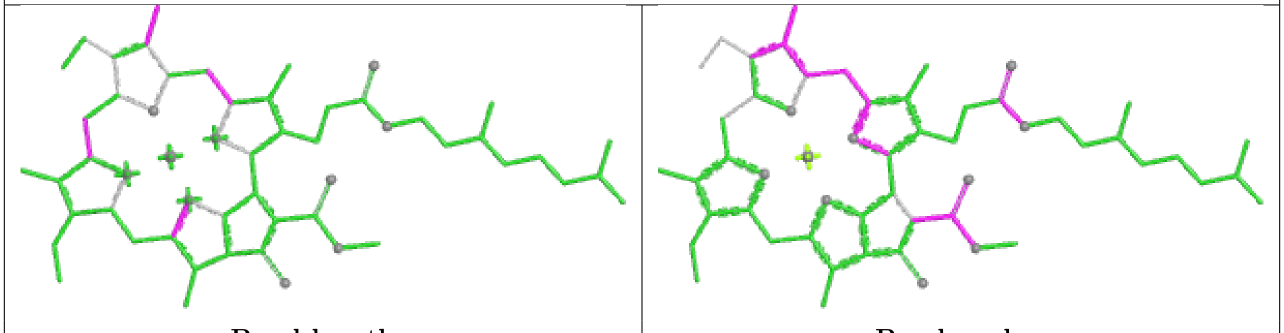
Bond angles



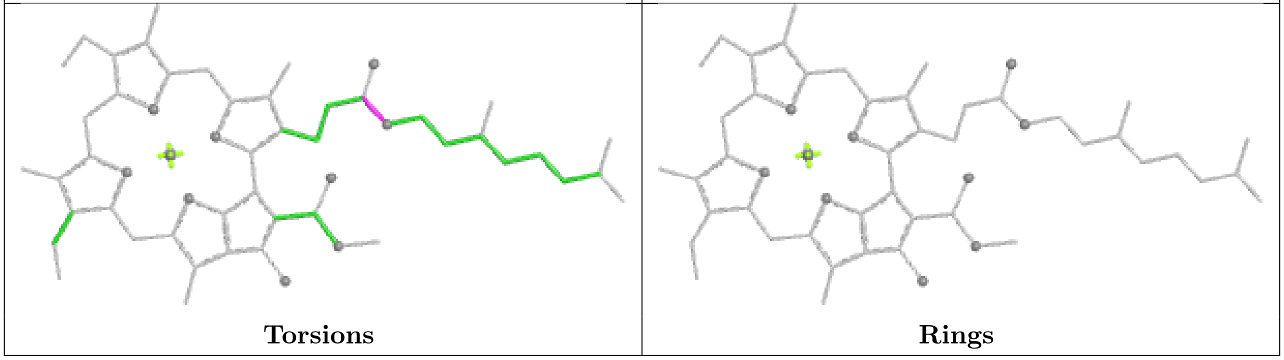
Torsions

Rings

Ligand CLA G 803

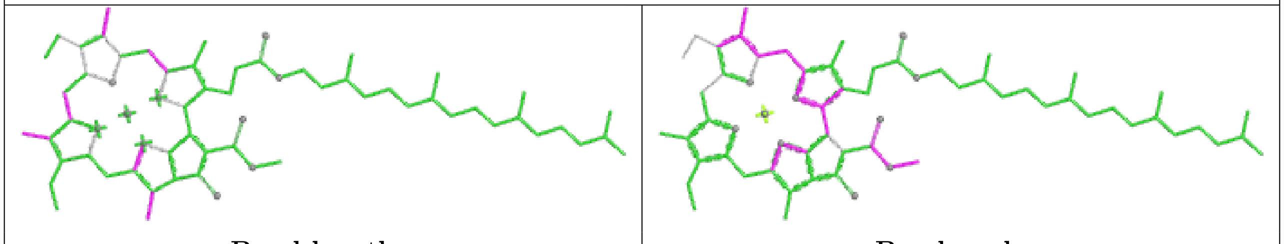


Bond lengths Bond angles

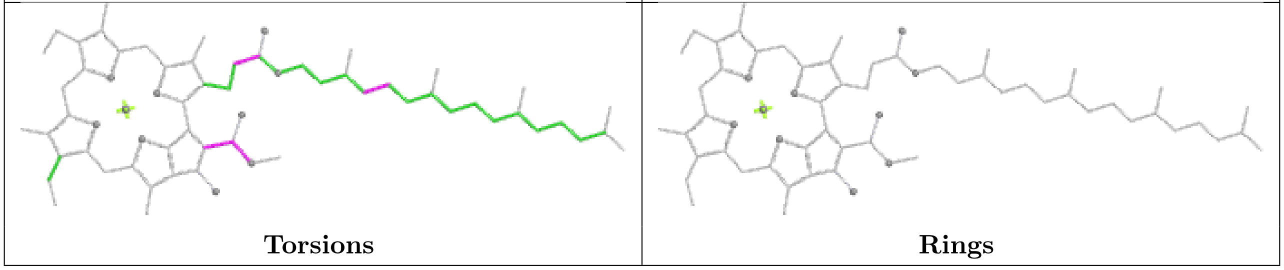


Torsions Rings

Ligand CLA A 801

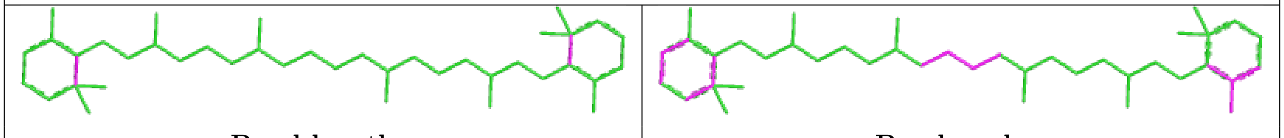


Bond lengths Bond angles

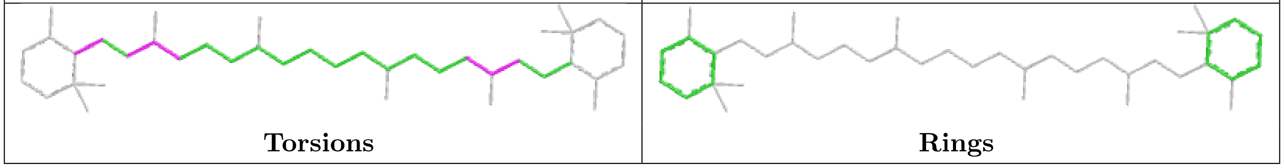


Torsions Rings

Ligand BCR I 101

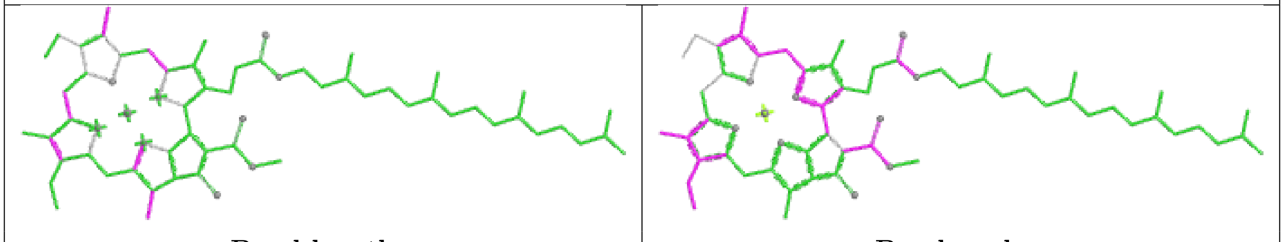


Bond lengths Bond angles



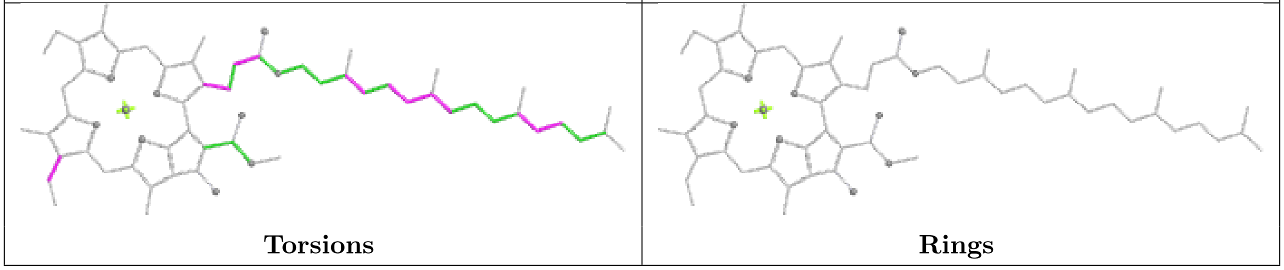
Torsions Rings

Ligand CLA H 2111



Bond lengths

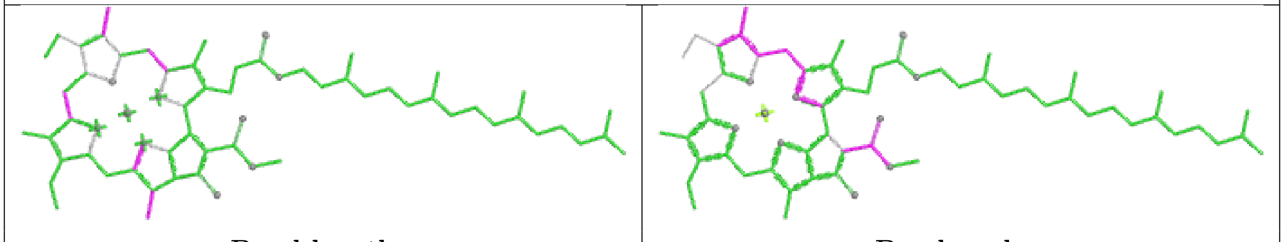
Bond angles



Torsions

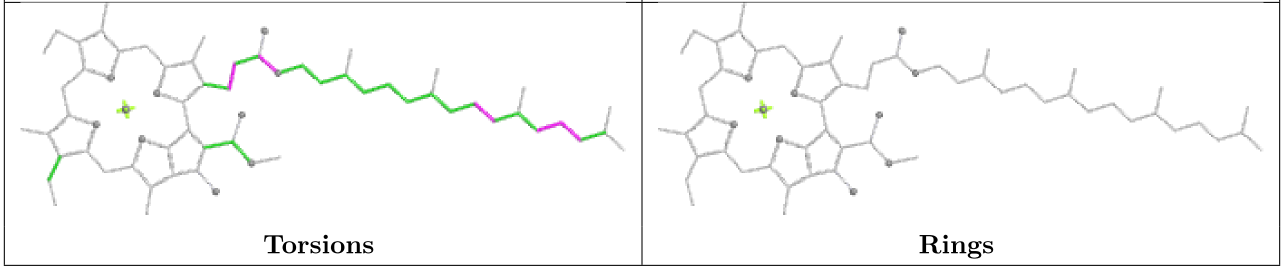
Rings

Ligand CLA l 205



Bond lengths

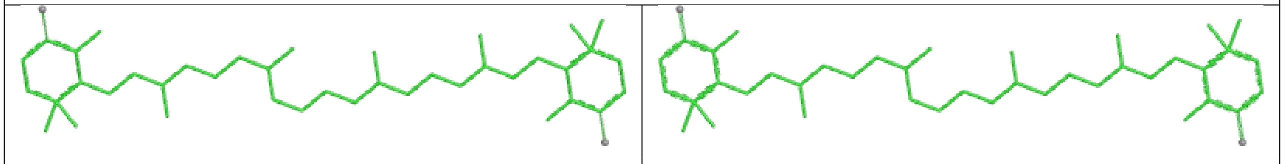
Bond angles



Torsions

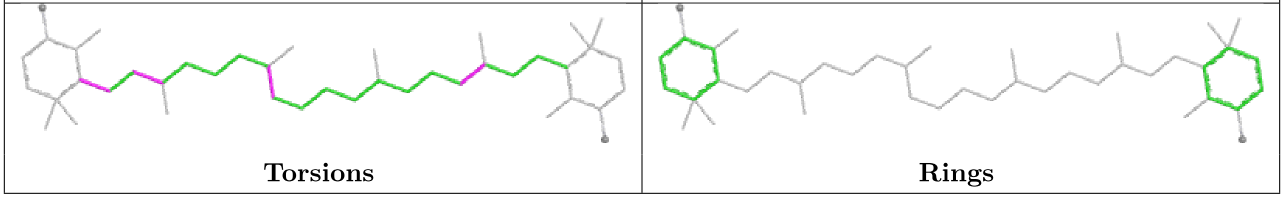
Rings

Ligand 45D a 852



Bond lengths

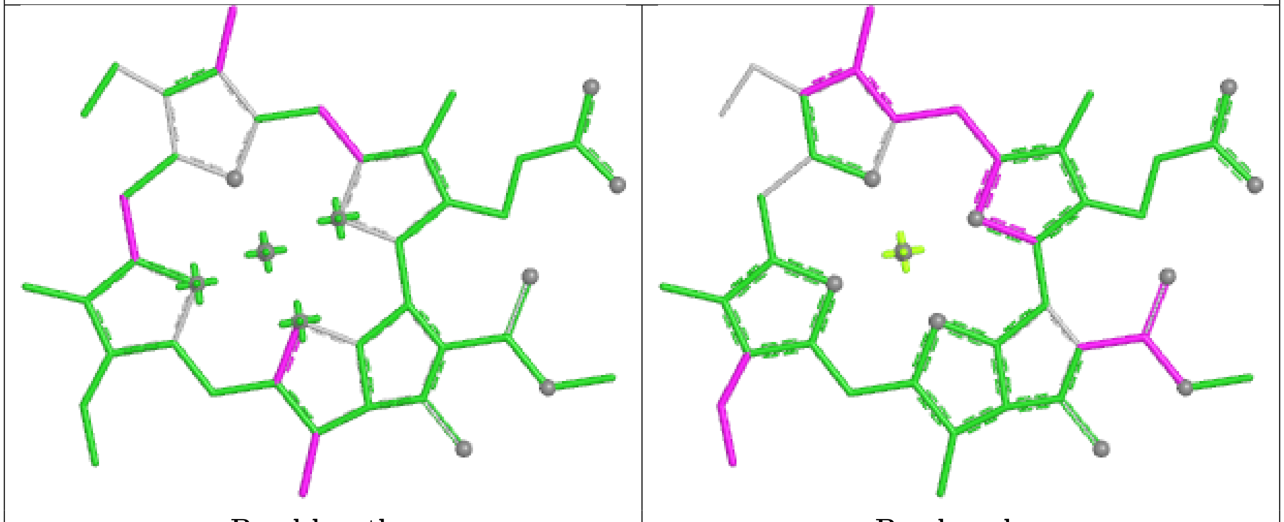
Bond angles



Torsions

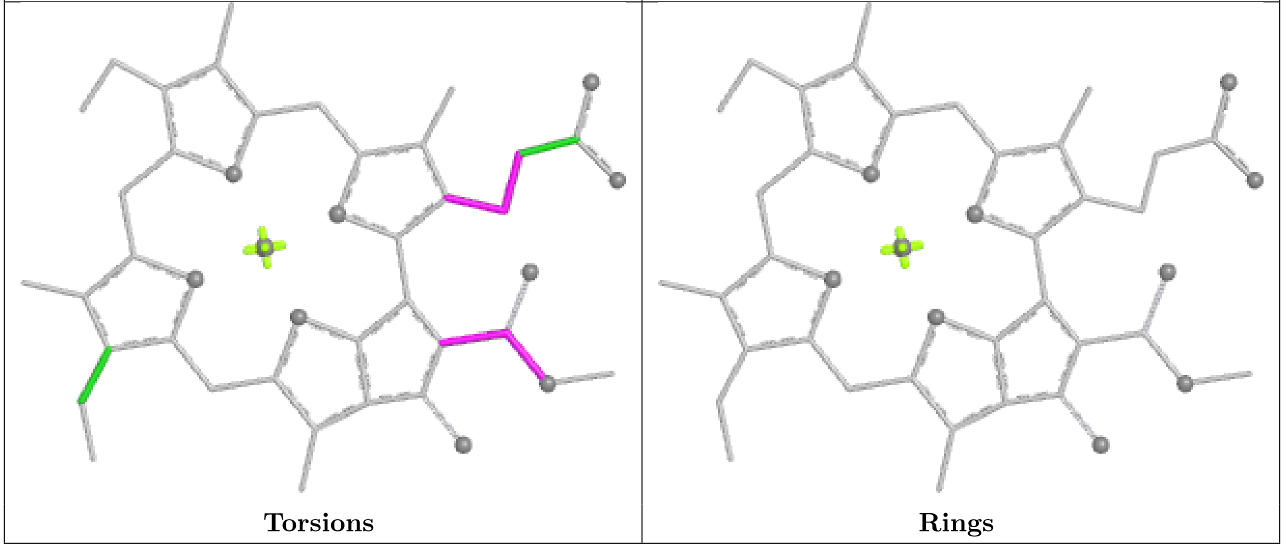
Rings

Ligand CLA b 2141



Bond lengths

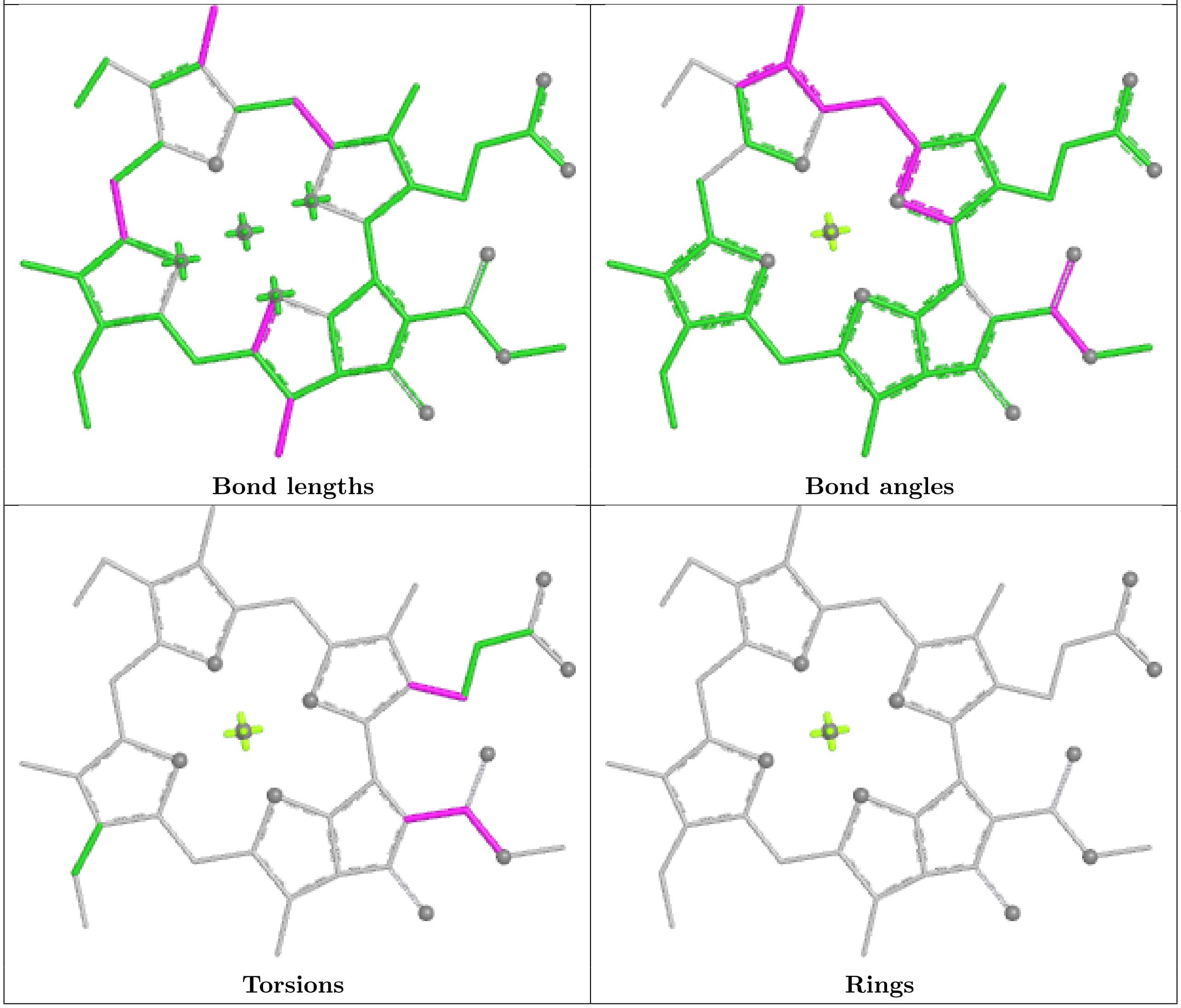
Bond angles



Torsions

Rings

Ligand CLA B 2137



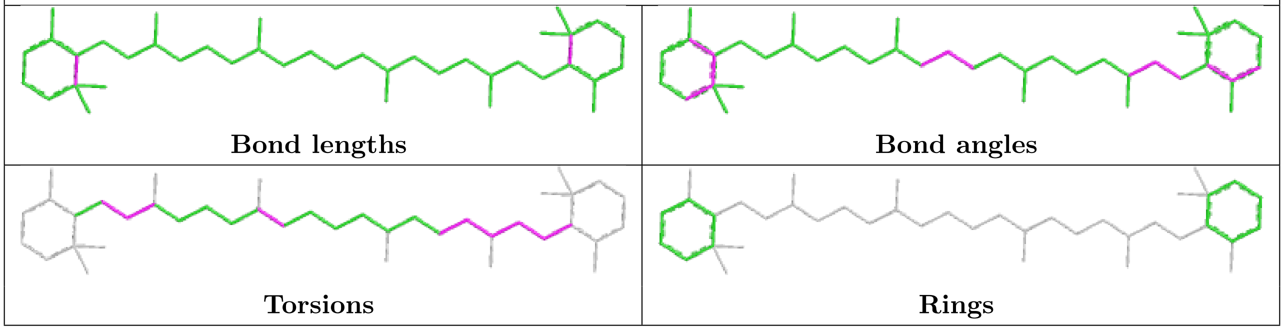
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR f 202



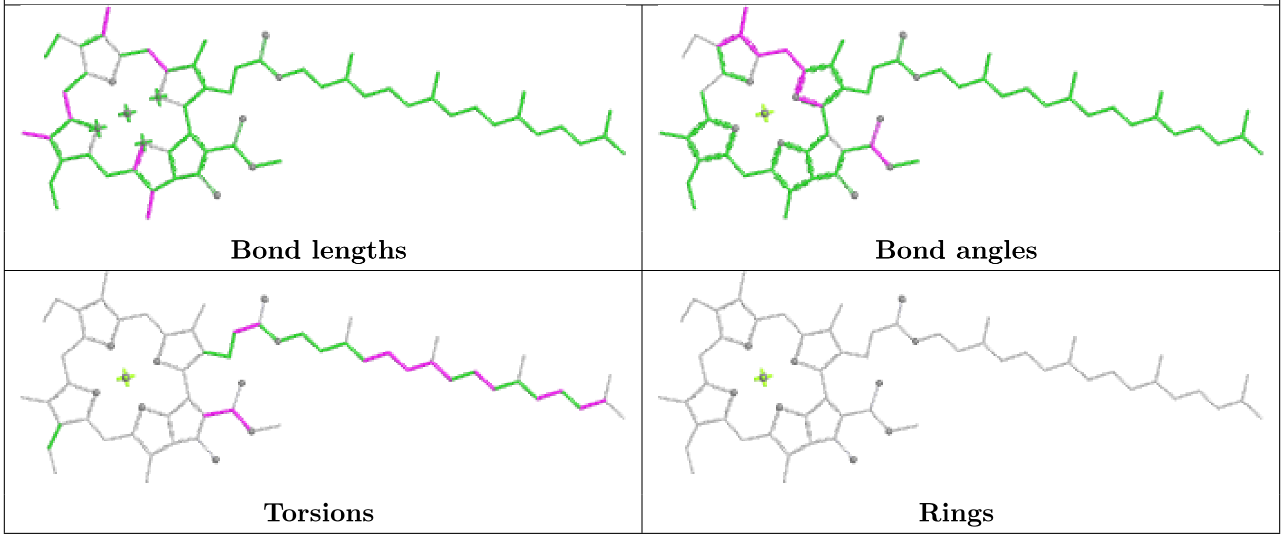
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 2108



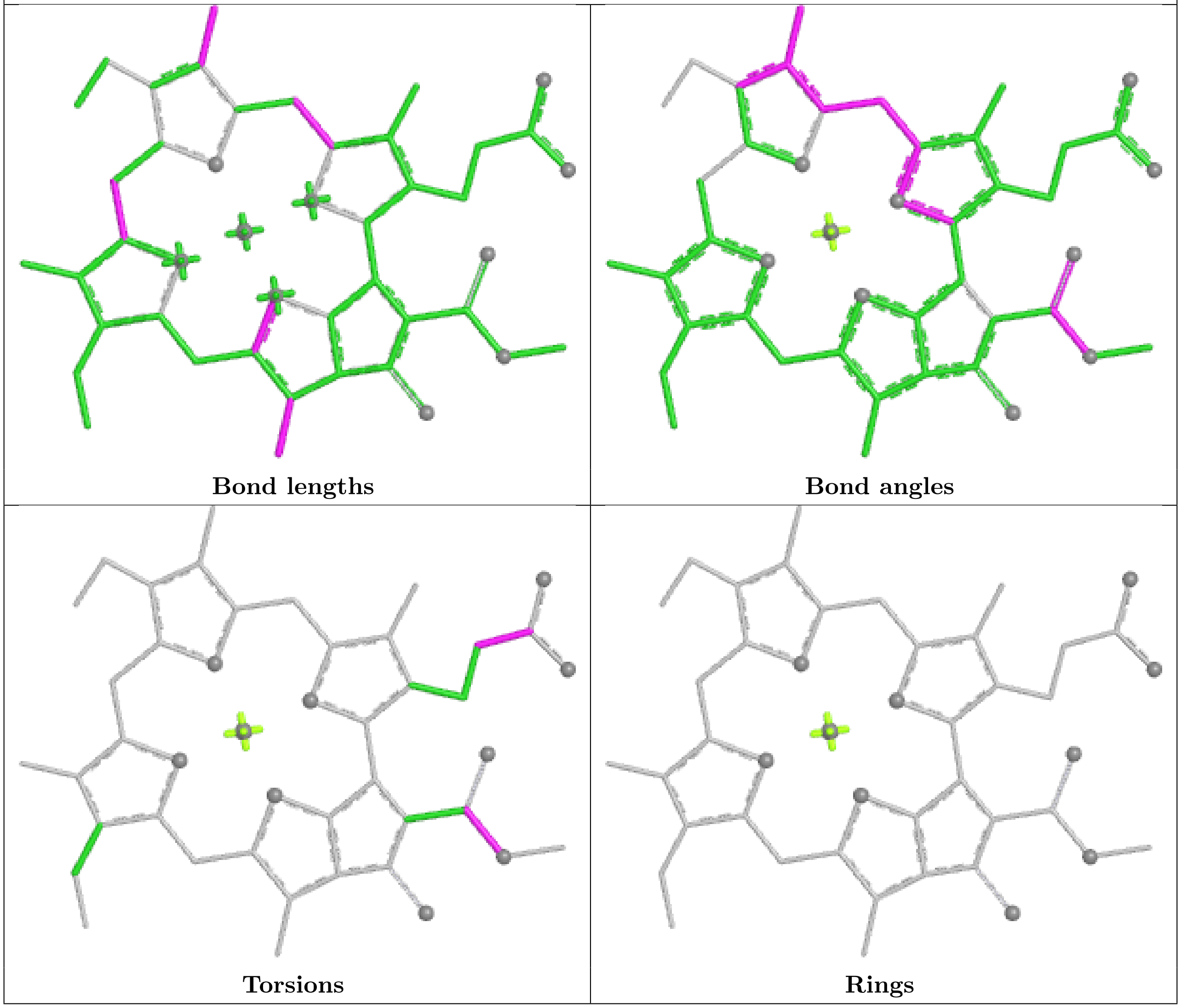
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 2135



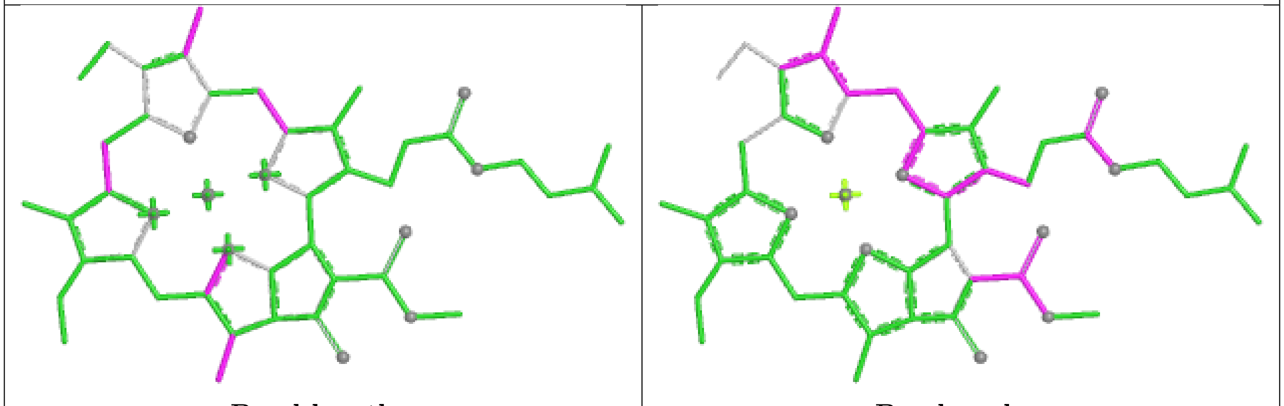
Bond lengths

Bond angles

Torsions

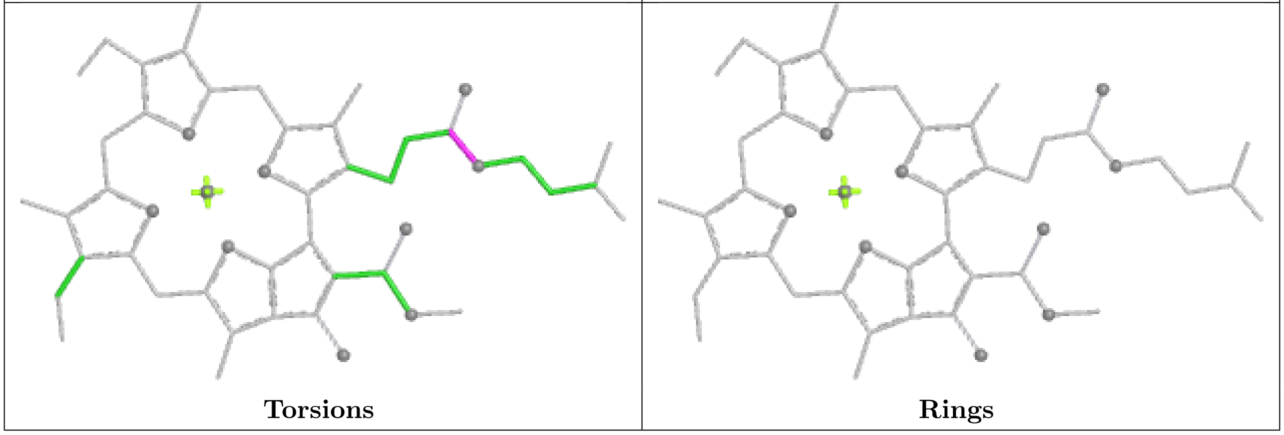
Rings

Ligand CLA H 2125



Bond lengths

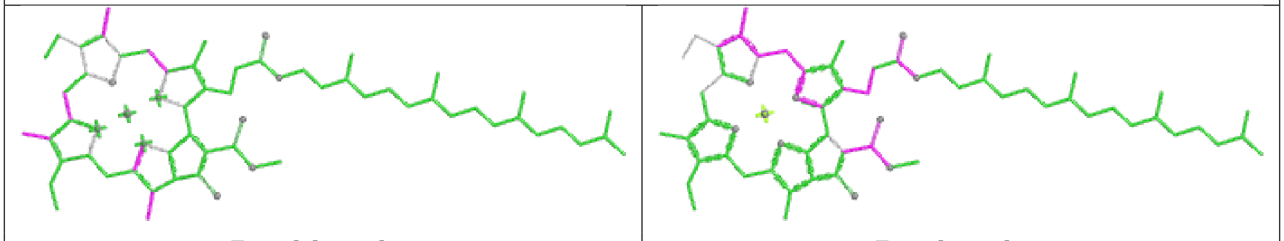
Bond angles



Torsions

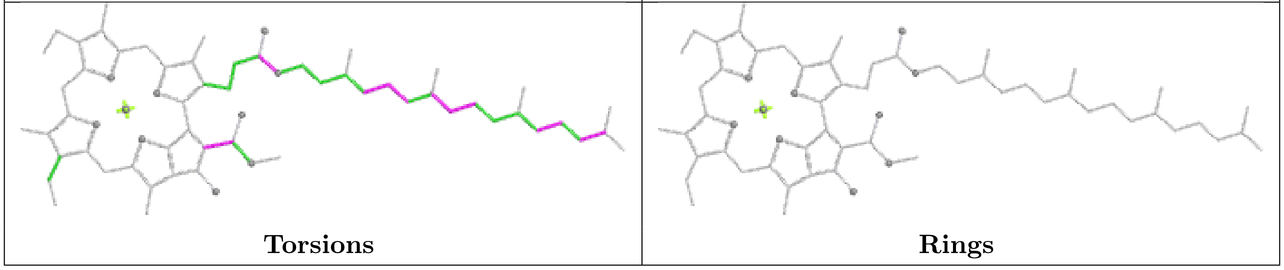
Rings

Ligand CLA B 2110



Bond lengths

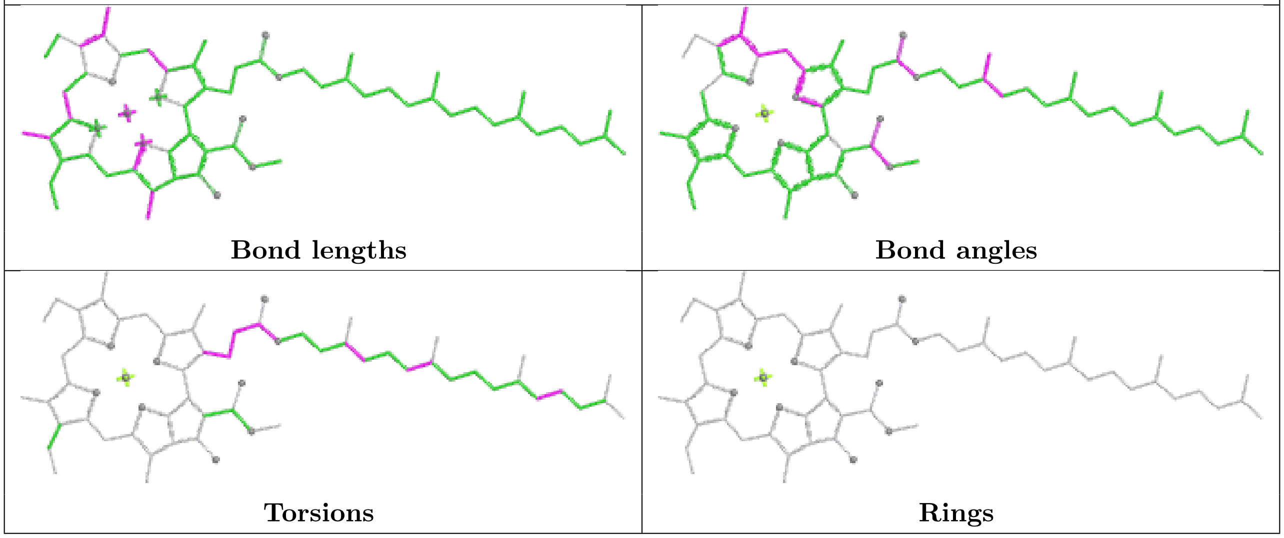
Bond angles



Torsions

Rings

Ligand CLA a 851



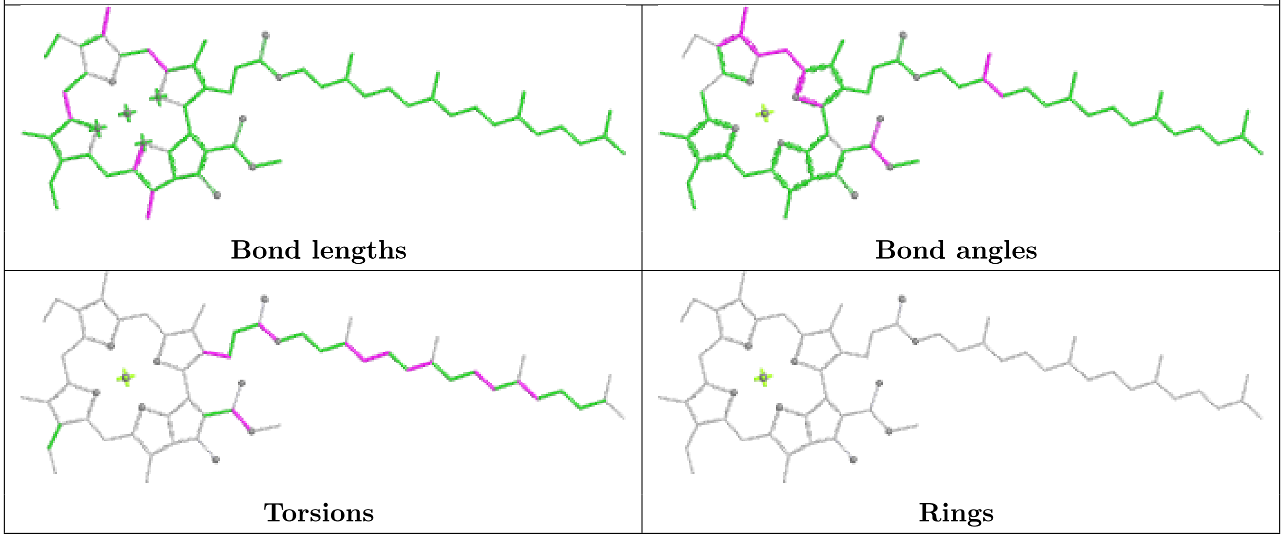
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 833



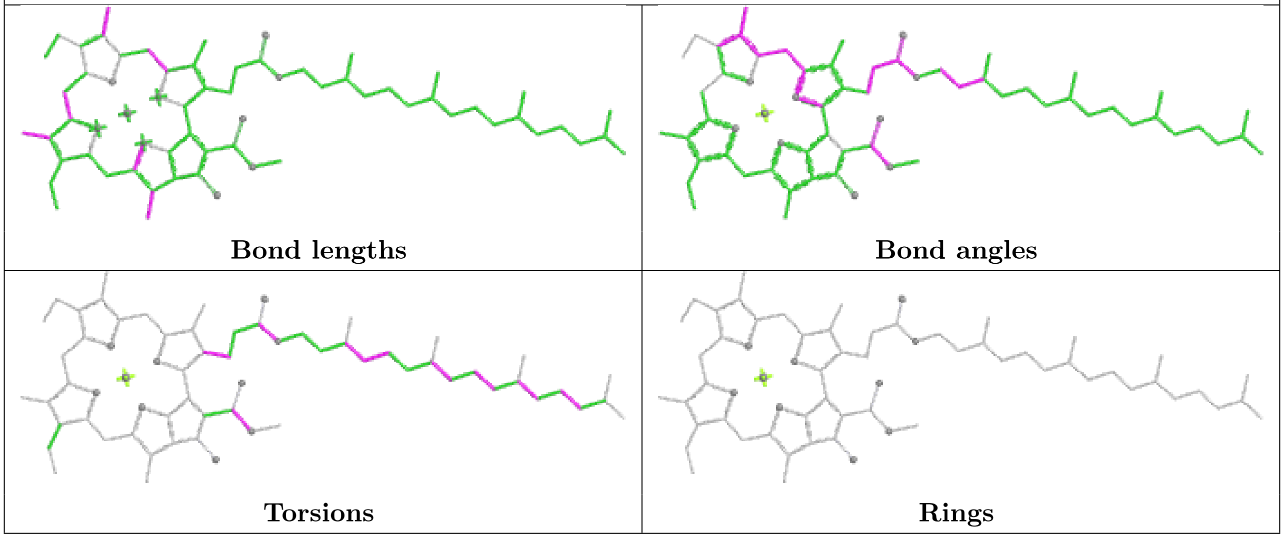
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 805



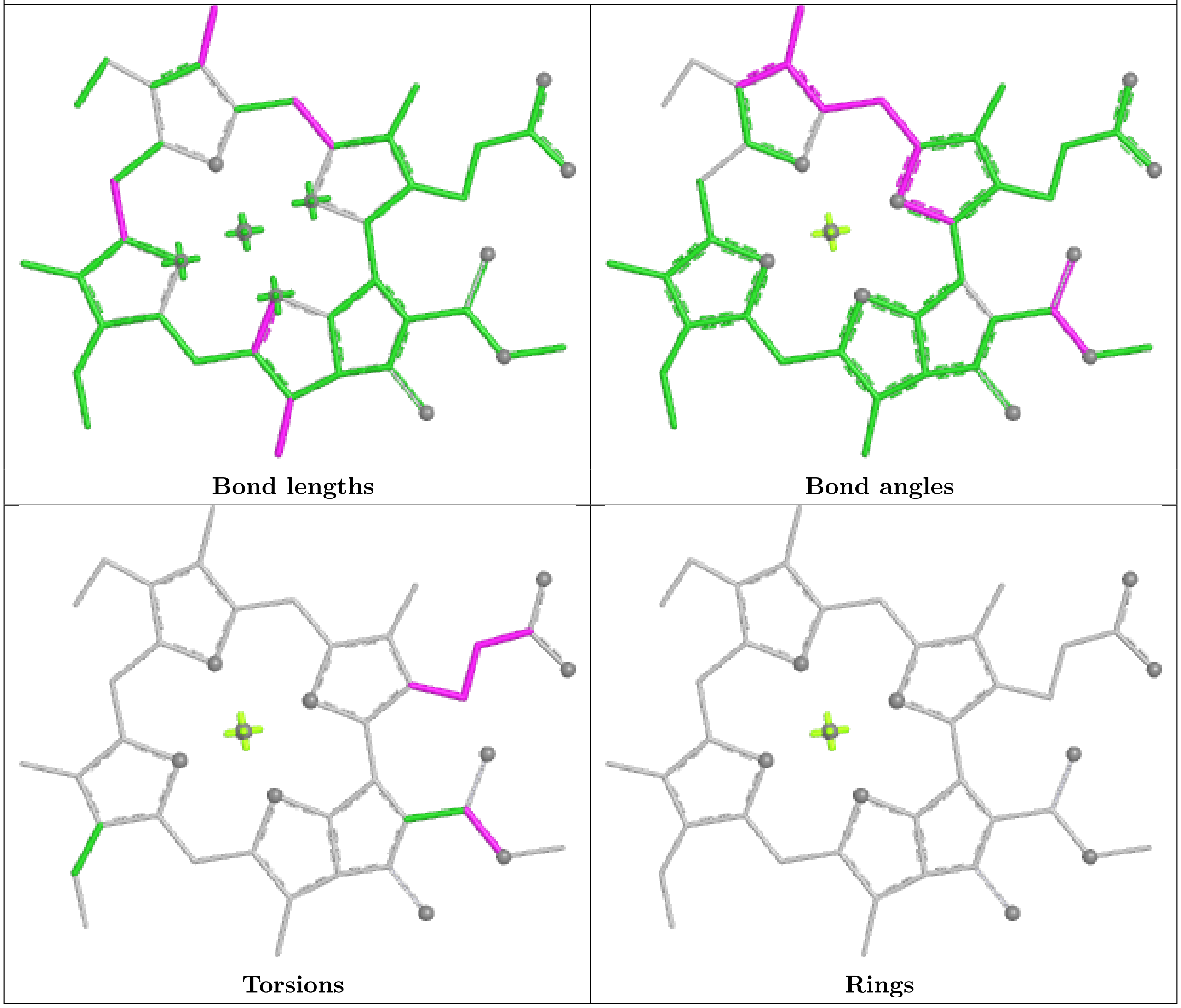
Bond lengths

Bond angles

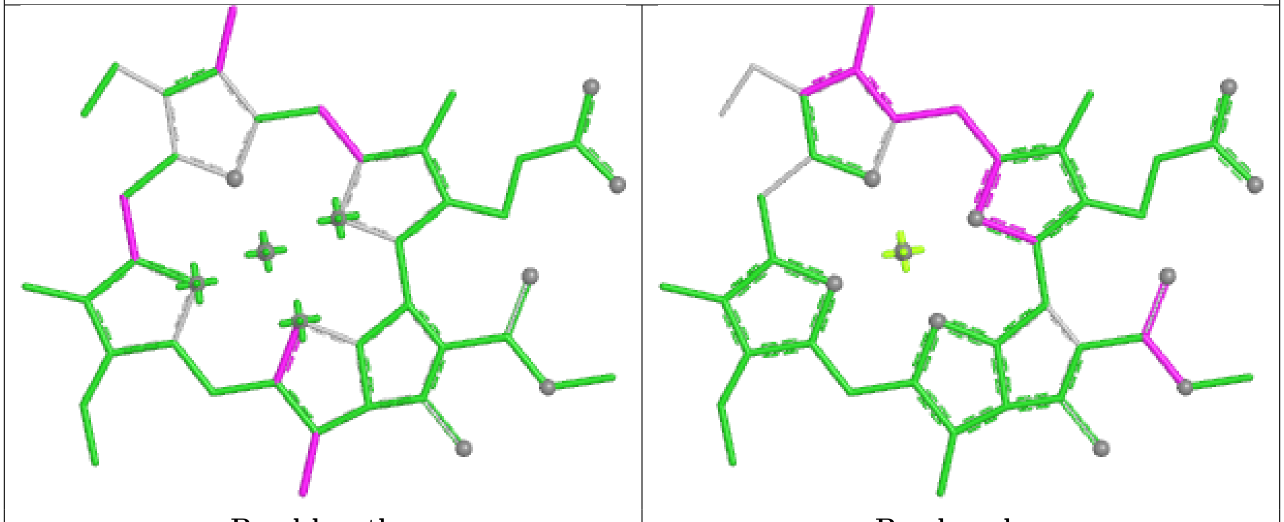
Torsions

Rings

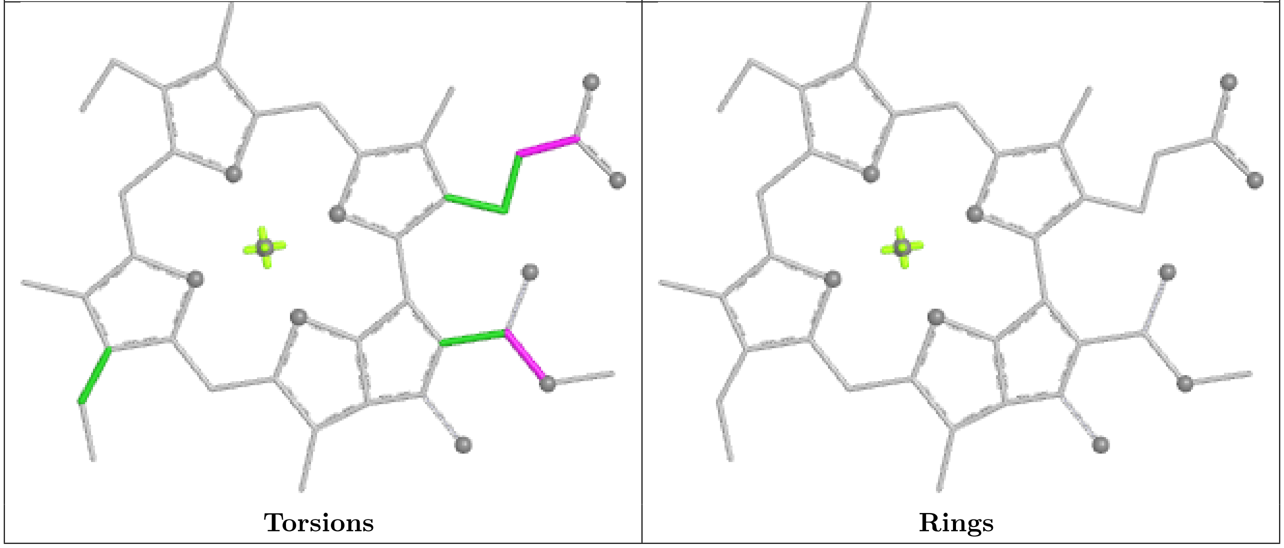
Ligand CLA H 2116



Ligand CLA b 2134

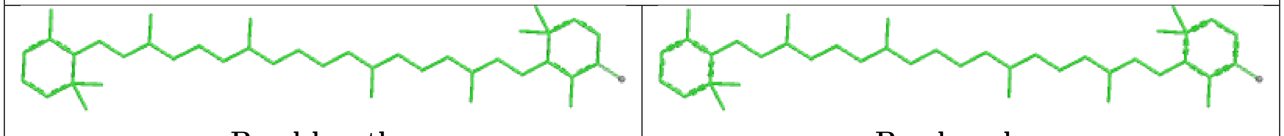


Bond lengths **Bond angles**

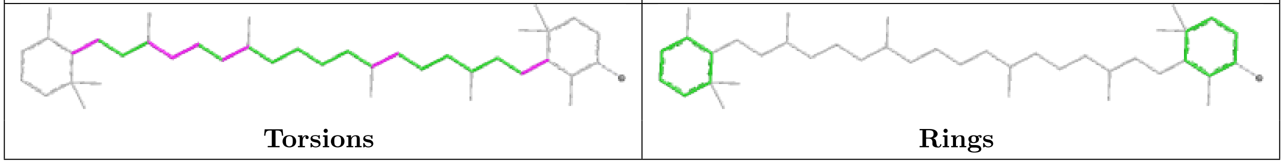


Torsions **Rings**

Ligand ECH V 101

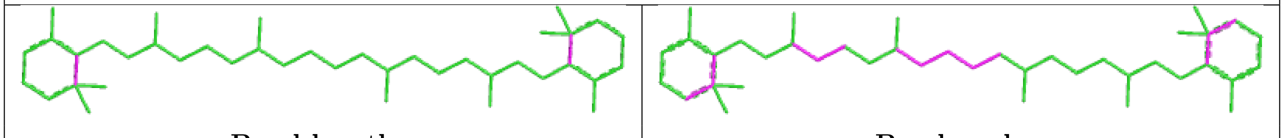


Bond lengths **Bond angles**



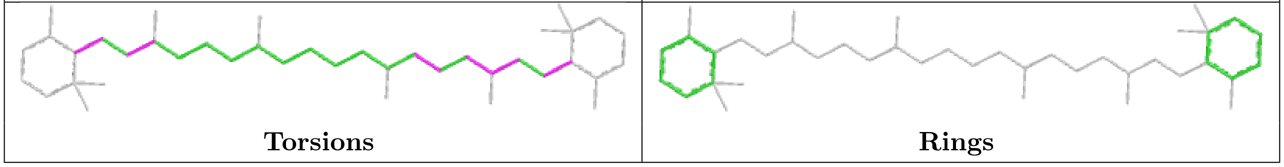
Torsions **Rings**

Ligand BCR l 206



Bond lengths

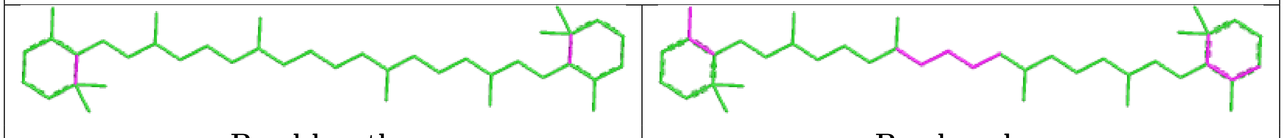
Bond angles



Torsions

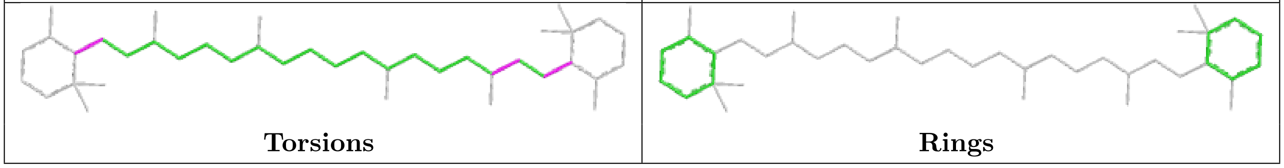
Rings

Ligand BCR B 2143



Bond lengths

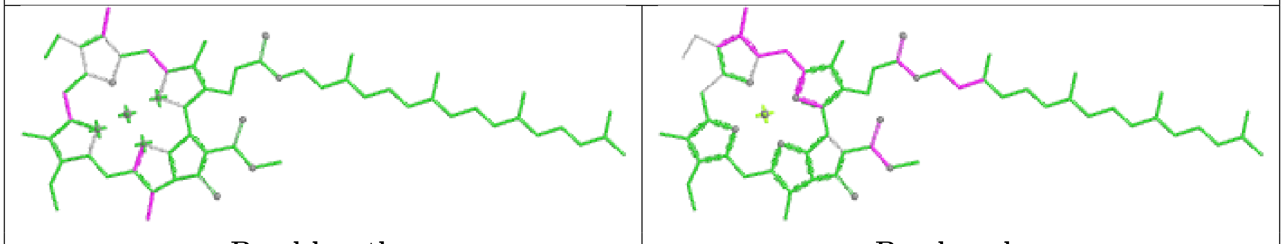
Bond angles



Torsions

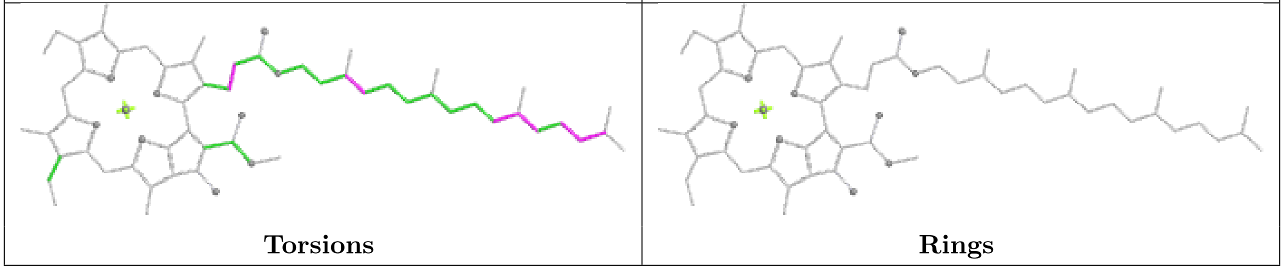
Rings

Ligand CLA a 818



Bond lengths

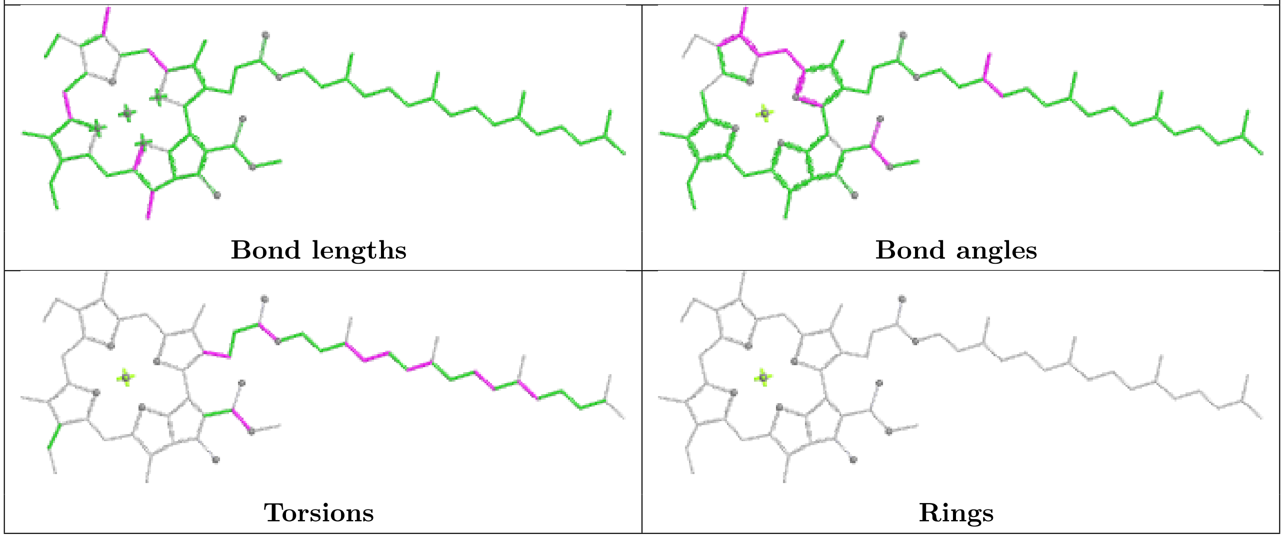
Bond angles



Torsions

Rings

Ligand CLA G 833



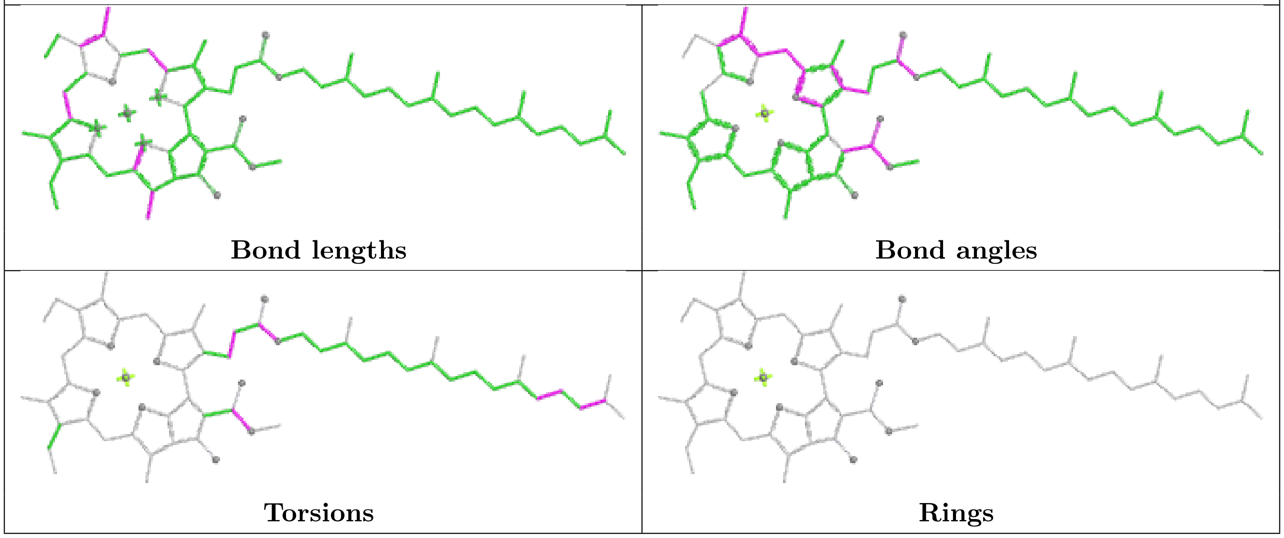
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 2139



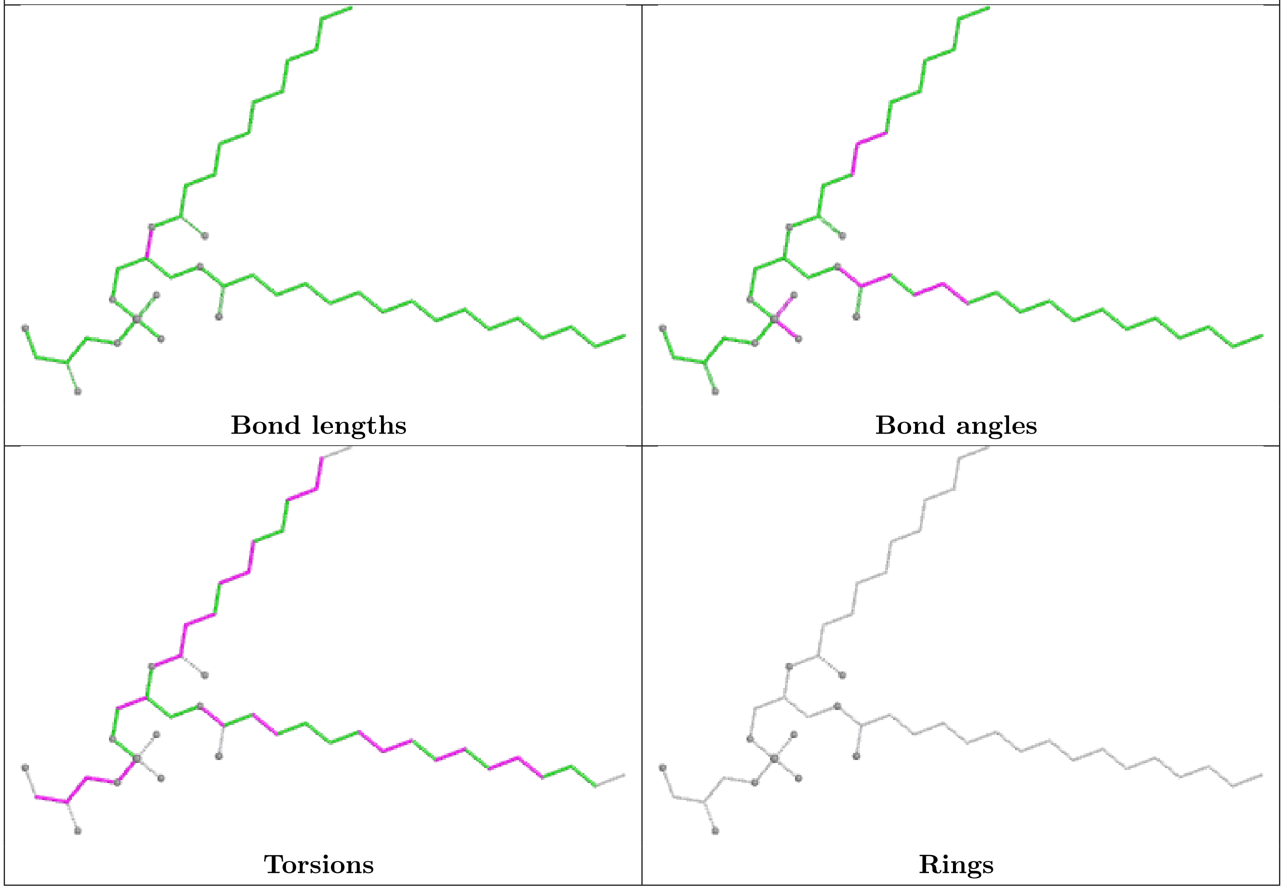
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG V 103



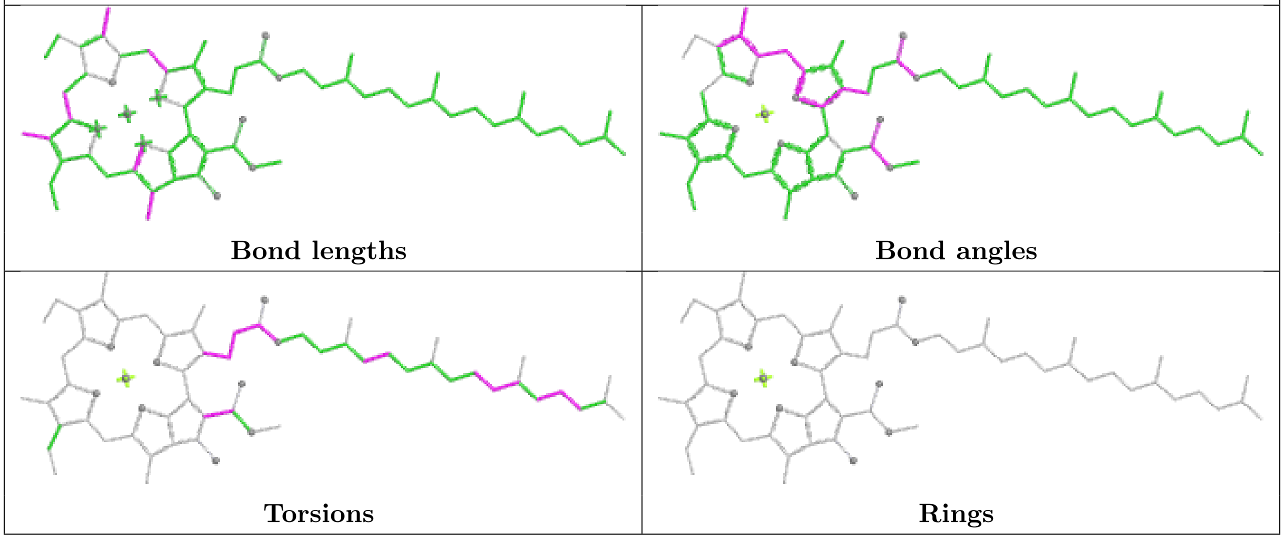
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 807

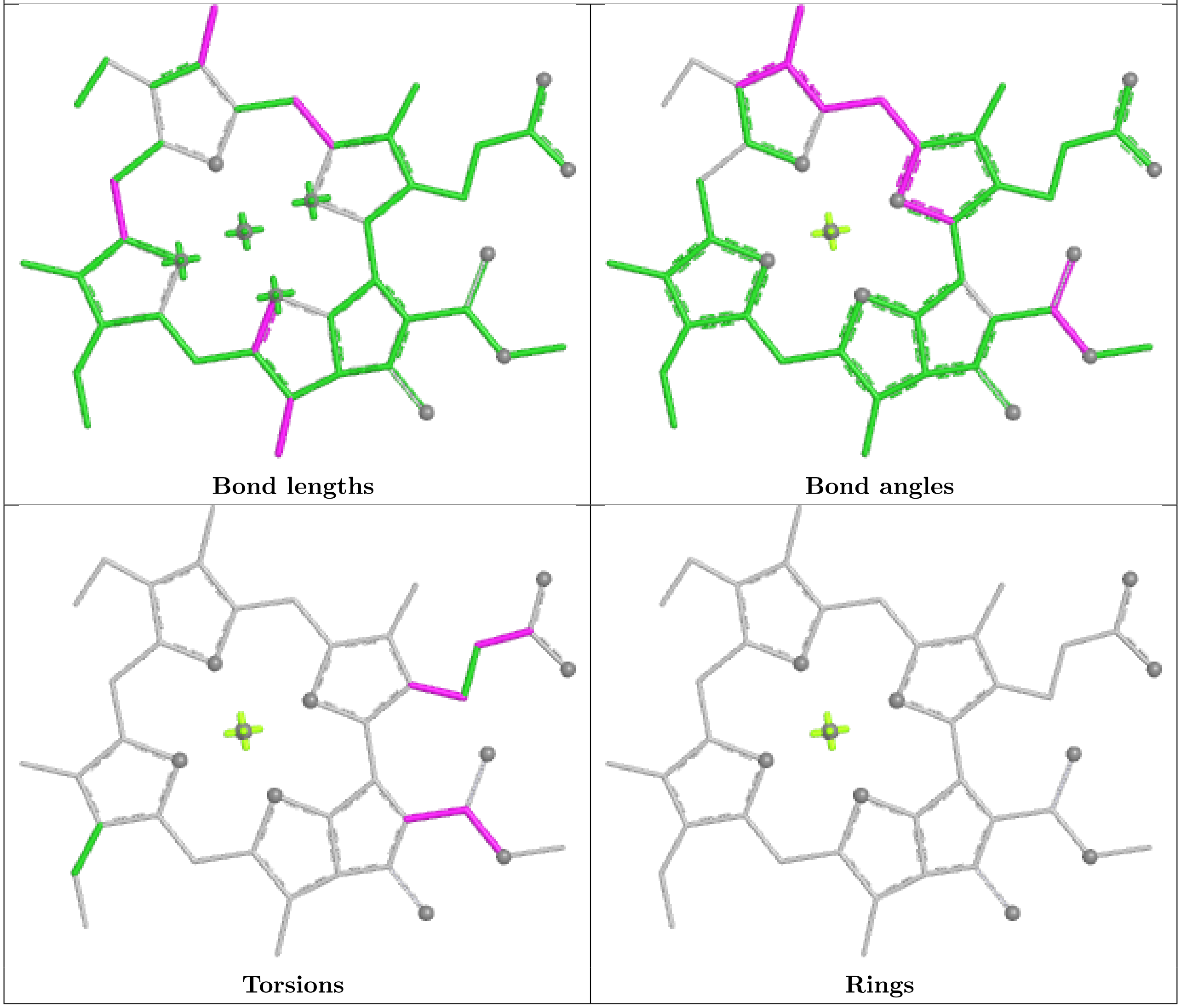


Bond lengths

Bond angles

Torsions

Rings



Ligand CLA K 4002

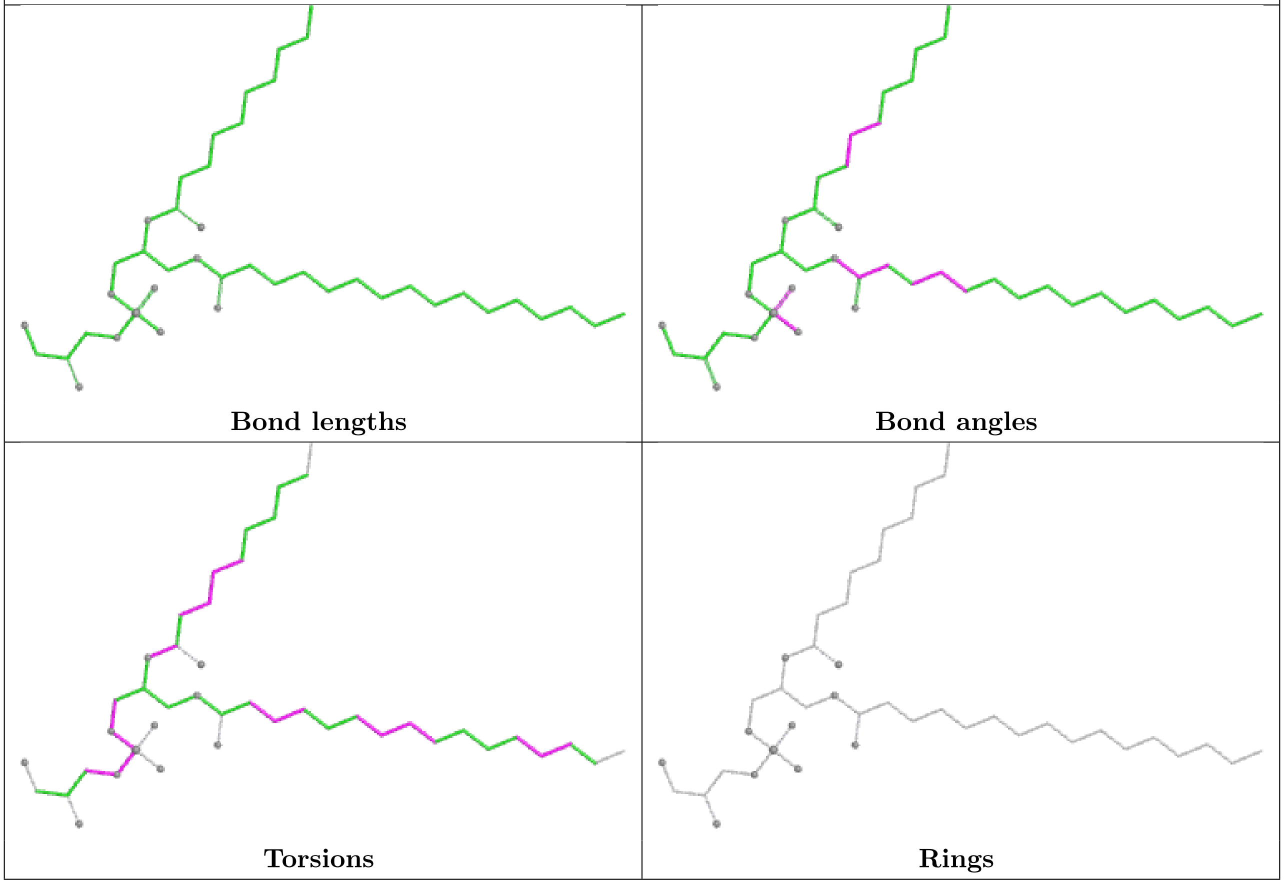
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG b 2148



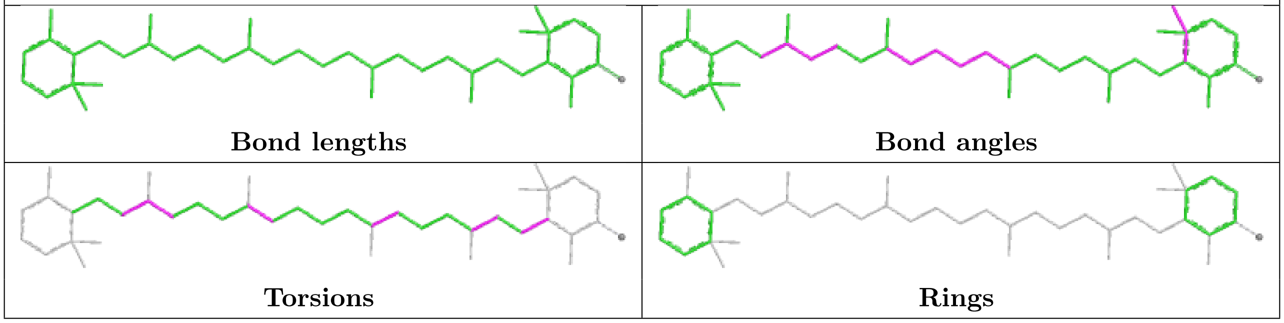
Bond lengths

Bond angles

Torsions

Rings

Ligand ECH b 2143



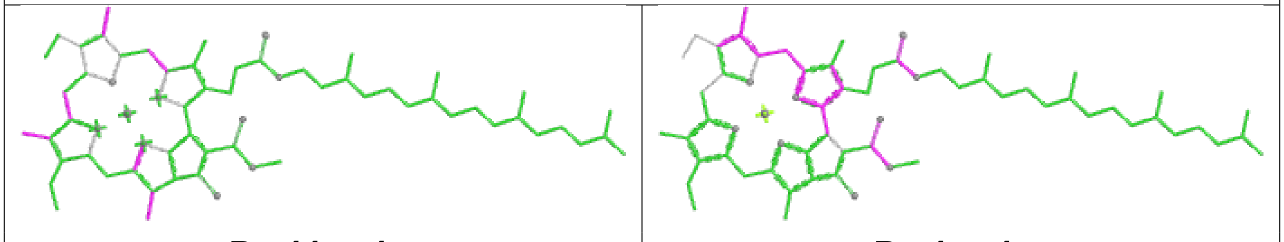
Bond lengths

Bond angles

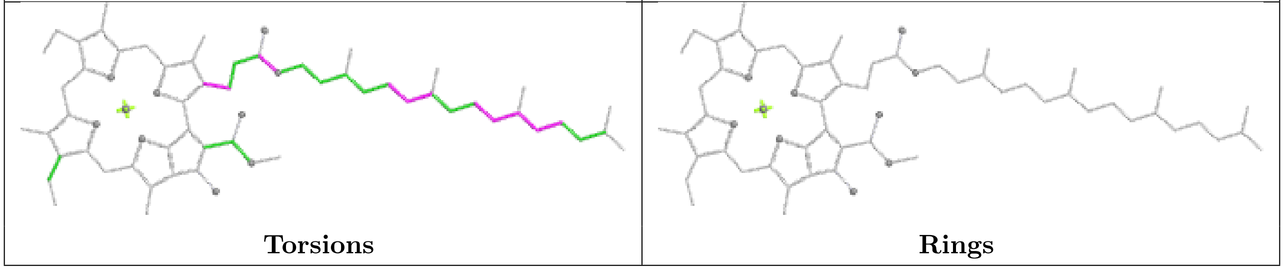
Torsions

Rings

Ligand CLA U 203

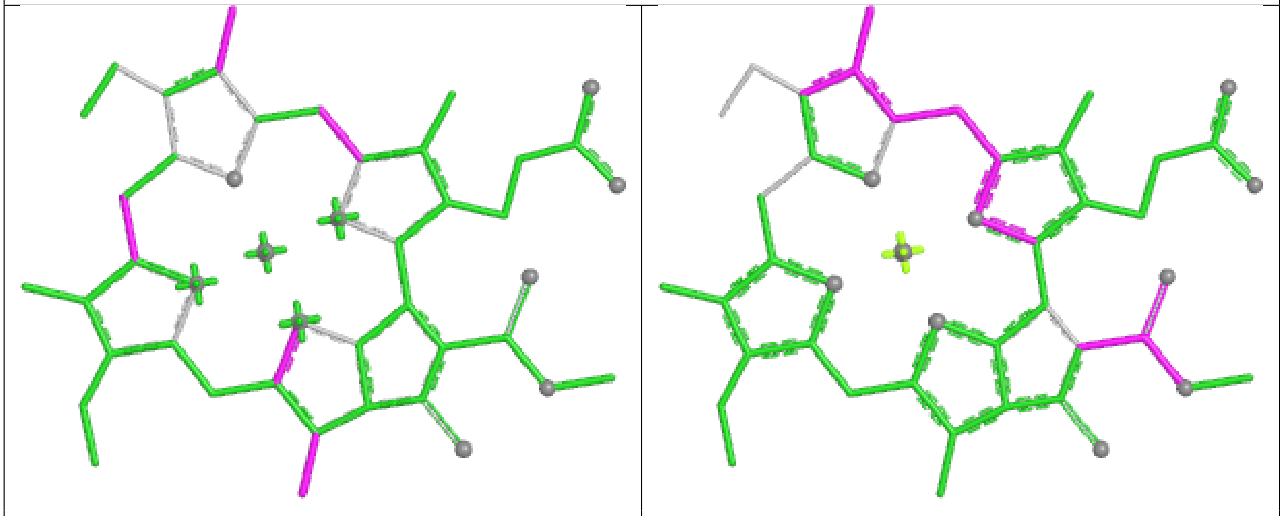


Bond lengths Bond angles

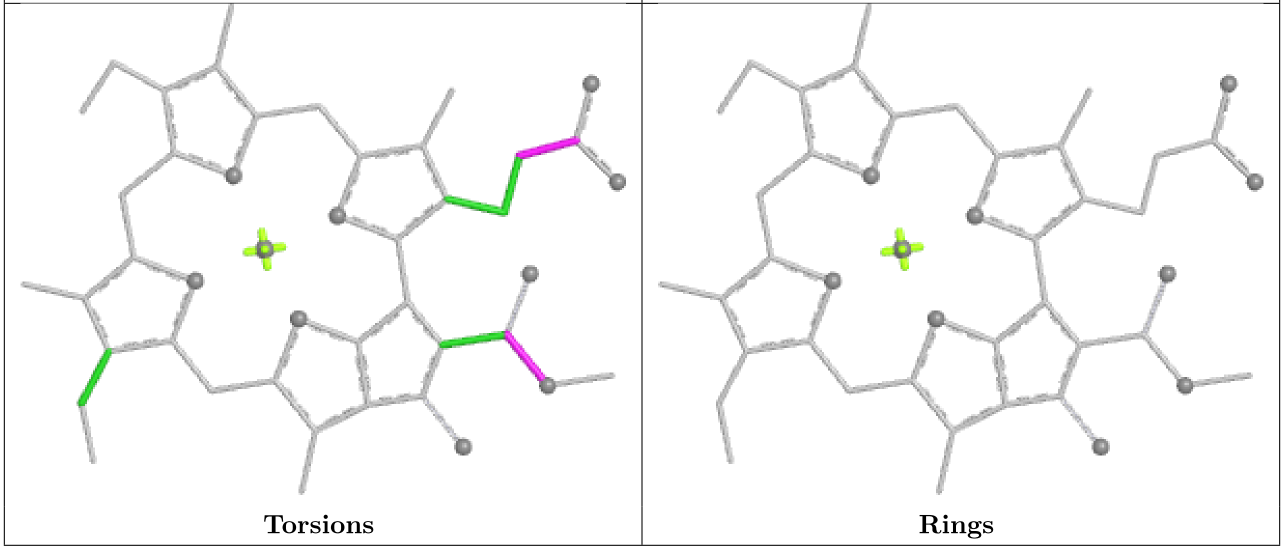


Torsions Rings

Ligand CLA H 2138

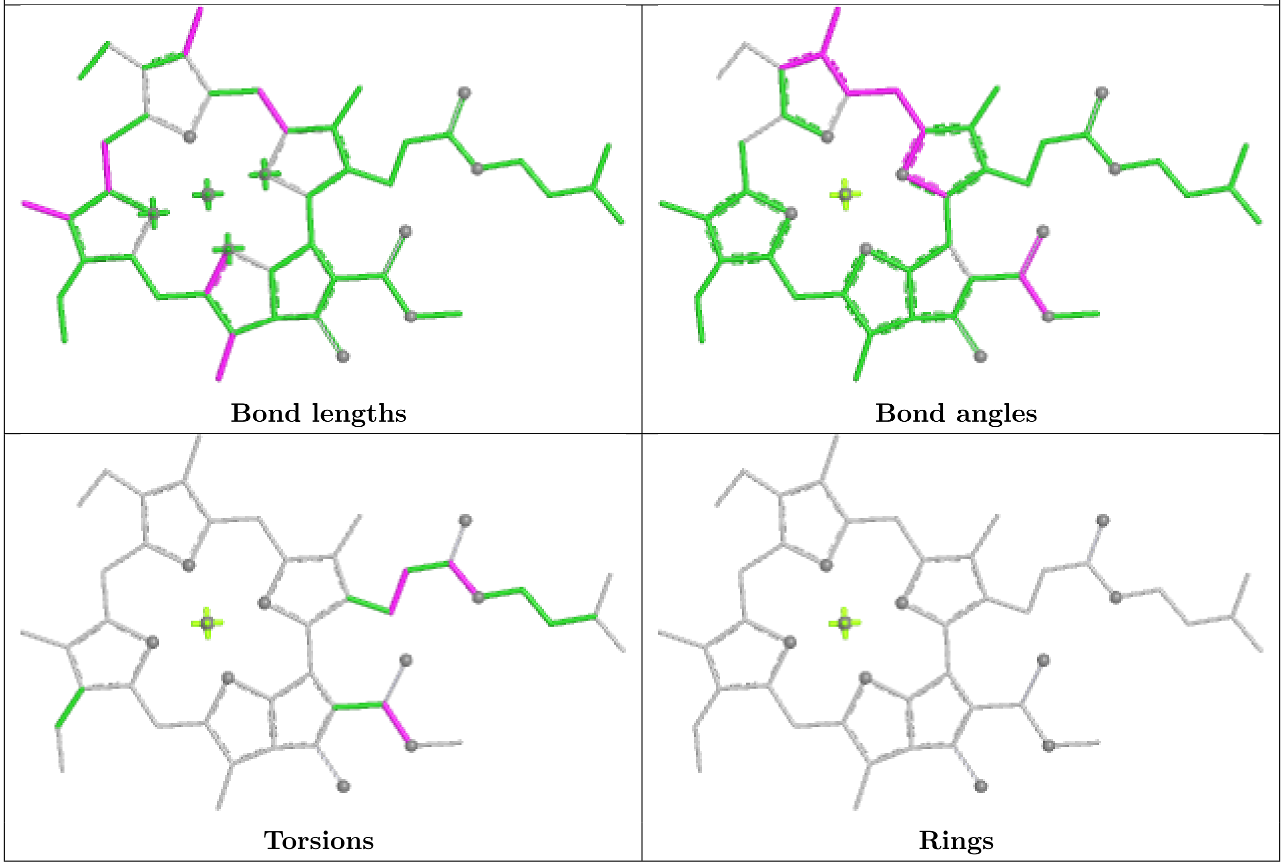


Bond lengths Bond angles



Torsions Rings

Ligand CLA B 2101



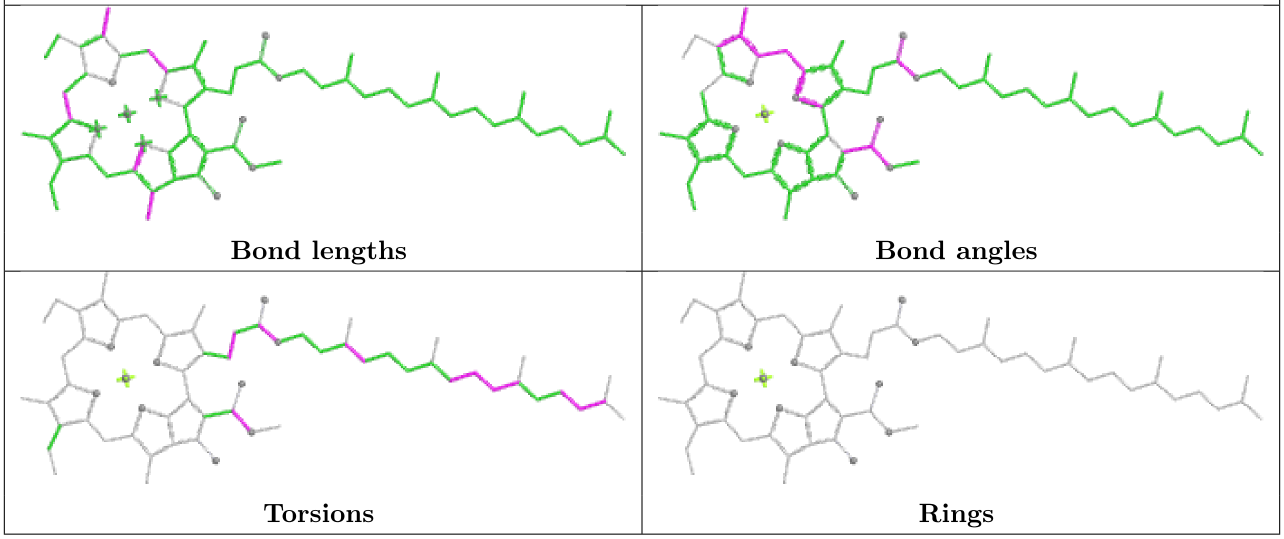
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 810



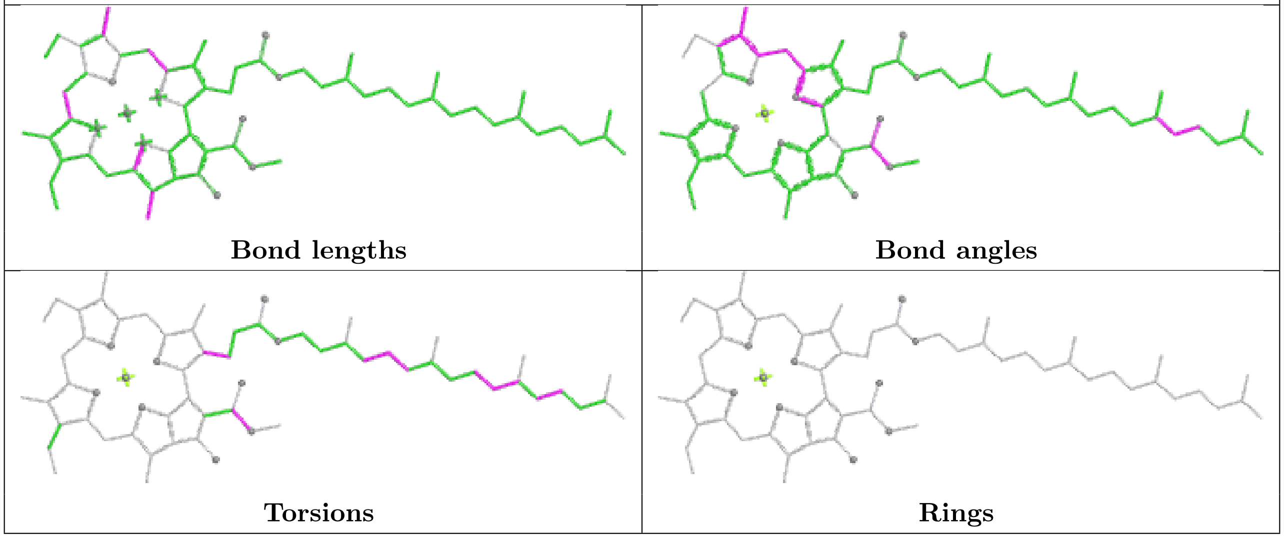
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 839



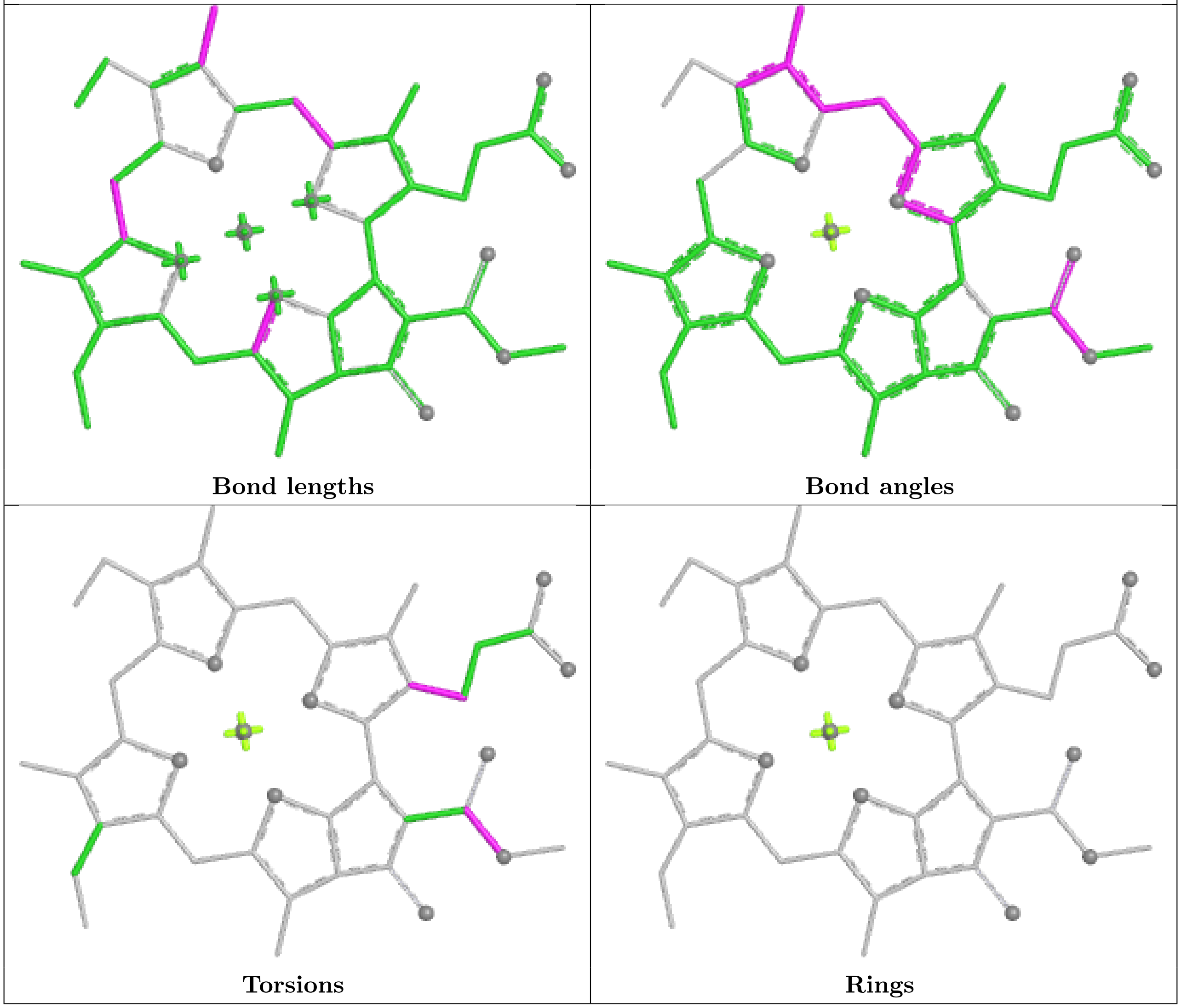
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 815



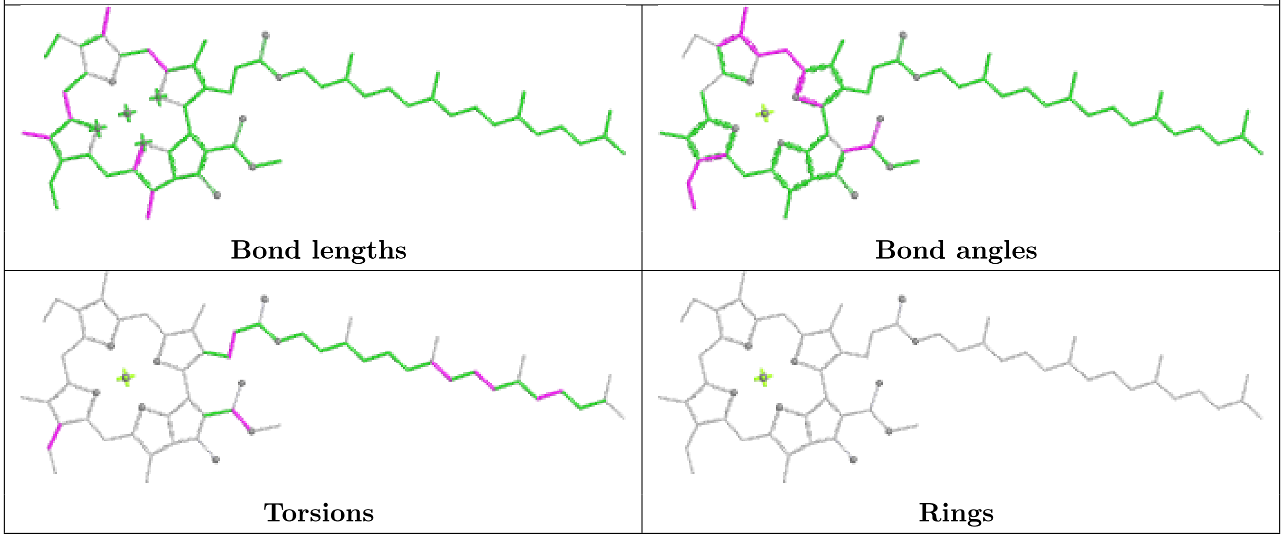
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 2104



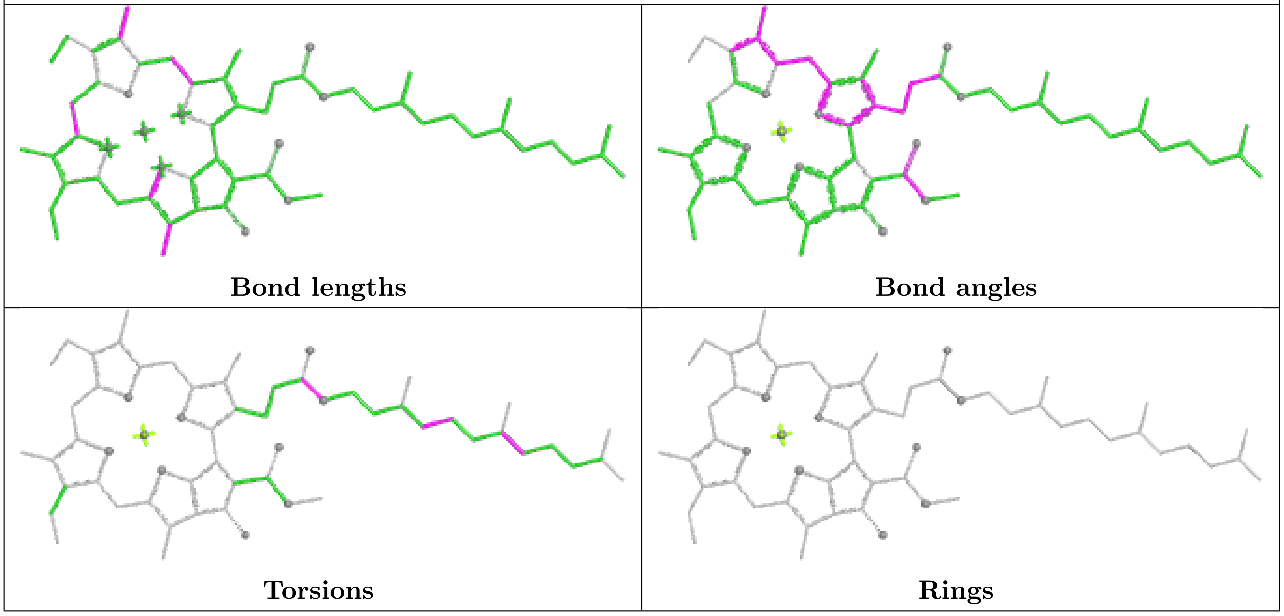
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 825



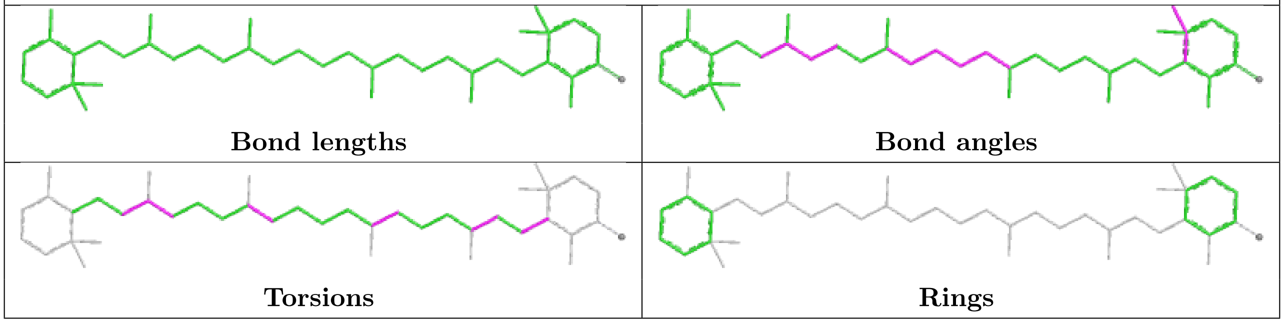
Bond lengths

Bond angles

Torsions

Rings

Ligand ECH B 2144



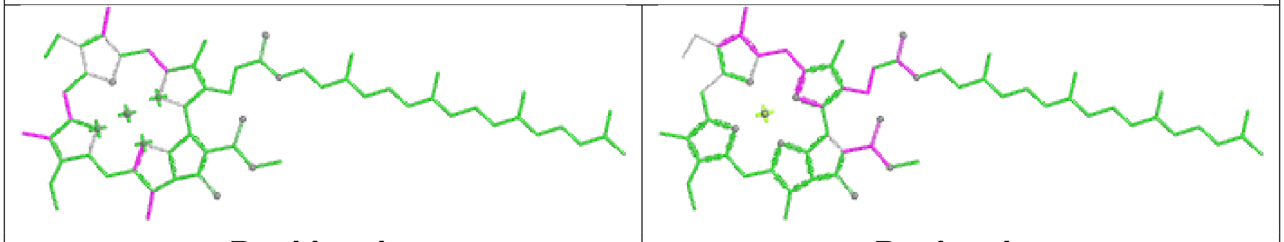
Bond lengths

Bond angles

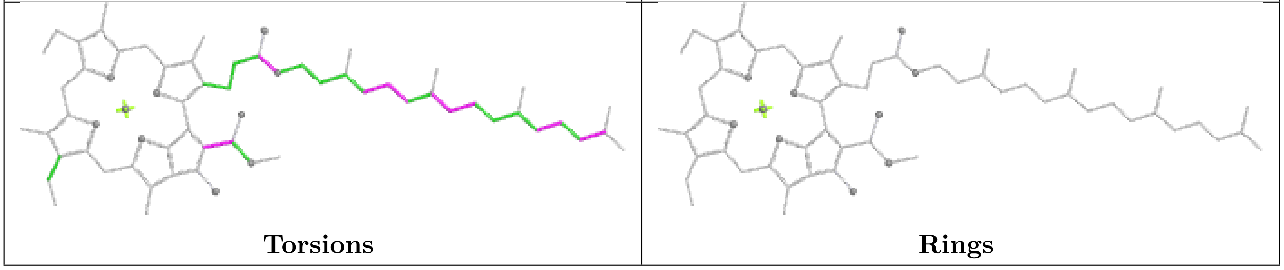
Torsions

Rings

Ligand CLA b 2109

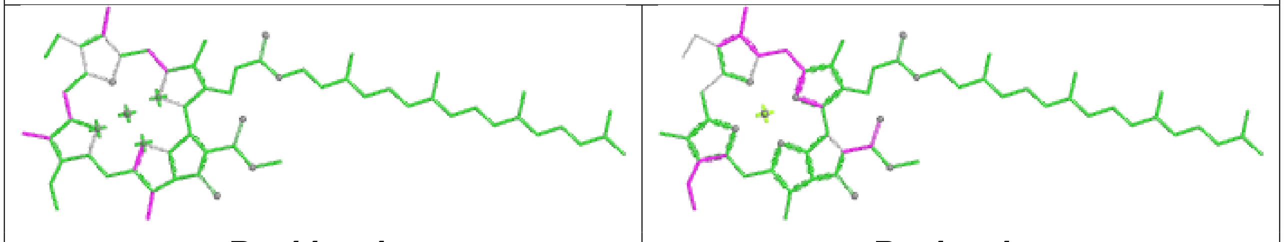


Bond lengths Bond angles

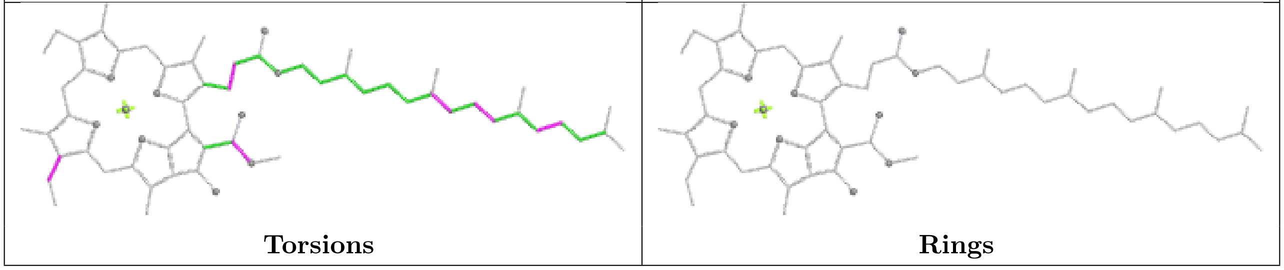


Torsions Rings

Ligand CLA b 2104

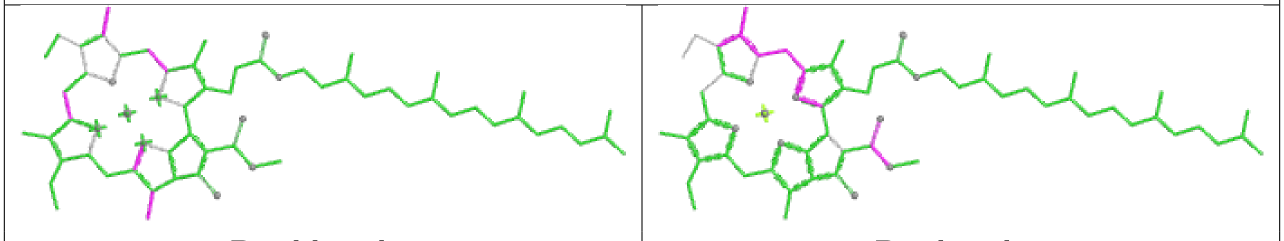


Bond lengths Bond angles

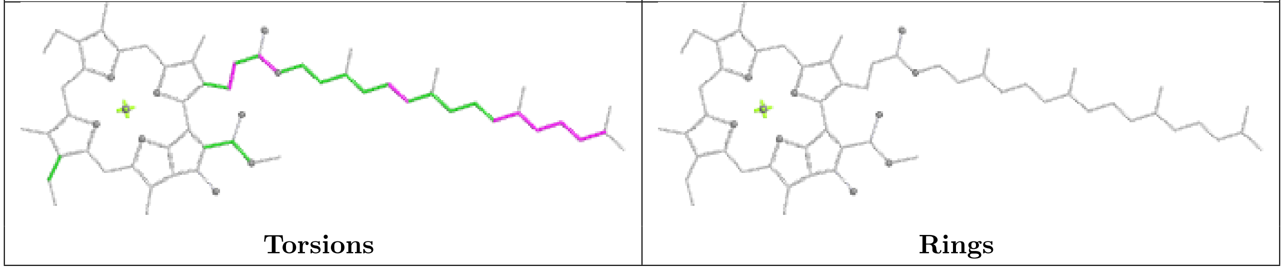


Torsions Rings

Ligand CLA G 828

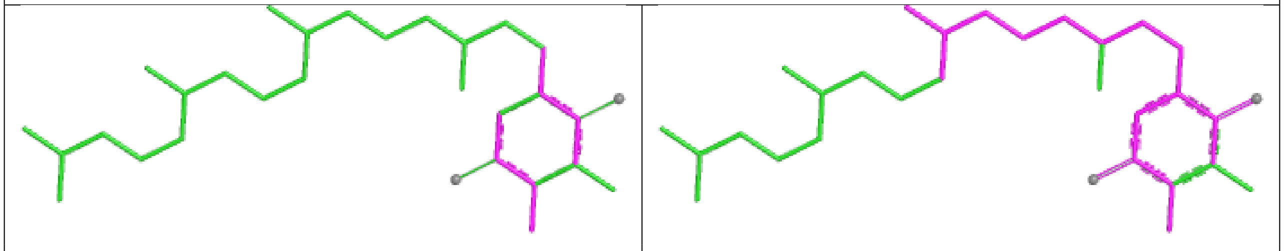


Bond lengths Bond angles



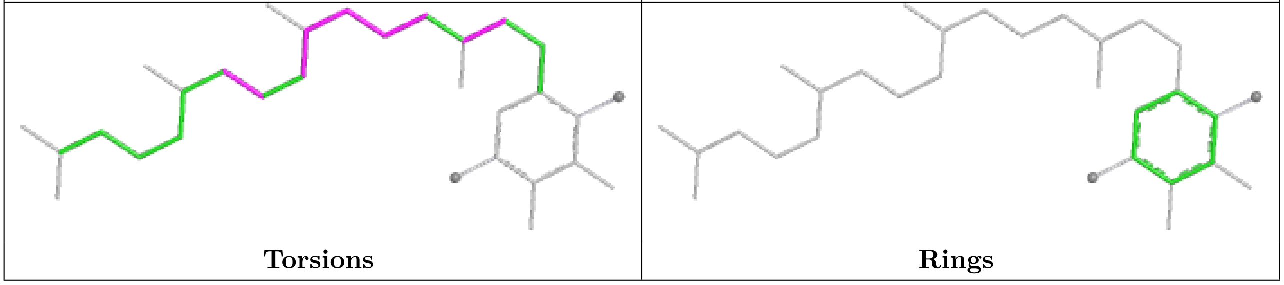
Torsions Rings

Ligand A1AGD B 2153



Bond lengths

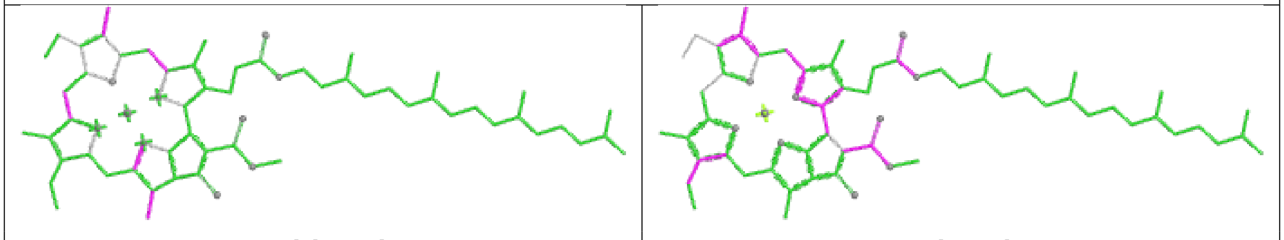
Bond angles



Torsions

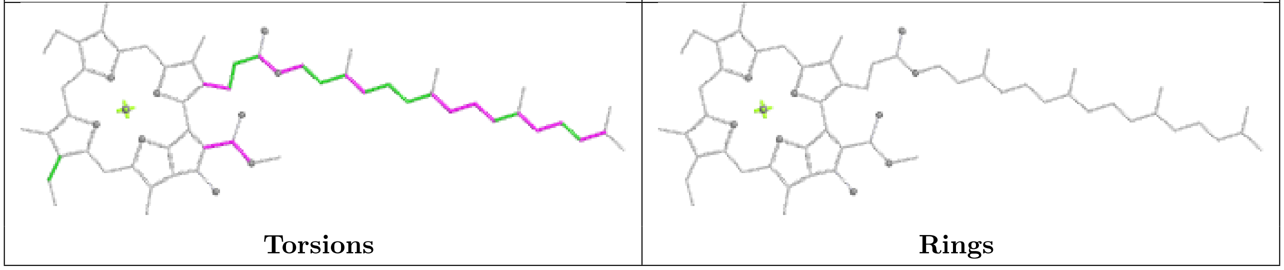
Rings

Ligand CLA G 824



Bond lengths

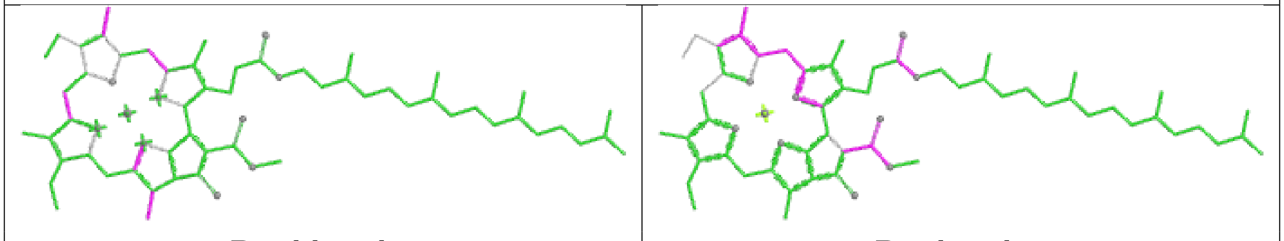
Bond angles



Torsions

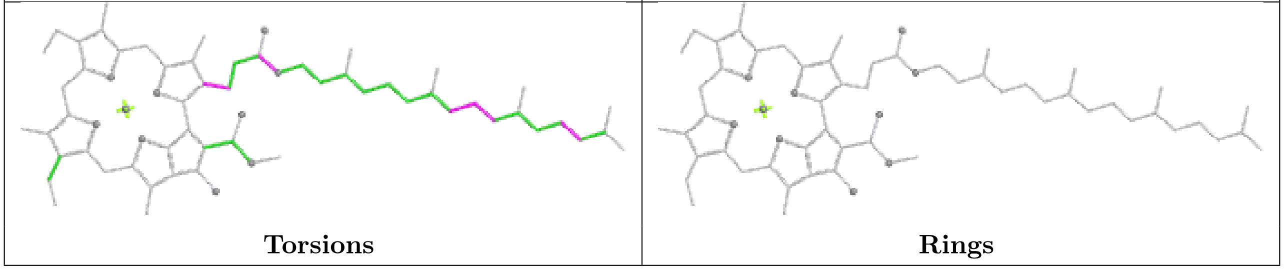
Rings

Ligand CLA A 802



Bond lengths

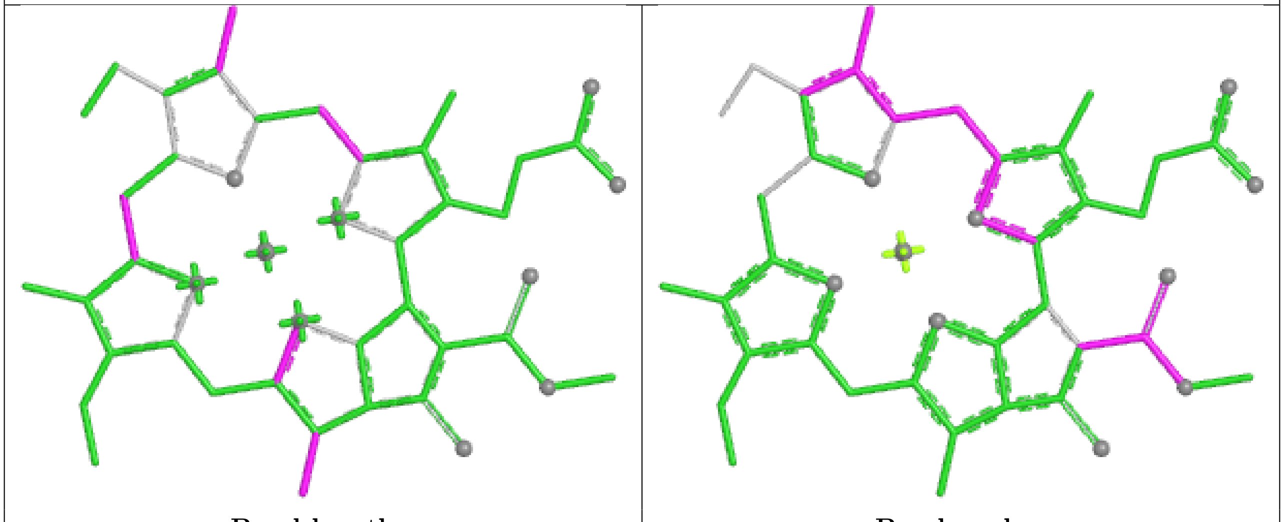
Bond angles



Torsions

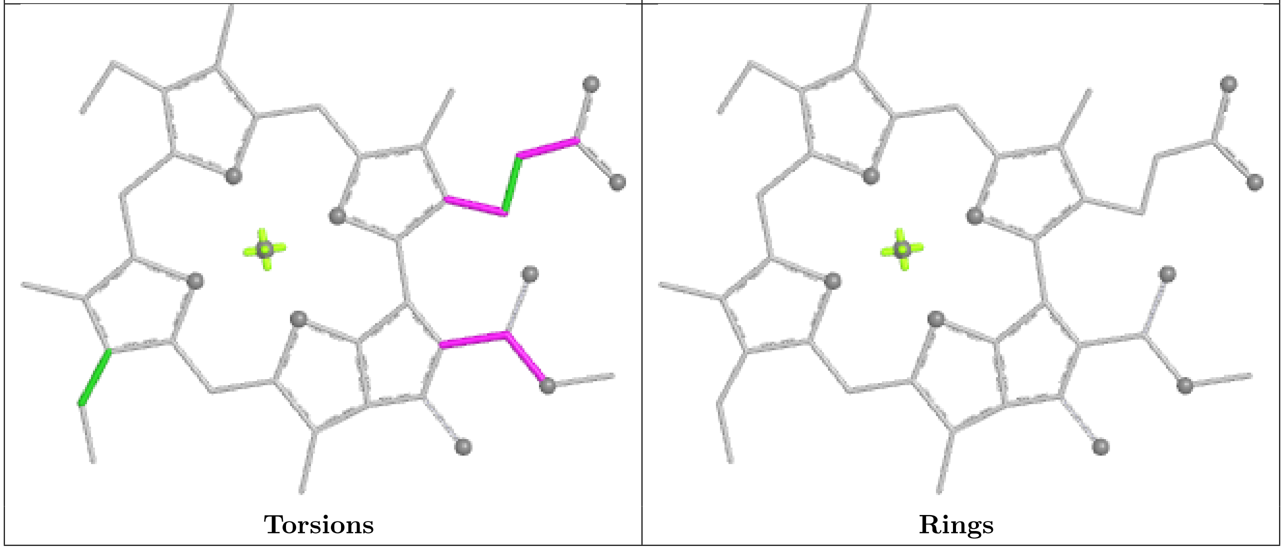
Rings

Ligand CLA S 103



Bond lengths

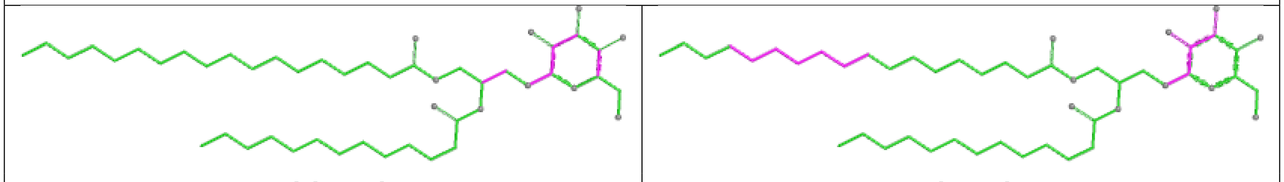
Bond angles



Torsions

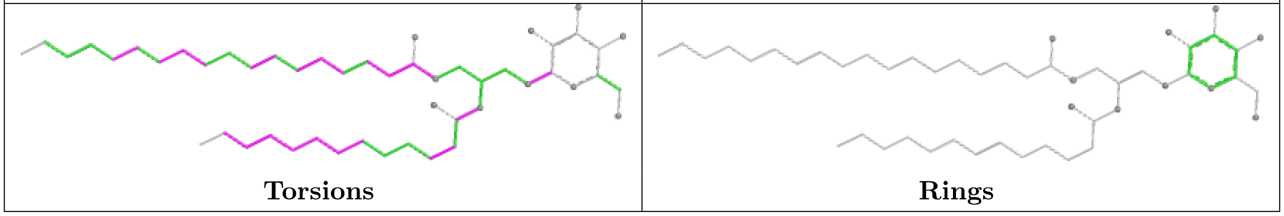
Rings

Ligand LMG a 847



Bond lengths

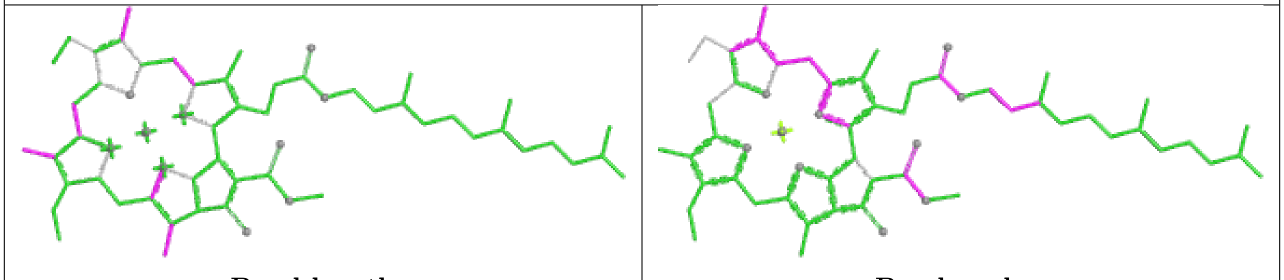
Bond angles



Torsions

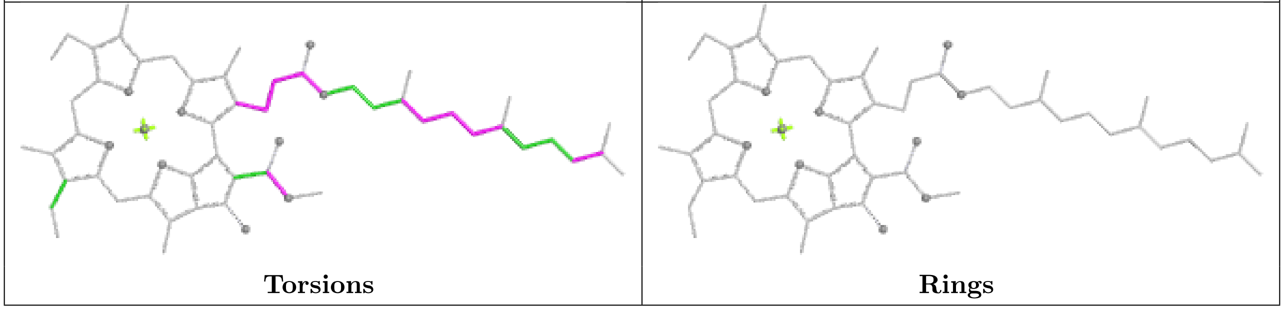
Rings

Ligand CLA A 817



Bond lengths

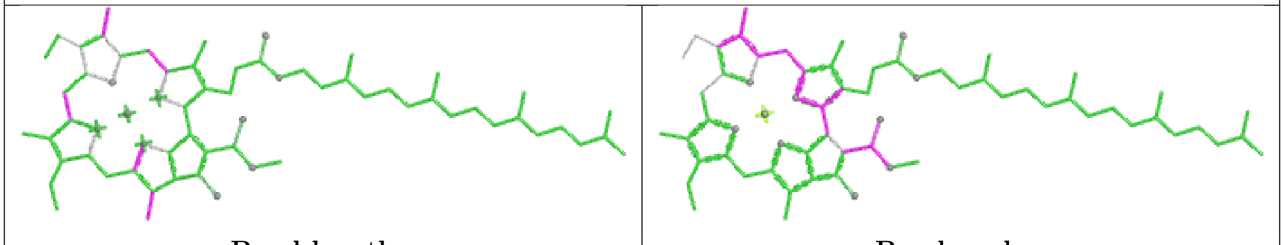
Bond angles



Torsions

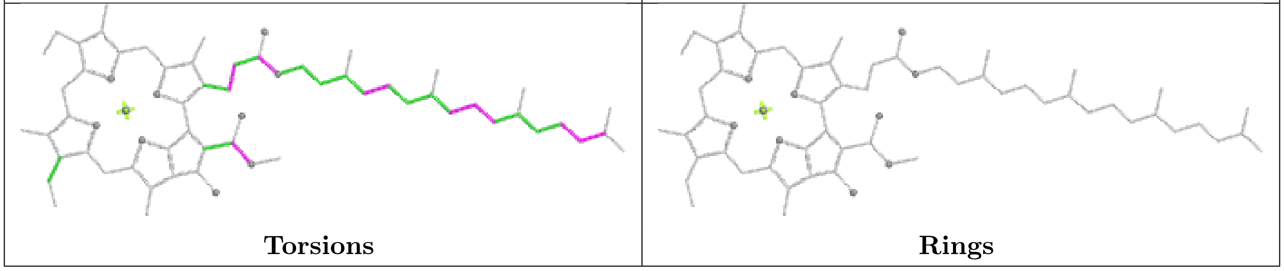
Rings

Ligand CLA G 837



Bond lengths

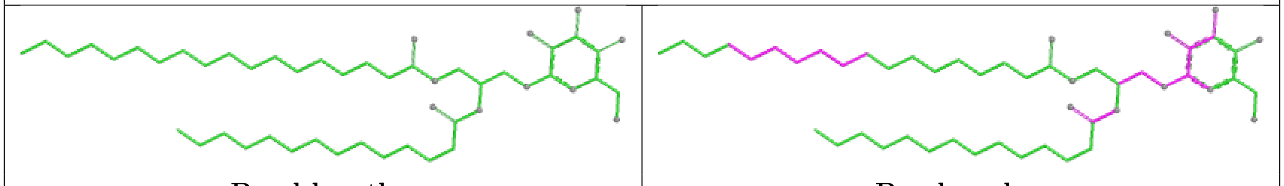
Bond angles



Torsions

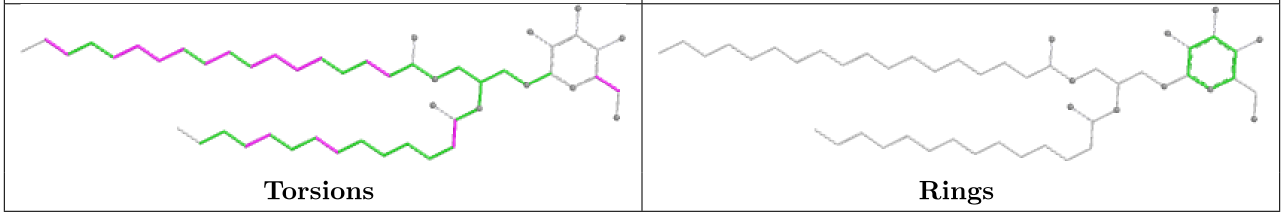
Rings

Ligand LMG B 2148



Bond lengths

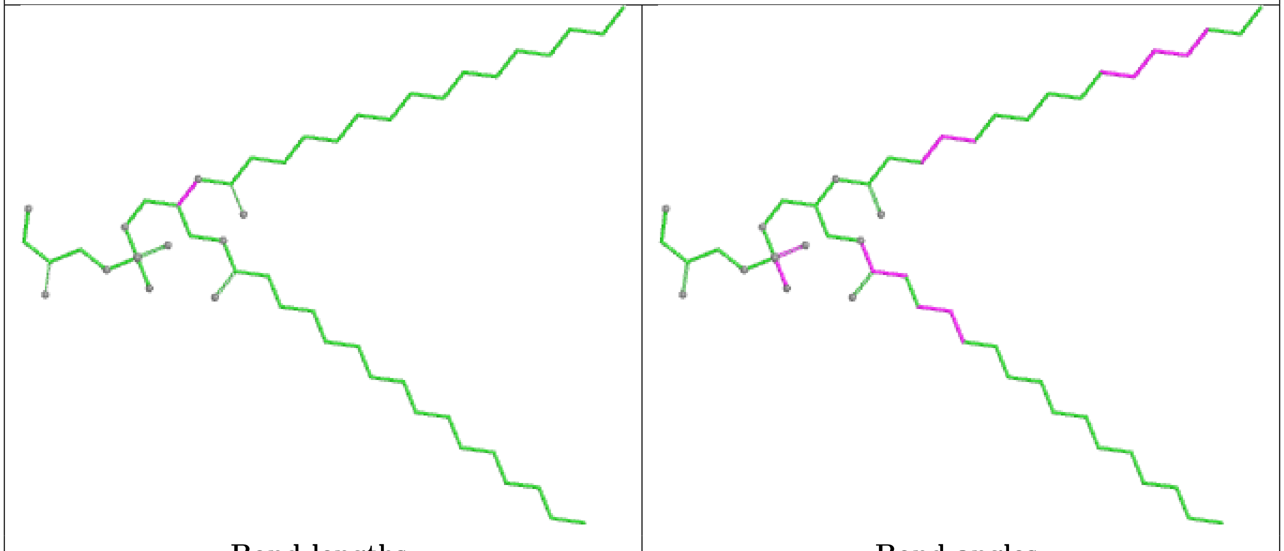
Bond angles



Torsions

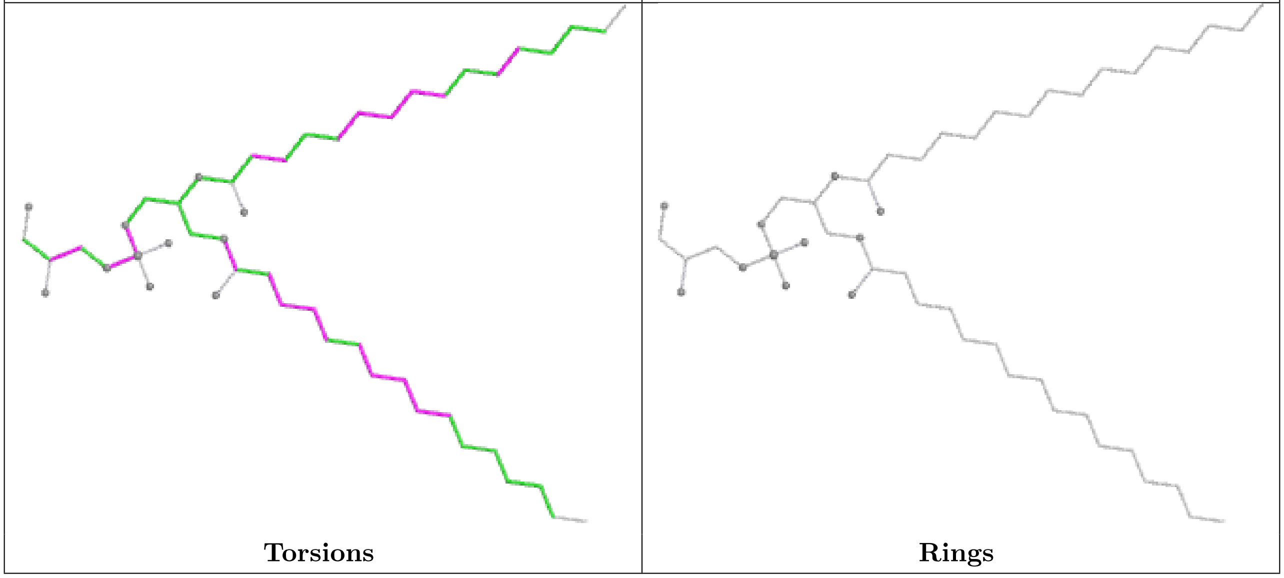
Rings

Ligand LHG a 848



Bond lengths

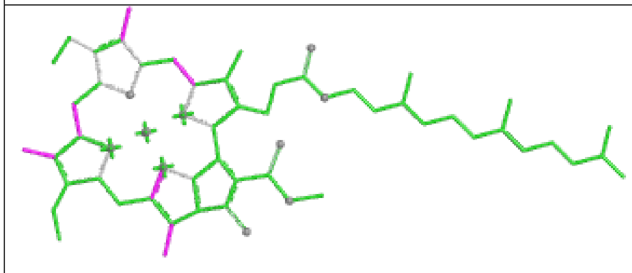
Bond angles



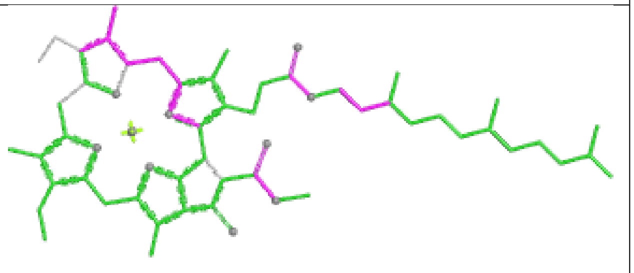
Torsions

Rings

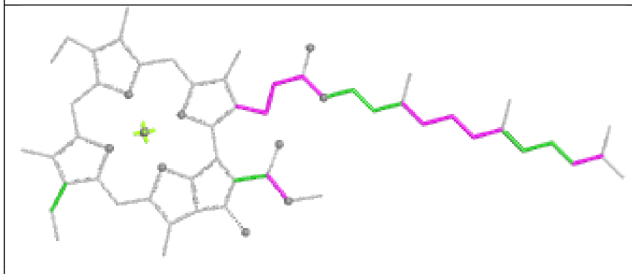
Ligand CLA G 817



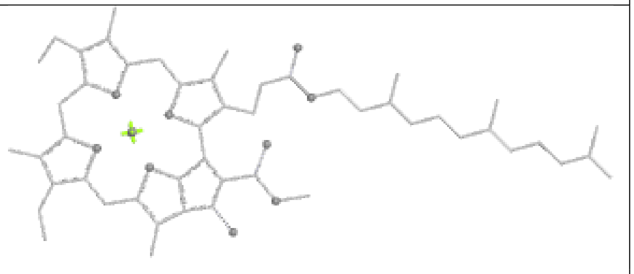
Bond lengths



Bond angles

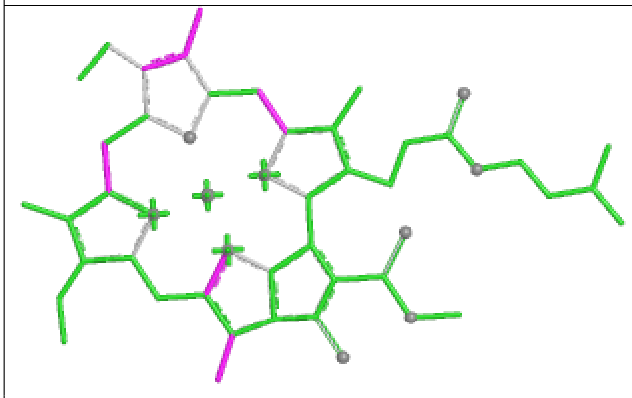


Torsions

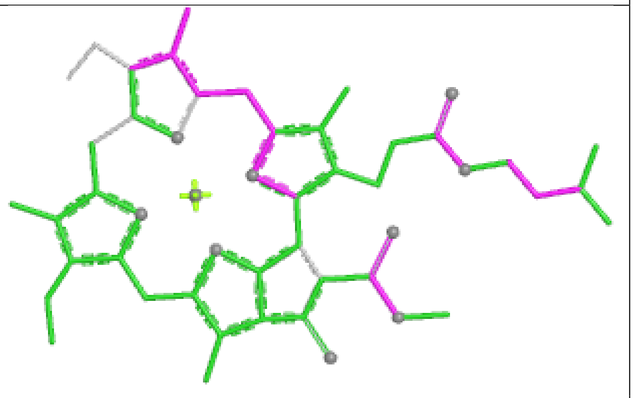


Rings

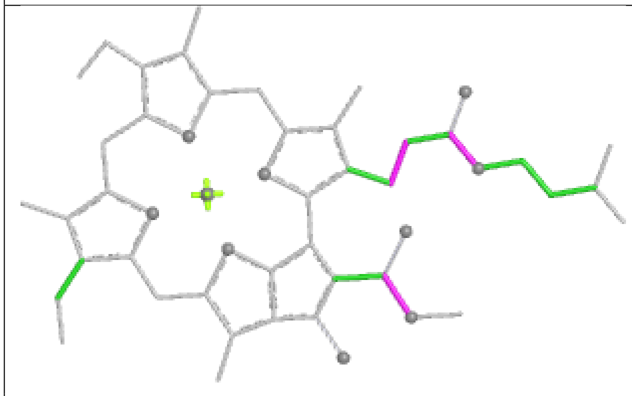
Ligand CLA B 2119



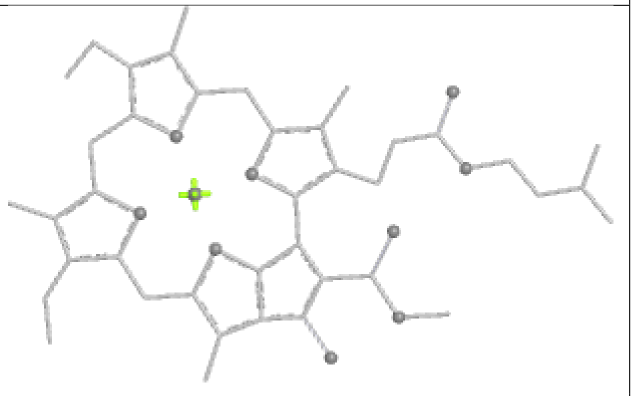
Bond lengths



Bond angles

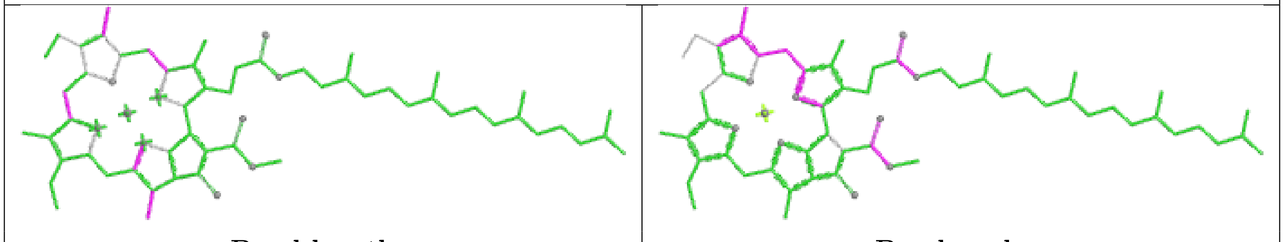


Torsions

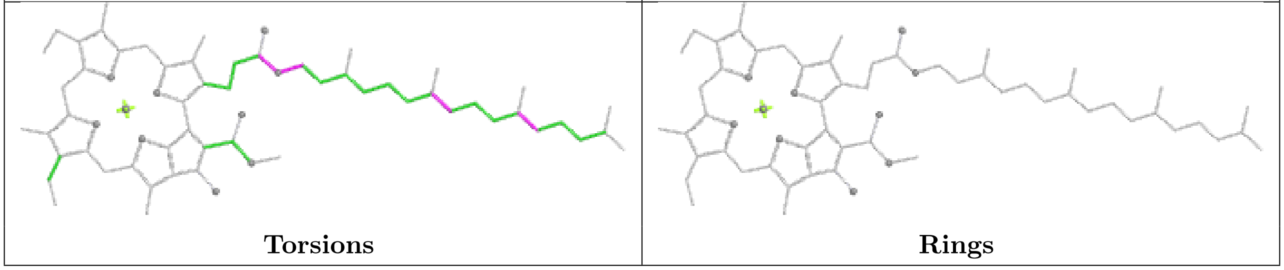


Rings

Ligand CLA H 2137

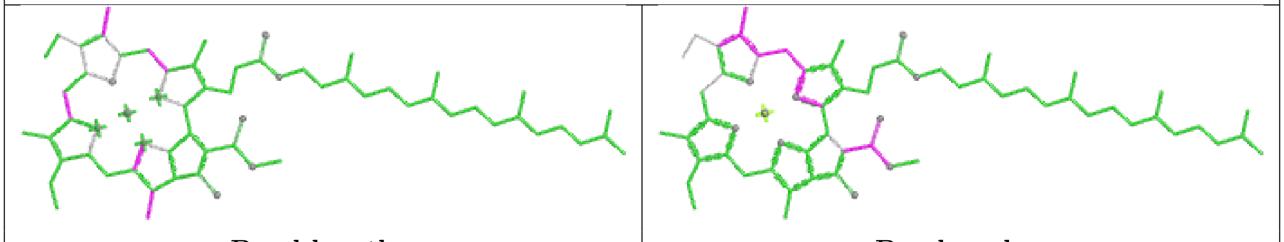


Bond lengths Bond angles

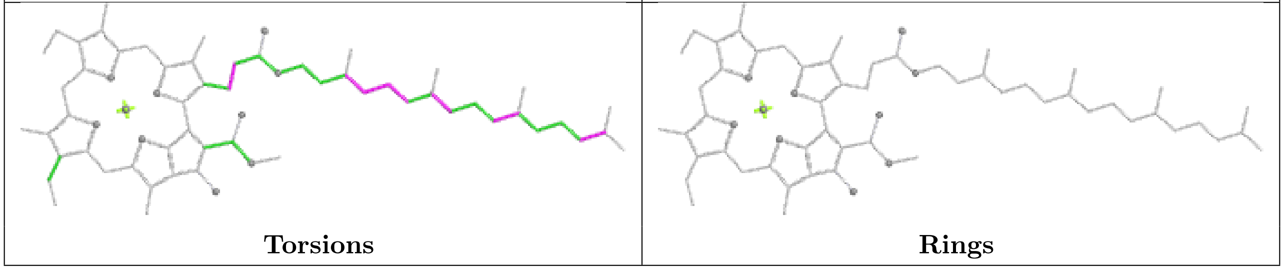


Torsions Rings

Ligand CLA H 2108

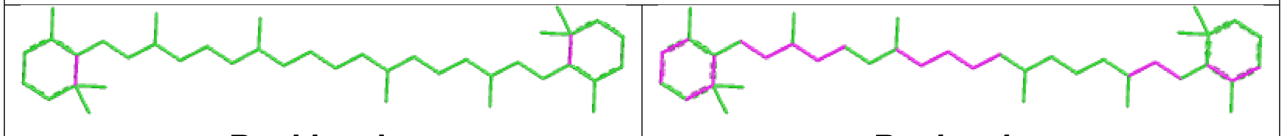


Bond lengths Bond angles

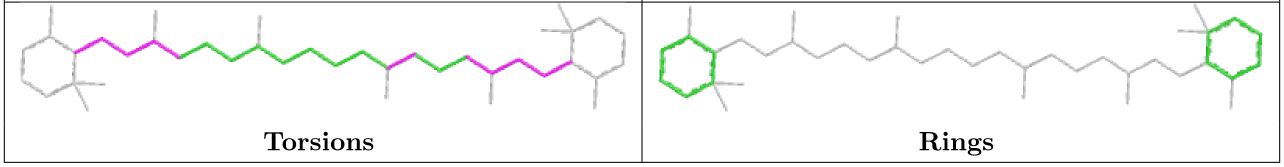


Torsions Rings

Ligand BCR J 101

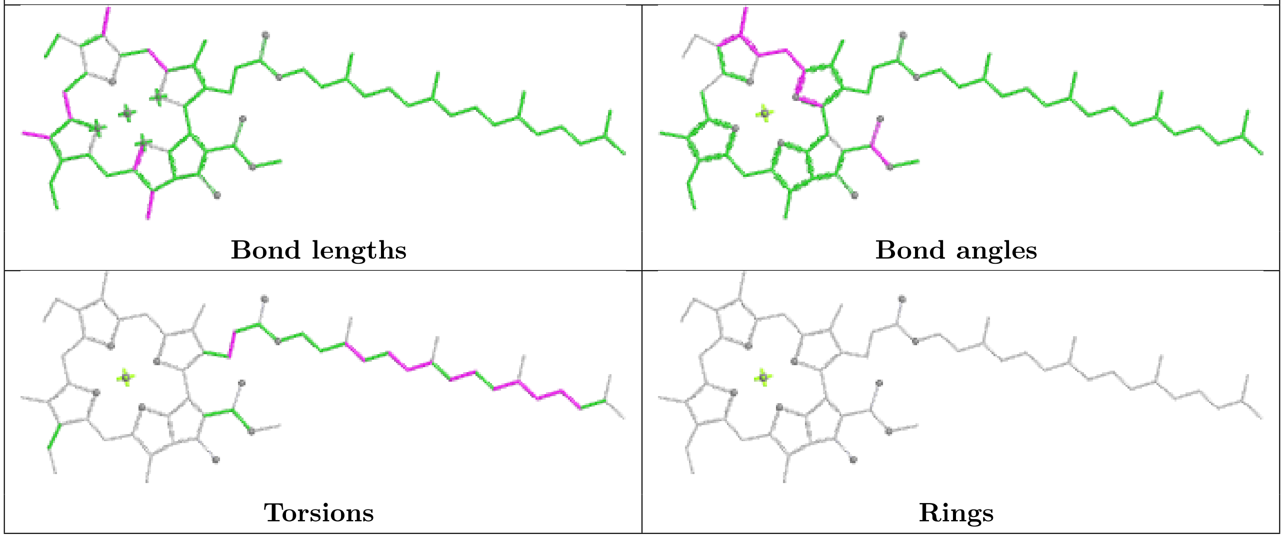


Bond lengths Bond angles



Torsions Rings

Ligand CLA a 836



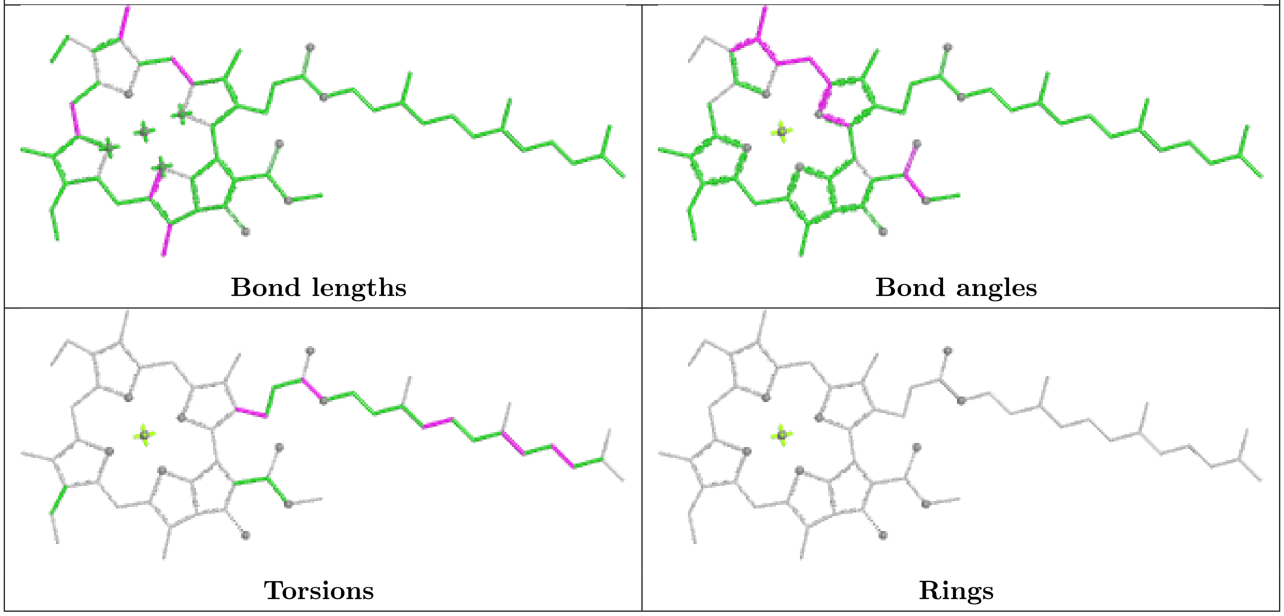
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 821



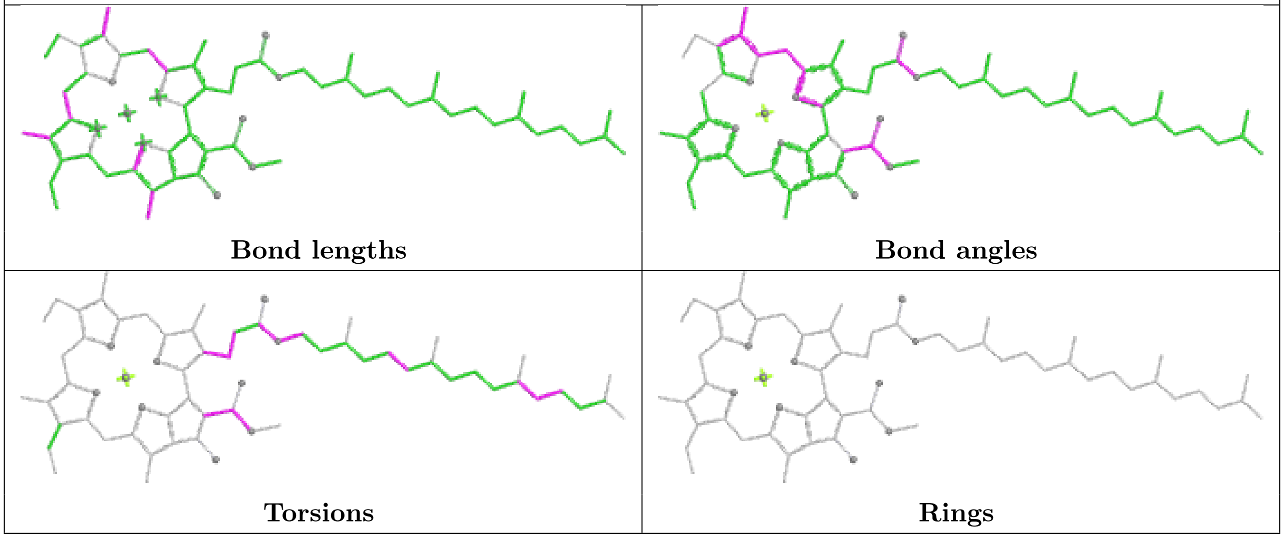
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA U 201



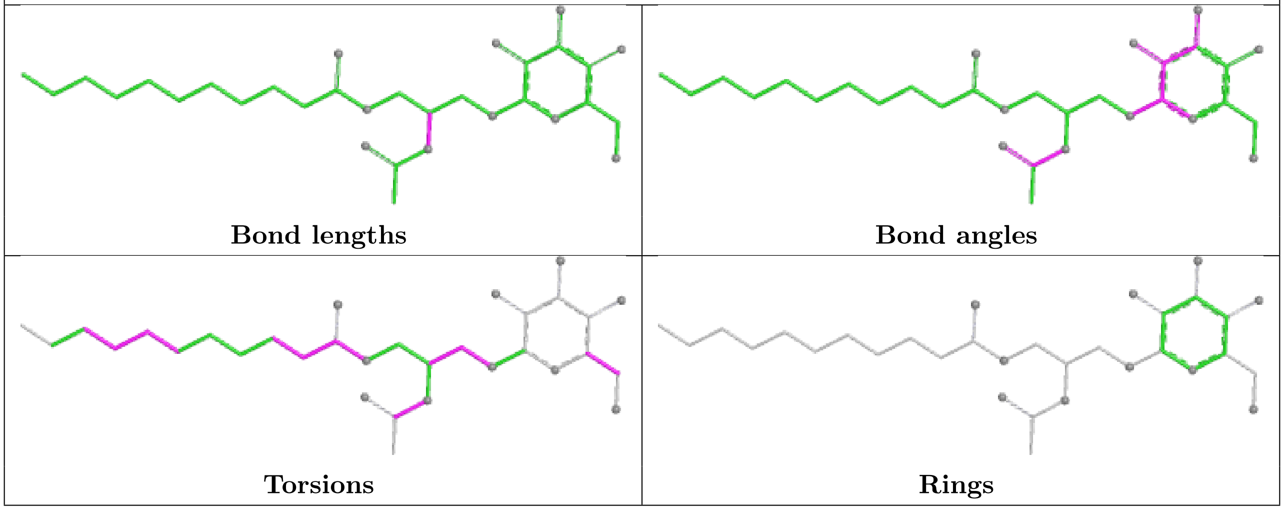
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG A 849

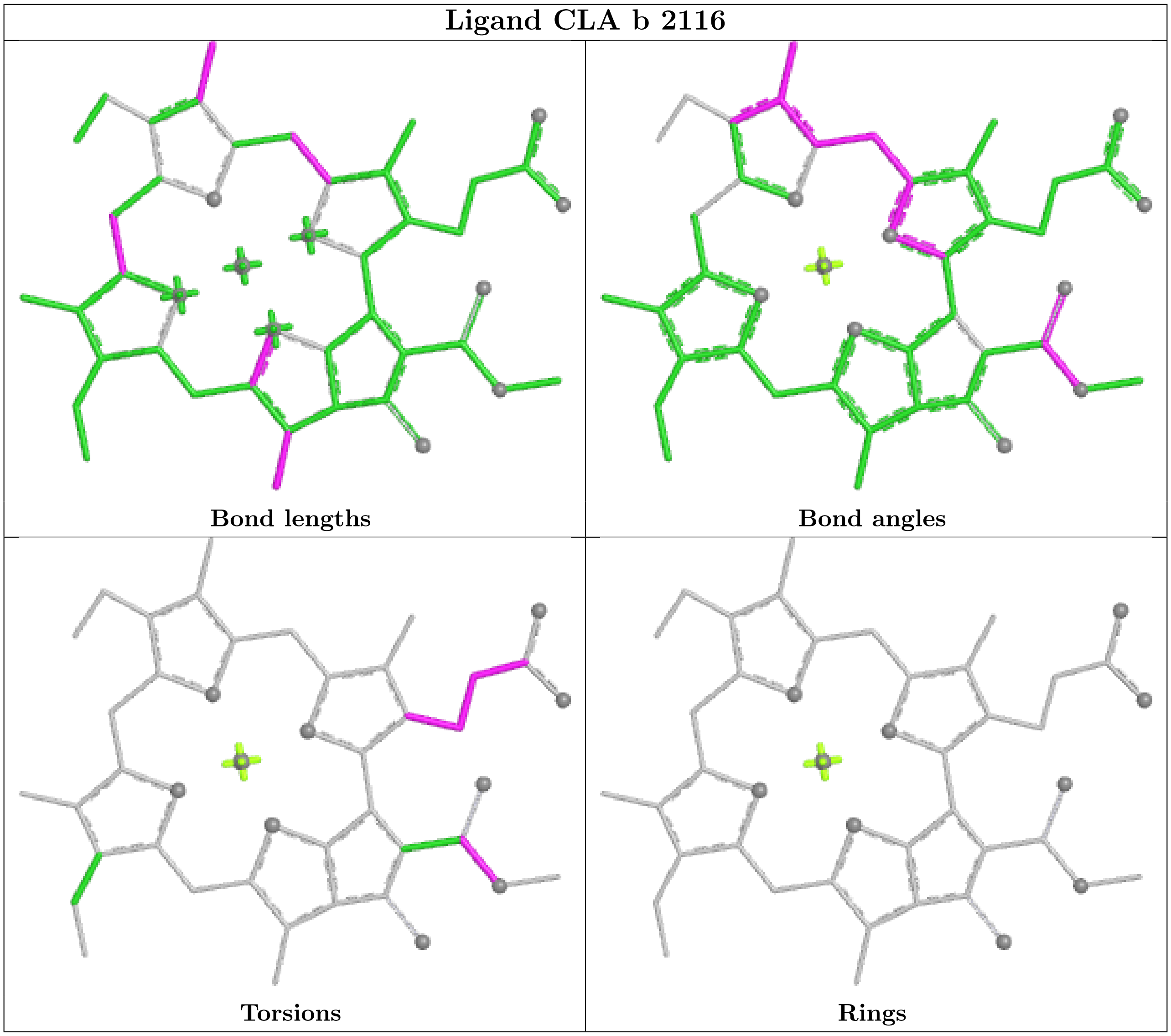


Bond lengths

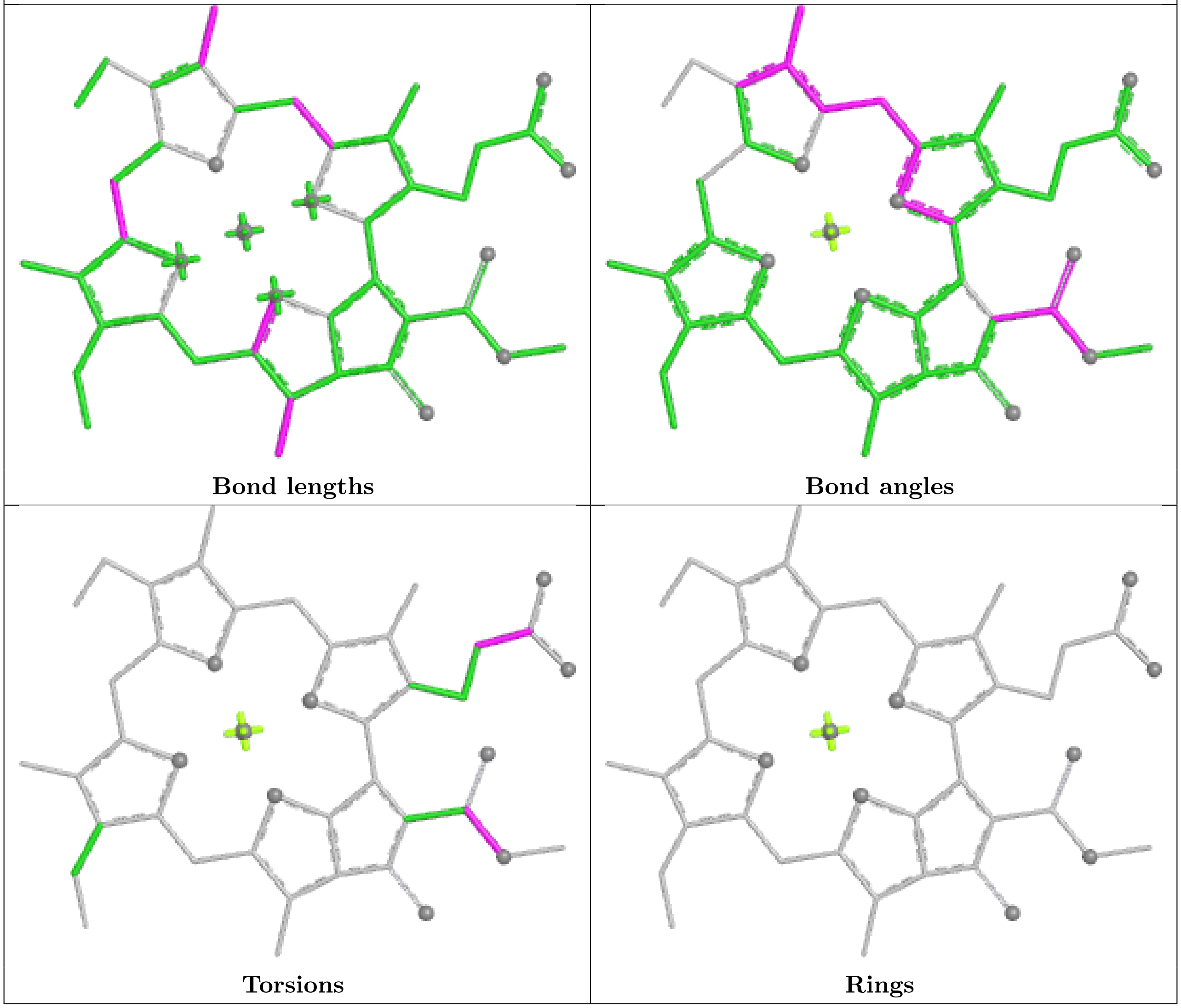
Bond angles

Torsions

Rings


Ligand CLA b 2116

Ligand CLA B 2139



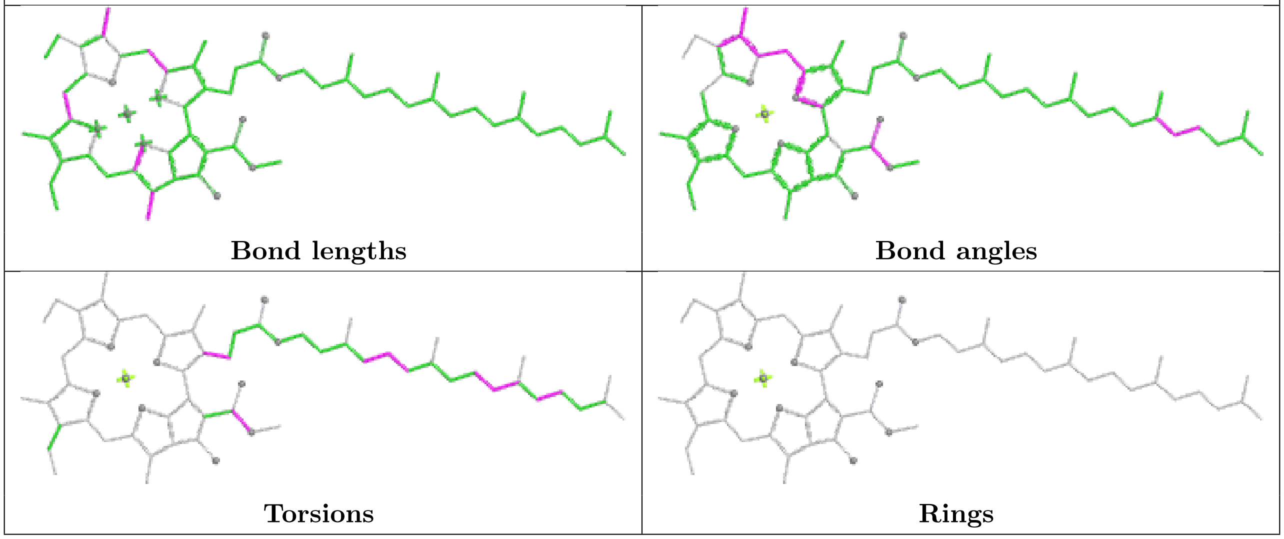
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 839



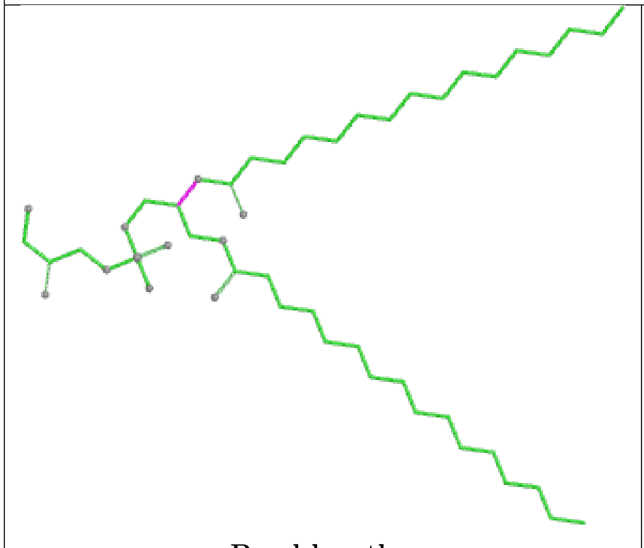
Bond lengths

Bond angles

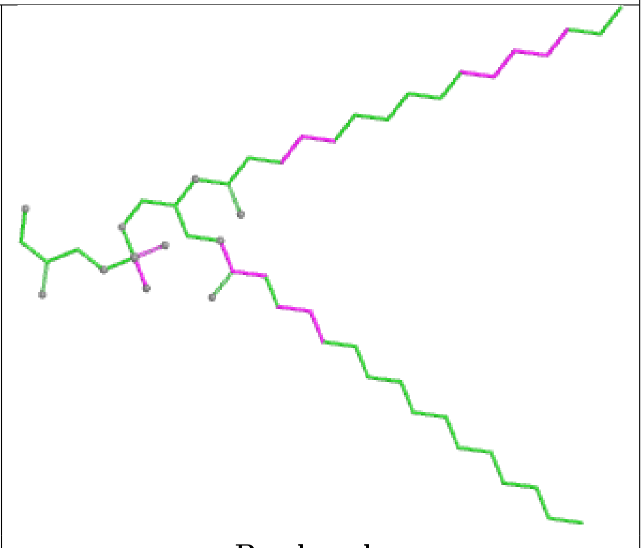
Torsions

Rings

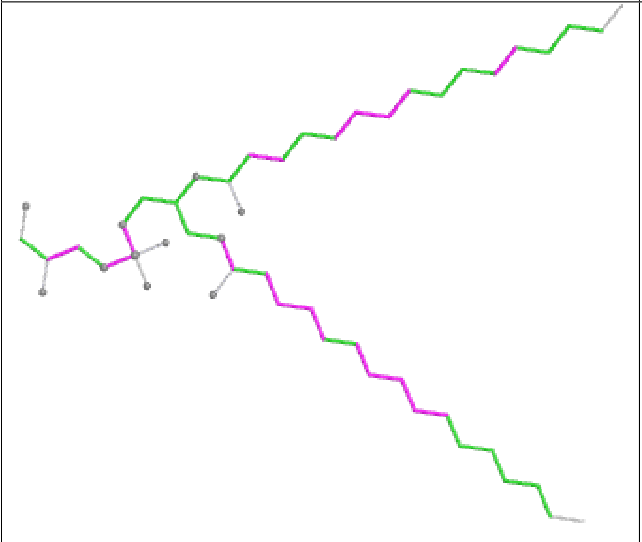
Ligand LHG G 848



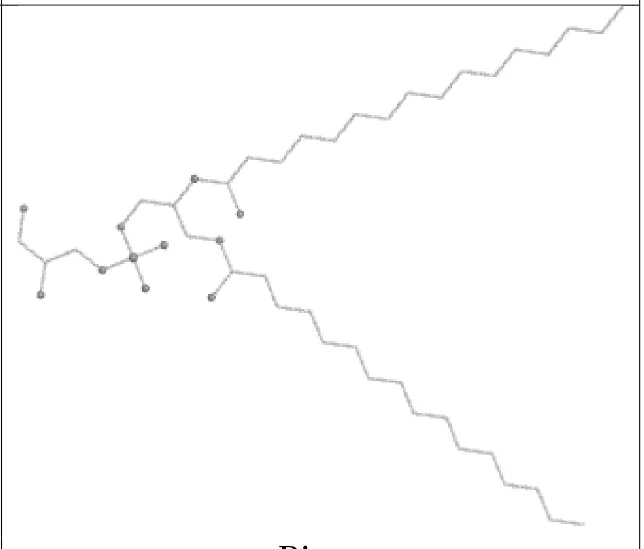
Bond lengths



Bond angles

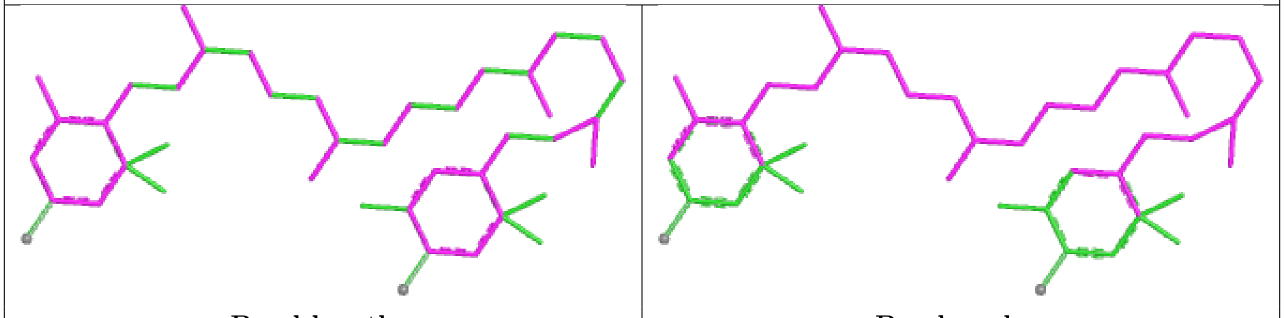


Torsions



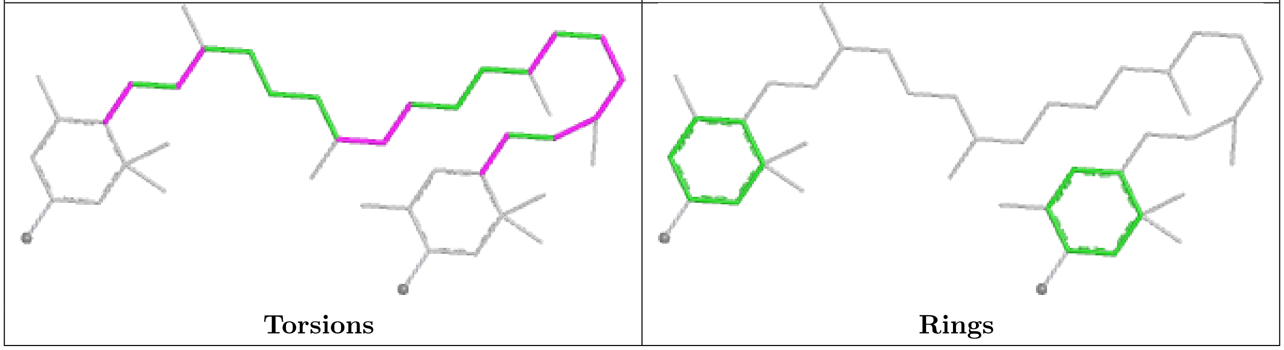
Rings

Ligand ZEX f 205



Bond lengths

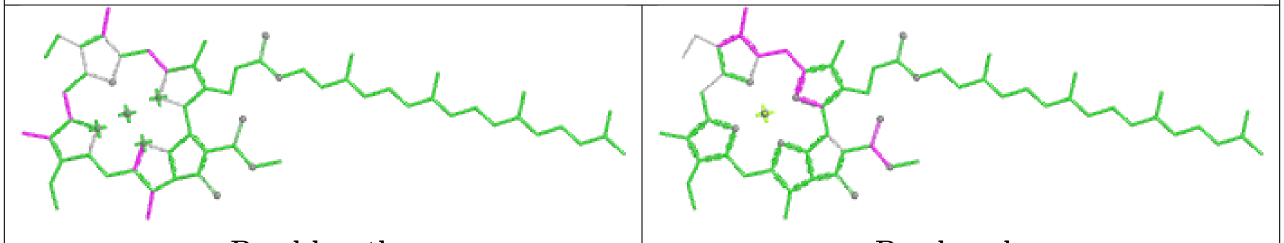
Bond angles



Torsions

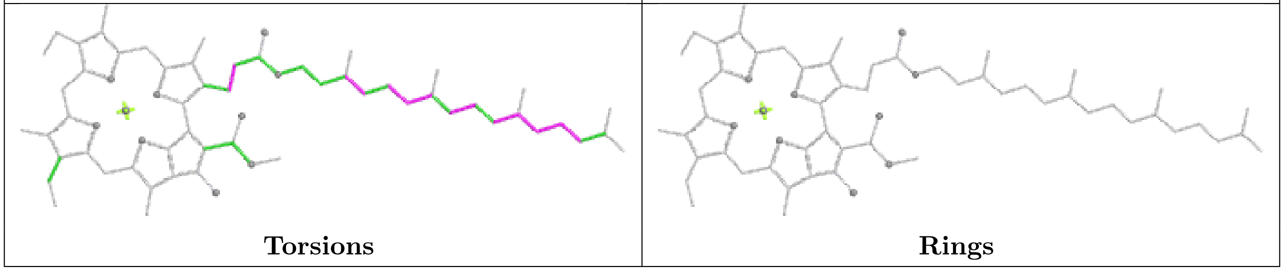
Rings

Ligand CLA G 836



Bond lengths

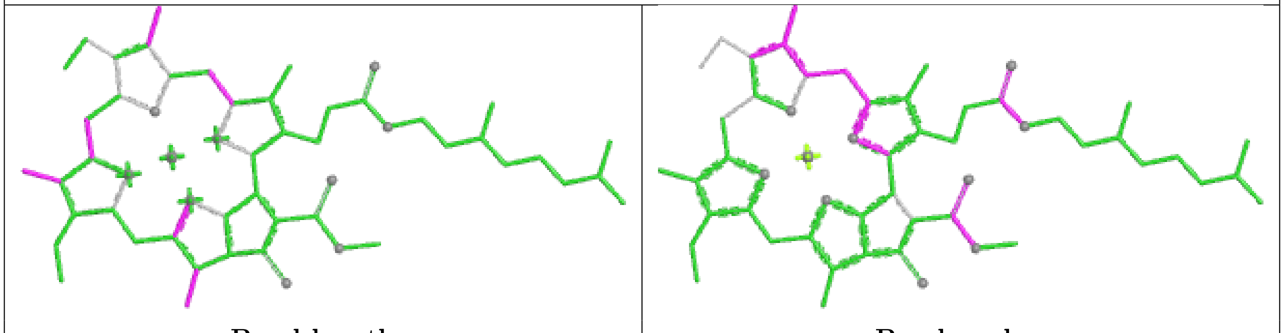
Bond angles



Torsions

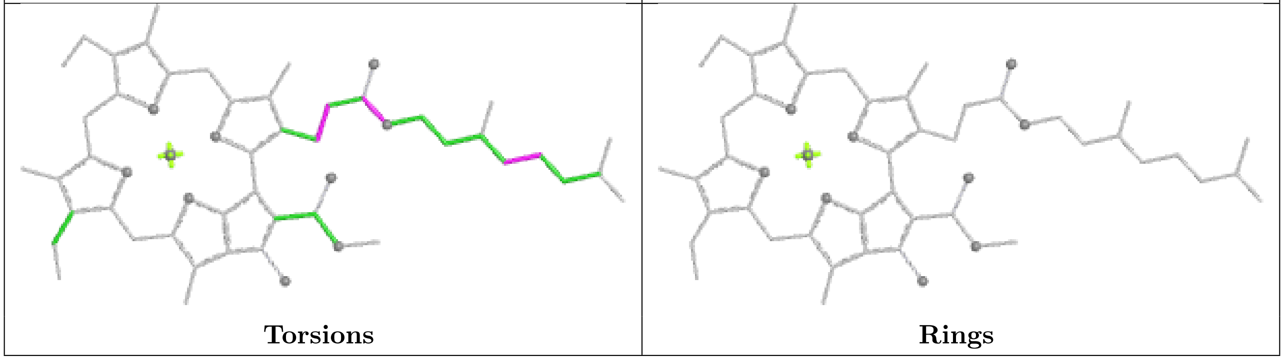
Rings

Ligand CLA A 816



Bond lengths

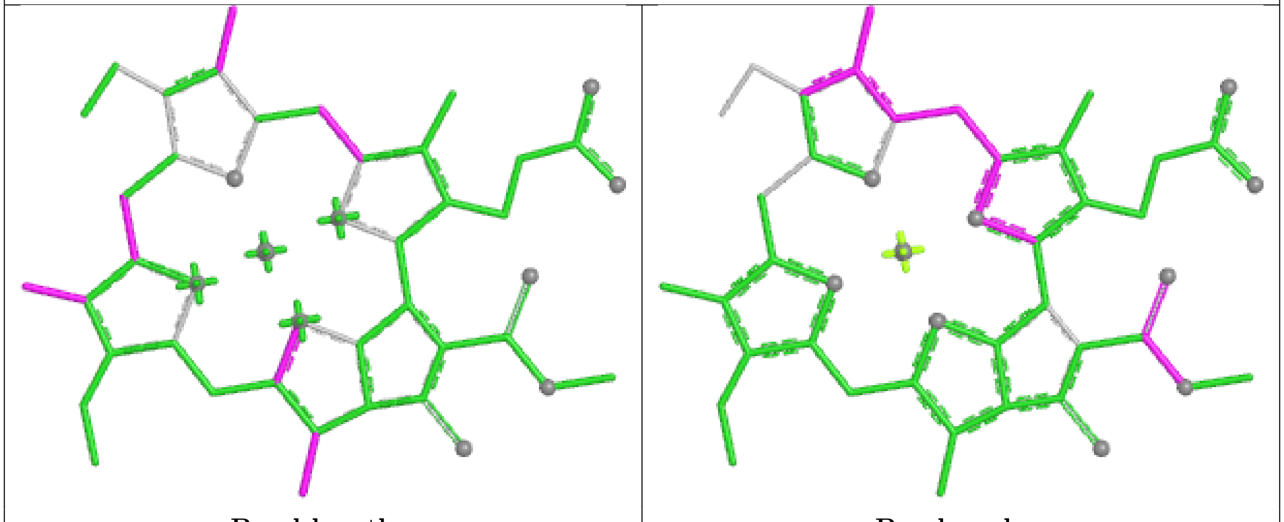
Bond angles



Torsions

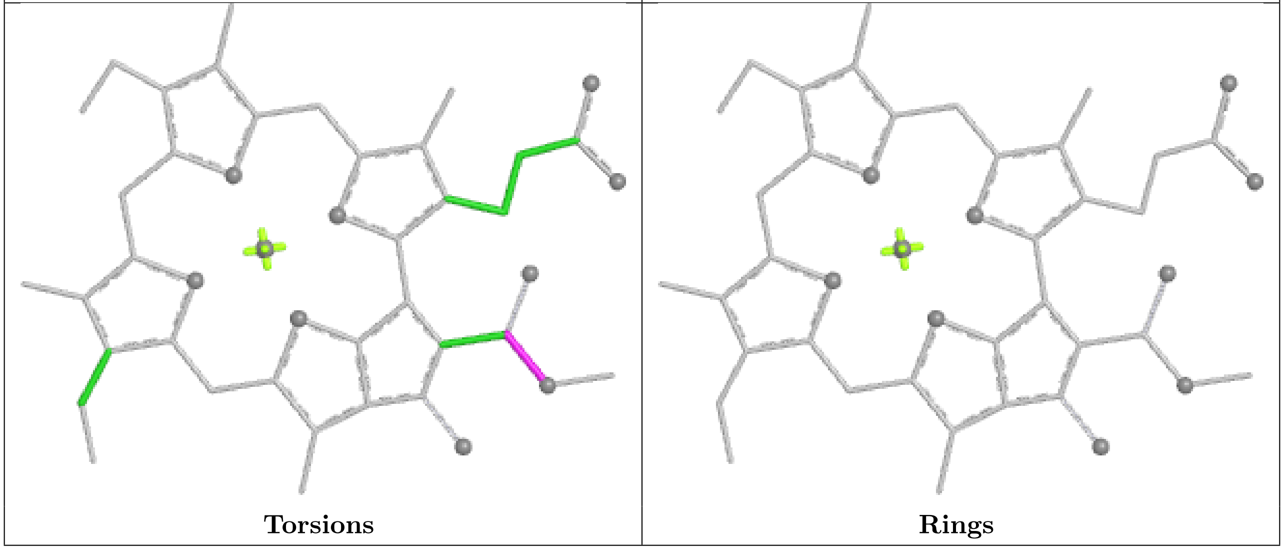
Rings

Ligand CLA B 2116



Bond lengths

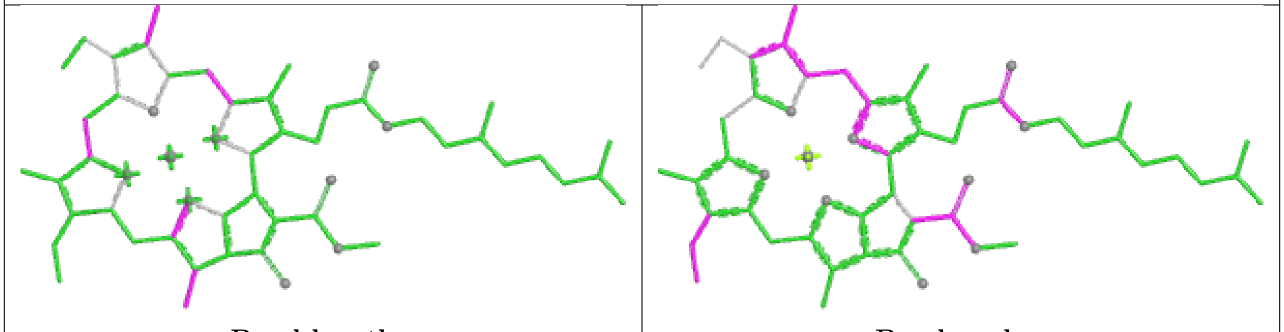
Bond angles



Torsions

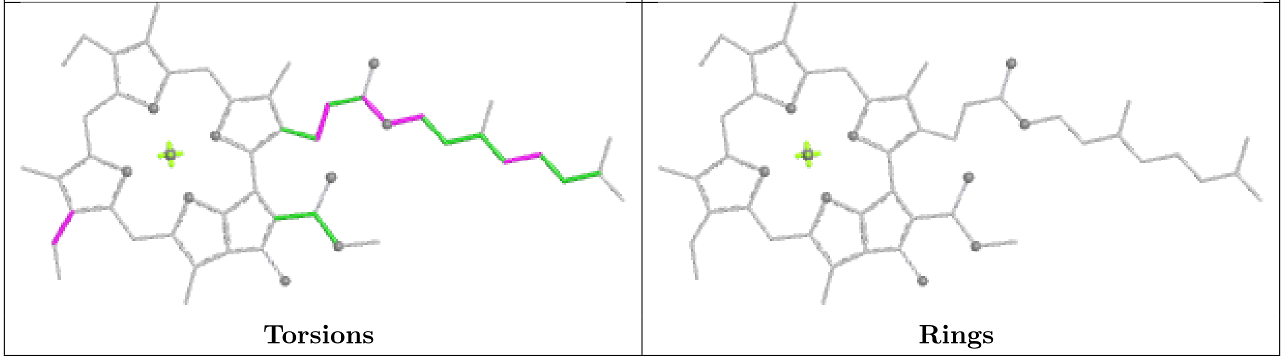
Rings

Ligand CLA A 830



Bond lengths

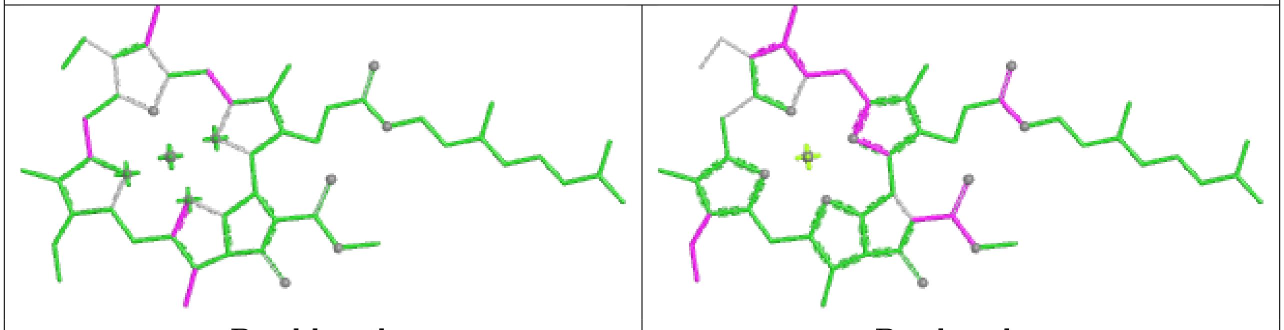
Bond angles



Torsions

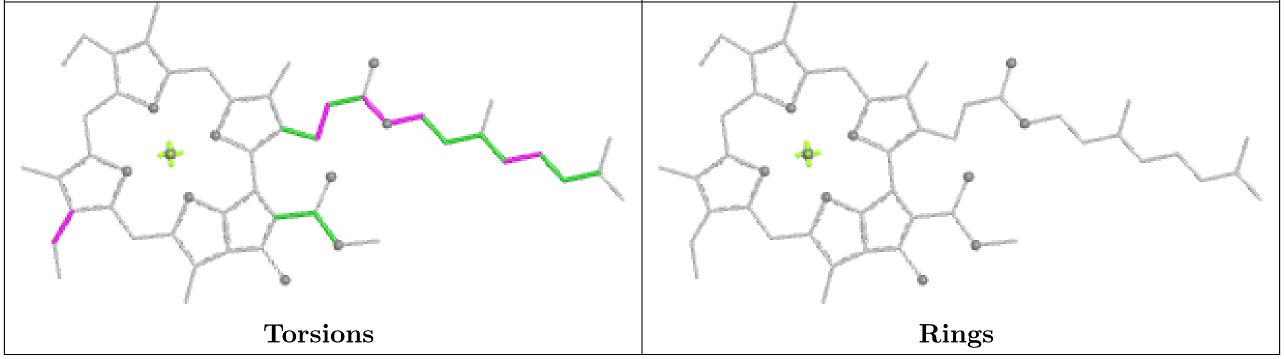
Rings

Ligand CLA a 830



Bond lengths

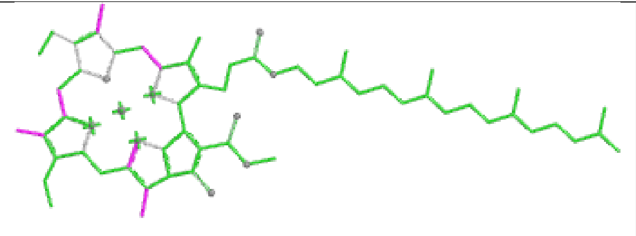
Bond angles



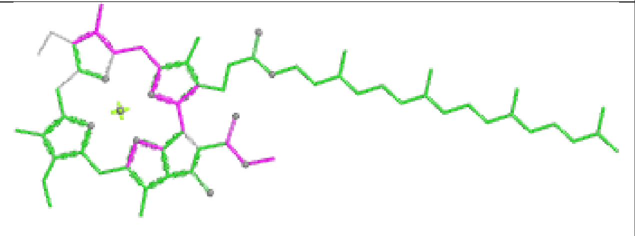
Torsions

Rings

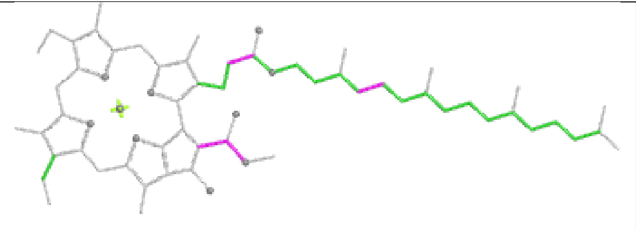
Ligand CLA G 801



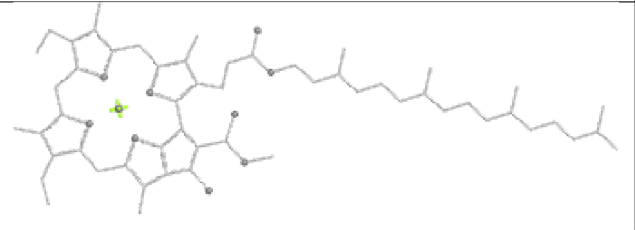
Bond lengths



Bond angles

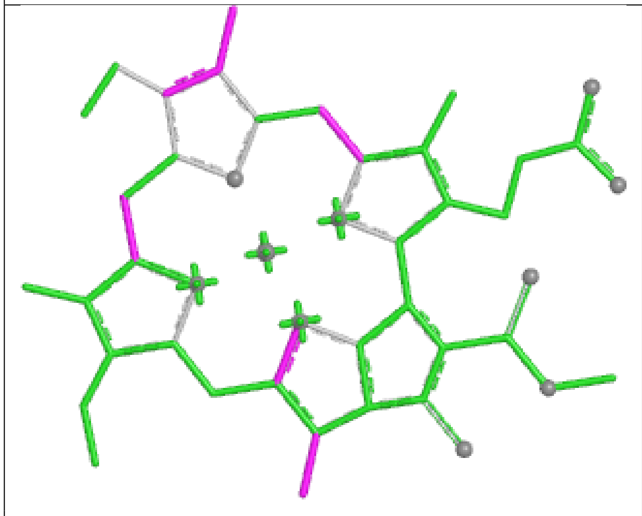


Torsions

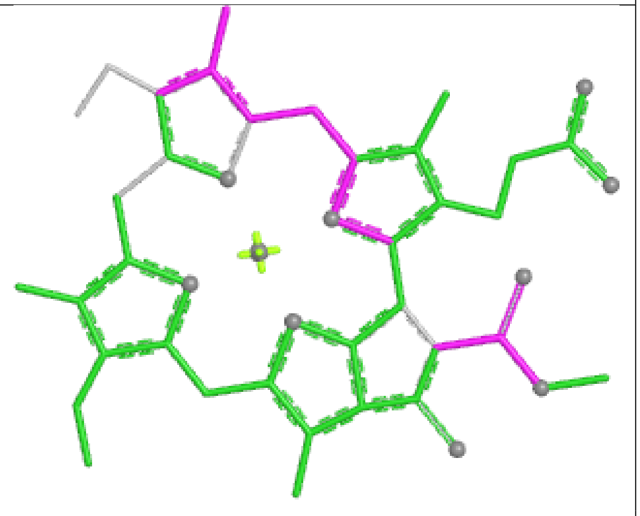


Rings

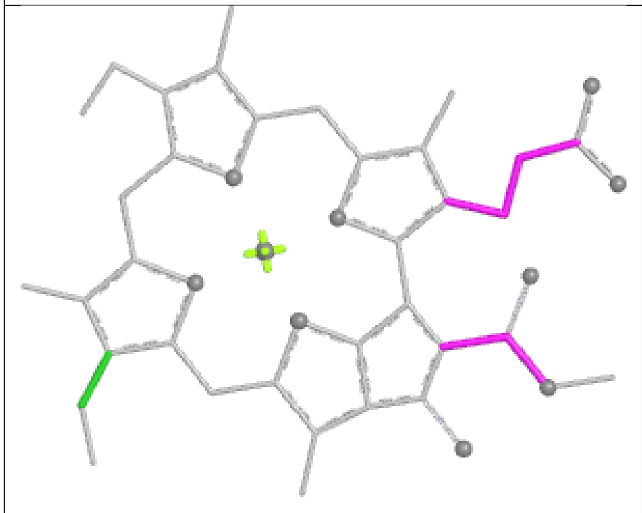
Ligand CLA B 2114



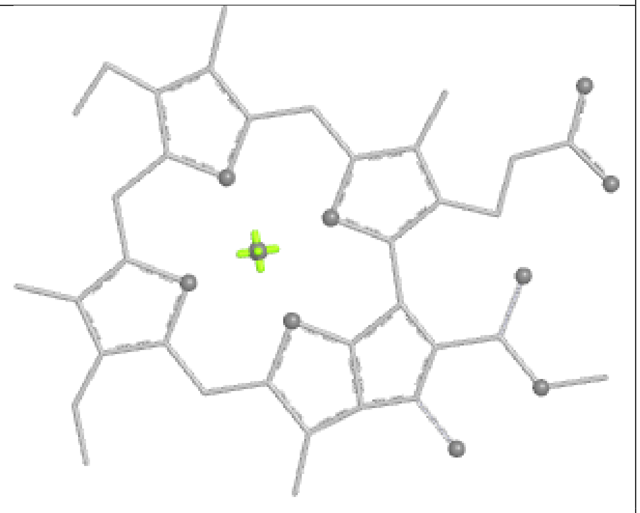
Bond lengths



Bond angles

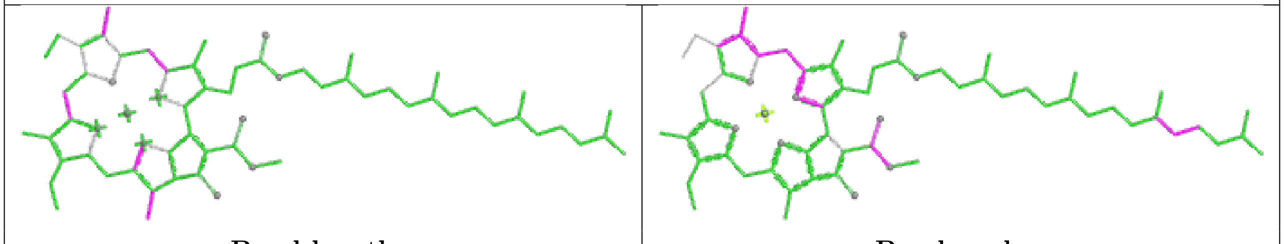


Torsions



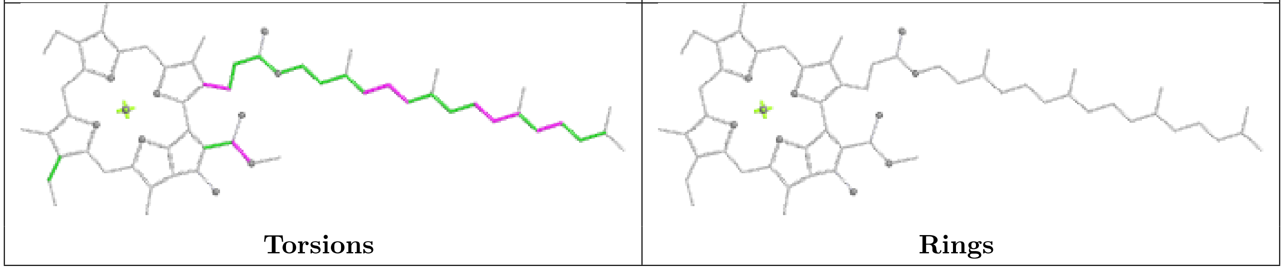
Rings

Ligand CLA G 839



Bond lengths

Bond angles



Torsions

Rings

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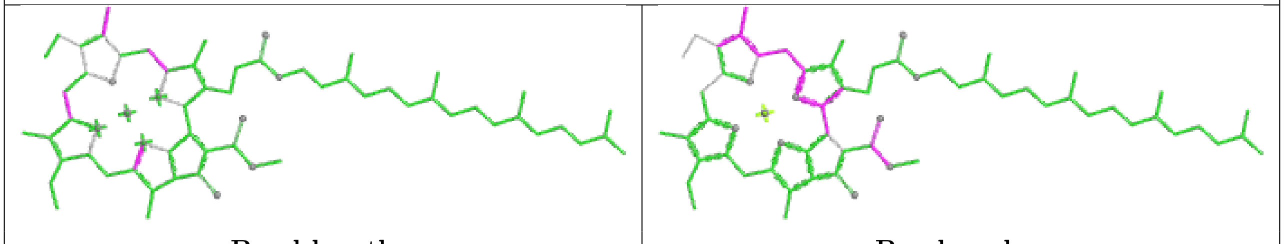
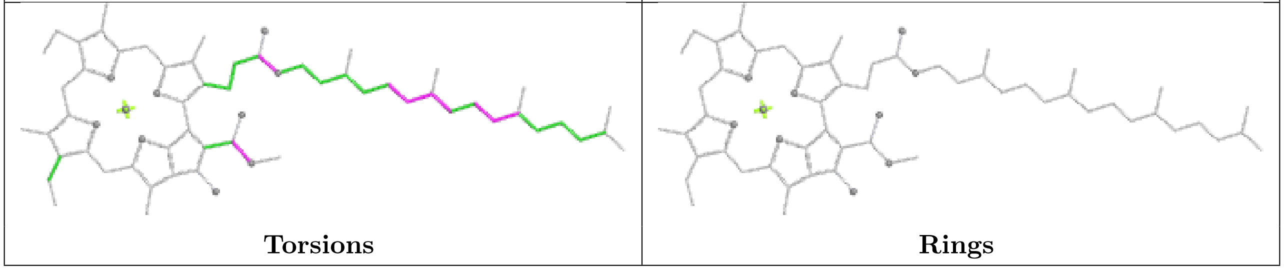


Bond lengths

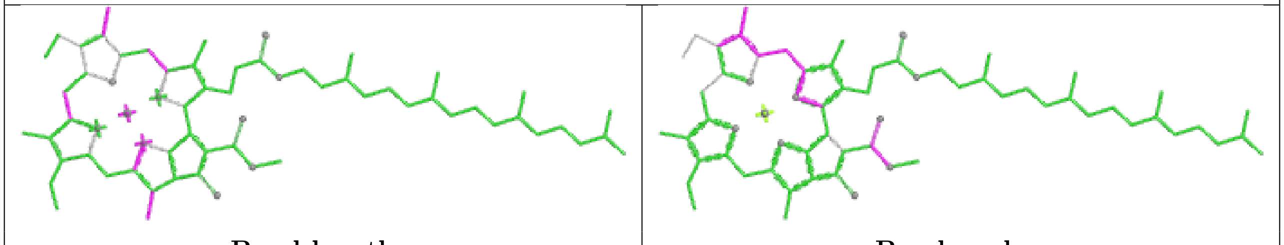
Bond angles



Torsions

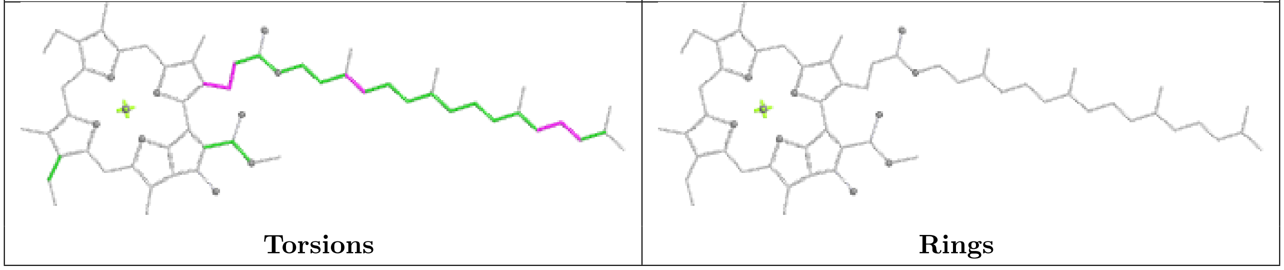
Rings

Ligand CLA A 850



Bond lengths

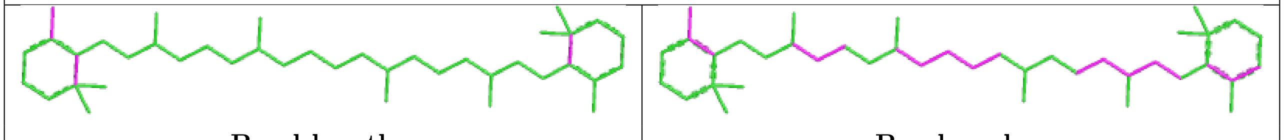
Bond angles



Torsions

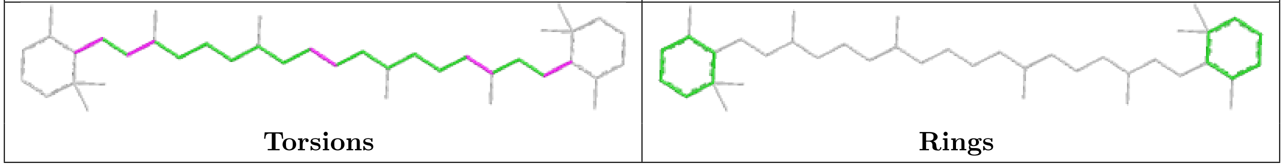
Rings

Ligand BCR j 104



Bond lengths

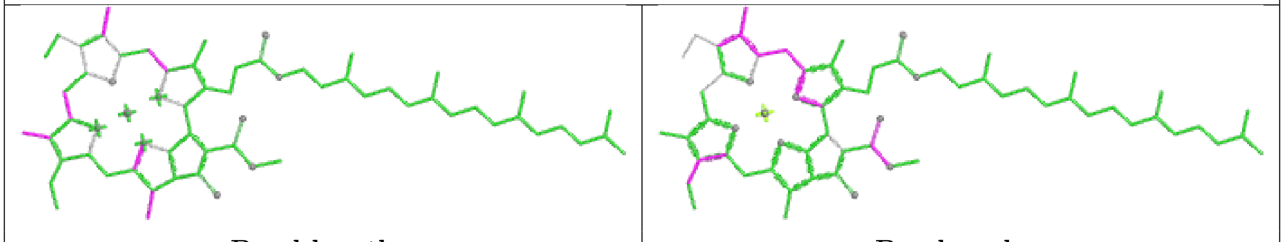
Bond angles



Torsions

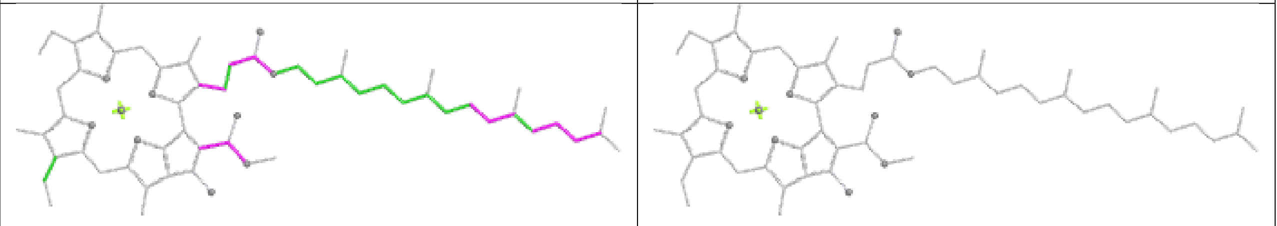
Rings

Ligand CLA a 804



Bond lengths

Bond angles



Torsions

Rings

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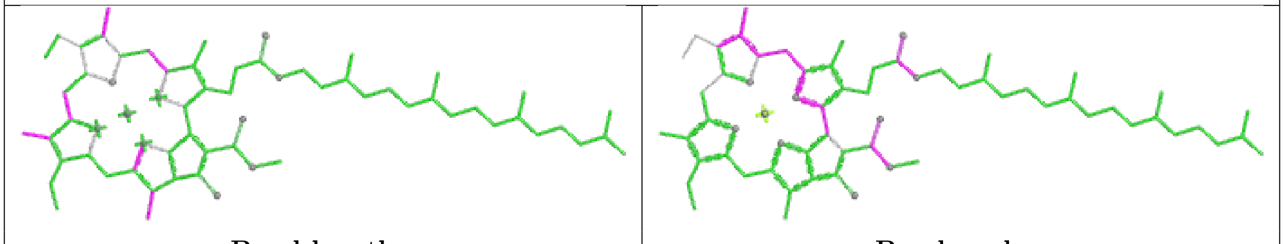
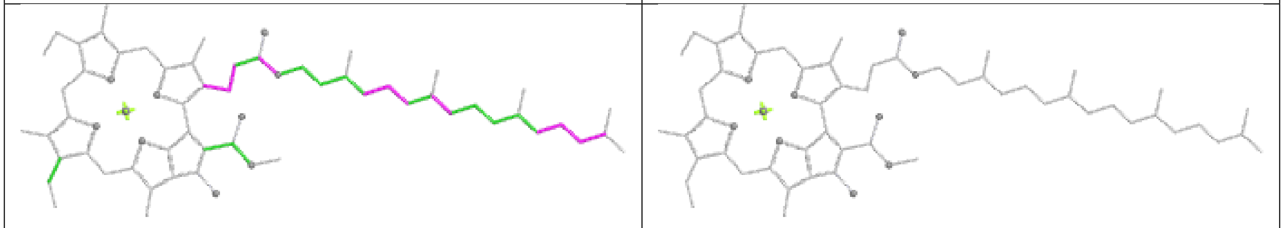


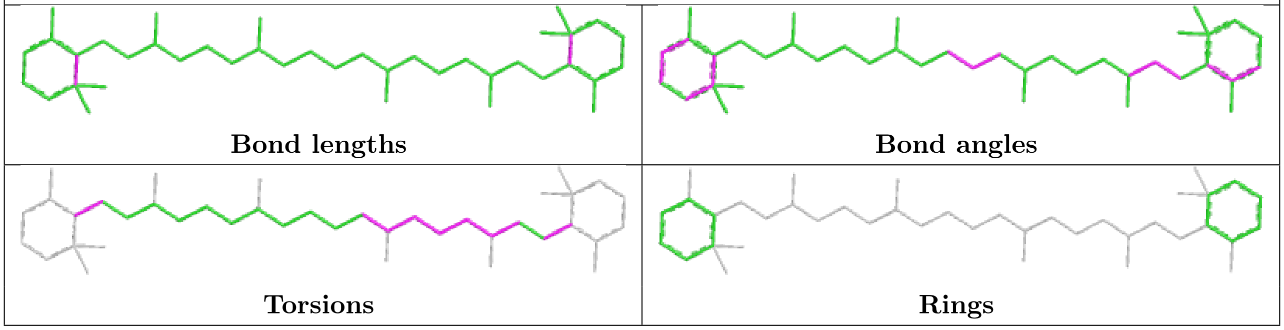
Bond lengths

Bond angles



Torsions

Rings



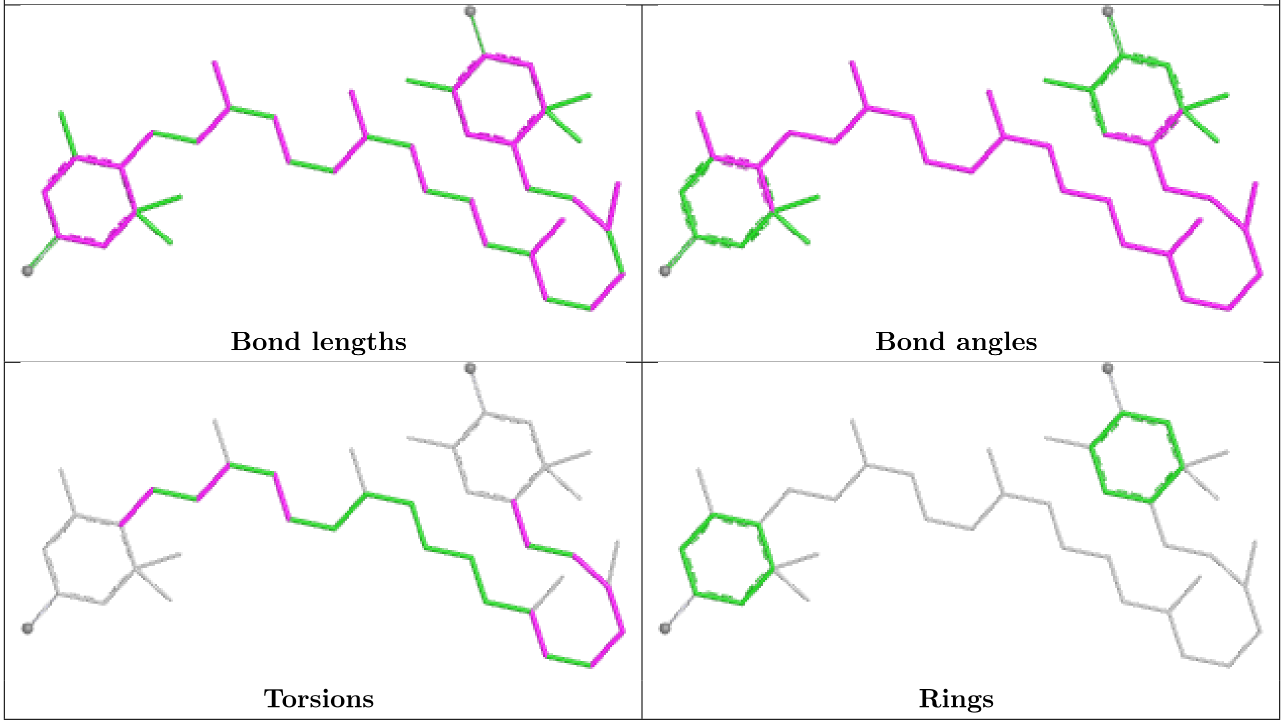
Ligand BCR a 842

Bond lengths

Bond angles

Torsions

Rings



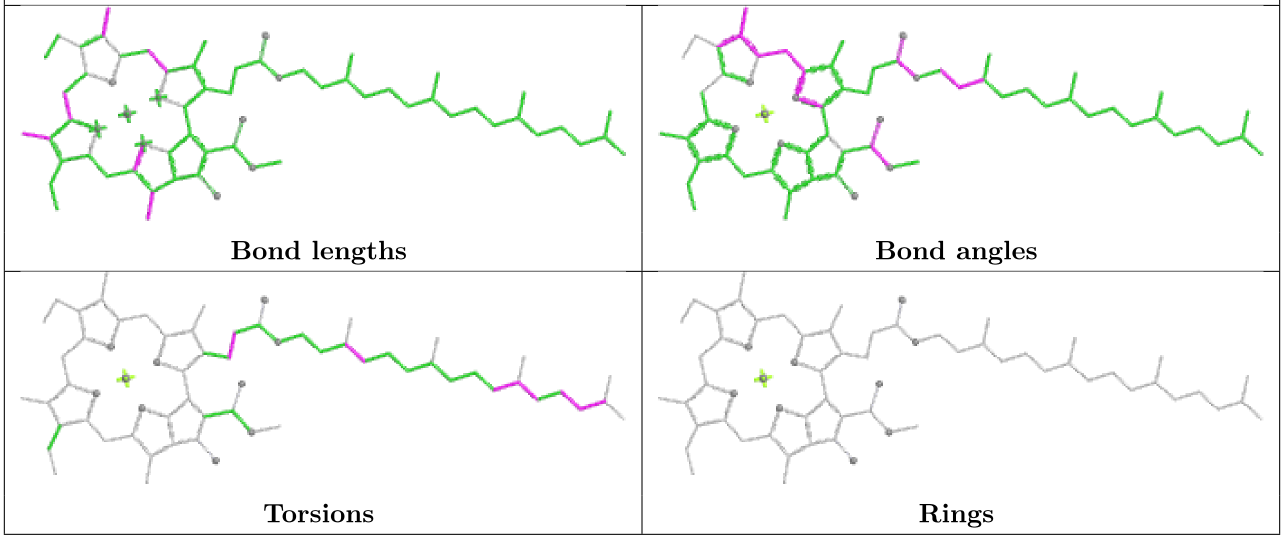
Ligand ZEX B 2152

Bond lengths

Bond angles

Torsions

Rings



Ligand CLA G 818

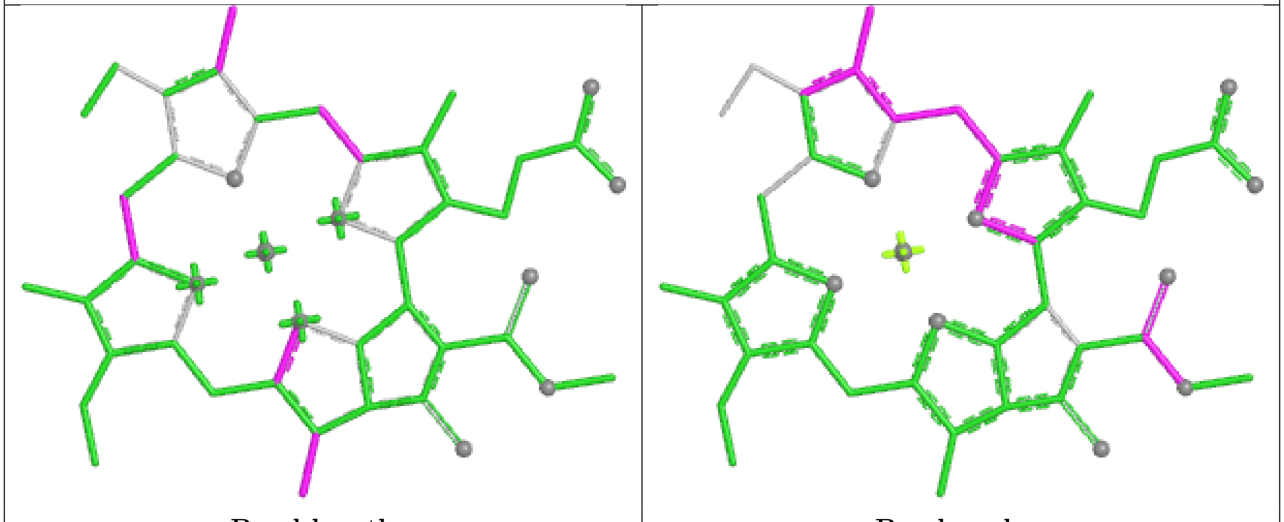
Bond lengths

Bond angles

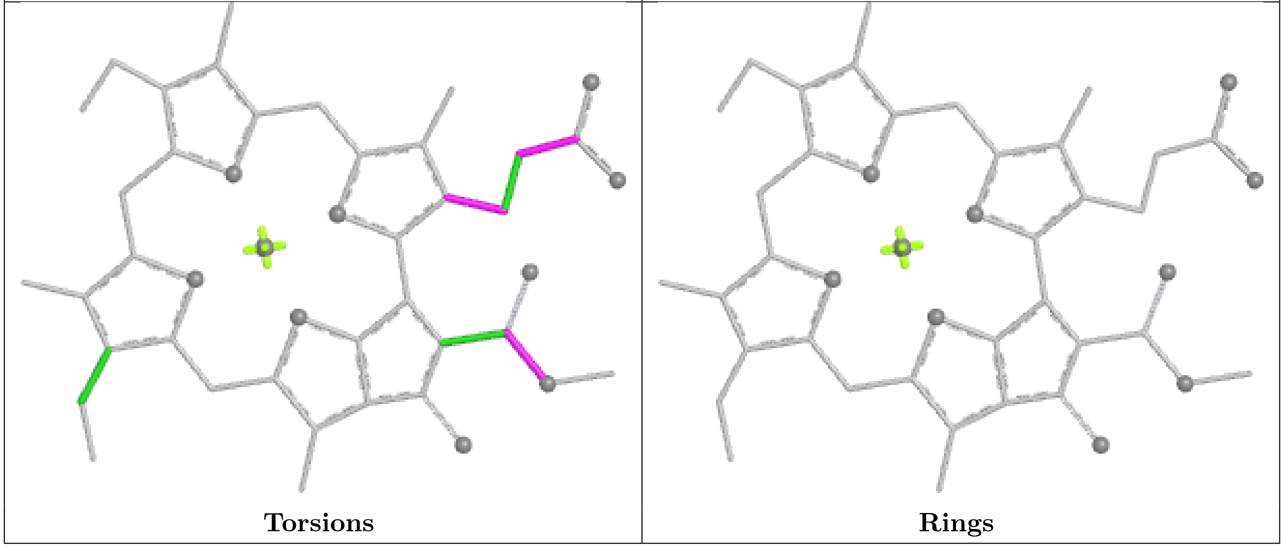
Torsions

Rings

Ligand CLA a 811

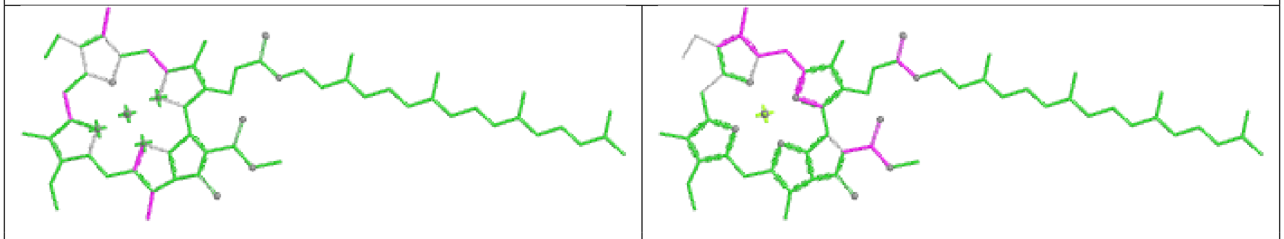


Bond lengths Bond angles

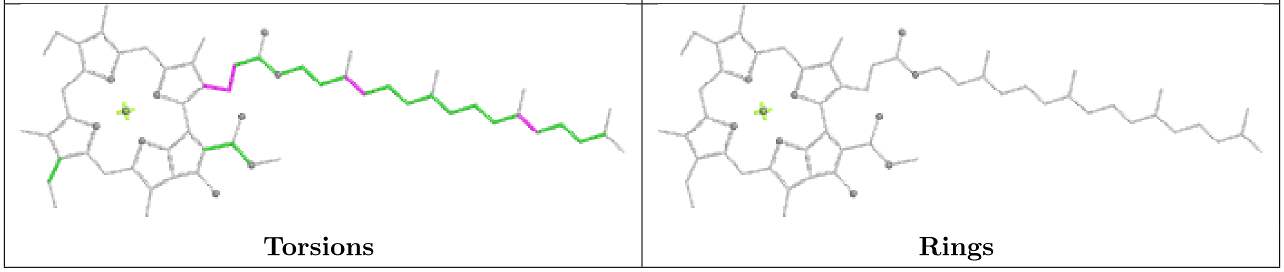


Torsions Rings

Ligand CLA U 204

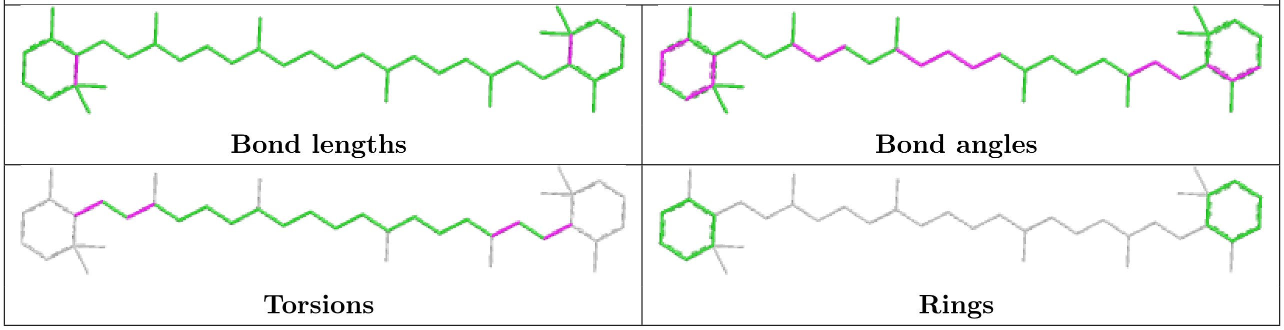


Bond lengths Bond angles



Torsions Rings

Ligand BCR A 844



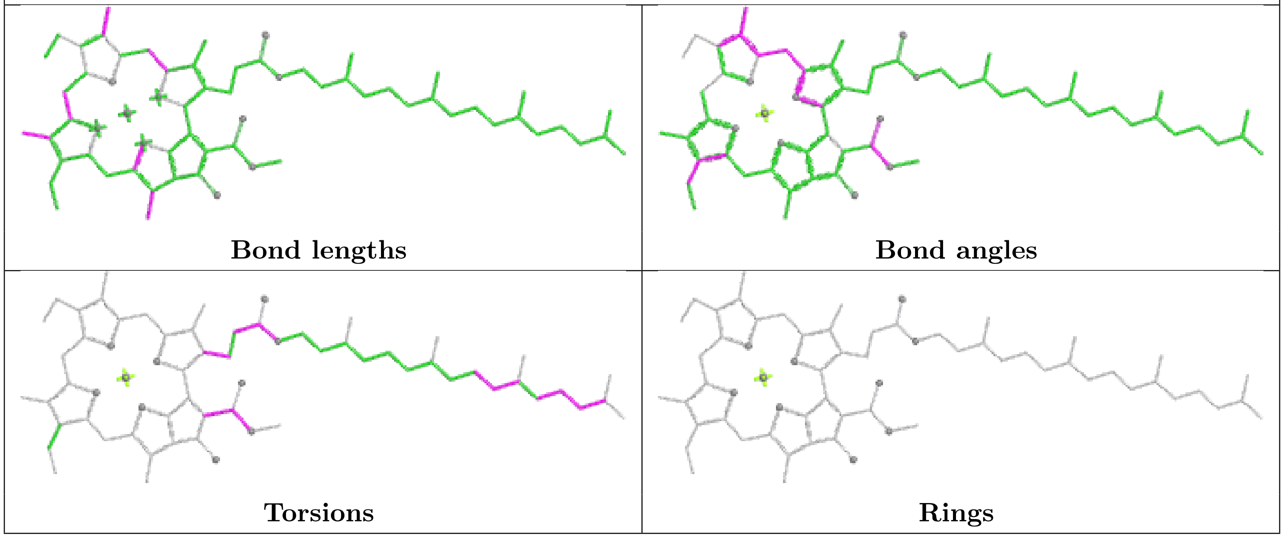
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 804



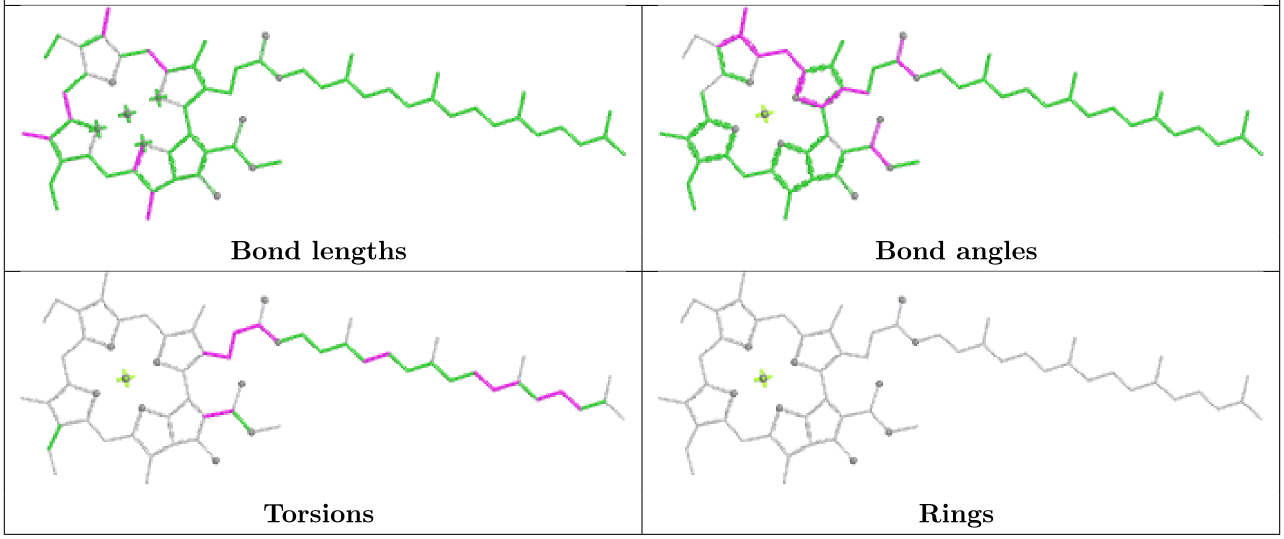
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 807



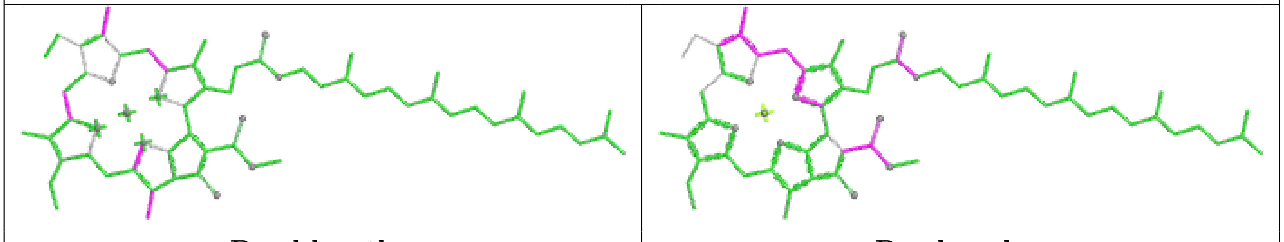
Bond lengths

Bond angles

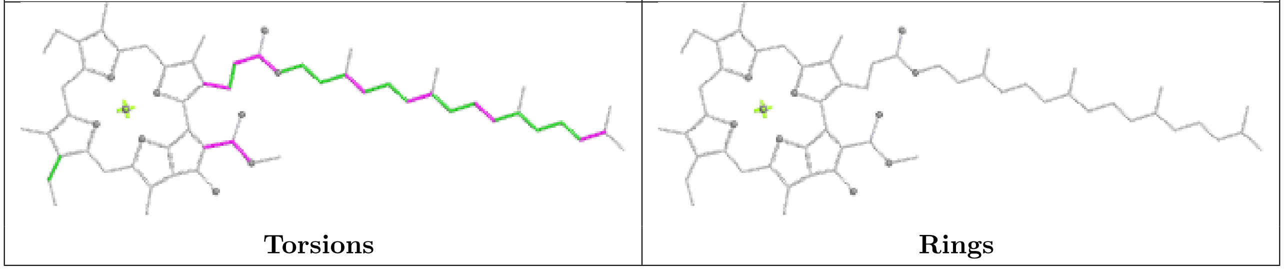
Torsions

Rings

Ligand CLA B 2134

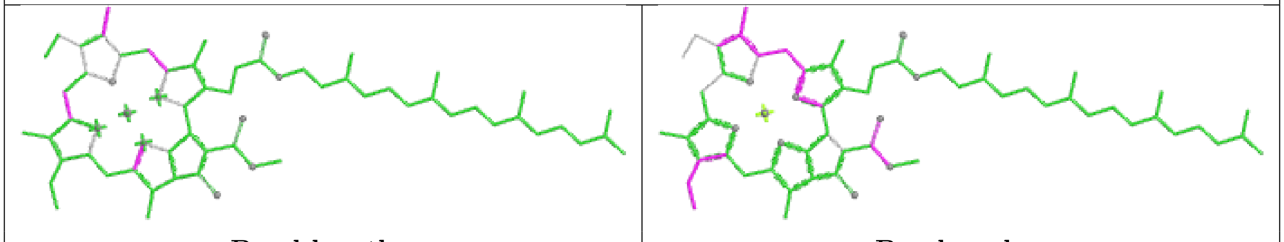


Bond lengths Bond angles

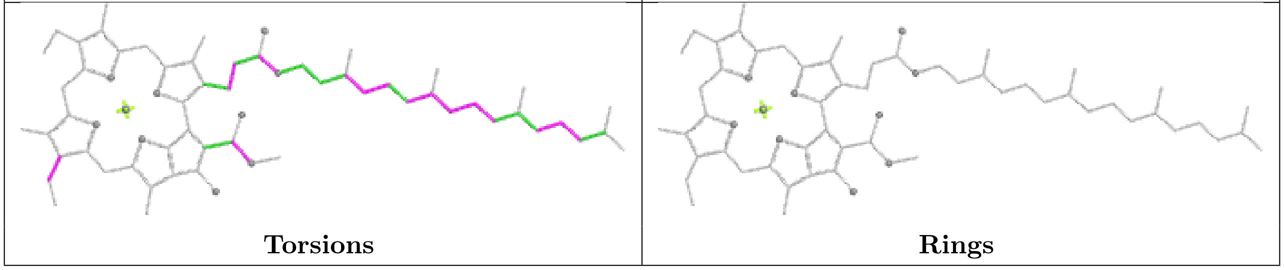


Torsions Rings

Ligand CLA H 2132

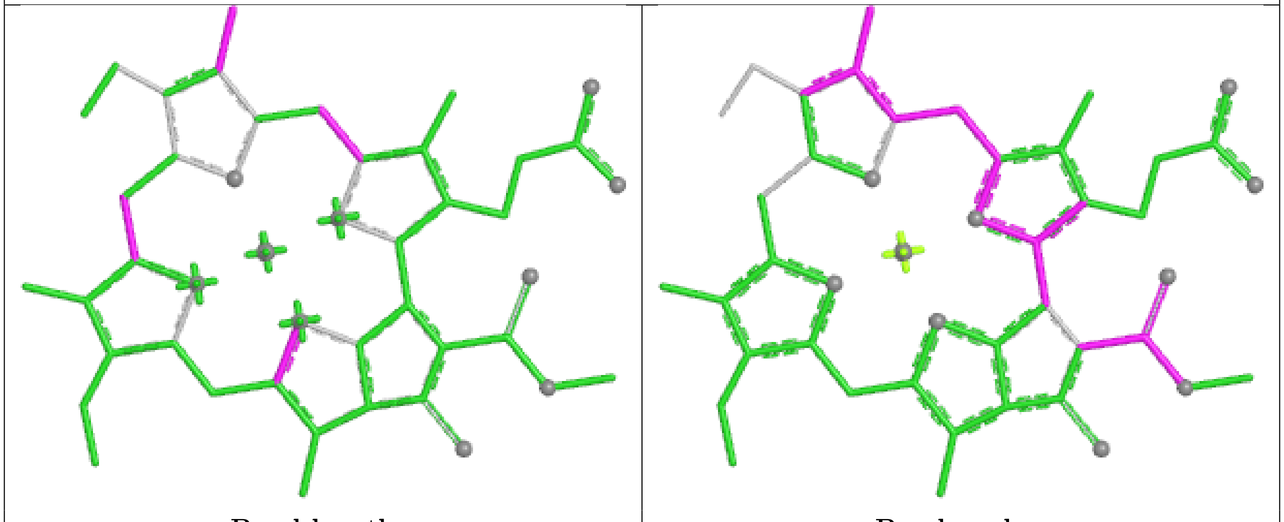


Bond lengths Bond angles

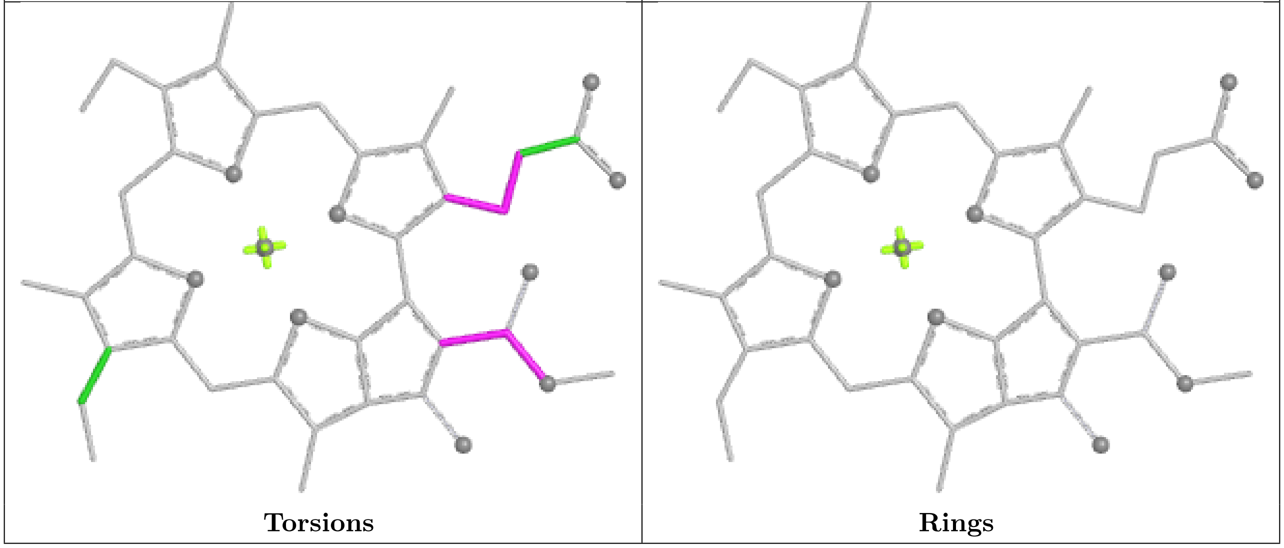


Torsions Rings

Ligand CLA S 102

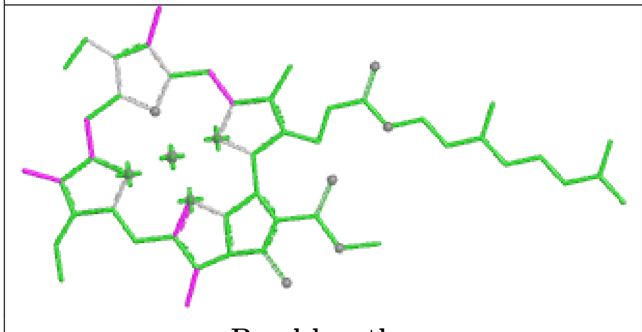


Bond lengths **Bond angles**

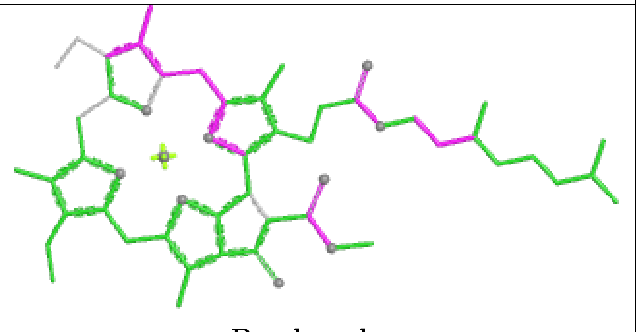


Torsions **Rings**

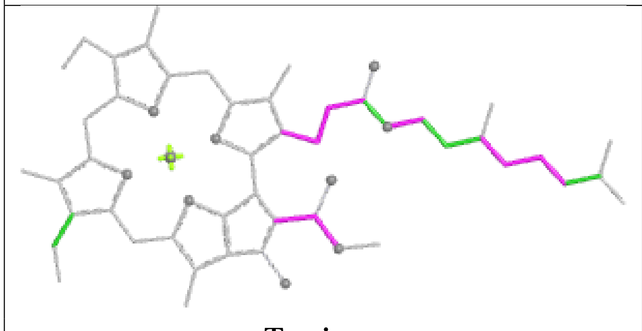
Ligand CLA B 2124



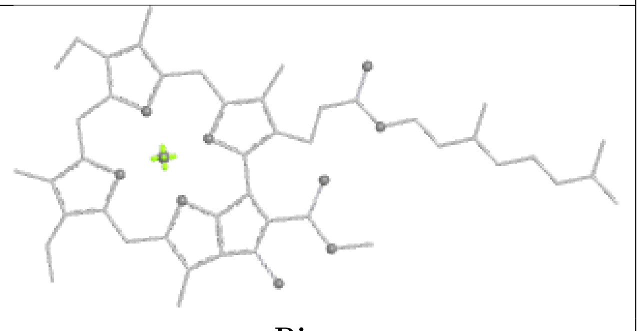
Bond lengths



Bond angles

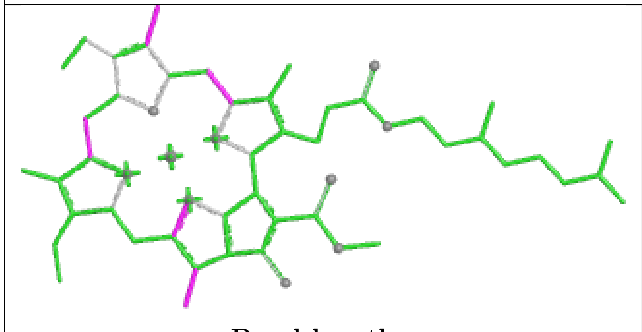


Torsions

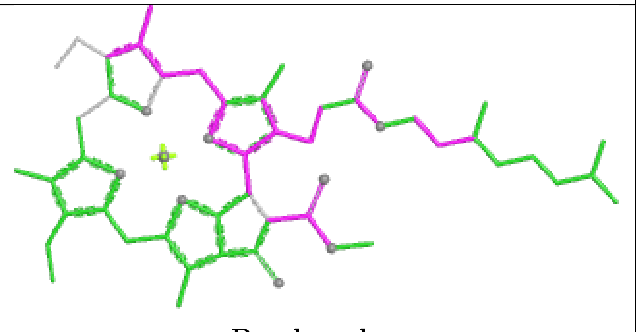


Rings

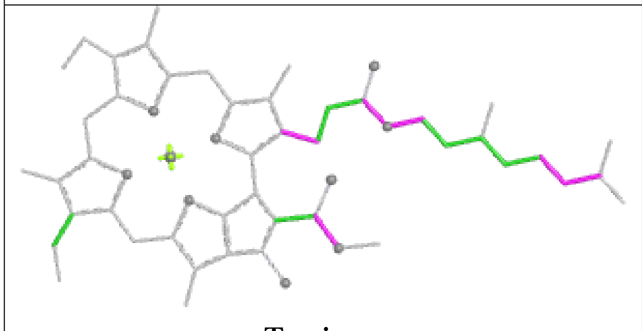
Ligand CLA G 834



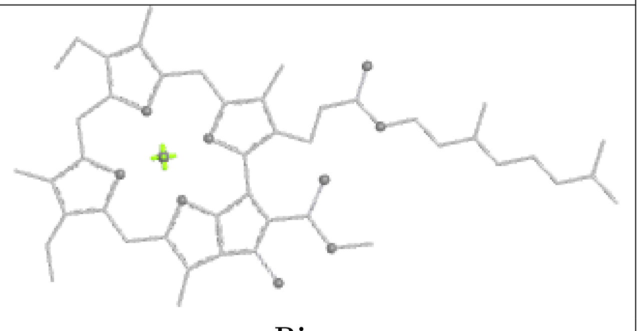
Bond lengths



Bond angles

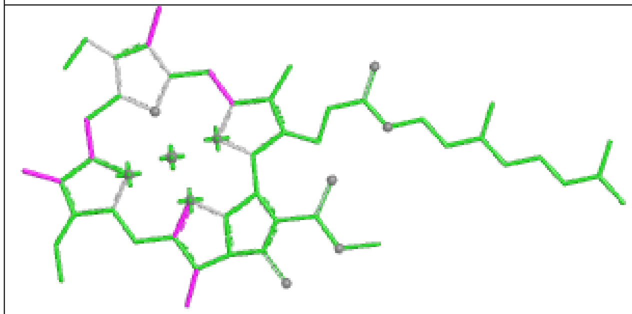


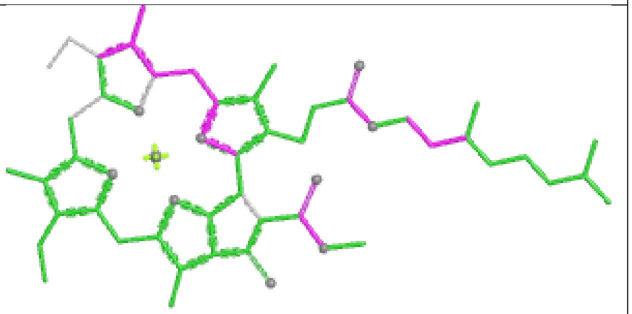
Torsions

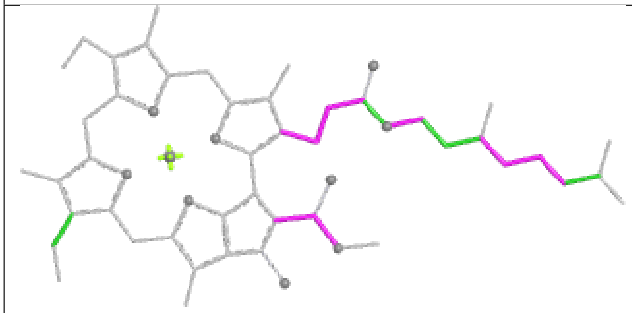


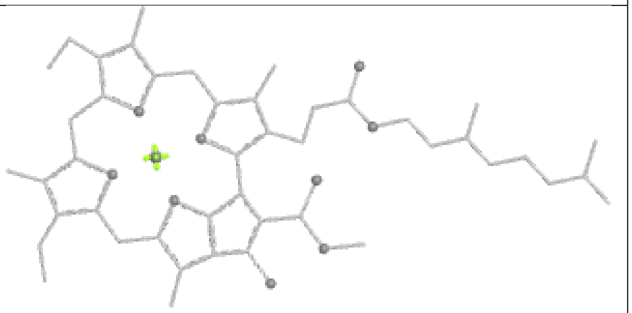
Rings

Ligand CLA b 2123

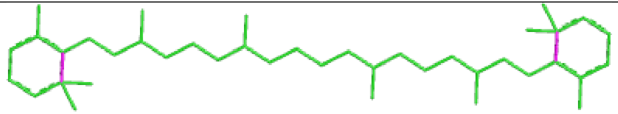

Bond lengths

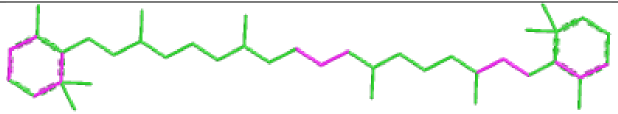

Bond angles

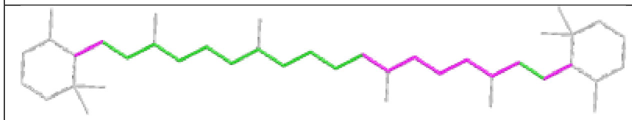

Torsions

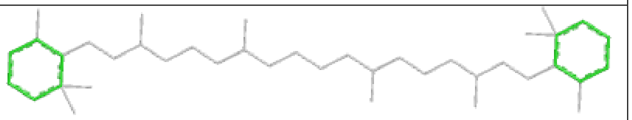

Rings

Ligand BCR A 842

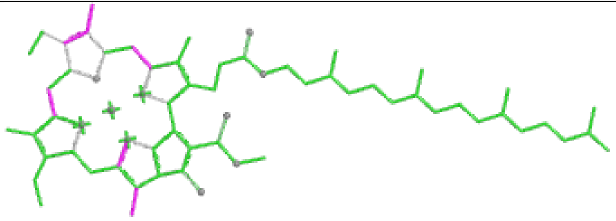

Bond lengths

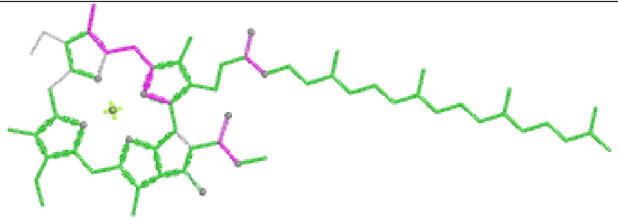

Bond angles

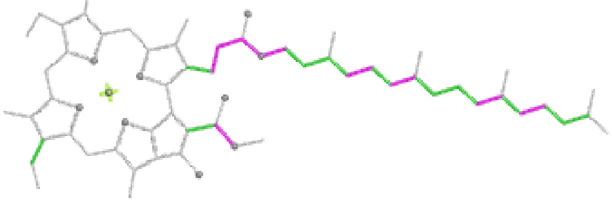

Torsions

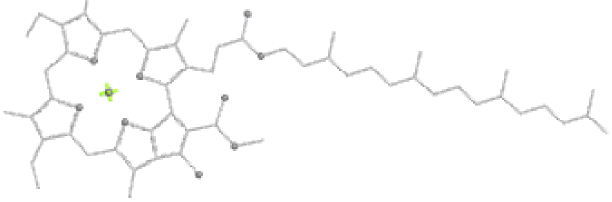

Rings

Ligand CLA B 2141

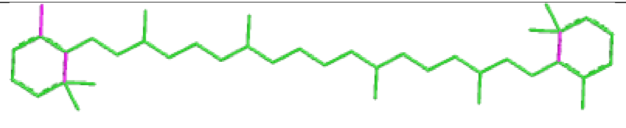
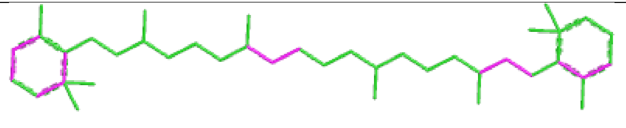
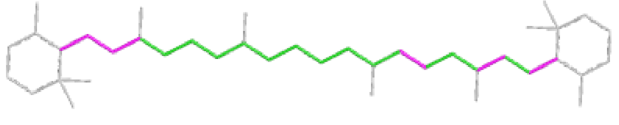
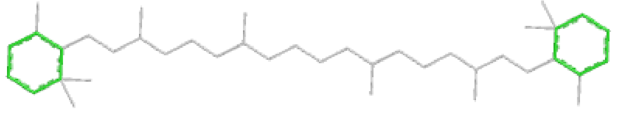

Bond lengths


Bond angles

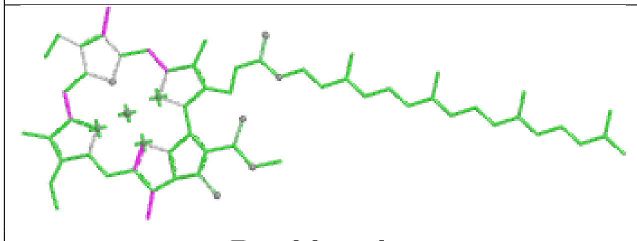
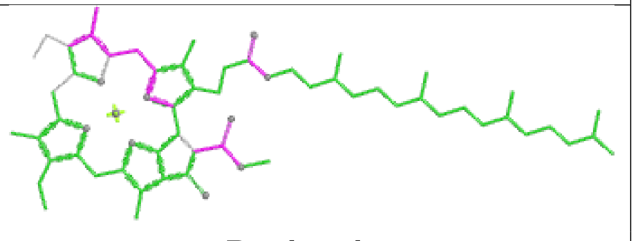
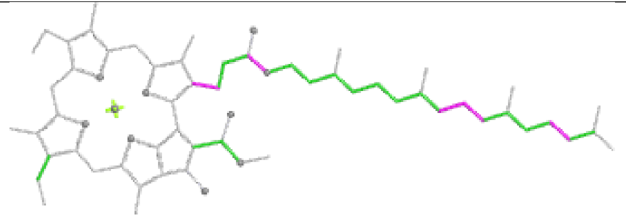
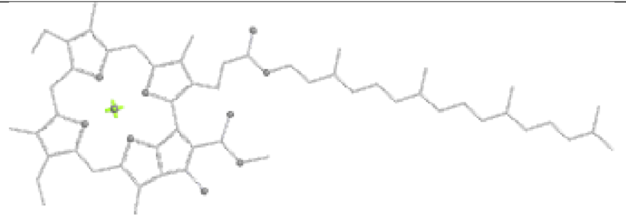

Torsions


Rings

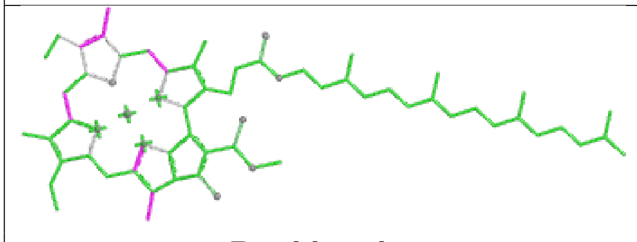
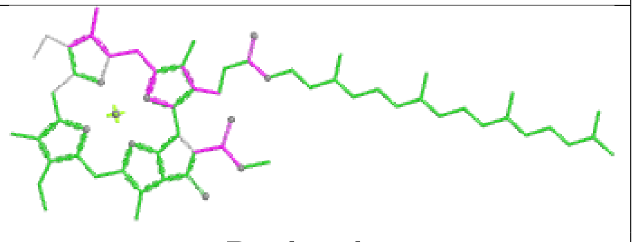
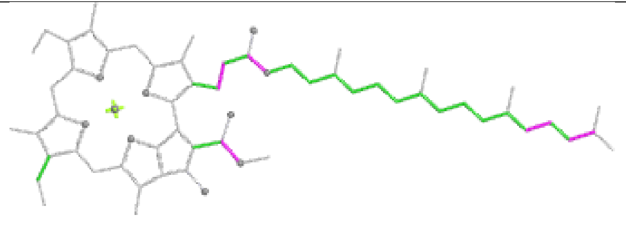
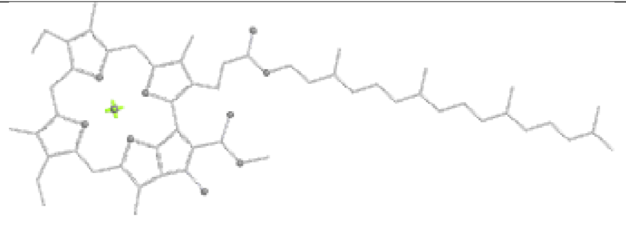
Ligand BCR K 4001

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

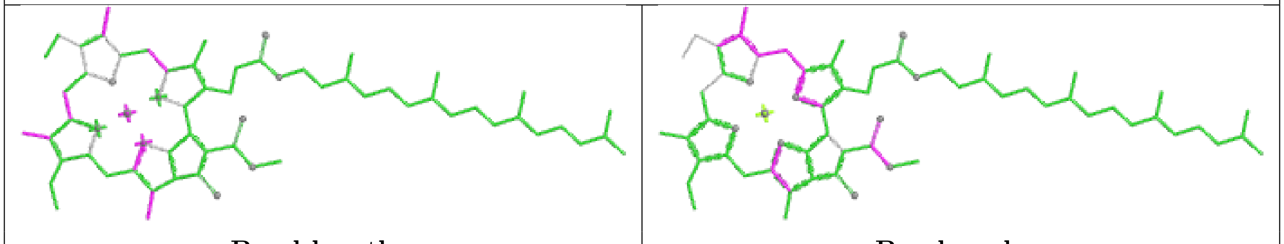
Ligand CLA a 802

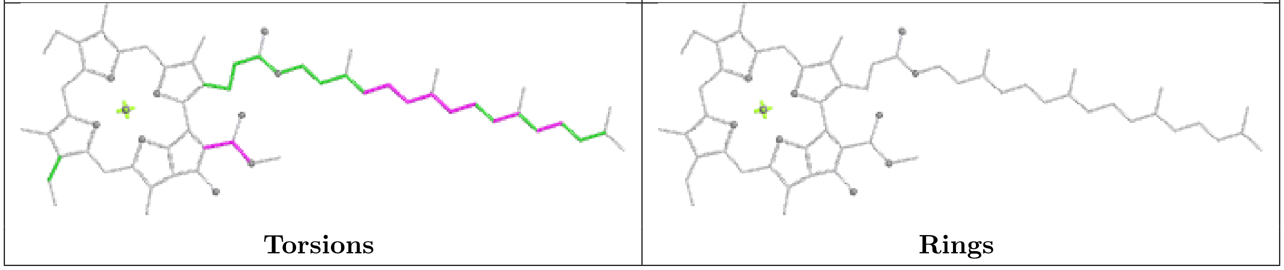
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA H 2139

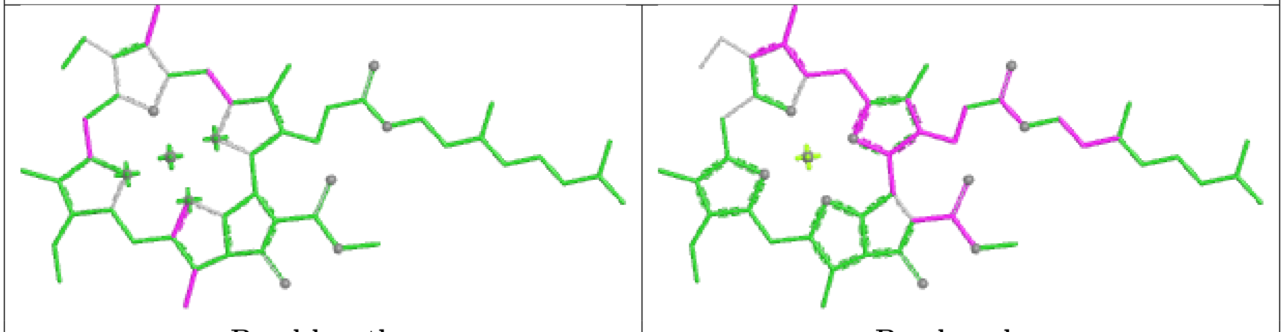
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

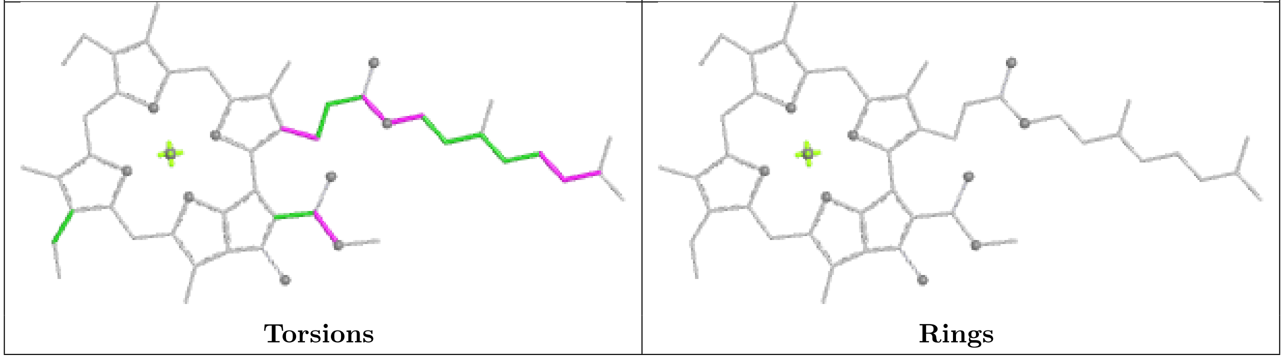
Ligand CLA b 2129


Bond lengths Bond angles

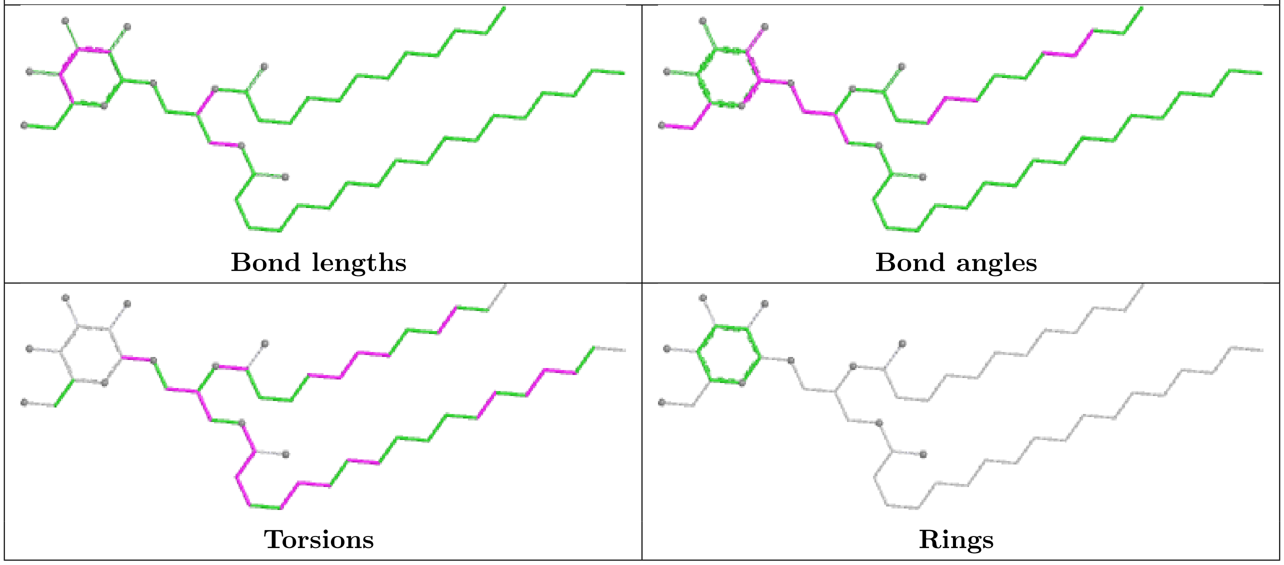

Torsions Rings

Ligand CLA a 834


Bond lengths Bond angles


Torsions Rings

Ligand DGD L 209



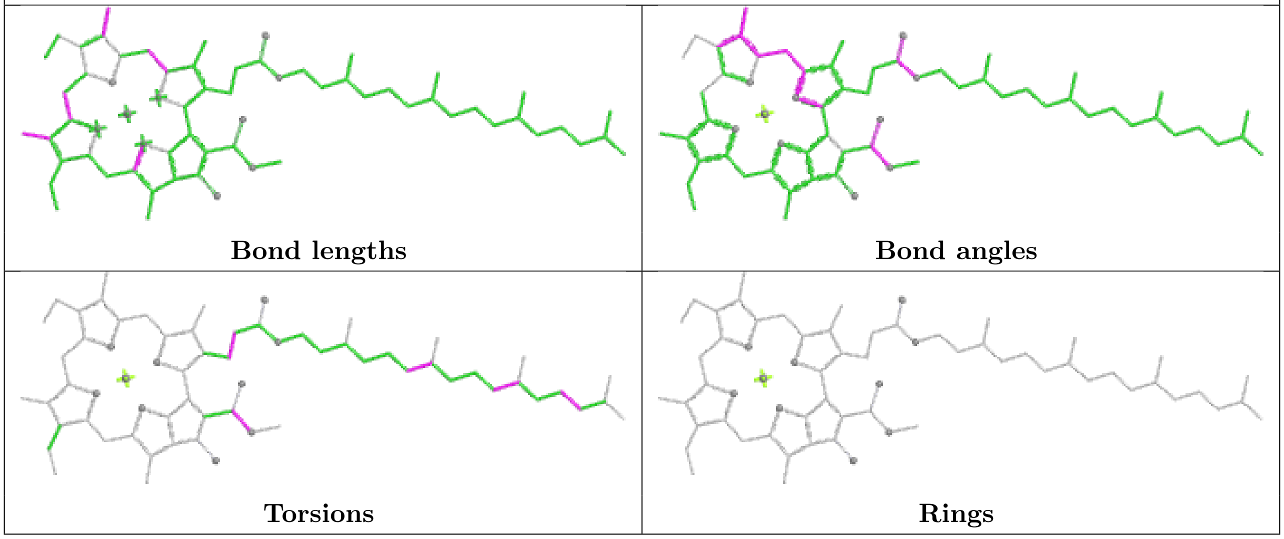
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 820



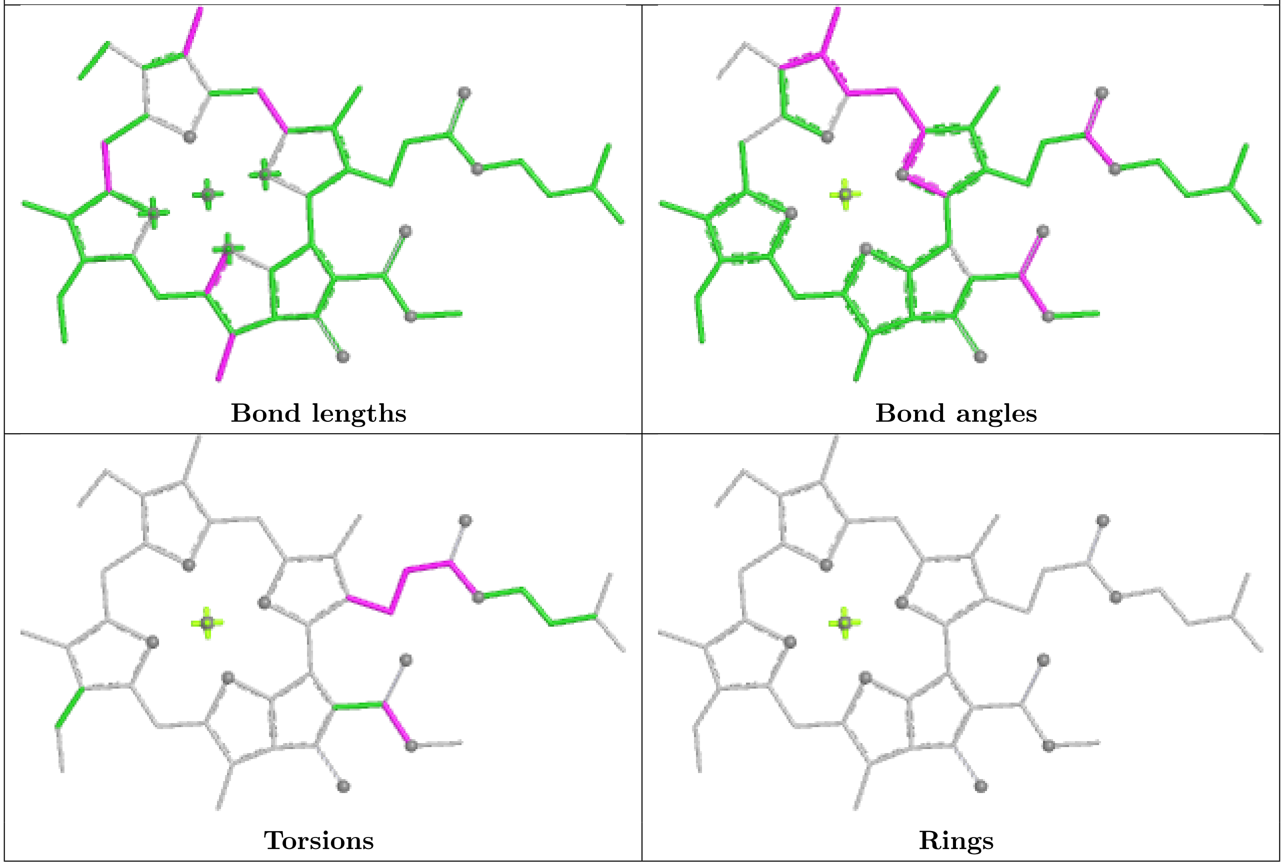
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 822



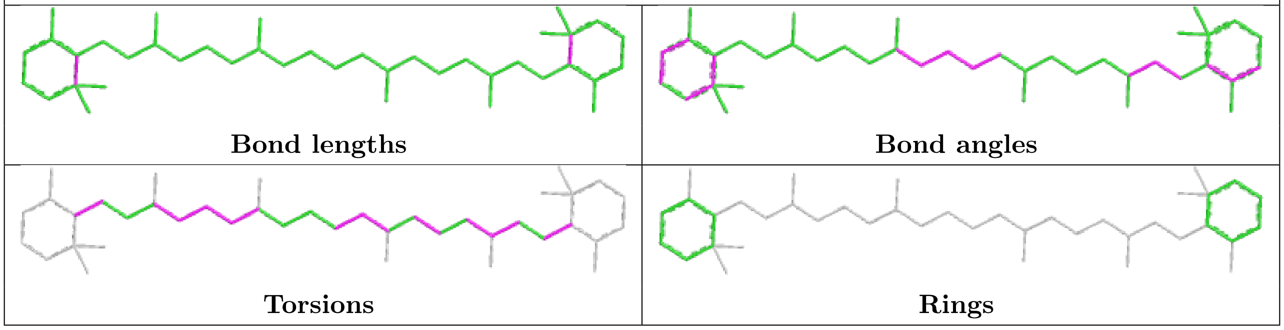
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR b 2146



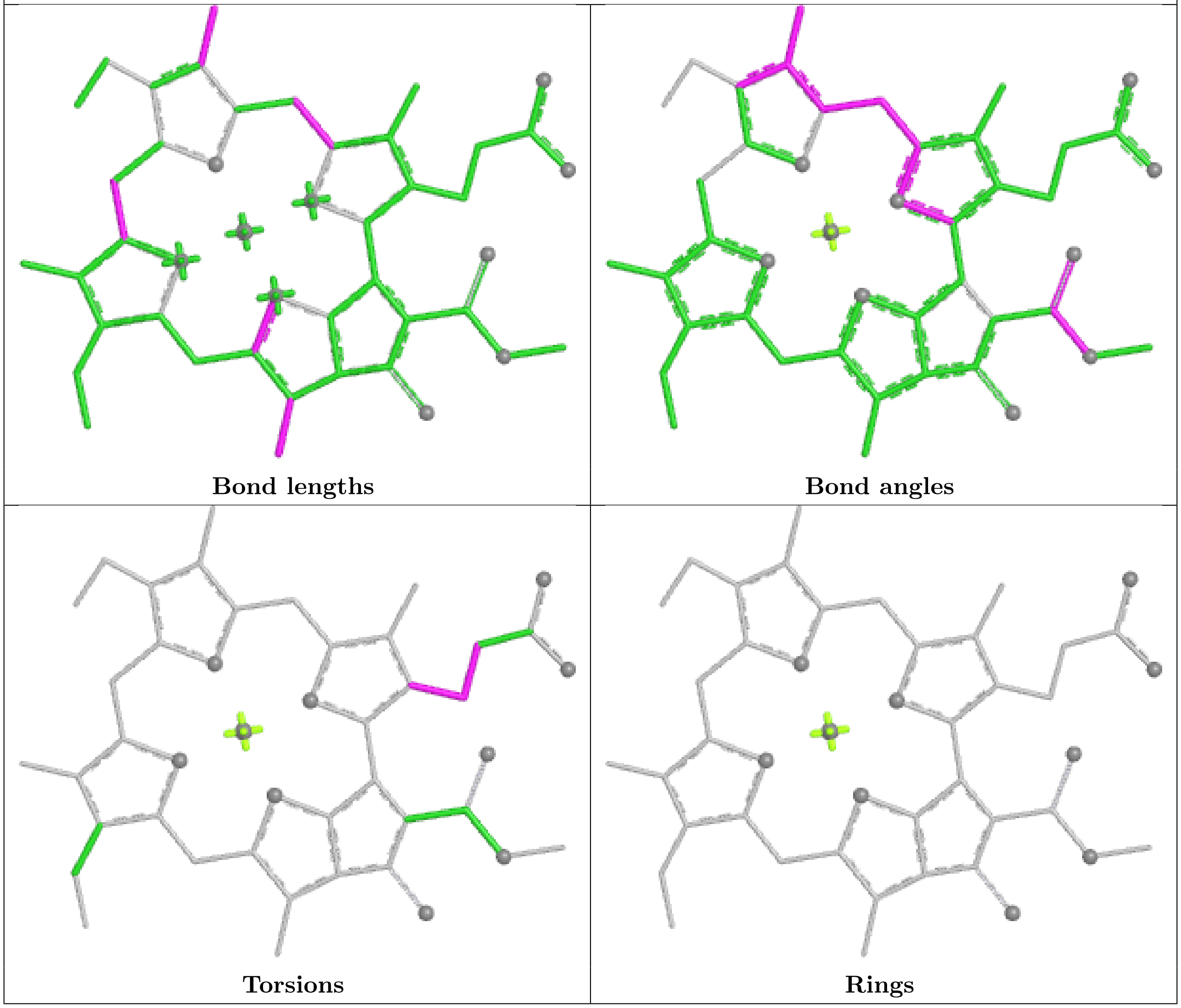
Bond lengths

Bond angles

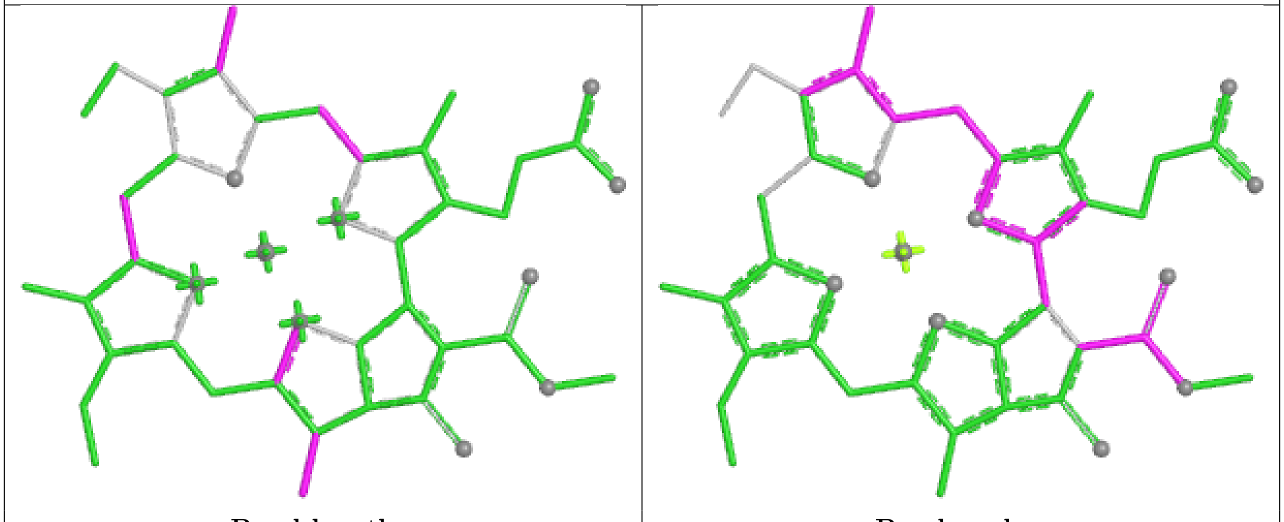
Torsions

Rings

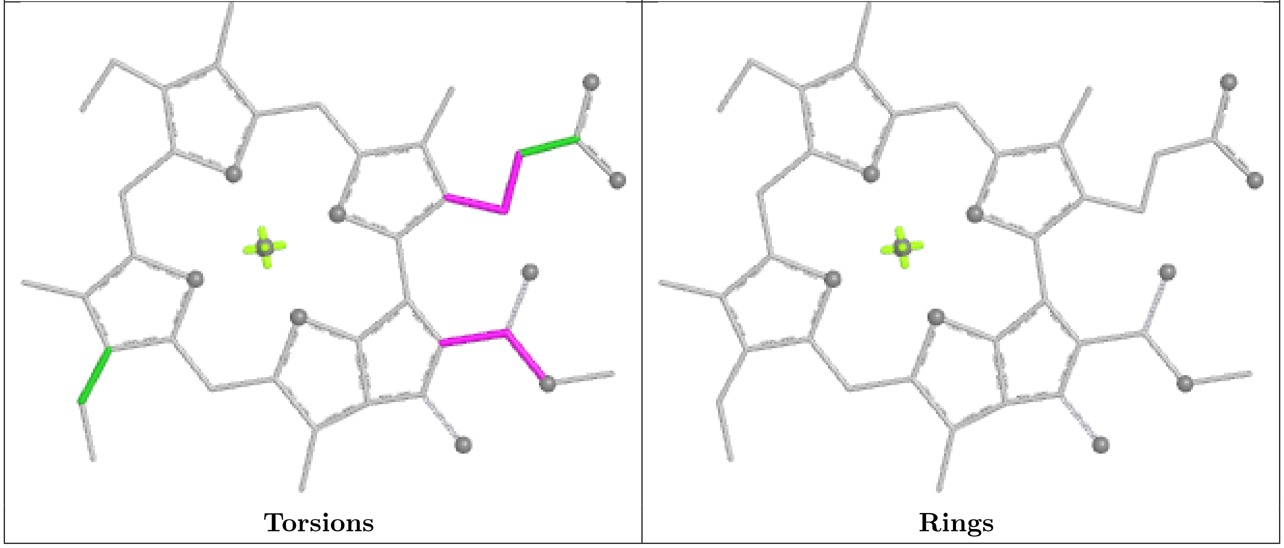
Ligand CLA F 204



Ligand CLA j 102

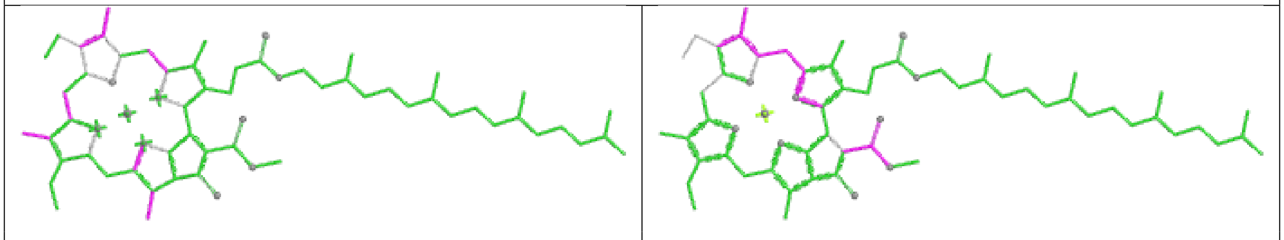


Bond lengths Bond angles

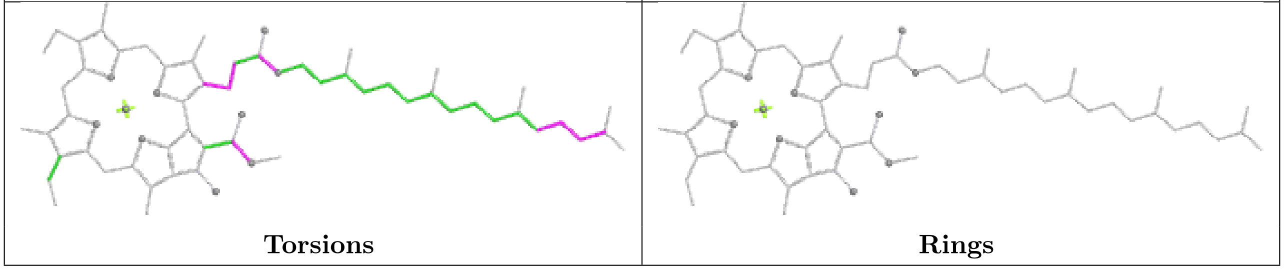


Torsions Rings

Ligand CLA H 2128

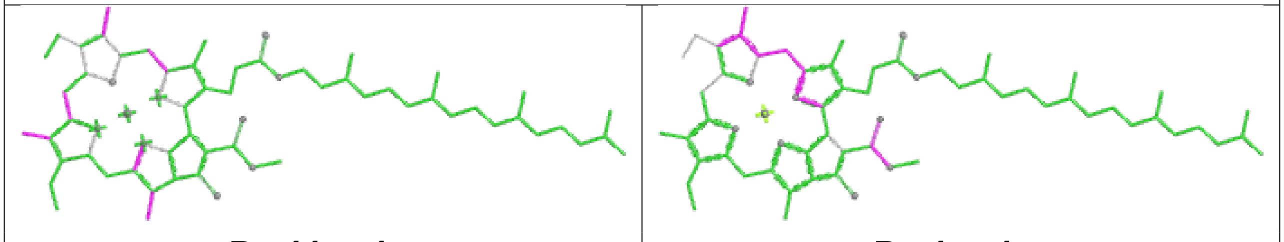


Bond lengths Bond angles



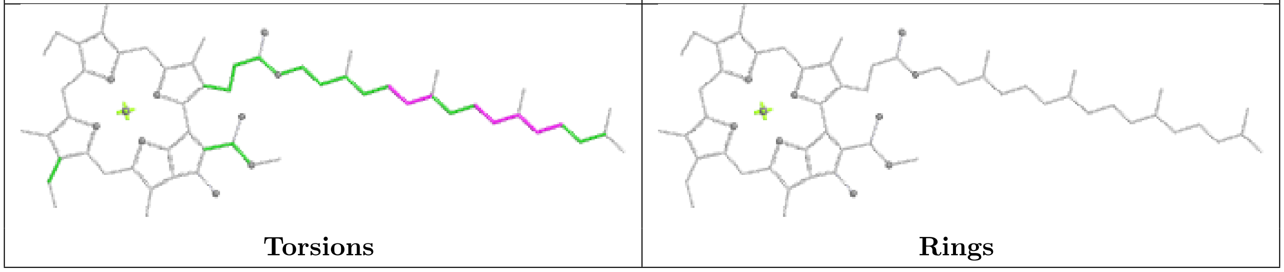
Torsions Rings

Ligand CLA b 2126



Bond lengths

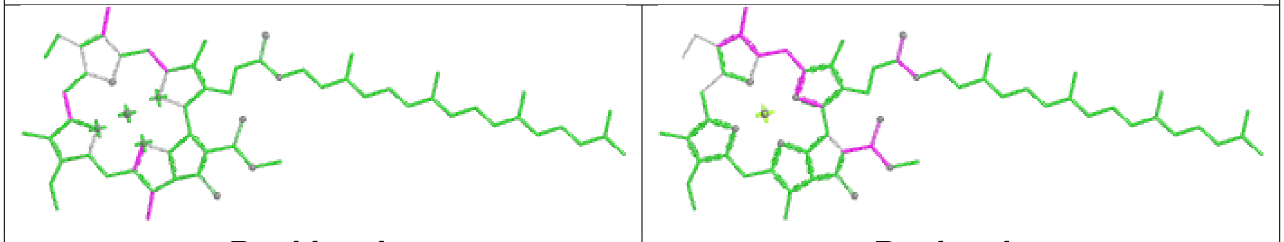
Bond angles



Torsions

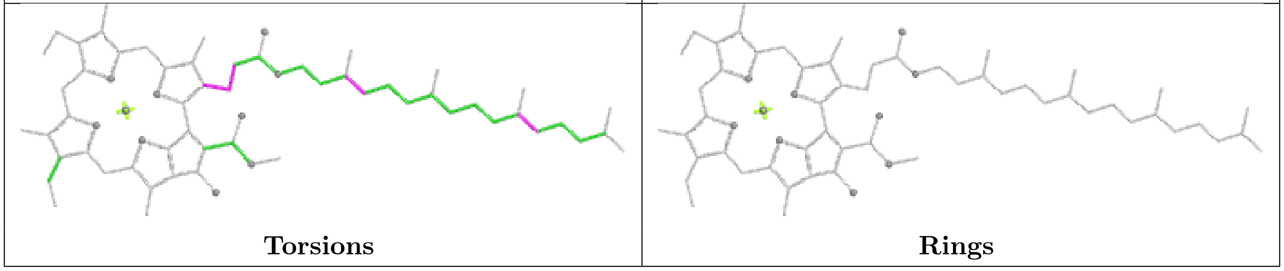
Rings

Ligand CLA L 204



Bond lengths

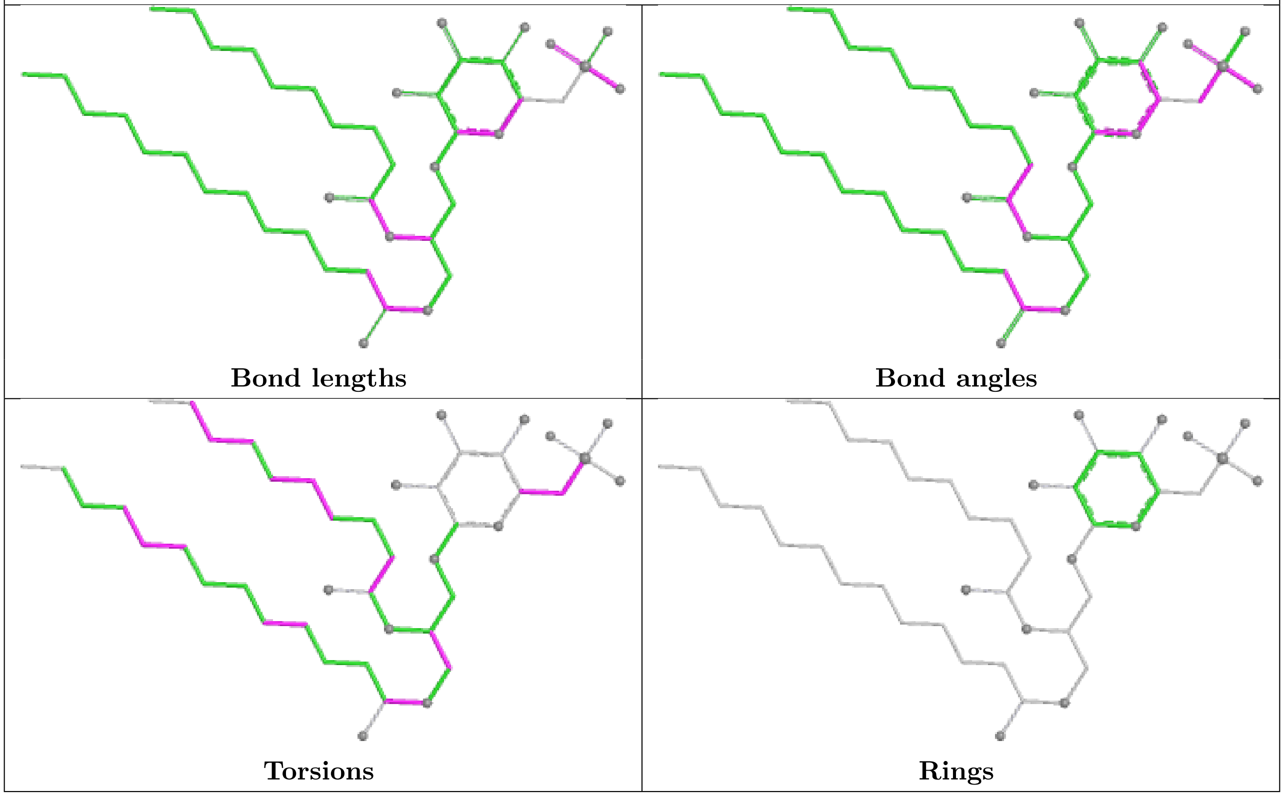
Bond angles



Torsions

Rings

Ligand SQD L 208



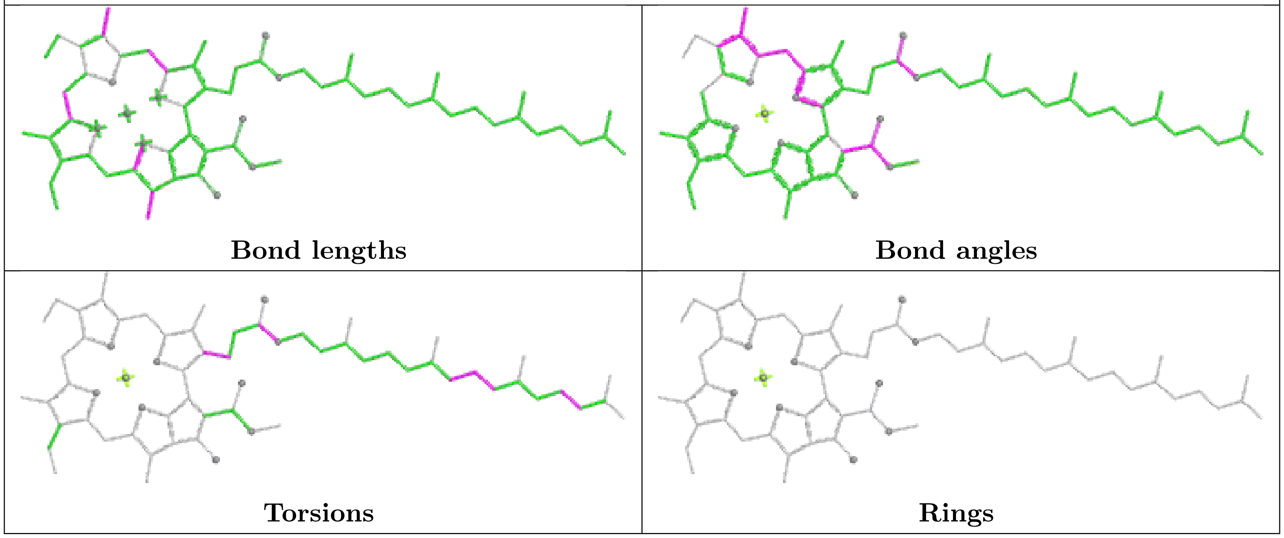
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 802



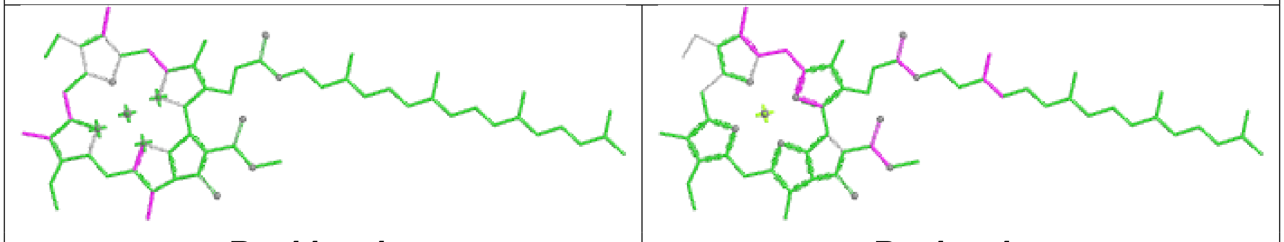
Bond lengths

Bond angles

Torsions

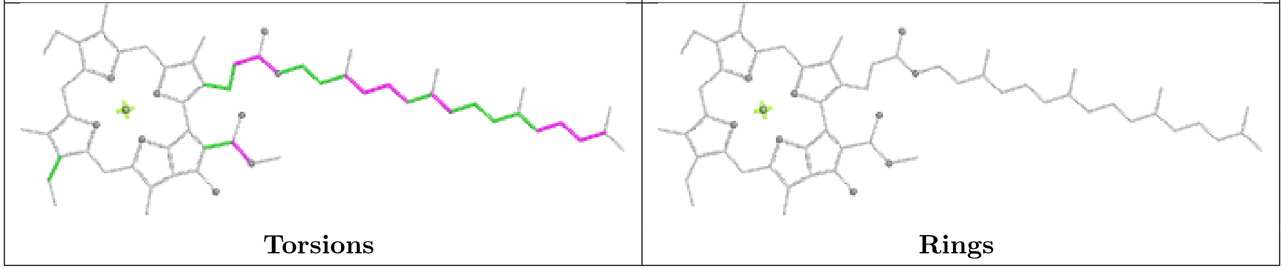
Rings

Ligand CLA B 2104



Bond lengths

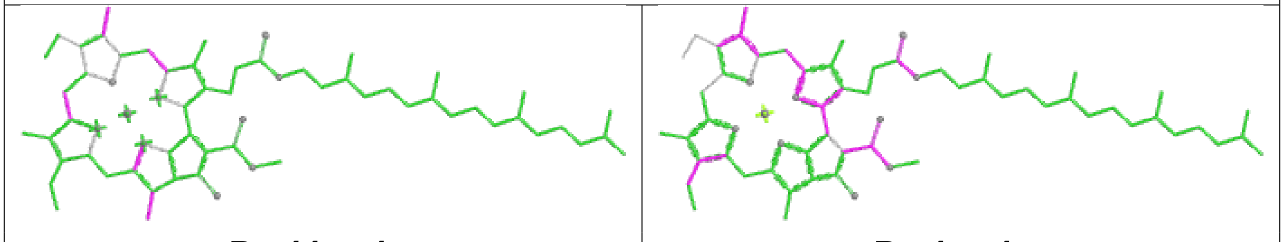
Bond angles



Torsions

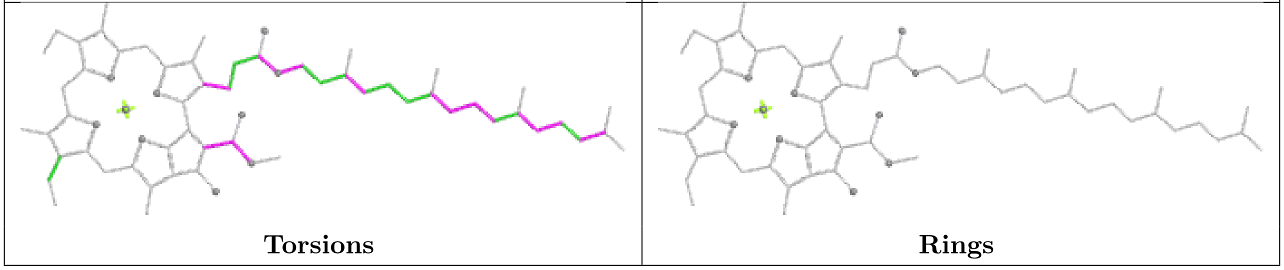
Rings

Ligand CLA a 824



Bond lengths

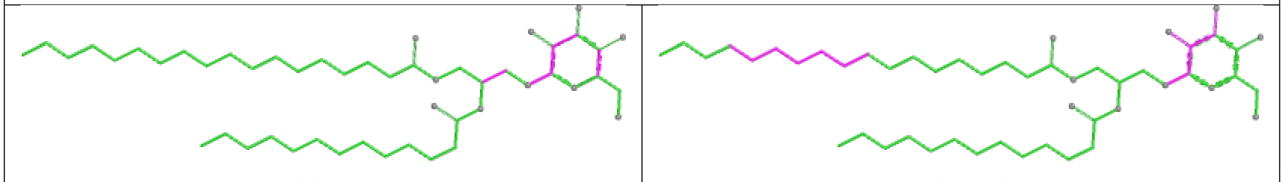
Bond angles



Torsions

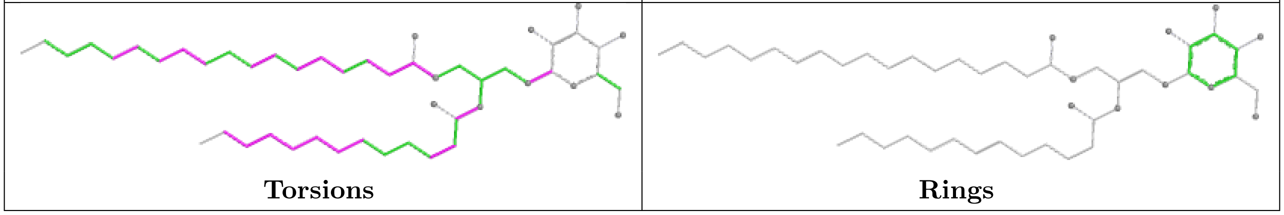
Rings

Ligand LMG G 847



Bond lengths

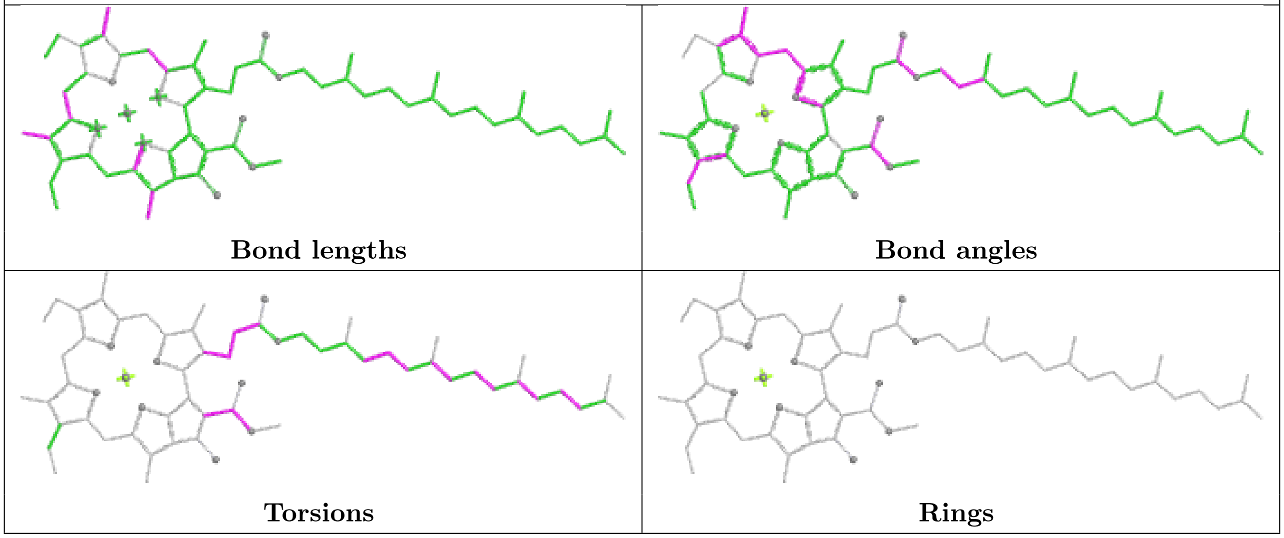
Bond angles



Torsions

Rings

Ligand CLA B 2115



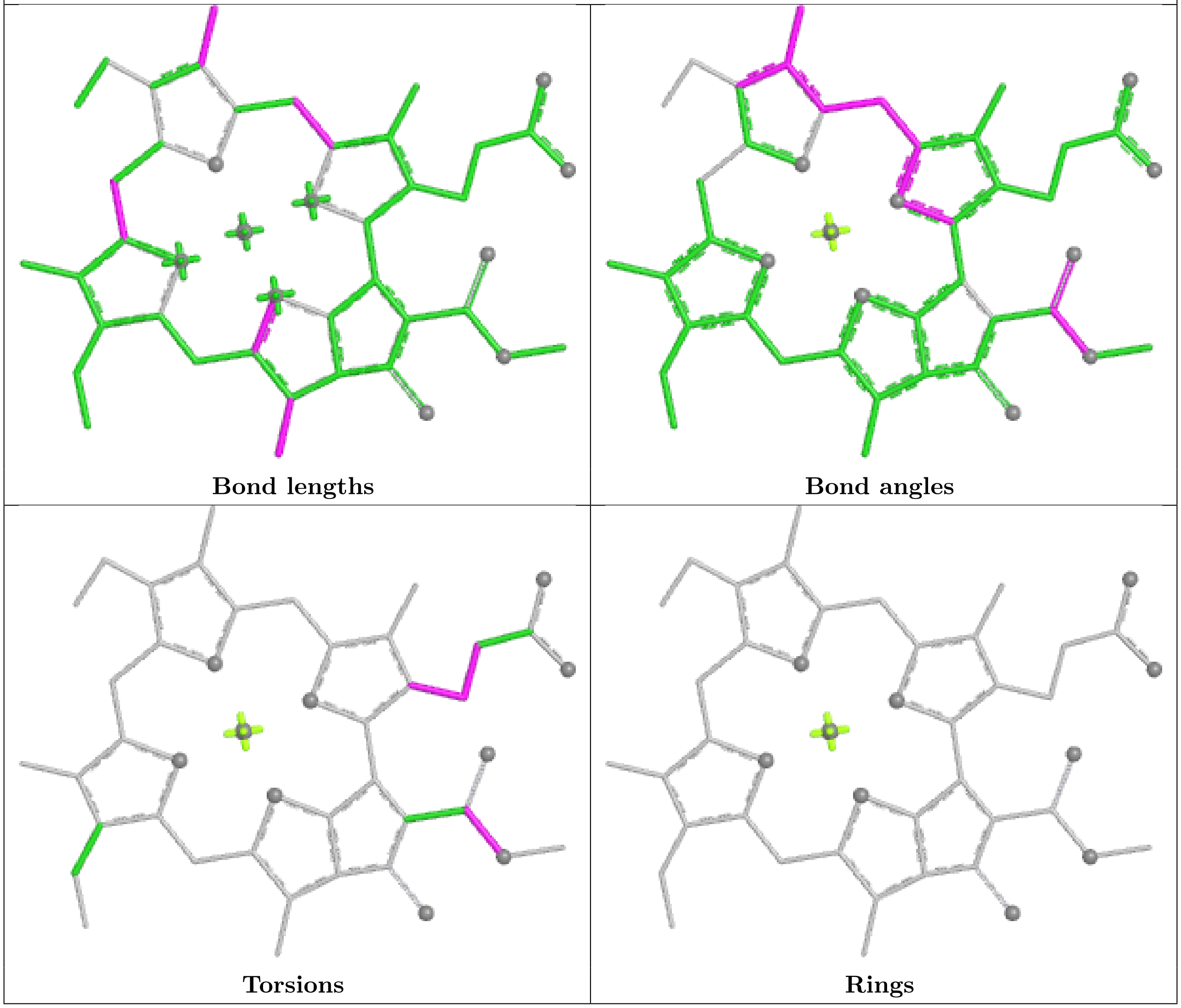
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 2122



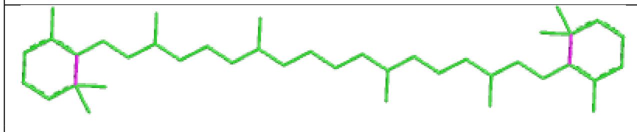
Bond lengths

Bond angles

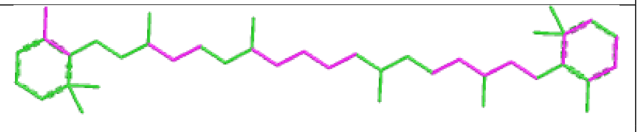
Torsions

Rings

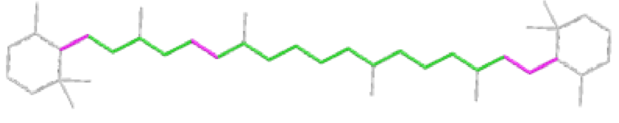
Ligand BCR L 207



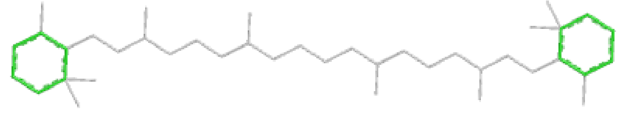
Bond lengths



Bond angles

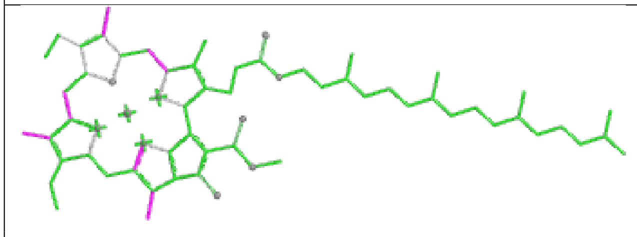


Torsions

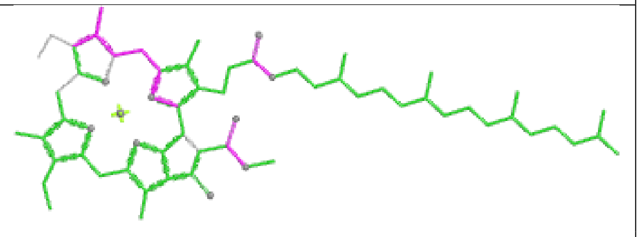


Rings

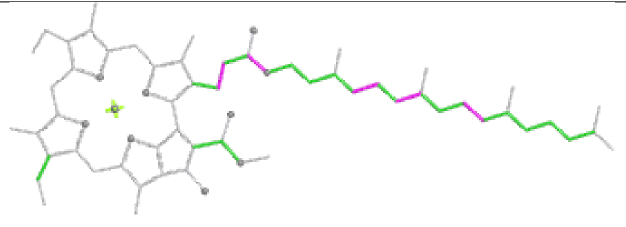
Ligand CLA b 2105



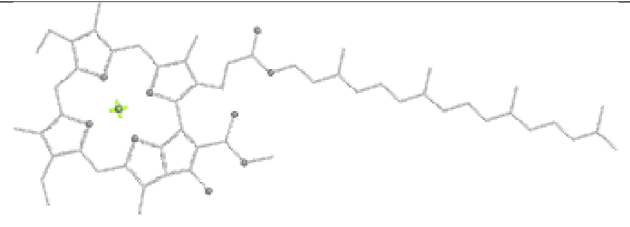
Bond lengths



Bond angles

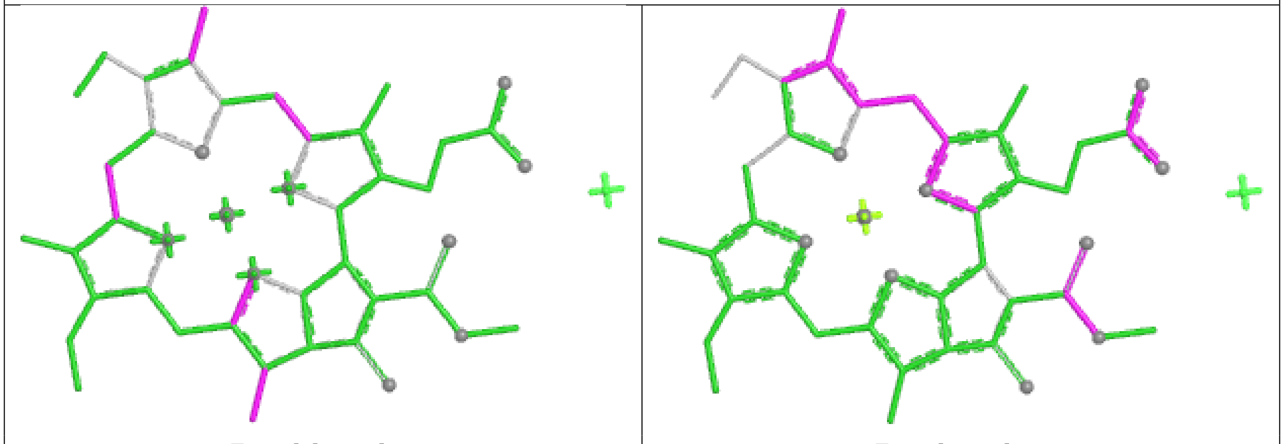


Torsions



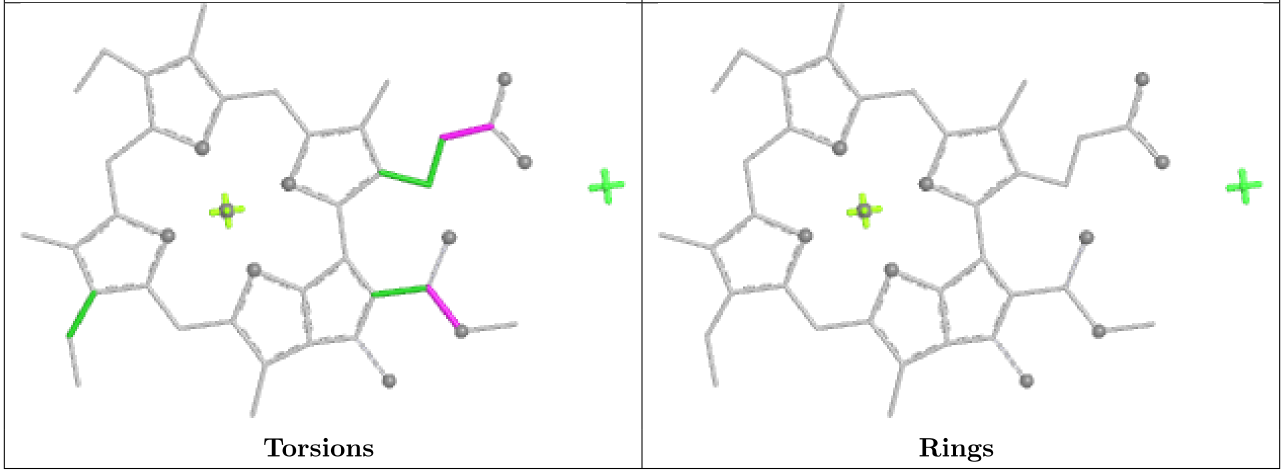
Rings

Ligand CLA F 203



Bond lengths

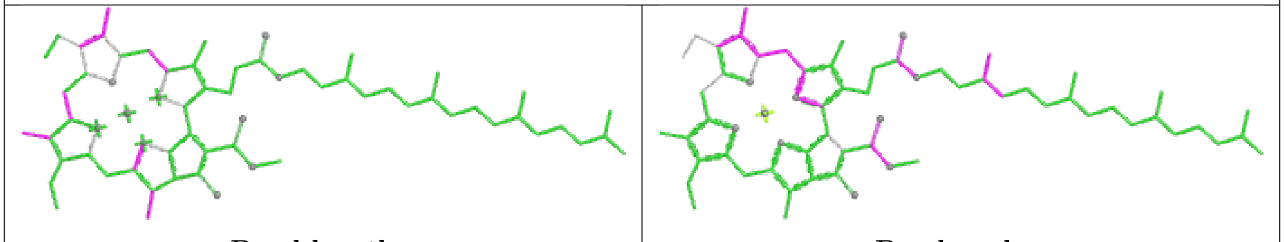
Bond angles



Torsions

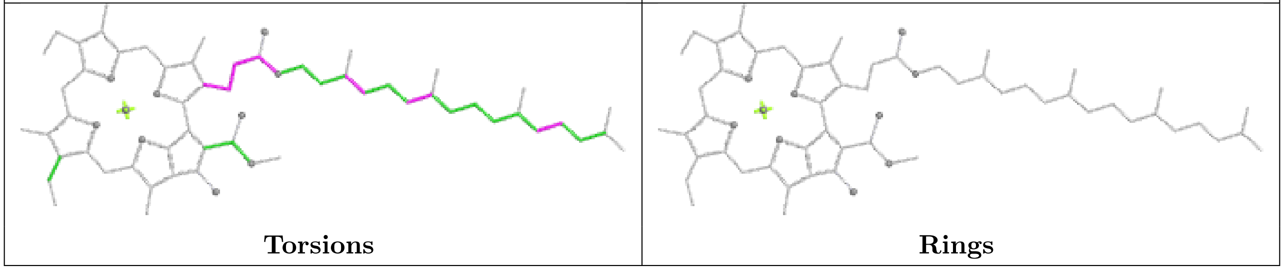
Rings

Ligand CLA G 851



Bond lengths

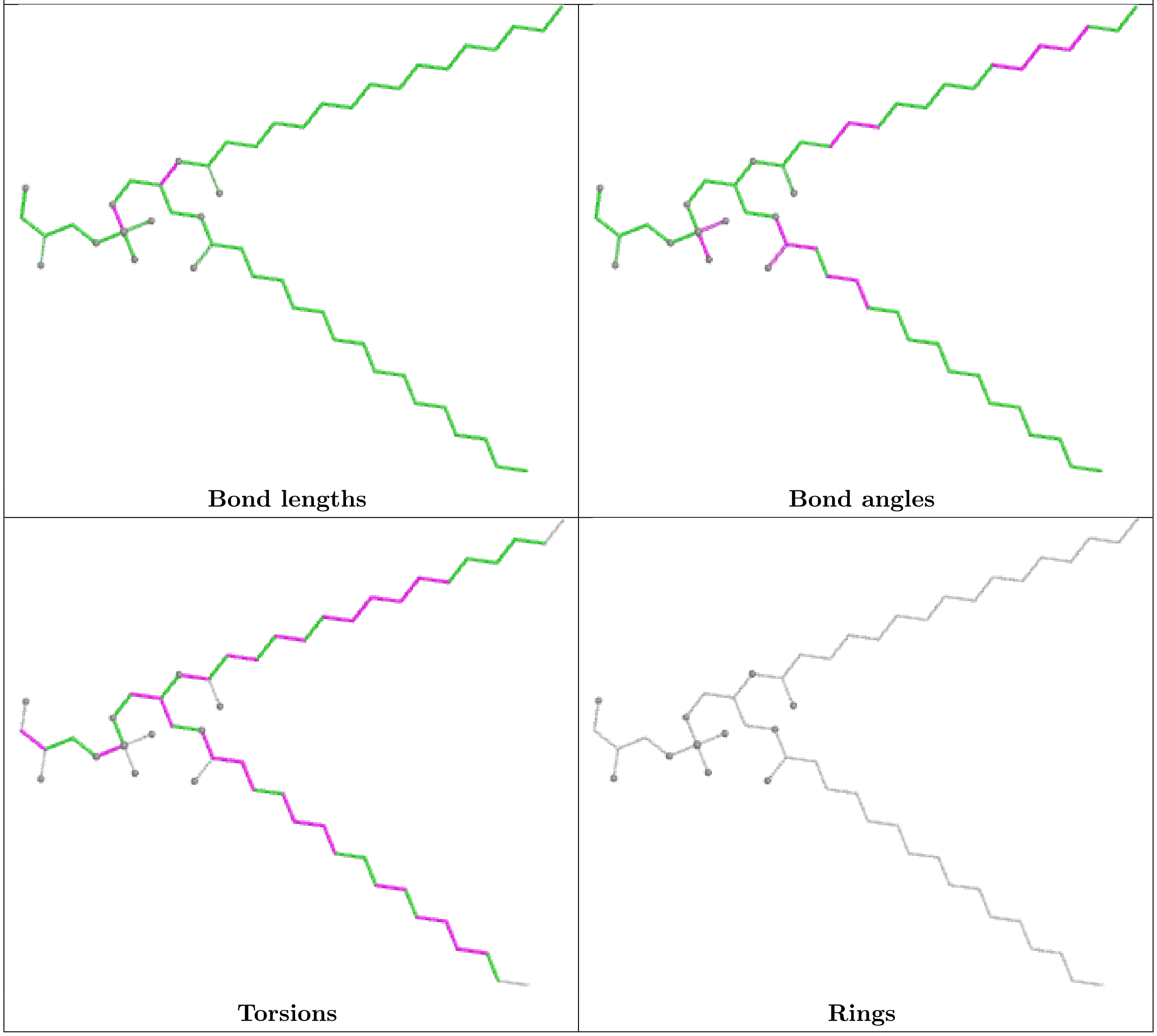
Bond angles



Torsions

Rings

Ligand LHG a 846



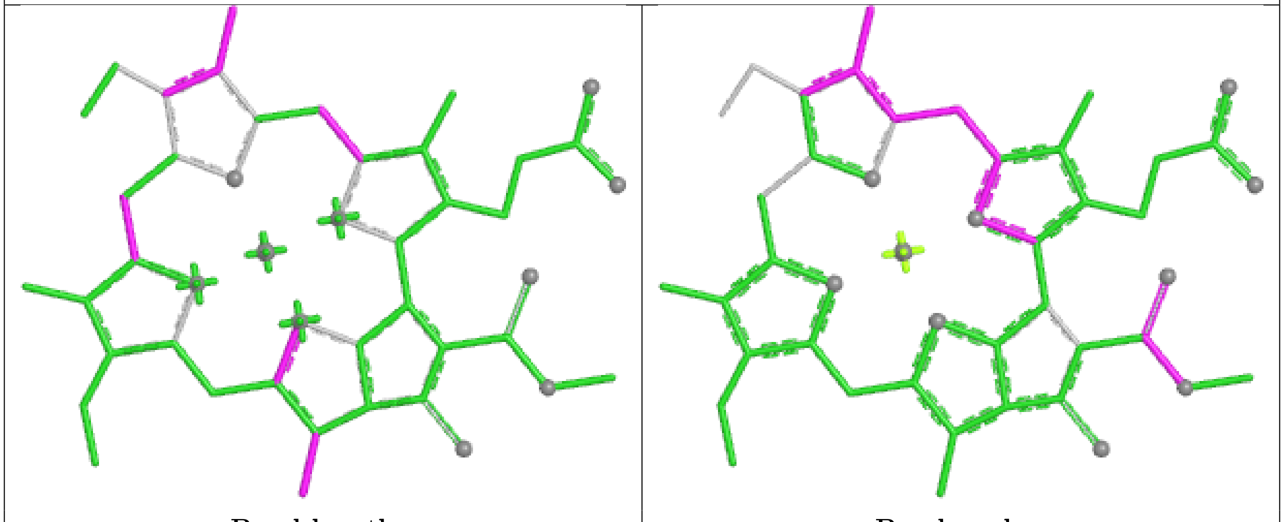
Bond lengths

Bond angles

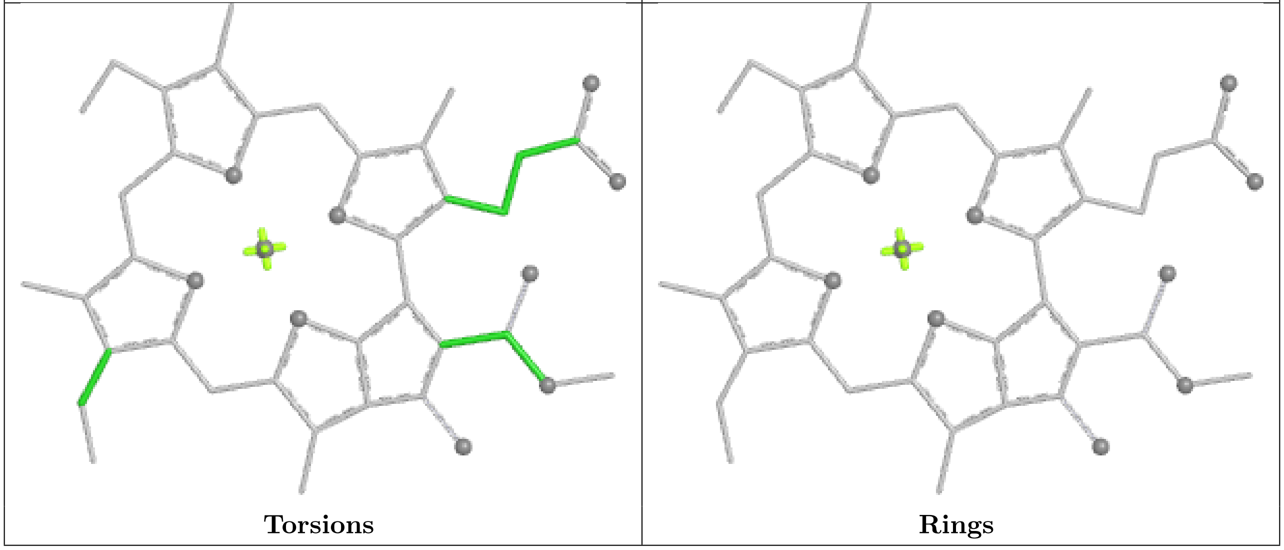
Torsions

Rings

Ligand CLA H 2130

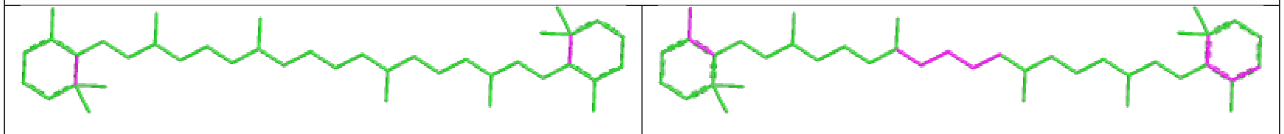


Bond lengths Bond angles

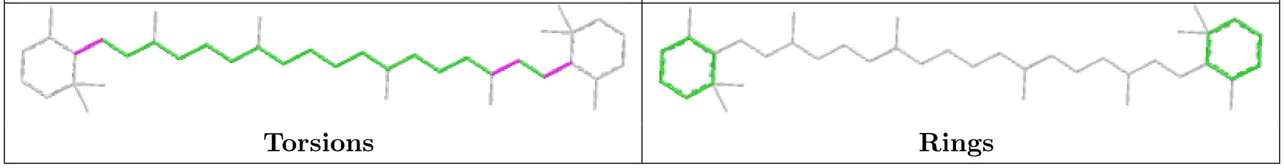


Torsions Rings

Ligand BCR H 2142

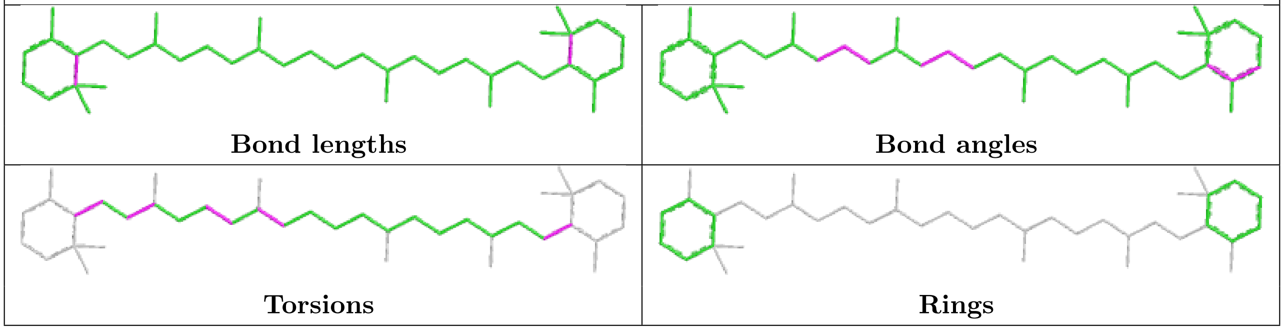


Bond lengths Bond angles



Torsions Rings

Ligand BCR H 2145



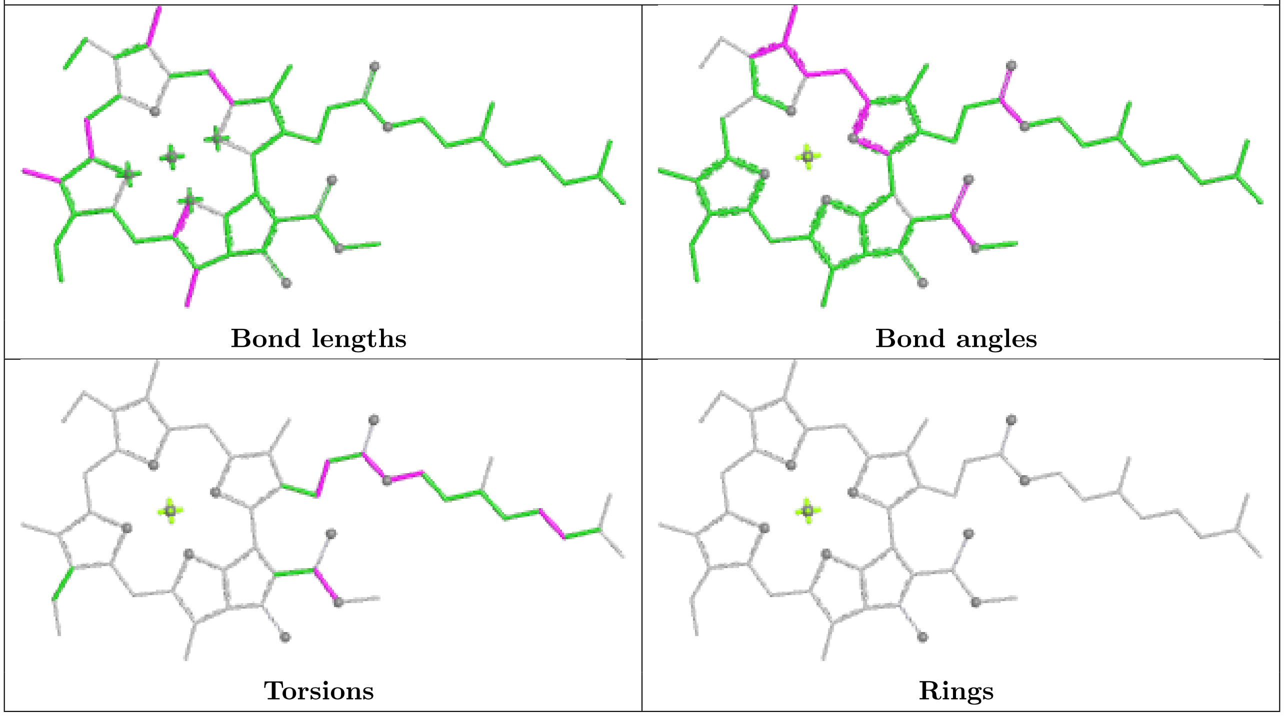
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 2131



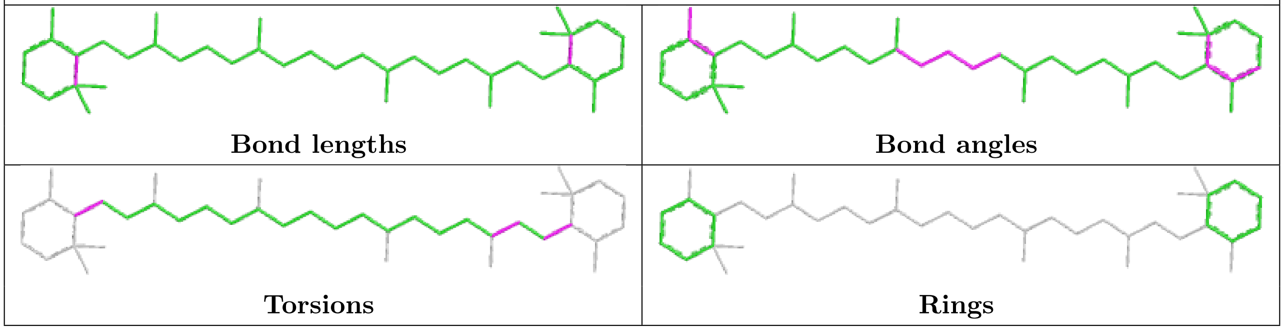
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR b 2142



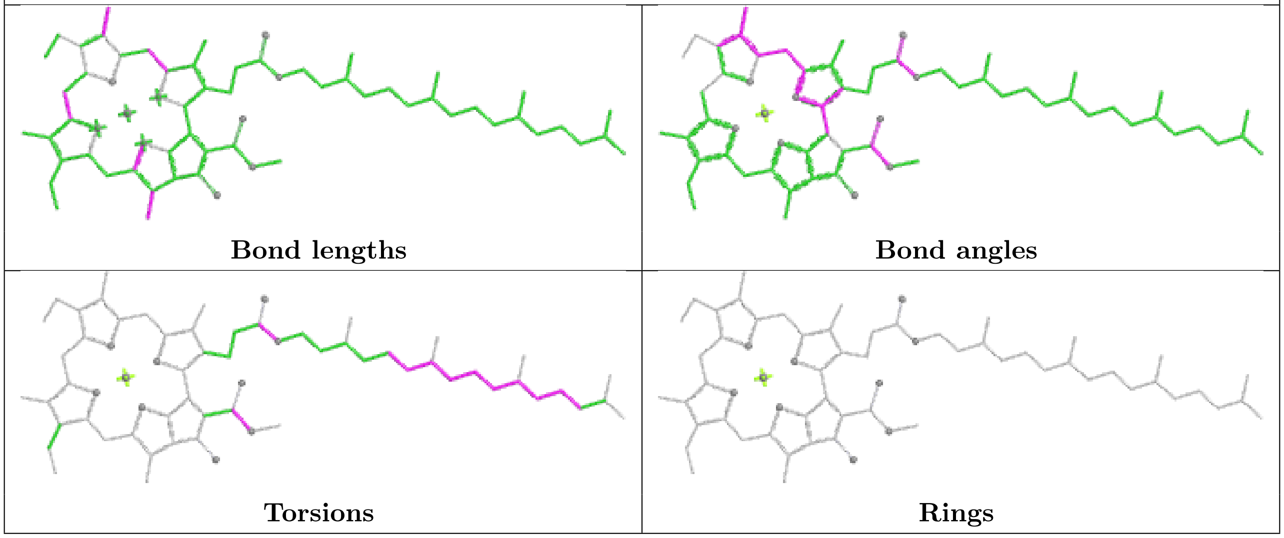
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 819



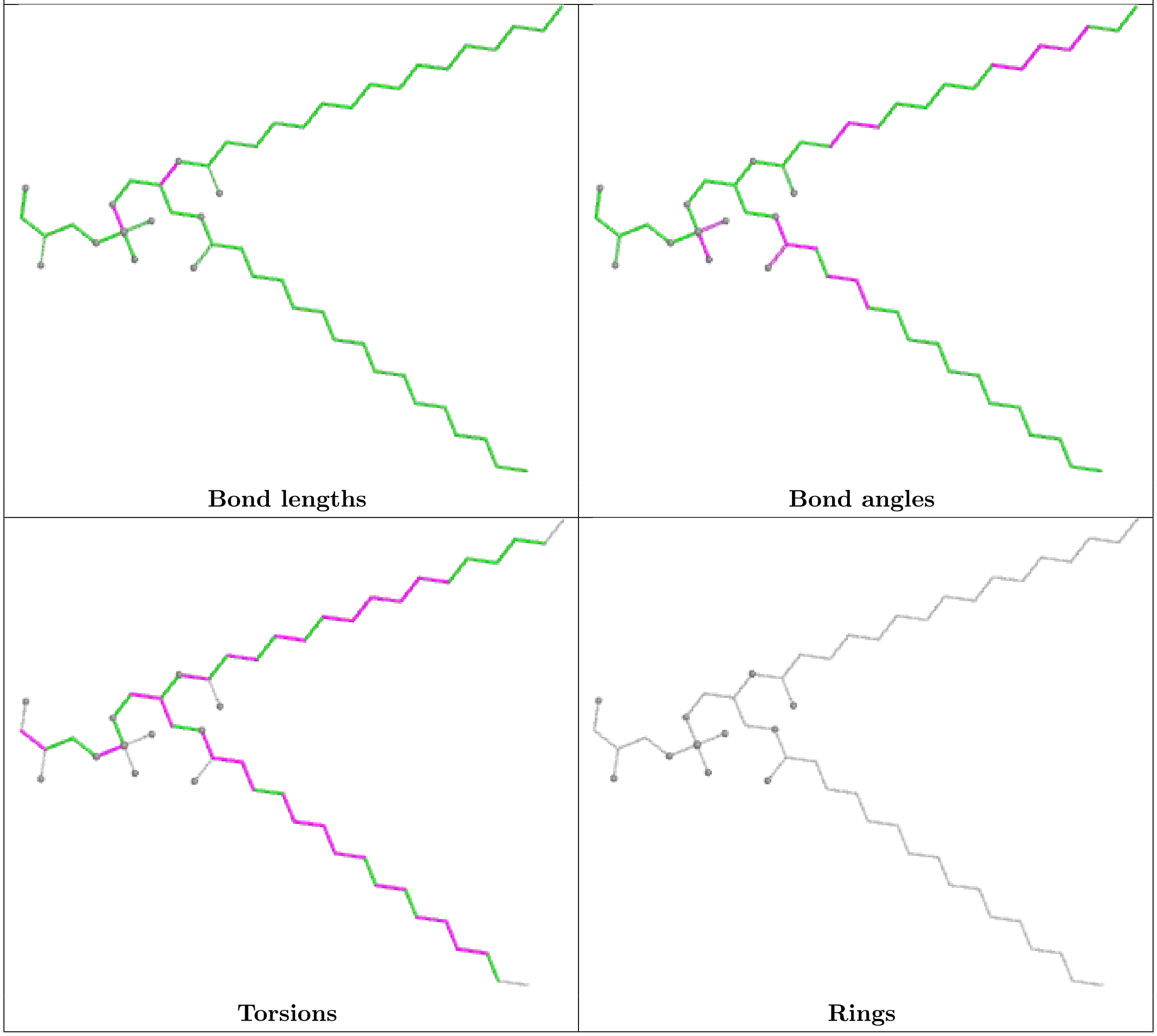
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG G 846



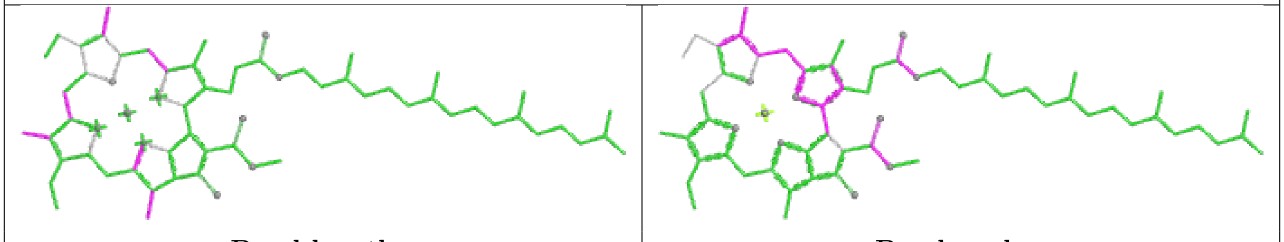
Bond lengths

Bond angles

Torsions

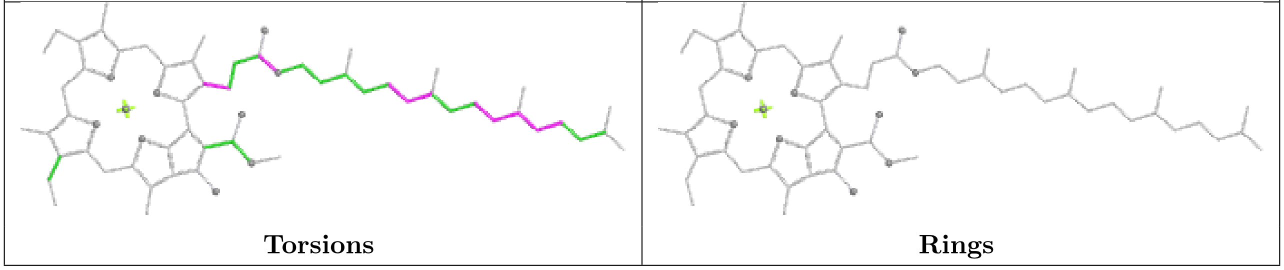
Rings

Ligand CLA L 203



Bond lengths

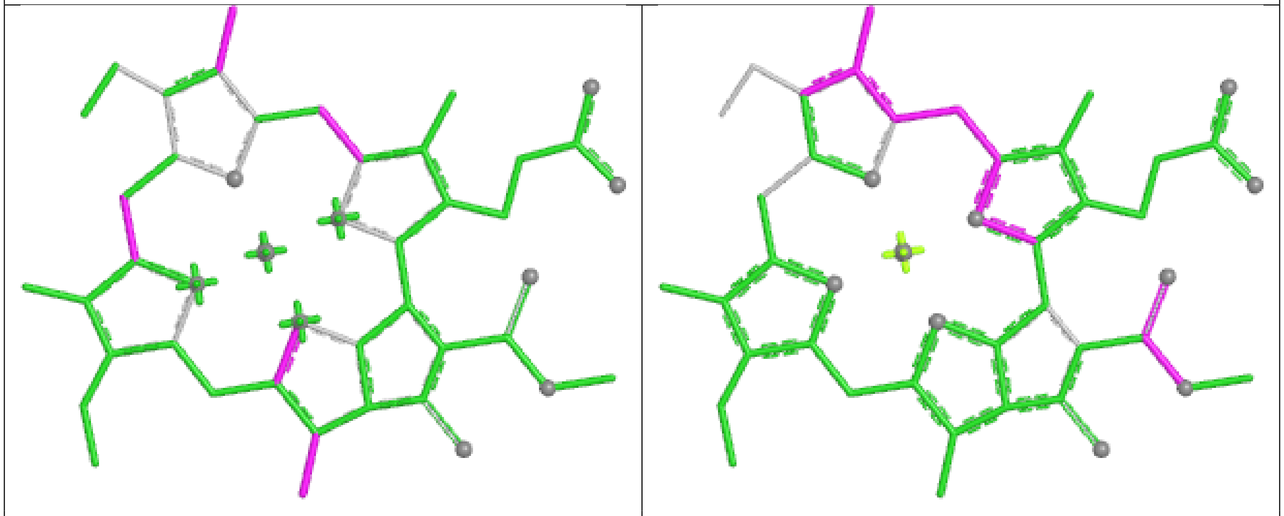
Bond angles



Torsions

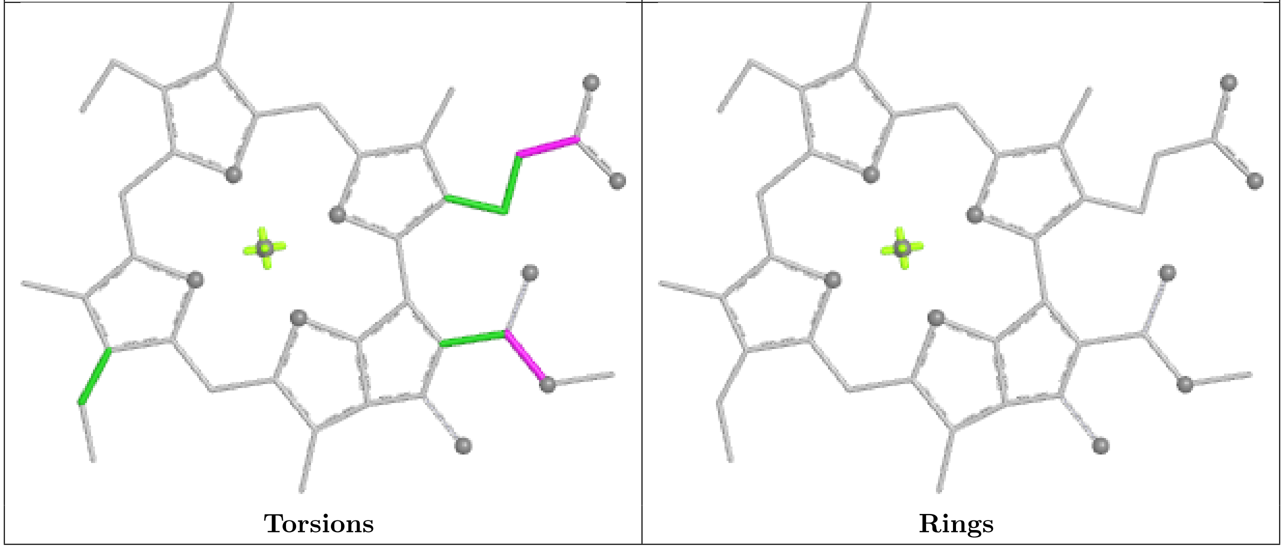
Rings

Ligand CLA H 2134



Bond lengths

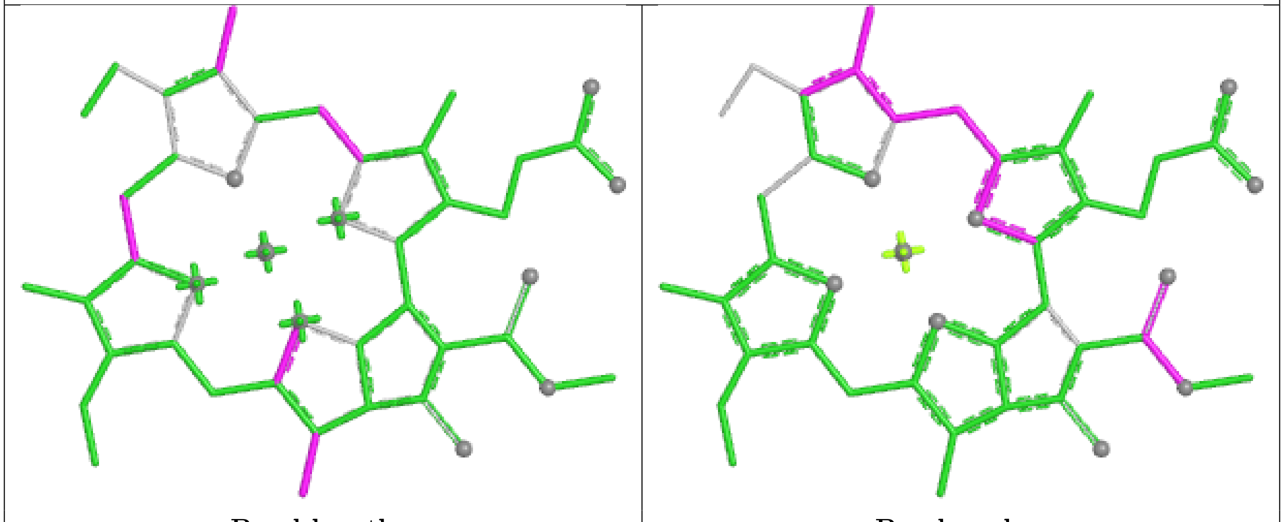
Bond angles



Torsions

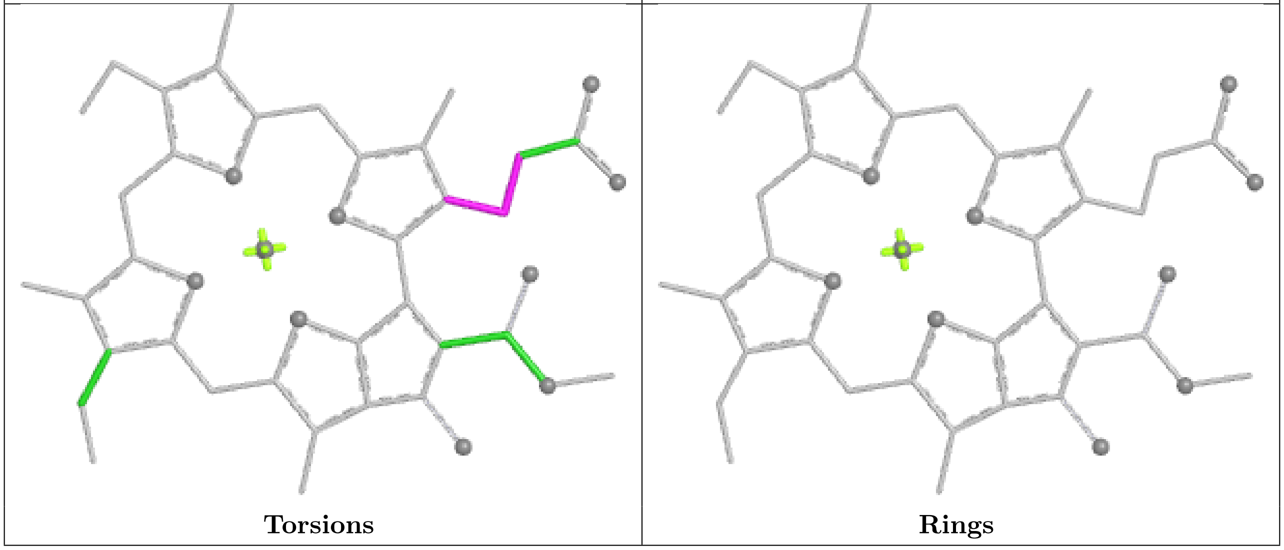
Rings

Ligand CLA f 204



Bond lengths

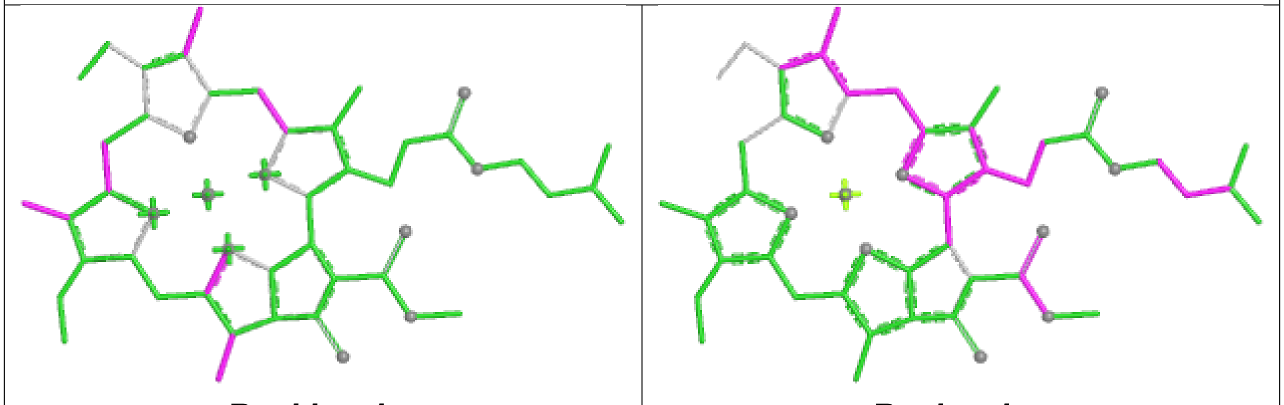
Bond angles

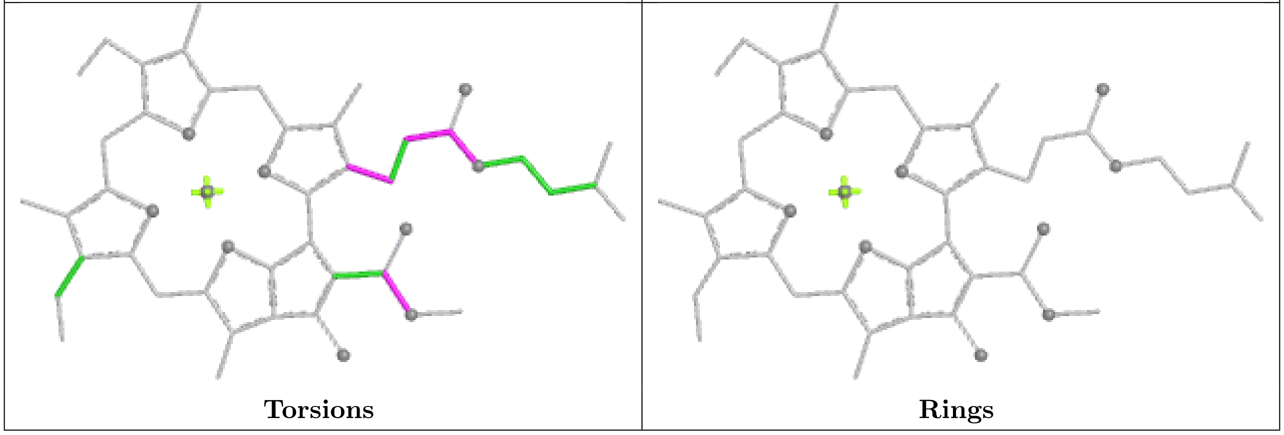


Torsions

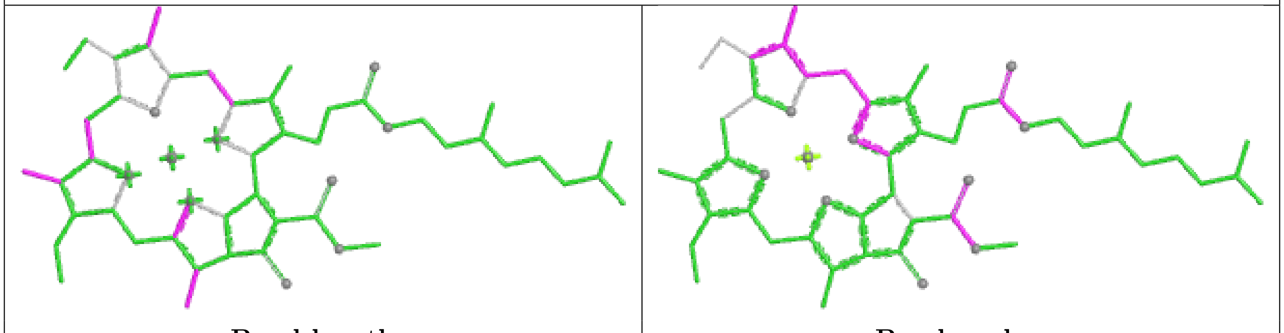
Rings

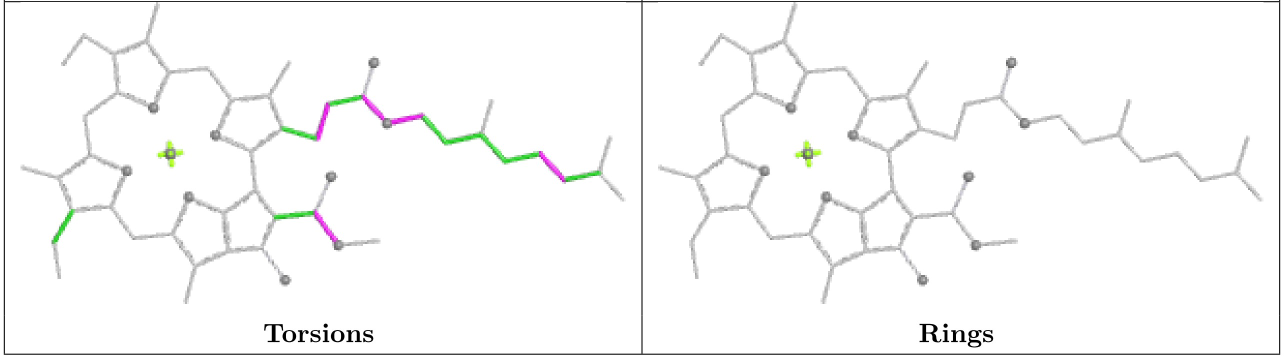
Ligand CLA G 809


Bond lengths
Bond angles

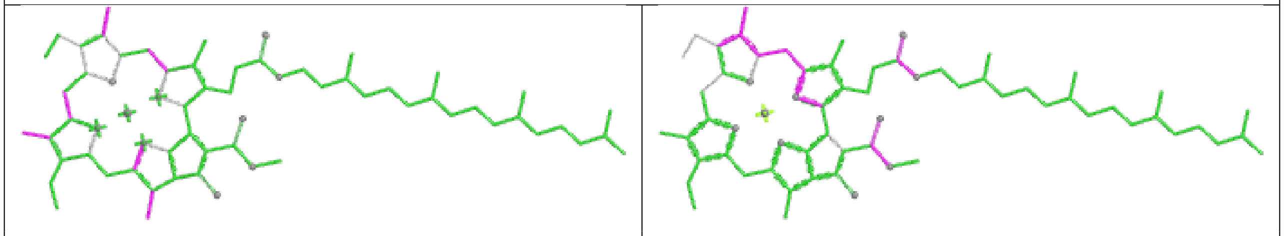

Torsions
Rings

Ligand CLA b 2131


Bond lengths
Bond angles

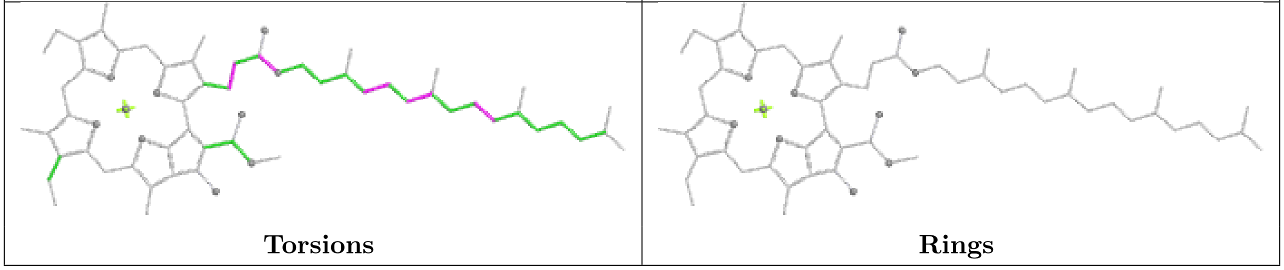

Torsions
Rings

Ligand CLA H 2105



Bond lengths

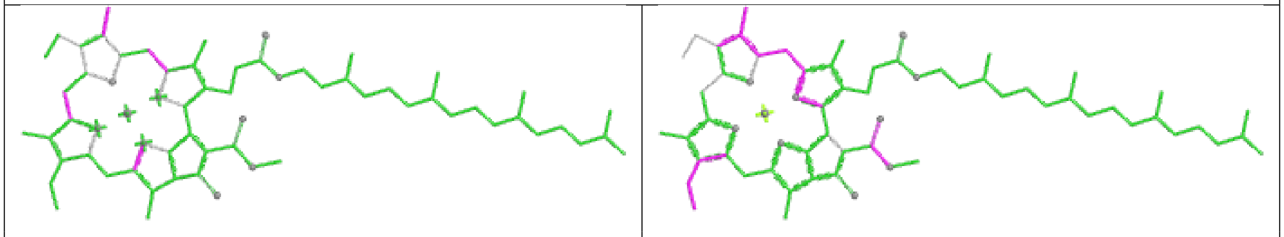
Bond angles



Torsions

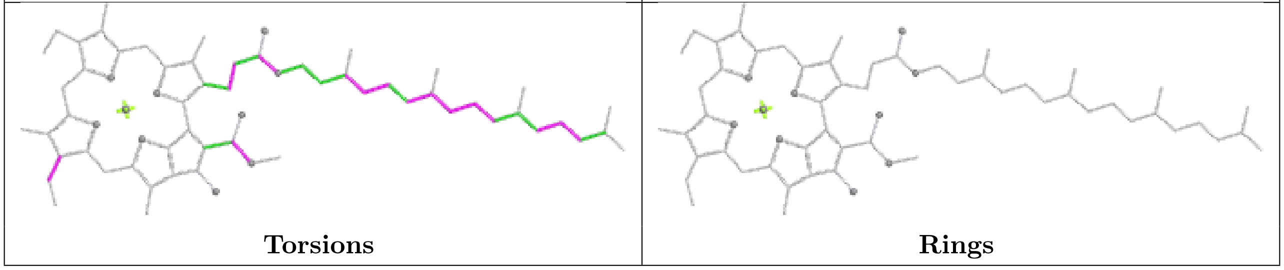
Rings

Ligand CLA b 2132



Bond lengths

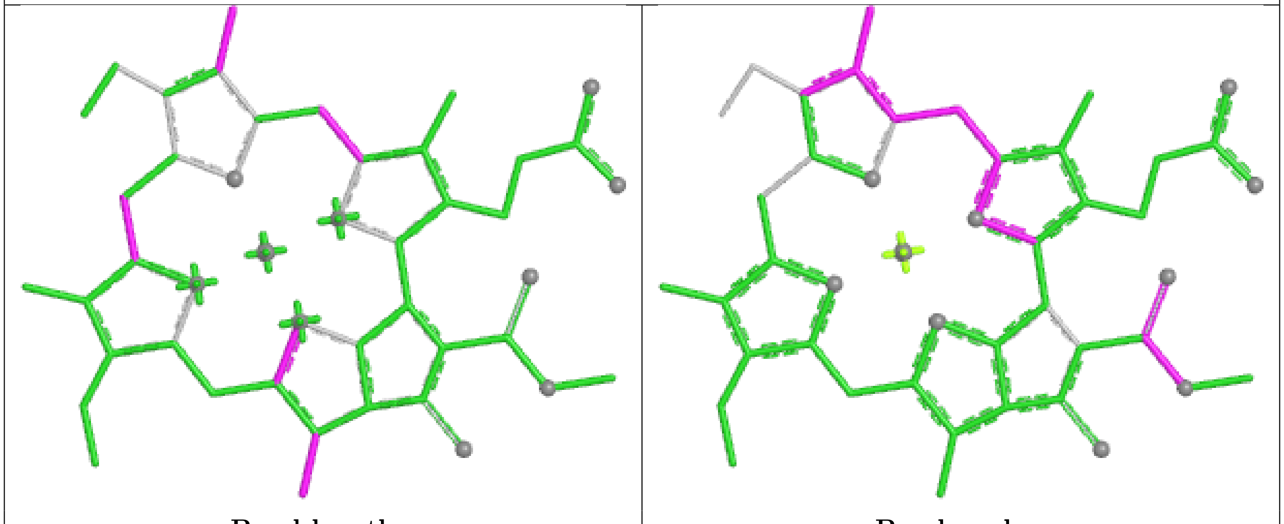
Bond angles



Torsions

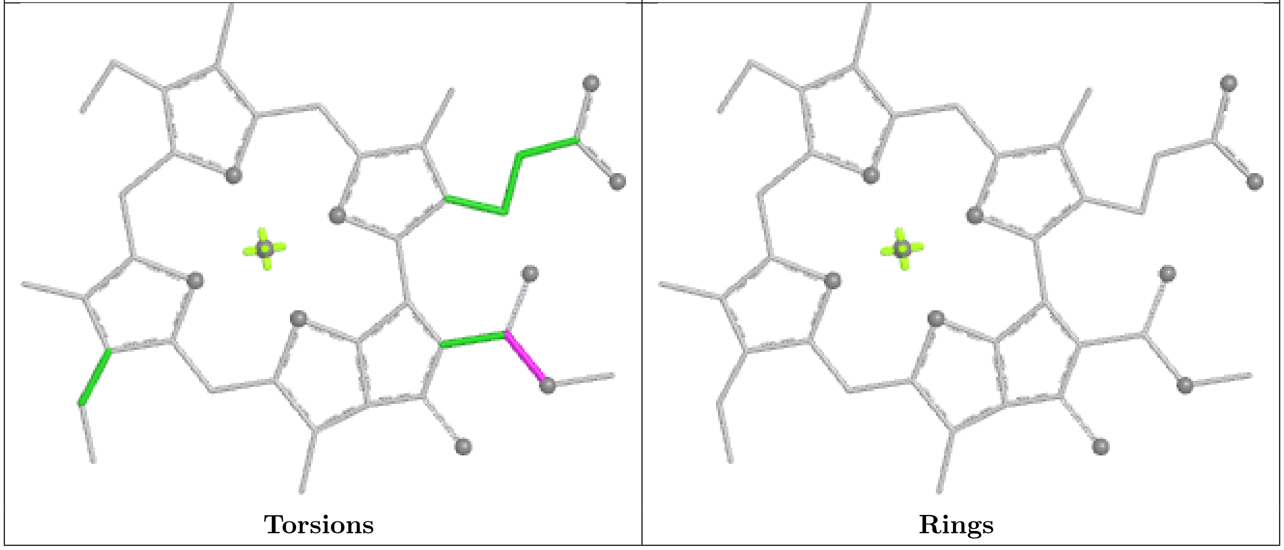
Rings

Ligand CLA b 2115



Bond lengths

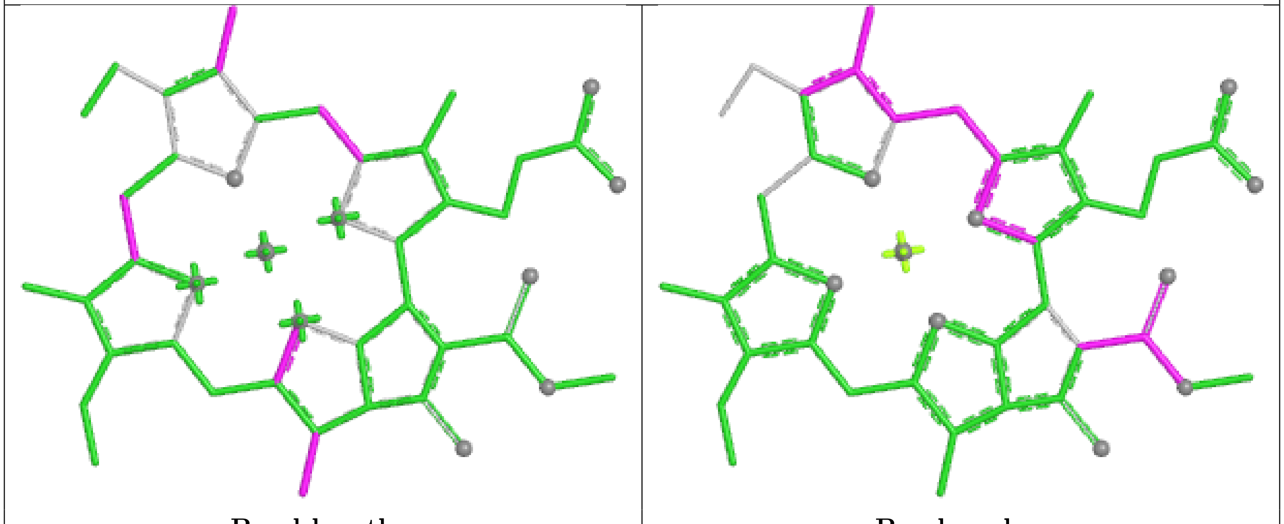
Bond angles



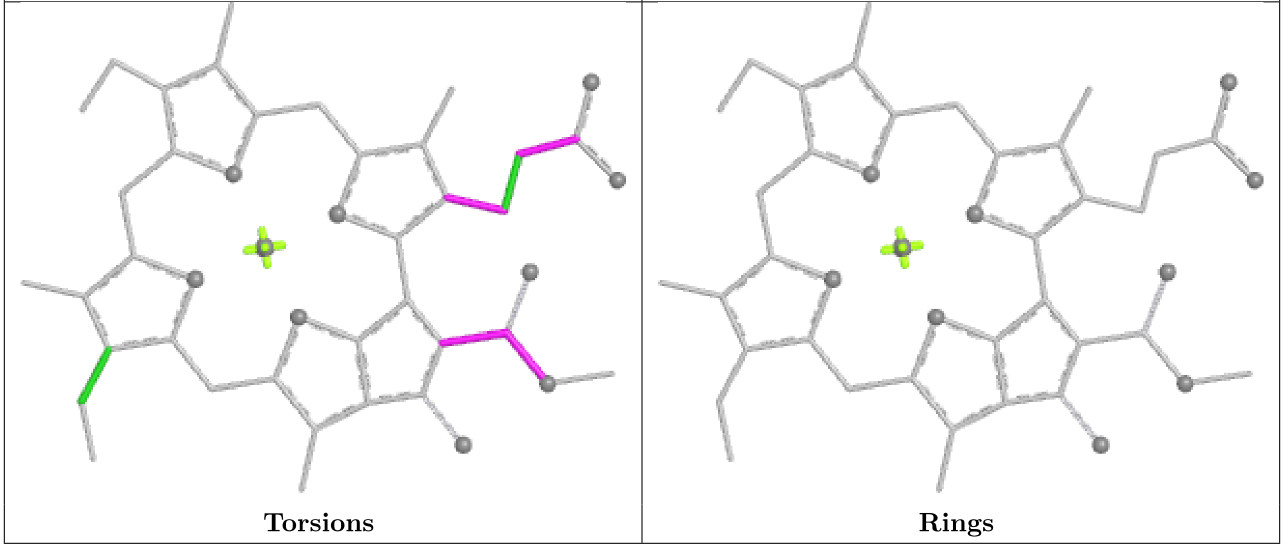
Torsions

Rings

Ligand CLA J 103

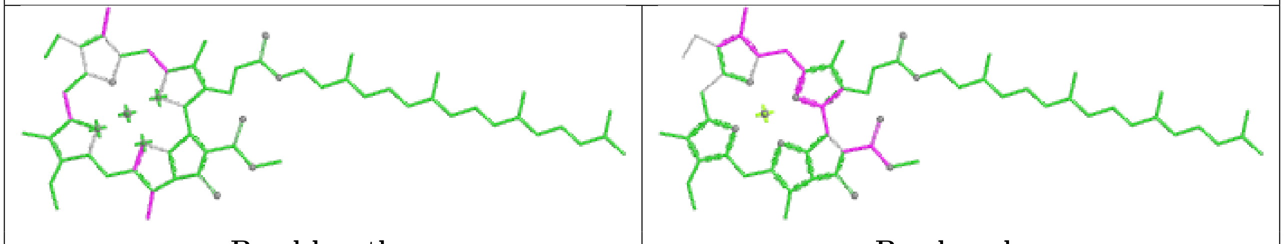


Bond lengths Bond angles

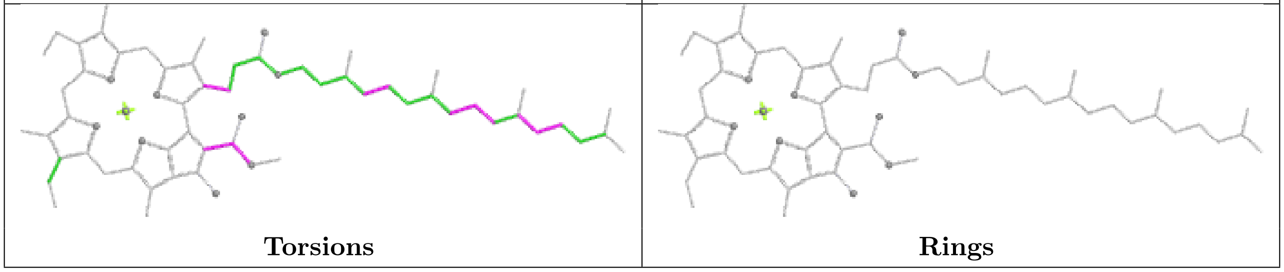


Torsions Rings

Ligand CLA G 812

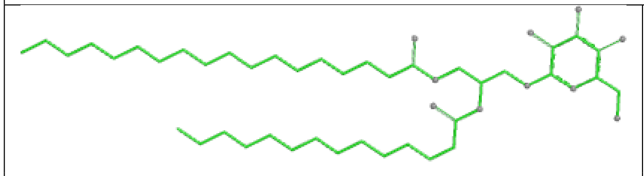


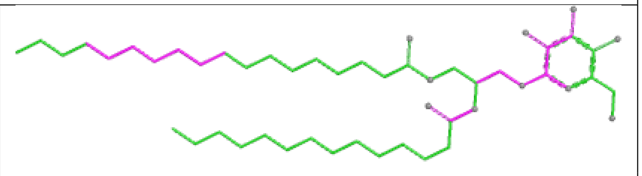
Bond lengths Bond angles

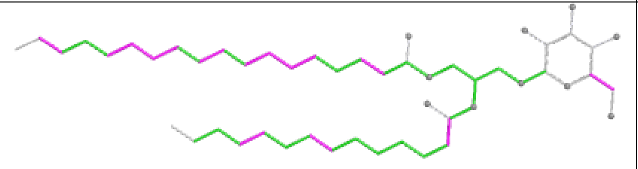


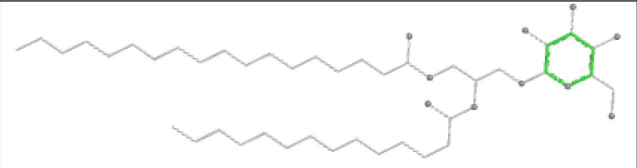
Torsions Rings

Ligand LMG b 2147

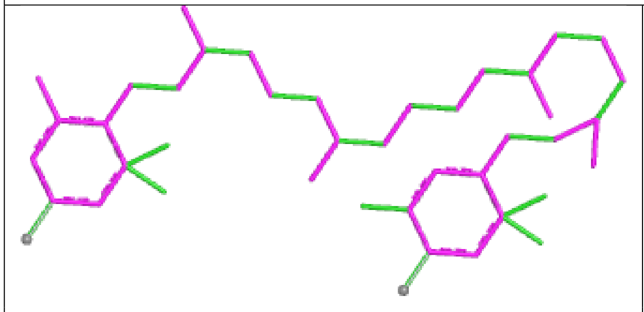

Bond lengths

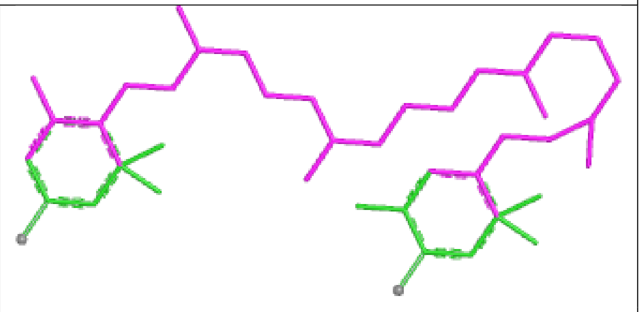

Bond angles

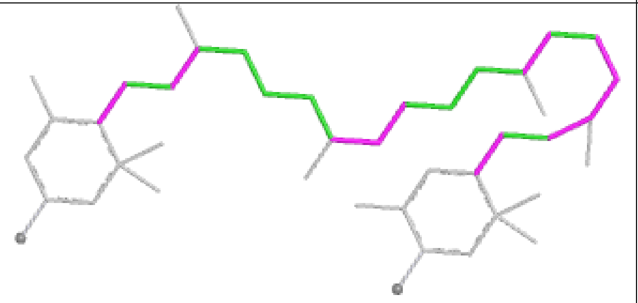

Torsions

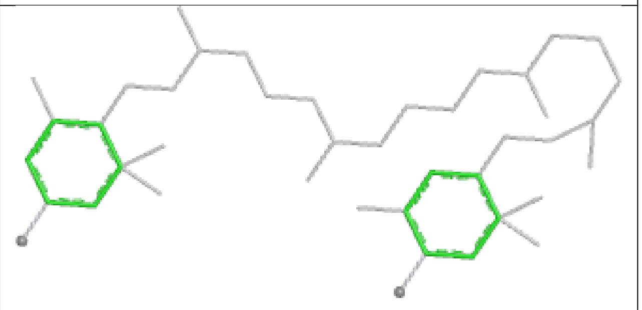

Rings

Ligand ZEX Q 205

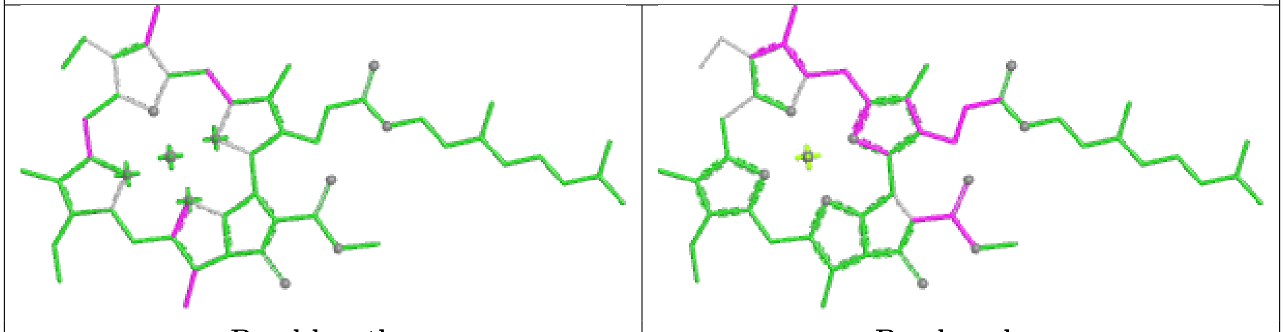

Bond lengths


Bond angles


Torsions

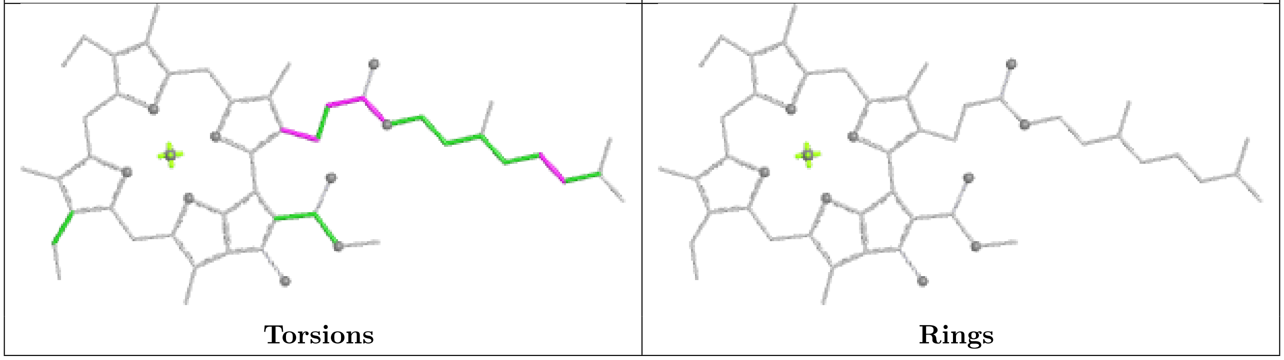

Rings

Ligand CLA A 854



Bond lengths

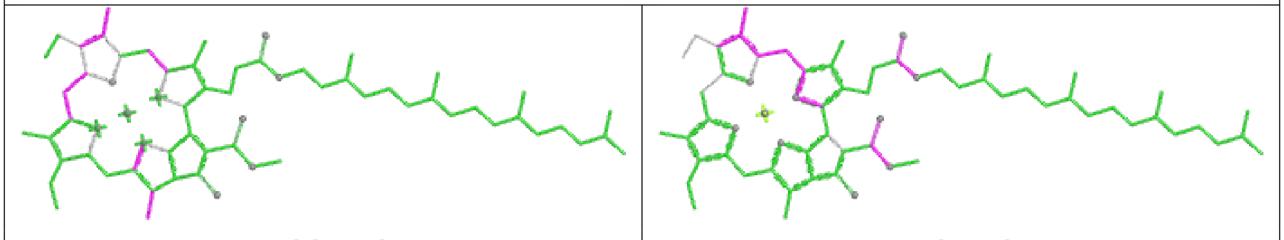
Bond angles



Torsions

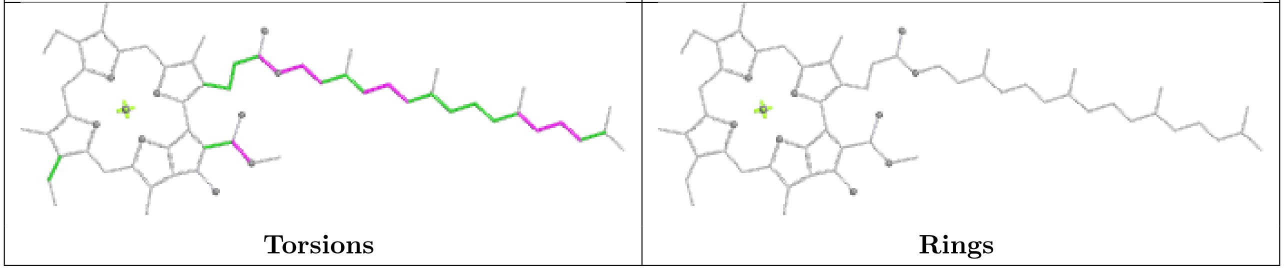
Rings

Ligand CLA b 2110



Bond lengths

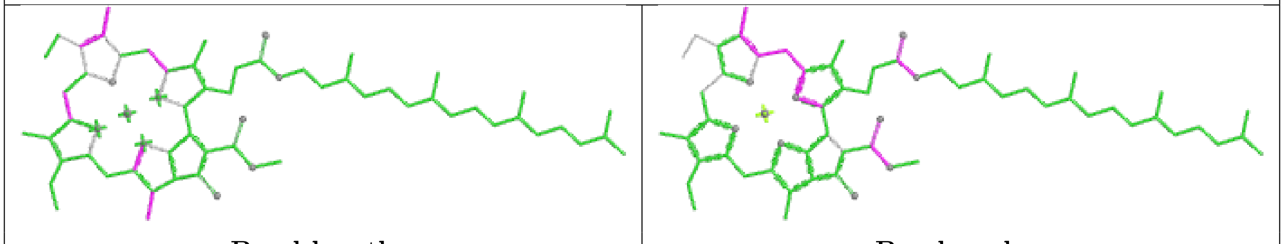
Bond angles



Torsions

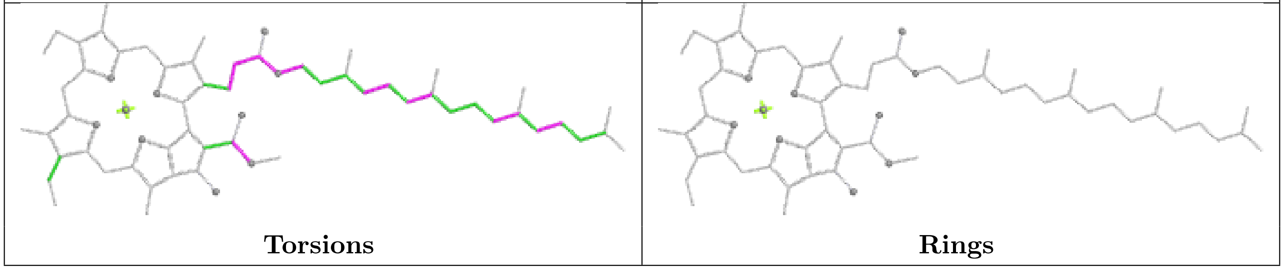
Rings

Ligand CLA b 2140



Bond lengths

Bond angles



Torsions

Rings

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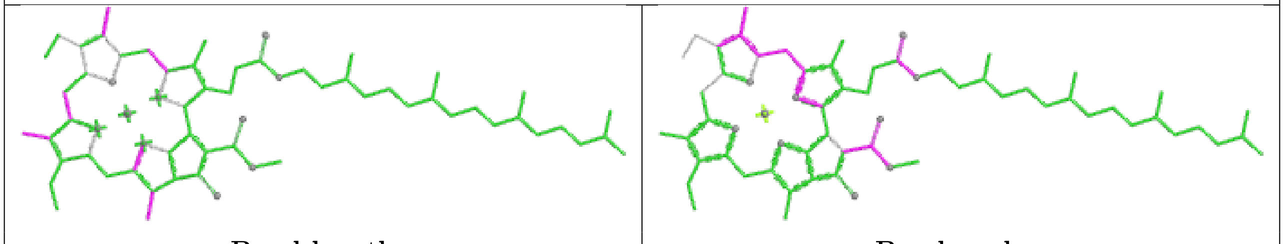
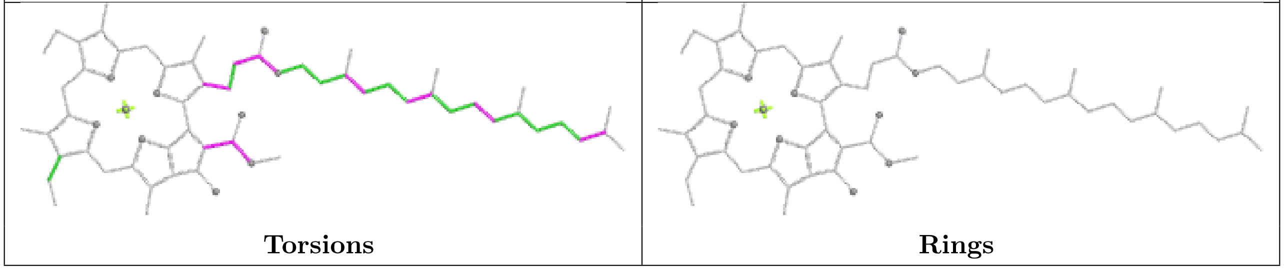


Bond lengths

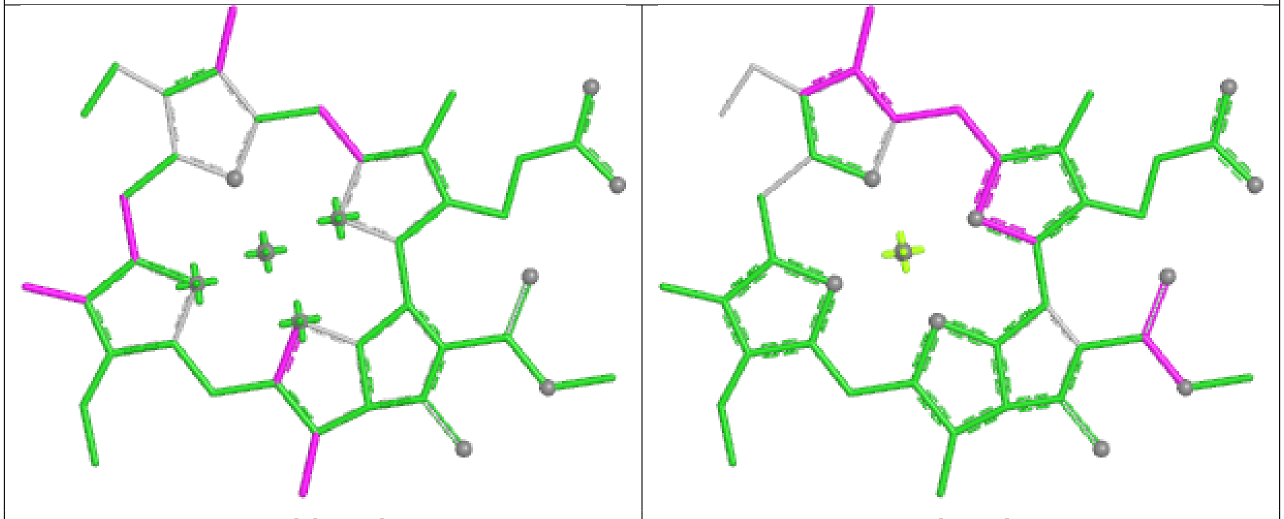
Bond angles



Torsions

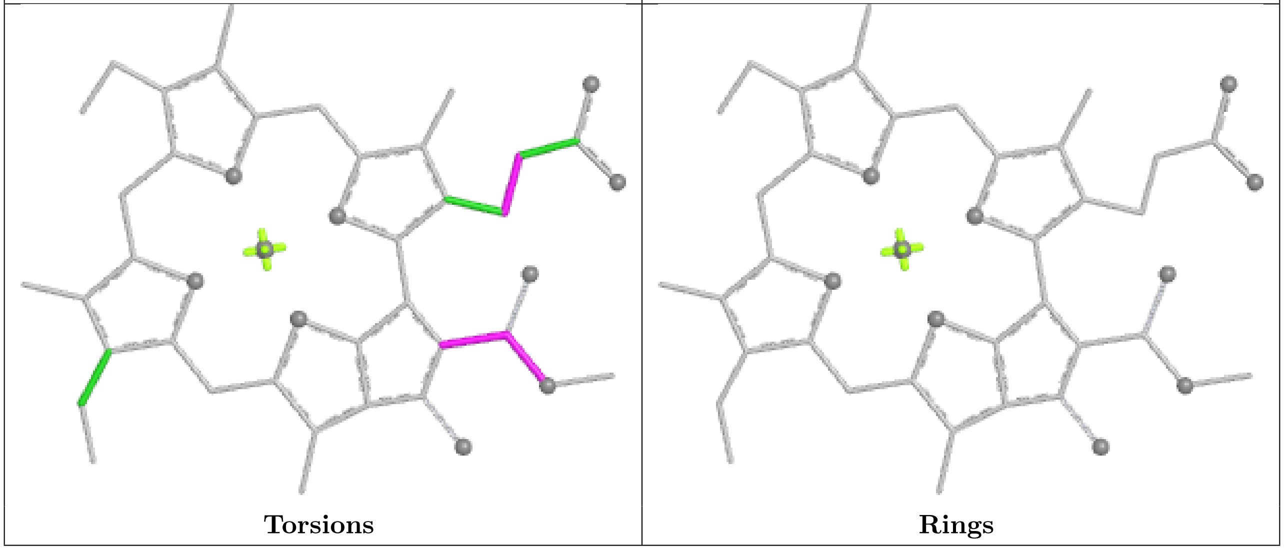
Rings

Ligand CLA G 814



Bond lengths

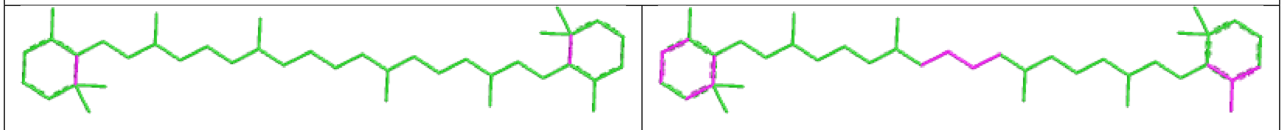
Bond angles



Torsions

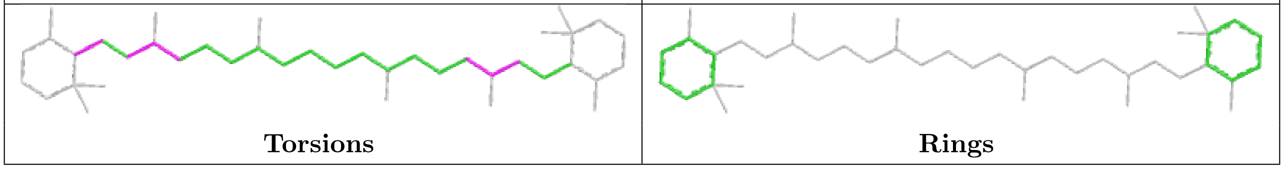
Rings

Ligand BCR i 101



Bond lengths

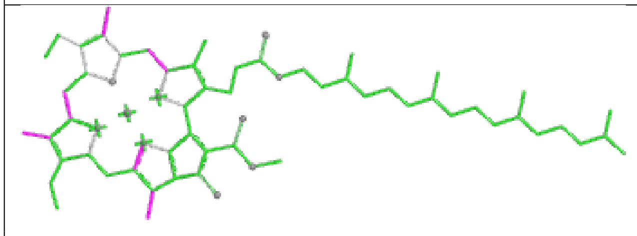
Bond angles



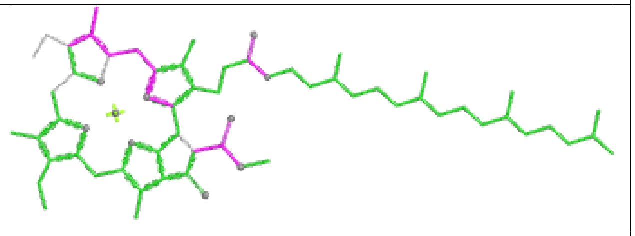
Torsions

Rings

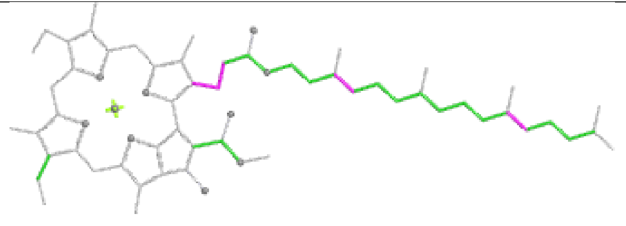
Ligand CLA l 204



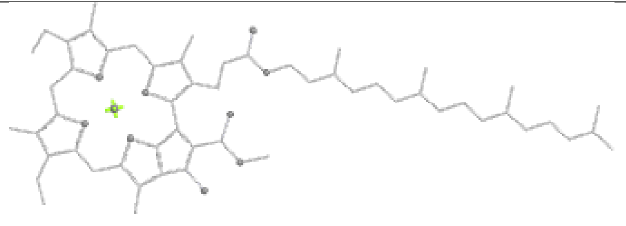
Bond lengths



Bond angles

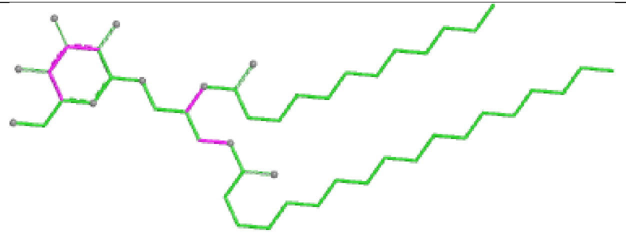


Torsions

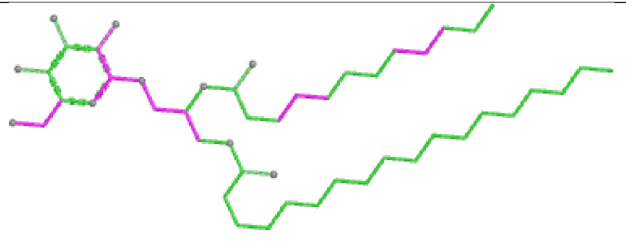


Rings

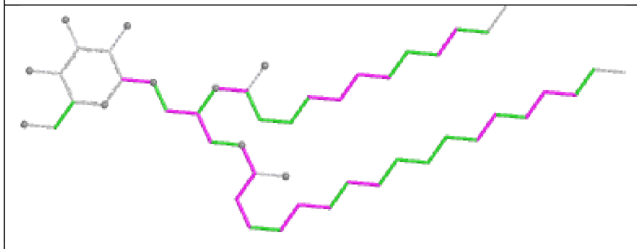
Ligand DGD U 209



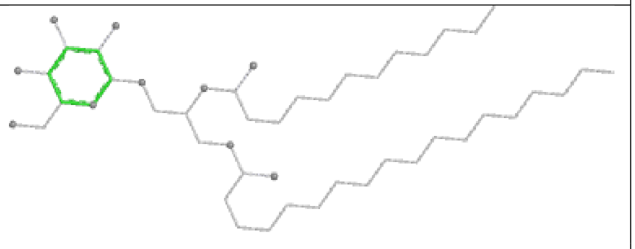
Bond lengths



Bond angles

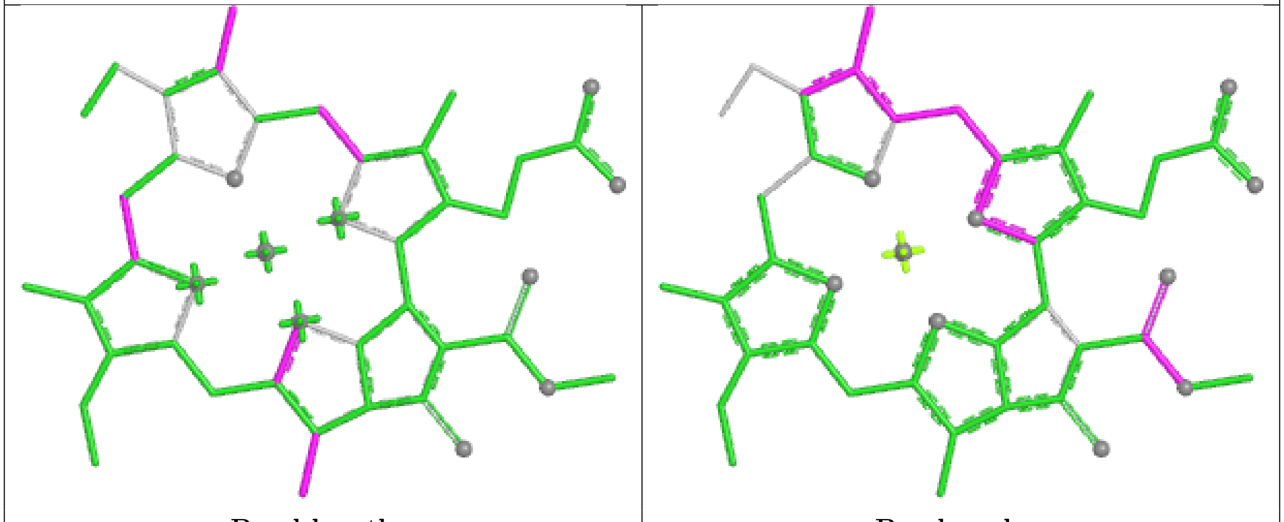


Torsions

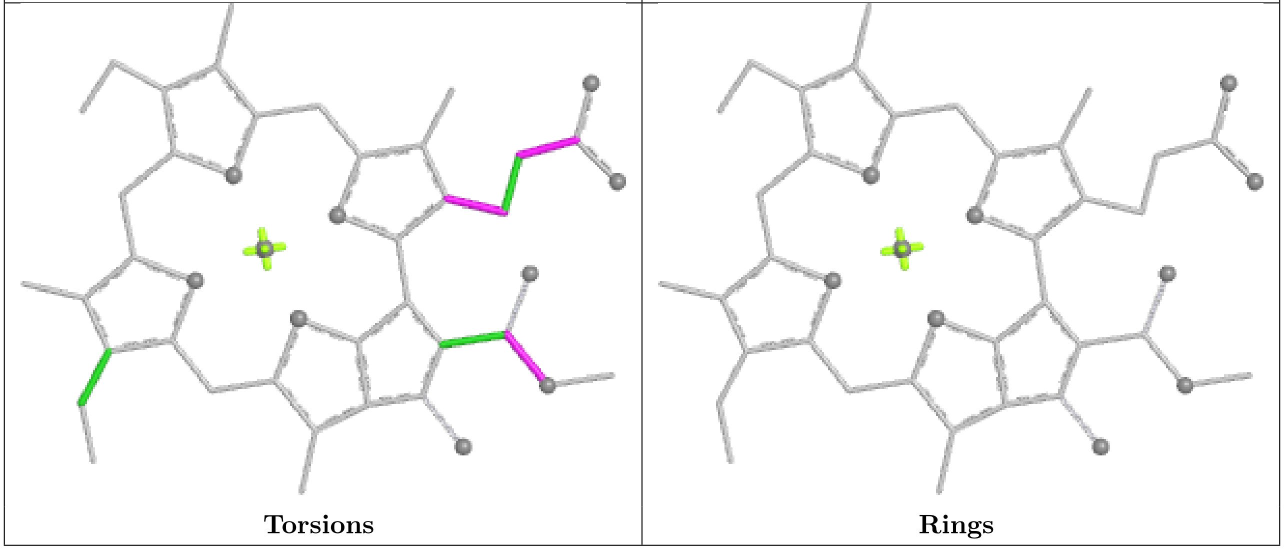


Rings

Ligand CLA A 811

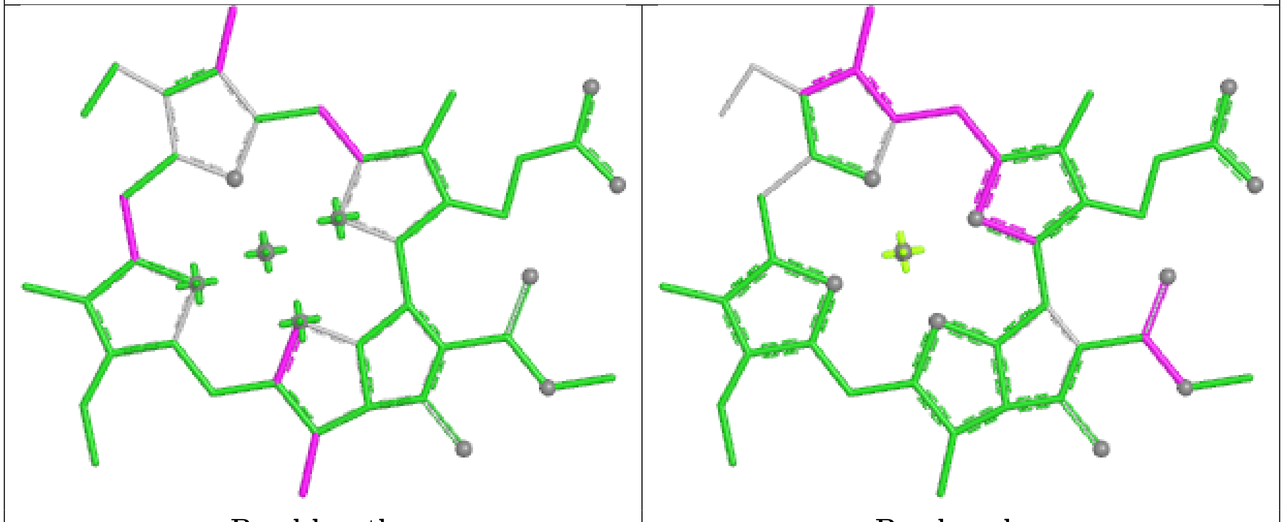


Bond lengths Bond angles

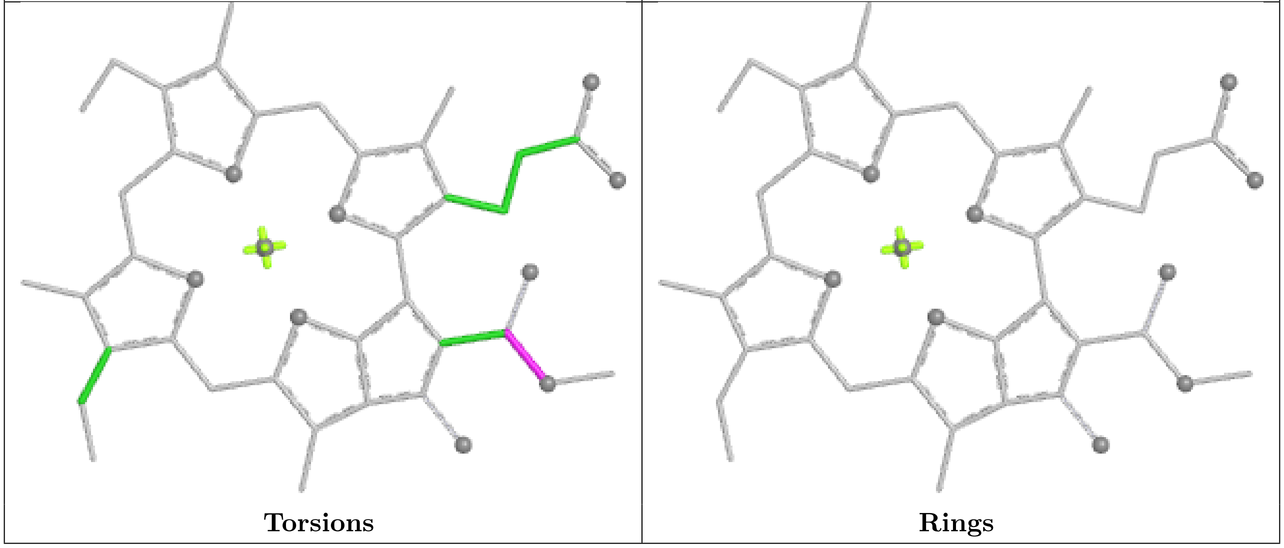


Torsions Rings

Ligand CLA H 2115

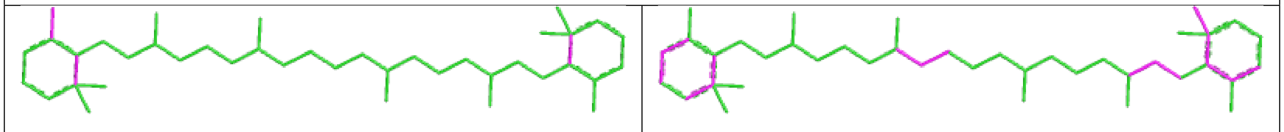


Bond lengths Bond angles

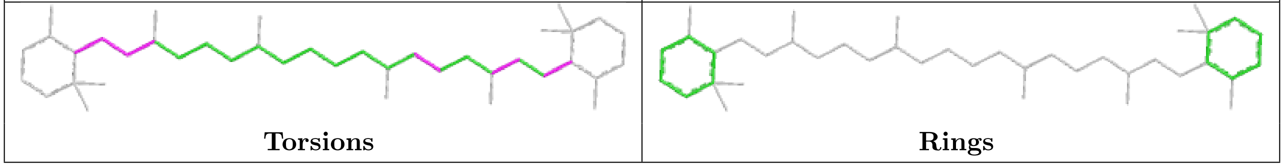


Torsions Rings

Ligand BCR T 4001

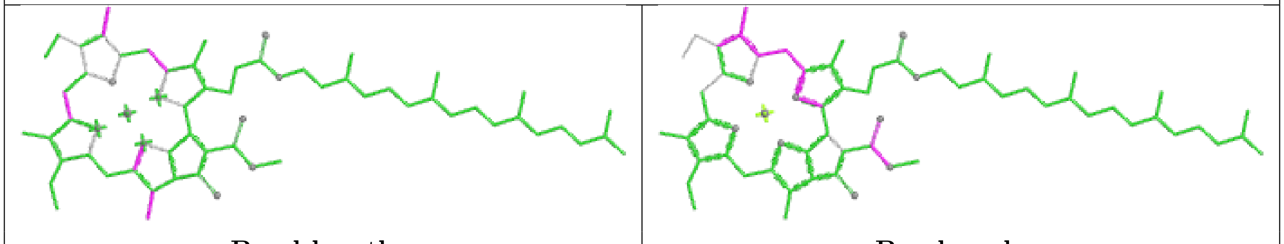


Bond lengths Bond angles



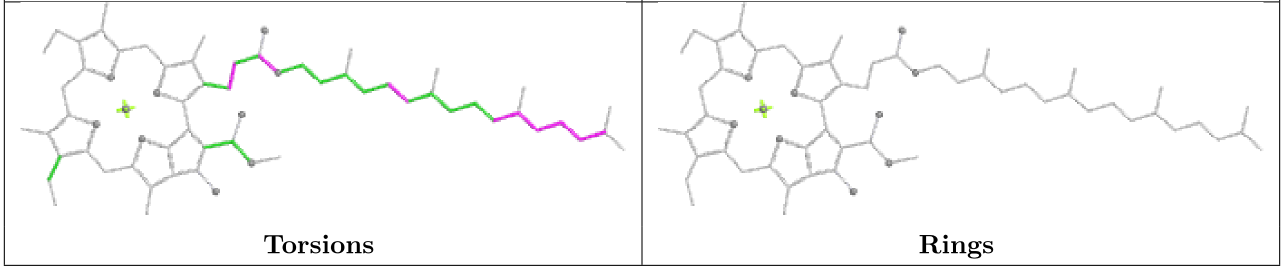
Torsions Rings

Ligand CLA a 828



Bond lengths

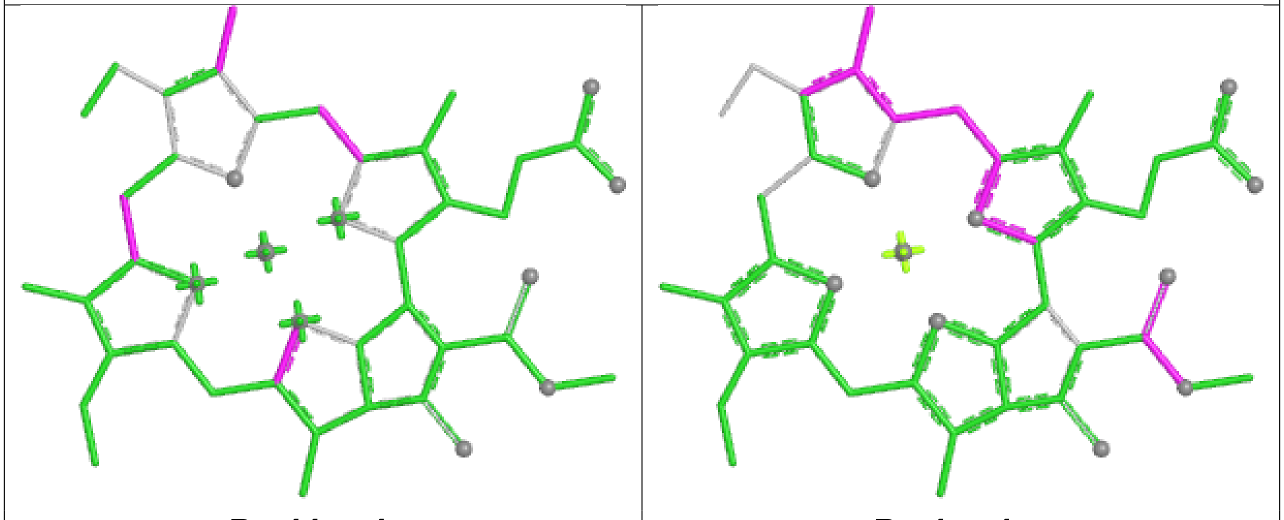
Bond angles



Torsions

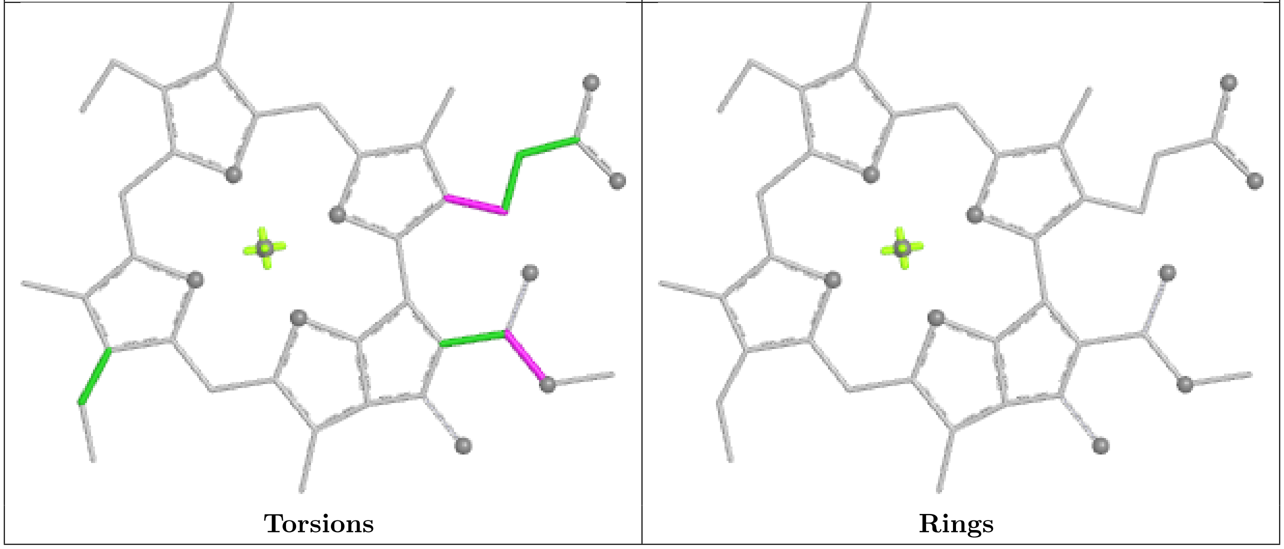
Rings

Ligand CLA G 815



Bond lengths

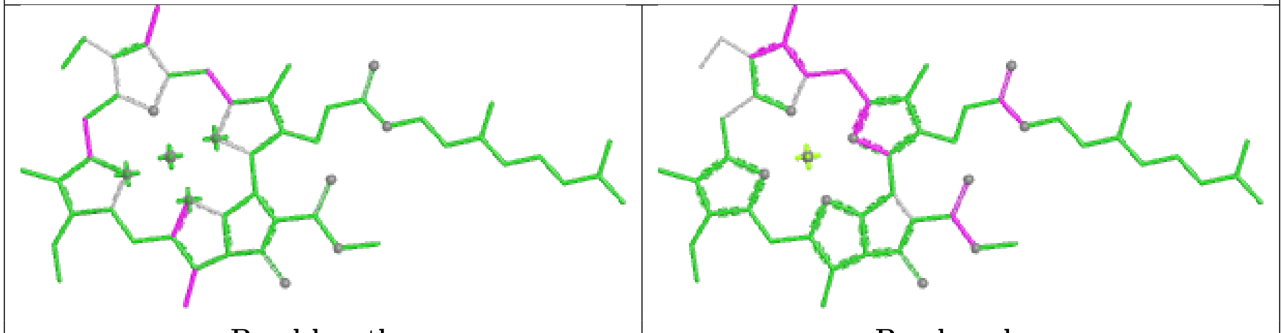
Bond angles



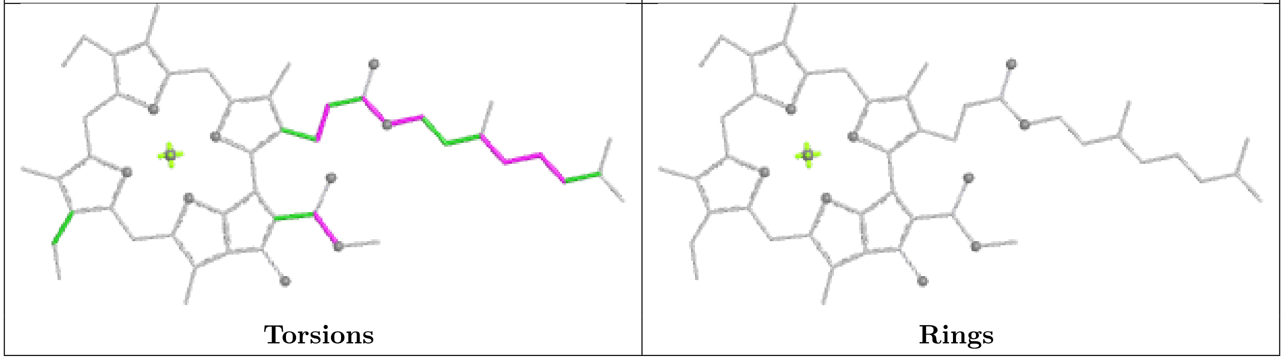
Torsions

Rings

Ligand CLA B 2122

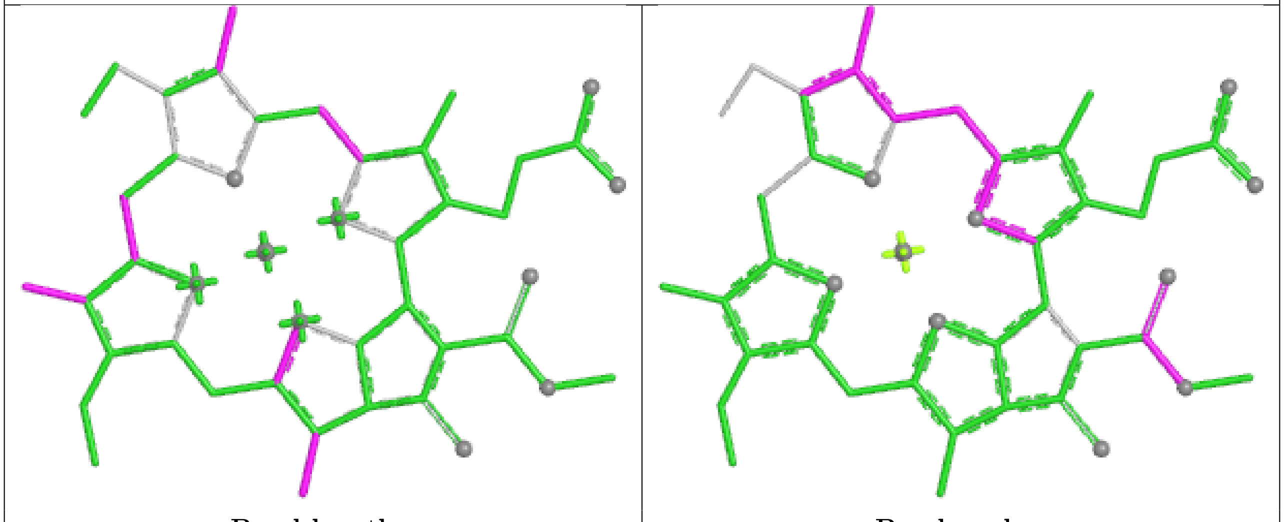


Bond lengths **Bond angles**

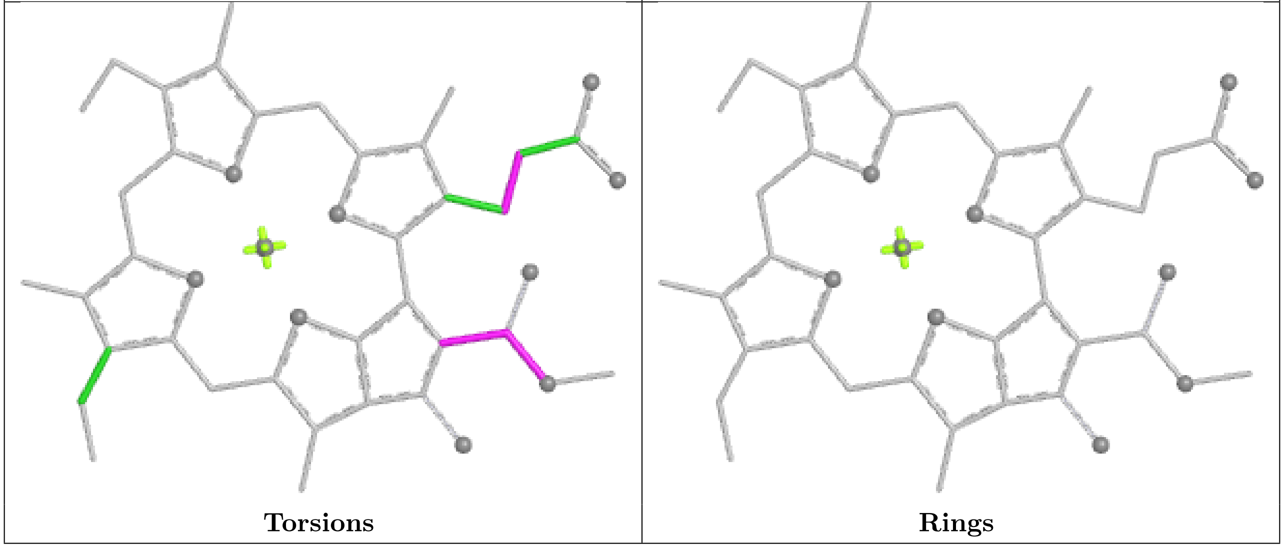


Torsions **Rings**

Ligand CLA A 814

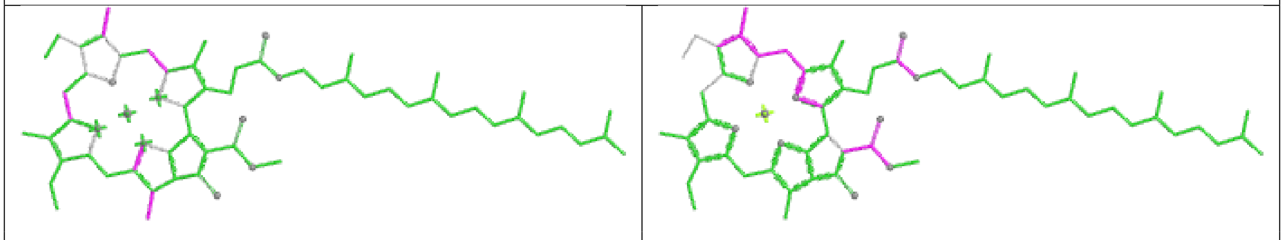


Bond lengths Bond angles

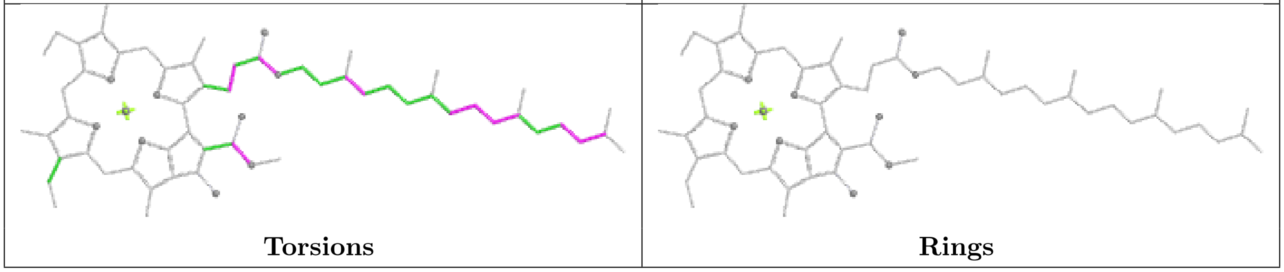


Torsions Rings

Ligand CLA a 810

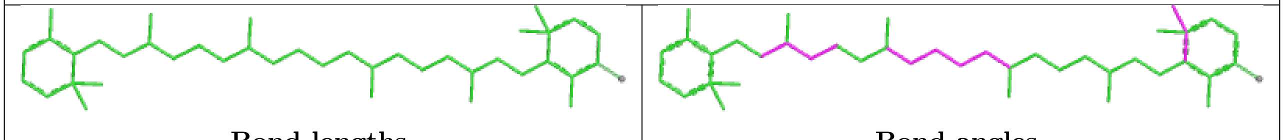


Bond lengths Bond angles

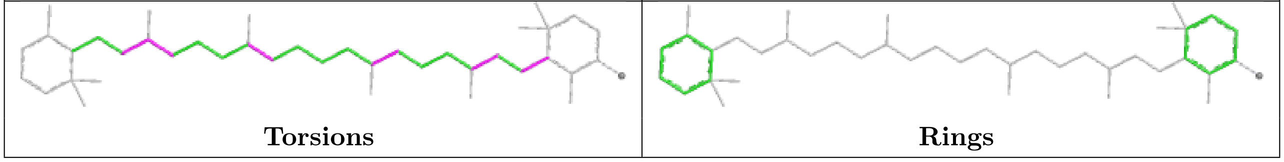


Torsions Rings

Ligand ECH H 2143

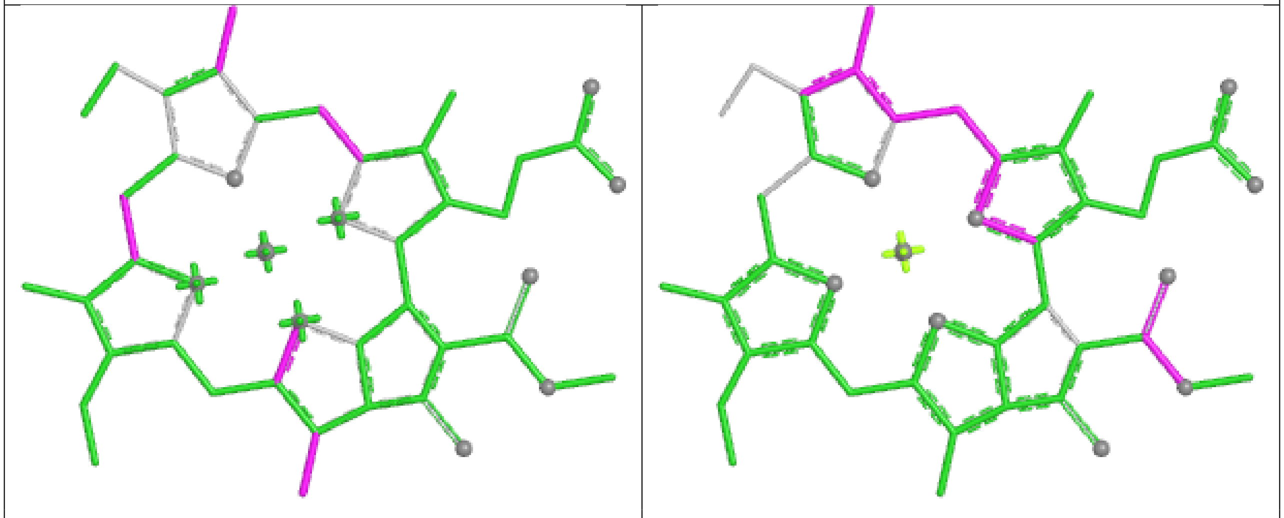


Bond lengths Bond angles

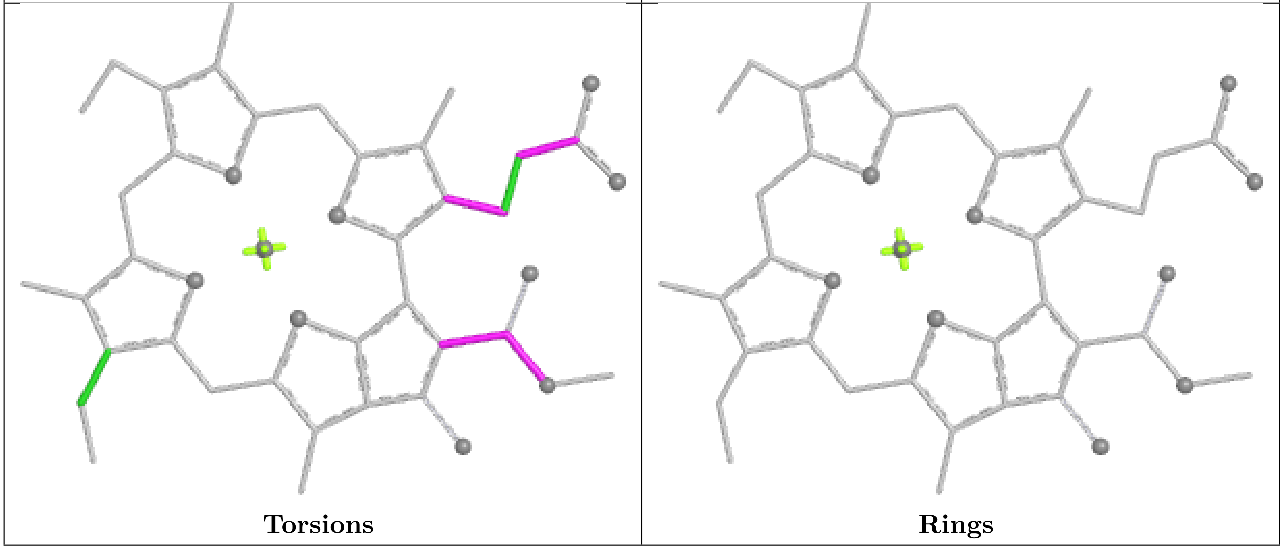


Torsions Rings

Ligand CLA k 4002

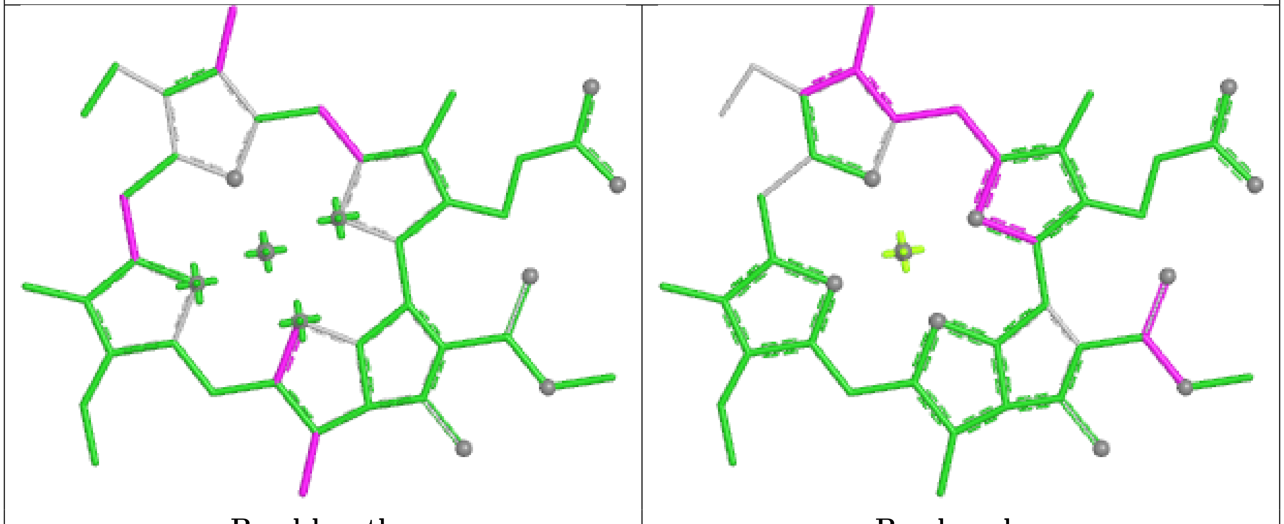


Bond lengths Bond angles



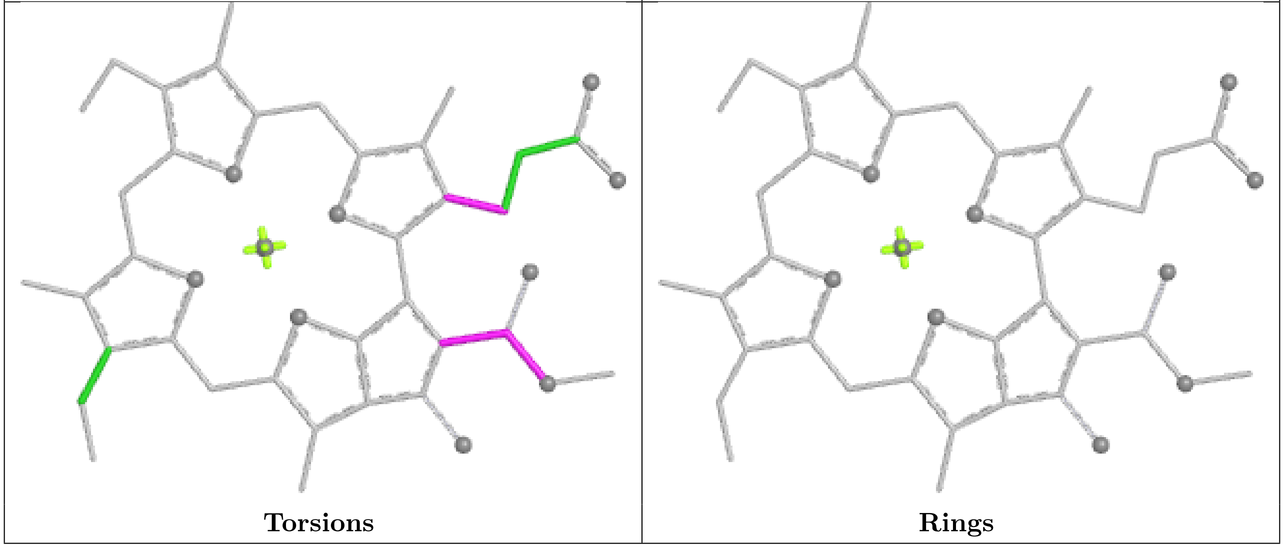
Torsions Rings

Ligand CLA H 2136



Bond lengths

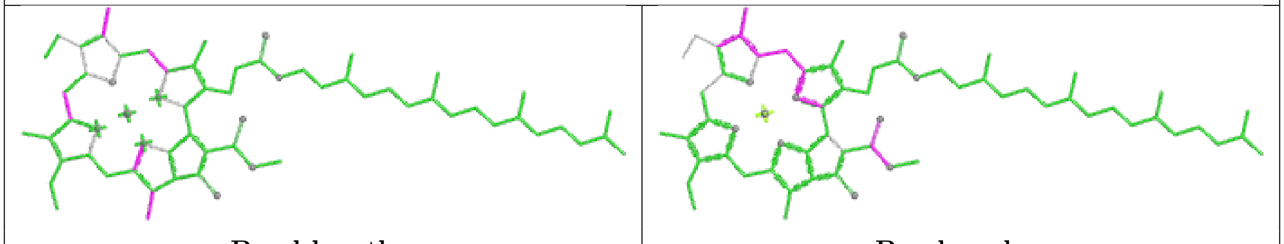
Bond angles



Torsions

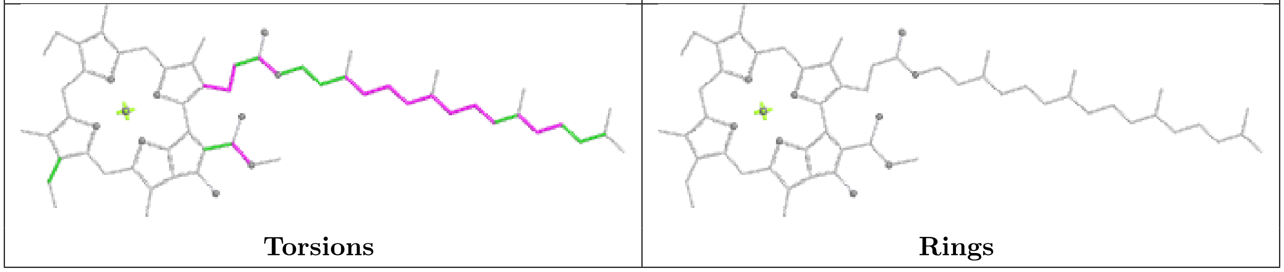
Rings

Ligand CLA Q 201



Bond lengths

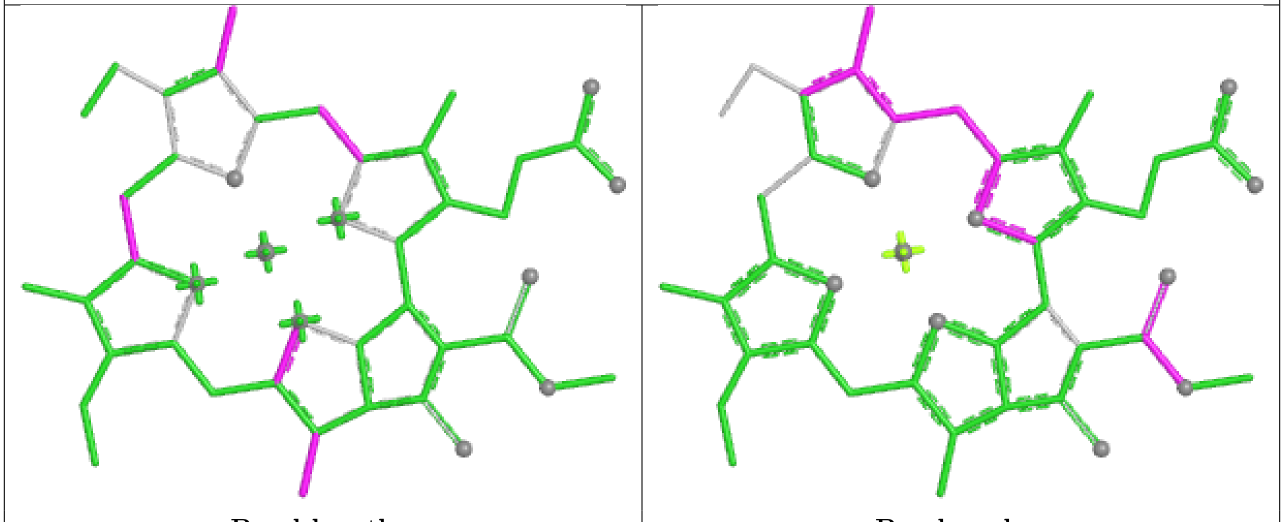
Bond angles



Torsions

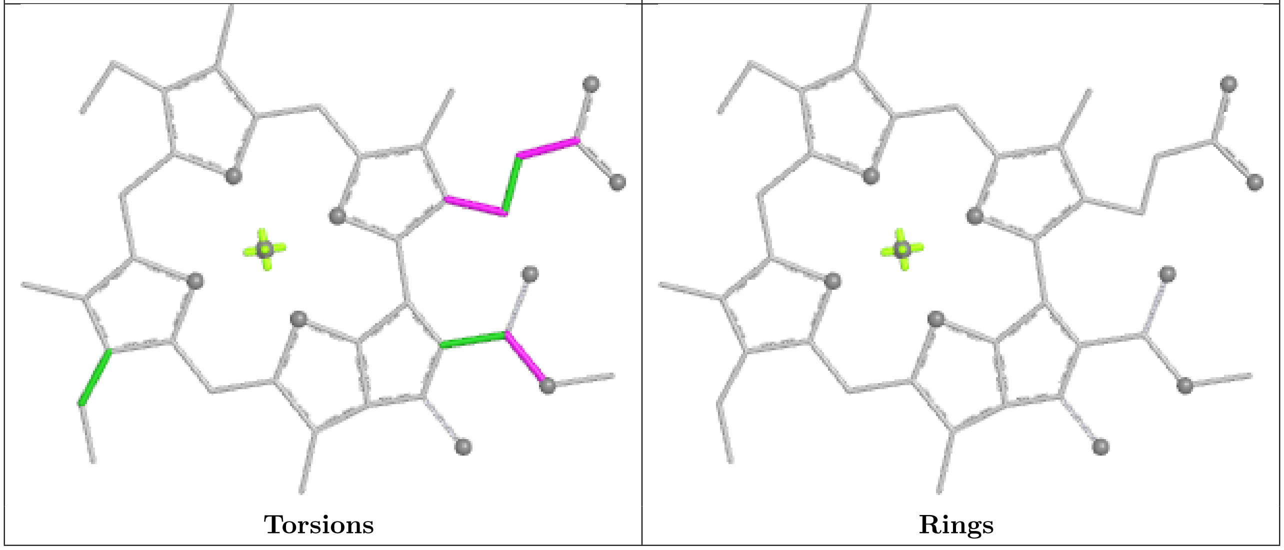
Rings

Ligand CLA G 811



Bond lengths

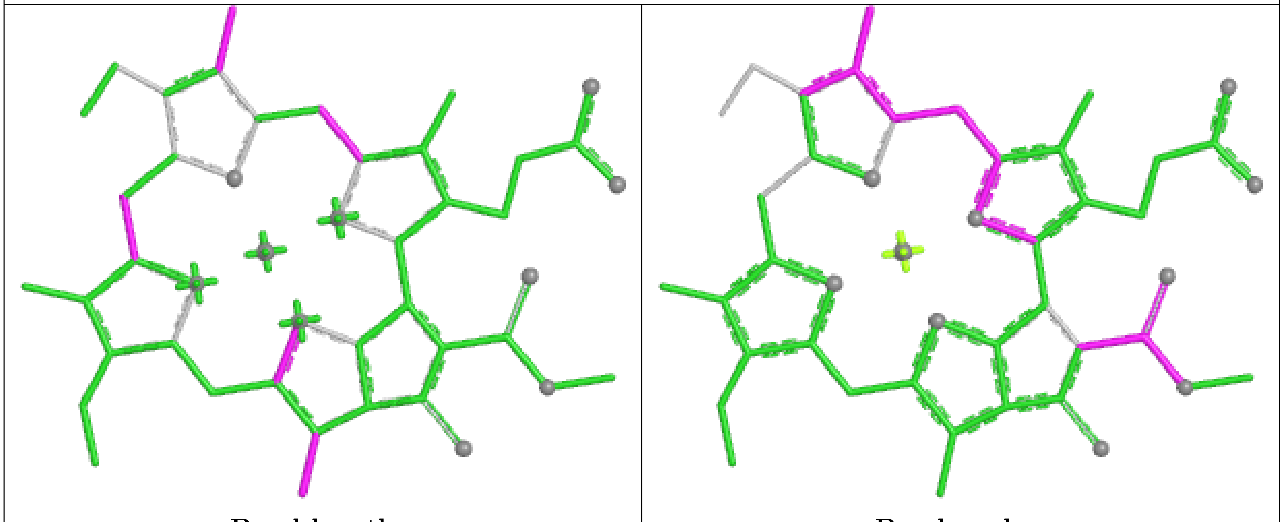
Bond angles



Torsions

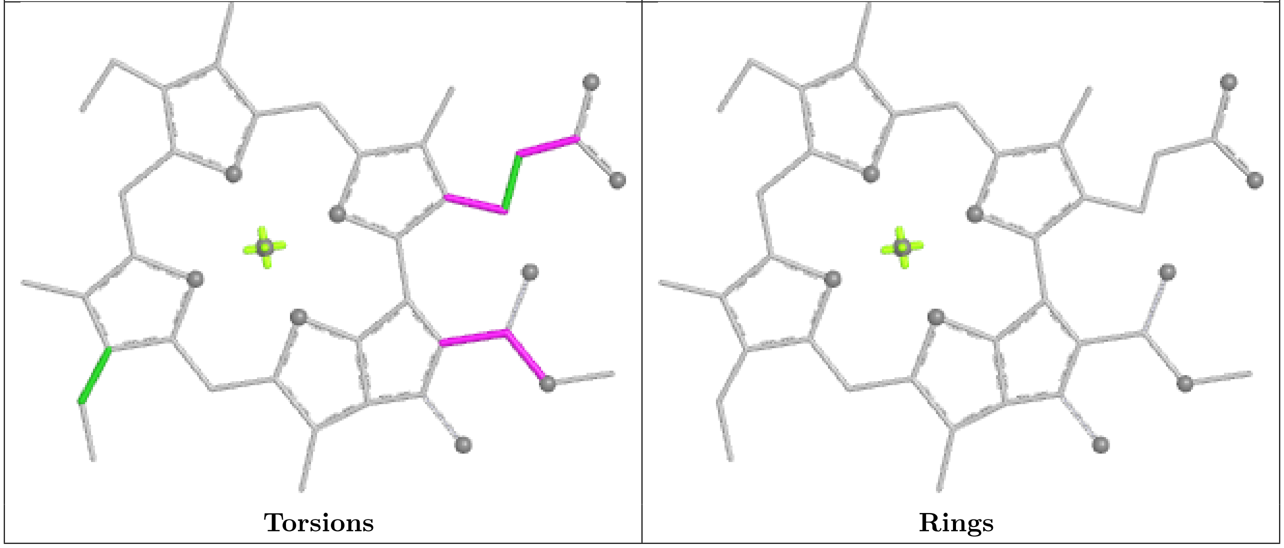
Rings

Ligand CLA j 103



Bond lengths

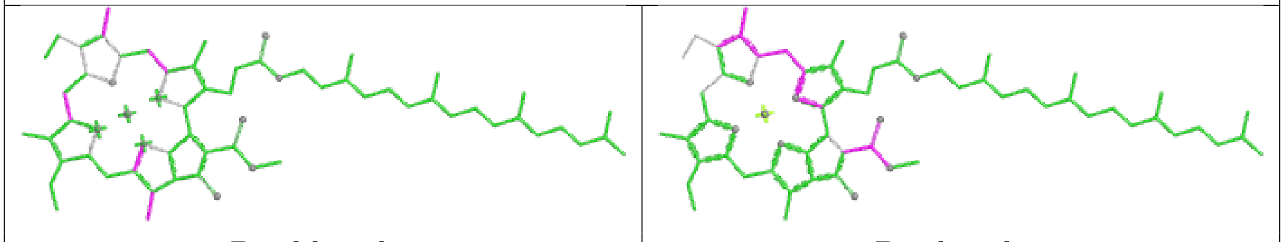
Bond angles



Torsions

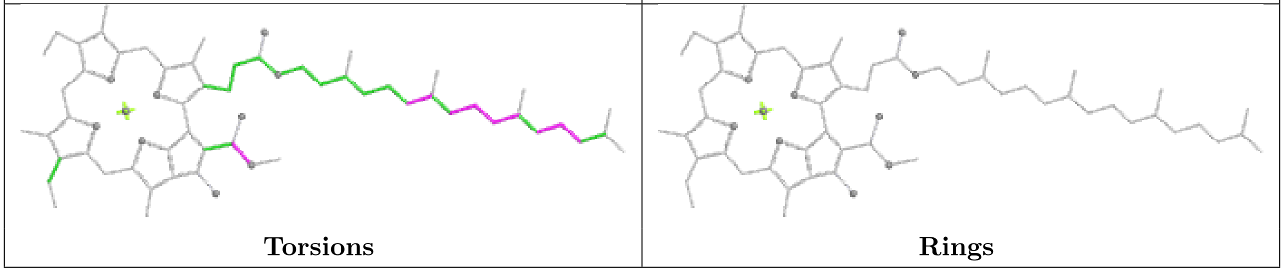
Rings

Ligand CLA a 832



Bond lengths

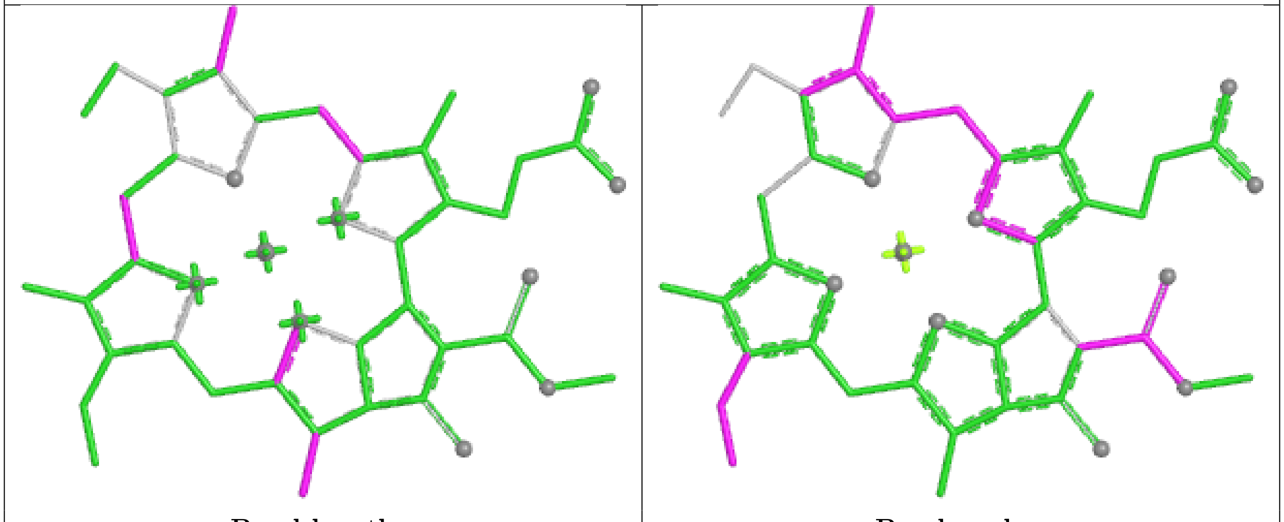
Bond angles



Torsions

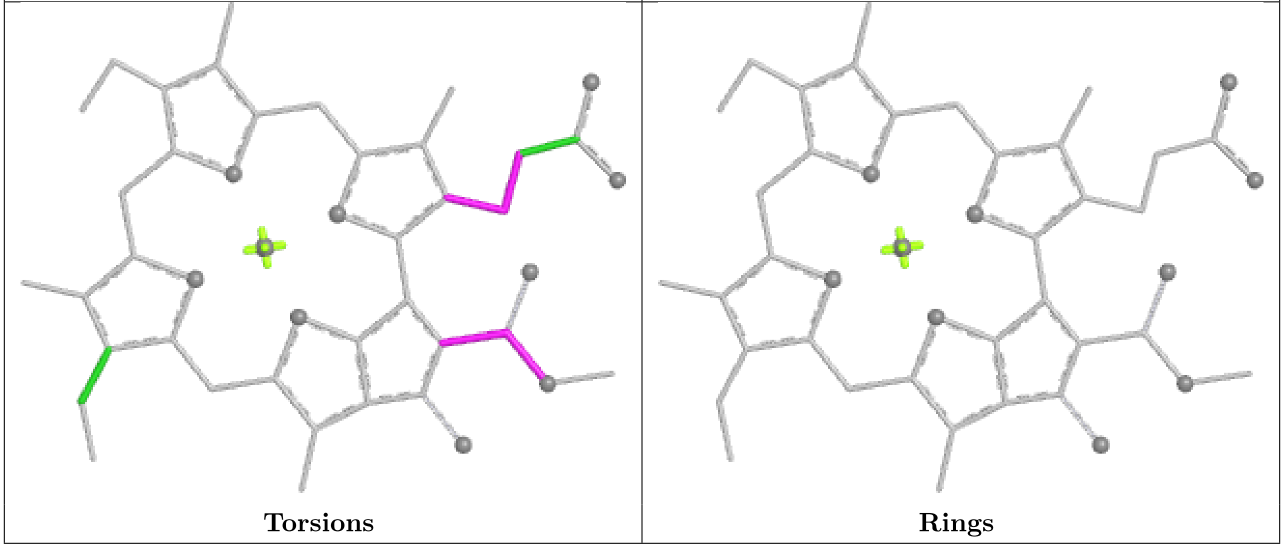
Rings

Ligand CLA H 2141



Bond lengths

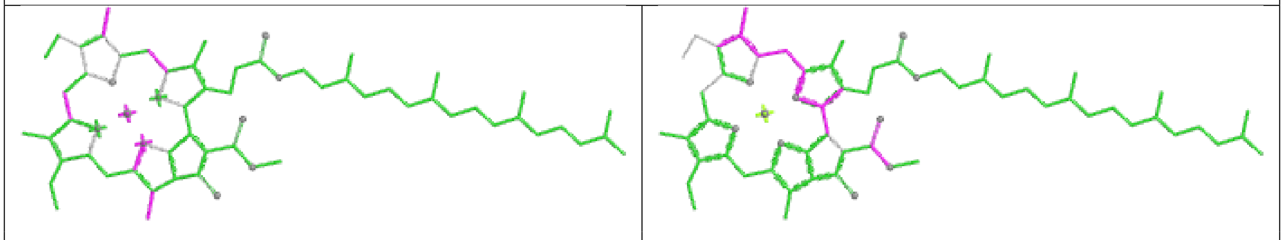
Bond angles



Torsions

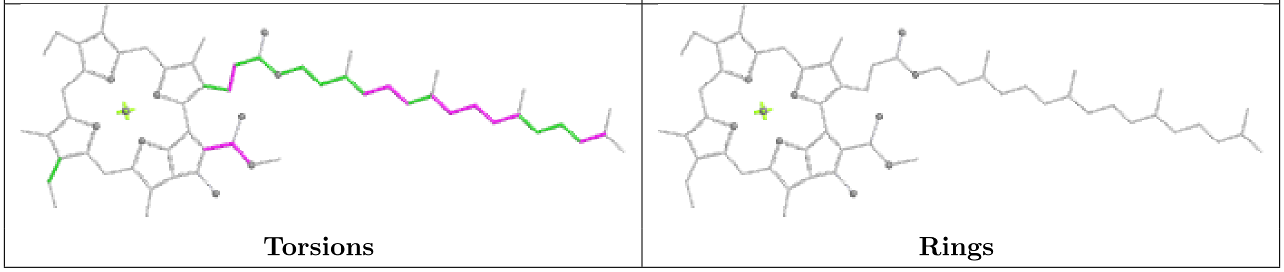
Rings

Ligand CLA H 2101



Bond lengths

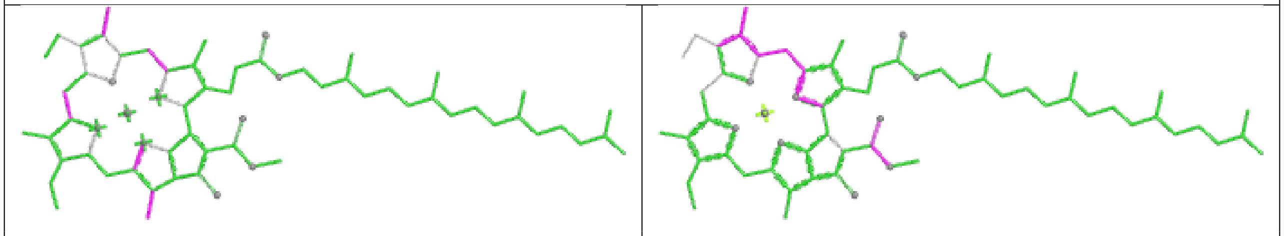
Bond angles



Torsions

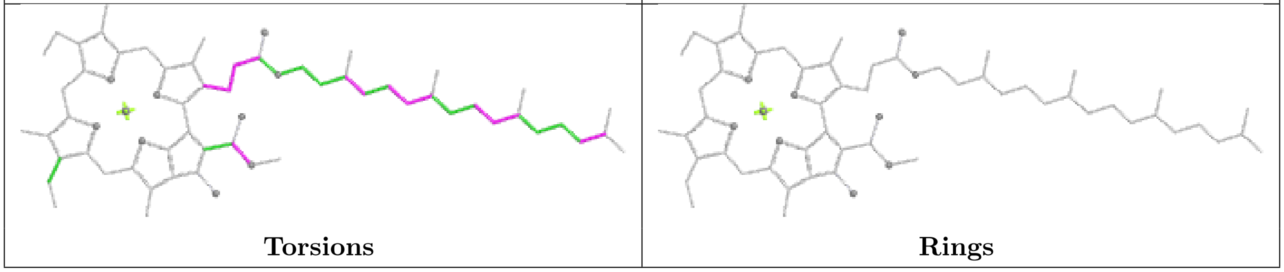
Rings

Ligand CLA B 2128



Bond lengths

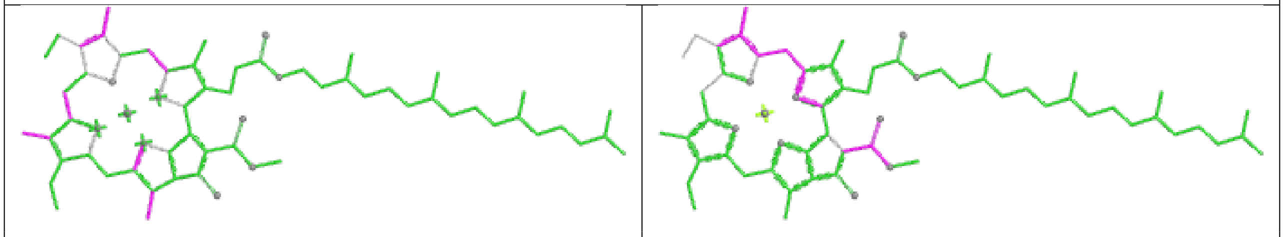
Bond angles



Torsions

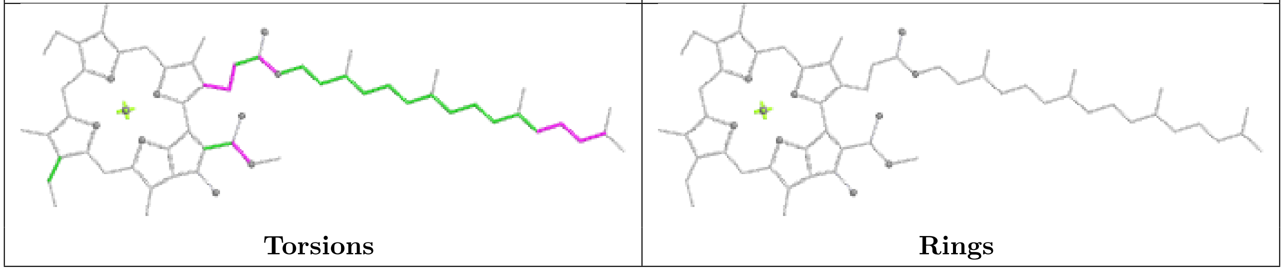
Rings

Ligand CLA B 2129



Bond lengths

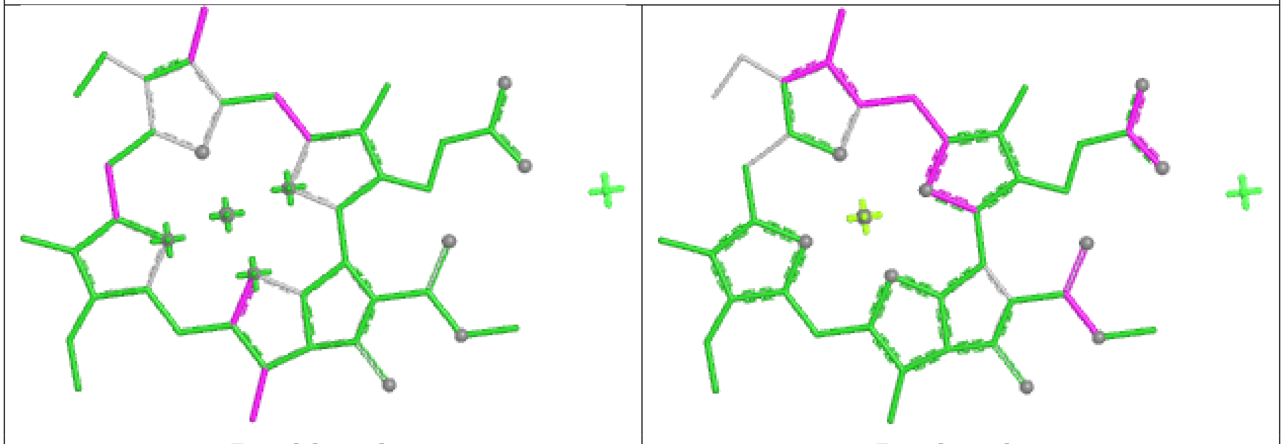
Bond angles



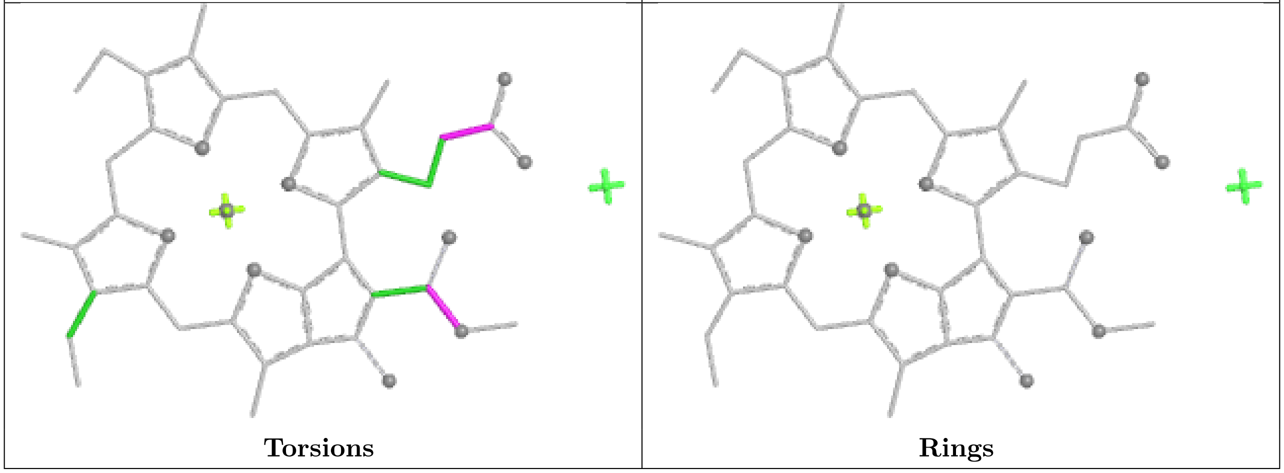
Torsions

Rings

Ligand CLA f 203

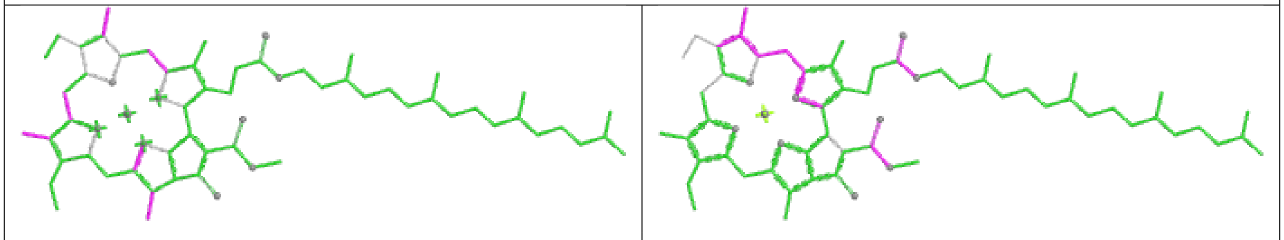


Bond lengths **Bond angles**

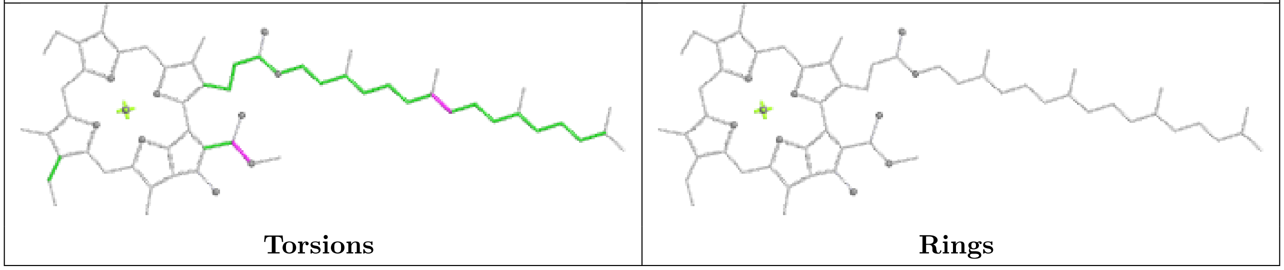


Torsions **Rings**

Ligand CLA a 838

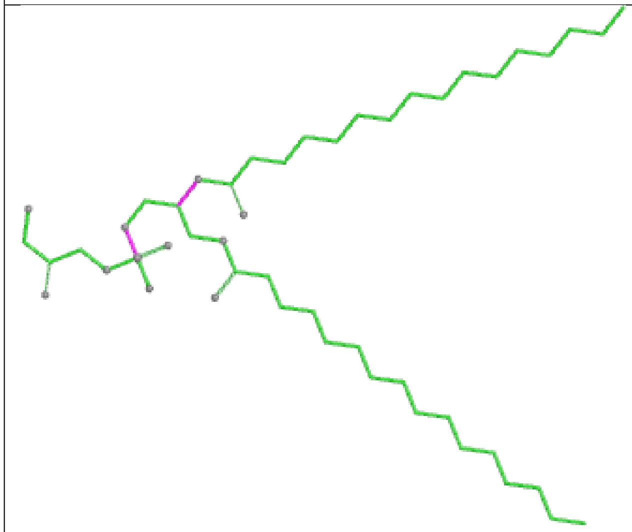


Bond lengths **Bond angles**

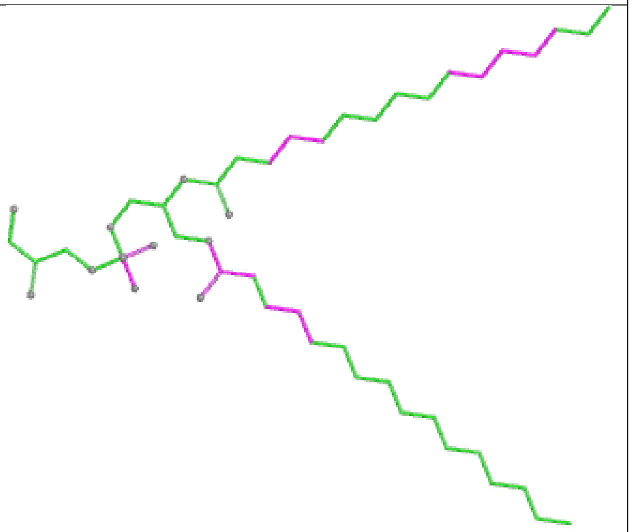


Torsions **Rings**

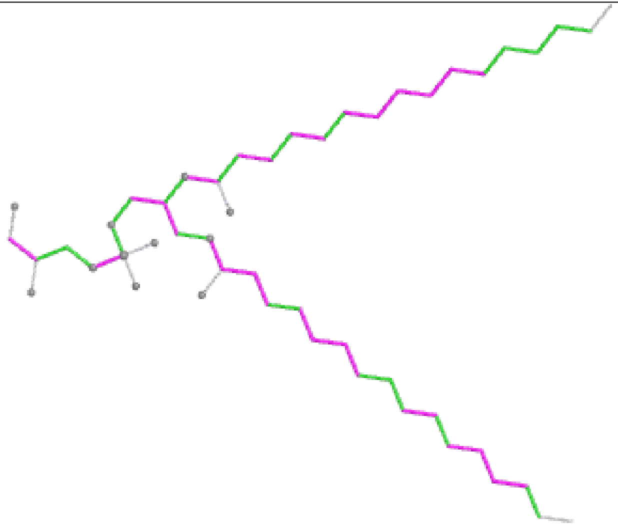
Ligand LHG A 846



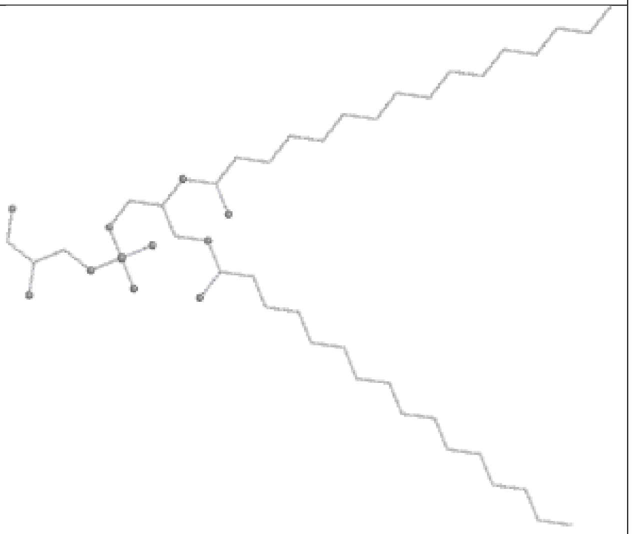
Bond lengths



Bond angles

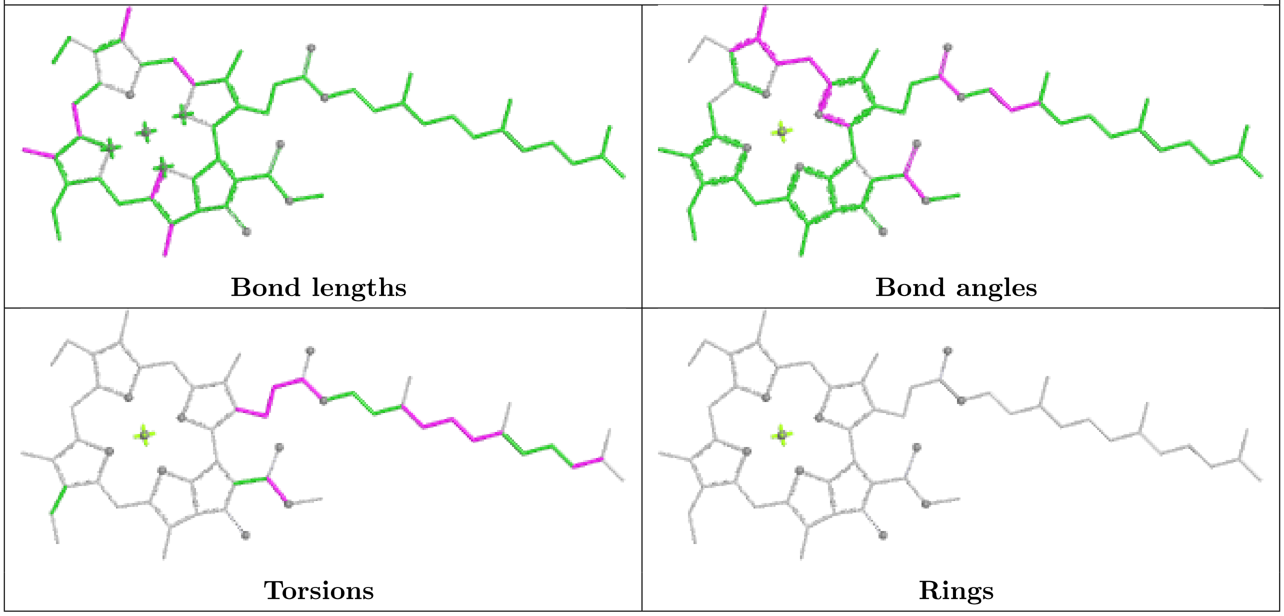


Torsions



Rings

Ligand CLA a 817



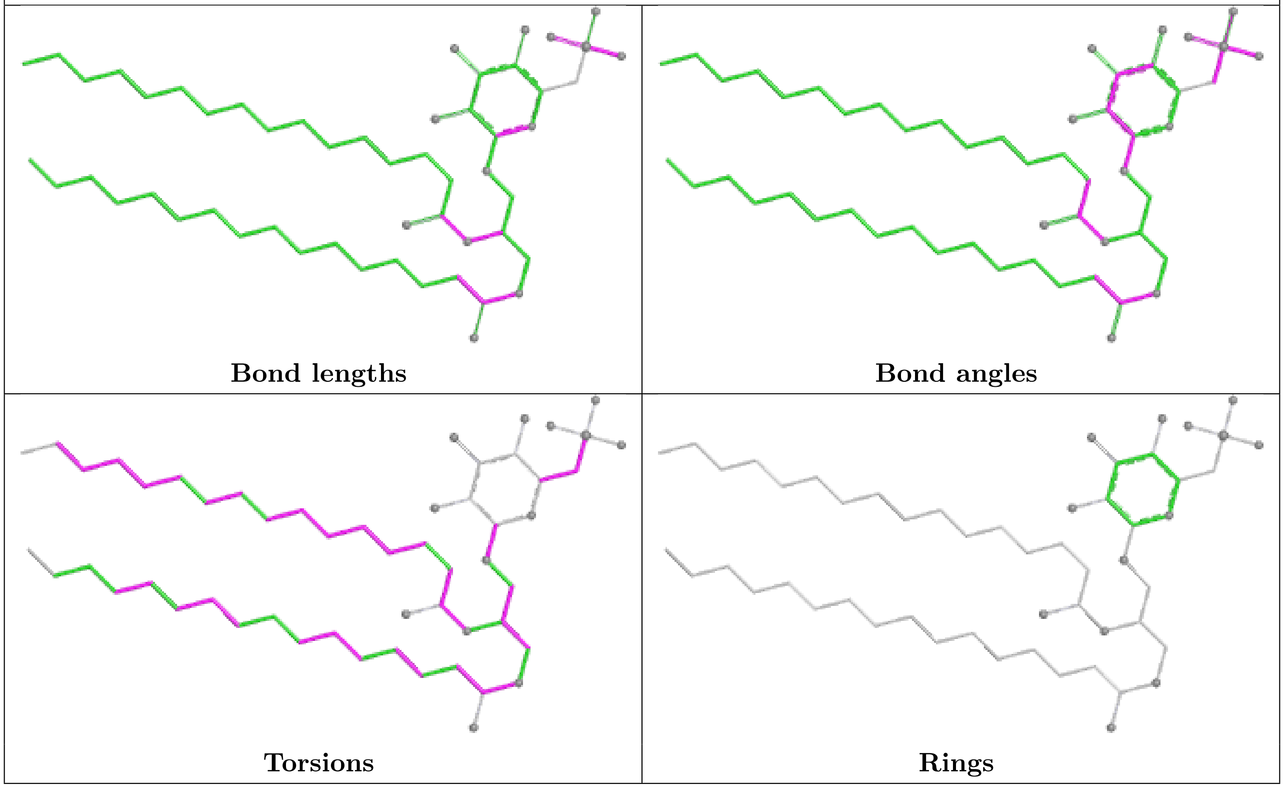
Bond lengths

Bond angles

Torsions

Rings

Ligand SQD m 102



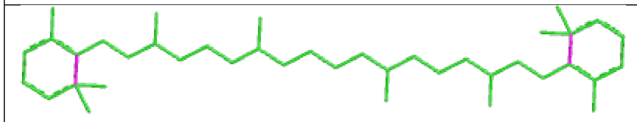
Bond lengths

Bond angles

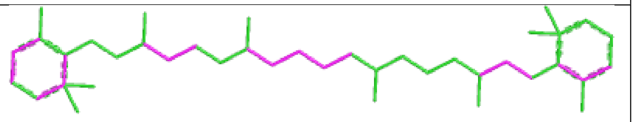
Torsions

Rings

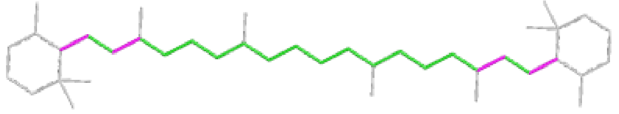
Ligand BCR G 844



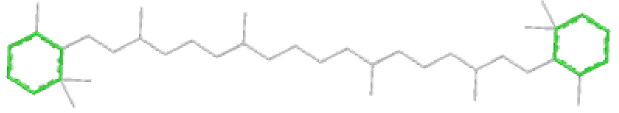
Bond lengths



Bond angles

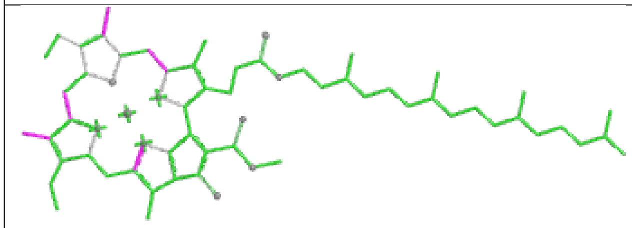


Torsions

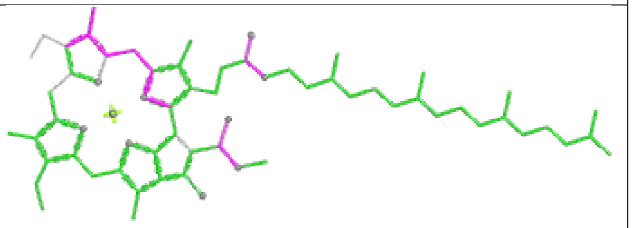


Rings

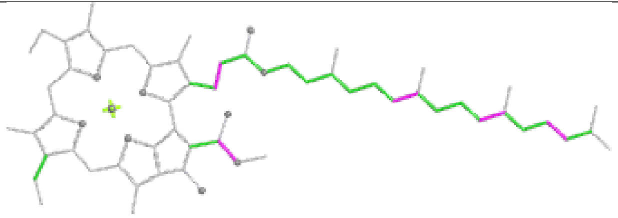
Ligand CLA a 820



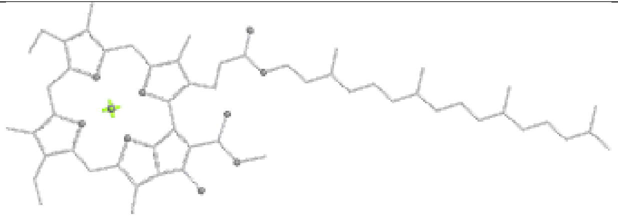
Bond lengths



Bond angles

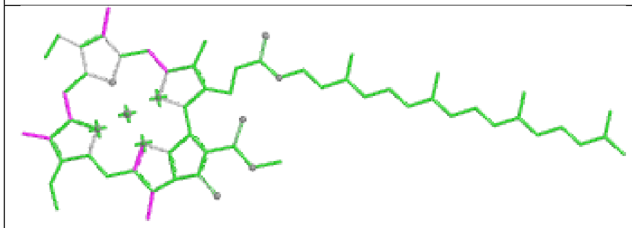


Torsions

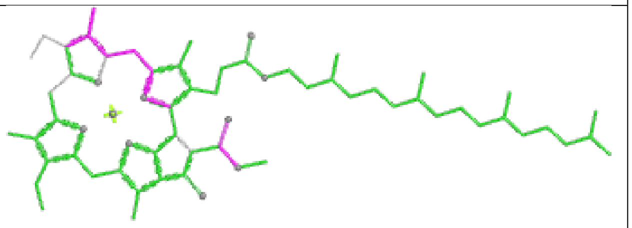


Rings

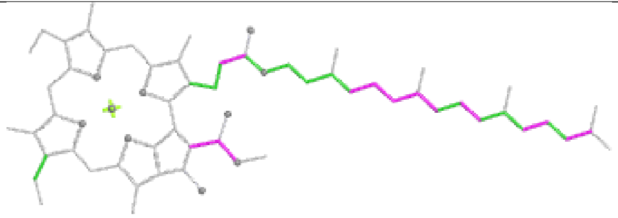
Ligand CLA b 2107



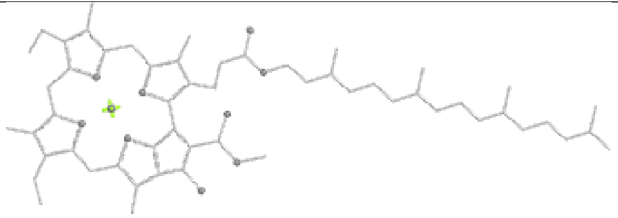
Bond lengths



Bond angles

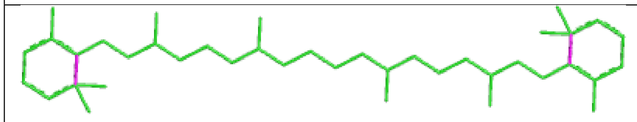


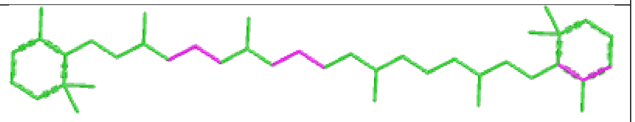
Torsions

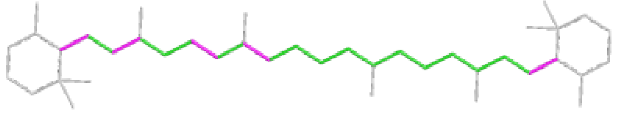


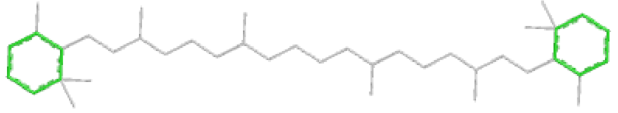
Rings

Ligand BCR B 2146

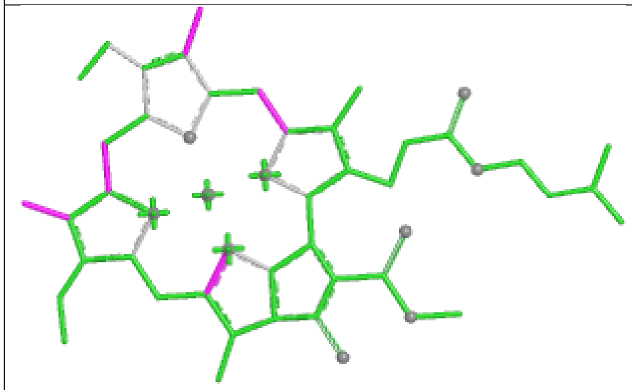

Bond lengths

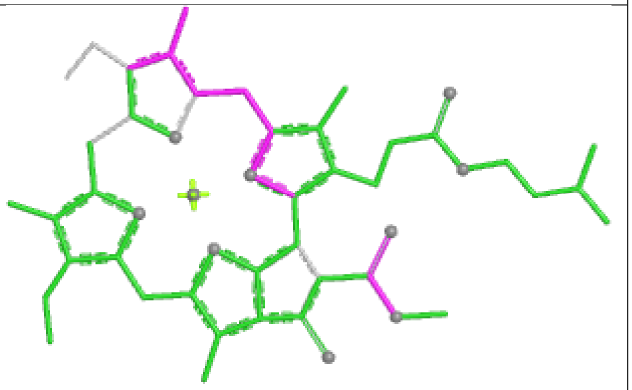

Bond angles

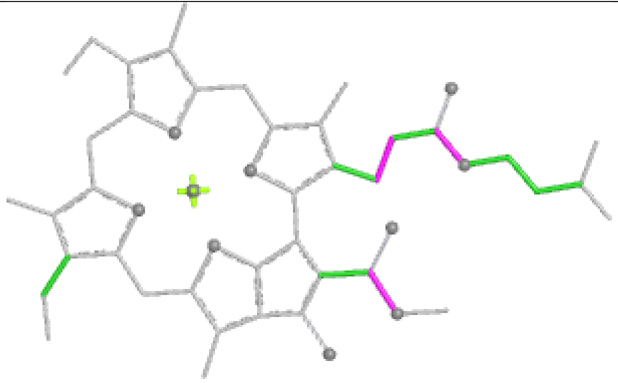

Torsions

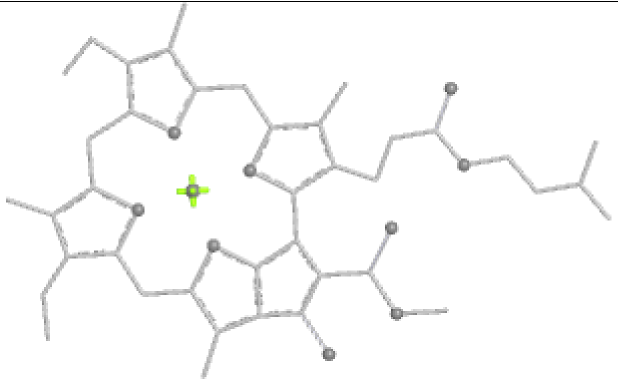

Rings

Ligand CLA H 2152

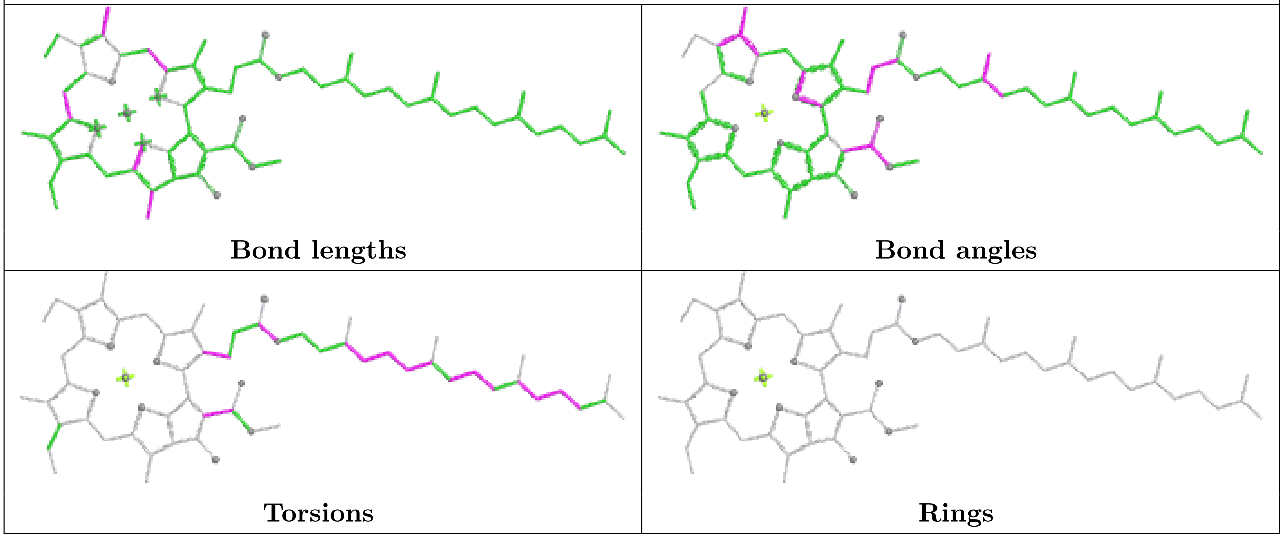

Bond lengths


Bond angles

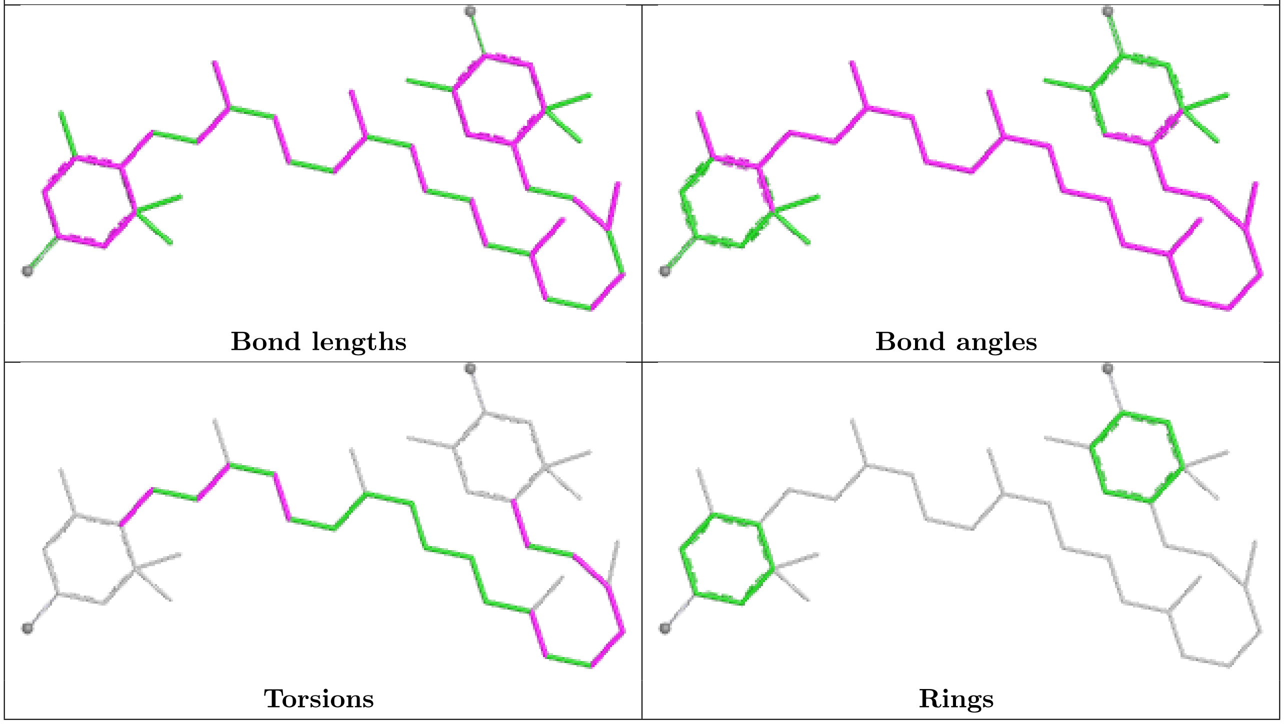

Torsions


Rings

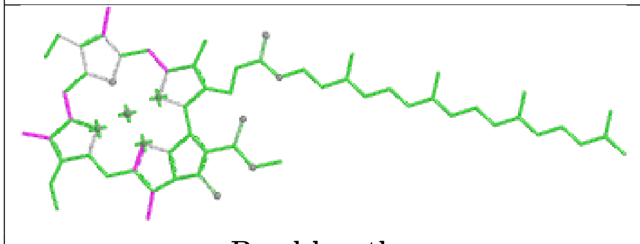
Ligand CLA B 2120

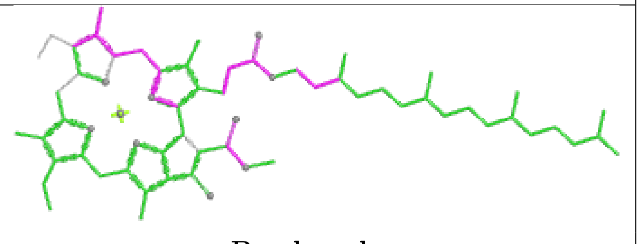


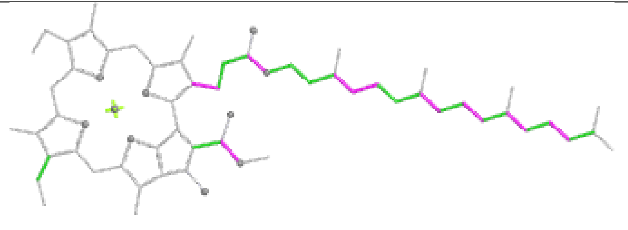
Ligand ZEX b 2151



Ligand CLA a 805


Bond lengths


Bond angles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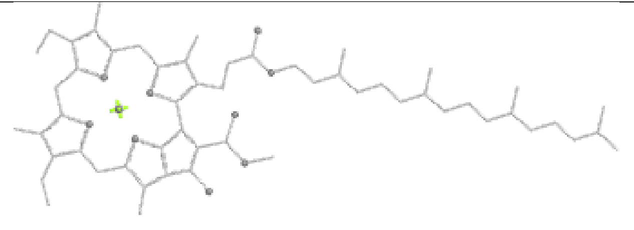
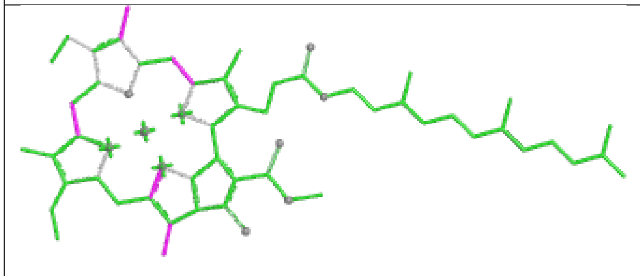

Rings

Ligand CLA a 831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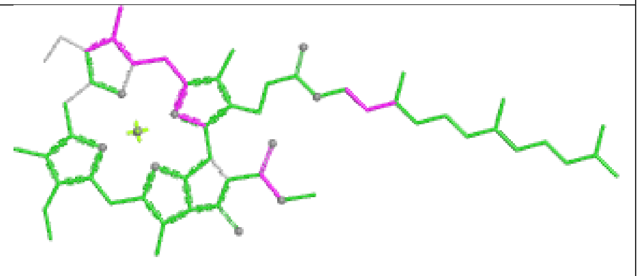
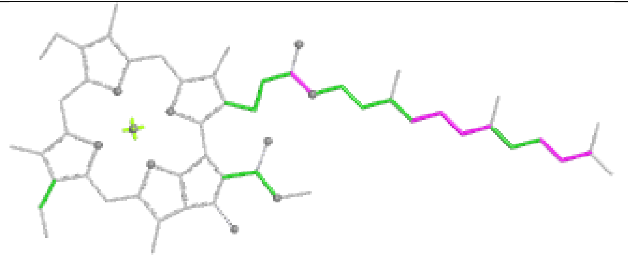
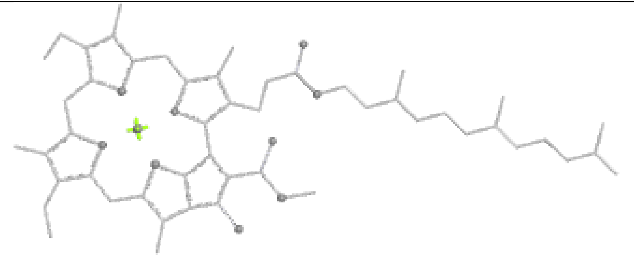
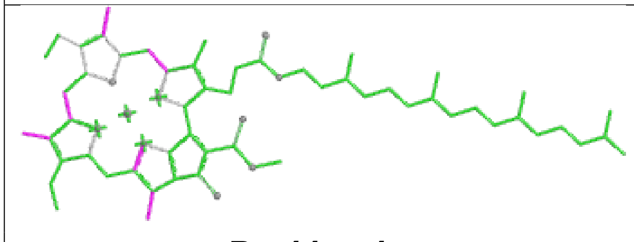

Bond angles

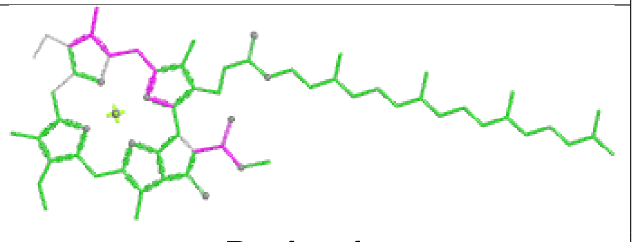

Torsions


Rings

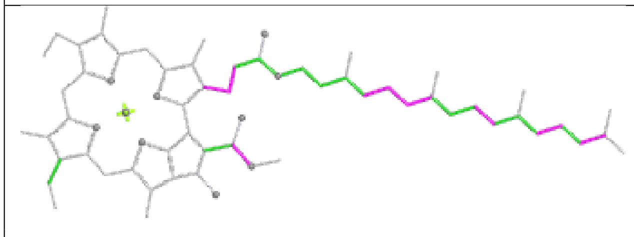
Ligand CLA A 829



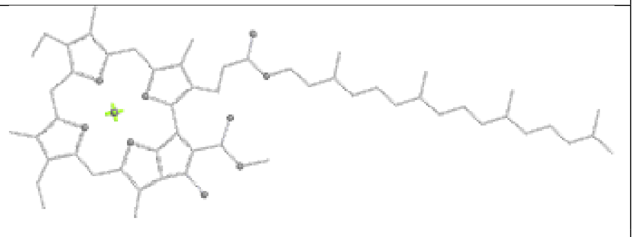
Bond lengths



Bond angles

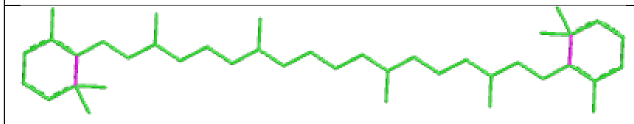


Torsions

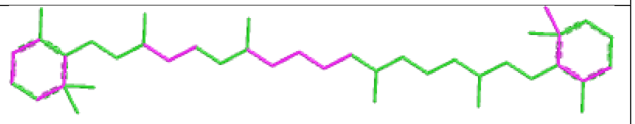


Rings

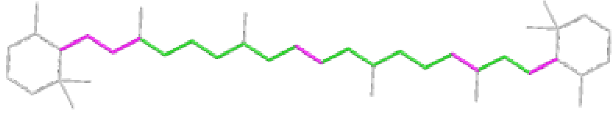
Ligand BCR B 2145



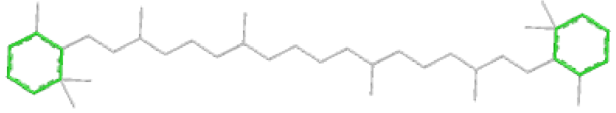
Bond lengths



Bond angles

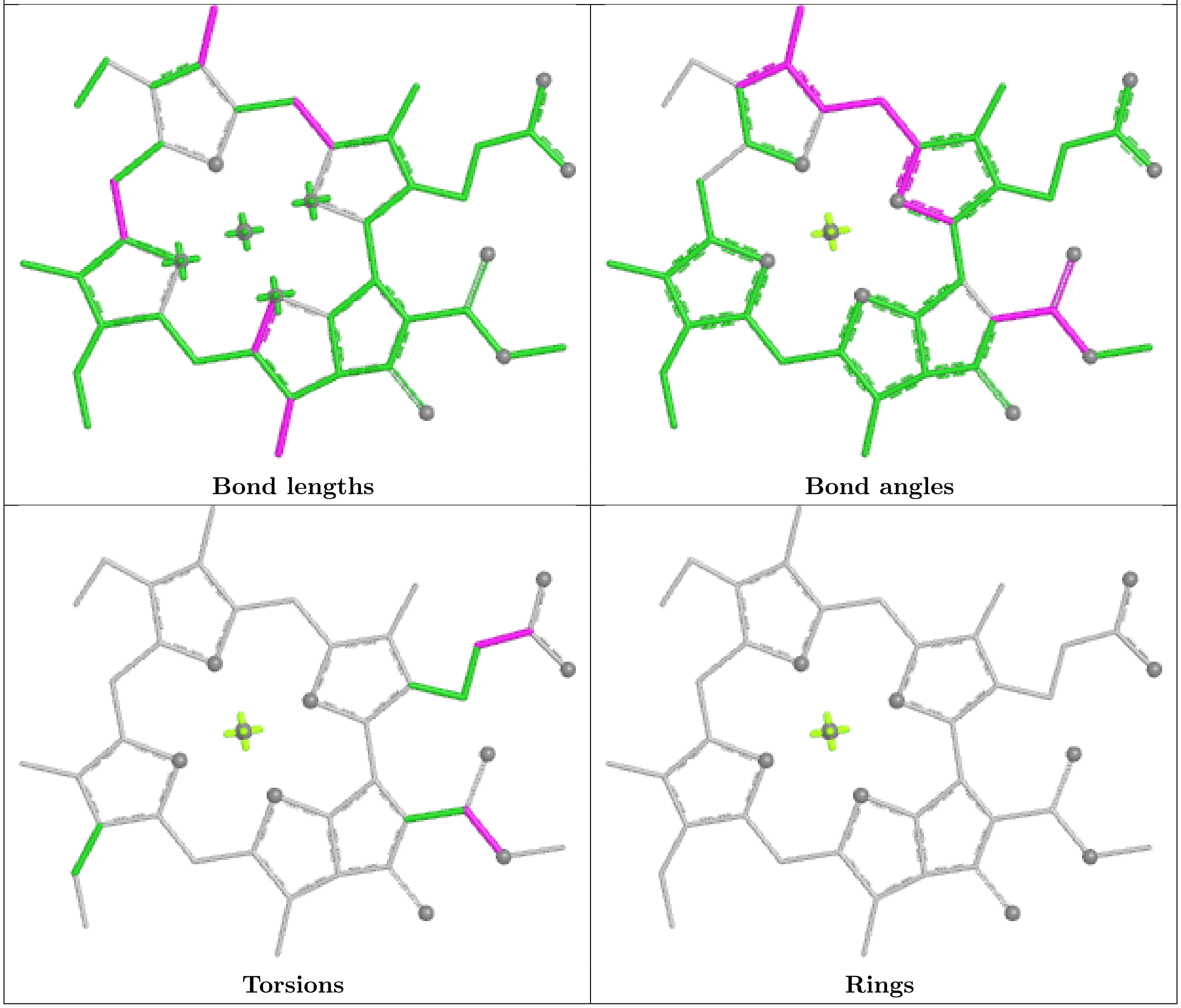


Torsions



Rings

Ligand CLA b 2138



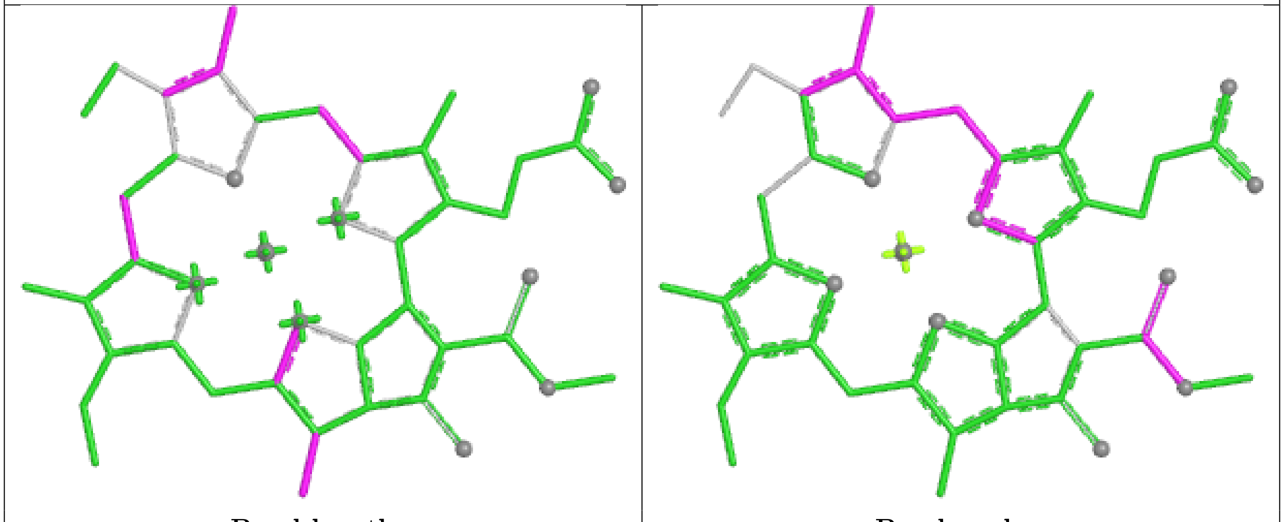
Bond lengths

Bond angles

Torsions

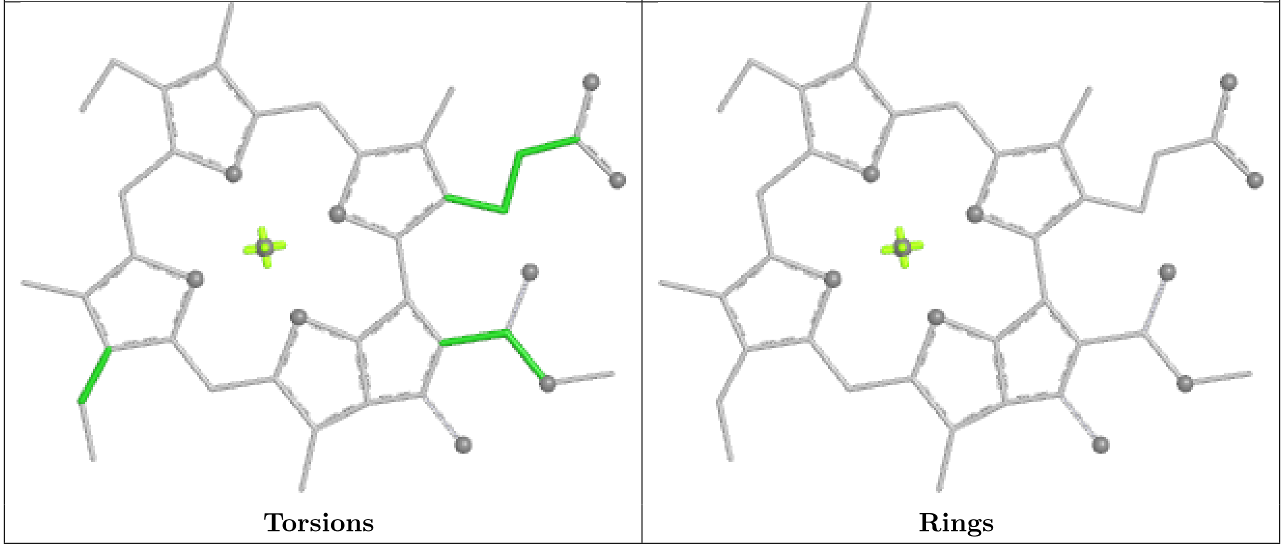
Rings

Ligand CLA B 2131



Bond lengths

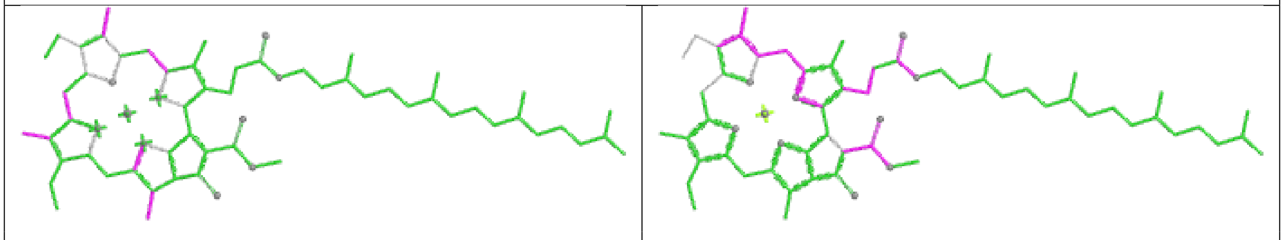
Bond angles



Torsions

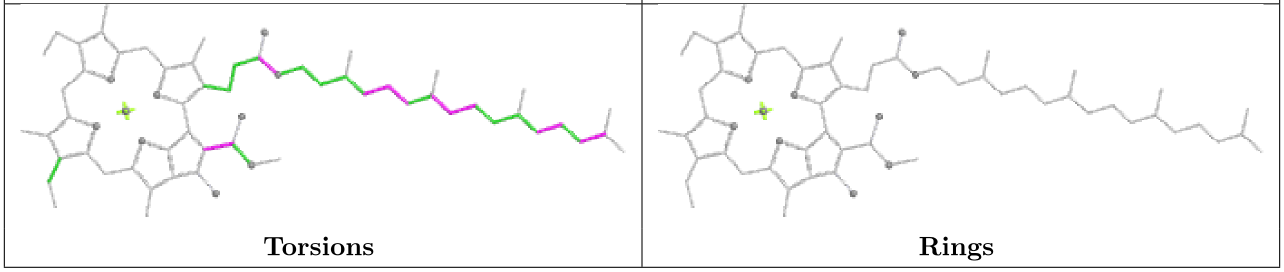
Rings

Ligand CLA H 2109



Bond lengths

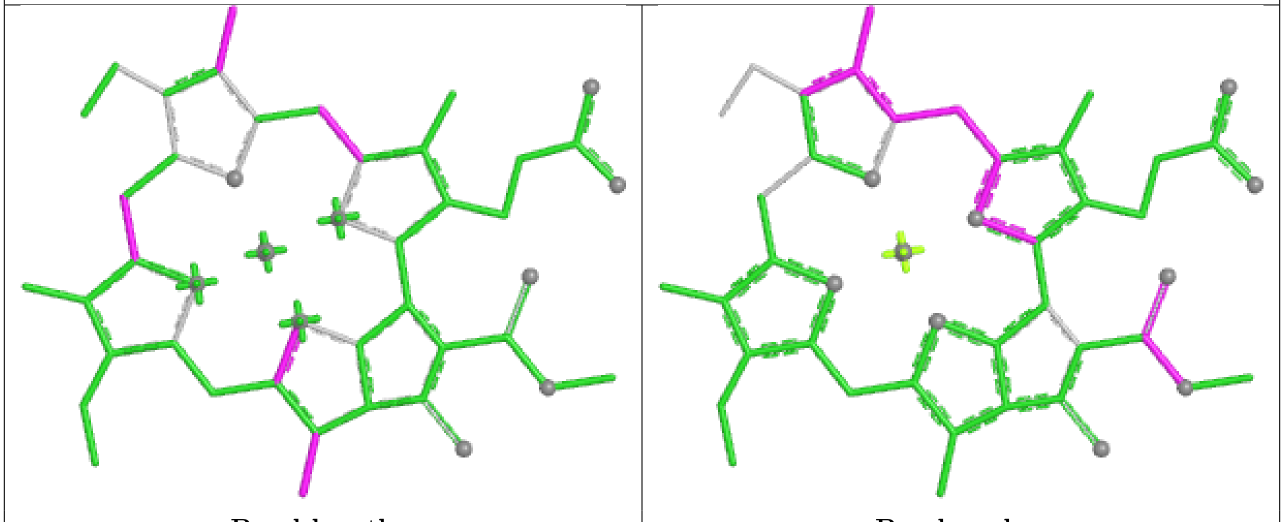
Bond angles



Torsions

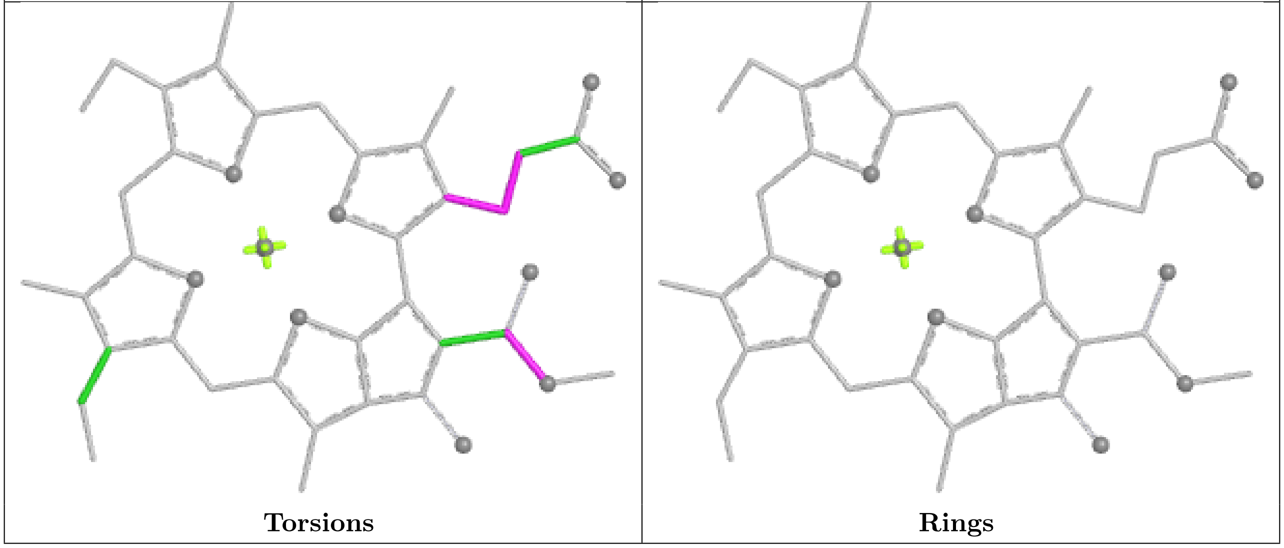
Rings

Ligand CLA H 2122



Bond lengths

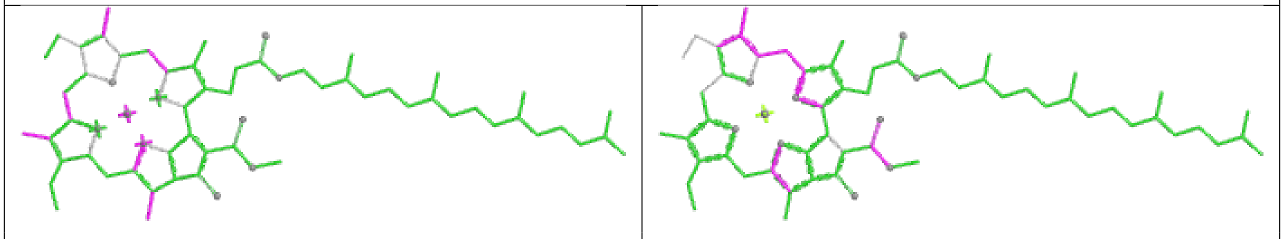
Bond angles



Torsions

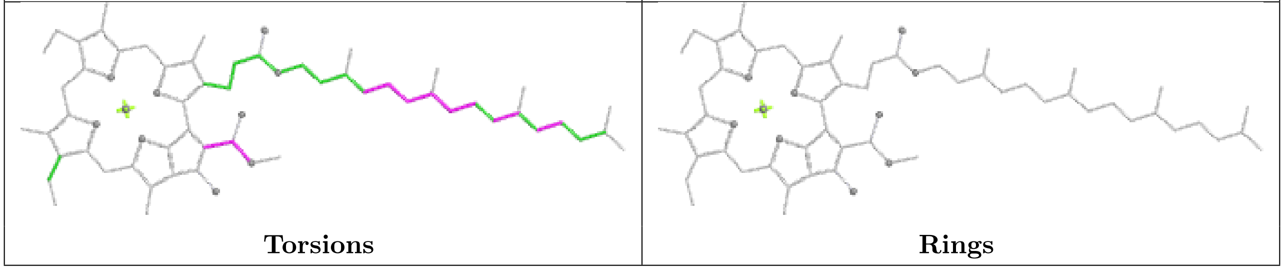
Rings

Ligand CLA B 2130



Bond lengths

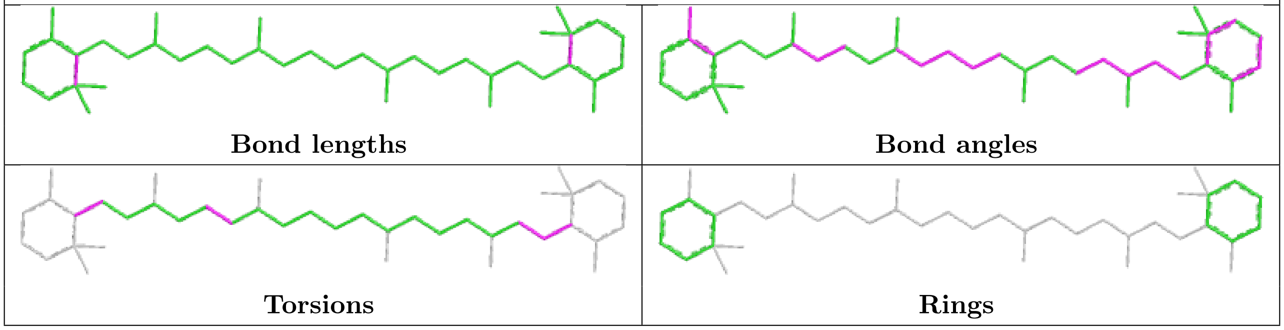
Bond angles



Torsions

Rings

Ligand BCR U 207



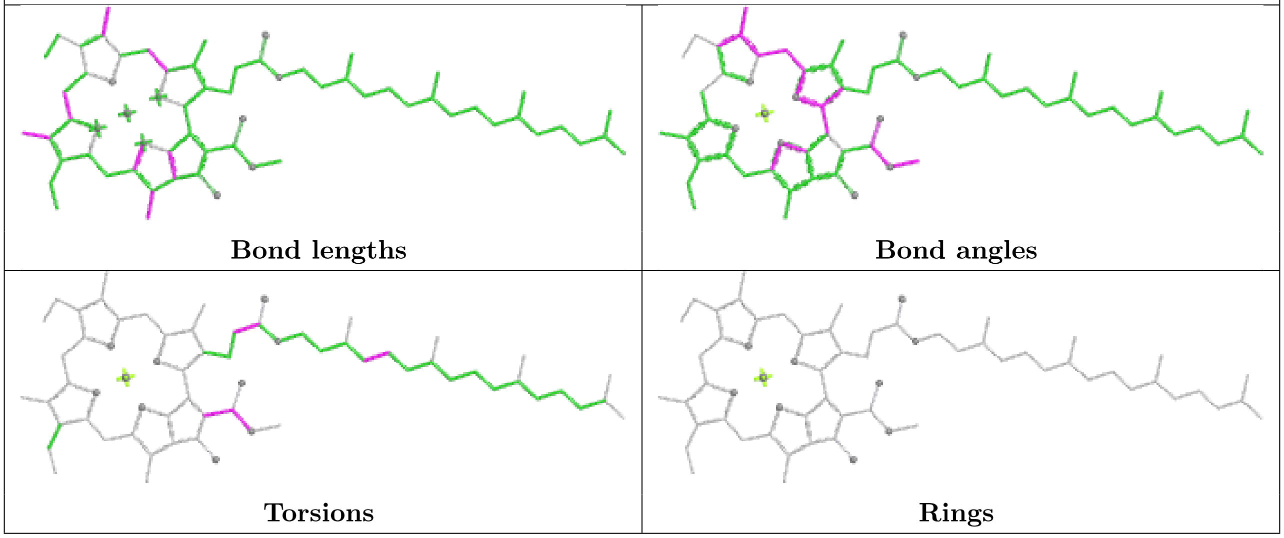
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 801



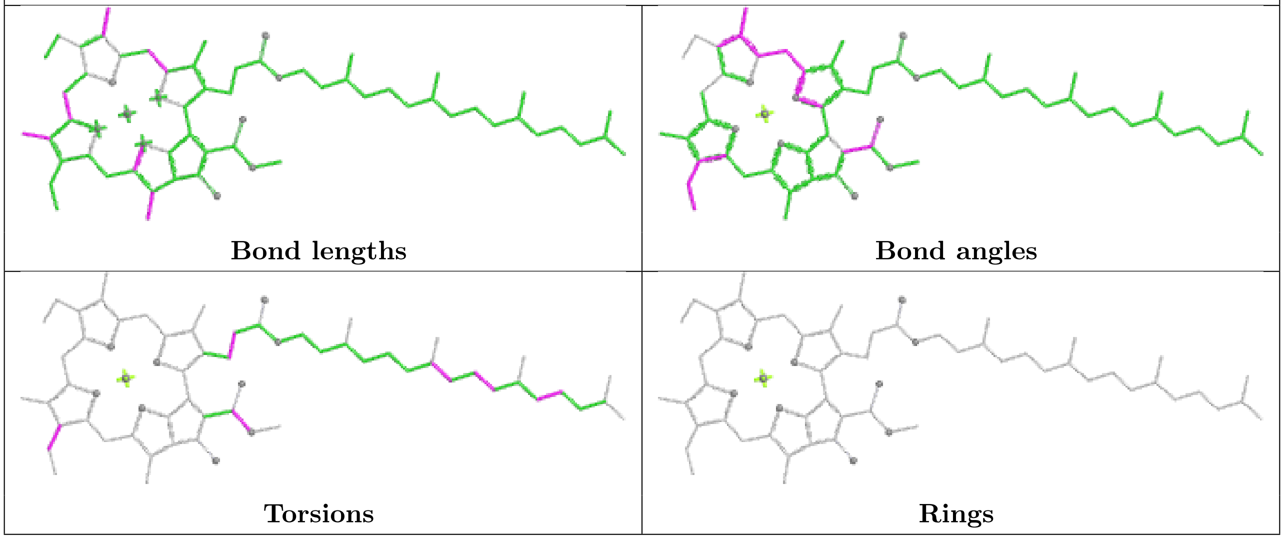
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 2105



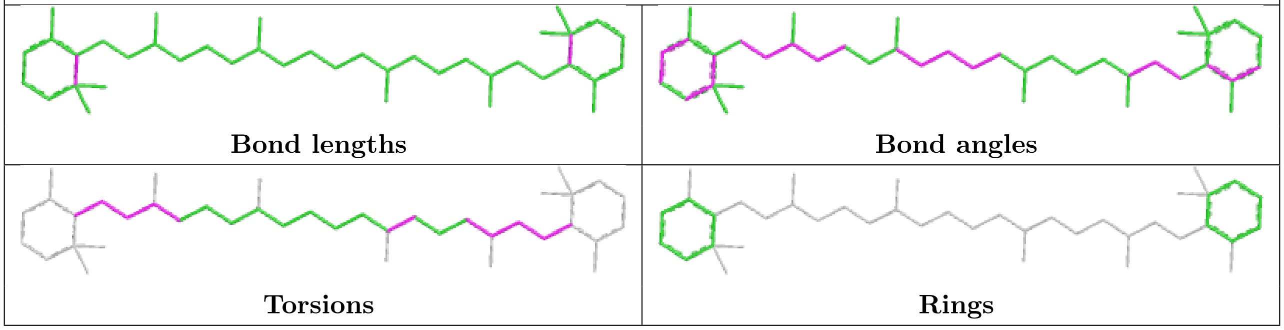
Bond lengths

Bond angles

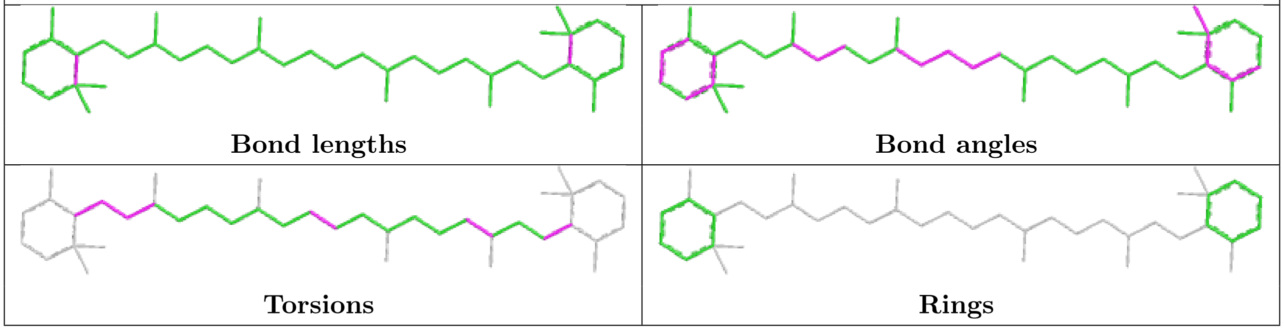
Torsions

Rings

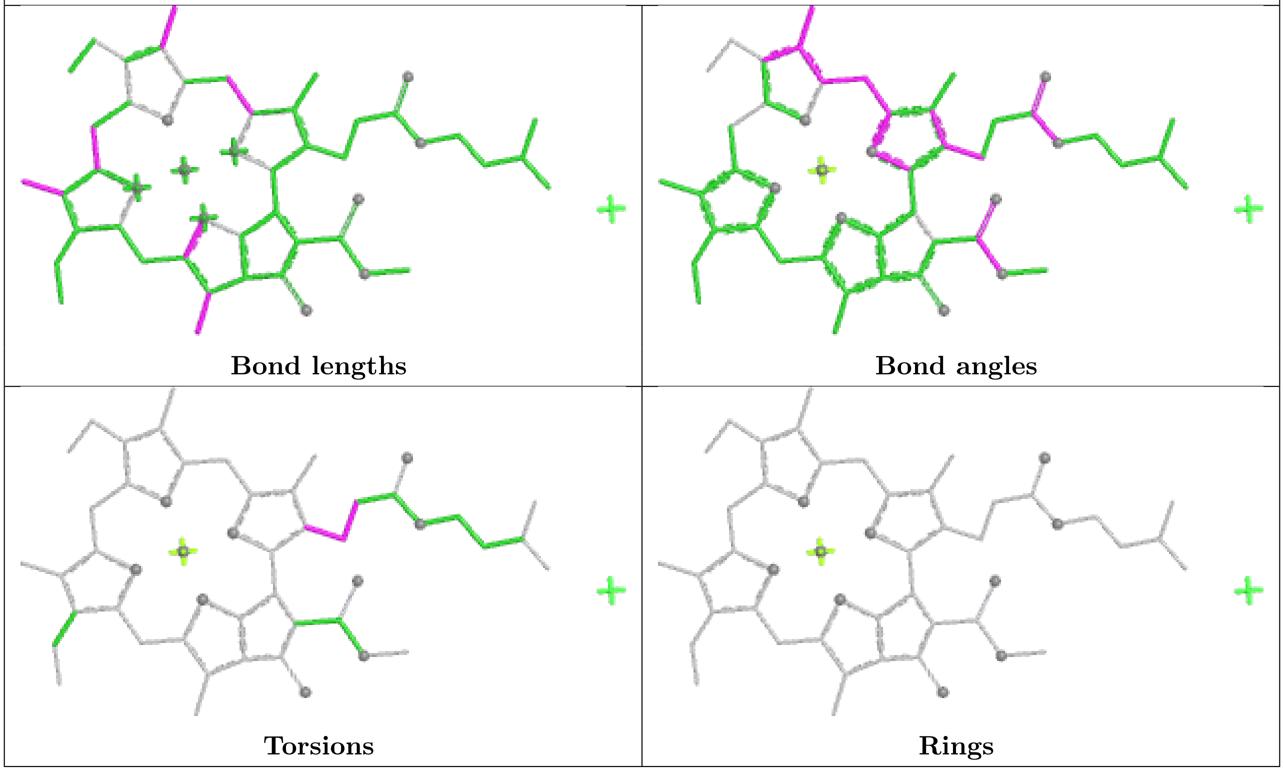
Ligand BCR j 101



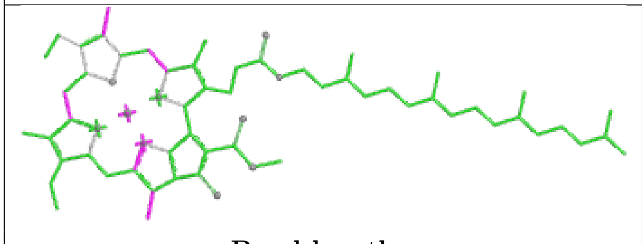
Ligand BCR H 2144



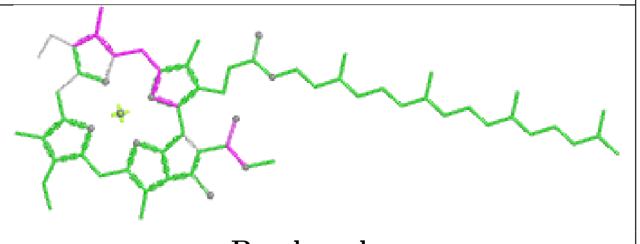
Ligand CLA A 808



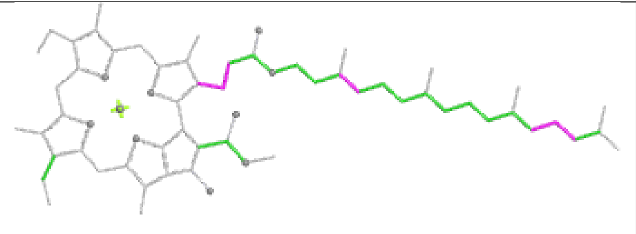
Ligand CLA a 850



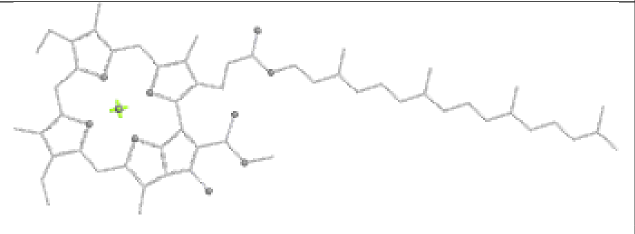
Bond lengths



Bond angles

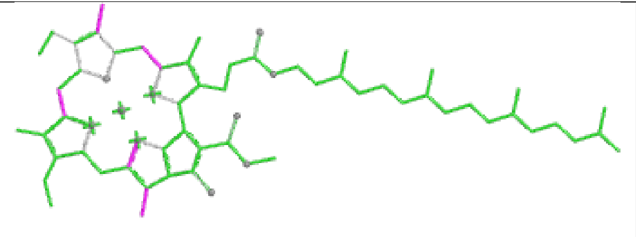


Torsions

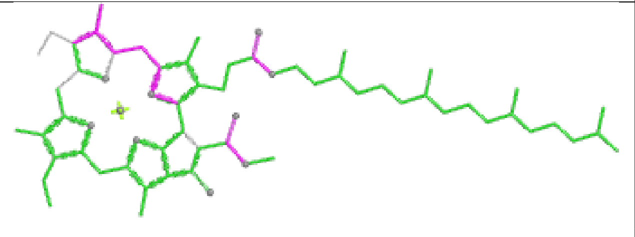


Rings

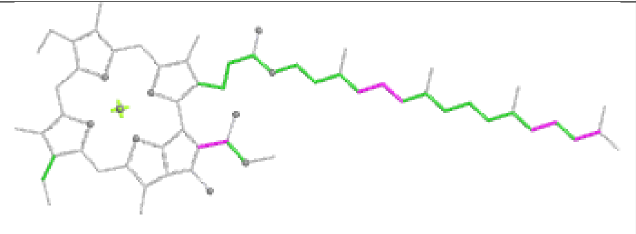
Ligand CLA b 2112



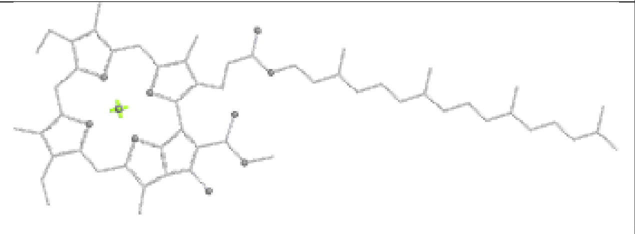
Bond lengths



Bond angles

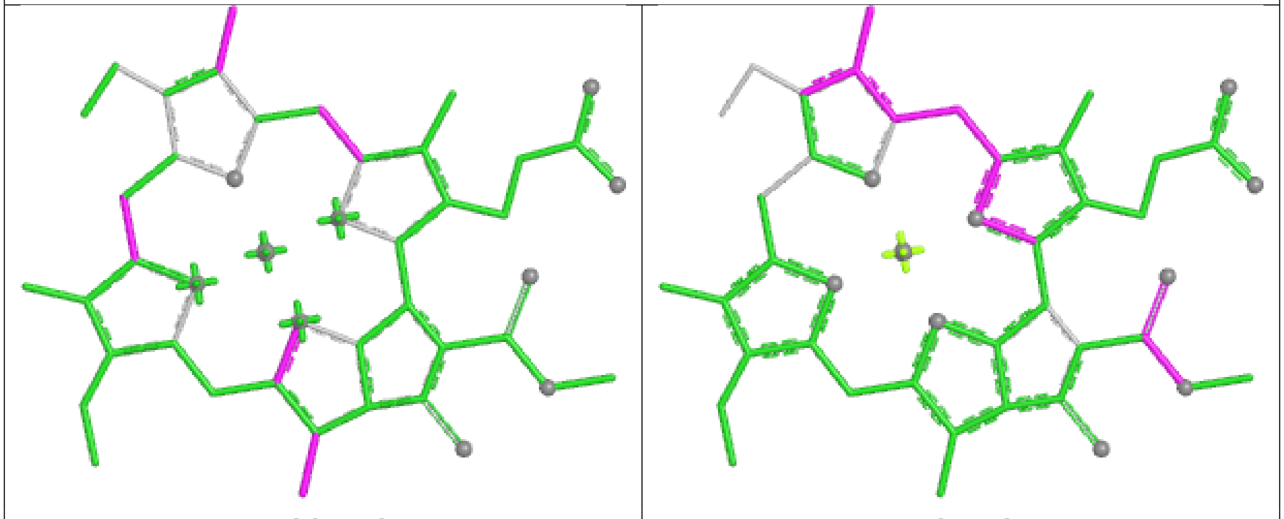


Torsions



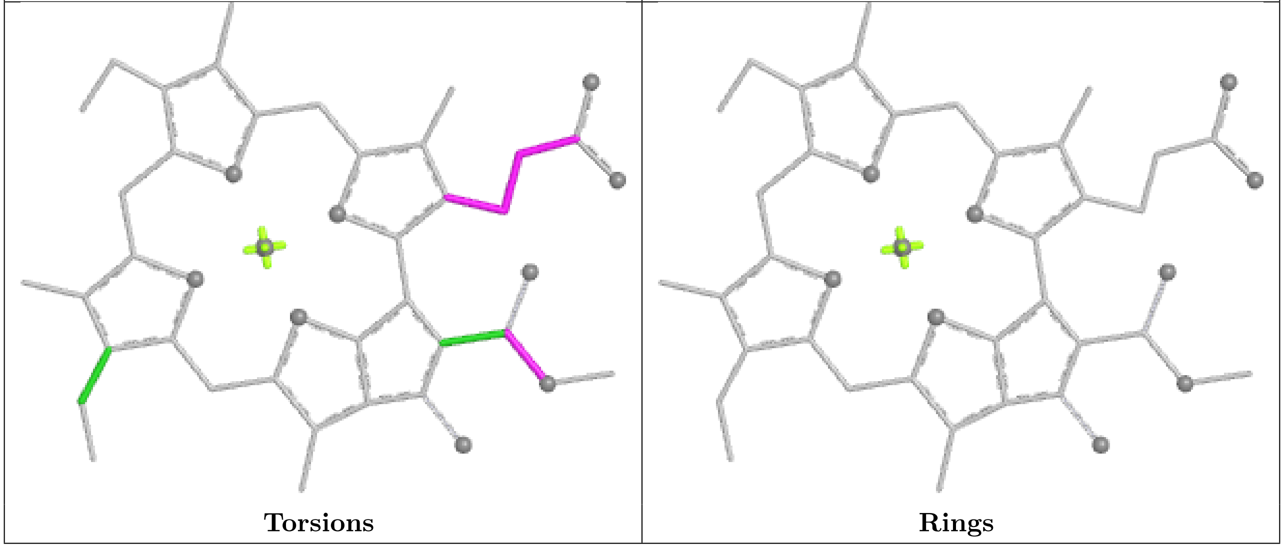
Rings

Ligand CLA b 2135



Bond lengths

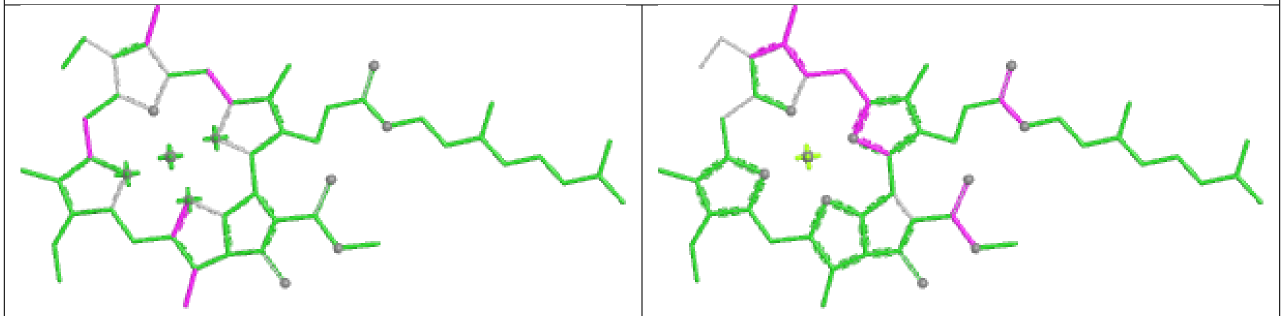
Bond angles



Torsions

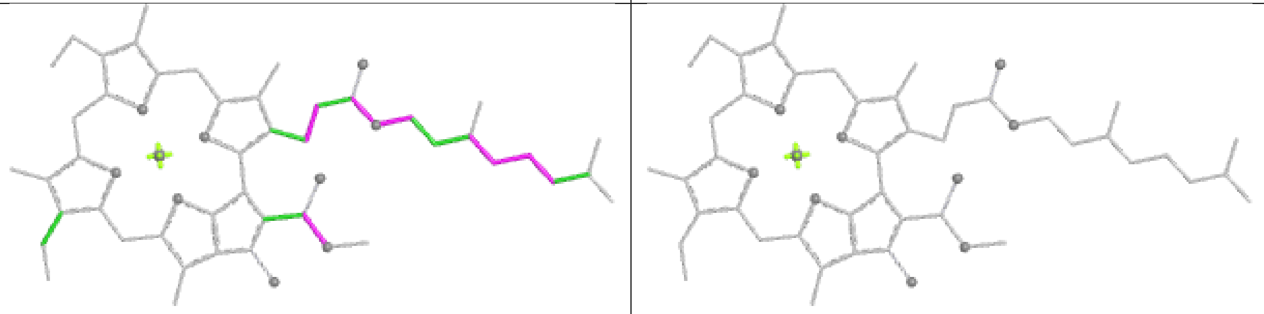
Rings

Ligand CLA b 2121



Bond lengths

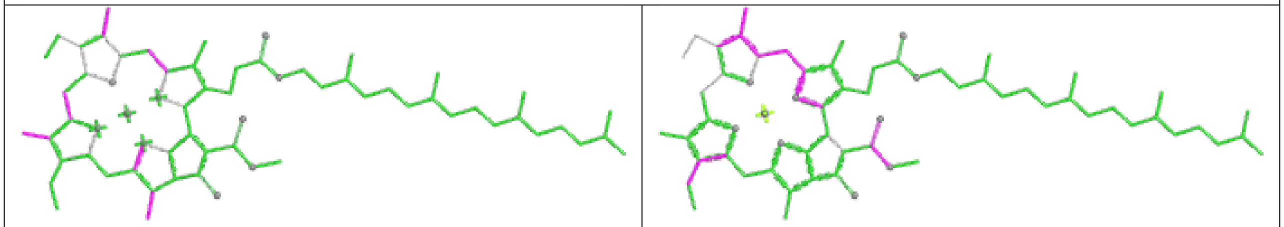
Bond angles



Torsions

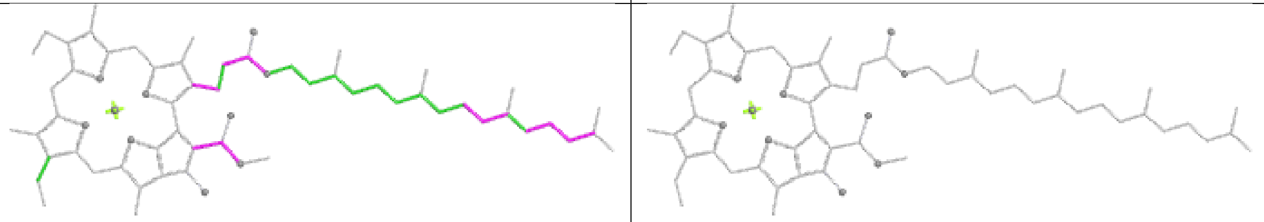
Rings

Ligand CLA A 804



Bond lengths

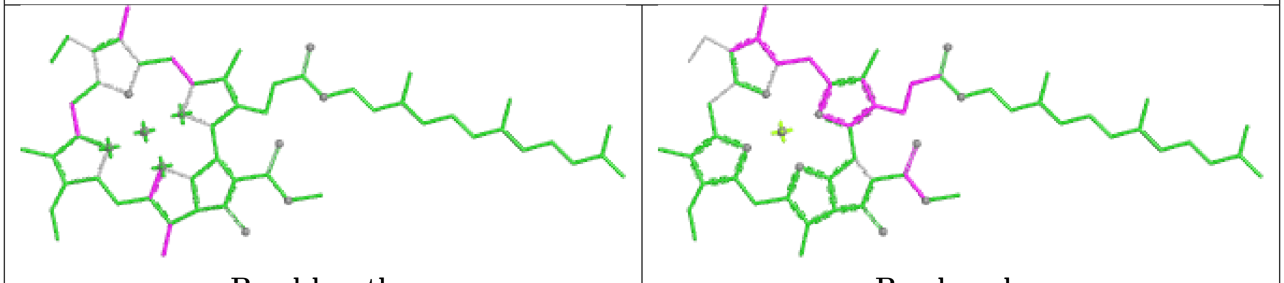
Bond angles



Torsions

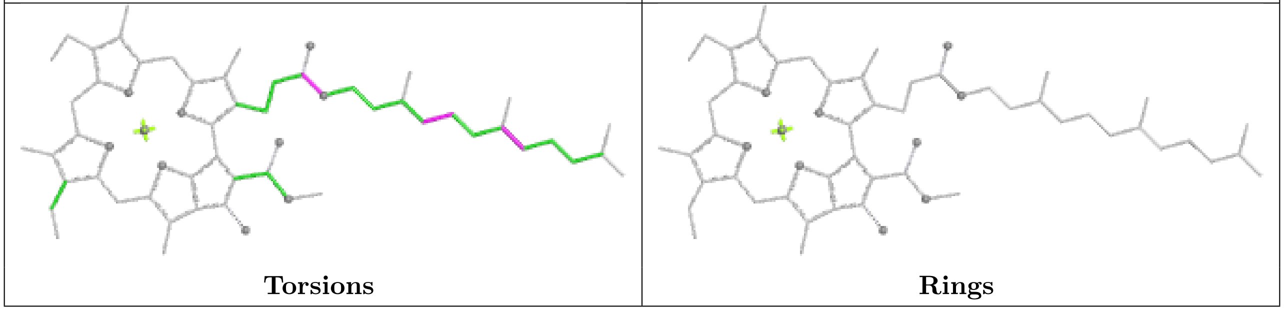
Rings

Ligand CLA a 825



Bond lengths

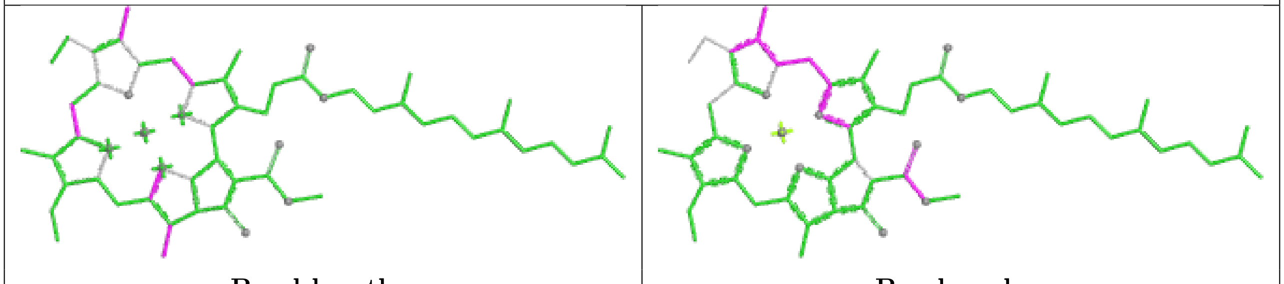
Bond angles



Torsions

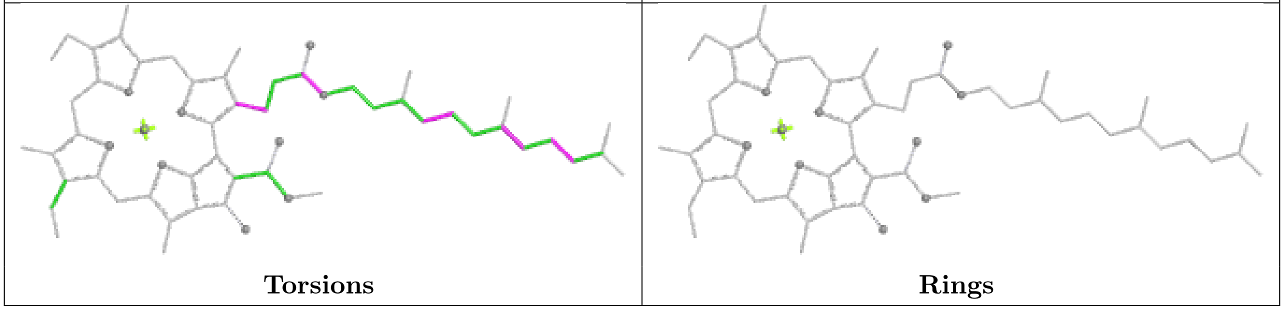
Rings

Ligand CLA A 821



Bond lengths

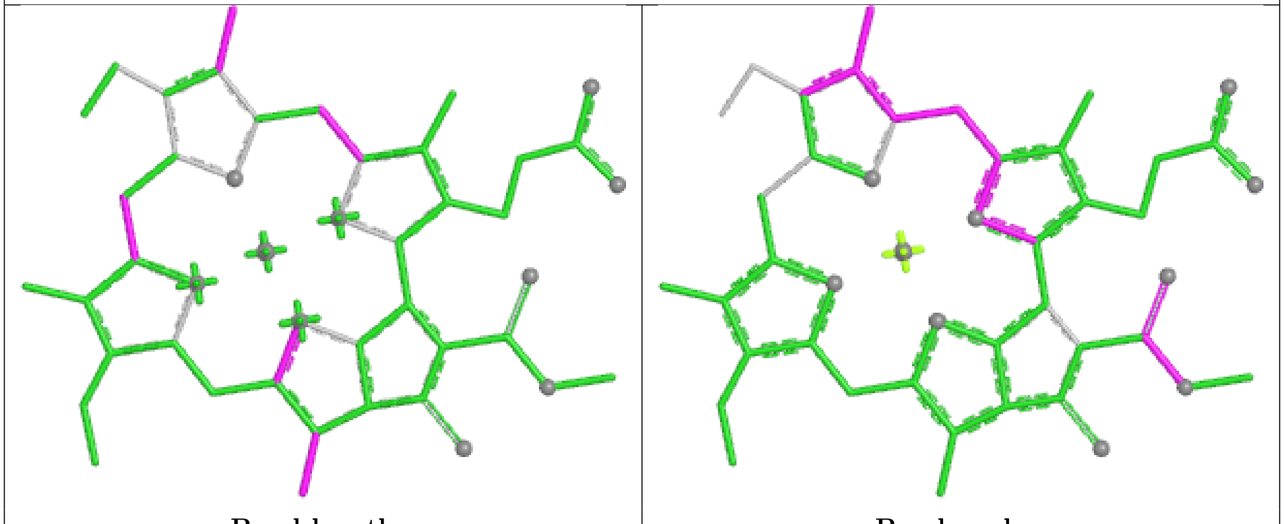
Bond angles



Torsions

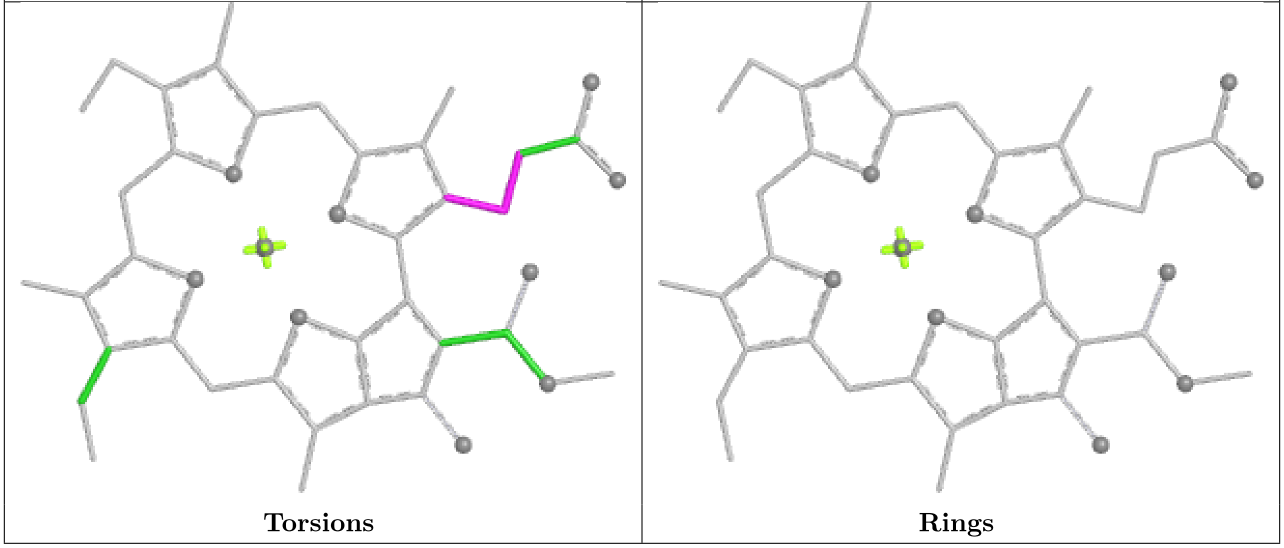
Rings

Ligand CLA Q 204



Bond lengths

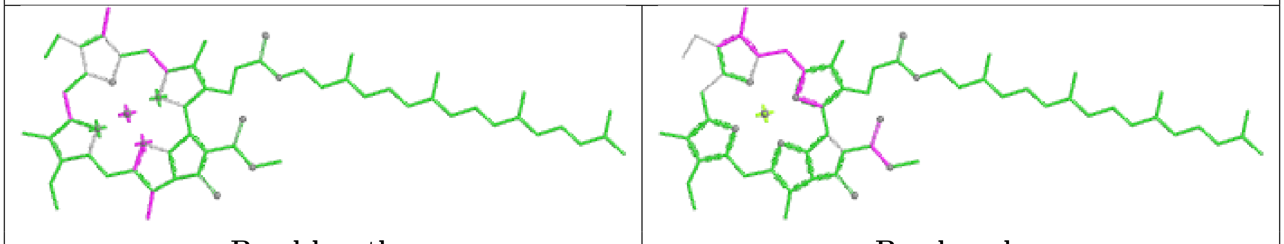
Bond angles



Torsions

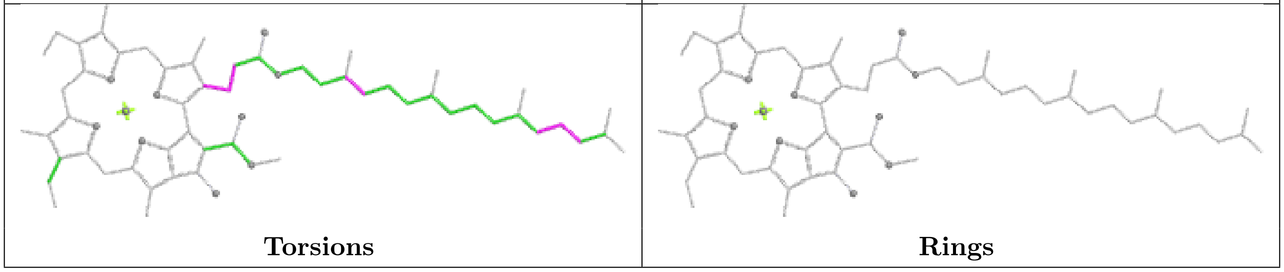
Rings

Ligand CLA G 850



Bond lengths

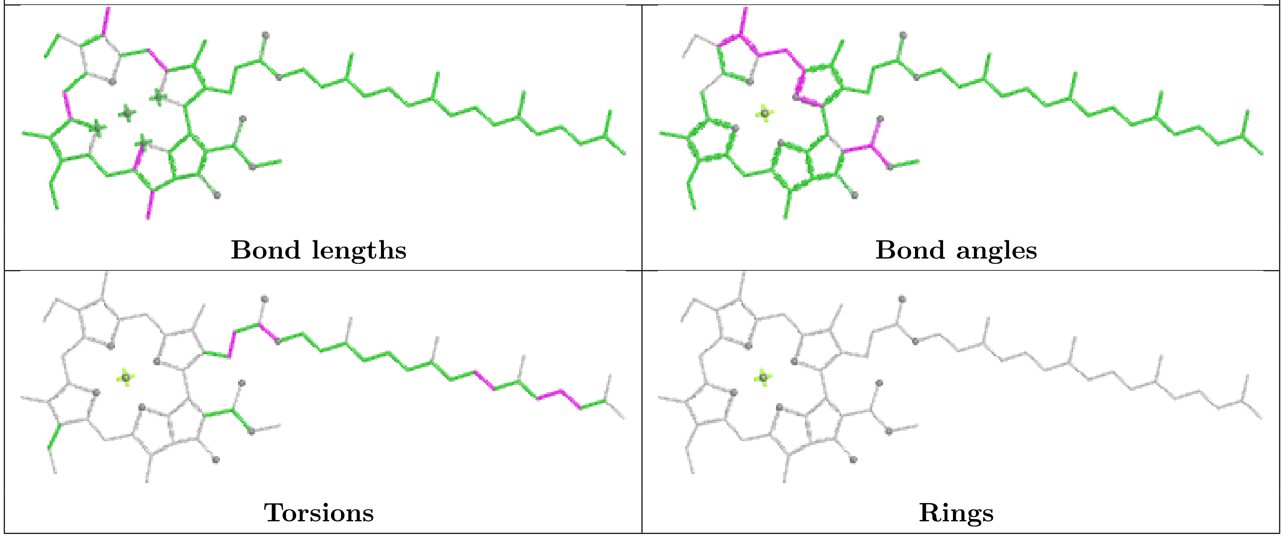
Bond angles



Torsions

Rings

Ligand CLA L 205



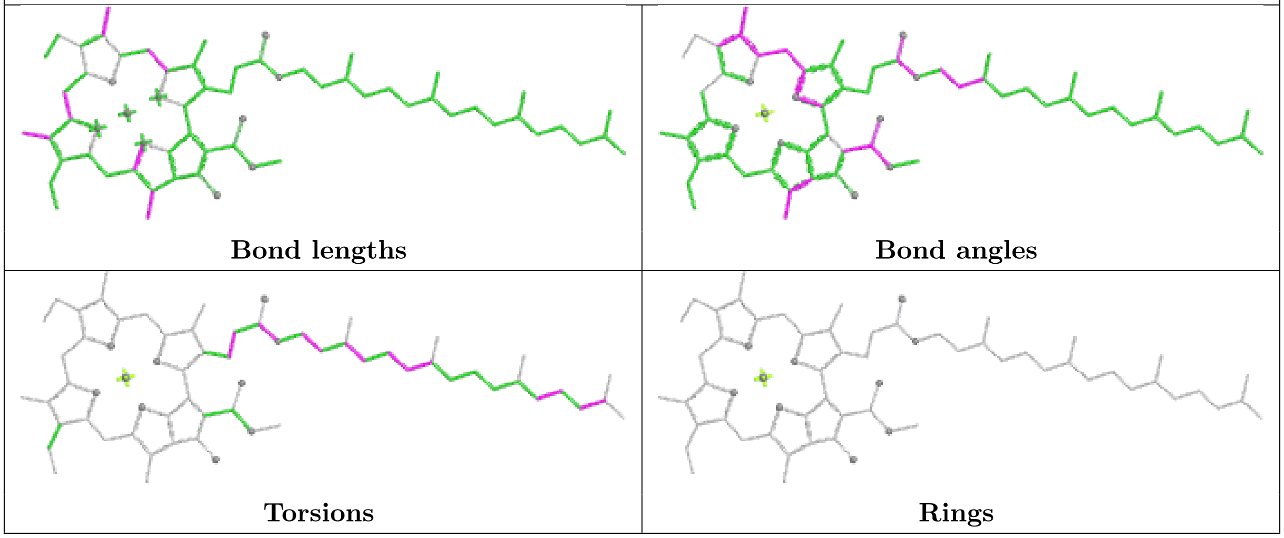
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 2103



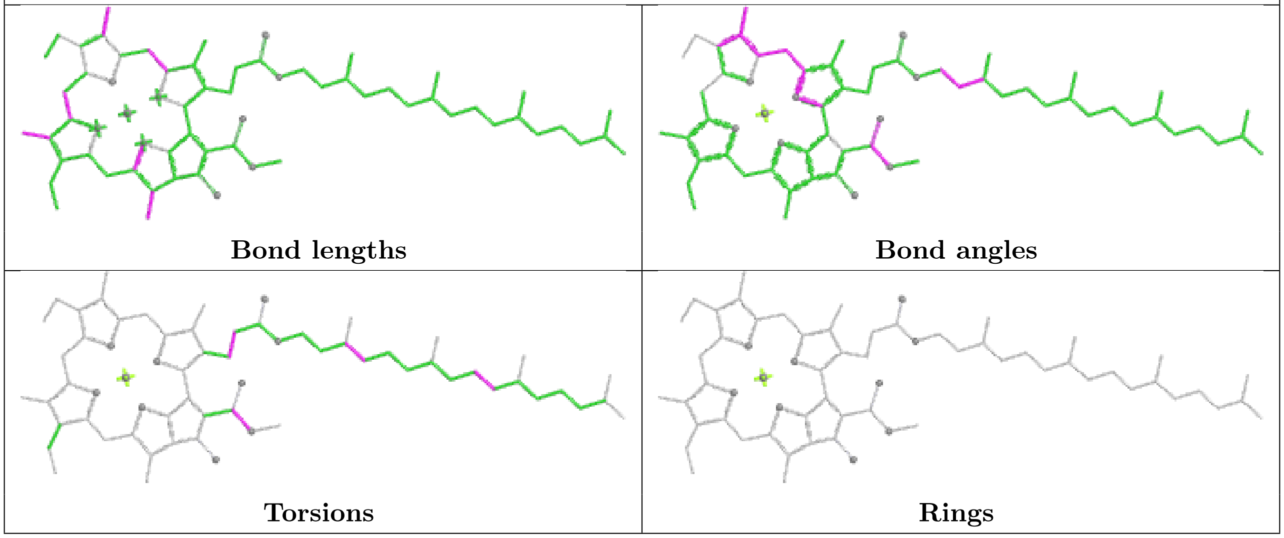
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 827



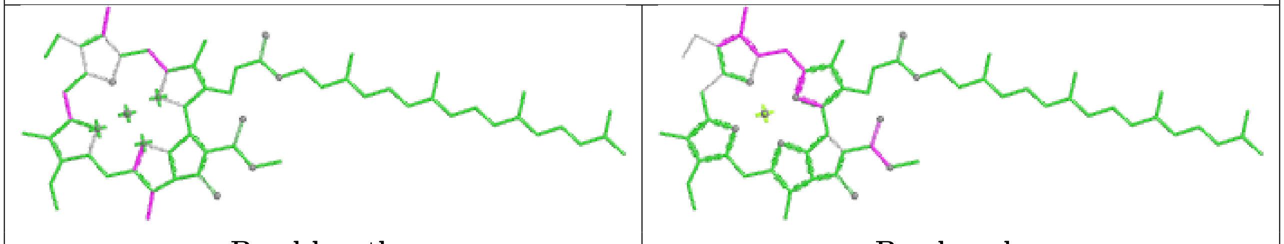
Bond lengths

Bond angles

Torsions

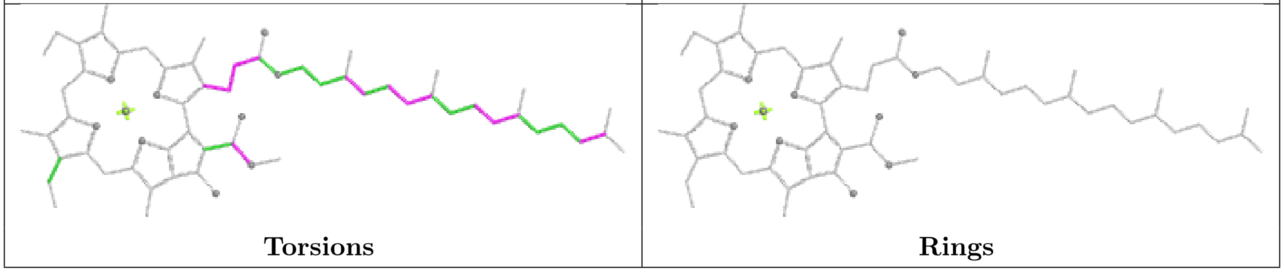
Rings

Ligand CLA b 2127



Bond lengths

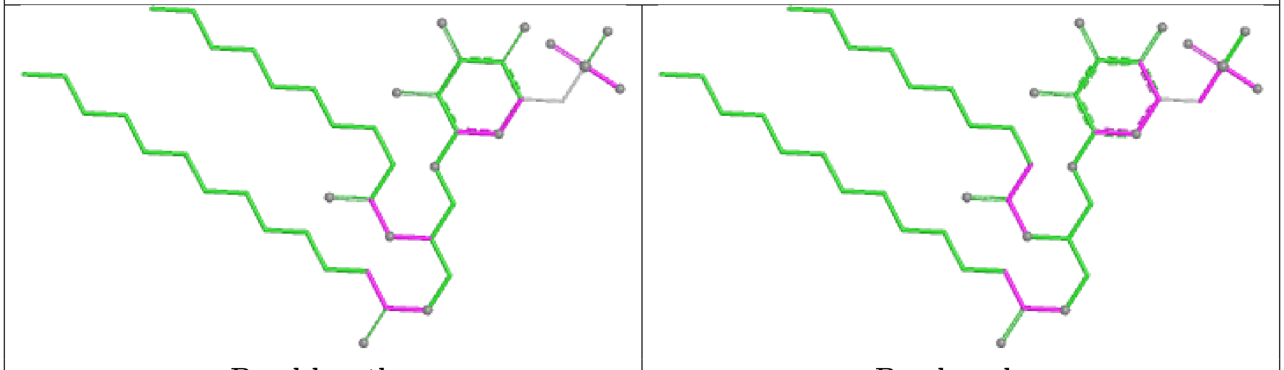
Bond angles



Torsions

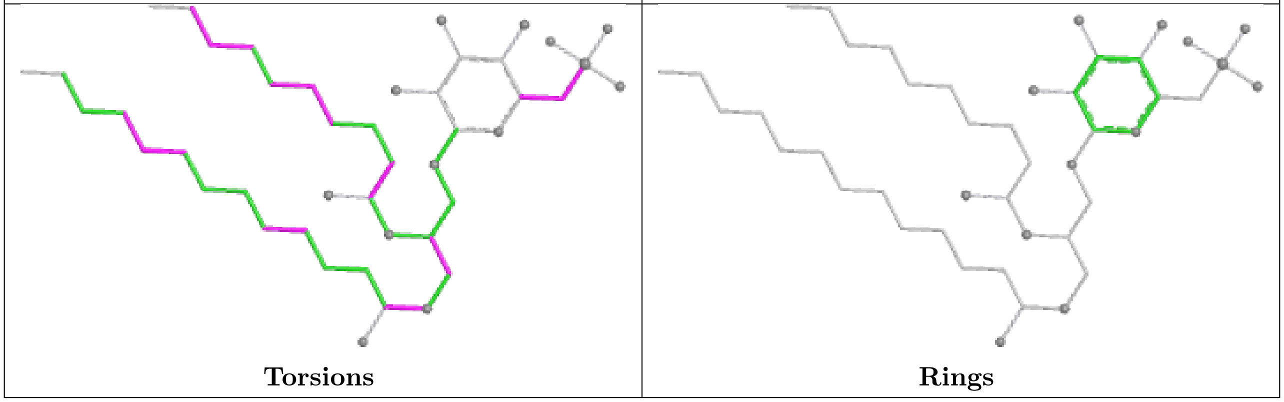
Rings

Ligand SQD U 208



Bond lengths

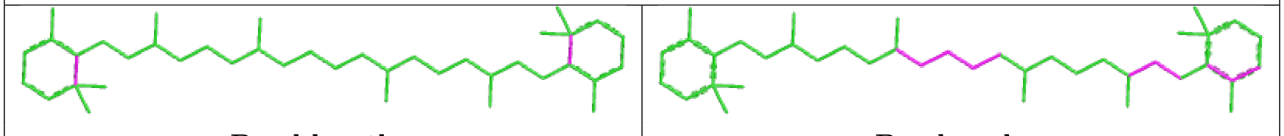
Bond angles



Torsions

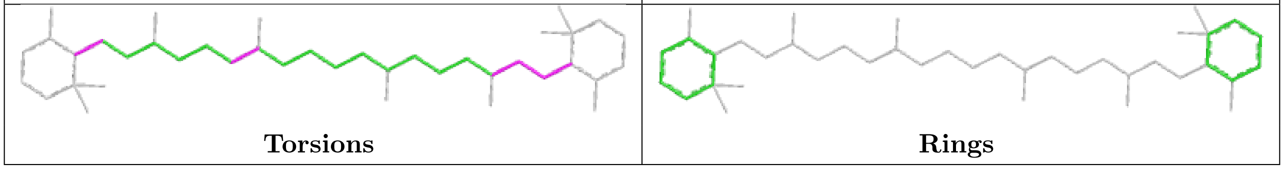
Rings

Ligand BCR A 845



Bond lengths

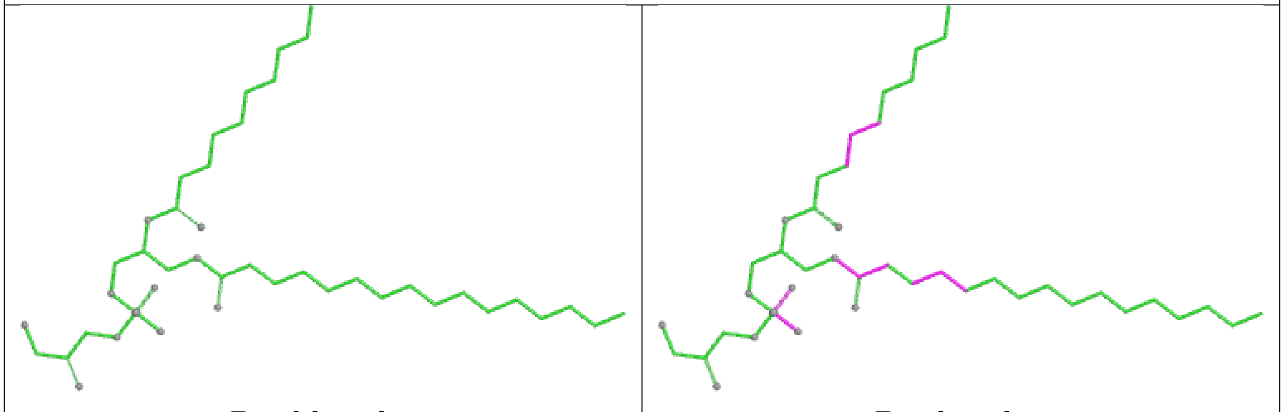
Bond angles



Torsions

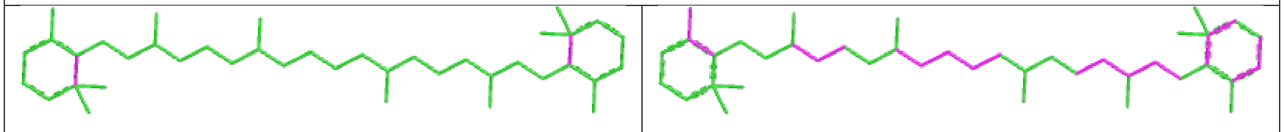
Rings

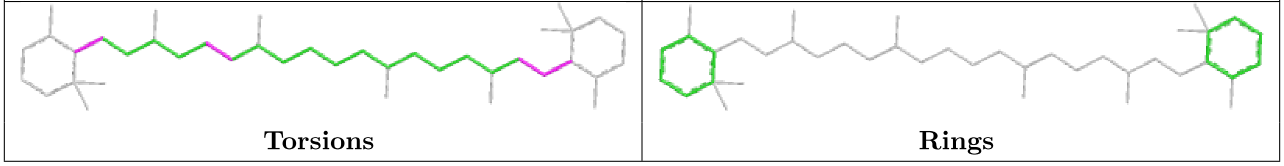
Ligand LHG B 2149


Bond lengths
Bond angles

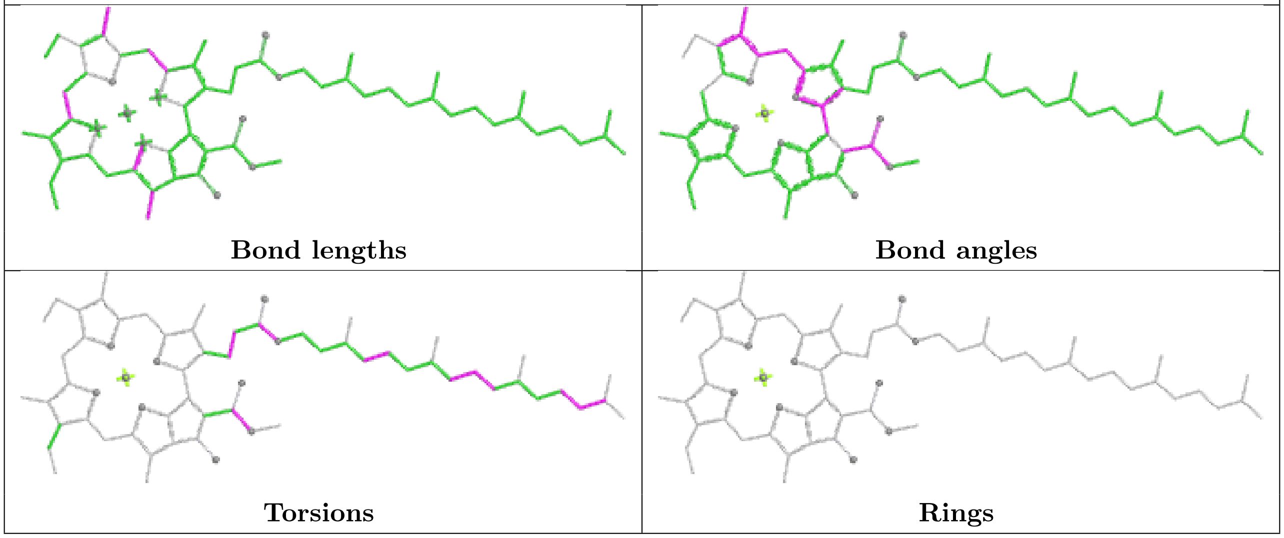

Torsions
Rings

Ligand BCR l 207


Bond lengths
Bond angles


Torsions
Rings

Ligand CLA a 837



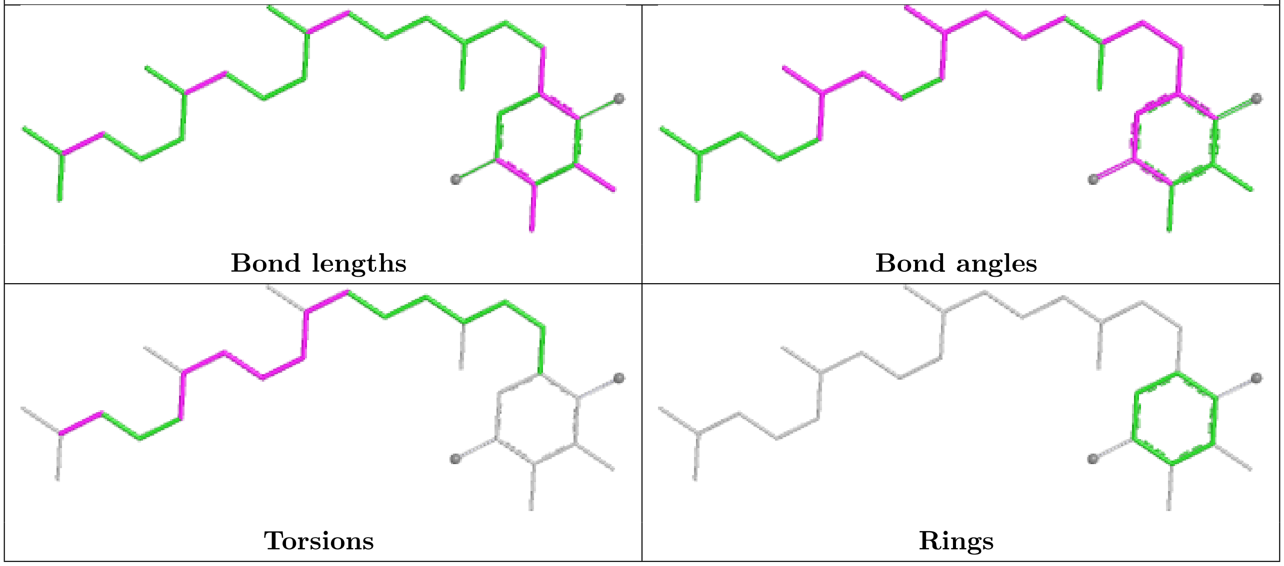
Bond lengths

Bond angles

Torsions

Rings

Ligand A1AGD A 840



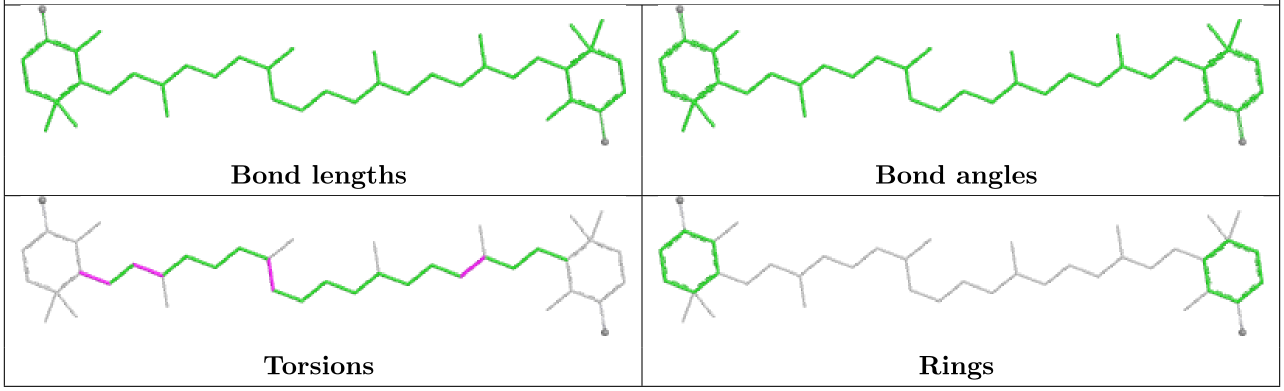
Bond lengths

Bond angles

Torsions

Rings

Ligand 45D A 852



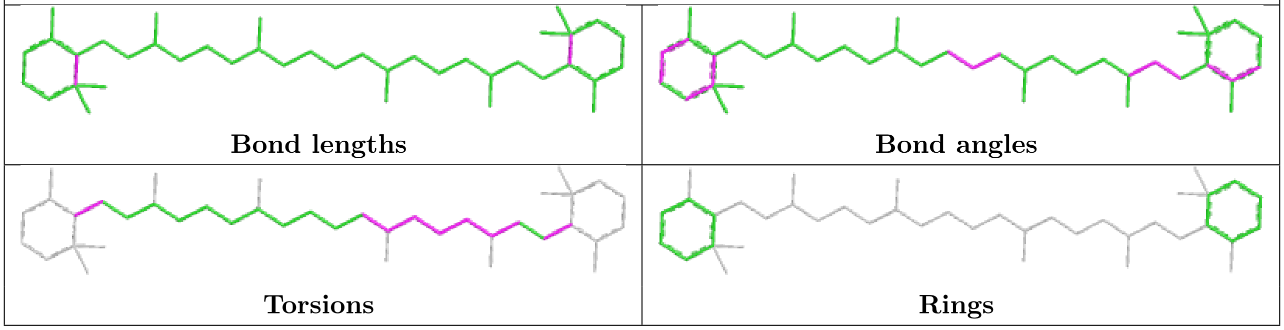
Bond lengths

Bond angles

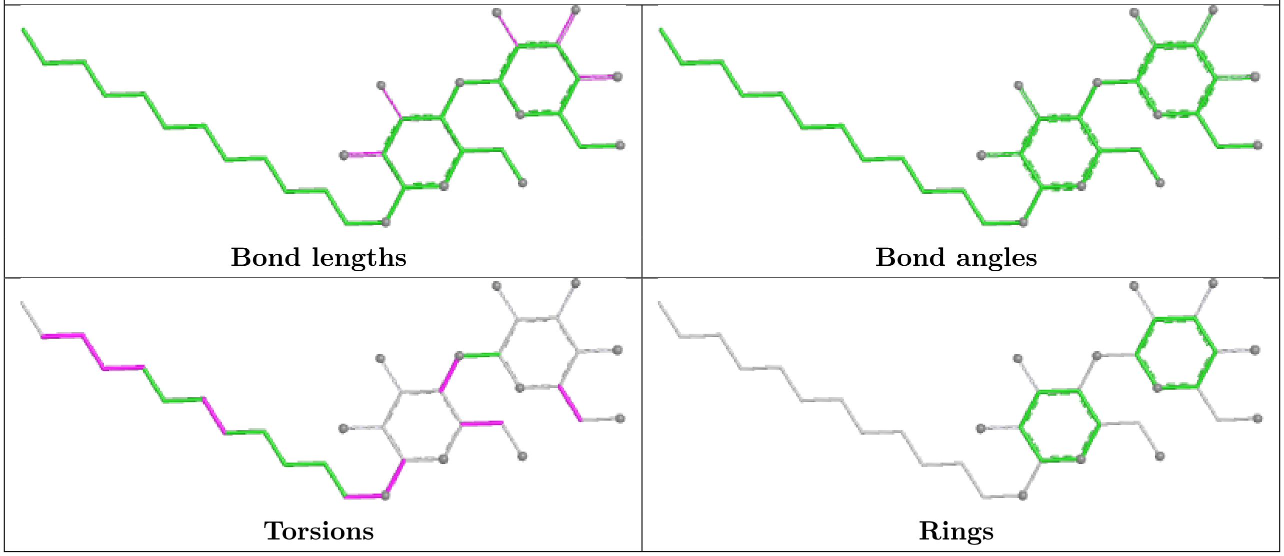
Torsions

Rings

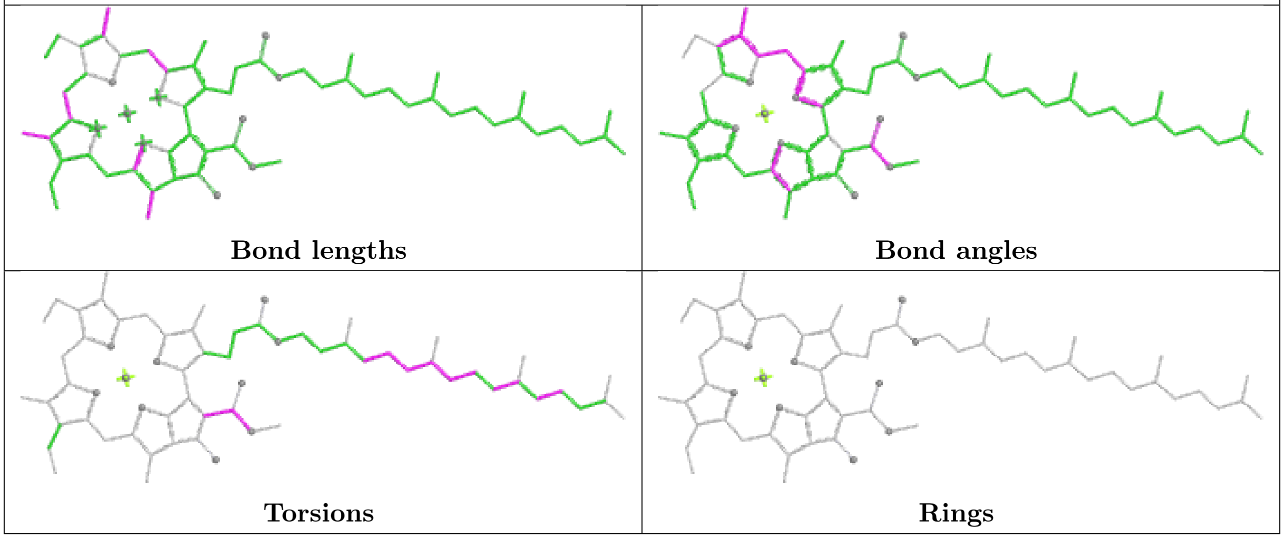
Ligand BCR G 842


Bond lengths
Bond angles
Torsions
Rings

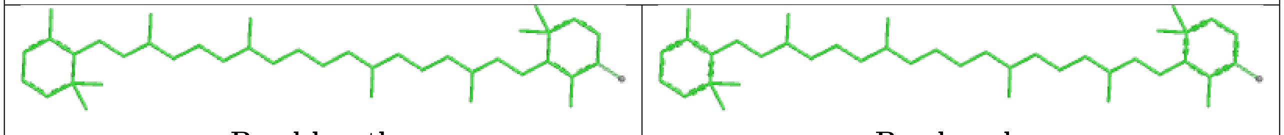
Ligand LMT l 210


Bond lengths
Bond angles
Torsions
Rings

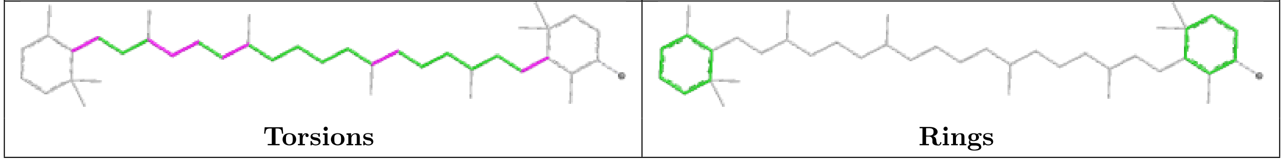
Ligand CLA H 2129


Bond lengths
Bond angles
Torsions
Rings

Ligand ECH m 101

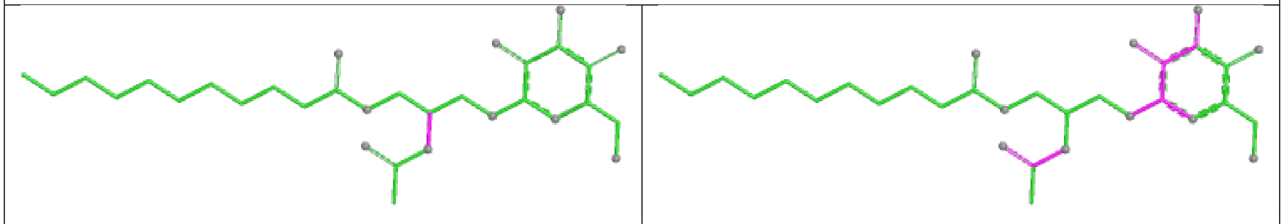


Bond lengths **Bond angles**

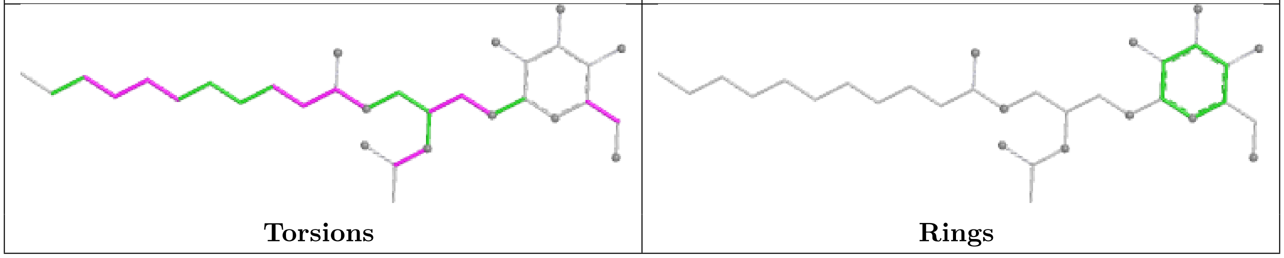


Torsions **Rings**

Ligand LMG G 849

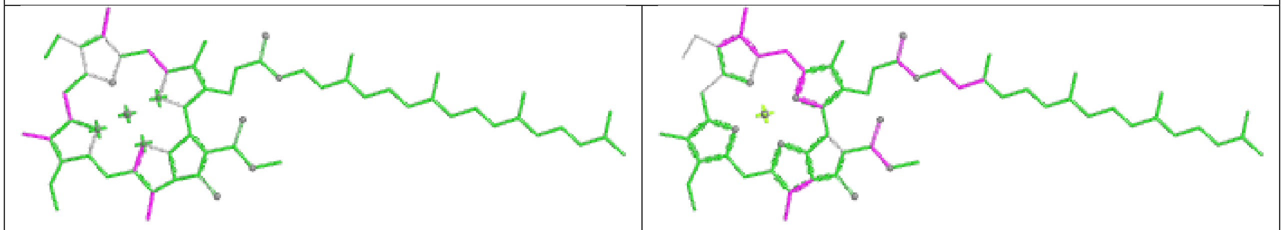


Bond lengths **Bond angles**

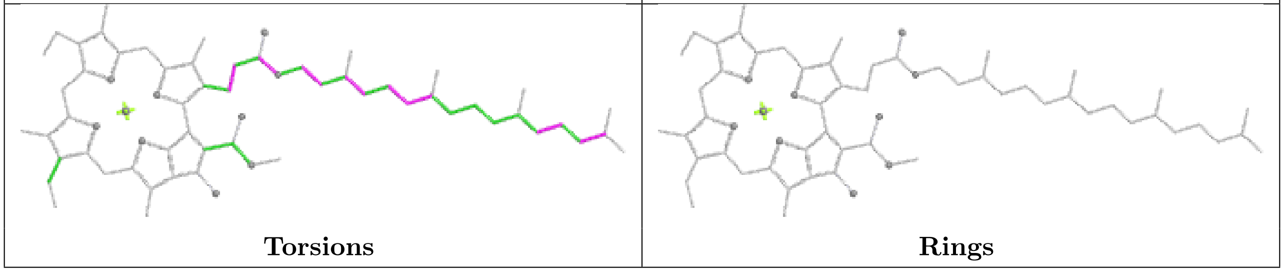


Torsions **Rings**

Ligand CLA H 2102

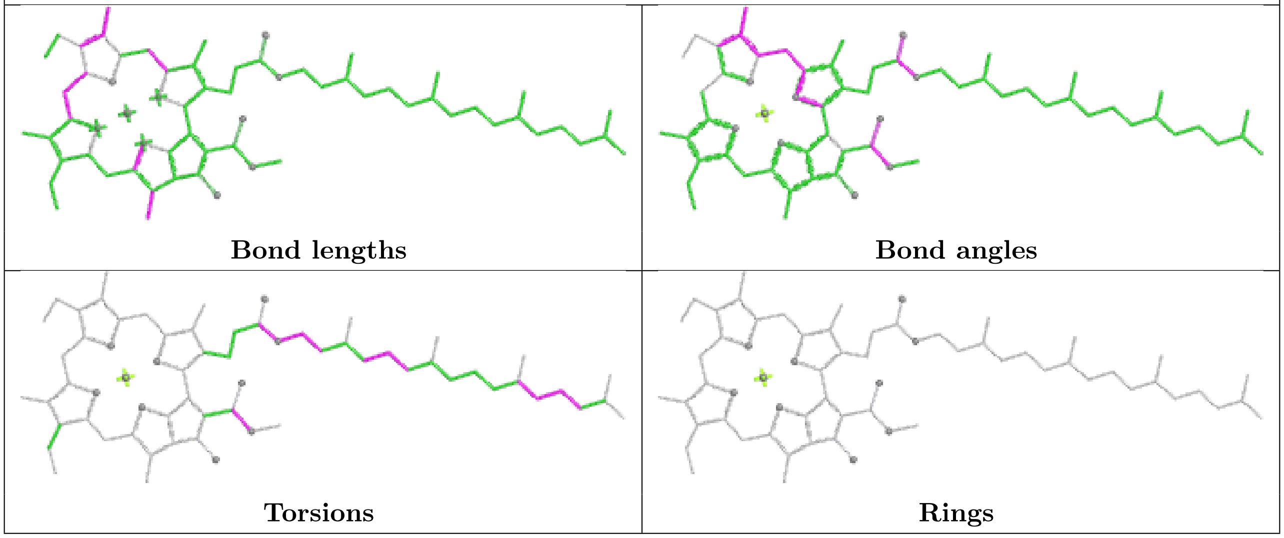


Bond lengths **Bond angles**

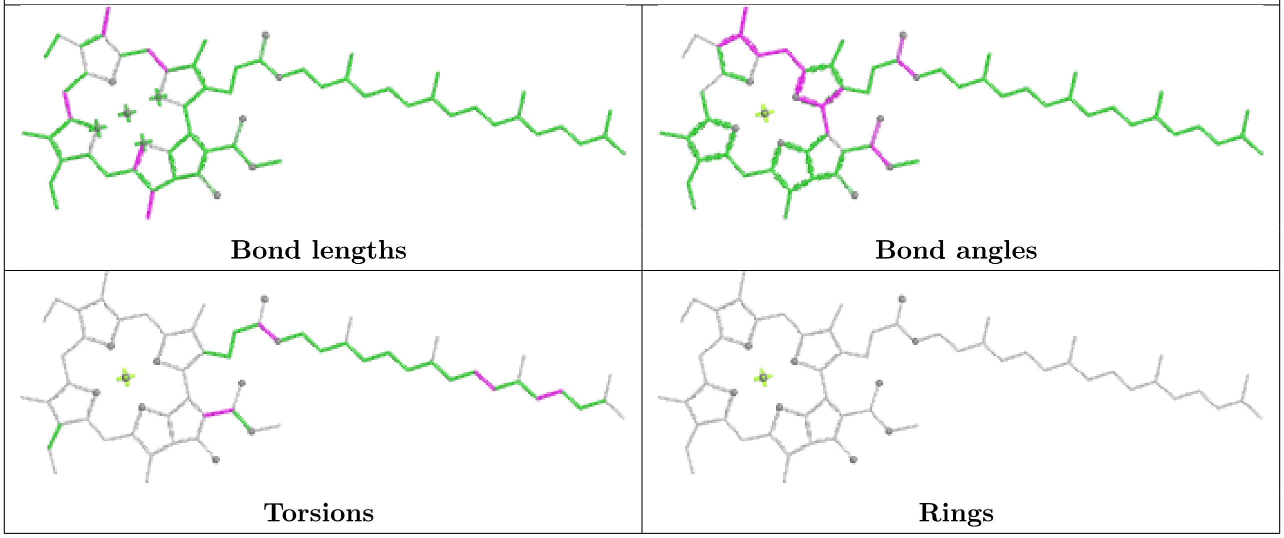


Torsions **Rings**

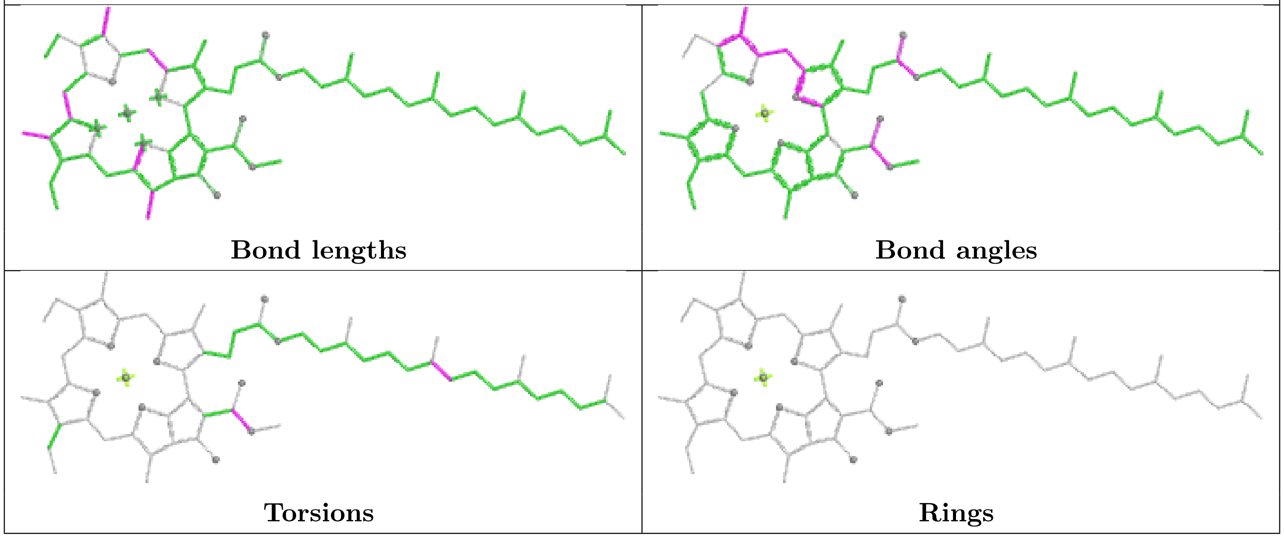
Ligand CLA B 2111



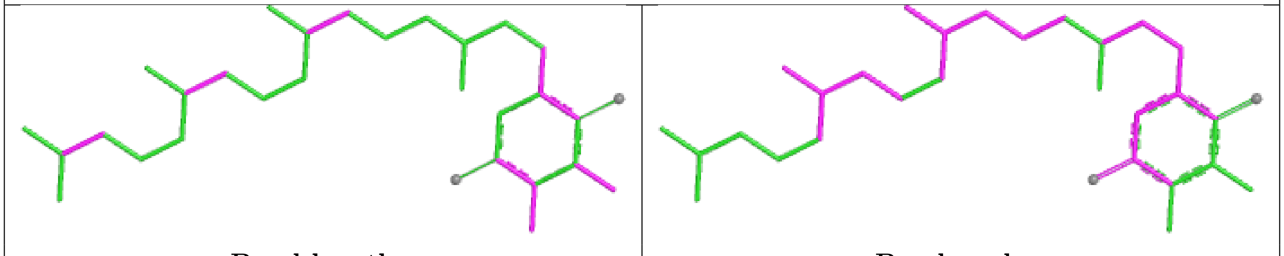
Ligand CLA b 2124



Ligand CLA A 838

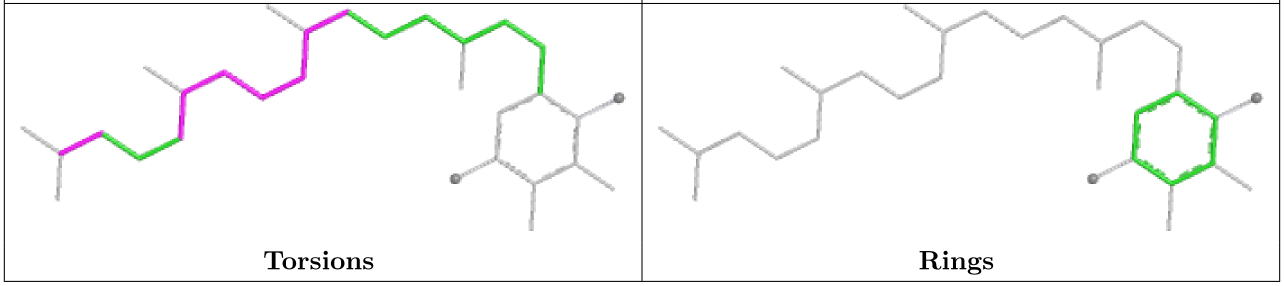


Ligand A1AGD a 840



Bond lengths

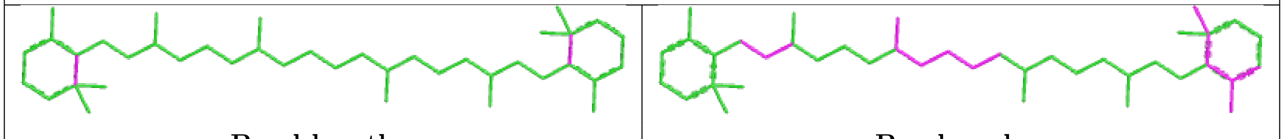
Bond angles



Torsions

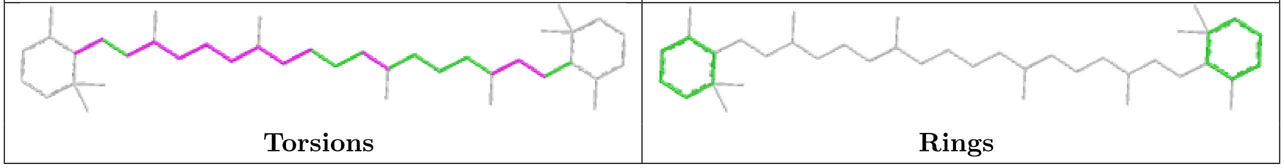
Rings

Ligand BCR a 843



Bond lengths

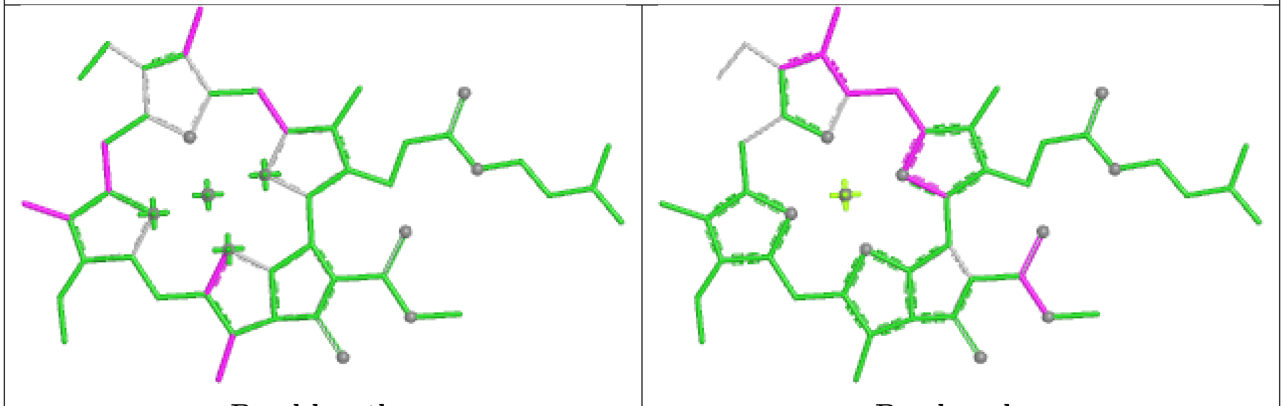
Bond angles



Torsions

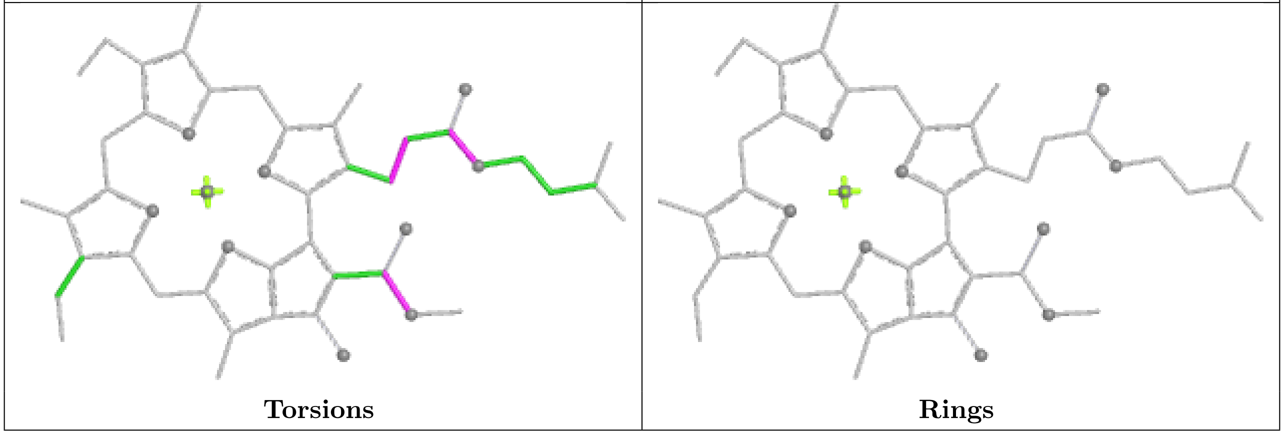
Rings

Ligand CLA b 2152



Bond lengths

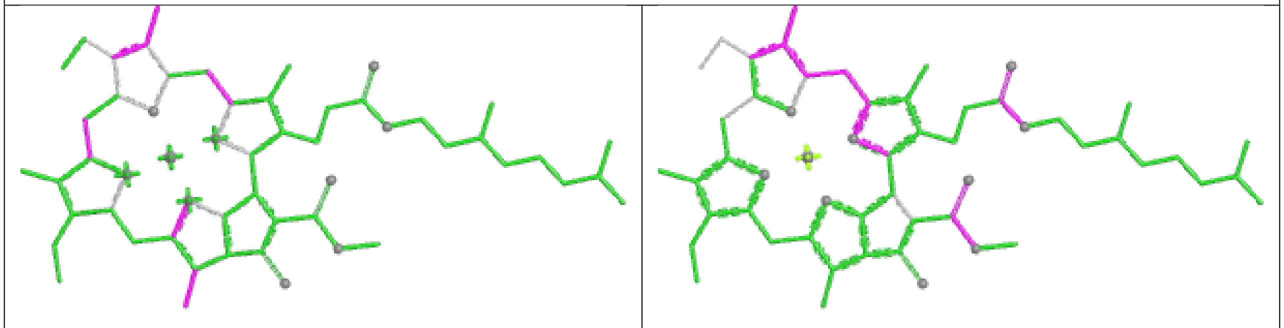
Bond angles



Torsions

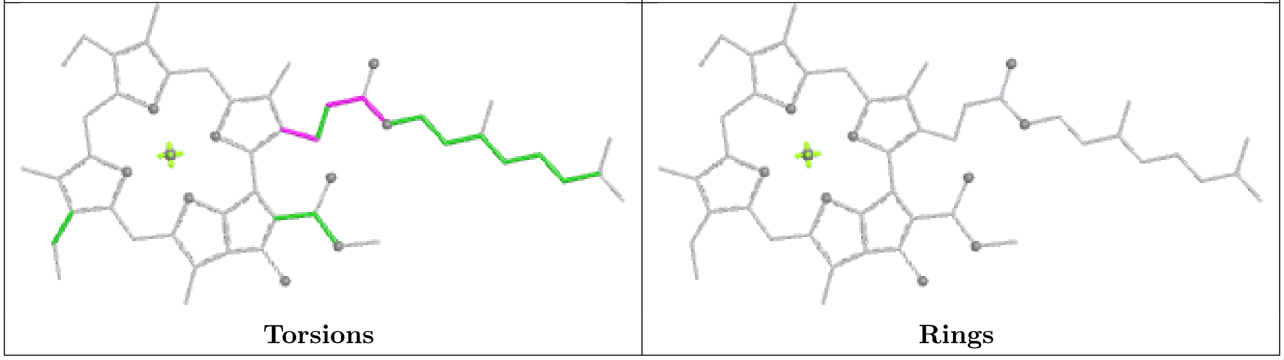
Rings

Ligand CLA H 2120



Bond lengths

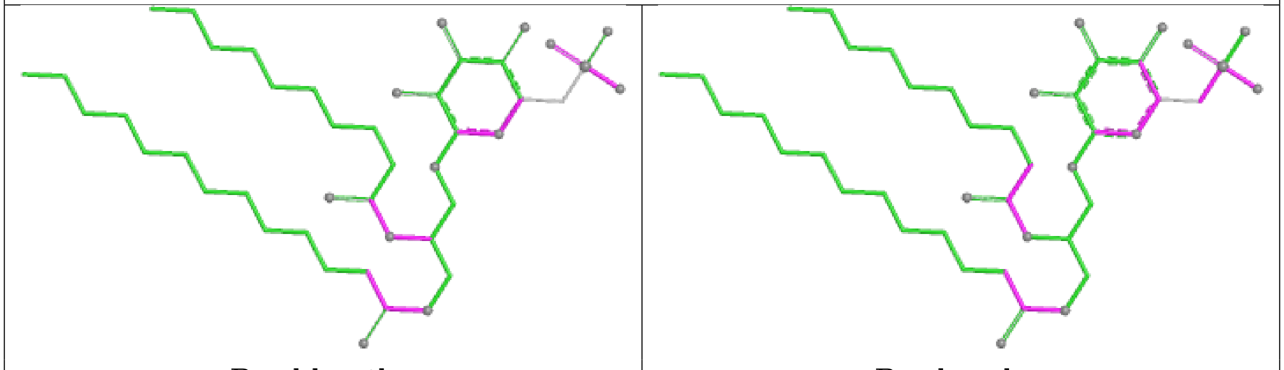
Bond angles



Torsions

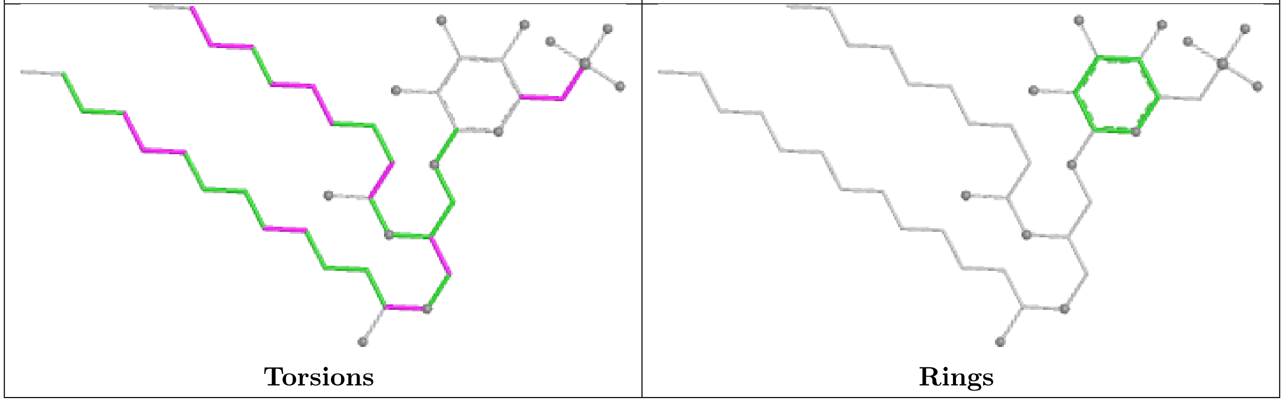
Rings

Ligand SQD l 208



Bond lengths

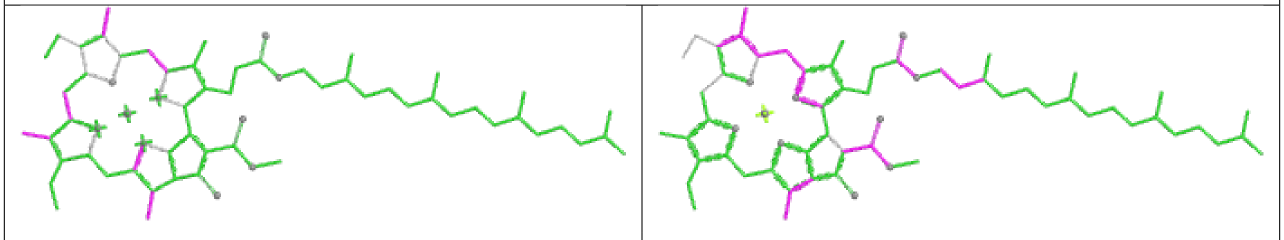
Bond angles



Torsions

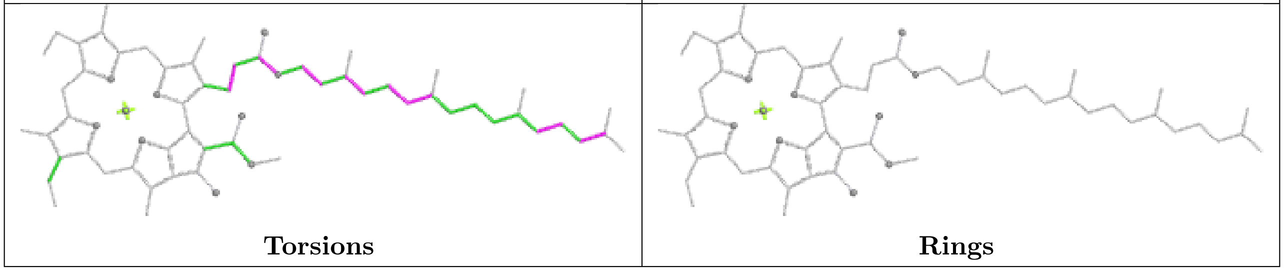
Rings

Ligand CLA b 2102



Bond lengths

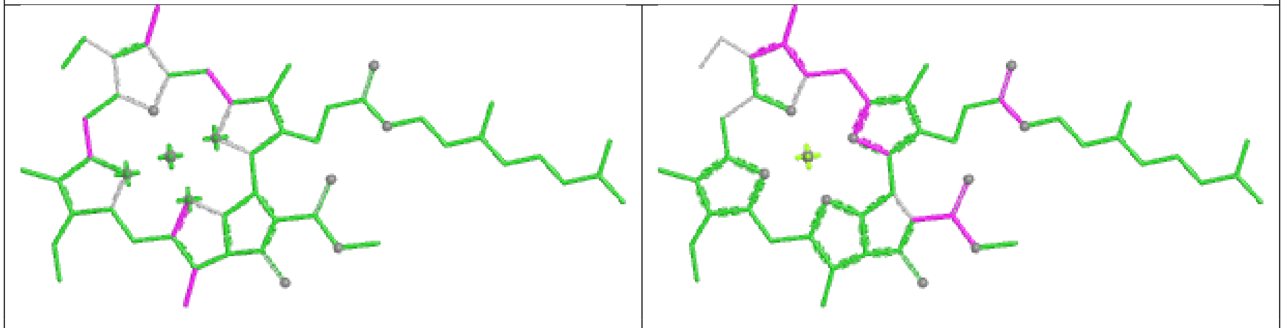
Bond angles



Torsions

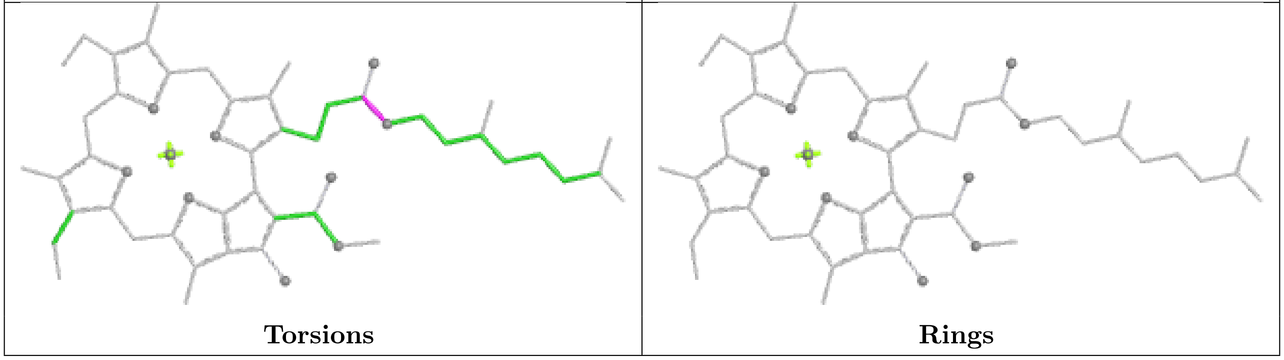
Rings

Ligand CLA a 803



Bond lengths

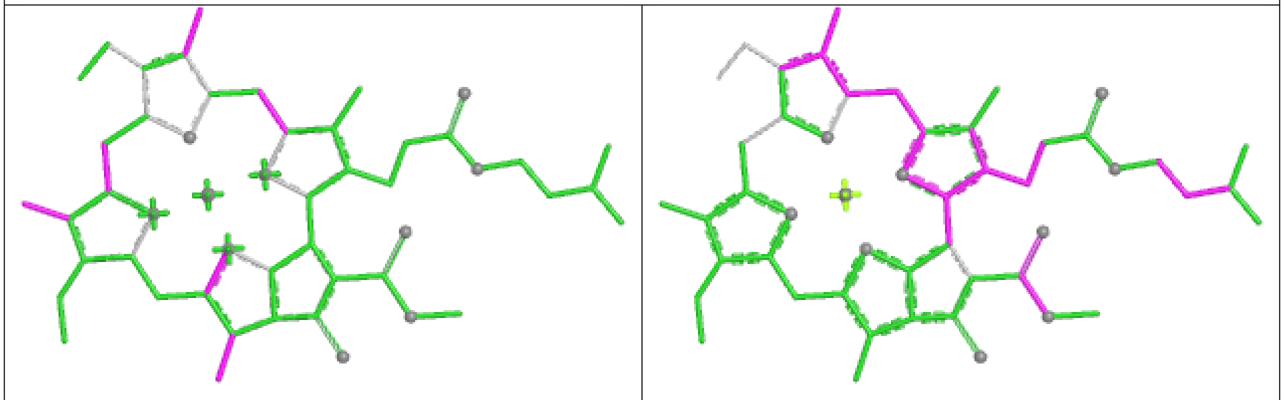
Bond angles



Torsions

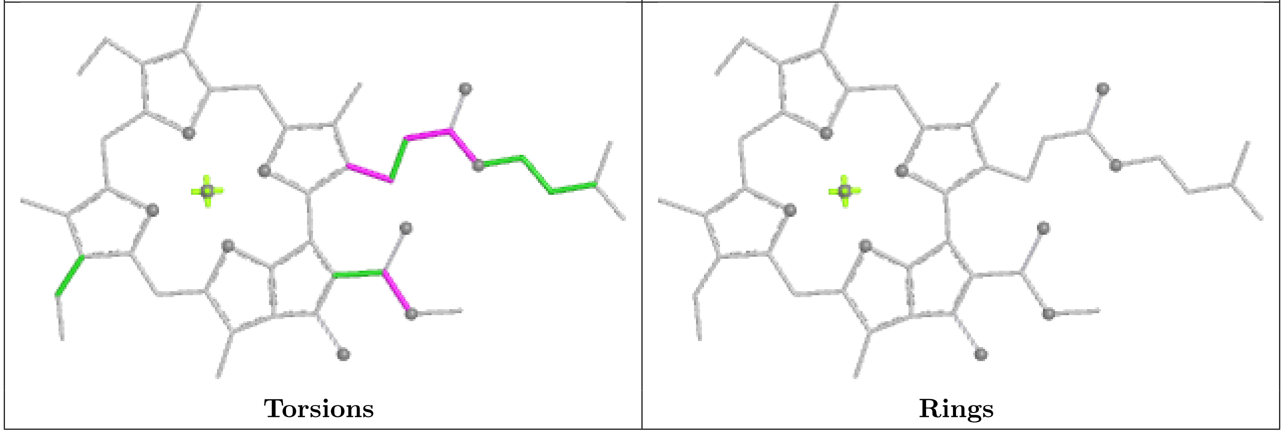
Rings

Ligand CLA a 809



Bond lengths

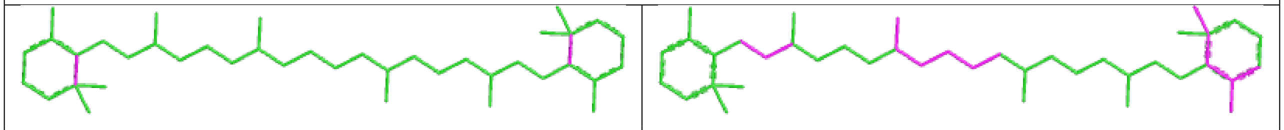
Bond angles



Torsions

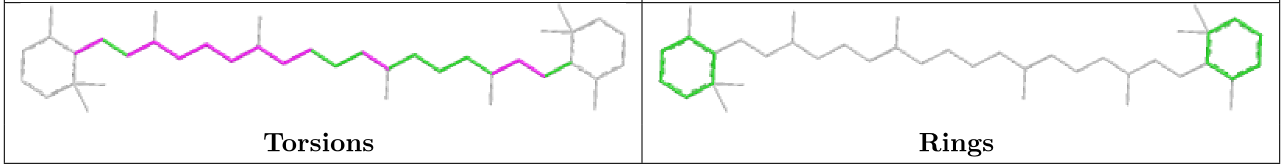
Rings

Ligand BCR G 843



Bond lengths

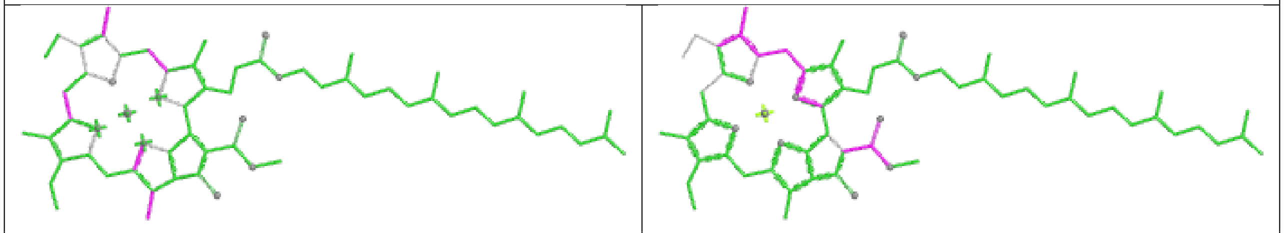
Bond angles



Torsions

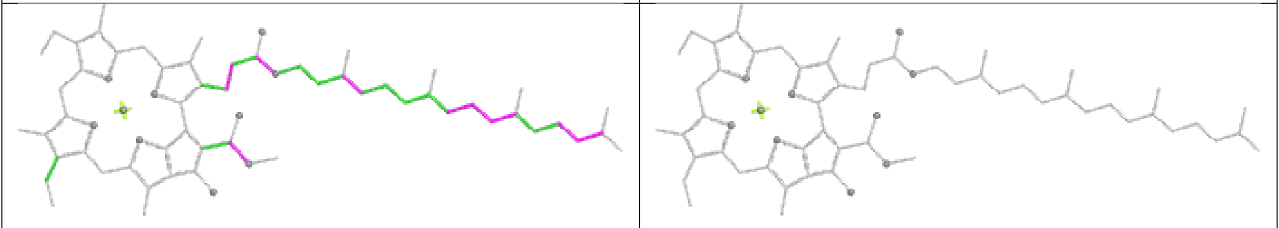
Rings

Ligand CLA A 810



Bond lengths

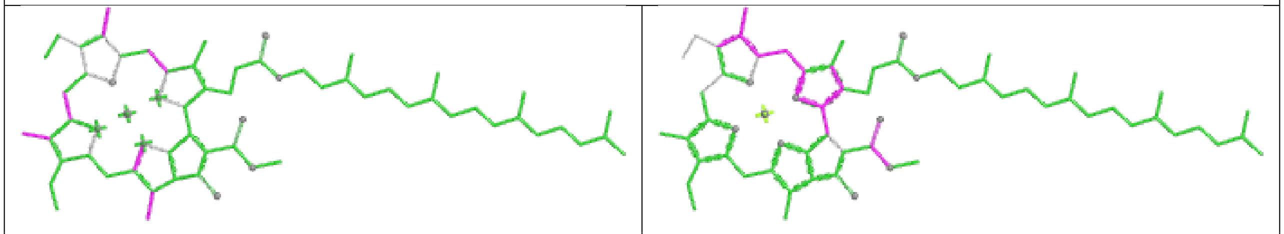
Bond angles



Torsions

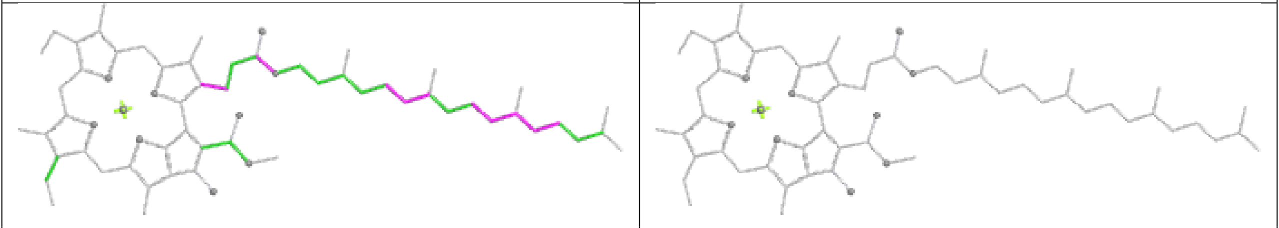
Rings

Ligand CLA l 203



Bond lengths

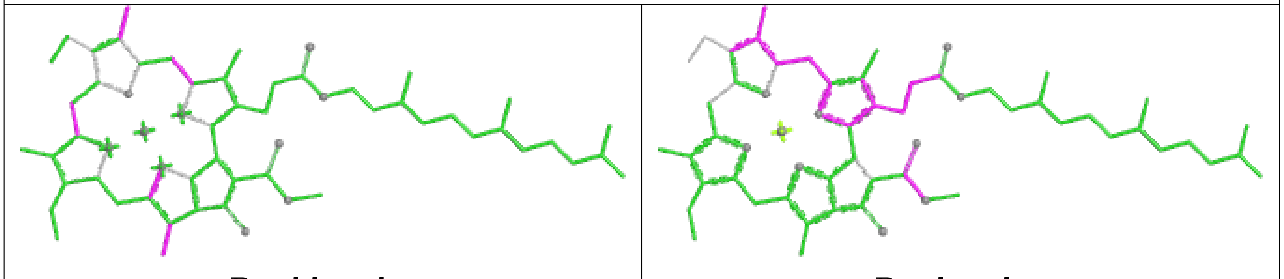
Bond angles



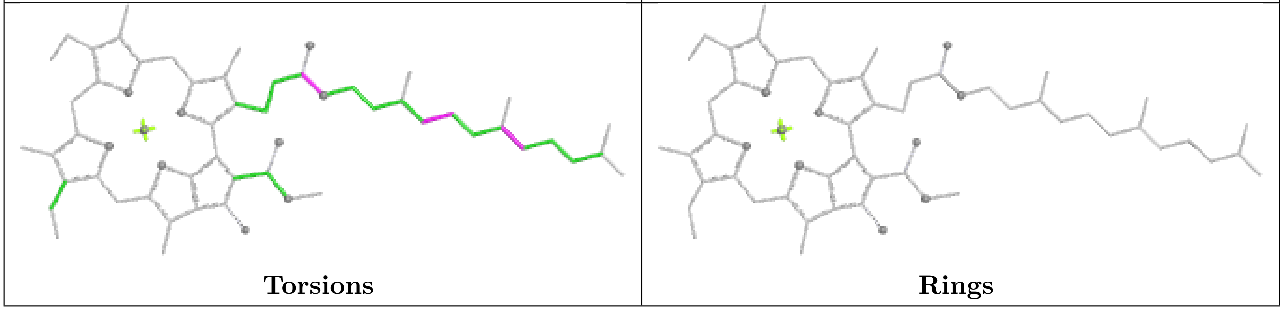
Torsions

Rings

Ligand CLA A 825

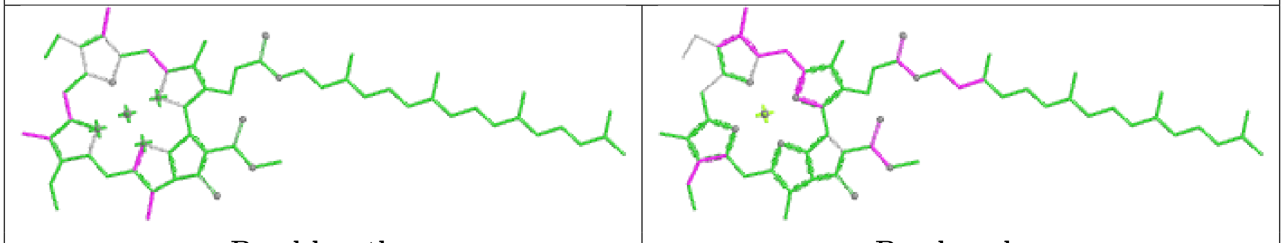


Bond lengths **Bond angles**

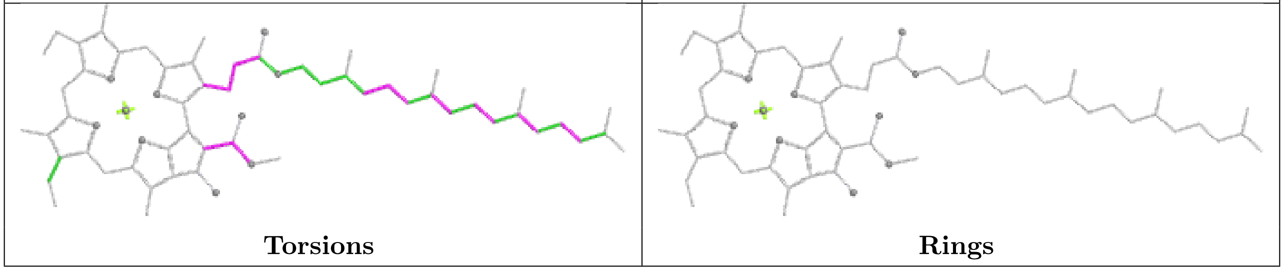


Torsions **Rings**

Ligand CLA H 2114

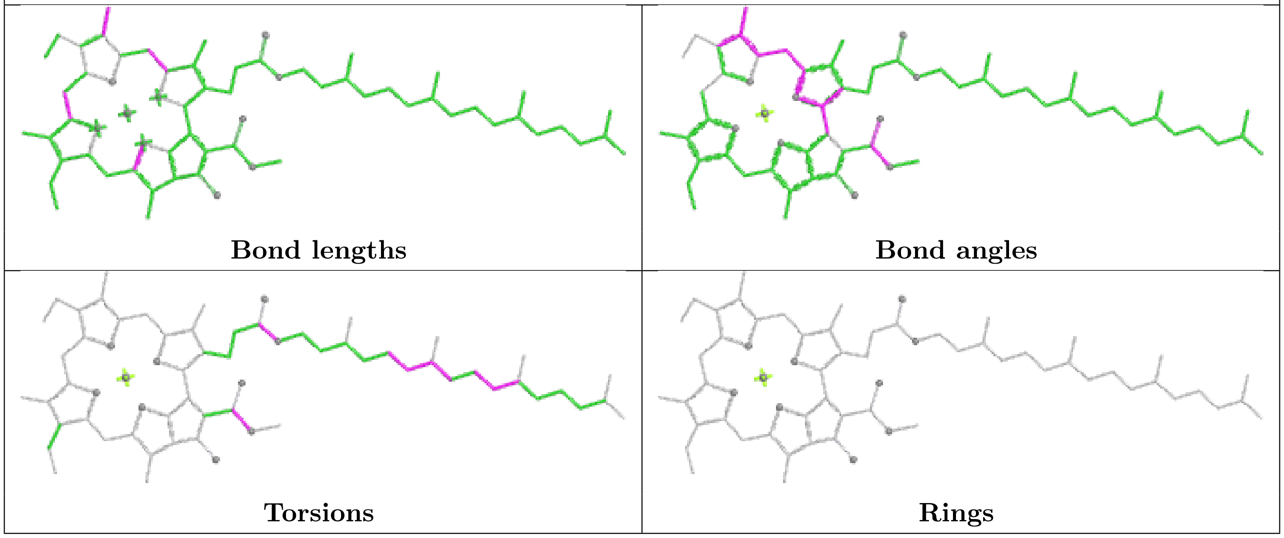


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA a 813



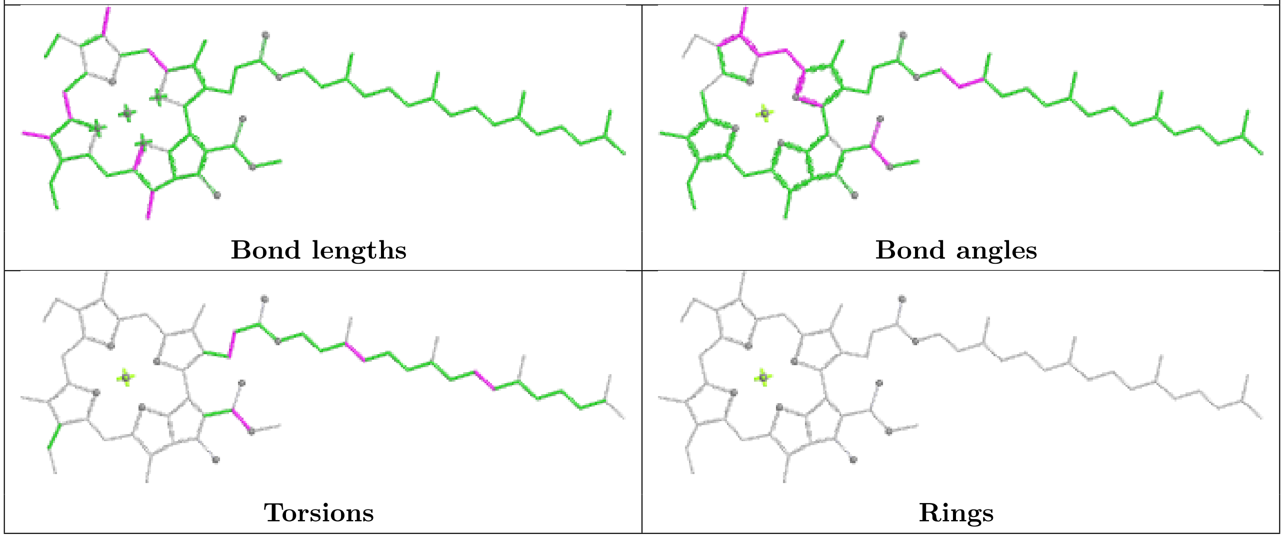
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 827



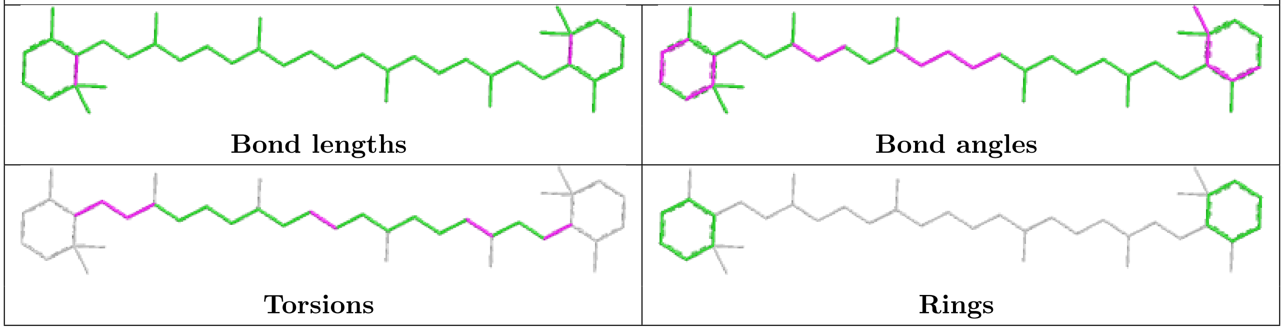
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR b 2144



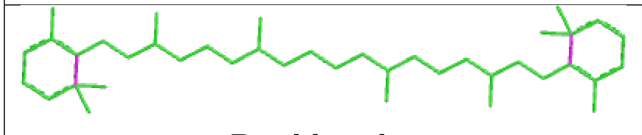
Bond lengths

Bond angles

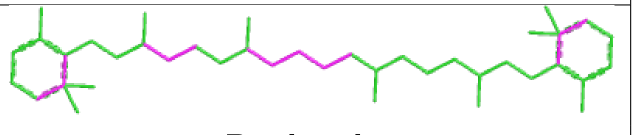
Torsions

Rings

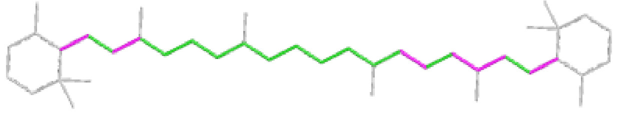
Ligand BCR L 206



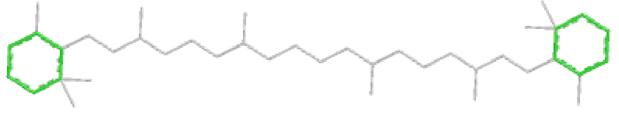
Bond lengths



Bond angles

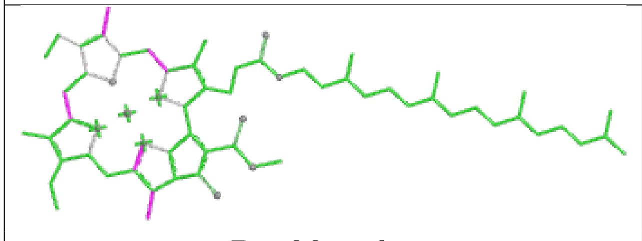


Torsions

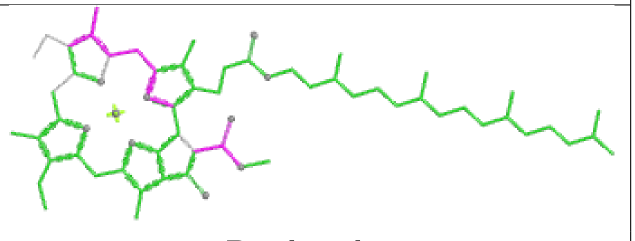


Rings

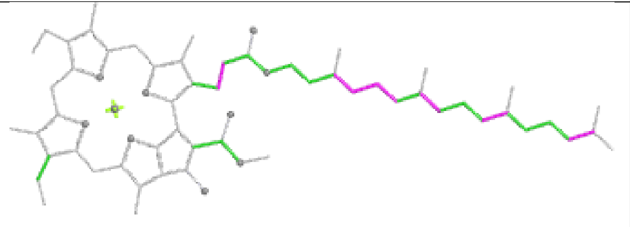
Ligand CLA B 2109



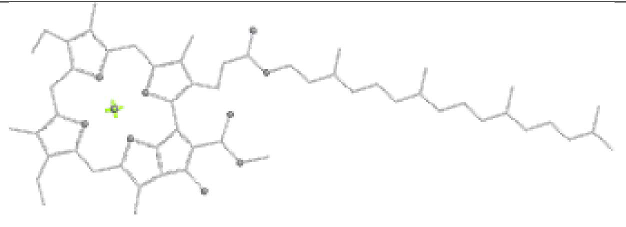
Bond lengths



Bond angles

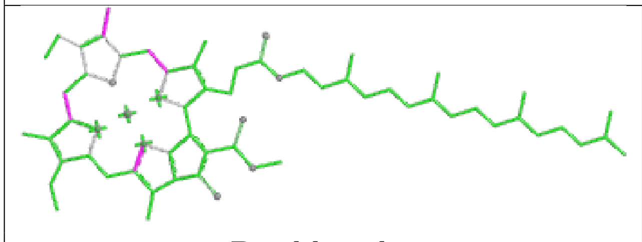


Torsions

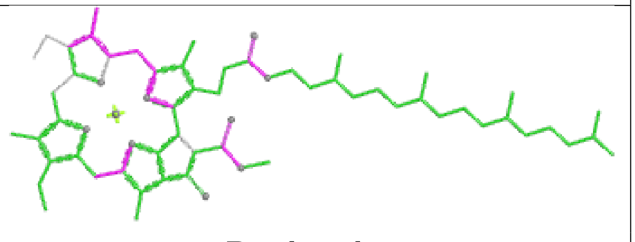


Rings

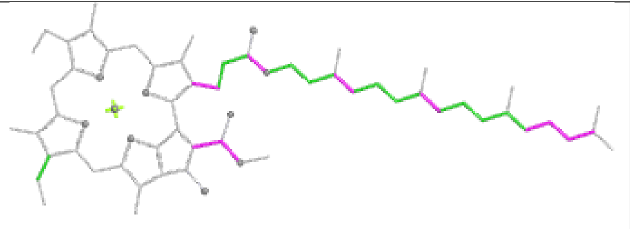
Ligand CLA b 2106



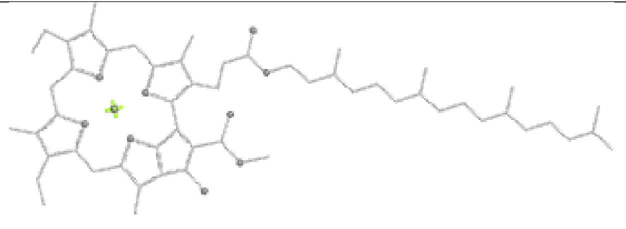
Bond lengths



Bond angles

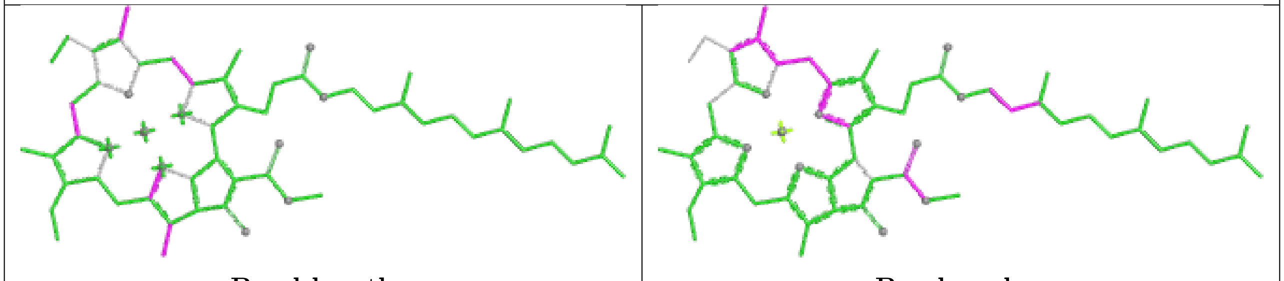


Torsions



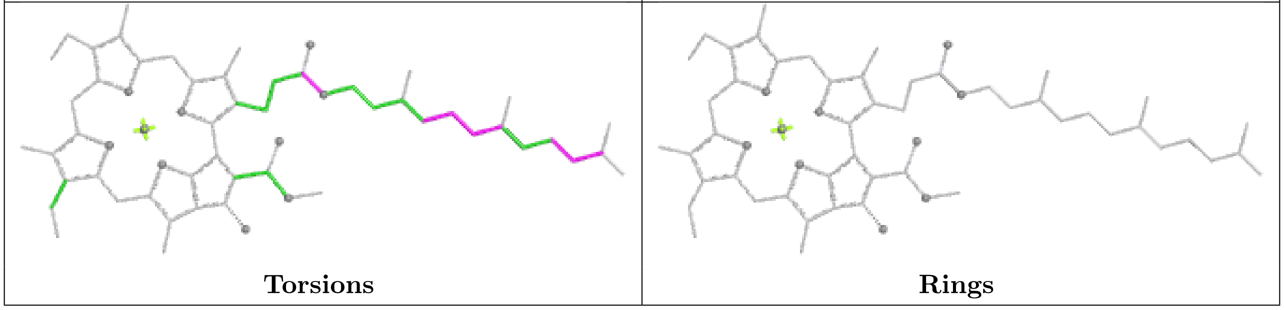
Rings

Ligand CLA G 831



Bond lengths

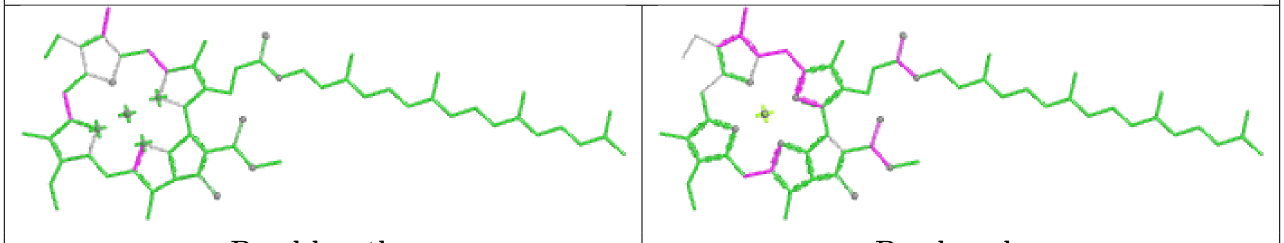
Bond angles



Torsions

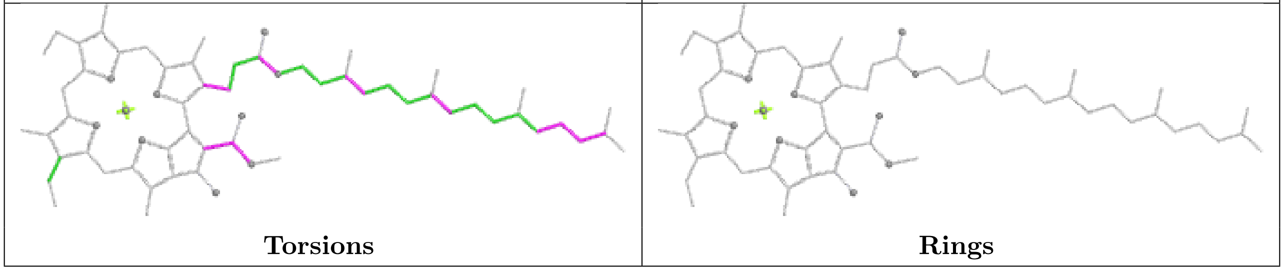
Rings

Ligand CLA B 2107



Bond lengths

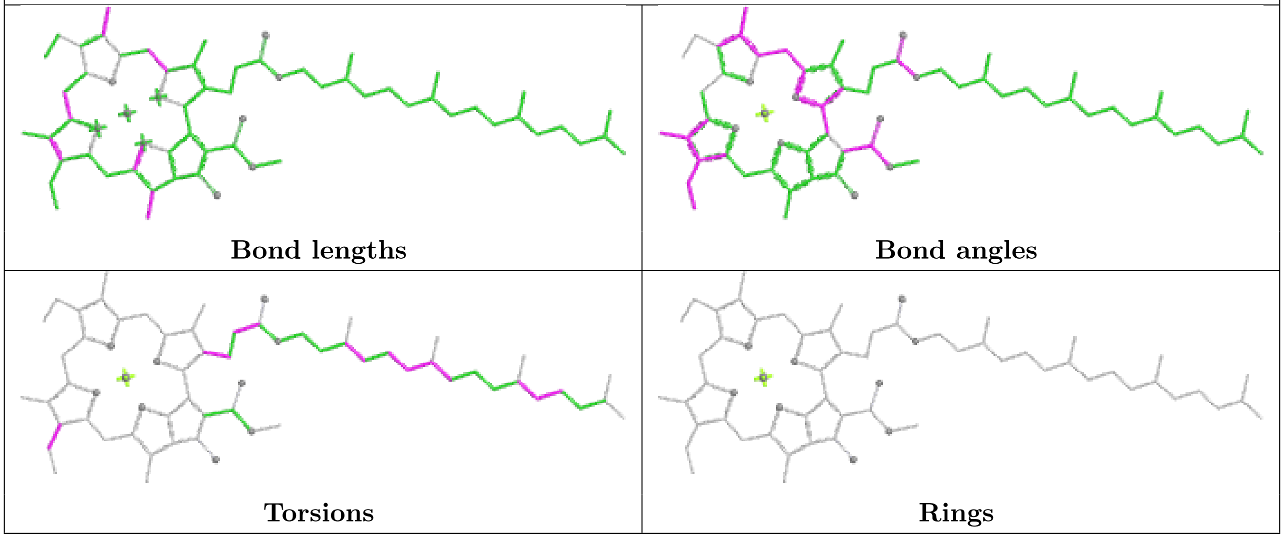
Bond angles



Torsions

Rings

Ligand CLA b 2111



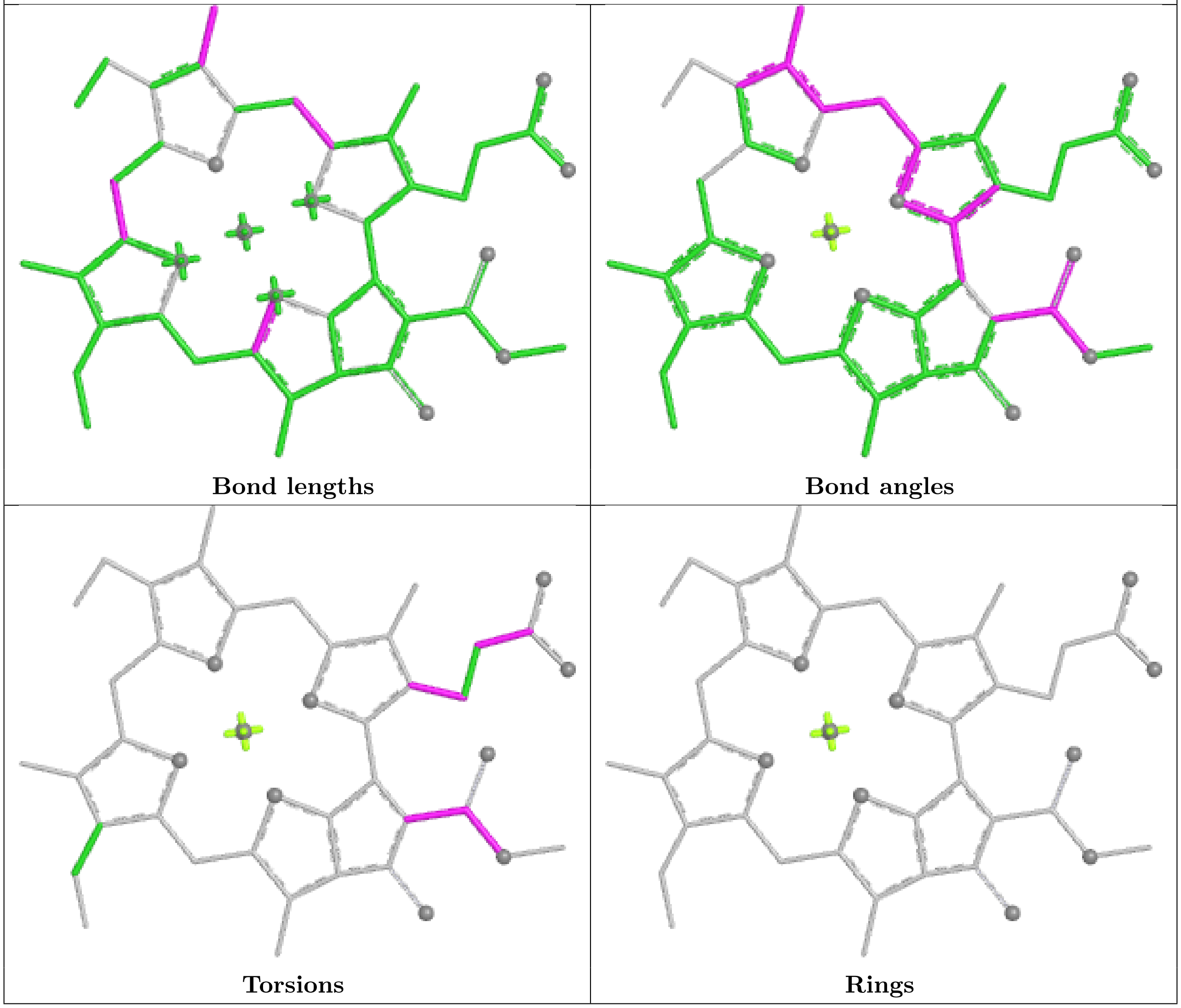
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA H 2117



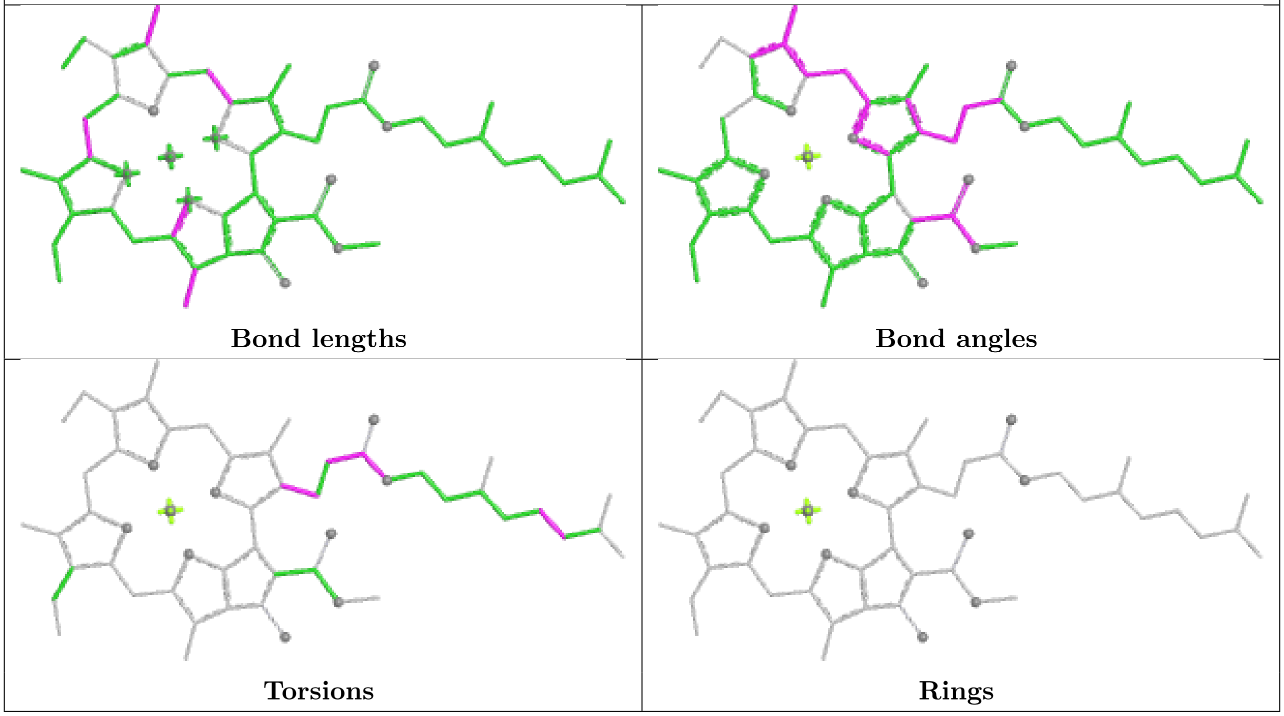
Bond lengths

Bond angles

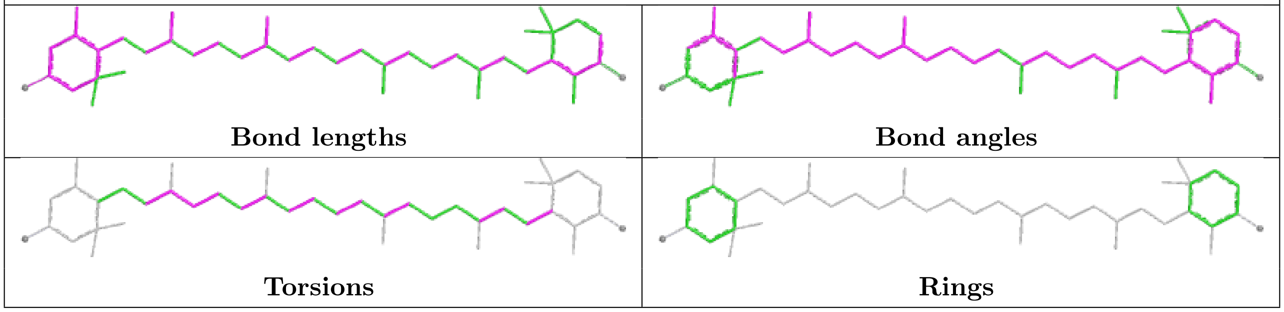
Torsions

Rings

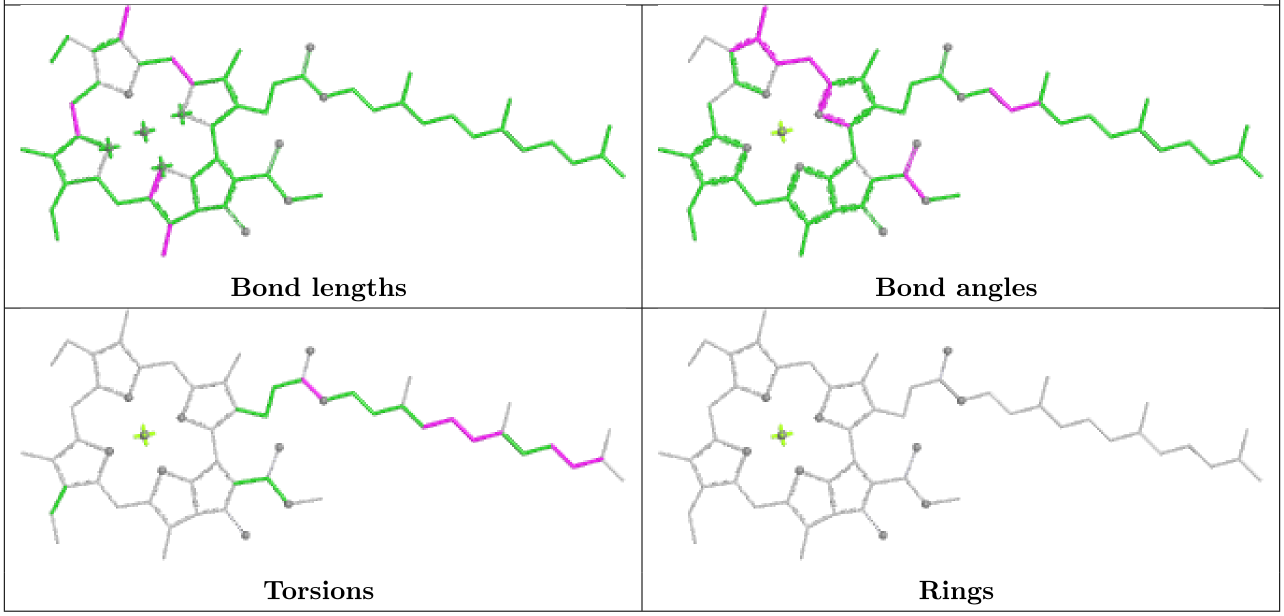
Ligand CLA a 854


Bond lengths
Bond angles
Torsions
Rings

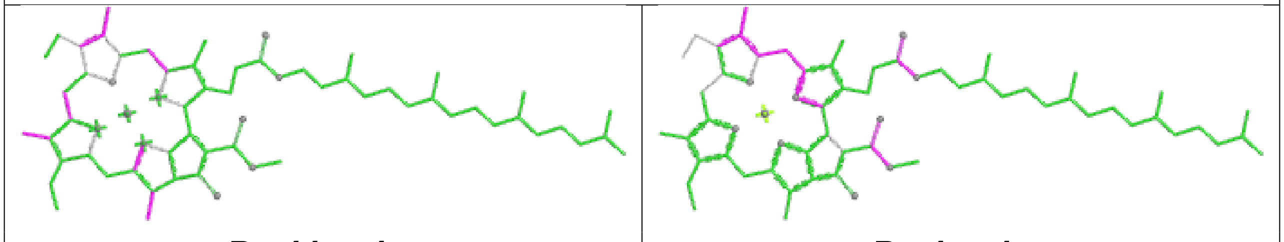
Ligand EQ3 B 2151


Bond lengths
Bond angles
Torsions
Rings

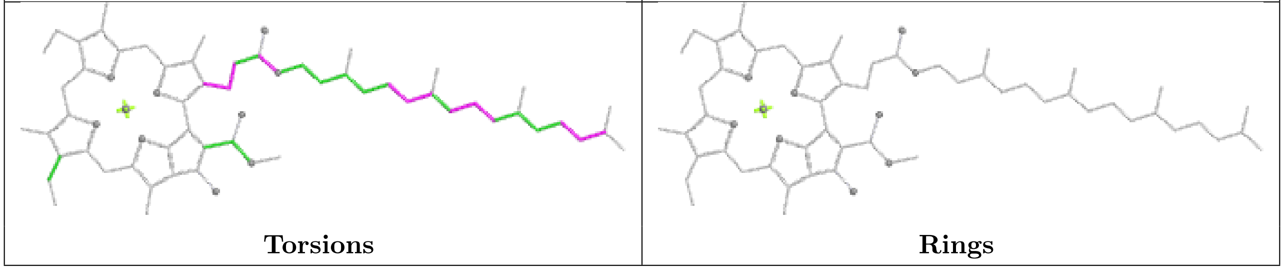
Ligand CLA A 831


Bond lengths
Bond angles
Torsions
Rings

Ligand CLA A 826

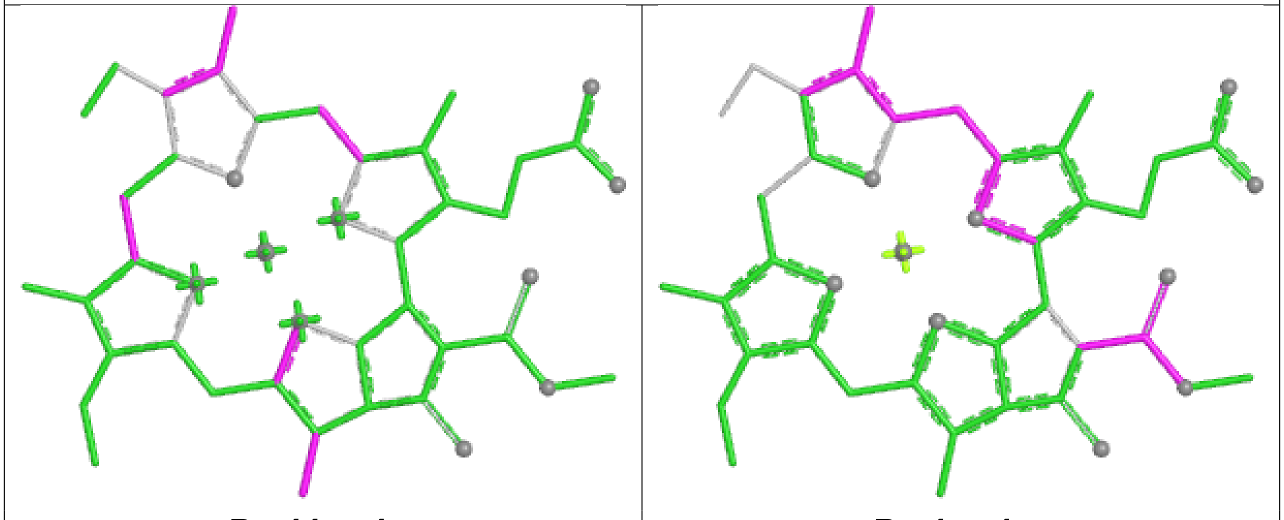


Bond lengths Bond angles

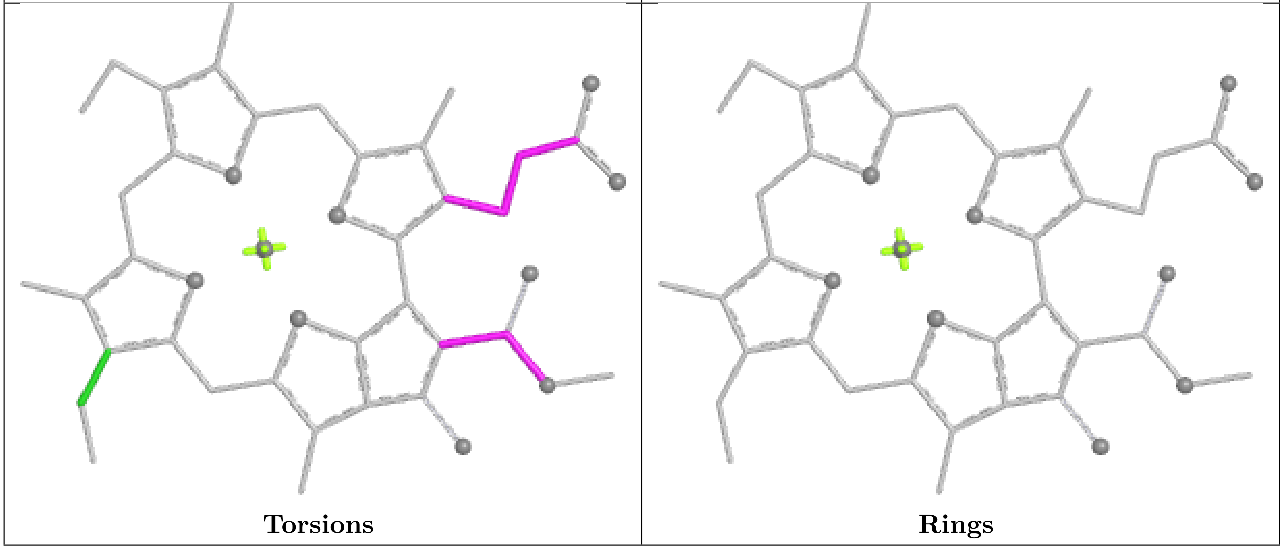


Torsions Rings

Ligand CLA H 2113

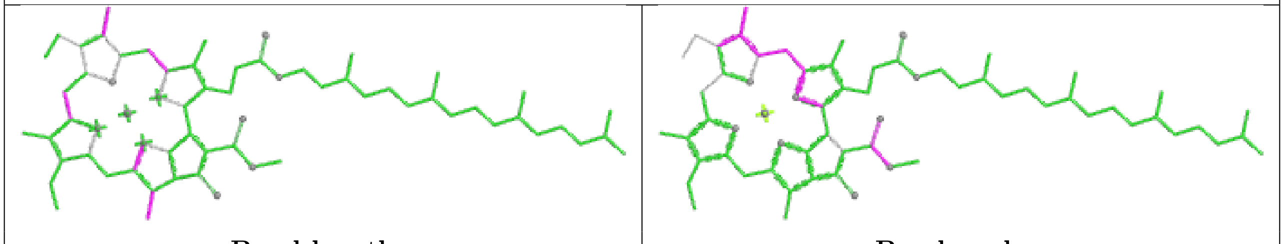


Bond lengths Bond angles

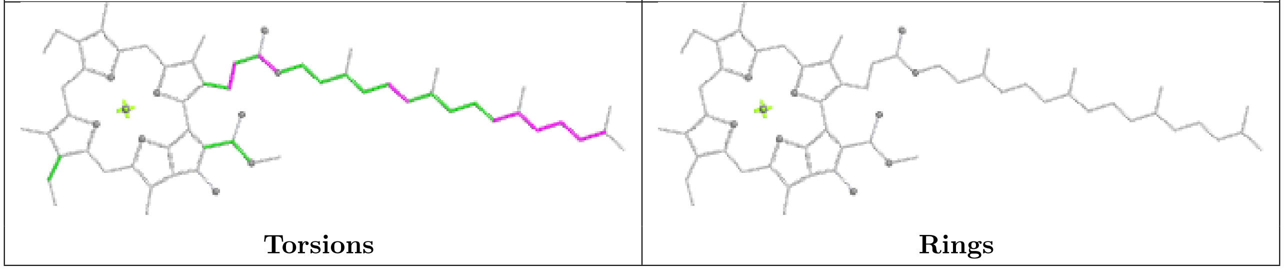


Torsions Rings

Ligand CLA A 828

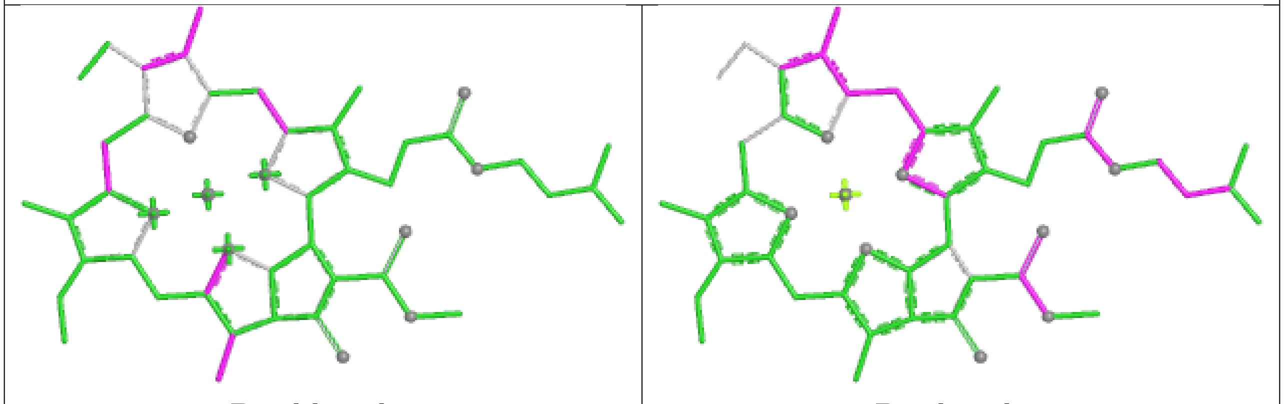


Bond lengths **Bond angles**

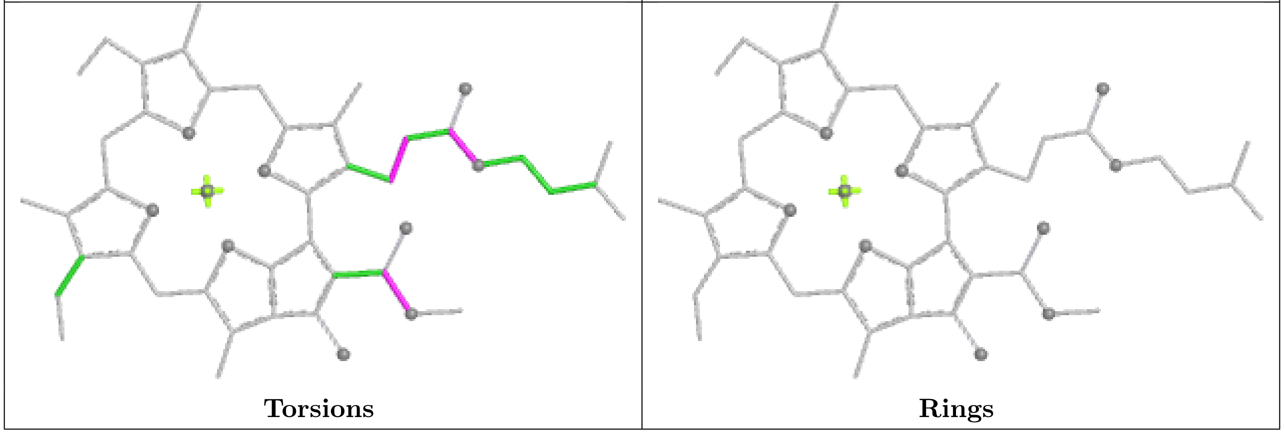


Torsions **Rings**

Ligand CLA b 2118

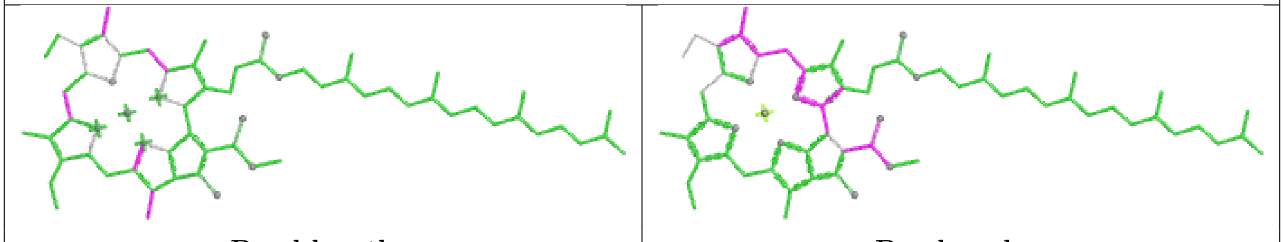


Bond lengths **Bond angles**

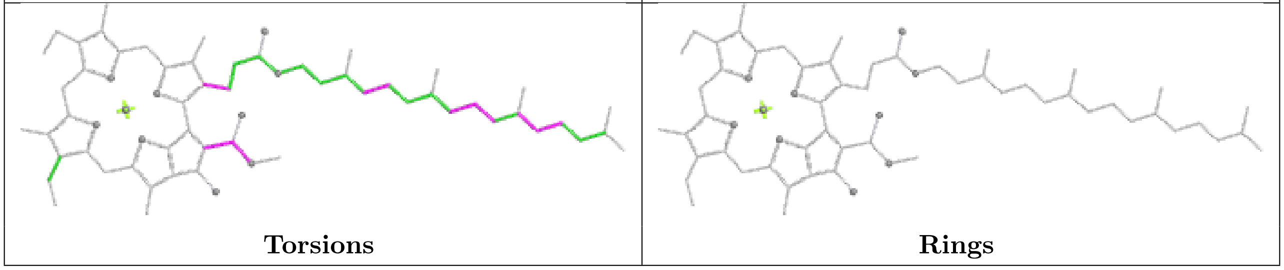


Torsions **Rings**

Ligand CLA a 812

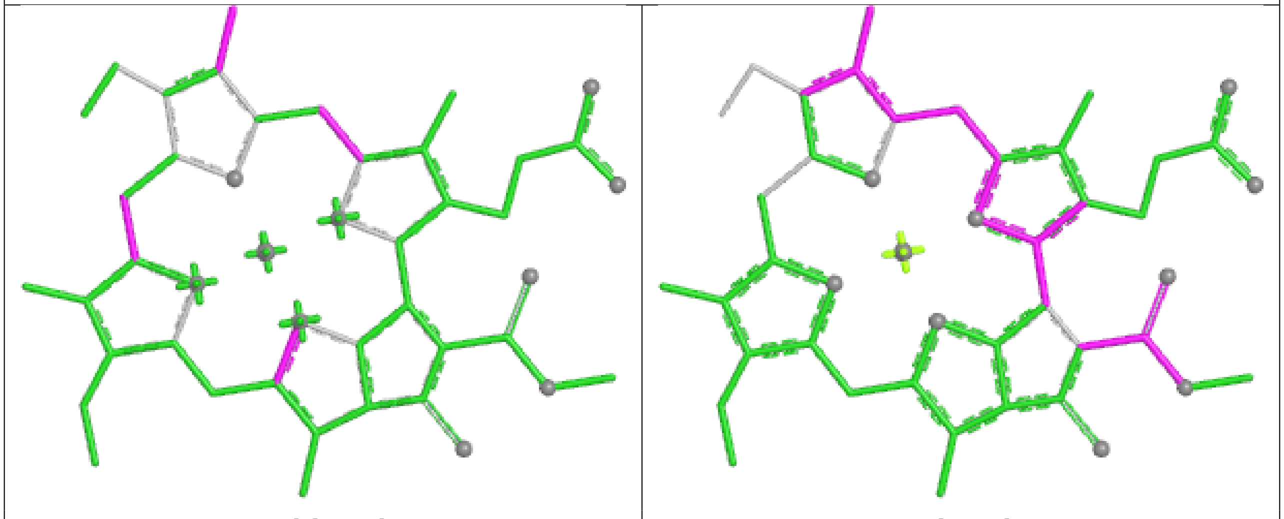


Bond lengths Bond angles

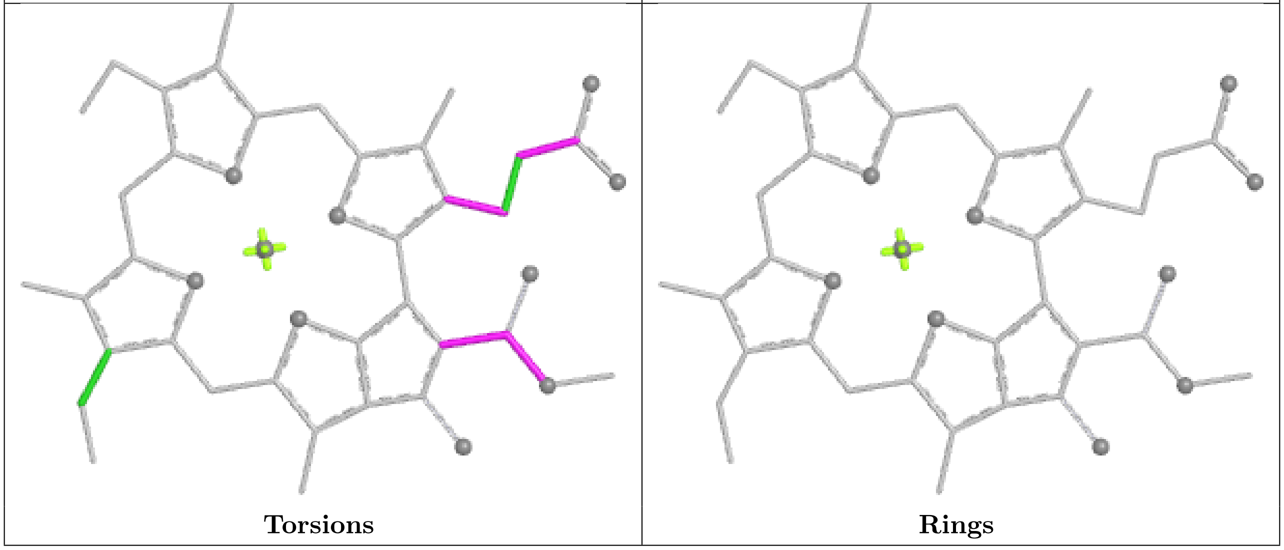


Torsions Rings

Ligand CLA b 2117

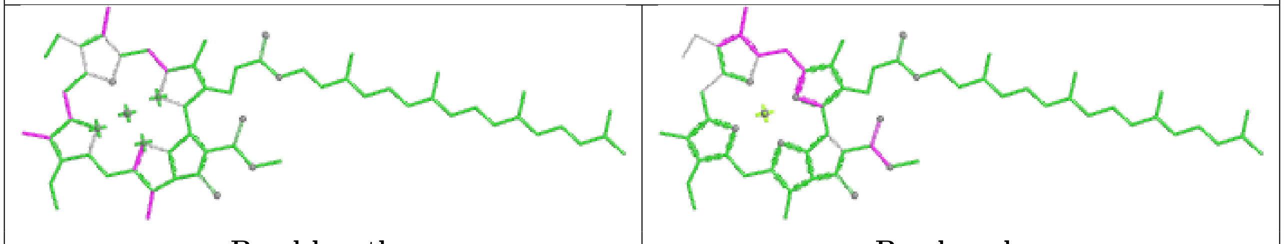


Bond lengths Bond angles



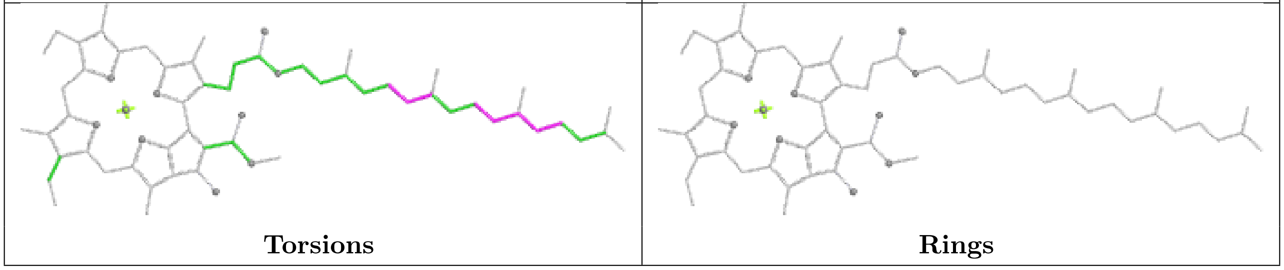
Torsions Rings

Ligand CLA H 2126



Bond lengths

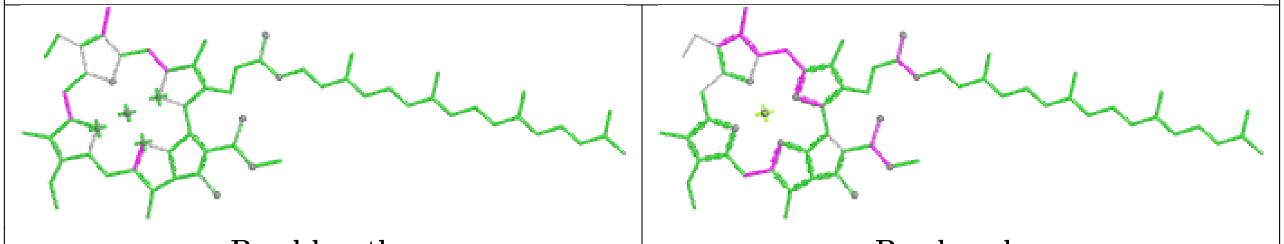
Bond angles



Torsions

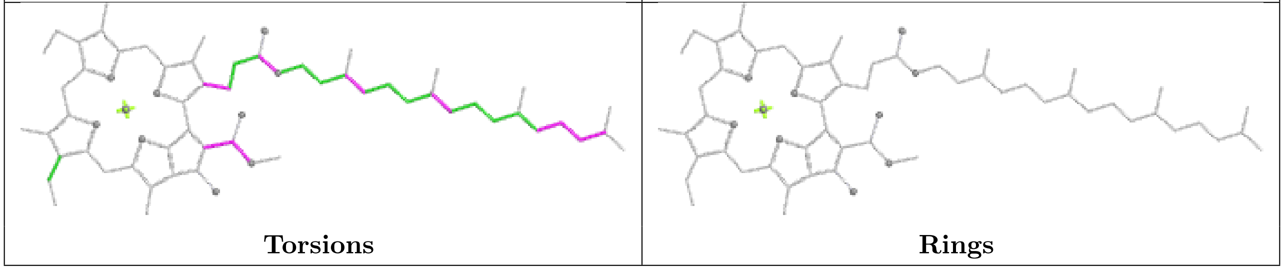
Rings

Ligand CLA H 2106



Bond lengths

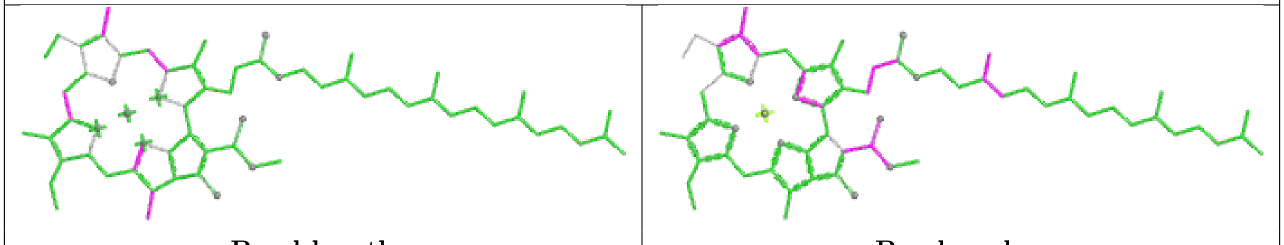
Bond angles



Torsions

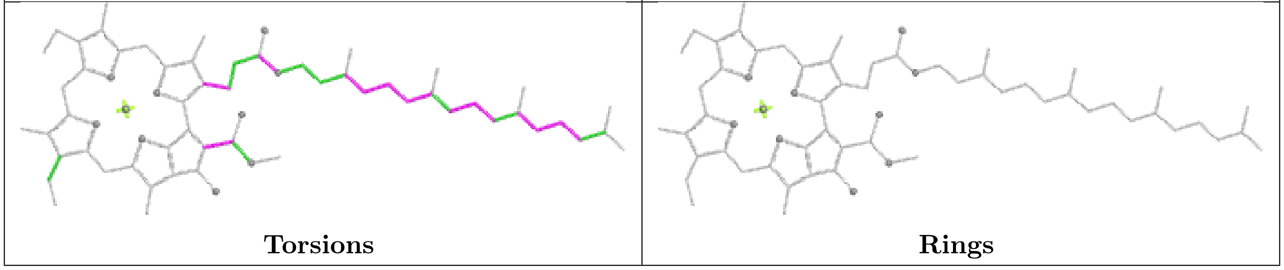
Rings

Ligand CLA b 2119



Bond lengths

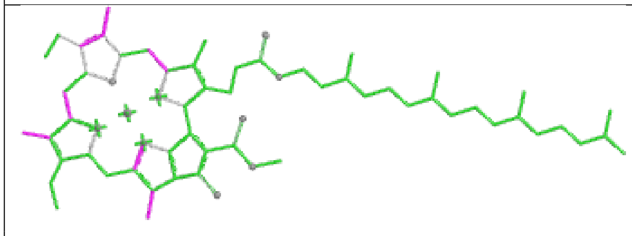
Bond angles



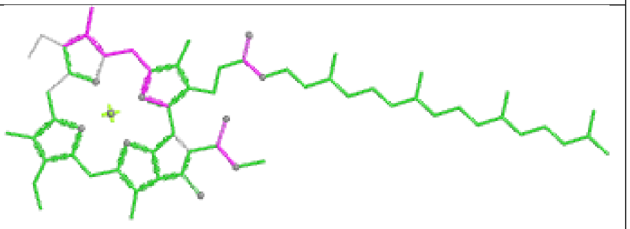
Torsions

Rings

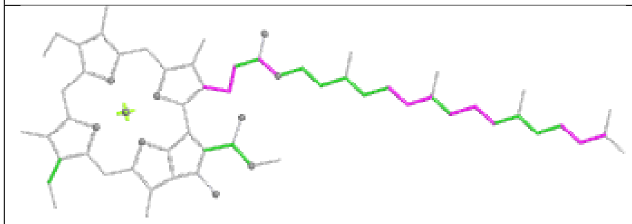
Ligand CLA a 826



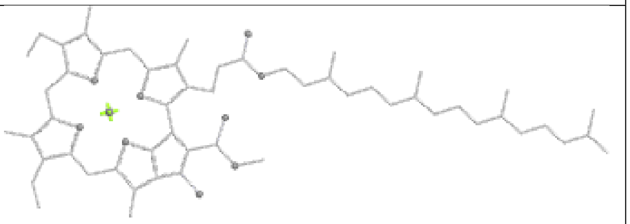
Bond lengths



Bond angles

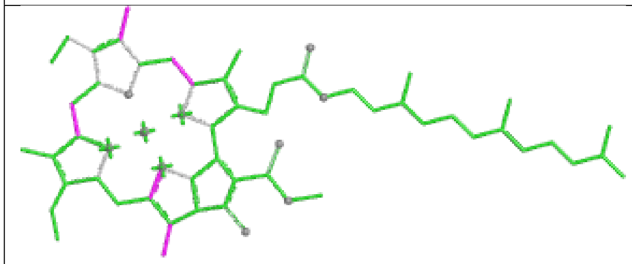


Torsions

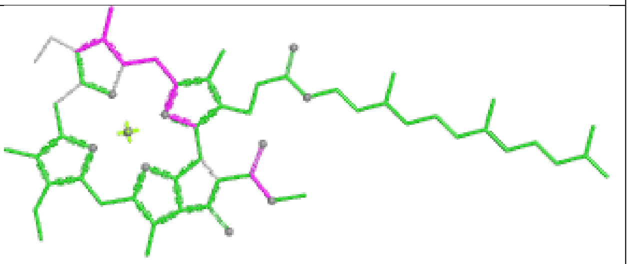


Rings

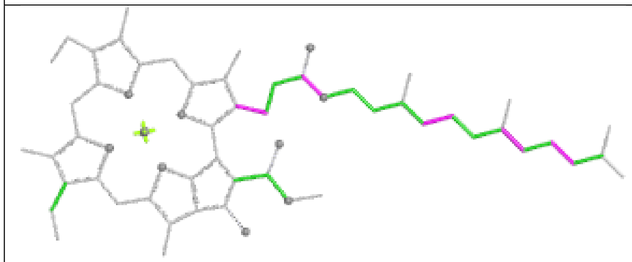
Ligand CLA G 821



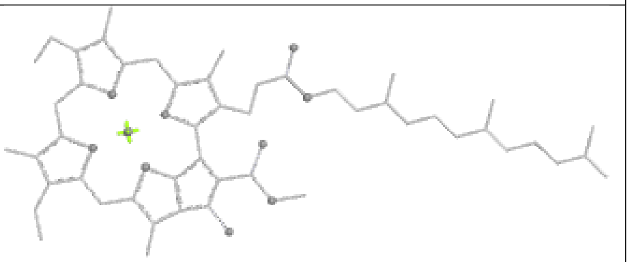
Bond lengths



Bond angles

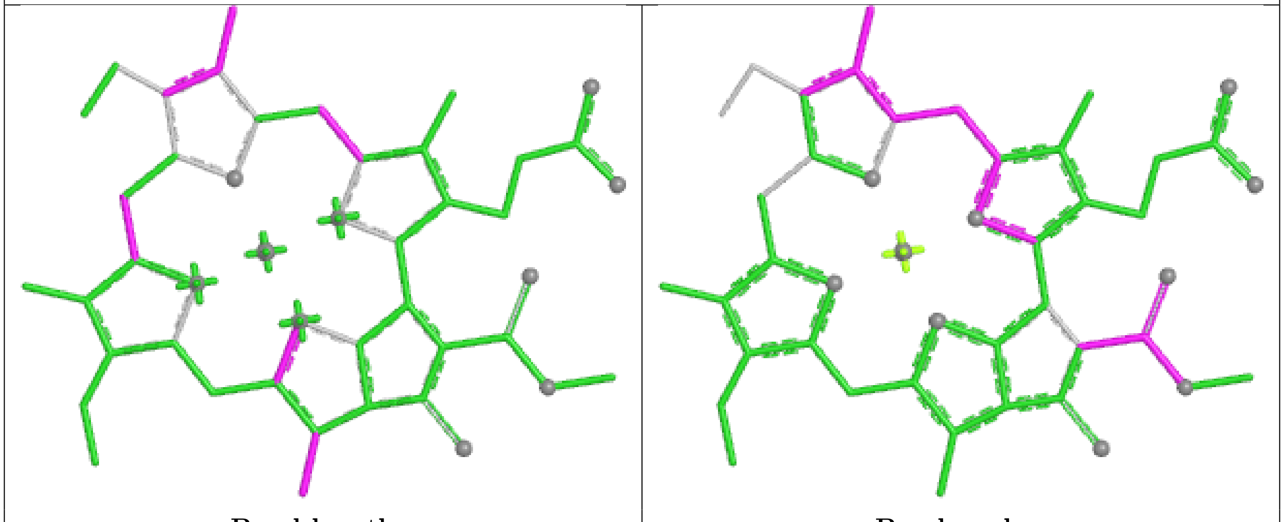


Torsions



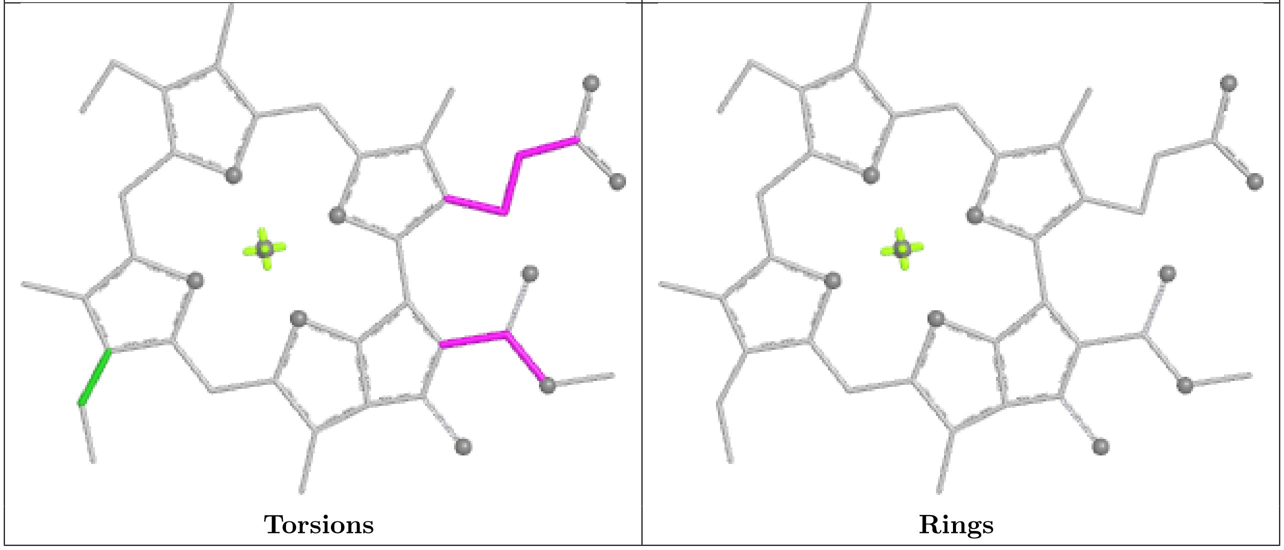
Rings

Ligand CLA b 2113



Bond lengths

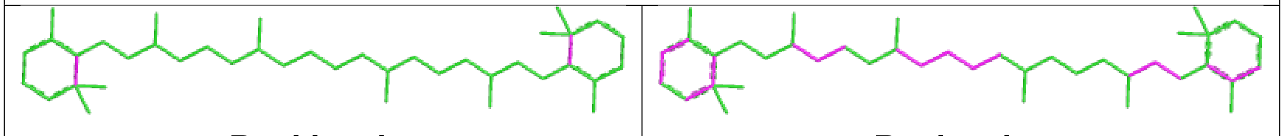
Bond angles



Torsions

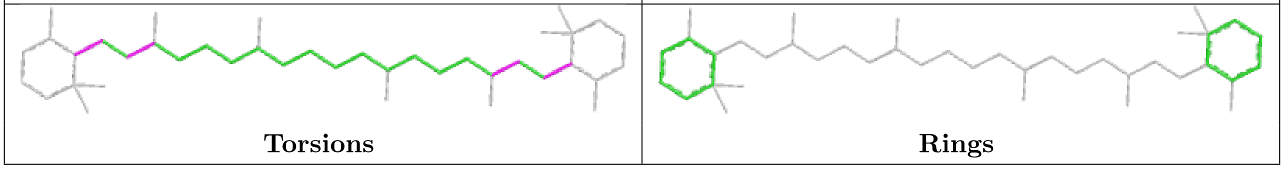
Rings

Ligand BCR a 844



Bond lengths

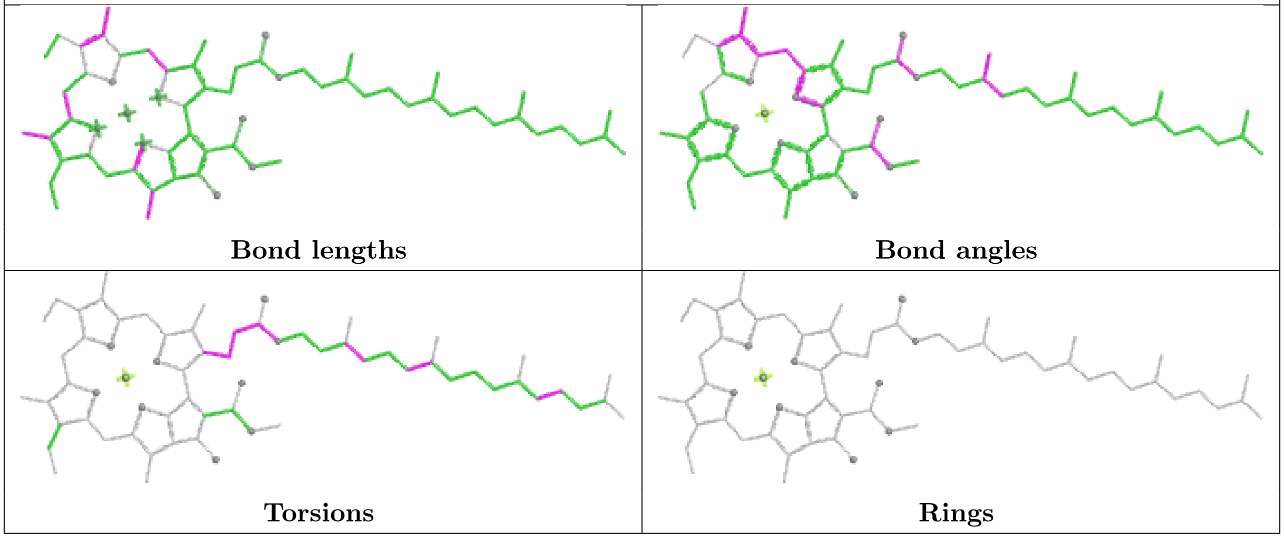
Bond angles



Torsions

Rings

Ligand CLA A 851



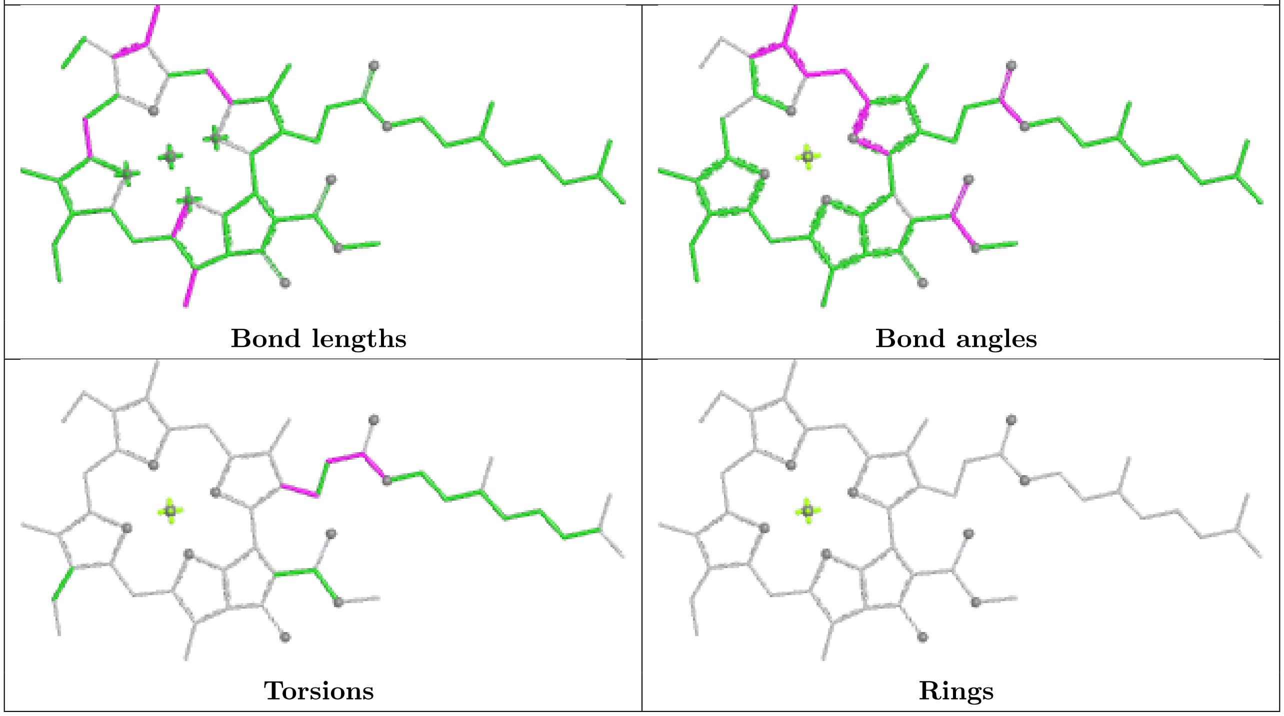
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 2121



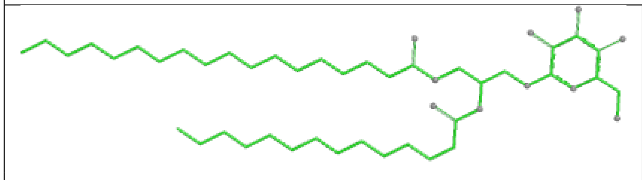
Bond lengths

Bond angles

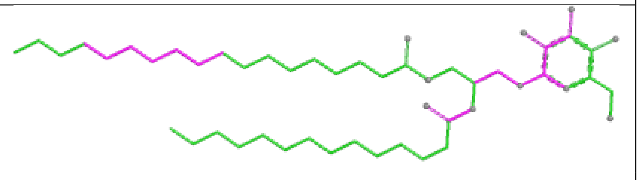
Torsions

Rings

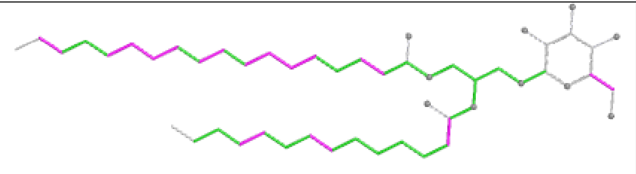
Ligand LMG H 2147



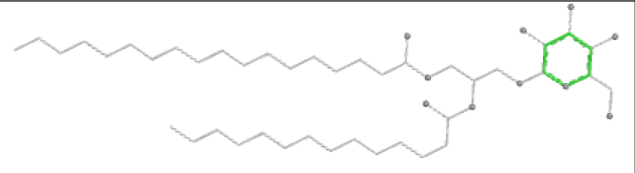
Bond lengths



Bond angles

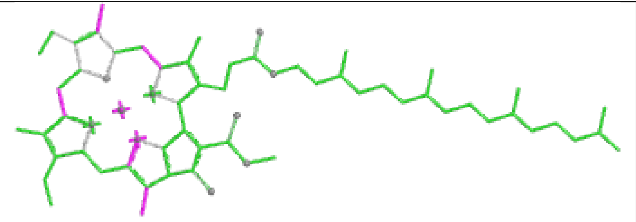


Torsions

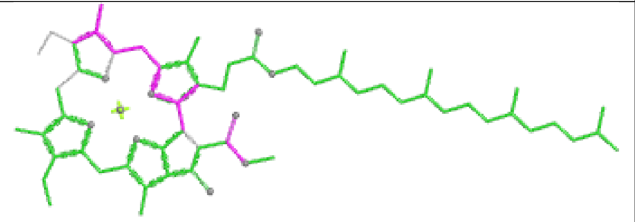


Rings

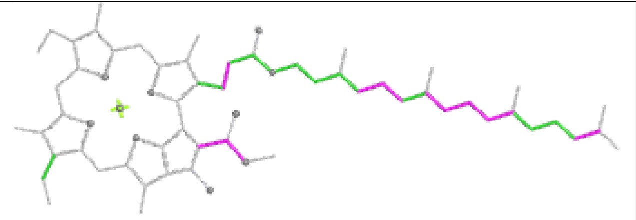
Ligand CLA B 2102



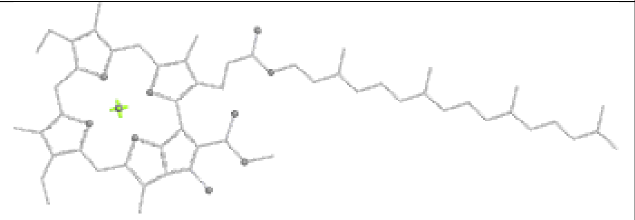
Bond lengths



Bond angles

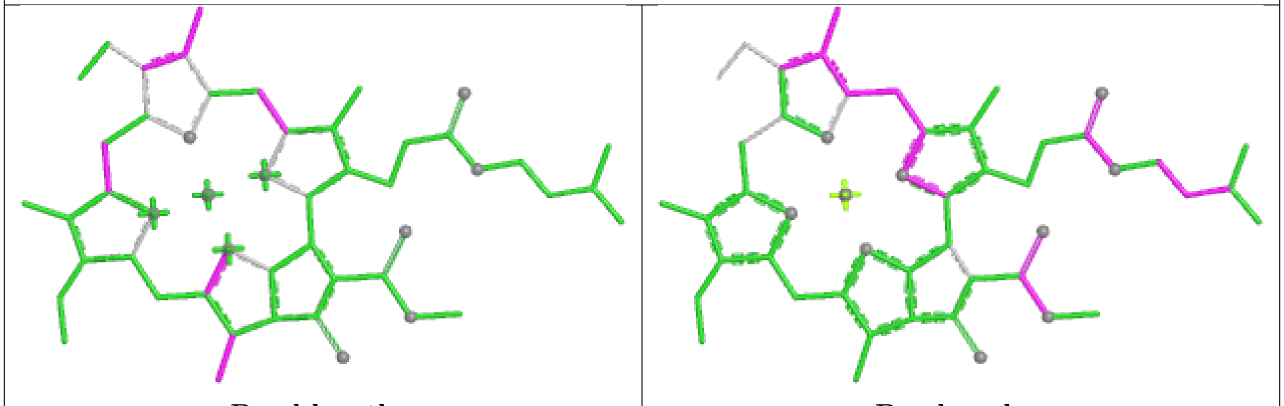


Torsions



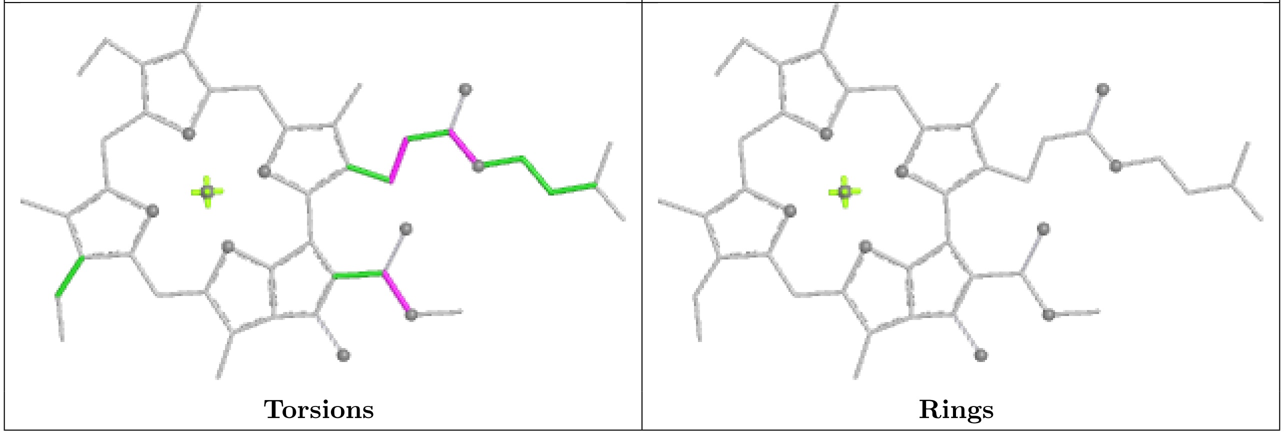
Rings

Ligand CLA H 2118



Bond lengths

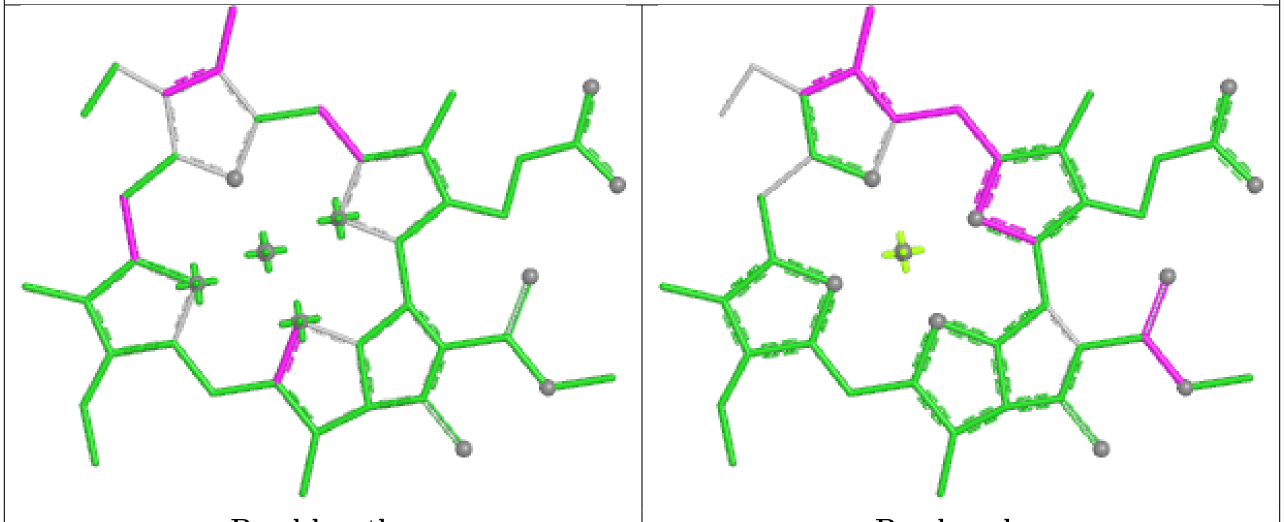
Bond angles



Torsions

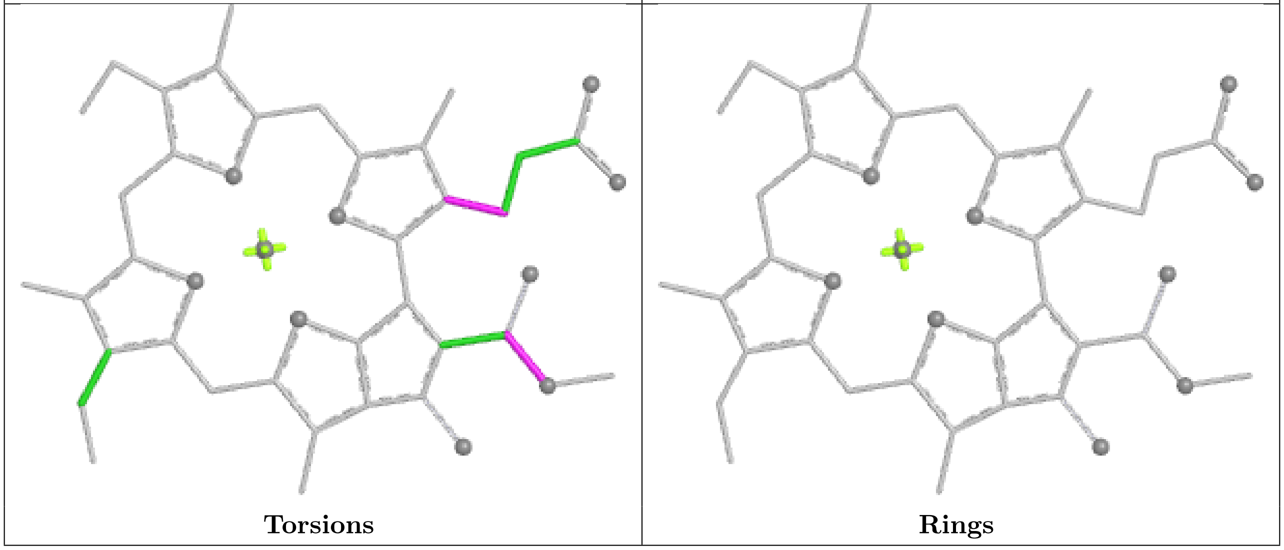
Rings

Ligand CLA a 815



Bond lengths

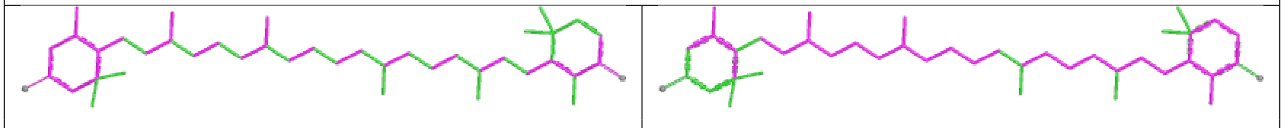
Bond angles



Torsions

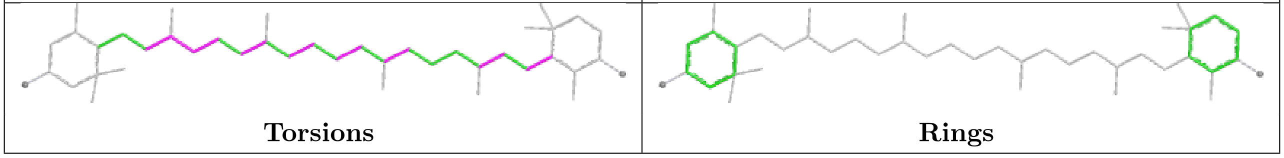
Rings

Ligand EQ3 H 2150



Bond lengths

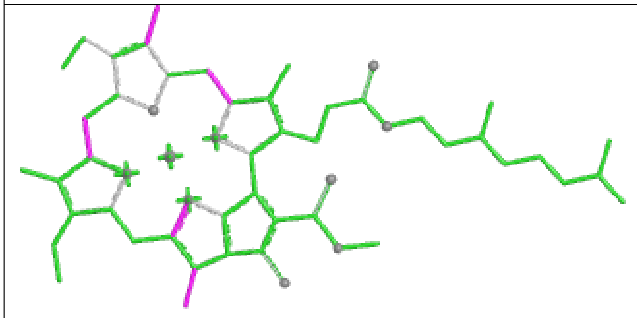
Bond angles



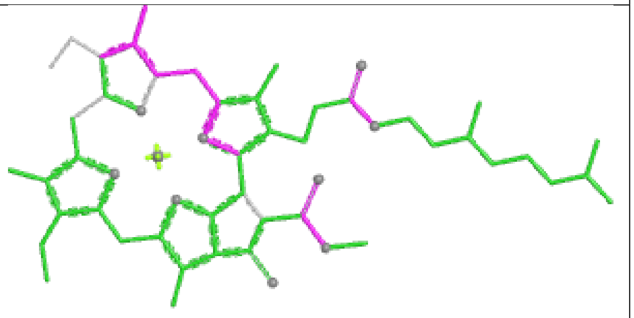
Torsions

Rings

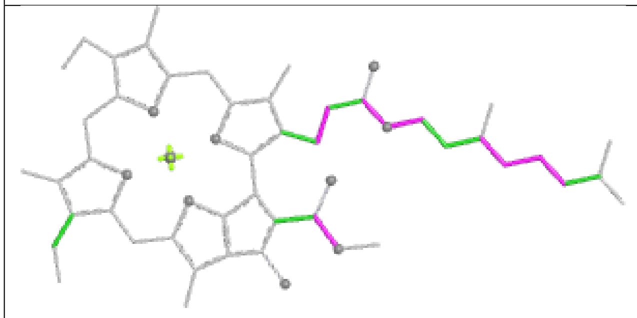
Ligand CLA H 2121



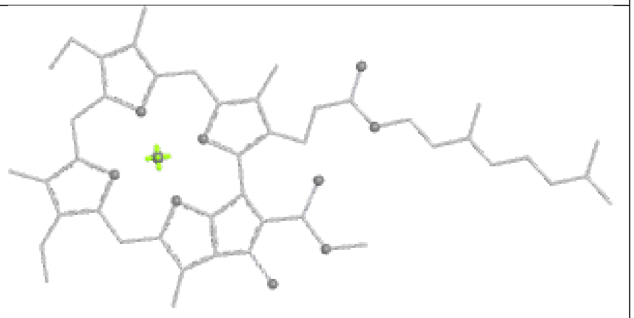
Bond lengths



Bond angles

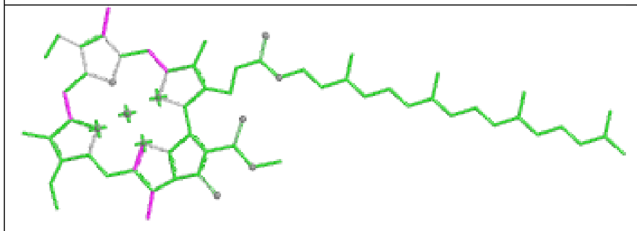


Torsions

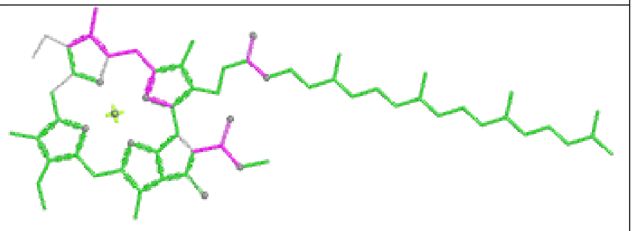


Rings

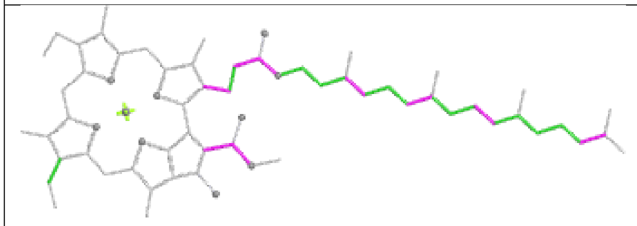
Ligand CLA H 2133



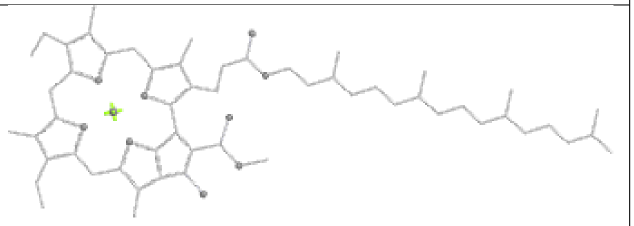
Bond lengths



Bond angles

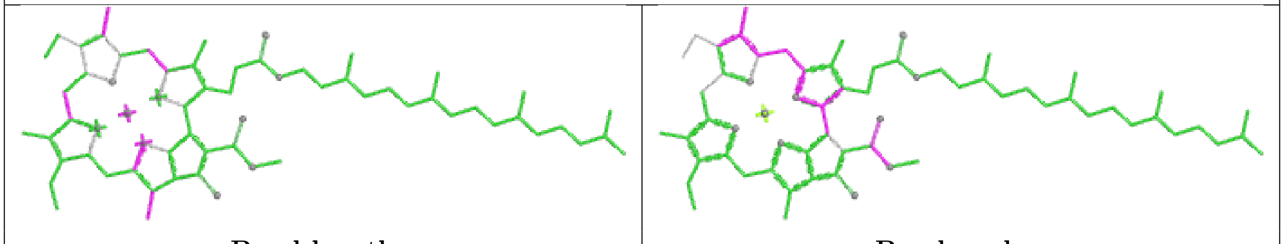


Torsions

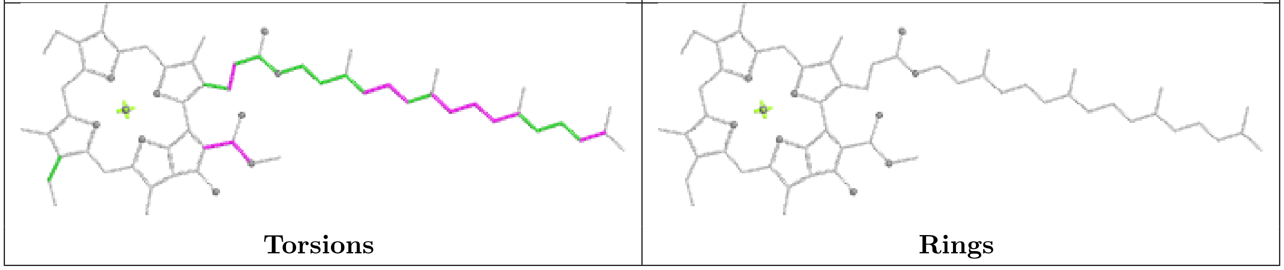


Rings

Ligand CLA b 2101

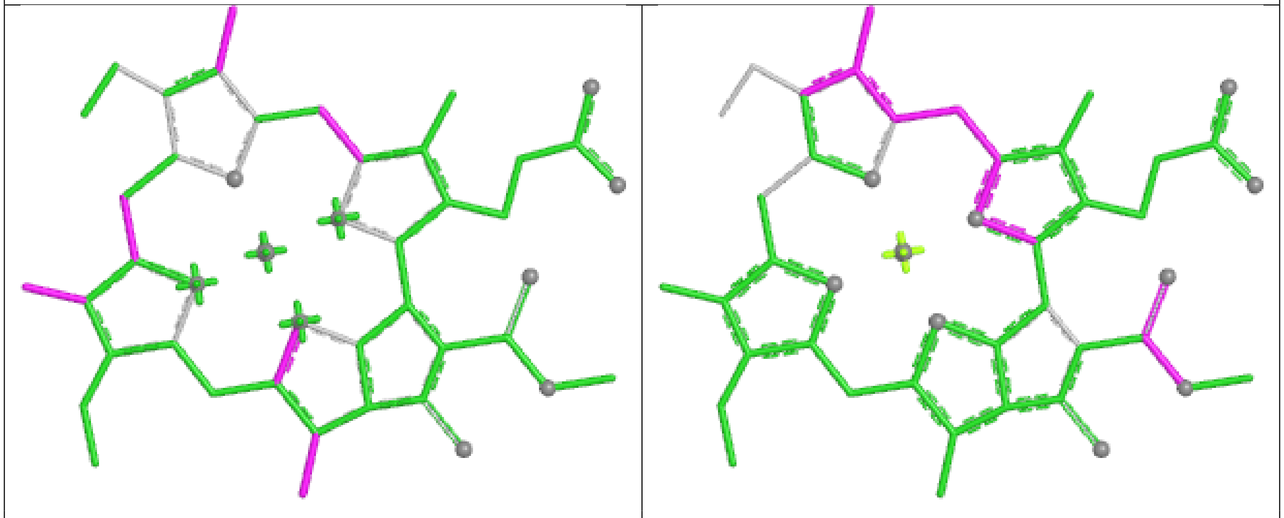


Bond lengths Bond angles

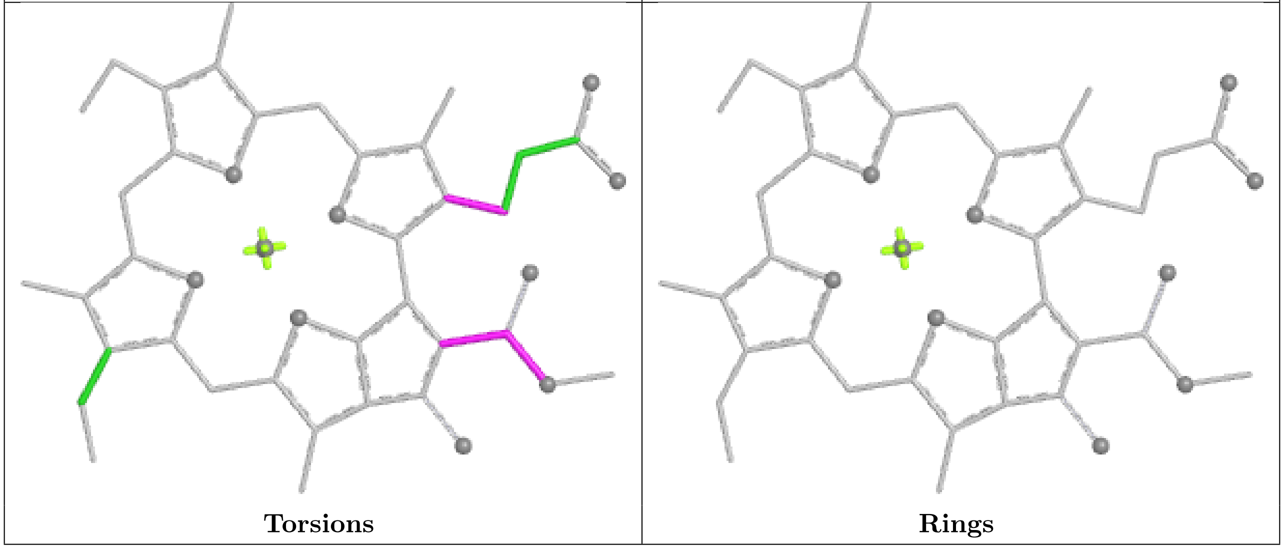


Torsions Rings

Ligand CLA b 2136

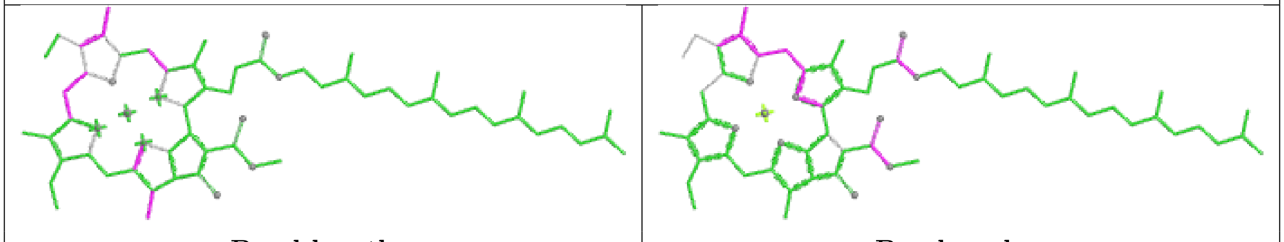


Bond lengths Bond angles



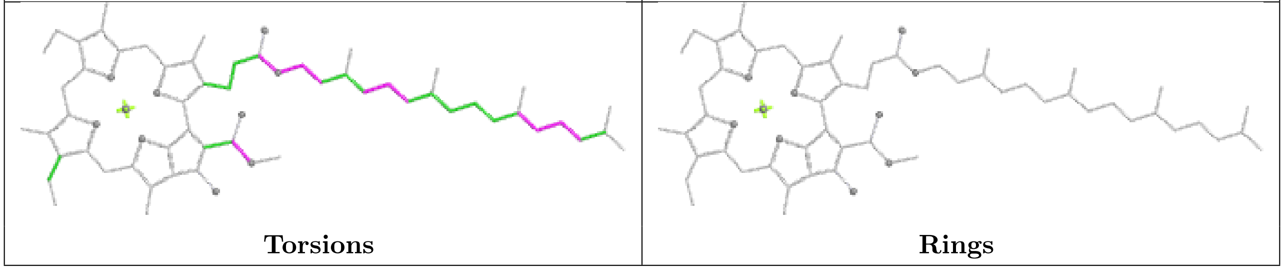
Torsions Rings

Ligand CLA H 2110



Bond lengths

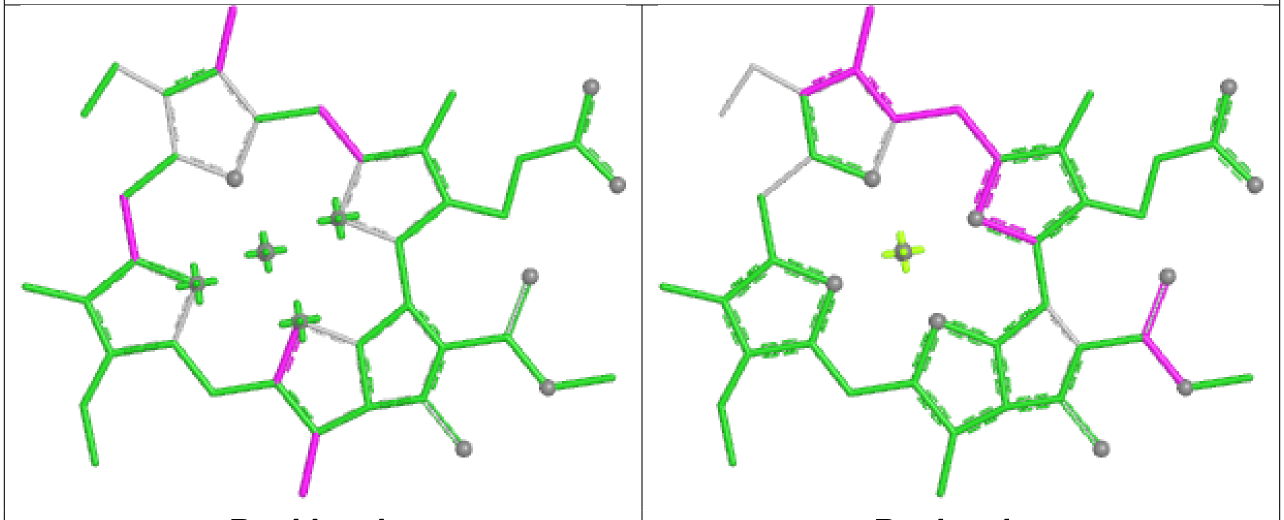
Bond angles



Torsions

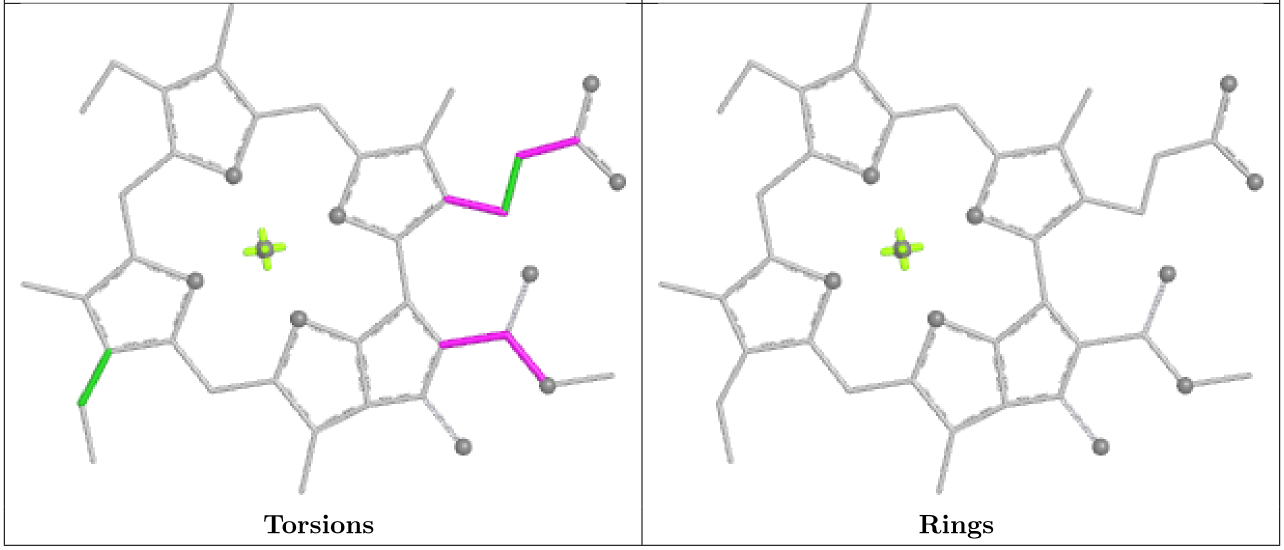
Rings

Ligand CLA T 4002



Bond lengths

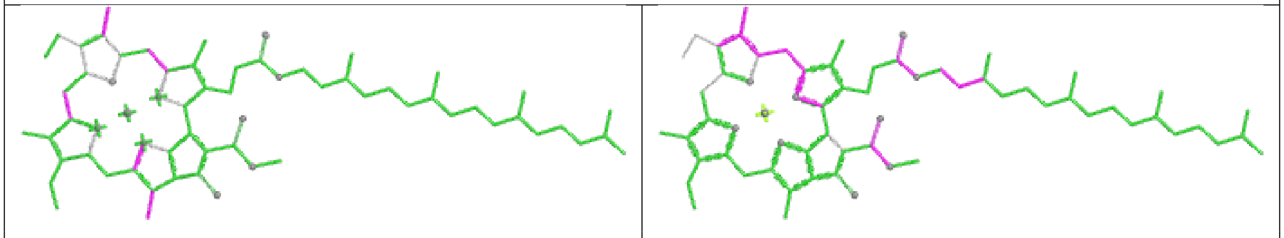
Bond angles



Torsions

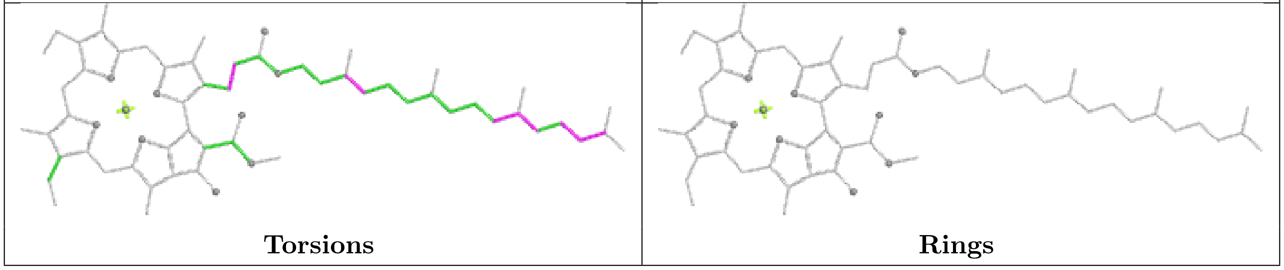
Rings

Ligand CLA A 818



Bond lengths

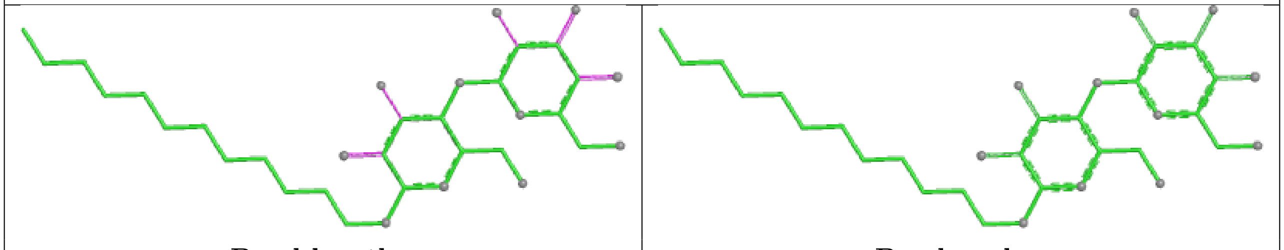
Bond angles



Torsions

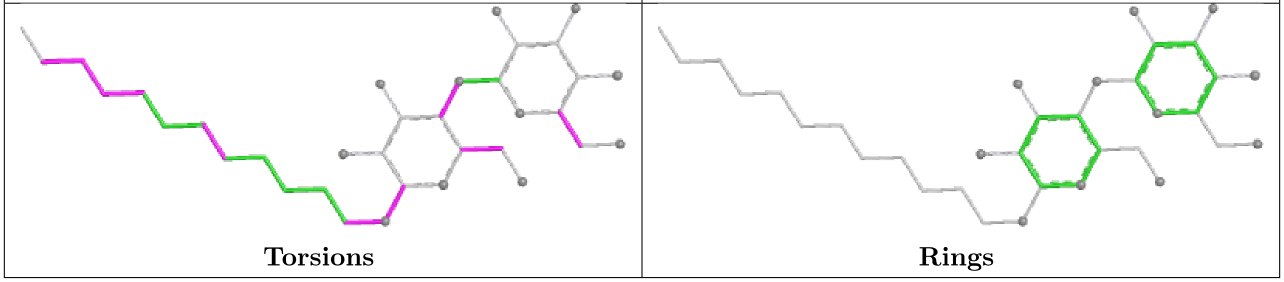
Rings

Ligand LMT L 210



Bond lengths

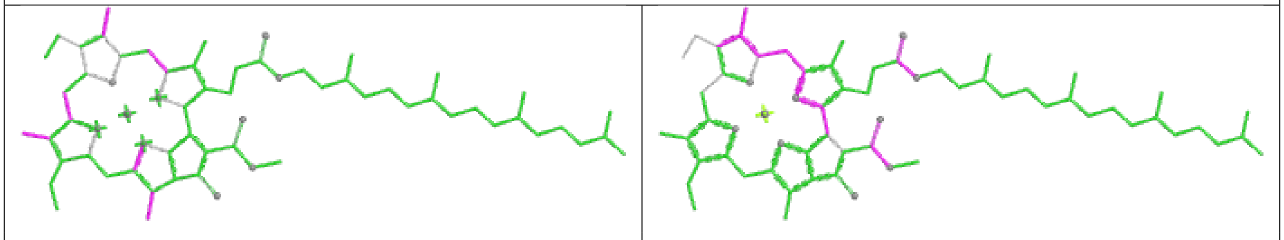
Bond angles



Torsions

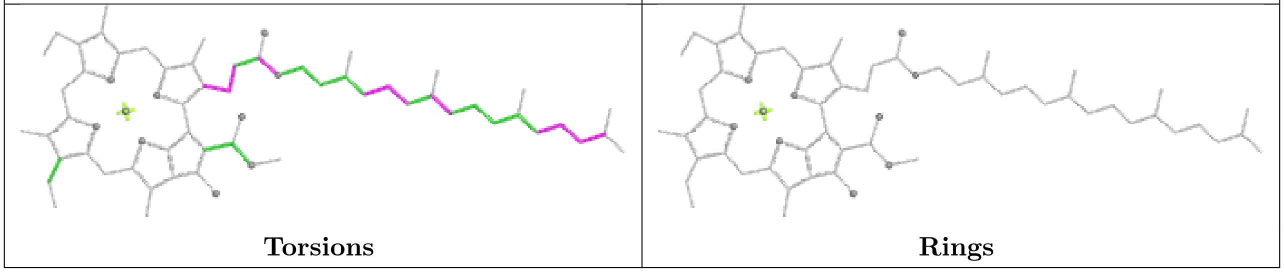
Rings

Ligand CLA A 835



Bond lengths

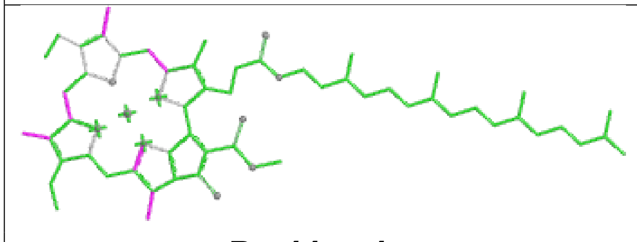
Bond angles



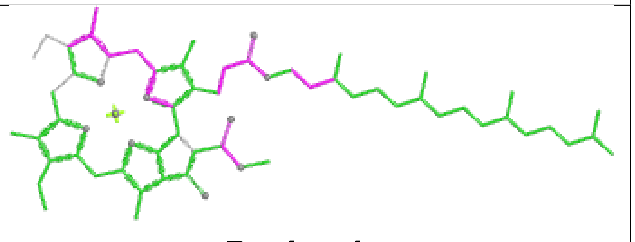
Torsions

Rings

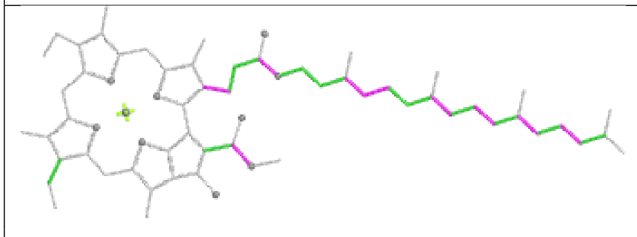
Ligand CLA A 805



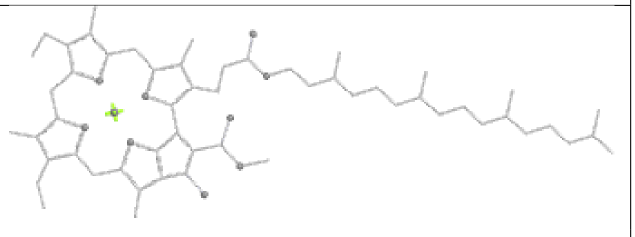
Bond lengths



Bond angles

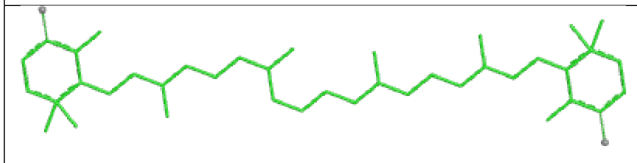


Torsions

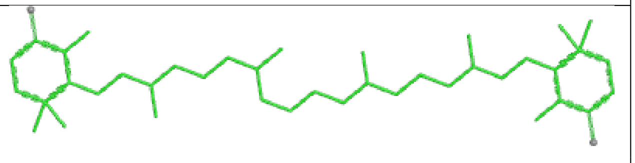


Rings

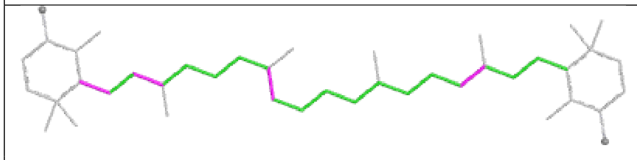
Ligand 45D G 852



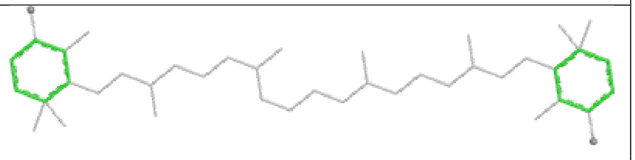
Bond lengths



Bond angles

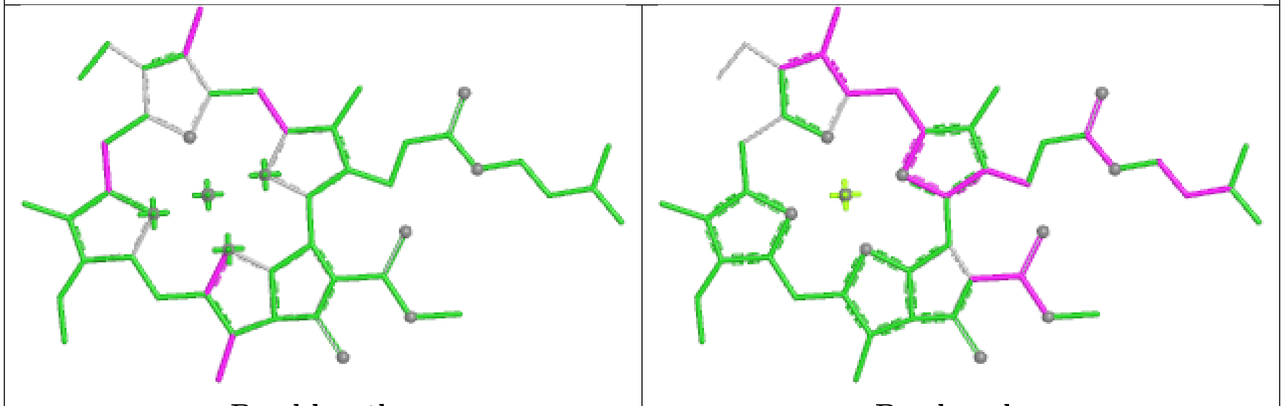


Torsions



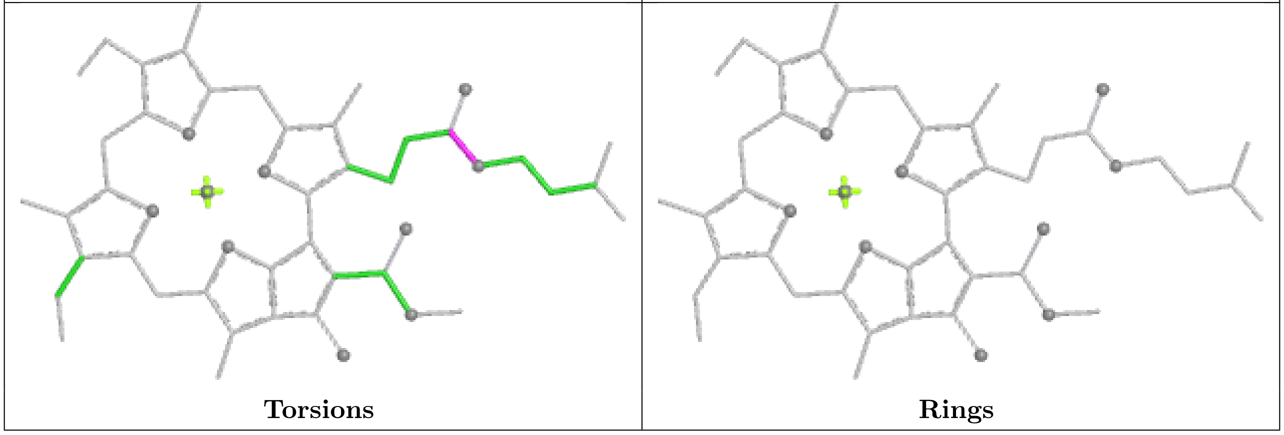
Rings

Ligand CLA b 2125



Bond lengths

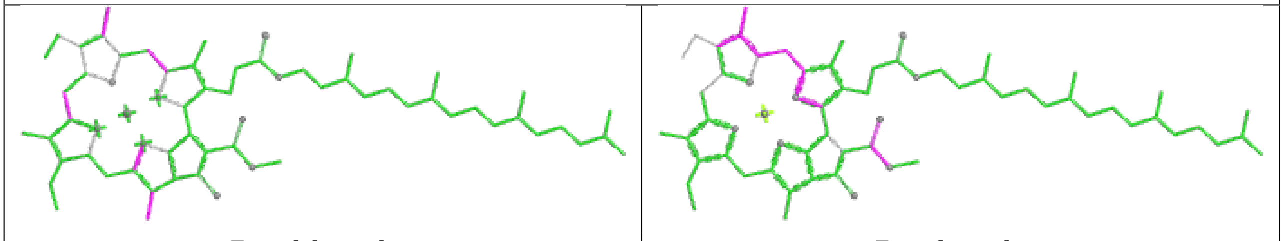
Bond angles



Torsions

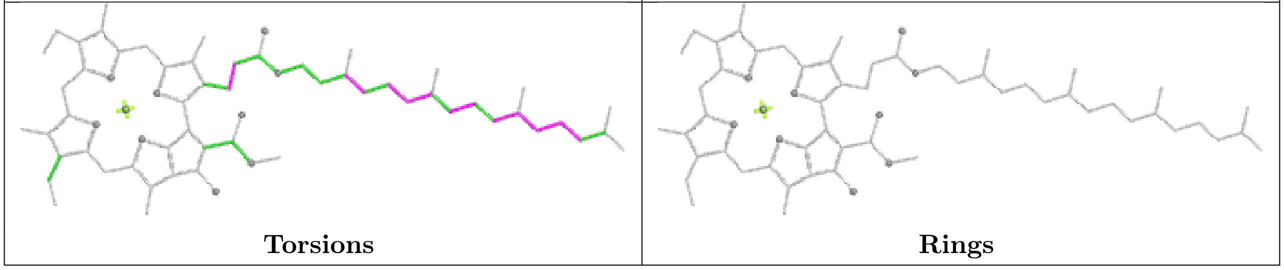
Rings

Ligand CLA A 836



Bond lengths

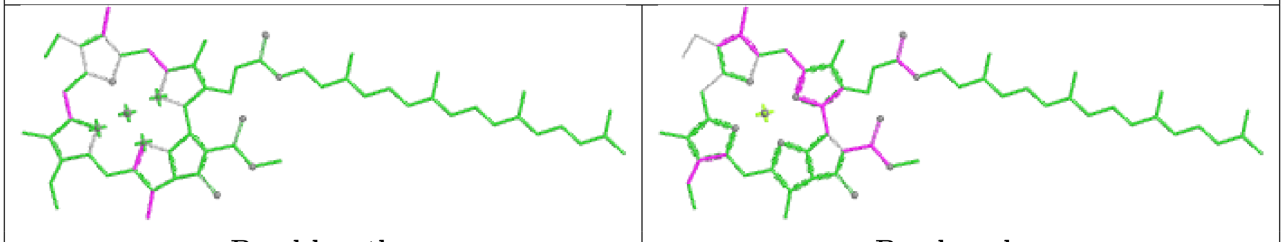
Bond angles



Torsions

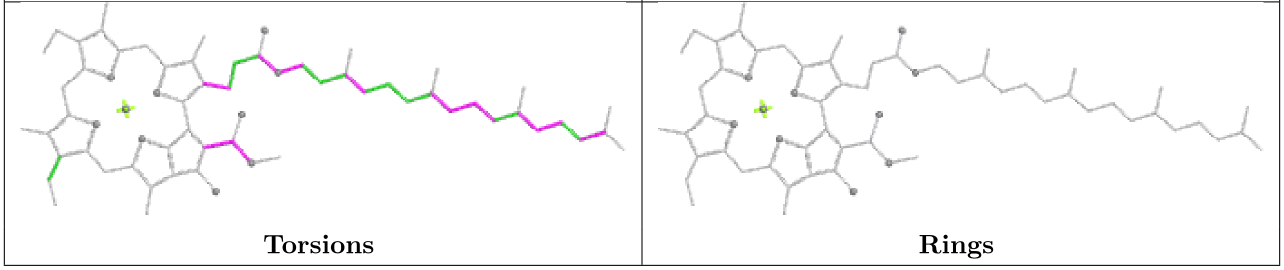
Rings

Ligand CLA A 824



Bond lengths

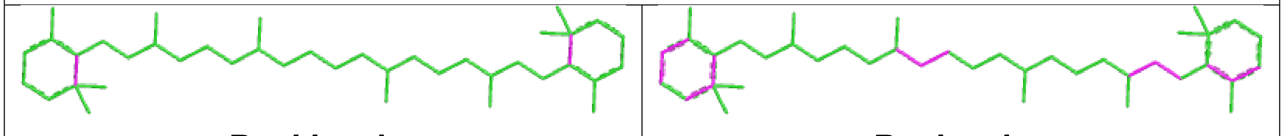
Bond angles



Torsions

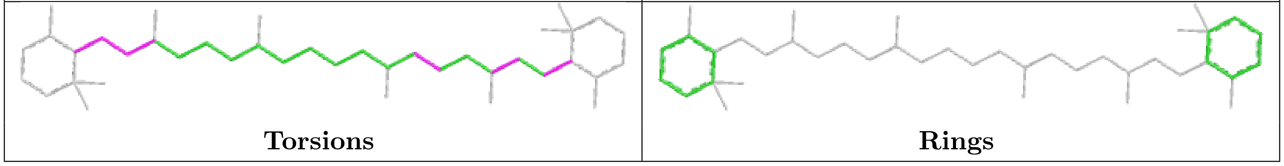
Rings

Ligand BCR k 4001



Bond lengths

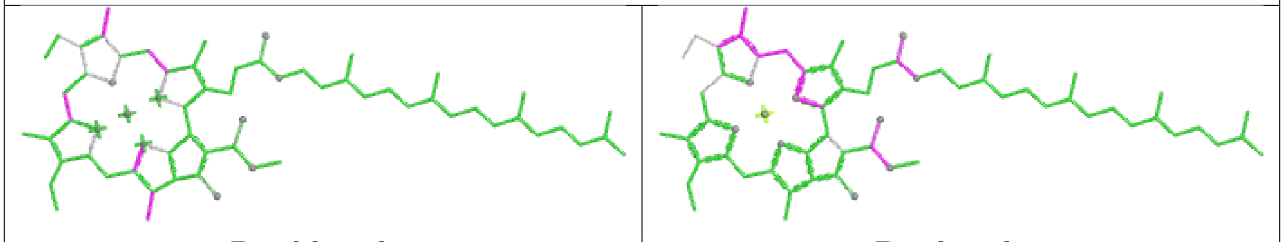
Bond angles



Torsions

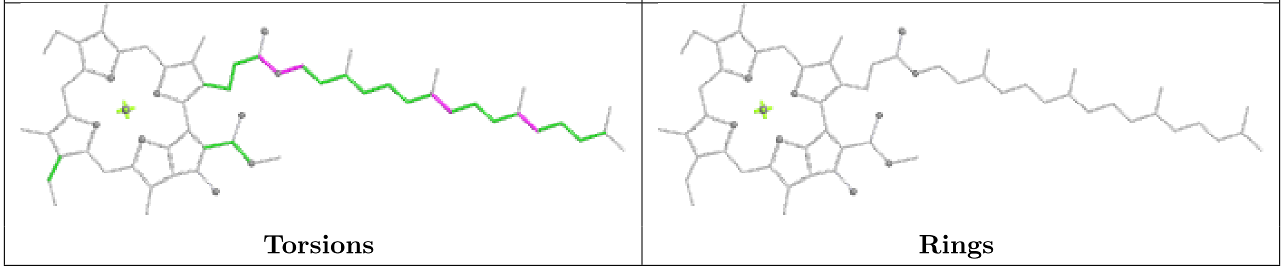
Rings

Ligand CLA B 2138



Bond lengths

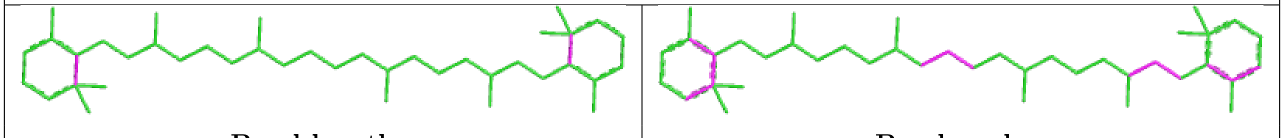
Bond angles



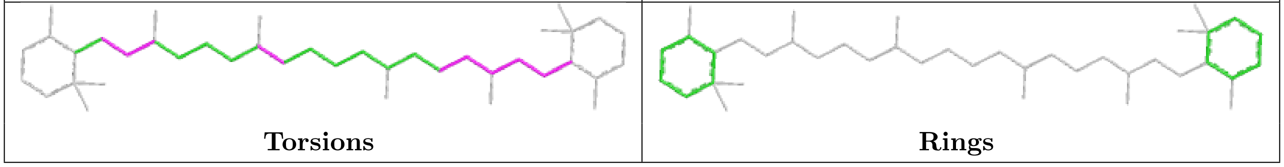
Torsions

Rings

Ligand BCR F 202

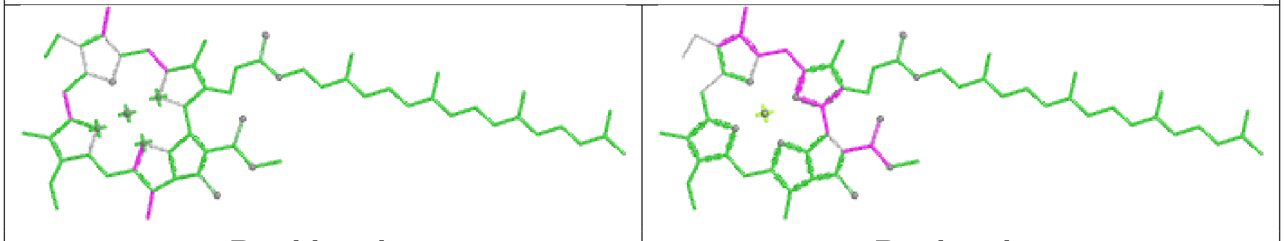


Bond lengths Bond angles

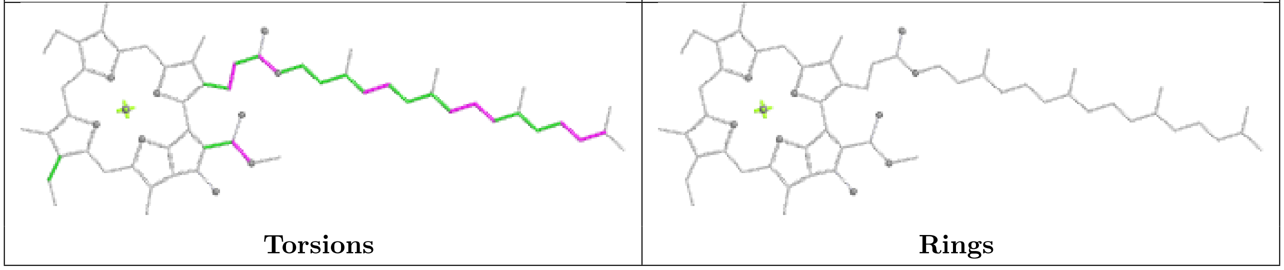


Torsions Rings

Ligand CLA A 837

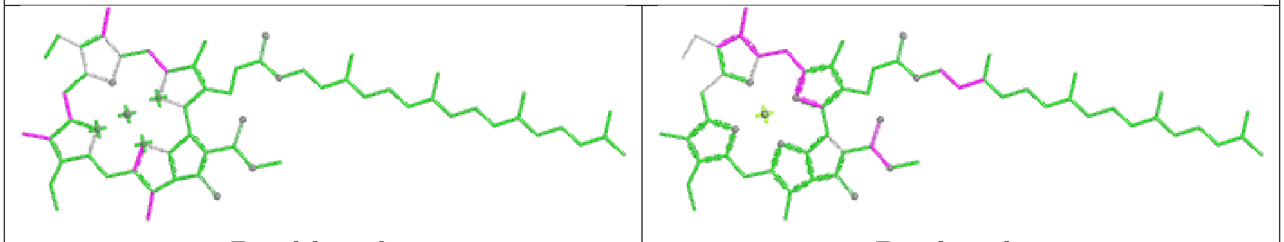


Bond lengths Bond angles

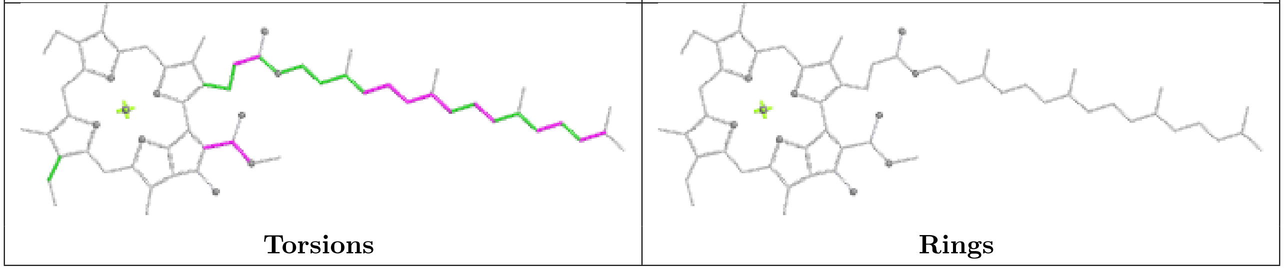


Torsions Rings

Ligand CLA H 2107

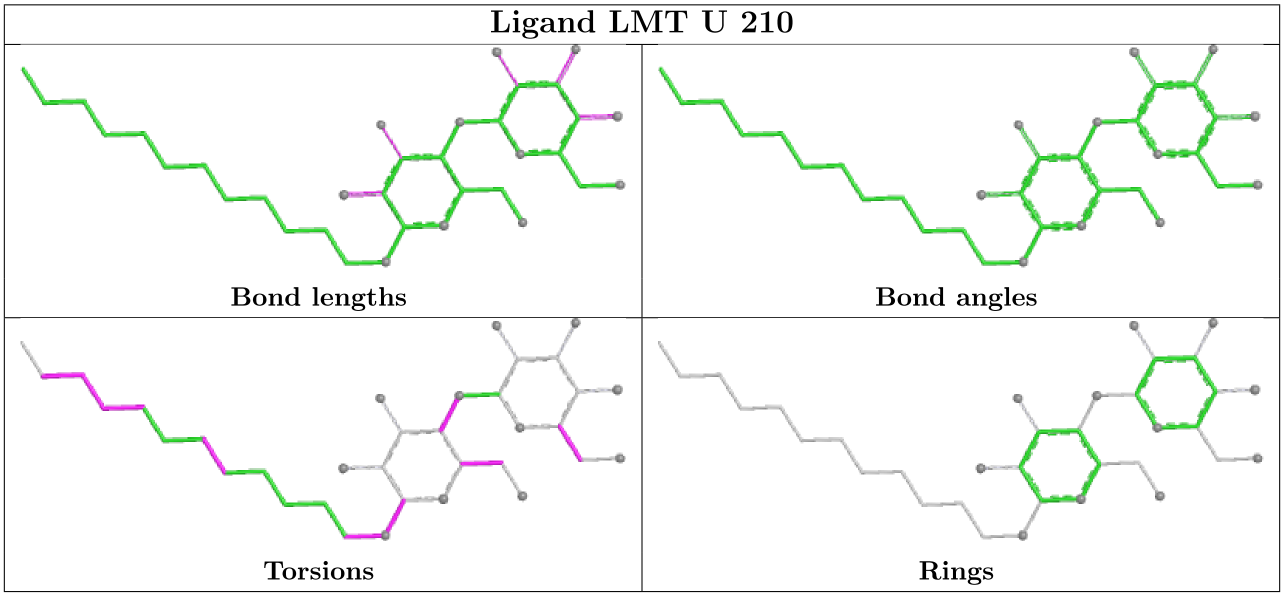


Bond lengths Bond angles



Torsions Rings

Ligand LMT U 210



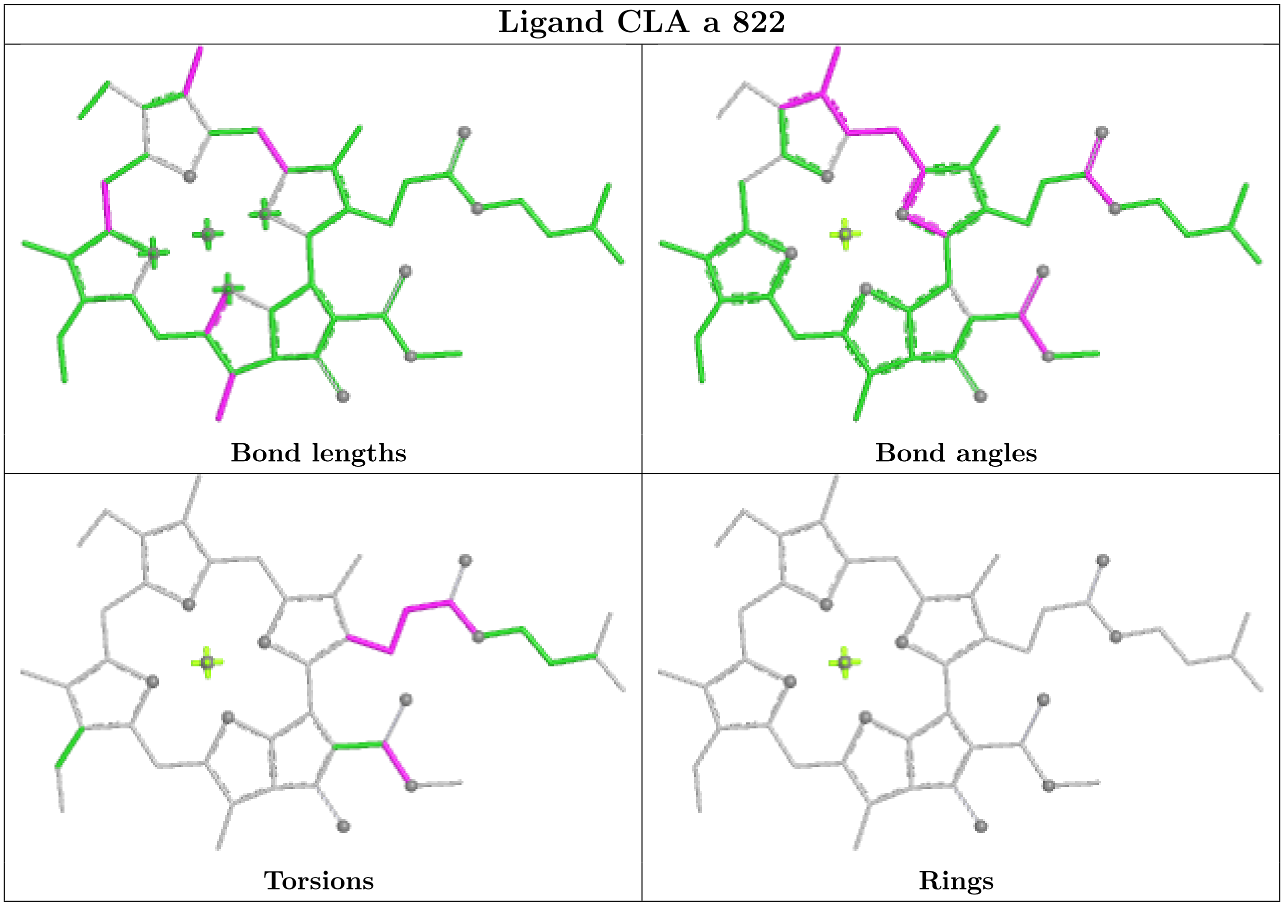
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 822



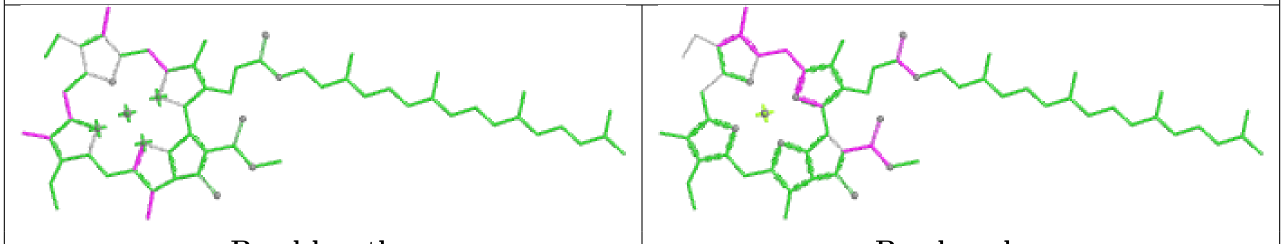
Bond lengths

Bond angles

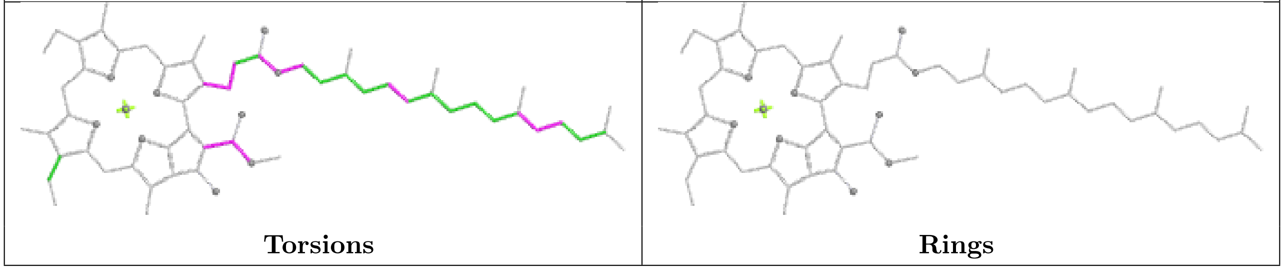
Torsions

Rings

Ligand CLA L 201

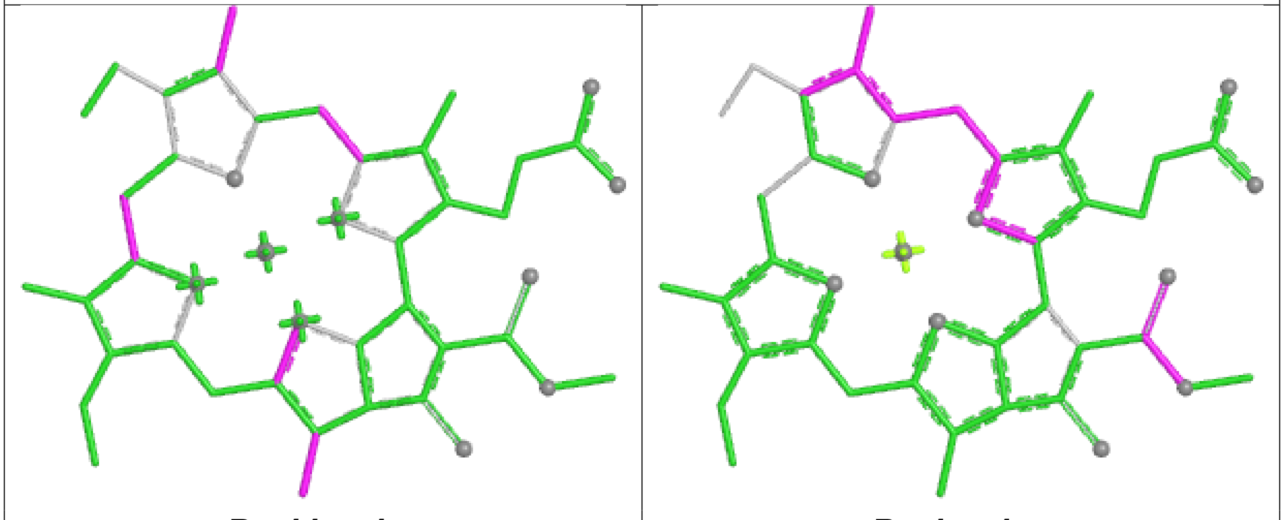


Bond lengths Bond angles

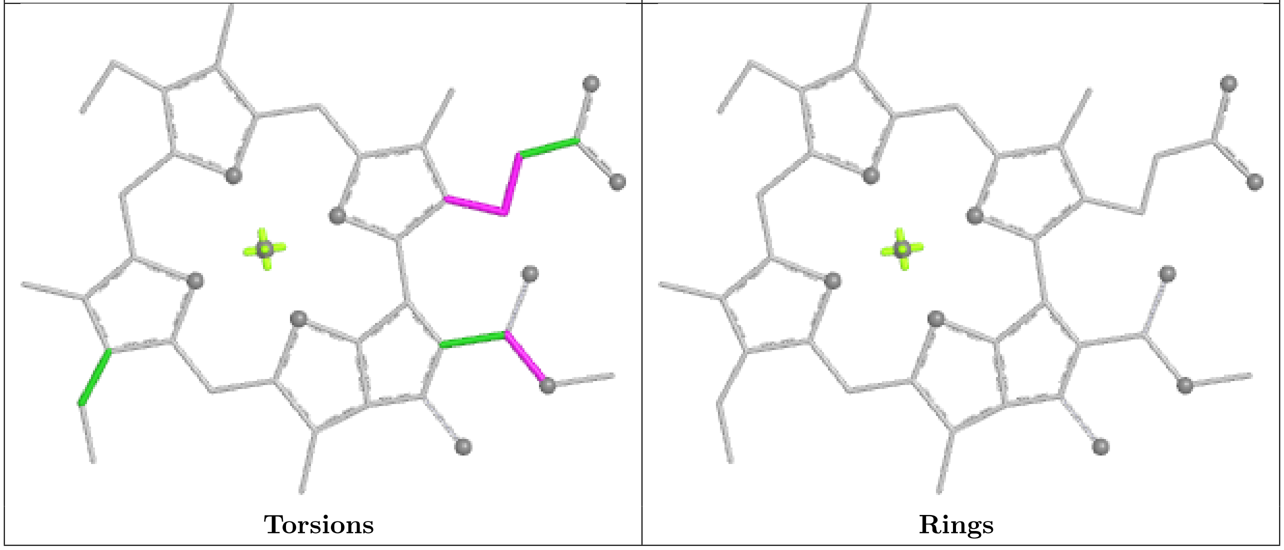


Torsions Rings

Ligand CLA B 2123

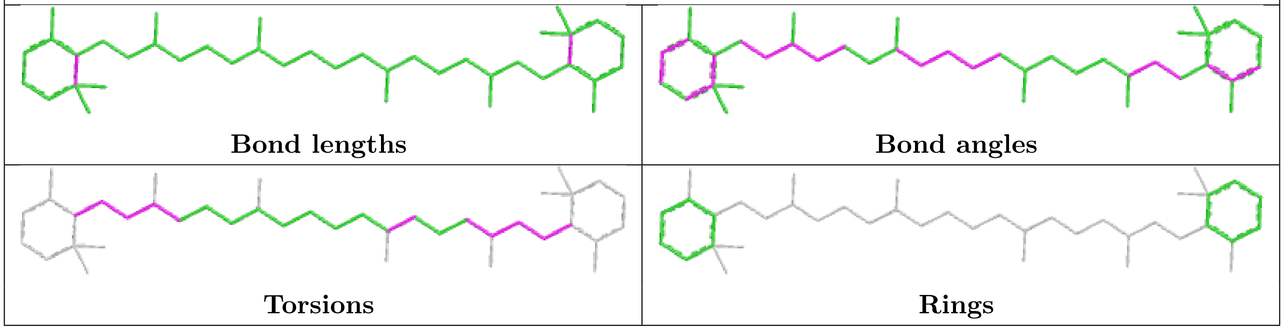


Bond lengths Bond angles

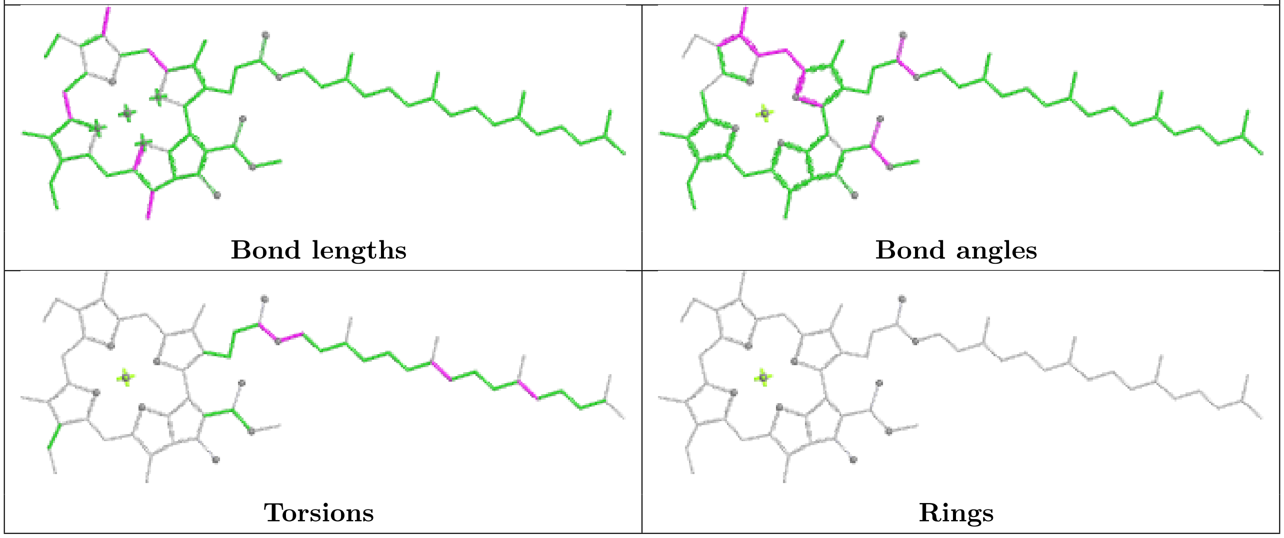


Torsions Rings

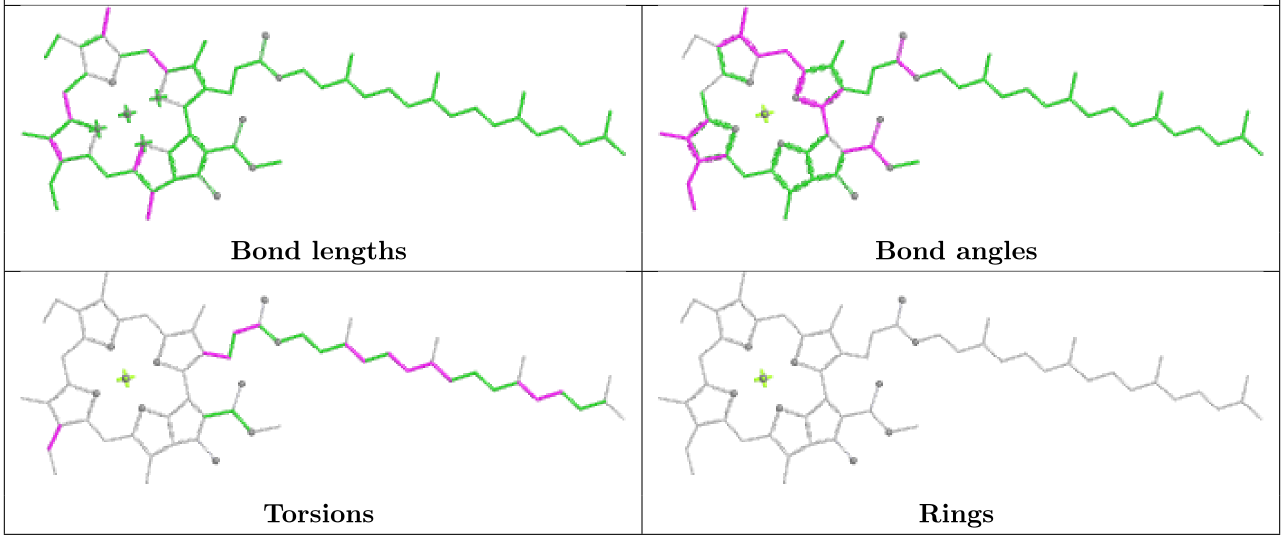
Ligand BCR S 101


Bond lengths
Bond angles
Torsions
Rings

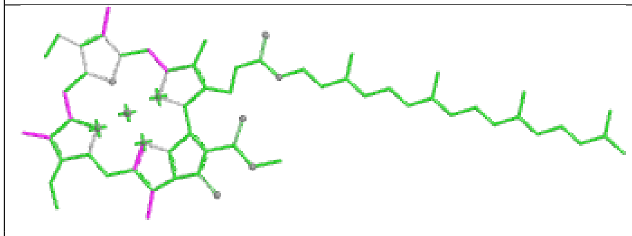
Ligand CLA b 2137


Bond lengths
Bond angles
Torsions
Rings

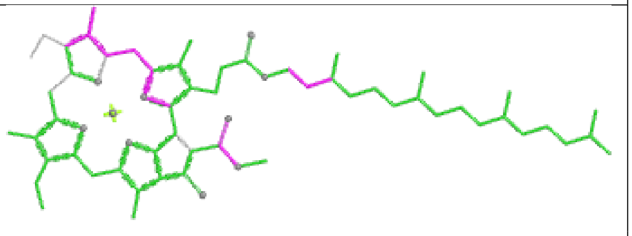
Ligand CLA B 2112


Bond lengths
Bond angles
Torsions
Rings

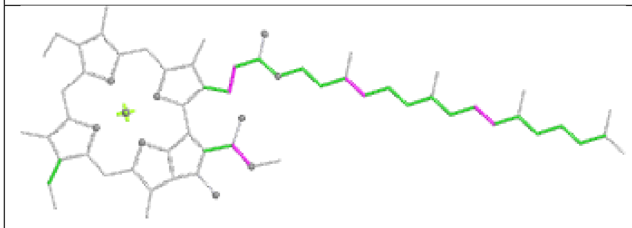
Ligand CLA a 827



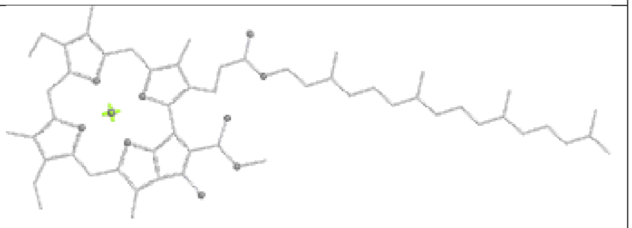
Bond lengths



Bond angles

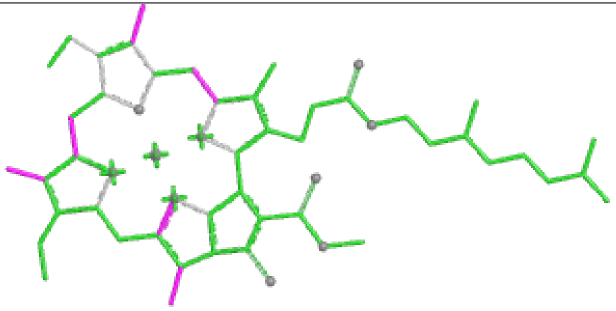


Torsions

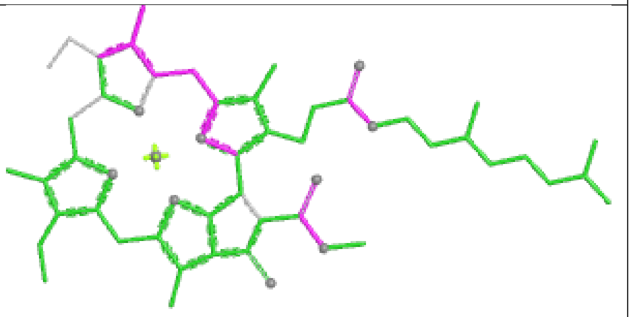


Rings

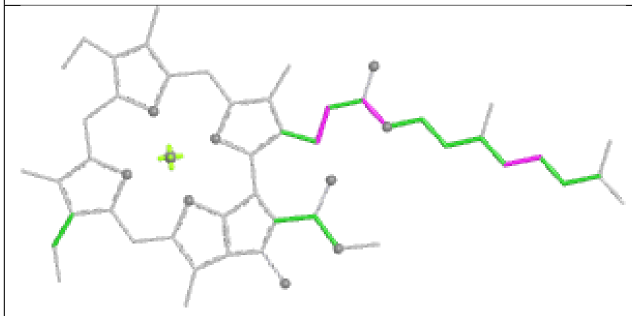
Ligand CLA a 816



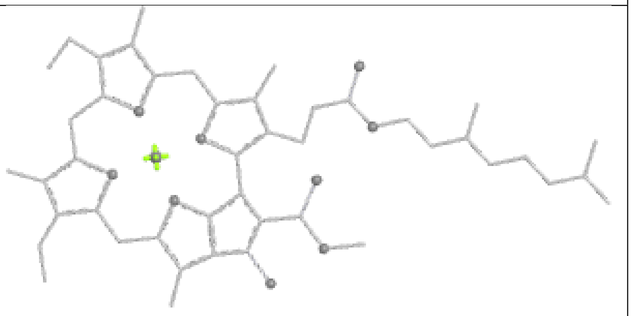
Bond lengths



Bond angles

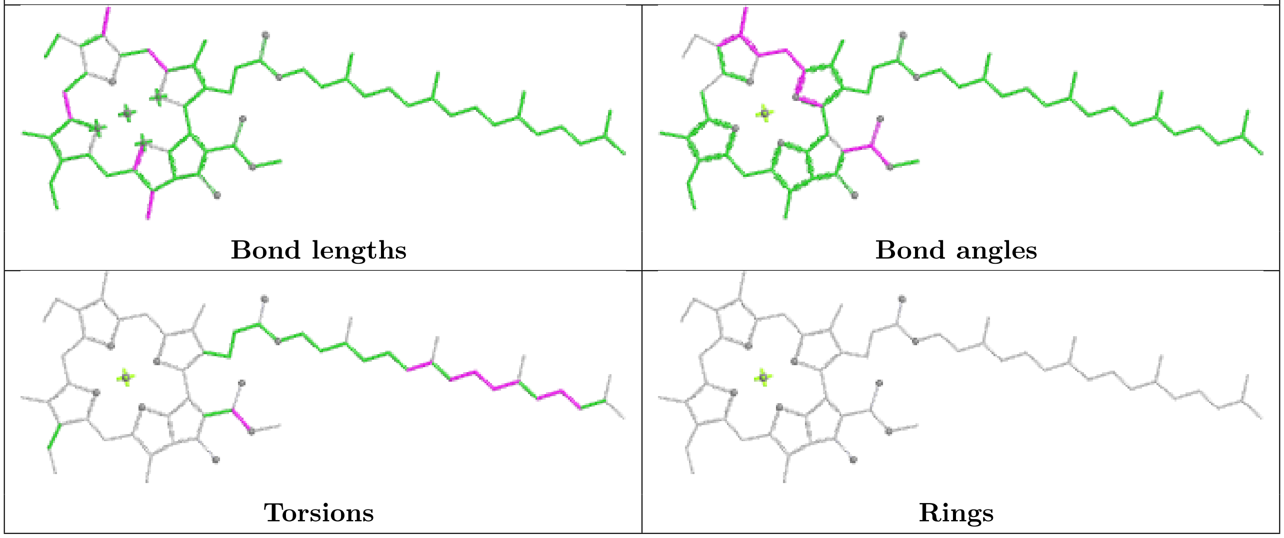


Torsions



Rings

Ligand CLA G 832



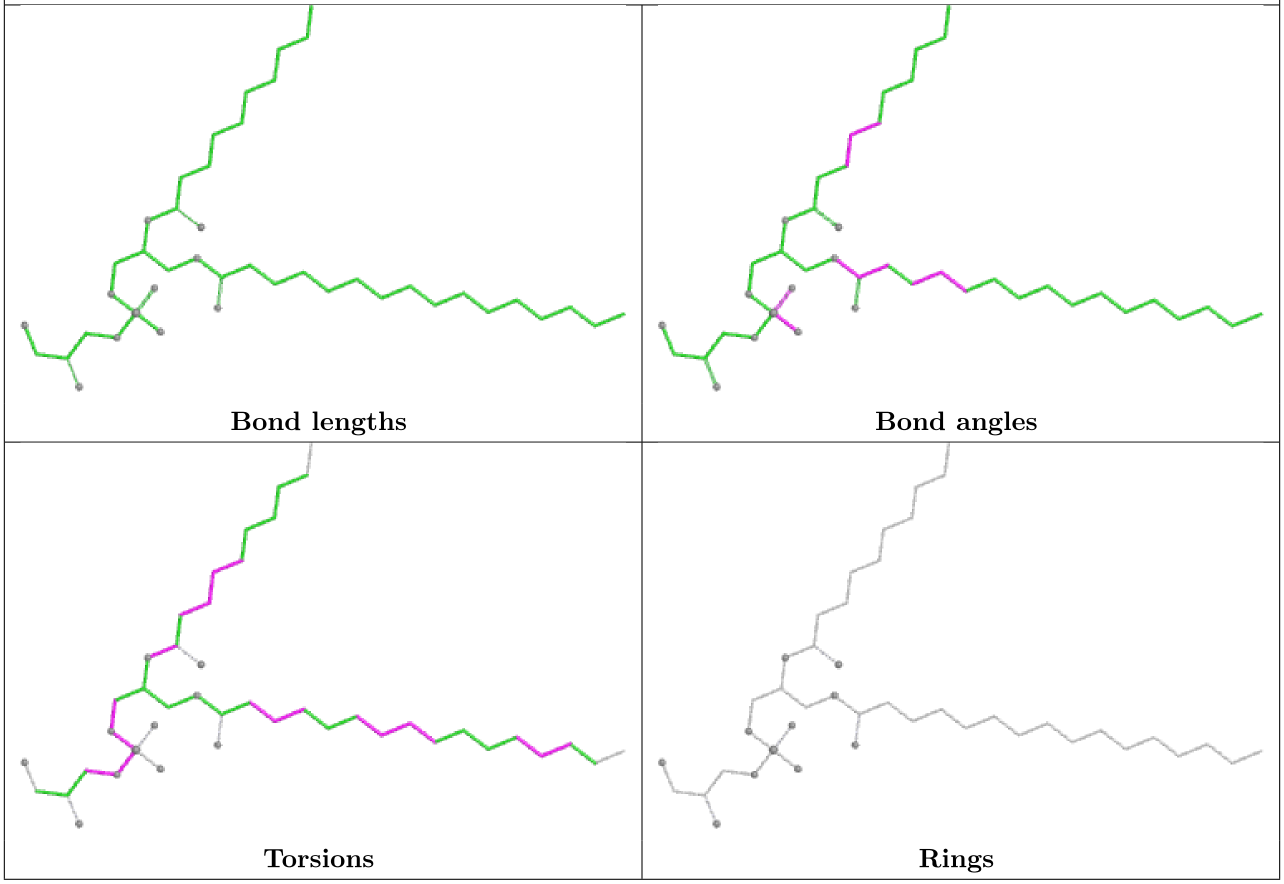
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG H 2148



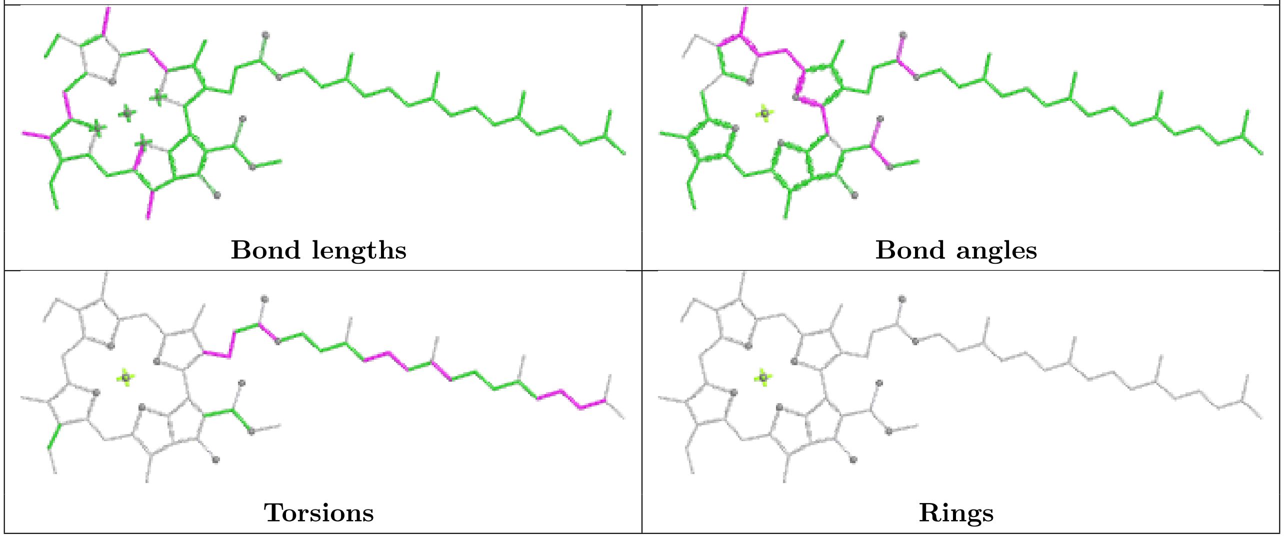
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA G 835



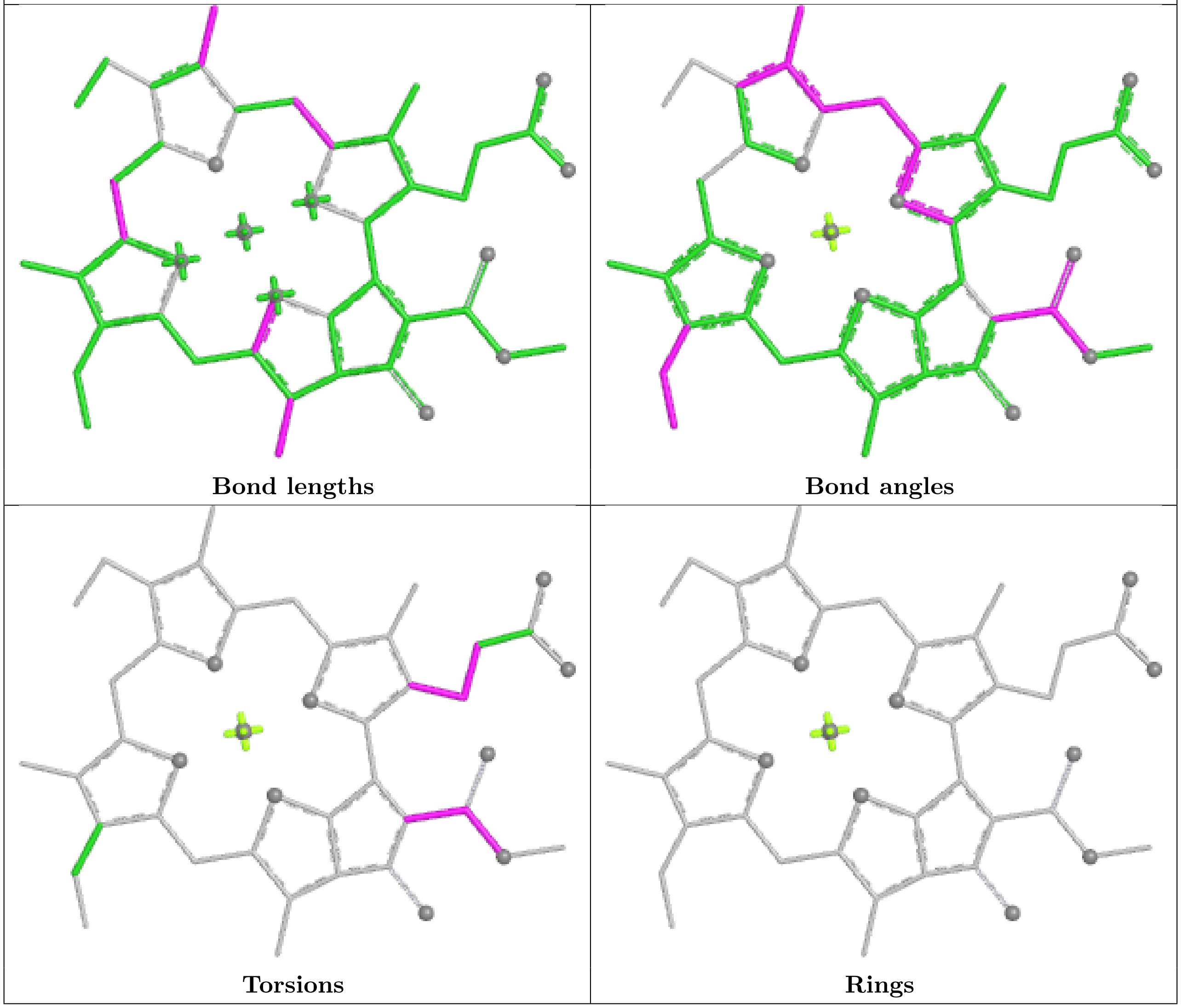
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 2142



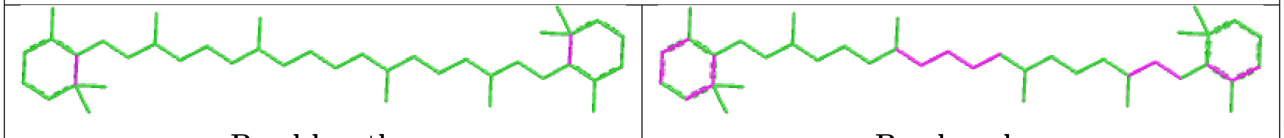
Bond lengths

Bond angles

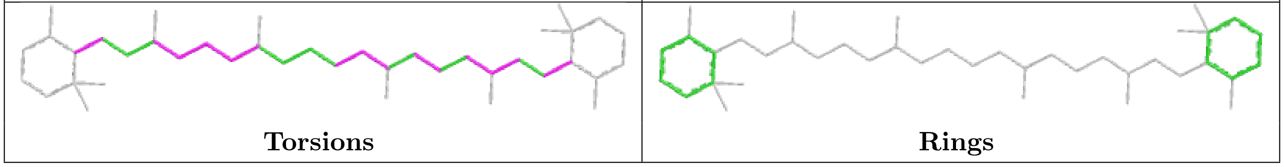
Torsions

Rings

Ligand BCR B 2147

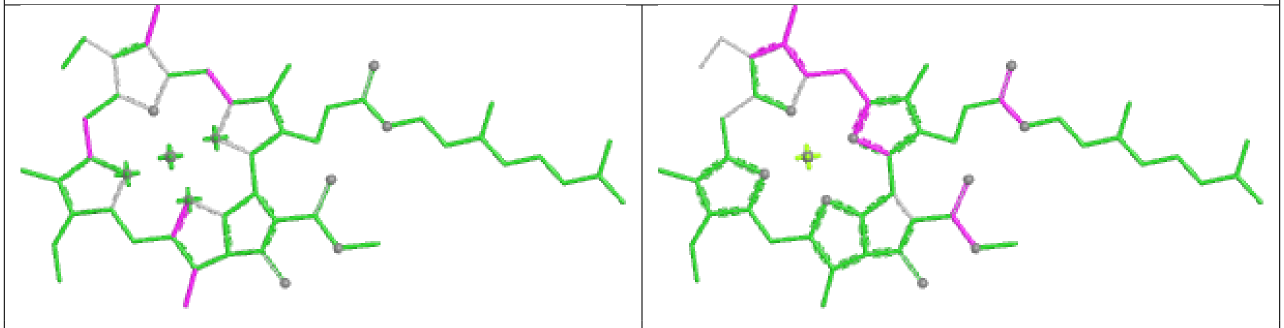


Bond lengths Bond angles

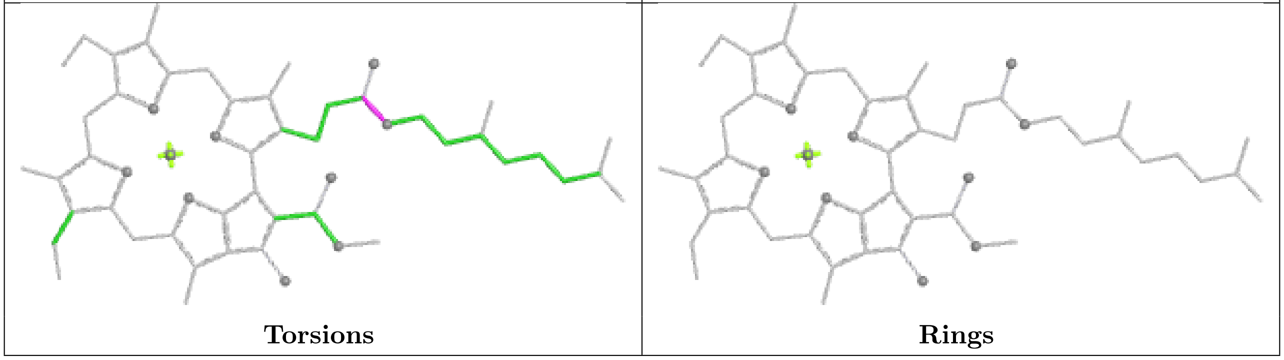


Torsions Rings

Ligand CLA A 803

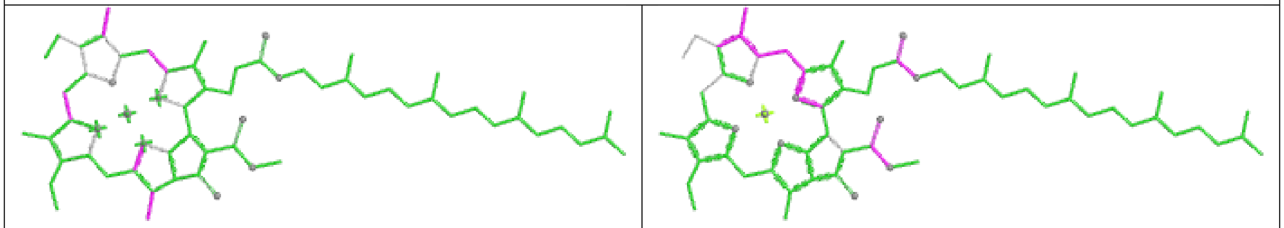


Bond lengths Bond angles

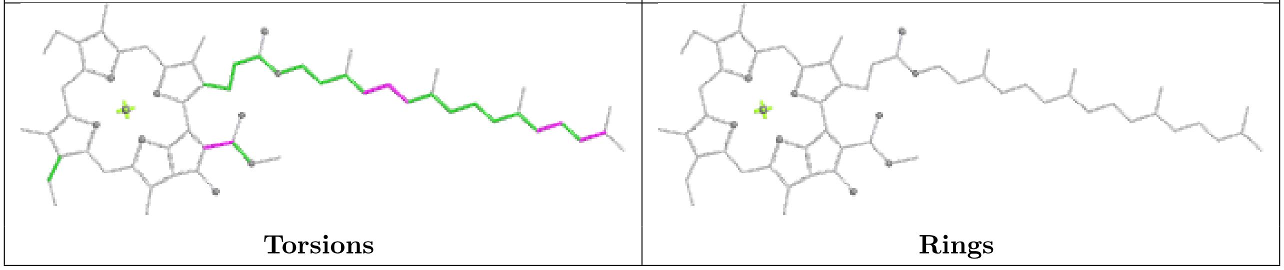


Torsions Rings

Ligand CLA B 2113

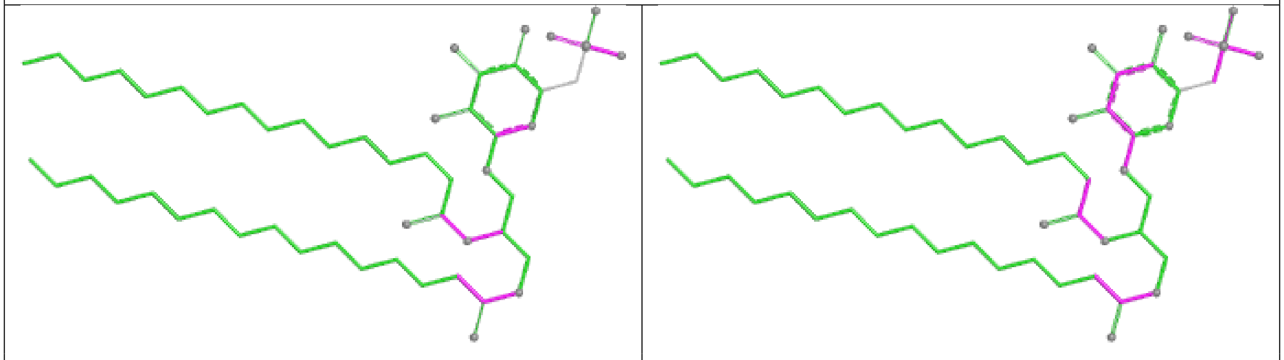


Bond lengths Bond angles



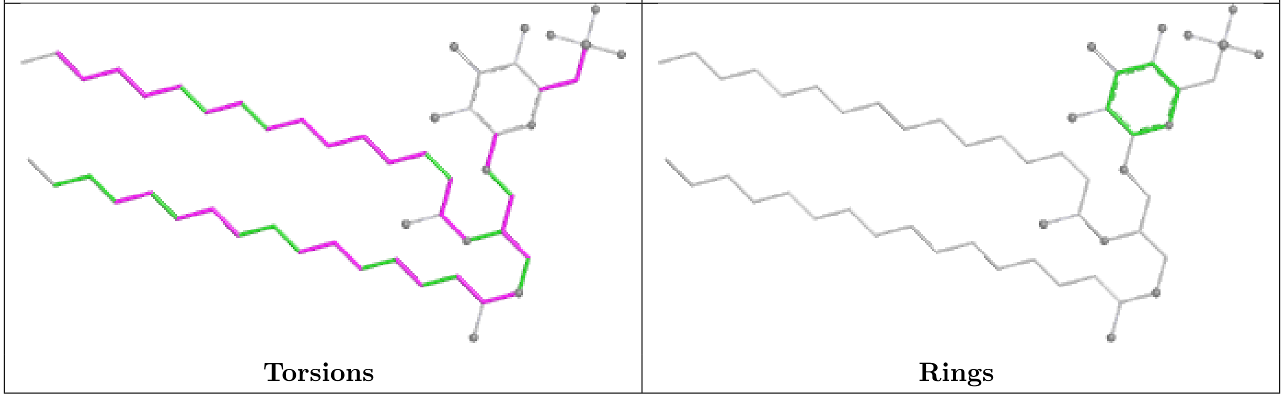
Torsions Rings

Ligand SQD V 102



Bond lengths

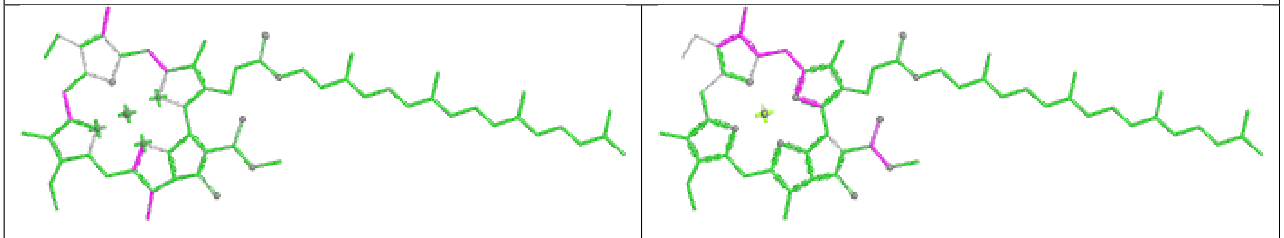
Bond angles



Torsions

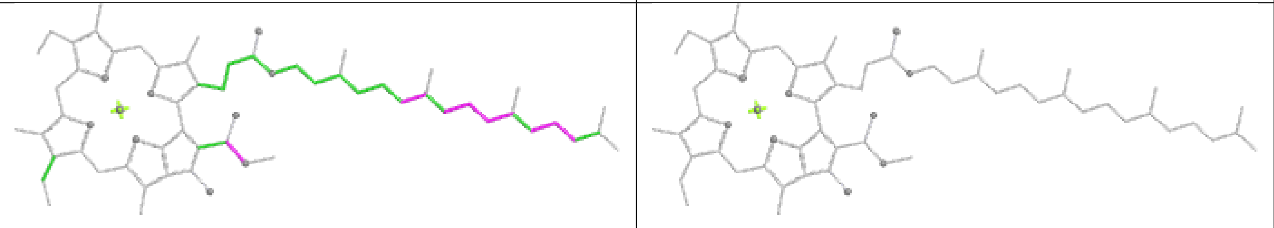
Rings

Ligand CLA A 832



Bond lengths

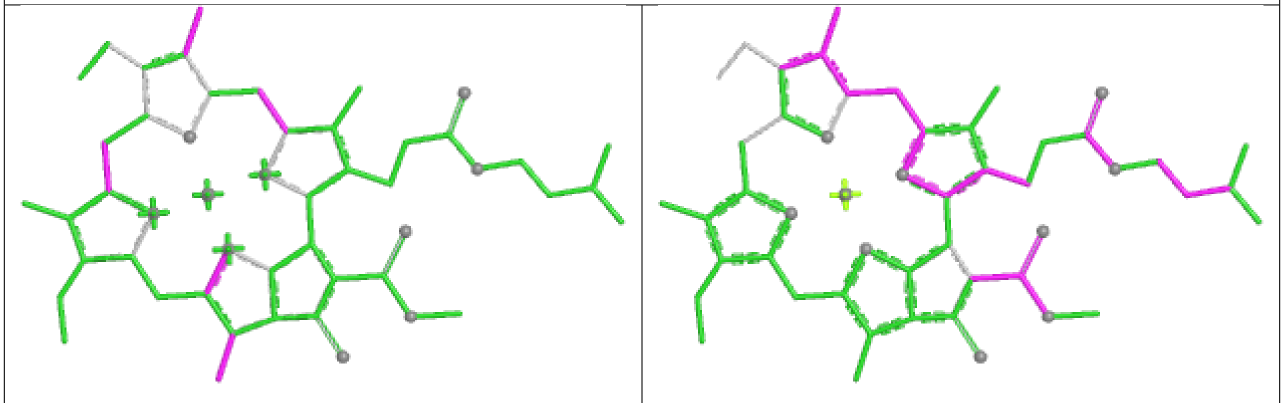
Bond angles



Torsions

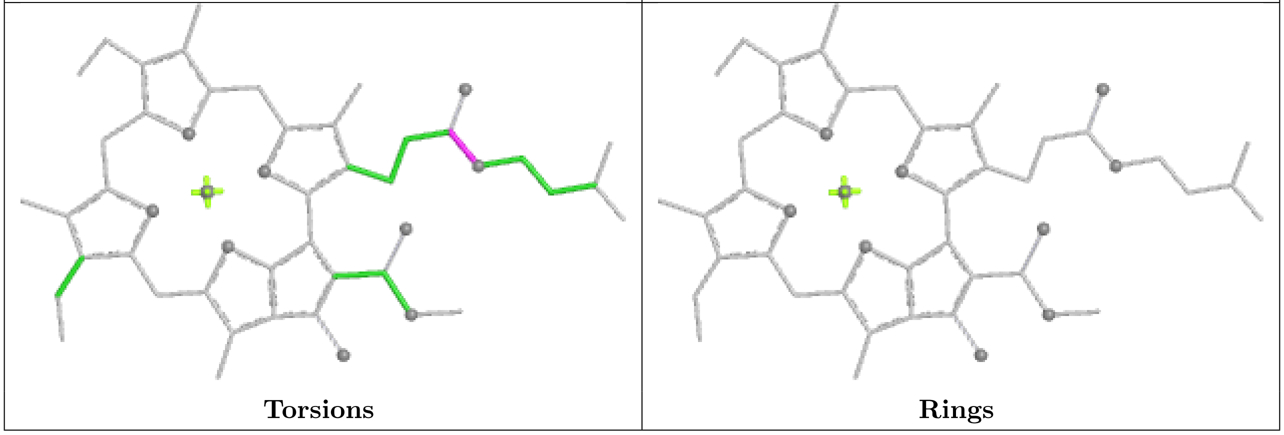
Rings

Ligand CLA B 2126



Bond lengths

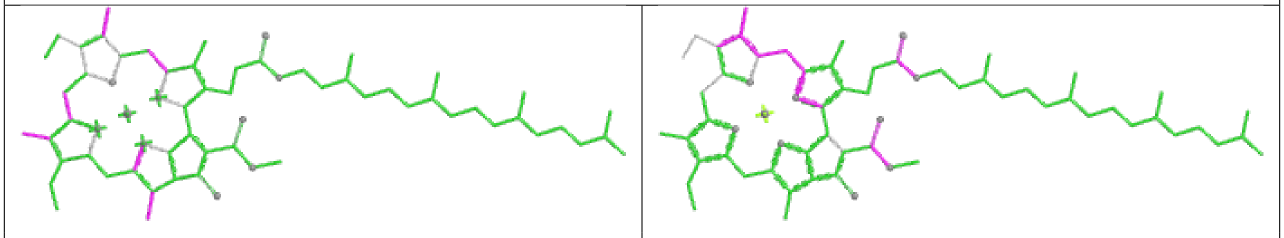
Bond angles



Torsions

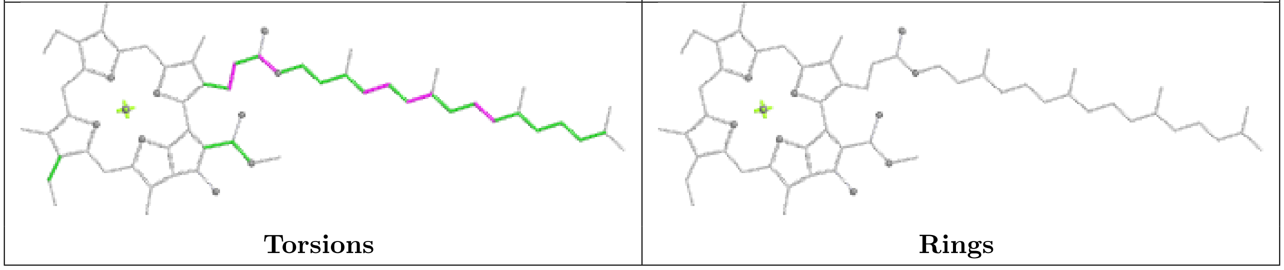
Rings

Ligand CLA B 2106



Bond lengths

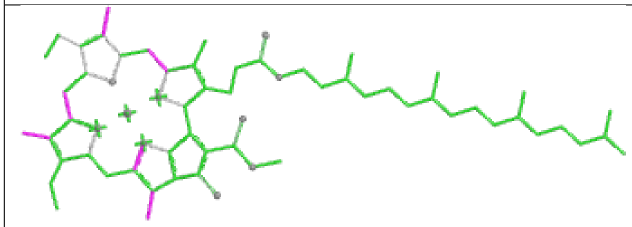
Bond angles

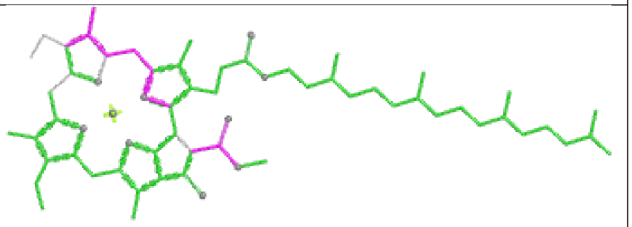


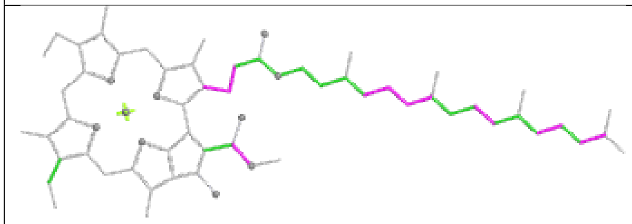
Torsions

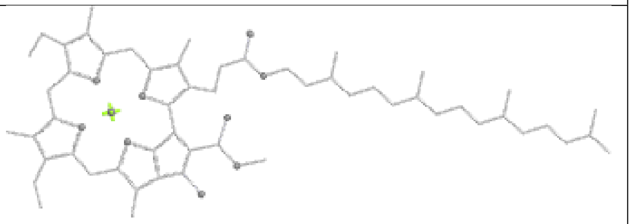
Rings

Ligand CLA a 829

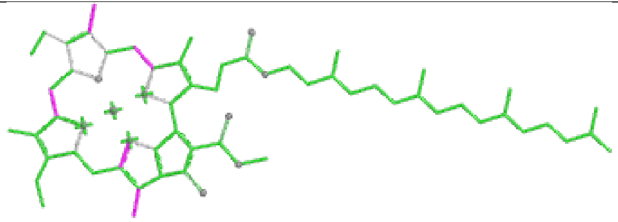

Bond lengths

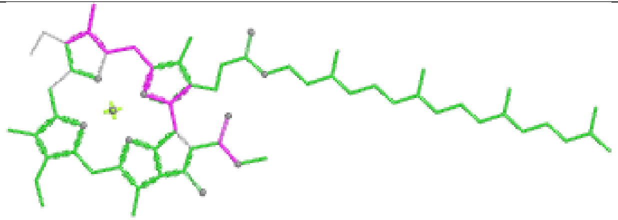

Bond angles

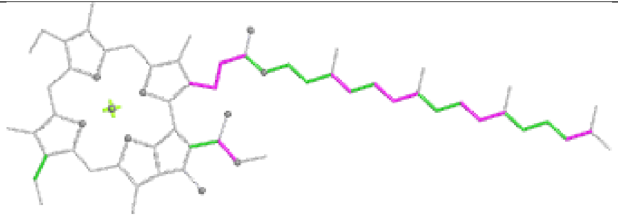

Torsions

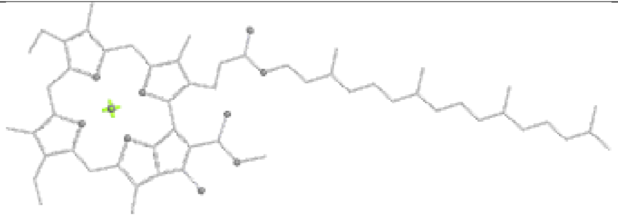

Rings

Ligand CLA H 2127

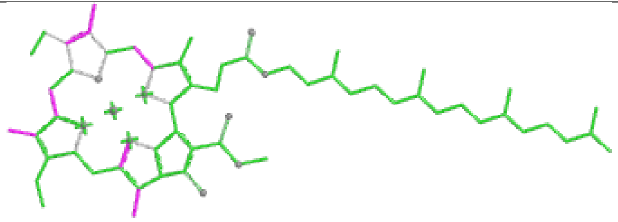

Bond lengths

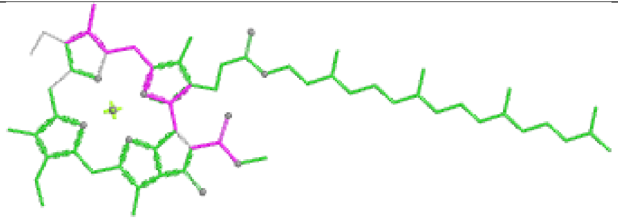

Bond angles

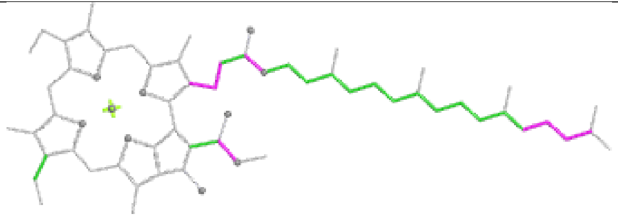

Torsions

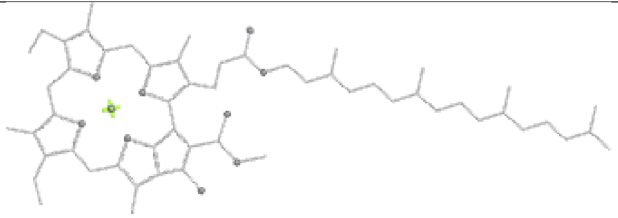

Rings

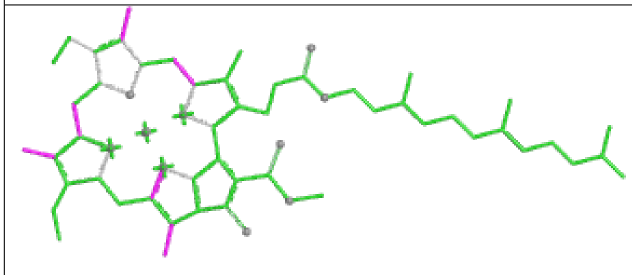
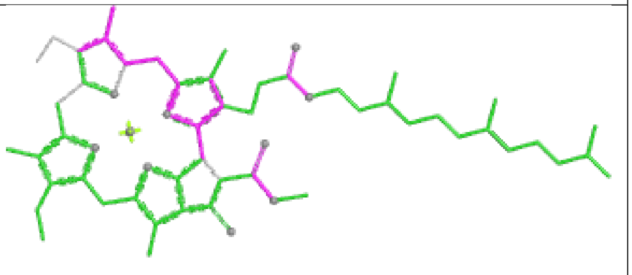
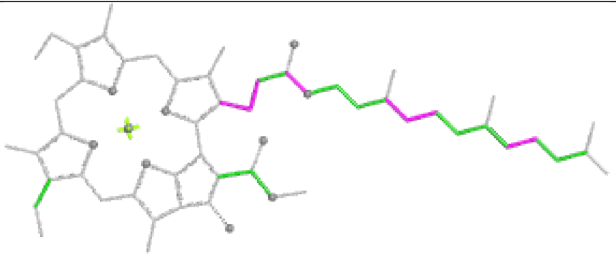
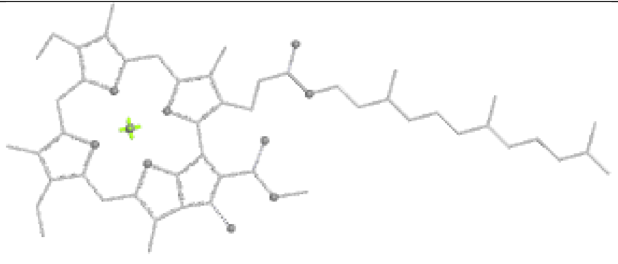
Ligand CLA b 2128

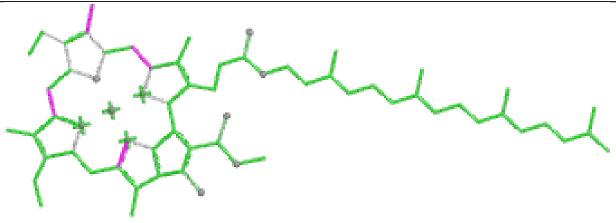
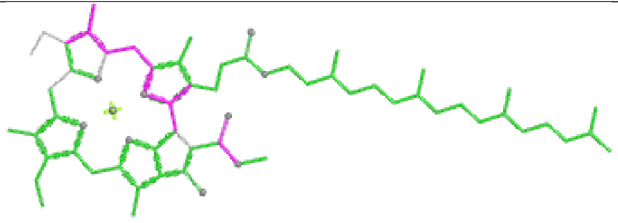
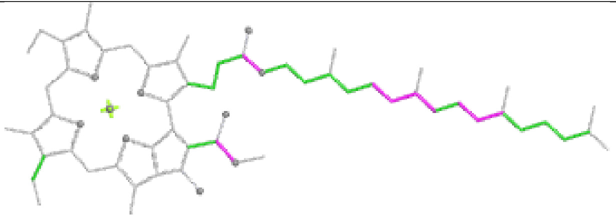
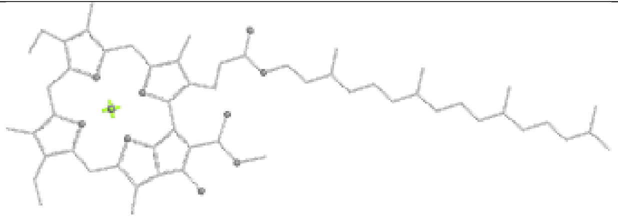

Bond lengths


Bond angles

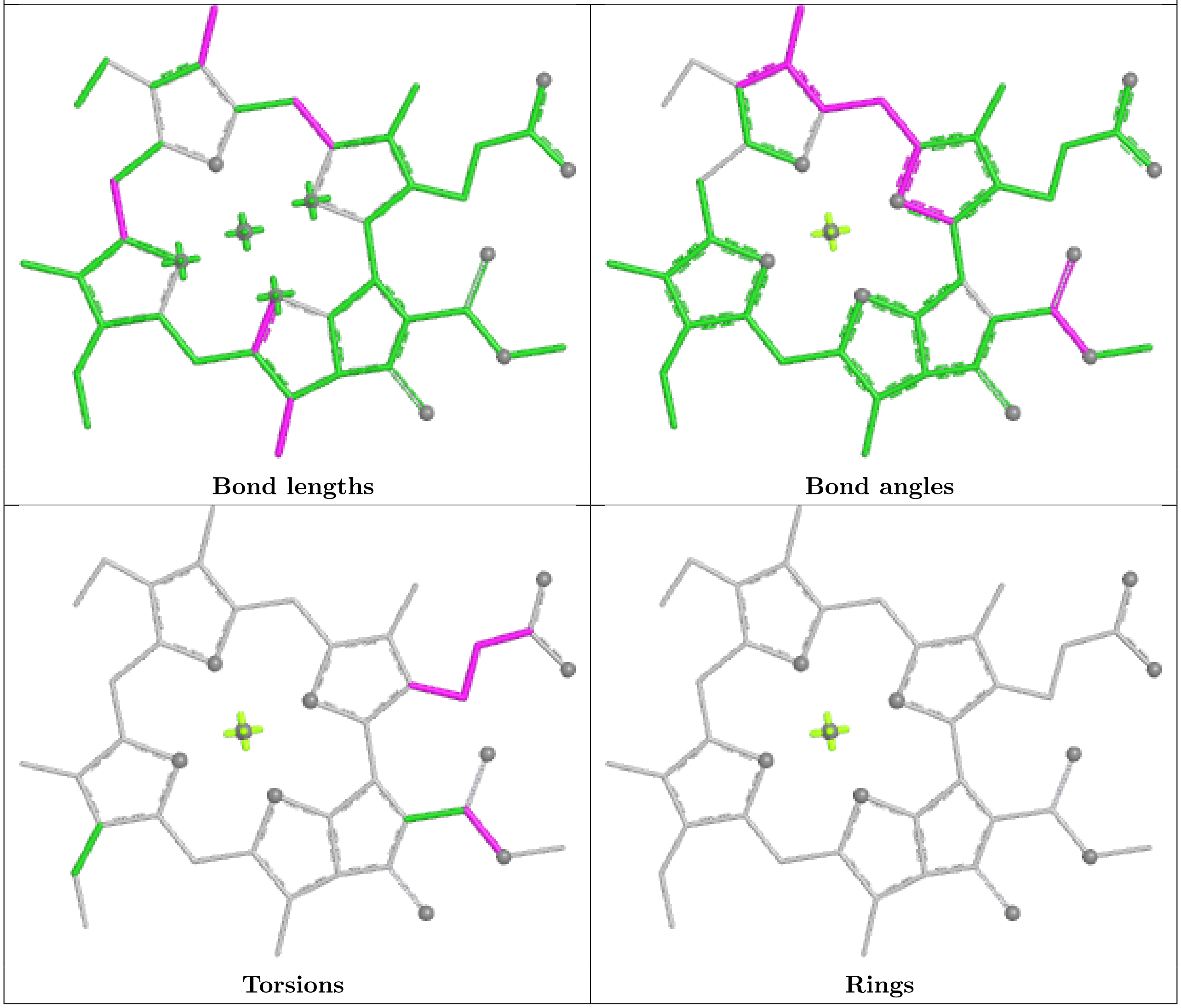

Torsions


Rings

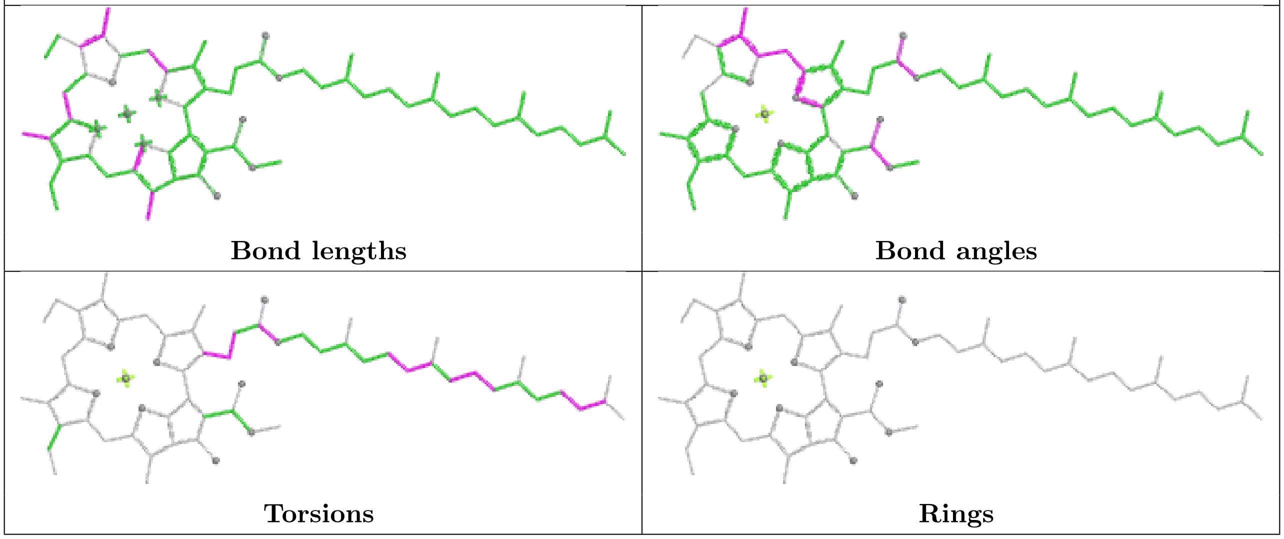
Ligand CLA a 823	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA A 813	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

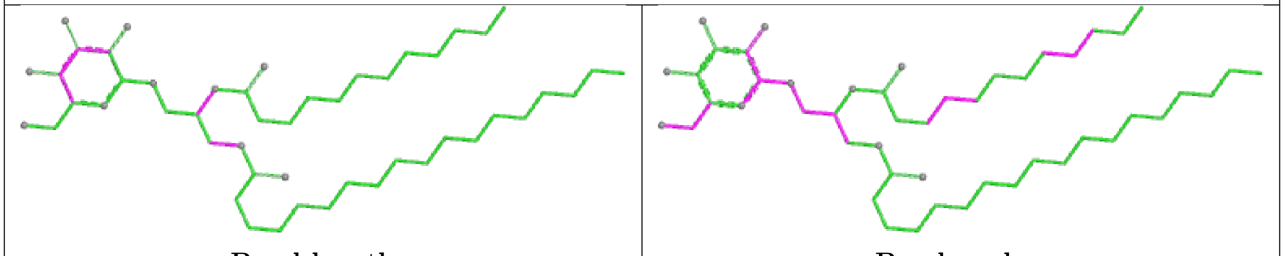
Ligand CLA B 2136


Bond lengths
Bond angles
Torsions
Rings

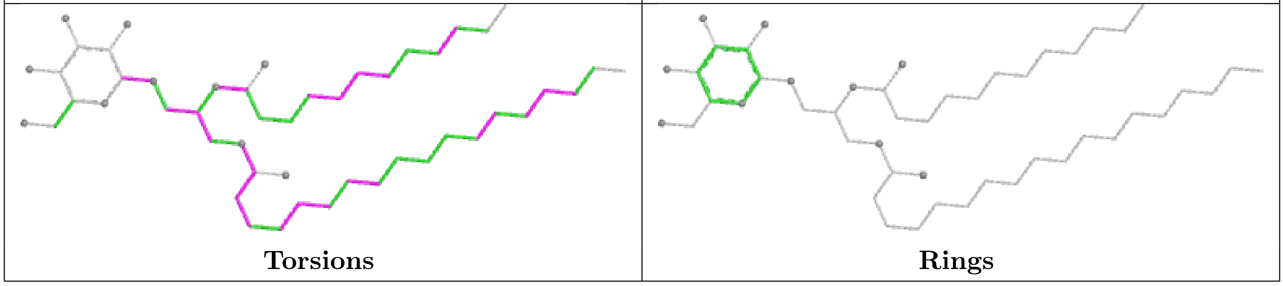
Ligand CLA G 826


Bond lengths
Bond angles
Torsions
Rings

Ligand DGD l 209

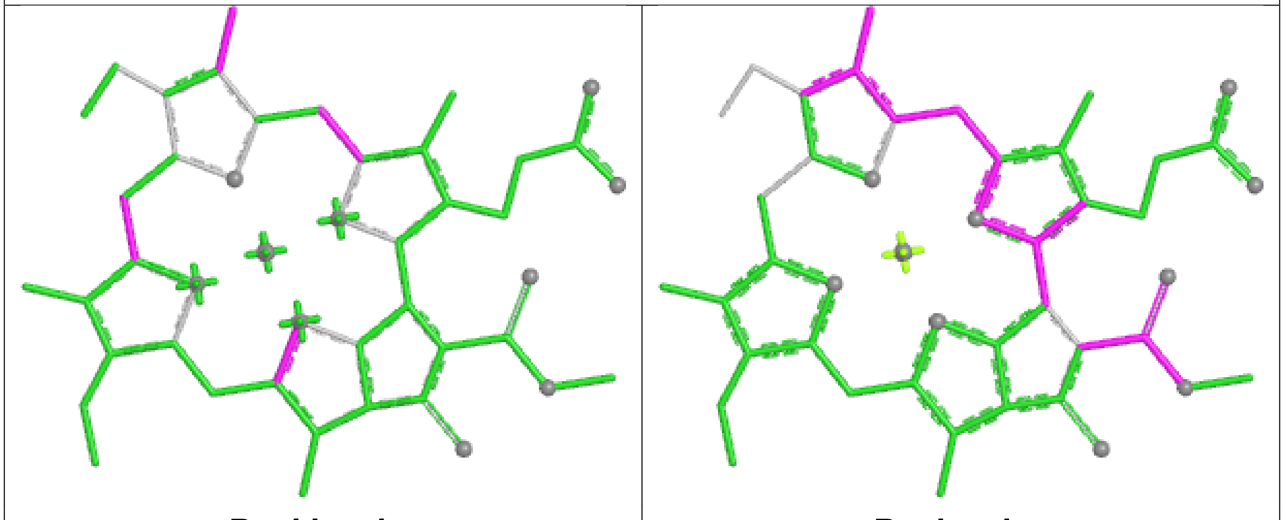


Bond lengths Bond angles

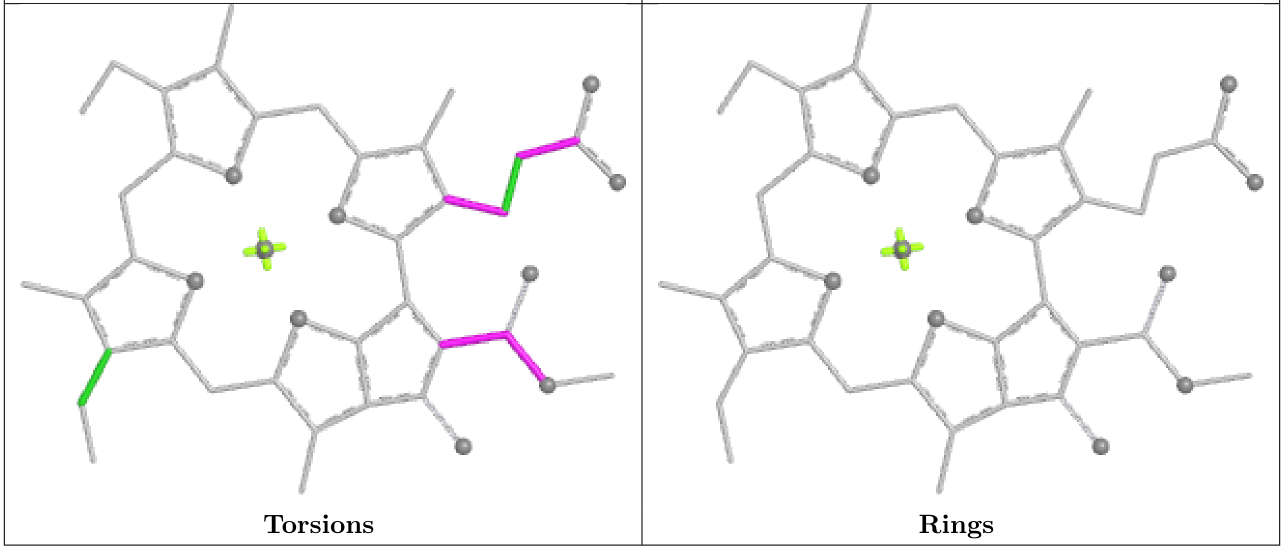


Torsions Rings

Ligand CLA B 2118

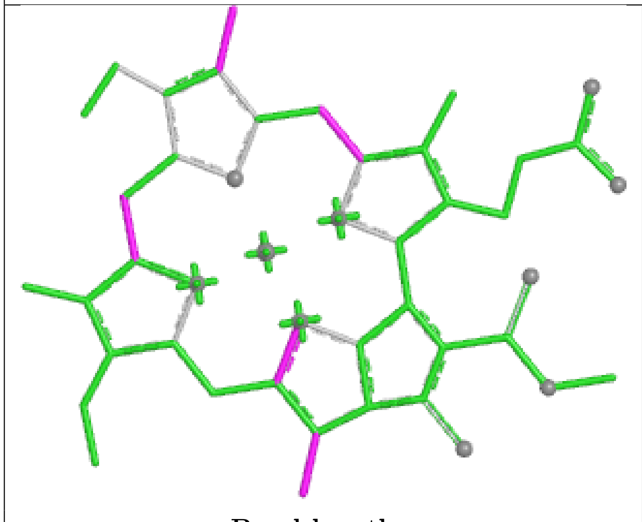


Bond lengths Bond angles

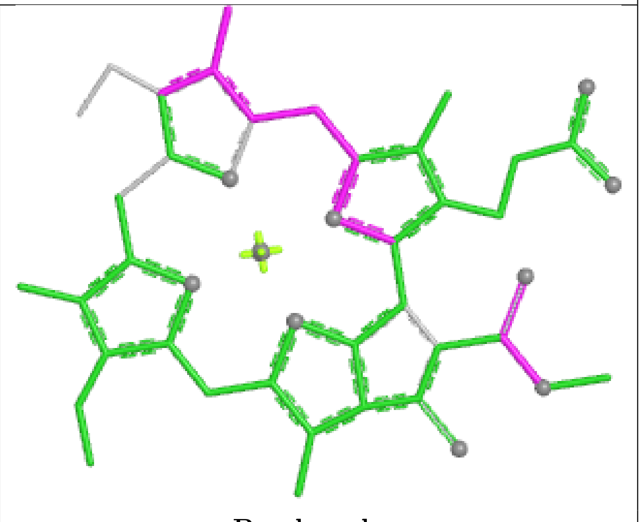


Torsions Rings

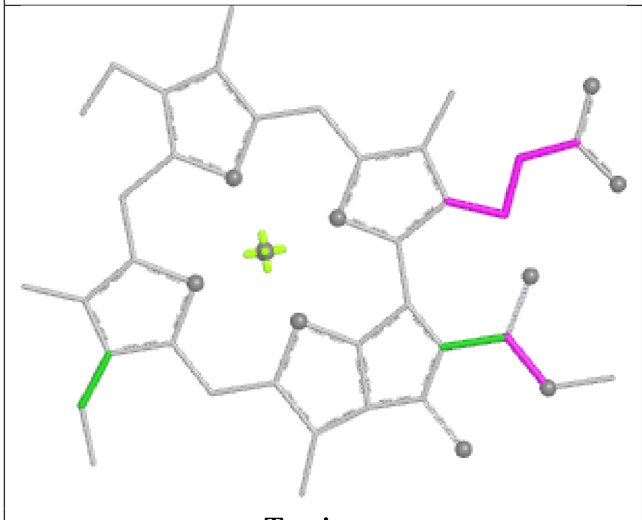
Ligand CLA B 2117



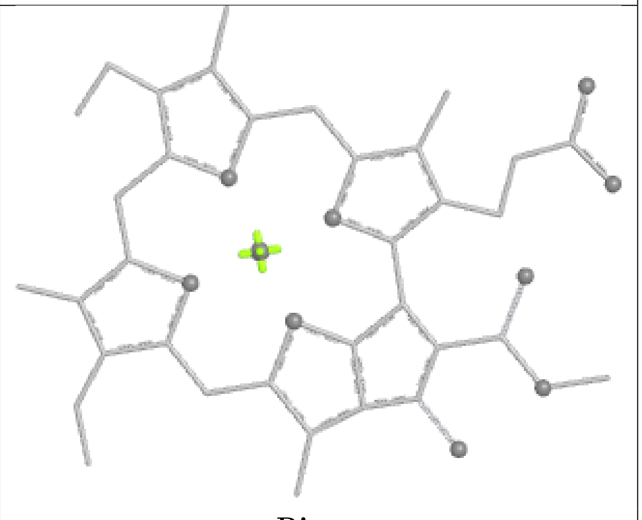
Bond lengths



Bond angles

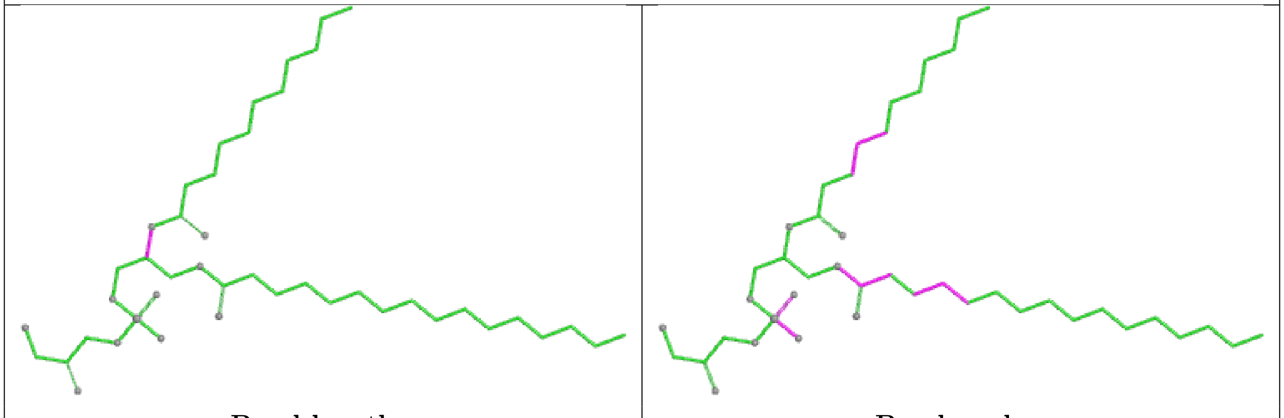


Torsions



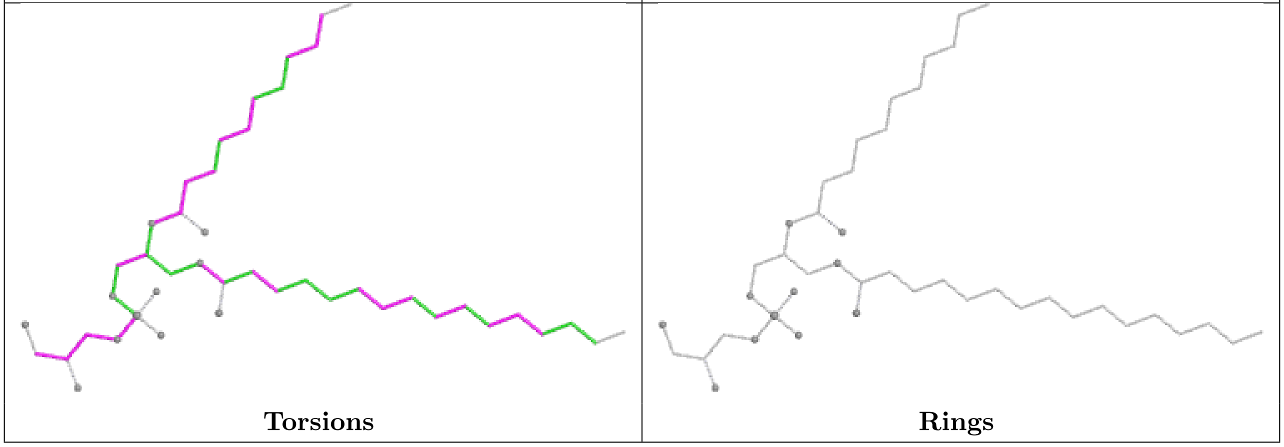
Rings

Ligand LHG m 103



Bond lengths

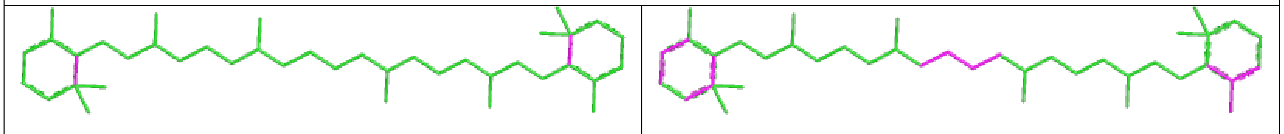
Bond angles



Torsions

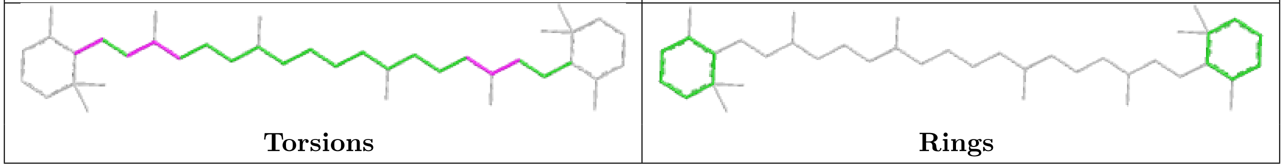
Rings

Ligand BCR R 101



Bond lengths

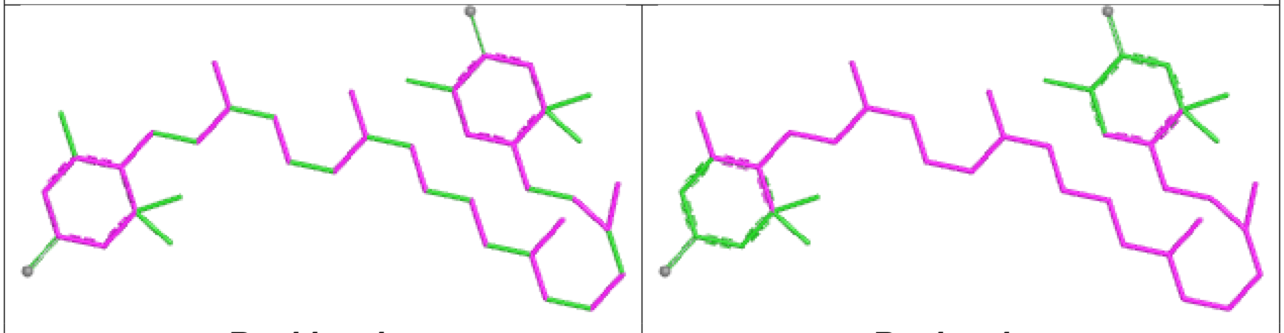
Bond angles



Torsions

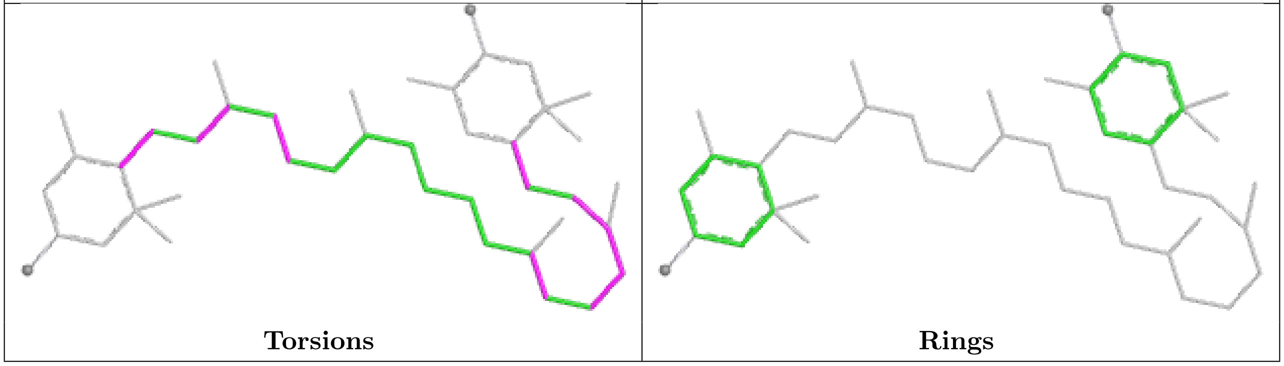
Rings

Ligand ZEX H 2151



Bond lengths

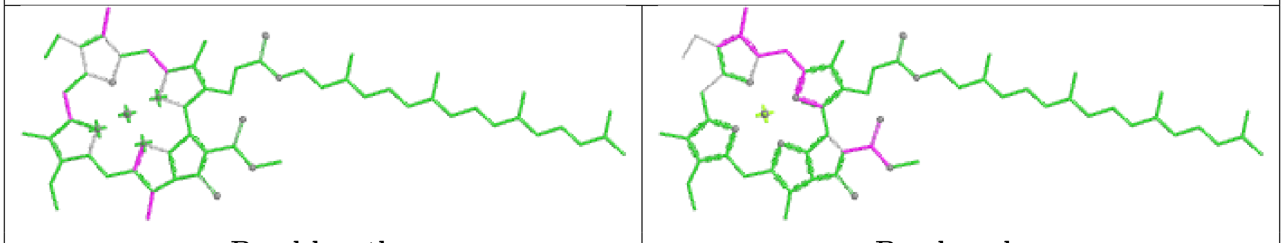
Bond angles



Torsions

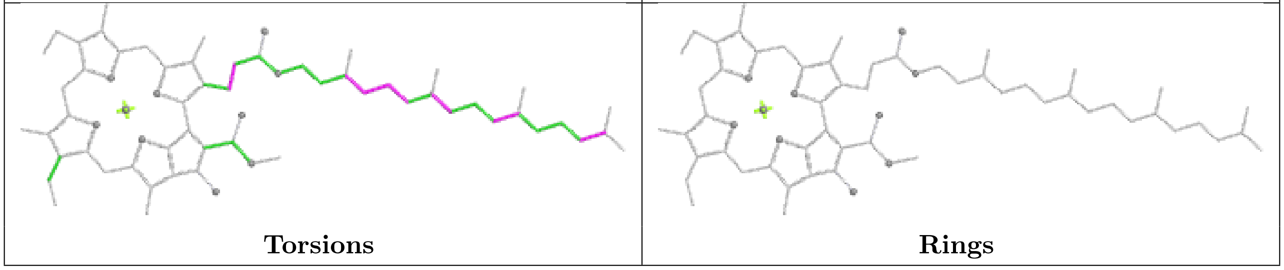
Rings

Ligand CLA b 2108



Bond lengths

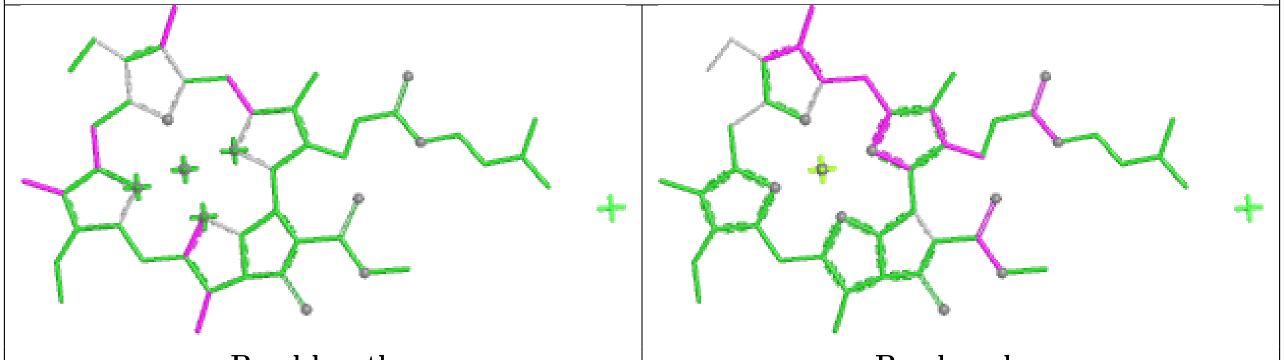
Bond angles



Torsions

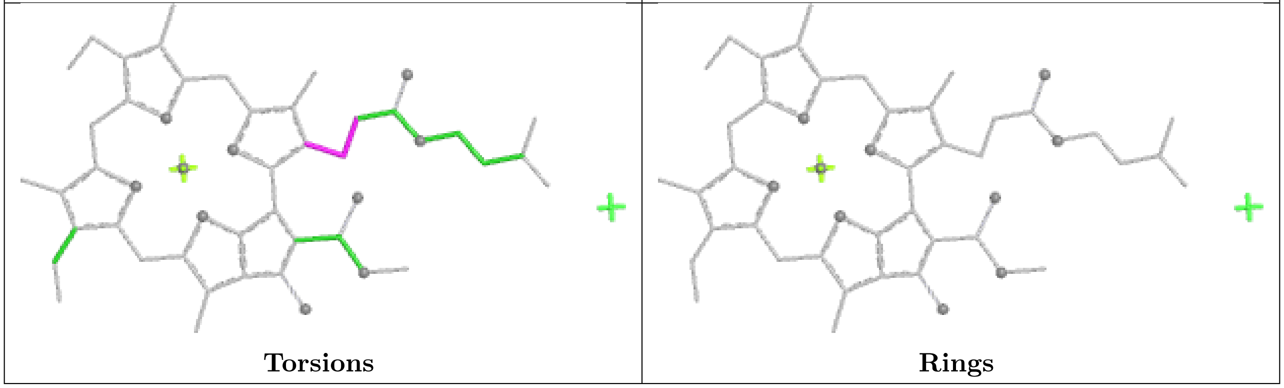
Rings

Ligand CLA a 808



Bond lengths

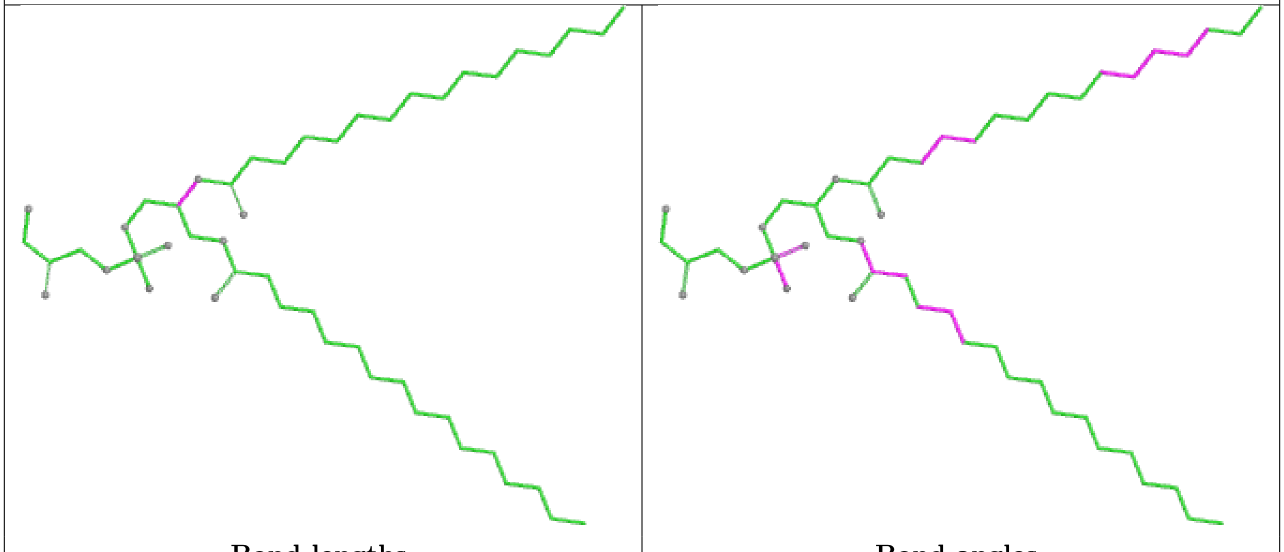
Bond angles



Torsions

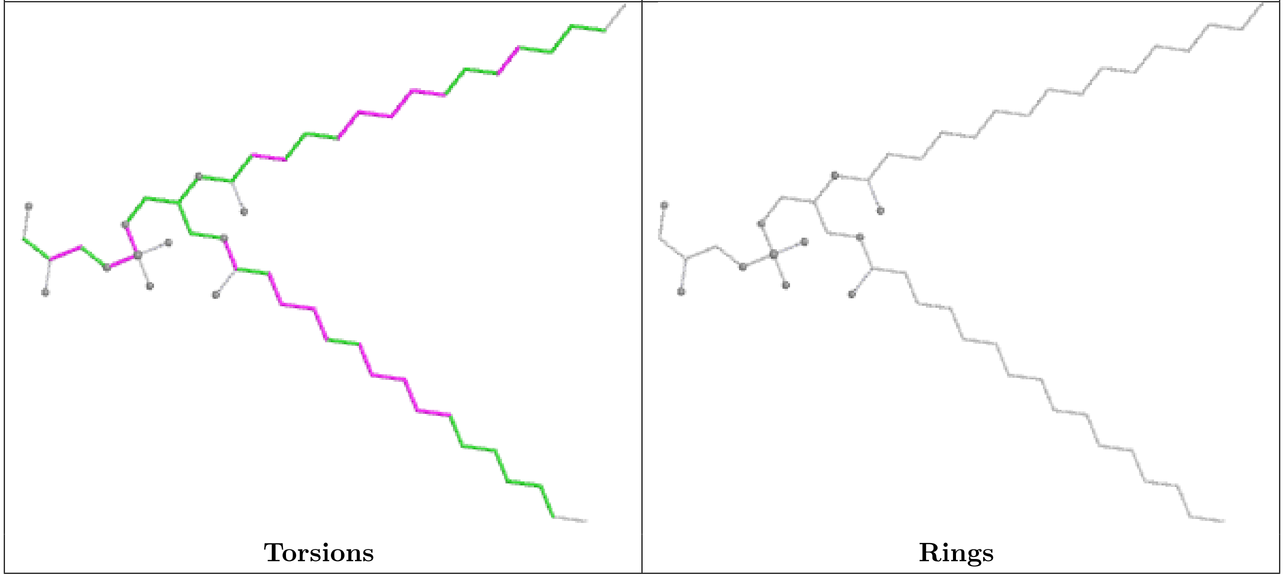
Rings

Ligand LHG A 848



Bond lengths

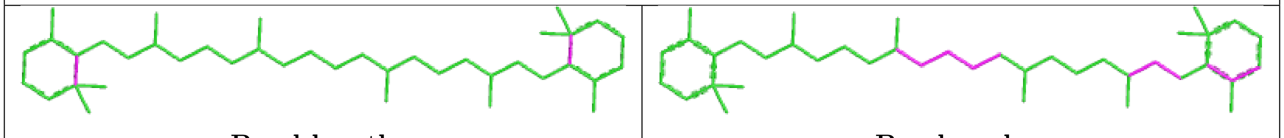
Bond angles



Torsions

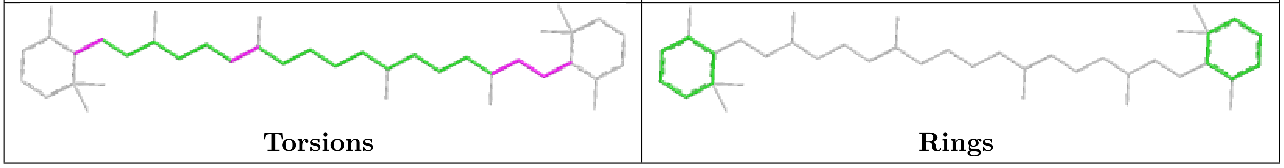
Rings

Ligand BCR G 845



Bond lengths

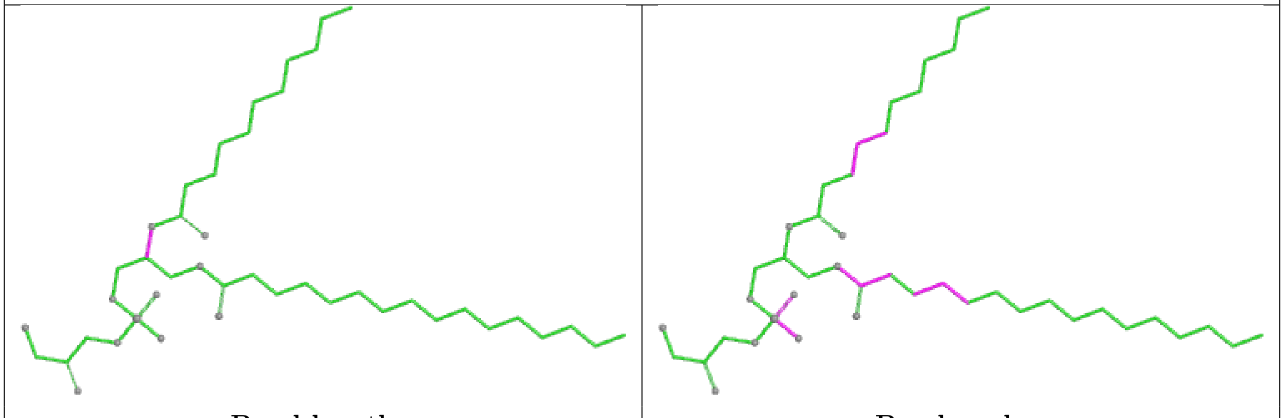
Bond angles



Torsions

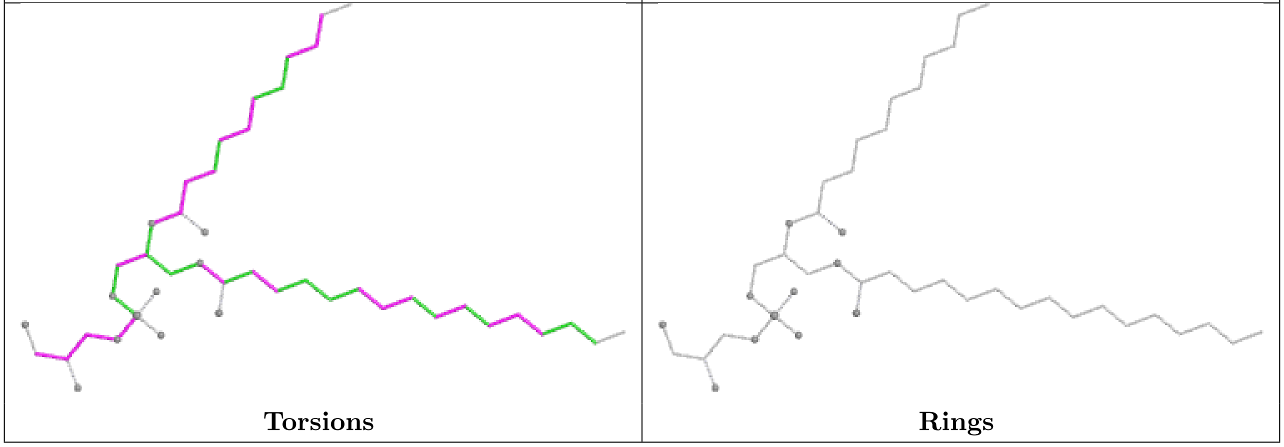
Rings

Ligand LHG M 102



Bond lengths

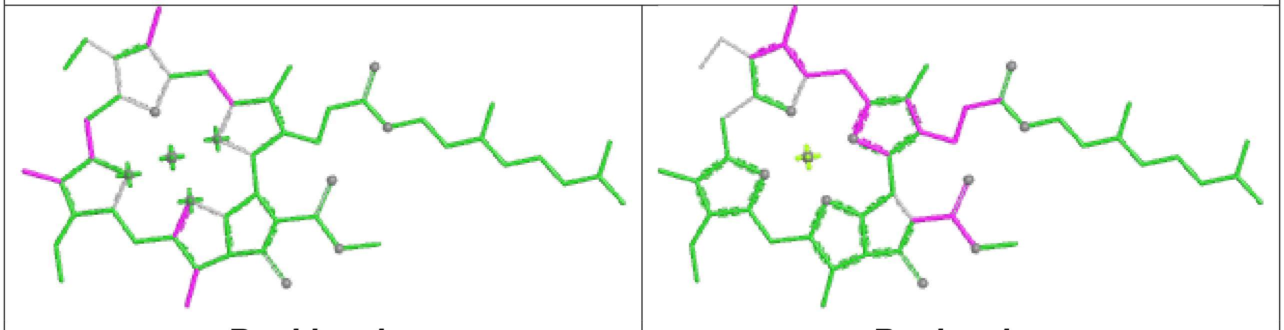
Bond angles



Torsions

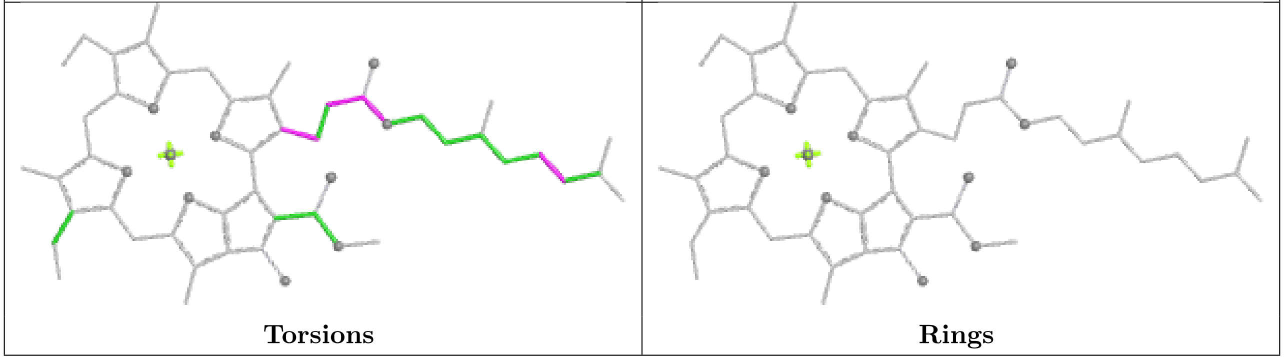
Rings

Ligand CLA G 854



Bond lengths

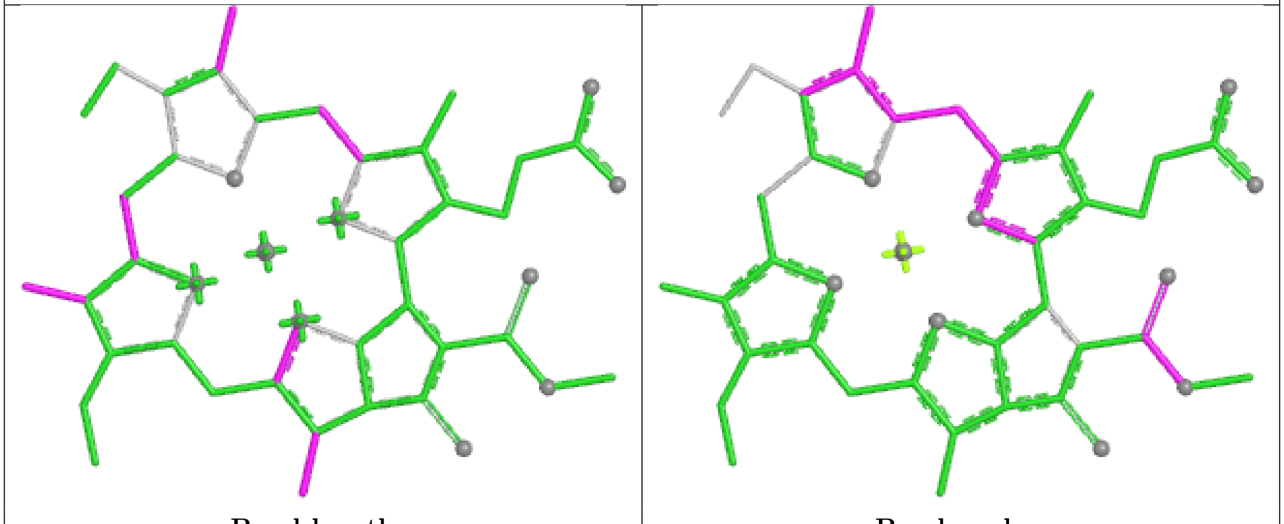
Bond angles



Torsions

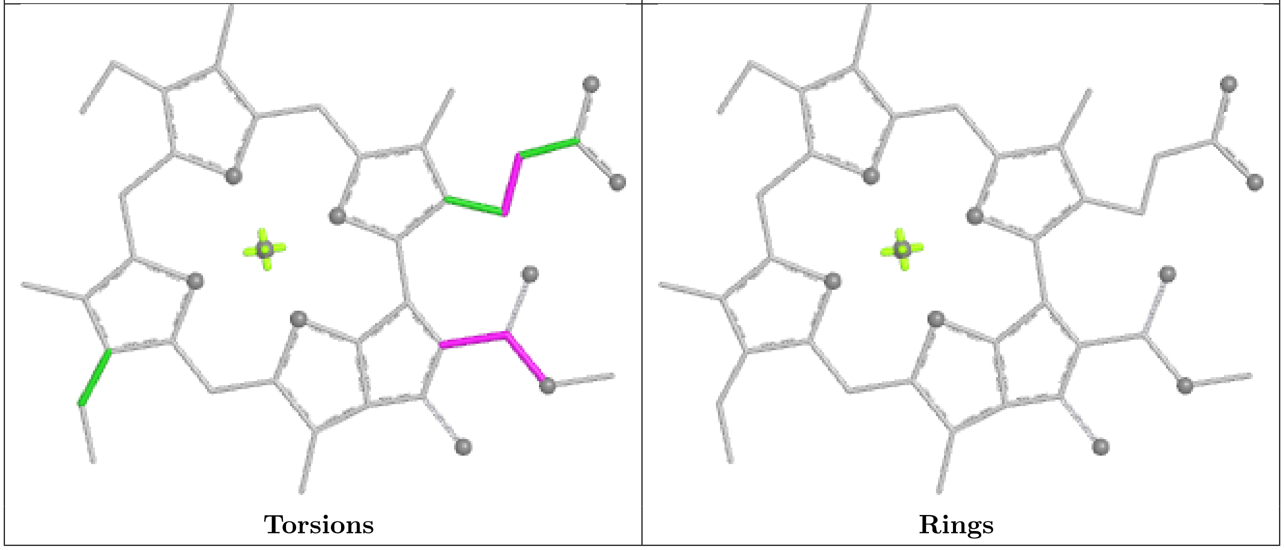
Rings

Ligand CLA a 814



Bond lengths

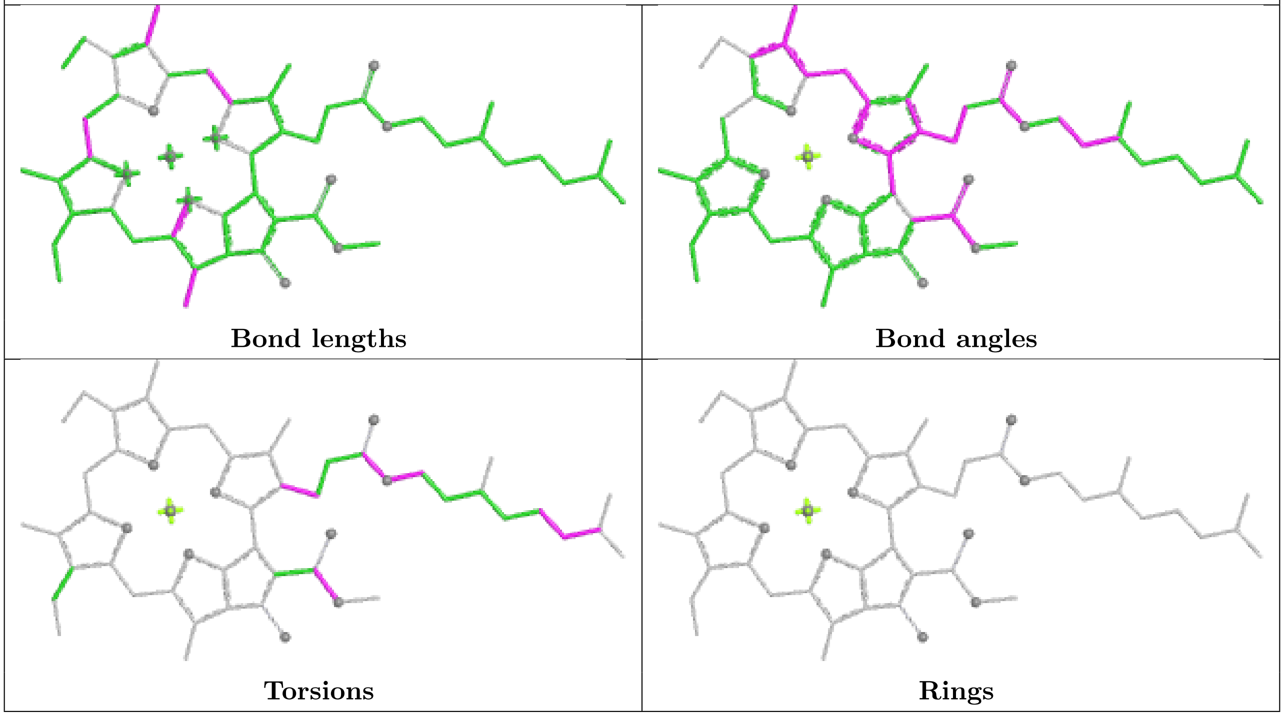
Bond angles



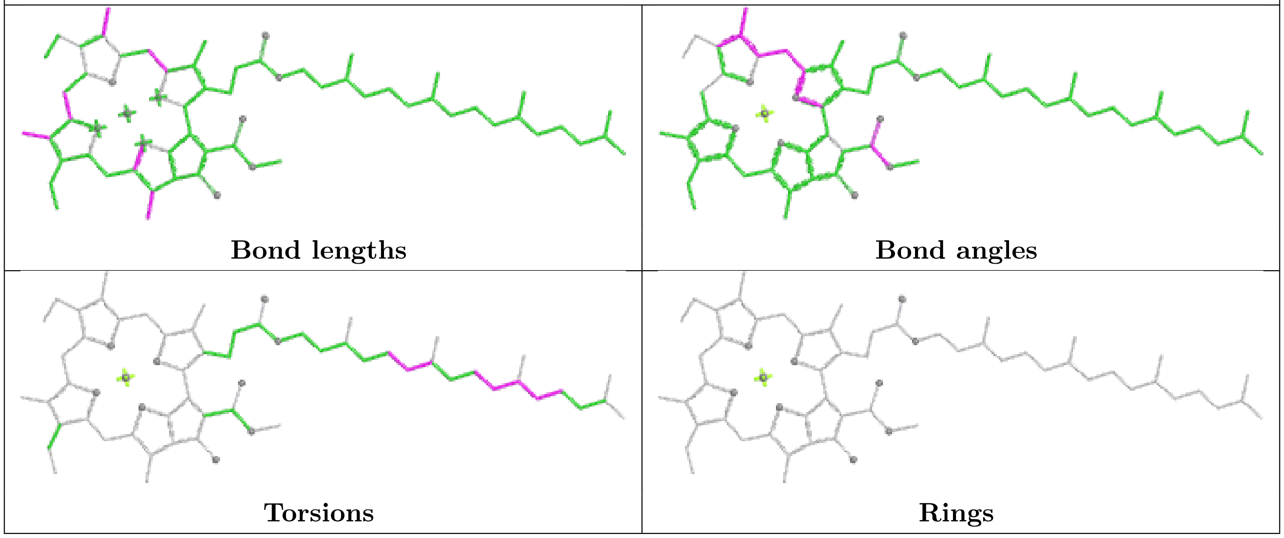
Torsions

Rings

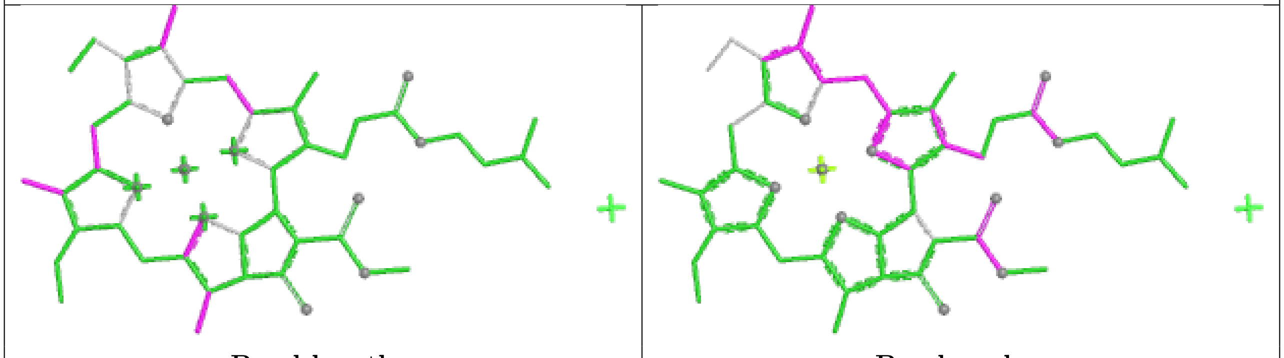
Ligand CLA A 834



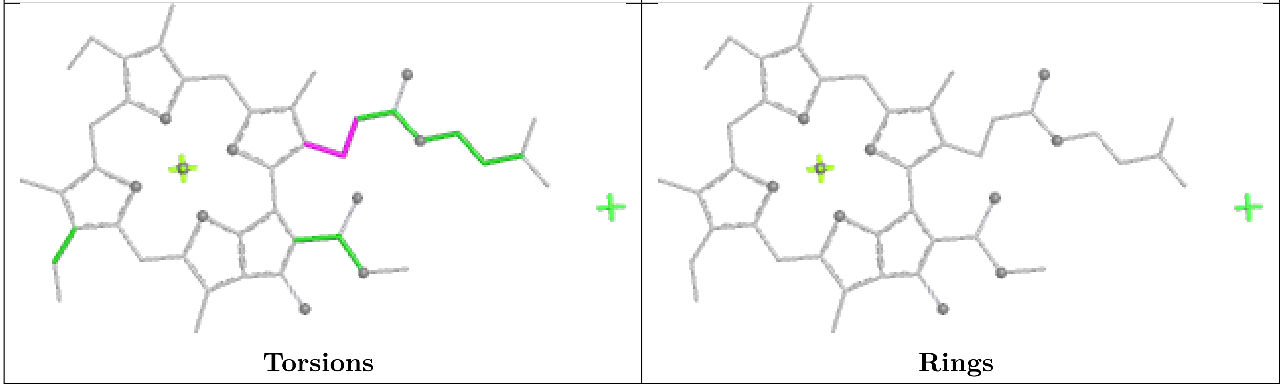
Ligand CLA B 2127



Ligand CLA G 808

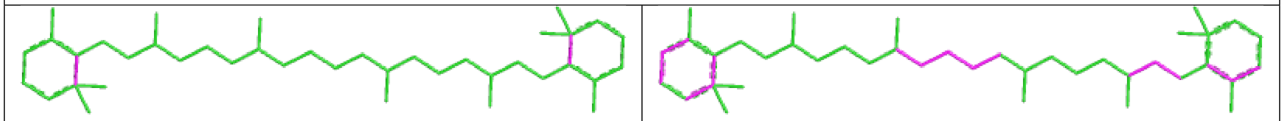


Bond lengths Bond angles

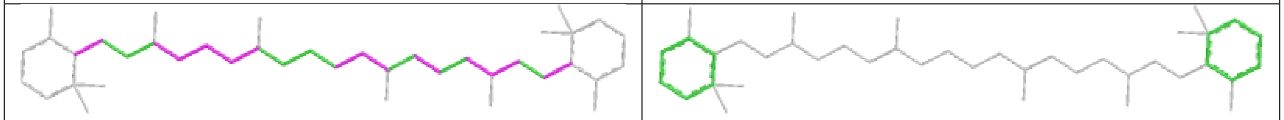


Torsions Rings

Ligand BCR H 2146

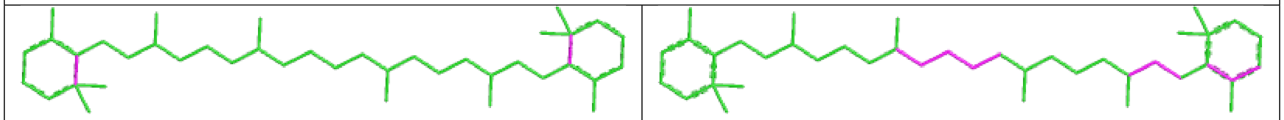


Bond lengths Bond angles

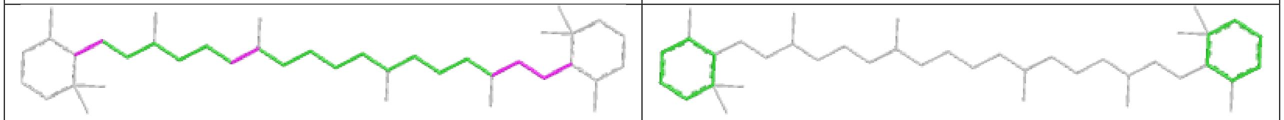


Torsions Rings

Ligand BCR a 845

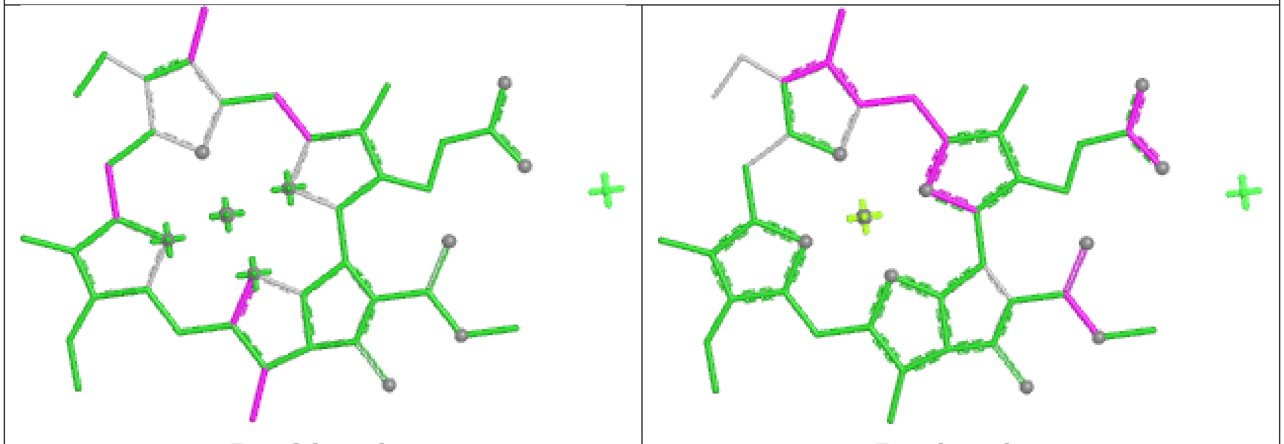


Bond lengths Bond angles

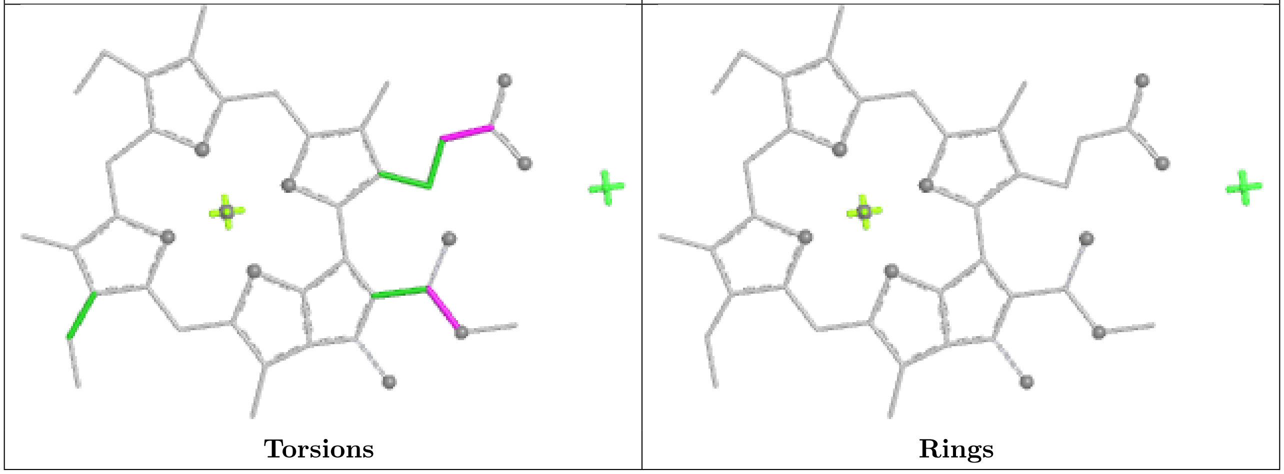


Torsions Rings

Ligand CLA Q 203

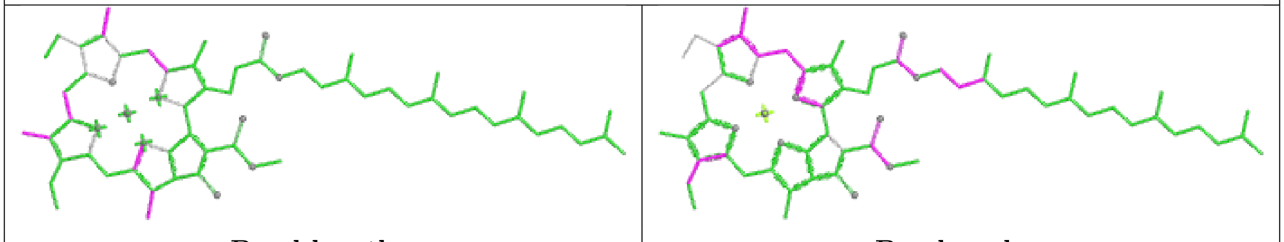


Bond lengths Bond angles

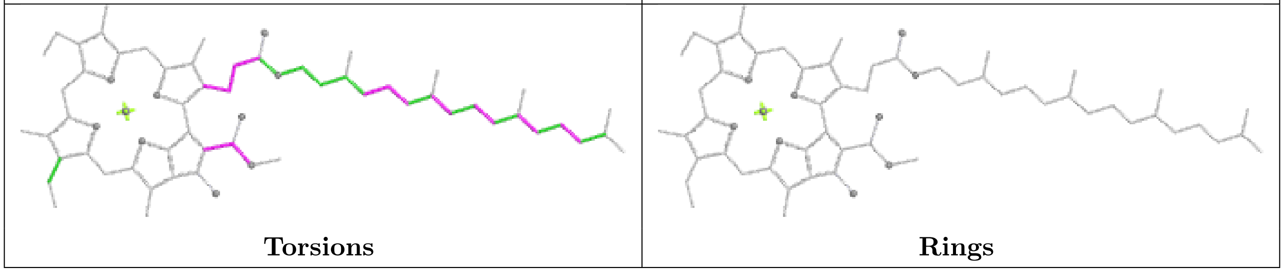


Torsions Rings

Ligand CLA b 2114

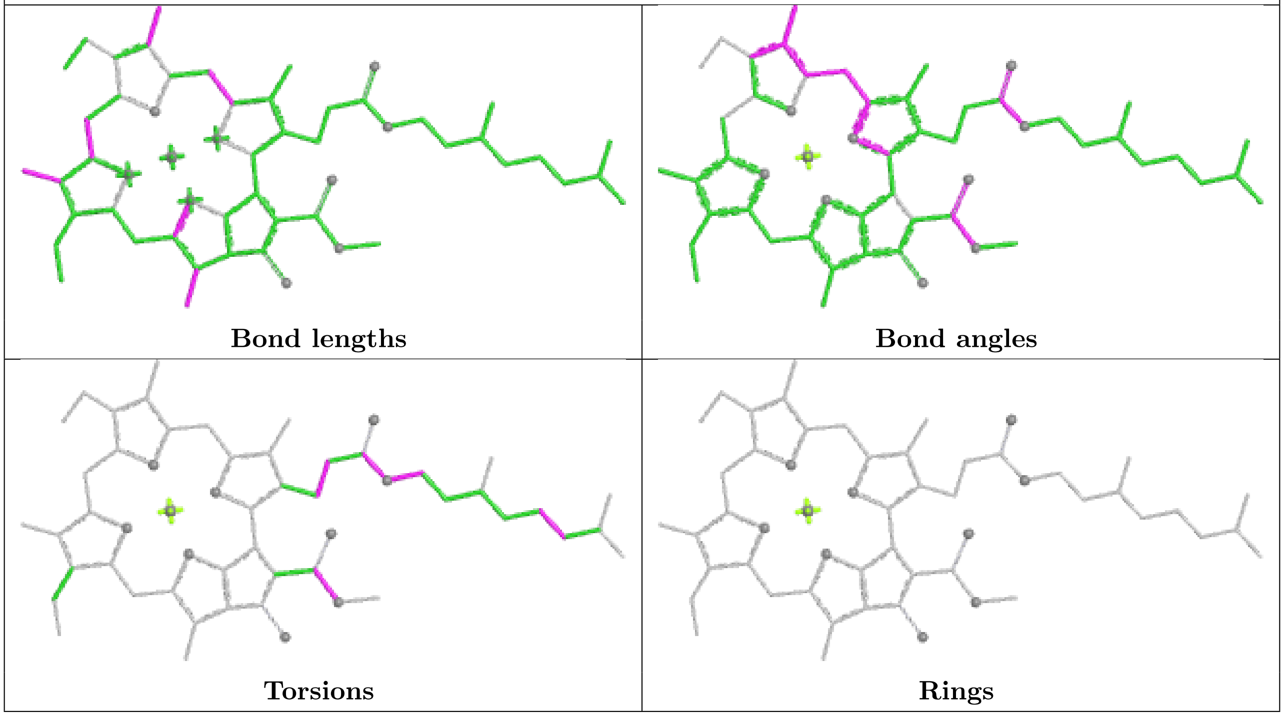


Bond lengths Bond angles



Torsions Rings

Ligand CLA B 2132



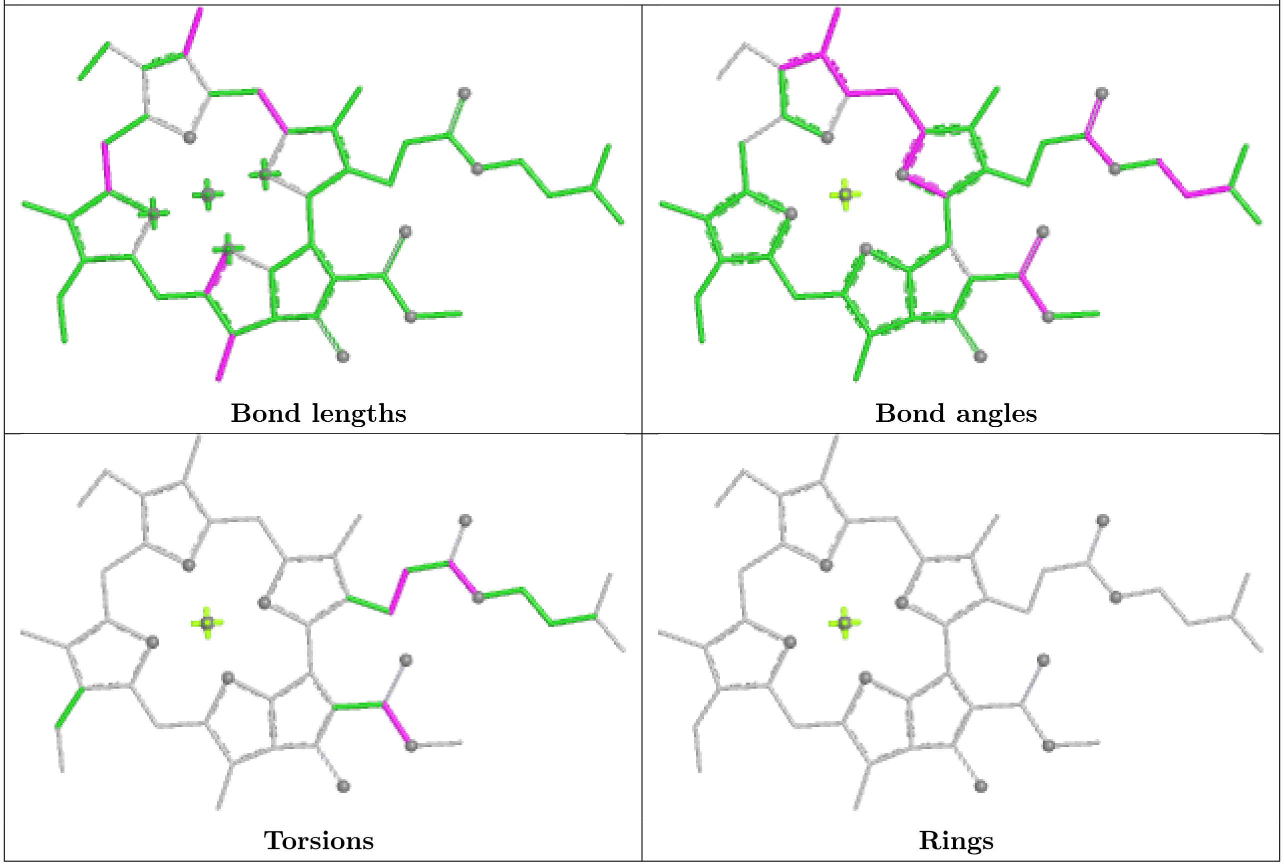
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 806



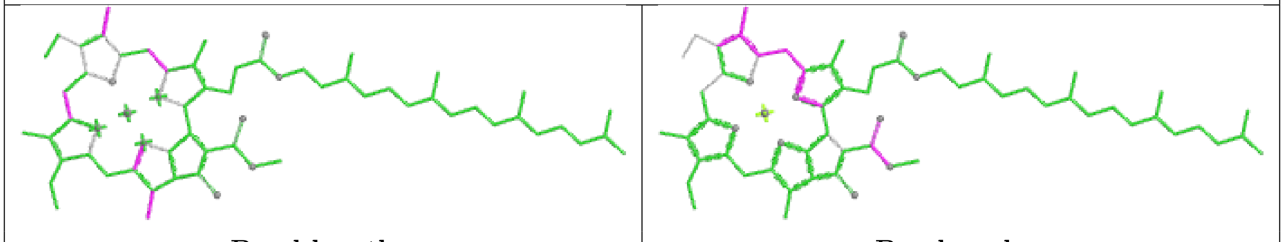
Bond lengths

Bond angles

Torsions

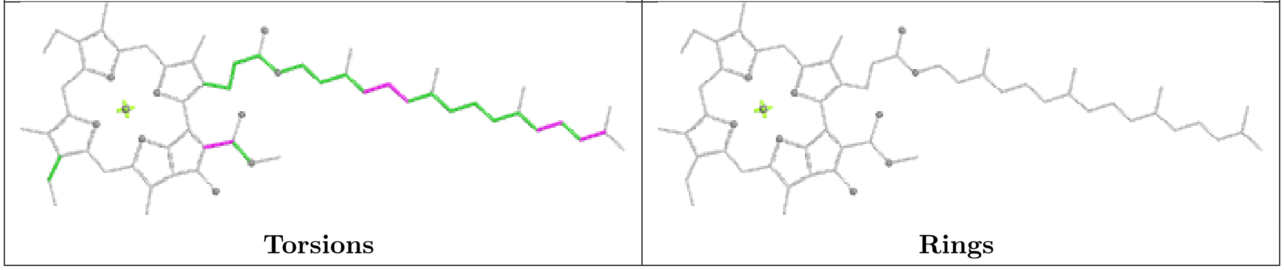
Rings

Ligand CLA H 2112



Bond lengths

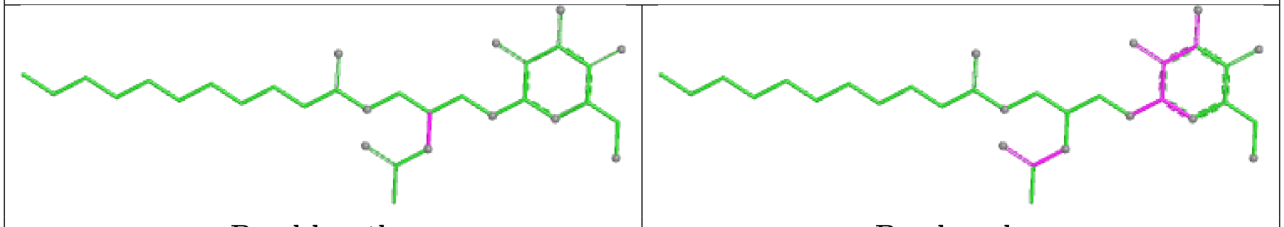
Bond angles



Torsions

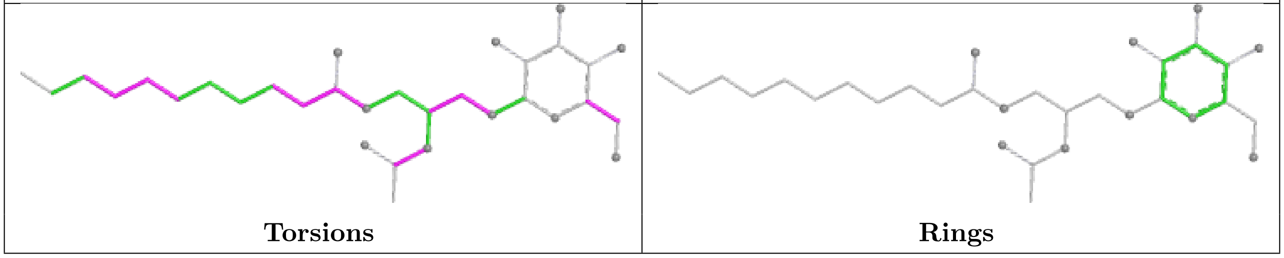
Rings

Ligand LMG a 849



Bond lengths

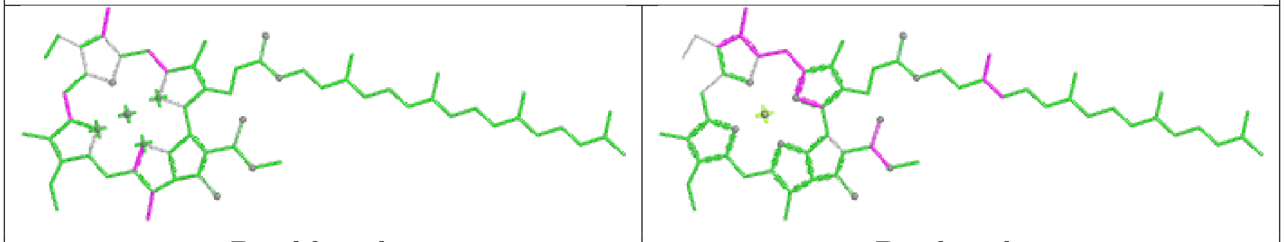
Bond angles



Torsions

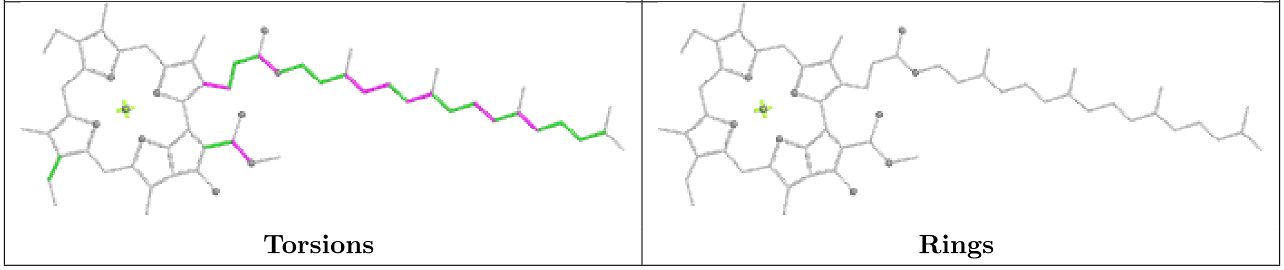
Rings

Ligand CLA A 833



Bond lengths

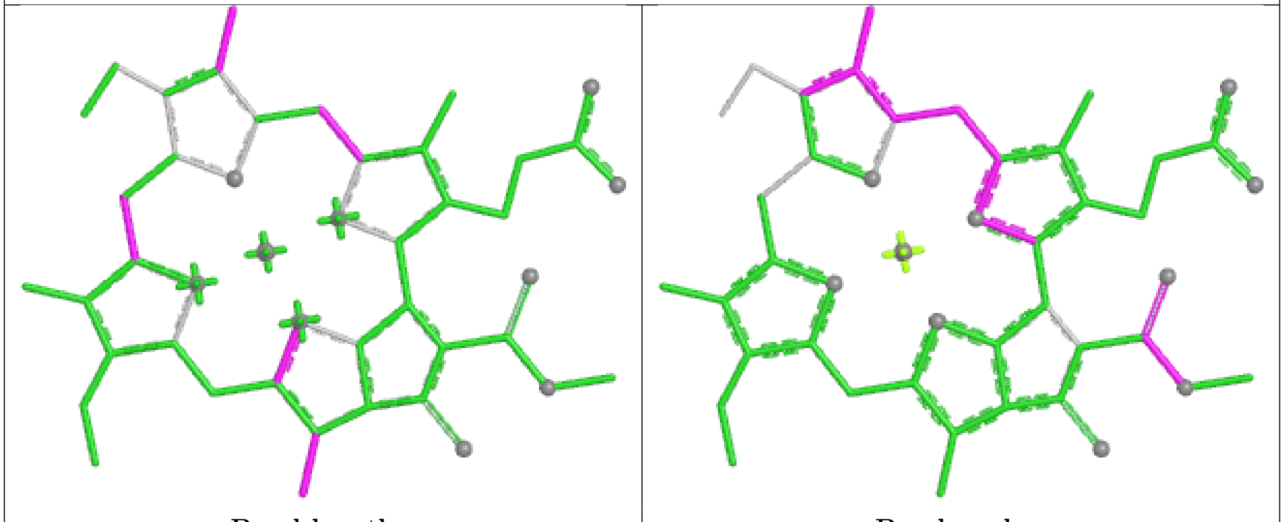
Bond angles



Torsions

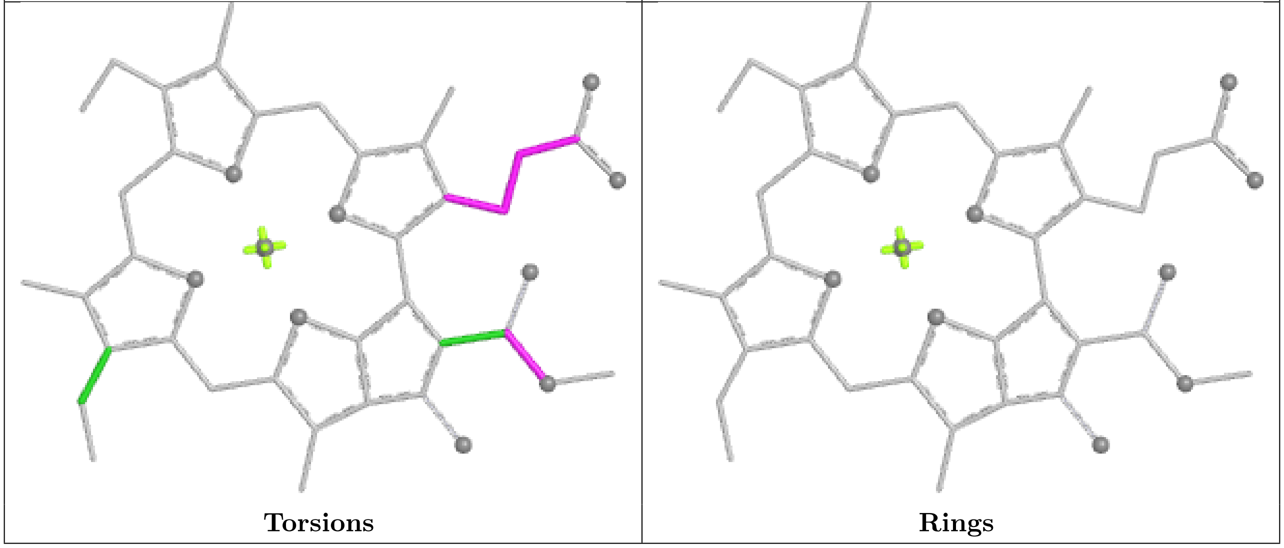
Rings

Ligand CLA H 2135



Bond lengths

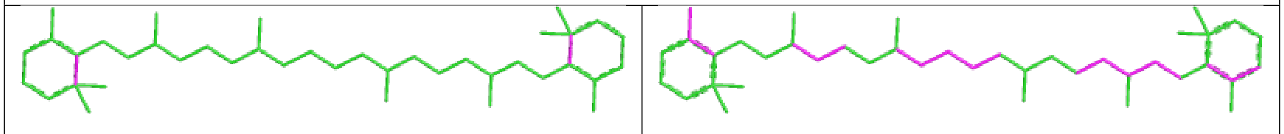
Bond angles



Torsions

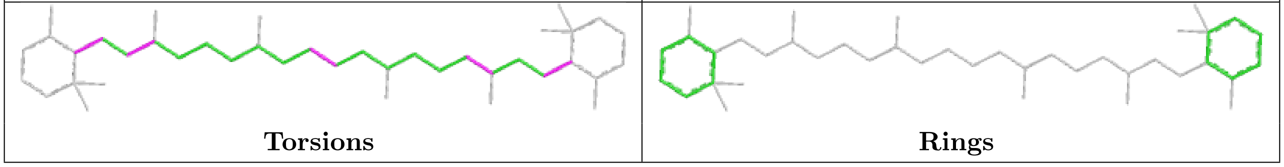
Rings

Ligand BCR S 104



Bond lengths

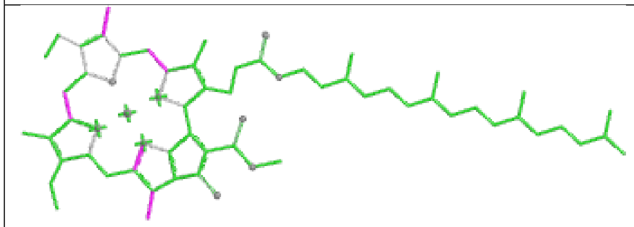
Bond angles



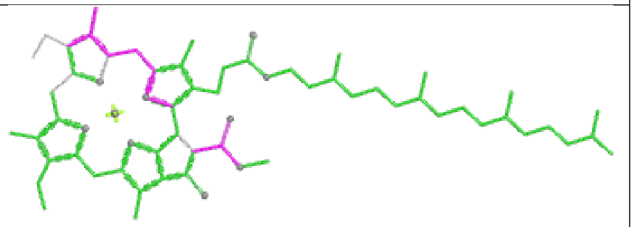
Torsions

Rings

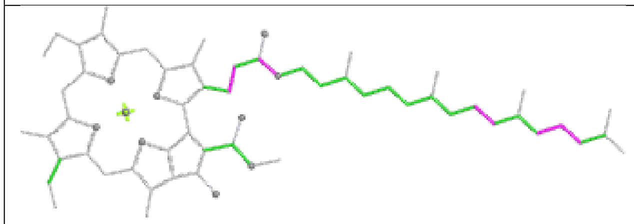
Ligand CLA U 205



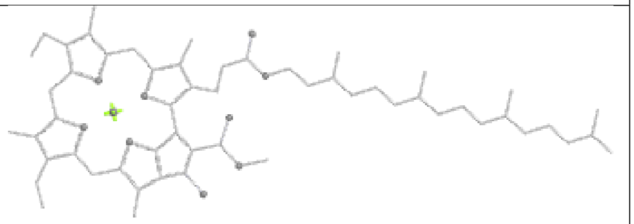
Bond lengths



Bond angles

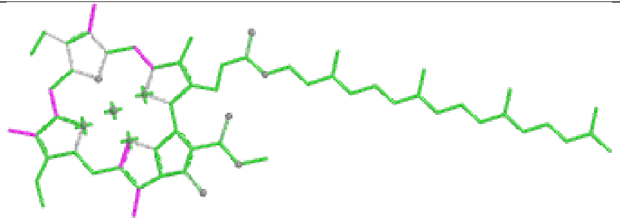


Torsions

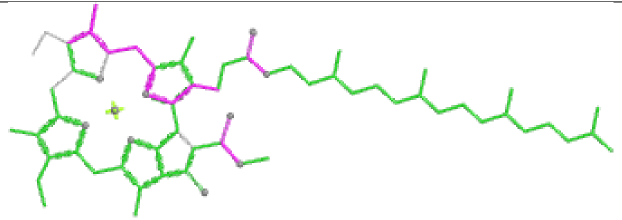


Rings

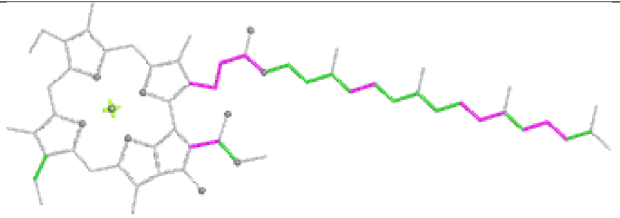
Ligand CLA A 807



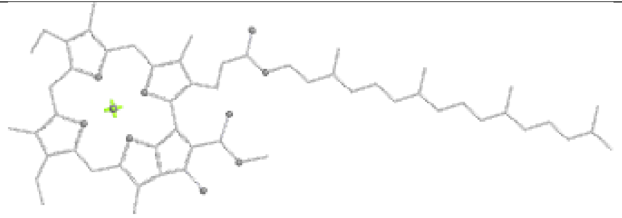
Bond lengths



Bond angles

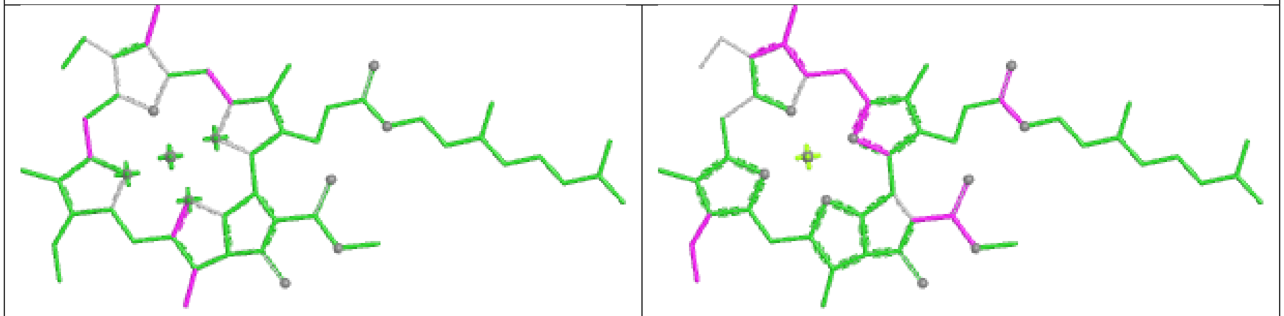


Torsions

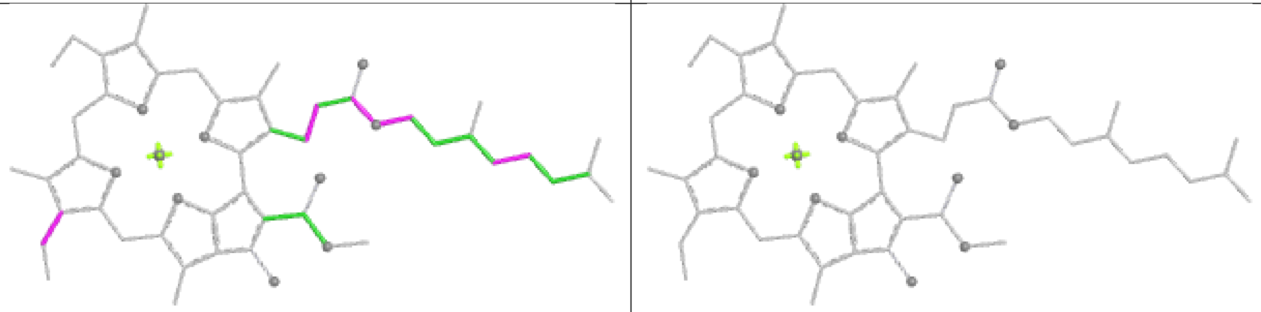


Rings

Ligand CLA G 830

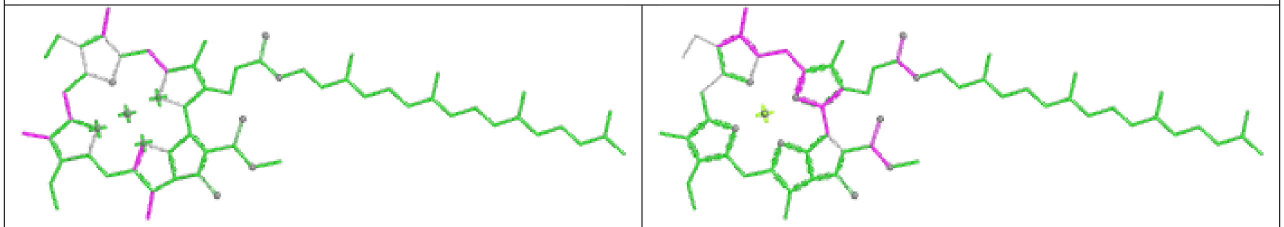


Bond lengths Bond angles

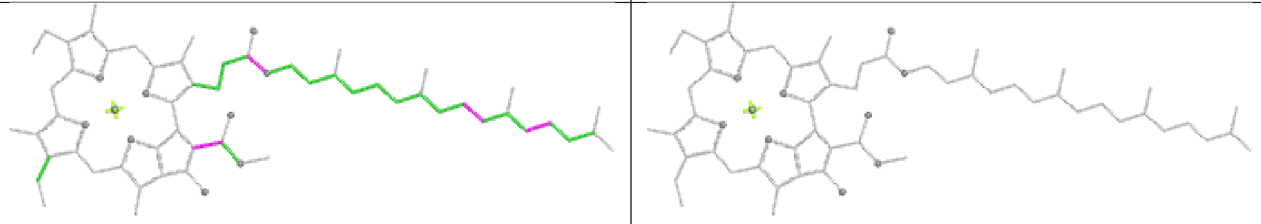


Torsions Rings

Ligand CLA H 2124

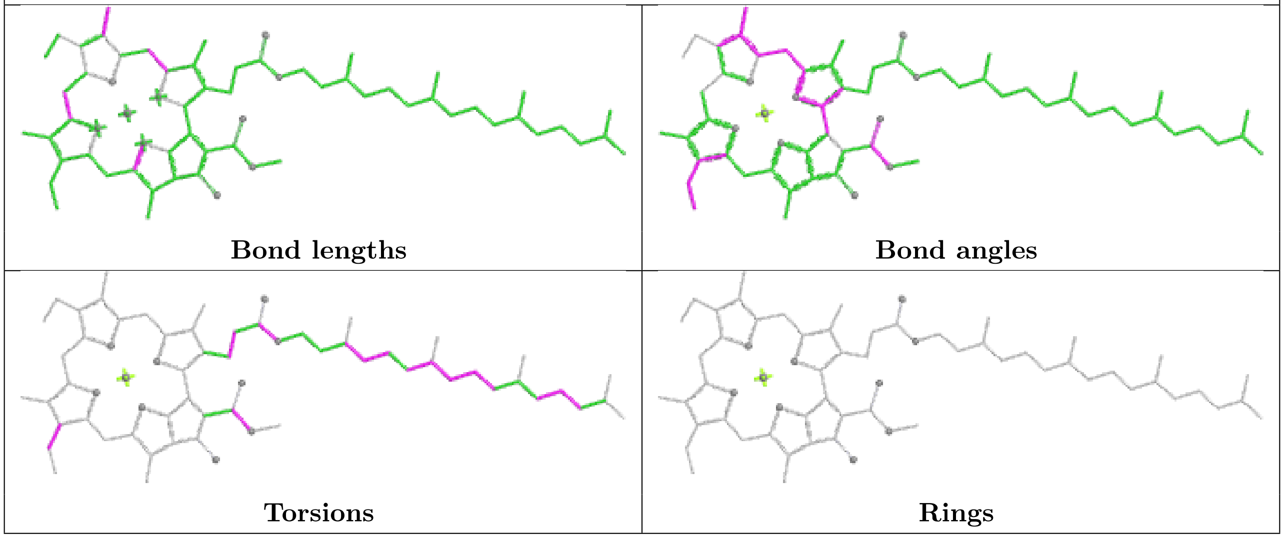


Bond lengths Bond angles



Torsions Rings

Ligand CLA B 2133



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

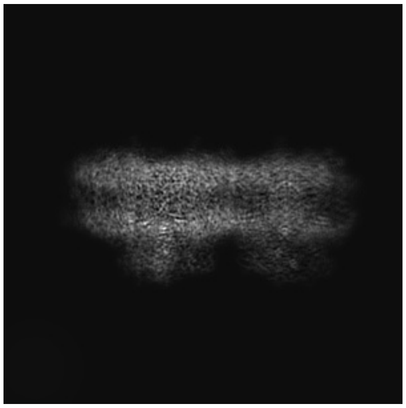
6 Map visualisation

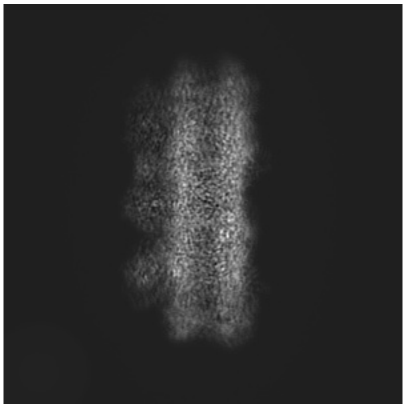
This section contains visualisations of the EMDB entry EMD-43843. These allow visual inspection of the internal detail of the map and identification of artifacts.

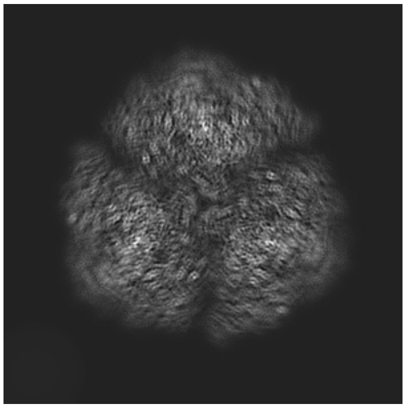
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

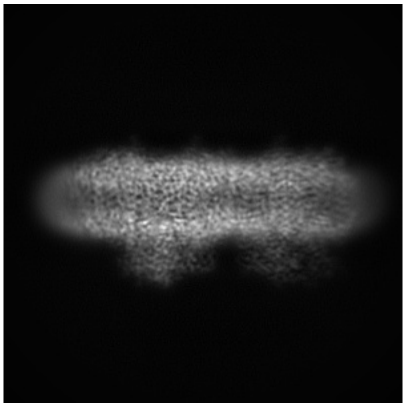
6.1.1 Primary map

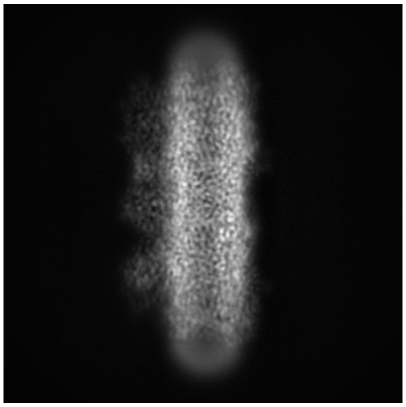

X

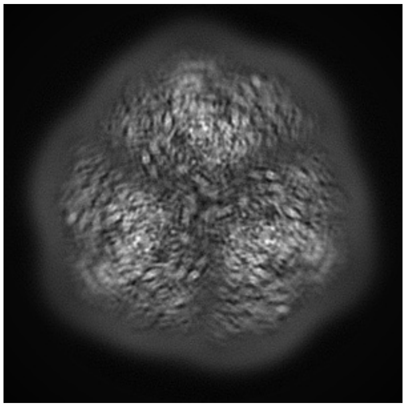

Y


Z

6.1.2 Raw map


X


Y


Z

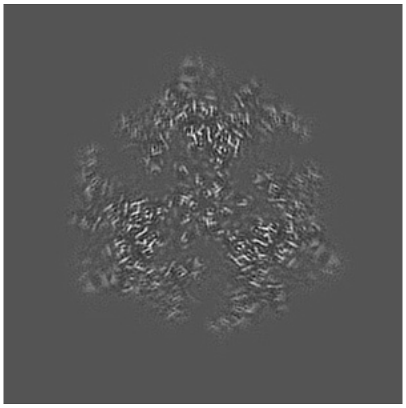
The images above show the map projected in three orthogonal directions.

6.2 Central slices

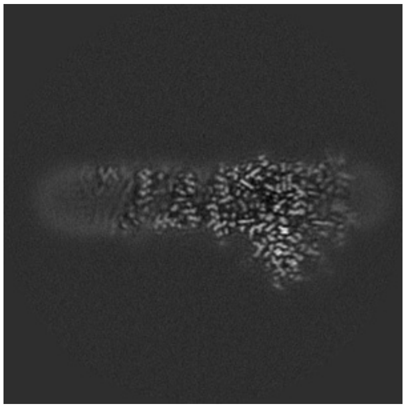
6.2.1 Primary map

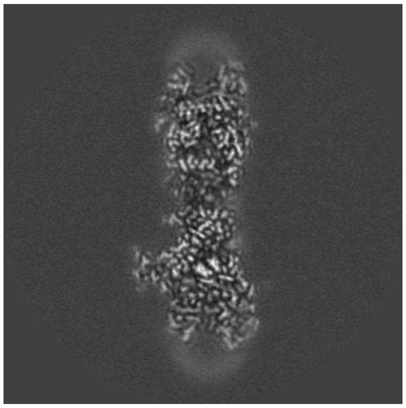

X Index: 160

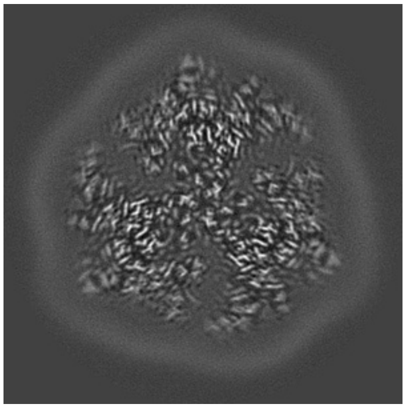

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160


Y Index: 160


Z Index: 160

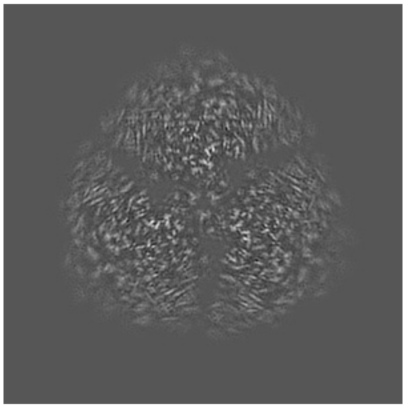
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map

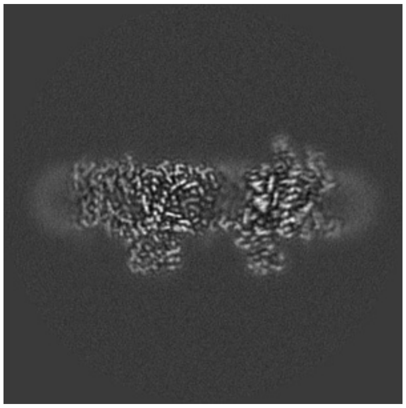
X Index: 107

Y Index: 128

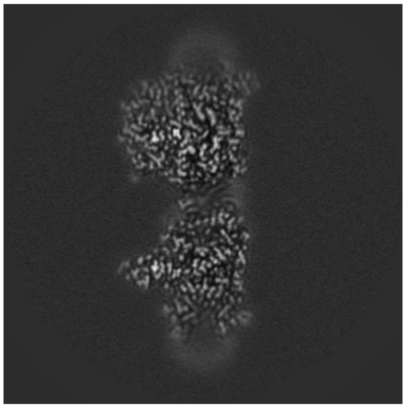


Z Index: 176

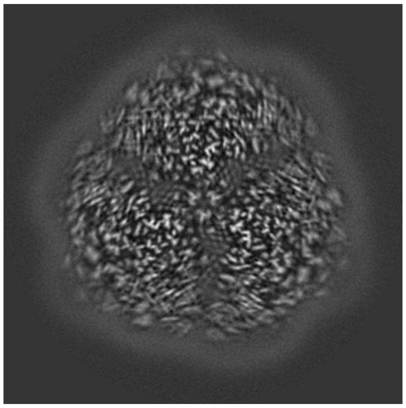
6.3.2 Raw map



X Index: 187



Y Index: 129

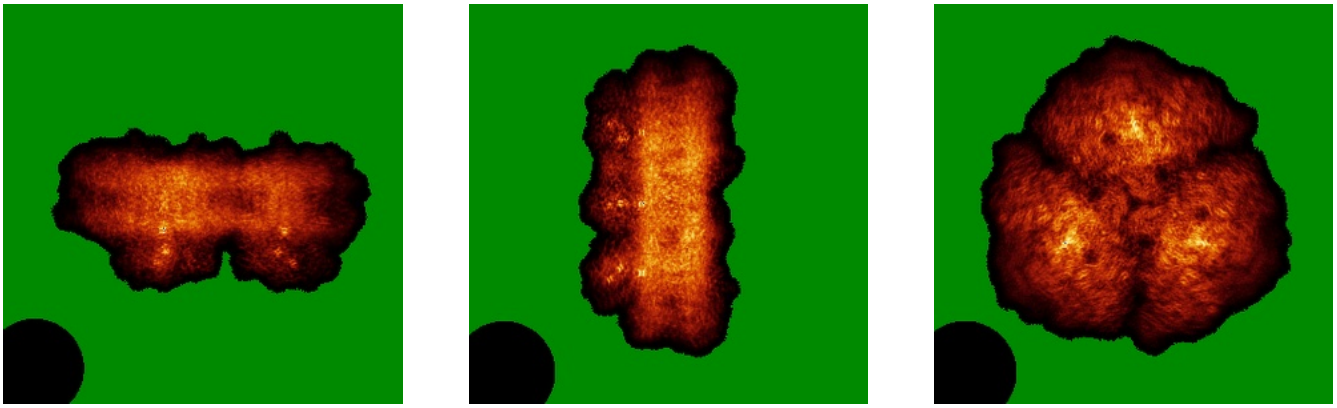


Z Index: 176

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

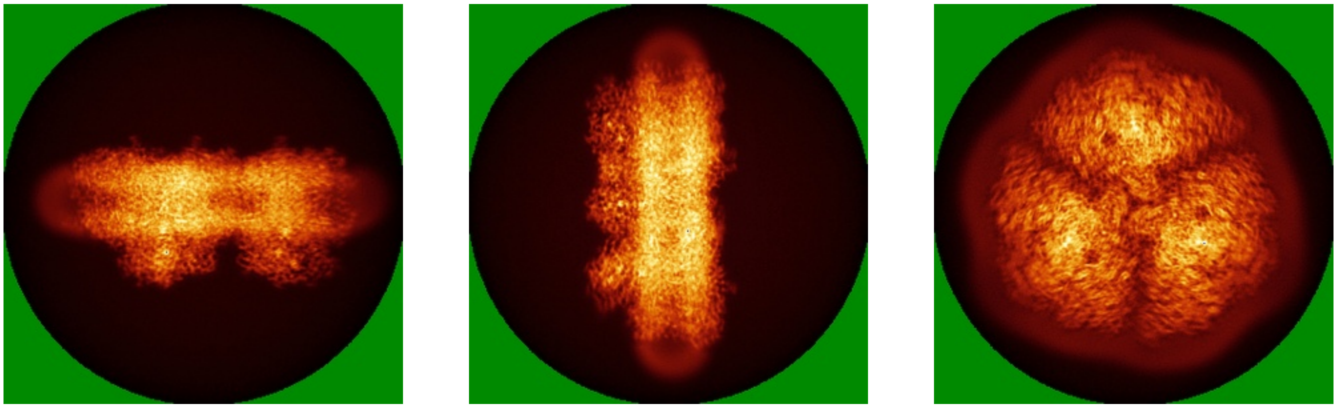
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

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 0.0149. 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.

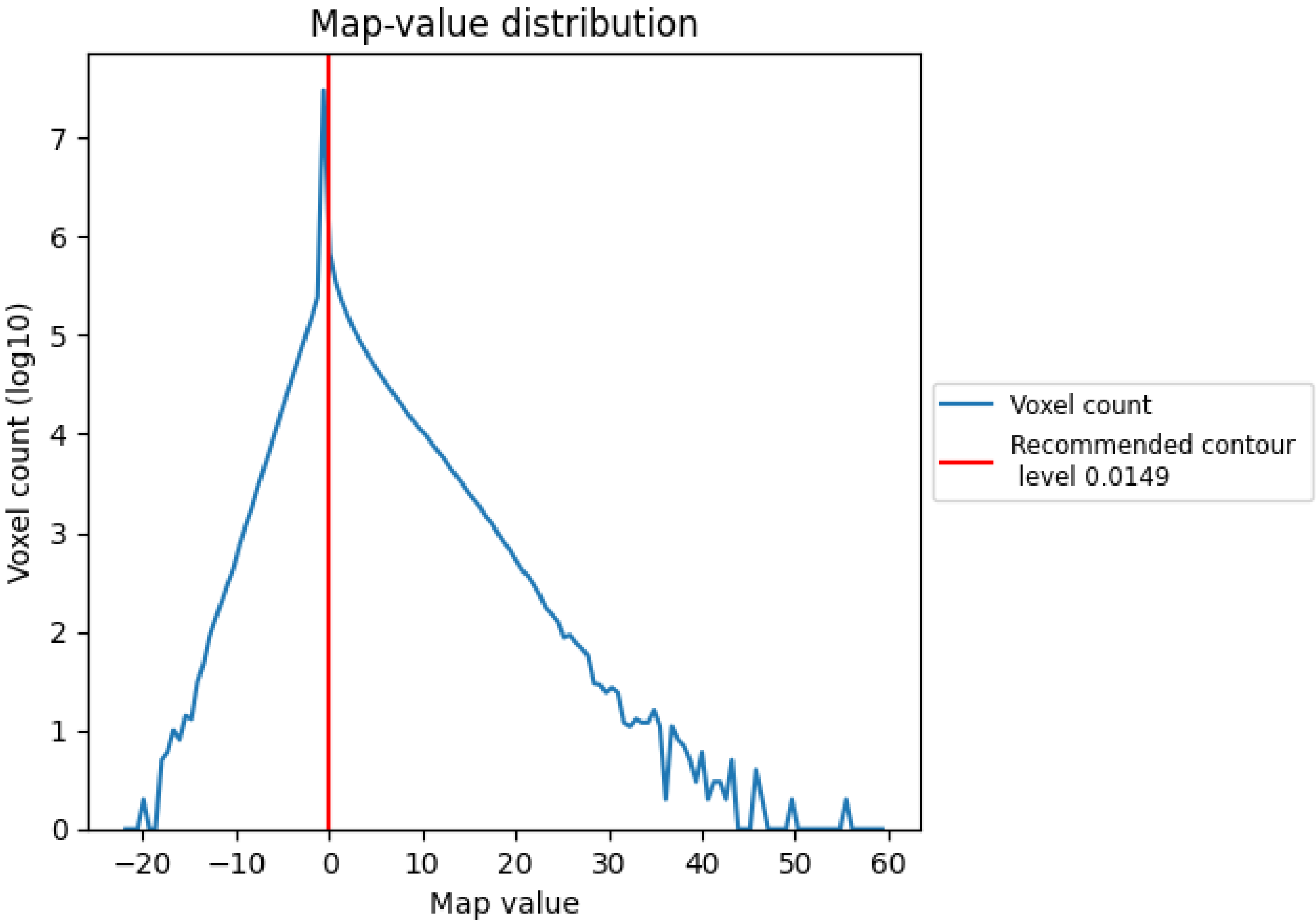
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

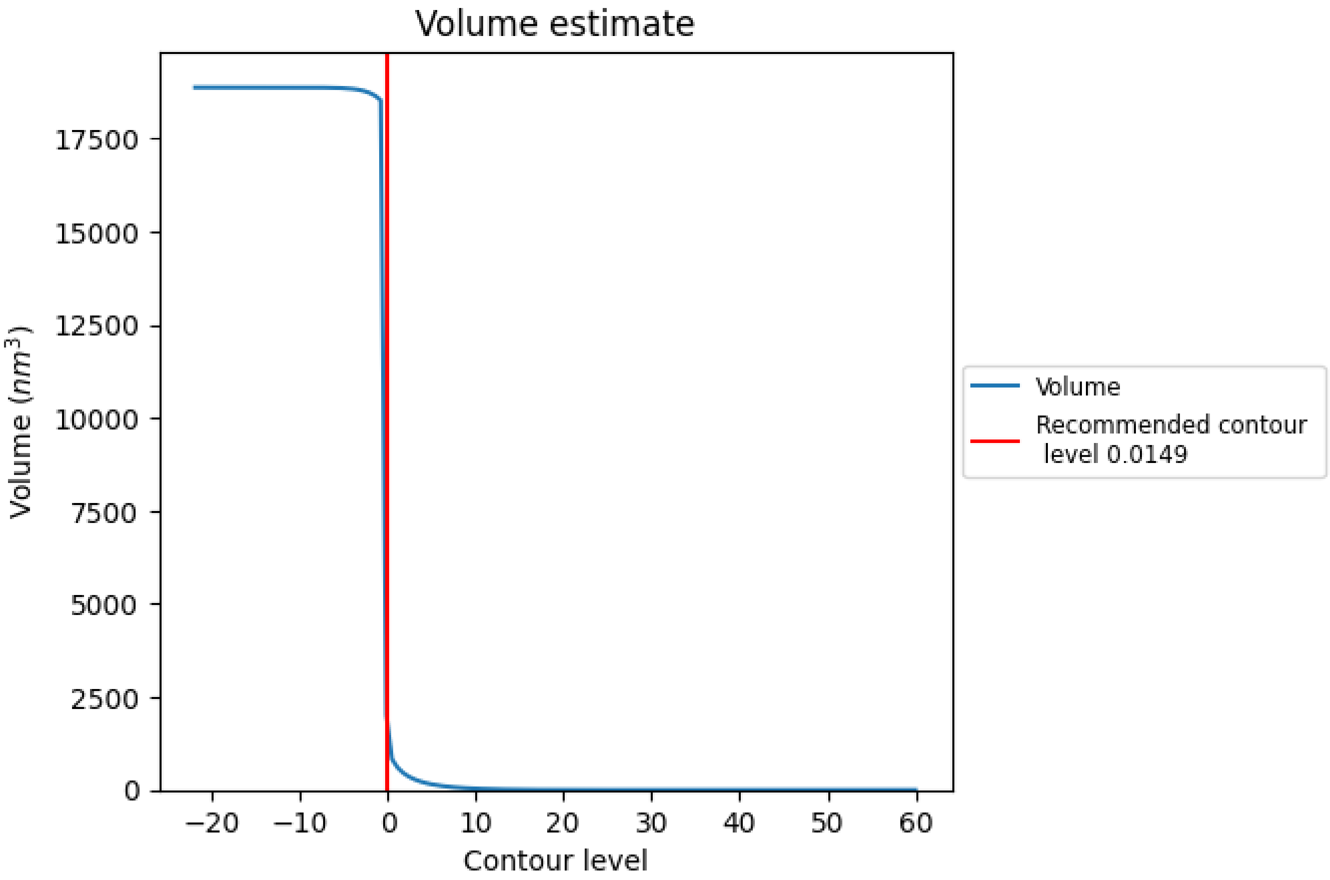
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

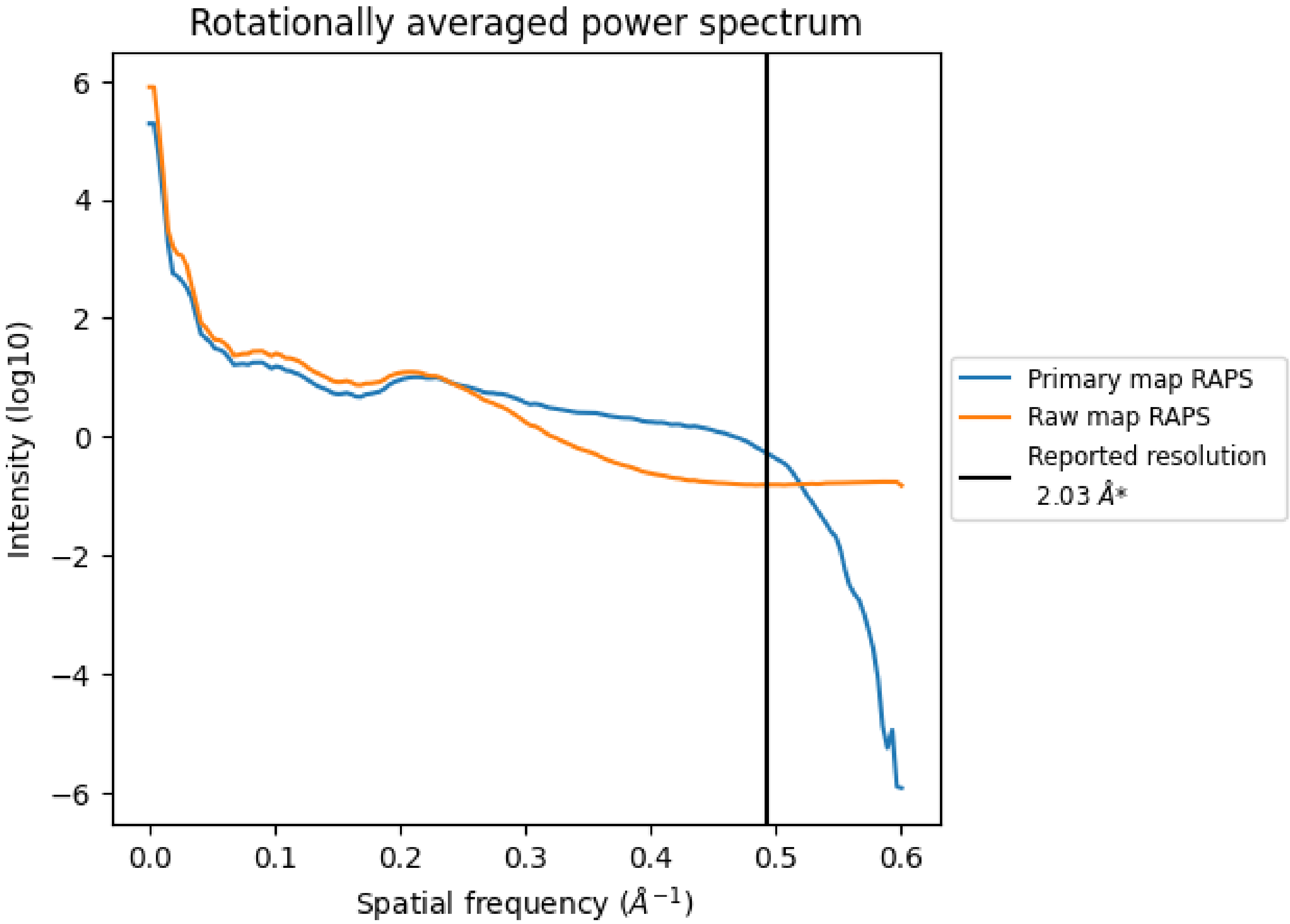
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1809 nm^3; this corresponds to an approximate mass of 1634 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 ⓘ

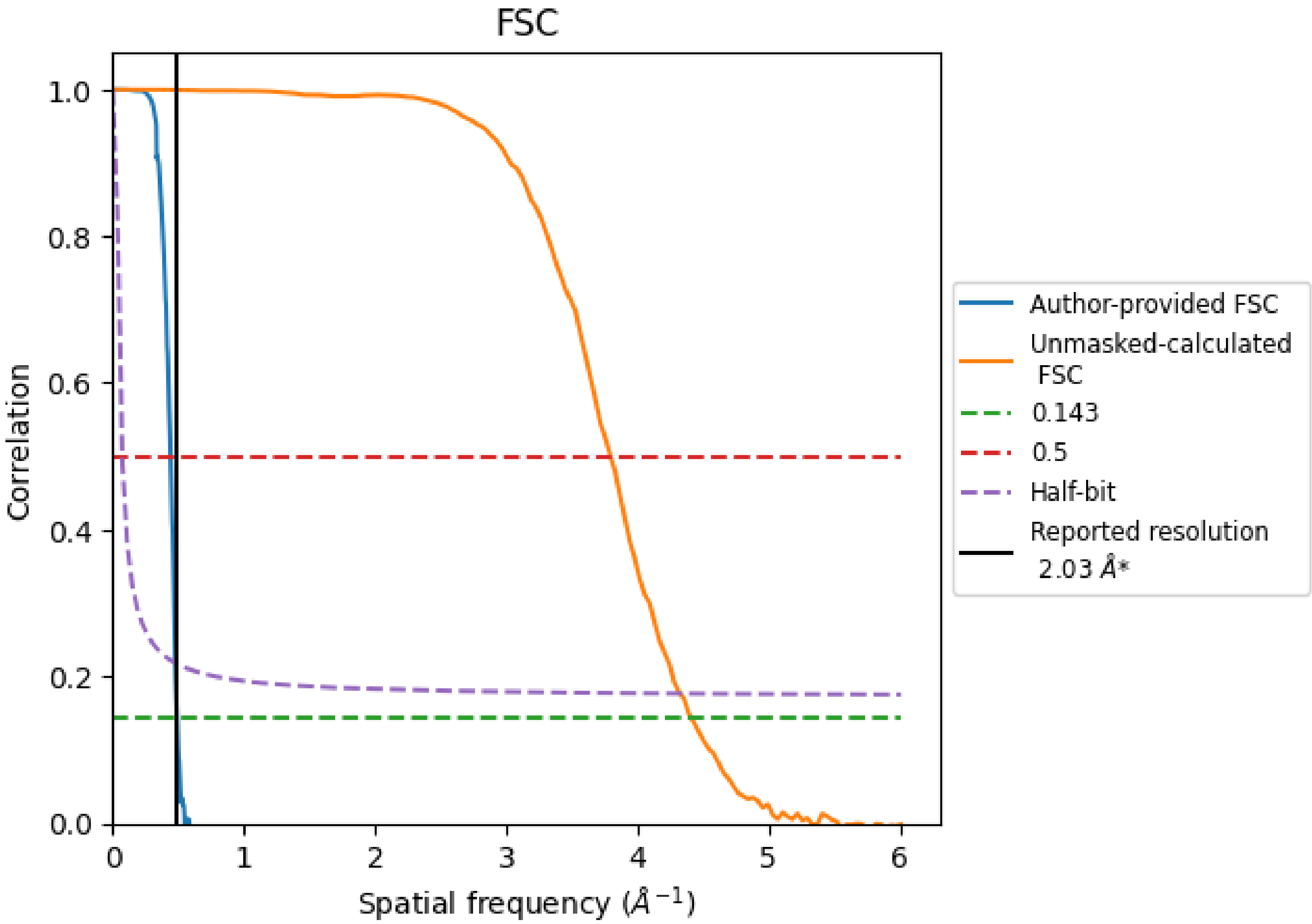


*Reported resolution corresponds to spatial frequency of 0.493 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.493 Å^{-1}

8.2 Resolution estimates ⓘ

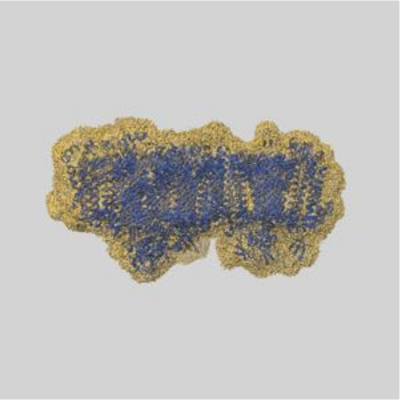
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.03	-	-
Author-provided FSC curve	2.03	2.26	2.06
Unmasked-calculated*	0.23	0.26	0.23

*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 0.23 differs from the reported value 2.03 by more than 10 %

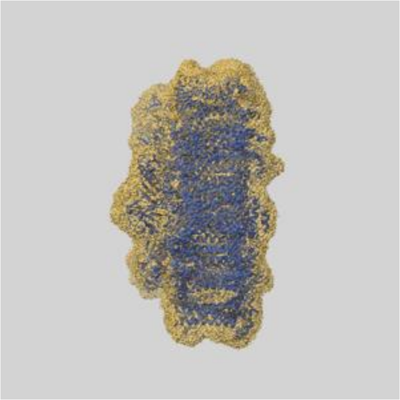
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43843 and PDB model 9AU4. Per-residue inclusion information can be found in section 3 on page 42.

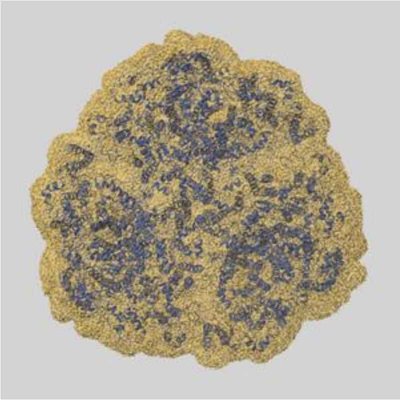
9.1 Map-model overlay



X



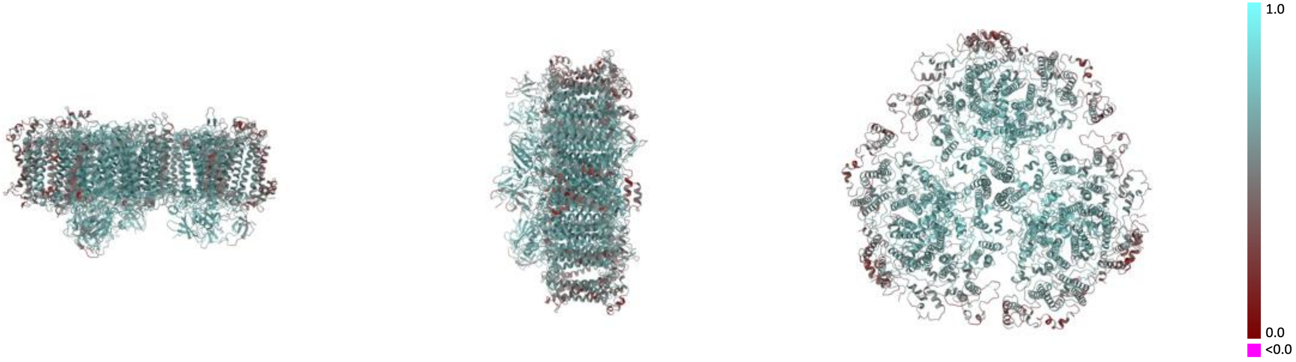
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

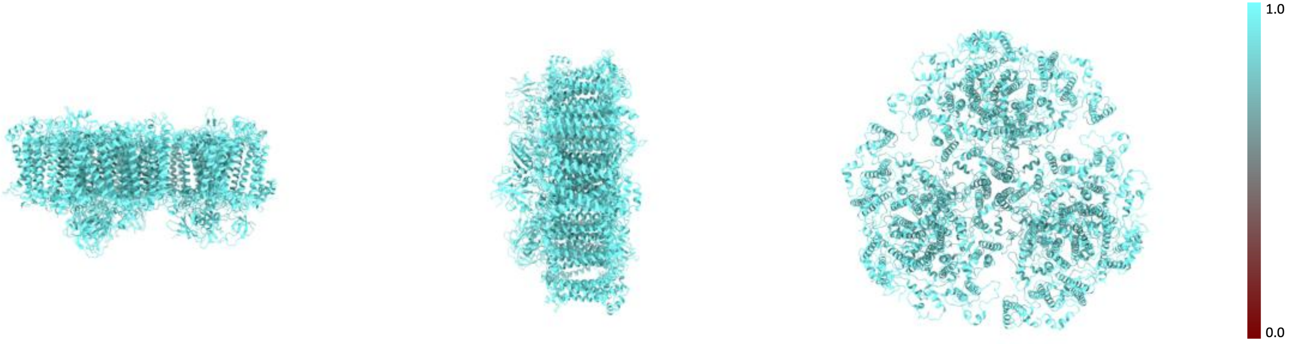
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

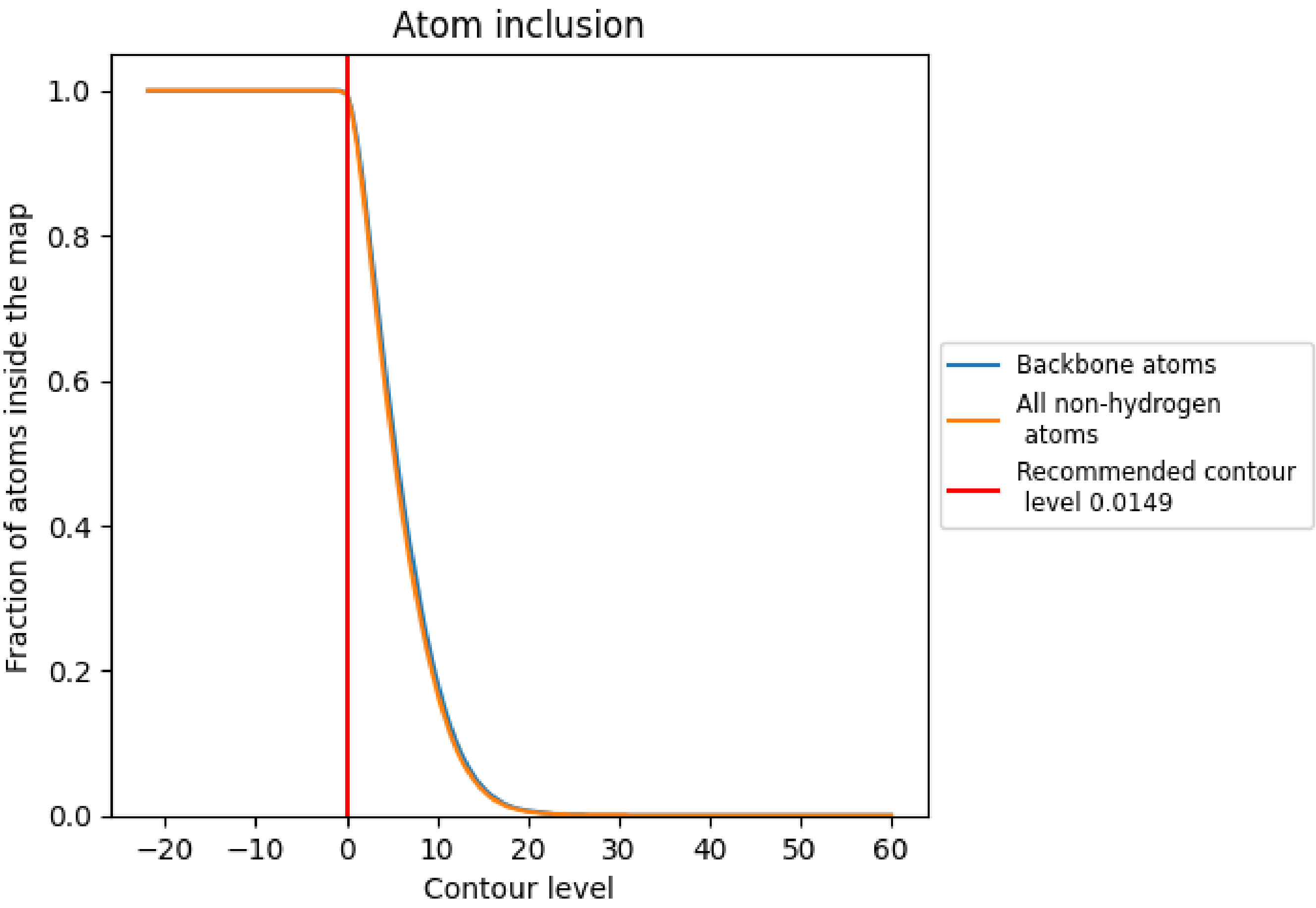
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0149).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9950	0.6100
A	0.9960	0.6240
B	0.9960	0.6230
C	0.9970	0.7170
D	1.0000	0.6860
E	0.9940	0.5800
F	0.9880	0.4410
G	0.9950	0.6180
H	0.9960	0.6180
I	1.0000	0.6990
J	0.9870	0.3880
K	0.9860	0.4140
L	0.9990	0.6850
M	1.0000	0.6520
N	0.9980	0.7120
O	0.9990	0.6740
P	0.9850	0.5580
Q	0.9810	0.4280
R	0.9970	0.6950
S	0.9830	0.3800
T	0.9820	0.3930
U	0.9980	0.6810
V	1.0000	0.6530
a	0.9960	0.6200
b	0.9960	0.6190
c	0.9970	0.7150
d	1.0000	0.6820
e	0.9960	0.5720
f	0.9880	0.4310
i	1.0000	0.6950
j	0.9810	0.3820
k	0.9880	0.3970
l	0.9980	0.6810
m	1.0000	0.6510