

Supporting Information

Regioselective (3+2) Cycloaddition Reactions of Zerumbone: Synthesis of Isoxazolines and Spiro-Pyrrolizidino-Oxindole, Conformational Diversity and Theoretical Insights

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1. General information:

All reactions were performed with the commercially available starting materials without any further purifications. Zerumbone was isolated from *Zingiber zerumbet* (L) Smith rhizomes purchased from Siddha Medicinal Plants Garden, Salem, India. Proton nuclear magnetic resonance (^1H NMR) spectra were recorded on a Bruker BBFO (500 MHz) spectrometer at SRM University and Gandhigram University. Chemical shifts were recorded in parts per million (ppm, δ) relative to chloroform ($\delta = 7.26$, singlet). ^1H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), multiplet, (m), broad singlet (bs), etc. Carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker BBFO (101 MHz) spectrometer. ^{13}C NMR data are reported with the solvent peak ($\text{CDCl}_3 = 77.16$) as the internal standard. High-resolution mass spectral analysis (HRMS) was performed on the Bruker Impact HD mass spectrometer. Single crystal X-ray diffractometer (SCXRD) analysis was carried out using Bruker, D8 Quest (NRC). Analytical thin-layer chromatography (TLC) was carried out on a Merck 60 F254 pre-coated silica gel plate (0.2 mm thickness). Visualization was performed using a UV lamp.

2. Extraction and isolation procedure for zerumbone:

Zerumbone **1** is a form of sesquiterpenes isolated from *Zingiber zerumbet* (L) Smith rhizomes. Further rhizomes were cleaned and chopped into small pieces. It was dried at room temperature for three days and powdered. One kilogram of the powdered rhizomes is extracted with methanol (3L) at room temperature, overnight with occasional shaking. The extraction is filtered and concentrated under reduced pressure to get 100 g of crude. This was further subjected to silica gel column chromatography using a hexane and ethyl acetate system. The desired Zerumbone **1** was eluted around 8:2 (Hexane: Ethyl acetate) and obtained **16 g of Zerumbone (1)**



Dried rhizomes



Powdered rhizomes



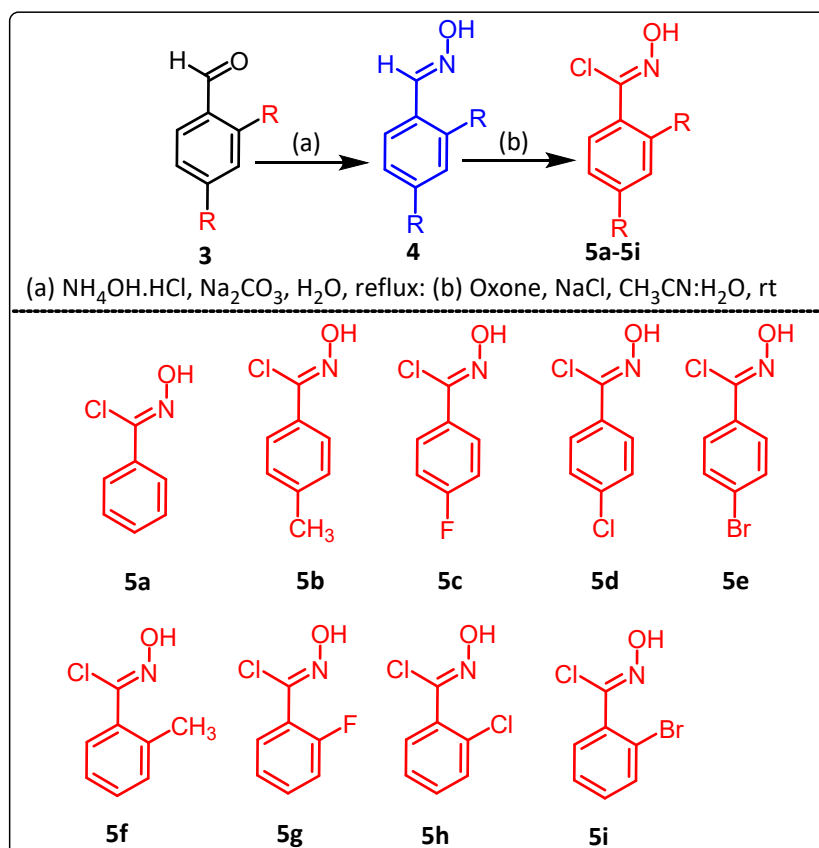
Purification



Zerumbone

3. General procedure for the synthesis of *N*-hydroxyimoyl chloride

The compound **3** was dissolved in H₂O followed by the addition of Na₂CO₃ (0.7 equiv), NH₄OH.HCl (1 equiv) reflux, 2 h. The reaction mixture was allowed to stir at 80 °C. The reaction completion was monitored by TLC chromatography (2-5 h). After completion, the reaction was extracted with ethyl acetate (3 x 10 mL). The combined ethyl acetate layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure to get a crude compound. The obtained crude **4** was used for the next step without further purification. Obtained aldoximes are further dissolved in MeCN: H₂O followed by the addition of Oxone (1.1 equiv) and NaCl (1.1 equiv). The reaction mixture was stirred at room temperature for 2-14 hours. After completion of the reaction the reaction mixture was concentrated in a vacuum and extracted with ethyl acetate (3 x 10 mL). The combined ethyl acetate layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure to get a crude compound. The obtained crude was purified using column chromatography by eluting hexane/ethyl acetate to afford the desired product. **5a-5i**



Scheme 1: Synthesis of *N*-hydroxyimoyl chloride

4. Optimization condition for isoxazoline and spirocycle derivatives

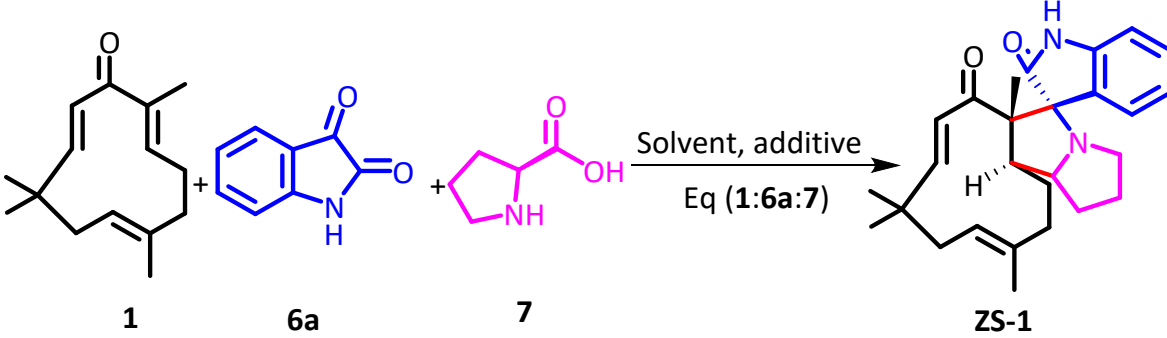
Table 1: Optimization condition for isoxazoline^{a, b, c}

S.No	Base(equivalent)	Solvent	Time (in hours)	Temperature (°C)	Yield (%) ^b
1	2,6-Lutidine (1)	1,4-dioxane	28	0 °C	Trace
2	2,6-Lutidine (1)	DMSO	36	0 °C-rt	Trace
3	Na ₂ CO ₃ (1)	1,4-dioxane	24	0 °C	Trace
4	DABCO (1)	1,4-dioxane	30	0 °C	Trace
5	TEA (1)	DMF	12	0 °C-rt	4
6	TEA (1)	DMF	12	0 °C	3
7	TEA (1)	DMF	24	0 °C-rt	18
8	TEA (0.5)	DMF	24	0 °C-rt	28
9	TEA (0.5)	DMF	20	0 °C	20
10	TEA (0.5)	DMF	30	0 °C-rt	26
11	DBU (1)	DMF	20	0 °C-rt	18

^a **Reaction condition:** **1** (0.45 mmol, 1 equiv), **5a** (0.7 mmol, 1.5equiv), Base, Solvent (0.25M),

^b isolated yield based on starting material recovered.

Table 2: Optimization condition for spirocycle^{a, b, c}

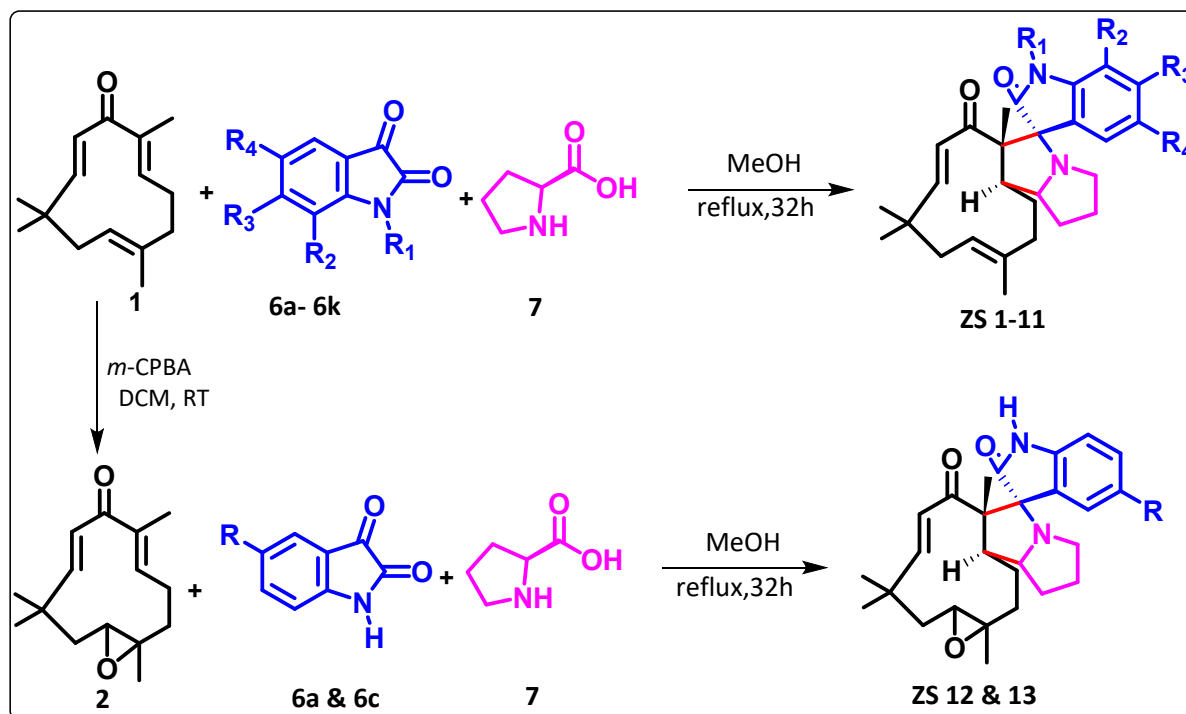
			
S. No	Solvent	Equiv (1:6a:7)	Yield % ^c (%) ^d
1	EtOAc	1:2.5:3	0
2	DMF	1:2.5:3	26(13.5)
3	DMSO	1:2.5:3	16.5(13.5)
4	Methanol(TEA) ^b	1:2.5:3	28(18)
5	Methanol (Cs ₂ CO ₃) ^b	1:2.5:3	23(15)
6	Methanol	1:1.5:3	26(19)
7	Methanol	1:2:2.5	28(22)
8	Methanol	1:2:2.5	32(27)
9	Methanol	1:3:3.5	23.7(17.7)

^a **Reaction condition:** **1** (0.45mmol, 1 equiv), **6a**, and **7** in MeOH (0.15 M) under reflux condition, ^b additives used, ^c isolated yield based on starting material recovered, ^d isolated yield

5. General procedure for the synthesis of zerumbone fused spirocyclic compounds

Isatin **6a** – **6k** (2.5 equiv, 1.1 mmol) and L-proline **7** (3 equiv, 1.3 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The reaction was allowed to stir for 32 h. The reaction was concentrated under reduced pressure to get a crude compound. The

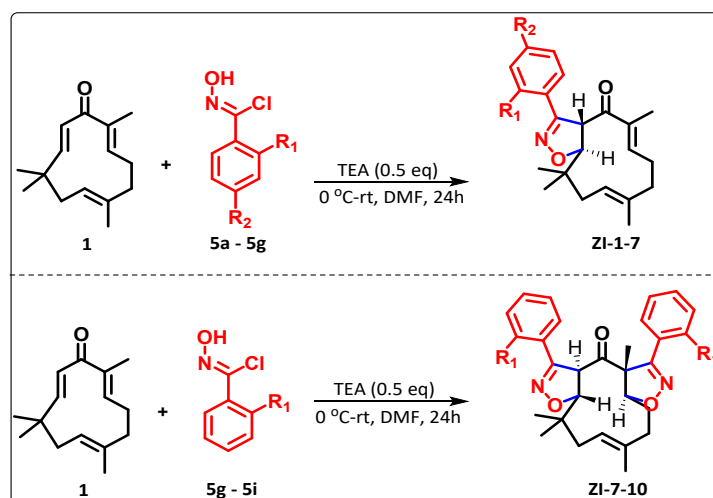
obtained crude was purified by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to afford the desired product.



Scheme 2: General procedure for spirocycle synthesis

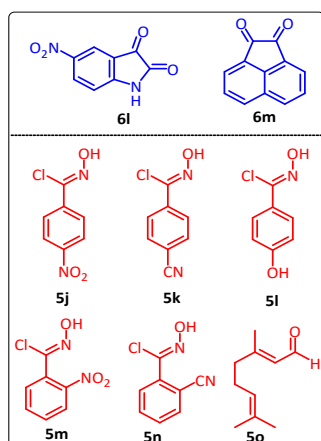
6. General procedure for the synthesis of zerumbone fused isoxazoline

Compound **5a-5i** (1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of Triethyl amine (0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min then compound **1** (1 equiv, 0.45 mmol) was added and warmed to rt. The reaction was allowed to stir for 24 hours. The reaction mixture was diluted with 10 mL of water and extracted with ethyl acetate (3 x 10 mL). The combined ethyl acetate layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure to get a crude compound. The obtained crude was purified using column chromatography by eluting (5:95 Hexanes/Ethyl acetate) to afford the desired product.

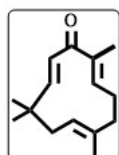


Scheme 3: General procedure for isoxazoline synthesis

7. Unsuccessful substrates for spirocycle & isoxazoline synthesis



8. ¹H and ¹³C NMR spectral data of zerumbone **1**

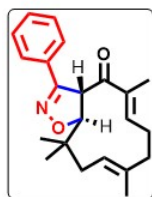


¹H NMR (500 MHz, CDCl₃) δ : 6.01 (dd, $J = 12.5, 1.5$ Hz, 1H), 5.97 (d, $J = 16.5$ Hz, 1H), 5.85 (d, $J = 16.5$ Hz, 1H), 5.24 (dd, $J = 12, 4$ Hz, 1H), 2.50 – 2.40 (m, 1H), 2.36 – 2.31 (m, 2H), 2.27 – 2.18 (m, 2H), 1.89 (d, $J = 13$ Hz, 1H), 1.79 (s, 3H), 1.53 (d, $J = 1.1$ Hz, 3H), 1.19 (s, 3H), 1.06 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ : 204.51, 160.89, 148.96, 138.05, 136.39, 127.26, 125.09, 42.51, 39.55, 37.97, 29.53, 24.41, 15.33, 11.89.

9. ¹H and ¹³C NMR spectral data of isoxazoline compounds

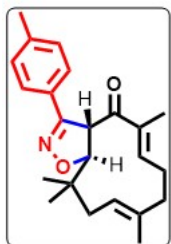
(5E,9E)-5,9,12,12-tetramethyl-3-phenyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one



Compound **5a** (107 mg, 1.5 equiv, 0.68 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (32 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-1** as a white solid 35 mg (28%(22%)). Mp (74-79 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.57 (dd, $J = 6.7, 2.9$ Hz, 2H), 7.37 – 7.26 (m, 3H), 6.39 (d, $J = 10$ Hz, 1H), 5.21 (d, $J = 10$ Hz, 1H), 5.06 (d, $J = 5$ Hz, 1H), 4.15 (d, $J = 5$ Hz, 1H), 2.64 – 2.55 (m, 1H), 2.49 – 2.41 (m, 1H), 2.38 – 2.35 (m, 2H), 2.24 (dd, $J = 15, 10$ Hz, 1H), 1.95 (d, $J = 15$ Hz, 1H), 1.83 (s, 3H), 1.50 (s, 3H), 1.17 (s, 3H), 0.97 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 199.32, 155.46, 147.15, 135.36, 134.84, 130.02, 129.12, 128.90 (2C), 126.70 (2C), 123.48, 93.92, 56.89, 40.77, 39.62, 39.49, 28.64, 25.56, 19.43, 15.72, 12.80.

HRMS (ESI): Calcd for C₂₂H₂₇NO₂K 376.1678 [M+K]; Found for C₂₂H₂₇NO₂K: 376.1666

(5E,9E)-5,9,12,12-tetramethyl-3-(p-tolyl)-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one

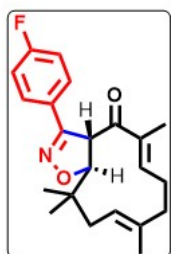


Compound **5b** (116 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (32 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to

give **ZI-2** as a white solid 32 mg (22%(21%)). Mp (91-96 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.46 (d, J = 10 Hz, 2H), 7.15 (d, J = 5 Hz, 2H), 6.37 (d, J = 10 Hz, 1H), 5.21 (d, J = 5 Hz, 1H), 5.04 (d, J = 5 Hz, 1H), 4.12 (d, J = 5 Hz, 1H), 2.63 – 2.54 (m, 1H), 2.46 - 2.41(m, 1H), 2.37 – 2.36 (m, 2H), 2.34 (s, 3H), 2.26 – 2.21 (m, 1H), 1.94 (d, J = 15 Hz, 1H), 1.82 (s, 3H), 1.49 (s, 3H), 1.16 (s, 3H), 0.96 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 199.38, 155.38, 146.92, 140.23, 135.39, 134.79, 129.59 (2C), 126.63 (2C), 126.29, 123.51, 93.68, 57.03, 40.77, 39.59, 39.48, 28.63, 25.55, 21.54, 19.43, 15.71, 12.81.

HRMS (ESI): Calcd for C₂₃H₃₀NO₂ 352.2276 [M+H]⁺; Found for C₂₃H₃₀NO₂: 352.2258

(5E,9E)-3-(4-fluorophenyl)-5,9,12,12-tetramethyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one

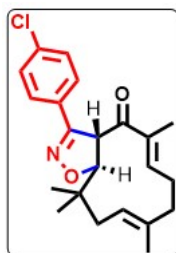


Compound **5c** (119 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (32 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1**(100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to

give **ZI-3** as a white solid 31 mg (21%(20%)). Mp (87-91°C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.57 – 7.53 (m, 2H), 7.06 – 7.01 (m, 2H), 6.37 (d, J = 5 Hz, 1H), 5.21 (d, J = 10 Hz, 1H), 5.03 (d, J = 4 Hz, 1H), 4.14 (d, J = 5 Hz, 1H), 2.65 – 2.56 (m, 1H), 2.46 – 2.35 (m, 3H), 2.26 – 2.21 (m, 1H), 1.95 (d, J = 15 Hz, 1H), 1.82 (s, 3H), 1.49 (s, 3H), 1.17 (s, 3H), 0.96 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 199.16, 163.72 (d, J = 251.4 Hz), 154.52, 147.31, 135.31, 134.91, 128.59 (d, J = 9.0 Hz), 125.42 (d, J = 4.0 Hz), 123.43, 116.16, 115.95, 94.05, 77.36, 56.92, 40.77, 39.62, 39.47, 28.64, 25.54, 19.42, 15.71, 12.78.

HRMS (ESI): Calcd for C₂₂H₂₆FNO₂K 394.1584 [M+K]⁺; Found for C₂₂H₂₆FNO₂K: 394.1572

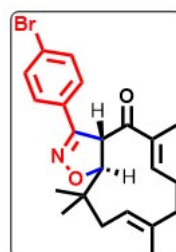
(5E,9E)-3-(4-chlorophenyl)-5,9,12,12-tetramethyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one.



Compound **5d** (130 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (32 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-4** as a white solid 30 mg (20%(19%)). Mp (77-82 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.49 (d, J = 10 Hz, 2H), 7.31 (d, J = 5 Hz, 2H), 6.37 (d, J = 10 Hz, 1H), 5.20 (d, J = 10 Hz, 1H), 5.02 (d, J = 5 Hz, 1H), 4.15 (d, J = 5 Hz, 1H), 2.64-2.56 (m, 1H), 2.45-2.42 (m, 1H), 2.338 – 2.35 (m, 2H), 2.26 – 2.21 (m, 1H), 1.94 (d, J = 15 Hz, 1H), 1.82 (s, 3H), 1.49 (s, 3H), 1.16 (s, 3H), 0.96 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 199.08, 154.61, 147.41, 135.94, 135.27, 134.94, 129.17 (2C), 127.88 (2C), 127.66, 123.39, 94.23, 56.66, 40.75, 39.62, 39.46, 28.62, 25.53, 19.39, 15.71, 12.76.

HRMS (ESI): Calcd for C₂₂H₂₇ClNO₂ 372.1730 [M+H]; Found for C₂₂H₂₇ClNO₂: 372.1738

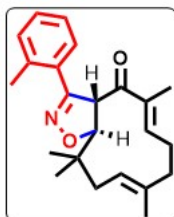
(5E,9E)-3-(4-bromophenyl)-5,9,12,12-tetramethyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one



Compound **5e** (160 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (32 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred to rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-5** as a white solid 35 mg (22%(19%)). Mp (82-86 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.47 – 7.41 (m, 4H), 6.38 (d, J = 10 Hz, 1H), 5.20 (d, J = 5 Hz, 1H), 5.03 (d, J = 5 Hz, 1H), 4.14 (d, J = 5 Hz, 1H), 2.61-2.54 (m, 1H), 2.44 - 2.40 (m, 1H), 2.36 – 2.34 (m, 2H), 2.22 (dd, J = 15, 10 Hz, 1H), 1.93 (d, J = 15 Hz, 1H), 1.80 (s, 3H), 1.48 (s, 3H), 1.15 (s, 3H), 0.95 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 199.07, 154.68, 147.51, 135.16, 134.91, 132.07 (2C), 128.06 (3C), 124.16, 123.30, 94.25, 56.54, 40.69, 39.57, 39.38, 28.58, 25.49, 19.34, 15.67, 12.71.

HRMS (ESI): Calcd for C₂₂H₂₇BrNO₂ 416.1225 [M+H]; Found for C₂₂H₂₇BrNO₂: 416.1198

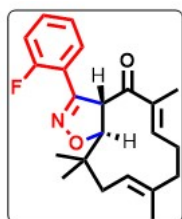
(5E,9E)-5,9,12,12-tetramethyl-3-(o-tolyl)-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one



Compound **5f** (116 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (32 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred to rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-6** as a white solid 33mg (23%(21%)). Mp (81-85 °C). ¹H NMR (400 MHz, CDCl₃) δ : 7.20 (d, J = 40 Hz, 4H), 6.25 (d, J = 8 Hz, 2H), 5.20 (d, J = 4 Hz, 2H), 5.10 (d, J = 3.2 Hz, 2H), 4.09 (d, J = 4 Hz, 2H), 2.62 (s, 3H), 2.36 - 2.34 (m, 1H), 2.32 – 2.26 (m, 2H), 2.22 (m, 2H), 1.96 (d, J = 16 Hz, 1H), 1.79 (s, 3H), 1.59 (s, 1H), 1.50 (s, 3H), 1.29 (d, J = 28 Hz, 1H), 1.19 (s, 3H), 1.03 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ : 199.61, 155.79, 146.70, 138.81, 135.55, 134.79, 131.90, 129.23, 128.23, 126.15, 125.79, 123.51, 92.60, 59.42, 40.84, 39.65, 39.49, 28.58, 25.53, 22.83, 19.79, 15.76, 12.75.

HRMS (ESI): Calcd for C₂₃H₃₀NO₂ 352.2276 [M+H]; Found for C₂₃H₃₀NO₂: 352.2272

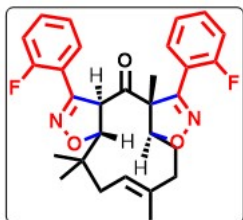
(5E,9E)-3-(2-fluorophenyl)-5,9,12,12-tetramethyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one



Compound **5g** (119 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (31 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-7** as a white solid 20 mg (15%(12%)). Mp (82-86 °C). ¹H NMR (500 MHz, CDCl₃) δ : 7.98 – 7.95 (m, 1H), 7.36-7.32 (m, 1H), 7.18 – 7.15 (m, 1H), 7.04-7.00 (m, 1H), 6.22 (d, J = 10 Hz, 1H), 5.19-5.15 (m, 2H), 4.16 (d, J = 3.5, 1H), 2.59-2.50 (m, 1H), 2.39 – 2.32 (m, 3H), 2.26 – 2.21 (m, 1H), 1.95 (d, J = 15 Hz, 1H), 1.79 (s, 3H), 1.50 (s, 3H), 1.17 (s, 3H), 0.99 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ : 199.53, 160.02 (d, J = 250 Hz), 151.96 (d, J = 3.0 Hz), 146.46, 135.15, 134.76, 131.69 (d, J = 8.0 Hz), 129.68 (d, J = 4.0 Hz), 124.87 (d, J = 3.0 Hz), 123.24, 117.11 (d, J = 11.1 Hz), 116.10, 93.49, 58.56, 40.91, 39.67, 39.45, 28.40, 25.45, 19.83, 15.76, 12.84.

HRMS (ESI): Calcd for C₂₂H₂₇FNO₂ 356.2025 [M+H]; Found for C₂₂H₂₇FNO₂: 356.1999

(E)-1,12-bis(2-fluorophenyl)-4,4,7,12a-tetramethyl-3a,4,5,8,9,9a,12a,13a-octahydro-13H-cycloundeca[2,1-d:4,5-d']diisoxazol-13-one

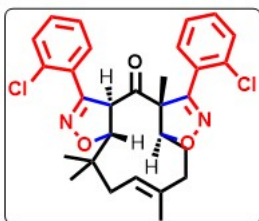


Compound **5g** (119 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (31 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100mg, 1 equiv, 0.45 mmol) was added and stirred rt.

The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-8** as a white solid 39 mg (19%(17%)). Mp (91-95 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.50 – 7.39 (m, 3H), 7.33 – 7.28 (m 1H), 7.24 – 7.17 (m, 2H), 7.12 (t, J = 7.5 Hz, 1H), 6.94 – 6.87 (m, 1H), 5.50 (d, J = 5 Hz, 1H), 5.26 – 5.21 (t, J = 7.5 Hz, 1H), 5.07 (d, J = 5 Hz, 1H), 4.17 (d, J = 5 Hz, 1H), 2.23 – 2.12 (m, 2H), 2.04 – 1.96 (m, 2H), 1.71 - 1.65 (m, 2H), 1.48 (s, 3H), 1.27 (s, 3H), 1.22 (s, 3H), 1.10 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 201.78, 160.79 (d, J = 248.46 Hz), 160.16 (d, J = 259.48 Hz), 158.88 (d, J = 8.1 Hz), 151.60, 135.51, 132.26 (d, J = 8.3 Hz), 131.23 (d, J = 8.6 Hz), 130.84 (d, J = 3.5 Hz), 130.17 (d, J = 3.6 Hz), 125.47, 125.00 (d, J = 3.3 Hz), 124.25 (d, J = 3.2 Hz), 118.72 (d, J = 14.0 Hz), 117.11 (d, J = 14.2 Hz), 116.36 (d, J = 21.2 Hz), 115.53 (d, J = 22.2 Hz), 93.67, 93.09, 56.99, 54.39, 40.91, 39.48, 38.35, 28.89, 22.12, 19.40, 16.94, 15.18.

HRMS (ESI): Calcd for C₂₉H₃₁F₂N₂O₃ 493. 2302 [M+H]⁺; Found for C₂₉H₃₁F₂N₂O₃: 493. 2301

(5E,9E)-3-(2-chlorophenyl)-5,9,12,12-tetramethyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one



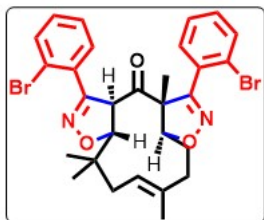
Compound **5h** (130 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (31 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column

chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-9** as a white solid 41 mg (20%(17%)). Mp (81-85 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.48 – 7.46 (m, 1H), 7.43 – 7.41 (m, 1H), 7.34 – 7.31 (m, 4H), 7.27 (s, 1H), 7.21 – 7.19 (m, 1H), 5.64 – 5.60 (m, 1H), 5.13 – 5.09 (m, 1H), 5.03 (s, 1H), 4.26 – 4.25 (m, 1H), 2.18 – 2.13 (m, 1H), 2.04 – 2.00 (m, 2H), 1.91 (s, 1H), 1.55 (s, 2H), 1.47 (s, 3H), 1.31 (s, 3H), 1.19 (s, 3H), 1.15 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 202.33, 160.83, 154.14, 135.58, 133.78, 133.13, 131.39 (2C), 130.97 130.65,

130.15, 130.10, 129.36, 128.45, 127.38, 126.70, 124.86, 93.44, 92.92, 56.98, 54.22, 41.06, 38.39, 38.29, 29.17, 21.51, 20.36, 16.41, 15.38.

HRMS (ESI): Calcd for $C_{29}H_{31}Cl_2N_2O_3$ 525.1711 [M+H]; Found for $C_{29}H_{31}Cl_2N_2O_3$: 525.1701

(5E,9E)-3-(2-bromophenyl)-5,9,12,12-tetramethyl-3a,7,8,11,12,12a-hexahydro-4H-cycloundeca[d]isoxazol-4-one



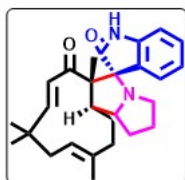
Compound **5i** (160 mg, 1.5 equiv, 0.7 mmol) was dissolved in DMF (0.25 M) at 0 °C followed by the addition of triethylamine (31 μ l, 0.5 equiv). The reaction mixture was allowed to stir under the 0 °C for 10 min, then compound **1** (100 mg, 1 equiv, 0.45 mmol) was added and stirred at rt. The crude material was purified by silica gel column chromatography (5:95 Ethyl acetate / Hexanes) to give **ZI-10** as a white solid 35 mg (15%(12%)).

Mp (87-92 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.65 (d, J = 5 Hz, 1H), 7.55 (d, J = 10 Hz, 1H), 7.38-7.28 (m, 3H), 7.25 – 7.20 (m, 2H), 7.13 (dd, J = 7.5, 1.5 Hz, 1H), 5.61 (d, J = 10 Hz, 1H), 5.11 (d, J = 10 Hz, 1H), 4.99 (t, J = 10 Hz, 1H), 4.33 (t, J = 10, 1H), 2.16 – 2.12 (m, 1H), 2.05 – 2.01 (m, 1H), 1.98 – 1.94 (m, 1H), 1.89-1.84 (m, 1H), 1.57 (s, 1H), 1.53 (d, J = 5 Hz, 1H), 1.48 (s, 3H), 1.31 (s, 3H), 1.18 (d, J = 2.5 Hz, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ : 202.64, 161.64, 155.26, 135.59, 133.30, 132.38, 132.10, 131.52, 131.49, 131.12, 130.84, 130.49, 127.85, 127.18, 124.67, 123.51, 122.43, 93.34, 92.92, 57.06, 53.96, 41.12, 38.29, 38.01, 29.29, 21.33, 20.83, 16.37, 15.50.

HRMS (ESI): Calcd for $C_{29}H_{31}Br_2N_2O_3$ 613.0701 [M+H]; Found for $C_{29}H_{31}Br_2N_2O_3$: 613.0721

10. ¹H and ¹³C NMR spectral data of Spirocyclic compounds

(5R,5aS,7E,11E)-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione



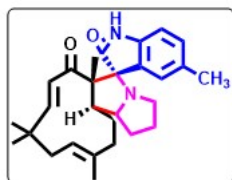
Isatin **6a** (167 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The solvent was evaporated under reduced

pressure and the crude material was purified by silica gel column chromatography (20:80 ethyl acetate / Hexanes) to give **ZS-1** as a white solid 51 mg (32% (27%)). Mp (132-136 °C). **¹H**

NMR (500 MHz, CDCl₃) δ : 8.00 (bs, 1H), 7.27 (m, 1H), 7.15 (td, J = 8, 1.5 Hz, 1H), 6.97 (td, J = 7.5, 1 Hz, 1H), 6.77 (d, J = 7.5 Hz, 1H), 5.79 (m, 2H), 5.12 (t, J = 15 Hz, 1H), 3.79 – 3.74 (m, 1H), 2.64 (m, 2H), 2.54 (dd, J = 15, 10 Hz, 1H), 2.36 (d, J = 13 Hz, 1H), 2.26 – 2.23 (m, 1H), 2.126–2.11 (m, 2H), 1.95 – 1.92 (m, 2H), 1.77 (s, 1H), 1.70 – 1.62 (m, 3H), 1.46 (s, 3H), 1.42 (s, 3H), 1.05 (s, 3H), 0.85 (s, 3H). **¹³C NMR (101MHz, CDCl₃)** δ : 201.19, 179.42, 147.85, 141.16, 137.42, 130.38, 129.46, 126.95, 126.17, 124.10, 121.17, 111.15, 77.76, 73.64, 69.56, 48.95, 45.93, 40.20, 38.78, 38.52, 32.78, 29.96, 29.25, 28.35, 27.00, 18.16, 14.46.

HRMS (ESI): Calcd for C₂₇H₃₅N₂O₂: 419.2704, [M+H]⁺; Found for C₂₇H₃₅N₂O₂: 419.2721.

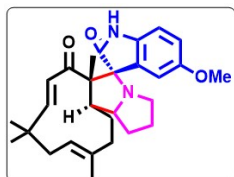
(5R,5aS,7E,11E)-5a,5',9,9,12-pentamethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione



Isatin **6b** (185 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The solvent was evaporated under reduced pressure and the crude material was purified by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-2** as a white solid 40 mg (22% (20%)). Mp (144–146 °C). **¹H NMR (400 MHz, CDCl₃)** δ : 8.15 (s, 1H), 7.07 (s, 1H), 6.95 (d, J = 8 Hz, 1H), 6.66 (d, J = 8 Hz, 1H), 5.80 (s, 2H), 5.11 (t, J = 6 Hz, 1H), 3.79 – 3.73 (m, 1H), 2.65 – 2.62 (m, 2H), 2.55 (dd, J = 16, 8 Hz, 1H), 2.32 (s, 3H), 2.27 – 2.20 (m, 1H), 2.14 – 2.10 (m, 2H), 1.95 – 1.89 (m, 3H), 1.73 – 1.59 (m, 3H), 1.48 (s, 3H), 1.41 (s, 3H), 1.05 (s, 3H), 0.86 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ : 201.08, 179.63, 147.66, 138.86, 137.35, 130.35, 130.23, 129.82, 127.71, 126.11, 124.07, 110.99, 77.99, 73.53, 69.48, 48.85, 45.99, 40.14, 38.57, 38.32, 32.89, 29.99, 29.12, 28.46, 27.05, 21.42, 18.20, 14.43.

HRMS (ESI): Calcd for C₂₈H₃₇N₂O₂ 433.2860 [M+H]⁺; Found for C₂₈H₃₇N₂O₂: 433.2869.

(5R,5aS,7E,11E)-5'-methoxy-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione.

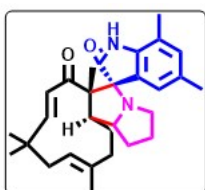


Isatin **6c** (203 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-3** as a white solid 48 mg (27% (23%)). Mp (152–156 °C). **¹H NMR (500 MHz, CDCl₃)** δ : 7.69 (s, 1H),

6.91 (s, 1H), 6.68 (s, 2H), 5.84 (s, 2H), 5.13 (t, $J = 7.75$ Hz, 1H), 3.76 (s, 3H), 2.68 – 2.56 (m, 3H), 2.35 (d, $J = 13.5$ Hz, 1H), 2.26 – 2.22 (m, 1H), 2.15 – 2.10 (m, 2H), 1.94 – 1.92 (m, 2H), 1.68 – 1.59 (m, 5H), 1.43 (s, 3H), 1.41 (s, 3H), 1.06 (s, 3H), 0.86 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 200.92, 179.38, 154.80, 147.85, 137.55, 134.64, 130.30, 127.71, 123.94, 115.59, 112.43, 111.21, 78.33, 73.68, 69.65, 55.76, 48.97, 45.95, 40.26, 38.73, 38.64, 32.82, 29.99, 29.27, 28.12, 26.67, 18.04, 14.50.

HRMS (ESI): Calcd for $\text{C}_{28}\text{H}_{37}\text{N}_2\text{O}_3$ 449.2804[M+H]; Found for $\text{C}_{28}\text{H}_{36}\text{N}_2\text{O}_3$ 449.2824.

(5R,5aS,7E,11E)-5a,5',7',9,9,12-hexamethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione

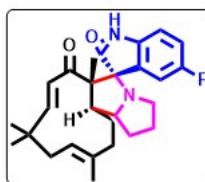


Isatin **6d** (201 mg, 2.5 eq, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-4** as a white solid 36 mg (21% (18%)). Mp (152-156 °C). ^1H NMR (500 MHz, CDCl_3) δ : 7.56 (s, 1H), 6.92 (s, 1H), 6.79 (s, 1H), 5.84 (d, $J = 16$ Hz, 1H), 5.77 (d, $J = 16$ Hz, 1H), 5.11 (t, $J = 7.5$ Hz, 1H), 3.77 – 3.72 (m, 1H), 2.66-2.60 (m, 2H), 2.53 (dd, $J = 15, 10$ Hz, 1H), 2.36 (d, $J = 15$ Hz, 1H), 2.30 (s, 3H), 2.25 – 2.22 (m, 1H), 2.10 (s, 3H), 1.96-1.88 (m, 3H), 1.79 – 1.64 (m, 3H), 1.61-1.58 (m, 2H), 1.50 (s, 3H), 1.41 (s, 3H), 1.06 (s, 3H), 0.87 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 201.38, 179.54, 147.53, 137.46, 137.20, 131.36, 130.54, 130.18, 125.53, 125.24, 124.13, 119.79, 78.01, 73.56, 69.50, 48.76, 45.98, 40.13, 38.60, 38.14, 32.83, 29.94, 29.05, 28.67, 27.07, 21.36, 18.29, 16.39, 14.44.

HRMS (ESI): Calcd for $\text{C}_{29}\text{H}_{39}\text{N}_2\text{O}_2$ 447.3011[M+H]; Found for $\text{C}_{29}\text{H}_{39}\text{N}_2\text{O}_2$: 447. 3021.

(5R,5aS,7E,11E)-5'-fluoro-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione



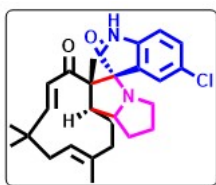
Isatin **6e** (189 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-5** as a white solid 54 mg (30% (27%)). Mp (131-135 °C) ^1H NMR (500 MHz, CDCl_3) δ : 8.44 (s, 1H), 7.01 (dd, $J = 8, 2.5$ Hz, 1H), 6.87 (td, $J = 8.5, 2.5$ Hz, 1H), 6.73 – 6.71 (m, 1H), 5.85 (s, 2H), 5.15

(t, $J = 7.75$ Hz, 1H), 3.79 – 3.74 (m, 1H), 2.67 (m, 1H), 2.59 – 2.49 (m, 2H), 2.37 (d, $J = 13.5$ Hz, 1H), 2.28 – 2.23 (m, 1H), 2.15 – 2.11 (m, 2H), 1.95 (m, 3H), 1.77 (s, 1H), 1.64 (m, 2H), 1.46 (s, 3H), 1.42 (s, 3H), 1.07 (s, 3H), 0.90 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 201.31, 179.39, 163.38 (d, $J = 198.9$ Hz), 148.33, 142.60 (d, $J = 12.1$ Hz), 137.40, 130.18, 127.85 (d, $J = 9.7$ Hz), 124.30, 121.58 (d, $J = 3.1$ Hz), 107.62 (d, $J = 18.1$ Hz), 99.63 (d, $J = 21.2$ Hz), 77.16, 73.50, 69.60, 48.86, 45.86, 40.17, 38.80, 38.44, 33.35, 32.83, 29.85, 29.11, 27.11, 18.31, 14.55.

HRMS (ESI): Calcd for $\text{C}_{27}\text{H}_{34}\text{FN}_2\text{O}_2$ 437.2604[M+H]; Found for $\text{C}_{27}\text{H}_{34}\text{FN}_2\text{O}_2$: 437.2615.

(5R,5aS,7E,11E)-5'-chloro-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione.

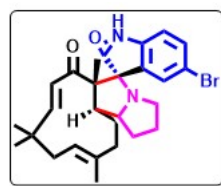


Isatin **6f** (208 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-6** as a white solid 39.5 mg (23% (19%)). Mp (137-141 °C). ^1H NMR (500 MHz, CDCl_3) δ : 8.58 (s, 1H), 7.22 (s, 1H), 7.13 (d, $J = 8.5$ Hz, 1H), 6.72 (d, $J = 8.0$ Hz, 1H), 5.83 (s, 2H), 5.15 (t, $J = 7$ Hz, 1H), 3.78 – 3.73 (m, 1H), 2.67 (s, 1H), 2.58 – 2.57 (m, 1H), 2.50 (dd, $J = 16.5, 7$ Hz, 1H), 2.39 (d, $J = 12.5$ Hz, 1H), 2.29 – 2.23 (m, 1H), 2.13 (s, 2H), 2.02 – 2.00 (m, 1H), 1.97 – 1.89 (m, 2H), 1.80 (s, 1H), 1.67 – 1.64 (m, 2H), 1.51 (s, 3H), 1.41 (s, 3H), 1.07 (s, 3H), 0.94 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 201.00, 179.21, 148.55, 139.87, 137.26, 129.84, 129.34, 128.35, 127.00, 126.76, 124.49, 112.12, 78.02, 73.37, 69.94, 48.79, 46.14, 40.11, 38.71, 38.15, 33.03, 29.96, 28.91, 28.81, 27.48, 18.46, 14.51.

HRMS (ESI): Calcd for $\text{C}_{27}\text{H}_{34}\text{ClN}_2\text{O}_2$ 453.2308[M+H]; Found for $\text{C}_{27}\text{H}_{34}\text{ClN}_2\text{O}_2$: 453.2293.

(5R,5aS,7E,11E)-5'-bromo-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione.



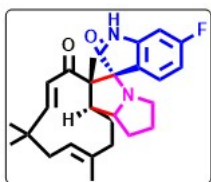
Isatin **6g** (260 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1'** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-7** as a white solid 69 mg (35% (30%)). Mp (146-150 °C). ^1H NMR (500 MHz, CDCl_3) δ : 8.29 (s, 1H), 7.01

(d, $J = 10$ Hz, 1H), 6.89 – 6.86 (m, 1H), 6.74 – 6.70 (m, 1H), 5.86 (s, 2H), 5.15 (t, $J = 7.5$ Hz, 1H), 3.79 – 3.75 (m, 1H), 2.69–2.66 (m, 1H), 2.58 – 2.48 (m, 2H), 2.38 (d, $J = 10$ Hz, 1H), 2.27 (s, 1H), 2.13– (m, 2H), 2.00 – 1.90 (m, 3H), 1.72 (s, 1H), 1.67 – 1.64 (m, 2H), 1.46 (s, 3H), 1.42 (s, 3H), 1.08 (s, 3H), 0.91 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 200.89, 179.37, 148.39, 137.48, 137.16, 129.90, 128.10, 124.24, 115.88, 115.65, 114.54, 111.54, 78.18, 73.53, 69.91, 49.00, 45.97, 40.18, 38.76, 38.51, 32.92, 29.92, 29.07, 28.42, 26.96, 18.21, 14.55.

HRMS (ESI): Calcd for $\text{C}_{27}\text{H}_{33}\text{BrN}_2\text{O}_2$ 498.1803 $[\text{M}+2\text{H}]$; Found for $\text{C}_{27}\text{H}_{33}\text{BrN}_2\text{O}_2$: 499.1795

(5R,5aS,7E,11E)-6'-fluoro-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione

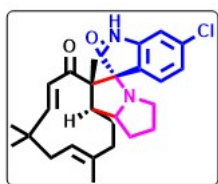


Isatin **6h** (189 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-8** as a white solid 39.7 mg (21% (20%)). mp (138–140 °C). ^1H NMR (500 MHz, CDCl_3) δ : 8.20 (s, 1H), 7.20 – 7.17 (m, 1H), 6.66 (td, $J = 10, 5$ Hz, 1H), 6.51 (dd, $J = 10, 5$ Hz, 1H), 5.85 (d, $J = 16$ Hz, 1H), 5.81 (d, $J = 16$ Hz, 1H), 5.13 (t, $J = 7.5$ Hz, 1H), 3.79 – 3.74 (m, 1H), 2.65–2.57 (m, 2H), 2.49 (dd, $J = 15, 5$ Hz, 1H), 2.38 (d, $J = 15$ Hz, 1H), 2.27 – 2.22 (m, 1H), 2.13 – 2.10 (m, 2H), 2.01–1.89 (m, 3H), 1.71 (s, 1H), 1.65–1.62 (m, 2H), 1.47 (s, 3H), 1.41 (s, 3H), 1.08 (s, 3H), 0.90 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 201.33, 179.54, 164.73 (d, $J = 248.46$ Hz), 148.32, 142.72 (d, $J = 12.0$ Hz), 137.39, 130.21, 127.81 (d, $J = 9.6$ Hz), 124.31, 121.59 (d, $J = 3.1$ Hz), 107.69 (d, $J = 22.2$ Hz), 99.71 (d, $J = 26.2$ Hz), 77.26, 73.50, 69.59, 48.88, 45.88, 40.18, 38.80, 38.43, 32.84, 29.86, 29.11, 28.54, 27.13, 18.32, 14.56.

HRMS (ESI): Calcd for $\text{C}_{27}\text{H}_{34}\text{FN}_2\text{O}_2$ 437.2604 $[\text{M}+\text{H}]$; Found for $\text{C}_{27}\text{H}_{34}\text{FN}_2\text{O}_2$: 437.2615.

(5R,5aS,7E,11E)-6'-chloro-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione



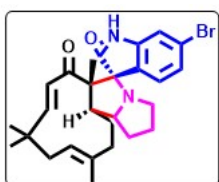
Isatin **6i** (206 mg, 2.5 equiv, 1.1 mmol) and L- proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-9** as a white

solid 57 mg (31% (27%)). Mp (126-129 °C). **¹H NMR (500 MHz, CDCl₃)** δ: 7.81 (s, 1H), 7.16 (d, *J* = 10 Hz, 1H), 6.95 (dd, *J* = 10, 5 Hz, 1H), 6.76 (s, 1H), 5.87 (d, *J* = 20 Hz, 1H), 5.82 (d, *J* = 20 Hz, 1H), 5.14 (t, *J* = 7.5 Hz, 1H), 3.80 – 3.73 (m, 1H), 2.68 – 2.55 (m, 3H), 2.48 (dd, *J* = 20, 10 Hz, 1H), 2.39 (d, *J* = 15 Hz, 1H), 2.28 – 2.22 (m, 1H), 2.14 – 2.09 (m, 2H), 2.00-1.93 (m, 3H), 1.69 – 1.60 (m, 5H), 1.47 (s, 3H), 1.42 (s, 3H), 1.09 (s, 3H), 0.91 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ: 201.27, 179.00, 148.42, 142.28, 137.44, 135.22, 130.14, 127.58, 124.78, 124.30, 121.15, 111.65, 77.28, 73.51, 69.81, 48.91, 45.89, 40.20, 38.85, 38.48, 32.79, 29.86, 29.04, 28.53, 27.09, 18.30, 14.55.

HRMS (ESI): Calcd for C₂₇H₃₄ClN₂O₂ 453.2308 [M+H]; Found for C₂₇H₃₄ClN₂O₂: 453.2312

(5R,5aS,7E,11E)-6'-bromo-5a,9,9,12-tetramethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione

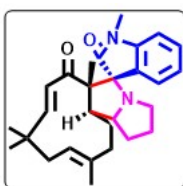


Isatin **6j** (260 mg, 2.5 equiv, 1.1 mmol) and L-proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified

by silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-10** as a white solid 71 mg (35% (31%)). Mp (144-148 °C). **¹H NMR (500 MHz, CDCl₃)** δ: 7.71 (s, 1H), 7.11 (s, 2H), 6.91 (s, 1H), 5.86 (d, *J* = 20 Hz, 1H), 5.81 (d, *J* = 20 Hz, 1H), 5.13 (t, *J* = 10 Hz, 1H), 3.79 – 3.73 (m, 1H), 2.67 – 2.55 (m, 2H), 2.51 (dd, *J* = 25, 10 Hz, 1H), 2.38 (d, *J* = 15 Hz, 1H), 2.28-2.21 (m, 1H), 2.13 – 2.10 (m, 1H), 1.98 – 1.91 (m, 2H), 1.68 – 1.58 (m, 5H), 1.46 (s, 3H), 1.41 (s, 3H), 1.10 (s, 3H), 0.91 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ: 201.24, 178.89, 148.43, 142.40, 137.45, 130.11, 127.90, 125.36, 124.30, 124.12, 123.10, 114.42, 77.36, 73.51, 69.81, 48.91, 45.89, 40.21, 38.86, 38.48, 32.77, 29.86, 29.04, 28.50, 27.09, 18.30, 14.54.

HRMS (ESI): Calcd for C₂₇H₃₅BrN₂O₂ 498.1803 [M+2H]; Found for C₂₇H₃₅BrN₂O₂: 499.1795.

(5R,5aS,7E,11E)-1',5a,9,9,12-pentamethyl-1,2,3,5a,9,10,13,14,14a,14b-decahydro-6H-spiro[cycloundeca[a]pyrrolizine-5,3'-indoline]-2',6-dione.



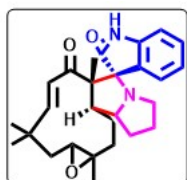
Isatin **6k** (185 mg, 2.5 equiv, 1.1 mmol) and L-proline **7** (158 mg, 3 equiv, 1.37 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone **1** (100 mg, 0.45 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified by

silica gel column chromatography (20:80 Ethyl acetate / Hexanes) to give **ZS-11** as a white solid 51 mg (28% (26%)). Mp (127-132 °C). **¹H NMR (500 MHz, CDCl₃)** δ: 7.28 (d, *J* = 5

Hz, 1H), 7.22 (td, $J = 10$, 1 Hz, 1H), 6.98 (td, $J = 7.5$, 1 Hz, 1H), 6.74 (d, $J = 5$ Hz, 1H), 5.76 (s, 2H), 5.10 (t, $J = 7.5$ Hz, 1H), 3.80 – 3.75 (m, 1H), 3.14 (s, 3H), 2.67 – 2.57 (m, 2H), 2.48 (dd, $J = 20$, 10 Hz, 1H), 2.36 (d, $J = 15$ Hz, 1H), 2.26 – 2.22 (m, 1H), 2.14 – 2.06 (m, 2H), 1.98 – 1.88 (m, 3H), 1.70 – 1.66 (m, 2H), 1.64 – 1.61 (m, 1H), 1.48 (s, 3H), 1.40 (s, 3H), 1.04 (s, 3H), 0.90 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 201.47, 192.88, 148.00, 144.38, 137.12, 130.21, 129.88, 126.41 (2C), 124.45, 121.21, 109.19, 77.36, 77.32, 73.74, 69.51, 48.46, 46.48, 40.06, 38.71, 38.12, 32.59, 29.77, 28.84, 27.40, 26.70, 18.53, 14.47.

HRMS (ESI): Calcd for $\text{C}_{28}\text{H}_{37}\text{N}_2\text{O}_2$ 433.2860 $[\text{M}+\text{H}]$; Found for $\text{C}_{28}\text{H}_{37}\text{N}_2\text{O}_2$: 433.2870.

(3R,6a'S,E)-3',3',6a',13a'-tetramethyl-1a',2',3',6a',9',10',11',11a',11b',12',13',13a'-dodecahydro-6'H-spiro[indoline-3,7'-oxireno[2',3':8,9]cycloundeca[1,2-a]pyrrolizine]-2,6'-dione.

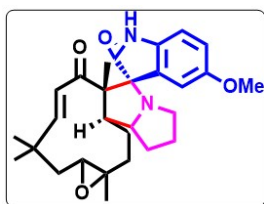


Isatin **6a** (157 mg, 2.5 equiv, 1 mmol) and L- proline **7** (148 mg, 3 equiv, 1.2 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone Epoxide **2** (100 mg, 0.4 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude material was purified by

silica gel column chromatography (30:70 Ethyl acetate / Hexanes) to give **ZS-12** as a white solid 13 mg (13% (7%)). Mp (112-118 °C). ^1H NMR (400 MHz, CDCl_3) δ : 8.33 (s, 1H), 7.25 – 7.19 (m, 2H), 7.02 (t, $J = 8$ Hz, 1H), 6.84 (d, $J = 8$ Hz, 1H), 5.82 (d, $J = 16$ Hz, 1H), 5.66 (d, $J = 16$ Hz, 1H), 5.29 (s, 1H), 3.71 (dd, $J = 12$, 8 Hz, 1H), 2.76 (d, $J = 8$ Hz, 1H), 2.64 (s, 1H), 2.59 – 2.49 (m, 3H), 2.31 – 2.25 (m, 1H), 2.19 (s, 1H), 2.11 (s, 2H), 1.71 (d, $J = 16$ Hz, 1H), 1.66 – 1.57 (m, 3H), 1.42 (s, 3H), 1.16 (s, 3H), 1.00 (d, $J = 5.4$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ : 203.67, 179.66, 147.28, 141.41, 130.40, 129.74, 127.03, 126.11, 121.33, 111.60, 77.37, 73.09, 69.20, 61.89, 61.00, 53.56, 51.96, 45.86, 38.19, 37.64, 36.55, 32.95, 30.36, 25.32, 23.82, 17.24, 14.31.

HRMS (ESI): Calcd for $\text{C}_{27}\text{H}_{35}\text{N}_2\text{O}_3$ 435.2653 $[\text{M}+\text{H}]$; Found for $\text{C}_{27}\text{H}_{35}\text{N}_2\text{O}_3$: 435.2647

(3R,6a'S,E)-5-methoxy-3',3',6a',13a'-tetramethyl-1a',2',3',6a',9',10',11',11a',11b',12',13',13a'-dodecahydro-6'H-spiro[indoline-3,7'-oxireno[2',3':8,9]cycloundeca[1,2-a]pyrrolizine]-2,6'-dione



Isatin **6c** (189 mg, 2.5 equiv, 1 mmol) and L- proline **7** (138 mg, 3 equiv, 1.2 mmol) were dissolved in methanol (0.15 M) followed by the addition of zerumbone Epoxide **2** (100 mg, 0.4 mmol, 1 equiv). The reaction mixture was allowed to stir under the reflux condition. The crude

material was purified by silica gel column chromatography (30:70 Ethyl acetate / Hexanes) to

give **ZS-13** as a white solid 10.5 mg (11% (5%)). Mp (112-118 °C). **¹H NMR (400 MHz, CDCl₃)** δ: 7.95 (s, 1H), 6.89 (s, 1H), 6.75 (s, 2H), 5.89 (d, *J* = 20 Hz, 1H), 5.74 (d, *J* = 20Hz, 1H), 3.82 (s, 1H), 3.78 (s, 3H), 2.78 (d, *J* = 15 Hz, 1H), 2.68 – 2.65 (m, 1H), 2.59 – 2.53 (m, 3H), 2.31 – 2.25 (m, 1H), 2.17 (s, 2H), 1.73 (d, *J* = 15 Hz, 1H), 1.65 – 1.58 (m, 3H), 1.41 (s, 3H), 1.29 (s, 1H), 1.25 (s, 2H), 1.15 (s, 3H), 1.01 (d, *J* = 2.6 Hz, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ: 203.24, 179.49, 154.98, 147.55, 134.45, 130.36, 127.83, 116.07, 112.00, 111.51, 77.83, 73.09, 69.34, 61.87, 61.06, 55.82, 55.65, 51.85, 45.80, 38.33, 37.71, 36.33, 32.98, 30.41, 24.87, 23.67, 17.23, 14.27.

HRMS (ESI): Calcd for C₂₈H₃₇N₂O₄ 465.2758 [M+H]⁺; Found for C₂₈H₃₇N₂O₄: 465.2755.

11. ^1H and ^{13}C NMR spectral images of Zerumbone:

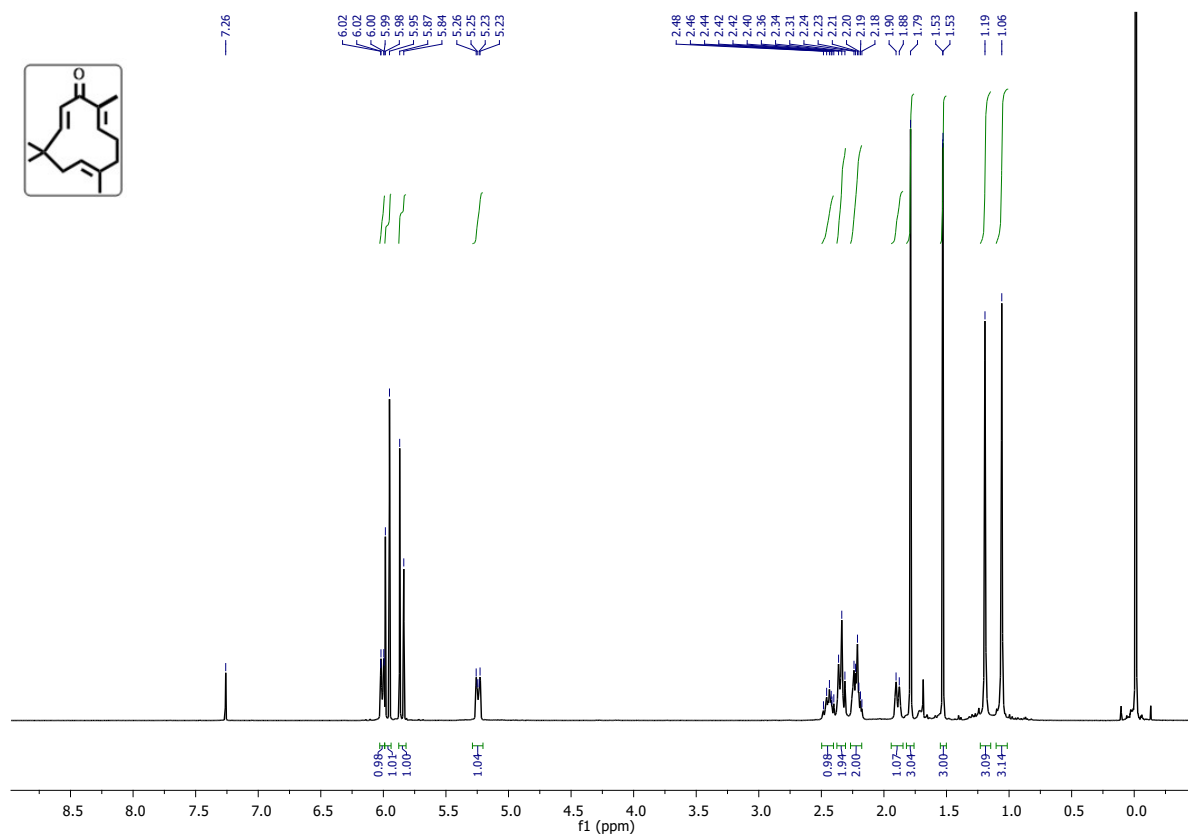


Figure S1: Compound -1 (^1H NMR (500 MHz, CDCl_3))

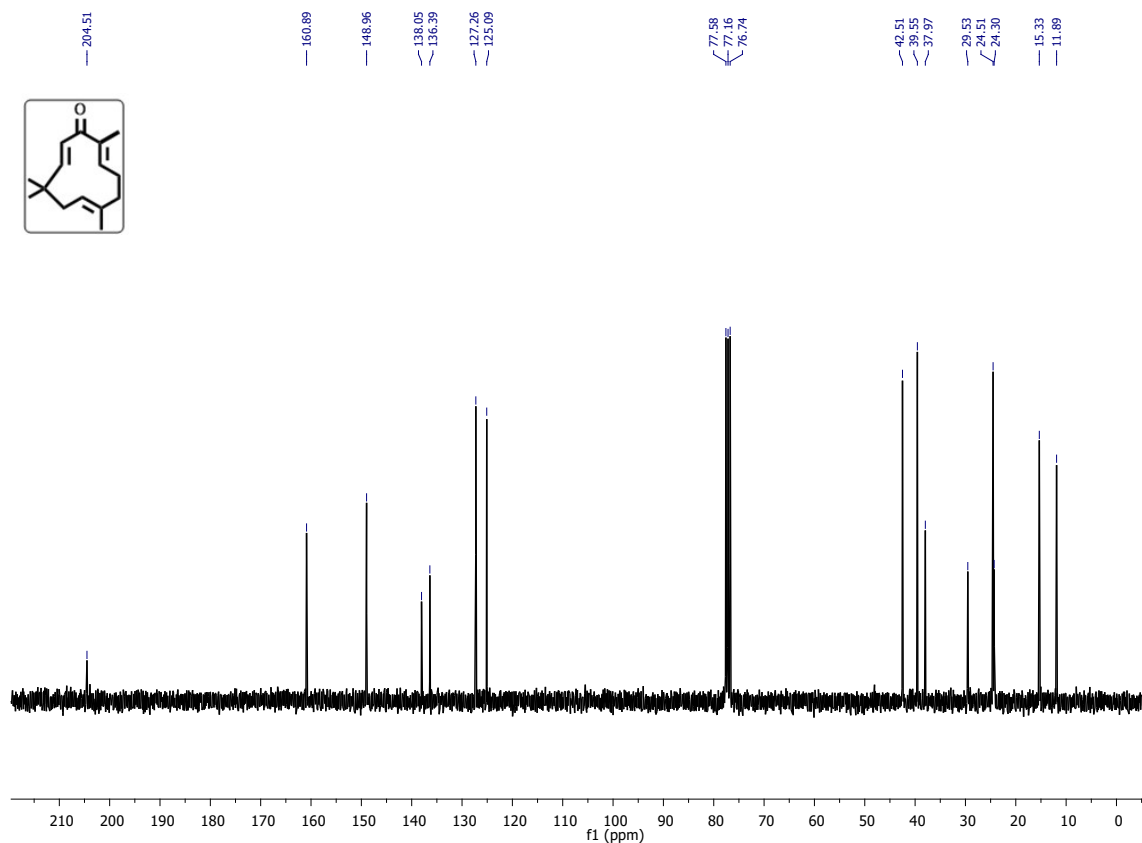


Figure S2: Compound -1 (^{13}C NMR (75 MHz, CDCl_3))

12. ^1H and ^{13}C NMR spectral images of Isoxazoline compounds:

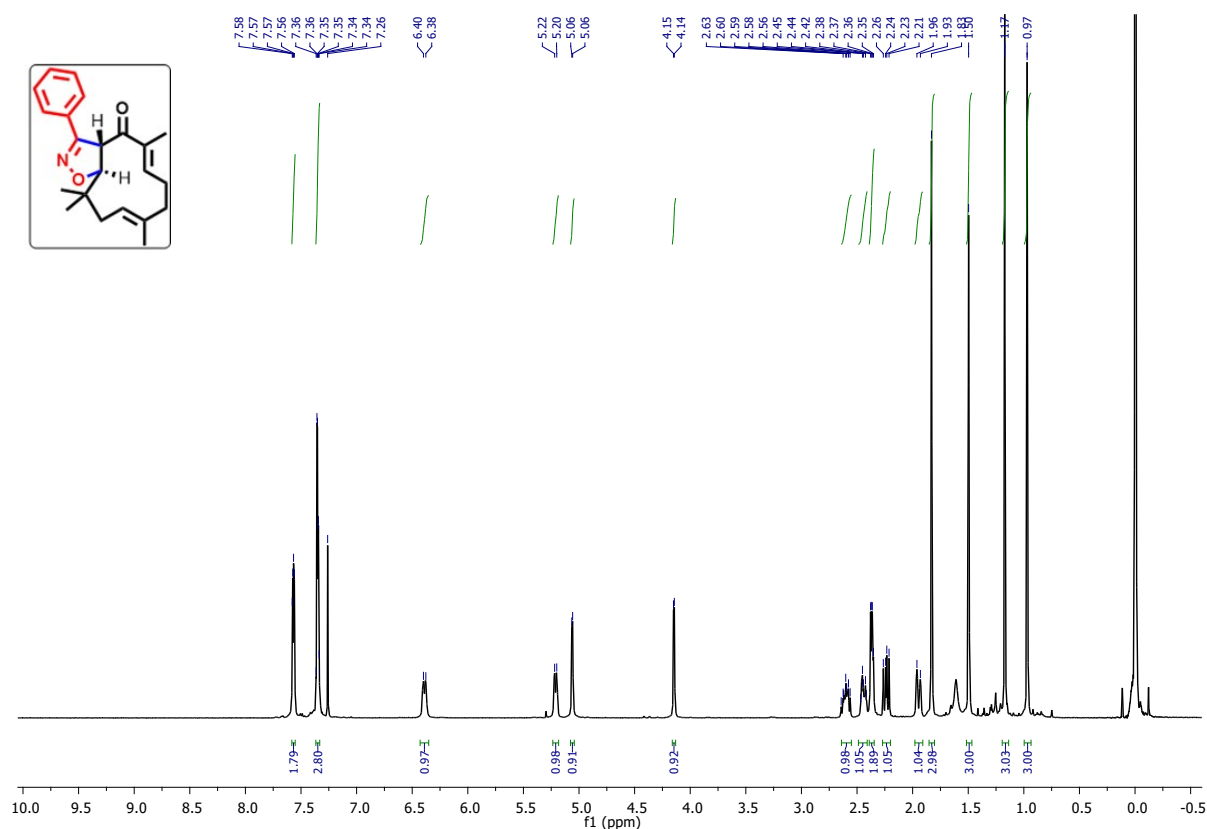


Figure S3: ZI-1 (^1H NMR (500 MHz, CDCl_3))

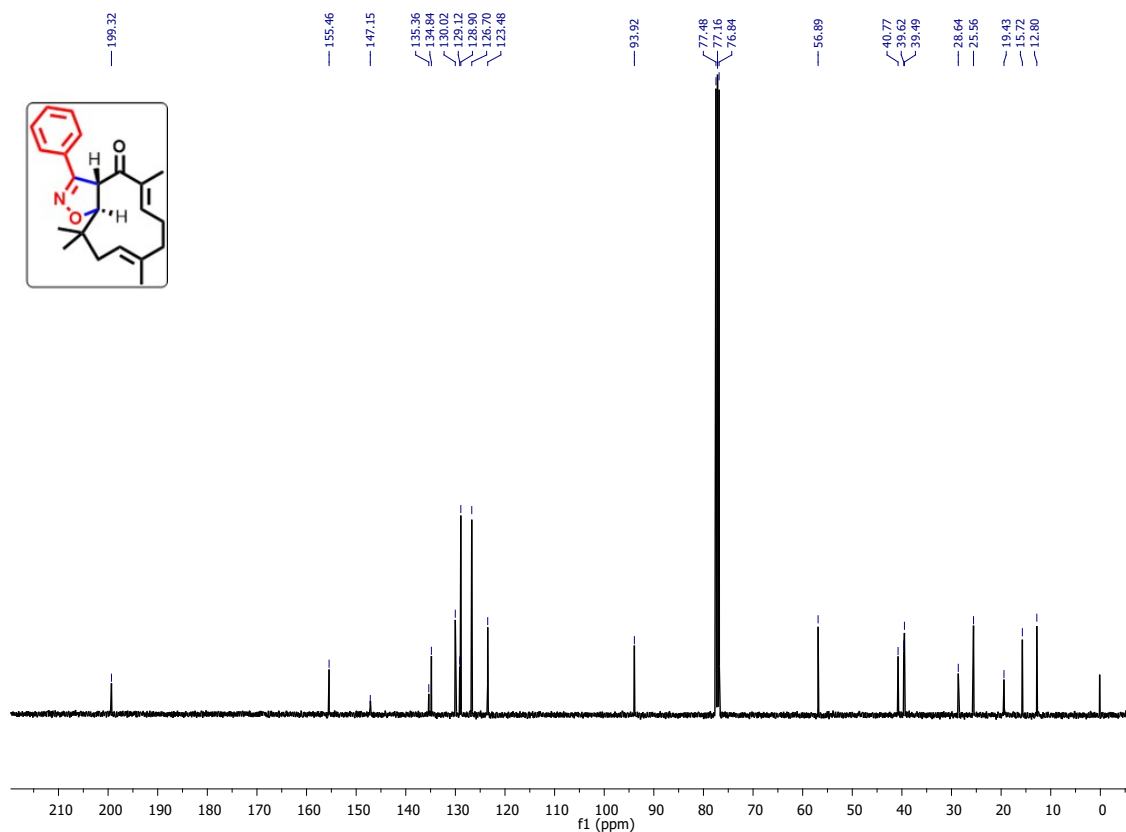
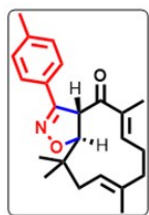


Figure S4: ZI-1 (^{13}C NMR (101 MHz, CDCl_3))



Chemical structure of compound 10a is shown in the top left corner. The structure is a complex bicyclic molecule with a p-tolyl group, a nitro group, and a ketone. The ¹³C NMR spectrum is displayed below the structure, showing peaks from 0 to 200 ppm. The peaks are labeled with their chemical shifts in ppm: 199.38, 155.38, 146.92, 140.23, 135.39, 134.79, 129.59, 126.63, 126.29, 123.51, 93.68, 77.48, 76.84, 57.03, 40.77, 39.59, 39.48, 28.63, 25.55, 21.54, 19.43, 15.71, and 12.81.

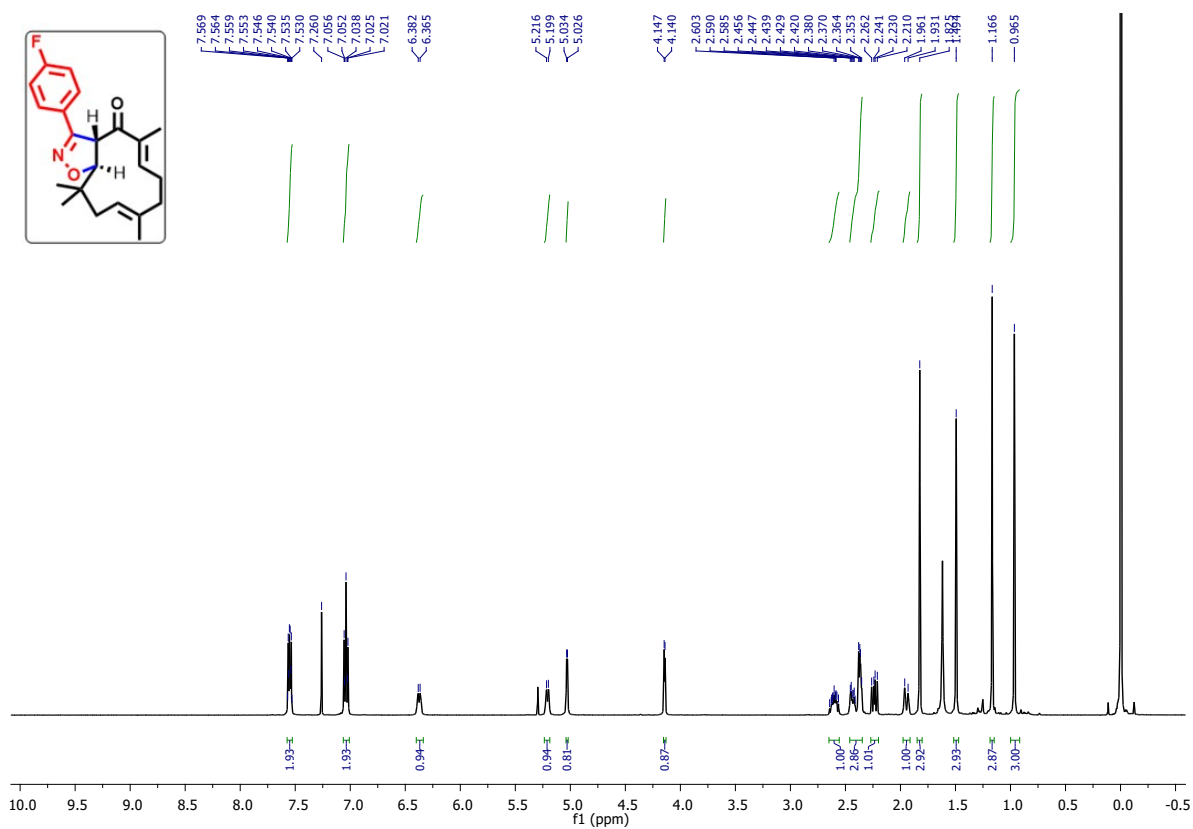


Figure S7: ZI-3 (¹H NMR (500 MHz, CDCl₃))

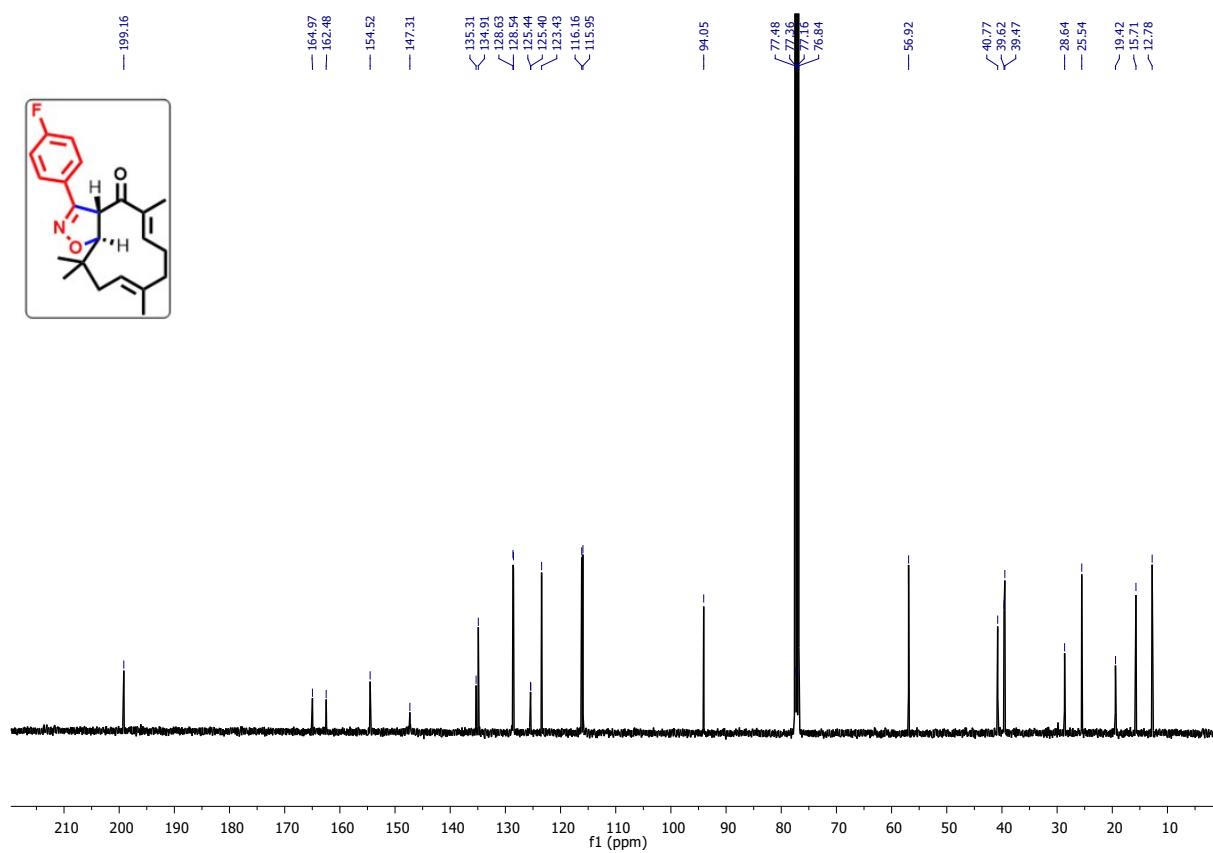


Figure S8: ZI-3 (¹³C NMR (101 MHz, CDCl₃))

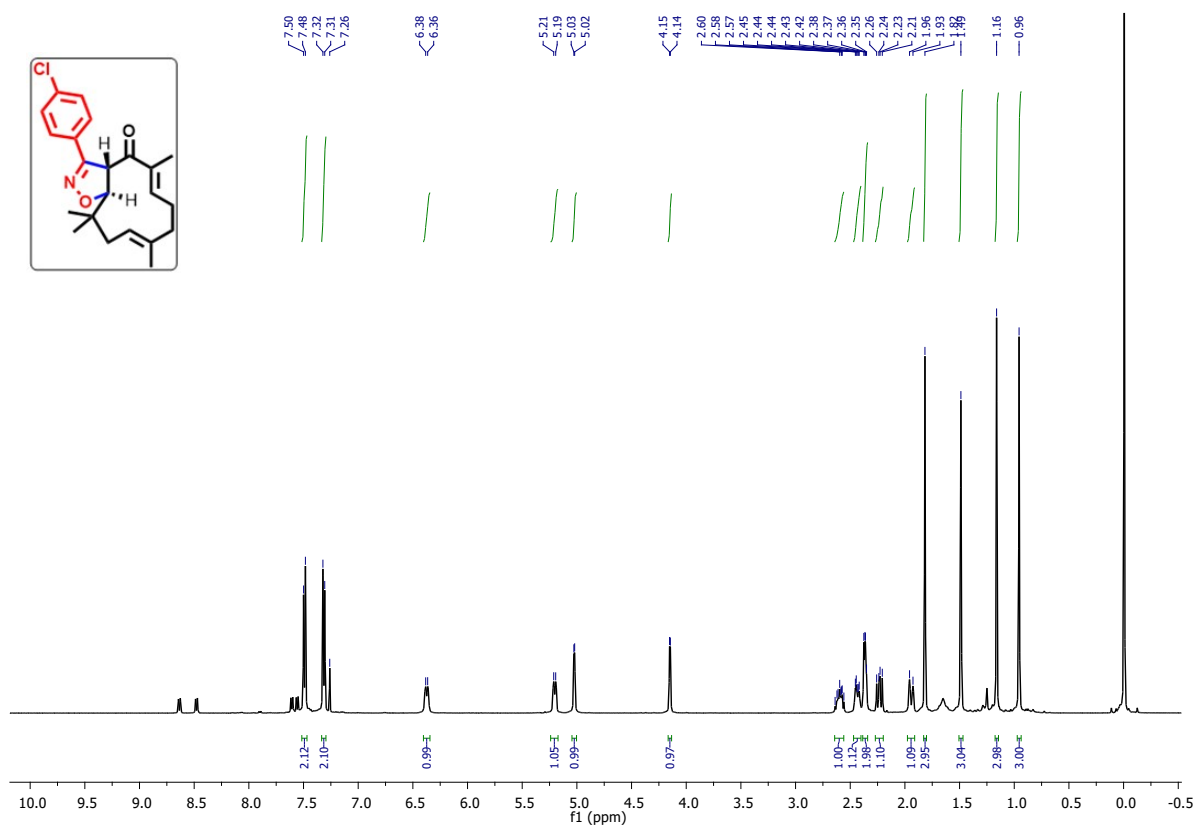


Figure S9: ZI-4 (¹H NMR (500 MHz, CDCl₃))

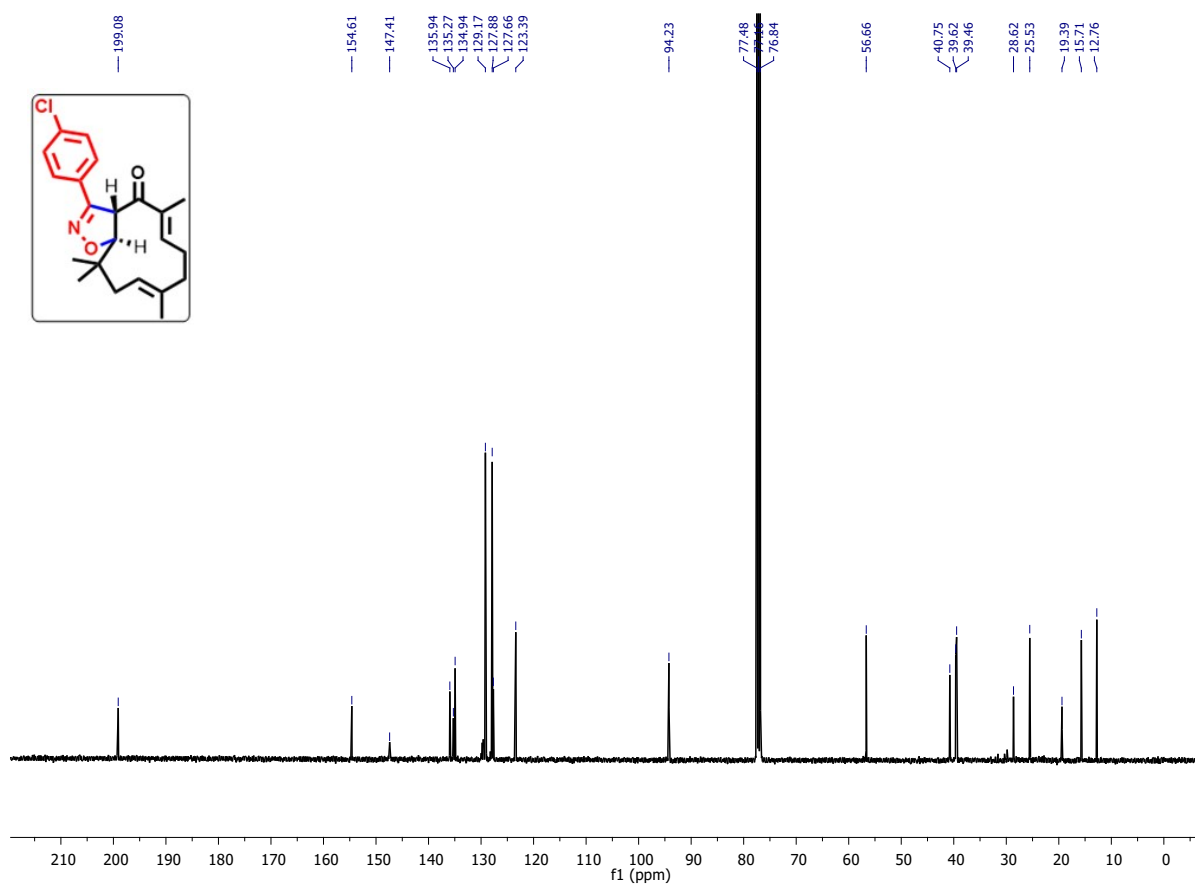


Figure S10: ZI-4 (¹³C NMR (101 MHz, CDCl₃))

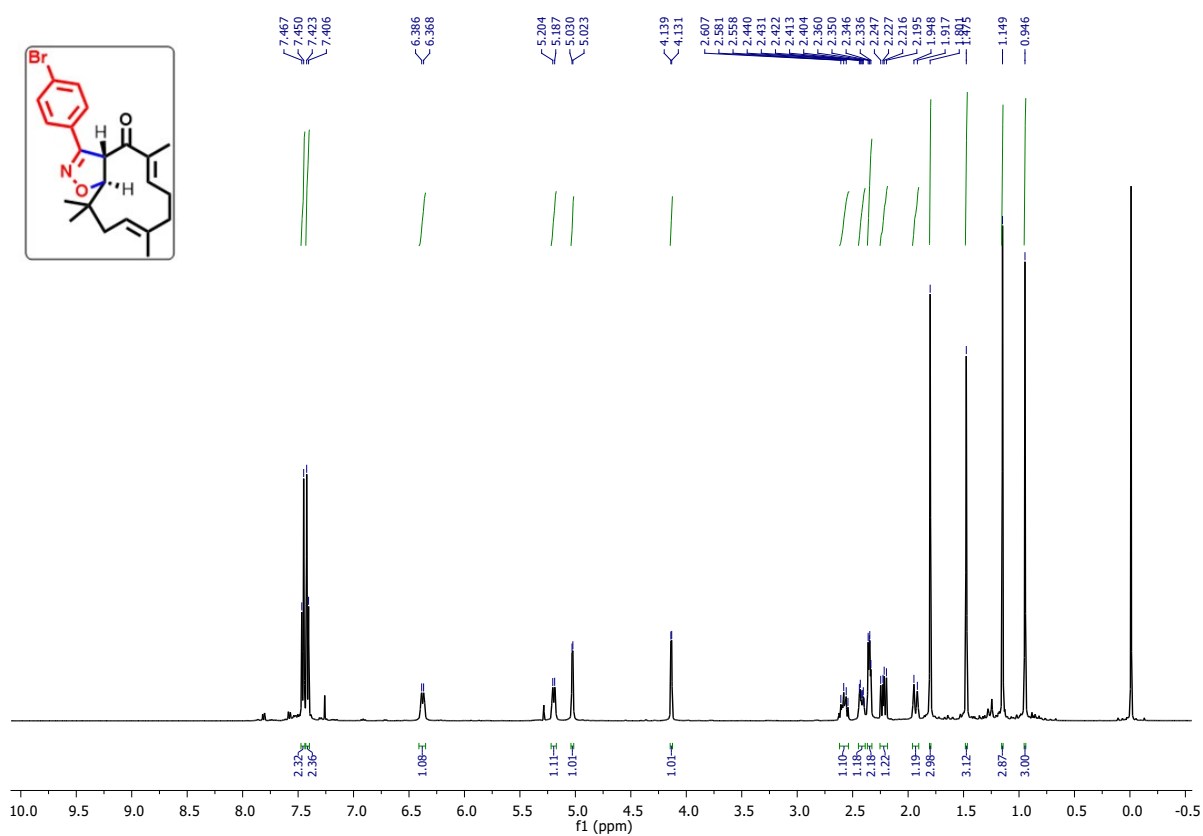


Figure S11: ZI-5 (¹H NMR (500 MHz, CDCl₃))

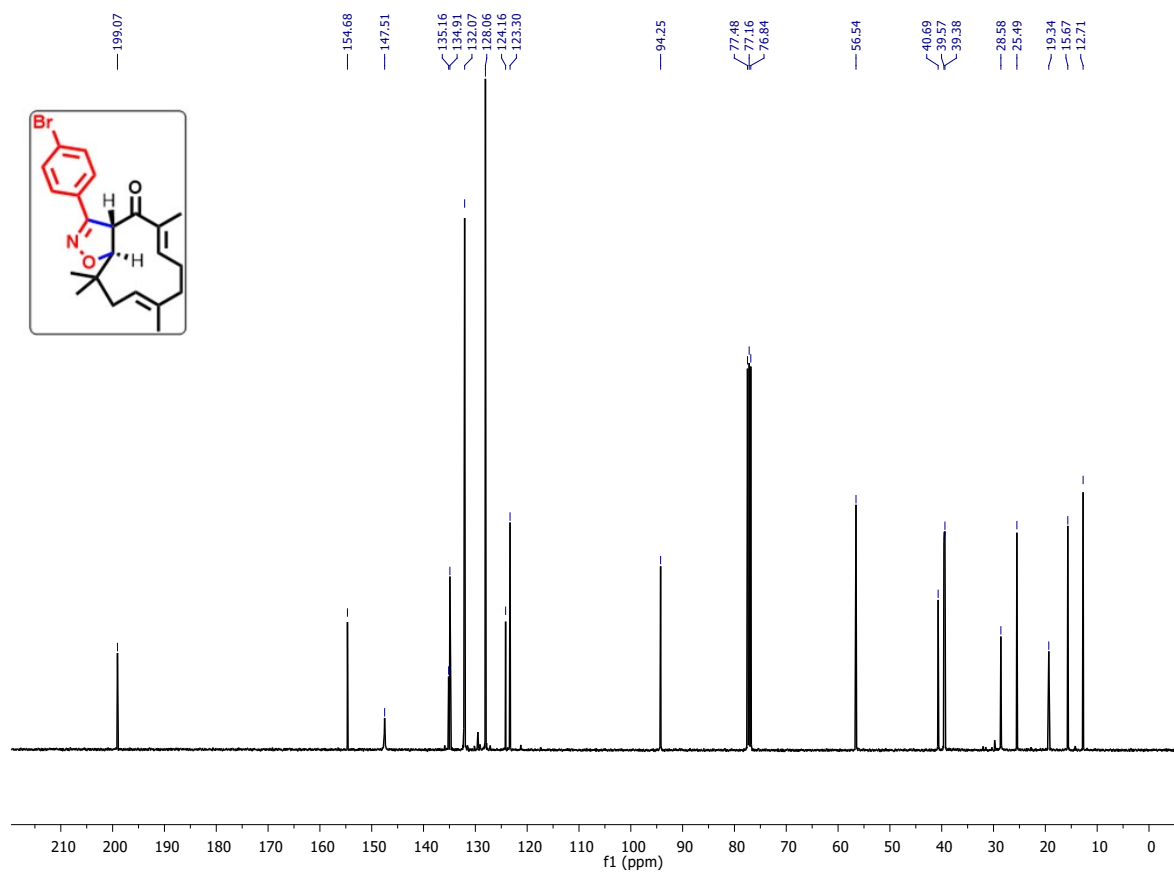


Figure S12: ZI-5 (¹³C NMR (101 MHz, CDCl₃))

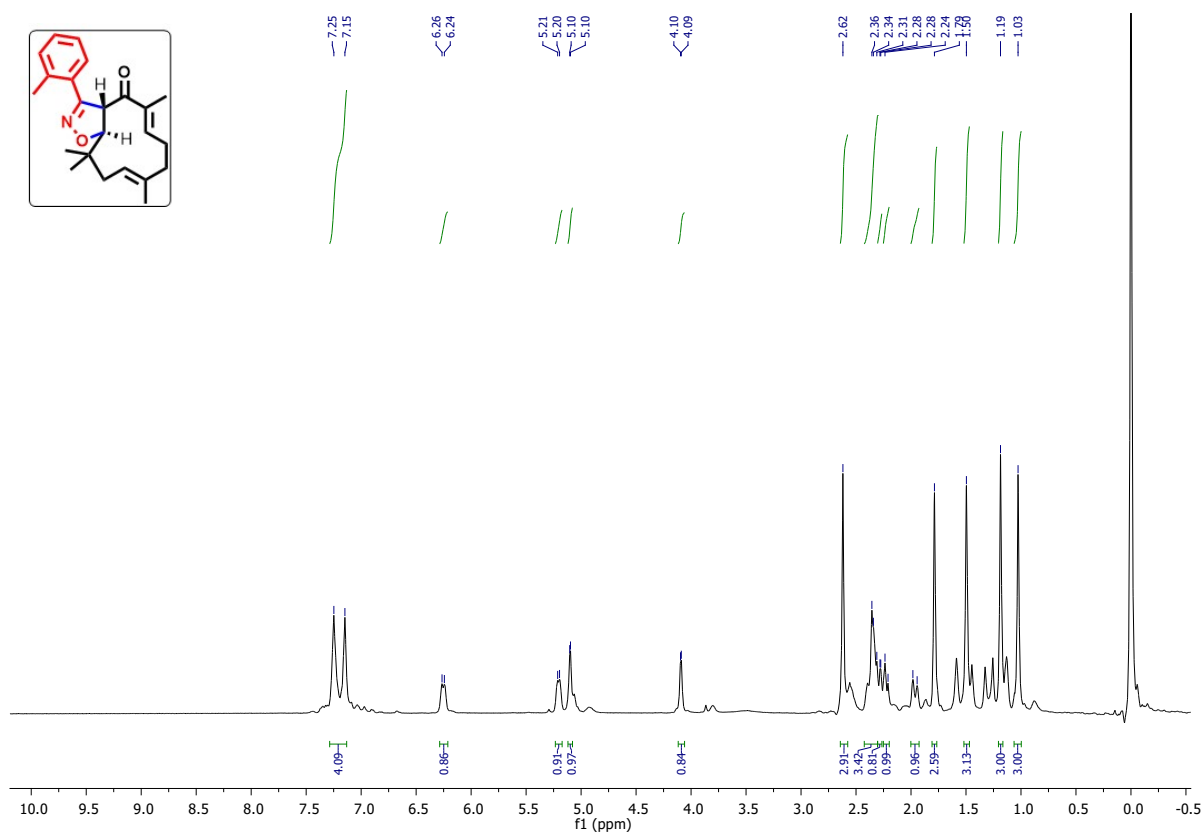


Figure S13: ZI-6 (¹H NMR (400 MHz, CDCl₃))

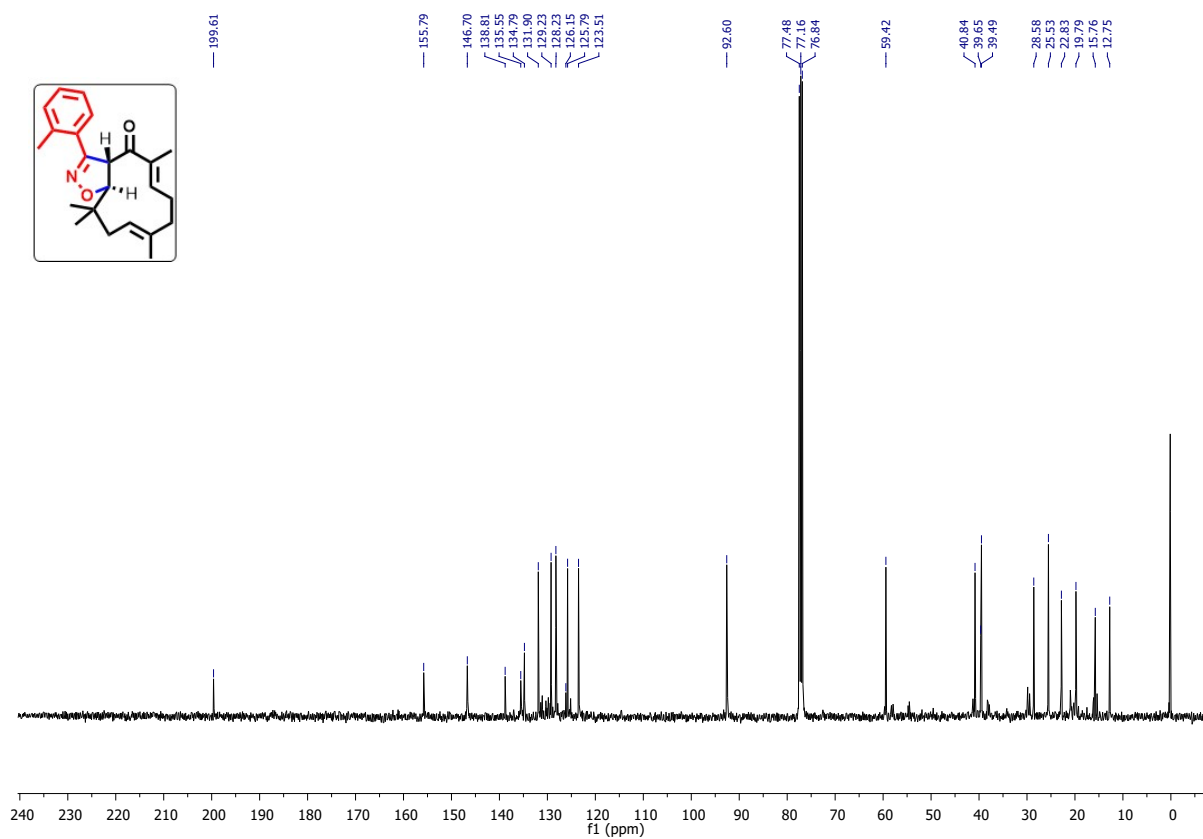


Figure S14: ZI-6 (¹³C NMR (101 MHz, CDCl₃))

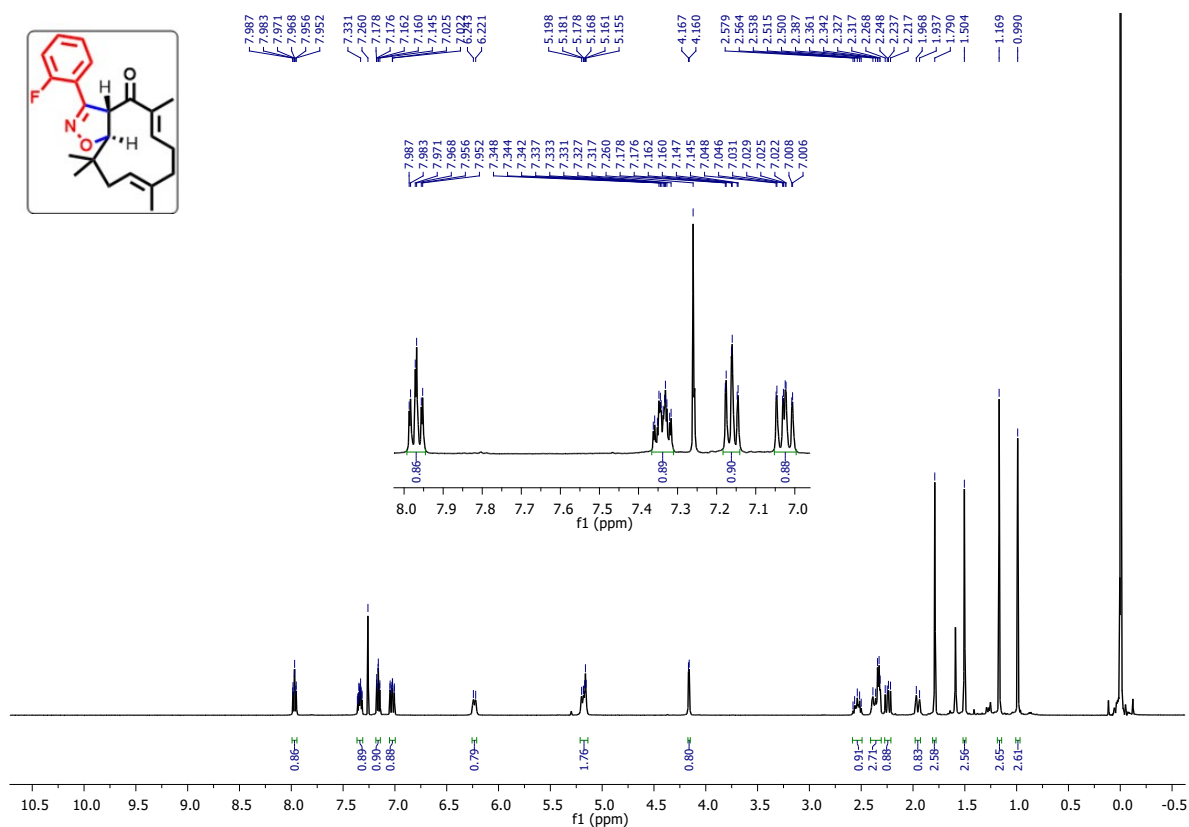


Figure S15: ZI-7 (¹H NMR (500 MHz, CDCl₃))

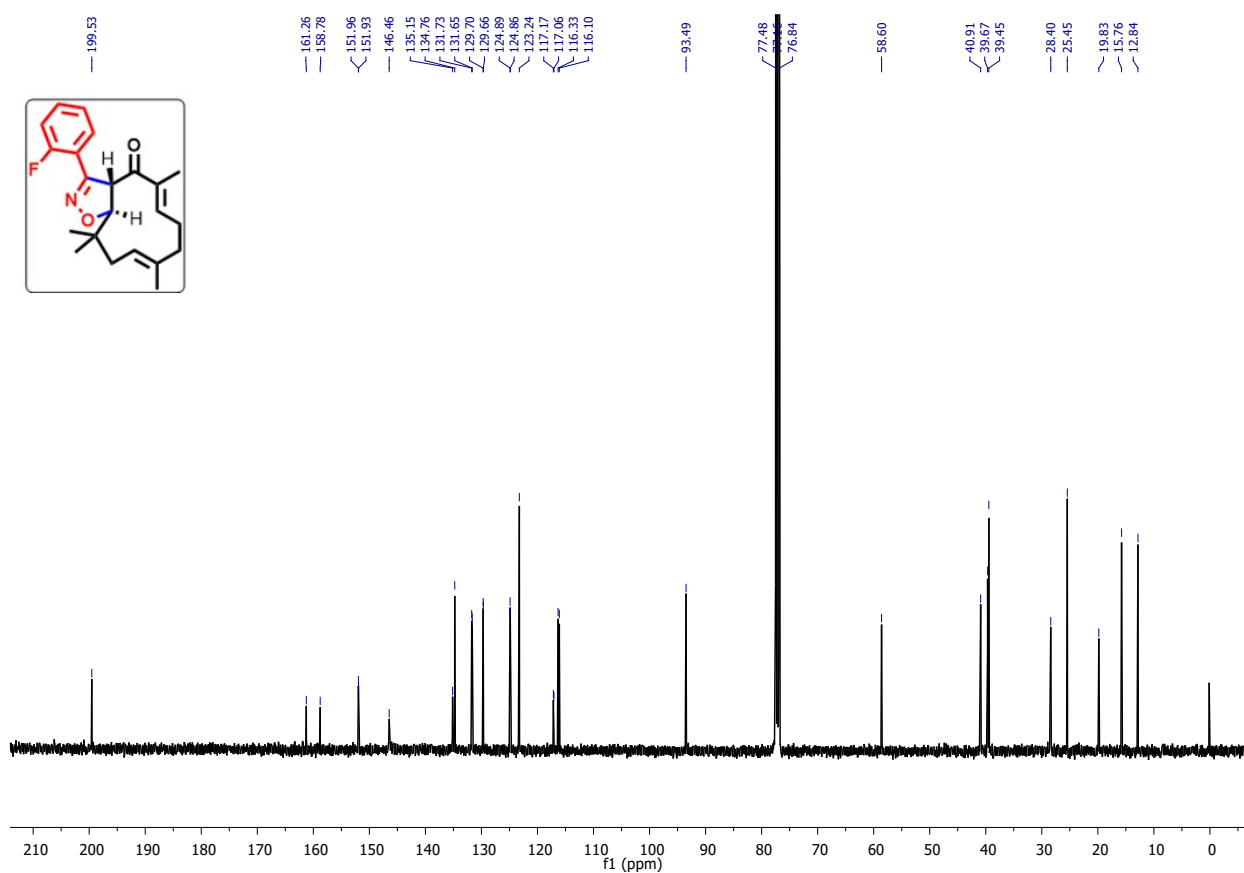


Figure S16: ZI-7 (¹³C NMR (101 MHz, CDCl₃))

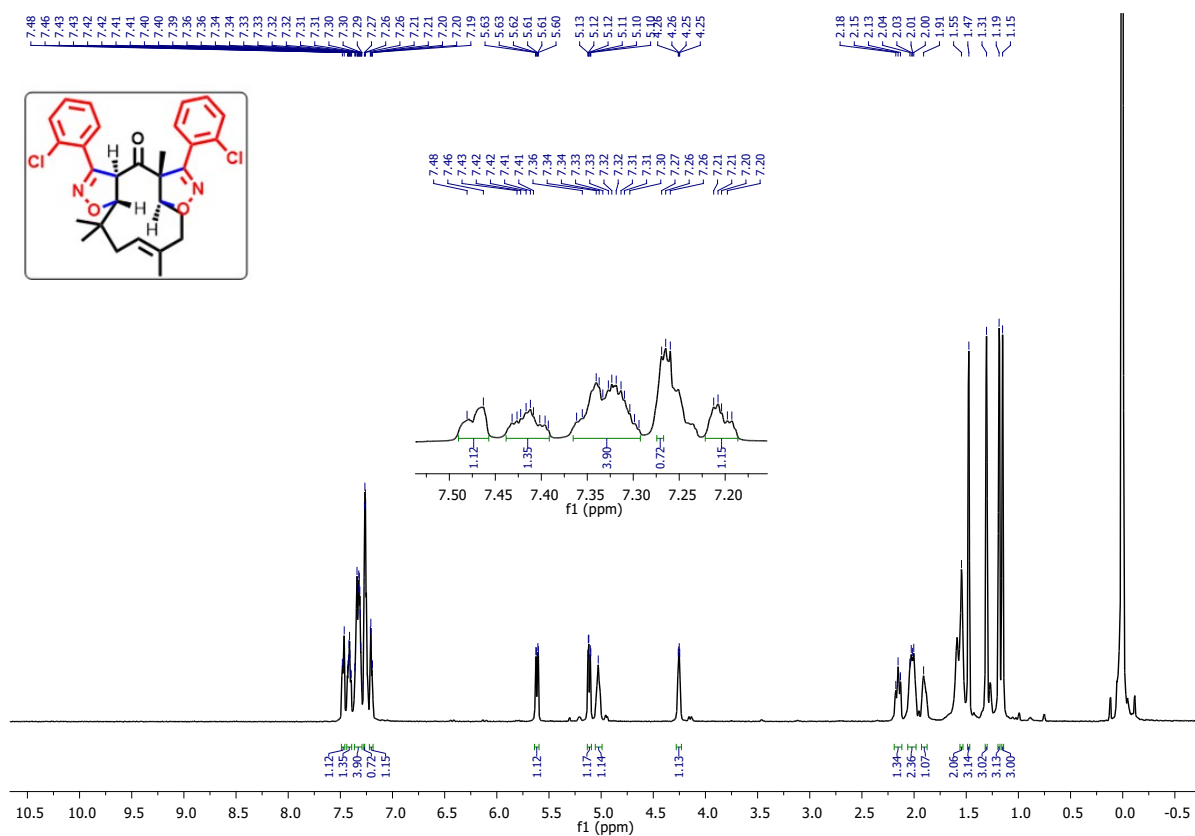


Figure S19: ZI-9 (¹H NMR (500 MHz, CDCl₃))

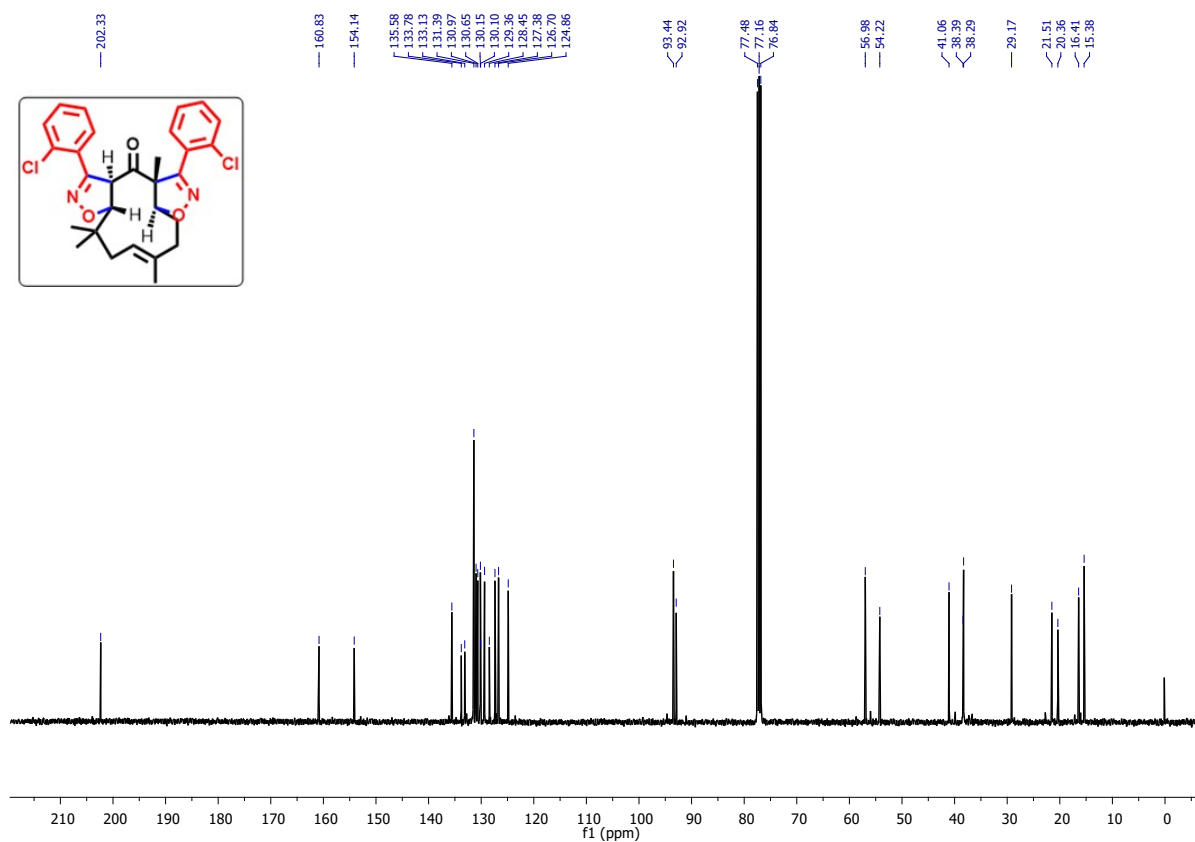
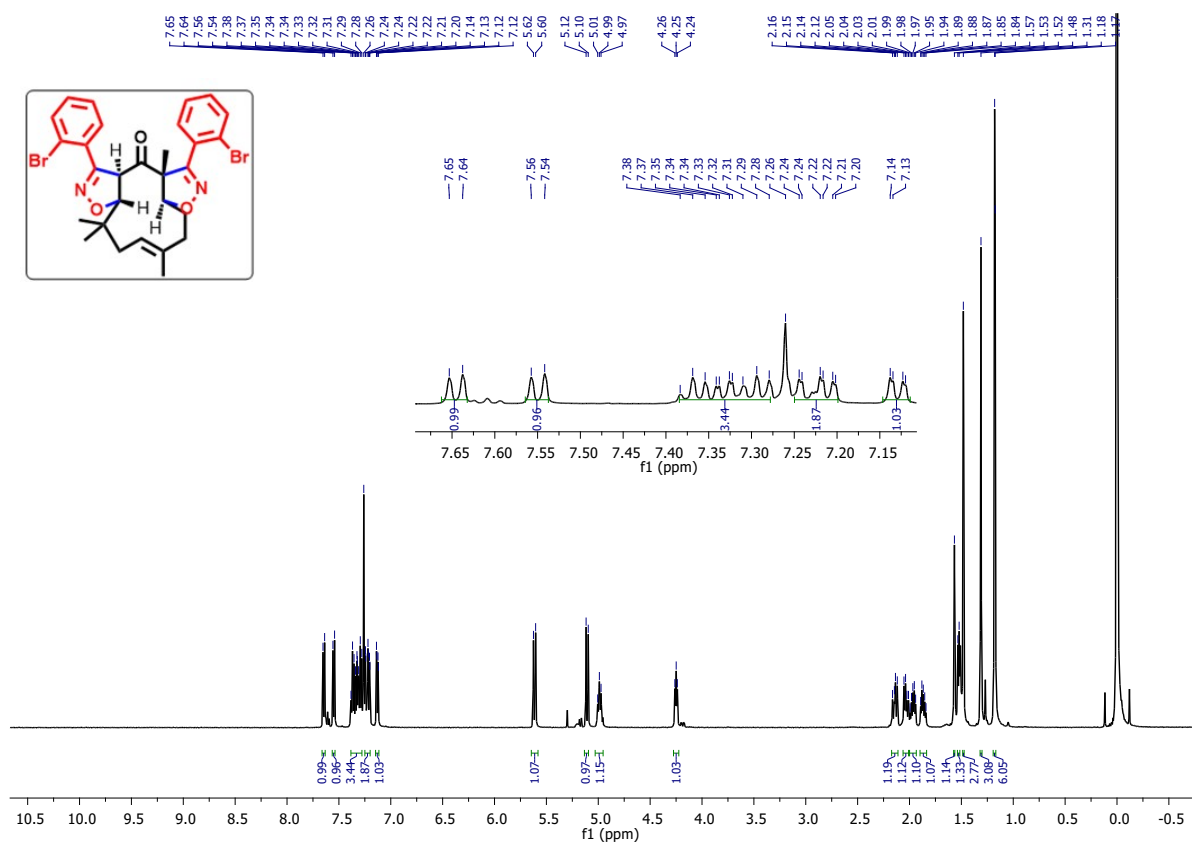


Figure S20: ZI-9 (¹³C NMR (101 MHz, CDCl₃))



13. ^1H and ^{13}C NMR spectral images of Spirocyclic compounds

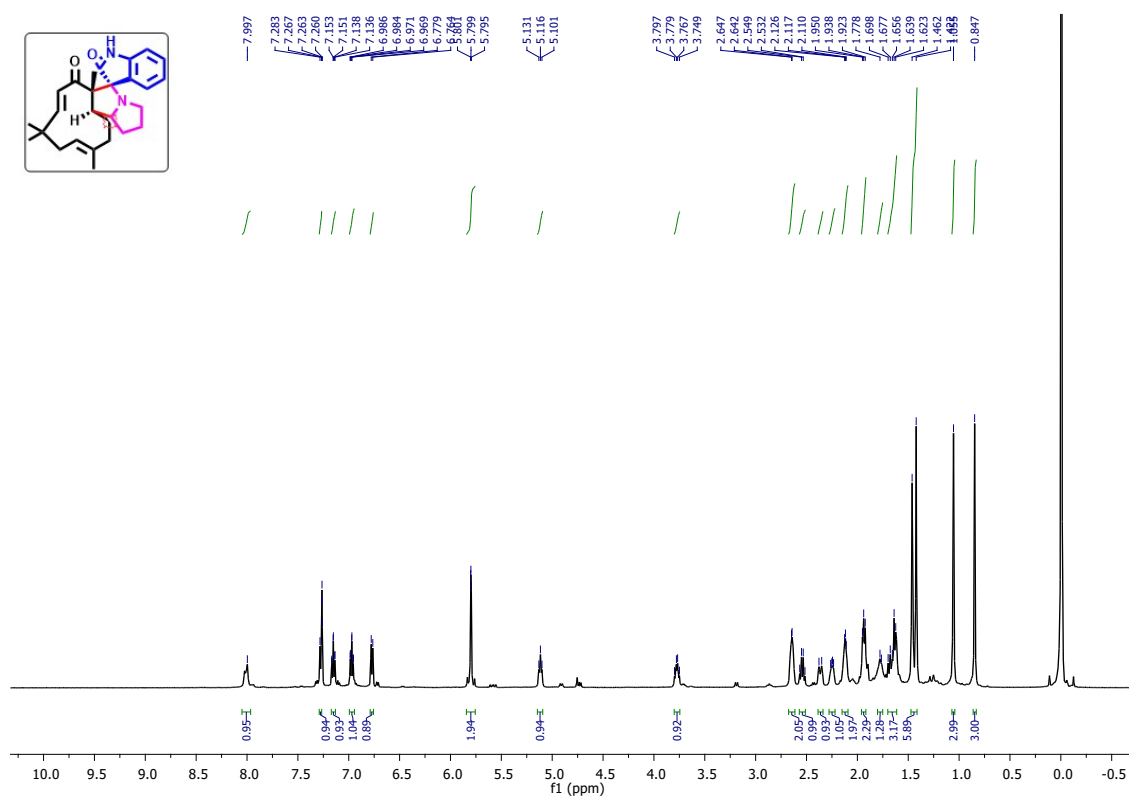


Figure S23: ZS-1 (^1H NMR (500 MHz, CDCl_3))

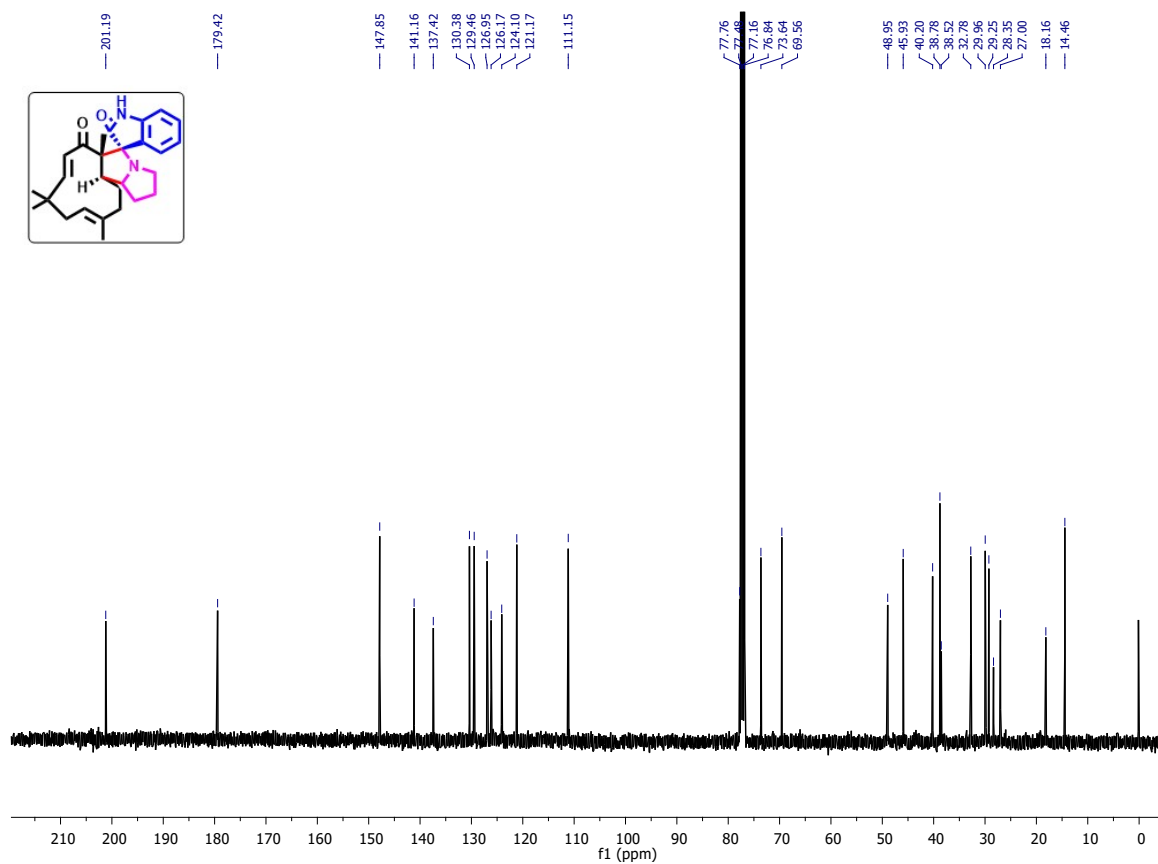


Figure S24: ZS-1 (^{13}C NMR (101 MHz, CDCl_3))

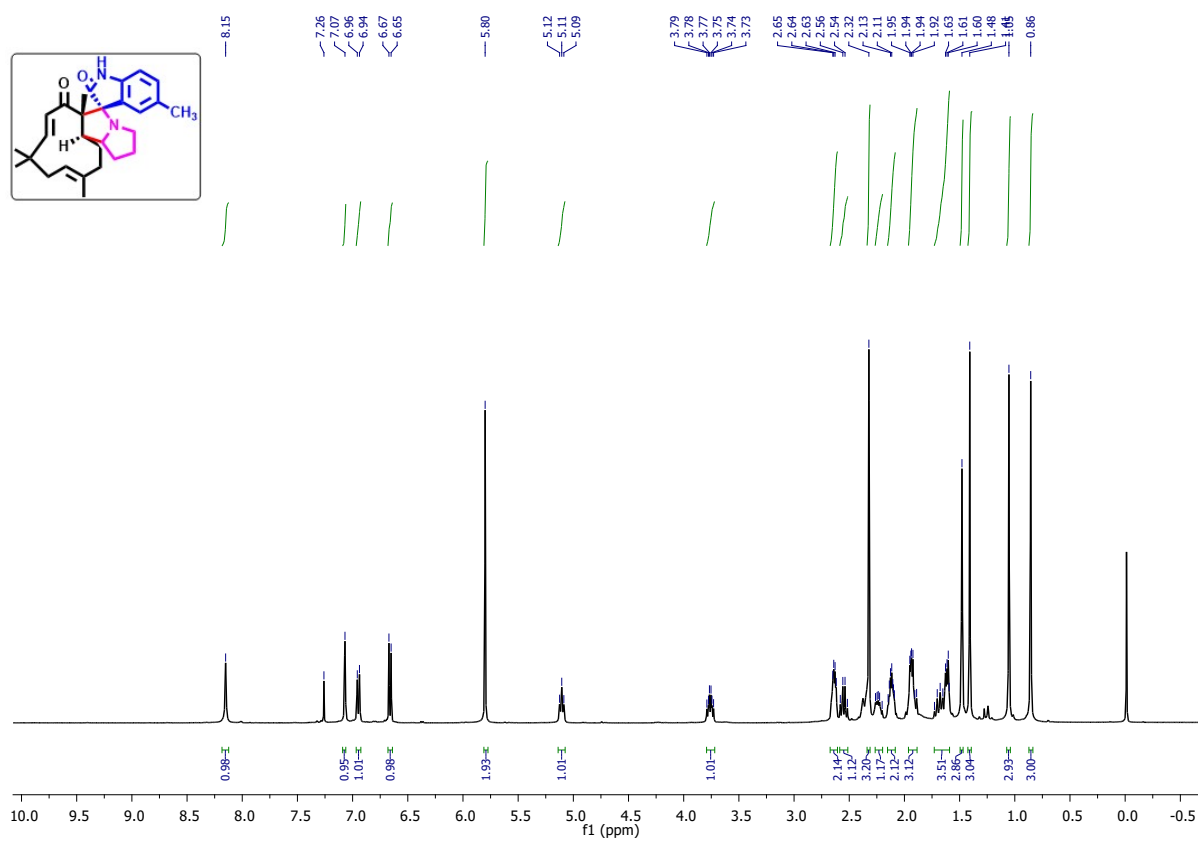


Figure S25: ZS-2 (¹H NMR (500 MHz, CDCl₃))

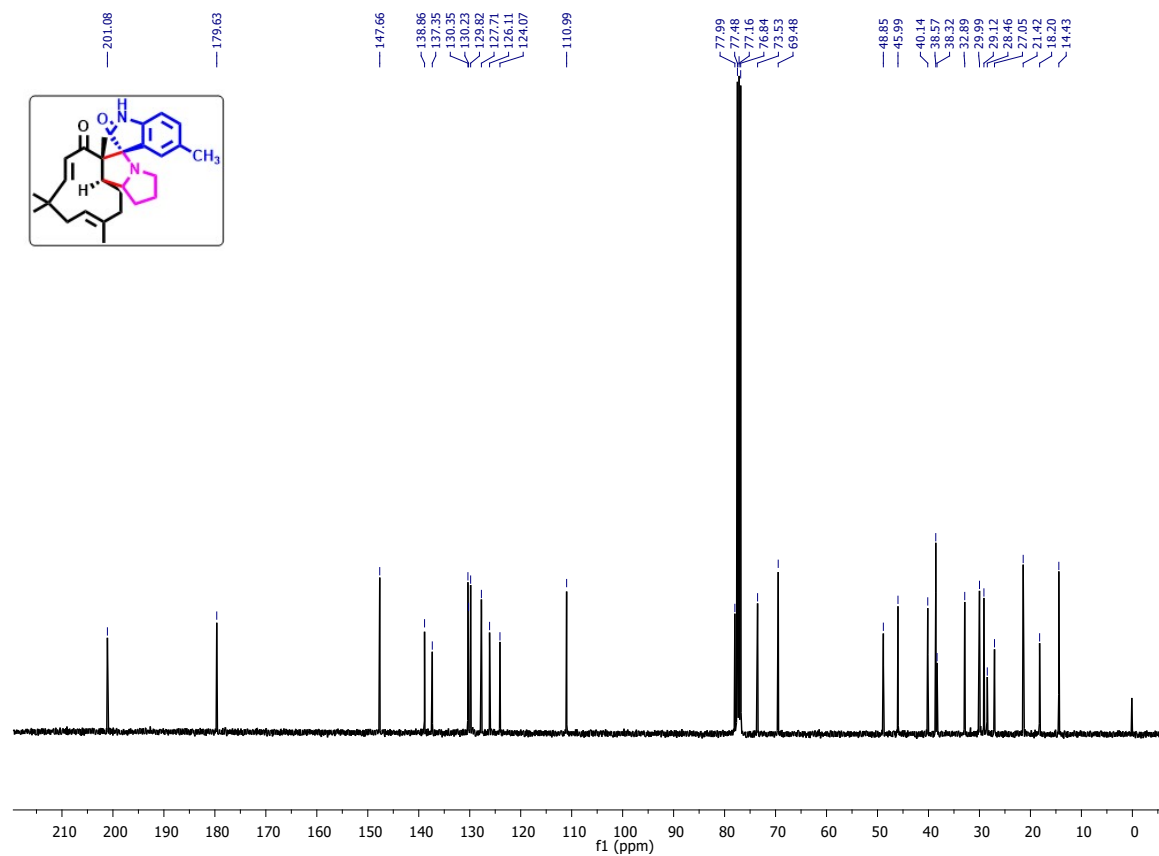


Figure S26: ZS-2 (¹³C NMR (101 MHz, CDCl₃))

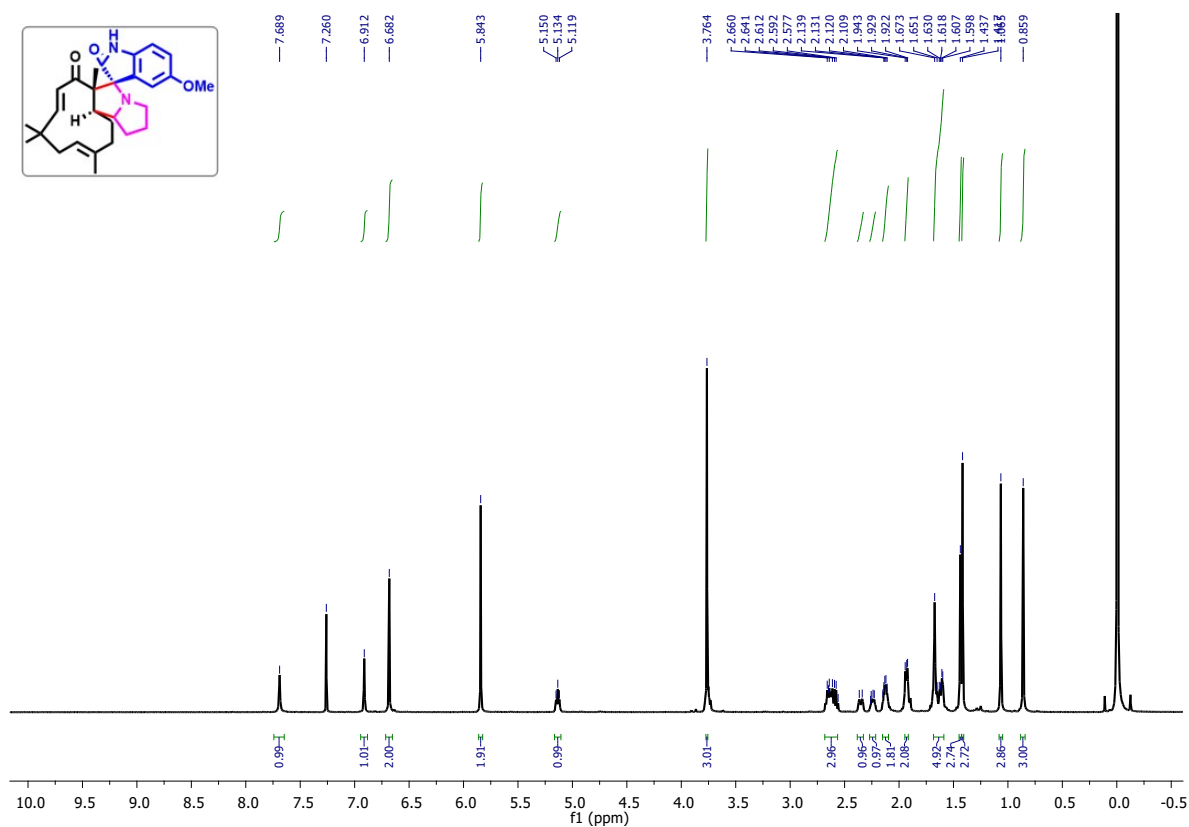


Figure S27: ZS-3 (¹H NMR (500 MHz, CDCl₃))

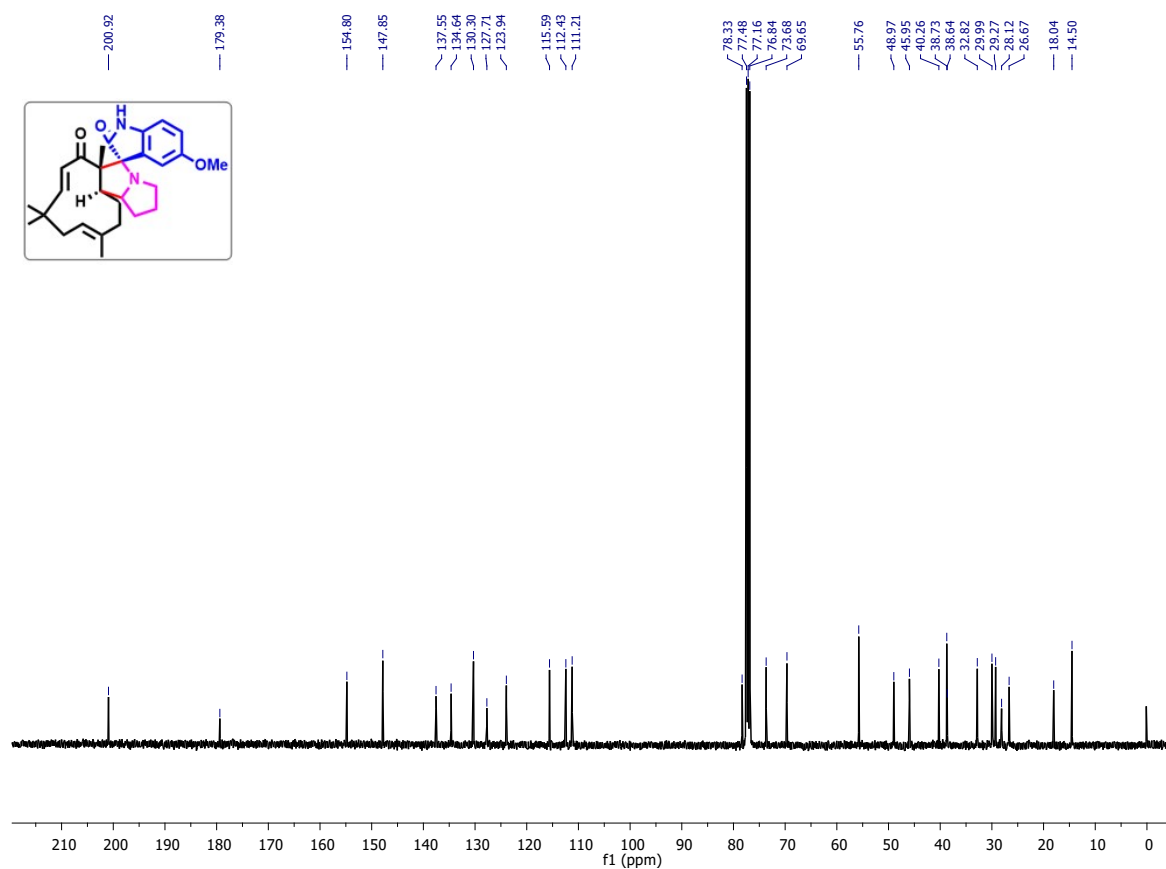


Figure S28: ZS-3 (¹³C NMR (101 MHz, CDCl₃))

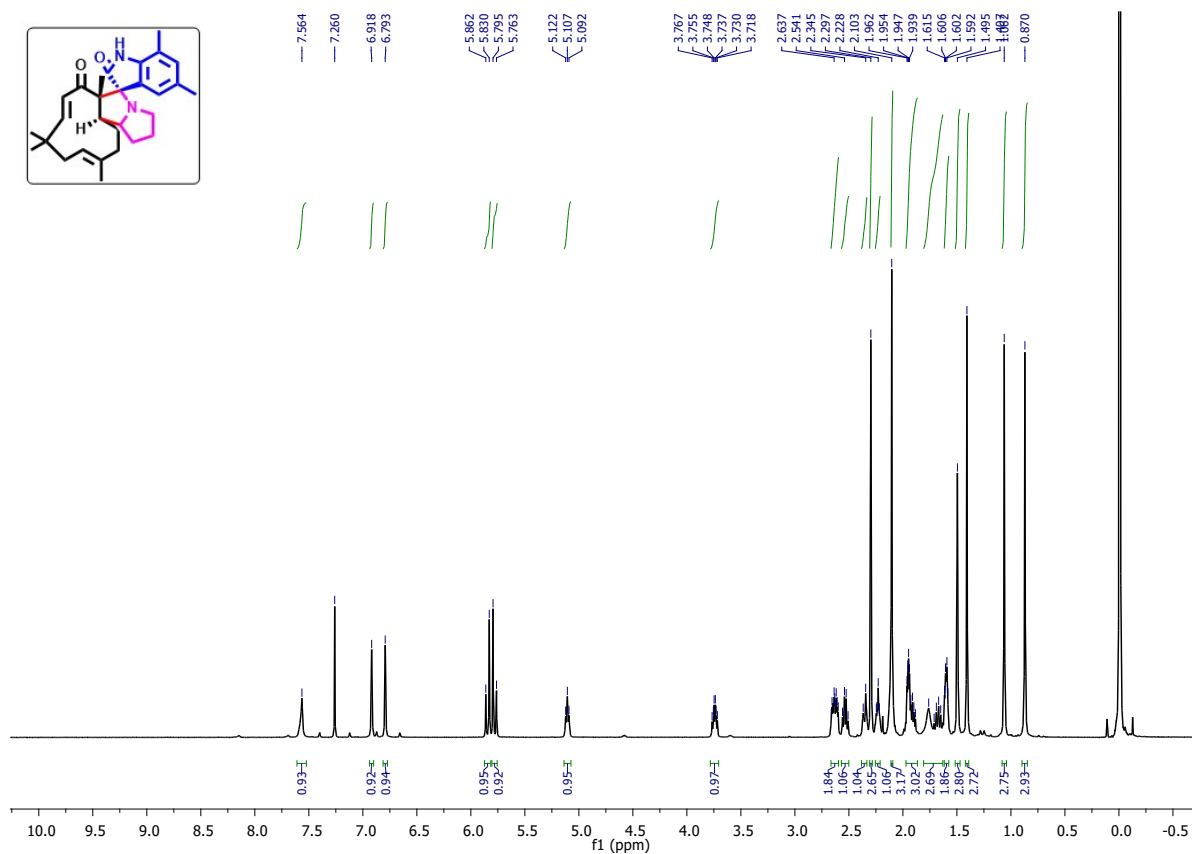


Figure S29: ZS-4 (¹H NMR (500 MHz, CDCl₃))

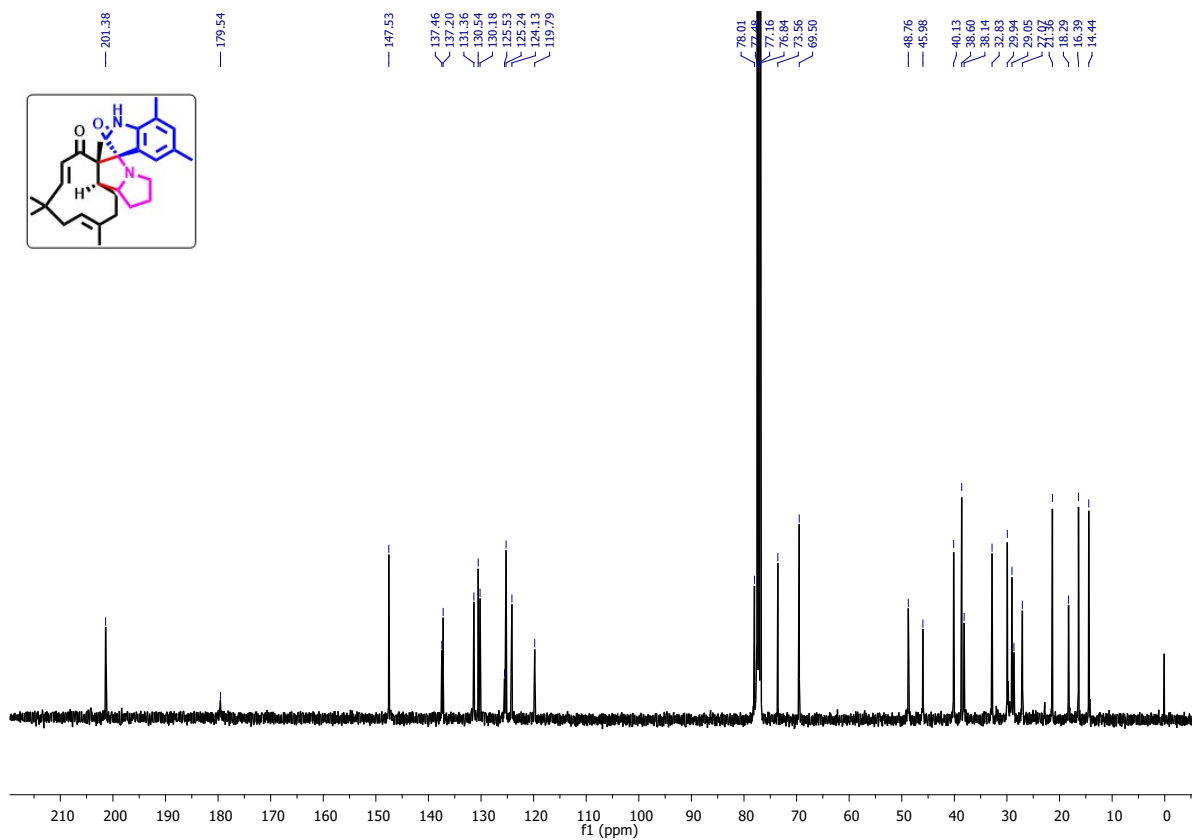
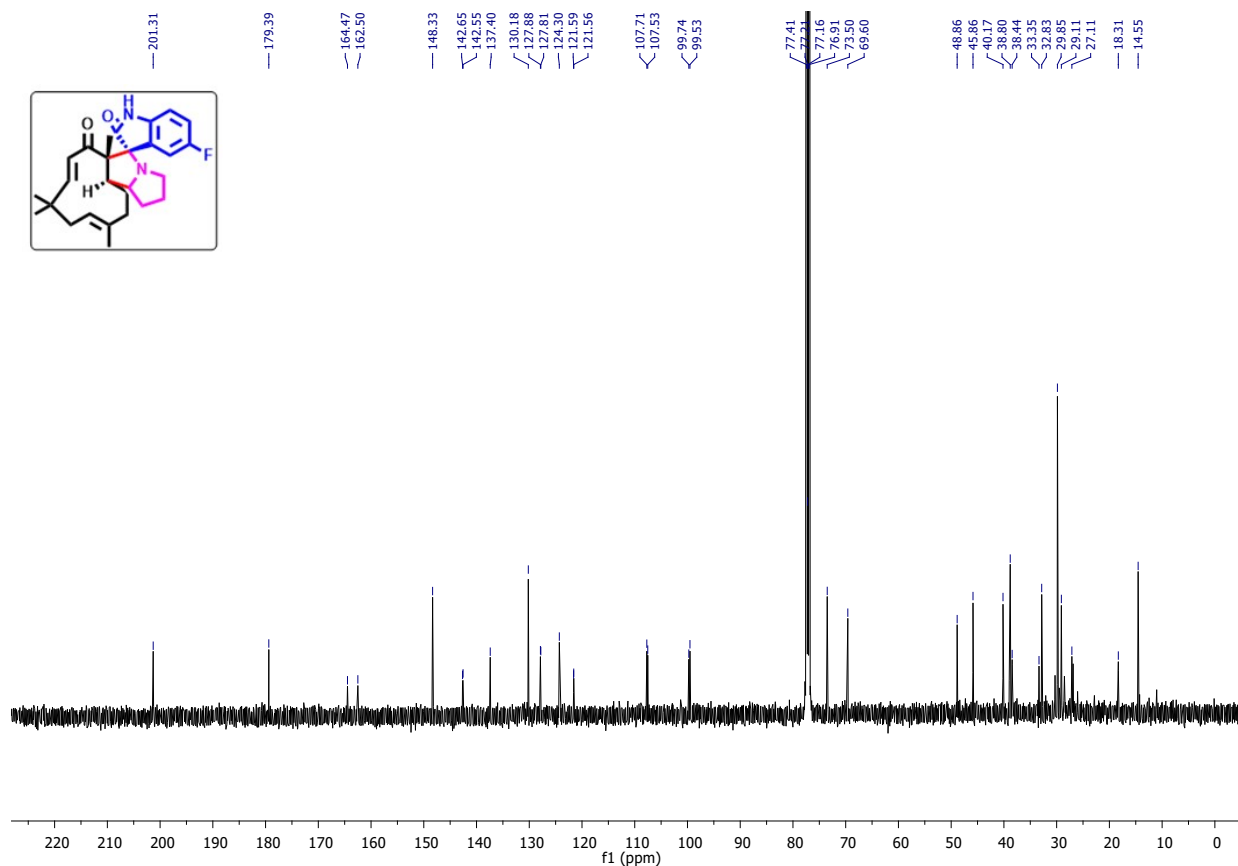
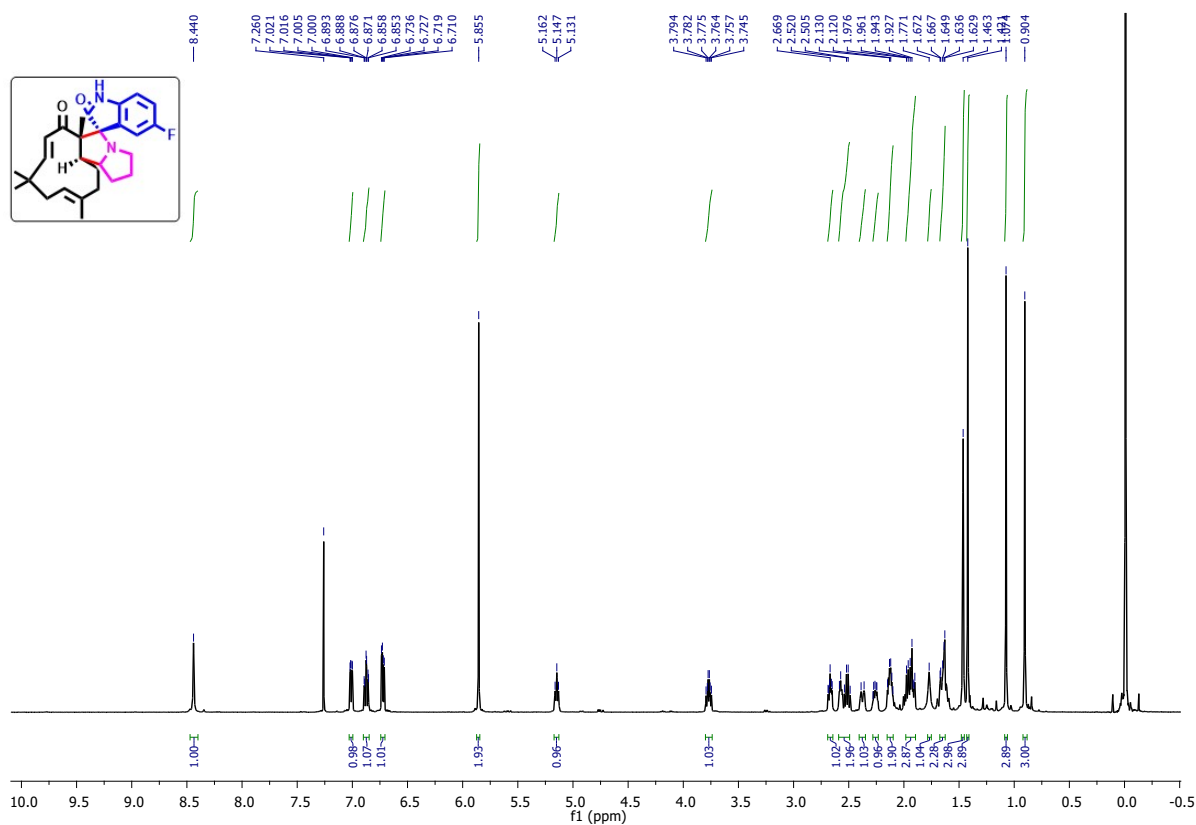


Figure S30: ZS-4 (¹³C NMR (101 MHz, CDCl₃))



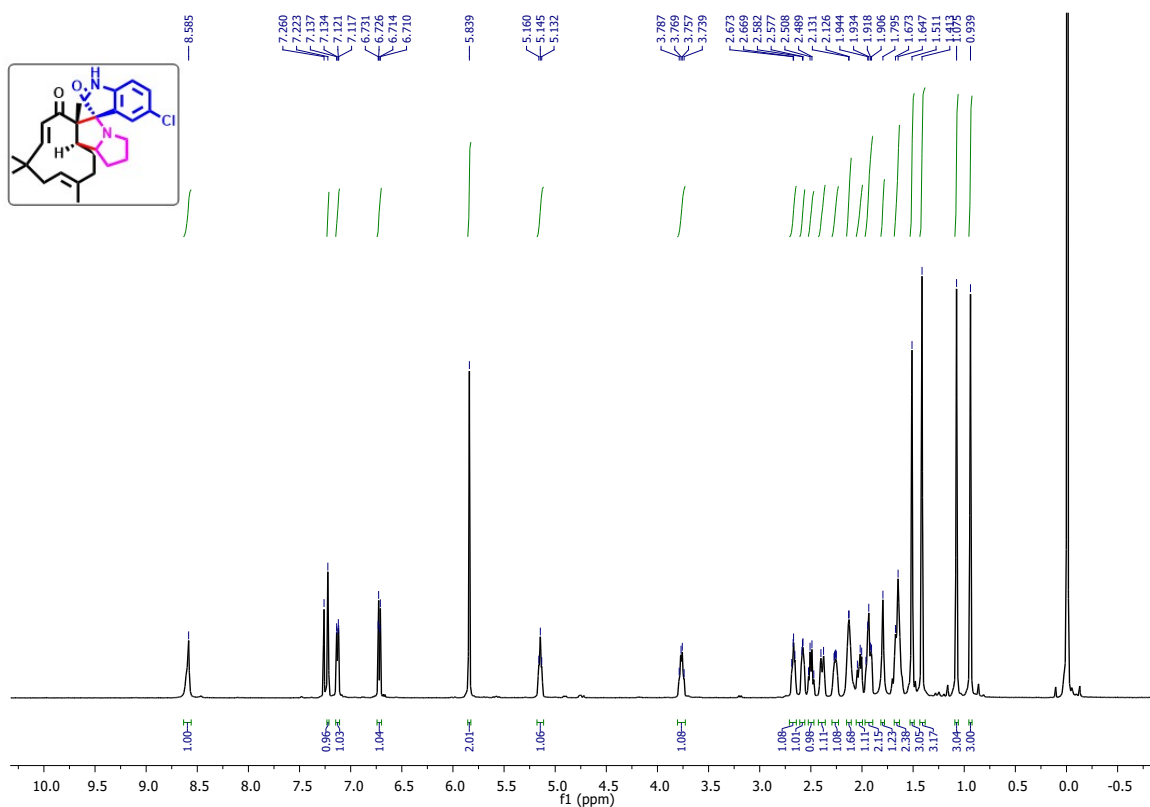


Figure S33: ZS-6 (¹H NMR (500 MHz, CDCl₃))

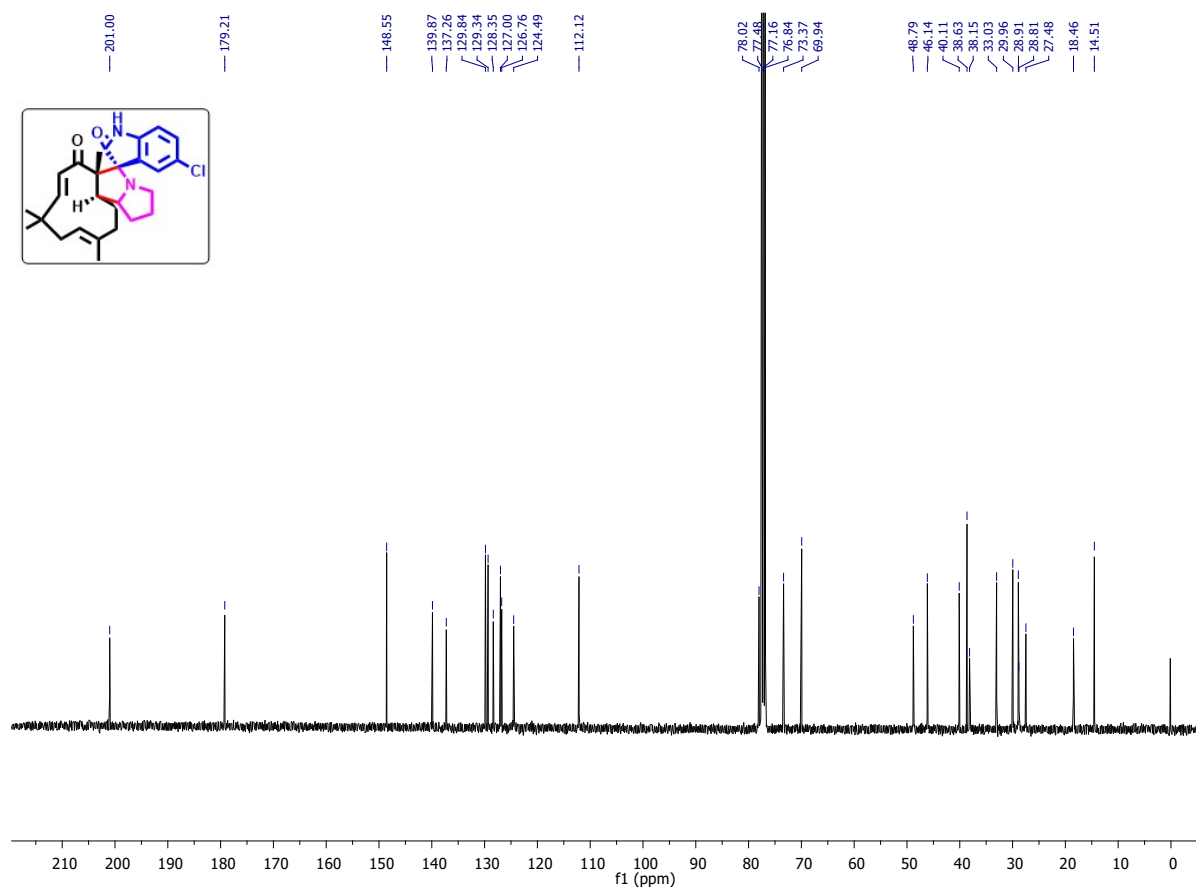
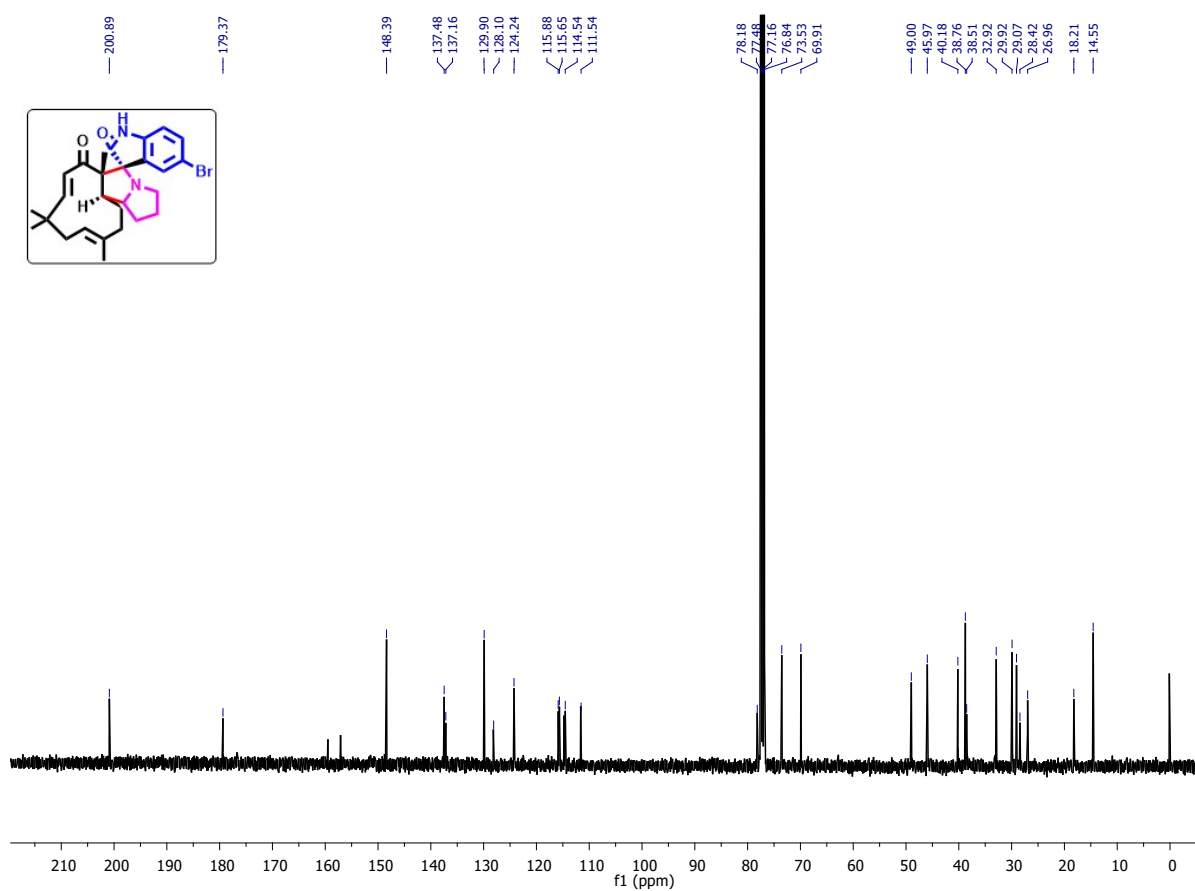
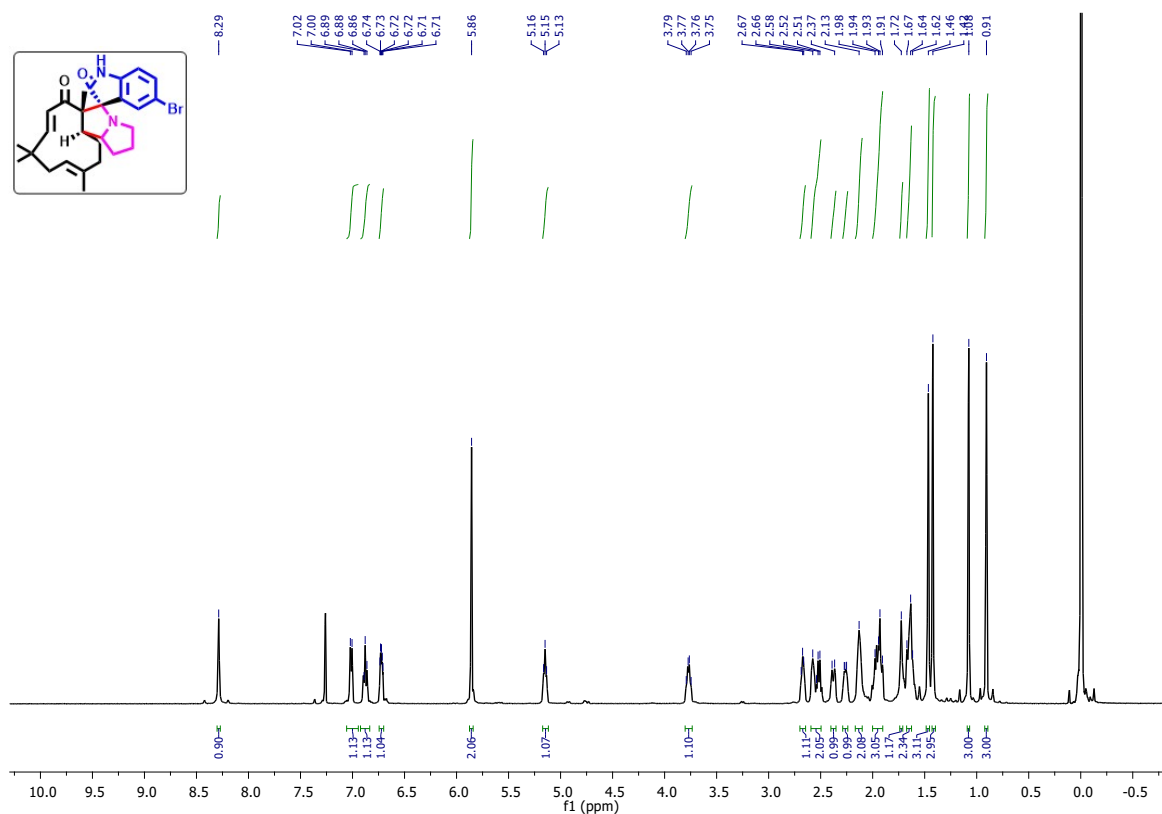


Figure S34: ZS-6 (¹³C NMR (101 MHz, CDCl₃))



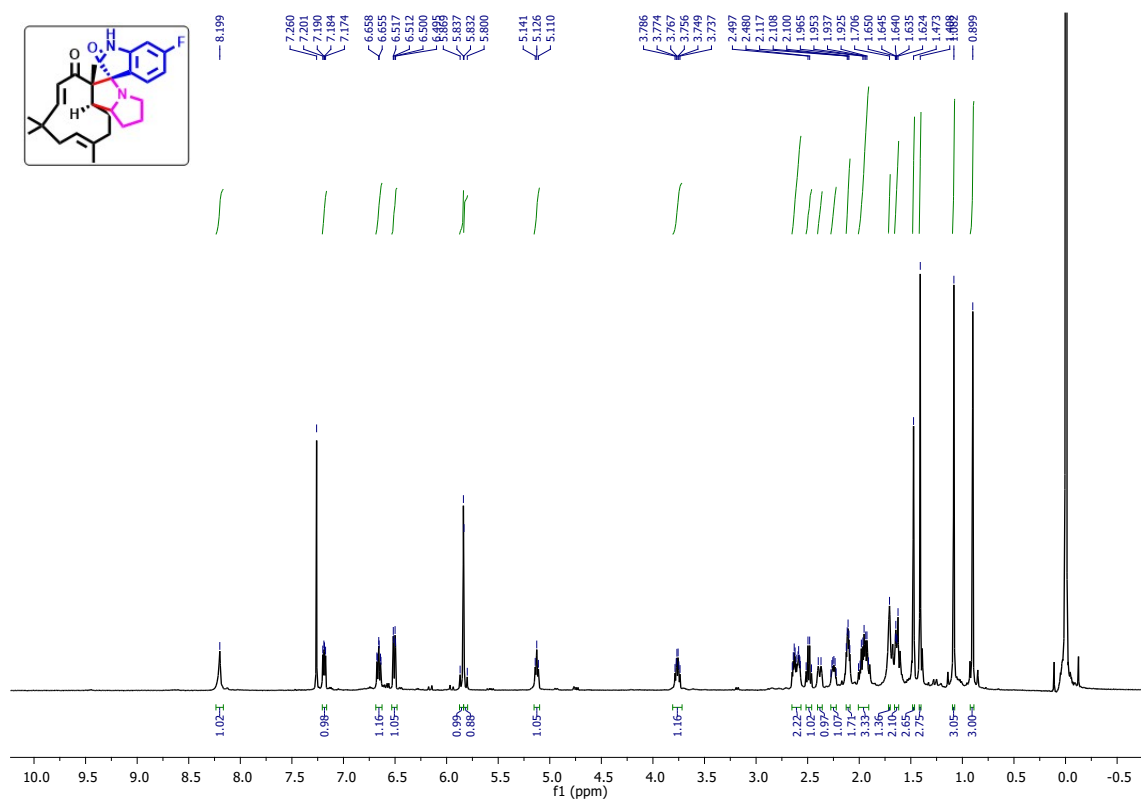


Figure S37: ZS-8 (¹H NMR (500 MHz, CDCl₃))

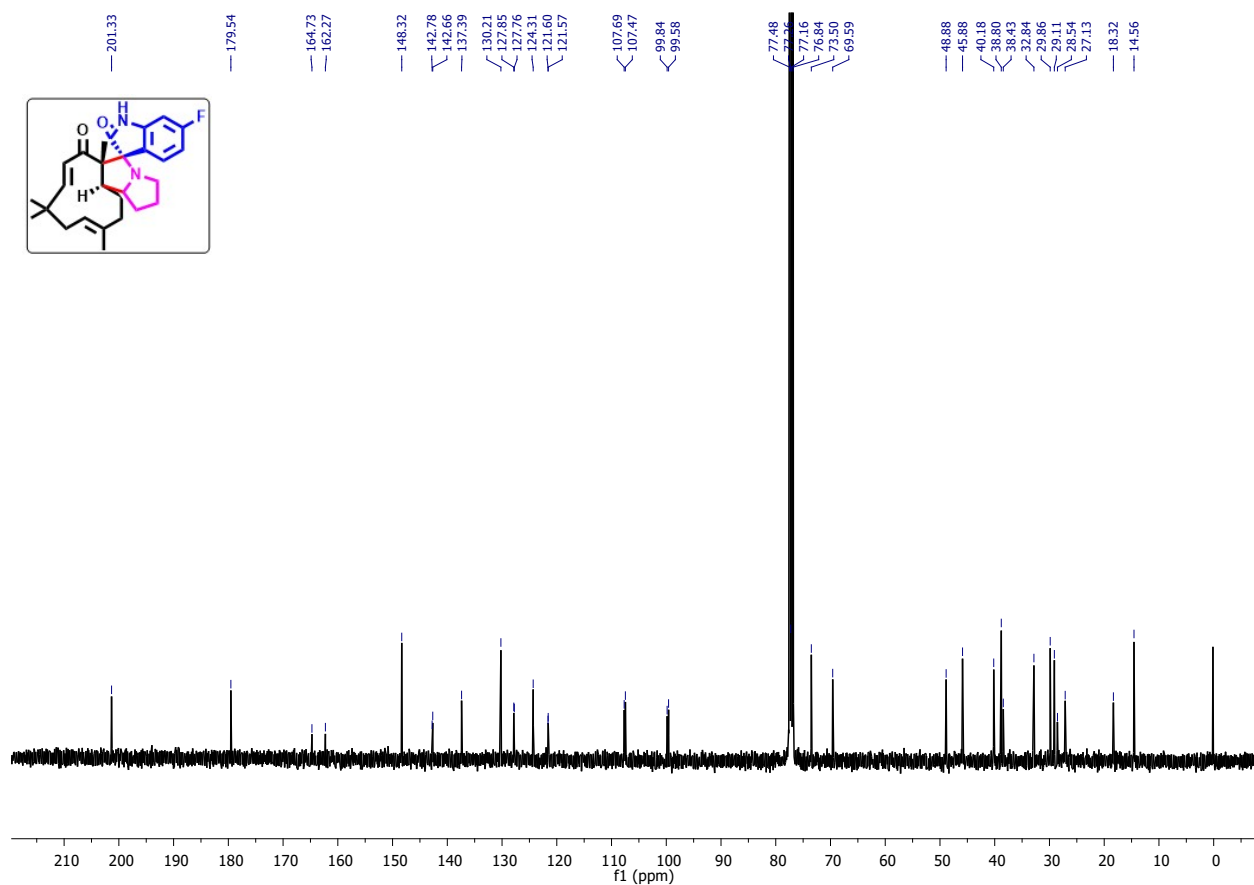


Figure S38: ZS-8 (¹³C NMR (101 MHz, CDCl₃))

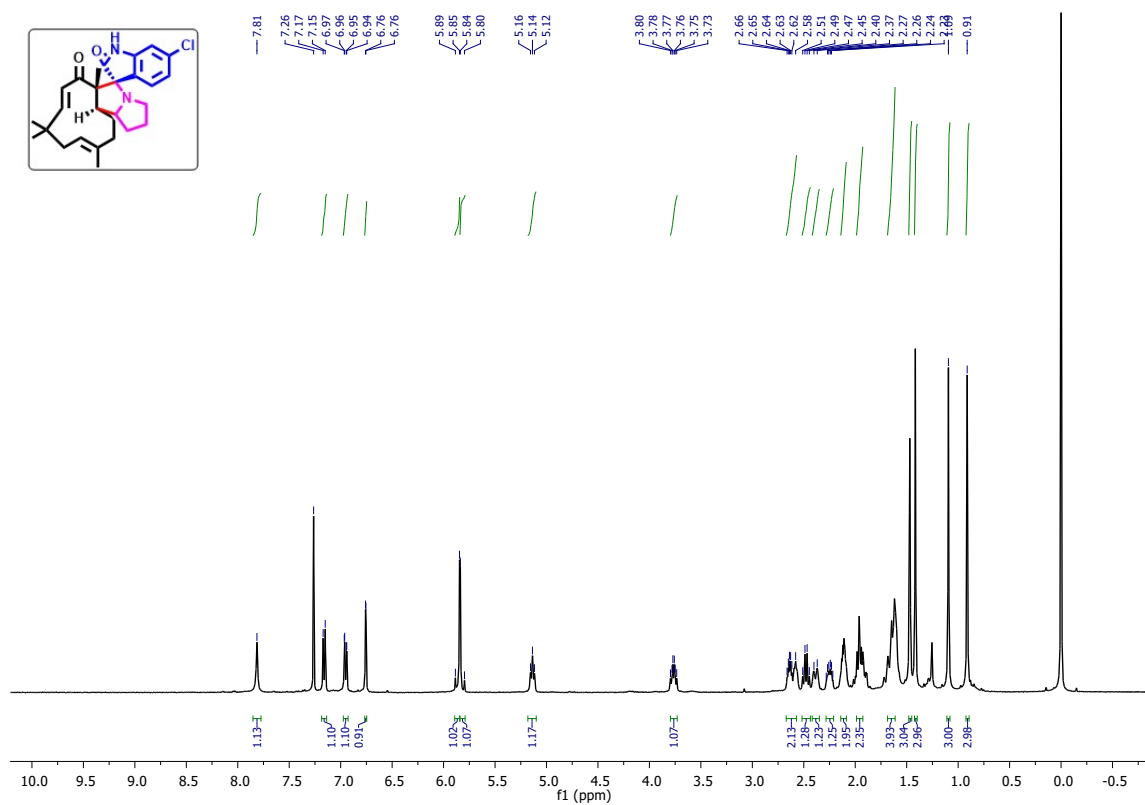


Figure S39: ZS-9 (¹H NMR (500 MHz, CDCl₃))

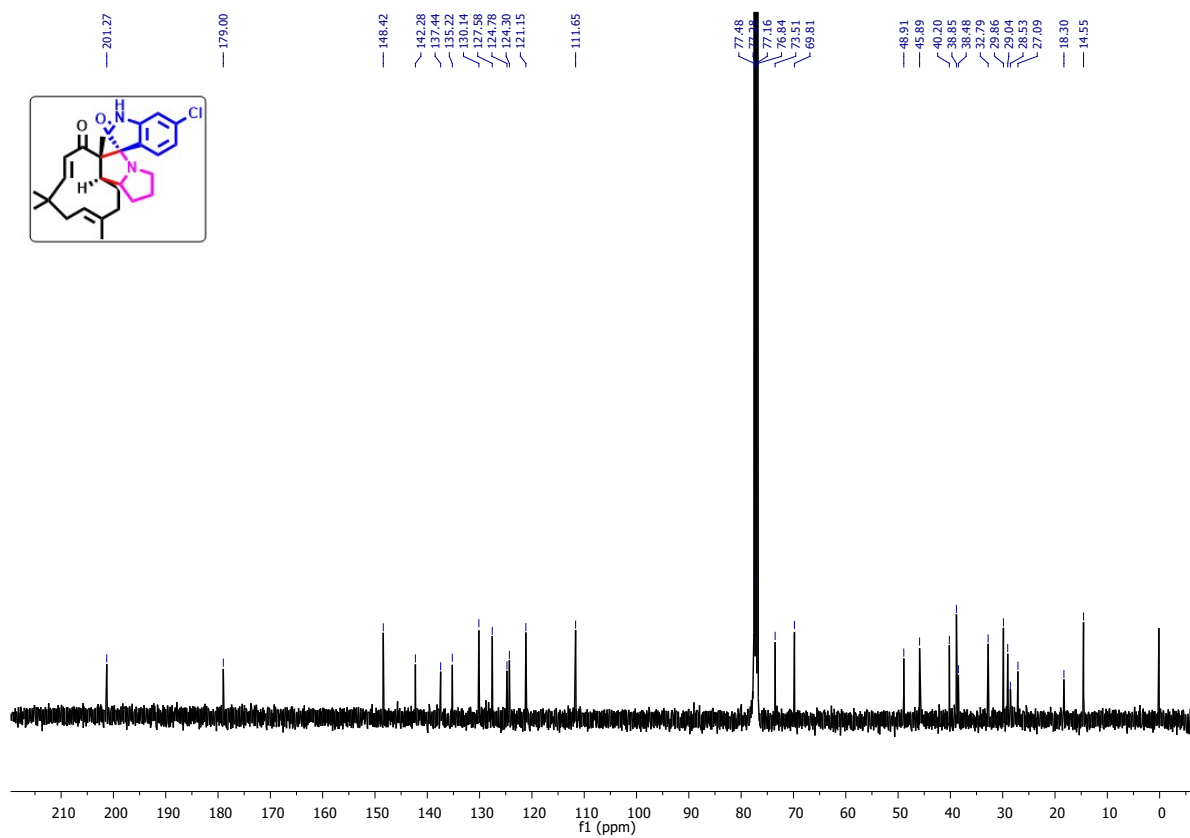


Figure S40: ZS-9 (¹³C NMR (101 MHz, CDCl₃))

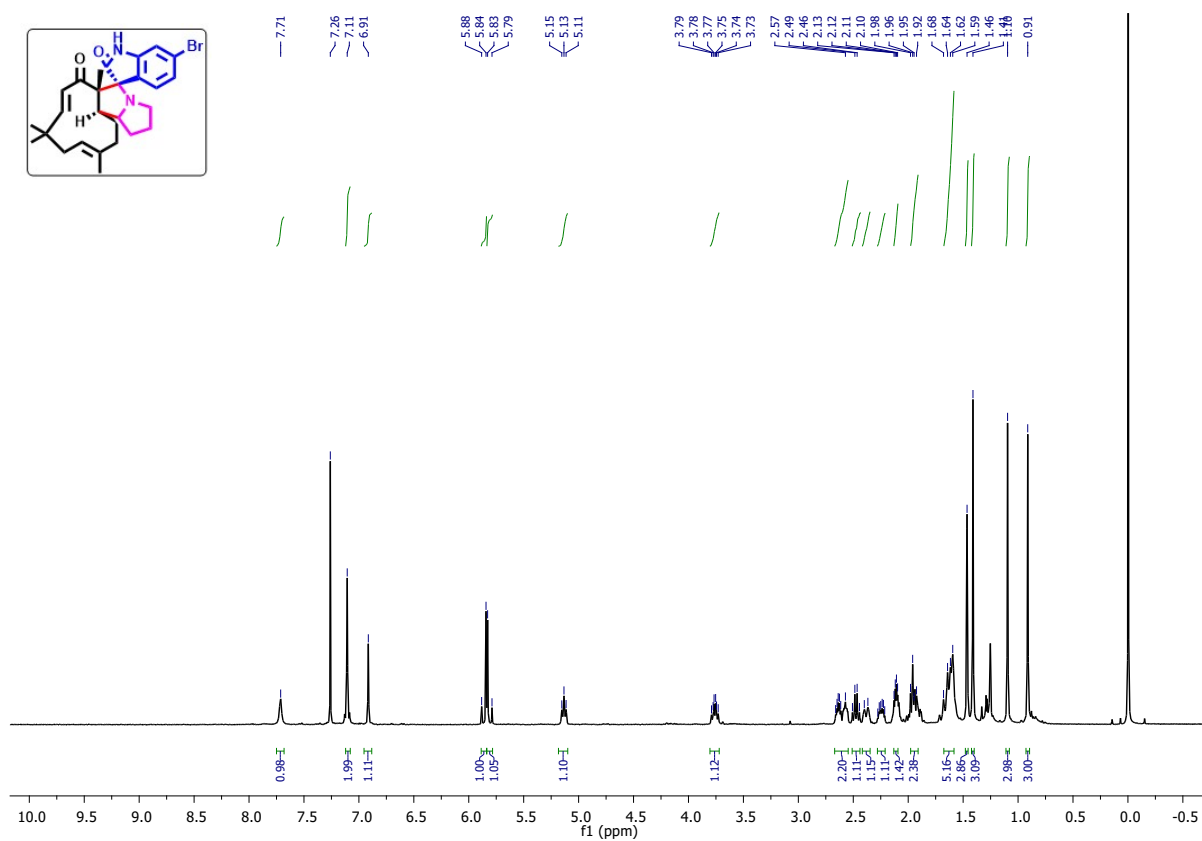


Figure 41: ZS-10 (¹H NMR (500 MHz, CDCl₃))

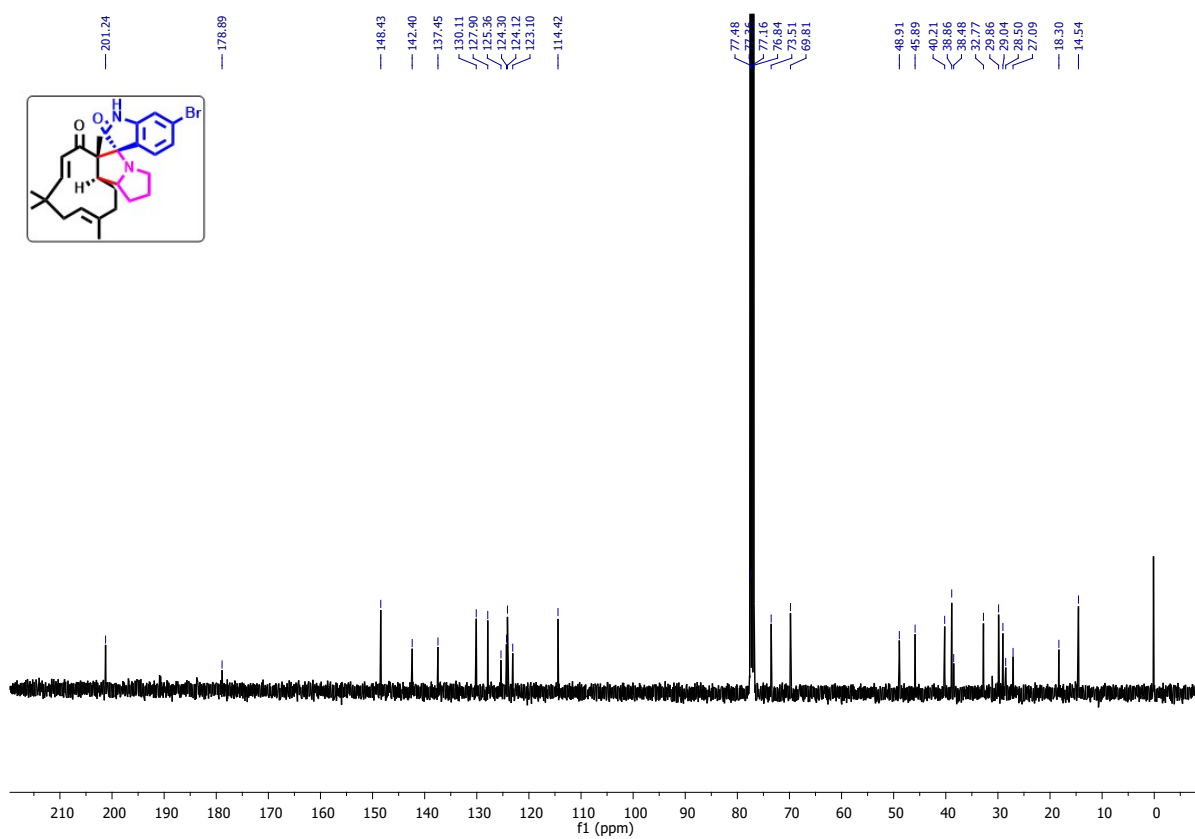
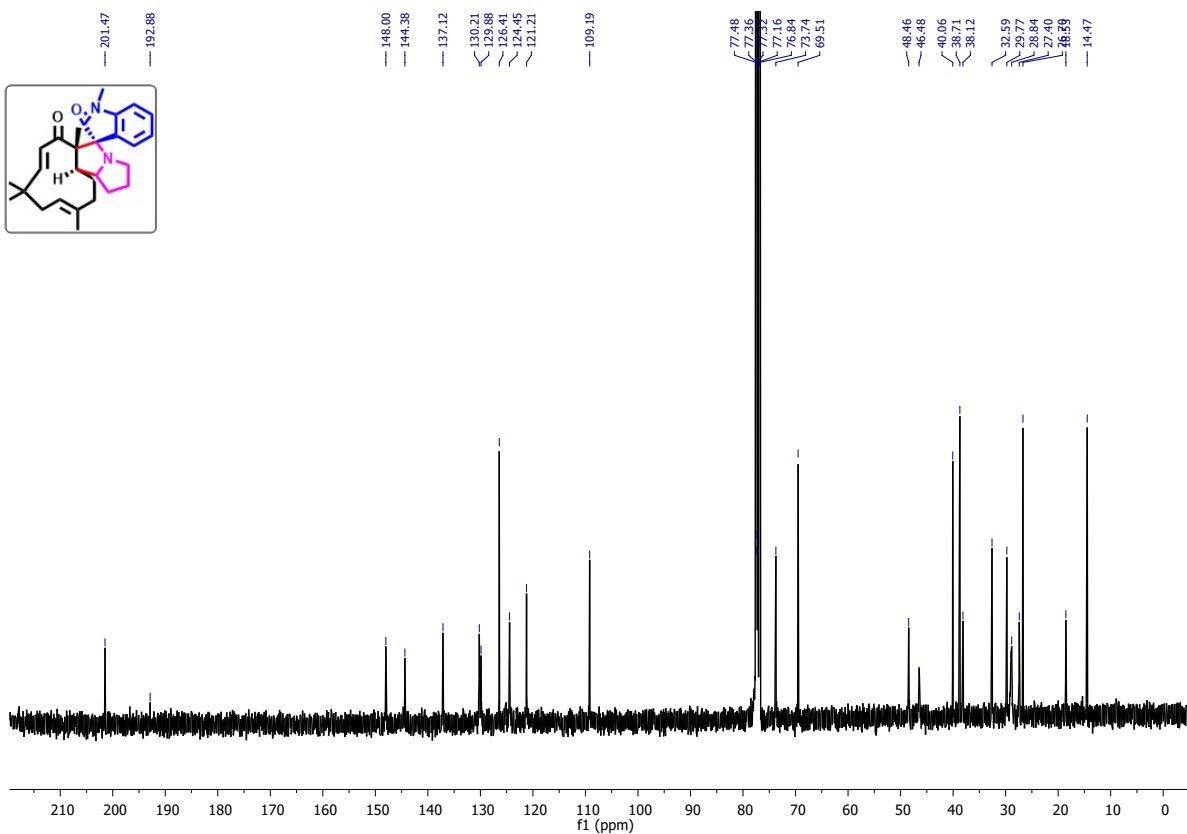
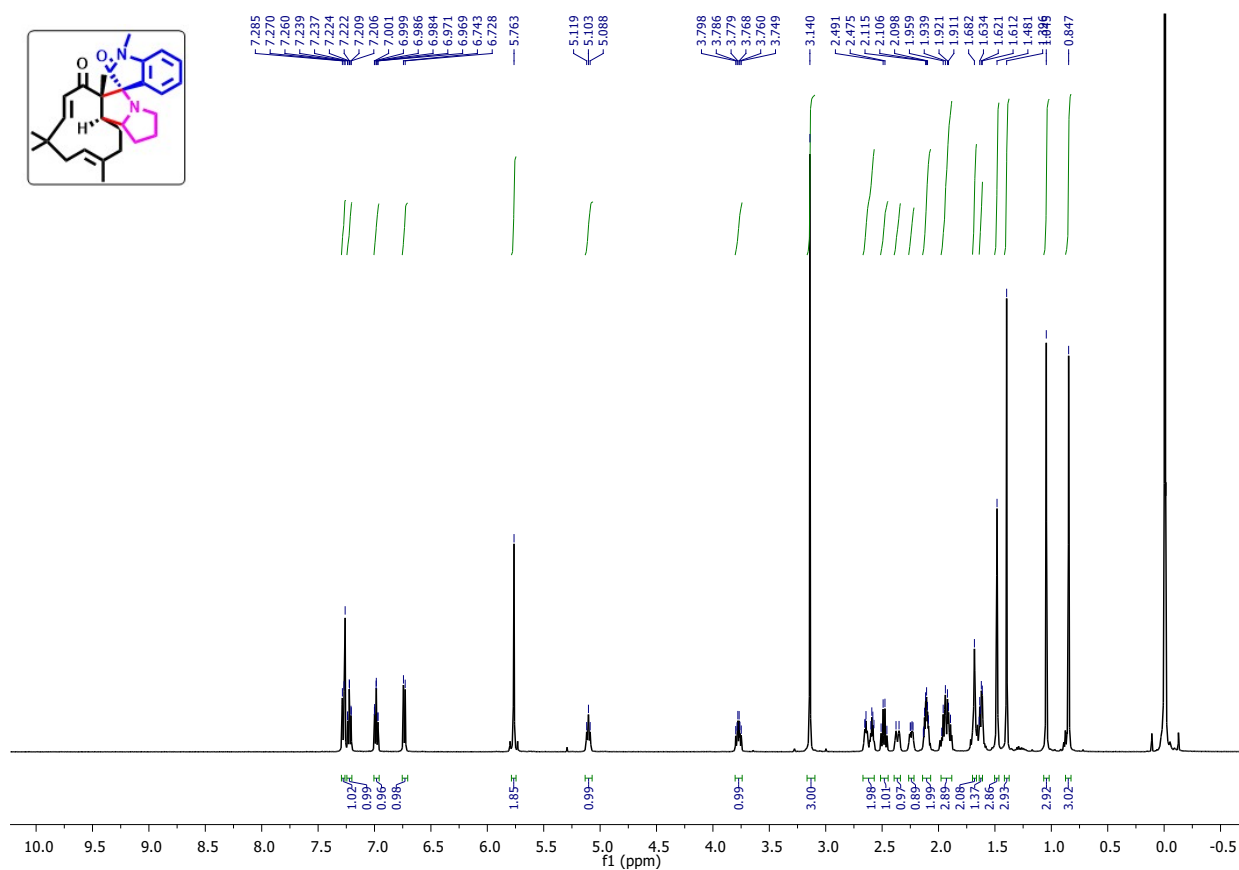


Figure S42: ZS-10 (¹³C NMR (101 MHz, CDCl₃))



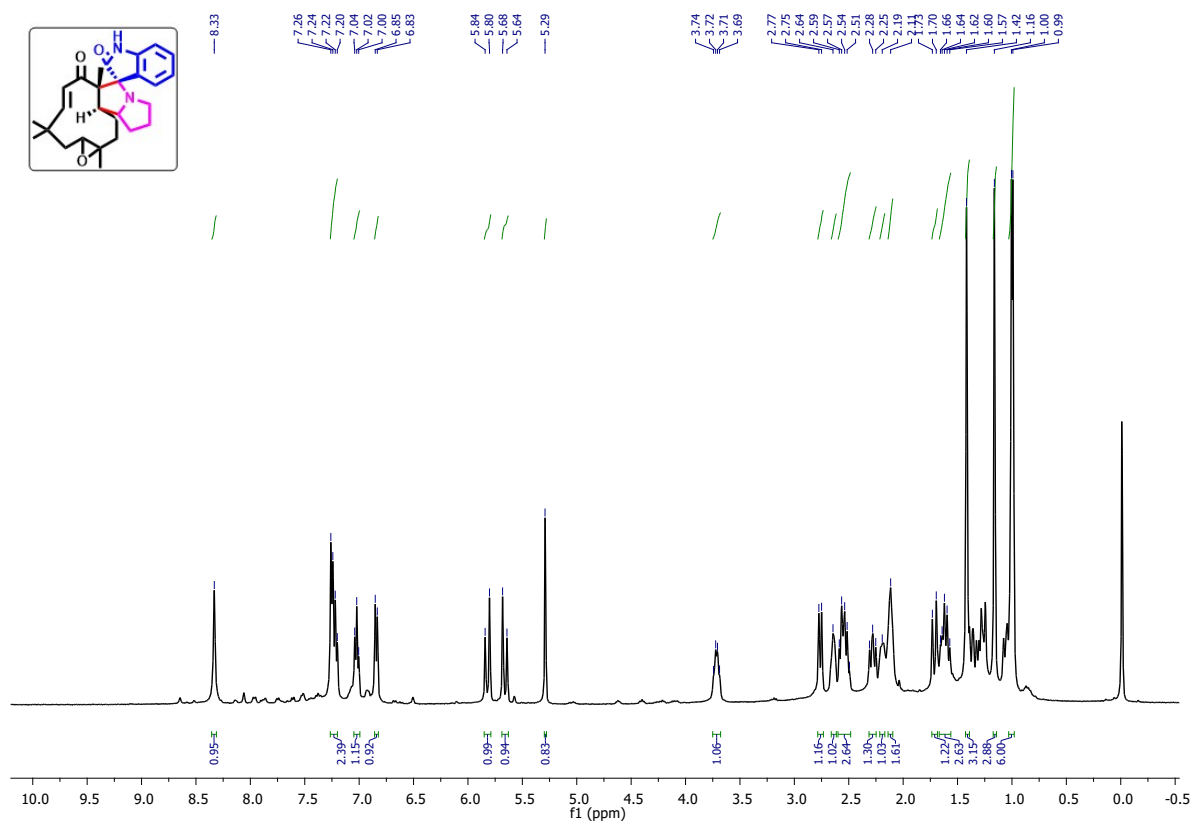


Figure S45: ZS-12 ^1H NMR (400 MHz, CDCl_3)

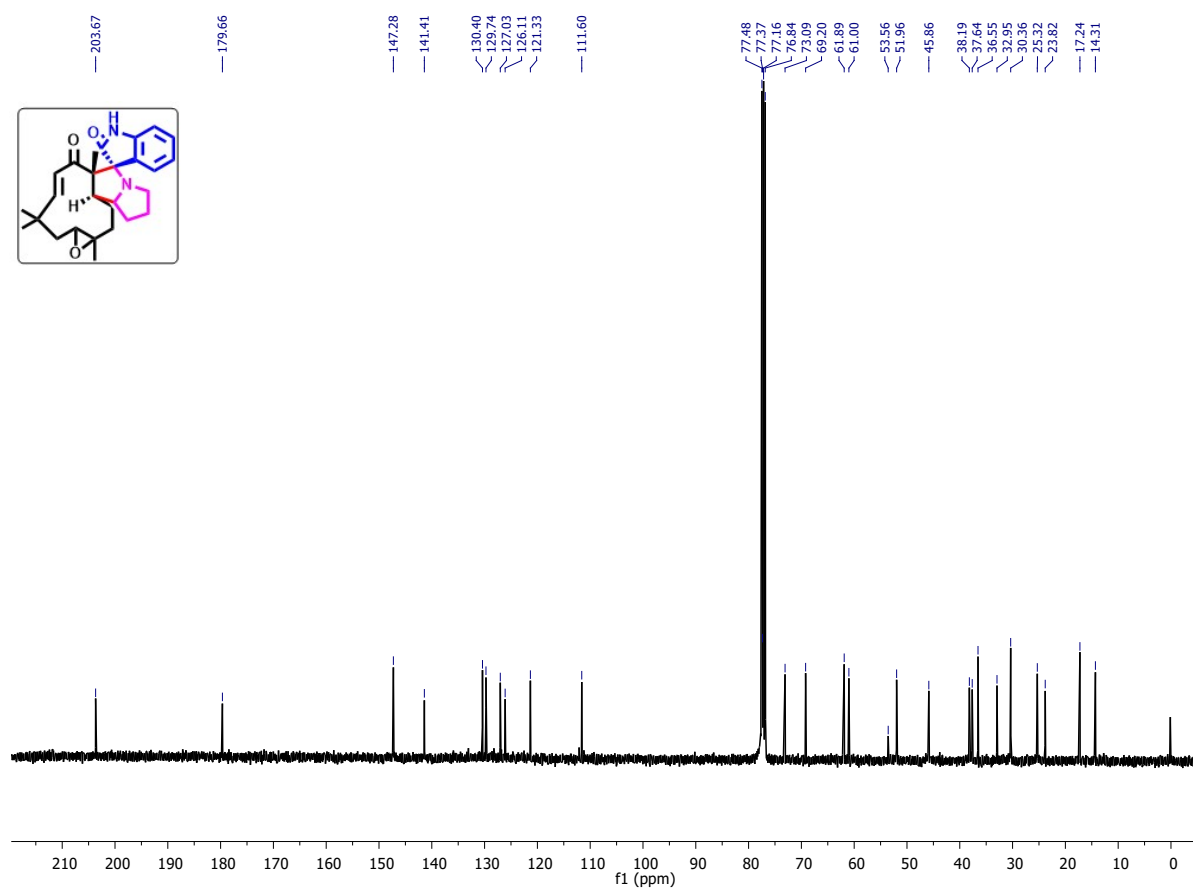


Figure S46: ZS-12 ^{13}C NMR (101 MHz, CDCl_3)

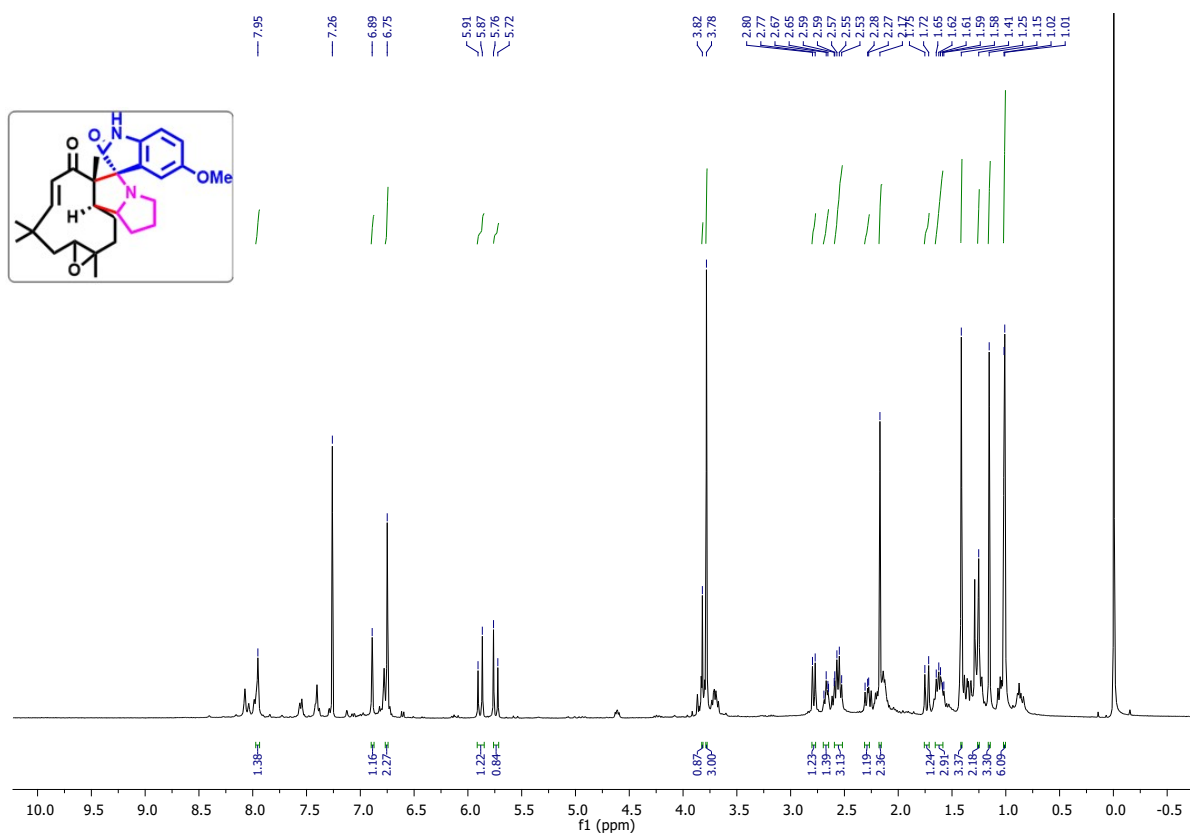


Figure S47: ZS-13 ¹H NMR (400 MHz, CDCl₃)

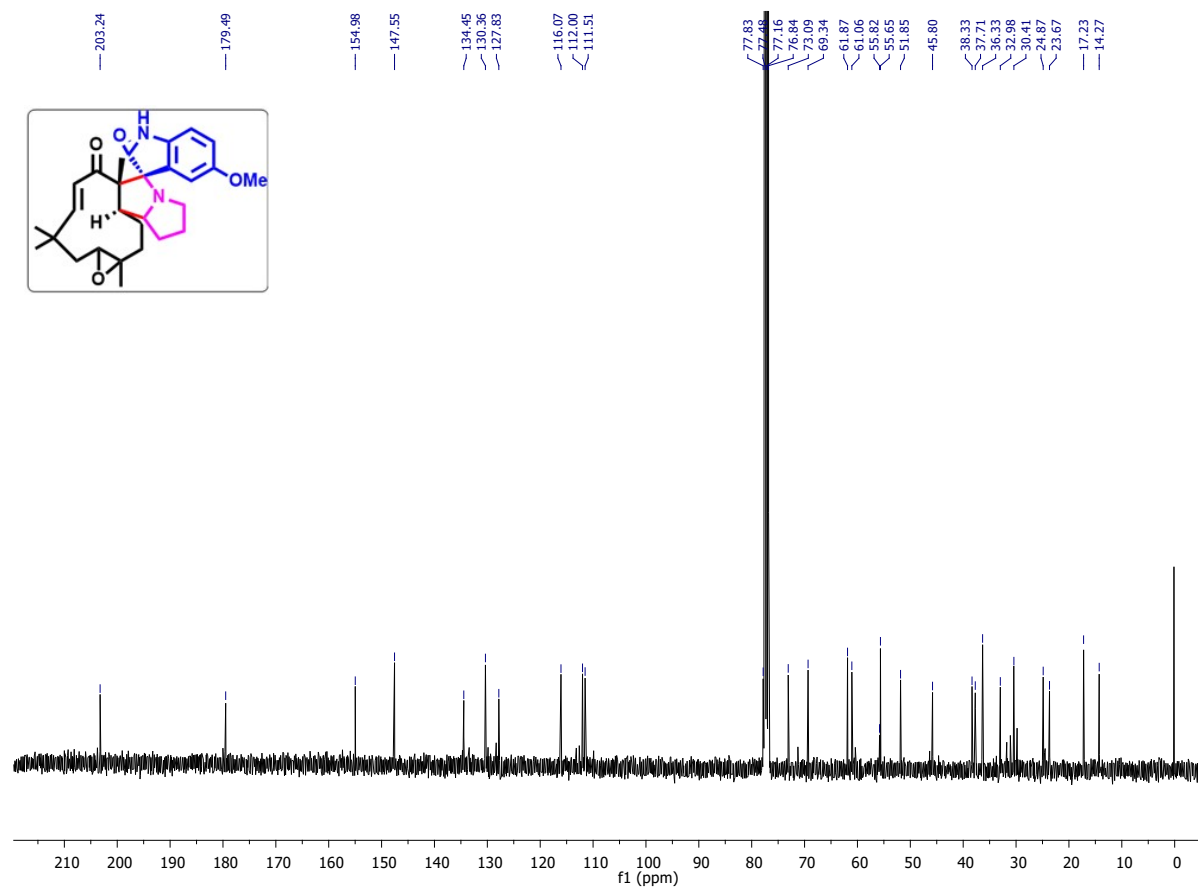


Figure S48: ZS-13 ¹³C NMR (101 MHz, CDCl₃)

14. ^{19}F NMR of fluorinated compounds

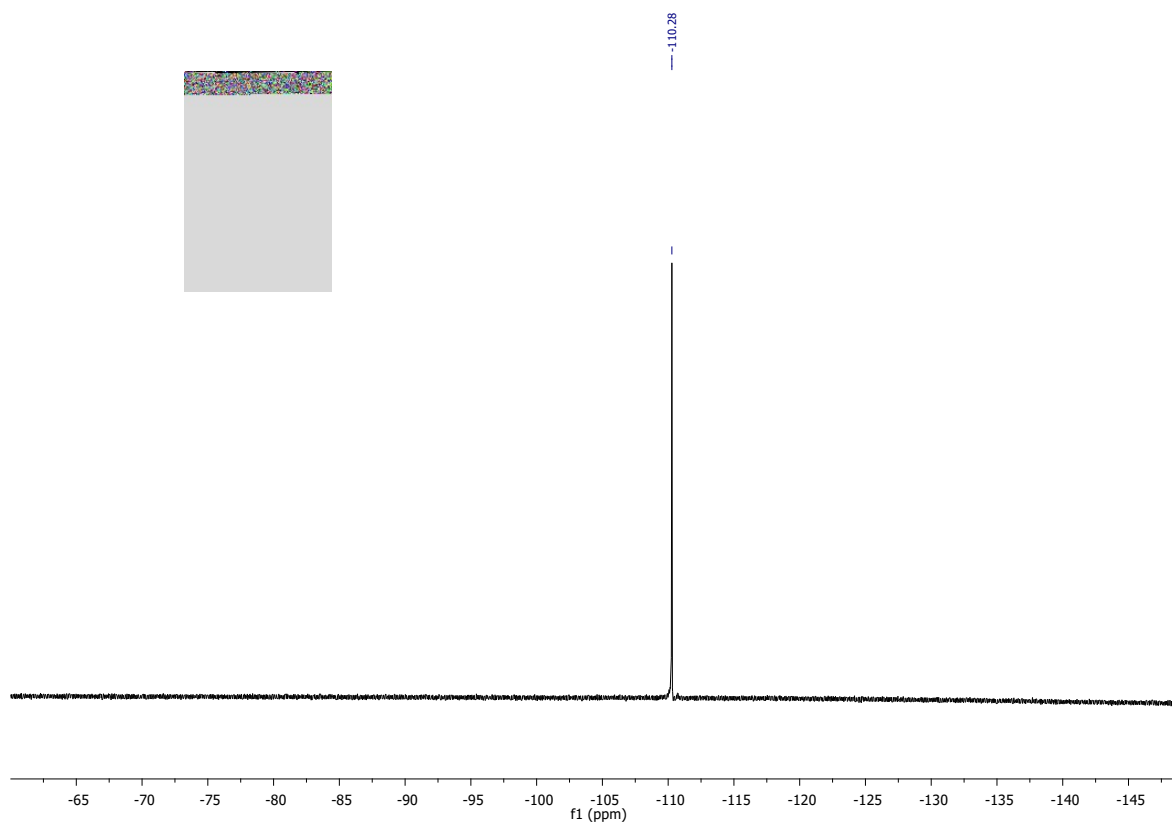


Figure S49: ZI-3 ^{19}F NMR (377 MHz, CDCl_3)

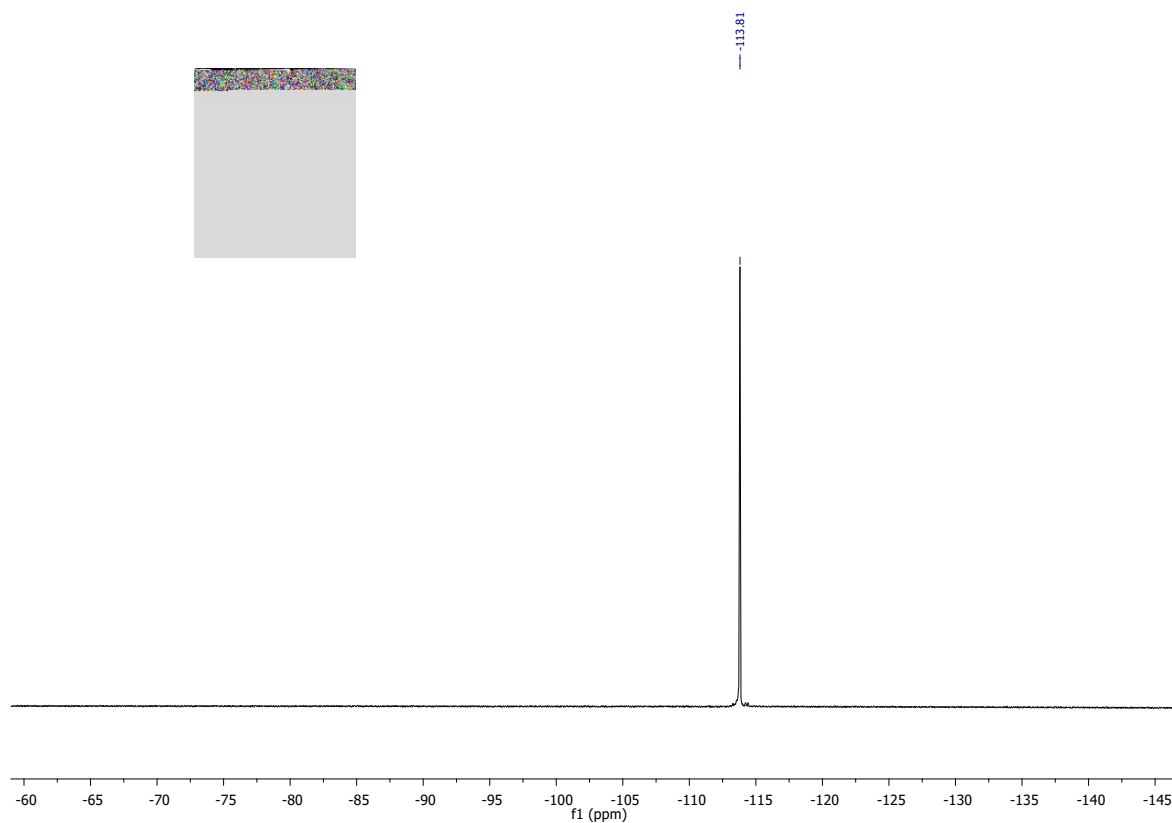


Figure S50: ZI-7 ^{19}F NMR (377 MHz, CDCl_3)

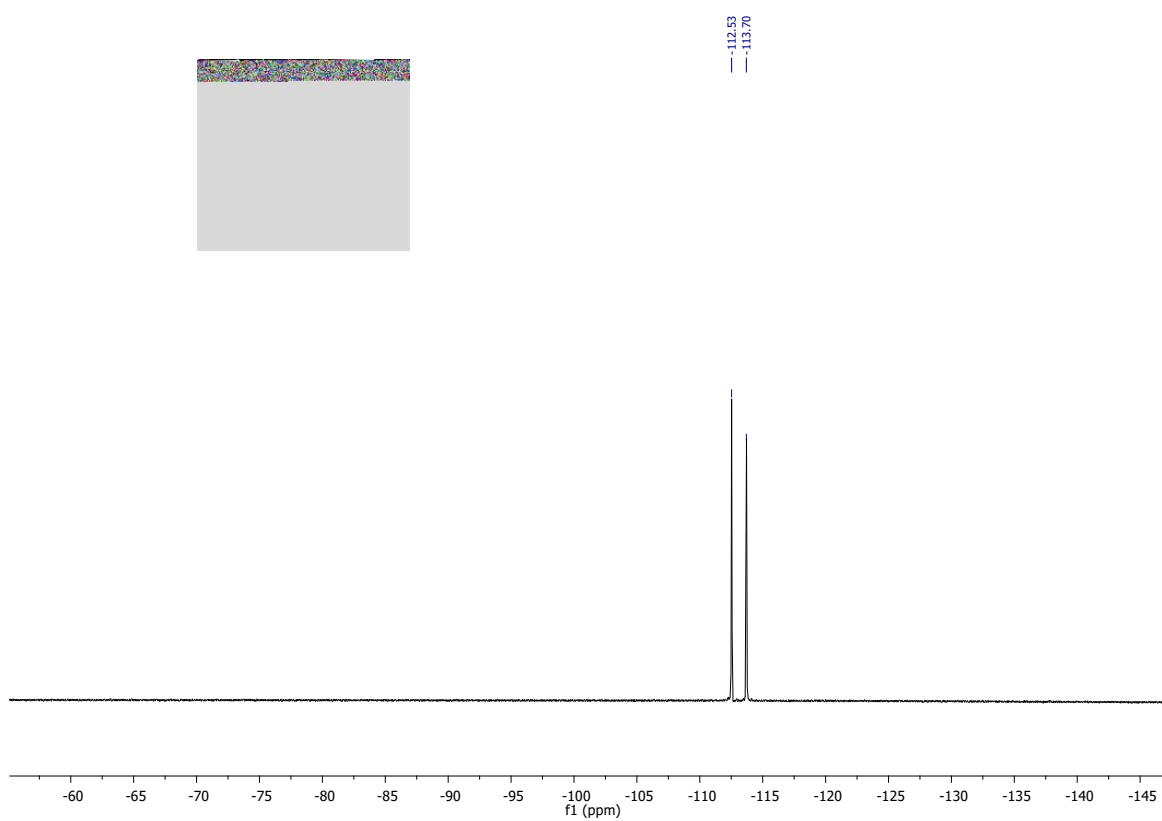


Figure S50: ZI-8 ^{19}F NMR (377 MHz, CDCl_3)

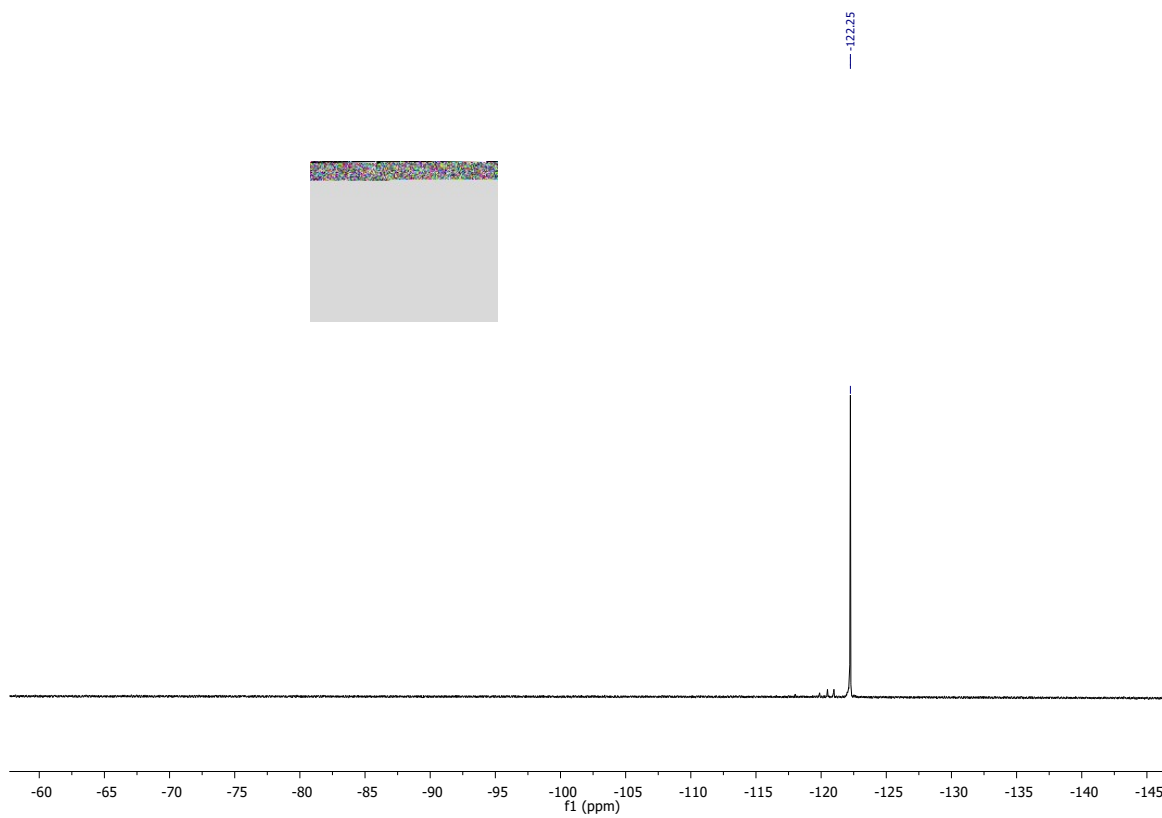


Figure S50: ZS-5 ^{19}F NMR (377 MHz, CDCl_3)

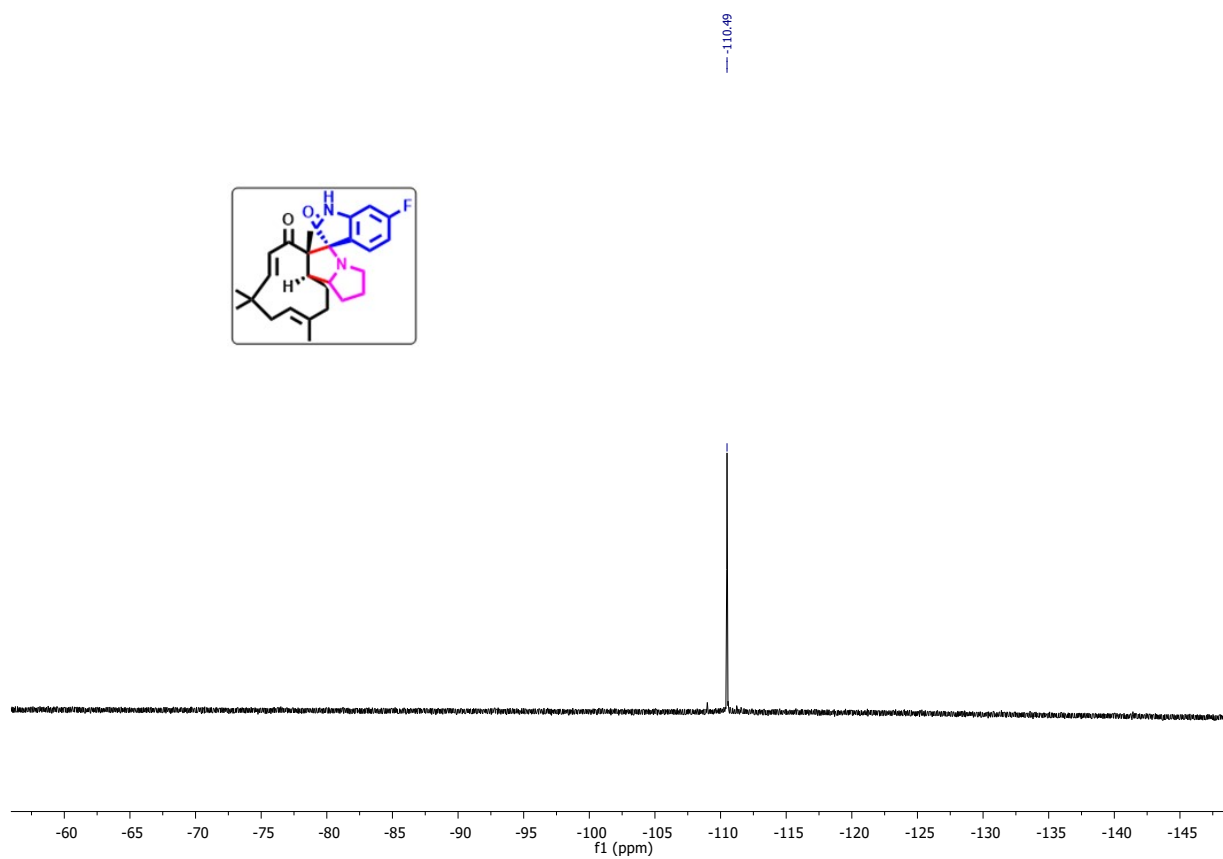


Figure S50: ZS-9 ^{19}F NMR (377 MHz, CDCl_3)

15. LC-MS data

<Chromatogram>

mAU

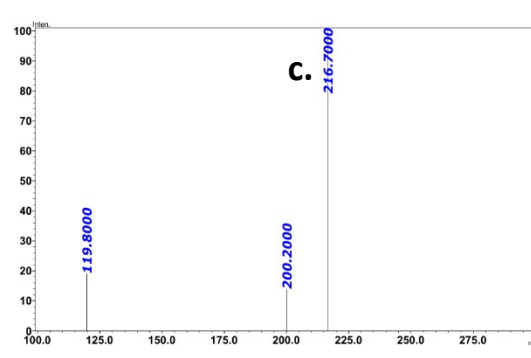
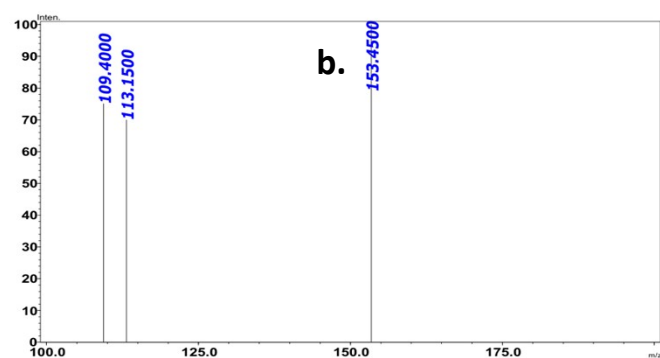
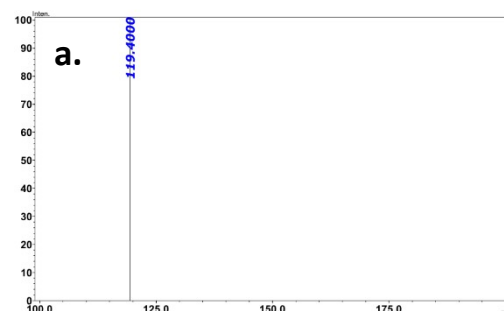
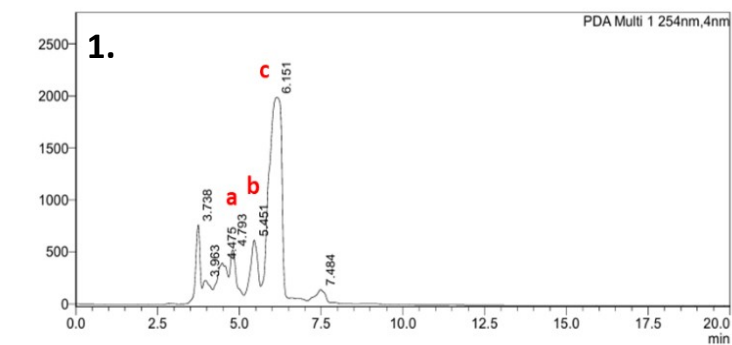
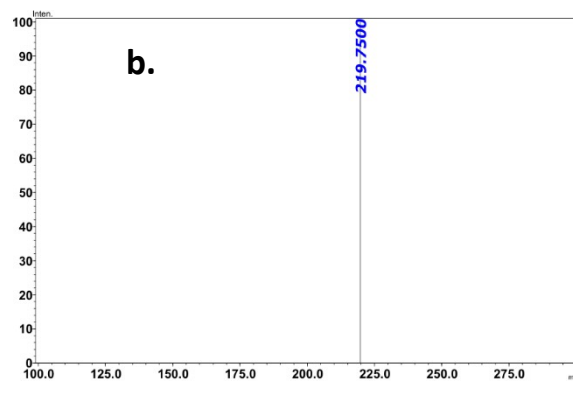
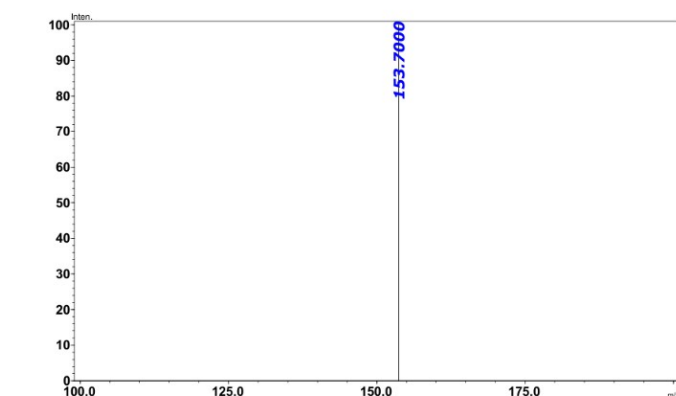
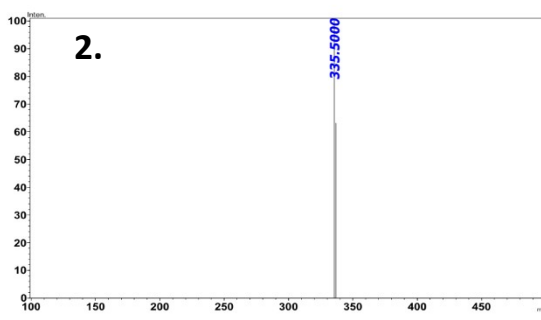
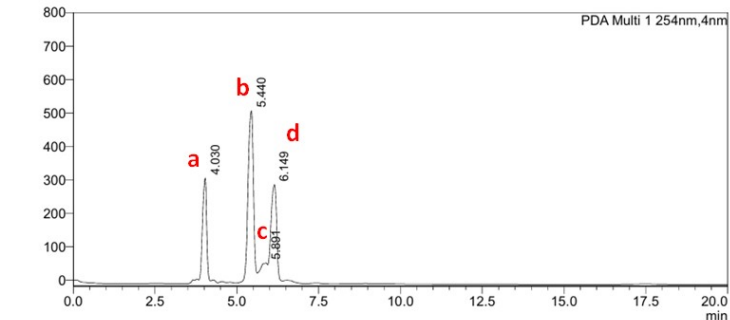


Figure S51: LC data at 0th hour. a. Mass data of 'a' at 0th hour, b. Mass data of 'b' at 0th hour, c. Mass data of 'c' at 0th hour

<Chromatogram>

mAU



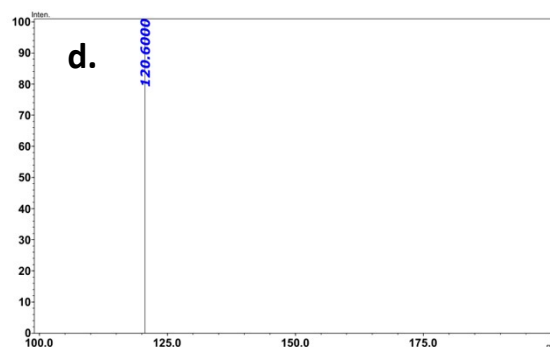


Figure S52: Mass data of 'a' at 12th hour, b. Mass data of 'b' at 12th hour, c. Mass data of 'c' at 12th hour, d. Mass data of 'd' at 12th hour

<Chromatogram>

mAU

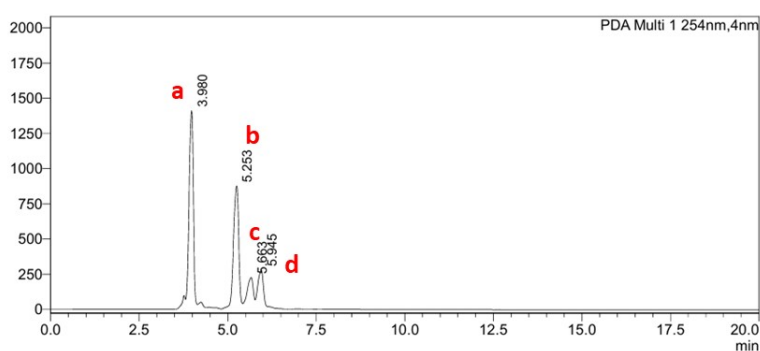
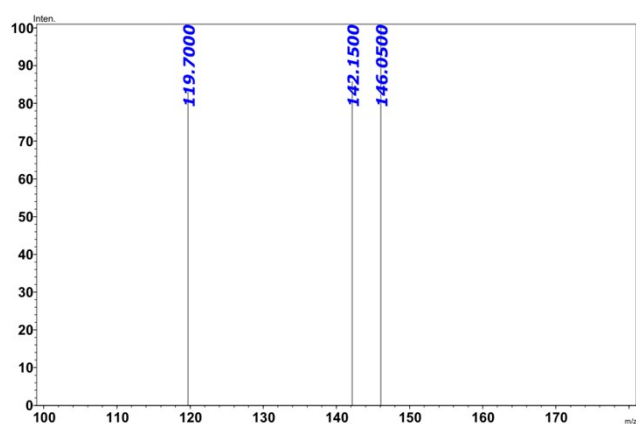
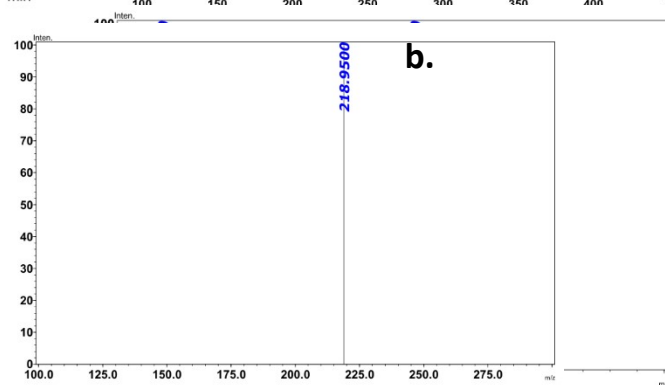
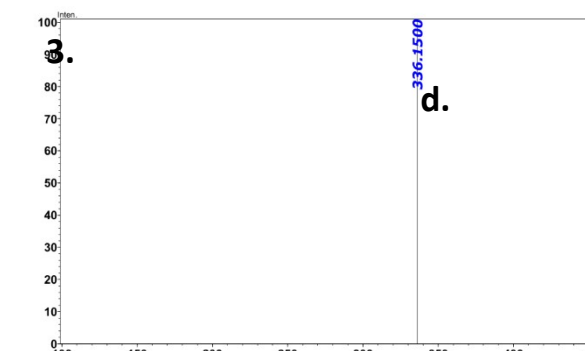


Figure S53: Mass data of 'a' at 12th hour, b. Mass data of 'b' at 12th hour, c. Mass data of 'c' at 12th hour, d. Mass data of 'd' at 12th hour

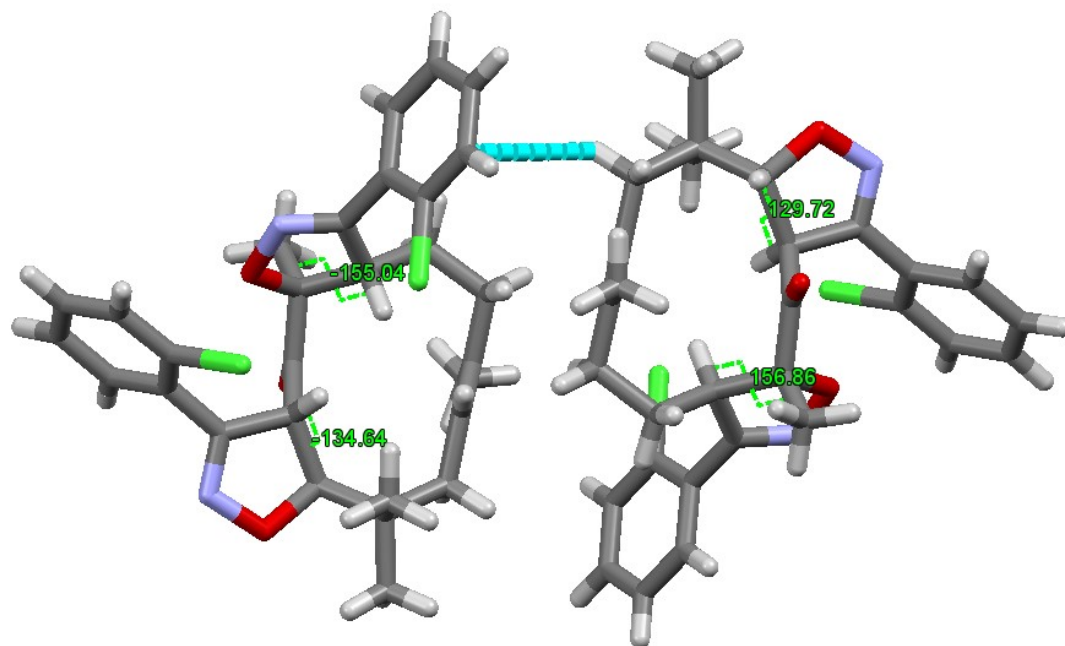


15. Crystallography data

Table 3: Crystallographic data

	ZI-1	ZI-9	ZI-10	ZS-1
CCDC number	2362922	2362919	2362921	2362920
Empirical formula	C ₂₂ H ₂₇ NO ₂	C ₂₉ H ₃₀ Cl ₂ N ₂ O ₃	C ₂₉ H ₃₀ Br ₂ N ₂ O ₂	C ₂₇ H ₃₄ N ₂ O ₂
Formula weight (g.mol ⁻¹)	337.465	350.319	588.130	418.583
Temperature (K)	296 K	299 K		273 K
Radiation, λ (Å)	Mo-K α (λ = 0.71073)	Mo-K α (λ = 0.71073)	Mo-K α (λ = 0.71073)	Mo-K α (λ = 0.71073)
Crystal Colour, habit	Block, Colourless	Block, Colourless	Block, colourless	Block, colourless
Crystal size (mm ³)	0.36 × 0.22 × 0.18	0.307 × 0.089 × 0.088	0.273 × 0.234 × 0.234	0.2 × 0.18 × 0.15
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	<i>P</i> 1 2 ₁ / <i>n</i> 1	<i>P</i> 1 <i>n</i> 1	<i>P</i> -1	<i>P</i> 1 2 ₁ / <i>c</i> 1
Unit cell dimensions				
<i>a</i> (Å)	8.6646(3)	9.2353(7)	9.343(2)	10.1096(18)
<i>b</i> (Å)	21.5471(7)	13.3183(10)	13.457(3)	9.5621(19)
<i>c</i> (Å)	10.7458(3)	22.4290(16)	22.540(5)	23.618(5)
α (°)	90	90	84.172(10)	90
β (°)	109.576(1)	100.025(2)	79.375(8)	94.613(7)
γ (°)	90	90	89.555(9)	90
Volume (Å ³)	1890.29(10)	2716.6(4)	2770.8(11)	2275.7(8)
<i>Z</i>	4	6	2	2
Calculated density (Mg.m ⁻³)	1.186	1.285	1.410	1.222
μ (mm ⁻¹)	0.075	0.272	2.958	0.077
F(000)	728.421	1105.786	1135.112	904.516
θ range (°)	2.63 to 28.27	2.27 to 20.66	2.24 to 21.15	2.30 to 26.36
Reflections collected	49003	67185	9297	18909
Independent reflections	4703	13184	5401	4356
Parameters/ restraints	241/0	657/2	657/0	284/0
GooF on F ²	1.0835	1.1443	1.0432	1.2831
R ₁ [<i>I</i> > 2 σ (<i>I</i>)] ^a	0.0673(3727)	0.0498(6752)	0.0559(3240)	0.1012(3571)
wR ₂ (all data) ^b	0.1397(4703)	0.1464(13184)	0.1229(5401)	0.2979(4356)
Maximum/minimum residual electron density (e.Å ⁻³)	0.3063/-0.3063	0.3232/-0.4641	0.6563/-0.9225	0.7561/- 0.8460

(a) Torsion angle of **ZI-9**



(b) Torsion angle of **ZI-10**

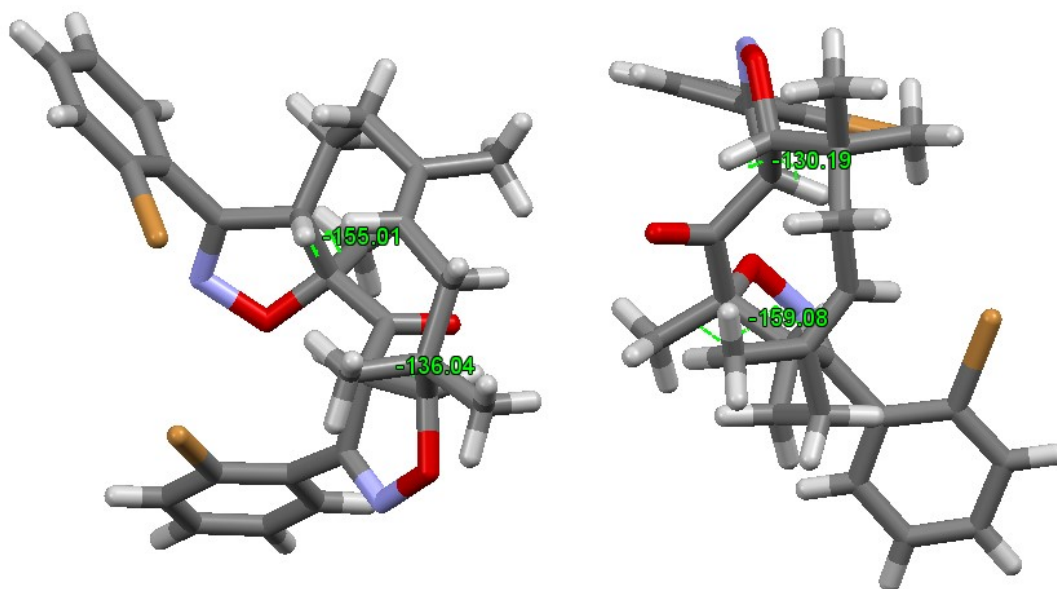


Figure S54: Torsion angles at C2 - C3 and C10 – C11 (a) Torsion angle of **ZI-9** (b) Torsion angle of **ZI-10**

Solid-state packing of Isoxazoline compounds

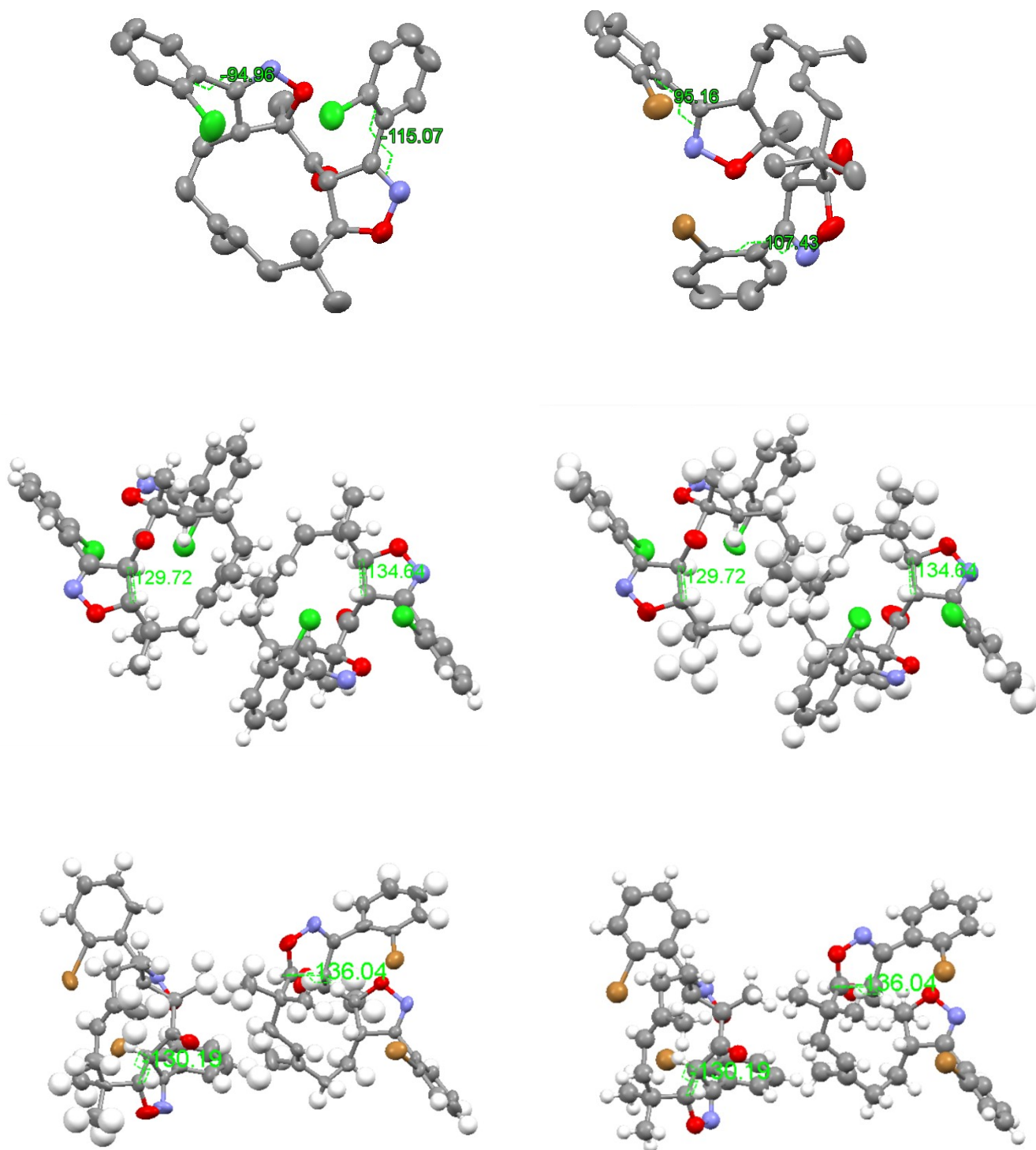
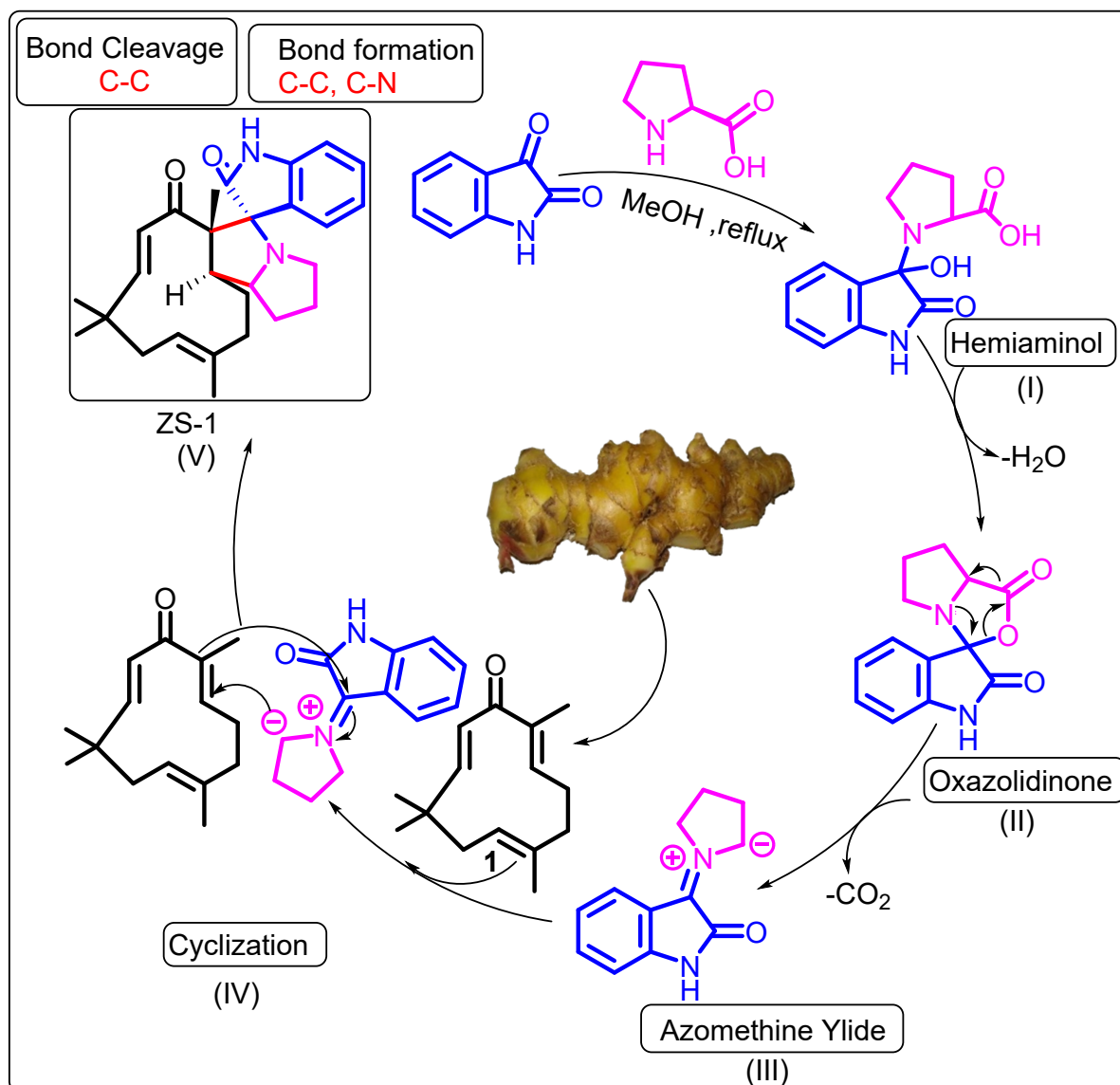


Figure S55: Conformational diversity in Solid-state packing

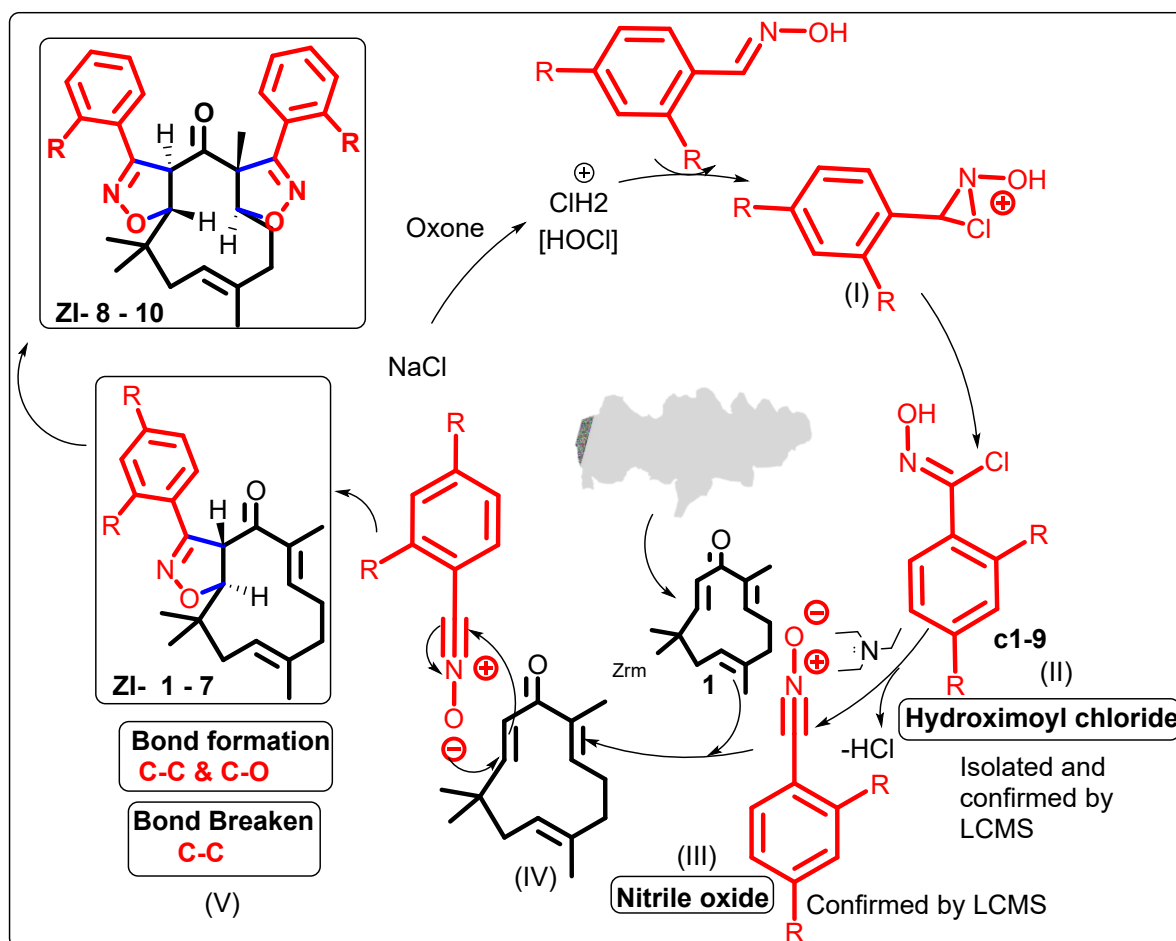
16. Mechanism

Mechanism -1



Scheme 4: Plausible reaction mechanism for Zerumbone fused Spirocycle compounds

Transitioning towards spirocycles synthesis involves a stepwise progression starting with a straightforward addition reaction between isatin and L-proline, yielding a hemiaminal intermediate (I). Upon the removal of water, this intermediate transforms into an oxazolidinone (II). Subsequently, an intramolecular cyclization event occurs, facilitating decarboxylation and leading to the generation of an azomethine ylide (III). This reactive intermediate undergoes further cyclisation processes through subsequent chemical transformations with zerumbone (IV), ultimately yielding the desired product **ZS-1** (V). This sequential series of reactions underscores a strategic approach toward the synthesis of intricate spirocycles, showcasing the intricate.



Scheme 5: Plausible reaction mechanism for Zerumbone fused Isoxazoline compounds

An outline of the catalytic cyclization mechanism is given in Scheme 4. First, a reaction between NaCl and Oxone produces hypochlorous acid, the active chlorine species. The production of the chlorine ion results from this hypochlorous acid's interaction with the aldoxime. Following this, the alkene and chlorine ion engage in an opening reaction (I) that yields N-hydroxybenzimidoyl chloride (II) (confirmed by LC-MS). In addition, triethylamine affords nitrile oxide (III) (confirmed by LC-MS) with the elimination of HCl. Subsequent chemical changes aid in the cyclization process (IV), which then proceeds further and culminates in beta elimination to produce the desired isoxazoline molecule **ZI-1** to **ZI-10** (V). This sequential process demonstrates the complexity of the cyclization pathway and emphasizes how crucial each reactive intermediate is to producing the desired end product.

17. Computational details

Methodology:

All quantum chemical calculations were carried out using the Gaussian 16 software suite¹, employing density functional theory (DFT) as the computational methodology. The B3LYP hybrid functional²⁻⁴, renowned for its accuracy and computational efficiency, was utilized in conjunction with the 6-31G(d,p) basis set for energy minimization^{5,6}. To improve the precision of the energy calculations and account for long-range interactions, the more sophisticated

triple-zeta valence polarized def2-TZVP basis set was employed⁷. This was complemented by Grimme's D3 dispersion corrections, ensuring highly accurate energy predictions and a robust treatment of non-covalent interactions⁸. Geometrical optimizations were conducted without any symmetry or constraints, allowing for the attainment of true minimum energy configurations. The polarized continuum model (PCM) was applied to account for solvent effects, effectively simulating solvent polarity⁹. Methanol was chosen as the solvent for reactions involving C-nucleophiles, while N,N-dimethylformamide (DMF) was used for reactions with O-nucleophiles. These analyses were critical in confirming that the structures corresponded to authentic minima or transition states on the potential energy surface (PES). Additionally, intrinsic reaction coordinate (IRC) calculations were systematically conducted to validate that the transition states connected the correct reactants and products, providing a comprehensive understanding of the reaction mechanism.

Interaction of **1** with Nucleophiles

The zerumbone **1** was optimized using various initial structural models to determine its ground state geometry accurately. The nucleophiles interact with **1** at the C2-C3 and C10-C11 double bonds. For each nucleophile, interactions are considered at both double bonds in two distinct orientations, as illustrated in Figure S67. Specifically, the nucleophile is allowed to approach **1** from both the top and bottom of the ring at the C10-C11 double bond. This methodology is consistently applied to both C- and O-nucleophiles at both double bonds. In doing so, we systematically explore all possible interaction configurations, ensuring that no potential conformational pathways are overlooked.

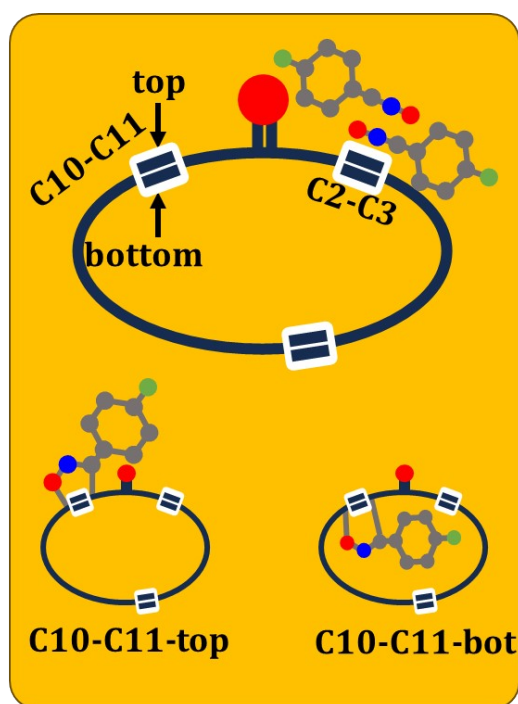


Fig S56. Possible ways of interaction of CNU and ONU with **1**.

Table 4. Cartesian coordinates of optimized geometries of all the transition states and intermediates computed at B3LYP-D3/6-31G(d,p) level of theory.

TS1				TS1p			
6	-3.632326000	-0.984889000	-0.956958000	6	-3.910701000	-0.759017000	-0.946558000
6	-4.124181000	0.344601000	-0.444319000	6	-4.132146000	0.517972000	-0.180771000
6	-2.575331000	-1.761236000	1.245051000	6	-2.545591000	-1.726336000	0.962880000
6	-3.537702000	-2.119283000	0.111921000	6	-3.663543000	-2.003346000	-0.031182000
6	-0.743492000	1.213820000	-0.026517000	6	-0.209892000	1.655081000	0.240639000
6	-1.290420000	-1.389730000	1.186081000	6	-1.319024000	-1.187286000	0.820885000
6	-0.423263000	-1.269071000	-0.040484000	6	-0.612262000	-0.816567000	-0.429954000
6	-0.142637000	0.058624000	-0.575636000	6	0.381523000	0.373761000	-0.444425000
1	-4.323837000	-1.346089000	-1.734441000	1	-4.802255000	-0.984976000	-1.549846000
6	-3.675457000	1.574809000	-0.742715000	6	-3.450836000	1.673315000	-0.249537000
6	-2.525538000	1.865793000	-1.686119000	6	-2.344084000	1.960118000	-1.244226000
6	-1.227559000	2.311712000	-0.959359000	6	-1.049625000	2.570430000	-0.664152000
1	-2.824503000	2.670760000	-2.371341000	1	-2.739646000	2.689078000	-1.967516000
1	-4.975796000	0.289236000	0.232680000	1	-4.951217000	0.478887000	0.537409000
1	-2.658926000	-0.879051000	-1.442442000	1	-3.079919000	-0.668376000	-1.646571000
8	0.020515000	-2.300140000	-0.579983000	8	-0.806019000	-1.436580000	-1.475001000
1	-1.452768000	1.008600000	0.772203000	1	-0.859221000	1.320728000	1.055104000
1	-0.473901000	2.556249000	-1.712951000	1	-0.439557000	2.934919000	-1.496741000
1	-1.432193000	3.232044000	-0.406573000	1	-1.314869000	3.461514000	-0.085498000
1	-2.299849000	0.995225000	-2.306917000	1	-2.107417000	1.065253000	-1.822618000
6	0.572432000	0.104123000	-1.900389000	6	0.768076000	0.618612000	-1.911962000
1	1.215271000	-0.767643000	-2.016404000	1	1.159047000	-0.290214000	-2.363687000
1	-0.143596000	0.104769000	-2.733873000	1	-0.101634000	0.908650000	-2.500797000
1	1.182894000	1.004810000	-2.005440000	1	1.511061000	1.409315000	-2.001170000
6	-3.066797000	-3.411736000	-0.596205000	6	-3.329789000	-3.230181000	-0.910261000
1	-2.995686000	-4.237023000	0.120471000	1	-3.185497000	-4.121615000	-0.290103000
1	-3.783712000	-3.700952000	-1.373978000	1	-4.160538000	-3.430373000	-1.597186000
1	-2.083725000	-3.276854000	-1.049609000	1	-2.421360000	-3.053913000	-1.485006000
6	-4.928953000	-2.394211000	0.721741000	6	-4.944775000	-2.326039000	0.770732000
1	-5.659659000	-2.615981000	-0.063354000	1	-5.785963000	-2.503092000	0.092871000
1	-4.884915000	-3.257321000	1.394985000	1	-4.802143000	-3.229264000	1.374101000
1	-5.301328000	-1.545525000	1.303169000	1	-5.221280000	-1.515116000	1.451095000
6	-4.309596000	2.797114000	-0.118698000	6	-3.824818000	2.829068000	0.651315000
1	-5.141874000	2.534744000	0.540477000	1	-4.737606000	2.622706000	1.216882000
1	-3.581794000	3.366407000	0.473764000	1	-3.028442000	3.045756000	1.374438000
1	-4.684571000	3.483519000	-0.889207000	1	-3.978559000	3.749951000	0.073630000
1	-3.007465000	-1.826131000	2.244224000	1	-2.820302000	-1.932724000	1.997941000
1	-0.772546000	-1.155808000	2.116192000	1	-0.802595000	-0.960538000	1.743337000
6	3.302346000	-1.621429000	0.401691000	6	2.881472000	-1.903967000	0.746495000
6	3.223942000	-0.288901000	-0.092609000	6	2.732407000	-0.840395000	-0.162137000
6	3.965912000	-0.043601000	-1.234602000	6	3.453273000	-0.890791000	-1.353981000
6	4.752610000	-0.932963000	-1.851119000	6	4.292281000	-1.982797000	-1.617642000
6	4.804609000	-2.238751000	-1.349066000	6	4.409363000	-3.027362000	-0.700002000
6	4.074193000	-2.599019000	-0.211042000	6	3.698754000	-3.000525000	0.504780000
6	1.864595000	-0.538003000	1.823063000	6	1.471193000	-0.456244000	1.831485000
1	3.949088000	1.044558000	-1.645767000	1	3.380808000	-0.099655000	-2.088520000
1	5.330436000	-0.671206000	-2.731819000	1	4.852816000	-2.010786000	-2.546282000
1	5.420570000	-2.983232000	-1.843844000	1	5.059373000	-3.869416000	-0.916684000
1	4.108605000	-3.608191000	0.186211000	1	3.785625000	-3.801752000	1.231141000
7	2.509917000	-1.727488000	1.536875000	7	2.107400000	-1.663743000	1.886982000
8	1.159214000	-0.344831000	2.823179000	8	0.840954000	0.047548000	2.752413000
6	2.256541000	0.392129000	0.740440000	6	1.734902000	0.160338000	0.413845000
1	2.368899000	-2.565489000	2.080438000	1	2.133767000	-2.220796000	2.730113000
6	0.658688000	2.092079000	1.247812000	6	1.023198000	2.375519000	0.921805000
6	2.555062000	2.779433000	0.003230000	6	3.230485000	2.218660000	-0.090544000
6	0.645726000	3.599427000	1.273250000	6	1.475261000	3.769838000	0.438407000
6	1.596207000	3.978035000	0.119752000	6	2.545907000	3.487996000	-0.623479000
1	2.731658000	2.494646000	-1.032959000	1	3.644975000	1.595868000	-0.882658000
1	3.522130000	2.950872000	0.484995000	1	4.068864000	2.492869000	0.565055000
1	-0.355581000	4.020180000	1.164761000	1	0.655587000	4.390003000	0.072803000
1	1.035137000	3.944560000	2.239969000	1	1.925896000	4.299571000	1.285150000
1	1.033052000	4.095435000	-0.808390000	1	2.078579000	3.300264000	-1.595477000

1	2.136485000	4.907861000	0.304306000	1	3.249310000	4.315458000	-0.751373000
7	1.867567000	1.688633000	0.739750000	7	2.205570000	1.513113000	0.701945000
1	0.306101000	1.527309000	2.099353000	1	0.797995000	2.419361000	1.990141000
TS2				TS2p			
6	-3.453052000	0.690582000	0.734508000	6	3.634309000	0.459276000	-0.449964000
6	-3.609118000	-0.115346000	-0.527710000	6	3.601205000	-0.206664000	0.901440000
6	-1.907580000	2.398686000	-0.494575000	6	2.063488000	2.325670000	0.386727000
6	-3.042562000	2.179733000	0.503773000	6	3.314404000	1.987919000	-0.416899000
6	-0.467953000	-2.119495000	-0.383540000	6	0.150833000	-2.037982000	-0.208058000
6	-0.836576000	1.644103000	-0.778699000	6	0.881451000	1.695141000	0.471790000
6	-0.497432000	0.357692000	-0.101829000	6	0.453841000	0.498695000	-0.300269000
6	-0.307510000	-0.827918000	-0.934994000	6	-0.225523000	-0.661936000	0.440045000
1	-4.408127000	0.716506000	1.281562000	1	4.644965000	0.363425000	-0.875239000
6	-3.366330000	-1.424585000	-0.697247000	6	3.202732000	-1.439062000	1.259588000
6	-2.914070000	-2.379972000	0.396787000	6	2.683826000	-2.555282000	0.358101000
6	-1.397192000	-2.368496000	0.793473000	6	1.586993000	-2.304944000	-0.695284000
1	-3.174405000	-3.395265000	0.076091000	1	2.335522000	-3.369878000	1.005313000
1	-3.941907000	0.443621000	-1.402099000	1	3.989310000	0.414804000	1.708478000
1	-2.734664000	0.212959000	1.400975000	1	2.970659000	-0.033250000	-1.156441000
8	-0.429781000	0.345350000	1.144202000	8	0.619551000	0.446861000	-1.516538000
1	-1.188044000	-3.340806000	1.248501000	1	1.531552000	-3.228495000	-1.286548000
1	-3.483571000	-2.196045000	1.315302000	1	3.550686000	-2.969312000	-0.177212000
6	-2.600856000	2.778343000	1.860251000	6	3.132315000	2.490405000	-1.868949000
1	-2.364997000	3.843812000	1.762451000	1	2.955394000	3.571215000	-1.889040000
1	-3.403259000	2.677365000	2.601122000	1	4.038004000	2.286731000	-2.452274000
1	-1.712045000	2.254671000	2.218789000	1	2.283366000	1.989661000	-2.337170000
6	-4.273866000	2.962656000	-0.007696000	6	4.502699000	2.747909000	0.215426000
1	-5.095288000	2.897582000	0.713394000	1	5.420258000	2.559771000	-0.351030000
1	-4.033139000	4.022163000	-0.148697000	1	4.318361000	3.827706000	0.209930000
1	-4.634133000	2.573941000	-0.965911000	1	4.678022000	2.448066000	1.253319000
6	-3.546106000	-2.066485000	-2.052459000	6	3.354183000	-1.874924000	2.702174000
1	-3.836912000	-1.342856000	-2.819706000	1	3.774216000	-1.087442000	3.334379000
1	-2.615892000	-2.550737000	-2.376451000	1	2.385890000	-2.173864000	3.123728000
1	-4.308499000	-2.856130000	-2.018108000	1	4.007688000	-2.754587000	2.774546000
1	-1.994714000	3.333079000	-1.050249000	1	2.165281000	3.210210000	1.015574000
1	-0.158678000	1.981151000	-1.560356000	1	0.151253000	2.068290000	1.185779000
6	-0.195541000	-0.691194000	-2.435228000	6	0.065608000	-0.583705000	1.951310000
1	0.353645000	0.200864000	-2.745348000	1	-0.515230000	0.213280000	2.426074000
1	0.331717000	-1.554132000	-2.851585000	1	-0.193535000	-1.523520000	2.440878000
1	-1.189522000	-0.643381000	-2.896802000	1	1.118715000	-0.377239000	2.129282000
1	-0.526764000	-2.906698000	-1.138602000	1	-0.074097000	-2.776038000	0.569591000
6	2.999410000	1.568184000	-0.936023000	6	-3.267567000	0.892783000	1.289779000
6	2.545932000	0.929701000	0.251862000	6	-2.405962000	0.785785000	0.185408000
6	2.351161000	1.711674000	1.397089000	6	-2.230730000	1.885510000	-0.648605000
6	2.618155000	3.083772000	1.344133000	6	-2.907105000	3.079742000	-0.362970000
6	3.066486000	3.686981000	0.164262000	6	-3.747925000	3.167432000	0.748942000
6	3.259122000	2.929981000	-0.998758000	6	-3.941346000	2.069159000	1.595940000
6	2.716349000	-0.643881000	-1.501487000	6	-2.540399000	-1.287720000	1.372913000
1	1.992987000	1.237871000	2.317999000	1	-1.573906000	1.823649000	-1.508509000
1	2.470797000	3.687475000	2.234335000	1	-2.774158000	3.939664000	-1.011322000
1	3.267019000	4.753825000	0.144317000	1	-4.264408000	4.098221000	0.962671000
1	3.599525000	3.389041000	-1.921547000	1	-4.597865000	2.130196000	2.457578000
7	3.093137000	0.616411000	-1.945315000	7	-3.320324000	-0.330860000	1.970776000
8	2.758942000	-1.666910000	-2.197547000	8	-2.457419000	-2.457143000	1.715148000
6	2.303206000	-0.455775000	-0.097211000	6	-1.803766000	-0.611301000	0.160847000
1	3.399498000	0.786533000	-2.891197000	1	-3.935566000	-0.532227000	2.746946000
6	1.469406000	-2.668783000	0.245631000	6	-0.897443000	-2.282372000	-1.335521000
6	1.978575000	-1.430942000	2.195575000	6	-2.693309000	-0.985661000	-2.233038000
6	1.473242000	-3.677260000	1.364342000	6	-0.560756000	-1.971049000	-2.833676000
6	1.430520000	-2.802507000	2.636040000	6	-1.557723000	-0.874843000	-3.264824000
1	1.325870000	-0.618557000	2.504159000	1	-3.240211000	-0.054882000	-2.076180000
1	2.998060000	-1.238296000	2.541784000	1	-3.425240000	-1.740386000	-2.557197000
1	0.642911000	-4.383970000	1.299245000	1	0.467167000	-1.640394000	-2.971378000
1	2.398467000	-4.265902000	1.312748000	1	-0.700484000	-2.879596000	-3.428481000
1	0.401762000	-2.693415000	2.983956000	1	-1.084227000	0.106221000	-3.185548000
1	2.016885000	-3.226781000	3.452854000	1	-1.912169000	-1.005066000	-4.292145000
7	2.001604000	-1.502686000	0.712351000	7	-2.050465000	-1.439658000	-1.004579000

1	1.760692000	-2.946959000	-0.757574000	1	-1.178918000	-3.343249000	-1.276420000
1	-1.226669000	-1.608828000	1.550530000	1	1.892177000	-1.533679000	-1.398433000
TS3				TS3p			
6	-2.516925000	0.253144000	1.754969000	6	-2.467730000	0.157596000	1.763757000
6	-3.613784000	0.734484000	0.834746000	6	-3.548876000	0.670810000	0.842800000
6	-0.615477000	1.130711000	0.293885000	6	-0.528444000	1.113457000	0.325628000
6	-1.181541000	1.083973000	1.732238000	6	-1.133541000	0.979965000	1.769072000
6	-2.412000000	-1.634338000	-1.153988000	6	-2.283787000	-1.665373000	-1.080648000
6	-0.215831000	0.014046000	-0.471134000	6	0.134159000	-0.103513000	-0.439602000
6	-0.244825000	-1.418904000	-0.068275000	6	-0.066832000	-1.549638000	0.003255000
6	-1.336937000	-2.267135000	-0.644296000	6	-1.324692000	-2.266586000	-0.349255000
1	-2.885727000	0.295022000	2.791960000	1	-2.846181000	0.193193000	2.796780000
6	-4.489363000	0.012035000	0.113073000	6	-4.429936000	-0.023371000	0.103207000
6	-4.534143000	-1.507354000	0.057890000	6	-4.487641000	-1.538788000	0.024714000
6	-3.827467000	-2.111472000	-1.201575000	6	-3.711578000	-2.106218000	-1.201527000
1	-5.581562000	-1.834690000	0.053879000	1	-5.533936000	-1.860423000	-0.046868000
1	-3.722774000	1.817219000	0.779738000	1	-3.640397000	1.755320000	0.802297000
1	-2.280998000	-0.795229000	1.560257000	1	-2.250850000	-0.892151000	1.564533000
8	0.486613000	-1.918239000	0.790326000	8	0.789556000	-2.137380000	0.662804000
1	-2.321430000	-0.568454000	-1.332842000	1	-2.085077000	-0.682107000	-1.492582000
1	-3.914769000	-3.200758000	-1.168926000	1	-3.813154000	-3.194900000	-1.213849000
1	-4.331368000	-1.761478000	-2.109969000	1	-4.151176000	-1.724976000	-2.128835000
1	-4.067968000	-1.944360000	0.945661000	1	-4.076261000	-1.994819000	0.929974000
6	-1.279790000	-3.730817000	-0.292736000	6	-1.471957000	-3.619642000	0.300041000
1	-1.439313000	-3.883545000	0.780526000	1	-1.557843000	-3.515587000	1.388214000
1	-2.027160000	-4.309402000	-0.839233000	1	-2.347034000	-4.160529000	-0.061384000
1	-0.288812000	-4.135770000	-0.519326000	1	-0.580552000	-4.225727000	0.117278000
6	-0.218991000	0.445343000	2.755517000	6	-0.179670000	0.320419000	2.782053000
1	0.703054000	1.026429000	2.848866000	1	0.686997000	0.954876000	2.980390000
1	-0.690884000	0.425849000	3.744521000	1	-0.694918000	0.180064000	3.738770000
1	0.060324000	-0.568861000	2.476695000	1	0.184208000	-0.651005000	2.446619000
6	-1.480555000	2.520696000	2.214745000	6	-1.464428000	2.393828000	2.308822000
1	-2.021127000	2.493735000	3.166888000	1	-1.957494000	2.307567000	3.282964000
1	-0.557219000	3.082334000	2.381442000	1	-0.564539000	2.997316000	2.451829000
1	-2.088201000	3.085345000	1.500906000	1	-2.132635000	2.952116000	1.648403000
6	-5.522117000	0.697568000	-0.752257000	6	-5.446332000	0.688430000	-0.758814000
1	-5.432421000	1.786879000	-0.715574000	1	-5.333157000	1.775313000	-0.717216000
1	-5.428129000	0.387736000	-1.801234000	1	-5.358777000	0.380083000	-1.808746000
1	-6.539291000	0.425759000	-0.440879000	1	-6.468843000	0.436664000	-0.448200000
6	2.135465000	0.536419000	-0.835030000	6	1.626996000	0.303543000	-0.714488000
7	1.774333000	1.852927000	-0.825465000	7	1.568267000	1.767263000	-0.819421000
6	2.865353000	-0.164139000	0.210673000	6	2.736406000	-0.117288000	0.248103000
6	3.269017000	0.160324000	1.507468000	6	3.069973000	0.307680000	1.525437000
6	3.250544000	-1.415863000	-0.331369000	6	3.602694000	-1.001819000	-0.410760000
6	4.007588000	-0.769551000	2.247314000	6	4.213434000	-0.209944000	2.152691000
1	3.026744000	1.121396000	1.946283000	1	2.459266000	1.032873000	2.044798000
6	3.977522000	-2.349094000	0.394430000	6	4.740914000	-1.529789000	0.182445000
6	4.347477000	-2.013469000	1.702980000	6	5.031627000	-1.128470000	1.492944000
1	4.318282000	-0.520934000	3.257543000	1	4.462776000	0.111672000	3.159099000
1	4.255193000	-3.302743000	-0.043560000	1	5.386138000	-2.217193000	-0.354908000
1	4.912762000	-2.726123000	2.295983000	1	5.912154000	-1.525416000	1.988902000
1	-1.148764000	1.865534000	-0.309229000	1	-1.379334000	1.412544000	-0.295792000
1	-0.312993000	0.144905000	-1.546399000	1	-0.286068000	-0.042058000	-1.446658000
6	1.102062000	2.400499000	0.228907000	6	0.564582000	2.229881000	0.167157000
6	1.621864000	2.672541000	-2.060128000	6	1.341505000	2.448945000	-2.120844000
6	0.747558000	3.825761000	-0.116857000	6	0.052600000	3.553702000	-0.422970000
6	0.628419000	3.768356000	-1.652046000	6	0.062294000	3.276633000	-1.932199000
1	1.285474000	2.045032000	-2.883253000	1	1.257799000	1.741500000	-2.945257000
1	2.608075000	3.077363000	-2.311458000	1	2.196169000	3.106831000	-2.329419000
1	-0.169693000	4.158400000	0.369958000	1	-0.929755000	3.834162000	-0.040090000
1	1.552445000	4.502969000	0.199284000	1	0.751403000	4.362287000	-0.179988000
1	-0.386999000	3.474375000	-1.934721000	1	-0.815974000	2.682575000	-2.211757000
1	0.848345000	4.722373000	-2.134615000	1	0.053500000	4.186998000	-2.537813000
6	2.187717000	-0.306994000	-2.051210000	6	2.039033000	-0.466221000	-2.011990000
7	2.809073000	-1.481695000	-1.649299000	7	3.149450000	-1.202605000	-1.723422000
8	1.730097000	-0.113260000	-3.183705000	8	1.431770000	-0.481922000	-3.076222000
1	2.934310000	-2.263721000	-2.274117000	1	3.578651000	-1.818240000	-2.400036000

1	1.410044000	2.130206000	1.227724000	1	1.055615000	2.393606000	1.131627000
	TS4				TS4p		
6	2.678439000	-0.979033000	1.545422000	6	2.704768000	-0.762432000	1.567055000
6	3.466177000	-1.062915000	0.265622000	6	3.437897000	-1.216020000	0.334860000
6	0.054197000	-1.315570000	0.923251000	6	0.064902000	-1.066171000	0.949446000
6	1.350410000	-1.784828000	1.663770000	6	1.300667000	-1.385666000	1.864187000
6	1.541252000	1.561843000	0.100191000	6	1.776180000	1.506596000	-0.625527000
6	-0.697915000	-0.122889000	1.194814000	6	-0.636947000	0.353496000	0.976767000
6	-0.356395000	1.248072000	1.621222000	6	0.138382000	1.673307000	1.211426000
6	0.812386000	2.027509000	1.128039000	6	1.363426000	2.112948000	0.502664000
1	3.324258000	-1.393936000	2.335279000	1	3.319088000	-1.057570000	2.432347000
6	4.099904000	-0.065159000	-0.372732000	6	4.114948000	-0.478197000	-0.559790000
6	4.042528000	1.391411000	0.054461000	6	4.233667000	1.033872000	-0.522866000
6	2.790602000	2.143021000	-0.484439000	6	3.093877000	1.749625000	-1.304762000
1	4.936183000	1.908484000	-0.313313000	1	5.193343000	1.330082000	-0.963539000
1	3.604683000	-2.067913000	-0.129885000	1	3.439382000	-2.293178000	0.175229000
1	2.492366000	0.055731000	1.828589000	1	2.637843000	0.322794000	1.606916000
8	-1.133658000	1.798734000	2.423690000	8	-0.292949000	2.372365000	2.132689000
1	1.258450000	0.598739000	-0.302230000	1	1.136624000	0.735051000	-1.039461000
1	2.890302000	3.206907000	-0.254438000	1	3.326769000	2.818581000	-1.363200000
1	2.763486000	2.053807000	-1.578197000	1	3.062866000	1.372188000	-2.332264000
1	4.053614000	1.483359000	1.145364000	1	4.233952000	1.404140000	0.506614000
6	1.039276000	3.337533000	1.835110000	6	2.098201000	3.241593000	1.184950000
1	1.165625000	3.175673000	2.910777000	1	2.467724000	2.926469000	2.168303000
1	1.914919000	3.868758000	1.459985000	1	2.948464000	3.594374000	0.600210000
1	0.161463000	3.981923000	1.722861000	1	1.420891000	4.081283000	1.364312000
6	0.971637000	-1.740864000	3.171793000	6	0.922279000	-0.915511000	3.290618000
1	0.032897000	-2.272040000	3.358120000	1	-0.049855000	-1.318622000	3.594894000
1	1.752898000	-2.212542000	3.778891000	1	1.667044000	-1.257360000	4.016701000
1	0.846178000	-0.708183000	3.511972000	1	0.867754000	0.175246000	3.356285000
6	1.601291000	-3.265743000	1.304716000	6	1.432120000	-2.926332000	1.895504000
1	2.466408000	-3.649686000	1.855853000	1	2.266949000	-3.227574000	2.537418000
1	0.735401000	-3.879924000	1.574518000	1	0.521090000	-3.386305000	2.293515000
1	1.789733000	-3.416515000	0.241143000	1	1.605832000	-3.345789000	0.901366000
6	4.923422000	-0.328970000	-1.611233000	6	4.779789000	-1.129886000	-1.749336000
1	4.851858000	-1.369345000	-1.941008000	1	4.617764000	-2.211216000	-1.771577000
1	4.602671000	0.313082000	-2.441985000	1	4.392307000	-0.712304000	-2.688418000
1	5.981191000	-0.096110000	-1.432013000	1	5.861523000	-0.942675000	-1.750802000
6	-1.650790000	0.166432000	-1.015033000	6	-1.537131000	0.302881000	-0.324258000
7	-0.609790000	-0.453185000	-1.625463000	7	-0.679534000	-0.430799000	-1.219023000
6	-2.915375000	-0.433428000	-0.583724000	6	-2.928100000	-0.268596000	-0.030694000
6	-3.370011000	-1.742015000	-0.408392000	6	-3.349584000	-1.506165000	0.442637000
6	-3.793823000	0.639702000	-0.292255000	6	-3.887726000	0.717043000	-0.310927000
6	-4.674453000	-1.958551000	0.052072000	6	-4.721046000	-1.741663000	0.626705000
1	-2.734273000	-2.592353000	-0.625661000	1	-2.638013000	-2.290781000	0.671968000
6	-5.084851000	0.437735000	0.176196000	6	-5.248992000	0.510957000	-0.128960000
6	-5.518036000	-0.883304000	0.348343000	6	-5.655343000	-0.743041000	0.346039000
1	-5.029704000	-2.975478000	0.185389000	1	-5.054429000	-2.707700000	0.992029000
1	-5.736543000	1.277928000	0.393481000	1	-5.969702000	1.291520000	-0.349868000
1	-6.522766000	-1.069867000	0.714681000	1	-6.713224000	-0.935706000	0.496227000
6	-0.071580000	-1.635742000	-1.149350000	6	-0.075872000	-1.566225000	-0.531625000
6	0.204513000	0.161357000	-2.710468000	6	-1.014803000	-0.857308000	-2.564540000
6	1.079300000	-2.009607000	-2.067875000	6	0.974525000	-1.979447000	-1.571719000
6	1.480436000	-0.682491000	-2.733947000	6	0.182012000	-1.800745000	-2.905565000
1	0.366212000	1.218613000	-2.512927000	1	-1.094554000	0.004499000	-3.234256000
1	-0.371661000	0.066200000	-3.637432000	1	-1.969625000	-1.408877000	-2.601375000
1	1.911584000	-2.471145000	-1.538940000	1	1.834942000	-1.315969000	-1.541780000
1	0.721486000	-2.736429000	-2.808482000	1	1.331184000	-3.004017000	-1.438203000
1	2.259217000	-0.203540000	-2.143172000	1	0.819387000	-1.374920000	-3.684493000
1	1.860263000	-0.817043000	-3.748433000	1	-0.189934000	-2.759859000	-3.276147000
6	-1.878844000	1.639375000	-1.097766000	6	-1.891410000	1.704585000	-0.911561000
7	-3.144150000	1.839625000	-0.572886000	7	-3.246390000	1.870440000	-0.785046000
8	-1.133661000	2.537727000	-1.489281000	8	-1.122467000	2.509535000	-1.410396000
1	-3.545864000	2.760306000	-0.477490000	1	-3.720371000	2.692105000	-1.133201000
1	-0.775343000	-2.431753000	-0.944394000	1	-0.785784000	-2.415312000	-0.494266000
1	-1.716353000	-0.312875000	1.513911000	1	-1.310922000	0.368597000	1.833487000
1	-0.636906000	-2.146890000	1.065502000	1	-0.695637000	-1.664890000	1.460453000

TSolBr				TSolBr_P			
6	3.824301000	0.492382000	-0.950868000	6	4.107570000	0.471854000	-0.865301000
6	4.320825000	-0.719188000	-0.201666000	6	4.318671000	-0.742574000	-0.000894000
6	2.842690000	1.780829000	1.051927000	6	2.743423000	1.715897000	0.908092000
6	3.797366000	1.830762000	-0.142906000	6	3.901962000	1.806666000	-0.074563000
6	1.027513000	-1.240797000	0.354248000	6	0.586271000	-1.620140000	0.516847000
6	1.536467000	1.490089000	1.087111000	6	1.492061000	1.240225000	0.765807000
6	0.646262000	1.149350000	-0.080245000	6	0.848781000	0.709546000	-0.458720000
6	0.293985000	-0.268935000	-0.318769000	6	-0.113152000	-0.481984000	-0.279107000
1	4.489739000	0.669630000	-1.810053000	1	5.001210000	0.622897000	-1.488451000
6	3.860934000	-1.980875000	-0.245655000	6	3.666945000	-1.917854000	-0.006225000
6	2.667274000	-2.439909000	-1.063604000	6	2.547047000	-2.291123000	-0.960093000
6	1.369573000	-2.583581000	-0.214584000	6	1.237107000	-2.742855000	-0.273159000
1	2.891630000	-3.416369000	-1.510930000	1	2.893264000	-3.128417000	-1.580922000
1	5.196897000	-0.545191000	0.421256000	1	5.133419000	-0.648202000	0.716532000
1	2.832464000	0.312881000	-1.373517000	1	3.277320000	0.333823000	-1.557312000
8	0.217852000	2.045888000	-0.811320000	8	1.063139000	1.148245000	-1.581770000
1	1.705459000	-0.891592000	1.123720000	1	1.328037000	-1.178759000	1.194303000
1	0.565758000	-2.973485000	-0.844503000	1	0.540682000	-3.129551000	-1.021626000
1	1.531794000	-3.302433000	0.593821000	1	1.437662000	-3.566803000	-0.418559000
1	2.468848000	-1.754164000	-1.892429000	1	2.330777000	-1.471373000	-1.650175000
6	-0.468525000	-0.564917000	-1.592915000	6	-0.710490000	-0.897159000	-1.633949000
1	-1.157329000	0.251374000	-1.815250000	1	-1.299324000	-0.074514000	-2.045068000
1	0.216433000	-0.657455000	-2.444447000	1	0.076373000	-1.134464000	-2.351559000
1	-1.043236000	-1.489033000	-1.513115000	1	-1.366064000	-1.761120000	-1.510695000
6	3.371222000	2.964235000	-1.107100000	6	3.646757000	2.954723000	-1.080390000
1	3.329511000	3.922234000	-0.578504000	1	3.519703000	3.907668000	-0.555992000
1	4.098166000	3.058587000	-1.922020000	1	4.506177000	3.052899000	-1.753394000
1	2.385415000	2.774392000	-1.534244000	1	2.750860000	2.757937000	-1.669172000
6	5.210408000	2.164289000	0.382061000	6	5.179435000	2.144568000	0.726534000
1	5.937142000	2.164525000	-0.436934000	1	6.046215000	2.192483000	0.060007000
1	5.219784000	3.158286000	0.842037000	1	5.077370000	3.118220000	1.217747000
1	5.549720000	1.450535000	1.138368000	1	5.387504000	1.402807000	1.503086000
6	4.518489000	-3.069136000	0.571592000	6	4.069495000	-3.009502000	0.961289000
1	5.347437000	-2.686582000	1.173487000	1	4.974900000	-2.745614000	1.514121000
1	3.800919000	-3.545310000	1.251888000	1	3.280304000	-3.209904000	1.696452000
1	4.904166000	-3.866472000	-0.077163000	1	4.251300000	-3.955226000	0.434696000
6	-1.527697000	-0.102780000	1.116613000	6	-1.275392000	-0.232590000	0.684890000
8	-0.335078000	-1.900896000	1.919723000	8	-0.473660000	-2.159711000	1.363117000
7	-1.249103000	-1.062875000	1.802636000	7	-1.459795000	-1.187343000	1.523498000
6	-2.561648000	0.785500000	0.682169000	6	-2.274502000	0.852084000	0.528801000
6	-3.679484000	0.311984000	-0.040737000	6	-3.588313000	0.598772000	0.095091000
6	-2.437930000	2.171698000	0.894806000	6	-1.915935000	2.188881000	0.766502000
6	-4.654092000	1.187670000	-0.505466000	6	-4.512633000	1.628745000	-0.073264000
6	-3.410647000	3.049870000	0.428987000	6	-2.830914000	3.226443000	0.602471000
1	-1.569126000	2.542584000	1.425476000	1	-0.908325000	2.415804000	1.094844000
6	-4.516405000	2.557595000	-0.267335000	6	-4.132139000	2.945265000	0.185695000
1	-5.508615000	0.804959000	-1.050730000	1	-5.516817000	1.400751000	-0.410897000
1	-3.305263000	4.114624000	0.605691000	1	-2.526910000	4.248704000	0.801088000
1	3.297944000	2.034512000	2.009080000	1	2.986047000	2.053889000	1.915526000
1	1.029186000	1.493283000	2.051516000	1	0.888153000	1.168224000	1.667941000
1	-5.277371000	3.238000000	-0.635382000	1	-4.853296000	3.745348000	0.053496000
35	-3.869750000	-1.553684000	-0.391679000	35	-4.161890000	-1.180049000	-0.337901000
TSolCl				TSolCl_P			
6	3.461965000	0.726906000	-0.885578000	6	3.725925000	0.710029000	-0.772777000
6	4.056900000	-0.456621000	-0.163792000	6	4.009987000	-0.518353000	0.049938000
6	2.285883000	1.825638000	1.124981000	6	2.195894000	1.754008000	0.995118000
6	3.270263000	2.021617000	-0.029904000	6	3.375902000	1.986154000	0.062556000
6	0.816748000	-1.345114000	0.258744000	6	0.348139000	-1.732830000	0.388985000
6	1.018430000	1.395471000	1.099751000	6	0.997329000	1.177059000	0.787141000
6	0.211473000	1.007758000	-0.112196000	6	0.445616000	0.645198000	-0.481103000
6	0.005461000	-0.428585000	-0.403079000	6	-0.422519000	-0.625497000	-0.384637000
1	4.133405000	1.006104000	-1.712372000	1	4.625200000	0.964322000	-1.352723000
6	3.731919000	-1.756138000	-0.268562000	6	3.460973000	-1.742552000	-0.026375000
6	2.618944000	-2.304105000	-1.143527000	6	2.411859000	-2.167270000	-1.037377000
6	1.319405000	-2.620353000	-0.345518000	6	1.122710000	-2.758894000	-0.420882000
1	2.960071000	-3.231718000	-1.620093000	1	2.850909000	-2.944204000	-1.677657000

1	4.890839000	-0.218805000	0.494820000	1	4.787883000	-0.386526000	0.801584000
1	2.508619000	0.464319000	-1.351190000	1	2.936566000	0.532295000	-1.502449000
8	-0.271398000	1.880482000	-0.838385000	8	0.666776000	1.142364000	-1.578236000
1	1.431643000	-0.956287000	1.061584000	1	1.024574000	-1.259095000	1.111458000
1	0.583129000	-3.070537000	-1.016368000	1	0.490058000	-3.171255000	-1.211063000
1	1.534437000	-3.348429000	0.442013000	1	1.370048000	-3.592132000	-0.244043000
1	2.372420000	-1.609361000	-1.951696000	1	2.150097000	-1.339455000	-1.701531000
6	-0.691193000	-0.752322000	-1.707439000	6	-0.934204000	-1.030984000	-1.776664000
1	-1.476645000	-0.021249000	-1.905353000	1	-1.579502000	-0.245728000	-2.176140000
1	0.012353000	-0.711340000	-2.547880000	1	-0.106883000	-1.168112000	-2.474764000
1	-1.138263000	-1.748109000	-1.686592000	1	-1.510528000	-1.956664000	-1.713145000
6	2.763030000	3.145093000	-0.966228000	6	3.056019000	3.150773000	-0.905106000
1	2.604400000	4.070955000	-0.403579000	1	2.827475000	4.065422000	-0.347956000
1	3.504446000	3.346933000	-1.747900000	1	3.926500000	3.352016000	-1.539886000
1	1.817568000	2.873823000	-1.438028000	1	2.202186000	2.903266000	-1.535801000
6	4.622864000	2.474745000	0.560714000	6	4.589583000	2.397986000	0.925871000
1	5.373469000	2.581150000	-0.229305000	1	5.471706000	2.550176000	0.296142000
1	4.514599000	3.445370000	1.056546000	1	4.384584000	3.336491000	1.452035000
1	5.007236000	1.769178000	1.302996000	1	4.834787000	1.643565000	1.679043000
6	4.473883000	-2.801681000	0.532147000	6	3.919243000	-2.836312000	0.913511000
1	5.241384000	-2.359404000	1.173311000	1	4.780910000	-2.522717000	1.508661000
1	3.789856000	-3.373255000	1.172315000	1	3.124878000	-3.128739000	1.611341000
1	4.958087000	-3.530978000	-0.130436000	1	4.195386000	-3.742440000	0.359088000
6	-1.870428000	-0.510608000	0.976258000	6	-1.638879000	-0.523525000	0.541827000
8	-0.515102000	-2.206619000	1.745157000	8	-0.687159000	-2.399947000	1.171510000
7	-1.507338000	-1.461960000	1.634241000	7	-1.761342000	-1.527791000	1.334005000
6	-2.974574000	0.307290000	0.576316000	6	-2.721369000	0.479108000	0.399256000
6	-4.077390000	-0.228918000	-0.127149000	6	-4.041771000	0.126735000	0.056825000
6	-2.940328000	1.695877000	0.810040000	6	-2.441341000	1.847045000	0.561178000
6	-5.119835000	0.588201000	-0.551873000	6	-5.038128000	1.091628000	-0.092086000
6	-3.979665000	2.514446000	0.382400000	6	-3.428589000	2.817926000	0.415337000
1	-2.086567000	2.115930000	1.327644000	1	-1.435564000	2.153668000	0.822092000
6	-5.067013000	1.960278000	-0.296068000	6	-4.731344000	2.438889000	0.092058000
1	-5.961000000	0.154515000	-1.079869000	1	-6.042847000	0.784633000	-0.358847000
1	-3.940719000	3.580799000	0.575623000	1	-3.179023000	3.864239000	0.555761000
1	2.678376000	2.087907000	2.107265000	1	2.371561000	2.071438000	2.022939000
1	0.481586000	1.303334000	2.043636000	1	0.368842000	1.019089000	1.661379000
1	-5.880888000	2.593546000	-0.633551000	1	-5.510074000	3.185410000	-0.025272000
17	-4.158290000	-1.948519000	-0.465884000	17	-4.496088000	-1.548923000	-0.255772000
TSolF				TSolF_P			
6	-3.200056000	0.891588000	0.881227000	6	3.451008000	1.103412000	-0.372731000
6	-3.892560000	-0.246698000	0.173817000	6	3.722519000	-0.116780000	0.464905000
6	-1.952213000	1.865978000	-1.149559000	6	1.439386000	1.838614000	1.051994000
6	-2.906019000	2.156822000	0.011113000	6	2.736471000	2.270738000	0.383882000
6	-0.739189000	-1.395239000	-0.245749000	6	0.329594000	-1.932856000	0.015996000
6	-0.722208000	1.338112000	-1.129543000	6	0.412715000	1.085713000	0.613361000
6	0.066339000	0.905454000	0.080016000	6	0.236169000	0.478318000	-0.722777000
6	0.144920000	-0.537553000	0.400383000	6	-0.487605000	-0.879196000	-0.779916000
1	-3.842378000	1.233377000	1.707712000	1	4.409920000	1.513423000	-0.722321000
6	-3.673998000	-1.567005000	0.293455000	6	3.394453000	-1.398307000	0.229253000
6	-2.607102000	-2.191813000	1.174373000	6	2.667751000	-1.898539000	-1.005940000
6	-1.337145000	-2.617928000	0.380094000	6	1.399712000	-2.731119000	-0.708997000
1	-3.019900000	-3.084302000	1.661249000	1	3.354155000	-2.545812000	-1.568584000
1	-4.705079000	0.051237000	-0.487174000	1	4.280993000	0.077981000	1.380409000
1	-2.268997000	0.556445000	1.345259000	1	2.883565000	0.856440000	-1.268640000
8	0.638617000	1.748457000	0.775547000	8	0.649362000	0.984904000	-1.761258000
1	-1.323342000	-0.971870000	-1.053954000	1	0.769967000	-1.445100000	0.897182000
1	-0.634835000	-3.111194000	1.057243000	1	1.001096000	-3.141705000	-1.639966000
1	-1.608538000	-3.340553000	-0.394993000	1	1.652300000	-3.588517000	-0.077256000
1	-2.306619000	-1.509577000	1.974874000	1	2.409904000	-1.073049000	-1.673528000
6	0.819252000	-0.902662000	1.706290000	6	-0.776611000	-1.302002000	-2.230252000
1	1.610973000	-0.185964000	1.929558000	1	-1.504577000	-0.633841000	-2.693645000
1	0.105949000	-0.873592000	2.538806000	1	0.134354000	-1.268817000	-2.829653000
1	1.255350000	-1.903118000	1.667703000	1	-1.182088000	-2.316347000	-2.246458000
6	-2.296648000	3.241247000	0.932269000	6	2.433849000	3.407503000	-0.622502000
1	-2.065693000	4.145549000	0.359692000	1	1.960733000	4.257118000	-0.119054000
1	-3.010541000	3.511788000	1.718808000	1	3.368837000	3.760495000	-1.072481000

1	-1.372916000	2.895224000	1.398391000	1	1.769530000	3.052607000	-1.411133000
6	-4.220115000	2.718234000	-0.573274000	6	3.670740000	2.830061000	1.480495000
1	-4.951113000	2.898177000	0.221814000	1	4.623029000	3.147822000	1.044631000
1	-4.033397000	3.670074000	-1.082040000	1	3.215822000	3.699549000	1.967160000
1	-4.671014000	2.039913000	-1.303445000	1	3.882068000	2.089029000	2.257099000
6	-4.498422000	-2.558750000	-0.494769000	6	3.789282000	-2.474471000	1.217005000
1	-5.228302000	-2.063834000	-1.141396000	1	4.442674000	-2.082795000	2.001009000
1	-3.862845000	-3.190972000	-1.127861000	1	2.912222000	-2.915033000	1.707349000
1	-5.039177000	-3.238943000	0.176268000	1	4.311186000	-3.298837000	0.714174000
6	2.004690000	-0.792789000	-0.974369000	6	-1.787126000	-0.983867000	0.035959000
8	0.517970000	-2.387827000	-1.716948000	8	-0.698607000	-2.835547000	0.508459000
7	1.570790000	-1.726657000	-1.613230000	7	-1.875827000	-2.103872000	0.676037000
6	3.148057000	-0.039019000	-0.568441000	6	-2.879751000	-0.000835000	0.008929000
6	4.083891000	-0.614711000	0.308393000	6	-4.016451000	-0.096479000	0.833837000
6	3.325099000	1.307654000	-0.939568000	6	-2.823750000	1.119341000	-0.845533000
6	5.179579000	0.087723000	0.782677000	6	-5.038314000	0.842180000	0.818440000
6	4.420829000	2.025822000	-0.471910000	6	-3.840838000	2.069516000	-0.878417000
1	2.595992000	1.771367000	-1.593664000	1	-1.971869000	1.251971000	-1.500327000
6	5.344322000	1.416729000	0.384283000	6	-4.952777000	1.933716000	-0.045480000
1	5.878077000	-0.403347000	1.450234000	1	-5.881629000	0.701329000	1.485133000
1	4.554238000	3.060103000	-0.769033000	1	-3.760962000	2.915124000	-1.553024000
1	-2.332501000	2.145444000	-2.131935000	1	1.337972000	2.181664000	2.081731000
1	-0.203109000	1.195149000	-2.076911000	1	-0.370643000	0.847966000	1.329147000
1	6.197123000	1.978470000	0.750990000	1	-5.749121000	2.670416000	-0.063270000
9	3.898504000	-1.891185000	0.695597000	9	-4.139693000	-1.129867000	1.690598000
TS1o2Br				TS1o2Br_P			
6	-3.473061000	0.852183000	1.071650000	6	-3.658633000	0.846250000	0.921264000
6	-4.240249000	0.029427000	0.067079000	6	-4.180730000	-0.270304000	0.056516000
6	-1.924837000	2.016152000	-0.612515000	6	-2.042505000	1.722755000	-0.855654000
6	-2.909815000	2.210244000	0.541713000	6	-3.143002000	2.093053000	0.129805000
6	-1.242528000	-1.513769000	-0.397393000	6	-0.746853000	-1.942884000	-0.486315000
6	-0.788414000	1.310500000	-0.656654000	6	-0.928259000	0.984508000	-0.709409000
6	-0.156405000	0.527043000	0.465906000	6	-0.403250000	0.342329000	0.522194000
6	-0.342408000	-0.945427000	0.501620000	6	0.227601000	-1.065418000	0.364095000
1	-4.141126000	1.102125000	1.910542000	1	-4.474465000	1.206997000	1.564984000
6	-4.220889000	-1.301265000	-0.115148000	6	-3.836270000	-1.569094000	0.039218000
6	-3.356613000	-2.267557000	0.673793000	6	-2.823443000	-2.213457000	0.966879000
6	-2.084989000	-2.718613000	-0.101026000	6	-1.648944000	-2.920761000	0.251210000
1	-3.944432000	-3.163021000	0.912262000	1	-3.344385000	-2.972830000	1.565356000
1	-4.924043000	0.595556000	-0.563741000	1	-4.962999000	0.028789000	-0.640491000
1	-2.651892000	0.274487000	1.504090000	1	-2.872753000	0.501837000	1.593559000
8	0.490991000	1.107107000	1.339881000	8	-0.506045000	0.827487000	1.640252000
1	-1.644036000	-0.858287000	-1.161009000	1	-1.369434000	-1.290547000	-1.107781000
1	-1.540160000	-3.454351000	0.496527000	1	-1.069100000	-3.501939000	0.972880000
1	-2.373053000	-3.208247000	-1.035712000	1	-2.032132000	-3.635601000	-0.483528000
1	-3.050205000	-1.832306000	1.629076000	1	-2.430238000	-1.484135000	1.679705000
6	0.041091000	-1.626010000	1.799275000	6	0.588043000	-1.624995000	1.751744000
1	0.934520000	-1.162982000	2.219335000	1	1.334185000	-0.983912000	2.224245000
1	-0.759077000	-1.523670000	2.542580000	1	-0.285082000	-1.653971000	2.404707000
1	0.232029000	-2.692063000	1.657051000	1	1.001248000	-2.632536000	1.663082000
6	-2.218394000	2.937353000	1.719501000	6	-2.620893000	3.148402000	1.133331000
1	-1.799206000	3.892866000	1.387653000	1	-2.266194000	4.040088000	0.605503000
1	-2.945726000	3.143770000	2.513160000	1	-3.431597000	3.454949000	1.804399000
1	-1.404658000	2.341988000	2.135731000	1	-1.799234000	2.744564000	1.724598000
6	-4.063732000	3.108276000	0.046250000	6	-4.304004000	2.726537000	-0.669112000
1	-4.817095000	3.237947000	0.830200000	1	-5.135530000	2.976706000	-0.002625000
1	-3.684102000	4.099382000	-0.224607000	1	-3.973176000	3.649847000	-1.156819000
1	-4.559350000	2.695306000	-0.837214000	1	-4.681344000	2.058605000	-1.448871000
6	-5.081119000	-1.947068000	-1.176809000	6	-4.511177000	-2.518541000	-0.926515000
1	-5.661749000	-1.210176000	-1.738650000	1	-5.330682000	-2.033678000	-1.463625000
1	-4.471974000	-2.512053000	-1.893876000	1	-3.807238000	-2.902203000	-1.675287000
1	-5.779417000	-2.667171000	-0.730489000	1	-4.914430000	-3.394060000	-0.401443000
6	1.643682000	-1.370054000	-0.627269000	6	1.482233000	-1.192157000	-0.517092000
8	0.030170000	-2.433140000	-1.876147000	8	0.116916000	-2.675275000	-1.407159000
7	1.160595000	-2.060848000	-1.498850000	7	1.379397000	-2.106269000	-1.418046000
6	2.836109000	-0.977463000	0.062877000	6	2.854634000	-0.739479000	-0.160126000
6	3.411123000	-1.856013000	1.003926000	6	3.784351000	-1.746787000	0.165857000

6	3.415075000	0.295915000	-0.105819000	6	3.303389000	0.587525000	-0.086013000
6	4.528408000	-1.475604000	1.738837000	6	5.086431000	-1.445963000	0.555089000
6	4.530910000	0.681471000	0.629333000	6	4.602859000	0.905295000	0.307711000
6	5.084016000	-0.207057000	1.553607000	6	5.495577000	-0.114635000	0.633202000
1	4.962626000	-2.164049000	2.455556000	1	5.774148000	-2.247949000	0.802006000
1	4.963249000	1.663662000	0.479944000	1	4.912203000	1.943104000	0.348124000
1	-2.191513000	2.539367000	-1.530680000	1	-2.209459000	2.090800000	-1.867992000
1	-0.226700000	1.287409000	-1.587657000	1	-0.339534000	0.785932000	-1.601190000
1	5.952347000	0.097918000	2.128416000	1	6.505298000	0.136588000	0.941433000
35	2.684157000	1.507673000	-1.381606000	35	2.163988000	2.041909000	-0.583654000
1	2.964027000	-2.833722000	1.143400000	1	3.456657000	-2.779153000	0.117263000
TS1o2Cl				TS1o2Cl_P			
6	3.237339000	0.953642000	-0.958653000	6	3.400188000	1.235606000	-0.543582000
6	3.996095000	-0.012166000	-0.083186000	6	3.730848000	0.162279000	0.458165000
6	1.764950000	1.958318000	0.889944000	6	1.277248000	1.973130000	0.698375000
6	2.737058000	2.255848000	-0.253286000	6	2.566349000	2.428143000	0.029941000
6	0.959115000	-1.497934000	0.270846000	6	0.512975000	-1.984362000	0.108164000
6	0.606388000	1.288183000	0.872704000	6	0.333695000	1.091858000	0.316362000
6	-0.068465000	0.664130000	-0.322014000	6	0.264224000	0.323654000	-0.945236000
6	0.055854000	-0.799877000	-0.526839000	6	-0.314101000	-1.100715000	-0.866655000
1	3.896022000	1.281659000	-1.777823000	1	4.337739000	1.673626000	-0.916352000
6	3.933146000	-1.353926000	-0.063852000	6	3.517402000	-1.162399000	0.387139000
6	3.015854000	-2.188754000	-0.938602000	6	2.894985000	-1.882107000	-0.795285000
6	1.747237000	-2.688057000	-0.187860000	6	1.686352000	-2.777255000	-0.439148000
1	3.565151000	-3.067559000	-1.299385000	1	3.659424000	-2.533959000	-1.239509000
1	4.715355000	0.448899000	0.592107000	1	4.230172000	0.522168000	1.357562000
1	2.386360000	0.461813000	-1.437118000	1	2.889911000	0.828032000	-1.415200000
8	-0.703300000	1.365655000	-1.112621000	8	0.655472000	0.752822000	-2.025028000
1	1.408639000	-0.947865000	1.088927000	1	0.848411000	-1.360584000	0.948833000
1	1.162317000	-3.328490000	-0.853314000	1	1.377518000	-3.350294000	-1.316979000
1	2.039718000	-3.294647000	0.674079000	1	1.971216000	-3.510369000	0.321944000
1	2.702009000	-1.631241000	-1.825625000	1	2.604962000	-1.175857000	-1.577166000
6	-0.406917000	-1.321554000	-1.870602000	6	-0.444543000	-1.709230000	-2.272588000
1	-1.293022000	-0.778811000	-2.201654000	1	-1.074666000	-1.088068000	-2.909079000
1	0.368101000	-1.174282000	-2.632844000	1	0.532798000	-1.762643000	-2.754981000
1	-0.640700000	-2.387877000	-1.832014000	1	-0.870019000	-2.713513000	-2.214002000
6	2.054527000	3.148030000	-1.317504000	6	2.229425000	3.404702000	-1.122742000
1	1.677031000	4.068969000	-0.861189000	1	1.668786000	4.267969000	-0.749009000
1	2.776376000	3.426034000	-2.094140000	1	3.156240000	3.775461000	-1.575428000
1	1.212461000	2.638026000	-1.787362000	1	1.633374000	2.904254000	-1.886366000
6	3.933910000	3.042591000	0.323055000	6	3.401947000	3.192166000	1.081682000
1	4.679163000	3.238016000	-0.454976000	1	4.348784000	3.527387000	0.646923000
1	3.598716000	4.007075000	0.719500000	1	2.860376000	4.076815000	1.433646000
1	4.426688000	2.506865000	1.139670000	1	3.628259000	2.573943000	1.955384000
6	4.795883000	-2.152280000	0.886279000	6	3.951668000	-2.060775000	1.524682000
1	5.415542000	-1.508833000	1.516980000	1	4.536270000	-1.514637000	2.269660000
1	4.185252000	-2.781558000	1.546257000	1	3.091298000	-2.504644000	2.040870000
1	5.457456000	-2.833815000	0.335618000	1	4.559151000	-2.897561000	1.156574000
6	-1.903805000	-1.226194000	0.654577000	6	-1.648277000	-1.202722000	-0.108716000
8	-0.308783000	-2.523940000	1.688097000	8	-0.484315000	-2.903238000	0.641917000
7	-1.426052000	-2.038840000	1.416887000	7	-1.711880000	-2.233711000	0.657362000
6	-3.097618000	-0.652208000	0.109559000	6	-2.793457000	-0.271585000	-0.228699000
6	-3.757474000	-1.305847000	-0.951324000	6	-3.340715000	0.014887000	-1.491937000
6	-3.596715000	0.593499000	0.543296000	6	-3.358679000	0.384646000	0.882500000
6	-4.879383000	-0.739976000	-1.546158000	6	-4.402080000	0.902532000	-1.644071000
6	-4.719913000	1.161849000	-0.049311000	6	-4.420716000	1.277511000	0.740354000
6	-5.356426000	0.493919000	-1.096963000	6	-4.944035000	1.535558000	-0.525360000
1	-5.378757000	-1.257559000	-2.357840000	1	-4.805182000	1.093896000	-2.632847000
1	-5.090514000	2.115898000	0.306798000	1	-4.826601000	1.767924000	1.617574000
1	2.064604000	2.359579000	1.857967000	1	1.105918000	2.418895000	1.678386000
1	0.062526000	1.165654000	1.806926000	1	-0.450491000	0.869645000	1.035005000
1	-6.229206000	0.943129000	-1.559273000	1	-5.770340000	2.230869000	-0.630844000
17	-2.824730000	1.435361000	1.873890000	17	-2.723068000	0.150335000	2.513057000
1	-3.371705000	-2.259480000	-1.293064000	1	-2.941459000	-0.488273000	-2.363303000
TS1o2F				TS1o2F_P			
6	-3.068825000	1.037298000	0.869651000	6	-3.339225000	1.182187000	0.358905000
6	-3.845861000	0.001164000	0.096586000	6	-3.625990000	0.009037000	-0.538067000

6	-1.609711000	1.899545000	-1.068087000	6	-1.250510000	1.909381000	-0.973252000
6	-2.585046000	2.276294000	0.049093000	6	-2.548335000	2.351584000	-0.312484000
6	-0.819544000	-1.504754000	-0.185351000	6	-0.372647000	-1.998470000	-0.099172000
6	-0.449157000	1.236386000	-0.999875000	6	-0.262626000	1.090377000	-0.564393000
6	0.219075000	0.690527000	0.235511000	6	-0.157563000	0.367402000	0.720825000
6	0.111593000	-0.757441000	0.529246000	6	0.531202000	-1.009069000	0.690727000
1	-3.712405000	1.433844000	1.670362000	1	-4.294939000	1.617156000	0.686833000
6	-3.785941000	-1.337378000	0.193817000	6	-3.370650000	-1.294066000	-0.331415000
6	-2.848712000	-2.096429000	1.115328000	6	-2.714722000	-1.865332000	0.913019000
6	-1.596151000	-2.655625000	0.379771000	6	-1.476785000	-2.746734000	0.628305000
1	-3.388485000	-2.942138000	1.559808000	1	-3.448578000	-2.497676000	1.431081000
1	-4.580211000	0.403610000	-0.599586000	1	-4.132404000	0.261619000	-1.469865000
1	-2.208785000	0.587697000	1.372489000	1	-2.819687000	0.873452000	1.263776000
8	0.848482000	1.443569000	0.983092000	8	-0.637738000	0.776618000	1.771273000
1	-1.293098000	-1.011410000	-1.026077000	1	-0.796611000	-1.466530000	-0.963406000
1	-0.997504000	-3.242927000	1.080895000	1	-1.099705000	-3.168627000	1.563333000
1	-1.906901000	-3.326739000	-0.426176000	1	-1.759892000	-3.595861000	-0.002090000
1	-2.515144000	-1.467141000	1.945479000	1	-2.439415000	-1.074260000	1.613071000
6	0.649096000	-1.203402000	1.872331000	6	0.869668000	-1.497268000	2.108525000
1	1.560758000	-0.655232000	2.114824000	1	1.644818000	-0.867871000	2.546634000
1	-0.075068000	-1.001563000	2.671168000	1	-0.011334000	-1.440256000	2.749524000
1	0.870517000	-2.273024000	1.880827000	1	1.225283000	-2.529804000	2.074276000
6	-1.905575000	3.264209000	1.027959000	6	-2.219992000	3.410949000	0.767976000
1	-1.541612000	4.146612000	0.491454000	1	-1.697581000	4.267394000	0.329021000
1	-2.624606000	3.600319000	1.784022000	1	-3.148610000	3.777908000	1.220126000
1	-1.054147000	2.804056000	1.531611000	1	-1.591386000	2.976918000	1.546739000
6	-3.792441000	2.998244000	-0.586918000	6	-3.426708000	3.016794000	-1.396332000
1	-4.539616000	3.246578000	0.174022000	1	-4.372413000	3.358565000	-0.964315000
1	-3.470203000	3.931634000	-1.060929000	1	-2.918170000	3.887031000	-1.825330000
1	-4.278572000	2.391523000	-1.356448000	1	-3.655797000	2.329500000	-2.216349000
6	-4.672030000	-2.212505000	-0.662620000	6	-3.774160000	-2.319171000	-1.368628000
1	-5.304139000	-1.624412000	-1.333737000	1	-4.369521000	-1.871571000	-2.168796000
1	-4.078152000	-2.900522000	-1.277751000	1	-2.899668000	-2.792678000	-1.832234000
1	-5.322822000	-2.839617000	-0.039240000	1	-4.361056000	-3.128129000	-0.914724000
6	2.018676000	-1.231311000	-0.723364000	6	1.778731000	-1.157439000	-0.195304000
8	0.409804000	-2.648523000	-1.563474000	8	0.585188000	-2.954727000	-0.630660000
7	1.522619000	-2.107953000	-1.395838000	7	1.784556000	-2.276911000	-0.841586000
6	3.198788000	-0.548643000	-0.298345000	6	2.947778000	-0.267710000	-0.311805000
6	4.087622000	-1.115591000	0.637641000	6	3.917073000	-0.500702000	-1.311861000
6	3.449398000	0.759838000	-0.740288000	6	3.165290000	0.843440000	0.511839000
6	5.190955000	-0.394632000	1.081726000	6	5.029011000	0.320102000	-1.453692000
6	4.541589000	1.492210000	-0.304787000	6	4.265427000	1.681594000	0.387868000
6	5.415282000	0.904832000	0.612439000	6	5.207399000	1.417081000	-0.603170000
1	5.874642000	-0.840768000	1.795523000	1	5.753837000	0.111420000	-2.233493000
1	4.692554000	2.497016000	-0.681665000	1	4.361249000	2.520328000	1.067905000
1	-1.901216000	2.242876000	-2.060627000	1	-1.102929000	2.326949000	-1.969482000
1	0.110856000	1.064937000	-1.916813000	1	0.535450000	0.886760000	-1.274125000
1	6.273661000	1.467986000	0.963534000	1	6.070548000	2.065227000	-0.712795000
1	3.895671000	-2.119589000	0.998960000	1	3.771709000	-1.341838000	-1.979524000
9	2.596771000	1.311632000	-1.625645000	9	2.272812000	1.134925000	1.492213000
TS1pBr				TS1pBr_P			
6	-3.964443000	1.366159000	0.861361000	6	-3.970701000	1.781661000	0.476749000
6	-4.894222000	0.328208000	0.283683000	6	-4.596310000	0.743098000	-0.414662000
6	-2.634168000	1.888489000	-1.279992000	6	-1.857536000	2.000827000	-0.972749000
6	-3.467758000	2.465115000	-0.133859000	6	-2.966887000	2.742261000	-0.241290000
6	-2.044628000	-1.466941000	-0.104221000	6	-1.857498000	-1.981470000	-0.175836000
6	-1.534809000	1.125972000	-1.233771000	6	-1.080508000	0.964002000	-0.606262000
6	-0.804838000	0.652134000	-0.003695000	6	-1.061986000	0.256695000	0.691668000
6	-0.982449000	-0.748213000	0.436433000	6	-0.765229000	-1.253784000	0.657261000
1	-4.493061000	1.900954000	1.665701000	1	-4.765540000	2.424909000	0.882078000
6	-4.931760000	-0.993467000	0.522568000	6	-4.646263000	-0.590717000	-0.259496000
6	-3.970157000	-1.738004000	1.431097000	6	-4.071241000	-1.352795000	0.920584000
6	-2.848532000	-2.482826000	0.648659000	6	-3.098854000	-2.491172000	0.535155000
1	-4.529024000	-2.480481000	2.014565000	1	-4.903857000	-1.811757000	1.470738000
1	-5.661858000	0.721056000	-0.381292000	1	-5.093129000	1.144963000	-1.297575000
1	-3.097708000	0.897234000	1.334138000	1	-3.481026000	1.328820000	1.337518000
8	-0.068153000	1.426689000	0.613509000	8	-1.284545000	0.802291000	1.767747000

1	-2.569222000	-1.005169000	-0.932263000	1	-2.153443000	-1.332115000	-1.011606000
1	-2.232065000	-3.049438000	1.351320000	1	-2.819320000	-3.056433000	1.427706000
1	-3.293509000	-3.198879000	-0.048398000	1	-3.594946000	-3.199166000	-0.136076000
1	-3.502641000	-1.060872000	2.151813000	1	-3.576721000	-0.677389000	1.622813000
6	-0.333029000	-1.124660000	1.750731000	6	-0.591749000	-1.820627000	2.076390000
1	0.629979000	-0.622157000	1.852811000	1	0.301513000	-1.409595000	2.550395000
1	-0.955593000	-0.815340000	2.599204000	1	-1.448253000	-1.563509000	2.701361000
1	-0.174830000	-2.203054000	1.824298000	1	-0.489967000	-2.907516000	2.032953000
6	-2.625936000	3.490446000	0.663717000	6	-2.337604000	3.686355000	0.811989000
1	-2.248760000	4.275849000	0.000500000	1	-1.650437000	4.395005000	0.337919000
1	-3.243537000	3.966090000	1.434313000	1	-3.126456000	4.262877000	1.308558000
1	-1.768234000	3.015468000	1.141969000	1	-1.788987000	3.113050000	1.559954000
6	-4.671612000	3.215791000	-0.742852000	6	-3.721722000	3.606502000	-1.276390000
1	-5.323782000	3.604961000	0.045895000	1	-4.537983000	4.153298000	-0.794294000
1	-4.325683000	4.063653000	-1.343816000	1	-3.046730000	4.339841000	-1.730856000
1	-5.271490000	2.575173000	-1.395748000	1	-4.146503000	3.002975000	-2.084115000
6	-5.968314000	-1.867077000	-0.146145000	6	-5.353083000	-1.446115000	-1.288263000
1	-6.615680000	-1.295584000	-0.817030000	1	-5.882118000	-0.836475000	-2.025465000
1	-5.497612000	-2.665848000	-0.733334000	1	-4.649645000	-2.087484000	-1.833772000
1	-6.600971000	-2.364858000	0.600393000	1	-6.079537000	-2.116607000	-0.811356000
6	0.733669000	-1.484726000	-0.973097000	6	0.439376000	-1.674103000	-0.192331000
8	-1.077291000	-2.812920000	-1.497535000	8	-1.133225000	-3.103266000	-0.758168000
7	0.085760000	-2.362443000	-1.501761000	7	0.200307000	-2.724660000	-0.903567000
6	2.046725000	-0.980297000	-0.695011000	6	1.782901000	-1.076559000	-0.157458000
6	2.992272000	-1.807130000	-0.056046000	6	2.791105000	-1.544966000	-1.022252000
6	2.378026000	0.353610000	-0.994729000	6	2.089875000	-0.027191000	0.724335000
6	4.256411000	-1.317788000	0.251442000	6	4.064683000	-0.990447000	-1.002692000
1	2.731528000	-2.830400000	0.190234000	1	2.567251000	-2.347438000	-1.715736000
6	3.640340000	0.848230000	-0.682920000	6	3.364613000	0.536946000	0.752496000
1	1.648245000	1.001242000	-1.464207000	1	1.342353000	0.364215000	1.403910000
6	4.565875000	0.006553000	-0.065653000	6	4.340559000	0.048908000	-0.111477000
1	4.989556000	-1.953058000	0.733936000	1	4.833629000	-1.356596000	-1.672909000
1	3.900925000	1.873583000	-0.916140000	1	3.589803000	1.345050000	1.438290000
35	6.300835000	0.684428000	0.362835000	35	6.093003000	0.819699000	-0.083400000
1	-2.988224000	2.150317000	-2.276901000	1	-1.680538000	2.359824000	-1.986664000
1	-1.092703000	0.794092000	-2.172846000	1	-0.410159000	0.554363000	-1.358380000
TS1pCl				TS1pCl_P			
6	-3.471776000	1.239192000	0.845607000	6	-3.528684000	1.608480000	0.481443000
6	-4.332546000	0.161429000	0.234717000	6	-4.082774000	0.523750000	-0.402173000
6	-2.129682000	1.869536000	-1.259492000	6	-1.446395000	1.976054000	-0.982220000
6	-3.017641000	2.379743000	-0.122823000	6	-2.603028000	2.637240000	-0.246920000
6	-1.381709000	-1.466064000	-0.122879000	6	-1.149519000	-1.991274000	-1.700390000
6	-0.990503000	1.168757000	-1.201593000	6	-0.593467000	1.000528000	-0.616206000
6	-0.261055000	0.714336000	0.036193000	6	-0.515184000	0.302674000	0.684684000
6	-0.369594000	-0.701267000	0.449464000	6	-0.109535000	-1.182385000	0.654752000
1	-4.043826000	1.731313000	1.647457000	1	-4.365531000	2.193206000	0.890871000
6	-4.302327000	-1.163875000	0.453760000	6	-4.034231000	-0.809535000	-0.242233000
6	-3.318059000	-1.869108000	1.369371000	6	-3.397923000	-1.522966000	0.936800000
6	-2.142304000	-2.537473000	0.597191000	6	-2.346645000	-2.588046000	0.549174000
1	-3.845555000	-2.651196000	1.929804000	1	-4.191403000	-2.040105000	1.493164000
1	-5.108336000	0.522328000	-0.438846000	1	-4.613297000	0.884851000	-1.283088000
1	-2.589578000	0.810703000	1.328001000	1	-3.000656000	1.195678000	1.339666000
8	0.418428000	1.517361000	0.681962000	8	-0.769414000	0.835822000	1.759955000
1	-1.916149000	-1.018048000	-0.952070000	1	-1.496541000	-1.368402000	-1.006387000
1	-1.509025000	-3.081802000	1.302516000	1	-2.021705000	-3.128588000	1.441669000
1	-2.534186000	-3.264401000	-0.120182000	1	-2.793158000	-3.332473000	-0.117403000
1	-2.902727000	-1.179382000	2.109884000	1	-2.950785000	-0.810549000	1.634244000
6	0.275233000	-1.065035000	1.769542000	6	0.111677000	-1.728685000	2.075298000
1	1.206852000	-0.512180000	1.898771000	1	0.973512000	-1.250067000	2.544026000
1	-0.379094000	-0.806106000	2.610879000	1	-0.759093000	-1.533855000	2.703083000
1	0.491776000	-2.134188000	1.827585000	1	0.294293000	-2.805093000	2.035680000
6	-2.250662000	3.437558000	0.707124000	6	-2.038746000	3.629854000	0.798556000
1	-1.904199000	4.252744000	0.063367000	1	-1.406839000	4.383893000	0.317670000
1	-2.909212000	3.866459000	1.471232000	1	-2.864751000	4.150479000	1.296458000
1	-1.377752000	3.003262000	1.196516000	1	-1.446733000	3.101494000	1.546538000
6	-4.249218000	3.071599000	-0.745914000	6	-3.425615000	3.438645000	-1.281026000
1	-4.938429000	3.410402000	0.034527000	1	-4.277131000	3.925954000	-0.795999000

1	-3.939472000	3.947378000	-1.326239000	1	-2.809150000	4.217632000	-1.742431000
1	-4.798260000	2.409098000	-1.421292000	1	-3.809401000	2.801826000	-2.083545000
6	-5.277587000	-2.081961000	-0.246749000	6	-4.683323000	-1.718180000	-1.263348000
1	-5.942105000	-1.536308000	-0.922359000	1	-5.258343000	-1.151387000	-2.000285000
1	-4.753689000	-2.845815000	-0.835339000	1	-3.938668000	-2.310242000	-1.809853000
1	-5.896377000	-2.623648000	0.480602000	1	-5.357492000	-2.436635000	-0.779531000
6	1.409747000	-1.321887000	-0.936151000	6	1.118676000	-1.516869000	-0.199238000
8	-0.318844000	-2.731204000	-1.523576000	8	-0.348218000	-3.059239000	-0.752282000
7	0.818922000	-2.221170000	-1.494820000	7	0.953720000	-2.584705000	-0.905646000
6	2.690532000	-0.760899000	-0.618224000	6	2.415143000	-0.822652000	-0.173094000
6	3.663708000	-1.557298000	0.017899000	6	3.449953000	-1.218352000	-1.042642000
6	2.961129000	0.595313000	-0.875645000	6	2.649697000	0.248594000	0.704488000
6	4.896005000	-1.015853000	0.363889000	6	4.679823000	-0.572810000	-1.031902000
1	3.449343000	-2.598406000	0.231668000	1	3.280990000	-2.036729000	-1.732996000
6	4.190805000	1.142935000	-0.525263000	6	3.879570000	0.904704000	0.724259000
1	2.209142000	1.218849000	-1.342485000	1	1.879089000	0.585816000	1.387171000
6	5.145378000	0.330795000	0.088419000	6	4.884022000	0.486778000	-0.144544000
1	5.651816000	-1.625748000	0.844499000	1	5.470999000	-0.882134000	-1.705113000
1	4.406583000	2.185773000	-0.725012000	1	4.050887000	1.729309000	1.406201000
17	6.700195000	1.020413000	0.531068000	17	6.439793000	1.311947000	-1.130320000
1	-2.476601000	2.128933000	-2.259545000	1	-1.301976000	2.342587000	-1.998624000
1	-0.510619000	0.879068000	-2.136098000	1	0.100484000	0.637413000	-1.370819000
TS1pF				TS1pF_P			
6	-3.225887000	1.141082000	0.829304000	6	-3.356565000	1.420942000	0.481842000
6	-4.033857000	0.048522000	0.174107000	6	-3.825470000	0.293673000	-0.397760000
6	-1.852417000	1.863509000	-1.225879000	6	-1.310040000	1.941869000	-0.985633000
6	-2.787281000	2.317311000	-0.102996000	6	-2.512473000	2.515066000	-0.249899000
6	-1.020427000	-1.473301000	-0.144074000	6	-0.709128000	-1.992715000	-0.162897000
6	-0.692580000	1.199105000	-1.152042000	6	-0.385381000	1.034140000	-0.619493000
6	0.018957000	0.739986000	0.094722000	6	-0.252463000	0.346016000	0.682363000
6	-0.051700000	-0.686680000	0.472049000	6	0.268189000	-1.102233000	0.654444000
1	-3.834458000	1.596039000	1.626218000	1	-4.235883000	1.941060000	0.889432000
6	-3.963760000	-1.279544000	0.365608000	6	-3.674100000	-1.031292000	-0.233030000
6	-2.978595000	-1.971779000	1.290075000	6	-2.984334000	-1.689554000	0.948060000
6	-1.763438000	-2.584492000	0.533143000	6	-1.856211000	-2.673903000	0.562986000
1	-3.493275000	-2.782316000	1.821310000	1	-3.735899000	-2.262538000	1.507971000
1	-4.805054000	0.397885000	-0.510736000	1	-4.381827000	0.609741000	-1.280047000
1	-2.341912000	0.732112000	1.325104000	1	-2.798179000	1.053044000	1.341261000
8	0.654027000	1.550333000	0.775987000	8	-0.548015000	0.859572000	1.756785000
1	-1.549552000	-1.024291000	-0.976216000	1	-1.104495000	-1.401857000	-1.001203000
1	-1.130257000	-3.124247000	1.242108000	1	-1.488990000	-3.183272000	1.457458000
1	-2.113615000	-3.307333000	-0.209524000	1	-2.246548000	-3.454030000	-0.098141000
1	-2.603812000	-1.284807000	2.054418000	1	-2.590818000	-0.942546000	1.641619000
6	0.576283000	-1.060572000	1.797153000	6	0.537012000	-1.625329000	2.075466000
1	1.490948000	-0.487190000	1.955542000	1	1.362084000	-1.080691000	2.538291000
1	-0.099952000	-0.835525000	2.630952000	1	-0.343178000	-1.495660000	2.707032000
1	0.819397000	-2.124824000	1.838203000	1	0.801135000	-2.684757000	2.037682000
6	-2.079808000	3.383188000	0.768566000	6	-2.023784000	3.549666000	0.792925000
1	-1.747543000	4.224327000	0.151211000	1	-1.451958000	4.348834000	0.309725000
1	-2.771967000	3.771280000	1.524755000	1	-2.886334000	4.006584000	1.291425000
1	-1.203767000	2.969588000	1.270249000	1	-1.392073000	3.069267000	1.540830000
6	-4.026077000	2.979099000	-0.744235000	6	-3.394429000	3.249834000	-1.284670000
1	-4.747245000	3.276000000	0.024317000	1	-4.280293000	3.671843000	-0.799912000
1	-3.732788000	3.877919000	-1.297250000	1	-2.839216000	4.072559000	-1.747940000
1	-4.533165000	2.312831000	-1.448123000	1	-3.729199000	2.584213000	-2.085788000
6	-4.890271000	-2.214005000	-0.378177000	6	-4.250863000	-1.990959000	-1.250922000
1	-5.556148000	-1.676170000	-1.058706000	1	-4.869659000	-1.473236000	-1.988526000
1	-4.326884000	-2.947240000	-0.969220000	1	-3.462388000	-2.523755000	-1.796896000
1	-5.508045000	-2.791466000	0.322031000	1	-4.865682000	-2.759134000	-0.764436000
6	1.781340000	-1.205987000	-0.889814000	6	1.515405000	-1.343335000	-0.204386000
8	0.117987000	-2.667660000	-1.537150000	8	0.168606000	-2.999816000	-0.739452000
7	1.236300000	-2.114129000	-1.479878000	7	1.430944000	-2.424522000	-0.904676000
6	3.020825000	-0.578778000	-0.541040000	6	2.751512000	-0.546392000	-0.188252000
6	4.002172000	-1.310176000	0.160381000	6	3.809984000	-0.862038000	-1.064067000
6	3.238253000	0.782198000	-0.831294000	6	2.903863000	0.543910000	0.685858000
6	5.193064000	-0.701306000	0.536375000	6	4.984414000	-0.120406000	-1.062310000
1	3.824324000	-2.352865000	0.398290000	1	3.700433000	-1.694045000	-1.750079000

6	4.426235000	1.397031000	-0.452666000	6	4.077440000	1.296155000	0.696771000
1	2.475914000	1.352142000	-1.347892000	1	2.111308000	0.818870000	1.371222000
6	5.381236000	0.642537000	0.222050000	6	5.098220000	0.949561000	-0.177895000
1	5.967119000	-1.243513000	1.066861000	1	5.804010000	-0.352981000	-1.732775000
1	4.620155000	2.441085000	-0.668705000	1	4.203750000	2.137325000	1.368519000
9	6.533007000	1.235948000	0.589320000	9	6.237221000	1.674597000	-0.175867000
1	-2.180613000	2.135318000	-2.228987000	1	-1.194927000	2.317051000	-2.002638000
1	-0.178683000	0.947565000	-2.079529000	1	0.333708000	0.724296000	-1.374217000
TS2o1Br				TS2o1Br_P			
6	-4.022709000	0.456078000	0.249650000	6	-3.995722000	0.228053000	0.092160000
6	-3.776160000	-0.609817000	-0.785486000	6	-3.507196000	-0.777503000	-0.918768000
6	-2.347402000	1.994212000	-0.997904000	6	-2.454421000	1.994720000	-0.977928000
6	-3.667707000	1.896920000	-0.239839000	6	-3.814897000	1.711989000	-0.355374000
6	-0.673176000	-2.096318000	0.519138000	6	-0.379126000	-1.879951000	1.036119000
6	-1.188024000	1.339191000	-0.826518000	6	-1.242905000	1.500606000	-0.677980000
6	-0.891553000	0.374413000	0.265642000	6	-0.903545000	0.621131000	0.465268000
6	-0.238751000	-0.924264000	-0.100785000	6	0.033791000	-0.595782000	0.231780000
1	-5.086881000	0.476803000	0.528181000	1	-5.071478000	0.082891000	0.270631000
6	-3.391559000	-1.878903000	-0.583977000	6	-3.007852000	-2.000824000	-0.685262000
6	-3.178772000	-2.516367000	0.781272000	6	-2.858401000	-2.625603000	0.695330000
6	-1.813870000	-2.217436000	1.490588000	6	-1.774951000	-2.053567000	1.636532000
1	-3.272781000	-3.601316000	0.661551000	1	-2.657828000	-3.694399000	0.560413000
1	-3.903851000	-0.291752000	-1.819900000	1	-3.583403000	-0.465505000	-1.959878000
1	-3.475564000	0.232010000	1.166208000	1	-3.514370000	0.072810000	1.057928000
8	-1.165785000	0.663994000	1.434603000	8	-1.274143000	0.878825000	1.605487000
1	-1.892177000	-1.306367000	2.077749000	1	-2.088915000	-1.115419000	2.090047000
1	-1.609113000	-3.035668000	2.186698000	1	-1.655467000	-2.764819000	2.461536000
1	-3.974471000	-2.213098000	1.470308000	1	-3.813059000	-2.564257000	1.231466000
6	-3.602291000	2.839732000	0.984620000	6	-4.001704000	2.635059000	0.871885000
1	-3.419675000	3.874464000	0.674980000	1	-3.937612000	3.689674000	0.583788000
1	-4.553514000	2.813847000	1.529196000	1	-4.988453000	2.466526000	1.318372000
1	-2.798098000	2.526575000	1.652993000	1	-3.232211000	2.429311000	1.618523000
6	-4.786335000	2.391975000	-1.185812000	6	-4.895073000	2.058104000	-1.405634000
1	-5.748762000	2.401636000	-0.664494000	1	-5.894460000	1.920974000	-0.981090000
1	-4.581349000	3.410003000	-1.534479000	1	-4.805293000	3.100863000	-1.728507000
1	-4.886666000	1.751674000	-2.068260000	1	-4.816086000	1.425325000	-2.295503000
6	-3.129250000	-2.792901000	-1.757996000	6	-2.605590000	-2.901212000	-1.830729000
1	-3.284047000	-2.288824000	-2.716333000	1	-2.692822000	-2.402787000	-2.800466000
1	-2.096819000	-3.165551000	-1.735281000	1	-1.571060000	-3.249037000	-1.718079000
1	-3.777563000	-3.678278000	-1.725196000	1	-3.232116000	-3.802682000	-1.851269000
6	1.624447000	-0.478585000	1.119644000	6	1.336701000	-0.270579000	0.965245000
8	0.948928000	-2.495101000	1.991886000	8	0.554369000	-1.921150000	2.169639000
7	1.632971000	-1.468449000	1.819135000	7	1.571718000	-0.990573000	1.994995000
6	2.311985000	0.728101000	0.758745000	6	2.243361000	0.835918000	0.571122000
6	3.392374000	0.718300000	-0.147822000	6	3.372123000	0.627556000	-0.233342000
6	1.856779000	1.968908000	1.246980000	6	1.955893000	2.149155000	0.975077000
6	4.015698000	1.899707000	-0.536489000	6	4.194532000	1.681239000	-0.627655000
6	2.476592000	3.151929000	0.858597000	6	2.768958000	3.212924000	0.587720000
1	1.004339000	1.979012000	1.915809000	1	1.085681000	2.324344000	1.598779000
6	3.554891000	3.116422000	-0.029121000	6	3.887416000	2.977791000	-0.213639000
1	4.848238000	1.868746000	-1.229317000	1	5.061086000	1.488196000	-1.249156000
1	2.118408000	4.099840000	1.245376000	1	2.530773000	4.219989000	0.913440000
1	-2.370222000	2.697055000	-1.830859000	1	-2.484211000	2.678281000	-1.826047000
1	-0.391778000	1.507555000	-1.547503000	1	-0.406097000	1.762094000	-1.321678000
6	0.406445000	-1.040958000	-1.475128000	6	0.276022000	-0.879943000	-1.260713000
1	1.125035000	-0.242225000	-1.675020000	1	0.864701000	-0.085027000	-1.724498000
1	0.944621000	-1.987707000	-1.560412000	1	0.836359000	-1.808524000	-1.381859000
1	-0.356312000	-1.007644000	-2.261368000	1	-0.673179000	-0.959334000	-1.791040000
1	-0.395647000	-3.021085000	0.018284000	1	-0.141275000	-2.747556000	0.407338000
1	4.040300000	4.036953000	-0.336586000	1	4.525706000	3.800187000	-0.520252000
35	4.014528000	-0.938020000	-0.863319000	35	3.809908000	-1.143577000	-0.822177000
TS2o1Cl				TS2o1Cl_P			
6	3.632966000	0.616540000	-0.395710000	6	3.624545000	0.438972000	-0.214195000
6	3.520589000	-0.394358000	0.714993000	6	3.278337000	-0.529270000	0.887937000
6	1.922442000	2.114008000	0.852774000	6	1.979949000	2.136903000	0.811941000
6	3.202909000	2.058512000	0.025309000	6	3.330136000	1.929869000	0.139579000
6	0.465686000	-2.166925000	-0.317963000	6	0.176950000	-2.044494000	-0.812019000

6	0.804938000	1.372300000	0.789837000	6	0.806440000	1.516356000	0.612688000
6	0.517932000	0.323564000	-0.224532000	6	0.494565000	0.528118000	-0.446451000
6	-0.020769000	-0.990766000	0.254249000	6	-0.315331000	-0.745551000	-0.078706000
1	4.675981000	0.691460000	-0.737712000	1	4.699415000	0.376086000	-0.439708000
6	3.217596000	-1.697028000	0.613776000	6	2.883813000	-1.805834000	0.765068000
6	2.977143000	-2.434158000	-0.695509000	6	2.728362000	-2.539204000	-0.560291000
6	1.559885000	-2.270756000	-1.343409000	6	1.551282000	-2.136347000	-1.476633000
1	3.150846000	-3.500737000	-0.515267000	1	2.636323000	-3.609401000	-0.343402000
1	3.681436000	-0.002206000	1.718883000	1	3.373506000	-0.136537000	1.899730000
1	3.053655000	0.296892000	-1.262834000	1	3.114356000	0.172119000	-1.139987000
8	0.707891000	0.556712000	-1.422558000	8	0.784650000	0.732409000	-1.620369000
1	1.543352000	-1.394780000	-1.986284000	1	1.754018000	-1.209631000	-2.009893000
1	1.377182000	-3.142445000	-1.978102000	1	1.457529000	-2.913743000	-2.243208000
1	3.712984000	-2.125415000	-1.445941000	1	3.645935000	-2.429945000	-1.150744000
6	3.003843000	2.913083000	-1.248463000	6	3.374846000	2.773906000	-1.156108000
1	2.761851000	3.950298000	-0.992544000	1	3.228115000	3.836995000	-0.937908000
1	3.924628000	2.918854000	-1.843560000	1	4.351149000	2.660542000	-1.641262000
1	2.191253000	2.501252000	-1.849754000	1	2.593639000	2.447777000	-1.845538000
6	4.332869000	2.689153000	0.871992000	6	4.421729000	2.445001000	1.105314000
1	5.262883000	2.728928000	0.296130000	1	5.408601000	2.366332000	0.638734000
1	4.075300000	3.712024000	1.167603000	1	4.251672000	3.496283000	1.361198000
1	4.525467000	2.117082000	1.785439000	1	4.442749000	1.873754000	2.038991000
6	3.086295000	-2.549035000	1.854445000	6	2.620405000	-2.653446000	1.988444000
1	3.257837000	-1.974917000	2.769557000	1	2.702950000	-2.080005000	2.916212000
1	2.083198000	-2.990895000	1.916069000	1	1.619820000	-3.102283000	1.952640000
1	3.792899000	-3.389067000	1.836565000	1	3.330252000	-3.489673000	2.038382000
6	-1.982972000	-0.762743000	-0.866594000	6	-1.678881000	-0.597540000	-0.757332000
8	-1.202545000	-2.774491000	-1.659611000	8	-0.803514000	-2.255776000	-1.885064000
7	-1.955072000	-1.794958000	-1.502933000	7	-1.895906000	-1.413778000	-1.717134000
6	-2.762066000	0.393334000	-0.523671000	6	-2.667716000	0.445837000	-0.388976000
6	-3.853931000	0.314826000	0.367702000	6	-3.758366000	0.183385000	0.453352000
6	-2.388966000	1.660319000	-1.015643000	6	-2.499908000	1.758499000	-0.858354000
6	-4.562602000	1.454826000	0.736398000	6	-4.657451000	1.185329000	0.817051000
6	-3.092199000	2.800833000	-0.643828000	6	-3.389650000	2.769378000	-0.500536000
1	-1.534083000	1.724589000	-1.678189000	1	-1.662477000	1.974310000	-1.513208000
6	-4.177336000	2.697300000	0.229895000	6	-4.467890000	2.481403000	0.337790000
1	-5.403174000	1.368432000	1.414993000	1	-5.491841000	0.949271000	1.467402000
1	-2.794504000	3.768107000	-1.033846000	1	-3.242679000	3.775632000	-0.878371000
1	1.940977000	2.867461000	1.640338000	1	1.986028000	2.882410000	1.606690000
1	0.040182000	1.531754000	1.546023000	1	-0.019816000	1.751543000	1.279679000
6	-0.587136000	-1.064803000	1.665748000	6	-0.463100000	-0.938124000	1.440293000
1	-1.355097000	-0.309498000	1.851939000	1	-1.090756000	-0.158338000	1.878210000
1	-1.039657000	-2.044160000	1.839129000	1	-0.938011000	-1.897661000	1.654308000
1	0.206204000	-0.921278000	2.408054000	1	0.512795000	-0.905469000	1.925355000
1	0.283634000	-3.075052000	0.252404000	1	0.053564000	-2.880198000	-0.111191000
1	-4.729154000	3.584021000	0.524130000	1	-5.166306000	3.261921000	0.621690000
17	-4.349738000	-1.238347000	1.019053000	17	-4.021569000	-1.443975000	1.081145000
TS2o1F				TS2o1F_P			
6	3.302891000	0.872047000	-0.504207000	6	3.338569000	0.721838000	-0.332060000
6	3.359617000	-0.121962000	0.625914000	6	3.172032000	-0.241651000	0.815049000
6	1.502145000	2.198601000	0.809050000	6	1.550517000	2.245655000	0.727950000
6	2.738569000	2.266604000	-0.082139000	6	2.882651000	2.178022000	-0.006371000
6	0.469903000	-2.238172000	-0.213294000	6	0.195544000	-2.175030000	-0.678203000
6	0.470301000	1.339600000	0.812869000	6	0.450993000	1.485837000	0.603899000
6	0.249860000	0.245197000	-0.169661000	6	0.212134000	0.430601000	-0.408842000
6	-0.117084000	-1.109159000	0.357976000	6	-0.417256000	-0.918797000	0.037735000
1	4.312530000	1.053551000	-0.901998000	1	4.399961000	0.781446000	-0.615176000
6	3.197055000	-1.451765000	0.561036000	6	2.932936000	-1.560477000	0.751972000
6	2.972285000	-2.238630000	-0.721928000	6	2.798155000	-2.355407000	-0.539907000
6	1.513740000	-2.246021000	-1.294618000	6	1.540008000	-2.124829000	-1.406447000
1	3.272679000	-3.275483000	-0.534852000	1	2.841433000	-3.420382000	-0.285248000
1	3.527955000	0.306318000	1.613706000	1	3.272098000	0.195074000	1.808185000
1	2.718898000	0.473275000	-1.334580000	1	2.817929000	0.362526000	-1.219928000
8	0.354923000	0.472267000	-1.378896000	8	0.420124000	0.626368000	-1.601123000
1	1.367933000	-1.391606000	-1.950065000	1	1.605191000	-1.198791000	-1.974348000
1	1.394634000	-3.146521000	-1.903745000	1	1.505558000	-2.932726000	-2.146010000
1	3.629444000	-1.866802000	-1.515557000	1	3.667424000	-2.164362000	-1.180709000

6	2.384207000	3.069798000	-1.355583000	6	2.762905000	2.975274000	-1.326680000
1	2.043738000	4.079483000	-1.101576000	1	2.499154000	4.020232000	-1.132175000
1	3.267902000	3.163866000	-1.997707000	1	3.721334000	2.962395000	-1.858385000
1	1.592113000	2.561306000	-1.908283000	1	1.994591000	2.533999000	-1.964561000
6	3.833130000	3.032890000	0.696436000	6	3.948596000	2.853932000	0.886019000
1	4.723230000	3.162885000	0.072757000	1	4.914624000	2.876321000	-0.372096000
1	3.479600000	4.027014000	0.990945000	1	3.665348000	3.886188000	1.118072000
1	4.132866000	2.503025000	1.606479000	1	4.082515000	2.323760000	1.834385000
6	3.224981000	-2.286415000	1.820153000	6	2.845064000	-2.389424000	2.012953000
1	3.379853000	-1.677564000	2.715590000	1	2.907809000	-1.777150000	2.917192000
1	2.281323000	-2.833824000	1.943196000	1	1.907444000	-2.958191000	2.050286000
1	4.018002000	-3.044424000	1.777115000	1	3.654854000	-3.130336000	2.044414000
6	-2.129819000	-1.108244000	-0.689383000	6	-1.810343000	-0.942273000	-0.592544000
8	-1.191723000	-3.067186000	-1.444970000	8	-0.798756000	-2.540421000	-1.695736000
7	-2.029029000	-2.156380000	-1.290686000	7	-1.966312000	-1.807167000	-1.522027000
6	-2.953793000	0.029963000	-0.406771000	6	-2.871692000	0.042076000	-0.275456000
6	-3.863626000	-0.004638000	0.661535000	6	-3.687460000	-0.107542000	0.847326000
6	-2.814150000	1.236318000	-1.121661000	6	-3.067638000	1.175655000	-1.078125000
6	-4.638725000	1.090601000	1.009617000	6	-4.667361000	0.813347000	1.190877000
6	-3.584240000	2.344600000	-0.783525000	6	-4.045590000	2.116655000	-0.755226000
1	-2.085538000	1.282342000	-1.922148000	1	-2.435680000	1.310722000	-1.949583000
6	-4.494660000	2.270478000	0.276532000	6	-4.843007000	1.934713000	0.377668000
1	-5.331774000	1.009473000	1.839015000	1	-5.273138000	0.641308000	2.073327000
1	-3.474102000	3.267619000	-1.342189000	1	-4.184599000	2.988363000	-1.385864000
1	1.477044000	2.964832000	1.584041000	1	1.504672000	3.012649000	1.500683000
1	-0.269702000	1.430224000	1.604388000	1	-0.366002000	1.644958000	1.304051000
6	-0.609524000	-1.214441000	1.795167000	6	-0.463520000	-1.077546000	1.566591000
1	-1.446360000	-0.544299000	2.007316000	1	-1.126530000	-0.342848000	2.026253000
1	-0.944898000	-2.233489000	2.003684000	1	-0.840914000	-2.067447000	1.831066000
1	0.195495000	-0.971966000	2.498234000	1	0.533565000	-0.948958000	1.988310000
1	0.421321000	-3.145543000	0.384437000	1	0.206723000	-2.993897000	0.052584000
1	-5.093292000	3.136115000	0.540496000	1	-5.604633000	2.664539000	0.632578000
9	-3.974629000	-1.144366000	1.372883000	9	-3.512768000	-1.198953000	1.630944000
TS2o2Br				TS2o2Br_P			
6	3.183461000	0.944432000	-1.127417000	6	3.292555000	0.809086000	-1.175019000
6	3.654783000	-0.221454000	-0.299893000	6	3.701113000	-0.454326000	-0.466893000
6	2.055237000	2.181764000	0.879145000	6	2.644244000	1.964208000	1.043537000
6	2.929734000	2.273642000	-0.359576000	6	3.307672000	2.103886000	-0.311606000
6	0.660566000	-2.355801000	0.688880000	6	0.352542000	-2.170976000	0.938096000
6	1.106676000	1.313559000	1.264691000	6	1.577890000	1.262173000	1.471882000
6	0.597325000	0.137246000	0.509573000	6	0.635726000	0.429461000	0.693521000
6	0.403451000	-1.128130000	1.295124000	6	-0.055204000	-0.746136000	1.410165000
1	3.951681000	1.176119000	-1.880788000	1	3.987815000	0.990024000	-2.008199000
6	3.269147000	-1.506428000	-0.395330000	6	3.082592000	-1.647183000	-0.507506000
6	2.232480000	-2.006419000	-1.379668000	6	1.815152000	-1.893027000	-1.296234000
6	0.909889000	-2.614703000	-0.772989000	6	0.621906000	-2.517294000	-0.535065000
1	2.696794000	-2.789872000	-1.992423000	1	2.051661000	-2.583678000	-2.118268000
1	4.429316000	0.009095000	0.432311000	1	4.625377000	-0.389689000	0.108515000
1	2.282025000	0.682996000	-1.678034000	1	2.306574000	0.701655000	-1.621368000
8	0.336639000	0.217004000	-0.690807000	8	0.330970000	0.672780000	-0.470304000
1	0.069747000	-2.213440000	-1.342618000	1	-0.287466000	-2.294733000	-1.098999000
1	0.912183000	-3.698522000	-0.911869000	1	0.723025000	-3.608126000	-0.526787000
1	1.951637000	-1.206006000	-2.061208000	1	1.475695000	-0.971923000	-1.763323000
6	2.226096000	3.254720000	-1.330516000	6	2.554340000	3.213290000	-1.087711000
1	2.059806000	4.229524000	-0.859958000	1	2.580132000	4.164056000	-0.545318000
1	2.843828000	3.410428000	-2.222519000	1	3.025594000	3.367468000	-2.065190000
1	1.258969000	2.848144000	-1.638914000	1	1.511862000	2.922715000	-1.238913000
6	4.283633000	2.886784000	0.070699000	6	4.767866000	2.555531000	-0.081735000
1	4.927767000	3.035272000	-0.801897000	1	5.268334000	2.723778000	-1.040311000
1	4.138923000	3.860108000	0.551989000	1	4.804663000	3.491121000	0.486782000
1	4.813904000	2.242003000	0.778511000	1	5.340528000	1.805216000	0.472804000
6	3.916574000	-2.566476000	0.465153000	6	3.689191000	-2.858350000	0.162655000
1	4.666451000	-2.143309000	1.139677000	1	4.598519000	-2.605634000	0.715106000
1	3.179779000	-3.100832000	1.075837000	1	2.995414000	-3.342724000	0.859154000
1	4.406939000	-3.324733000	-0.159584000	1	3.946255000	-3.619092000	-0.586683000
6	-1.834826000	-1.099446000	1.100704000	6	-1.545725000	-0.852761000	1.069787000
8	-1.354480000	-3.312191000	0.727196000	8	-0.866421000	-2.923637000	1.274380000

7	-2.037195000	-2.281611000	0.884256000	7	-1.965286000	-2.064467000	1.066704000
6	-2.450432000	0.191373000	0.966648000	6	-2.459344000	0.283962000	0.819475000
6	-2.587803000	1.038682000	2.081450000	6	-2.835581000	1.130327000	1.873446000
6	-2.830816000	0.681809000	-0.302348000	6	-2.939853000	0.580295000	-0.465290000
6	-3.096108000	2.325953000	1.939014000	6	-3.663424000	2.229866000	1.654817000
6	-3.341834000	1.967747000	-0.446975000	6	-3.767173000	1.677964000	-0.697105000
6	-3.470694000	2.788683000	0.675601000	6	-4.128370000	2.503537000	0.367850000
1	-3.199828000	2.965200000	2.809003000	1	-3.945427000	2.866572000	2.486782000
1	-3.631702000	2.325633000	-1.427872000	1	-4.121462000	1.883976000	-1.700420000
1	2.244541000	2.994983000	1.581188000	1	3.137018000	2.545914000	1.823105000
1	0.665714000	1.468391000	2.245918000	1	1.372139000	1.321870000	2.534555000
6	0.540928000	-1.069926000	2.811200000	6	0.072046000	-0.713779000	2.954632000
1	-0.131997000	-0.339943000	3.268004000	1	-0.354714000	0.197523000	3.379347000
1	0.306528000	-2.045317000	3.244668000	1	-0.454116000	-1.571508000	3.378293000
1	1.562338000	-0.802314000	3.104843000	1	1.121570000	-0.776942000	3.253970000
1	0.929993000	-3.162143000	1.363732000	1	1.140265000	-2.560096000	1.585727000
1	-3.864354000	3.792811000	0.555908000	1	-4.771937000	3.358244000	0.185827000
35	-2.654778000	-0.418716000	-1.848897000	35	-2.453561000	-0.508784000	-1.964153000
1	-2.295450000	0.667876000	3.057550000	1	-2.483043000	0.911059000	2.875418000
TS2o2Cl				TS2o2Cl_P			
6	3.121623000	1.117397000	-0.807813000	6	3.375792000	0.861959000	-0.357163000
6	3.534885000	0.131741000	0.253036000	6	3.375794000	-0.189451000	0.722361000
6	1.537852000	2.245942000	0.910327000	6	1.578345000	2.186367000	0.943126000
6	2.527870000	2.443548000	-0.233616000	6	2.852225000	2.255749000	0.110810000
6	0.765547000	-2.274538000	0.046434000	6	0.393532000	-2.201661000	-0.684857000
6	0.623793000	1.286263000	1.125447000	6	0.516897000	1.370113000	0.846561000
6	0.301343000	0.174446000	0.189814000	6	0.277038000	0.362891000	-0.213917000
6	0.203141000	-1.211897000	0.756010000	6	-0.221059000	-1.053350000	0.190866000
1	3.991340000	1.405716000	-1.417002000	1	4.403730000	1.020219000	-0.716087000
6	3.497443000	-1.207553000	0.190185000	6	3.218285000	-1.515151000	0.583660000
6	3.064098000	-2.008335000	-1.029566000	6	3.010224000	-2.236105000	-0.741975000
6	1.521265000	-2.176409000	-1.248823000	6	1.678528000	-2.021212000	-1.495296000
1	3.509561000	-3.006009000	-0.948877000	1	3.124562000	-3.310692000	-0.560331000
1	3.882183000	0.572129000	1.187383000	1	3.543242000	0.182931000	1.732623000
1	2.408921000	0.661134000	-1.495678000	1	2.810212000	0.527117000	-1.226313000
8	0.126159000	0.410249000	-1.007595000	8	0.409096000	0.637742000	-1.399738000
1	1.135356000	-1.346814000	-1.835162000	1	1.650846000	-1.057293000	-1.998415000
1	1.359856000	-3.088744000	-1.830032000	1	1.633506000	-2.778201000	-2.286627000
1	3.473957000	-1.561877000	-1.941958000	1	3.814409000	-1.962976000	-1.436097000
6	1.814633000	3.206860000	-1.374251000	6	2.580436000	3.133376000	-1.134128000
1	1.438506000	4.174570000	-1.024933000	1	2.265613000	4.141127000	-0.843137000
1	2.515963000	3.394689000	-2.195826000	1	3.494058000	3.224973000	-1.732809000
1	0.974865000	2.617691000	-1.747203000	1	1.795471000	2.685301000	-1.746404000
6	3.686190000	3.319263000	0.298374000	6	3.939453000	2.940379000	0.970712000
1	4.394947000	3.542190000	-0.505463000	1	4.860036000	3.062656000	0.391582000
1	3.309318000	4.270826000	0.688929000	1	3.611055000	3.933223000	1.296387000
1	4.235531000	2.822711000	1.104909000	1	4.178362000	2.358135000	1.866433000
6	3.903495000	-2.039190000	1.384583000	6	3.312641000	-2.430254000	1.783569000
1	4.197504000	-1.420330000	2.237279000	1	3.423889000	-1.876891000	2.720534000
1	3.077714000	-2.686812000	1.706600000	1	2.424175000	-3.068792000	1.867007000
1	4.740032000	-2.706109000	1.138108000	1	4.170085000	-3.108799000	1.683357000
6	-1.995953000	-1.462837000	0.171415000	6	-1.676833000	-1.157230000	-0.282339000
8	-1.008495000	-3.320441000	-0.756416000	8	-0.653795000	-2.516916000	-1.662744000
7	-1.897650000	-2.512988000	-0.431853000	7	-1.857688000	-1.939691000	-1.279093000
6	-2.882204000	-0.366333000	0.445225000	6	-2.813126000	-0.403623000	0.306381000
6	-3.244994000	-0.070973000	1.774135000	6	-3.326412000	-0.792951000	1.555085000
6	-3.352265000	0.485851000	-0.579914000	6	-3.409858000	0.699449000	-0.327758000
6	-4.032608000	1.035663000	2.072666000	6	-4.380567000	-0.106606000	2.153464000
6	-4.144097000	1.591857000	-0.282853000	6	-4.464601000	1.396146000	0.262841000
6	-4.475546000	1.869889000	1.044296000	6	-4.946701000	0.992840000	1.507304000
1	-4.302478000	1.243891000	3.102224000	1	-4.759067000	-0.432678000	3.116439000
1	-4.497445000	2.227855000	-1.086161000	1	-4.901081000	2.243938000	-0.252596000
1	1.610820000	3.005806000	1.688652000	1	1.546214000	2.899371000	1.766670000
1	0.075282000	1.304072000	2.063967000	1	-0.254152000	1.434940000	1.611126000
6	0.089395000	-1.365375000	2.266300000	6	-0.069307000	-1.320457000	1.697487000
1	-0.700804000	-0.747532000	2.697648000	1	-0.709474000	-0.664246000	2.289345000
1	-0.121603000	-2.405909000	2.525960000	1	-0.344160000	-2.352591000	1.929964000

1	1.028503000	-1.078419000	2.753520000	1	0.961516000	-1.150643000	2.006564000
1	0.968768000	-3.170736000	0.628310000	1	0.491632000	-3.084323000	-0.038355000
1	-5.087887000	2.737223000	1.268052000	1	-5.766855000	1.537252000	1.964030000
17	-2.985760000	0.146574000	-2.260015000	17	-2.847907000	1.249303000	-1.904764000
1	-2.907992000	-0.732214000	2.563635000	1	-2.896358000	-1.657273000	2.048864000
TS2o2F				TS2o2F_P			
6	3.081734000	1.086418000	-0.640256000	6	3.465470000	0.422226000	-0.335093000
6	3.347989000	0.108876000	0.473754000	6	3.211339000	-0.398080000	0.903743000
6	1.295441000	2.238880000	0.849768000	6	1.822615000	2.172166000	0.564878000
6	2.425579000	2.420511000	-0.159364000	6	3.139229000	1.937282000	-0.162317000
6	0.614339000	-2.291819000	-0.074749000	6	0.057130000	-2.132994000	-0.549956000
6	0.358325000	1.283370000	0.955221000	6	0.648305000	1.527638000	0.481629000
6	0.156953000	0.160616000	-0.001137000	6	0.261566000	0.457168000	-0.473542000
6	-0.011354000	-1.219577000	0.562276000	6	-0.495531000	-0.791790000	0.062761000
1	4.024577000	1.365456000	-1.134049000	1	4.526815000	0.354631000	-0.616882000
6	3.311042000	-1.230827000	0.418717000	6	2.831405000	-1.682503000	0.975162000
6	3.037330000	-2.042475000	-0.839243000	6	2.610415000	-2.585218000	-0.230696000
6	1.535938000	-2.205383000	-1.258941000	6	1.442136000	-2.260293000	-1.183625000
1	3.461981000	-3.041432000	-0.690460000	1	2.472635000	-3.610186000	0.132198000
1	3.572047000	0.556637000	1.441665000	1	3.365361000	0.124869000	1.847113000
1	2.461961000	0.626838000	-1.411009000	1	2.909782000	0.026518000	-1.184728000
8	0.126289000	0.384099000	-1.213594000	8	0.498955000	0.537000000	-1.671991000
1	1.236005000	-1.377165000	-1.895088000	1	1.643199000	-1.382193000	-1.793745000
1	1.448485000	-3.120134000	-1.852001000	1	1.361659000	-3.099632000	-1.883943000
1	3.566778000	-1.607945000	-1.694068000	1	3.522009000	-2.604806000	-0.840881000
6	1.868182000	3.174411000	-1.389452000	6	3.080006000	2.605241000	-1.555686000
1	1.456410000	4.147676000	-1.101113000	1	2.908654000	3.683253000	-1.466120000
1	2.669287000	3.349661000	-2.117242000	1	4.030454000	2.457310000	-2.081485000
1	1.079037000	2.584865000	-1.859714000	1	2.272324000	2.171872000	-2.148404000
6	3.510565000	3.297182000	0.508174000	6	4.262429000	2.607544000	0.660534000
1	4.316928000	3.510290000	-0.200743000	1	5.223706000	2.501168000	0.148097000
1	3.091275000	4.253539000	0.839265000	1	4.065178000	3.677105000	0.790463000
1	3.950421000	2.806116000	1.382375000	1	4.359532000	2.163212000	1.656421000
6	3.548346000	-2.052439000	1.664323000	6	2.661535000	-2.364710000	2.313087000
1	3.731599000	-1.426754000	2.542655000	1	2.801387000	-1.675286000	3.150682000
1	2.681004000	-2.690169000	1.879256000	1	1.664997000	-2.815133000	2.404041000
1	4.404297000	-2.728193000	1.537731000	1	3.381204000	-3.186842000	2.422716000
6	-2.134576000	-1.447638000	-0.242663000	6	-1.909949000	-0.851683000	-0.539472000
8	-1.066827000	-3.282328000	-1.127219000	8	-0.886596000	-2.462103000	-1.618872000
7	-1.981726000	-2.476278000	-0.868053000	7	-2.068723000	-1.761167000	-1.431733000
6	-3.032042000	-0.377191000	0.079428000	6	-3.093173000	-0.089553000	-0.089279000
6	-3.662601000	-1.426312000	1.336814000	6	-4.267215000	-0.771116000	-0.277081000
6	-3.236232000	0.672865000	-0.832569000	6	-3.119416000	1.304547000	-0.006912000
6	-4.462008000	0.800841000	1.654760000	6	-5.396963000	-0.079913000	0.710612000
6	-4.028715000	1.769225000	-0.528572000	6	-4.225819000	2.018305000	0.429094000
6	-4.640228000	1.830670000	0.725304000	6	-5.375353000	1.314909000	0.791959000
1	-4.945639000	0.851617000	2.624057000	1	-6.289372000	-0.629149000	0.991511000
1	-4.157036000	2.550339000	-1.269060000	1	-4.176281000	3.100651000	0.464290000
1	1.269376000	3.008622000	1.621332000	1	1.859537000	2.968613000	1.307974000
1	-0.308633000	1.312342000	1.813518000	1	-0.132828000	1.814354000	1.178566000
6	-0.309066000	-1.357238000	2.048381000	6	-0.559107000	-0.835900000	1.598785000
1	-1.161695000	-0.752747000	2.367707000	1	-1.178576000	-0.026806000	1.992751000
1	-0.528476000	-2.399275000	2.295331000	1	-1.000976000	-1.778712000	1.931483000
1	0.555515000	-1.043516000	2.644676000	1	0.439956000	-0.742508000	2.025921000
1	0.720848000	-3.194158000	0.523328000	1	-0.061493000	-2.907001000	0.221445000
1	-5.259962000	2.686100000	0.973278000	1	-6.249606000	1.858315000	1.135185000
9	-2.652137000	0.603725000	-2.040685000	9	-2.019270000	2.000004000	-0.390755000
1	-3.520423000	-1.099264000	2.047575000	1	-4.269967000	-1.854294000	0.224674000
TS2pBr				TS2pBr_P			
6	3.746375000	1.712327000	-0.525555000	6	4.287801000	1.123566000	-0.383918000
6	4.065149000	0.930182000	0.721382000	6	4.228050000	0.371250000	0.921149000
6	1.489333000	2.413101000	0.543665000	6	2.232656000	2.438200000	0.393077000
6	2.685293000	2.837634000	-0.302937000	6	3.564972000	2.506448000	-0.338177000
6	2.207589000	-2.176410000	0.047885000	6	1.671724000	-2.281402000	-0.294999000
6	0.840614000	1.239915000	0.619367000	6	1.287758000	1.482541000	0.399660000
6	1.110162000	0.045437000	-0.224335000	6	1.213013000	0.278951000	-0.465392000
6	1.211892000	-1.286754000	0.453974000	6	0.761141000	-1.072584000	0.151328000

1	4.651604000	2.210415000	-0.903663000	1	5.334765000	1.321374000	-0.657046000
6	4.397013000	-0.365806000	0.817874000	6	4.190678000	-0.957221000	1.101614000
6	4.574583000	-1.308293000	-0.363561000	6	4.250905000	-1.979578000	-0.024607000
6	3.268315000	-1.911939000	-0.983800000	6	3.033677000	-2.094614000	-0.965940000
1	5.213386000	-2.136260000	-0.036934000	1	4.425254000	-2.965328000	0.421564000
1	3.988416000	1.489895000	1.653256000	1	4.212368000	0.992510000	1.816071000
1	3.414988000	1.044158000	-1.321374000	1	3.878104000	0.523979000	-1.196819000
8	1.225445000	0.168989000	-1.448155000	8	1.446096000	0.330684000	-1.667832000
1	2.876956000	-1.245324000	-1.747607000	1	2.982288000	-1.265291000	-1.668816000
1	3.532310000	-2.851569000	-1.477262000	1	3.183380000	-2.994457000	-1.573114000
1	5.114118000	-0.804876000	-1.173108000	1	5.124890000	-1.777091000	-0.655472000
6	2.168032000	3.317751000	-1.679246000	6	3.337475000	3.013401000	-1.781238000
1	1.468509000	4.153164000	-1.566824000	1	2.885453000	4.010883000	-1.816071000
1	3.006814000	3.661302000	-2.296058000	1	4.297199000	3.079021000	-2.306566000
1	1.658109000	2.499646000	-2.191192000	1	2.679296000	2.332013000	-2.322797000
6	3.364040000	4.028663000	0.412705000	6	4.460999000	3.521206000	0.407679000
1	4.194286000	4.411159000	-0.189401000	1	5.416949000	3.636154000	-0.112501000
1	2.653684000	4.848167000	0.566877000	1	3.980946000	4.504557000	0.454712000
1	3.760818000	3.743124000	1.392403000	1	4.671019000	3.202545000	1.433842000
6	4.621938000	-0.997100000	2.171977000	6	4.156960000	-1.547936000	2.492339000
1	4.474002000	-0.285076000	2.989045000	1	4.079460000	-0.779789000	3.267199000
1	3.932505000	-1.837186000	2.327341000	1	3.311150000	-2.237277000	2.609470000
1	5.635581000	-1.410697000	2.254233000	1	5.062318000	-2.138703000	2.684861000
6	-0.585632000	-2.143049000	-0.642270000	6	-0.553393000	-1.514867000	-0.509137000
8	1.063232000	-3.673341000	-1.125426000	8	0.856533000	-3.017369000	-1.266075000
7	-0.060847000	-3.133593000	-1.105737000	7	-0.447394000	-2.559625000	-1.249354000
6	-1.821392000	-1.432095000	-0.454391000	6	-1.883323000	-0.907929000	-0.306509000
6	-2.783023000	-1.918739000	0.451132000	6	-3.014225000	-1.741281000	-0.237017000
6	-2.042784000	-0.208638000	-1.114479000	6	-2.064831000	0.478796000	-0.188446000
6	-3.958382000	-1.208639000	0.675783000	6	-4.288181000	-1.209930000	-0.059679000
1	-2.606703000	-2.853462000	0.971776000	1	-2.886464000	-2.815183000	-0.313164000
6	-3.213927000	0.506986000	-0.887298000	6	-3.334651000	1.023734000	-0.006425000
1	-1.290108000	0.178509000	-1.790844000	1	-1.224327000	1.156350000	-0.265370000
6	-4.159662000	-0.002240000	0.003849000	6	-4.434960000	0.171962000	0.057336000
1	-4.704033000	-1.584347000	1.366278000	1	-5.152564000	-1.861208000	-0.003119000
1	-3.389712000	1.447457000	-1.395778000	1	-3.463090000	2.096394000	0.077654000
35	-5.768684000	0.981787000	0.318313000	35	-6.182543000	0.912739000	0.316429000
1	1.127107000	3.192825000	1.213858000	1	2.050407000	3.271219000	1.071562000
1	0.057326000	1.134328000	1.365951000	1	0.481718000	1.589720000	1.120440000
6	0.676704000	-1.415979000	1.873479000	6	0.608946000	-1.013652000	1.681826000
1	-0.363147000	-1.088902000	1.963812000	1	-0.208731000	-0.352172000	1.976630000
1	0.724442000	-2.458332000	2.199466000	1	0.384121000	-2.008096000	2.075168000
1	1.274617000	-0.817238000	2.569947000	1	1.529784000	-0.652327000	2.142891000
1	2.441208000	-2.971350000	0.752465000	1	1.784869000	-2.939181000	0.576472000
TS2pCl				TS2pCl_P			
6	3.370002000	1.481755000	-0.538459000	6	3.784298000	0.938229000	-0.399400000
6	3.634639000	0.645615000	0.685896000	6	3.687549000	0.162080000	0.889356000
6	1.221798000	2.388622000	0.598439000	6	1.843987000	2.386559000	0.436386000
6	2.435414000	2.705006000	-0.270209000	6	3.168782000	2.370040000	-0.311383000
6	1.453246000	-2.237662000	0.001236000	6	0.924899000	-2.264521000	-0.336218000
6	0.457240000	1.287117000	0.669372000	6	0.829877000	1.504863000	0.436249000
6	0.582426000	0.089262000	-0.202900000	6	0.656546000	0.326728000	-0.449588000
6	0.562882000	-1.260216000	0.447923000	6	0.117210000	-0.999909000	0.150371000
1	4.312906000	1.892107000	-0.929620000	1	4.839120000	1.063174000	-0.685084000
6	3.834071000	-0.679208000	0.750080000	6	3.555448000	-1.164057000	1.040285000
6	3.886689000	-1.609804000	-0.452793000	6	3.523244000	-2.161012000	-0.109556000
6	2.511070000	-2.061347000	-1.051945000	6	2.284553000	-2.166634000	-1.030086000
1	4.443005000	-2.506216000	-0.157408000	1	3.633879000	-3.166867000	0.311324000
1	3.636311000	1.190579000	1.629580000	1	3.730950000	0.761520000	1.798157000
1	2.953927000	0.867352000	-1.337856000	1	3.318955000	0.389962000	-1.218594000
8	0.680708000	0.226649000	-1.426751000	8	0.874475000	0.385781000	-1.654529000
1	2.173677000	-1.340989000	-1.792276000	1	2.282912000	-1.321768000	-1.716147000
1	2.664694000	-3.011941000	-1.570459000	1	2.355800000	-3.062821000	-1.656624000
1	4.457484000	-1.147958000	-1.265691000	1	4.398539000	-2.006492000	-0.752022000
6	1.939481000	3.262238000	-1.625171000	6	2.961550000	2.926611000	-1.739159000
1	1.330438000	4.161314000	-1.481585000	1	2.585435000	3.954658000	-1.708041000
1	2.795199000	3.532037000	-2.255268000	1	3.916600000	2.932924000	-2.276920000

1	1.338805000	2.509797000	-2.139473000	1	2.247223000	2.309103000	-2.286278000
6	3.249052000	3.805993000	0.448966000	6	4.148733000	3.296215000	0.444146000
1	4.099872000	4.113897000	-0.167021000	1	5.103833000	3.351049000	-0.087282000
1	2.630141000	4.690370000	0.635517000	1	3.745404000	4.311639000	0.520814000
1	3.637215000	3.461823000	1.413157000	1	4.347264000	2.938093000	1.459521000
6	4.022581000	-1.358764000	2.086229000	6	3.499808000	-1.783564000	2.417690000
1	3.968670000	-0.652479000	2.919727000	1	3.490031000	-1.030340000	3.210784000
1	3.252399000	-2.125277000	2.242923000	1	2.608188000	-2.412641000	2.533617000
1	4.988833000	-1.877587000	2.135618000	1	4.362831000	-2.442427000	2.581505000
6	-1.337733000	-1.907815000	-0.618144000	6	-1.239335000	-1.329256000	-0.490404000
8	0.134481000	-3.588943000	-1.166886000	8	0.038180000	-2.918150000	-1.303435000
7	-0.927506000	-2.937705000	-1.110585000	7	-1.227919000	-2.364884000	-1.250285000
6	-2.490878000	-1.079875000	-0.388580000	6	-2.514724000	-0.627491000	-0.245747000
6	-3.478698000	-1.486670000	0.527985000	6	-3.698186000	-1.377408000	-0.126318000
6	-2.600719000	0.173678000	-1.019437000	6	-2.592299000	0.769488000	-0.134927000
6	-4.572377000	-0.668141000	0.791576000	6	-4.923824000	-0.755650000	0.093049000
1	-3.387052000	-2.445270000	1.026351000	1	-3.649808000	-2.458157000	-0.196637000
6	-3.688952000	0.998215000	-0.753690000	6	-3.811983000	1.405265000	0.088850000
1	-1.826086000	0.497699000	-1.704045000	1	-1.708945000	1.384217000	-0.251167000
6	-4.664255000	0.566909000	0.147380000	6	-4.967290000	0.634283000	0.202187000
1	-5.339772000	-0.980176000	1.490163000	1	-5.830700000	-1.341576000	0.188637000
1	-3.780883000	1.962825000	-1.238808000	1	-3.862826000	2.485013000	0.166802000
17	-6.040254000	1.608533000	0.484405000	17	-6.512089000	1.430392000	0.493726000
1	0.957802000	3.187721000	1.291283000	1	1.732275000	3.217743000	1.132171000
1	-0.315672000	1.247405000	1.433032000	1	0.040398000	1.658178000	1.167031000
6	0.050834000	-1.363772000	1.878028000	6	-0.002883000	-0.959173000	1.684443000
1	-0.947069000	-0.933303000	2.001414000	1	-0.764833000	-0.245573000	2.006021000
1	-0.001907000	-2.412248000	2.182955000	1	-0.292885000	-1.941806000	2.064504000
1	0.724159000	-0.844955000	2.569815000	1	0.949799000	-0.674476000	2.134298000
1	1.621383000	-3.066114000	0.685584000	1	1.004518000	-2.945964000	0.520611000
TS2pF				TS2pF_P			
6	3.231843000	1.237648000	-0.550372000	6	3.549857000	0.745593000	-0.418528000
6	3.432552000	0.350145000	0.649657000	6	3.413706000	-0.051080000	0.853970000
6	1.211206000	2.337585000	0.648805000	6	1.739081000	2.319667000	0.480068000
6	2.436755000	2.545253000	-0.235699000	6	3.048415000	2.217943000	-0.288198000
6	0.947917000	-2.274024000	-0.047111000	6	0.455973000	-2.230395000	-0.379887000
6	0.336322000	1.321010000	0.711295000	6	0.660194000	1.518719000	0.476663000
6	0.321044000	0.134584000	-0.185758000	6	0.386019000	0.375989000	-0.430395000
6	0.176581000	-1.218123000	0.440502000	6	-0.242004000	-0.919343000	0.150228000
1	4.204358000	1.556020000	-0.954635000	1	4.606579000	0.795543000	-0.719774000
6	3.493710000	-0.989377000	0.680502000	6	3.184023000	-1.366725000	0.977603000
6	3.424503000	-1.891248000	-0.543239000	6	3.058060000	-2.331503000	-0.193131000
6	1.997374000	-2.185657000	-1.119814000	6	1.809195000	-2.221192000	-1.093100000
1	3.892016000	-2.846638000	-0.280514000	1	3.097228000	-3.352332000	0.203781000
1	3.510408000	0.869431000	1.604534000	1	3.516487000	0.521658000	1.775118000
1	2.736950000	0.688455000	-1.352282000	1	3.030641000	0.254176000	-1.241360000
8	0.409229000	0.287396000	-1.408710000	8	0.588917000	0.446274000	-1.637472000
1	1.721424000	-1.418873000	-1.838724000	1	1.862594000	-1.363232000	-1.760571000
1	2.041123000	-3.135834000	-1.659626000	1	1.802378000	-3.105588000	-1.740093000
1	4.022556000	-1.470747000	-1.358996000	1	3.933243000	-2.229825000	-0.846281000
6	1.979233000	3.184685000	-1.567627000	6	2.865285000	2.822606000	-1.699614000
1	1.469412000	4.138141000	-1.391802000	1	2.569826000	3.875409000	-1.639399000
1	2.847598000	3.379887000	-2.207858000	1	3.810486000	2.768532000	-2.251918000
1	1.295042000	2.511557000	-2.087471000	1	2.098119000	2.274910000	-2.249491000
6	3.374264000	3.536673000	0.492084000	6	4.107585000	3.047803000	0.472339000
1	4.243234000	3.766920000	-0.132443000	1	5.057084000	3.040099000	-0.071802000
1	2.856012000	4.477133000	0.708755000	1	3.785802000	4.089572000	0.576405000
1	3.738616000	3.131029000	1.441547000	1	4.290708000	2.652913000	1.476895000
6	3.638134000	-1.716709000	1.996805000	6	3.103198000	-2.012293000	2.341741000
1	3.674503000	-1.028986000	2.846629000	1	3.163426000	-1.279273000	3.151363000
1	2.796304000	-2.403558000	2.154024000	1	2.168093000	-2.574371000	2.459313000
1	4.546481000	-2.333107000	2.012826000	1	3.915920000	-2.738431000	2.475753000
6	-1.807897000	-1.640190000	-0.588638000	6	-1.631641000	-1.126519000	-0.471671000
8	-0.524730000	-3.446927000	-1.211173000	8	-0.492638000	-2.787772000	-1.347290000
7	-1.515195000	-2.692790000	-1.116670000	7	-1.713420000	-2.139395000	-1.257091000
6	-2.857546000	-0.697229000	-0.316877000	6	-2.843193000	-0.335320000	-0.179288000
6	-3.849242000	-1.001893000	0.636676000	6	-4.073572000	-0.999495000	-0.022182000

6	-2.856320000	0.564162000	-0.945209000	6	-2.813120000	1.063961000	-0.060692000
6	-4.840931000	-0.074390000	0.937905000	6	-5.242507000	-0.291433000	0.241647000
1	-3.838805000	-1.967007000	1.130699000	1	-4.103637000	-2.080415000	-0.099850000
6	-3.841949000	1.496976000	-0.642363000	6	-3.974693000	1.785361000	0.207728000
1	-2.074364000	0.804788000	-1.655335000	1	-1.890071000	1.610619000	-0.206122000
6	-4.816944000	1.158215000	0.291744000	6	-5.170244000	1.092636000	0.355415000
1	-5.619594000	-0.288088000	1.660851000	1	-6.194660000	-0.793711000	0.369980000
1	-3.865597000	2.472293000	-1.114432000	1	-3.962750000	2.865764000	0.294604000
9	-5.773181000	2.060956000	0.585516000	9	-6.298613000	1.786321000	0.621258000
1	1.043308000	3.144852000	1.361909000	1	1.700961000	3.142446000	1.193583000
1	-0.424322000	1.346293000	1.487854000	1	-0.107485000	1.716995000	1.219858000
6	-0.310433000	-1.297039000	1.880724000	6	-0.332613000	-0.905509000	1.686631000
1	-1.258308000	-0.773204000	2.034582000	1	-1.031910000	-0.143375000	2.037598000
1	-0.459425000	-2.340676000	2.170144000	1	-0.691666000	-1.871680000	2.049817000
1	0.425642000	-0.859375000	2.564688000	1	0.646451000	-0.705706000	2.125221000
1	1.043362000	-3.129878000	0.617239000	1	0.495359000	-2.936665000	0.459710000
TS3o1Br				TS3o1Br_P			
6	-3.036161000	-1.272333000	-0.805841000	6	-2.763825000	-1.290572000	-0.795300000
6	-4.146169000	-0.895555000	0.144464000	6	-3.934441000	-1.035445000	0.124130000
6	-1.220647000	-1.114648000	0.973362000	6	-0.979737000	-1.034348000	1.061028000
6	-1.782806000	-1.967929000	-0.161783000	6	-1.500138000	-1.910530000	-0.116978000
6	-2.493710000	1.954785000	0.090612000	6	-2.512873000	1.949803000	0.140827000
6	-0.515655000	0.071461000	0.915086000	6	-0.191880000	0.304327000	0.851242000
6	-0.322873000	0.908846000	-0.333681000	6	-0.297549000	1.083125000	-0.467368000
6	-1.369308000	1.922028000	-0.652413000	6	-1.492090000	1.917169000	-0.739870000
1	-3.425536000	-1.984743000	-1.549408000	1	-3.069870000	-2.018216000	-1.561992000
6	-4.882275000	0.229380000	0.156497000	6	-4.772685000	0.014422000	0.153840000
6	-4.710928000	1.383204000	-0.818965000	6	-4.688861000	1.217337000	-0.769519000
6	-3.821353000	2.542294000	-0.264513000	6	-3.909186000	2.412605000	-0.142122000
1	-5.696639000	1.797523000	-1.063805000	1	-5.702657000	1.558084000	-1.012166000
1	-4.387642000	-1.646479000	0.896033000	1	-4.134972000	-1.831671000	0.839447000
1	-2.698143000	-0.399144000	-1.366770000	1	-2.486421000	-0.386772000	-1.338694000
8	0.618527000	0.744924000	-1.106654000	8	0.596537000	0.988124000	-1.303516000
1	-2.526209000	1.328058000	0.974761000	1	-2.394549000	1.449102000	1.096109000
1	-3.751902000	3.328363000	-1.020784000	1	-3.934076000	3.255695000	-0.837791000
1	-4.296560000	2.974755000	0.623563000	1	-4.400147000	2.732690000	0.782301000
1	-4.270115000	1.039343000	-1.758984000	1	-4.207661000	0.954969000	-1.716259000
6	-1.138146000	2.703153000	-1.919607000	6	-1.519209000	2.544091000	-2.110184000
1	-1.167616000	2.042271000	-2.793121000	1	-1.606309000	1.772315000	-2.883799000
1	-1.880443000	3.490825000	-2.056970000	1	-2.347715000	3.242766000	-2.228713000
1	-0.142891000	3.157603000	-1.908164000	1	-0.581377000	3.072264000	-2.302454000
6	-0.749924000	-2.212586000	-1.282870000	6	-0.415955000	-2.148460000	-1.183204000
1	0.161572000	-2.648015000	-0.866928000	1	0.507467000	-2.507945000	-0.722759000
1	-1.165743000	-2.908222000	-2.020162000	1	-0.759477000	-2.907569000	-1.894015000
1	-0.478582000	-1.292846000	-1.801613000	1	-0.175643000	-1.244806000	-1.743840000
6	-2.198271000	-3.337907000	0.415660000	6	-1.881064000	-3.287688000	0.482470000
1	-2.687401000	-3.942021000	-0.355663000	1	-2.401464000	-3.885828000	-0.272348000
1	-1.320885000	-3.880360000	0.773989000	1	-0.988658000	-3.830514000	0.797554000
1	-2.894005000	-3.236538000	1.254656000	1	-2.536103000	-3.198479000	1.354382000
6	-5.954628000	0.442473000	1.199171000	6	-5.892882000	0.079479000	1.165612000
1	-6.011043000	-0.388632000	1.907648000	1	-5.883506000	-0.775600000	1.847045000
1	-5.771480000	1.361414000	1.771196000	1	-5.826054000	0.993601000	1.769623000
1	-6.940031000	0.562584000	0.730271000	1	-6.869791000	0.111064000	0.665769000
6	1.583328000	-0.538114000	1.329308000	6	1.219283000	-0.157405000	1.149386000
8	0.551398000	-2.582276000	1.606779000	8	-0.009255000	-1.840169000	1.820947000
7	1.442528000	-1.720703000	1.561487000	7	1.275430000	-1.310242000	1.701892000
6	2.592574000	0.463789000	1.114977000	6	2.440181000	0.649867000	0.937951000
6	2.637097000	1.599183000	1.942201000	6	2.578434000	1.865511000	1.624457000
6	3.510533000	0.373172000	0.048617000	6	3.467823000	0.267882000	0.063956000
6	3.578459000	2.601419000	1.726548000	6	3.710824000	2.661241000	1.462142000
1	1.921488000	1.680446000	2.753500000	1	1.787548000	2.179702000	2.298909000
6	4.458156000	1.368681000	-0.166215000	6	4.606661000	1.053099000	-0.105957000
6	4.489712000	2.483422000	0.675037000	6	4.728031000	2.251192000	0.599081000
1	3.601831000	3.469608000	2.376379000	1	3.798320000	3.594525000	2.008594000
1	5.159064000	1.277747000	-0.987726000	1	5.384441000	0.734213000	-0.790107000
1	-1.584892000	-1.388493000	1.959049000	1	-1.815995000	-0.857374000	1.742379000
1	-0.523085000	0.662666000	1.829766000	1	-0.482001000	0.987866000	1.658742000

1	5.226586000	3.260483000	0.499437000	1	5.614662000	2.862406000	0.464047000
35	3.458605000	-1.120679000	-1.133870000	35	3.311216000	-1.328818000	-0.982468000
TS3o1Cl				TS3o1Cl_P			
6	-2.916463000	1.173750000	0.837197000	6	-2.594567000	1.174893000	0.954499000
6	-3.905899000	0.775141000	-0.230131000	6	-3.704909000	1.000620000	-0.054717000
6	-0.947215000	1.258308000	-0.777151000	6	-0.704573000	1.220814000	-0.810631000
6	-1.667401000	1.994061000	0.351228000	6	-1.326949000	1.924791000	0.431108000
6	-2.064792000	-1.949440000	-0.166539000	6	-2.155576000	-1.907544000	-0.392849000
6	-0.177924000	0.112440000	-0.735685000	6	0.133745000	-0.098863000	-0.715486000
6	-0.012552000	-0.785890000	0.474094000	6	-0.029717000	-1.044761000	0.482748000
6	-1.006052000	-1.879598000	0.665285000	6	-1.197946000	-1.952866000	0.555869000
1	-3.423974000	1.811497000	1.577243000	1	-2.970411000	1.785398000	1.789260000
6	-4.555535000	-0.394403000	-0.362689000	6	-4.492427000	-0.065843000	-0.274212000
6	-4.387670000	-1.583594000	0.569974000	6	-4.404302000	-1.381417000	0.479158000
6	-3.368882000	-2.647243000	0.047270000	6	-3.545915000	-2.450095000	-0.263388000
1	-5.357842000	-2.077822000	0.702808000	1	-5.413860000	-1.786975000	0.617267000
1	-4.131955000	1.547281000	-0.964835000	1	-3.906090000	1.879082000	-0.665876000
1	-2.563556000	0.295806000	1.381408000	1	-2.306603000	0.218748000	1.392972000
8	0.868670000	-0.608138000	1.313015000	8	0.794121000	-1.021167000	1.393125000
1	-2.074184000	-1.279497000	-1.019026000	1	-1.997036000	-1.286892000	-1.268522000
1	-3.303357000	-3.462072000	0.772784000	1	-3.575160000	-3.384183000	0.304149000
1	-3.733590000	-3.069136000	-0.896441000	1	-3.972658000	-2.650286000	-1.251093000
1	-4.059271000	-1.260152000	1.561728000	1	-3.981527000	-1.236825000	1.477676000
6	-0.813543000	-2.711111000	1.906365000	6	-1.292173000	-2.751453000	1.830837000
1	-0.940904000	-2.099274000	2.806354000	1	-1.496922000	-2.092709000	2.683011000
1	-1.514507000	-3.545787000	1.953538000	1	-2.076382000	-3.507734000	1.787565000
1	0.205790000	-3.107312000	1.942329000	1	-0.338113000	-3.242572000	2.039549000
6	-0.758819000	2.236880000	1.574781000	6	-0.311326000	2.075233000	1.578470000
1	0.127288000	2.800501000	1.274240000	1	0.607397000	2.545827000	1.216743000
1	-1.303136000	2.816898000	2.328241000	1	-0.731312000	2.714834000	2.361846000
1	-0.430429000	1.305748000	2.037454000	1	-0.046145000	1.118855000	2.030140000
6	-2.131369000	3.366416000	-0.181707000	6	-1.740432000	3.348603000	-0.019521000
1	-2.714607000	3.892764000	0.581082000	1	-2.329233000	3.827391000	0.769369000
1	-1.268629000	3.983129000	-0.443100000	1	-0.859569000	3.962562000	-0.213103000
1	-2.756059000	3.270177000	-1.075420000	1	-2.341835000	3.340312000	-0.933414000
6	-5.512262000	-0.624482000	-1.508960000	6	-5.555825000	-0.030859000	-1.347060000
1	-5.565077000	0.236985000	-2.180475000	1	-5.549089000	0.909874000	-1.904294000
1	-5.212880000	-1.497607000	-2.103293000	1	-5.418838000	-0.849815000	-2.064979000
1	-6.524300000	-0.835505000	-1.139439000	1	-6.554500000	-0.166380000	-0.911815000
6	1.904727000	0.846106000	-0.956783000	6	1.539189000	0.456637000	-0.848231000
8	0.799157000	2.865499000	-1.113286000	8	0.267367000	2.149901000	-1.409979000
7	1.722240000	2.037789000	-1.090013000	7	1.565792000	1.669307000	-1.263328000
6	2.935068000	-0.149649000	-0.832566000	6	2.774964000	-0.326648000	-0.659673000
6	2.898676000	-1.285129000	-1.661780000	6	2.841909000	-1.613815000	-1.221139000
6	3.955357000	-0.064588000	0.137746000	6	3.895851000	0.127224000	0.056893000
6	3.850463000	-2.292063000	-1.539306000	6	3.980391000	-2.404586000	-1.099724000
1	2.110520000	-1.362728000	-2.402746000	1	1.984728000	-1.991136000	-1.769827000
6	4.915787000	-1.065409000	0.256908000	6	5.041541000	-0.658058000	0.187083000
6	4.859978000	-2.180535000	-0.581005000	6	5.085968000	-1.923269000	-0.396833000
1	3.805911000	-3.158778000	-2.189927000	1	4.003175000	-3.390890000	-1.551134000
1	5.694599000	-0.973426000	1.005127000	1	5.886240000	-0.279536000	0.751262000
1	-1.236615000	1.581544000	-1.772895000	1	-1.493693000	1.096885000	-1.556509000
1	-0.084607000	-0.417637000	-1.682295000	1	-0.071044000	-0.678487000	-1.623682000
1	5.607128000	-2.960608000	-0.478166000	1	5.979668000	-2.529741000	-0.291806000
17	4.040464000	1.314223000	1.219807000	17	3.887932000	1.685114000	0.884951000
TS3o1F				TS3o1F_P			
6	-2.827123000	1.059397000	0.865071000	6	-2.612393000	1.069957000	0.961075000
6	-3.755243000	0.665633000	-0.257651000	6	-3.592827000	0.885235000	-0.173151000
6	-0.811466000	1.334298000	-0.668996000	6	-0.557697000	1.383588000	-0.589281000
6	-1.608237000	1.968926000	0.469543000	6	-1.355596000	1.936187000	0.629822000
6	-1.775164000	-1.959679000	-0.261532000	6	-1.848885000	-1.894142000	-0.485499000
6	0.011079000	0.225975000	-0.663203000	6	0.318018000	0.083146000	-0.547924000
6	0.188333000	-0.723498000	0.504920000	6	0.131987000	-0.927640000	0.594867000
6	-0.747895000	-1.877731000	0.607812000	6	-0.962257000	-1.924655000	0.530712000
1	-3.394612000	1.628946000	1.617101000	1	-3.120343000	1.596449000	1.783136000
6	-4.336357000	-0.527680000	-0.471696000	6	-4.286751000	-0.212314000	-0.519076000
6	-4.137758000	-1.752476000	0.407498000	6	-4.197005000	-1.553219000	0.188537000

6	-3.045936000	-2.734492000	-0.127798000	6	-3.201216000	-2.537153000	-0.498573000
1	-5.084141000	-2.302283000	0.479699000	1	-5.188250000	-2.022177000	0.203173000
1	-3.995622000	1.461349000	-0.962064000	1	-3.778426000	1.778687000	-0.767331000
1	-2.446087000	0.173508000	1.376513000	1	-2.302800000	0.109158000	1.373271000
8	1.031168000	-0.540738000	1.381784000	8	0.873409000	-0.884023000	1.572576000
1	-1.794106000	-1.247318000	-1.078698000	1	-1.675880000	-1.209147000	-1.398767000
1	-2.960578000	-3.579245000	0.560477000	1	-3.215304000	-3.488686000	0.039429000
1	-3.355671000	-3.128109000	-1.102883000	1	-3.521470000	-2.733118000	-1.526753000
1	-3.861814000	-1.463194000	1.425418000	1	-3.889548000	-1.429046000	1.230946000
6	-0.548791000	-2.760995000	1.811581000	6	-1.084775000	-2.800612000	1.751079000
1	-0.746783000	-2.206966000	2.736000000	1	-1.388657000	-2.207106000	2.621196000
1	-1.197653000	-3.637822000	1.788493000	1	-1.810838000	-3.602169000	1.612736000
1	0.491367000	-3.095888000	1.867295000	1	-0.114952000	-3.240582000	1.998354000
6	-0.757636000	2.191979000	1.737667000	6	-0.474539000	2.060352000	1.886155000
1	0.105779000	2.817625000	1.500935000	1	0.446593000	2.601897000	1.651489000
1	-1.359239000	2.699290000	2.500021000	1	-1.008817000	2.624647000	2.657616000
1	-0.394835000	1.255277000	2.161757000	1	-0.203137000	1.091143000	2.304666000
6	-2.126969000	3.342120000	-0.007672000	6	-1.822966000	3.362738000	0.243026000
1	-2.760060000	3.797455000	0.761053000	1	-2.511559000	3.743050000	1.004225000
1	-1.290055000	4.014641000	-0.208522000	1	-0.972377000	4.043078000	0.177939000
1	-2.718230000	3.261425000	-0.925360000	1	-2.338274000	3.387357000	-0.721877000
6	-5.238253000	-0.748499000	-1.663355000	6	-5.228310000	-0.189896000	-1.700428000
1	-5.313574000	0.142202000	-2.293307000	1	-5.220423000	0.774346000	-2.215936000
1	-4.871654000	-1.573473000	-2.288057000	1	-4.963561000	-0.965520000	-2.430624000
1	-6.249925000	-1.030291000	-1.343331000	1	-6.257648000	-0.402994000	-1.383886000
6	2.059066000	1.064394000	-0.795748000	6	1.716111000	0.673570000	-0.591404000
8	0.868919000	3.041731000	-0.838643000	8	0.427669000	2.411345000	-0.961189000
7	1.828536000	2.254059000	-0.848934000	7	1.726041000	1.934391000	-0.843331000
6	3.119713000	0.100211000	-0.703747000	6	2.953658000	-0.111605000	-0.490105000
6	3.205199000	-0.982546000	-1.595790000	6	2.956092000	-1.484979000	-0.796844000
6	4.055258000	0.171339000	0.339719000	6	4.177648000	0.447206000	-0.091444000
6	4.206132000	-1.939791000	-1.451901000	6	4.119405000	-2.246625000	-0.722729000
1	2.478133000	-1.060722000	-2.396959000	1	2.031706000	-1.961397000	-1.105828000
6	5.062980000	-0.768021000	0.492196000	6	5.347663000	-0.294769000	-0.003960000
6	5.133531000	-1.831301000	-0.411084000	6	5.319226000	-1.652180000	-0.324703000
1	4.263659000	-2.768711000	-2.148964000	1	4.087799000	-3.301853000	-0.972457000
1	5.765961000	-0.662415000	1.310667000	1	6.257020000	0.201013000	0.316855000
1	-1.080961000	1.700347000	-1.655525000	1	-1.250545000	1.312015000	-1.432275000
1	0.161073000	-0.247788000	-1.632162000	1	0.161314000	-0.446281000	-1.493655000
1	5.914859000	-2.575585000	-0.297356000	1	6.229622000	-2.239117000	-0.260452000
9	3.971951000	1.192891000	1.212242000	9	4.237811000	1.754880000	0.239568000
TS3o2Br				TS3o2Br_P			
6	3.401625000	1.033156000	-0.569280000	6	-2.951829000	1.235094000	0.905402000
6	3.954294000	0.418649000	0.693205000	6	-3.967027000	0.751269000	-0.103555000
6	1.077474000	1.360714000	0.417905000	6	-1.018778000	1.447190000	-0.788164000
6	2.193861000	2.021811000	-0.388788000	6	-1.828509000	2.160219000	0.332039000
6	1.861971000	-1.967596000	-0.172251000	6	-1.876374000	-1.827410000	-0.098190000
6	0.216171000	0.340009000	0.069387000	6	0.050341000	0.343131000	-0.498832000
6	0.272433000	-0.442586000	-1.224141000	6	-0.013875000	-0.500355000	-0.780746000
6	1.112533000	-1.672128000	-1.253459000	6	-0.957169000	-1.638567000	0.869729000
1	4.194846000	1.614670000	-1.063898000	1	-3.471399000	1.841472000	1.662460000
6	4.364275000	-0.847281000	0.885425000	6	-4.525570000	-0.464022000	-0.235373000
6	4.325672000	-1.935203000	-0.176617000	6	-4.221103000	-1.665165000	0.642582000
6	3.063039000	-2.852352000	-0.086279000	6	-3.144530000	-2.612887000	0.029772000
1	5.214931000	-2.569465000	-0.076047000	1	-5.141225000	-2.242648000	0.793503000
1	4.049391000	1.099083000	1.538913000	1	-4.310777000	1.513094000	-0.801322000
1	3.107351000	0.255011000	-1.276056000	1	-2.505471000	0.400400000	1.447880000
8	-0.299435000	-0.066286000	-2.246671000	8	0.691547000	-0.208575000	1.742800000
1	1.712454000	-1.364048000	0.715917000	1	-1.816174000	-1.225497000	-0.998910000
1	3.105636000	-3.594183000	-0.887884000	1	-3.030454000	-3.485273000	0.678519000
1	3.070800000	-3.391201000	0.868296000	1	-3.477156000	-2.969954000	-0.950118000
1	4.357741000	-1.502958000	-1.180658000	1	-3.876182000	-1.353118000	1.632805000
6	1.176468000	-2.378233000	-2.582308000	6	-0.916252000	-2.384072000	2.178246000
1	1.665789000	-1.748090000	-3.333602000	1	-1.229696000	-1.735215000	3.003599000
1	1.718274000	-3.323192000	-2.518872000	1	-1.556351000	-3.266676000	2.170864000
1	0.166730000	-2.576760000	-2.953937000	1	0.109148000	-2.695453000	2.397983000
6	1.735316000	2.462131000	-1.794878000	6	-0.925411000	2.642195000	1.481938000

1	0.886364000	3.144301000	-1.712668000	1	-0.109417000	3.258630000	1.093018000
1	2.555179000	2.981741000	-2.303223000	1	-1.507281000	3.257108000	2.176620000
1	1.435706000	1.616877000	-2.415085000	1	-0.488464000	1.816089000	2.043617000
6	2.666344000	3.276140000	0.376419000	6	-2.482914000	3.410319000	-0.306981000
1	3.511548000	3.741816000	-0.141112000	1	-3.196470000	3.852823000	0.395471000
1	1.857079000	4.006950000	0.442891000	1	-1.726683000	4.159062000	-0.548107000
1	2.986228000	3.038762000	1.396061000	1	-3.018319000	3.176292000	-1.231865000
6	4.883680000	-1.298814000	2.230205000	6	-5.532034000	-0.732574000	-1.330263000
1	4.850371000	-0.498077000	2.974227000	1	-5.681896000	0.137230000	-1.975660000
1	4.297060000	-2.142544000	2.616525000	1	-5.212429000	-1.571134000	-1.962339000
1	5.919685000	-1.653679000	2.152363000	1	-6.503515000	-1.018785000	-0.906596000
6	-1.746237000	1.341067000	-0.146495000	6	1.328646000	1.154089000	-0.623130000
8	-0.459420000	3.188212000	0.352621000	8	-0.212303000	2.458305000	-1.488009000
7	-1.453693000	2.497549000	0.071028000	7	1.138857000	2.285451000	-1.204353000
6	-2.834510000	0.463444000	-0.489022000	6	2.689437000	0.812709000	-0.163113000
6	-3.383887000	-0.426844000	0.452315000	6	3.266325000	-0.467477000	-0.222896000
6	-3.333880000	0.435450000	-1.804358000	6	3.481602000	1.846064000	0.374060000
6	-4.407882000	-1.304061000	0.108070000	6	4.559021000	-0.713890000	0.236399000
6	-4.365356000	-0.429713000	-2.152727000	6	4.776678000	1.616160000	0.826113000
6	-4.900064000	-1.299247000	-1.198155000	6	5.317082000	0.330792000	0.763322000
1	-4.815783000	-1.978303000	0.851816000	1	4.968351000	-1.715397000	0.173638000
1	-4.745745000	-0.433713000	-3.168596000	1	5.356658000	2.435586000	1.237838000
1	1.101419000	1.593722000	1.478774000	1	-1.731048000	1.075408000	-1.528998000
1	-0.210745000	-0.217276000	0.900848000	1	0.030007000	-0.348337000	-1.346211000
1	-5.699260000	-1.982325000	-1.467040000	1	6.322040000	0.134604000	1.122697000
35	-2.718873000	-0.441697000	2.245473000	35	2.322986000	-1.963434000	-0.975126000
1	-2.885853000	1.092929000	-2.539348000	1	3.047188000	2.837002000	0.442092000
TS3o2Cl				TS3o2Cl_P			
6	3.107810000	0.956577000	-0.753301000	6	2.645671000	1.165820000	-0.994909000
6	3.772352000	0.548048000	0.538332000	6	3.704647000	0.862033000	0.038505000
6	0.851769000	1.386971000	0.349865000	6	0.727552000	1.385036000	0.719359000
6	1.888934000	1.940089000	-0.626534000	6	1.454602000	2.044157000	-0.488840000
6	1.689515000	-1.973876000	0.202491000	6	1.828278000	-1.864154000	0.321999000
6	-0.006760000	0.313814000	0.219020000	6	-0.261727000	0.180965000	0.568924000
6	-0.015889000	-0.655106000	-0.943675000	6	-0.154657000	-0.770656000	-0.628611000
6	0.854753000	-1.859790000	-0.850204000	6	0.906725000	-1.803890000	-0.660480000
1	3.844144000	1.471934000	-1.389066000	1	3.106402000	1.741318000	-1.811782000
6	4.232415000	-0.667136000	0.883658000	6	4.359882000	-0.287149000	0.275149000
6	4.144183000	-1.903644000	0.002683000	6	4.145303000	-1.585749000	-0.482126000
6	2.917508000	-2.815791000	0.328910000	6	3.156346000	-2.552497000	0.237087000
1	5.055451000	-2.501367000	0.127068000	1	5.107515000	-2.099707000	-0.595787000
1	3.912307000	1.349537000	1.263032000	1	3.989920000	1.711248000	0.657408000
1	2.784123000	0.076802000	-1.312561000	1	2.266757000	0.251352000	-1.452949000
8	-0.666285000	-0.448624000	-1.967825000	8	-0.925333000	-0.648620000	-1.577151000
1	1.589829000	-1.243630000	0.997690000	1	1.705064000	-1.232133000	1.195146000
1	2.921010000	-3.671686000	-0.350852000	1	3.102873000	-3.488240000	-0.326053000
1	3.010829000	-3.200758000	1.351034000	1	3.529509000	-2.791307000	1.237779000
1	4.088753000	-1.628219000	-1.054224000	1	3.765911000	-1.396678000	-1.490556000
6	0.841717000	-2.759558000	-2.058076000	6	0.957241000	-2.607572000	-1.934578000
1	1.253895000	-2.242033000	-2.931672000	1	1.236416000	-1.969635000	-2.781156000
1	1.415860000	-3.672951000	-1.895362000	1	1.669626000	-3.430812000	-1.876418000
1	-0.186122000	-3.032274000	-2.315405000	1	-0.032396000	-3.012100000	-2.163770000
6	1.317740000	2.161265000	-2.042898000	6	0.495027000	2.328572000	-1.658636000
1	0.461986000	2.838350000	-1.997388000	1	-0.366508000	2.908104000	-1.313673000
1	2.085600000	2.609233000	-2.683425000	1	1.009883000	2.918539000	-2.424194000
1	0.992416000	1.229790000	-2.507035000	1	0.124714000	1.416150000	-2.127024000
6	2.380924000	3.301146000	-0.090193000	6	2.010003000	3.404149000	0.003536000
1	3.174252000	3.698559000	-0.731888000	1	2.672341000	3.828559000	-0.757735000
1	1.559132000	4.020627000	-0.071170000	1	1.197145000	4.108930000	0.185172000
1	2.778990000	3.222320000	0.926487000	1	2.577895000	3.312621000	0.934087000
6	4.865250000	-0.901571000	2.235226000	6	5.392302000	-0.370993000	1.375487000
1	4.865980000	0.001741000	2.851559000	1	5.477385000	0.565230000	1.933851000
1	4.333628000	-1.686752000	2.788548000	1	5.144799000	-1.168027000	2.088455000
1	5.901903000	-1.247082000	2.129280000	1	6.380279000	-0.619318000	0.966373000
6	-2.002502000	1.243248000	-0.018368000	6	-1.593985000	0.904875000	0.654718000
8	-0.732405000	3.162088000	0.135901000	8	-0.137905000	2.398553000	1.340078000
7	-1.724705000	2.422747000	0.022432000	7	-1.478001000	2.100170000	1.114212000

6	-3.096818000	0.311979000	-0.102291000	6	-2.935734000	0.417422000	0.279644000
6	-3.604428000	-0.322096000	1.048479000	6	-3.410063000	-0.883947000	0.518579000
6	-3.642454000	-0.034029000	-1.352101000	6	-3.816166000	1.314636000	-0.354116000
6	-4.639248000	-1.249540000	0.964795000	6	-4.691080000	-1.280143000	0.137901000
6	-4.681642000	-0.953790000	-1.441552000	6	-5.100009000	0.934634000	-0.731332000
6	-5.178019000	-1.560589000	-0.284695000	6	-5.538376000	-0.368536000	-0.490408000
1	-5.016386000	-1.718847000	1.865949000	1	-5.019432000	-2.292821000	0.342061000
1	-5.098388000	-1.204183000	-2.411218000	1	-5.751339000	1.650407000	-1.221995000
1	0.945378000	1.775106000	1.360156000	1	1.482529000	1.142480000	1.471223000
1	-0.359986000	-0.120432000	1.152857000	1	-0.166919000	-0.422613000	1.476690000
1	-5.984206000	-2.284026000	-0.349673000	1	-6.534007000	-0.680860000	-0.788179000
17	-2.931154000	0.060694000	2.627499000	17	-2.415009000	-2.080676000	1.356301000
1	-3.220969000	0.421761000	-2.239259000	1	-3.459989000	2.318049000	-0.558103000
TS3o2F				TS3o2F P			
6	-2.816927000	1.069323000	0.926350000	6	-2.561214000	1.045733000	1.016840000
6	-3.743278000	0.717559000	-0.211872000	6	-3.579017000	0.820656000	-0.076467000
6	-0.787043000	1.392970000	-0.579741000	6	-0.582223000	1.443834000	-0.602935000
6	-1.599282000	1.994442000	0.564854000	6	-1.363128000	1.973934000	0.635886000
6	-1.749281000	-1.900029000	-0.314763000	6	-1.690710000	-1.861663000	-0.488162000
6	0.049440000	0.295851000	-0.587380000	6	0.383274000	0.210629000	-0.556158000
6	0.201800000	-0.702774000	0.541638000	6	0.263689000	-0.823508000	0.572045000
6	-0.731627000	-1.863601000	0.568381000	6	-0.780543000	-1.872538000	0.506562000
1	-3.386377000	1.610702000	1.697506000	1	-3.058335000	1.543882000	1.862820000
6	-4.319354000	-0.467615000	-0.478191000	6	-4.224457000	-0.308533000	-0.414282000
6	-4.116729000	-1.729967000	0.344828000	6	-4.032358000	-1.654829000	0.261705000
6	-3.020337000	-2.681723000	-0.233410000	6	-3.011474000	-2.568196000	-0.482758000
1	-5.061127000	-2.286054000	0.390505000	1	-4.995192000	-2.178250000	0.304424000
1	-3.988521000	1.541716000	-0.880941000	1	-3.840809000	1.711389000	-0.645397000
1	-2.435474000	0.165736000	1.405674000	1	-2.187931000	0.098841000	1.408370000
8	1.022721000	-0.561560000	1.446570000	8	1.011774000	-0.756020000	1.543659000
1	-1.760056000	-1.145303000	-1.093202000	1	-1.568167000	-1.152562000	-1.300176000
1	-2.939612000	-3.561733000	0.409805000	1	-2.963859000	-3.534562000	0.026306000
1	-3.322324000	-3.023393000	-1.230267000	1	-3.352928000	-2.750715000	-1.506609000
1	-3.842992000	-1.486306000	1.375274000	1	-3.691716000	-1.532671000	1.294093000
6	-0.541904000	-2.811547000	1.723486000	6	-0.833014000	-2.780143000	1.708652000
1	-0.748482000	-2.310225000	2.675561000	1	-1.144427000	-2.222166000	2.599365000
1	-1.188265000	-3.687093000	1.645952000	1	-1.522636000	-3.612899000	1.567812000
1	0.498644000	-3.146997000	1.768941000	1	0.162460000	-3.178195000	1.923462000
6	-0.757119000	2.188723000	1.843271000	6	-0.447484000	2.155678000	1.860016000
1	0.101987000	2.828650000	1.628460000	1	0.428261000	2.755053000	1.593918000
1	-1.365409000	2.670060000	2.617052000	1	-0.988512000	2.685467000	2.651094000
1	-0.387355000	1.243521000	2.241832000	1	-0.099116000	1.205888000	2.266164000
6	-2.120037000	3.377639000	0.119651000	6	-1.916358000	3.370313000	0.253573000
1	-2.766795000	3.807191000	0.891900000	1	-2.604991000	3.718530000	1.030043000
1	-1.284493000	4.060536000	-0.049671000	1	-1.105394000	4.094604000	0.162710000
1	-2.697132000	3.320176000	-0.808597000	1	-2.456002000	3.360850000	-0.698116000
6	-5.221073000	-0.638302000	-1.678341000	6	-5.215267000	-0.318000000	-1.555023000
1	-5.299506000	0.279128000	-2.268276000	1	-5.283231000	0.654320000	-2.050552000
1	-4.852161000	-1.433651000	-2.339050000	1	-4.938563000	-1.063817000	-2.311393000
1	-6.231719000	-0.937169000	-1.370791000	1	-6.216727000	-0.595063000	-1.200807000
6	2.118330000	1.168650000	-0.593746000	6	1.731637000	0.904223000	-0.588472000
8	0.876043000	3.115973000	-0.736041000	8	0.318140000	2.519460000	-1.049076000
7	1.845541000	2.348788000	-0.689245000	7	1.649053000	2.150438000	-0.892982000
6	3.279710000	0.340248000	-0.396540000	6	3.048158000	0.287027000	-0.377832000
6	3.294597000	-1.010738000	-0.766961000	6	3.276023000	-1.072490000	-0.619123000
6	4.447802000	0.863894000	0.195541000	6	4.147530000	1.048164000	0.058715000
6	4.396696000	-1.827710000	-0.566906000	6	4.510874000	-1.677289000	-0.439370000
6	5.567333000	0.061879000	0.390978000	6	5.399936000	0.467369000	0.239104000
6	5.543240000	-1.284789000	0.013798000	6	5.583714000	-0.896861000	-0.006837000
1	4.342184000	-2.866391000	-0.872130000	1	4.613990000	-2.736648000	-0.645301000
1	6.457424000	0.486032000	0.843398000	1	6.230555000	1.075722000	0.581423000
1	-1.045602000	1.781542000	-1.560411000	1	-1.301896000	1.302939000	-1.413805000
1	0.246851000	-0.136496000	-1.564591000	1	0.282553000	-0.328542000	-1.503088000
1	6.412987000	-1.913700000	0.171857000	1	6.556216000	-1.355428000	-0.139302000
9	2.192205000	-1.550868000	-1.336596000	9	2.247075000	-1.843254000	-1.060092000
1	4.454824000	1.906195000	0.494511000	1	3.994510000	2.101667000	0.264916000
TS3pBr				TS3pBr P			

6	-4.109994000	0.619026000	0.799530000	6	-3.904270000	0.689236000	0.832684000
6	-4.852563000	0.074758000	-0.396068000	6	-4.688100000	0.247170000	-0.380369000
6	-2.095713000	1.362905000	-0.573084000	6	-1.861010000	1.502922000	-0.546565000
6	-3.087335000	1.777324000	0.512807000	6	-2.870679000	1.833877000	0.593269000
6	-2.364312000	-2.072196000	-0.297942000	6	-2.334781000	-2.040657000	-0.392022000
6	-1.060288000	0.452217000	-0.527286000	6	-0.730418000	0.416184000	-0.447855000
6	-0.768160000	-0.475974000	0.634751000	6	-0.721529000	-0.570476000	0.731823000
6	-1.439942000	-1.804827000	0.646724000	6	-1.541050000	-1.803847000	0.672952000
1	-4.836749000	1.032098000	1.515814000	1	-4.606454000	1.083414000	1.582757000
6	-5.149872000	-1.206793000	-0.673225000	6	-5.070621000	-0.994818000	-0.722451000
6	-4.756035000	-2.390227000	0.196891000	6	-4.747921000	-2.246390000	0.076084000
6	-3.446392000	-3.102054000	-0.273629000	6	-3.485742000	-2.996277000	-0.450740000
1	-5.566420000	-3.129317000	0.189305000	1	-5.599854000	-2.935481000	-0.031715000
1	-5.208258000	0.824142000	-1.102496000	1	-5.006973000	1.051452000	-1.041794000
1	-3.586519000	-0.182499000	1.324022000	1	-3.411073000	-0.158453000	1.308757000
8	-0.043919000	-0.147263000	1.572773000	8	-0.056130000	-0.312509000	1.731082000
1	-2.479333000	-1.351767000	-1.099921000	1	-2.275456000	-1.372918000	-1.244668000
1	-3.230820000	-3.932464000	0.403471000	1	-3.321922000	-3.886895000	0.161400000
1	-3.597415000	-3.518757000	-1.276166000	1	-3.653206000	-3.327565000	-1.480598000
1	-4.618211000	-2.082853000	1.237328000	1	-4.587024000	-2.008774000	1.131552000
6	-1.136657000	-2.667353000	1.843612000	6	-1.529182000	-2.626976000	1.935539000
1	-1.508791000	-2.200405000	2.762323000	1	-2.024986000	-2.087283000	2.750913000
1	-1.580085000	-3.660348000	1.756304000	1	-2.029536000	-3.587122000	1.806577000
1	-0.054859000	-2.775966000	1.966775000	1	-0.500526000	-2.804919000	2.260237000
6	-2.395837000	2.133163000	1.845757000	6	-2.156290000	2.158373000	1.917886000
1	-1.672622000	2.936252000	1.687525000	1	-1.373498000	2.904442000	1.753500000
1	-3.144668000	2.474825000	2.568873000	1	-2.874176000	2.574957000	2.631996000
1	-1.871381000	1.281327000	2.279680000	1	-1.700419000	1.279419000	2.373703000
6	-3.850948000	3.025356000	0.020910000	6	-3.634060000	3.107031000	0.146301000
1	-4.618902000	3.311679000	0.747037000	1	-4.443508000	3.317302000	0.852435000
1	-3.164218000	3.865611000	-0.104324000	1	-2.966736000	3.970235000	0.122426000
1	-4.345174000	2.852204000	-0.940282000	1	-4.073870000	3.001958000	-0.850201000
6	-5.899846000	-1.574047000	-1.932146000	6	-5.857878000	-1.241781000	-1.987698000
1	-6.120749000	-0.699099000	-2.549782000	1	-6.021435000	-0.322874000	-2.557308000
1	-5.323247000	-2.281025000	-2.542825000	1	-5.340711000	-1.956473000	-2.640888000
1	-6.847141000	-2.074709000	-1.692907000	1	-6.836110000	-1.684567000	-1.759471000
6	0.791702000	1.718593000	-0.496041000	6	0.511380000	1.284400000	-0.476424000
8	-0.801850000	3.396293000	-0.586757000	8	-1.100364000	2.738123000	-0.807578000
7	0.293995000	2.823505000	-0.546443000	7	0.262814000	2.526136000	-0.694458000
6	2.083902000	1.086417000	-0.406884000	6	1.895047000	0.801108000	-0.369095000
6	2.252637000	-0.263682000	-0.753643000	6	2.198178000	-0.555967000	-0.561884000
6	3.197247000	1.827288000	0.036062000	6	2.945918000	1.695167000	-0.097826000
6	3.504350000	-0.865658000	-0.663647000	6	3.512469000	-1.013944000	-0.492819000
1	1.408740000	-0.850241000	-1.095746000	1	1.411321000	-1.271085000	-0.776875000
6	4.450926000	1.231837000	0.122715000	6	4.261642000	1.250604000	-0.024940000
1	3.073191000	2.869228000	0.309490000	1	2.724287000	2.744271000	0.062876000
6	4.592261000	-0.111740000	-0.226458000	6	4.532105000	-0.104064000	-0.223736000
1	3.630085000	-1.907880000	-0.931887000	1	3.737035000	-2.062942000	-0.645877000
1	5.305951000	1.804881000	0.461735000	1	5.065674000	1.944974000	0.189544000
35	6.315061000	-0.936170000	-0.100307000	35	6.341983000	-0.725234000	-0.117527000
1	-2.364625000	1.700806000	-1.569823000	1	-2.440974000	1.308374000	-1.453057000
1	-0.751518000	0.057438000	-1.494026000	1	-0.746280000	-0.163357000	-1.375709000
TS3pCl				TS3pCl P			
6	-3.476083000	0.765917000	0.811051000	6	-3.228998000	0.800406000	0.906050000
6	-4.258023000	0.280502000	-0.384797000	6	-4.104665000	0.447005000	-0.273016000
6	-1.421323000	1.376452000	-0.566917000	6	-1.193552000	1.482706000	-0.550636000
6	-2.376806000	1.852190000	0.526151000	6	-2.128878000	1.874074000	0.632521000
6	-1.924932000	-2.034131000	-0.306311000	6	-1.907953000	-1.992923000	-0.464991000
6	-0.451148000	0.396256000	-0.530790000	6	-0.122662000	0.335297000	-0.488044000
6	-0.218284000	-0.555484000	0.625645000	6	-0.163398000	-0.684541000	0.661718000
6	-0.981849000	-1.833841000	0.636489000	6	-1.066519000	-1.856453000	0.580686000
1	-4.170217000	1.224380000	1.532063000	1	-3.861119000	1.227270000	1.699279000
6	-4.644432000	-0.975944000	-0.666839000	6	-4.586323000	-0.754868000	-0.632638000
6	-4.331239000	-2.187771000	0.196892000	6	-4.307148000	-2.053696000	0.104009000
6	-3.075655000	-2.986773000	-0.280997000	6	-3.126127000	-2.861950000	-0.515823000
1	-5.191026000	-2.868762000	0.189082000	1	-5.204188000	-2.684108000	0.080690000
1	-4.562196000	1.056252000	-1.086797000	1	-4.405672000	1.291736000	-0.890802000

1	-3.007418000	-0.072632000	1.329367000	1	-2.775562000	-0.091687000	1.338987000
8	0.532850000	-0.282546000	1.560398000	8	0.533825000	-0.505316000	1.656537000
1	-1.991891000	-1.305803000	-1.106627000	1	-1.827957000	-1.297054000	-1.293260000
1	-2.915604000	-3.832339000	0.392749000	1	-2.999704000	-3.791307000	0.045587000
1	-3.258775000	-3.388700000	-1.284209000	1	-3.361275000	-3.129168000	-1.550976000
1	-4.169051000	-1.895239000	1.238093000	1	-4.077795000	-1.867655000	1.157222000
6	-0.736311000	-2.718541000	1.830421000	6	-1.077218000	-2.727900000	1.810443000
1	-1.073035000	-2.229519000	2.751318000	1	-1.516194000	-2.190190000	2.658997000
1	-1.247692000	-3.678158000	1.741722000	1	-1.642494000	-3.647888000	1.659018000
1	0.335656000	-2.901981000	1.950386000	1	-0.054733000	-2.984584000	2.099873000
6	-1.656017000	2.150882000	1.857562000	6	-1.338829000	2.136498000	1.927600000
1	-0.877931000	2.901111000	1.699972000	1	-0.515457000	2.830546000	1.735171000
1	-2.375474000	2.541196000	2.585865000	1	-1.996065000	2.593273000	2.674804000
1	-1.192024000	1.261449000	2.284795000	1	-0.923473000	1.224796000	2.357019000
6	-3.054272000	3.153071000	0.045178000	6	-2.819774000	3.201469000	0.227363000
1	-3.797522000	3.487273000	0.776518000	1	-3.591106000	3.453530000	0.961971000
1	-2.311626000	3.944580000	-0.078297000	1	-2.097354000	4.018639000	0.193665000
1	-3.563330000	3.020340000	-0.914705000	1	-3.296068000	3.141858000	-0.755944000
6	-5.420881000	-1.284543000	-1.925442000	6	-5.455706000	-0.903889000	-1.859043000
1	-5.581708000	-0.393640000	-2.538836000	1	-5.585953000	0.043264000	-2.389608000
1	-4.896109000	-2.027208000	-2.540487000	1	-5.025038000	-1.628475000	-2.562183000
1	-6.400212000	-1.719149000	-1.686069000	1	-6.448435000	-1.287695000	-1.590199000
6	1.484083000	1.530882000	-0.503361000	6	1.163289000	1.137363000	-0.508753000
8	0.010573000	3.315931000	-0.577675000	8	-0.372822000	2.667982000	-0.854193000
7	1.064028000	2.667839000	-0.546289000	7	0.978931000	2.389011000	-0.734416000
6	2.729870000	0.810206000	-0.424314000	6	2.521392000	0.587052000	-0.396961000
6	2.803466000	-0.546745000	-0.777465000	6	2.763798000	-0.777513000	-0.619887000
6	3.894029000	1.470433000	0.015304000	6	3.608824000	1.424795000	-0.093430000
6	4.010959000	-1.234019000	-0.696879000	6	4.054536000	-1.297320000	-0.550101000
1	1.919518000	-1.072576000	-1.117212000	1	1.946607000	-1.449253000	-0.859744000
6	5.104407000	0.790527000	0.092407000	6	4.902211000	0.918986000	-0.019210000
1	3.843438000	2.517189000	0.293455000	1	3.433179000	2.478543000	0.091581000
6	5.150994000	-0.558495000	-0.262936000	6	5.112367000	-0.441738000	-0.249062000
1	4.065227000	-2.281447000	-0.969385000	1	4.234673000	-2.351334000	-0.726733000
1	5.999833000	1.300332000	0.428604000	1	5.736244000	1.568463000	0.220641000
17	6.680314000	-1.424668000	-0.159293000	17	6.748326000	-1.091481000	-0.149714000
1	-1.670788000	1.737695000	-1.560505000	1	-1.823926000	1.319950000	-1.429261000
1	-0.174304000	-0.013427000	-1.500944000	1	-0.175217000	-0.217858000	-1.431278000
TS3pF				TS3pF_P			
6	-3.115152000	0.896592000	0.827427000	6	-2.883343000	0.893490000	0.910686000
6	-3.935489000	0.465839000	-0.363634000	6	-3.775795000	0.584939000	-0.268469000
6	-1.037118000	1.384406000	-0.563488000	6	-0.817320000	1.481182000	-0.545282000
6	-1.953930000	1.914765000	0.537656000	6	-1.733314000	1.913746000	0.638909000
6	-1.750559000	-1.991611000	-0.313104000	6	-1.702629000	-1.959127000	-0.464599000
6	-0.131174000	0.343900000	-0.537521000	6	0.193392000	0.280216000	-0.488143000
6	0.049040000	-0.624257000	0.614072000	6	0.104484000	-0.737040000	0.661038000
6	-0.790024000	-1.854913000	0.623344000	6	-0.852542000	-1.865772000	0.578803000
1	-3.773996000	1.392869000	1.556549000	1	-3.494039000	1.348159000	1.705327000
6	-4.401502000	-0.762850000	-0.647751000	6	-4.316463000	-0.591267000	-0.629017000
6	-4.157905000	-1.995896000	0.208351000	6	-4.101409000	-1.902995000	0.106287000
6	-2.958804000	-2.870141000	-0.282838000	6	-2.961712000	-2.767822000	-0.514568000
1	-5.058896000	-2.621453000	0.204922000	1	-5.028429000	-2.488434000	0.082645000
1	-4.196541000	1.262139000	-1.059964000	1	-4.034951000	1.444095000	-0.885348000
1	-2.694301000	0.028270000	1.337747000	1	-2.472907000	-0.020330000	1.341290000
8	0.816786000	-0.399949000	1.548189000	8	0.807445000	-0.591209000	1.657231000
1	-1.777984000	-1.256352000	-1.109403000	1	-1.592116000	-1.265215000	-1.290999000
1	-2.847271000	-3.727165000	0.386194000	1	-2.880601000	-3.702540000	0.046319000
1	-3.174571000	-3.255116000	-1.286238000	1	-3.210536000	-3.022766000	-1.549658000
1	-3.969462000	-1.718770000	1.249361000	1	-3.862970000	-1.729320000	1.159617000
6	-0.591843000	-2.758923000	1.811721000	6	-0.901524000	-2.738619000	1.806614000
1	-0.895481000	-2.256080000	2.736667000	1	-1.307778000	-2.181032000	2.658591000
1	-1.159138000	-3.686379000	1.720301000	1	-1.513958000	-3.628064000	1.656173000
1	0.467997000	-3.005578000	1.926147000	1	0.107934000	-3.048216000	2.090149000
6	-1.207088000	2.165403000	1.864506000	6	-0.931647000	2.135769000	1.934394000
1	-0.385173000	2.866237000	1.702060000	1	-0.075243000	2.788741000	1.742379000
1	-1.895861000	2.598031000	2.598611000	1	-1.565729000	2.623394000	2.682153000
1	-0.795668000	1.248185000	2.286785000	1	-0.561538000	1.204277000	2.362675000

6	-2.553669000	3.256190000	0.064888000	6	-2.359880000	3.273513000	0.236660000
1	-3.270005000	3.633229000	0.802292000	1	-3.116667000	3.561999000	0.973041000
1	-1.764453000	4.000813000	-0.061552000	1	-1.598488000	4.054485000	0.202416000
1	-3.076459000	3.158070000	-0.891792000	1	-2.840396000	3.238318000	-0.745796000
6	-5.206164000	-1.016351000	-1.900955000	6	-5.192636000	-0.696027000	-1.855188000
1	-5.315820000	-0.114310000	-2.509360000	1	-5.276425000	0.256985000	-2.384648000
1	-4.734289000	-1.787716000	-2.523470000	1	-4.798360000	-1.440123000	-2.559325000
1	-6.208906000	-1.389602000	-1.655015000	1	-6.202930000	-1.030932000	-1.586365000
6	1.871018000	1.351737000	-0.523979000	6	1.519934000	1.013820000	-0.514995000
8	0.507766000	3.223574000	-0.584311000	8	0.061116000	2.624325000	-0.843518000
7	1.522366000	2.512355000	-0.566251000	7	1.399704000	2.274163000	-0.735040000
6	3.064172000	0.546333000	-0.447840000	6	2.846341000	0.389001000	-0.412690000
6	3.048634000	-0.802765000	-0.840363000	6	3.010863000	-0.987183000	-0.641688000
6	4.262817000	1.112457000	0.031429000	6	3.980319000	1.165637000	-0.111833000
6	4.203922000	-1.574660000	-0.761683000	6	4.271198000	-1.578107000	-0.580450000
1	2.134057000	-1.252852000	-1.206945000	1	2.155125000	-1.610062000	-0.878947000
6	5.422285000	0.348477000	0.105556000	6	5.244186000	0.588660000	-0.046870000
1	4.276710000	2.151607000	0.340544000	1	3.861658000	2.226567000	0.077442000
6	5.371379000	-0.984481000	-0.290951000	6	5.366888000	-0.777346000	-0.283105000
1	4.209174000	-2.616793000	-1.059407000	1	4.410144000	-2.638379000	-0.758189000
1	6.353777000	0.767832000	0.468311000	1	6.125083000	1.174738000	0.189774000
9	6.494081000	-1.730026000	-0.213819000	9	6.592288000	-1.344034000	-0.215398000
1	-1.273269000	1.761265000	-1.554499000	1	-1.455353000	1.352730000	-1.424274000
1	0.109054000	-0.081139000	-1.510792000	1	0.108136000	-0.268843000	-1.431246000
TS4o1Br				TS4o1Br_P			
6	3.158711000	0.494034000	0.415648000	6	3.159530000	0.353514000	0.228860000
6	2.414317000	1.756025000	0.055559000	6	2.528273000	1.666136000	-0.172009000
6	2.112730000	-1.223064000	-1.324727000	6	1.797711000	-1.199841000	-1.434816000
6	3.346815000	-0.572175000	-0.701758000	6	3.168082000	-0.790393000	-0.830258000
6	0.219702000	-0.031829000	1.466890000	6	0.179628000	0.278381000	1.531935000
6	1.003203000	-1.882695000	-0.810376000	6	0.579332000	-1.788174000	-0.636054000
6	0.662450000	-2.276811000	0.606703000	6	0.611722000	-2.041806000	0.896819000
6	0.455170000	-1.329098000	1.731912000	6	0.369636000	-0.997407000	1.918001000
1	4.180754000	0.772093000	0.717294000	1	4.220544000	0.531217000	0.463007000
6	1.621105000	2.472091000	0.868560000	6	1.832261000	2.506856000	0.611310000
6	1.300020000	2.060135000	2.296409000	6	1.549007000	2.257128000	2.084515000
6	0.057661000	1.122753000	2.401550000	6	0.192121000	1.529866000	2.343219000
1	1.106138000	2.952418000	2.902889000	1	1.529743000	3.213645000	2.619946000
1	2.563679000	2.125682000	-0.955295000	1	2.663174000	1.954206000	-1.211269000
1	2.715437000	0.016751000	1.288251000	1	2.717228000	-0.019695000	1.152345000
8	0.532702000	-3.488506000	0.805634000	8	0.864310000	-3.192421000	1.249852000
1	0.231908000	2.68422000	0.428099000	1	0.150271000	0.484647000	0.471943000
1	-0.072893000	0.812997000	3.441337000	1	0.076117000	1.349685000	3.414453000
1	-0.838773000	1.679786000	2.104878000	1	-0.636479000	2.167666000	2.014830000
1	2.152894000	1.549958000	2.754299000	1	2.345773000	1.659547000	2.537371000
6	0.461741000	-1.957003000	3.101538000	6	0.459261000	-1.472186000	3.344951000
1	0.309085000	-1.220529000	3.891379000	1	0.215416000	-0.680181000	4.053870000
1	-0.321938000	-2.717443000	3.174474000	1	-0.221583000	-2.312676000	3.510267000
1	1.4111769000	-2.470579000	3.285204000	1	1.467264000	-1.839442000	3.565897000
6	4.152823000	-1.746291000	-0.079233000	6	3.794648000	-2.042683000	-0.181437000
1	4.343130000	-2.530902000	-0.818309000	1	3.842294000	-2.873281000	-0.894099000
1	5.119399000	-1.386097000	0.290102000	1	4.816949000	-1.821529000	0.141149000
1	3.608449000	-2.193976000	0.758292000	1	3.231605000	-2.380721000	0.691171000
6	4.184096000	0.034452000	-1.849709000	6	4.060329000	-0.371896000	-2.023526000
1	5.106987000	0.473407000	-1.457597000	1	5.061664000	-0.111095000	-1.666685000
1	4.462086000	-0.735175000	-2.577742000	1	4.162858000	-1.193059000	-2.741225000
1	3.629442000	0.810766000	-2.381349000	1	3.651948000	0.488362000	-2.558149000
6	0.944531000	3.733796000	0.391652000	6	1.211645000	3.760690000	0.043210000
1	1.125588000	3.919201000	-0.670890000	1	1.445732000	3.887689000	-1.017471000
1	-0.139827000	3.680144000	0.545219000	1	0.118709000	3.729923000	0.140139000
1	1.294093000	4.607017000	0.958303000	1	1.548975000	4.655427000	0.581969000
6	-0.694537000	-0.621477000	-1.543311000	6	-0.534569000	-0.899112000	-1.164513000
8	1.073851000	0.544921000	-2.453149000	8	1.229043000	-0.059264000	-2.160925000
7	-0.090894000	0.222896000	-2.177209000	7	-0.145130000	-0.006916000	-2.003832000
6	-1.980496000	-0.905651000	-0.970674000	6	-1.940307000	-1.016975000	-0.736177000
6	-2.790773000	0.101021000	-0.398872000	6	-2.781297000	0.077703000	-0.451474000
6	-2.422567000	-2.239249000	-0.890033000	6	-2.470615000	-2.305542000	-0.540136000

6	-4.002037000	-0.213102000	0.209721000	6	-4.091630000	-0.109451000	-0.013459000
6	-3.628712000	-2.556549000	-0.274909000	6	-3.778688000	-2.501757000	-0.107610000
1	-1.798151000	-3.021029000	-1.307269000	1	-1.841341000	-3.166409000	-0.739706000
6	-4.419372000	-1.543918000	0.272214000	6	-4.593415000	-1.400047000	0.153338000
1	-4.608459000	0.575911000	0.638545000	1	-4.710654000	0.752624000	0.205779000
1	-3.950500000	-3.590967000	-0.222562000	1	-4.157125000	-3.509634000	0.025879000
1	0.634667000	-2.665926000	-1.469960000	1	0.425337000	-2.802993000	-1.011049000
1	2.310229000	-1.504218000	-2.355252000	1	2.030080000	-1.945448000	-2.203422000
1	-5.361048000	-1.783612000	0.754996000	1	-5.613959000	-1.536427000	0.495966000
35	-2.239127000	1.928912000	-0.432722000	35	-2.173926000	1.897766000	-0.569018000
TS4o1Cl				TS4o1Cl_P			
6	3.058868000	0.211833000	0.401530000	6	3.105711000	-0.572482000	0.250537000
6	2.540695000	1.552385000	-0.057371000	6	3.249233000	0.705647000	-0.540500000
6	1.739544000	-1.414441000	-1.239460000	6	1.057234000	-1.687970000	-0.991823000
6	3.064710000	-0.945317000	-0.639159000	6	2.516897000	-1.809585000	-0.494629000
6	0.057234000	0.257271000	1.425099000	6	0.438702000	1.105913000	1.051754000
6	0.531966000	-1.844187000	-0.701889000	6	-0.200676000	-1.629507000	-0.070933000
6	0.121848000	-2.083345000	0.731888000	6	-0.183833000	-1.228310000	1.429297000
6	0.053955000	-1.038316000	1.785569000	6	0.002106000	0.159681000	1.907309000
1	4.112047000	0.330329000	0.700478000	1	4.110616000	-0.889305000	0.569584000
6	1.861894000	2.441078000	0.685772000	6	3.044533000	1.964936000	-0.121854000
6	1.465729000	2.189454000	2.131359000	6	2.565793000	2.342258000	1.269957000
6	0.078761000	1.489866000	2.268939000	6	1.012264000	2.446189000	1.375399000
1	1.423542000	3.141141000	2.673708000	1	2.990491000	3.313831000	1.548675000
1	2.757070000	1.819449000	-1.088173000	1	3.592723000	0.579864000	-1.564994000
1	2.535373000	-0.121407000	1.296616000	1	2.545520000	-0.404414000	1.170653000
8	-0.200953000	-3.242603000	1.007875000	8	-0.346852000	-2.137623000	2.241036000
1	0.146614000	0.470158000	0.368730000	1	0.556866000	0.843975000	0.010062000
1	-0.120495000	1.286290000	3.323954000	1	0.741644000	2.793236000	2.375378000
1	-0.701171000	2.173535000	1.910835000	1	0.649115000	3.187726000	0.653906000
1	2.213231000	1.572326000	2.638657000	1	2.911870000	1.621564000	2.017310000
6	-0.080663000	-1.558512000	3.192891000	6	-0.173920000	0.345868000	3.392727000
1	-0.134614000	-0.752022000	3.925249000	1	-0.138926000	1.397204000	3.680219000
1	-0.979102000	-2.176752000	3.284321000	1	-1.130574000	-0.073820000	3.717648000
1	0.767746000	-2.202757000	3.448317000	1	0.605859000	-0.190782000	3.944006000
6	3.651696000	-2.195489000	0.073458000	6	2.572363000	-3.019036000	0.463270000
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1	3.032640000	-2.485601000	0.928314000	1	2.017147000	-2.833790000	1.386202000
6	4.000379000	-0.571983000	-1.810509000	6	3.383740000	-2.130643000	-1.734544000
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1	4.145317000	-1.426136000	-2.480572000	1	3.093353000	-3.092744000	-2.169616000
1	3.591046000	0.249721000	-2.402408000	1	3.280924000	-1.370518000	-2.512260000
6	1.375434000	3.745082000	0.102346000	6	3.239016000	3.134735000	-1.057533000
1	1.625115000	3.837936000	-0.958395000	1	3.518842000	2.814391000	-2.065016000
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1	1.804627000	4.603952000	0.634961000	1	4.016402000	3.814245000	-0.683948000
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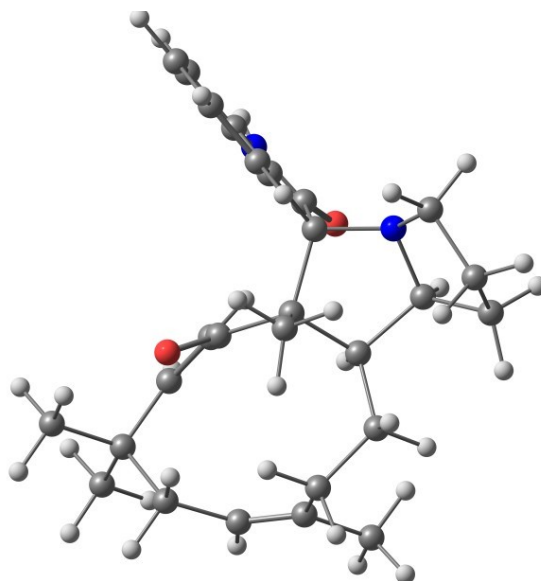
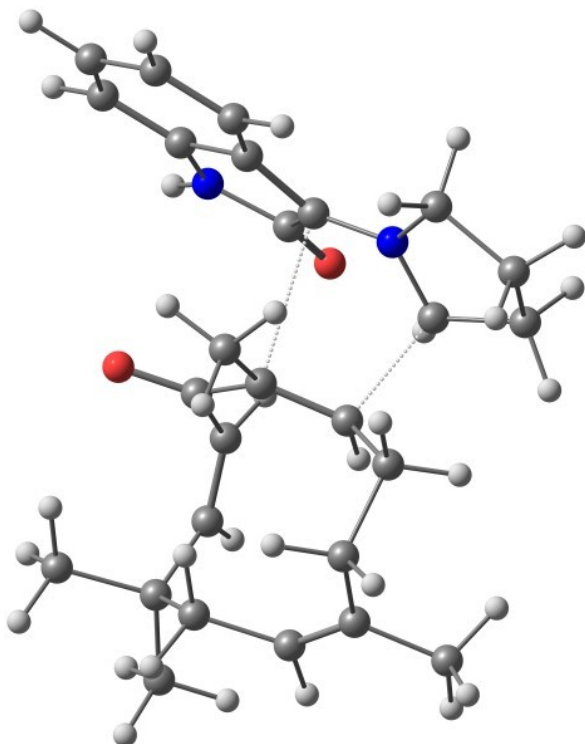
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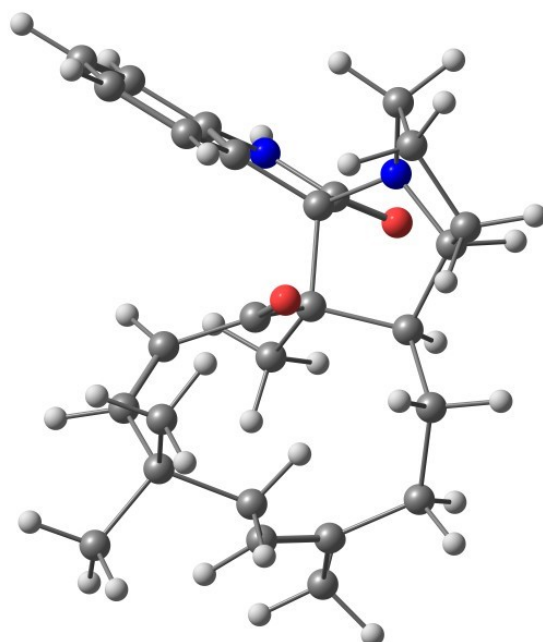
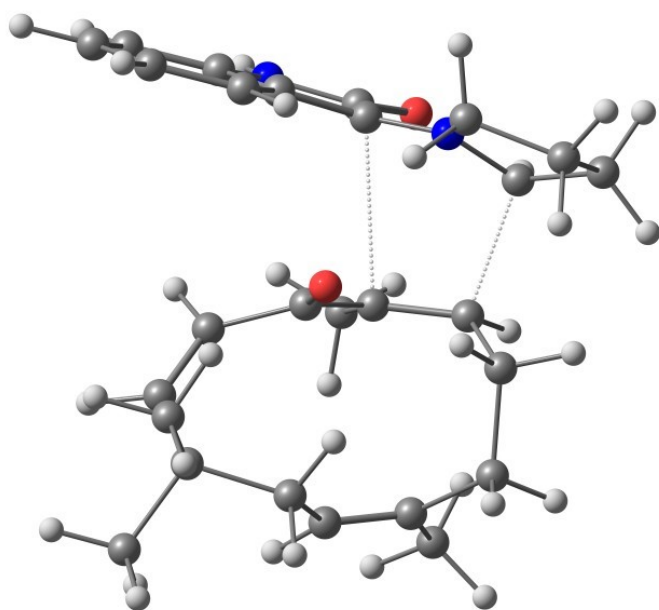
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1	0.137027000	-2.527030000	-0.995975000	1	-0.321623000	-2.366236000	0.539682000
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TS4pF				TS4pF_P			
6	3.204308000	0.068114000	0.351863000	6	3.182354000	-0.595043000	0.321387000
6	2.892613000	1.389582000	-0.304783000	6	3.462423000	0.429961000	-0.750640000
6	1.644699000	-1.577962000	-1.044322000	6	0.996449000	-1.737333000	-0.632235000
6	3.031743000	-1.214792000	-0.512513000	6	2.445457000	-1.897984000	-0.116707000
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6	0.403611000	-1.774578000	-0.452786000	6	-0.231818000	-1.366605000	0.252007000
6	-0.011550000	-1.724237000	0.995823000	6	-0.137732000	-0.592547000	1.594644000
6	0.067915000	-0.517939000	1.858875000	6	0.208480000	0.841604000	1.705030000
1	4.265475000	0.070722000	0.646113000	1	4.148616000	-0.940488000	0.720140000
6	2.346516000	2.466149000	0.282466000	6	3.395125000	1.767547000	-0.656594000
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6	0.419968000	2.028419000	1.918769000	6	1.424422000	2.807419000	0.622654000
1	1.990639000	3.506679000	2.132942000	1	3.482870000	3.483887000	0.631317000
1	3.159916000	1.472262000	-1.354843000	1	3.792989000	0.022540000	-1.703779000
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8	-0.482266000	-2.769133000	1.457513000	8	-0.382890000	-1.239106000	2.613198000
1	0.343633000	0.706845000	0.209899000	1	0.774801000	0.969334000	-0.305790000
1	0.170713000	2.033131000	2.982807000	1	1.194028000	3.424241000	1.494508000
1	-0.242667000	2.749752000	1.423073000	1	1.143548000	3.375635000	-0.272060000
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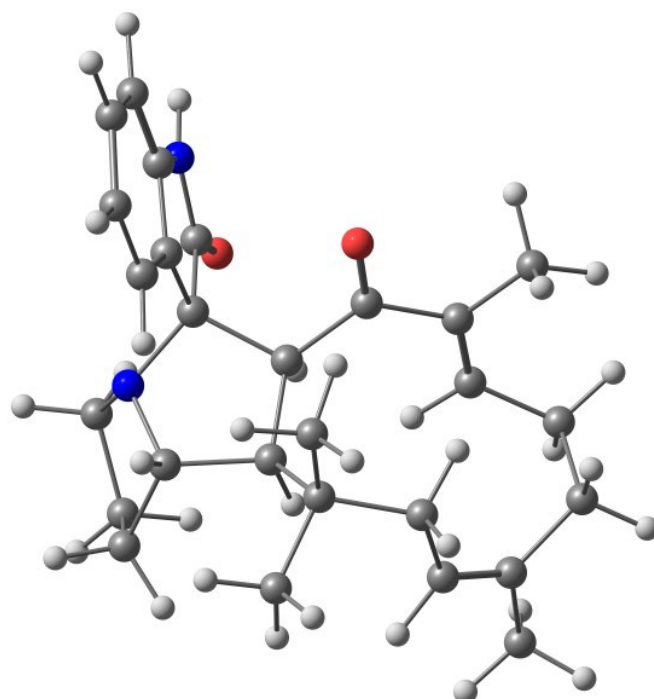
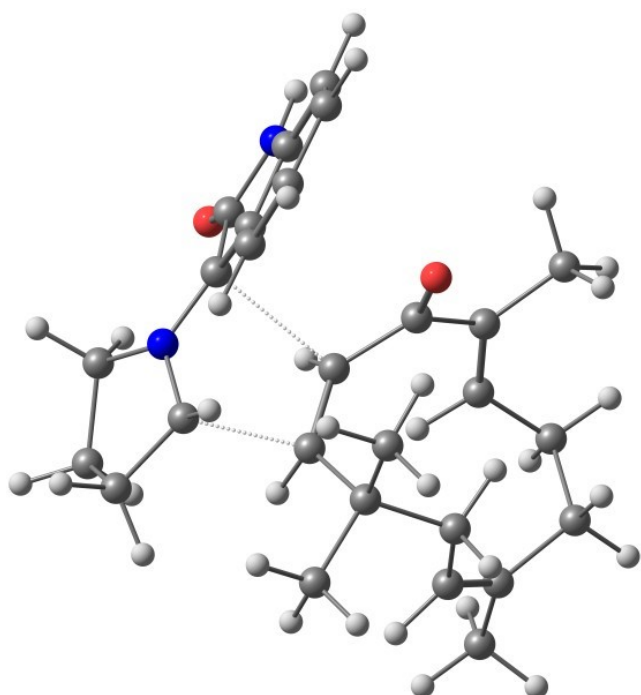
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6	3.452898000	-2.419708000	0.374087000	6	2.391174000	-2.849898000	1.097551000
1	3.375548000	-3.362129000	-0.177180000	1	1.863272000	-3.776700000	0.847554000
1	4.491762000	-2.302252000	0.701794000	1	3.405857000	-3.118089000	1.407759000
1	2.816840000	-2.493248000	1.261922000	1	1.883856000	-2.392551000	1.950960000
6	3.989635000	-1.146419000	-1.722808000	6	3.243792000	-2.591382000	-1.245311000
1	5.008745000	-0.923670000	-1.391226000	1	4.296288000	-2.688850000	-0.960833000
1	4.012122000	-2.103260000	-2.255267000	1	2.851436000	-3.596179000	-1.433925000
1	3.680088000	-0.377228000	-2.433917000	1	3.190880000	-2.033393000	-2.182983000
6	2.071110000	3.729726000	-0.495720000	6	3.718437000	2.645701000	-1.842434000
1	2.345206000	3.630305000	-1.549821000	1	3.963880000	2.061067000	-2.733456000
1	1.006283000	3.994470000	-0.447562000	1	2.870917000	3.298439000	-2.090408000
1	2.620169000	4.582633000	-0.075407000	1	4.564807000	3.309708000	-1.622593000
6	-0.896682000	-0.285281000	-1.537642000	6	-1.069012000	-0.686036000	-0.821275000
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7	-0.070324000	0.208996000	-2.278223000	7	-0.409133000	-0.404879000	-1.894572000
6	-2.257541000	-0.129706000	-1.095376000	6	-2.485382000	-0.331250000	-0.672250000
6	-2.900806000	1.117575000	-1.234805000	6	-3.152649000	0.401764000	-1.673700000
6	-2.940559000	-1.198382000	-0.488176000	6	-3.198052000	-0.712123000	0.477822000
6	-4.207610000	1.286431000	-0.792925000	6	-4.491270000	0.744081000	-1.533091000
1	-2.369161000	1.944881000	-1.691376000	1	-2.609670000	0.703080000	-2.562230000
6	-4.245218000	-1.030039000	-0.033806000	6	-4.541111000	-0.370860000	0.631628000
1	-2.448338000	-2.153822000	-0.354217000	1	-2.711159000	-1.274225000	1.266430000
6	-4.856496000	0.207912000	-0.197833000	6	-5.163794000	0.350395000	-0.378087000
1	-4.721816000	2.235197000	-0.894954000	1	-5.017039000	1.308642000	-2.294789000
1	-4.787630000	-1.839756000	0.440299000	1	-5.101059000	-0.657017000	1.514501000
9	-6.121771000	0.372763000	0.239748000	9	-6.464670000	0.684081000	-0.237740000
1	-0.182816000	-2.546094000	-0.948079000	1	-0.705010000	-2.300337000	0.560822000
1	1.728615000	-2.104563000	-1.990898000	1	0.722066000	-2.714411000	-1.056547000

Transition state product for ZS-1

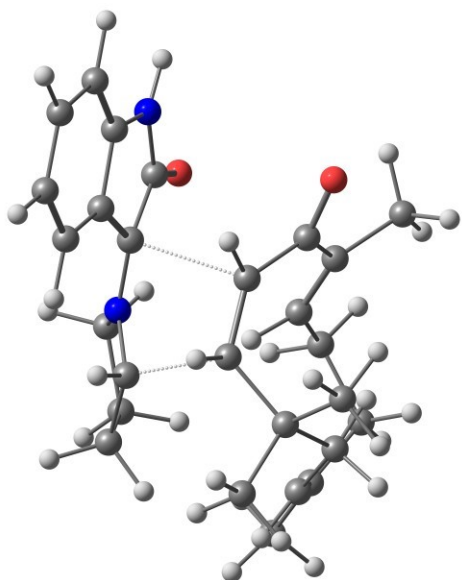




TS2C



TS3C



TS4C

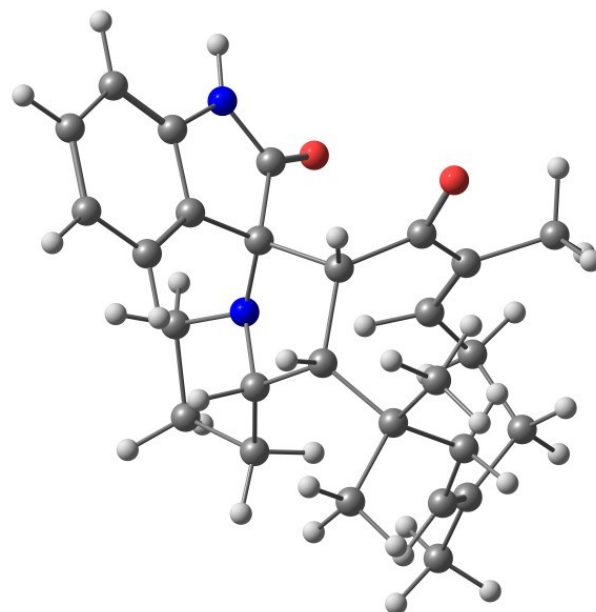
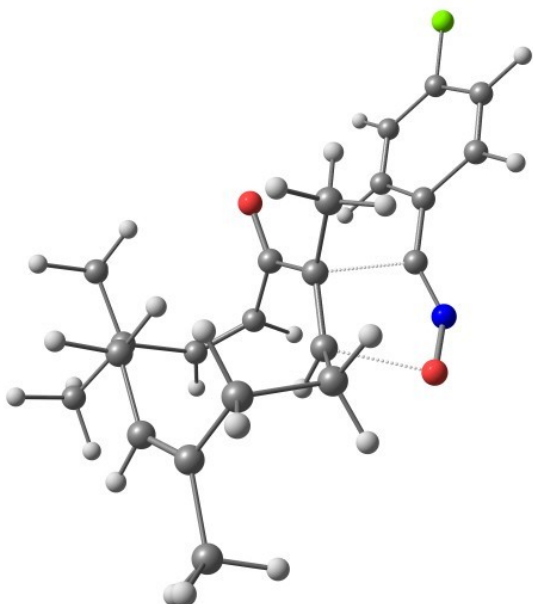
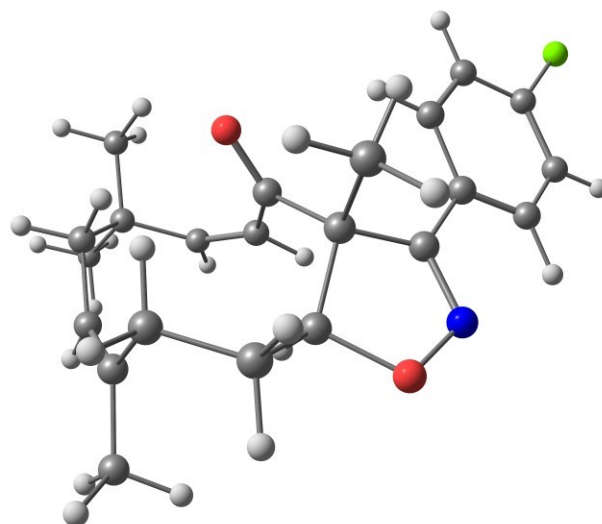


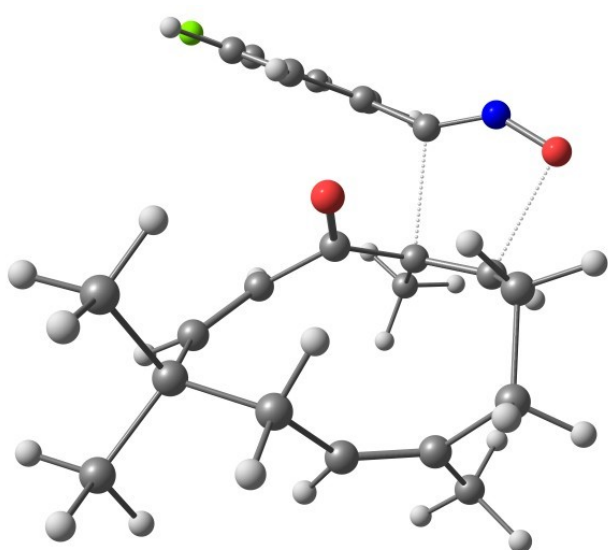
Figure S57: Four possible transitions and its product of ZS-1

Transition state and product for ZI-4

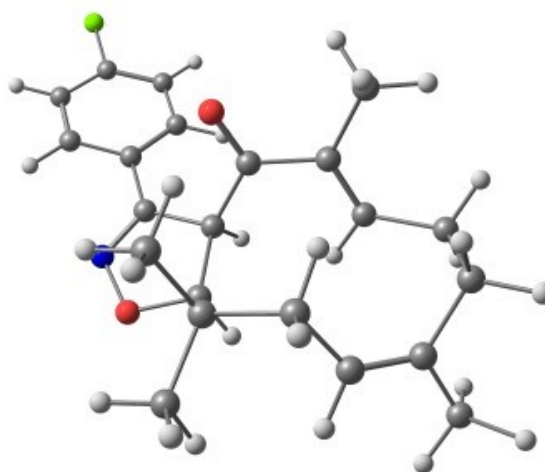
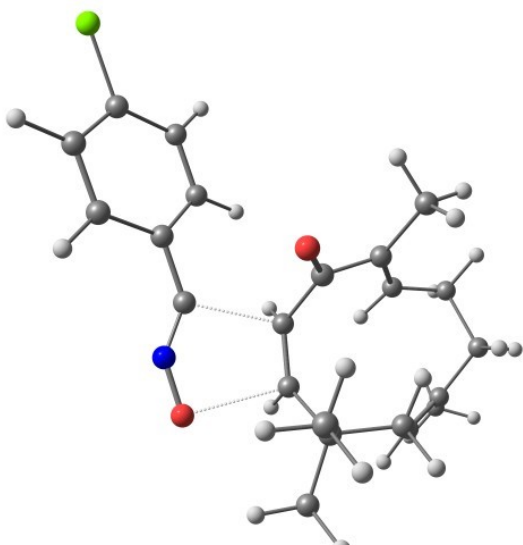
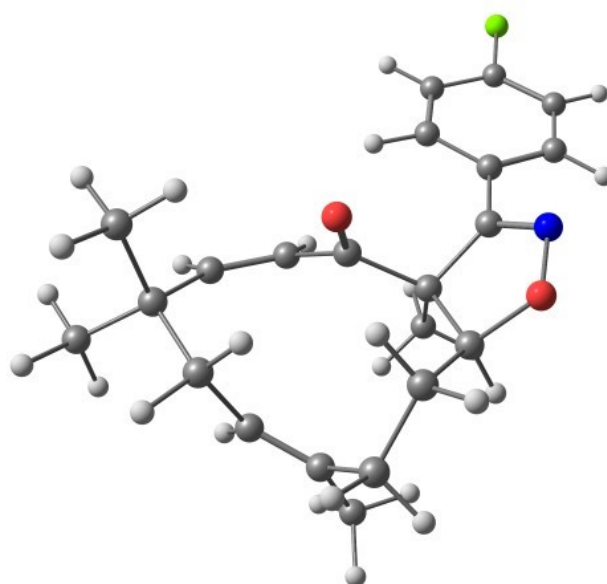


TS1pCl

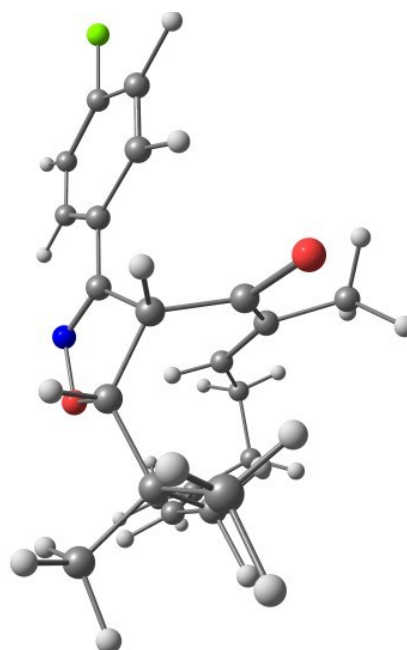
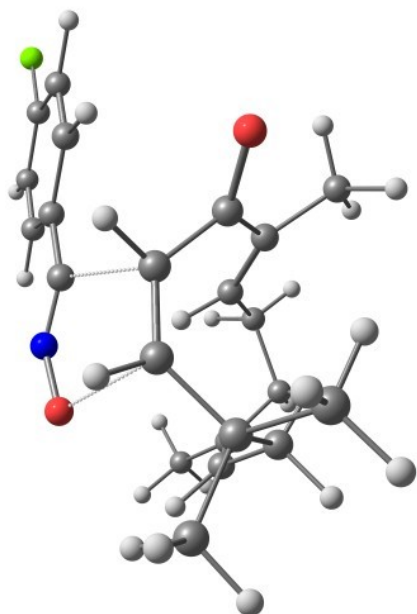




TS2pCl



TS3pCl



TS4pCl

Figure S58: Four possible transitions and products of **ZI-4**

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