Electronic Supporting Information for

On the Brassard's Rule of regioselectivity in Diels-Alder reactions between haloquinones and polar dienes

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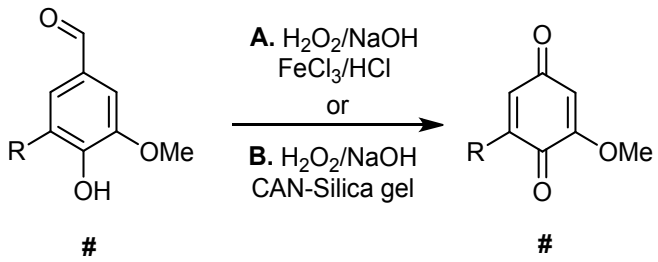
Contents	Page

Synthesis of 2-halo-6-metoxy-1,4-benzoquinones Q1-3:



**#**

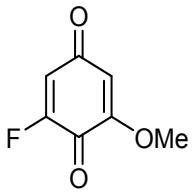
Method A. Oxidation with H_2O_2/$FeCl_3$

A solution of 5-halovainillin (1 mmol) in 4% aqueous NaOH (1.5 mL) was added to a solution of H_2O_2 (30%, 0.2 mL) in water (1.5 mL). Once reaction was over (20 to 30 min according to TLC monitoring), concentrated HCl (0.37 mL) was added, followed by $FeCl_3 \cdot 6H_2O$ (1.12 mmol) dissolved in a small volume of water.[1] The precipitate was filtered and recrystallized from methanol or purified by chromatography column.

Method B. H_2O_2/CAN-silica gel

A solution of 5-halovanillin (2 mmol) in 4% aqueous NaOH (3.0 mL) was added to a solution of H_2O_2 (30%, 0.4 mL) in water (3.0 mL). After the reaction was over, concentrated HCl (0.6 mL) was added and then filtered. Silica-gel supported CAN [2] (2.5 mmol-3 g) was prepared and suspended in 12 mL CH_2Cl_2. The solid hydroquinone (1 mmol) was dissolved in 1.25 mL of CH_2Cl_2 and added to the suspension. After the reaction was over (10 to 20 min according to TLC monitoring), the reaction mixture was filtered through celite and washed with 70 mL CH_2Cl_2. The filtrate was dried with anhydrous Na_2SO_4 and the solvent evaporated.

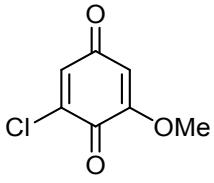
2-fluoro-6-methoxy-1,4-benzoquinone (**Q1**):



Q1

Obtained as a yellow solid and purified by column chromatography over silica gel using *n*-hexane/acetone (9:1), with a yield of 16% (Method **A**) and 28% (Method **B**) after flash chromatography. Recrystallized from acetone. **M.p.** 124.5-125.5; **^{1}H NMR** (400 MHz, $CDCl_3$). δ(ppm) 6.37 (dd, 1H, J=9.0, 2.3 Hz), 5.93 (d, 1H, J=2.2 Hz), 3.86 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ(ppm) 185.9 (C-4, C=O), 174.4 (C-1, C=O), 160.2 (C-F), 157.7 (C-6, C-O), 115.2 (C-3), 107.8 (C-5), 56.99 (OCH_3) ppm; **^{19}F NMR** (282 MHz, $CDCl_3$) δ(ppm) -116.32 ppm; **GC-MS:** m/z 156 (M^+); **IR (ATR).** υ(cm^{-1})= 1784, 1699, 1660, 1629, 1601, 1458, 1441, 1392, 1376; **Elem. Anal.:** Calculated for $C_7H_5FO_3$: C: 53.86; H: 3.23; F: 12.17; O, 30.75; found: C, 53.90; H, 2.95.

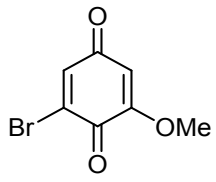
2-chloro-6-methoxy-1,4-benzoquinone (**Q2**):



Q2

Obtained as a yellow solid and purified by column chromatography over silica gel using CH_2Cl_2/MeOH (9:1), with a yield of 50% (for Method **A**) and 92 % (for Method **B**) after flash chromatography. **m.p.** 158.9-159.9 °C (MeOH) (lit.[5] m.p. = 155-157 °C); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.91 (d, 1H, J=2.3 Hz, H-3), 5.95 (d, 1H, J=2.2 Hz, H-5), 3.84 (s, 3H, OCH_3) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 184.67 (C-4, C=O), 174.71 (C-1, C=O), 158.76 (C-6), 141.67 (C-Cl), 133.07 (C-3), 107.79 (C-5), 56.25 (OCH_3) ppm.

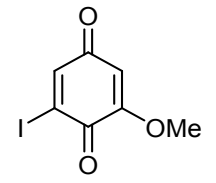
2-bromo-6-methoxy-1,4-benzoquinone (**Q3**)**:**



Q3

Obtained as a yellow-orange solid and purified by column chromatography over silica gel using CH_2Cl_2/MeOH (9:1), with a yield of 59% (for Method **A**) and 95 % (for Method **B**) after flash chromatography. **M.p** 162.0-163.0 °C (MeOH) (lit.[1] m.p. = 161-162 °C); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.21 (d, 1H, *J*=2.3 Hz, H-3) 5.96 (d, 1H *J*=2.2 Hz, H-5), 3.85 (s, 3-H, OCH_3) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 184.35 (C-4, C=O), 174.26 (C-1, C=O), 157.99 (C-6), 138.21 (C-3), 134.00 (C-Br), 107.36 (C-5), 56.53 (OCH_3) ppm.

Synthesis of 2-iodo-6-methoxy-1,4-benzoquinone(**Q4**)**:**

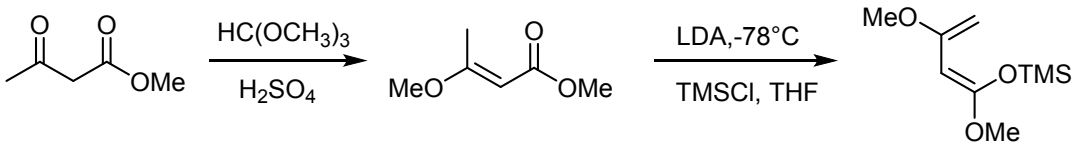


Q4

NaI (416 mg, 2.77mmol) was added to a solution of **Q3** (500 mg, 2.31 mmol) in glacial acetic acid (40 mL), the mixture was stirred at a temperature between 50-60 ° C (under nitrogen and protected from light). After 3 days a second addition of NaI (416 mg, 2.77 mmol) was made under the same conditions. The reaction was cooled and the solvent was evaporated. The residue was dissolved in CH_2Cl_2 (50 mL) and washed with water (2 x 25 mL). The aqueous phases were combined and extracted with CH_2Cl_2 (2 x 25 mL). The organic phases were combined and washed with a saturated $NaHCO_3$ solution (1 x 150 mL), a solution of 10% $Na_2S_2O_3$ (1 x 30 mL) and a saturated NaCl solution (1 x 150 mL), dried with anhydrous Na_2SO_4 and evaporated. The residue was purified by flash chromatography eluted with a hexane:acetone (9:1) system. The product obtained had a 2_I :1_{Br} proportion according to ^{1}H NMR and was obtained as a reddish

yellow solid. **M.p.**: 146.1-146.7 °C (Acetone). **^{1}H NMR** (400 MHz, $CDCl_3$) δ(ppm) 7.55 (d, 1H, J=2.3 Hz, H-3), 5.96 (d, 1H J=2.07 Hz, H-5), 3.84 (s, 3H, OCH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ(ppm) 185.03 (C-4, C=O), 175.60 (C-1, C=O), 157.01 (C-6), 146.81 (C-3), 115.16 (C-I), 107.79 (C-5), 56.82 (OCH_3); **GC-MS:** m/z 264 (M^+).

Procedure for the synthesis of Brassard's diene:



Methyl acetoacetate **2** **Brassard's diene**

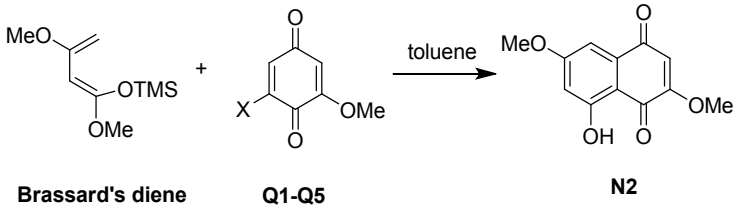
(*E*)-3-Methoxy-2-butenoic acid methyl ester (**2**): A solution of methyl acetoacetate (10.7 g, 92.6 mmol) and trimethyl orthoformate (9.8 g, 92.6 mmol) was cooled to 0°C, and concentrated H_2SO_4 (0.16 mL) was added dropwise. The solution was stirred at room temperature for 24 h, filtered over K_2CO_3 and distilled under reduced pressure (100 ° C, 80 mmHg) affording ester **2** (8.4 g, 70%)[4] as a colorless oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ(ppm): 5.01 (s, 1-H), 3.66 (s, 3-H), 3.62 (s, 3-H), 2.28 (s, 3-H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ(ppm): 173.39 (C-3), 168.45 (C=O), 90.57 (C-2), 55.52 (O-CH_3), 50.88 (OCH_3), 19.01 (CH_3).

(*Z*)-1,3-dimethoxy-1-[(trimethylsilyl)oxi]-1,3-butadiene (**Brassard's diene**): A solution of diisopropylamine (8.5 mL, 60.6 mmol) in anhydrous THF (50 mL) was cooled to -78 °C under nitrogen, and *n*-butyllithium (2.1M in hexane, 28 mL, 59 mmol) was added dropwise over 10 min. The yellow solution was stirred for 30 min. Ester **2** (5.85 g, 44 mmol) was added slowly to the solution, and kept at -78°C for 30 min more. Freshly distilled TMSCl solution (10 mL, 79 mmol) was slowly added and stirred for 10 min at -78 ° C. After this time, the reaction mixture was gradually brought to room temperature while stirring for 1 h. The mixture was diluted with hexane (50 mL) and filtered through celite three times. The filtrate was concentrated to a yellow oil which was distilled under reduced pressure (5 mmHg, 70 ° C). Diene was obtained as a clear oil (5.55 g, 61%) and stored under nitrogen

in cold.[4] **^{1}H NMR** (300 MHz, $CDCl_3$) δ(ppm): 4.34 (d, 1H, J=1.8Hz), 4.03 (d, 1H, J=1.5Hz), 3.98 (t, 1H, J=1.6Hz) 3.57 (s, 3H), 3.56 (s, 3H) 0.25 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ(ppm): 158.86 (C-1, C-3), 78.71 (C-4), 75.60 (C-2), 55.16 (OCH_3), 54.22 (OCH_3), 0.7 (3xCH_3).

Synthesis of naphthoquinone N2:

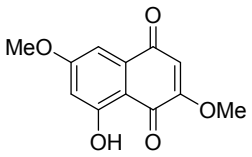
A solution of 2-halo-6-methoxy-1,4-benzoquinone (**Q1**-**Q4**) (100mg) and **Brassard's diene** (1.5 eq.) in 5 mL of toluene was refluxed for 0.3-2.5 h according to TLC monitoring. After the reaction was completed, the solvent was evaporated and the residue purified by flash chromatography. The products obtained were yellow-orange in color.



Scheme S1. Synthesis of naphtoquinone **N2.**

Table 1. Synthesis naphthoquinones: cycloaddition and aromatization.

X	Time (h)	Naphthoquinone	% R
F	2	**N2**	51
Cl	2.5	**N2**	60
Br	2	**N2**	71
I	0.3	**N2**	74



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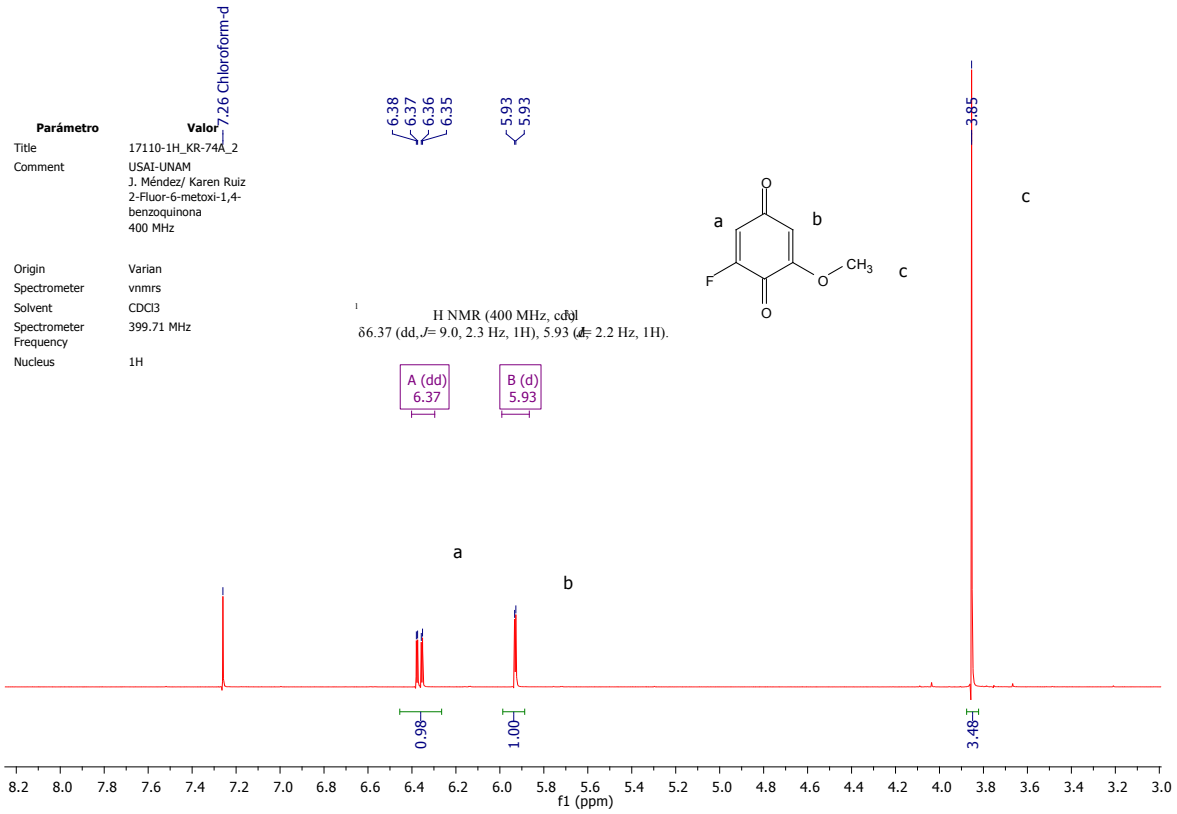
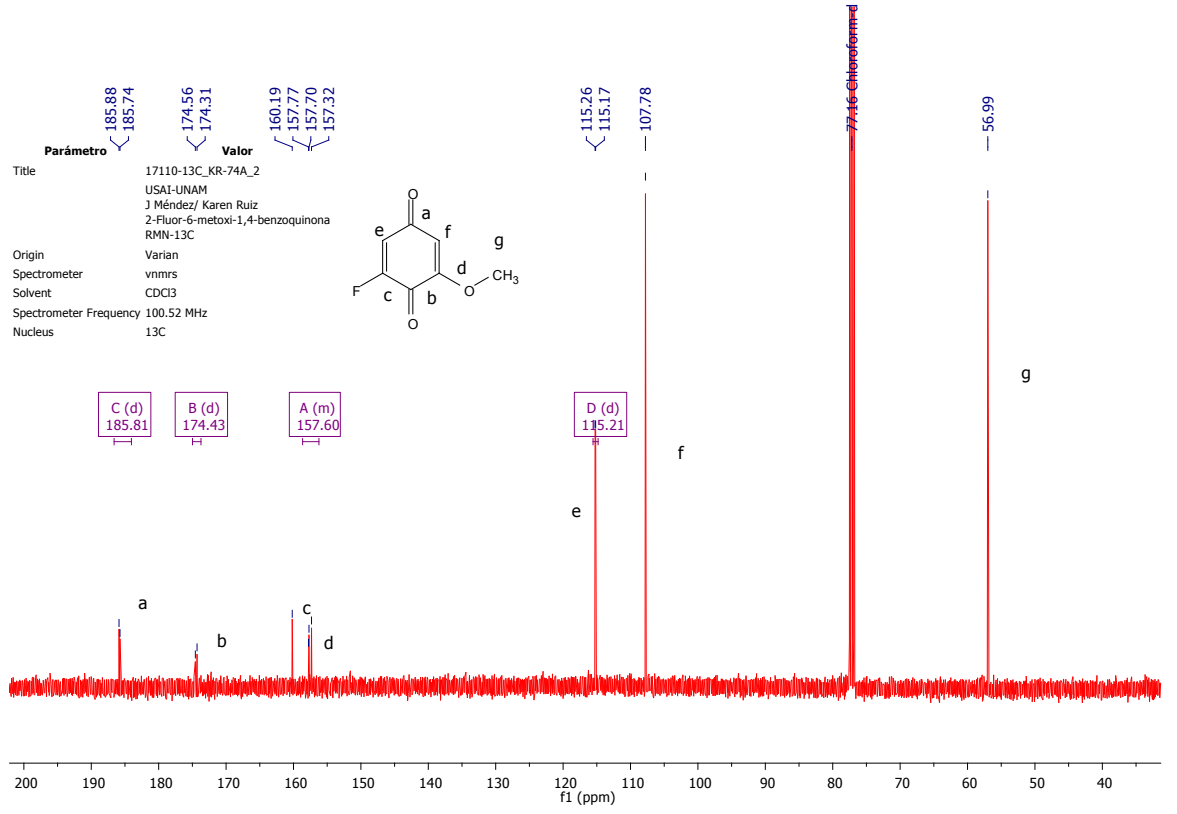
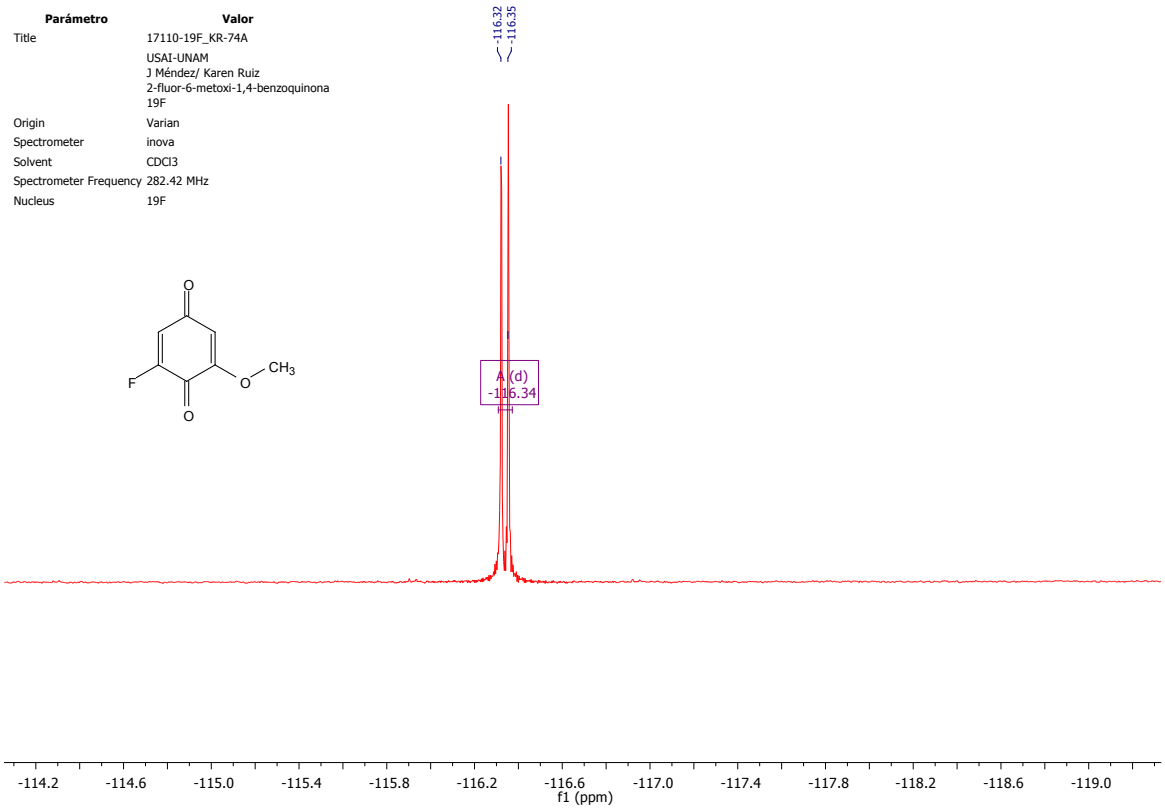
2,6-dimethoxy-8-hidroxy-1,4-naphthoquinone (N2): Obtained as a yellow-orange solid and purified by column chromatography over silica gel using CH_2Cl_2/MeOH (95:5) with a yield of 51-74 %R. **M.p.** 251.9-252.6 °C (MeOH); **^{1}H NMR** (400 MHz, $CDCl_3$) δ(ppm): 12.01 (s, 1H, -OH), 7.18 (d, 1H, J=2.5Hz, H-5), 6.61 (d, 1H, J=2.4 Hz, H-7), 6.09 (s, 1H, H-3), 3.91 (s, 3H, a), 3.90 (s, 3H, q); **^{13}C NMR** (100 MHz, $CDCl_3$) δ(ppm): 183.63, 182.66, 166.61, 164.77, 160.58, 133.63, 109.61, 108.65, 107.88, 105.23, 56.43, 55.95; **GC-MS:** m/z 234 (M^+); **IR (ATR).** υ=1639, 1615, 1595, 1579, 1389, 1319, 1234 cm^{-1}. **Anal. Calcd.** for $C_{12}H_{10}O_5$:C, 61.54; H, 4.30; O, 34.16; found: C, 53.90; H, 2.95.

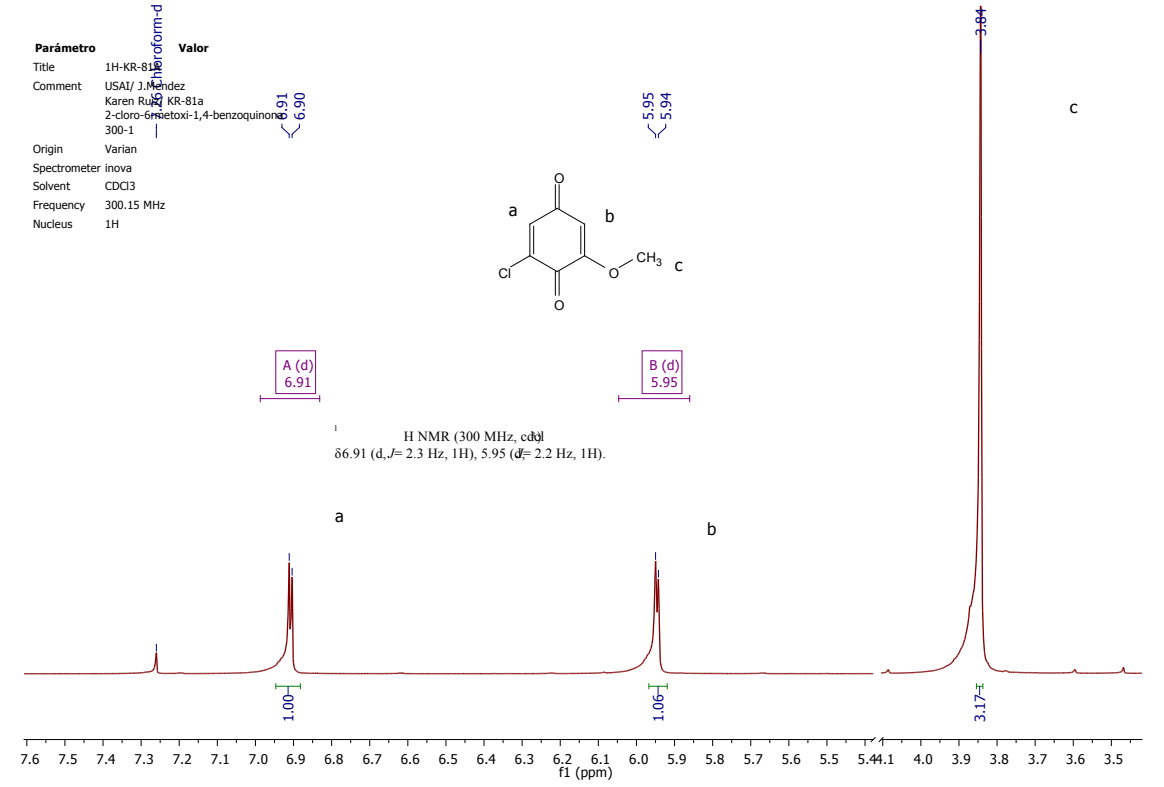
NMR Spectroscopy for compound Q1

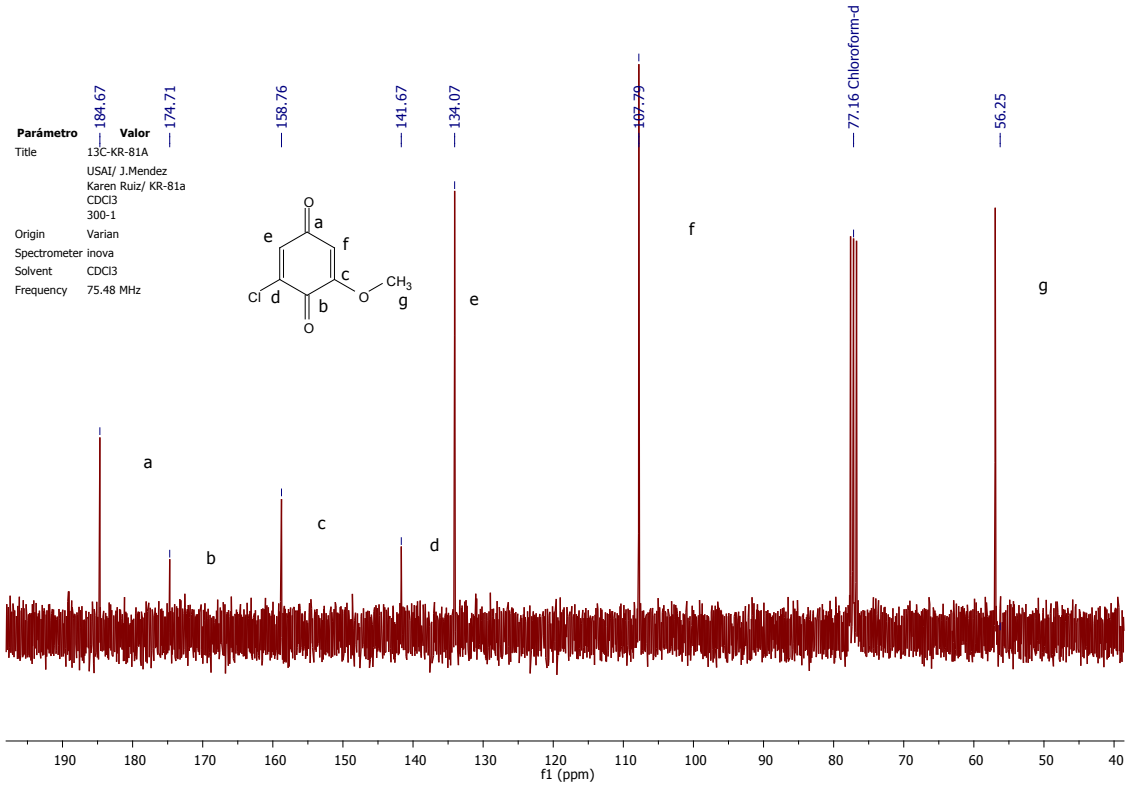




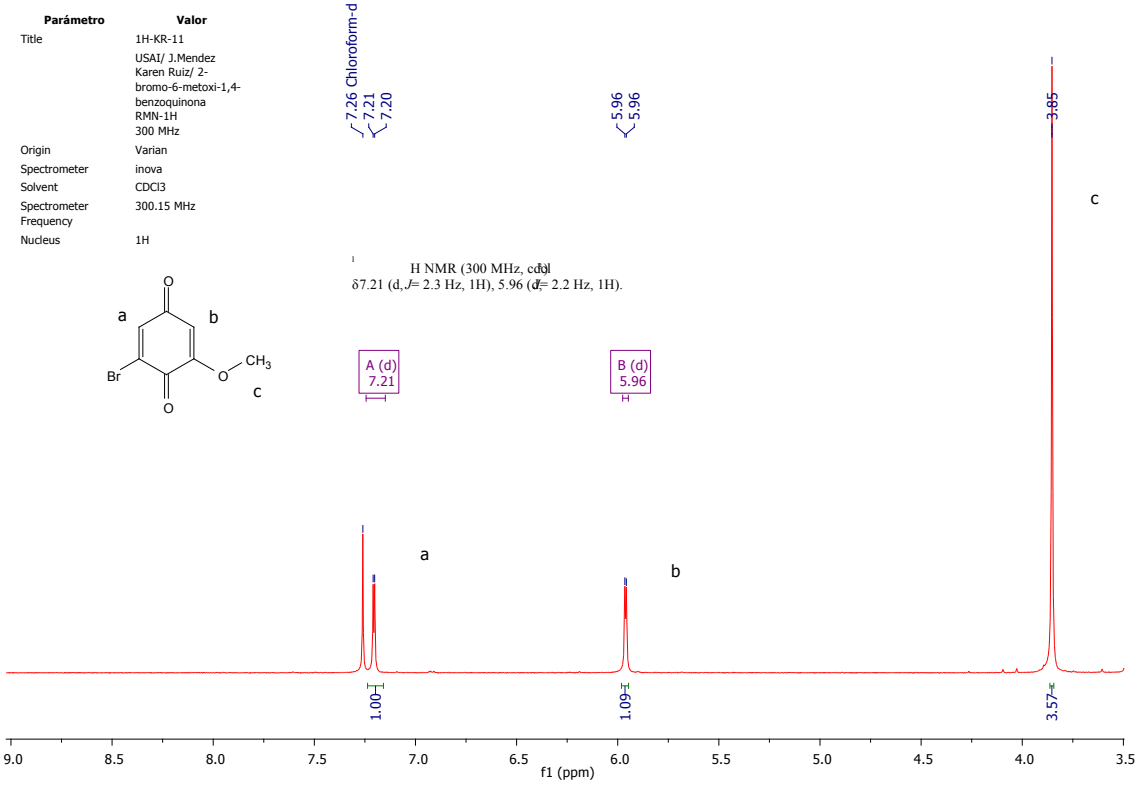


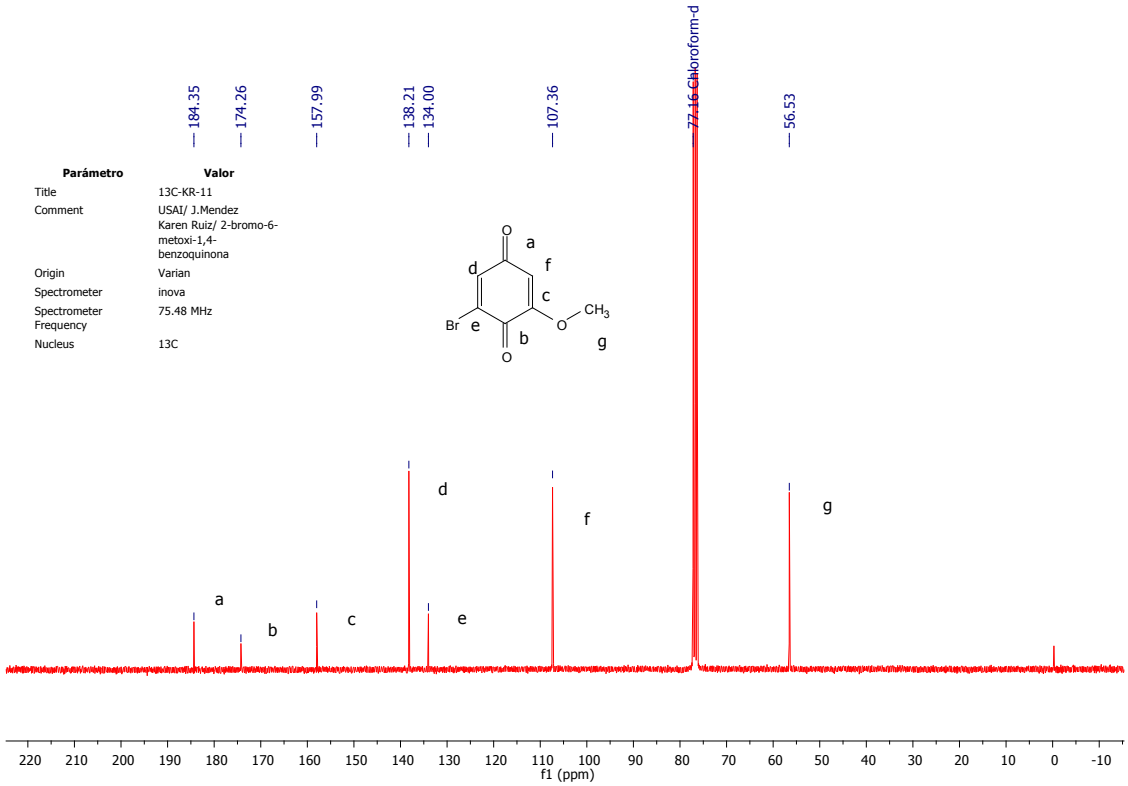
NMR Spectroscopy for compound Q2



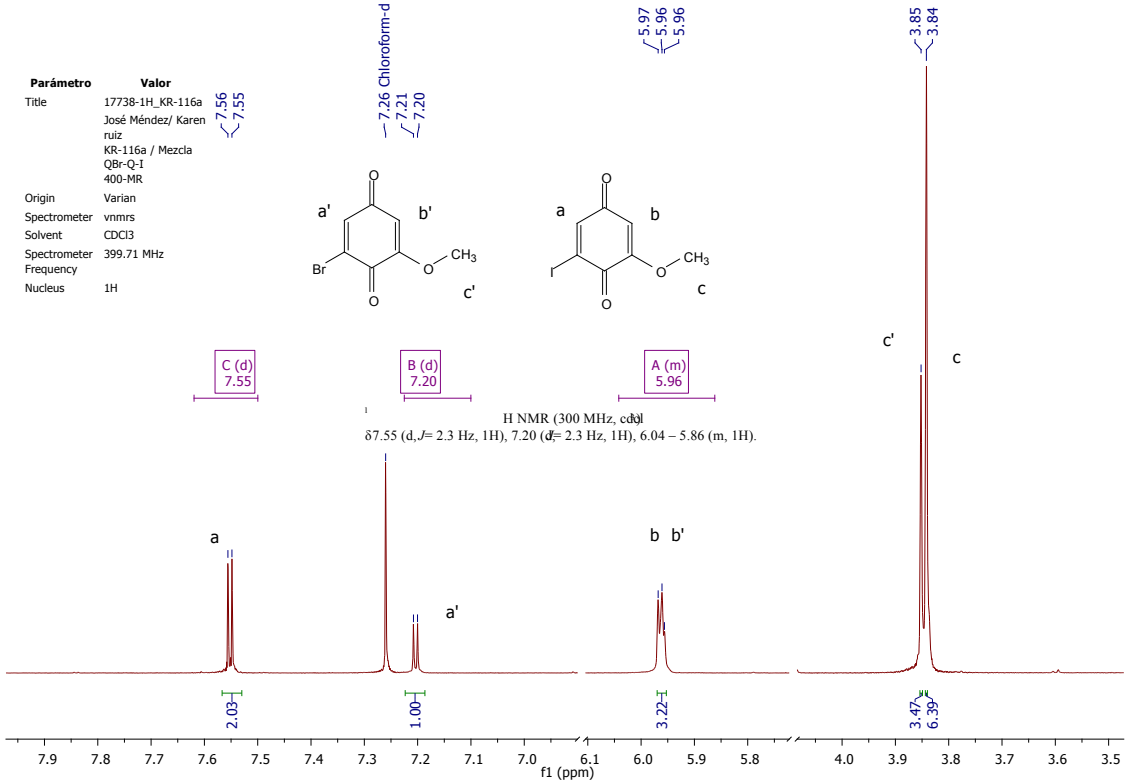


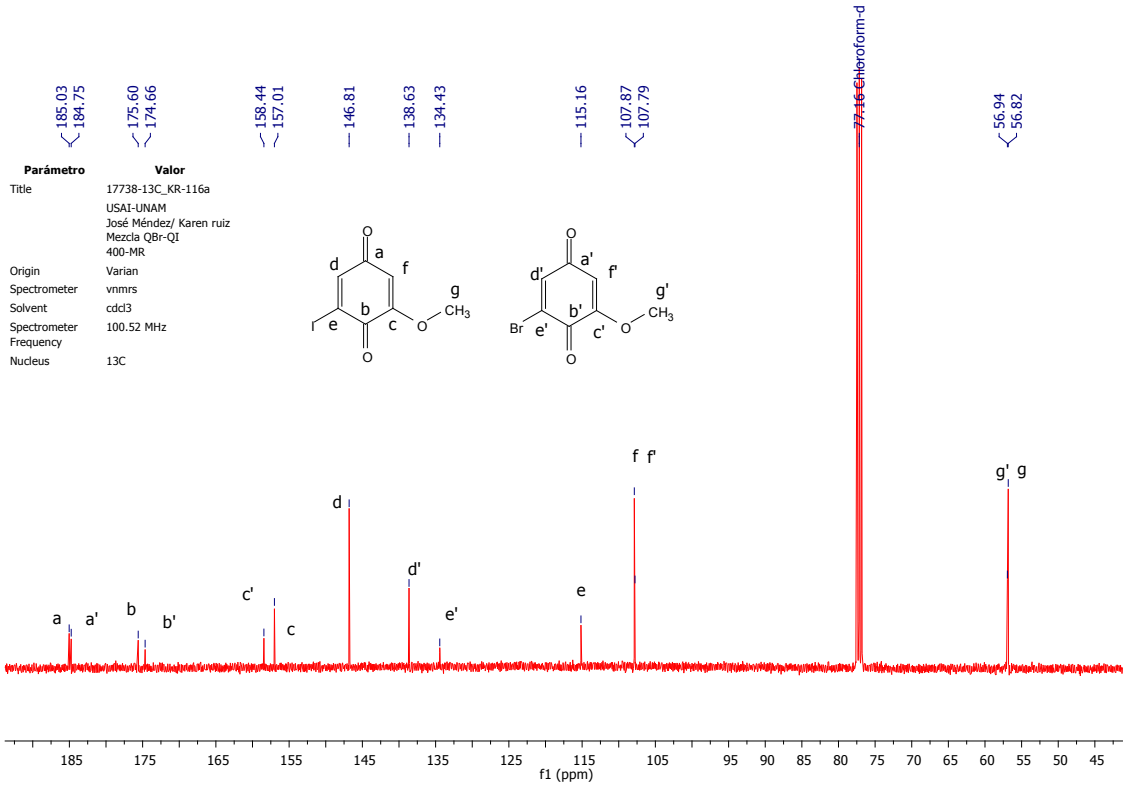
NMR Spectroscopy for compound Q3



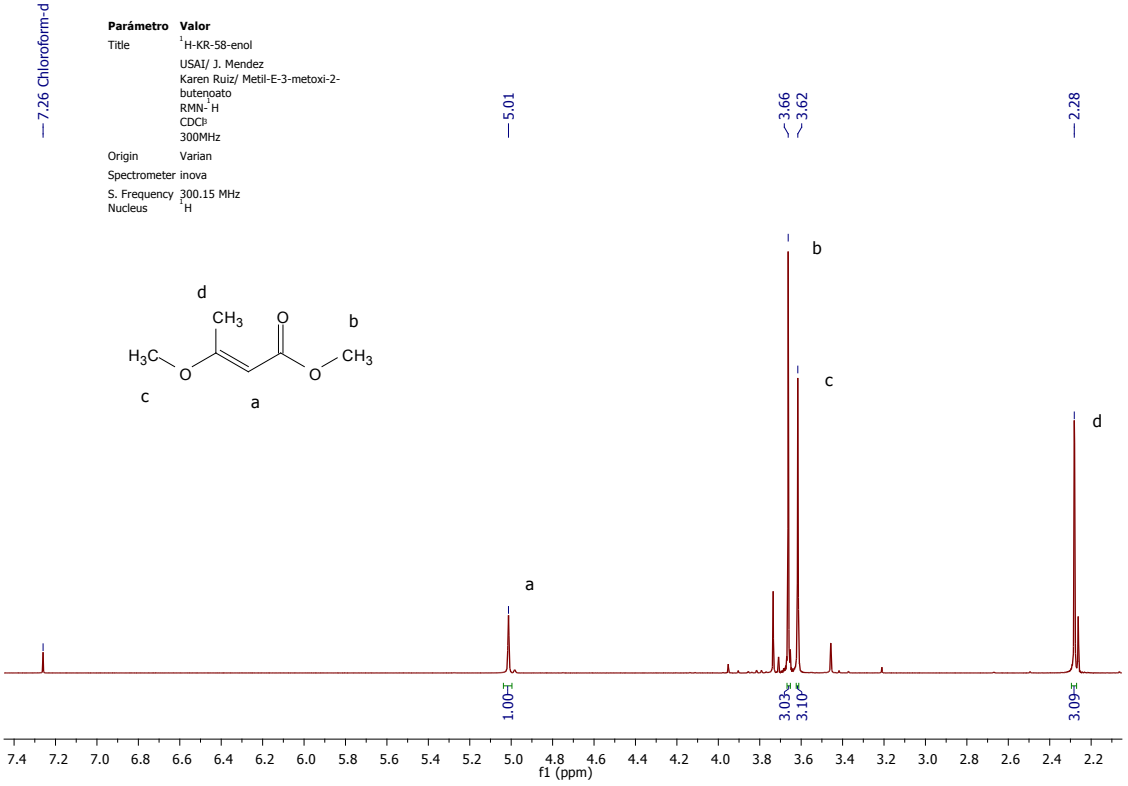


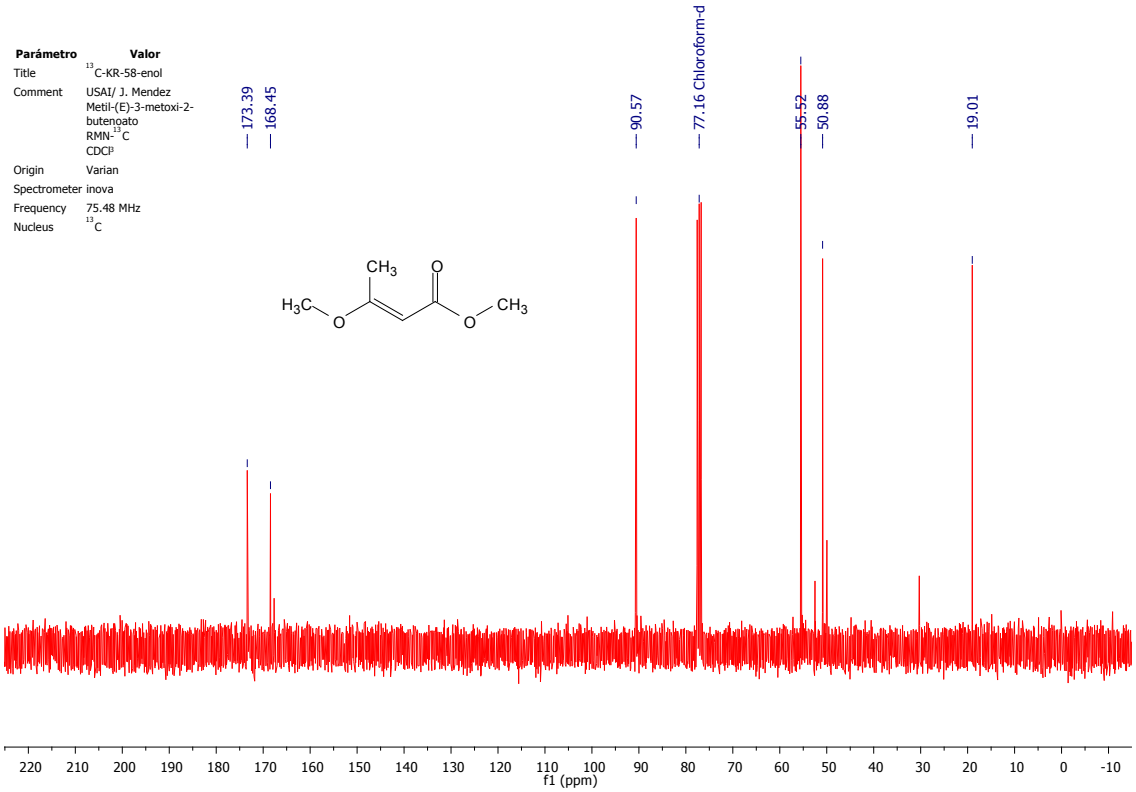
NMR Spectroscopy for compound Q4



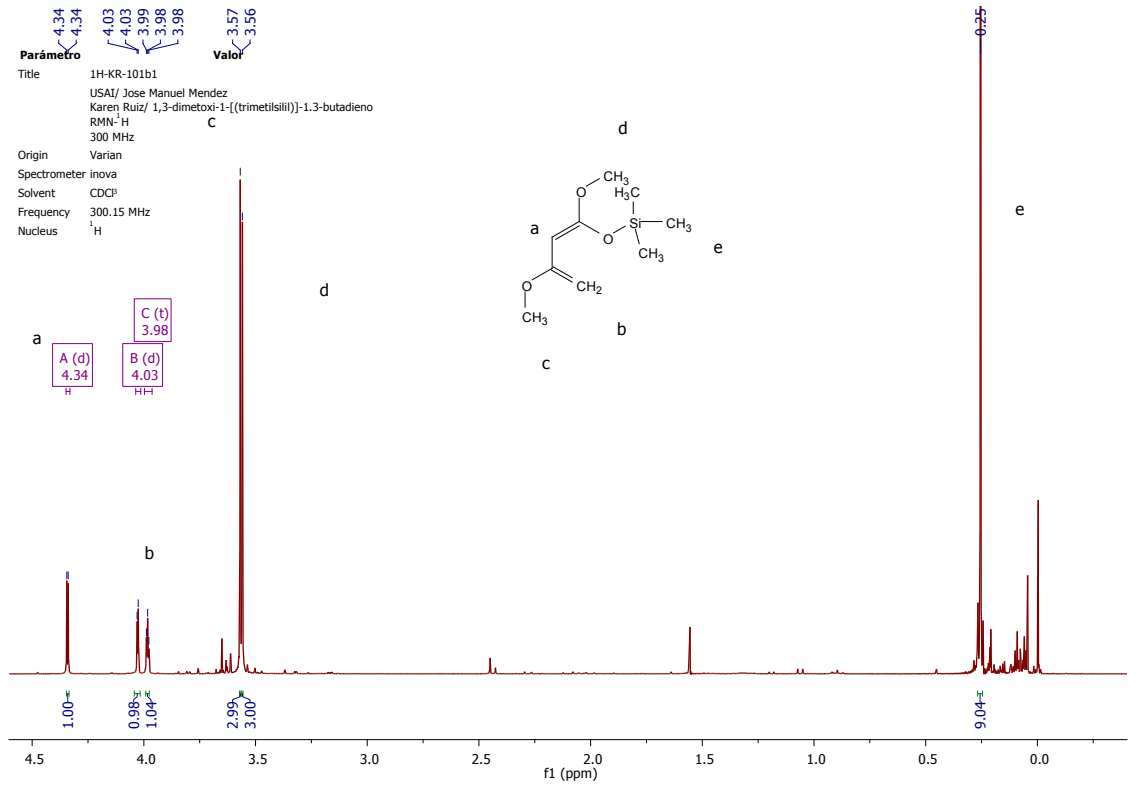


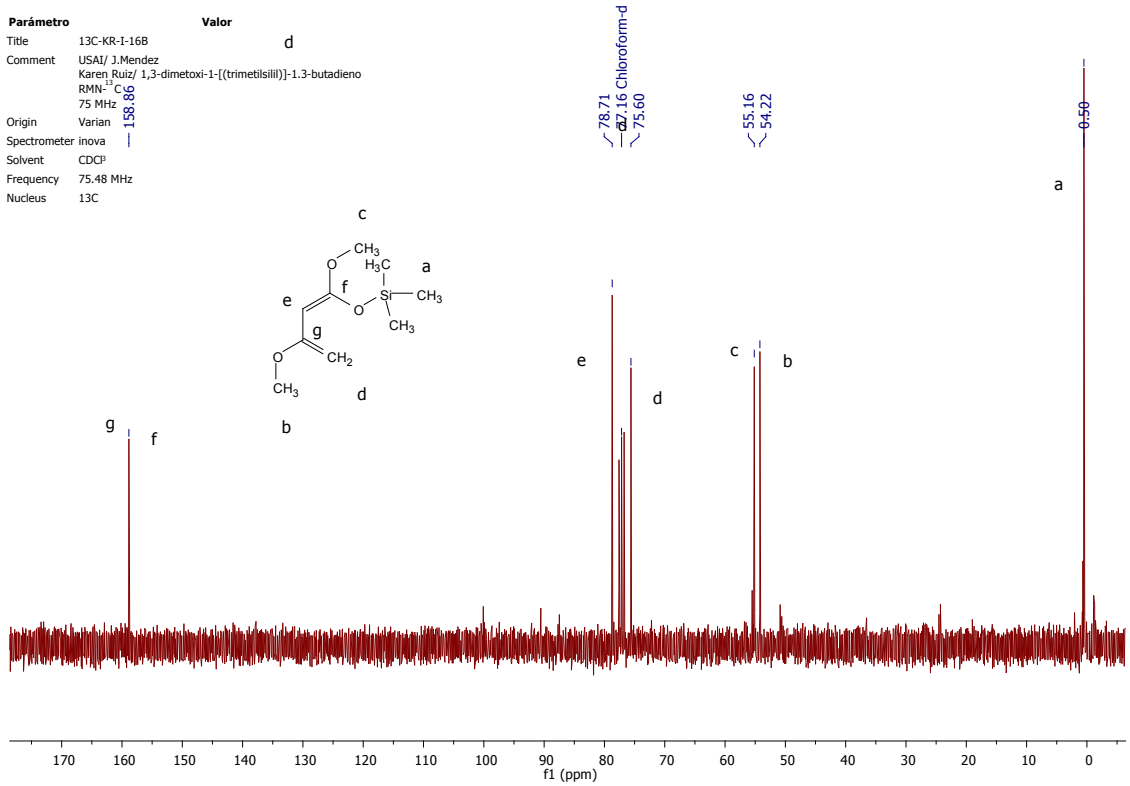
NMR Spectroscopy for ester 2



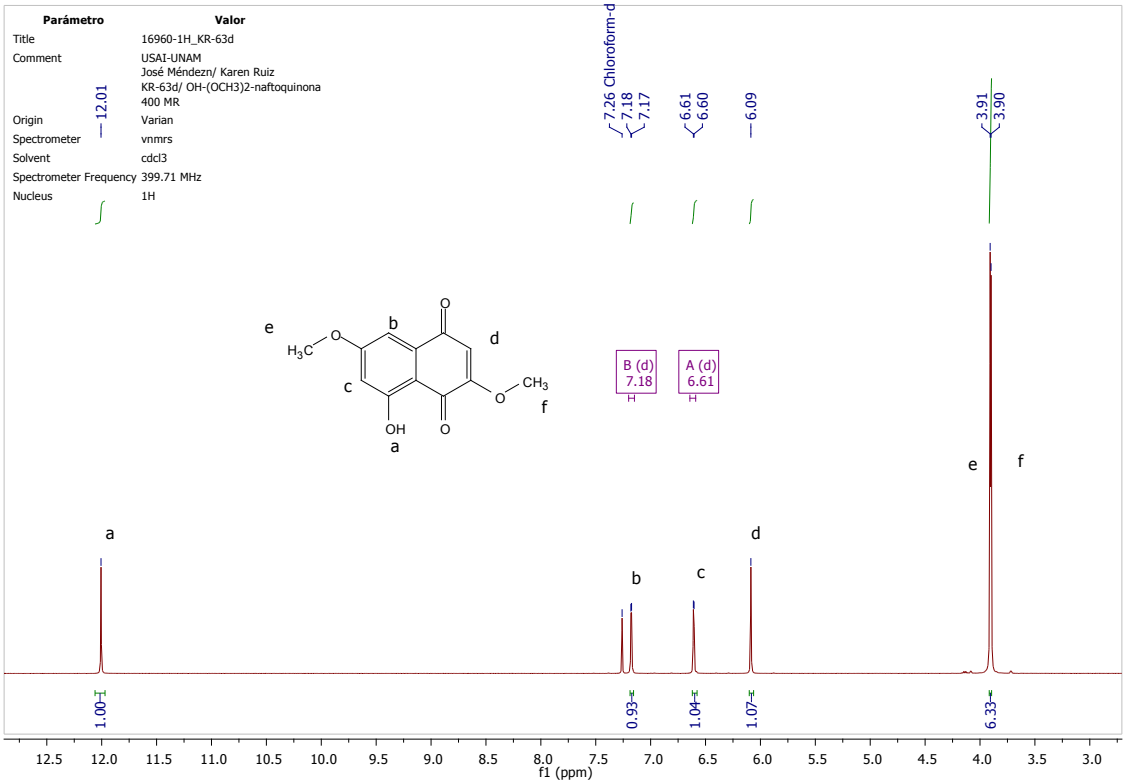


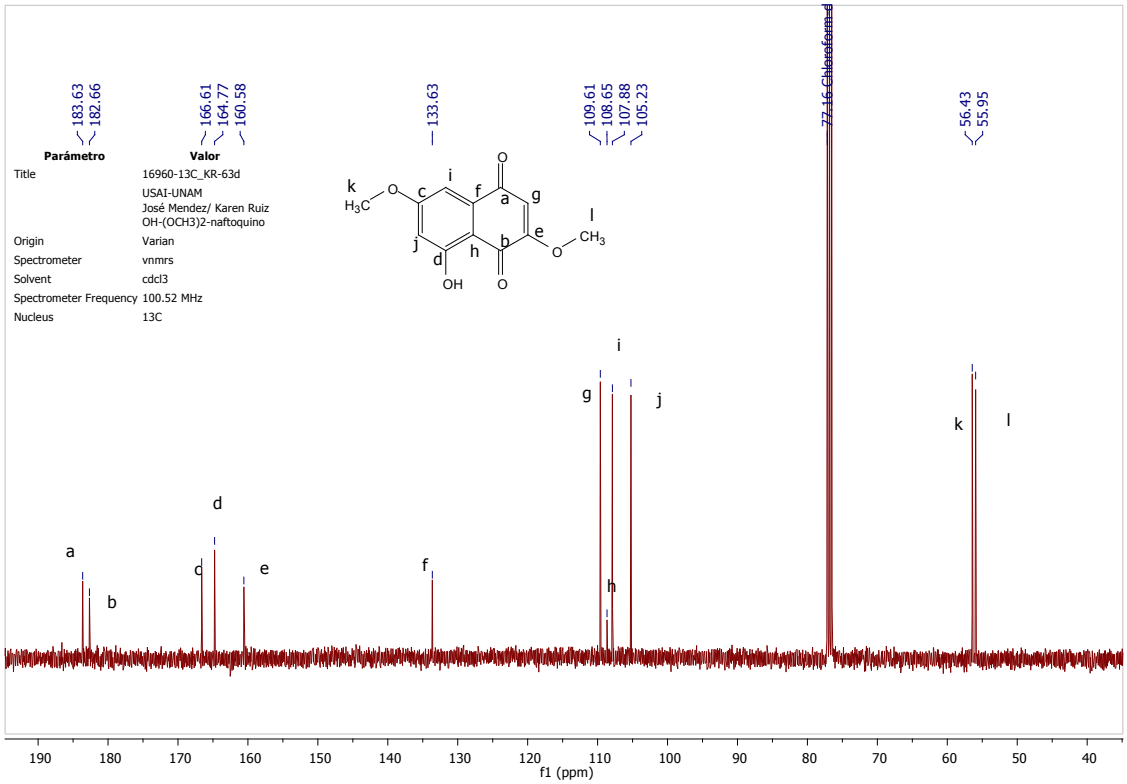
NMR Spectroscopy for Brassard's diene



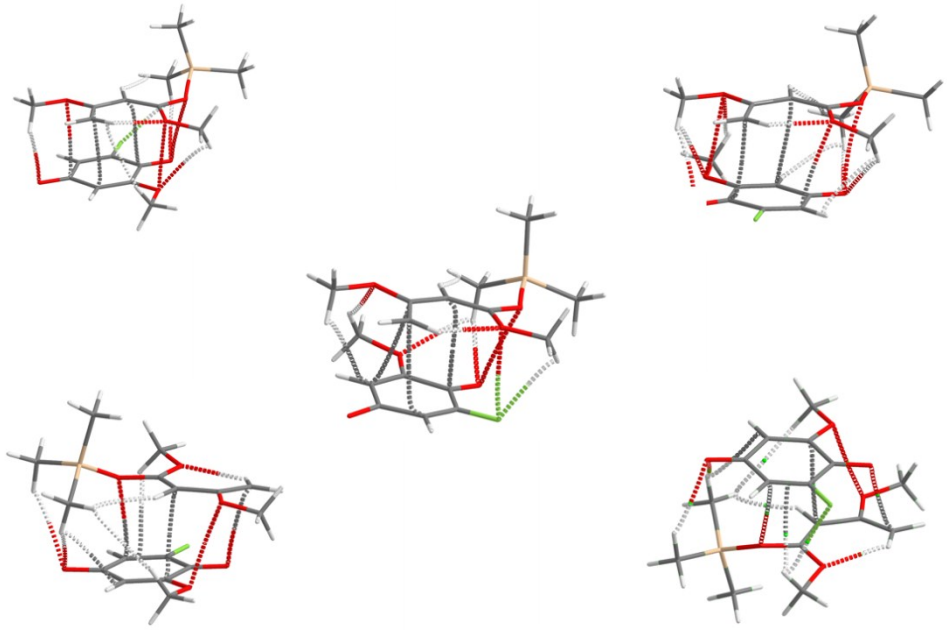


NMR Spectroscopy for compound N2

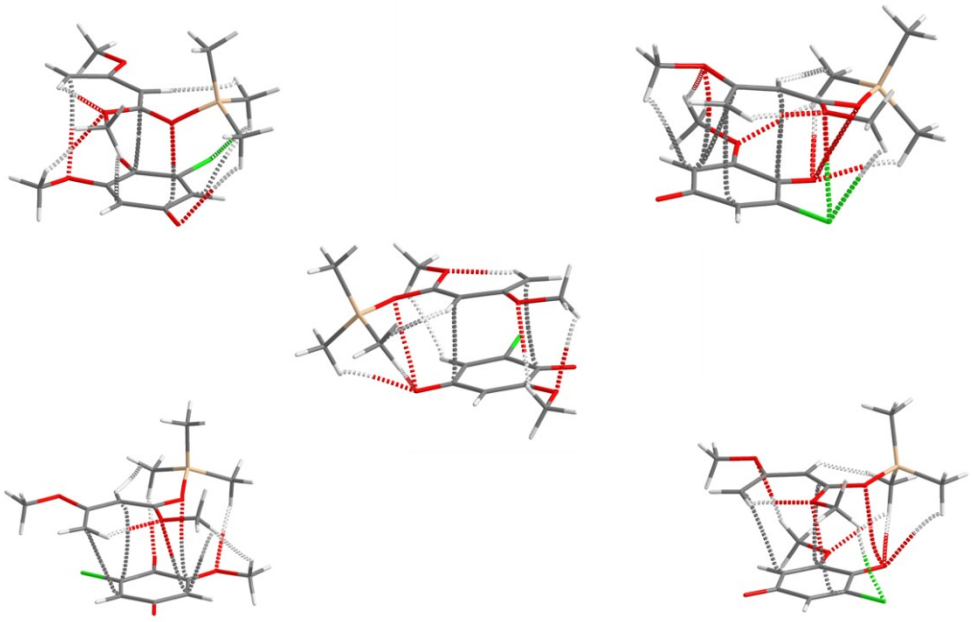




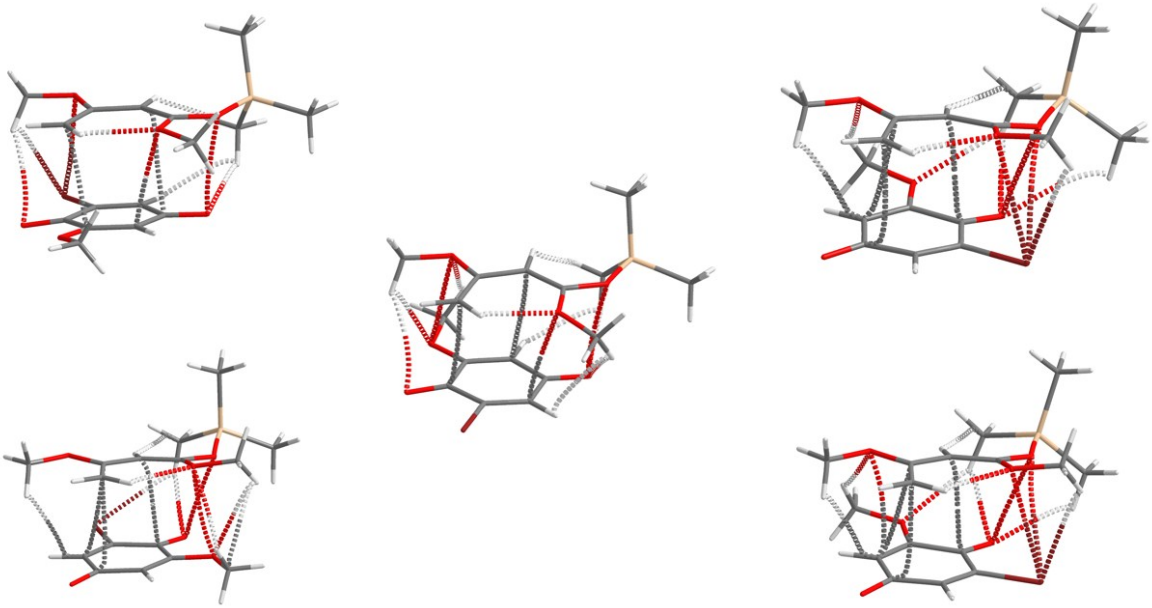
Topological analysis of the electron density for π-complexes between Brassard's diene and fluoroquinone Q1



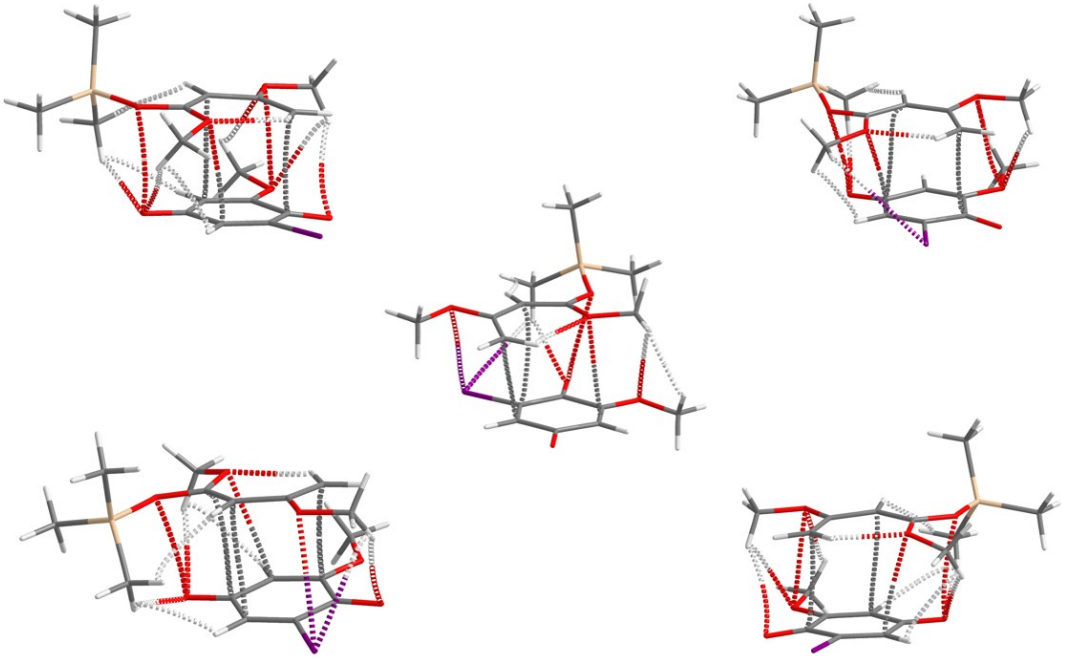
Topological analysis of the electron density for π-complexes between Brassard's diene and chloroquinone Q2



Topological analysis of the electron density for π-complexes between Brassard's diene and bromoquinone Q3

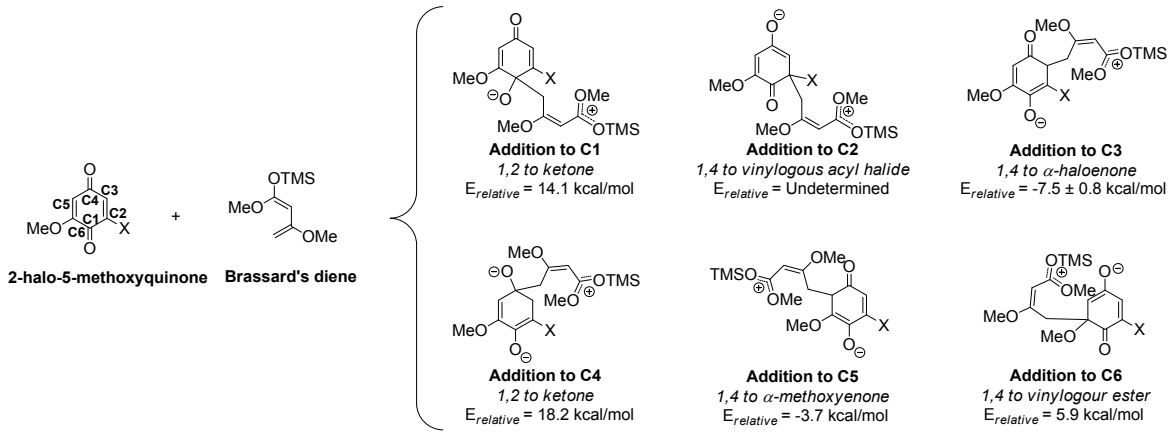


Topological analysis of the electron density for π-complexes between Brassard's diene and iodoquinone Q4



Sampling of addition routes

Virtually every carbon atom at the 1,4-benzoquinone core is a potential 1,2 or 1,4 electrophile. The corresponding set of possible products is shown in Figure SX. The random sampling method applied, yielded geometries close to addition to every electrophilic carbon. The corresponding addition products were built and optimized at the M06-2X/6-31+G(d) level, with PCM implicit toluene solvation. Energies shown were computed using the 6-311++G(2d,2p) basis set.



Scheme S2. Comparison between DFT energies of the probable addition products at every quinone position shows the observed regiochemistry is linked to the lowest-energy nucleophilic intermediate. Energies shown are relative to the corresponding stacked supermolecule.

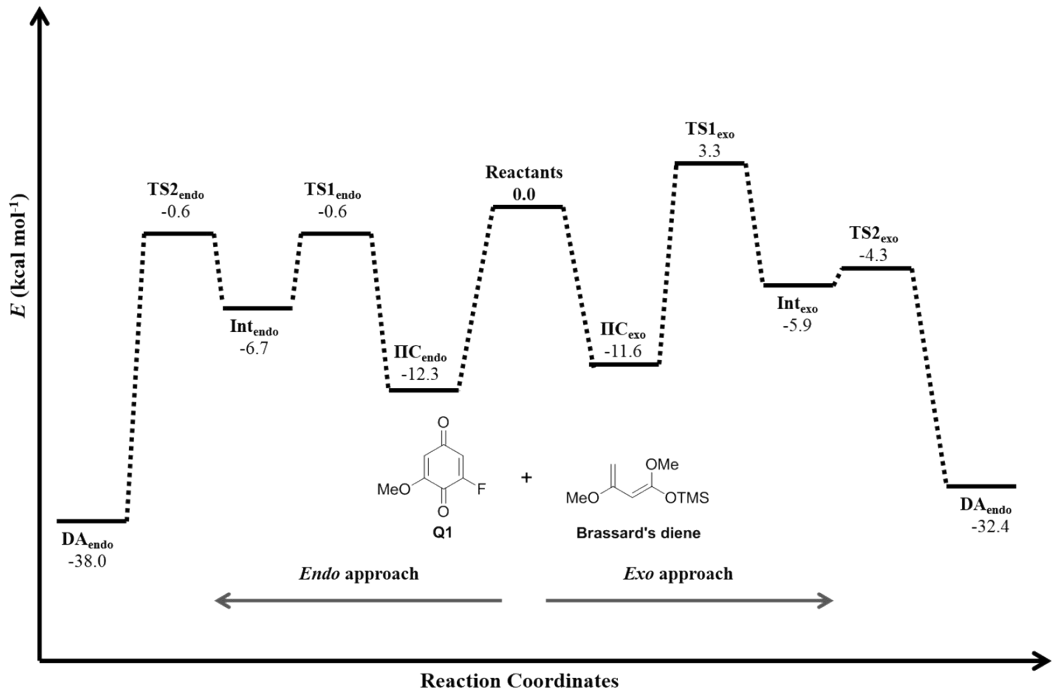
As seen, the only observed regioisomer is theoretically linked to a transient, lower-energy intermediate, derived from 1,4-addition of an activated diene to a α-haloenone system. The most probable competing addition would be, within this analysis, to the C5 electrophilic position. Products associated with this route were not observed in any case, and have not been reported up to date.

Addition to atom C2 was not determined since all attempts of modelling this reaction led to halogen elimination, an experimentally unobserved outcome.

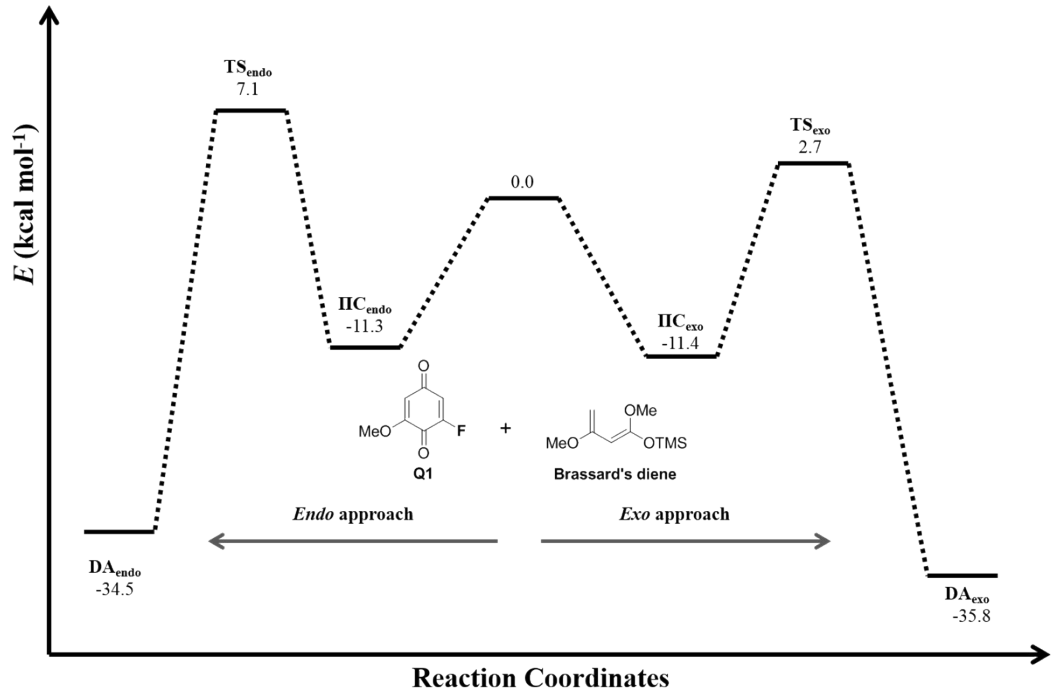
All alternative addition products are strongly disfavored, so addition to position C3 of the studied quinones is the main result. In the vast majority of reported cases, this is the only observed product.

Energy profiles and IRCs for the reaction between Brassard's diene and Q1

N2 routes

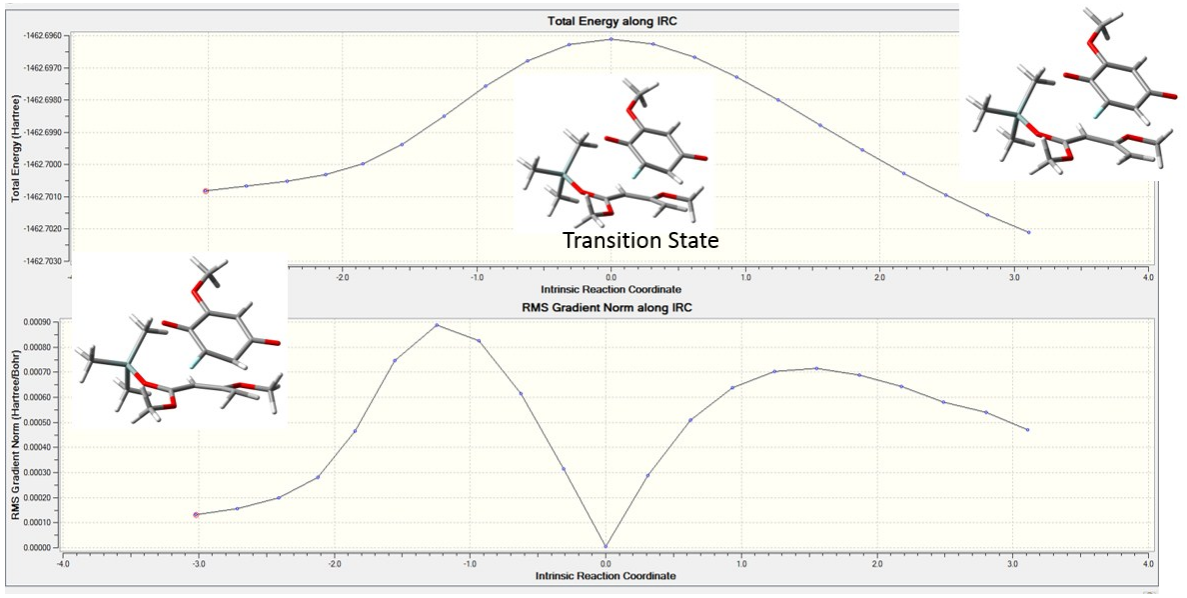


N1 routes

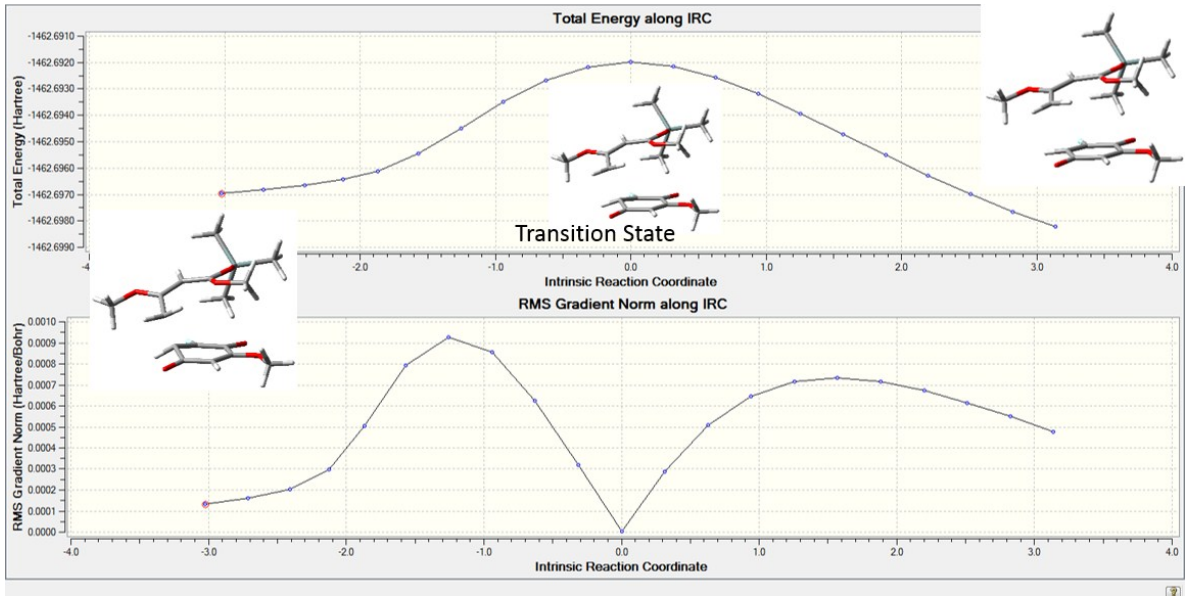


***N2* route with fluoroquinone Q1**

Endo approach

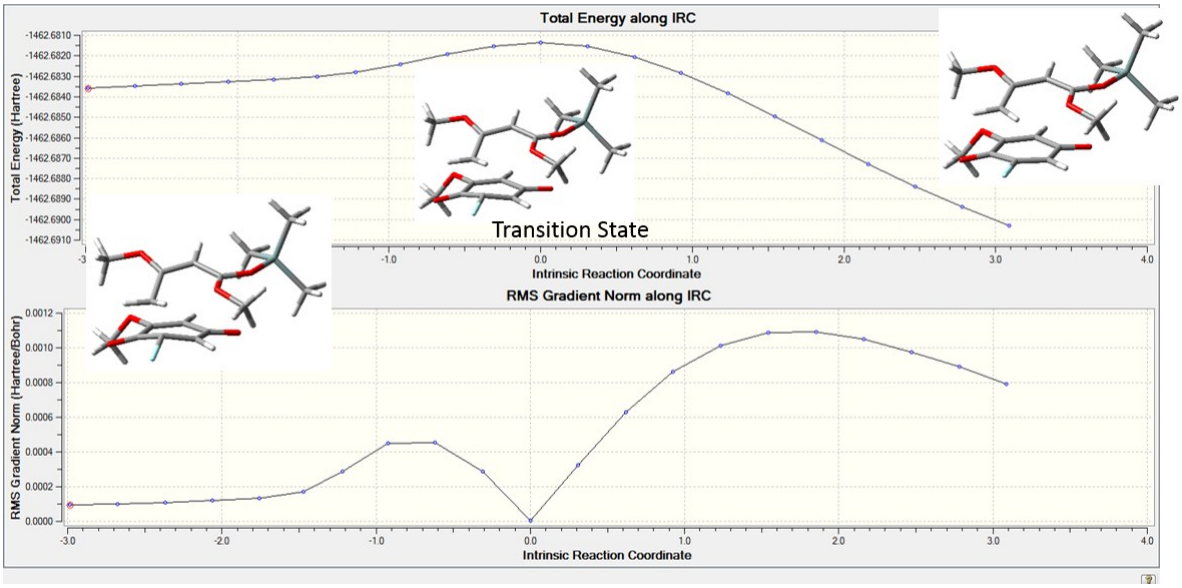


Exo approach

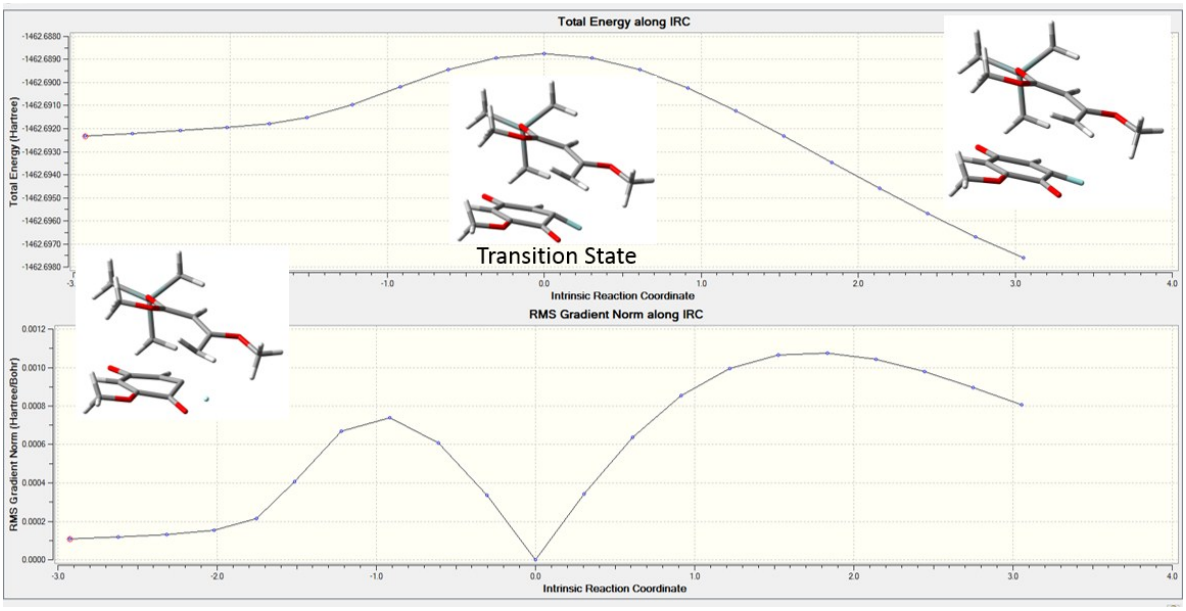


_N1_ route with fluoroquinone Q1

Endo approach

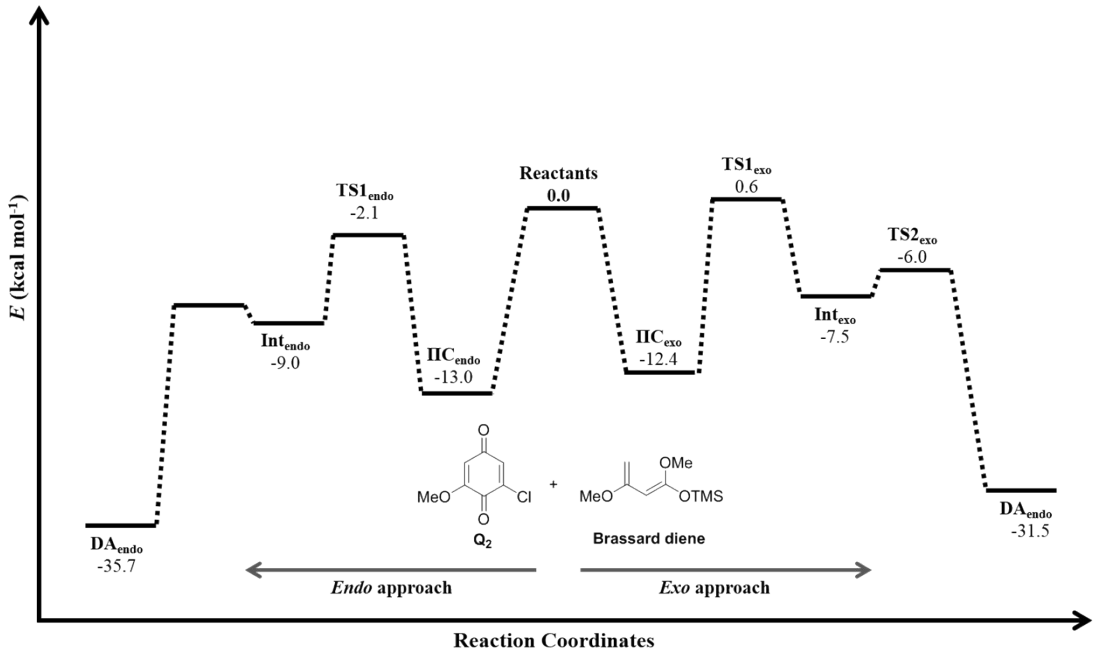


Endo approach

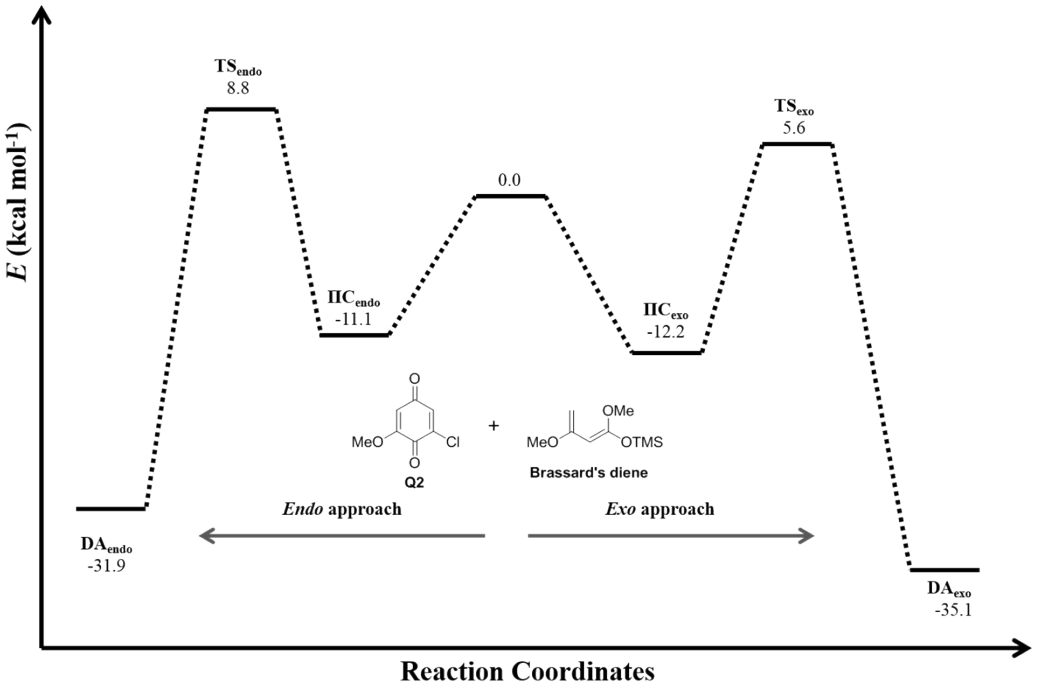


Energy profiles and IRCs for the reaction between Brassard's diene and Q2

N2 routes

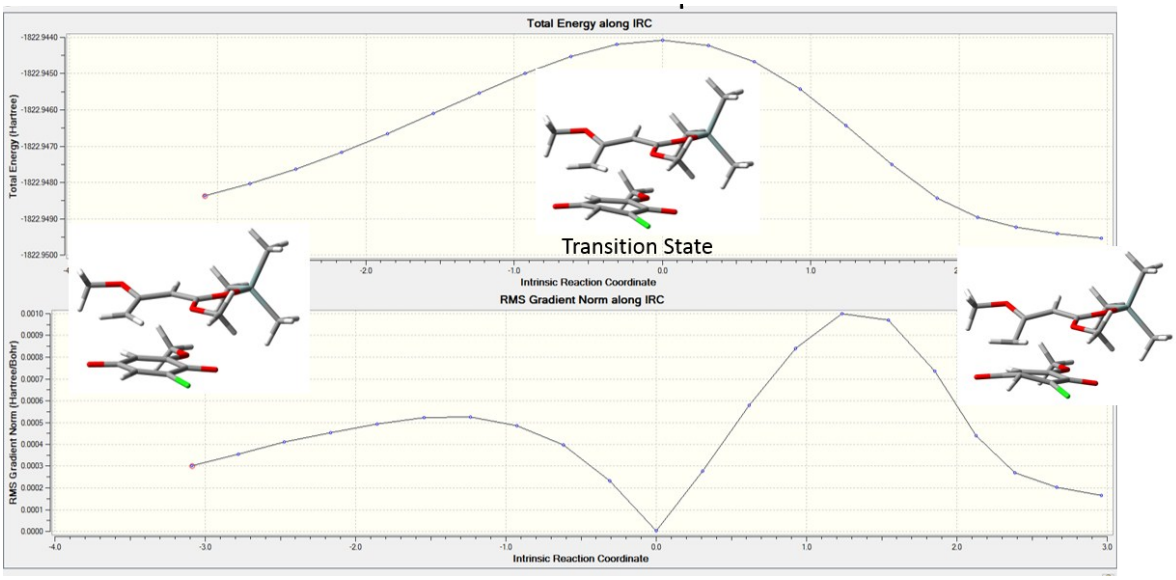


N1 routes

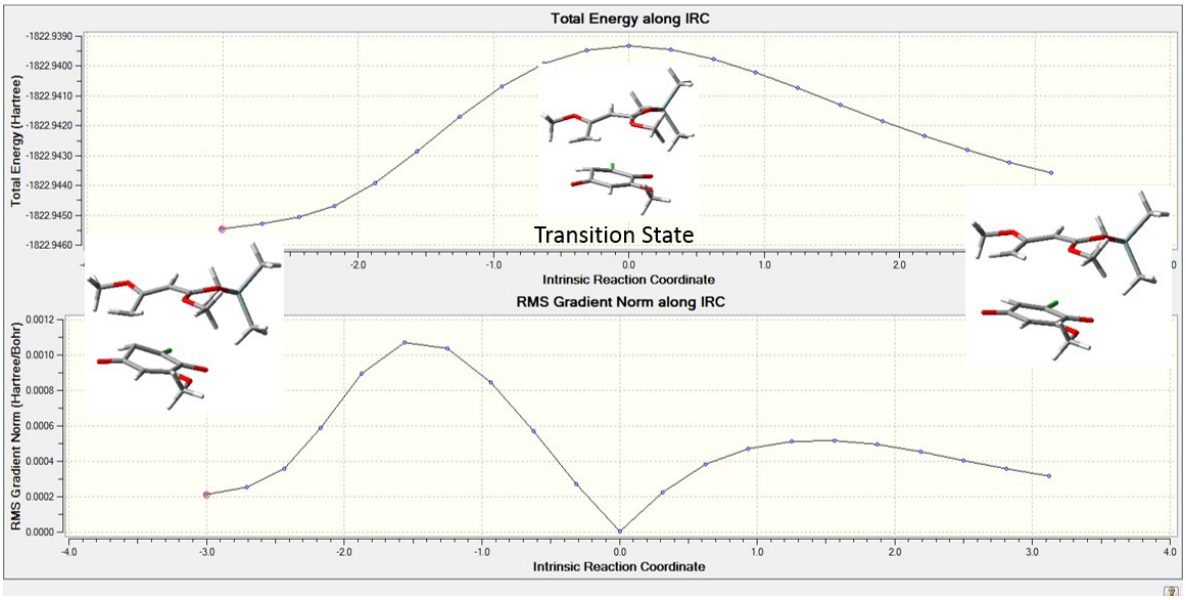


_N2_ route with chloroquinone Q2

Endo approach

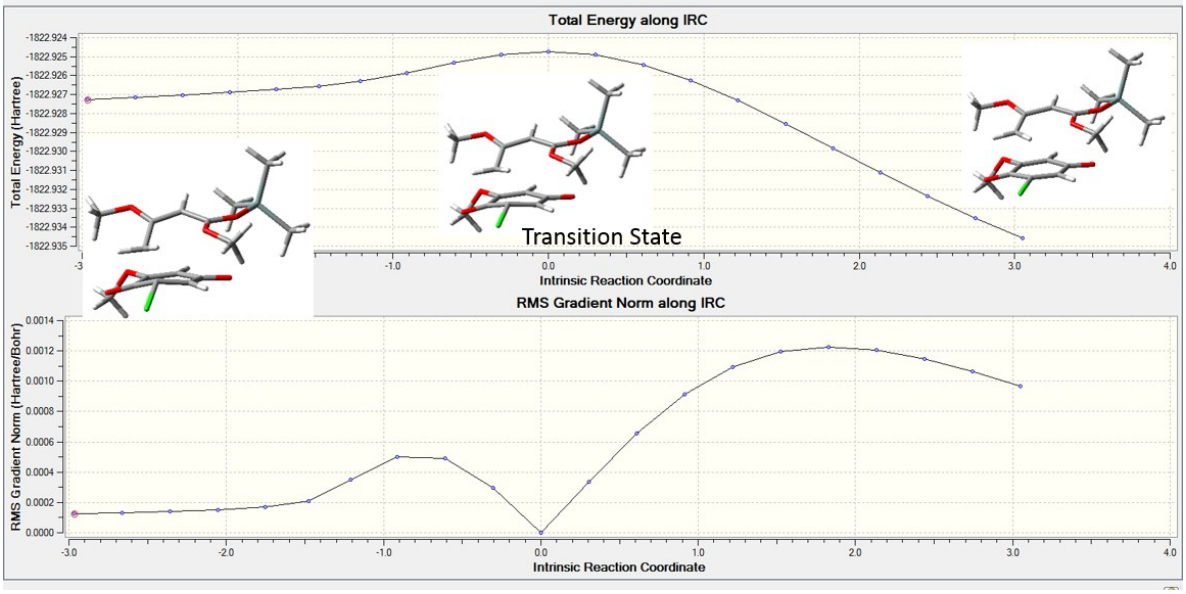


Exo approach

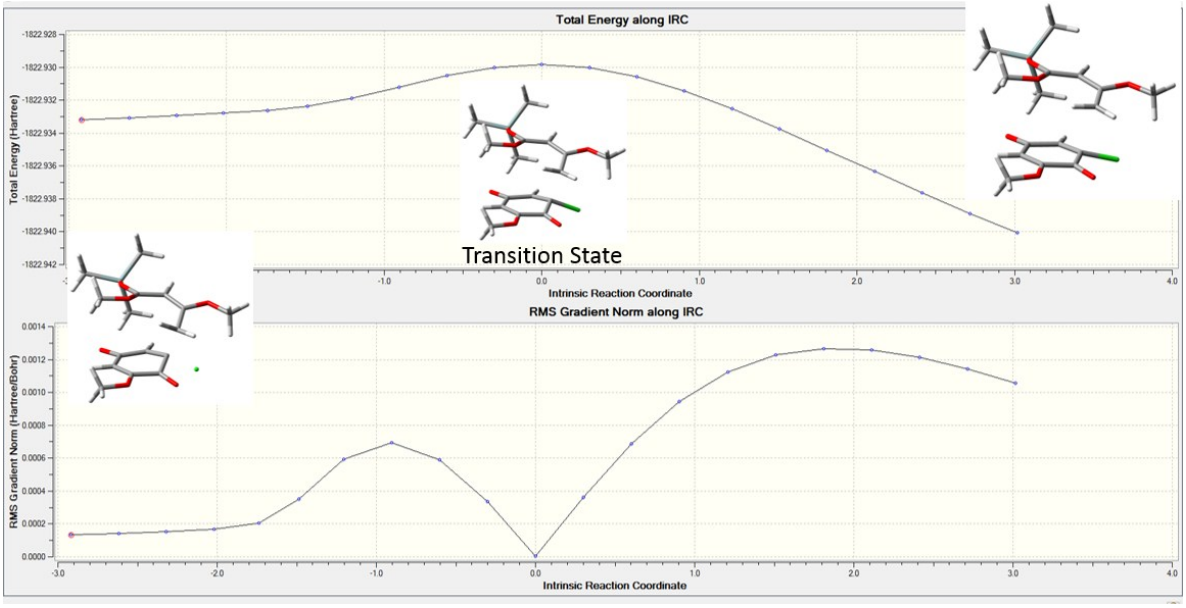


_N1_ route with chloroquinone Q2

Endo approach

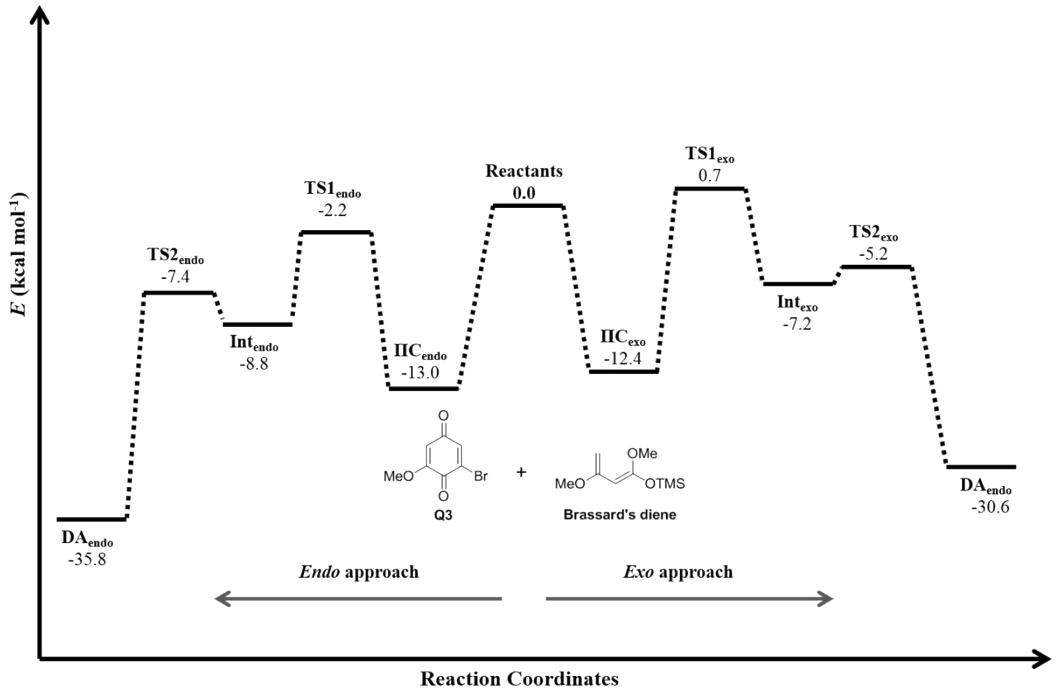


Exo approach

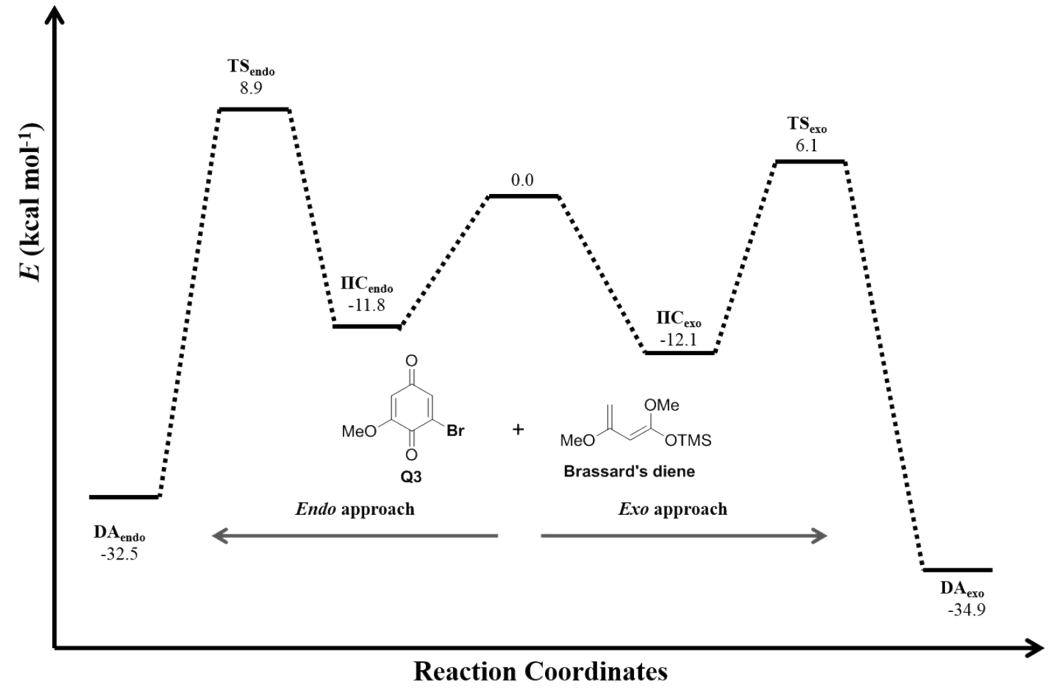


Energy profiles and IRCs for the reaction between Brassard's diene and Q3

N2 routes

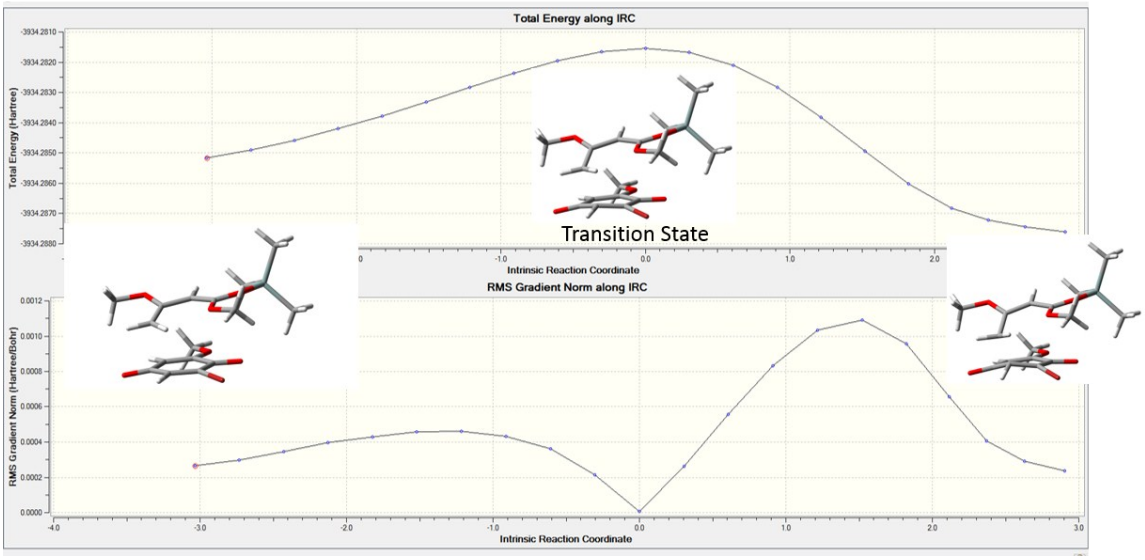


N1 routes

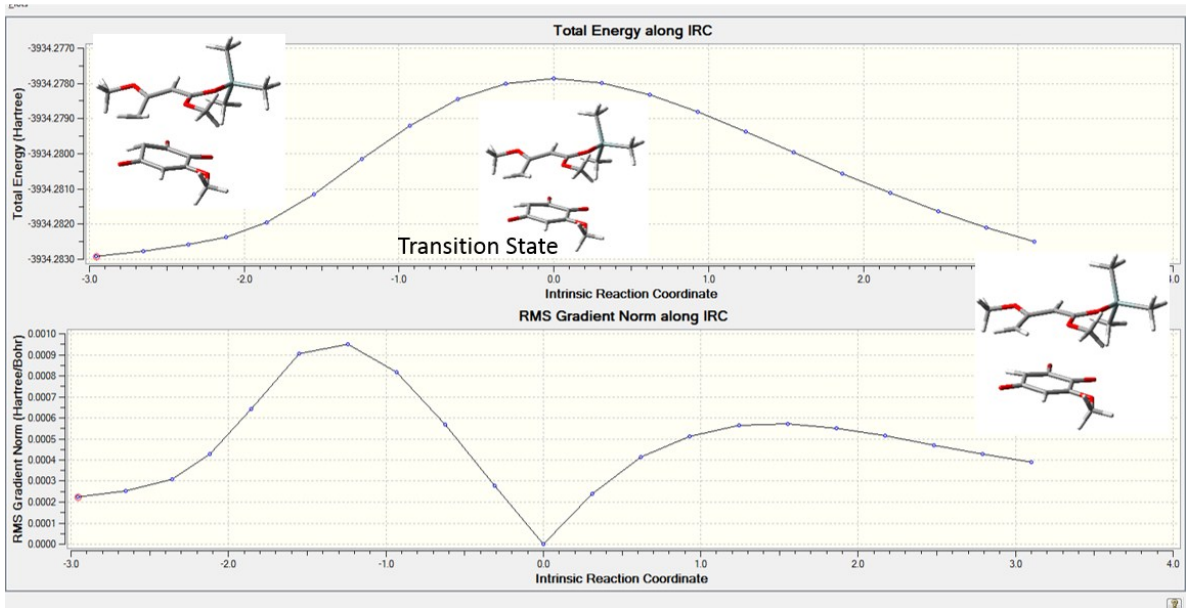


_N2_ route with bromoquinone Q3

Endo approach

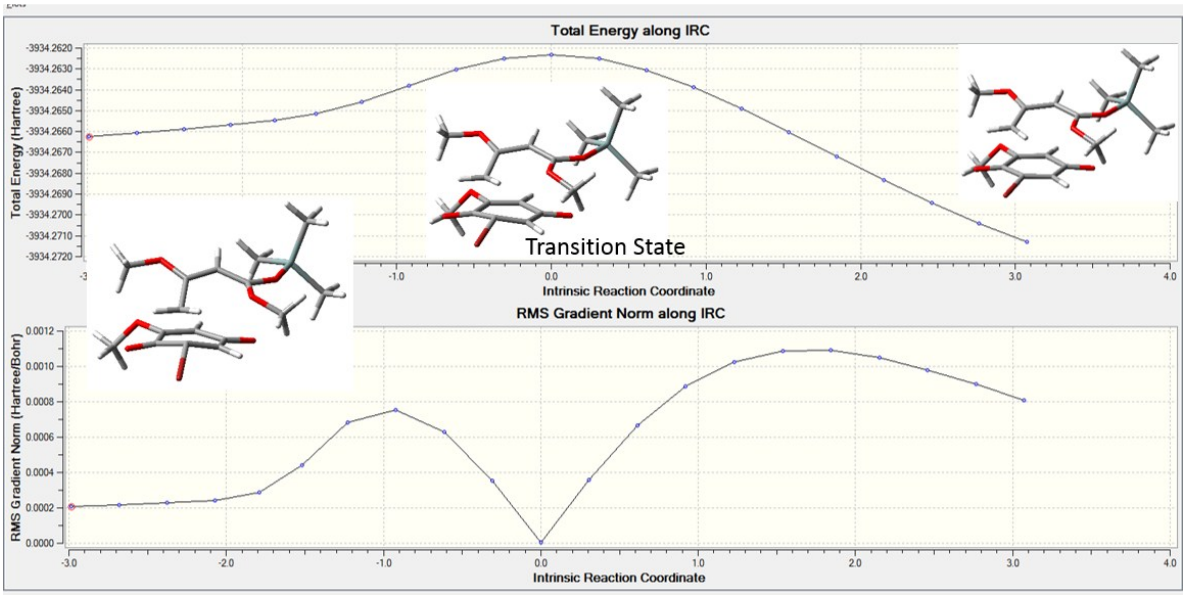


Exo approach

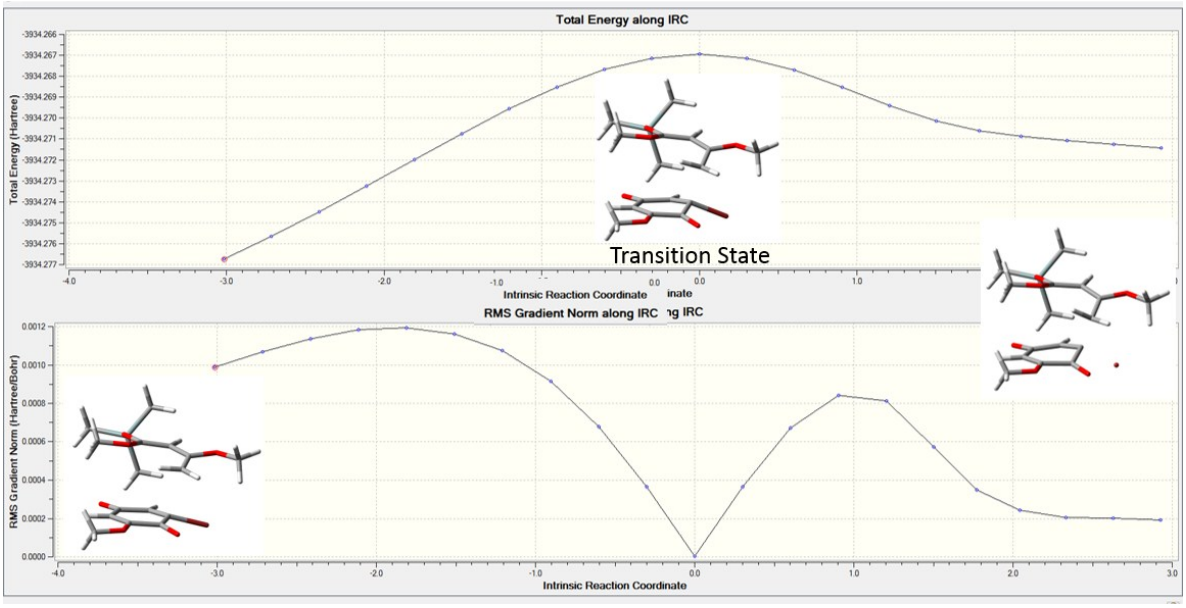


***N1* route with bromoquinone Q3**

Endo approach

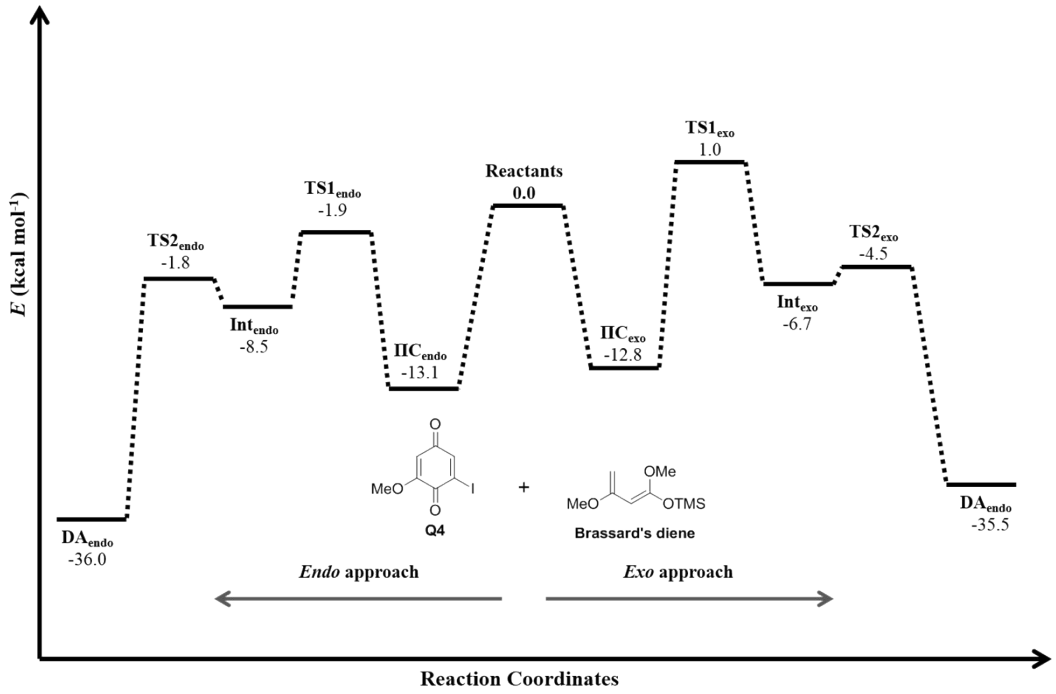


Exo approach

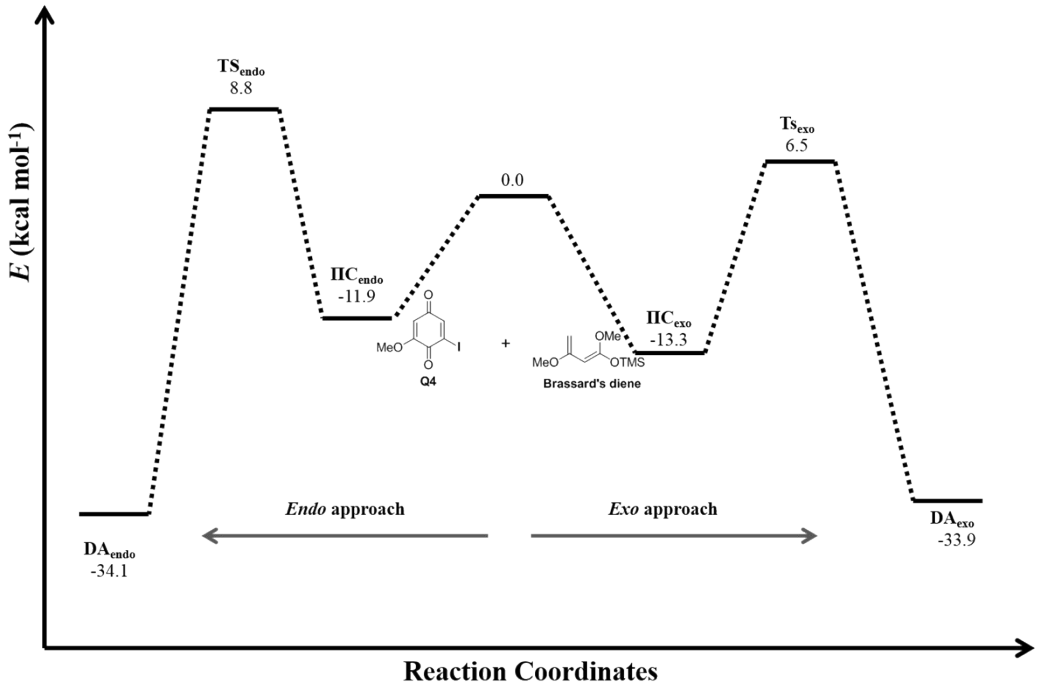


Energy profiles and IRCs for the reaction between Brassard's diene and Q4

N2 routes

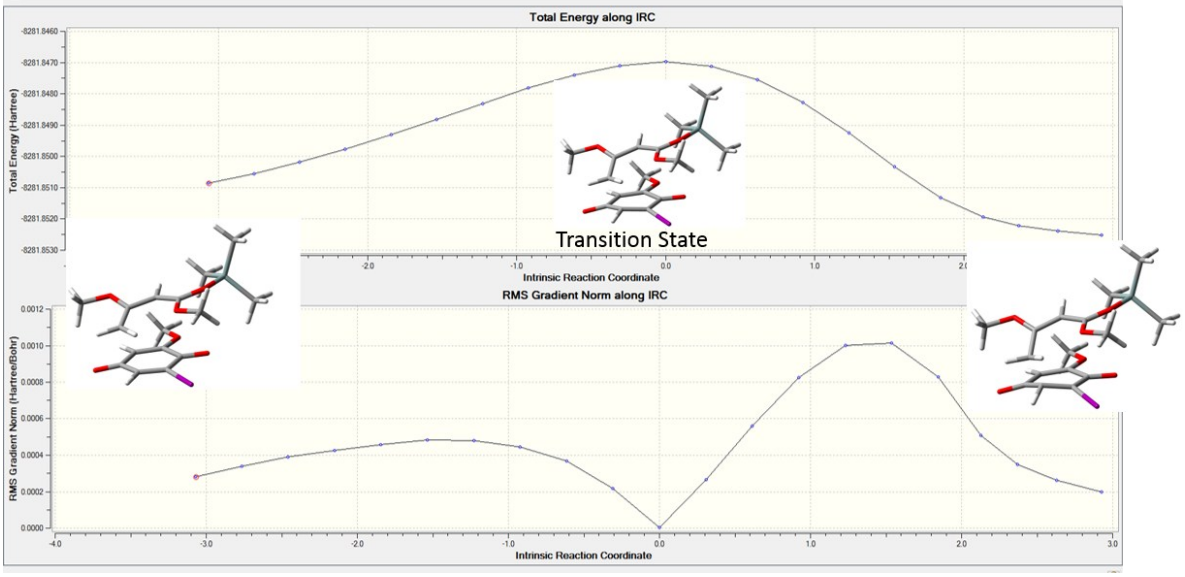


N1 routes

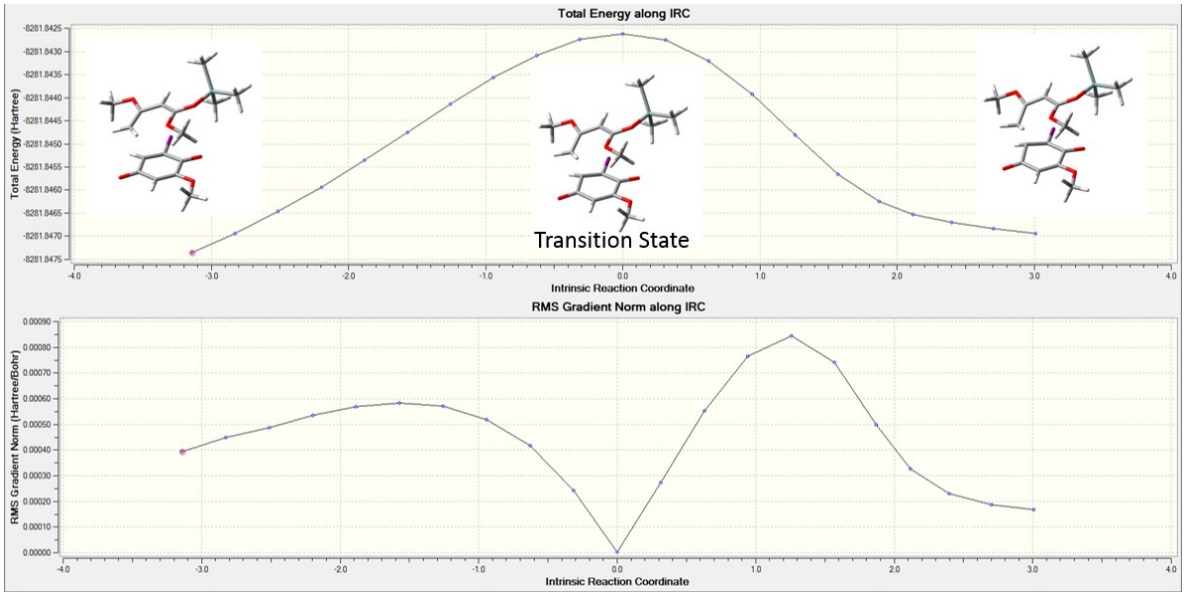


_N2_ route with iodoquinone Q4

Endo approach

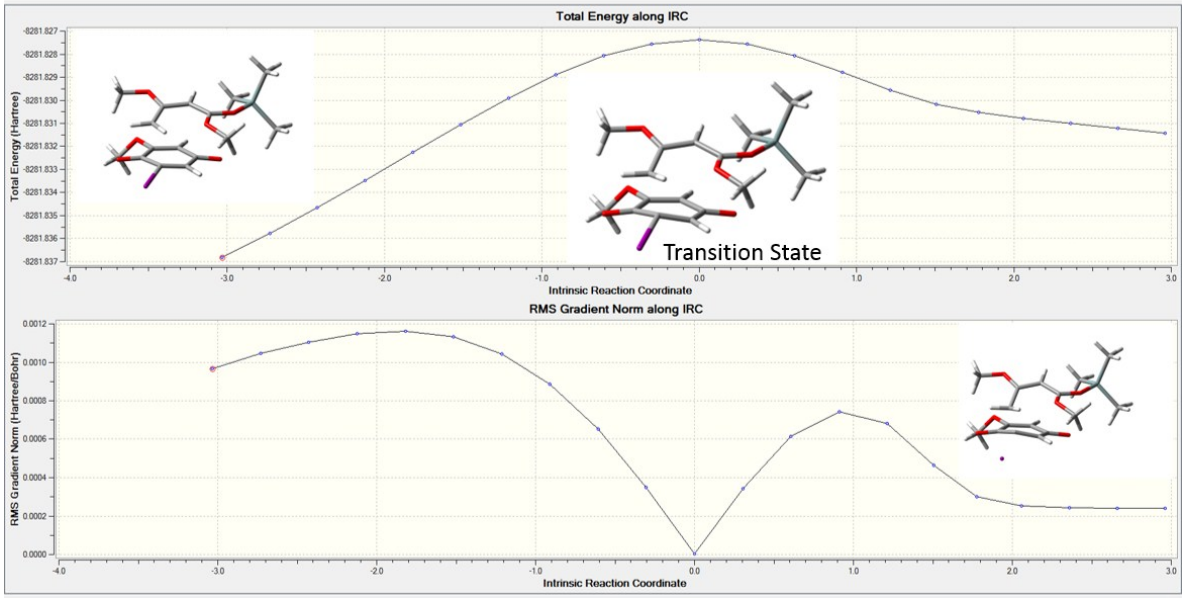


Exo approach

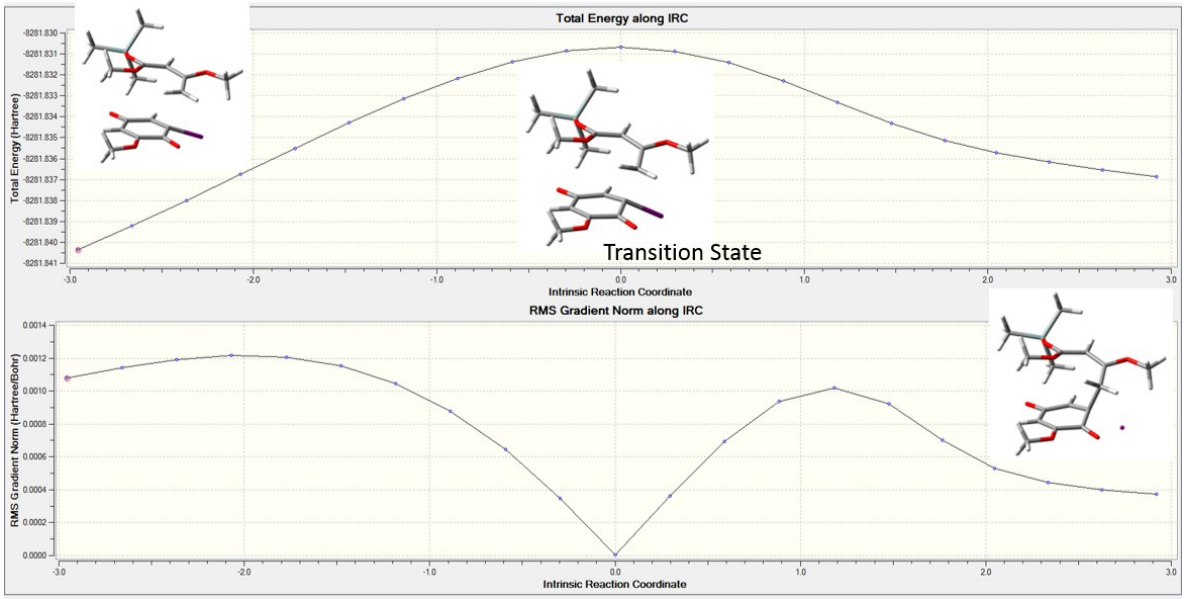


N1 route with iodoquinone Q4

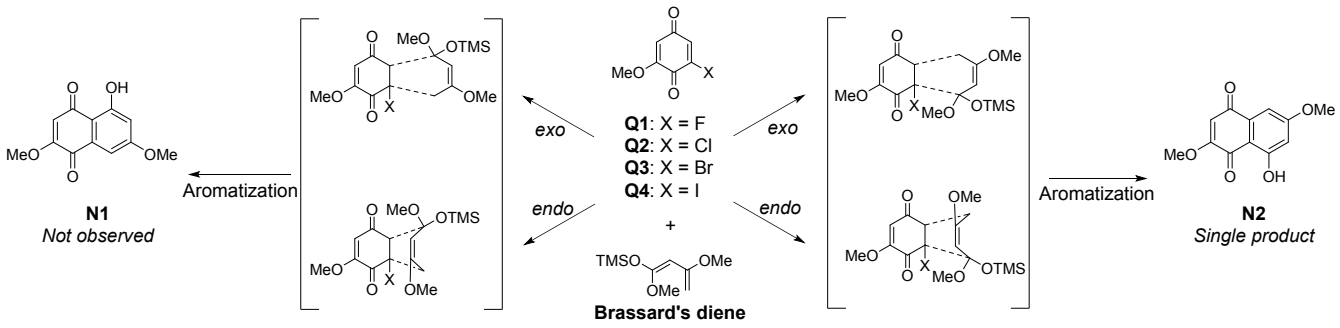
Endo approach



Exo approach



Global Electron-Density Transfer (GEDT) Indices for Transition States



Computed through Natural Population Analysis at the M062X 6-31+G(d) level

Cycloadduct	Approach	Halogen	GEDT (e)
N1	*Exo*	F	0.53
		Cl	0.56
		Br	0.56
		I	0.40
	Endo	F	0.57
		Cl	0.62
		Br	0.60
		I	0.55
N2	*Exo*	F	0.55
		Cl	0.54
		Br	0.55
		I	0.48
	Endo	F	0.54
		Cl	0.55
		Br	0.56
		I	0.49

Coordinates list for all calculated species.

1) Reactants structures.

Brassard diene:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-3.193348	1.061879	-0.060391
6	-2.423702	-0.039220	-0.038241
6	-0.083080	0.868128	-0.081406
6	-0.982809	-0.133545	-0.080766
1	-0.600142	-1.140145	-0.115957
8	-2.927939	-1.320448	0.031787
8	-0.469133	2.157388	-0.064888
8	1.246876	0.714884	-0.097844
6	-4.333496	-1.445580	0.072042
1	-4.792669	-1.043424	-0.832672
1	-4.540797	-2.506186	0.142688
1	-4.751565	-0.932181	0.937710
6	0.549125	3.145989	0.090668
1	1.225638	3.152047	-0.758288
1	0.021331	4.089311	0.149487
1	1.118358	2.981321	1.001196
14	2.180014	-0.697266	0.006545
6	1.774322	-1.594172	1.583919
1	0.790578	-2.057119	1.563342
1	2.501835	-2.382426	1.773208
1	1.798002	-0.918094	2.436358
6	1.889473	-1.754635	-1.494540
1	0.863125	-2.108613	-1.565717
1	2.105620	-1.209518	-2.411207
1	2.532512	-2.633387	-1.479225
6	3.902904	-0.009798	0.032493
1	4.646612	-0.794385	0.158895
1	4.135084	0.515464	-0.891632
1	4.032894	0.696370	0.850474
1	-2.733332	2.030021	-0.122745
1	-4.268057	1.013800	-0.022646

Quinone H:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.225611	1.378850	0.000011
6	-1.244948	1.586261	-0.000015
6	-2.093542	0.553960	-0.000015
6	-1.600702	-0.855335	0.000022
6	-0.146755	-1.085196	0.000012
6	0.719229	-0.049194	0.000010
1	-3.172892	0.676397	-0.000036
1	0.165285	-2.123415	0.000010
8	-2.394533	-1.780371	-0.000024
8	1.001599	2.308236	-0.000005
8	2.048253	-0.117293	0.000008
6	2.633079	-1.409520	0.000009
1	3.709780	-1.248656	0.000009
1	2.336221	-1.965368	0.896374
1	2.336221	-1.965370	-0.896355
1	-1.569003	2.622880	-0.000035

Quinone_F: ***Q1***

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.181001	-1.151332	-0.000052
6	1.564728	-0.585724	-0.000052
6	1.826663	0.720182	0.000000
6	0.704123	1.695546	0.000285
6	-0.680305	1.183383	0.000062
6	-0.937650	-0.140778	0.000006
1	2.838636	1.111275	-0.000089
1	-1.456599	1.940038	0.000019
8	0.934010	2.891601	-0.000173
8	-0.018020	-2.340337	0.000170
8	-2.129827	-0.731449	-0.000033
6	-3.270328	0.113641	-0.000005
1	-4.132768	-0.550477	-0.000063
1	-3.279725	0.742935	0.896751
1	-3.279686	0.743045	-0.896684
9	2.521271	-1.506094	-0.000123

Quinone_Cl: **Q2**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.209516	-0.946799	-0.000428
6	-1.354678	0.022815	-0.000034
6	-1.156376	1.344457	0.000050
6	0.220437	1.915109	0.000120
6	1.365569	0.992045	-0.000071
6	1.175791	-0.343321	-0.000165
1	-1.974922	2.057870	0.000184
1	2.345321	1.455701	-0.000057
8	0.372804	3.123811	-0.000183
8	-0.371724	-2.140680	0.000219
8	2.113143	-1.286893	-0.000149
6	3.465738	-0.857902	0.000029
1	4.065422	-1.766282	-0.000010
1	3.679719	-0.265731	-0.896629
1	3.679547	-0.265925	0.896855
17	-2.926509	-0.679056	0.000209

Quinone_Br: ***Q4***

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.224675	-0.846396	0.000029
6	-0.787789	0.258429	0.000041
6	-0.423595	1.543628	0.000130
6	1.013649	1.937997	0.000828
6	2.032520	0.878675	0.000238
6	1.674252	-0.421361	0.000143
1	-1.143115	2.356401	-0.000061
1	3.063198	1.213914	0.000070
8	1.315202	3.118522	-0.000426
8	-0.082491	-2.011821	0.000570
8	2.486189	-1.474334	-0.000012
6	3.881801	-1.216699	-0.000050
1	4.363444	-2.193011	-0.000202
1	4.167592	-0.655974	-0.896784
1	4.167689	-0.656211	0.896801
35	-2.573231	-0.283706	-0.000258

Quinone_I: **Q5**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.658659	-0.809841	0.000078
6	0.306018	0.334623	0.000033
6	-0.120888	1.601179	0.000037
6	-1.577403	1.932560	0.000120
6	-2.547771	0.829999	0.000078
6	-2.129366	-0.452261	0.000073
1	0.550433	2.454395	-0.000009
1	-3.592646	1.117856	0.000059
8	-1.927594	3.099558	0.000005
8	-0.307300	-1.963474	0.000088
8	-2.891643	-1.541825	0.000058
6	-4.297569	-1.350261	0.000047
1	-4.733552	-2.347789	0.000032
1	-4.609491	-0.803343	0.896650
1	-4.609470	-0.803324	-0.896553
53	2.342658	-0.167695	-0.000079

2) Flaviolin (**N1**) endo structures.

Int1_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.086607	-1.637567	0.419192
6	-1.237378	-1.993535	-0.394946
6	-2.458055	-1.454808	-0.186151
6	-2.619084	-0.491036	0.929001
6	-1.424212	0.426233	1.147680
6	-0.076260	-0.296640	1.128473
1	-1.123173	-2.831153	-1.067918
6	-1.576322	1.561695	0.101035
6	-0.658507	1.429333	-1.063232
6	1.022267	0.628142	0.498757
6	0.592088	1.006258	-0.881792
1	1.286568	0.963508	-1.703516
8	-3.637498	-0.397960	1.574432
8	0.856610	-2.403377	0.515251
8	-1.089508	1.726918	-2.321151
8	1.070444	1.850787	1.236061
8	2.237671	-0.015354	0.585662
6	-2.207808	2.593002	-2.462468
1	-2.095428	3.492410	-1.859933
1	-2.241938	2.866261	-3.509082
1	-3.142324	2.096301	-2.203594
6	1.584535	1.747172	2.556455
1	1.669544	2.763869	2.920941
1	0.906613	1.201655	3.214137
1	2.562633	1.270778	2.566205
14	3.390346	-0.500616	-0.526969
6	2.690352	-1.570788	-1.884417
1	1.870180	-1.096899	-2.422429
1	3.467036	-1.790040	-2.618011
1	2.321693	-2.516612	-1.494018

6	4.199206	1.010999	-1.267735
1	3.546742	1.545201	-1.956607
1	4.499953	1.717504	-0.495587
1	5.094188	0.736956	-1.826164
6	4.578769	-1.456448	0.528592
1	5.362353	-1.926426	-0.063152
1	5.060912	-0.819128	1.267443
1	4.049094	-2.242350	1.064392
1	0.205511	-0.491786	2.162338
8	-3.509120	-1.938720	-0.857813
6	-4.766725	-1.247529	-0.827718
1	-5.313728	-1.634699	-1.677978
1	-5.299832	-1.452092	0.092263
1	-4.631135	-0.174706	-0.939503
1	-1.347318	2.476498	0.645661
1	-2.618163	1.632408	-0.204259
9	-1.591241	1.012879	2.398004

Int1_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.391067	-1.527787	1.766544
6	-0.486850	-2.404283	0.615080
6	-0.937577	-2.000428	-0.590862
6	-1.348686	-0.589024	-0.790139
6	-1.659454	0.182618	0.499209
6	-0.559873	-0.025989	1.533379
1	-0.203667	-3.435148	0.766965
6	-1.990278	1.630671	0.231208
6	-0.759757	2.449982	0.071479
6	0.736933	0.693540	1.030218
6	0.443855	2.037115	0.455101
1	1.284020	2.706636	0.366926
8	-1.461964	-0.071103	-1.879691
8	-0.205919	-1.976545	2.884366
8	-0.886499	3.728626	-0.389291
8	1.671149	0.962373	2.047811
8	1.279519	-0.179186	0.054942
6	-1.940115	4.002748	-1.306330
1	-2.918305	3.958491	-0.827937
1	-1.767254	5.012970	-1.654734
1	-1.916208	3.320553	-2.155085
6	2.147705	-0.137417	2.820209
1	2.362607	-1.003575	2.194687
1	3.067206	0.204008	3.283856
1	1.430421	-0.419726	3.586329
14	2.631095	-0.062858	-0.931119
6	2.061502	-0.902734	-2.489787
1	1.249245	-0.344132	-2.955712
1	2.859947	-1.001379	-3.224073
1	1.687503	-1.903555	-2.277012
6	3.171045	1.689893	-1.252579
1	2.395887	2.284828	-1.732410
1	3.467482	2.196519	-0.335078
1	4.038690	1.693066	-1.912686
6	4.022641	-1.006752	-0.128907
1	4.868429	-1.111942	-0.807337
1	4.389236	-0.509560	0.768422
1	3.707789	-2.010874	0.153255
1	-0.854340	0.434352	2.475384
8	-0.937389	-2.873360	-1.605806
6	-1.802391	-2.680144	-2.737581

1	-1.885640	-3.659133	-3.191899
1	-2.783972	-2.336234	-2.424689
1	-1.369841	-1.973047	-3.435530
1	-2.576780	2.026092	1.061705
1	-2.624273	1.674931	-0.651315
17	-3.215322	-0.595448	1.100443

Int1_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.336791	-1.654361	-1.369872
6	0.490238	-2.321325	-0.086969
6	0.852177	-1.682783	1.043228
6	1.110230	-0.226369	1.025204
6	1.354308	0.383022	-0.347741
6	0.372244	-0.126742	-1.385589
1	0.306124	-3.385317	-0.070695
6	1.445100	1.884529	-0.272526
6	0.083873	2.465456	-0.099000
6	-1.054854	0.481396	-1.122897
6	-1.017320	1.826129	-0.484936
1	-1.968189	2.327869	-0.402977
8	1.130918	0.451122	2.031592
8	0.205353	-2.296618	-2.395777
8	-0.046249	3.733722	0.378321
8	-1.761243	0.695336	-2.327344
8	-1.724106	-0.469084	-0.323939
6	0.951113	4.228813	1.265751
1	0.591285	5.195907	1.593156
1	1.073410	3.577756	2.129958
1	1.908331	4.362513	0.765519
6	-2.119777	-0.461364	-3.079174
1	-2.527634	-1.240901	-2.437868
1	-2.882765	-0.136020	-3.778045
1	-1.269643	-0.866308	-3.624056
14	-3.019142	-0.340429	0.735890
6	-2.318024	-0.074870	2.438956
1	-1.720259	0.836604	2.477623
1	-3.098641	0.010981	3.194138
1	-1.668339	-0.899077	2.733850
6	-4.195638	1.028668	0.259930
1	-3.909321	1.988401	0.686054
1	-4.251850	1.147554	-0.821514
1	-5.201726	0.811686	0.617873
6	-3.844028	-2.000563	0.592134
1	-4.609973	-2.139464	1.353758
1	-4.322731	-2.130002	-0.376910
1	-3.117871	-2.804591	0.706305
1	0.690132	0.202085	-2.373391
8	0.892891	-2.360165	2.200507
6	1.832312	-1.956782	3.214430
1	2.025193	-2.853386	3.789663
1	2.755981	-1.604449	2.764271
1	1.413519	-1.182403	3.846865
1	1.898243	2.275088	-1.183864
1	2.102770	2.146086	0.551834
35	3.222827	-0.276178	-0.814184

Int1_I:

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
6	0.353636	-1.702078	-1.231537
6	0.413009	-2.323945	0.103800
6	0.578996	-1.603982	1.228080
6	0.714863	-0.109806	1.157639
6	1.080359	0.472371	-0.207316
6	0.237527	-0.174667	-1.313504
1	0.327651	-3.405278	0.148574
6	1.025521	1.990810	-0.201197
6	-0.394414	2.478168	-0.294056
6	-1.261351	0.293522	-1.189266
6	-1.388845	1.730200	-0.765141
1	-2.378886	2.164792	-0.874160
8	0.548596	0.594124	2.130064
8	0.412509	-2.384445	-2.236061
8	-0.634551	3.788545	-0.001350
8	-1.932745	0.250308	-2.420962
8	-1.858360	-0.566629	-0.256461
6	-0.050495	4.295172	1.192661
1	-0.575895	5.225529	1.409979
1	-0.186021	3.592119	2.022653
1	1.015116	4.511274	1.058140
6	-2.148079	-1.013271	-3.035468
1	-2.403483	-1.778837	-2.294457
1	-2.990202	-0.871326	-3.715866
1	-1.266937	-1.334985	-3.596760
14	-3.325507	-0.408808	0.567303
6	-3.183598	0.889179	1.915478
1	-3.226638	1.909447	1.520856
1	-3.996643	0.771944	2.642136
1	-2.232949	0.777044	2.450337
6	-4.700294	-0.003585	-0.641815
1	-4.547003	0.964331	-1.130394
1	-4.761819	-0.764126	-1.428164
1	-5.667727	0.027232	-0.126384
6	-3.542607	-2.110241	1.313815
1	-4.463448	-2.175551	1.904197
1	-3.585984	-2.874865	0.530200
1	-2.699368	-2.351227	1.971330
1	0.601558	0.146500	-2.294728
8	0.538925	-2.200725	2.430089
6	1.379184	-1.712015	3.482252
1	1.585163	-2.577093	4.113378
1	2.319217	-1.322054	3.079808
1	0.868671	-0.934809	4.051022
1	1.587263	2.394838	-1.052064
1	1.507930	2.350325	0.711220
53	3.216077	-0.055591	-0.477211

π_complex_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.241022	0.721008	-1.732903
6	1.036560	-0.496407	-1.677461
6	2.262110	-0.540337	-1.111129
6	2.845807	0.660230	-0.465965
6	1.969991	1.849519	-0.471966
6	0.780105	1.906254	-1.073273
1	0.632583	-1.381234	-2.146611
6	1.408013	0.407320	2.203293
6	0.691071	-0.608627	1.674703

6	-1.425962	0.529640	0.931639
6	-0.603398	-0.544442	1.061703
1	-0.942158	-1.469124	0.624964
8	3.976741	0.707901	-0.008648
8	-0.834283	0.774749	-2.334338
8	1.153537	-1.893984	1.584383
8	-1.103490	1.719252	1.456998
8	-2.579315	0.518660	0.289510
6	2.454594	-2.144214	2.085069
1	2.497914	-1.989659	3.163323
1	2.667390	-3.180688	1.852476
1	3.193829	-1.505266	1.600123
6	-1.980670	2.816363	1.174823
1	-2.953380	2.662184	1.631860
1	-1.495874	3.680398	1.610282
1	-2.103977	2.945698	0.103951
14	-3.522727	-0.782791	-0.306410
6	-2.591669	-1.824801	-1.525068
1	-1.879104	-2.500758	-1.056633
1	-3.292830	-2.441846	-2.086841
1	-2.052209	-1.198519	-2.234092
6	-4.050881	-1.763218	1.181789
1	-3.193327	-2.187808	1.702197
1	-4.596341	-1.150843	1.896553
1	-4.695782	-2.592741	0.895932
6	-4.912730	0.141774	-1.108015
1	-5.654513	-0.530285	-1.534902
1	-5.422931	0.787452	-0.396587
1	-4.537762	0.771363	-1.912884
1	0.201750	2.815890	-1.103795
8	2.912168	-1.720845	-1.080908
6	4.345322	-1.762986	-1.163471
1	4.573895	-2.749918	-1.547964
1	4.724069	-1.006497	-1.843219
1	4.804084	-1.623192	-0.189741
1	0.977499	1.389695	2.259625
1	2.389993	0.266837	2.621214
9	2.495200	2.913293	0.135771

π_complex_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.035974	0.255295	-1.686711
6	0.797758	-0.970705	-1.527717
6	2.056192	-0.973074	-1.041691
6	2.716500	0.274181	-0.581658
6	1.880337	1.495204	-0.678582
6	0.655131	1.492662	-1.220834
1	0.344254	-1.897411	-1.844383
6	1.411143	0.388182	2.176373
6	0.610721	-0.626008	1.780292
6	-1.451879	0.573943	0.971600
6	-0.699017	-0.535359	1.204604
1	-1.112132	-1.472553	0.873813
8	3.874020	0.300656	-0.198816
8	-1.078485	0.280569	-2.218698
8	0.990456	-1.940845	1.798133
8	-1.049572	1.783865	1.384841
8	-2.594929	0.579510	0.317144
6	2.294840	-2.222371	2.277464
1	2.395246	-1.928000	3.322454

1	2.422175	-3.293287	2.181046
1	3.053336	-1.713289	1.680754
6	-1.797598	2.914351	0.920813
1	-2.799201	2.915897	1.340399
1	-1.243885	3.778509	1.264190
1	-1.864947	2.912144	-0.164939
14	-3.654843	-0.638413	-0.257669
6	-2.811138	-2.114698	-0.998395
1	-2.298225	-2.751998	-0.281858
1	-3.568804	-2.732157	-1.482483
1	-2.104498	-1.804618	-1.765155
6	-4.661274	-1.122570	1.227561
1	-4.023170	-1.501814	2.024373
1	-5.226068	-0.283661	1.628486
1	-5.371522	-1.910960	0.982953
6	-4.605416	0.290007	-1.546006
1	-5.359693	-0.334632	-2.020531
1	-5.109111	1.162109	-1.135782
1	-3.919800	0.629182	-2.320342
1	0.086346	2.401285	-1.335318
8	2.687607	-2.156362	-0.896104
6	4.084113	-2.257033	-1.221171
1	4.222808	-3.276175	-1.563408
1	4.352049	-1.566288	-2.013914
1	4.704628	-2.062173	-0.352619
1	1.042963	1.396709	2.151192
1	2.405214	0.227470	2.556701
17	2.612280	2.946606	-0.114467

π_Complex_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.183629	-0.069829	-1.683131
6	-0.331340	1.279224	-1.542245
6	-1.568022	1.526274	-1.060932
6	-2.450119	0.433468	-0.577063
6	-1.861213	-0.921904	-0.658104
6	-0.662136	-1.161306	-1.201049
1	0.287759	2.099577	-1.872049
6	-1.160036	0.153973	2.178665
6	-0.183668	0.993179	1.768000
6	1.608875	-0.586682	0.969261
6	1.087038	0.648828	1.201456
1	1.681060	1.487744	0.881363
8	-3.588991	0.637384	-0.190062
8	1.270348	-0.319077	-2.213862
8	-0.310083	2.356503	1.761818
8	0.970569	-1.693172	1.371614
8	2.736430	-0.814336	0.327817
6	-1.535632	2.886395	2.237425
1	-1.684695	2.635794	3.288142
1	-1.460830	3.960160	2.120497
1	-2.378780	2.516726	1.652007
6	1.455344	-2.948036	0.876973
1	2.377151	-3.231080	1.375742
1	0.672754	-3.661084	1.105935
1	1.626249	-2.901307	-0.195389
14	3.998047	0.190323	-0.254390
6	3.417278	1.742187	-1.088360
1	2.999718	2.485936	-0.413702
1	4.270684	2.207670	-1.582828

1	2.681121	1.506628	-1.853941
6	5.026051	0.585696	1.242419
1	4.439599	1.134282	1.978672
1	5.410512	-0.307766	1.729603
1	5.877002	1.213094	0.982200
6	4.815498	-0.947050	-1.464272
1	5.650024	-0.470119	-1.974162
1	5.193313	-1.845615	-0.980833
1	4.091763	-1.250929	-2.219078
1	-0.272299	-2.161217	-1.304597
8	-1.967531	2.809374	-0.948098
6	-3.321730	3.159525	-1.278229
1	-3.272343	4.183271	-1.630648
1	-3.708401	2.521871	-2.067127
1	-3.969921	3.086747	-0.411498
1	-0.987447	-0.906190	2.170419
1	-2.105505	0.504405	2.555698
35	-2.954171	-2.340863	-0.004905

π_Complex_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.496668	0.480334	-1.739978
6	-0.051705	1.826918	-1.539532
6	-1.277238	2.019200	-1.017445
6	-2.141080	0.857554	-0.592388
6	-1.536292	-0.501701	-0.751694
6	-0.326639	-0.675897	-1.294847
1	0.561836	2.674330	-1.828373
6	-0.970829	0.448756	2.276640
6	0.032418	1.206706	1.782995
6	1.657501	-0.526756	0.943910
6	1.265811	0.755124	1.157669
1	1.903083	1.541608	0.777281
8	-3.268867	1.029507	-0.180203
8	1.579345	0.288934	-2.278494
8	-0.002720	2.574441	1.741586
8	0.922828	-1.557488	1.394257
8	2.735913	-0.895858	0.264940
6	-1.137916	3.213379	2.282923
1	-1.227924	3.004682	3.356553
1	-0.987941	4.280918	2.120457
1	-2.054118	2.893084	1.771295
6	1.368689	-2.881811	1.122661
1	2.349215	-3.062141	1.570499
1	0.620324	-3.531372	1.575831
1	1.424179	-3.065701	0.045874
14	4.172534	-0.123334	-0.248097
6	3.990968	1.697789	-0.639085
1	3.899635	2.318942	0.257630
1	4.904027	2.011879	-1.161603
1	3.146144	1.889592	-1.306693
6	5.372617	-0.345537	1.173616
1	4.988507	0.131818	2.082585
1	5.541467	-1.405147	1.392787
1	6.342112	0.110697	0.942366
6	4.647984	-1.101734	-1.761308
1	5.615743	-0.773060	-2.156384
1	4.719212	-2.170809	-1.534388
1	3.888785	-0.961674	-2.537339
1	0.119009	-1.655877	-1.440601

8	-1.705954	3.272187	-0.786492
6	-3.066684	3.636578	-1.044307
1	-3.036879	4.703499	-1.269681
1	-3.463107	3.088225	-1.903269
1	-3.692659	3.445704	-0.172124
1	-0.878854	-0.626497	2.287098
1	-1.873383	0.882301	2.687556
53	-2.702903	-2.119727	-0.103542

3) Flaviolin (**N1**) exo structures.

DA_adduct_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.641403	-1.532930	1.013588
6	-2.002882	-1.801819	0.582389
6	-2.790186	-0.848461	0.034325
6	-2.376414	0.581673	-0.010904
6	-1.191314	0.907943	0.901912
6	-0.108579	-0.135524	0.801399
1	-2.323391	-2.830077	0.656981
6	-0.684870	2.322054	0.760005
6	0.429442	2.449956	-0.221349
6	0.609922	0.000759	-0.572955
6	1.026587	1.410100	-0.804670
1	1.782496	1.571811	-1.558026
8	-2.989222	1.420557	-0.620510
8	0.079115	-2.406965	1.469011
8	0.905806	3.697046	-0.494109
8	-0.339300	-0.302229	-1.616822
8	1.648984	-0.908035	-0.665446
6	0.070967	4.816887	-0.225980
1	-0.845827	4.780203	-0.813012
1	-0.174538	4.901664	0.831463
1	0.646324	5.684674	-0.521296
6	-0.288181	-1.610208	-2.170491
1	-0.356042	-2.395100	-1.415645
1	-1.145230	-1.672345	-2.833100
1	0.627487	-1.762321	-2.738067
14	3.161120	-0.981017	0.054782
6	3.133809	-0.430391	1.833947
1	2.453087	-1.032283	2.433260
1	4.130119	-0.538465	2.262944
1	2.859505	0.619185	1.943310
6	3.579912	-2.782069	-0.088465
1	4.559907	-3.011302	0.326669
1	2.842738	-3.378080	0.446331
1	3.578203	-3.108920	-1.126995
6	4.347750	0.086553	-0.908293
1	5.373400	-0.065467	-0.572636
1	4.318366	-0.140507	-1.972854
1	4.127728	1.146498	-0.789444
1	-1.525101	2.954111	0.474676
1	-0.353296	2.653185	1.745034
9	-1.761487	0.803709	2.201430
1	0.625808	0.060415	1.580368
8	-3.992661	-1.031715	-0.510571
6	-4.487132	-2.368175	-0.547620
1	-3.801753	-3.014439	-1.093436
1	-4.631040	-2.751085	0.460723
1	-5.437601	-2.317855	-1.060524

DA_adduct_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.514284	-1.596394	0.891447
6	-1.829115	-1.932752	0.373731
6	-2.637824	-1.009389	-0.191388
6	-2.298944	0.443969	-0.200666
6	-1.165313	0.832440	0.748658
6	-0.039867	-0.174229	0.698389
1	-2.100224	-2.976616	0.422414
6	-0.704065	2.264359	0.580754
6	0.378081	2.411110	-0.434223
6	0.722440	-0.034110	-0.661810
6	1.051739	1.385235	-0.952343
1	1.799729	1.554984	-1.712395
8	-2.915135	1.250861	-0.848662
8	0.220631	-2.429011	1.398274
8	0.764032	3.671764	-0.777777
8	-0.146803	-0.445078	-1.733983
8	1.824785	-0.871767	-0.660248
6	-0.167393	4.735215	-0.612554
1	-1.088079	4.546286	-1.162289
1	-0.397012	4.916289	0.436005
1	0.320282	5.611397	-1.020875
6	0.029535	-1.761552	-2.239858
1	-0.028397	-2.527773	-1.465486
1	-0.780558	-1.903541	-2.947610
1	0.985388	-1.863808	-2.749353
14	3.291953	-0.814467	0.149808
6	3.116269	-0.229828	1.910420
1	2.449355	-0.869548	2.485628
1	4.091458	-0.255264	2.397291
1	2.759700	0.798428	1.981080
6	3.846856	-2.582451	0.084066
1	4.814912	-2.728927	0.560070
1	3.124013	-3.216216	0.594848
1	3.927789	-2.936042	-0.942436
6	4.450898	0.322716	-0.765198
1	5.457569	0.271761	-0.350603
1	4.520541	0.064442	-1.820533
1	4.130356	1.361571	-0.698749
1	-1.573530	2.864152	0.318116
1	-0.342176	2.638625	1.539250
17	-1.974414	0.732885	2.403151
1	0.672046	0.051450	1.488774
8	-3.804914	-1.239986	-0.791757
6	-4.210628	-2.600049	-0.916525
1	-3.479425	-3.163300	-1.493161
1	-4.339043	-3.058823	0.061551
1	-5.158050	-2.576025	-1.436584

DA_adduct_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.192445	-1.568125	0.793131
6	-1.361955	-2.144237	0.164487
6	-2.209528	-1.406808	-0.587369
6	-2.086418	0.076733	-0.711129
6	-1.136649	0.722560	0.289467

6	0.099564	-0.113452	0.509507
1	-1.486353	-3.209318	0.287441
6	-0.850044	2.184269	-0.003961
6	0.420374	2.406837	-0.754759
6	1.010551	0.011921	-0.759956
6	1.284423	1.440851	-1.062180
1	2.161090	1.657247	-1.653573
8	-2.742550	0.716065	-1.494692
8	0.583237	-2.235116	1.462077
8	0.748645	3.691607	-1.071096
8	0.270750	-0.493083	-1.891839
8	2.147867	-0.756008	-0.609230
6	-0.298852	4.647830	-1.188694
1	-1.002168	4.372188	-1.972092
1	-0.834207	4.786496	-0.250868
1	0.185656	5.578769	-1.453792
6	0.602267	-1.791578	-2.361302
1	0.626716	-2.540013	-1.568076
1	-0.179101	-2.043097	-3.073237
1	1.567164	-1.793212	-2.866302
14	3.483636	-0.622310	0.401095
6	3.070600	0.100435	2.066769
1	2.356687	-0.514309	2.611284
1	3.979030	0.161684	2.666509
1	2.679661	1.115655	1.992987
6	4.064305	-2.377680	0.545218
1	4.942127	-2.467977	1.183032
1	3.273969	-2.991207	0.974347
1	4.316511	-2.794815	-0.428043
6	4.753883	0.457776	-0.431830
1	5.690989	0.448358	0.124365
1	4.973889	0.117593	-1.442424
1	4.431147	1.495908	-0.495087
1	-1.700729	2.577841	-0.561500
1	-0.802907	2.744561	0.929600
35	-2.252632	0.688385	1.996698
1	0.662237	0.285920	1.349269
8	-3.234747	-1.875027	-1.297667
6	-3.422295	-3.288512	-1.294502
1	-4.274088	-3.473809	-1.934313
1	-2.540019	-3.789168	-1.689237
1	-3.628383	-3.646816	-0.287837

DA_adduct_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.00180504	1.75577000	-0.82834800
6	-0.84164000	2.76440000	-0.21741100
6	-1.70483000	2.46473000	0.77872300
6	-1.97997000	1.05699000	1.20297000
6	-1.42249000	-0.00616040	0.27954900
6	-0.05807090	0.36628700	-0.23790400
1	-0.70329800	3.77569000	-0.56900500
6	-1.50207000	-1.40440000	0.85362200
6	-0.28121300	-1.78292000	1.62423000
6	0.98708300	0.23139900	0.93212200
6	0.85116500	-1.08192000	1.61457000
1	1.68859000	-1.39378000	2.22185000
8	-2.64034000	0.79913500	2.18221000
8	0.77754100	2.01215000	-1.73715000
8	-0.29632000	-2.96244000	2.30567000
8	0.69970800	1.21222000	1.94249000

8	2.25451000	0.47667500	0.44342800
6	-1.55177000	-3.55438000	2.60693000
1	-2.10889000	-3.81894000	1.70842000
1	-1.32267000	-4.45929000	3.15785000
1	-2.16191000	-2.90353000	3.23261000
6	1.48312000	2.39470000	1.92915000
1	1.51977000	2.87605000	0.95160500
1	1.00900000	3.06594000	2.64143000
1	2.50469000	2.19083000	2.24592000
14	3.26251000	-0.41239200	-0.55374600
6	2.32026000	-1.43789000	-1.79534000
1	1.25740000	-1.20290000	-1.79511000
1	2.70003000	-1.23883000	-2.79738000
1	2.44298000	-2.50680000	-1.61529000
6	4.28343000	0.89889600	-1.37929000
1	5.04653000	0.46967900	-2.02718000
1	3.64255000	1.54004000	-1.98144000
1	4.78526000	1.52498000	-0.64292700
6	4.29810000	-1.53702000	0.51454500
1	5.06336000	-2.04321000	-0.07321360
1	4.80161000	-0.98063700	1.30345000
1	3.68912000	-2.30621000	0.98802400
1	-2.38833000	-1.45312000	1.48474000
1	-1.63968000	-2.13496000	0.05457330
1	0.25551900	-0.33501500	-1.00391000
8	-2.42537000	3.33651000	1.48451000
6	-2.19724000	4.71396000	1.21285000
1	-2.47831000	4.96278000	0.19029800
1	-2.82057000	5.26580000	1.90560000
1	-1.14829000	4.96591000	1.37244000
53	-2.89935000	0.03768600	-1.42328000

π_complex_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.319650	0.719022	1.652005
6	1.230594	1.616336	0.968748
6	2.437640	1.201932	0.522443
6	2.931086	-0.183037	0.767396
6	1.963268	-1.061200	1.439637
6	0.758396	-0.666274	1.859009
1	0.877104	2.625379	0.821925
6	1.661961	-0.399122	-2.008175
6	0.715288	-1.203188	-1.476662
6	-1.198808	0.375274	-1.047119
6	-0.601276	-0.843453	-1.031263
1	-1.171548	-1.654245	-0.607771
8	4.060026	-0.540271	0.496351
8	-0.783976	1.101496	2.050543
8	0.912468	-2.533193	-1.217190
8	-0.594325	1.446228	-1.584726
8	-2.388512	0.639134	-0.543056
6	2.182472	-3.074153	-1.549527
1	2.978966	-2.583203	-0.991834
1	2.140549	-4.119841	-1.271681
1	2.377661	-2.983870	-2.618018
6	-1.245866	2.709710	-1.400469
1	-1.454135	2.888831	-0.349207
1	-0.551789	3.447533	-1.782257
1	-2.173468	2.751111	-1.964185
14	-3.579509	-0.312309	0.228552
6	-2.875431	-1.369171	1.579085

1	-2.249276	-0.763117	2.232144
1	-3.691910	-1.771480	2.179700
1	-2.293384	-2.215678	1.221371
6	-4.671212	1.014626	0.919532
1	-5.519630	0.609531	1.467370
1	-4.098797	1.633259	1.609764
1	-5.062210	1.662896	0.137942
6	-4.385423	-1.323513	-1.105570
1	-5.175629	-1.953077	-0.699713
1	-4.831599	-0.693652	-1.872903
1	-3.670197	-1.979381	-1.598986
1	1.434237	0.633043	-2.201155
1	2.638062	-0.758545	-2.283757
9	2.392487	-2.310438	1.630273
1	0.094512	-1.342301	2.375253
8	3.337839	1.933051	-0.139012
6	2.950050	3.253960	-0.491019
1	3.774798	3.662606	-1.059846
1	2.049026	3.233827	-1.105592
1	2.776897	3.858579	0.397644

π_complex_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.264700	0.852473	-1.613365
6	-1.182200	1.793350	-1.007788
6	-2.365425	1.390026	-0.498232
6	-2.850620	-0.017525	-0.626991
6	-1.886209	-0.948184	-1.248901
6	-0.693910	-0.547439	-1.709778
1	-0.844388	2.815855	-0.943409
6	-1.480596	0.023584	2.105361
6	-0.570352	-0.885096	1.693491
6	1.381108	0.544331	0.989613
6	0.746271	-0.641907	1.173717
1	1.288780	-1.529920	0.892958
8	-3.973609	-0.337638	-0.297686
8	0.846356	1.196073	-2.028615
8	-0.809952	-2.231092	1.657210
8	0.819692	1.704756	1.356675
8	2.574397	0.686267	0.442887
6	-2.080793	-2.672167	2.110150
1	-2.885137	-2.227071	1.525232
1	-2.087975	-3.745923	1.968515
1	-2.222499	-2.435992	3.164412
6	1.462189	2.903259	0.895828
1	1.590002	2.876479	-0.183956
1	0.795190	3.706636	1.182183
1	2.427001	3.034257	1.375452
14	3.672643	-0.441012	-0.217385
6	2.848014	-1.523677	-1.477514
1	2.355180	-0.903623	-2.225358
1	3.592826	-2.133266	-1.988474
1	2.108761	-2.203489	-1.058725
6	4.906175	0.687135	-1.014479
1	5.728933	0.136941	-1.465971
1	4.424363	1.266990	-1.800426
1	5.332224	1.388639	-0.300304
6	4.377551	-1.406042	1.205910
1	5.106750	-2.136616	0.859355
1	4.883485	-0.754403	1.915378

1	3.609859	-1.950061	1.752581
1	-1.214151	1.063867	2.135522
1	-2.462567	-0.254058	2.446798
17	-2.412421	-2.579412	-1.394912
1	-0.008510	-1.236194	-2.179149
8	-3.255848	2.155581	0.137372
6	-2.873523	3.502666	0.384710
1	-3.682986	3.943992	0.951680
1	-1.952454	3.535194	0.968491
1	-2.734693	4.045629	-0.549035

π_complex_Br:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	0.042353	0.850425	-1.653525
6	-0.661853	2.019127	-1.174781
6	-1.861886	1.913484	-0.565135
6	-2.586075	0.609824	-0.445131
6	-1.834465	-0.557229	-0.941759
6	-0.623921	-0.450559	-1.502286
1	-0.153426	2.963847	-1.288919
6	-1.065507	0.836677	2.194470
6	-0.356515	-0.276123	1.906084
6	1.759707	0.649472	0.902831
6	0.939909	-0.360548	1.292935
1	1.291932	-1.365329	1.122731
8	-3.724411	0.554993	-0.027837
8	1.165864	0.921530	-2.160514
8	-0.820371	-1.544401	2.122128
8	1.436444	1.933779	1.109900
8	2.919490	0.489565	0.292959
6	-2.103358	-1.668933	2.716326
1	-2.870454	-1.199345	2.100844
1	-2.297423	-2.732469	2.779994
1	-2.115055	-1.228546	3.713020
6	2.243319	2.915946	0.442595
1	2.290044	2.710261	-0.624521
1	1.746621	3.859988	0.628441
1	3.246862	2.937808	0.855406
14	3.768761	-0.905456	-0.202185
6	2.705530	-1.999342	-1.257537
1	2.221478	-1.398807	-2.026900
1	3.329397	-2.737627	-1.762030
1	1.939590	-2.543449	-0.708974
6	5.141432	-0.160191	-1.197600
1	5.856823	-0.913821	-1.520728
1	4.742934	0.320789	-2.089265
1	5.687608	0.591607	-0.631489
6	4.367050	-1.752853	1.339641
1	4.931754	-2.651409	1.096531
1	5.021079	-1.105769	1.920628
1	3.545487	-2.053102	1.986667
1	-0.627604	1.802871	2.025060
1	-2.048420	0.800622	2.630688
35	-2.720582	-2.238864	-0.803856
1	-0.091388	-1.310579	-1.877987
8	-2.567104	2.913412	-0.030713
6	-1.948330	4.193918	-0.021309
1	-2.634381	4.853667	0.493649
1	-0.999999	4.154036	0.516278
1	-1.779376	4.551787	-1.035864

π_complex_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.401072	0.920427	-1.661922
6	-0.073492	2.215566	-1.234444
6	-1.251080	2.350751	-0.590318
6	-2.186137	1.201296	-0.383069
6	-1.665366	-0.105887	-0.822227
6	-0.472120	-0.234761	-1.414469
1	0.583387	3.051956	-1.415380
6	-0.560358	1.296370	2.195492
6	-0.066214	0.063862	1.956204
6	2.134093	0.547397	0.833706
6	1.161750	-0.279729	1.297179
1	1.324947	-1.336749	1.161558
8	-3.307902	1.375854	0.051615
8	1.496210	0.769485	-2.214238
8	-0.719330	-1.088355	2.296801
8	2.054846	1.874828	0.993992
8	3.224599	0.155286	0.207070
6	-1.943444	-0.945025	2.994674
1	-2.680532	-0.400111	2.403298
1	-2.305435	-1.951531	3.176558
1	-1.793331	-0.428716	3.944181
6	2.974766	2.668295	0.235983
1	2.946927	2.390901	-0.815743
1	2.641080	3.691689	0.366173
1	3.987245	2.560935	0.615734
14	3.787128	-1.396981	-0.200918
6	2.536067	-2.315079	-1.218060
1	2.165319	-1.663636	-2.008546
1	3.009540	-3.177859	-1.686783
1	1.687558	-2.678378	-0.641620
6	5.294592	-0.980946	-1.197502
1	5.843577	-1.876536	-1.483431
1	5.016678	-0.455399	-2.109764
1	5.973068	-0.340926	-0.635885
6	4.203633	-2.263693	1.392080
1	4.575460	-3.269868	1.202806
1	4.975078	-1.725627	1.939924
1	3.335406	-2.351756	2.042159
1	0.021042	2.160537	1.937471
1	-1.505888	1.453995	2.683438
53	-2.942986	-1.753316	-0.538920
1	-0.094919	-1.189312	-1.749120
8	-1.754538	3.489231	-0.104500
6	-0.915052	4.631512	-0.184960
1	-1.451065	5.436929	0.304088
1	0.029578	4.450969	0.331594
1	-0.713615	4.899191	-1.223125

TS1_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.416493	-1.250300	-1.067603
6	1.575990	-1.974205	-0.468003
6	2.746193	-1.360410	-0.210003

6	2.939999	0.090289	-0.556903
6	1.678002	0.842695	-0.890503
6	0.577799	0.130200	-1.373403
1	1.412385	-3.029704	-0.273803
6	1.478905	1.603196	0.920297
6	0.209008	2.213701	0.827697
6	-1.186701	0.170107	1.112297
6	-1.010795	1.514607	0.817597
1	-1.885893	2.054910	0.474997
8	4.025701	0.617785	-0.547603
8	-0.641810	-1.886895	-1.245003
8	0.056614	3.503602	0.482197
8	-0.258204	-0.519197	1.757297
8	-2.291704	-0.482488	0.889497
6	1.190017	4.363397	0.453197
1	1.898916	4.049294	-0.316503
1	0.794722	5.350499	0.215597
1	1.678318	4.386795	1.433297
6	-0.508210	-1.905996	2.035397
1	-0.779612	-2.433395	1.118897
1	0.433689	-2.278900	2.435997
1	-1.302110	-1.995592	2.780497
14	-3.526503	-0.441283	-0.323903
6	-2.956400	0.348215	-1.910603
1	-2.196003	-0.283988	-2.378003
1	-3.820200	0.414519	-2.584503
1	-2.557396	1.359013	-1.783103
6	-3.934311	-2.242581	-0.539703
1	-4.744912	-2.381977	-1.263503
1	-3.043414	-2.760985	-0.910303
1	-4.242613	-2.698479	0.407197
6	-4.911599	0.533623	0.474297
1	-5.797199	0.546127	-0.171303
1	-5.202001	0.092925	1.433897
1	-4.619295	1.574122	0.655797
1	1.532202	0.716495	1.539797
1	2.358008	2.237792	0.971197
9	1.946207	2.023094	-1.527603
1	-0.231299	0.667803	-1.851503
8	3.860690	-1.907915	0.299097
6	3.813984	-3.291414	0.587197
1	4.797983	-3.552119	0.975097
1	3.047183	-3.505811	1.342297
1	3.603182	-3.869114	-0.320403

TS1_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.214139	-1.339279	1.039709
6	-1.284078	-2.183883	0.441879
6	-2.497430	-1.686298	0.138325
6	-2.843723	-0.249757	0.432821
6	-1.668292	0.639440	0.776459
6	-0.501680	0.035322	1.272637
1	-1.025436	-3.227261	0.290255
6	-1.509364	1.324814	-1.071214

6	-0.294604	2.052408	-1.047506
6	1.267810	0.115879	-1.139906
6	0.970200	1.459096	-0.934896
1	1.791393	2.094539	-0.621864
8	-3.980087	0.148400	0.360777
8	0.887983	-1.871222	1.287121
8	-0.257131	3.385285	-0.870227
8	0.434070	-0.676835	-1.795805
8	2.412048	-0.424980	-0.842465
6	-1.428985	4.157311	-1.101620
1	-2.191923	3.953945	-0.346462
1	-1.107507	5.195985	-1.030537
1	-1.825397	3.959187	-2.103301
6	0.826813	-2.041340	-2.013387
1	1.104562	-2.511522	-1.068147
1	-0.054277	-2.515600	-2.444009
1	1.661413	-2.075560	-2.717623
14	3.612947	-0.229372	0.389641
6	2.958688	0.598342	1.923846
1	2.259995	-0.070552	2.433772
1	3.809025	0.791543	2.590540
1	2.465972	1.556739	1.732209
6	4.156067	-1.980873	0.696205
1	4.960787	-2.024028	1.438552
1	3.300102	-2.550781	1.073060
1	4.518423	-2.450675	-0.224548
6	4.936557	0.809182	-0.432877
1	5.814967	0.892958	0.217500
1	5.261303	0.361408	-1.378087
1	4.583443	1.825019	-0.643415
1	-1.477279	0.383744	-1.607956
1	-2.438634	1.872579	-1.196218
1	0.241008	0.640114	1.775629
8	-3.542643	-2.352489	-0.376452
6	-3.368072	-3.738196	-0.596342
1	-4.317133	-4.103598	-0.986304
1	-2.570584	-3.919318	-1.327916
1	-3.125353	-4.250865	0.341886
17	-2.169920	2.110877	1.643507

TS1_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.142035	1.470256	-1.051856
6	-0.778267	2.504818	-0.507643
6	-2.028817	2.202868	-0.109461
6	-2.574734	0.802863	-0.247998
6	-1.536699	-0.259069	-0.509516
6	-0.322601	0.123628	-1.096139
1	-0.379907	3.514036	-0.472511
6	-1.418291	-0.765678	1.405295
6	-0.326708	-1.666754	1.417319
6	1.496290	0.007476	1.188949
6	0.998404	-1.291097	1.162788
1	1.690662	-2.075308	0.876266
8	-3.751581	0.575388	-0.112026
8	1.282111	1.818459	-1.417856

8	-0.499543	-3.001659	1.403146
8	0.834042	0.979468	1.799440
8	2.681416	0.340052	0.768421
6	-1.729038	-3.552420	1.858840
1	-2.537425	-3.362203	1.148292
1	-1.553513	-4.625211	1.935769
1	-1.987498	-3.145551	2.842433
6	1.437361	2.282265	1.847435
1	1.723338	2.607689	0.845552
1	0.664835	2.927732	2.263825
1	2.309907	2.258586	2.504574
14	3.767001	-0.205630	-0.464100
6	2.911656	-1.071963	-1.875006
1	2.311882	-0.356876	-2.444449
1	3.689764	-1.475608	-2.535767
1	2.277541	-1.908057	-1.563571
6	4.587367	1.375132	-0.996196
1	5.346365	1.189515	-1.764324
1	3.825244	2.043370	-1.411131
1	5.074360	1.874802	-0.152061
6	4.925454	-1.368951	0.436441
1	5.728585	-1.703144	-0.230468
1	5.388159	-0.880256	1.300210
1	4.401153	-2.262206	0.794608
1	-1.235647	0.210920	1.837861
1	-2.412541	-1.160398	1.592004
1	0.309275	-0.619512	-1.561406
8	-2.949848	3.045714	0.381183
6	-2.576137	4.405272	0.489457
1	-3.442588	4.923687	0.898275
1	-1.719789	4.519973	1.165916
1	-2.322152	4.817336	-0.494155
35	-2.282984	-1.876736	-1.255231

TS1_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.03566810	1.54379000	-1.03595000
6	-0.94757000	2.58239000	-0.63609400
6	-2.18619000	2.25336000	-0.23705700
6	-2.70078000	0.81450000	-0.18207900
6	-1.63176000	-0.20970100	-0.51360900
6	-0.42595000	0.16200300	-1.02028000
1	-0.58592400	3.60407000	-0.70085900
6	-1.40409000	-0.62923400	1.47911000
6	-0.48276300	-1.66779000	1.50420000
6	1.65366000	-0.42691800	1.22153000
6	0.91068400	-1.58040000	1.21697000
1	1.41412000	-2.51195000	0.93476200
8	-3.84003000	0.55549000	0.09536730
8	1.17804000	1.86085000	-1.34211000
8	-0.79923200	-2.97671000	1.72246000
8	1.18349000	0.69647100	1.82105000
8	2.87601000	-0.34868100	0.77339300
6	-2.15788000	-3.32656000	2.10368000
1	-2.85968000	-3.06502000	1.29999000
1	-2.08051000	-4.41391000	2.22166000
1	-2.41632000	-2.83889000	3.04649000
6	1.97184000	1.92016000	1.73818000
1	2.04520000	2.23416000	0.68452500
1	1.35999000	2.61321000	2.32625000

1	2.95708000	1.76113000	2.18366000
14	4.05172000	-0.27894800	-0.45344700
6	3.28308000	-0.92680500	-2.00169000
1	2.47148000	-0.23576400	-2.31296000
1	4.02251000	-0.96104700	-2.81870000
1	2.84919000	-1.93076000	-1.89254000
6	4.53284000	1.49686000	-0.65846700
1	5.32898000	1.57727000	-1.41824000
1	3.65612000	2.06352000	-1.03582000
1	4.89095000	1.97675000	0.25976800
6	5.45630000	-1.32326000	0.15673400
1	6.25939000	-1.33829000	-0.59925500
1	5.87913000	-0.93424500	1.09529000
1	5.13913000	-2.36245000	0.33563400
1	-1.04743000	0.37022300	1.72002000
1	-2.42928000	-0.77993000	1.78624000
1	0.28065500	-0.56952300	-1.41306000
8	-3.18512000	3.07838000	0.17269500
6	-2.92750000	4.50918000	0.15618900
1	-3.88443000	4.90687000	0.51947800
1	-2.10993000	4.75362000	0.83917000
1	-2.72154000	4.84285000	-0.86486000
53	-2.46098000	-2.04692000	-1.31432000

4) *Isoflaviolin* (**N2**) endo structures.

Int1_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.115310	0.959094	-1.403760
6	-0.731761	2.019505	-0.540830
6	-1.968031	1.943189	0.032231
6	-2.840759	0.841435	-0.225125
6	-2.312769	-0.279091	-1.111313
6	-1.045768	-0.001545	-1.763419
6	-2.279559	-1.630490	-0.235578
6	-1.523333	-1.456467	1.010714
6	0.773868	-1.554349	0.063425
6	-0.158391	-1.281626	1.072875
1	0.244665	-0.913944	2.004035
8	-3.973773	0.750110	0.245860
8	1.089302	1.044490	-1.756014
8	-2.136239	-1.268744	2.188963
8	0.483756	-2.389581	-0.909975
8	1.992863	-1.132813	0.079563
6	-3.546930	-1.504606	2.326477
1	-3.781484	-2.540672	2.091635
1	-3.751364	-1.317510	3.371932
1	-4.117134	-0.823637	1.703299
6	1.450427	-2.476152	-1.990108
1	2.345971	-2.972875	-1.630850
1	0.959714	-3.065060	-2.751192
1	1.674924	-1.478837	-2.356407
14	2.984669	0.054793	0.839241
6	2.016031	1.474611	1.514378
1	1.154650	1.194834	2.118794
1	2.667944	2.084012	2.141246
1	1.671967	2.088547	0.686532
6	3.828352	-0.919577	2.181307
1	3.125257	-1.303509	2.918299
1	4.373370	-1.768923	1.773440
1	4.547657	-0.299823	2.713624

6	4.126432	0.552073	-0.521490
1	4.845129	1.298953	-0.189601
1	4.686595	-0.295824	-0.911546
1	3.538743	0.976553	-1.333931
1	-3.085667	-0.500593	-1.849246
1	-1.826939	-2.384286	-0.870958
1	-3.311044	-1.905124	-0.047879
8	0.084495	3.067706	-0.405841
6	-0.346291	4.144313	0.419501
1	-0.546338	3.796056	1.431887
1	0.472912	4.851170	0.430646
1	-1.239142	4.614060	0.011774
1	-2.371360	2.734949	0.644699
9	-0.704986	-0.931873	-2.707307

Int1_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.155150	0.716207	-1.476053
6	-0.731558	1.939203	-0.818819
6	-1.943276	1.995298	-0.198968
6	-2.824573	0.869665	-0.185259
6	-2.334602	-0.418695	-0.831346
6	-1.096581	-0.306869	-1.595423
6	-2.255723	-1.540456	0.322928
6	-1.469545	-1.068028	1.467838
6	0.811092	-1.420946	0.544954
6	-0.106893	-0.862788	1.442084
1	0.309620	-0.241071	2.219903
8	-3.939313	0.894318	0.333797
8	1.022804	0.740044	-1.894967
8	-2.054644	-0.597136	2.578629
8	0.510909	-2.520286	-0.114944
8	2.027702	-1.014783	0.409405
6	-3.451235	-0.833572	2.823667
1	-3.656926	-1.901060	2.831596
1	-3.625206	-0.426013	3.810792
1	-4.064340	-0.321744	2.089165
6	1.519578	-3.029586	-1.020350
1	2.354753	-3.415437	-0.444016
1	1.024193	-3.819077	-1.566652
1	1.845536	-2.246815	-1.695874
14	3.058307	0.313006	0.798787
6	2.131750	1.866541	1.168574
1	1.312668	1.755601	1.877067
1	2.823424	2.598554	1.586671
1	1.733733	2.269760	0.241534
6	3.978563	-0.320914	2.285941
1	3.316802	-0.504895	3.130513
1	4.499518	-1.251075	2.066715
1	4.726525	0.399232	2.612447
6	4.115685	0.453946	-0.705694
1	4.846414	1.254498	-0.605937
1	4.659775	-0.467118	-0.906823
1	3.482228	0.672438	-1.563993
1	-3.147976	-0.787194	-1.457092
1	-1.804698	-2.410845	-0.144132
1	-3.274851	-1.781889	0.602248
8	0.085511	2.987543	-0.949183
6	-0.320724	4.223343	-0.370622
1	-0.474564	4.113580	0.701800
1	0.492476	4.912683	-0.555246

1	-1.233738	4.589134	-0.835910
1	-2.325254	2.901726	0.245962
17	-0.768295	-1.633338	-2.673314

Int1_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.187707	-0.022641	-1.492340
6	0.640664	-1.454671	-1.606078
6	1.793470	-1.955919	-1.083320
6	2.731700	-1.110018	-0.412979
6	2.344335	0.348214	-0.208928
6	1.183503	0.799512	-0.965437
6	2.190463	0.575248	1.385608
6	1.278439	-0.410928	1.970270
6	-0.889828	0.643280	1.365330
6	-0.086050	-0.427435	1.769299
1	-0.601136	-1.350736	1.984491
8	3.808406	-1.511987	0.023770
8	-0.944701	0.289953	-1.917557
8	1.735847	-1.516067	2.577564
8	-0.470503	1.883256	1.518612
8	-2.112422	0.522460	0.974235
6	3.104967	-1.591834	3.010355
1	3.313648	-0.797005	3.722142
1	3.181180	-2.551751	3.503768
1	3.783389	-1.556188	2.163283
6	-1.373785	2.932688	1.097354
1	-2.220604	2.972767	1.775403
1	-0.785539	3.837383	1.149870
1	-1.704060	2.754333	0.080006
14	-3.261921	-0.635139	0.407529
6	-2.491345	-2.234290	-0.096979
1	-1.876934	-2.707291	0.666803
1	-3.290419	-2.935932	-0.341681
1	-1.896053	-2.090749	-0.995126
6	-4.366468	-0.834556	1.890702
1	-3.836108	-1.262166	2.740055
1	-4.783332	0.119016	2.209745
1	-5.202385	-1.494625	1.666450
6	-4.077717	0.253051	-0.986938
1	-4.884273	-0.334309	-1.421679
1	-4.501276	1.201956	-0.662017
1	-3.339499	0.451966	-1.761337
1	3.225888	0.945608	-0.440243
1	1.822060	1.589584	1.501870
1	3.185483	0.510270	1.811033
8	-0.220905	-2.173308	-2.331067
6	0.076280	-3.548434	-2.549969
1	0.141976	-4.084721	-1.604596
1	-0.748041	-3.932444	-3.135670
1	1.009236	-3.660677	-3.098899
1	2.090136	-2.985277	-1.216002
35	1.021136	2.700883	-1.179521

Int1_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	-0.158086	0.098427	-1.430186
6	-0.360279	1.557536	-1.742434
6	-1.385389	2.320321	-1.276965
6	-2.413055	1.758641	-0.459302
6	-2.257596	0.307121	-0.028023
6	-1.232886	-0.455884	-0.737109
6	-2.047983	0.329828	1.573842
6	-0.938419	1.219711	1.931226
6	0.955930	-0.323611	1.500567
6	0.386381	0.942459	1.673940
1	1.073678	1.773812	1.658537
8	-3.386762	2.401866	-0.068711
8	0.871771	-0.467393	-1.861480
8	-1.151964	2.479177	2.338686
8	0.337221	-1.390323	1.970295
8	2.138324	-0.535335	1.042271
6	-2.452369	2.871509	2.802228
1	-2.747947	2.258223	3.652056
1	-2.331580	3.899758	3.123502
1	-3.186113	2.816418	2.002930
6	1.037028	-2.646188	1.868060
1	1.917598	-2.625503	2.505506
1	0.329762	-3.387860	2.215649
1	1.316814	-2.847131	0.839821
14	3.438029	0.238287	0.216800
6	2.983127	1.882383	-0.488846
1	2.571907	2.579917	0.237905
1	3.889760	2.336008	-0.892287
1	2.281367	1.753360	-1.307667
6	4.685611	0.405950	1.588832
1	4.319361	1.057930	2.381419
1	4.921481	-0.559045	2.034571
1	5.616445	0.833409	1.219801
6	3.905178	-1.014979	-1.053184
1	4.769619	-0.696937	-1.633171
1	4.146192	-1.970779	-0.590092
1	3.058749	-1.151961	-1.723585
1	-3.240684	-0.154709	-0.118020
1	-1.856819	-0.699461	1.858236
1	-2.985165	0.653461	2.011309
8	0.575153	2.005818	-2.584718
6	0.520231	3.373564	-2.967441
1	0.607013	4.024093	-2.097085
1	1.365282	3.525565	-3.628690
1	-0.407431	3.597508	-3.493614
1	-1.506280	3.355571	-1.558080
53	-1.405470	-2.555073	-0.659550

Int2_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.630519	-1.473444	0.702253
6	2.224779	-1.059546	-0.603268
6	1.486634	-0.969325	-1.730638
6	0.050804	-1.159819	-1.695855
6	-0.516238	-1.873685	-0.469508
6	0.114327	-1.354454	0.824313
6	-2.030768	-1.853694	-0.442975
6	-2.576085	-0.614239	0.167638
6	-0.390456	0.088429	1.142915
6	-1.848913	0.224173	0.904916

1	-2.327291	1.068841	1.378337
8	-0.671702	-0.821659	-2.618944
8	2.318265	-1.934847	1.577541
8	-3.910120	-0.353836	0.057052
8	-0.212863	0.461893	2.481608
8	0.384476	0.903900	0.278757
6	-4.610839	-0.921889	-1.043138
1	-4.672693	-2.005786	-0.967068
1	-5.609102	-0.505765	-0.997854
1	-4.148916	-0.648376	-1.991844
6	1.120741	0.549008	2.975183
1	1.812185	0.887122	2.202568
1	1.097307	1.285334	3.771570
1	1.452485	-0.407697	3.370167
14	0.035459	2.453515	-0.277409
6	-1.463380	2.478724	-1.383160
1	-2.399974	2.420461	-0.831930
1	-1.486046	3.395210	-1.973678
1	-1.439864	1.640633	-2.080156
6	-0.166416	3.609580	1.168659
1	-0.992684	3.302749	1.808358
1	0.727810	3.637331	1.789067
1	-0.367642	4.628383	0.839994
6	1.572475	2.813584	-1.267165
1	1.624491	3.850206	-1.596029
1	2.470125	2.603707	-0.685276
1	1.598366	2.186814	-2.159090
1	-0.187632	-2.911631	-0.564031
1	-2.411356	-2.710297	0.115544
1	-2.367934	-1.963060	-1.471500
8	3.532517	-0.836067	-0.488820
6	4.238641	-0.485678	-1.677258
1	3.844352	0.435282	-2.102101
1	5.265714	-0.341139	-1.371788
1	4.177646	-1.288060	-2.409497
1	1.908247	-0.665590	-2.677092
9	-0.289284	-2.176144	1.861337

Int2_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.423372	-1.615708	0.258747
6	2.046014	-1.022406	-0.967243
6	1.325422	-0.582009	-2.019182
6	-0.119994	-0.629971	-2.007004
6	-0.770676	-1.523443	-0.952042
6	-0.092110	-1.403368	0.421384
6	-2.266452	-1.307461	-0.905592
6	-2.613399	-0.092068	-0.128888
6	-0.418788	-0.006740	1.082595
6	-1.788597	0.466464	0.756157
1	-2.141509	1.293700	1.352396
8	-0.795429	-0.054131	-2.843775
8	2.100906	-2.237866	1.034057
8	-3.862553	0.439162	-0.237847
8	-0.373633	-0.001386	2.481233
8	0.598569	0.833998	0.560380
6	-4.581843	0.212883	-1.444615
1	-4.874649	-0.830738	-1.548880
1	-5.473450	0.822582	-1.369733
1	-4.005876	0.523718	-2.315937

6	0.879315	-0.273579	3.102346
1	1.687436	0.289147	2.635632
1	0.769399	0.044859	4.132891
1	1.110615	-1.335083	3.076721
14	0.582767	2.496680	0.310505
6	-0.159459	2.877300	-1.352643
1	-1.206518	2.581438	-1.406222
1	-0.107448	3.944308	-1.569383
1	0.355397	2.354674	-2.157753
6	-0.315023	3.395907	1.672640
1	-1.394162	3.385958	1.532240
1	-0.107720	2.953301	2.646523
1	-0.011163	4.441407	1.711399
6	2.402881	2.886642	0.333223
1	2.613307	3.911932	0.033984
1	2.829348	2.737194	1.323887
1	2.940187	2.227299	-0.347614
1	-0.579890	-2.542449	-1.298477
1	-2.759947	-2.171376	-0.456750
1	-2.614573	-1.227532	-1.931665
8	3.373503	-1.006108	-0.863464
6	4.102501	-0.510070	-1.983020
1	3.849853	0.531165	-2.176540
1	5.146458	-0.589474	-1.712731
1	3.897824	-1.107795	-2.868652
1	1.781634	-0.132560	-2.888040
17	-0.736069	-2.710752	1.471163

Int2_Br:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	1.124109	-1.709324	-0.114747
6	2.007924	-1.095775	-1.155650
6	1.555300	-0.245749	-2.099222
6	0.158891	0.128008	-2.151001
6	-0.815074	-0.786490	-1.405232
6	-0.299564	-1.141589	-0.004896
6	-2.215210	-0.216952	-1.418943
6	-2.395486	0.821509	-0.374606
6	-0.375638	0.120888	0.932956
6	-1.590839	0.939581	0.679741
1	-1.823725	1.668450	1.441707
8	-0.240787	1.064843	-2.821422
8	1.547254	-2.614729	0.557803
8	-3.488078	1.634887	-0.428925
8	-0.424279	-0.158682	2.304658
8	0.820886	0.815037	0.611731
6	-4.027856	1.925475	-1.714572
1	-4.507174	1.054653	-2.158021
1	-4.772210	2.694245	-1.551131
1	-3.258747	2.303683	-2.388073
6	0.697836	-0.816604	2.885827
1	1.636304	-0.393029	2.527648
1	0.614641	-0.648140	3.954068
1	0.675878	-1.884372	2.681094
14	1.172698	2.440153	0.883976
6	0.348532	3.518858	-0.388332
1	-0.731775	3.558106	-0.256110
1	0.722337	4.541274	-0.328822
1	0.534699	3.155983	-1.398420
6	0.690340	2.944784	2.610479

1	-0.385538	2.899260	2.768894
1	1.151541	2.307230	3.362741
1	1.002675	3.969212	2.811591
6	3.021580	2.448300	0.665375
1	3.462279	3.417696	0.892251
1	3.493878	1.713018	1.316262
1	3.291618	2.200484	-0.360553
1	-0.815453	-1.714129	-1.983548
1	-2.945597	-1.011873	-1.254639
1	-2.393215	0.190962	-2.410266
8	3.266606	-1.509302	-1.011177
6	4.205250	-1.067070	-1.987713
1	4.337606	0.011511	-1.932599
1	5.135785	-1.564761	-1.752431
1	3.876216	-1.344350	-2.987027
1	2.207276	0.227231	-2.817199
35	-1.466298	-2.570801	0.742537

Int2_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.139133	-1.959540	-0.261909
6	1.069063	-2.135700	-1.159127
6	1.467641	-1.193112	-2.036470
6	0.758817	0.087209	-2.117265
6	-0.679159	0.119782	-1.572863
6	-0.760761	-0.551215	-0.183708
6	-1.254029	1.529944	-1.623006
6	-0.878972	2.338339	-0.416529
6	-0.020201	0.356462	0.873566
6	-0.367360	1.807905	0.694897
1	-0.177505	2.442301	1.556610
8	1.252270	1.051328	-2.673011
8	-0.559541	-2.916309	0.336970
8	-1.189969	3.665678	-0.408182
8	-0.330674	0.091098	2.209830
8	1.339462	0.097596	0.619248
6	-1.081889	4.371471	-1.634529
1	-1.866705	4.077377	-2.340273
1	-1.208263	5.424620	-1.382115
1	-0.096760	4.219465	-2.091349
6	0.016179	-1.173001	2.757356
1	0.964486	-1.539718	2.349631
1	0.124513	-1.012566	3.832035
1	-0.773143	-1.906933	2.571282
14	2.687288	1.018912	1.067793
6	2.745937	2.659995	0.165182
1	2.046902	3.390876	0.583025
1	3.757544	3.080433	0.227170
1	2.497755	2.520959	-0.893465
6	2.684030	1.258621	2.926806
1	1.779913	1.783378	3.254310
1	2.716530	0.296033	3.449510
1	3.553064	1.846526	3.244758
6	4.090106	-0.086661	0.501358
1	5.065940	0.302460	0.812343
1	3.976683	-1.095912	0.913814
1	4.089487	-0.160838	-0.592642
1	-1.249894	-0.510096	-2.270126
1	-2.349157	1.491129	-1.687133
1	-0.883570	2.001201	-2.537165

8	1.650340	-3.315813	-0.949741
6	2.798932	-3.619701	-1.723940
1	3.595239	-2.891583	-1.531252
1	3.116670	-4.612285	-1.408838
1	2.551653	-3.625593	-2.791434
1	2.355002	-1.290773	-2.652158
53	-2.852806	-0.768842	0.381406

π_complex_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.459302	-0.107388	-1.728392
6	-1.359924	1.006232	-1.326423
6	-2.623953	0.787345	-0.909865
6	-3.157945	-0.558833	-0.772663
6	-2.251880	-1.678891	-1.061684
6	-1.022273	-1.444091	-1.525334
6	-1.853034	-1.234239	2.068119
6	-1.180785	-0.088764	1.837099
6	0.987592	-0.902649	0.844762
6	0.118468	0.065446	1.248268
1	0.429766	1.084271	1.081907
8	-4.321664	-0.761115	-0.436714
8	0.649446	0.076126	-2.203416
8	-1.698471	1.161465	2.085768
8	0.695522	-2.199231	0.996298
8	2.137684	-0.671035	0.244856
6	-3.025841	1.210126	2.582865
1	-3.093853	0.744161	3.566042
1	-3.275604	2.261789	2.663726
1	-3.718695	0.715870	1.900544
6	1.685114	-3.148022	0.572122
1	2.579792	-3.063607	1.182765
1	1.226193	-4.115515	0.721081
1	1.936857	-3.003303	-0.472033
14	3.174166	0.686687	0.169582
6	2.311110	2.264964	-0.281526
1	1.751594	2.708684	0.540099
1	3.066022	2.993493	-0.581563
1	1.635474	2.125149	-1.123422
6	3.934550	0.787731	1.863941
1	3.163840	0.927288	2.621242
1	4.480339	-0.120077	2.114039
1	4.627132	1.622740	1.952822
6	4.351803	0.162994	-1.158012
1	5.122885	0.910205	-1.333560
1	4.846732	-0.773393	-0.908501
1	3.816757	0.013779	-2.094481
1	-2.629299	-2.679488	-0.923467
1	-1.384597	-2.178571	1.864052
1	-2.849434	-1.247172	2.474449
8	-0.750218	2.192981	-1.435093
6	-1.458052	3.321960	-0.933264
1	-1.762793	3.148531	0.098530
1	-0.762242	4.149792	-0.982073
1	-2.330549	3.536247	-1.547959
1	-3.293742	1.589921	-0.643323
9	-0.188131	-2.446830	-1.830972

π_complex_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.479623	0.254599	-1.616969
6	1.460763	-0.844880	-1.396904
6	2.724745	-0.611894	-0.982833
6	3.171572	0.723205	-0.633032
6	2.176849	1.804832	-0.708039
6	0.946335	1.588745	-1.196538
6	1.829725	0.788679	2.318215
6	1.228790	-0.328110	1.858677
6	-1.021709	0.525790	1.119897
6	-0.050127	-0.427053	1.217373
1	-0.258469	-1.372736	0.733911
8	4.326973	0.955924	-0.284211
8	-0.612553	0.047678	-2.119073
8	1.827294	-1.566076	1.851017
8	-0.864644	1.728232	1.684661
8	-2.132162	0.390271	0.424364
6	3.179904	-1.616947	2.273962
1	3.270343	-1.370589	3.336192
1	3.499160	-2.645478	2.114671
1	3.801217	-0.934622	1.685237
6	-1.989139	2.616659	1.652846
1	-2.842954	2.171300	2.165478
1	-1.653099	3.504209	2.181710
1	-2.262751	2.868686	0.629522
14	-3.141259	-0.920064	-0.006167
6	-2.212152	-2.445272	-0.505461
1	-1.723388	-2.952059	0.330348
1	-2.919828	-3.161880	-0.937832
1	-1.463234	-2.230728	-1.271386
6	-4.153374	-1.216789	1.527455
1	-3.504548	-1.400523	2.389493
1	-4.781100	-0.355229	1.770107
1	-4.814866	-2.082633	1.435214
6	-4.098142	-0.201460	-1.415963
1	-4.867658	-0.882584	-1.788353
1	-4.592364	0.731219	-1.134095
1	-3.420783	0.022354	-2.243945
1	2.508173	2.787388	-0.393944
1	1.304762	1.730545	2.293623
1	2.827325	0.783176	2.734431
8	0.922270	-2.041798	-1.665493
6	1.717069	-3.180374	-1.346934
1	2.004585	-3.155638	-0.292808
1	1.087069	-4.042391	-1.549500
1	2.608290	-3.216592	-1.979082
1	3.450988	-1.405936	-0.854216
17	-0.197710	2.870553	-1.376063

π_complex_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.484917	0.441154	-1.457095
6	1.511106	-0.637035	-1.544360
6	2.762900	-0.484379	-1.068338
6	3.161092	0.722729	-0.371166
6	2.129516	1.755389	-0.168182
6	0.907976	1.629189	-0.701534

6	1.890935	-0.042785	2.462120
6	1.332910	-1.029833	1.732811
6	-0.972069	-0.135517	1.275076
6	0.046635	-1.021187	1.097407
1	-0.116666	-1.796329	0.365872
8	4.307535	0.898730	0.032416
8	-0.605757	0.326712	-1.988749
8	1.983367	-2.196408	1.404999
8	-0.877673	0.852418	2.172583
8	-2.085011	-0.129323	0.570889
6	3.337670	-2.301921	1.816537
1	3.417316	-2.320146	2.903255
1	3.699861	-3.241164	1.414424
1	3.931700	-1.475706	1.424736
6	-2.063115	1.620154	2.423989
1	-2.859054	0.980470	2.795835
1	-1.776188	2.336350	3.182019
1	-2.390823	2.130794	1.524249
14	-3.038941	-1.330182	-0.181702
6	-2.055503	-2.575445	-1.140595
1	-1.480892	-3.246431	-0.503588
1	-2.744799	-3.196415	-1.714205
1	-1.377487	-2.094960	-1.844474
6	-3.940980	-2.142998	1.228459
1	-3.234062	-2.521692	1.966028
1	-4.607673	-1.450731	1.739820
1	-4.540783	-2.988661	0.896650
6	-4.115411	-0.300138	-1.277286
1	-4.857364	-0.897680	-1.802379
1	-4.641635	0.466430	-0.712471
1	-3.498760	0.201696	-2.021203
1	2.433203	2.629632	0.386004
1	1.322828	0.842988	2.677983
1	2.887225	-0.110327	2.863294
8	1.015450	-1.733198	-2.132361
6	1.832582	-2.900651	-2.100156
1	2.116879	-3.129865	-1.073227
1	1.220179	-3.694646	-2.507161
1	2.721609	-2.773504	-2.714990
1	3.512634	-1.255227	-1.155442
35	-0.400066	3.014168	-0.550615

π_complex_l:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.475140	0.390162	-1.393903
6	1.723142	-0.408718	-1.552266
6	2.910975	0.002133	-1.067932
6	3.024309	1.221585	-0.293397
6	1.781390	1.967098	-0.025389
6	0.613719	1.597191	-0.566876
6	2.001166	0.011385	2.458282
6	1.677888	-1.035106	1.674512
6	-0.780212	-0.688059	1.288061
6	0.418164	-1.280093	1.036343
1	0.429644	-2.003226	0.237867
8	4.104282	1.641874	0.116034
8	-0.563545	0.052233	-1.938171
8	2.571918	-2.006577	1.293838
8	-0.913128	0.205003	2.276683
8	-1.869548	-0.887168	0.579537

6	3.922173	-1.796648	1.668288
1	4.046031	-1.841448	2.751302
1	4.491595	-2.598344	1.209046
1	4.283583	-0.831933	1.309273
6	-2.245719	0.598853	2.618871
1	-2.831404	-0.261600	2.936451
1	-2.133220	1.294347	3.441635
1	-2.735734	1.086066	1.780978
14	-2.514185	-2.227985	-0.246547
6	-1.264048	-3.178013	-1.234635
1	-0.564175	-3.728201	-0.607482
1	-1.790152	-3.908633	-1.850055
1	-0.704564	-2.518334	-1.895051
6	-3.228815	-3.278286	1.115833
1	-2.454891	-3.521022	1.844519
1	-4.027015	-2.754539	1.639701
1	-3.633815	-4.218151	0.745071
6	-3.782432	-1.416400	-1.323419
1	-4.367256	-2.143541	-1.883498
1	-4.468895	-0.813622	-0.731451
1	-3.284944	-0.757866	-2.033435
1	1.887052	2.846659	0.591713
1	1.248198	0.732746	2.714694
1	2.990020	0.153004	2.857856
8	1.491787	-1.547859	-2.217615
6	2.560169	-2.486129	-2.257529
1	2.908913	-2.703632	-1.247481
1	2.149065	-3.379075	-2.713618
1	3.386866	-2.116632	-2.864067
1	3.817901	-0.565515	-1.205645
53	-1.148309	2.731293	-0.326947

TS1_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.347992	0.722417	-1.560703
6	-1.058771	1.784486	-0.766312
6	-2.293895	1.623921	-0.227904
6	-3.055799	0.424012	-0.463603
6	-2.353402	-0.697765	-1.156978
6	-1.155998	-0.406665	-1.808458
6	-2.080480	-1.917038	0.385155
6	-1.316985	-1.235644	1.350256
6	0.937287	-1.397421	0.287033
6	0.039210	-0.908747	1.216725
1	0.421694	-0.184571	1.918089
8	-4.218617	0.293028	-0.090933
8	0.815102	0.897219	-1.960660
8	-1.870528	-0.629397	2.426959
8	0.638919	-2.437844	-0.474224
8	2.140409	-0.932888	0.116266
6	-3.226687	-0.929744	2.766750
1	-3.357611	-2.001524	2.910682
1	-3.406461	-0.412577	3.700437
1	-3.914359	-0.567668	2.008229
6	1.566638	-2.756105	-1.535158
1	2.478810	-3.170477	-1.117315
1	1.053041	-3.491166	-2.138043
1	1.779470	-1.868178	-2.120542
14	3.125032	0.353570	0.680142
6	2.170398	1.906077	0.979938

1	1.401446	1.823682	1.745455
1	2.859167	2.689401	1.297978
1	1.702699	2.225400	0.051217
6	3.903973	-0.313384	2.230722
1	3.156241	-0.542158	2.988524
1	4.468998	-1.223225	2.040011
1	4.589107	0.410846	2.668691
6	4.302004	0.539967	-0.731940
1	5.052797	1.304452	-0.544468
1	4.825173	-0.389483	-0.946507
1	3.745558	0.826405	-1.623303
1	-3.021061	-1.392789	-1.649241
1	-1.565883	-2.680807	-0.172455
1	-3.103467	-2.158499	0.631594
8	-0.326597	2.896854	-0.677703
6	-0.846217	3.963091	0.107397
1	-0.983049	3.643891	1.139542
1	-0.107957	4.753178	0.056762
1	-1.793449	4.316708	-0.294367
1	-2.793288	2.403316	0.326952
9	-0.640807	-1.374295	-2.617232

TS1_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.372553	0.271259	-1.578297
6	-1.160623	1.479607	-1.143617
6	-2.426688	1.427484	-0.667961
6	-3.120767	0.169502	-0.556427
6	-2.307529	-1.062616	-0.771911
6	-1.095154	-0.944073	-1.460456
6	-2.023166	-1.550906	1.149074
6	-1.309173	-0.496140	1.745772
6	0.985715	-1.027715	0.926942
6	0.031866	-0.189696	1.475845
1	0.355675	0.809940	1.720286
8	-4.308369	0.088826	-0.256498
8	0.776929	0.412359	-2.013703
8	-1.907358	0.476497	2.473297
8	0.754756	-2.327767	0.811248
8	2.171785	-0.654853	0.556626
6	-3.270967	0.300946	2.866814
1	-3.389686	-0.616431	3.441159
1	-3.499299	1.153974	3.492966
1	-3.934348	0.290175	2.006820
6	1.814841	-3.138835	0.268577
1	2.648316	-3.168518	0.964784
1	1.380764	-4.121768	0.154268
1	2.136747	-2.749728	-0.690449
14	3.166630	0.738295	0.403420
6	2.220510	2.324800	0.424476
1	1.750846	2.545226	1.382108
1	2.919015	3.137466	0.220618
1	1.468872	2.336276	-0.362284
6	4.282357	0.591866	1.883976
1	3.714948	0.612422	2.813426
1	4.855472	-0.332815	1.867251
1	4.993268	1.415548	1.926567
6	4.031507	0.431983	-1.198122
1	4.765907	1.204343	-1.417174
1	4.551060	-0.524196	-1.188859

1	3.301761	0.413044	-2.005242
1	-2.908079	-1.939187	-0.970331
1	-1.461244	-2.444066	0.933756
1	-3.037016	-1.731232	1.475600
8	-0.457699	2.602072	-1.320943
6	-1.044479	3.821156	-0.879297
1	-1.255846	3.779306	0.189327
1	-0.308735	4.587649	-1.084231
1	-1.959703	4.033399	-1.427391
1	-2.989919	2.311841	-0.411644
17	-0.358007	-2.386330	-2.093633

TS1_Br:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	0.382749	0.061666	-1.474596
6	1.149482	-1.236763	-1.509703
6	2.408336	-1.385634	-1.036179
6	3.110849	-0.274240	-0.446446
6	2.308036	0.958075	-0.183576
6	1.112502	1.127208	-0.890223
6	1.993896	0.664879	1.769832
6	1.253722	-0.524907	1.897889
6	-1.018967	0.334551	1.342581
6	-0.085047	-0.672539	1.509649
1	-0.425820	-1.678926	1.322418
8	4.294004	-0.328396	-0.125187
8	-0.753529	0.109314	-1.960540
8	1.823848	-1.716537	2.192895
8	-0.770237	1.561265	1.779914
8	-2.201462	0.169987	0.835944
6	3.181264	-1.737294	2.642828
1	3.300231	-1.120239	3.531898
1	3.384856	-2.771852	2.888676
1	3.862924	-1.404411	1.865403
6	-1.823265	2.535749	1.647514
1	-2.648463	2.273824	2.304377
1	-1.374755	3.469941	1.954009
1	-2.160007	2.596361	0.619021
14	-3.217111	-1.024219	0.129133
6	-2.303290	-2.517811	-0.459822
1	-1.865960	-3.111211	0.341992
1	-3.011272	-3.163686	-0.981034
1	-1.529454	-2.242664	-1.173557
6	-4.366346	-1.439154	1.531255
1	-3.822848	-1.840203	2.385611
1	-4.918041	-0.565312	1.871792
1	-5.096421	-2.190837	1.235859
6	-4.034194	-0.085480	-1.233961
1	-4.775700	-0.687034	-1.755384
1	-4.536607	0.801714	-0.853199
1	-3.283210	0.233571	-1.954364
1	2.921845	1.832737	-0.020168
1	1.448111	1.582201	1.914073
1	3.002813	0.682879	2.155653
8	0.438382	-2.200541	-2.102132
6	1.005884	-3.504788	-2.140987
1	1.199129	-3.868967	-1.131996
1	0.267728	-4.128787	-2.628425
1	1.928637	-3.511391	-2.716936
1	2.958939	-2.309536	-1.127520

35	0.340319	2.882258	-0.989130

TS1_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.47990000	0.10414900	-1.59487000
6	-1.48093000	1.19383000	-1.32246000
6	-2.74039000	0.96118000	-0.88770500
6	-3.16567000	-0.37536800	-0.55543600
6	-2.08509000	-1.40020000	-0.46130600
6	-0.90846600	-1.18323000	-1.18749000
6	-1.81869000	-1.25112000	1.52181000
6	-1.23529000	0.00159119	1.78340000
6	1.14400000	-0.51227400	1.26397000
6	0.07994470	0.35190500	1.44296000
1	0.29671000	1.40374000	1.34296000
8	-4.33096000	-0.66281200	-0.29655500
8	0.58083500	0.39224800	-2.16593000
8	-1.94368000	1.07335000	2.20573000
8	1.03579000	-1.78677000	1.62092000
8	2.32434000	-0.16498300	0.86099400
6	-3.30657000	0.88325700	2.58018000
1	-3.38518000	0.15163800	3.38356000
1	-3.64423000	1.84931000	2.93709000
1	-3.91663000	0.57032900	1.73486000
6	2.21574000	-2.59997000	1.52017000
1	2.96969000	-2.25170000	2.22157000
1	1.89107000	-3.59885000	1.78129000
1	2.60781000	-2.58721000	0.50894200
14	3.15465000	1.07610000	0.00768171
6	2.10443000	2.56544000	-0.30062200
1	1.76728000	3.04537000	0.61753900
1	2.70917000	3.29408000	-0.84167900
1	1.25058000	2.31714000	-0.92778100
1	4.54531000	1.44837000	1.18589000
1	4.17837000	1.87104000	2.12001000
1	5.11121000	0.55004900	1.42697000
1	5.23885000	2.16832000	0.75336100
6	3.71875000	0.21688000	-1.52741000
1	4.34814000	0.85733200	-2.14253000
1	4.28806000	-0.67823900	-1.27952000
1	2.84480000	-0.07447470	-2.10852000
1	-2.46827000	-2.40976000	-0.40004500
1	-1.15616000	-2.09695000	1.56572000
1	-2.81411000	-1.44673000	1.89359000
8	-0.98349000	2.40031000	-1.61474000
6	-1.80410000	3.52207000	-1.32075000
1	-2.09831000	3.51871000	-0.27032900
1	-1.19937000	4.39572000	-1.53267000
1	-2.69482000	3.53199000	-1.94910000
1	-3.48001000	1.74187000	-0.79550400
53	0.35631400	-2.79960000	-1.68060000

TS2_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.132608	1.300427	1.362840
6	0.354934	2.289764	0.329851

6	1.588892	2.235665	-0.265214
6	2.533984	1.184619	0.021359
6	2.153007	0.130643	1.071826
6	0.775529	0.238842	1.601964
6	2.500730	-1.314618	0.532766
6	1.767371	-1.569688	-0.740323
6	-0.485820	-1.466111	0.307468
6	0.401083	-1.505317	-0.818507
1	-0.050189	-1.447562	-1.810222
8	3.641981	1.118601	-0.543133
8	-1.247145	1.462717	1.917667
8	2.409267	-1.708978	-1.932681
8	-0.279866	-2.356171	1.301807
8	-1.733914	-1.025639	0.216479
6	3.851002	-1.779789	-1.973714
1	4.212546	-2.661749	-1.422424
1	4.091421	-1.895895	-3.036486
1	4.300989	-0.856483	-1.585278
6	-1.295370	-2.430297	2.340623
1	-2.186871	-2.939213	1.944978
1	-0.836661	-3.030109	3.134732
1	-1.552684	-1.430508	2.707388
14	-2.781113	-0.411782	-1.002593
6	-1.997397	0.957162	-2.008362
1	-1.047480	0.669827	-2.480169
1	-2.692943	1.254010	-2.810366
1	-1.818768	1.834802	-1.373734
6	-3.239710	-1.873150	-2.088769
1	-2.379439	-2.261116	-2.656456
1	-3.652730	-2.701559	-1.491970
1	-4.006707	-1.571276	-2.820544
6	-4.218409	0.219639	-0.000637
1	-4.993400	0.653012	-0.651833
1	-4.682921	-0.581883	0.592409
1	-3.866378	0.998661	0.693068
1	2.850372	0.294504	1.915261
1	2.206031	-2.029150	1.311803
1	3.585139	-1.373758	0.396292
8	-0.552816	3.263868	0.116231
6	-0.185425	4.340007	-0.762824
1	-0.012074	3.971262	-1.785561
1	-1.039974	5.025767	-0.752947
1	0.714048	4.855813	-0.393057
1	1.920450	2.978902	-0.991010
9	0.638111	-0.419258	2.814376

TS2_CI:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.370541	1.107663	1.371041
6	-0.075661	2.267554	0.468980
6	1.097484	2.432426	-0.189730
6	2.176803	1.490955	-0.072038
6	2.037956	0.344233	0.919375
6	0.661558	0.119772	1.448391
6	2.628993	-0.941387	0.278675
6	1.950093	-1.152566	-1.027038
6	-0.245568	-1.435105	0.040861
6	0.602112	-1.229088	-1.105733
1	0.128470	-1.163381	-2.074878
8	3.204749	1.598170	-0.732968

8	-1.464852	1.045534	1.926485
8	2.612245	-1.104103	-2.197343
8	0.042811	-2.504280	0.802407
8	-1.529117	-1.139843	0.000477
6	4.038837	-1.002999	-2.211752
1	4.492938	-1.877459	-1.750154
1	4.303742	-0.972187	-3.260272
1	4.368313	-0.091918	-1.720627
6	-1.008047	-2.990690	1.656550
1	-1.736595	-3.532015	1.056688
1	-0.520686	-3.658897	2.353445
1	-1.496209	-2.180352	2.186294
14	-2.621596	-0.532822	-1.151366
6	-2.011182	1.033920	-1.940725
1	-0.960757	0.998729	-2.227701
1	-2.587299	1.235856	-2.844415
1	-2.152872	1.874482	-1.265794
6	-2.836772	-1.887382	-2.411531
1	-1.936363	-2.061330	-2.998506
1	-3.102845	-2.828835	-1.933692
1	-3.634389	-1.644374	-3.112373
6	-4.134855	-0.240135	-0.132506
1	-4.942085	0.190718	-0.721427
1	-4.501751	-1.158816	0.319155
1	-3.895886	0.452754	0.672849
1	2.690497	0.609395	1.755940
1	2.449029	-1.769329	0.961201
1	3.698813	-0.822545	0.161575
8	-1.100678	3.121102	0.426349
6	-0.937127	4.307266	-0.346222
1	-0.809796	4.065087	-1.400586
1	-1.849937	4.871032	-0.205674
1	-0.084280	4.883593	0.005515
1	1.278999	3.271286	-0.844769
17	0.702208	-0.747720	2.983793

TS2_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.272345	0.511122	-1.522933
6	-0.048433	1.965600	-1.355490
6	-1.185107	2.425692	-0.780485
6	-2.202868	1.539216	-0.289523
6	-2.049546	0.042169	-0.536820
6	-0.702307	-0.401187	-1.004427
6	-2.507911	-0.711861	0.742630
6	-1.687678	-0.213343	1.877937
6	0.378175	-1.082160	0.878527
6	-0.338375	-0.271268	1.830459
1	0.242140	0.282153	2.554778
8	-3.196942	1.956401	0.295352
8	1.349375	0.199732	-2.027830
8	-2.221932	0.468999	2.907582
8	0.019673	-2.379103	0.825469
8	1.652525	-0.874670	0.630774
6	-3.643562	0.555445	3.046480
1	-4.079988	-0.435148	3.157225
1	-3.798254	1.118004	3.958143
1	-4.082497	1.080933	2.204073
6	0.997434	-3.304233	0.320174
1	1.749914	-3.487327	1.085665

1	0.447168	-4.210870	0.108540
1	1.469625	-2.931988	-0.581617
14	2.858736	0.209254	1.141780
6	2.336968	1.977112	0.940898
1	1.343169	2.190195	1.334167
1	3.036997	2.628094	1.465520
1	2.357069	2.251801	-0.111326
6	3.205599	-0.213231	2.922381
1	2.362314	-0.016524	3.581836
1	3.463282	-1.265875	3.030118
1	4.049392	0.362813	3.300338
6	4.262174	-0.221955	0.019545
1	5.120604	0.426641	0.182443
1	4.591685	-1.250302	0.155414
1	3.944120	-0.108730	-1.015519
1	-2.785908	-0.186603	-1.311691
1	-2.361002	-1.778001	0.582964
1	-3.564696	-0.531615	0.897932
8	0.911605	2.735039	-1.870581
6	0.723624	4.146126	-1.824632
1	0.683987	4.498844	-0.794677
1	1.585563	4.567575	-2.325002
1	-0.186612	4.431862	-2.346963
1	-1.387066	3.480385	-0.663478
35	-0.834312	-2.038757	-2.060236

TS2_I:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	-0.139133	-1.959540	-0.261909
6	1.069063	-2.135700	-1.159127
6	1.467641	-1.193112	-2.036470
6	0.758817	0.087209	-2.117265
6	-0.679159	0.119782	-1.572863
6	-0.760761	-0.551215	-0.183708
6	-1.254029	1.529944	-1.623006
6	-0.878972	2.338339	-0.416529
6	-0.020201	0.356462	0.873566
6	-0.367360	1.807905	0.694897
1	-0.177505	2.442301	1.556610
8	1.252270	1.051328	-2.673011
8	-0.559540	-2.916309	0.336970
8	-1.189970	3.665678	-0.408182
8	-0.330674	0.091098	2.209830
8	1.339462	0.097596	0.619248
6	-1.081890	4.371471	-1.634529
1	-1.866706	4.077377	-2.340273
1	-1.208264	5.424620	-1.382115
1	-0.096761	4.219465	-2.091349
6	0.016179	-1.173001	2.757356
1	0.964486	-1.539718	2.349631
1	0.124513	-1.012566	3.832035
1	-0.773143	-1.906933	2.571282
14	2.687288	1.018912	1.067793
6	2.745937	2.659995	0.165182
1	2.046901	3.390876	0.583025
1	3.757544	3.080434	0.227170
1	2.497755	2.520959	-0.893465
6	2.684030	1.258621	2.926806
1	1.779913	1.783378	3.254310
1	2.716530	0.296033	3.449510

1	3.553064	1.846527	3.244758
6	4.090106	-0.086660	0.501358
1	5.065940	0.302461	0.812343
1	3.976683	-1.095911	0.913814
1	4.089487	-0.160837	-0.592642
1	-1.249894	-0.510096	-2.270126
1	-2.349157	1.491128	-1.687133
1	-0.883570	2.001201	-2.537165
8	1.650341	-3.315813	-0.949741
6	2.798933	-3.619701	-1.723940
1	3.595240	-2.891582	-1.531252
1	3.116671	-4.612285	-1.408838
1	2.551654	-3.625593	-2.791434
1	2.355002	-1.290773	-2.652158
53	-2.852806	-0.768843	0.381406

5) *Isoflaviolin* (**N2**) exo structures.

Int1_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.829449	-1.560412	-0.057443
6	-1.572657	-1.948075	-0.423629
6	-0.508462	-1.031218	-1.000641
6	-0.985513	0.233671	-1.223735
6	-3.264262	-0.185938	-0.232109
6	-2.200115	0.832078	-0.640848
8	-4.402027	0.197290	0.002668
8	0.653505	-1.489068	-1.233169
6	0.875452	0.433703	1.227867
6	0.628795	1.786962	0.880451
1	1.501110	2.370912	0.609348
6	-0.604042	2.354601	0.673611
6	-1.895972	1.614643	0.718832
1	-2.741920	2.271789	0.929421
1	-1.843884	0.871331	1.513364
8	-0.565210	3.634165	0.305965
8	0.007428	-0.246331	1.935455
6	0.260077	-1.655447	2.128639
1	-0.689724	-2.058609	2.477717
1	1.035862	-1.777470	2.887369
1	0.562474	-2.111028	1.183142
8	1.989617	-0.147781	0.990644
14	3.247738	-0.132255	-0.243082
6	-1.749180	4.308383	-0.115438
1	-2.249965	3.758513	-0.915344
1	-1.407404	5.271416	-0.491227
1	-2.429405	4.462868	0.726814
6	3.625403	-1.934002	-0.482052
1	4.479145	-2.062055	-1.157617
1	2.746717	-2.421573	-0.915398
1	3.875419	-2.413211	0.470958
6	4.622688	0.756529	0.675245
1	4.850880	0.265472	1.627310
1	4.361152	1.800022	0.885485
1	5.539491	0.762148	0.074199
6	2.769230	0.784664	-1.782595
1	2.416685	1.803410	-1.594974
1	1.981886	0.233001	-2.300952
1	3.660391	0.848885	-2.420861
1	-2.663452	1.539560	-1.337704
9	-0.182658	1.170717	-1.822435

1	-3.575883	-2.250781	0.317905
8	-1.123387	-3.201185	-0.320384
6	-2.011549	-4.197229	0.150736
1	-2.889695	-4.273527	-0.499601
1	-1.450689	-5.131058	0.128998
1	-2.335672	-3.979095	1.175931

Int1_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.132851	2.260183	-0.046534
6	-0.915656	2.239414	0.560578
6	-0.287851	1.024877	1.181147
6	-1.144032	-0.069834	1.183880
6	-2.942533	1.077658	-0.156681
6	-2.367236	-0.224644	0.396300
8	-4.035207	1.061531	-0.711092
8	0.871194	1.104951	1.649838
6	0.647135	-0.432397	-1.263452
6	0.200657	-1.734175	-1.000436
1	0.964235	-2.450439	-0.725601
6	-1.109062	-2.131447	-0.868717
6	-2.248049	-1.205086	-0.890418
1	-3.197147	-1.725505	-0.990638
1	-2.155173	-0.564385	-1.762323
8	-1.265258	-3.437382	-0.614602
8	-0.121366	0.415983	-1.931906
6	0.440927	1.710645	-2.227433
1	-0.390288	2.283006	-2.628062
1	1.226285	1.602989	-2.975809
1	0.842424	2.175478	-1.329362
8	1.839049	-0.016448	-1.012789
14	3.188039	-0.410588	0.019886
6	-2.509659	-3.888905	-0.073753
1	-2.793460	-3.280267	0.785329
1	-2.326767	-4.911095	0.242959
1	-3.292679	-3.877487	-0.832203
6	3.825474	1.262945	0.463926
1	4.703383	1.199695	1.112305
1	3.050620	1.817638	0.999748
1	4.114826	1.832502	-0.422564
6	4.300494	-1.307093	-1.174125
1	4.531875	-0.695147	-2.048738
1	3.848557	-2.234351	-1.535113
1	5.251153	-1.576379	-0.706858
6	2.736571	-1.474637	1.454484
1	2.278452	-2.424208	1.174464
1	2.054761	-0.943968	2.118733
1	3.647944	-1.715174	2.012202
1	-3.150069	-0.685224	1.007632
17	-0.703539	-1.484173	2.106910
1	-2.551510	3.162015	-0.477635
8	-0.112236	3.305295	0.672539
6	-0.597900	4.545627	0.177826
1	-1.546591	4.809619	0.648553
1	0.159327	5.283028	0.428224
1	-0.730515	4.506613	-0.906586

Int1_Br:

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
6	0.371545	3.088510	-0.081122
6	1.086793	2.221224	0.684262
6	0.553055	0.932700	1.237877
6	-0.786636	0.727404	0.929050
6	-0.935480	2.747110	-0.569020
6	-1.627135	1.516189	0.023155
8	-1.499219	3.385057	-1.453284
8	1.310485	0.213472	1.925099
6	0.365858	-0.576441	-1.455147
6	-0.832461	-1.289604	-1.318984
1	-0.746786	-2.353065	-1.139136
6	-2.082163	-0.726837	-1.249997
6	-2.327241	0.723688	-1.182940
1	-3.391618	0.937078	-1.168059
1	-1.948901	1.191618	-2.092837
8	-3.080825	-1.618523	-1.188734
8	0.351358	0.602085	-2.059811
6	1.624098	1.210051	-2.355056
1	1.375319	2.211556	-2.692559
1	2.116748	0.646713	-3.146868
1	2.260055	1.240962	-1.473111
8	1.533457	-1.046018	-1.168841
14	2.170142	-2.329691	-0.168304
6	-4.379915	-1.199114	-0.765250
1	-4.316856	-0.664515	0.183201
1	-4.941412	-2.118735	-0.630843
1	-4.862640	-0.586276	-1.527441
6	3.706465	-1.535830	0.474969
1	4.265626	-2.204371	1.133483
1	3.427450	-0.651567	1.056240
1	4.377236	-1.231418	-0.332356
6	2.476875	-3.672512	-1.418632
1	3.130244	-3.346358	-2.231003
1	1.544015	-4.022368	-1.868782
1	2.951291	-4.541113	-0.954368
6	1.009663	-2.876655	1.152642
1	0.044806	-3.244729	0.799821
1	0.826815	-2.061485	1.855317
1	1.482294	-3.696985	1.703755
1	-2.480592	1.918543	0.585823
35	-1.735590	-0.620751	1.927321
1	0.799026	4.003474	-0.474344
8	2.363809	2.404520	1.040611
6	2.974448	3.636823	0.684702
1	2.420283	4.478929	1.104082
1	3.974595	3.603475	1.107667
1	3.037539	3.747619	-0.401015

Int1_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.183595	-2.963492	0.075743
6	1.550630	-2.003831	-0.815068
6	0.678237	-0.862254	-1.246221
6	-0.597829	-0.916809	-0.698305
6	-0.028755	-2.845950	0.829351
6	-1.073407	-1.830853	0.349863
8	-0.252285	-3.520074	1.831794
8	1.133511	-0.037513	-2.073072

6	0.685844	0.605602	1.559257
6	-0.629740	1.076713	1.619769
1	-0.771017	2.136956	1.483959
6	-1.750874	0.293922	1.732730
6	-1.771277	-1.178297	1.623330
1	-2.790505	-1.536515	1.688884
1	-1.253866	-1.612215	2.478052
8	-2.873174	0.997824	1.927012
8	0.974799	-0.558291	2.114898
6	2.360719	-0.940220	2.172684
1	2.349895	-1.969209	2.510291
1	2.879255	-0.307567	2.887821
1	2.831442	-0.859392	1.198114
8	1.691646	1.291827	1.136676
14	1.914148	2.674435	0.109524
6	-4.148439	0.388853	1.725315
1	-4.197076	-0.070633	0.739102
1	-4.860824	1.202329	1.788726
1	-4.368134	-0.342680	2.500296
6	3.448948	2.183736	-0.794721
1	3.754087	2.947080	-1.507771
1	3.240744	1.267697	-1.349314
1	4.281490	2.008485	-0.114355
6	2.157565	4.050329	1.339373
1	2.988804	3.852002	2.013801
1	1.264933	4.201203	1.945517
1	2.365301	4.990904	0.830937
6	0.486178	2.966082	-1.015901
1	-0.450871	3.192786	-0.512229
1	0.343473	2.094705	-1.654810
1	0.732148	3.817388	-1.652735
1	-1.865449	-2.465248	-0.063212
53	-2.095789	0.268368	-1.610476
1	1.852571	-3.756240	0.374643
8	2.741013	-1.963958	-1.425672
6	3.623858	-3.051191	-1.193713
1	3.166004	-3.992556	-1.495539
1	4.501876	-2.862374	-1.799630
1	3.908862	-3.115038	-0.142681

Int2_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-3.168624	0.411759	-0.049068
6	-2.656487	-0.807088	-0.349729
6	-1.292286	-0.972012	-0.903744
6	-0.368659	0.215922	-0.755637
6	-2.373558	1.624122	-0.123703
6	-1.050223	1.568936	-0.884078
8	-2.799588	2.699265	0.347285
8	-0.917260	-2.024908	-1.435104
6	0.504570	0.087649	0.526944
6	1.452984	1.219615	0.629725
1	2.390231	1.085530	1.143939
6	1.142365	2.418012	0.132241
6	-0.128673	2.760072	-0.583266
1	0.148187	3.239485	-1.521571
1	-0.705710	3.496838	-0.014625
8	2.125262	3.410333	0.189079
8	-0.482287	0.216391	1.629361
6	-0.910897	-1.020709	2.280673

1	-1.872436	-0.773527	2.720467
1	-0.194456	-1.308675	3.043748
1	-1.022139	-1.841649	1.575339
8	1.076842	-1.175541	0.577617
14	2.532161	-1.968375	0.009019
6	1.704455	4.811855	0.250923
1	1.059394	5.066331	-0.584847
1	2.626051	5.368903	0.203575
1	1.187682	4.999138	1.190098
6	2.003350	-3.760773	0.224732
1	2.810666	-4.474109	0.075143
1	1.201243	-3.994674	-0.476251
1	1.595827	-3.887826	1.226654
6	3.932829	-1.424402	1.169007
1	3.838358	-1.809346	2.182027
1	3.951432	-0.336902	1.230532
1	4.905583	-1.727802	0.782441
6	2.970791	-1.412285	-1.739077
1	2.956775	-0.323132	-1.762038
1	2.272645	-1.764167	-2.494614
1	3.974578	-1.735205	-2.016763
1	-1.331880	1.650946	-1.938629
9	0.568177	0.134339	-1.877990
1	-4.173883	0.551310	0.311629
8	-3.279291	-2.006659	-0.183577
6	-4.624804	-2.035955	0.390638
1	-5.360668	-1.836602	-0.381610
1	-4.725446	-3.039073	0.781645
1	-4.708113	-1.316967	1.202596

Int2_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.522281	2.941514	-0.190915
6	0.632576	2.505308	0.355838
6	0.778038	1.136589	0.922337
6	-0.395361	0.194391	0.732592
6	-1.728229	2.127070	-0.207364
6	-1.734132	0.925575	0.731804
8	-2.715175	2.456897	-0.836412
8	1.811979	0.793536	1.449602
6	-0.239161	-0.631303	-0.604963
6	-1.454362	-1.453599	-0.838398
1	-1.317272	-2.314538	-1.479366
6	-2.660760	-1.142853	-0.370611
6	-2.930297	0.009531	0.527475
1	-3.268340	-0.359021	1.501743
1	-3.740953	0.622513	0.122096
8	-3.702927	-1.944996	-0.738417
8	-0.213456	0.341999	-1.672870
6	1.048756	0.704340	-2.191780
1	0.844419	1.493740	-2.915930
1	1.533616	-0.135817	-2.696883
1	1.739073	1.097401	-1.434967
8	0.868701	-1.425292	-0.630139
14	2.407336	-1.909815	-0.201001
6	-4.932121	-1.831301	-0.040633
1	-4.811654	-2.027956	1.027358
1	-5.575625	-2.595633	-0.468959
1	-5.399048	-0.854274	-0.184871
6	3.708373	-0.624762	-0.571837

1	4.684338	-1.013394	-0.261080
1	3.557394	0.310468	-0.029295
1	3.784561	-0.401807	-1.638870
6	2.670081	-3.362241	-1.337210
1	2.622393	-3.064502	-2.387444
1	1.907262	-4.130039	-1.186642
1	3.643099	-3.834099	-1.174713
6	2.525091	-2.461486	1.566185
1	1.749667	-3.188552	1.814580
1	2.441209	-1.631240	2.267631
1	3.492295	-2.947926	1.731817
1	-1.830217	1.380045	1.726675
17	-0.395520	-0.959059	2.124037
1	-0.609256	3.908925	-0.672744
8	1.788413	3.174916	0.413536
6	1.800927	4.483443	-0.146948
1	1.106209	5.138333	0.381645
1	2.818571	4.841392	-0.023380
1	1.546289	4.449610	-1.208825

Int2_Br:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	-0.235823	3.087081	-0.147971
6	0.849816	2.512294	0.412246
6	0.859751	1.089453	0.851257
6	-0.378441	0.276083	0.549489
6	-1.497651	2.378191	-0.301377
6	-1.654536	1.108690	0.531183
8	-2.414544	2.840740	-0.952189
8	1.854552	0.611533	1.350926
6	-0.220678	-0.477561	-0.824486
6	-1.471403	-1.209507	-1.152818
1	-1.359341	-2.052929	-1.821806
6	-2.675123	-0.820694	-0.742119
6	-2.907746	0.317787	0.184039
1	-3.360397	-0.055672	1.109026
1	-3.624597	1.017059	-0.257472
8	-3.754757	-1.517386	-1.204782
8	-0.109936	0.571550	-1.819650
6	1.181884	0.891345	-2.288908
1	1.042575	1.745393	-2.952736
1	1.623713	0.063268	-2.851004
1	1.879804	1.180564	-1.493544
8	0.840685	-1.330222	-0.880516
14	2.355470	-1.926997	-0.506886
6	-4.986564	-1.398431	-0.512429
1	-4.894600	-1.706262	0.532122
1	-5.667642	-2.075985	-1.021080
1	-5.392475	-0.385055	-0.561751
6	3.726770	-0.686524	-0.756230
1	4.676608	-1.153733	-0.473668
1	3.619690	0.205081	-0.135542
1	3.827379	-0.377716	-1.799595
6	2.542263	-3.275994	-1.778017
1	2.523619	-2.873373	-2.793798
1	1.733442	-4.007358	-1.708190
1	3.483548	-3.819395	-1.658119
6	2.440418	-2.649596	1.199526
1	1.608308	-3.328067	1.396276
1	2.432153	-1.882580	1.974220

1	3.365247	-3.226601	1.305880
1	-1.779763	1.494938	1.551210
35	-0.559222	-1.072819	2.013771
1	-0.220713	4.096353	-0.543992
8	2.049824	3.077193	0.581237
6	2.194448	4.420651	0.133485
1	1.527599	5.087320	0.683130
1	3.229712	4.682319	0.330862
1	1.991414	4.492165	-0.937451

Int2_I:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	3.322340	0.507820	-0.642775
6	3.036588	-0.572439	0.112603
6	1.696047	-0.758334	0.791185
6	0.610527	0.265451	0.449943
6	2.353136	1.602289	-0.812246
6	1.201761	1.660337	0.203314
8	2.530722	2.481847	-1.629466
8	1.522552	-1.702175	1.519357
6	-0.201558	-0.211735	-0.818665
6	-1.104728	0.880422	-1.316106
1	-1.882919	0.587570	-2.014943
6	-0.925205	2.175496	-1.053566
6	0.157759	2.713345	-0.162851
1	-0.283346	3.120383	0.754968
1	0.667241	3.532770	-0.681824
8	-1.743171	3.076678	-1.670654
8	0.731610	-0.436055	-1.870641
6	1.175264	-1.765009	-2.096495
1	2.024986	-1.673901	-2.777093
1	0.390080	-2.361554	-2.571896
1	1.490576	-2.277303	-1.181222
8	-0.845936	-1.388177	-0.499483
14	-2.395879	-1.998308	-0.767632
6	-2.127679	4.215005	-0.917028
1	-2.623121	3.916688	0.015500
1	-2.831915	4.763766	-1.542532
1	-1.272974	4.861391	-0.690005
6	-2.323001	-3.666526	0.067183
1	-3.283439	-4.189683	-0.002537
1	-2.072164	-3.547420	1.126795
1	-1.554954	-4.300422	-0.389080
6	-2.700074	-2.198187	-2.612209
1	-1.973178	-2.886041	-3.058143
1	-2.651267	-1.254589	-3.165797
1	-3.697351	-2.624783	-2.775781
6	-3.727217	-0.926095	0.003983
1	-3.652462	0.124990	-0.292505
1	-3.675530	-0.969710	1.096566
1	-4.713116	-1.296497	-0.303570
1	1.694808	1.976333	1.134219
1	4.256991	0.620910	-1.181206
8	3.838552	-1.614498	0.340265
6	5.124438	-1.587104	-0.254995
1	5.692381	-0.716701	0.092536
1	5.618259	-2.505110	0.059980
1	5.041939	-1.561728	-1.347874
53	-0.733061	0.363916	2.175087

π_complex_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.994646	2.160017	0.123371
6	0.794897	2.065138	-0.486289
6	0.487573	0.965988	-1.441289
6	1.574131	0.005476	-1.650896
6	3.059681	1.194559	-0.136704
6	2.770983	0.096216	-1.061576
8	4.166274	1.312297	0.380124
8	-0.576468	0.907277	-2.035613
6	-0.692167	-0.395584	1.069063
6	-0.030272	-1.455284	0.534280
1	-0.507469	-1.947625	-0.302052
6	1.253165	-1.990851	0.901388
6	2.172163	-1.446110	1.722519
1	3.139914	-1.896306	1.890778
1	1.962106	-0.521622	2.237231
8	1.454936	-3.147498	0.191037
8	-0.174000	0.289349	2.100973
6	-0.971667	1.335178	2.659600
1	-0.338518	1.793804	3.414198
1	-1.872903	0.931137	3.125399
1	-1.254433	2.062913	1.900306
8	-1.838106	0.084277	0.617618
14	-3.134163	-0.633095	-0.238060
6	2.720985	-3.762200	0.304942
1	3.516613	-3.084492	-0.020204
1	2.692345	-4.631423	-0.347862
1	2.920707	-4.087001	1.330408
6	-4.114544	0.866400	-0.702483
1	-5.047406	0.611491	-1.210912
1	-3.533782	1.501962	-1.375613
1	-4.371451	1.464487	0.174649
6	-3.978578	-1.725252	1.008648
1	-4.306570	-1.166098	1.887790
1	-3.303728	-2.512356	1.355320
1	-4.857870	-2.220588	0.588673
6	-2.596816	-1.606915	-1.722477
1	-2.240988	-2.609609	-1.478143
1	-1.816715	-1.089570	-2.285931
1	-3.450547	-1.731422	-2.396249
1	3.560045	-0.621258	-1.246945
9	1.280102	-0.990130	-2.491743
1	2.250607	2.958315	0.809424
8	-0.238580	2.912950	-0.365345
6	0.006130	4.104310	0.369762
1	0.843642	4.655243	-0.064889
1	-0.903996	4.692307	0.292314
1	0.223457	3.886483	1.419329

π_complex_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.843494	2.341751	-0.089550
6	-0.682162	2.118657	0.559351
6	-0.462454	0.907504	1.400897
6	-1.599929	-0.022841	1.471937

6	-2.954376	1.405141	0.011781
6	-2.752545	0.197787	0.821192
8	-4.034310	1.624170	-0.528103
8	0.578775	0.753733	2.015351
6	0.785063	-0.242852	-1.198170
6	0.065051	-1.331271	-0.819029
1	0.492340	-1.942563	-0.036111
6	-1.226708	-1.760187	-1.279883
6	-2.100155	-1.076619	-2.047444
1	-3.077952	-1.461874	-2.298712
1	-1.835101	-0.107659	-2.440813
8	-1.495545	-2.985846	-0.727097
8	0.333563	0.581109	-2.157065
6	1.188094	1.656570	-2.551292
1	0.607092	2.220706	-3.275943
1	2.099620	1.278389	-3.018543
1	1.452300	2.281790	-1.699188
8	1.931060	0.129386	-0.655474
14	3.148554	-0.732663	0.183031
6	-2.786245	-3.519740	-0.932596
1	-3.556735	-2.843070	-0.549719
1	-2.815310	-4.455697	-0.379556
1	-2.975536	-3.719978	-1.991585
6	4.169133	0.662942	0.843514
1	5.064041	0.311825	1.362900
1	3.583930	1.251699	1.554477
1	4.493995	1.336119	0.047324
6	4.005313	-1.740639	-1.124489
1	4.388367	-1.119897	-1.937663
1	3.318720	-2.469079	-1.563747
1	4.848881	-2.303363	-0.716320
6	2.494480	-1.816509	1.538245
1	2.100460	-2.771124	1.184411
1	1.715729	-1.314203	2.116776
1	3.309409	-2.050259	2.231222
1	-3.590679	-0.484308	0.884894
17	-1.360650	-1.428432	2.442379
1	-2.028579	3.223973	-0.690216
8	0.391314	2.923929	0.576376
6	0.233431	4.200717	-0.027984
1	-0.594671	4.741962	0.436150
1	1.166125	4.728898	0.149209
1	0.051027	4.114027	-1.102905

π_complex_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.284522	2.765981	-0.139003
6	0.257778	2.199831	-0.806078
6	0.331666	0.812315	-1.352737
6	1.599090	0.112595	-1.110116
6	2.527819	2.041537	0.083514
6	2.612468	0.666997	-0.430429
8	3.487192	2.559339	0.645774
8	-0.595814	0.346983	-1.992816
6	-1.036986	0.045667	1.319435
6	-0.118973	-0.955340	1.270277
1	-0.343807	-1.783677	0.611779
6	1.154949	-1.038806	1.930283
6	1.817329	-0.057459	2.576492
1	2.801666	-0.201706	2.998567

1	1.365744	0.914703	2.697850
8	1.667154	-2.293244	1.722225
8	-0.836872	1.124736	2.092687
6	-1.882869	2.097341	2.142637
1	-1.485964	2.899142	2.759480
1	-2.780138	1.681078	2.604938
1	-2.126917	2.463414	1.146023
8	-2.149890	0.084774	0.608252
14	-3.119361	-1.134054	-0.100204
6	2.994386	-2.529693	2.140883
1	3.688187	-1.830129	1.664032
1	3.230204	-3.545063	1.830417
1	3.094071	-2.452019	3.227891
6	-4.246481	-0.113607	-1.155440
1	-5.010304	-0.718647	-1.649874
1	-3.672267	0.394622	-1.934189
1	-4.760972	0.653213	-0.572353
6	-3.968285	-1.961561	1.332885
1	-4.534649	-1.253447	1.941913
1	-3.238193	-2.445688	1.986812
1	-4.662895	-2.737622	1.000809
6	-2.160367	-2.361910	-1.105104
1	-1.667884	-3.130182	-0.505872
1	-1.406921	-1.871574	-1.725970
1	-2.846562	-2.881688	-1.781740
1	3.548602	0.151237	-0.258453
35	1.724364	-1.655050	-1.816512
1	1.257646	3.779529	0.242498
8	-0.917592	2.777151	-1.099790
6	-1.026063	4.168754	-0.829865
1	-0.255618	4.721565	-1.373560
1	-2.009973	4.461846	-1.185692
1	-0.938051	4.380821	0.239031

π_complex_I:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.372869	3.067413	-0.509974
6	-0.367854	2.136702	-1.141608
6	0.116459	0.739138	-1.354173
6	1.473546	0.465168	-0.865444
6	1.709961	2.760979	-0.028726
6	2.205588	1.389755	-0.230022
8	2.425979	3.615157	0.483184
8	-0.581642	-0.073323	-1.937678
6	-1.384872	0.164422	1.298745
6	-0.255699	-0.544059	1.552891
1	-0.191453	-1.522937	1.106853
6	0.894632	-0.140262	2.309971
6	1.192457	1.090525	2.770942
1	2.110679	1.301116	3.291137
1	0.501551	1.899998	2.627771
8	1.729390	-1.219408	2.435646
8	-1.550938	1.394105	1.811036
6	-2.799822	2.038684	1.570256
1	-2.697394	3.024850	2.008543
1	-3.615393	1.505184	2.055772
1	-3.008931	2.111562	0.506570
8	-2.380158	-0.241407	0.537288
14	-2.915911	-1.769641	0.010040
6	2.995751	-0.987778	3.013743

1	3.541902	-0.216138	2.467039
1	3.534687	-1.927373	2.952850
1	2.912569	-0.686217	4.059900
6	-4.057358	-1.273863	-1.362696
1	-4.562145	-2.132036	-1.803149
1	-3.484167	-0.779071	-2.145727
1	-4.819165	-0.578245	-1.015029
6	-3.774404	-2.516476	1.483978
1	-4.581953	-1.886571	1.852523
1	-3.064549	-2.661596	2.297847
1	-4.194854	-3.492661	1.245491
6	-1.556397	-2.875102	-0.597410
1	-0.981840	-3.332482	0.205056
1	-0.874348	-2.329256	-1.247512
1	-1.999430	-3.682894	-1.180300
1	3.205846	1.200094	0.128382
53	2.206268	-1.482636	-1.216212
1	0.035918	4.082213	-0.365455
8	-1.583311	2.324006	-1.680626
6	-2.060247	3.662690	-1.703811
1	-1.353133	4.314761	-2.215453
1	-2.995858	3.639017	-2.249890
1	-2.230214	4.042682	-0.695315

TS1_F:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	2.875027	-1.431357	-0.005238
6	1.674585	-1.920502	0.390607
6	0.631234	-1.095413	1.092516
6	1.051041	0.221574	1.358684
6	3.255028	-0.063116	0.281025
6	2.185052	0.828934	0.823115
8	4.380050	0.369360	0.070189
8	-0.463541	-1.599857	1.400301
6	-0.879562	0.365593	-1.137031
6	-0.670616	1.671739	-0.744980
1	-1.519018	2.179297	-0.306016
6	0.543009	2.372729	-0.725754
6	1.807284	1.791221	-0.908740
1	2.684688	2.422978	-0.979690
1	1.838272	0.941149	-1.574915
8	0.387046	3.635728	-0.265152
8	0.023764	-0.286478	-1.869046
6	-0.266546	-1.662955	-2.179283
1	0.648846	-2.038408	-2.628300
1	-1.087309	-1.718243	-2.895332
1	-0.512182	-2.221587	-1.277675
8	-1.973250	-0.303006	-0.911276
14	-3.292696	-0.175634	0.196877
6	1.542419	4.454583	-0.140696
1	2.250295	4.042493	0.580995
1	1.182845	5.413710	0.221445
1	2.032574	4.585411	-1.108170
6	-3.755378	-1.952444	0.408174
1	-4.644359	-2.071394	1.032166
1	-2.936065	-2.494150	0.886357
1	-3.959826	-2.432952	-0.551101
6	-4.566394	0.797636	-0.746640
1	-4.801116	0.331606	-1.705813
1	-4.230230	1.816797	-0.954979

1	-5.501169	0.878825	-0.185622
6	-2.833524	0.632404	1.790368
1	-2.538848	1.679371	1.706538
1	-2.019961	0.084798	2.267193
1	-3.701589	0.596739	2.456719
1	2.559947	1.703723	1.344520
9	0.221894	1.017518	2.089264
1	3.635598	-2.042171	-0.476371
8	1.264019	-3.183751	0.226996
6	2.174217	-4.084304	-0.389249
1	3.093518	-4.165144	0.193640
1	1.665900	-5.044245	-0.417254
1	2.413918	-3.761283	-1.405359

TS1_Cl:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	-2.480606	1.940684	-0.142587
6	-1.285304	2.123397	0.464098
6	-0.539356	1.033633	1.185812
6	-1.270761	-0.173566	1.297470
6	-3.161185	0.664629	-0.072401
6	-2.411400	-0.472912	0.548470
8	-4.292118	0.495797	-0.507543
8	0.588036	1.266142	1.643226
6	0.828209	-0.342223	-1.247763
6	0.455241	-1.627684	-0.921404
1	1.223260	-2.255509	-0.500190
6	-0.832488	-2.179830	-0.975318
6	-2.015672	-1.448883	-1.172397
1	-2.943429	-1.983606	-1.304734
1	-1.924568	-0.592639	-1.816654
8	-0.834300	-3.479989	-0.610764
8	0.002267	0.459644	-1.919478
6	0.462623	1.794334	-2.197495
1	-0.409467	2.308982	-2.580925
1	1.244635	1.770310	-2.949642
1	0.823243	2.273714	-1.292997
8	1.997728	0.171161	-1.002430
14	3.323969	-0.127690	0.064135
6	-2.086839	-4.134487	-0.441588
1	-2.673277	-3.648060	0.335268
1	-1.849533	-5.145811	-0.139317
1	-2.650045	-4.156955	-1.372360
6	3.811137	1.591478	0.537023
1	4.686460	1.598676	1.183780
1	2.987868	2.055201	1.079381
1	4.037066	2.203868	-0.333460
6	4.559572	-0.979216	-1.033386
1	4.761637	-0.404198	-1.935070
1	4.202080	-1.960143	-1.344391
1	5.509799	-1.129096	-0.523978
6	2.855916	-1.146211	1.528691
1	2.619309	-2.184306	1.306683
1	2.007037	-0.697137	2.041972
1	3.697814	-1.148802	2.222705
1	-3.066619	-1.241742	0.933297
17	-0.609369	-1.449452	2.282905
1	-3.015696	2.735464	-0.638970
8	-0.611721	3.280498	0.508647
6	-1.237953	4.415419	-0.075847

1	-2.207054	4.601261	0.382536
1	-0.573348	5.249332	0.108494
1	-1.369405	4.282137	-1.150239

TS1_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.061308	2.462668	-0.104237
6	-0.896381	2.344027	0.573473
6	-0.391778	1.049197	1.154917
6	-1.312513	-0.016092	1.031610
6	-2.933473	1.322993	-0.285962
6	-2.420035	-0.007334	0.179670
8	-4.038670	1.410404	-0.802802
8	0.716877	1.030112	1.706309
6	0.921894	-0.110261	-1.427806
6	0.343271	-1.354356	-1.309323
1	0.980482	-2.145984	-0.950573
6	-1.001321	-1.687898	-1.521110
6	-2.050322	-0.762458	-1.655974
1	-3.032418	-1.121893	-1.921999
1	-1.789394	0.157471	-2.148523
8	-1.215366	-3.012167	-1.370899
8	0.271432	0.892283	-2.017569
6	0.951752	2.156804	-2.097660
1	0.230845	2.826673	-2.549329
1	1.835954	2.072304	-2.721031
1	1.233445	2.504882	-1.107802
8	2.130270	0.184056	-1.052527
14	3.356709	-0.458263	-0.023230
6	-2.556216	-3.489671	-1.375336
1	-3.139866	-3.017326	-0.588161
1	-2.485076	-4.552028	-1.186012
1	-3.029208	-3.320531	-2.341063
6	4.103698	1.097047	0.642288
1	4.955446	0.894284	1.288914
1	3.359189	1.632335	1.229898
1	4.441902	1.753931	-0.156795
6	4.470116	-1.369587	-1.200950
1	4.789606	-0.734628	-2.025125
1	3.970475	-2.237077	-1.630230
1	5.365637	-1.731578	-0.699092
6	2.686823	-1.541388	1.308807
1	2.214374	-2.456527	0.958692
1	1.962791	-0.986230	1.903491
1	3.510281	-1.831302	1.963244
1	-3.217588	-0.704039	0.398044
35	-0.918879	-1.663568	1.941026
1	-2.421455	3.404050	-0.489838
8	-0.049236	3.348899	0.829554
6	-0.439997	4.649205	0.405690
1	-1.393425	4.929607	0.848224
1	0.337135	5.319294	0.749340
1	-0.519997	4.698799	-0.680051

TS1_I: -isoflaviolin-exo

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	-3.08510000	0.39523500	0.07859780
6	-2.30264000	-0.26342100	-0.80577500
6	-1.07837000	0.33328000	-1.45001000
6	-0.88536000	1.70254000	-1.14617000
6	-2.80986000	1.77264000	0.42366600
6	-1.53530000	2.36103000	-0.10009800
6	-3.56624000	2.44606000	1.11129000
6	-0.40072000	-0.37393500	-2.20983000
6	0.82952600	-0.34384900	0.98106500
6	1.39304000	0.91432400	0.99573800
1	2.38395000	0.99840900	0.58001300
6	0.79663400	2.10947000	1.42352000
6	-0.57069000	2.28360000	1.68933000
1	-0.90352600	3.21685000	2.11508000
1	-1.07243000	1.42455000	2.09462000
8	1.66130000	3.14488000	1.36531000
8	-0.30780700	-0.58600100	1.62613000
6	-0.83438300	-1.91793000	1.55271000
1	-1.82638000	-1.84682000	1.98407000
1	-0.21721200	-2.59567000	2.13605000
1	-0.88997100	-2.26069000	0.52373200
8	1.35921000	-1.38634000	0.41575200
14	2.57431000	-1.70344000	-0.76056400
6	1.14969000	4.45983000	1.53558000
1	0.39508300	4.68052000	0.78141000
1	1.99576000	5.12317000	1.40345000
1	0.73154800	4.59756000	2.53285000
6	1.84993000	-3.17938000	-1.61319000
1	2.50974000	-3.55517000	-2.39295000
1	0.90688300	-2.89152000	-2.07749000
1	1.65848000	-3.99386000	-0.91589100
6	4.07858000	-2.08941000	0.26382700
1	3.89007000	-2.89708000	0.96923300
1	4.39294000	-1.21651000	0.83543800
1	4.91863000	-2.38762000	-0.36182700
6	2.84301000	-0.29615100	-1.92053000
1	3.28090000	0.58730100	-1.46135000
1	1.89820000	-0.01315740	-2.38238000
1	3.52141000	-0.62560700	-2.70812000
1	-1.56462000	3.44163000	-0.12195800
53	0.59440400	2.76676000	-2.22076000
1	-3.97688000	-0.03543910	0.50660200
8	-2.51697000	-1.51303000	-1.24132000
6	-3.68513000	-2.16515000	-0.76687800
1	-4.58038000	-1.60311000	-1.03096000
1	-3.70291000	-3.13584000	-1.24892000
1	-3.65123000	-2.29447000	0.31570400

TS2_F:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.929020	0.937030	-0.014425
6	-2.531172	-0.249465	-0.546217
6	-1.185095	-0.469624	-1.150947
6	-0.327824	0.637933	-1.050006
6	-2.032040	2.055914	0.123651
6	-0.698204	1.996052	-0.615002
8	-2.310190	3.029568	0.813168
8	-0.878454	-1.571994	-1.636556
6	0.666204	-0.064969	0.948310
6	1.803131	0.751339	0.666707

1	2.761063	0.256577	0.556415
6	1.700852	2.057700	0.326208
6	0.396524	2.753018	0.216220
1	0.516397	3.756021	-0.184239
1	-0.021699	2.892477	1.215776
8	2.867018	2.681213	0.051588
8	-0.270048	0.440194	1.777784
6	-1.187277	-0.492092	2.366173
1	-2.014981	0.110980	2.731371
1	-0.696800	-1.008061	3.193318
1	-1.535312	-1.227629	1.640797
8	0.719145	-1.370289	0.903318
14	1.703752	-2.507691	0.054009
6	2.860160	3.971891	-0.546441
1	2.330454	3.962569	-1.501618
1	3.906555	4.209203	-0.715489
1	2.426324	4.723810	0.114580
6	0.591591	-3.981038	-0.031071
1	1.078245	-4.837285	-0.503281
1	-0.297994	-3.729568	-0.612964
1	0.272118	-4.294162	0.965702
6	3.144527	-2.782495	1.205568
1	2.818586	-3.079915	2.205078
1	3.760427	-1.886901	1.319809
1	3.800822	-3.573030	0.832141
6	2.294776	-1.898536	-1.586464
1	2.825716	-0.946791	-1.528651
1	1.459088	-1.769398	-2.274642
1	2.986920	-2.634635	-2.008485
1	-0.852295	2.596583	-1.524004
9	0.745861	0.646857	-1.902277
1	-3.900709	1.063639	0.450522
8	-3.275094	-1.358009	-0.593445
6	-4.600431	-1.272642	-0.086724
1	-5.167416	-0.501657	-0.612388
1	-5.048008	-2.246877	-0.260314
1	-4.591985	-1.055557	0.984840

TS2_Cl:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.973503	-2.389250	-0.114422
6	-2.298242	-1.224400	0.499510
6	-1.289548	-0.309486	1.116800
6	0.061316	-0.728004	0.964675
6	-0.602680	-2.781832	-0.338493
6	0.474616	-2.065238	0.465152
8	-0.310894	-3.675379	-1.121991
8	-1.654141	0.743259	1.648344
6	0.458227	0.410347	-0.945321
6	1.877864	0.364669	-0.769751
1	2.417319	1.298726	-0.735630
6	2.523602	-0.785352	-0.478747
6	1.837132	-2.091296	-0.298512
1	2.499973	-2.794414	0.191080
1	1.626954	-2.526968	-1.276037
8	3.863716	-0.679729	-0.338635
8	-0.064940	-0.512917	-1.787965
6	-1.328163	-0.208228	-2.391914
1	-1.671029	-1.144439	-2.816569
1	-1.188309	0.535243	-3.173387

1	-2.047508	0.166936	-1.667949
8	-0.221420	1.526778	-0.892652
14	-0.068561	3.085013	-0.191185
6	4.617287	-1.766311	0.187334
1	4.272699	-2.048774	1.179908
1	5.633458	-1.399677	0.256229
1	4.591472	-2.627470	-0.476431
6	-1.834644	3.621805	-0.081274
1	-1.924856	4.620818	0.341818
1	-2.392451	2.933045	0.551288
1	-2.305210	3.639329	-1.063053
6	0.891571	4.063561	-1.454121
1	0.407032	4.059994	-2.428823
1	1.899735	3.673803	-1.589006
1	0.993142	5.103473	-1.146234
6	0.810981	3.091876	1.431447
1	1.809123	2.661807	1.369910
1	0.255078	2.547453	2.190135
1	0.922756	4.126474	1.759463
1	0.611883	-2.709292	1.340419
17	1.152229	-0.131764	2.210697
1	-2.716408	-3.013422	-0.588533
8	-3.537528	-0.741289	0.628861
6	-4.604815	-1.553087	0.153084
1	-4.598994	-2.523540	0.646178
1	-5.512736	-1.017545	0.394749
1	-4.535507	-1.696198	-0.925164

TS2_Br:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.539225	-2.756579	-0.168382
6	-2.036909	-1.704893	0.526147
6	-1.187780	-0.602033	1.072615
6	0.196666	-0.718736	0.772740
6	-0.145377	-2.845511	-0.534003
6	0.831998	-1.932487	0.199611
8	0.250400	-3.646192	-1.369377
8	-1.716576	0.345040	1.660133
6	0.144883	0.474099	-1.155522
6	1.550855	0.735028	-1.131778
1	1.878700	1.763288	-1.141600
6	2.455863	-0.249430	-0.936815
6	2.098688	-1.668387	-0.675043
1	2.943141	-2.176577	-0.224656
1	1.924238	-2.183053	-1.622462
8	3.749537	0.142522	-0.962492
8	-0.249911	-0.549405	-1.950792
6	-1.598975	-0.520489	-2.435013
1	-1.763659	-1.500364	-2.866477
1	-1.695211	0.250404	-3.196365
1	-2.313969	-0.325875	-1.639880
8	-0.754468	1.409982	-1.011330
14	-0.924283	2.986167	-0.365602
6	4.778070	-0.755672	-0.562410

1	4.664458	-1.043432	0.481609
1	5.699586	-0.201703	-0.680152
1	4.803800	-1.642876	-1.192134
6	-2.750626	3.071511	-0.090015
1	-3.060807	4.047362	0.279178
1	-3.042629	2.322876	0.644566
1	-3.300629	2.874939	-1.008703
6	-0.355871	4.104958	-1.742480
1	-0.881991	3.894760	-2.672222
1	0.710190	4.000111	-1.940120
1	-0.532235	5.150825	-1.496052
6	0.062932	3.261094	1.168112
1	1.128275	3.094500	1.021730
1	-0.270920	2.606399	1.970040
1	-0.064897	4.295130	1.490167
1	1.173554	-2.555924	1.032981
35	1.356318	0.150416	2.070778
1	-2.178092	-3.516009	-0.593773
8	-3.330237	-1.502873	0.795037
6	-4.249474	-2.494913	0.353161
1	-4.005884	-3.468285	0.774673
1	-5.221134	-2.172024	0.700906
1	-4.249311	-2.563326	-0.735026

TS2_I:

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	3.322340	0.507820	-0.642775
6	3.036588	-0.572439	0.112603
6	1.696047	-0.758334	0.791185
6	0.610527	0.265451	0.449943
6	2.353136	1.602289	-0.812246
6	1.201761	1.660337	0.203314
8	2.530722	2.481847	-1.629466
8	1.522552	-1.702175	1.519357
6	-0.201558	-0.211735	-0.818665
6	-1.104728	0.880422	-1.316106
1	-1.882919	0.587570	-2.014943
6	-0.925205	2.175496	-1.053566
6	0.157759	2.713345	-0.162851
1	-0.283346	3.120383	0.754968
1	0.667241	3.532770	-0.681824
8	-1.743171	3.076678	-1.670654
8	0.731610	-0.436055	-1.870641
6	1.175264	-1.765009	-2.096495
1	2.024986	-1.673901	-2.777093
1	0.390080	-2.361554	-2.571896
1	1.490576	-2.277303	-1.181222
8	-0.845936	-1.388177	-0.499483
14	-2.395879	-1.998308	-0.767632
6	-2.127679	4.215005	-0.917028
1	-2.623121	3.916688	0.015500
1	-2.831915	4.763766	-1.542532
1	-1.272974	4.861391	-0.690005
6	-2.323001	-3.666526	0.067183
1	-3.283439	-4.189683	-0.002537
1	-2.072164	-3.547420	1.126795
1	-1.554954	-4.300422	-0.389080
6	-2.700074	-2.198187	-2.612209
1	-1.973178	-2.886041	-3.058143
1	-2.651267	-1.254589	-3.165797
1	-3.697351	-2.624783	-2.775781

6	-3.727217	-0.926095	0.003983	8	3.838552	-1.614498	0.340265
1	-3.652462	0.124990	-0.292505	6	5.124438	-1.587104	-0.254995
1	-3.675530	-0.969710	1.096566	1	5.692381	-0.716701	0.092536
1	-4.713116	-1.296497	-0.303570	1	5.618259	-2.505110	0.059980
1	1.694808	1.976333	1.134219	1	5.041939	-1.561728	-1.347874
1	4.256991	0.620910	-1.181206	53	-0.733061	0.363916	2.175087

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