Supporting Information

Six-Step Total Synthesis of Isohirsut-4-ene Through [5+2+1] Cycloaddition and Transannular Epoxide-Alkene Cyclization

Jing Liu‡[1], Yi Zhou‡[2], and Zhi-Xiang Yu[1,2]*

1. Department of Chemistry, Renmin University of China, Beijing 100872, China
2. Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China

*Email: yuzx@pku.edu.cn

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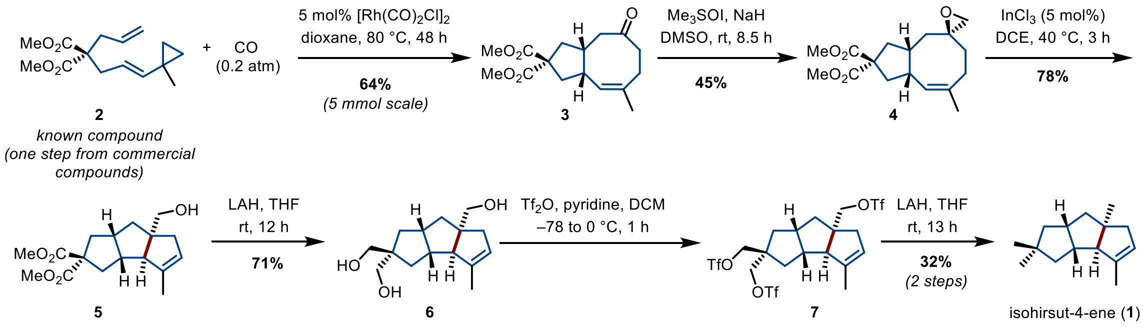
1. General Information

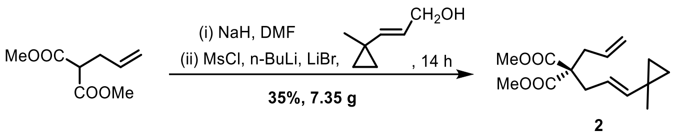
All chemicals were used as received without further purification. DCE (with molecular sieves, water ≤30 ppm) was purchased from J&K. Reactions were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using Thermostat-controlled silicone oil baths. Analytical TLCs were performed with 0.25 mm silica gel HSGF254. The TLC plates were visualized by ultraviolet light and treatment with anisaldehyde-H_2SO_4 or phosphomolybdic acid stain followed by gentle heating. Purification of products was accomplished by flash chromatography on silica gel (200-300 mesh) and the purified compounds show a single spot by analytical TLC. Organic solutions were concentrated using a Büchi or Eyela rotary evaporator with a desktop vacuum pump. Nuclear magnetic resonance (NMR) spectra were measured on Bruker ARX 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz), Bruker AVANCE III 500 (^{1}H at 500 MHz; ^{13}C at 126 MHz) NMR spectrometers. Data for ^{1}H NMR spectra are reported as follows: chemical shift δ (ppm) referenced to either $CHCl_3$ (7.26 ppm) or $CHDCl_2$ (5.32 ppm) or CHD_2OD (3.31 ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets), coupling constant J (Hz), and integration. Data for ^{13}C{1H} NMR spectra are reported in terms of chemical shift δ (ppm) referenced to either $CDCl_3$ (77.16 ppm) or CD_2Cl_2 (53.84 ppm) or CD_3OD (49.00 ppm). High-resolution mass spectra (HRMS) were recorded on Bruker Solarix XR Fourier transform ion cyclotron resonance (FTICR) mass spectrometer (electrospray ionization, ESI) and Hybrid Quadrupole-Orbitrap GC-MS/MS System (Q Exactive GC). Single crystal X-ray diffractometer was measured on XtaLAB PRO 007HF(Mo). All crystal compounds were obtained by adding *n*-hexane to their dichloromethane solutions and then stilling for several days.

2. Total Synthesis of Isohirsut-4-ene

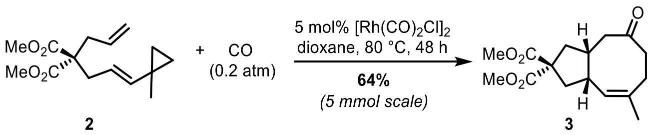
Scheme S1. total synthesis of isohirsut-4-ene.



Detailed synthesis procedures:



Compound **2** was obtained (35% yield, 7.35 g) according to literature.[1]



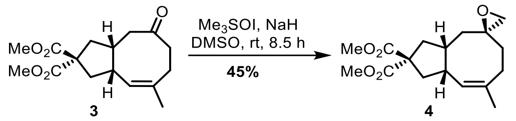
Preparation of 3: The catalyst of $[Rh(CO)_2Cl]_2$ (97.2 mg, 0.25 mmol, 5 mol% to ene-VCP) and substrates **2** (1.33g, 5 mmol) were added in glass flask (500 mL) and sealed, then displaced gas with CO/N_2 (1:4, *V/V*). The super-dried dioxane (100 mL, 0.05 M) was added and bubbled with balloon pressured mix gas of CO and N_2 (1:4, *V/V*) for 10 min. The solution was heated to 80 °C in an oil bath with stirring under a positive pressure of 0.2 atm CO. After stirring for 48 h, TLC indicated the absence of the starting material. Then the resulting solution was cooled to room temperature. Solvent was evaporated and the residue was purified by flash column chromatography on silica gel (eluted with petroleum ether/ethyl acetate = 8/1) to afford cycloadduct **3** as a yellow oil**.** Run 1: **3** (907.6 mg, 62%). Run 2: **3** (970.0 mg, 66%). The average yield of two runs was 64%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.15 (d, J = 9.0 Hz, 1H), 3.73 (s, 3H), 3.71 (s, 3H), 2.76 – 2.68 (m, 1H), 2.58 – 2.48 (m, 2H), 2.47 – 2.37 (m, 2H), 2.34 (d, J = 10.8 Hz, 2H), 2.31 – 2.23 (m, 2H), 2.23 – 2.16 (m, 1H), 2.03 (ddd, J = 13.5, 6.0, 3.2 Hz, 1H), 1.84 (s, 3H), 1.80 – 1.74 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 213.0, 173.1, 173.0, 137.2, 126.6, 59.2, 53.0, 53.0, 45.4, 43.5, 41.1, 40.1, 39.9, 28.9, 24.3.

HRMS (ESI−FTICR, *m/z*): $[M + H]^+$ calculated for $C_{16}H_{23}O_5^+$: 295.1540; found: 295.1537.



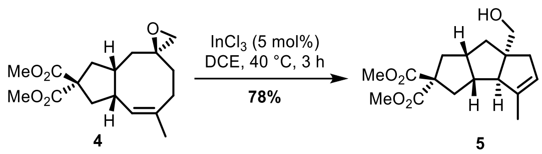
Preparation of 4: Me_3SOI (550.2 mg, 2.5 mmol, 2.5 equiv.) and NaH (60% weight in mineral oil, 100.0 mg, 2.5 mmol, 2.5 equiv.) were added in 50 mL reaction tube. Then DMSO (10 mL) was added under Argon. The resulting mixture was stirred at room temperature for 3 hours. Then a solution of **3** (294.0 mg, 1.00 mmol, 1.0 equiv.) in DMSO (10 mL) was added (1 mL THF was used to transfer the residual substrate due to the low solubility of **3** in DMSO). After stirring at room temperature for 5.5 hours, TLC indicated the absence of substrate. Then the reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 10:1 petroleum ether/EtOAc) afforded the title compound **4** as a colorless oil. Run 1: **4** (140.3 mg, 46%). Run 2: **4** (132.3.0 mg, 43%). The average yield of two runs was 45%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.5.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 5.08 (dt, J = 8.4, 1.5 Hz, 1H), 3.69 (s, 3H), 3.68 (s, 3H), 3.15 – 3.02 (m, 1H), 2.61 – 2.54 (m, 2H), 2.54 – 2.48 (m, 2H), 2.27 (dd, J = 14.3, 2.0 Hz, 1H), 2.22 – 2.13 (m, 2H), 1.89 (ddd, J = 14.1, 12.8, 2.2 Hz, 1H), 1.77(t, J=1.5 Hz, 3H), 1.81 – 1.74 (m, 1H), 1.71 – 1.60 (m, 2H), 1.50 (dd, J = 13.8, 3.7 Hz, 1H), 1.32 (ddd, J = 14.2, 6.6, 2.0 Hz, 1H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 173.5, 138.3, 126.7, 59.5, 59.1, 59.0, 53.0, 52.9, 42.7, 40.6, 40.2, 40.2, 36.9, 34.4, 29.3, 24.3.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{17}H_{25}O_5^+$: 309.1697; found: 309.1696.



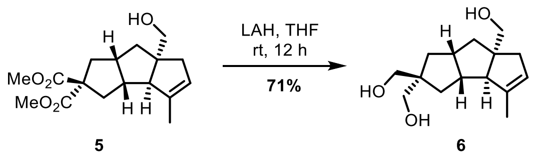
Preparation of 5: Substrate **4** (123.3 mg, 0.4 mmol, 1.0 equiv.) was added in the reaction flask (25 mL) which was then moved to glovebox, charged with $InCl_3$ (4.4 mg, 0.1 mmol, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (8 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). The reaction was monitored by TLC. After 3 h, the reaction mixture was finally cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel (eluted with petroleum ether/ethyl acetate = 5/1 ~ 4/1) to afford the pure product **5** as a light yellow oil. Run 1: **5** (93.6 mg, 76%). Run 2: **5** (98.6 mg, 80%). The average yield of two runs was 78%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.13 (dd, J = 3.6 Hz, 3.6Hz, 1H), 3.72 (s, 3H), 3.71 (s, 3H), 3.50 (s, 2H), 2.60 (ddd, J = 10.6, 7.5, 3.0 Hz, 1H), 2.54 – 2.41 (m, 3H), 2.38 – 2.24 (m, 2H), 2.17 – 2.08 (m, 2H), 2.02 (dd, J = 13.2, 11.2 Hz, 1H), 1.71 (dd, J = 12.9, 7.4 Hz, 1H), 1.66 (s, 3H), 1.58 – 1.51 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.3, 173.3, 141.9, 123.0, 70.3, 61.9, 61.1, 58.3, 52.9, 52.9, 49.6, 43.5, 43.4, 42.6, 40.2, 38.8, 15.9.

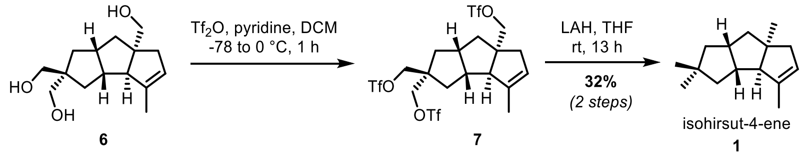
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{17}H_{25}O_5^+$: 309.1697; found: 309.1694.



Preparation of 6: To a solution of **5** (88.2 mg, 0.29 mmol, 1.0 equiv.) in THF (10mL) was added LAH (65.9 mg, 1.7 mmol, 6.0 equiv.) slowly at 0 °C. Then the resulting mixture was warmed to room temperature and stirred for 12 h. The reaction mixture was quenched by saturated potassium sodium tartrate and extracted by EA. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation to afford crude product. Then recrystallization using EA/PE as solvent gave pure **6** as white solid. Run 1: **6** (52.7 mg, 73%). Run 2: **6** (49.7 mg, 69%). The average yield of two runs was 71%.

TLC (9:1 DCM/MeOH, R_f): 0.4. m.p.=121.5-123.0 °C.

^{1}H NMR (400 MHz, CD_3OD) δ 5.10 (s, 1H), 4.89 (s, 3H), 3.56 – 3.48 (m, 2H), 3.43 – 3.37 (m, 4H), 2.55 – 2.44 (m, 1H), 2.40 (s, 1H), 2.33 – 2.22 (m, 2H), 2.13 – 2.04 (m, 1H), 1.73 (dd, J = 13.0, 7.7 Hz, 1H), 1.67 (s, 3H), 1.66 – 1.62 (m, 2H), 1.61 – 1.55 (m, 1H), 1.42 – 1.32 (m, 2H).
^{13}C NMR (101 MHz, MeOD) δ 143.2, 123.3, 70.4, 69.3, 67.0, 62.6, 59.1, 52.4, 50.1, 44.6, 44.5, 44.3, 38.5, 37.0, 16.0.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{15}H_{25}O_3^+$: 253.1798; found: 253.1793.



Preparation of 1: A 25 mL reaction flask was charged with a stir bar and **6** (25.2 mg, 0.1 mmol, 1.0 equiv.) and placed under an atmosphere of argon. Super-dried CH_2Cl_2 (2.0 mL) and pyridine (0.3 mL) were added. Then the solution was cooled to −78 °C and triflic anhydride (75.6 µL, 0.45 mmol, 4.5 equiv) was added dropwise, and then the reaction mixture was warmed to 0 °C. After stirring for 1 h at °C, the flask was moved to a −78 °C bath, 1 mL brine and 1 mL 1 N HCl was added and allowed to freeze in the flask. The flask was removed from the cold bath, and as soon as the mixture had thawed slightly, it was transferred to a separatory funnel and extracted with 3 × 10 mL of CH_2Cl_2. The organic layers were combined and washed with 1N HCl, saturated $NaHCO_3$, and brine. The collected organic layers were then dried over Na_2SO_4, then filtered and concentrated under vacuum, affording a yellow liquid which was used in the next step without further purification or isolation.

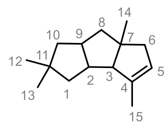
A 25 mL reaction flask was charged with a stir bar and LAH (38.0 mg, 0.1 mmol, 10.0 equiv.) and placed under an atmosphere of argon. THF (1.5 mL) was added and the solution was cooled to 0 °C before adding the solution of the above liquid (**7**) in THF (1.5 mL). Another 1 mL THF was used to transfer the residual liquid. The resulting mixture was stirred for 13 h in a 25 °C oil bath, then saturated potassium sodium tartrate was added carefully. The mixture was extracted with 3 × 10 mL of EA. The organic layers were combined and washed with brine, then filtered and concentrated under vacuum. The crude mixture was purified by flash column chromatography with silica gel (eluted with petroleum ether or n-hexane) to afford pure product isohirsut-4-ene **1** as a colorless oil. Run 1: **1** (6.1 mg, 30%). Run 2: **6** (6.8 mg, 33%). The average yield of two runs was 32%.

TLC (petroleum ether, R_f): 0.9.

^{1}H NMR (500 MHz, $CDCl_3$) δ 5.07 (t, *J* = 1.9 Hz, 1H), 2.61 – 2.47 (m, 1H), 2.40 – 2.30 (m, 1H), 2.27 – 2.15 (m, 1H), 2.12 (s, 1H), 2.05 – 1.96 (m, 1H), 1.82 (dd, *J* = 12.8, 7.8 Hz, 1H), 1.68 (s, 3H), 1.63 (ddd, *J* = 12.9, 8.3, 1.5 Hz, 2H), 1.58 (ddd, *J* = 12.3, 7.6, 1.5 Hz, 2H), 1.34 (dd, *J* = 8.8, 4.0 Hz, 2H), 1.30 (d, *J* = 12.1 Hz, 2H), 1.29 – 1.23 (m, 2H), 1.17 (s, 3H), 1.07 (s, 3H), 0.92 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 143.0, 121.9, 66.9, 53.1, 50.2, 49.0, 49.0, 47.7, 47.6, 44.5, 41.8, 30.7, 29.6, 29.3, 16.1.
HRMS (EI−GC-MS, *m*/*z*): $[M]^{+\cdot}$ calculated for $C_{15}H_{24}^{+\cdot}$: 204.1873; found: 204.1873.

3. NMR Comparison between Isohirsut-4-ene Obtained from Total Synthesis and Isohirsut-4-ene Isolated from Bacteria.

Table S1. Chemical shifts for each atom in isohirsut-4-ene obtained from bacteria[2] and total synthesis (this work).



	Reported *Exp. δ (p.p.m)*	This work *δ(p.p.m)*	Difference (this work minus Reported *Exp.*)
C1	48.8	49.0	0.2
C10	47.4	47.6	0.2
C11	41.6	41.8	0.2
C12 or C13	29.2	29.3	0.1
C12 or C13	30.5	30.7	0.2
C14	29.4	29.6	0.2
C15	15.9	16.1	0.2
C2	50.1	50.2	0.1
C3	66.7	66.9	0.2
C4	142.8	143.0	0.2
C5	121.8	121.9	0.1
C6	47.5	47.7	0.2
C7	52.9	53.1	0.2
C8	48.9	49.0	0.1
C9	44.3	44.5	0.2
			MAD 0.17
H1	1.58	1.58	0
H1	1.30	1.30	0
H10	1.27	1.26	-0.01
H10	1.64	1.63	-0.01
H12 or H13	0.92	0.92	0
H12 or H13	1.06	1.07	0.01
H14	1.17	1.17	0
H15	1.68	1.68	0
H2	2.34	2.35	0.01
H3	2.11	2.12	0.01
H5	5.06	5.07	0.01
H6	2.01	2.00	-0.01
H7	2.19	2.20	0.01
H8	1.81	1.82	0.01
H8	1.32	1.34	0.02
H9	2.52	2.53	0.01
			MAD 0.01

MAD, mean absolute deviation

As shown in **Table S1**, the chemical shifts for each atom in product **1** are fully consistent with the reported literature[2] (MAD=0.17 for ^{13}C NMR and 0.01 for ^{1}H NMR). Thus, we concluded that a six-step total synthesis of the natural product isohirsut-4-ene was achieved. This work also demonstrated the relative configuration of isohirsut-4-ene (*cis-anti-cis* fused rings) and supported the computational prediction.

4. Corey-Chaykovsky Reaction

4.1. DFT study on the stereoselectivity of Corey-Chaykovsky reaction

DFT calculations were performed with Gaussian 09[3]. The functional M06-2X[4] and a basis set 6-31+G(d) were employed for optimizing the geometries of minima and transition states in the gas phase. Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. Pruned integration grids with 99 radial shells and 590 angular points per shell were used. Based on the gas-phase optimized structures, single-point energy was computed at the same level under SMD[5] model to account for solvation effects of dimethyl sulfoxide (DMSO). All discussed energy differences were based on the Gibbs energies in DMSO at 298 K. For all transition states and intermediates, we have manually searched for their conformations and the most stable ones are present here.

A preliminary DFT calculation was carried out to study the diastereoselectivity of Corey-Chaykovsky reaction in this work. To simplify the computations, we chose **8a'** as the model substrate (**Figure S1**). According to our DFT study on the mechanism of Corey-Chaykovsky reaction[6], we calculated the nucleophilic transition states of **8a'** shown in **Figure S1**. Firstly, **S1** undergoes the nucleophilic addition to the carbonyl group of **8a'** via either **8a'-TS1** or **8a'-TS2**, DFT calculation indicated that the nucleophilic transition state **8a'-TS1** (leading to **9m**) is favored over **8a'-TS2** (leading to **9n)** by 3.5 kcal/mol of Gibbs free energy. These two processes (from **8a'** to **8a'-INT1** and **8a'-INT2**) are endergonic by 6.5 kcal/mol and 10.4 kcal/mol, respectively, indicating that the first nucleophilic additions are reversible. In the second steps, intermediate **8a'-INT1** undergoes a nucleophilic substitution reaction via **8a'-TS3** to afford epoxide **9m**, requiring an activation free energy of 7.6 kcal/mol, while **8a'-INT2** undergoes a nucleophilic substitution reaction via **8a'-TS4** to afford epoxide **9n**, requiring an activation free energy of 8.7 kcal/mol. As shown in **Figure S1**, the second step was found to be both rate-determining and stereo-determining.

Thus, the diastereoselectivity of this Corey-Chaykovsky reaction is determined by the energy difference between **8a'-TS3** and **8a'-TS4**. Our calculations showed that **8a'-TS3** (leading to **9m**) is favored over **8a'-TS4** (leading to **9n**) by 5.0 kcal/mol, suggesting that **9m** is formed exclusively. This is consistent with our experiments, where **9a** was obtained as a single isomer. We attribute such a high diastereoselectivity to the different ring strains of the eight-membered rings in the transition states. As shown in **Figure S1**, the H···H distance in **8a'-TS4** is 1.97 Å and the angle of C1-C2(sp^3)-C3 is 120°. The corresponding values in **8a'-TS3** are 2.02 Å and 115°, indicating that there is more severe ring strain in **8a'-TS4** than that in **8a'-TS3**.

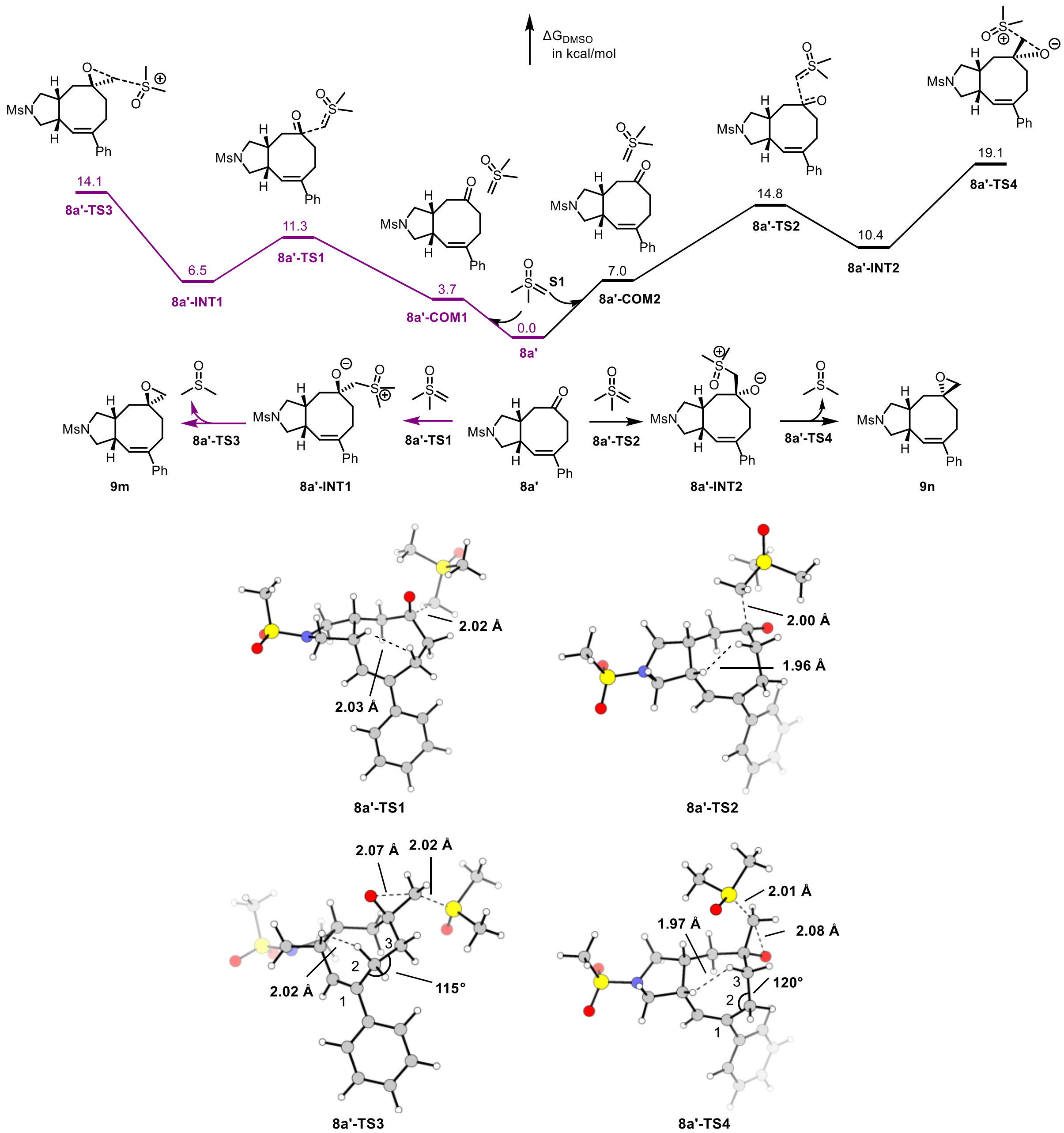
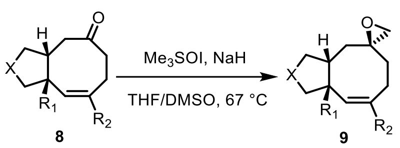


Figure S1. Gibbs energy profiles for the two nucleophilic steps of Corey-Chaykovsky reaction of **8a'**. Color scheme: H, white; C, gray; O, red; S, yellow; N, blue.

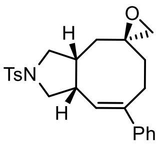
4.2. Experiments for Corey-Chaykovsky reaction.

Substrates 8a-8f were prepared through [5+2+1] cycloaddition and reported by literature[7].



General Procedure: Me_3SOI (1.35 equiv.) and NaH (60% weight in mineral oil, 1.35 equiv.) were added in a 25 mL reaction tube. Then THF (1 mL) was added under argon atmosphere. The resulting mixture was stirred in an oil bath at 67 °C for 2 h. Then a solution of substrate **8** (1.0 equiv.) in DMSO (1 mL) was added

(2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C. After TLC indicated the absence of substrate, the reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9**.



9a

Me_3SOI (59.7 mg, 0.27 mmol, 1.35 equiv.) and NaH (11.7 mg, 0.27 mmol, 60% weight in mineral oil, 1.35 equiv.) were added in 25 mL reaction tube. Then THF (1 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 2.5 h. Then a solution of substrate **8a** (79.5 mg, 0.20 mmol, 1.0 equiv.) in DMSO (1 mL) was added (2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 2 hours. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9a** as a white foam. Run 1: **9a** (64.8 mg, 79%). Run 2: **9a** (64.5 mg, 79%). The average yield of two runs was 79%.

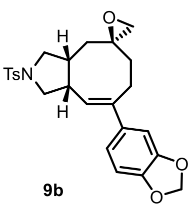
At 1.8 mmol scale: Me_3SOI (534.8 mg, 2.43 mmol, 1.35 equiv.) and NaH (97.2 mg, 2.43 mmol, 60% weight in mineral oil, 1.35 equiv.) were added in 100 mL reaction tube. Then THF (9 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 3 h. Then a solution of substrate **8a** (711.9 mg, 1.80 mmol, 1.0 equiv.) in DMSO (9 mL) was added (2 × 0.5 mL THF was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 6 hours. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9a** as a white foam. Run 1: **9a** (565.7 mg, 77%). Run 2: **9a** (541.9 mg, 74%). The average yield of two runs was 76%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.3.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.73 (d, J = 7.9 Hz, 2H), 7.37 (d, J = 7.9 Hz, 2H), 7.32 – 7.20 (m, 5H), 5.13 (d, J = 8.9 Hz, 1H), 3.52 – 3.44 (m, 2H), 3.35 (dd, J = 9.4, 7.8 Hz, 1H), 3.30 – 3.24 (m, 1H), 2.81 – 2.69 (m, 2H), 2.60 (d, J = 5.5 Hz, 1H), 2.53 (d, J = 5.5 Hz, 1H), 2.51 – 2.46 (m, 1H), 2.42 (s, 3H), 2.39 – 2.31 (m, 1H), 2.02 (ddd, J = 13.7, 13.6, 2.2 Hz, 1H), 1.58 (d, J = 8.2 Hz, 2H), 1.40 (ddd, J = 14.3, 6.3, 1.9 Hz, 1H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 144.1, 142.5, 142.2, 134.2, 130.1, 128.6, 127.8, 127.5, 126.8, 126.1, 59.3, 58.5, 54.5, 51.9, 41.5, 41.0, 38.3, 32.3, 27.2, 21.7.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{24}H_{28}NO_3S^+$: 410.1784; found: 410.1784.



9b

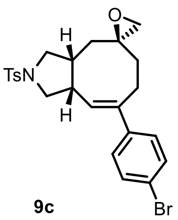
Me_3SOI (59.4 mg, 0.27 mmol, 1.35 equiv.) and NaH (11.8 mg, 0.27 mmol, 60% weight in mineral oil, 1.35

equiv.) were added in 25 mL reaction tube. Then THF (1 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 2 h. Then a solution of substrate **8b** (88.0 mg, 0.20 mmol, 1.0 equiv.) in DMSO (1 mL) was added (2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 2 hours. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9b** as a white solid. Run 1: **9b** (68.8 mg, 76%). Run 2: **9b** (65.6 mg, 72%). The average yield of two runs was 74%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.2. m.p.=196.2-198.0 °C.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.73 (d, J = 8.1 Hz, 2H), 7.38 (d, J = 8.1 Hz, 2H), 6.77 – 6.63 (m, 3H), 5.96 (s, 2H), 4.99 (d, J = 9.0 Hz, 1H), 3.51 – 3.40 (m, 2H), 3.35 (dd, J = 9.4, 7.8 Hz, 1H), 3.27 – 3.19 (m, 1H), 2.79 – 2.67 (m, 2H), 2.58 (d, J = 5.5 Hz, 1H), 2.52 (d, J = 5.5 Hz, 1H), 2.42 (s, 3H), 2.40 – 2.30 (m, 2H), 1.97 (ddd, J = 13.7, 13.6, 2.1 Hz, 1H), 1.59 – 1.49 (m, 2H), 1.37 (ddd, J = 14.3, 6.3, 1.9 Hz, 1H). **^{13}C NMR** (101 MHz, CD_2Cl_2) δ 148.1, 147.3, 144.2, 142.1, 136.5, 134.2, 130.2, 127.8, 125.7, 119.6, 108.2, 106.7, 101.7, 59.3, 58.5, 54.5, 51.9, 41.6, 40.9, 38.2, 32.3, 27.4, 21.6.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{25}H_{28}NO_5S^+$: 454.1683; found: 454.1677.



9c

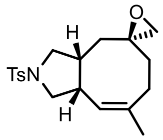
Me_3SOI (59.4 mg, 0.27 mmol, 1.35 equiv.) and NaH (10.8 mg, 0.27 mmol, 60% weight in mineral oil, 1.35 equiv.) were added in 25 mL reaction tube. Then THF (1 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 2 h. Then a solution of substrate **8c** (94.9 mg, 0.20 mmol, 1.0 equiv.) in DMSO (1 mL) was added (2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 2.5 h. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9c** as a white solid. Run 1: **9c** (70.3 mg, 72%). Run 2: **9c** (67.1 mg, 69%). The average yield of two runs was 71%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.2. m.p.=188.6-190.1 °C.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.73 (d, J = 8.2 Hz, 2H), 7.42 (d, J = 8.6 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 7.10 (d, J = 8.6 Hz, 2H), 5.17 (d, J = 8.9 Hz, 1H), 3.45 (d, J = 2.9 Hz, 2H), 3.34 (dd, J = 9.5, 7.9 Hz, 1H), 3.30 – 3.21 (m, 1H), 2.83 – 2.68 (m, 2H), 2.59 (d, J = 5.5 Hz, 1H), 2.52 (d, J = 5.5 Hz, 1H), 2.43 (s, 3H), 2.46 – 2.31 (m, 2H), 2.02 – 1.94 (m, 1H), 1.61 – 1.50 (m, 2H), 1.39 (ddd, J = 14.3, 6.2, 1.9 Hz, 1H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 144.1, 141.6, 141.2, 134.2, 131.7, 130.1, 127.9, 127.8, 127.6, 121.3, 59.3, 58.4, 54.4, 51.9, 41.5, 41.0, 38.1, 32.3, 27.1, 21.7.

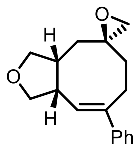
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{24}H_{27}BrNO_3S^+$: 488.0890; found: 488.0890.



9d

Me_3SOI (50.5 mg, 0.27 mmol, 1.35 equiv.) and NaH (9.2 mg, 0.23 mmol, 60% weight in mineral oil, 1.35 equiv.) were added in 25 mL reaction tube. Then THF (1 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 2 h. Then a solution of substrate **8d** (56.3 mg, 0.17 mmol, 1.0 equiv.) in DMSO (1 mL) was added (2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 4 h. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9d** as a white solid. Run 1: **9d** (35.1 mg, 60%). Run 2: **9d** (37.5 mg, 63%). The average yield of two runs was 62%.
TLC (3:1 petroleum ether/EtOAc, R_f): 0.4. m.p.=136.1-138.1 °C.

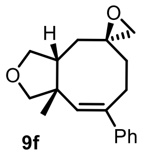
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.69 (d, J = 8.2 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 4.64 (d, J = 8.6 Hz, 1H), 3.35 – 3.29 (m, 2H), 3.25 (dd, J = 9.5, 8.1 Hz, 1H), 3.11 – 3.04 (m, 1H), 2.66 (dd, J = 11.2, 9.5 Hz, 1H), 2.54 (d, J = 5.6 Hz, 1H), 2.51 – 2.45 (m, 2H), 2.44 (s, 3H), 2.19 (dddd, J = 13.3, 8.0, 6.6, 4.0 Hz, 1H), 1.85 (ddd, J = 14.6, 12.9, 2.2 Hz, 1H), 1.76 (ddd, J = 13.9, 6.5, 2.3 Hz, 1H), 1.68 (s, 3H), 1.55 (dd, J = 13.8, 11.5 Hz, 1H), 1.46 (dd, J = 13.8, 4.6 Hz, 1H), 1.29 (ddd, J = 14.3, 6.6, 2.1 Hz, 1H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 143.9, 139.5, 134.2, 130.0, 127.8, 123.5, 59.1, 58.5, 54.5, 51.8, 41.0, 40.0, 36.7, 32.4, 29.1, 24.2, 21.6.
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{19}H_{26}NO_3S^+$: 348.1628; found: 348.1621.



9e

Me_3SOI (59.4 mg, 0.27 mmol, 1.35 equiv.) and NaH (10.8 mg, 0.27 mmol, 60% weight in mineral oil, 1.35 equiv.) were added in 25 mL reaction tube. Then THF (1 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 2 h. Then a solution of substrate **8e** (50.0 mg, 0.21 mmol, 1.0 equiv.) in DMSO (1 mL) was added (2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 2 h. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9e** as a white foam. Run 1: **9e** (41.8 mg, 79%). Run 2: **9e** (41.1 mg, 78%). The average yield of two runs was 79%.
TLC (3:1 petroleum ether/EtOAc, R_f): 0.4.
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.49 – 7.41 (m, 2H), 7.36 – 7.30 (m, 2H), 7.28 – 7.22 (m, 1H), 5.84 (d, J = 7.8 Hz, 1H), 4.02 (dd, J = 8.4, 4.9 Hz, 1H), 3.90 (dd, J = 8.4, 1.3 Hz, 1H), 3.84 (dd, J = 8.0 Hz, 8.0 Hz, 1H), 3.40 – 3.32 (m, 1H), 3.24 (dd, J = 10.6, 7.8 Hz, 1H), 2.96 – 2.87 (m, 1H), 2.71 – 2.53 (m, 2H), 2.63 (d, J = 5.5 Hz, 1H), 2.57 (d, J = 5.5 Hz, 1H), 2.09 (ddd, J = 14.6, 12.8, 2.1 Hz, 1H), 1.76 (dd, J = 13.9, 11.9 Hz, 1H), 1.57 – 1.46 (m, 2H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 142.7, 142.3, 129.0, 128.7, 127.4, 126.2, 75.0, 72.3, 59.1, 59.1, 42.6, 42.2, 38.1, 31.7, 27.4.
HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{17}H_{21}O_2^+$: 257.1536; found: 257.1543.



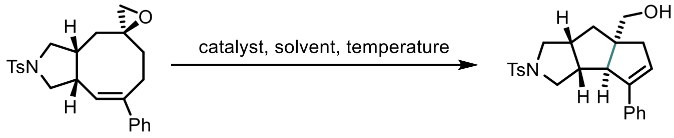
9f

Me_3SOI (59.4 mg, 0.27 mmol, 1.35 equiv.) and NaH (10.8 mg, 0.27 mmol, 60% weight in mineral oil, 1.35 equiv.) were added in 25 mL reaction tube. Then THF (1 mL) was added under Argon. The resulting mixture was stirred in an oil bath at 67 °C for 2 h. Then a solution of substrate **8f** (51.3 mg, 0.20 mmol, 1.0 equiv.) in DMSO (1 mL) was added (2 × 0.5 mL DMSO was used to transfer the residual substrate from the container). The mixture was stirred at 67 °C for 2 h. The reaction system was quenched by water at room temperature and extracted with EA. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography afforded **9f** as a colorless oil. Run 1: **9f** (46.0 mg, 85%). Run 2: **9f** (45.5 mg, 84%). The average yield of two runs was 85%.
TLC (3:1 petroleum ether/EtOAc, R_f): 0.2.
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.42 – 7.38 (m, 2H), 7.35 – 7.29 (m, 2H), 7.28 – 7.23 (m, 1H), 5.75 (s, 1H), 4.32 (dd, J = 8.7, 7.0 Hz, 1H), 3.68 (d, J = 8.0 Hz, 1H), 3.61 (d, J = 8.0 Hz, 1H), 3.42 (dd, J = 8.7, 3.4 Hz, 1H), 3.03 – 2.96 (m, 1H), 2.67 – 2.56 (m, 2H), 2.55 (s, 2H), 2.19 (dd, J = 14.6, 9.7 Hz, 1H), 1.86 (ddd, J = 14.7, 12.0, 2.6 Hz, 1H), 1.60 – 1.52 (m, 1H), 1.33 (s, 3H), 1.24 (ddd, J = 14.7, 1.5 Hz, 1.5 Hz, 1H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 143.2, 141.0, 130.6, 128.7, 127.5, 126.8, 79.6, 78.6, 59.4, 57.8, 47.7, 45.7, 39.9, 35.2, 26.9, 26.7.
HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{18}H_{23}O_2^+$: 271.1693; found: 271.1687.

5. Epoxide-Alkene Cyclization

5.1. Reaction optimization

Table S2: Reaction Optimization for the Epoxide-Alkene Cyclization.



Entry	Catalyst	Loading (equivalent)	Solvent	Temperature (°C)	Time (h)	Yield (%)
1	$InCl_3$	0.1	DCE	60	1	87
2	BF_3•Et_2O	1.2	DCM	-78	4.5	69
3	$TiCl_4$	2.0	DCM	-78	2	mixture
4	Cp_2TiCl_2/Zn	3.0	THF	rt	1	63
5	SmI_2	4.0	THF	-78	3.5	mixture
6	TfOH	10.0	DCE	60	0.3	21
7	$InCl_3$	0.05	DCE	60	1.5	85
8	$InCl_3$	0.01	DCE	60	18	trace
9	$InCl_3$	0.01	DCE	60	48	80
10	**$InCl_3$**	**0.05**	**DCE**	**40**	**1.5**	**91**
11	$InCl_3$	0.05	DCE	25	6.5	89
12	$InCl_3$	0.05	$PhCF_3$	60	1.5	79
13	$InCl_3$	0.05	CH_3CN	60	1.5	trace
14	$InCl_3$	0.05	Dioxane	60	1.5	NR
15	$InCl_3$	0.05	THF	60	1.5	NR

9a was chose as the model substrate. Different catalysts were screened for the epoxide-alkene cyclization. We firstly tested $InCl_3$, which was previously shown to be efficient in transannular ene reaction.[7] We were happy to find that this Lewis acid also showed great reactivity toward the present epoxide-alkene cyclization. In this case, the desired product **10a** was obtained in 87% yield with 10 mol% $InCl_3$ (**Table S2**, entry 1). The widely used Lewis acids of $BF_3·Et_2O$ and $TiCl_4$ were also tested: $BF_3·Et_2O$ afforded **10a** in 69% yield (**Table S2**, entry 2), while $TiCl_4$ gave a complex mixture (**Table S2**, entry 3). Cp_2TiCl_2 combined with the reductant Zn also worked well, giving the desired product in 63% yield, though the mechanism was not clear at this stage (ionic pathway or radical pathway, **Table S2**, entry 4). Using another redox catalyst of

SmI_2 afforded a complex mixture (**Table 2**, entry 5). Besides, Brønsted acid of TfOH was also effective in this reaction, even though the reaction yield was low (21%, **Table 2**, entry 6). Thus, we chose $InCl_3$ as the catalyst for further optimization. Reducing the catalyst loading to 5 mol% had little effect on the product yield (85%, entry 7). But using 1 mol% $InCl_3$ required 2 days to get a comparable yield (entry 8, entry 9). Different solvents and temperatures were also screened, finding that the optimal temperature was 40 °C and the best solvent was DCE (entry 10-15). Considering the reaction time, catalyst cost, and product yield, we chose entry 10 (5 mol% $InCl_3$, DCE as solvent, 40 °C) as the standard reaction conditions.

5.2. DFT study on the stereoselectivity of epoxide-alkene cyclization.

DFT calculations were performed with Gaussian 09[3]. The functional M06-2X[4] and a basis set def2-SVP[8] with corresponding effective core potential[9] were employed for optimizing the geometries of minima and transition states in the gas phase. Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and evaluate its zero-point energy and thermal corrections at 298 K. Pruned integration grids with 99 radial shells and 590 angular points per shell were used. Based on the gas-phase optimized structures, single-point energies were computed at the same level under SMD[5] model to account for solvation effects of dichloroethane (DCE). All discussed energy differences were based on the Gibbs energies in DCE at 298 K. For all transition states and intermediates, we have manually searched for their conformations and the most stable ones are present here.

5.2.1 $InCl_3$ as the catalytic species

Experimentally, substrates **9a** underwent epoxide-alkene cyclization to afford **10a** as a sole isomer. To understand the high stereoselectivity of epoxide-alkene cyclization in this work, preliminary DFT calculations have been carried out. To simplify the calculations, we chose two model substrates **9m** and **9n** for investigation (**Figure S2).** For substrate **9m**, the reaction starts from forming complex **A**. It's believed that epoxide-alkene cyclization undergoes via either a stepwise or concerted pathway.[10] Here, DFT calculations showed that, the concerted cyclization step for **A** through **TS1** requires an activation free energy of 28.8 kcal/mol. This transition state **TS1** leads directly to the linear triquinane product, with the *cis-anti-cis* configuration observed experimentally. However, the $InCl_3$-initiated heterolysis of C-O bond via **TS2**, which gives a carbocation **INT1**, is favored over **TS1** by 3.4 kcal/mol. Then, **INT1** can undergo a cation-alkene cyclization through two pathways: one via the cyclization transition state **TS3** leading to product **10m**, is much favored over the other via **TS4** leading to product **10n**, by 34.0 kcal/mol in terms of Gibbs free energy. Thus, only **10m** can be obtained through this stepwise pathway, which is consistent with our experiments.

We also computed the reaction of **9n**, which is the diastereomer of **9m** and was not observed in the epoxidation reaction experimentally. This reaction starts from forming complex **B**. DFT calculations indicated that, the $InCl_3$-inititated heterolysis of C-O bond for **B** (via **TS5)** gives the same carbocation **INT1** from reaction of **A**, requiring an activation free energy of 27.2 kcal/mol. Interestingly the concerted cyclization of **B** via **TS6** is impossible, requiring an activation free energy of 59.7 kcal/mol. As a result, **B** could also undergo epoxide-alkene cyclization through a stepwise pathway, in which a carbocation **INT1** is firstly formed, followed by cyclization to give **10m** as the sole isomer via **TS3**. Therefore, we predicted that this epoxide-alkene cyclization reaction is stereoselective, proceeding through a stepwise pathway, and the different configurations of epoxides cannot alter the relative configuration of the tricyclic products.

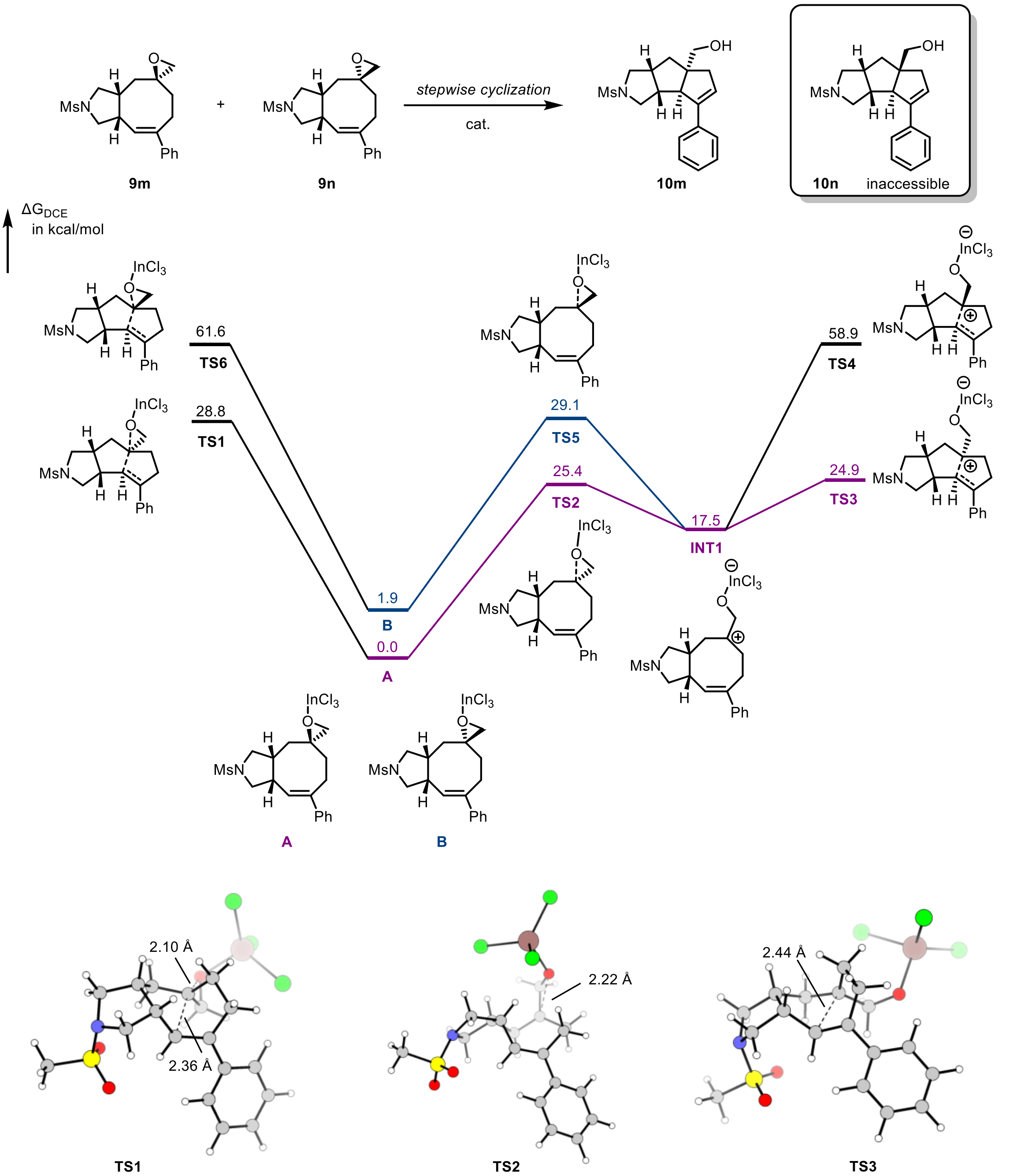


Figure S2. Gibbs energy profile for the cyclization step of different diastereomers **A** and **B**. Color scheme: H, white; C, gray; O, red; S, yellow; N, blue; In, brown; Cl, green.

5.2.2 $InCl_2^+$ as the possible catalytic species

In light of our previous work proposing that $InCl_3$ could dissociate into its cationic species as the real catalytic species,[11] we also considered this possibility using $InCl_2^+$ as the catalytic species for the cyclization reaction (**Figure S3**). For **9m**, the reaction starts from forming complex **C**. Both concerted and stepwise pathways for epoxide-alkene cyclization have been investigated. Our calculations indicated that the concerted cyclization via **TS7** requires an activation free energy of 14.2 kcal/mol, while the $InCl_2^+$-initiated heterolysis of C-O bond via **TS8** requires an activation free energy of 14.6 kcal/mol, which gives a carbocation **INT2**. Then **INT2** undergoes a cation-alkene cyclization through two different pathways, but the cyclization transition state **TS9** (leading to **10m**) is much favored over **TS10** (leading to **10n**) by 41.4

kcal/mol in terms of Gibbs free energy, indicating only **10m** can be obtained. This result is similar to the results from the DFT calculations using $InCl_3$ as the catalyst (**Figure S2**) and agrees with our experimental observation. The small energy difference between **TS7** and **TS8** ($\Delta\Delta G^‡$ = 0.4 kcal/mol) indicates both concerted and stepwise cyclization of **C** could happen to afford the same tricyclic product with *cis-anti-cis* configuration.

For **9n**, its reaction starts from forming complex **D**. We found that the stepwise mechanism via **TS11** ($\Delta G^‡$ = 14.4 kcal/mol) and **TS9** to give **10m** as the major product is possible. It is interesting to find that the concerted cyclization of **D** via **TS12** is impossible, requiring an activation free energy of 44.9 kcal/mol. Therefore, we conclude that this epoxide-alkene cyclization reaction is stereoselective, proceeding through a stepwise pathway (in contrast, both the concerted and stepwise pathways for **C** are possible).

In the above calculations, we have considered two possibilities of the real catalytic species from $InCl_3$: one possibility is a neutral species of $InCl_3$ and the other is a cationic species of $InCl_2^+$. At this moment, we didn't have computational or experimental evidence to confirm the exact form of the catalytic species. Here calculations were just used to show how the epoxide-alkene cyclization takes place and what the stereochemistry of this reaction is.

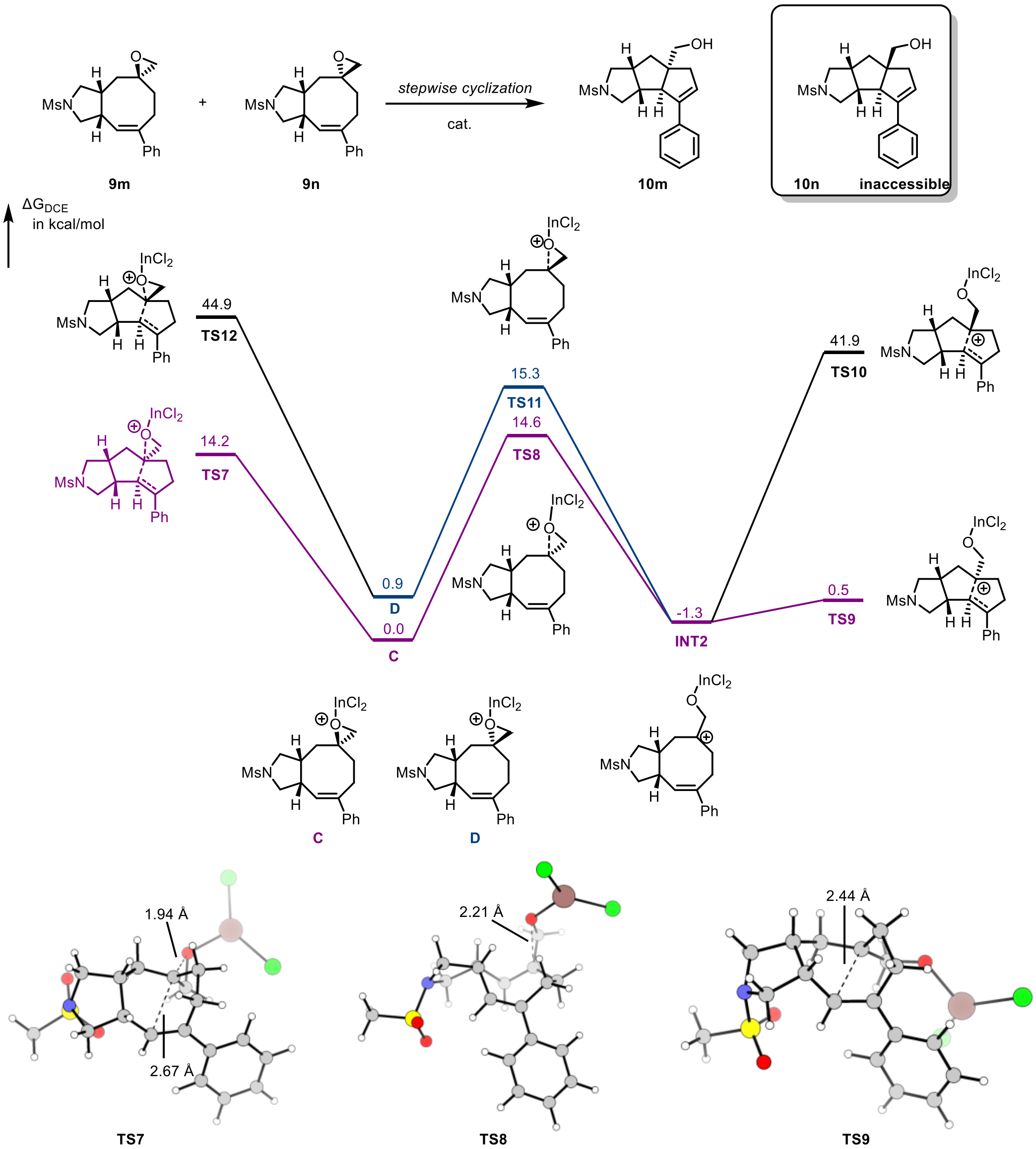
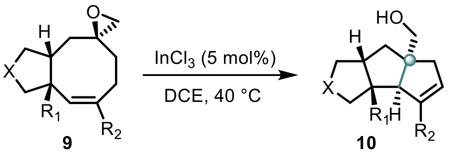


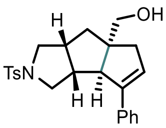
Figure S3. Gibbs energy profile for the cyclization step of different diastereomer **C** and **D**. Color scheme:

H, white; C, gray; O, red; S, yellow; N, blue; In, brown; Cl, green.

5.3. Experiments for epoxide-alkene cyclization.



General Procedure: Substrate **9** (1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). The reaction was monitored by TLC. The reaction mixture was finally cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10.**



10a

Substrate **9a** (20.1 mg, 0.05 mmol, 1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (0.6 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 1.5 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10a** as a colorless oil. Run 1: **10a** (18.3 mg, 91%). Run 2: **10a** (17.9 mg, 89%). The average yield of two runs was 90%.

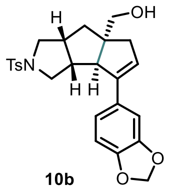
At 1.2 mmol scale: Substrate **9a** (491.5 mg, 1.2 mmol, 1.0 equiv.) was added in the reaction flask (100 mL) which was then moved to glovebox, charged with $InCl_3$ (13.3 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (24 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 10 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10a** as a colorless oil. Run 1: **10a** (436.3 mg, 89%). Run 2: **10a** (425.6 mg, 87%). The average yield of two runs was 88%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 7.6 Hz, 2H), 7.34 – 7.28 (m, 4H), 7.31 (d, J = 7.6 Hz, 2H), , 7.25 – 7.20 (m, 1H), 6.01 (dd, J = 3.0 Hz, 3.0 Hz, 1H), 3.58 – 3.42 (m, 3H), 3.28 (dd, J = 10.1, 1.4 Hz, 1H), 3.25 – 3.14 (m, 3H), 3.14 (s, 1H), 2.72 – 2.60 (m, 1H), 2.51 (dd, J = 18.3, 2.9 Hz, 1H), 2.46 – 2.37 (m, 4H), 2.32 (ddd, J = 18.2, 2.7 Hz, 2.7 Hz, 1H), 1.67 (dd, J = 12.9, 7.2 Hz, 1H), 1.64 (s, 1H), 1.38 (dd, J = 12.9, 11.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5, 143.5, 135.5, 133.6, 129.7, 128.6, 127.7, 127.4, 126.0, 124.7, 69.2, 57.4, 57.0, 52.6, 52.5, 49.0, 43.6, 43.1, 40.4, 21.7.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{24}H_{28}NO_3S^+$: 410.1784; found: 410.1785.



10b

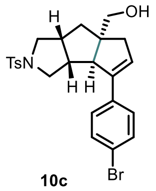
Substrate **9b** (22.7 mg, 0.05 mmol, 1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (0.6 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 1.5 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10b** as a colorless oil. Run 1: **10b** (20.4 mg, 90%). Run 2: **10b** (20.2 mg, 89%). The average yield of two runs was 90%.

TLC (1:1 petroleum ether/EtOAc, R_f): 0.7.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.1 Hz, 2H), 7.32 (d, J = 8.1 Hz, 2H), 6.85 (d, J = 1.5 Hz, 1H), 6.76 – 6.71 (m, 2H), 5.94 (s, 2H), 5.83 (dd, J = 3.7 Hz, 3.7 Hz, 1H), 3.58 – 3.42 (m, 3H), 3.30 – 3.20 (m, 2H), 3.15 (dd, J = 9.7, 8.5 Hz, 1H), 3.05 (d, J = 2.5 Hz, 1H), 2.70 – 2.61 (m, 1H), 2.48 (dd, J = 18.2, 2.9 Hz, 1H), 2.42 (s, 3H), 2.41 – 2.36 (m, 1H), 2.30 (ddd, J = 18.2, 2.7 Hz, 2.7 Hz, 1H), 1.65 (dd, J = 12.9, 7.1 Hz, 1H), 1.57 (s, 1H), 1.35 (dd, J = 12.9, 11.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 147.0, 143.5, 143.1, 133.7, 130.0, 129.7, 127.7, 123.3, 119.6, 108.3, 106.3, 101.2, 69.2, 57.4, 57.2, 52.6, 52.5, 49.1, 43.5, 43.1, 40.3, 21.7.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{25}H_{28}NO_5S^+$: 454.1683; found: 454.1681.



10c

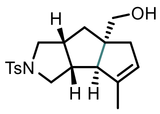
Substrate **9c** (24.4 mg, 0.05 mmol, 1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (0.6 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 2 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10c** as a colorless oil. Run 1: **10c** (18.9 mg, 77%). Run 2: **10c** (17.8 mg, 73%). The average yield of two runs was 75%.

TLC (1:1 petroleum ether/EtOAc, R_f): 0.7.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.69 (d, J = 8.2 Hz, 2H), 7.43 (d, J = 8.6 Hz, 2H), 7.34 (d, J = 8.2 Hz, 2H), 7.21 (d, J = 8.6 Hz, 2H), 6.04 (dd, J = 3.0 Hz, 3.0 Hz, 1H), 3.51 (dd, J = 9.5 Hz, 9.5 Hz, 1H), 3.47 – 3.40 (m, 2H), 3.26 – 3.18 (m, 2H), 3.14 – 3.08 (m, 2H), 2.69 – 2.58 (m, 1H), 2.47 (dd, J = 18.3, 2.9 Hz, 1H), 2.42 (s, 3H), 2.35 – 2.28 (m, 2H), 1.64 (dd, J = 12.9, 7.2 Hz, 1H), 1.52 (s, 1H), 1.32 (dd, J = 12.9, 11.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 142.6, 134.4, 133.6, 131.8, 129.7, 127.8, 127.6, 125.6, 121.2, 69.0, 57.5, 57.0, 52.6, 52.5, 48.9, 43.7, 43.2, 40.4, 21.7.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{24}H_{27}BrNO_3S^+$: 488.0890; found: 488.0889.



10d

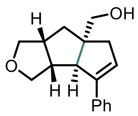
Substrate **9d** (17.4 mg, 0.05 mmol, 1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (0.6 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 2.5 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10d** as a colorless oil. Run 1: **10d** (14.5 mg, 83%). Run 2: **10c** (15.1 mg, 87%). The average yield of two runs was 85%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.1.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.1 Hz, 2H), 7.32 (d, J = 8.1 Hz, 2H), 5.14 (dd, J = 2.0 Hz, 2.0 Hz, 1H), 3.44 (dd, J = 9.4 Hz, 9.4 Hz, 1H), 3.38 (s, 2H), 3.31 – 3.21 (m, 2H), 3.01 (dd, J = 9.8, 8.4 Hz, 1H), 2.66 – 2.53 (m, 1H), 2.46 – 2.41 (m, 1H), 2.43 (s, 3H), 2.35 (ddd, J = 7.9, 7.9 Hz, 7.4 Hz, 1H), 2.30 – 2.23 (m, 1H), 2.08 (dddd, J = 16.9, 2.5 Hz, 2.5 Hz, 2.5 Hz, 1H), 1.62 (s, 3H), 1.57 (dd, J = 13.0, 7.3 Hz, 1H), 1.49 (s, 1H), 1.24 (dd, J = 10.0, 3.0 Hz, 1H).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 143.5, 140.7, 133.8, 129.7, 127.7, 123.8, 69.5, 60.4, 57.5, 52.5, 52.5, 47.8, 43.6, 43.0, 40.7, 21.7, 15.7.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{19}H_{26}NO_3S^+$: 348.1628; found: 348.1627.



10e

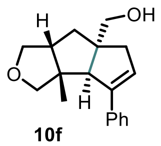
Substrate **9e** (13.2 mg, 0.05 mmol, 1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (0.6 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 7 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10e** as a colorless oil. Run 1: **10e** (11.8 mg, 89%). Run 2: **10e** (12.0 mg, 91%). The average yield of two runs was 90%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.1.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 4H), 7.25–7.21 (m, 1H), 6.04 (dd, J = 3.2 Hz, 3.2 Hz, 1H), 3.97 (dd, J = 8.5 Hz, 8.5 Hz, 1H), 3.86 – 3.76 (m, 2H), 3.72 (dd, J = 8.7, 5.7 Hz, 1H), 3.66 – 3.59 (m, 2H), 3.15 (s, 1H), 2.90 – 2.78 (m, 1H), 2.62 – 2.48 (m, 2H), 2.43 (ddd, J = 18.0, 2.6 Hz, 2.6 Hz, 1H), 1.90 (dd, J = 13.0, 7.8 Hz, 1H), 1.81 (dd, J = 13.0, 9.3 Hz, 1H), 1.71 (s, 1H).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 144.7, 135.9, 128.6, 127.3, 126.1, 124.5, 74.3, 73.9, 69.5, 58.6, 58.3, 50.8, 45.3, 43.2, 41.2.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{17}H_{21}O_2^+$: 257.1536; found: 257.1534.



10f

Substrate **9f** (14.0 mg, 0.05 mmol, 1.0 equiv.) was added in the reaction flask (10 mL) which was then moved to glovebox, charged with $InCl_3$ (0.6 mg, 5 mol%,) and sealed with a rubber stopper. After that, the flask was moved from the glovebox to the hood for the reaction. Super-dried DCE (1 mL, 0.05 M) was added under argon to the flask in the hood and then the mixture was heated in the oil bath (40 °C). After stirring for 2 h, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was purified by flash column chromatography with silica gel to afford the pure product **10f** as a colorless oil. Run 1: **10f** (13.4 mg, 96%). Run 2: **10f** (14.0 mg, 100%). The average yield of two runs was 98%.

TLC (3:1 petroleum ether/EtOAc, R_f): 0.1.

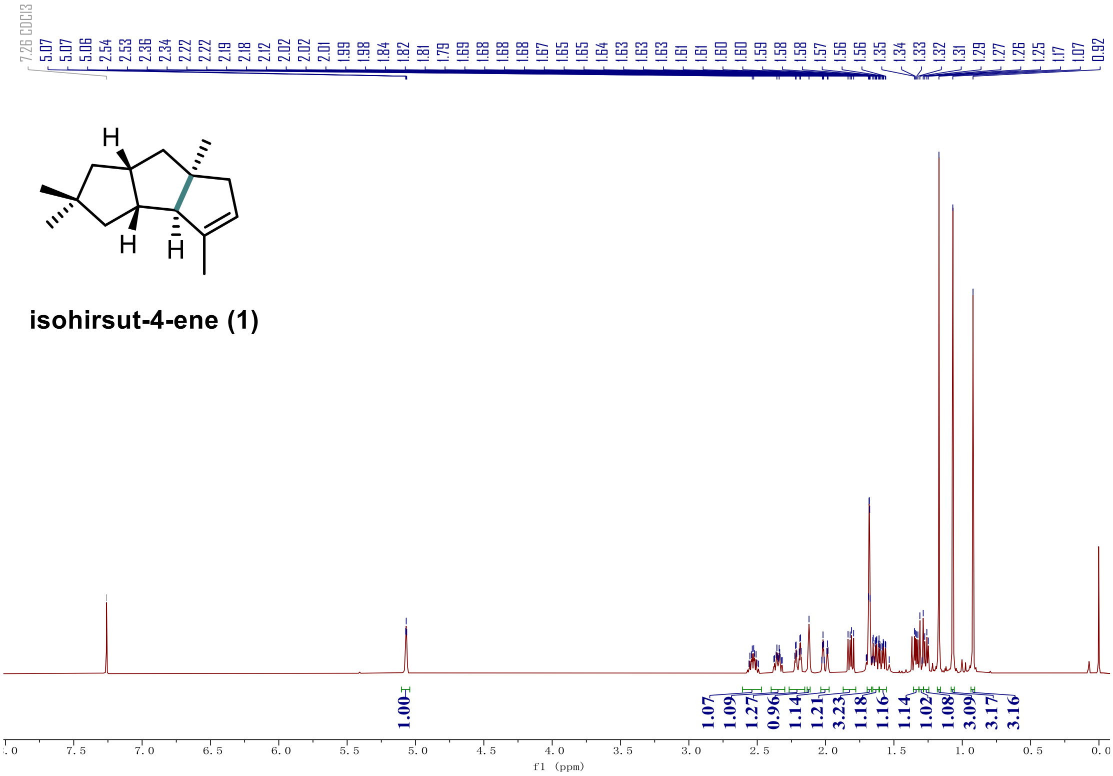
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.37 (m, 2H), 7.33 – 7.29 (m, 2H), 7.24 – 7.19 (m, 1H), 6.10 (dd, J = 2.7 Hz, 2.7 Hz, 1H), 3.94 (dd, J = 8.7, 6.2 Hz, 1H), 3.86 (d, J = 8.2 Hz, 1H), 3.79 (dd, J = 8.7, 2.4 Hz, 1H), 3.63 – 3.50 (m, 3H), 3.23 (d, J = 2.1 Hz, 1H), 2.52 – 2.35 (m, 3H), 1.89 (dd, J = 13.0, 7.5 Hz, 1H), 1.75 (dd, J = 13.0, 9.8 Hz, 1H), 1.68 (s, 1H), 0.84 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 137.2, 128.6, 127.2, 126.4, 126.0, 80.8, 73.2, 69.8, 59.6, 58.7, 54.7, 53.5, 42.6, 38.9, 22.6.

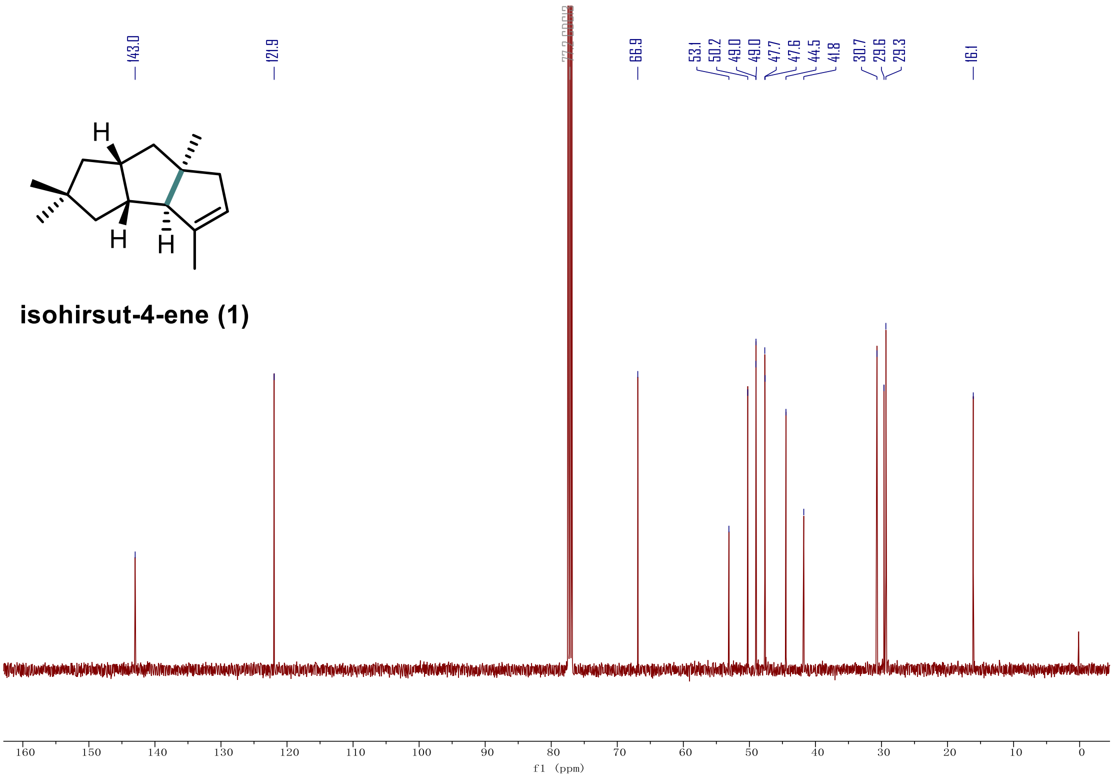
HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{18}H_{23}O_2^+$: 271.1693; found: 271.1688.

6. NMR Spectra and Crystal Structures of New Compounds.

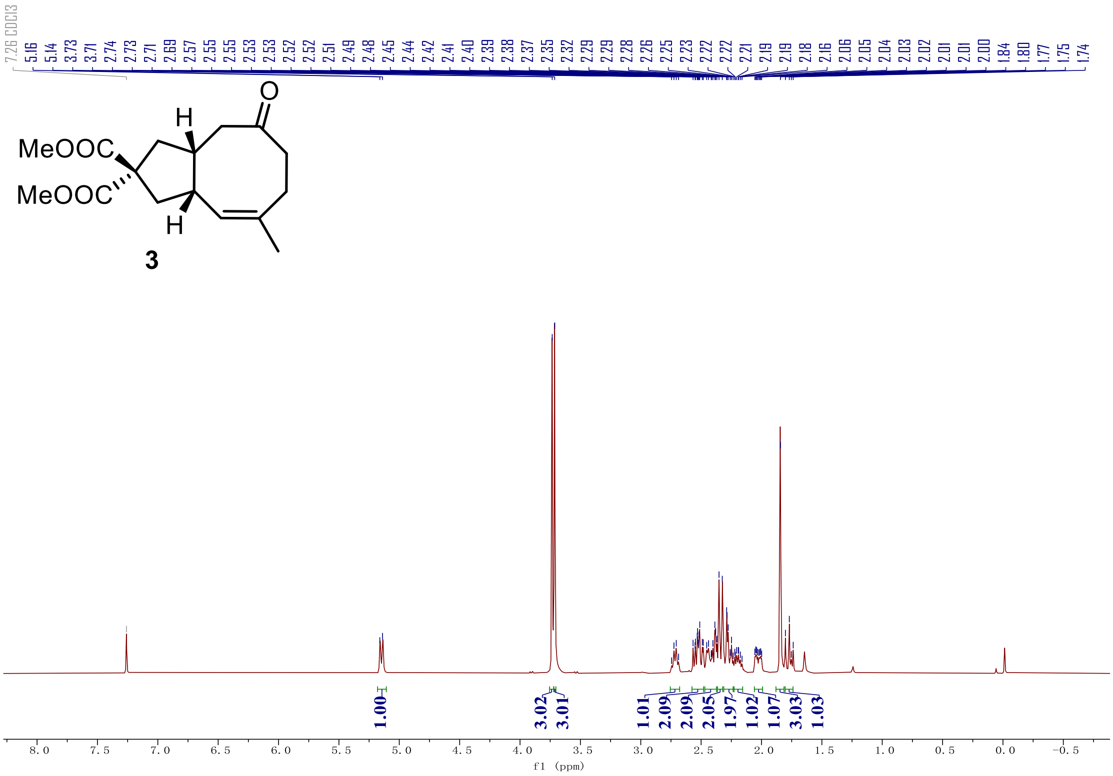
^{1}H NMR in $CDCl_3$, 500 MHz



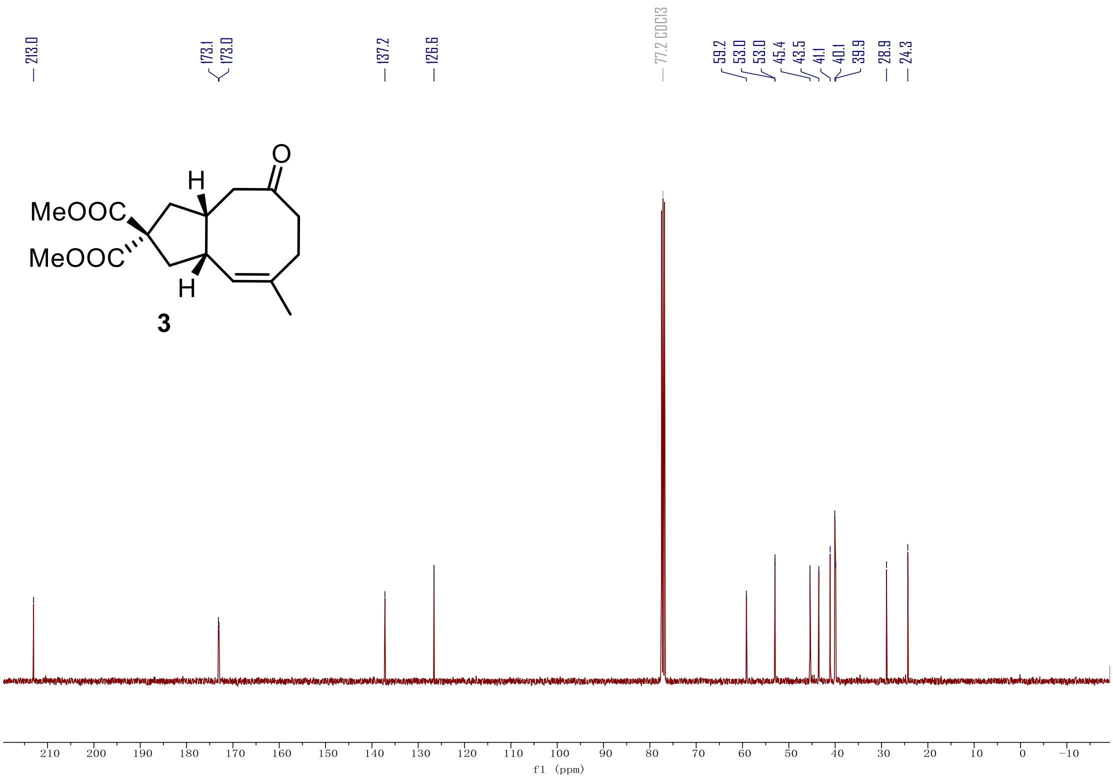
^{13}C NMR in $CDCl_3$, 126 MHz



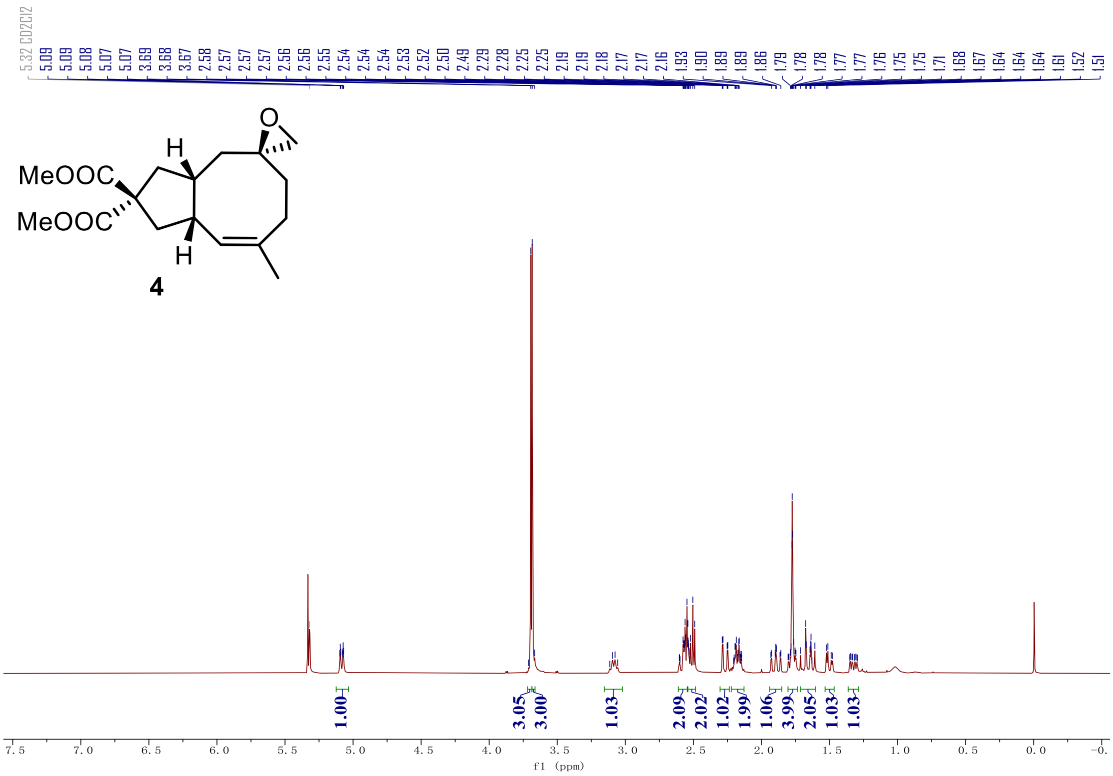
^{1}H NMR in $CDCl_3$, 400 MHz



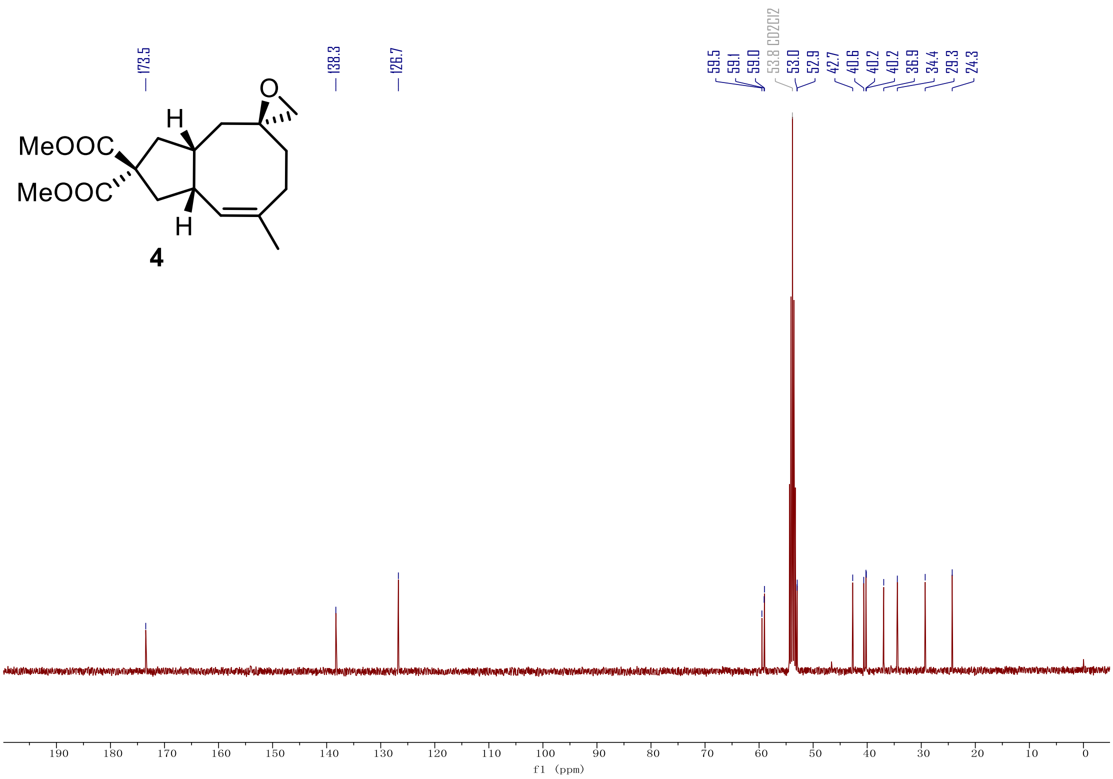
^{13}C NMR in $CDCl_3$, 101 MHz



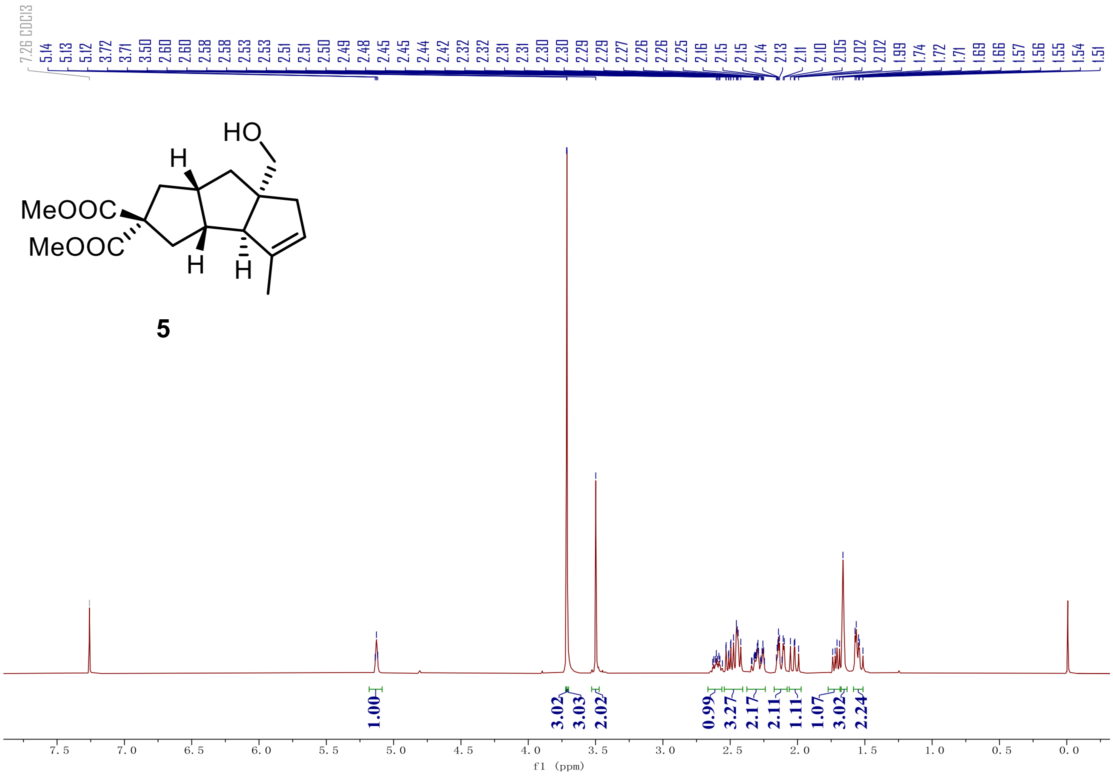
^{1}H NMR in CD_2Cl_2, 400 MHz



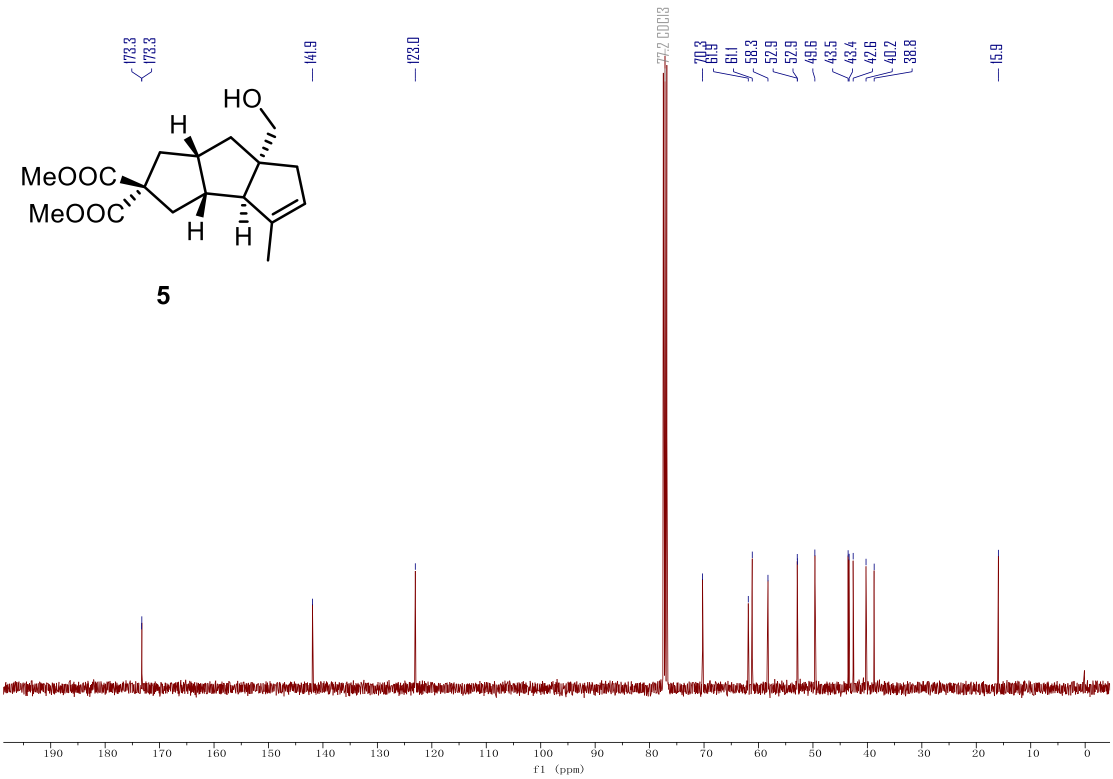
^{13}C NMR in CD_2Cl_2, 101 MHz



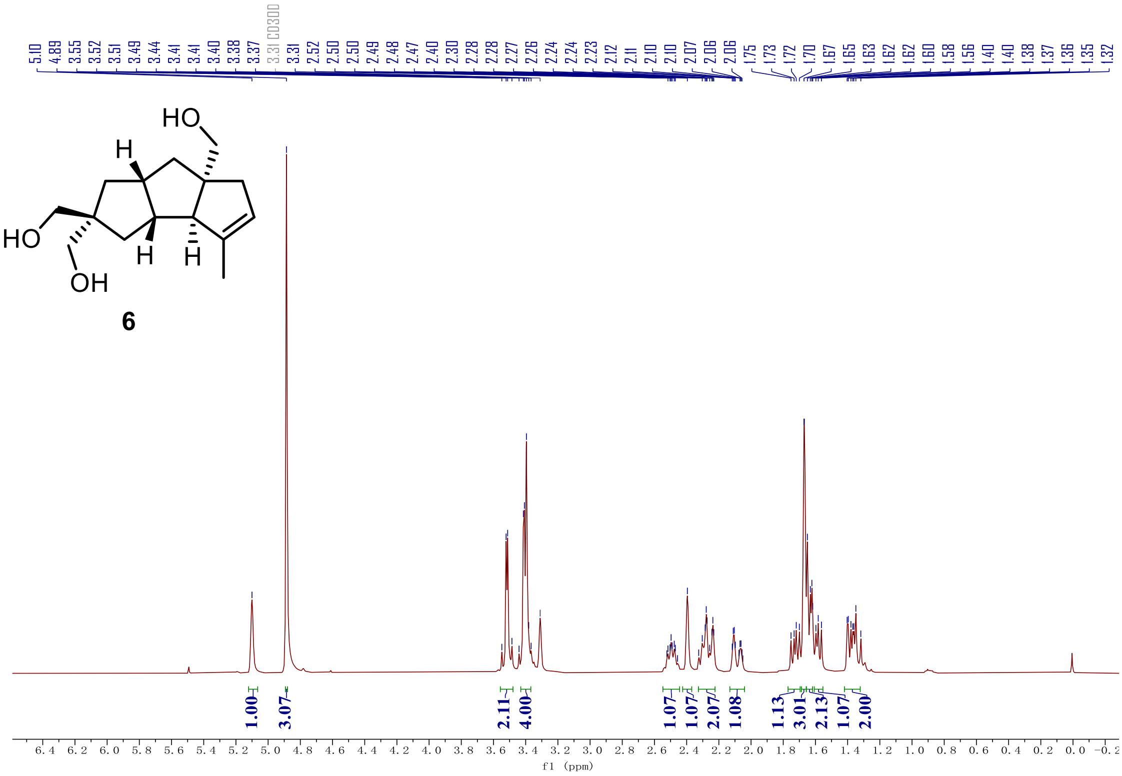
^{1}H NMR in $CDCl_3$, 400 MHz



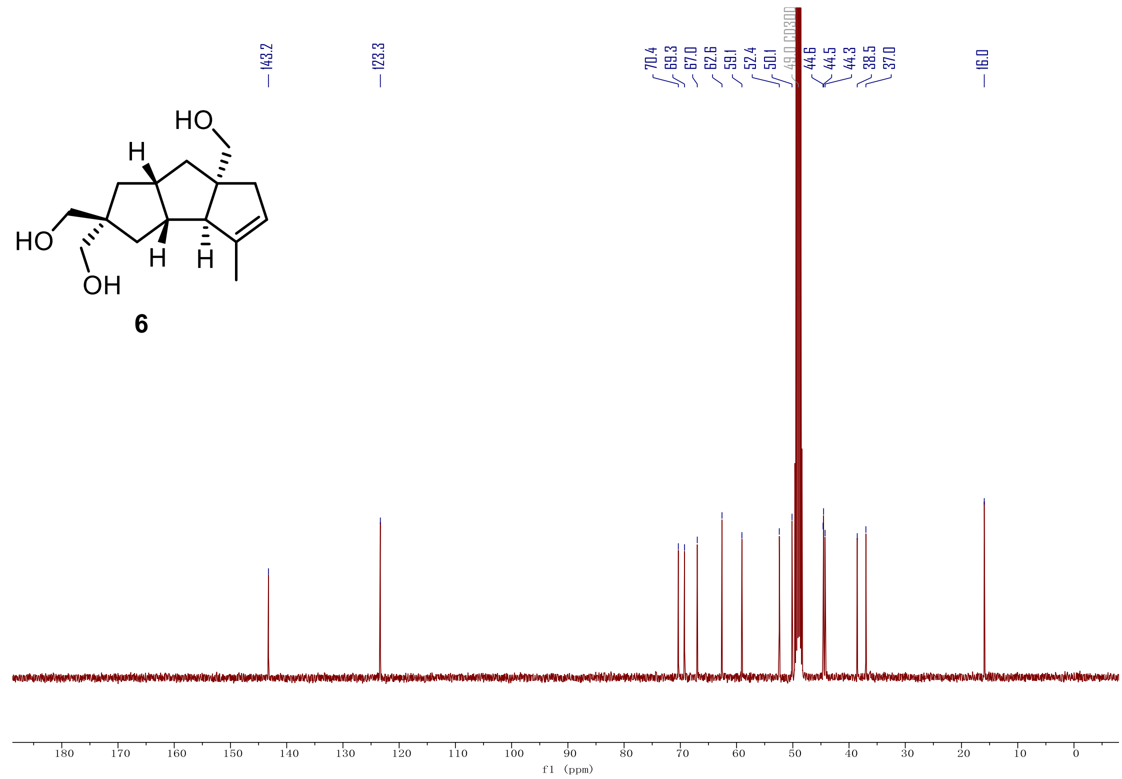
^{13}C NMR in $CDCl_3$, 101 MHz



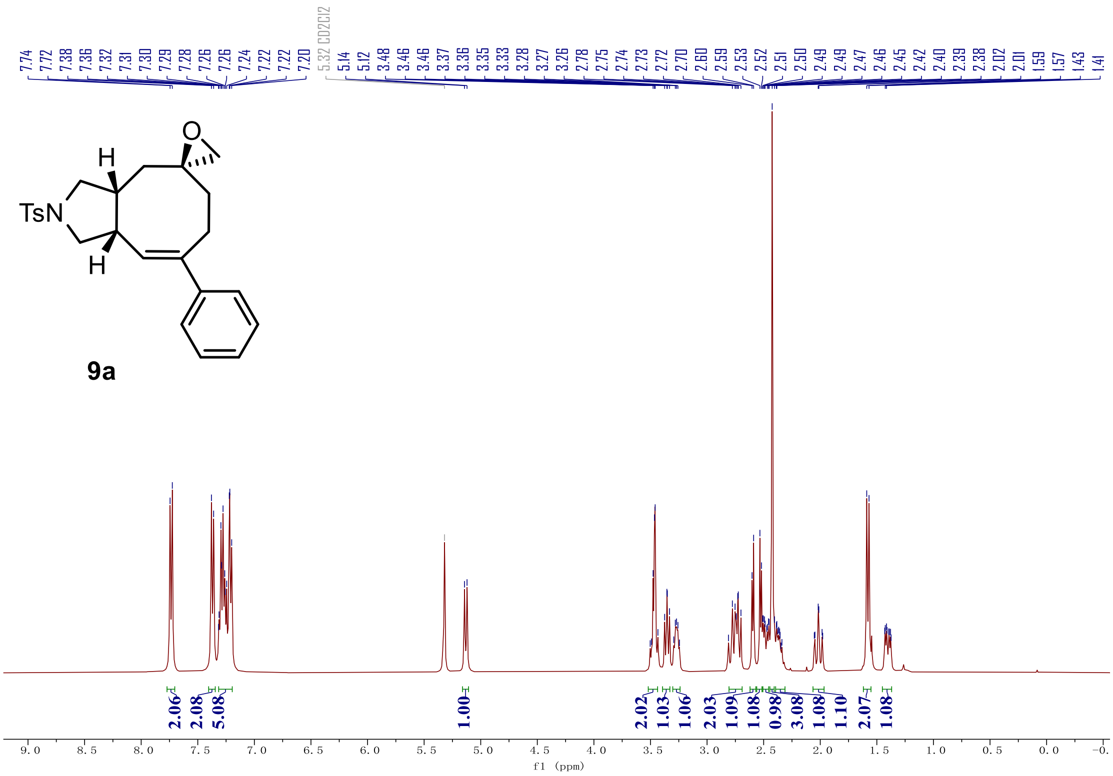
[1]H NMR in CD_3OD, 400 MHz



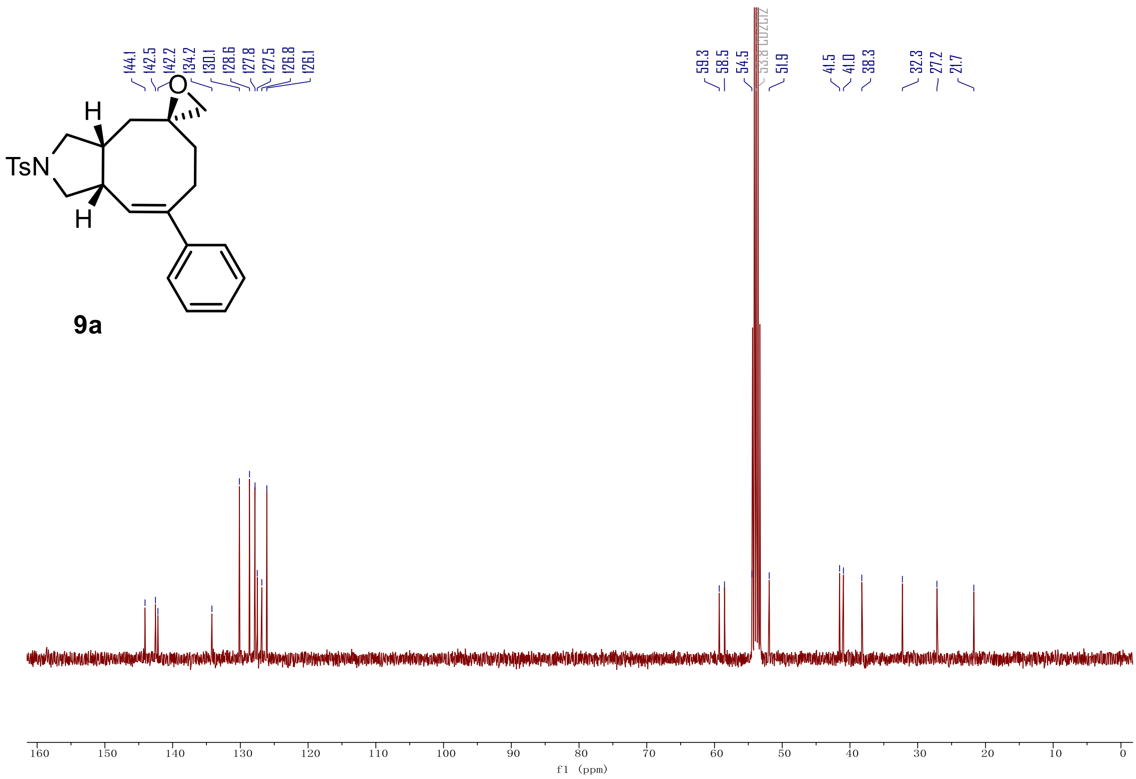
[13]C NMR in CD_3OD, 101 MHz



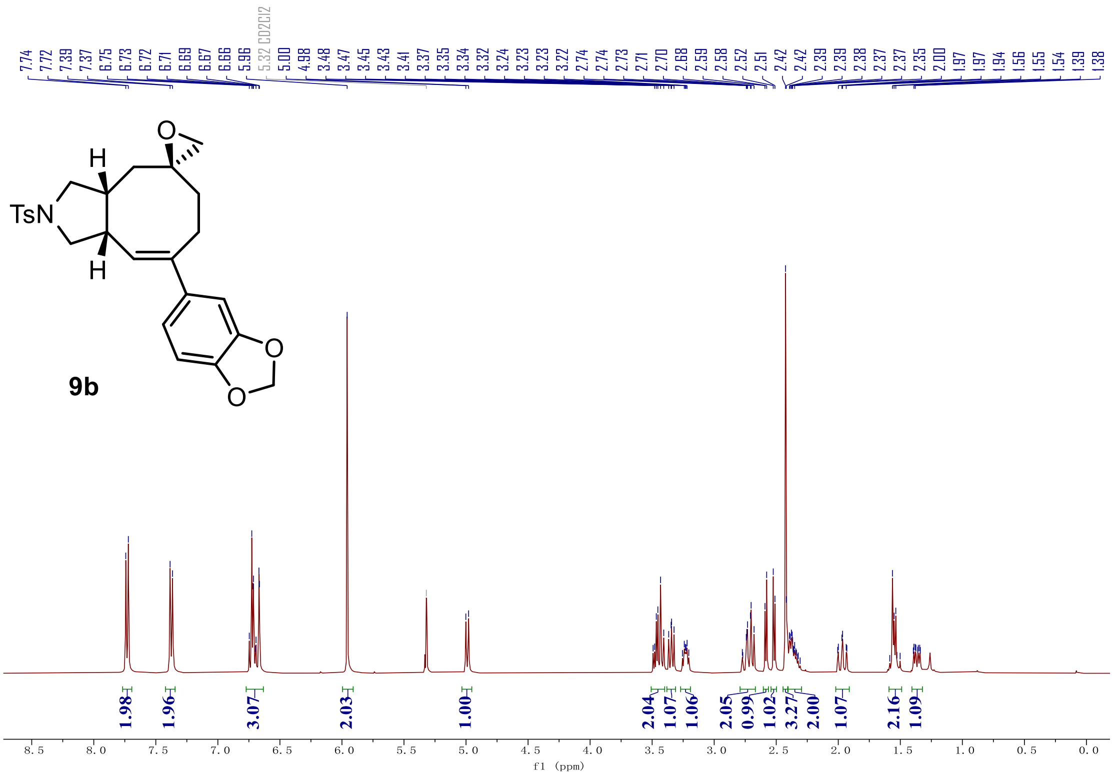
[1]H NMR in CD_2Cl_2, 400 MHz



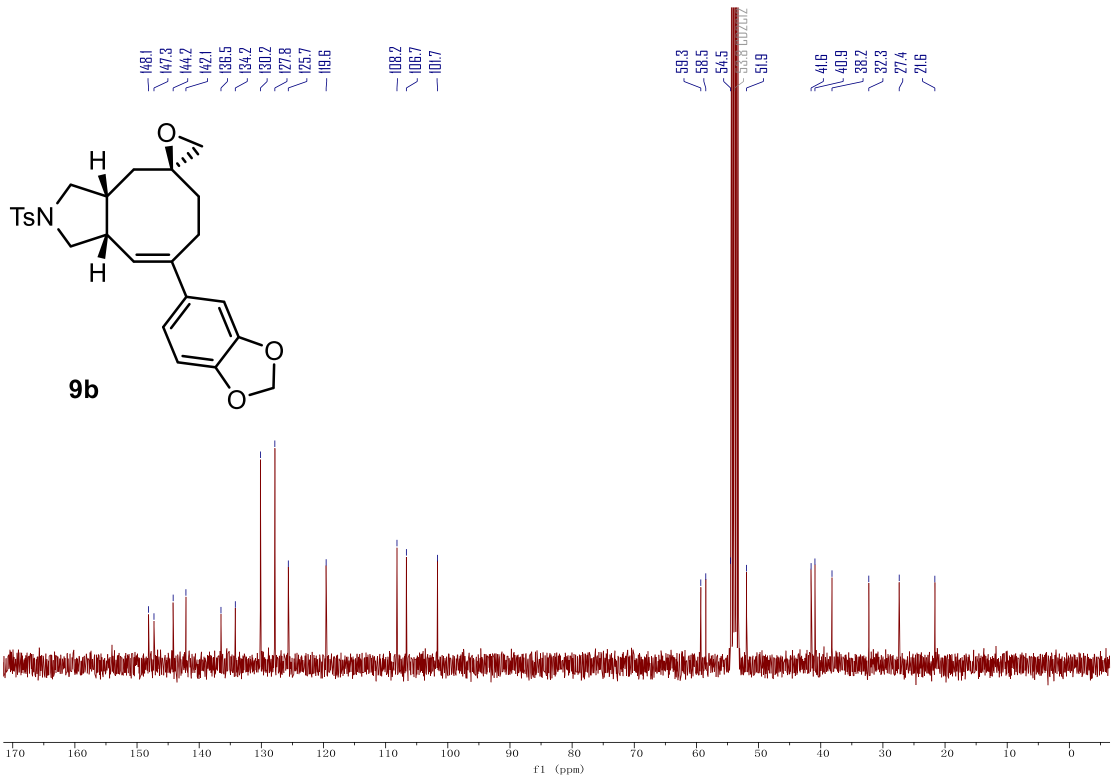
[13]C NMR in CD_2Cl_2, 101 MHz



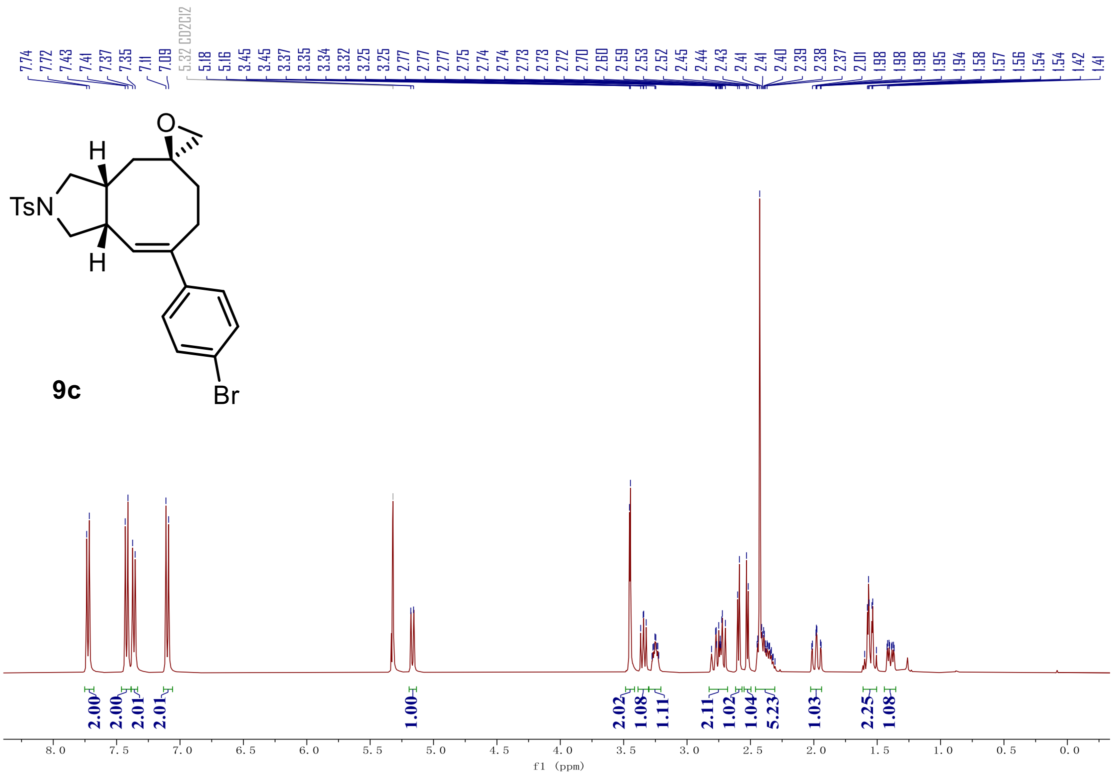
[1]H NMR in CD_2Cl_2, 400 MHz



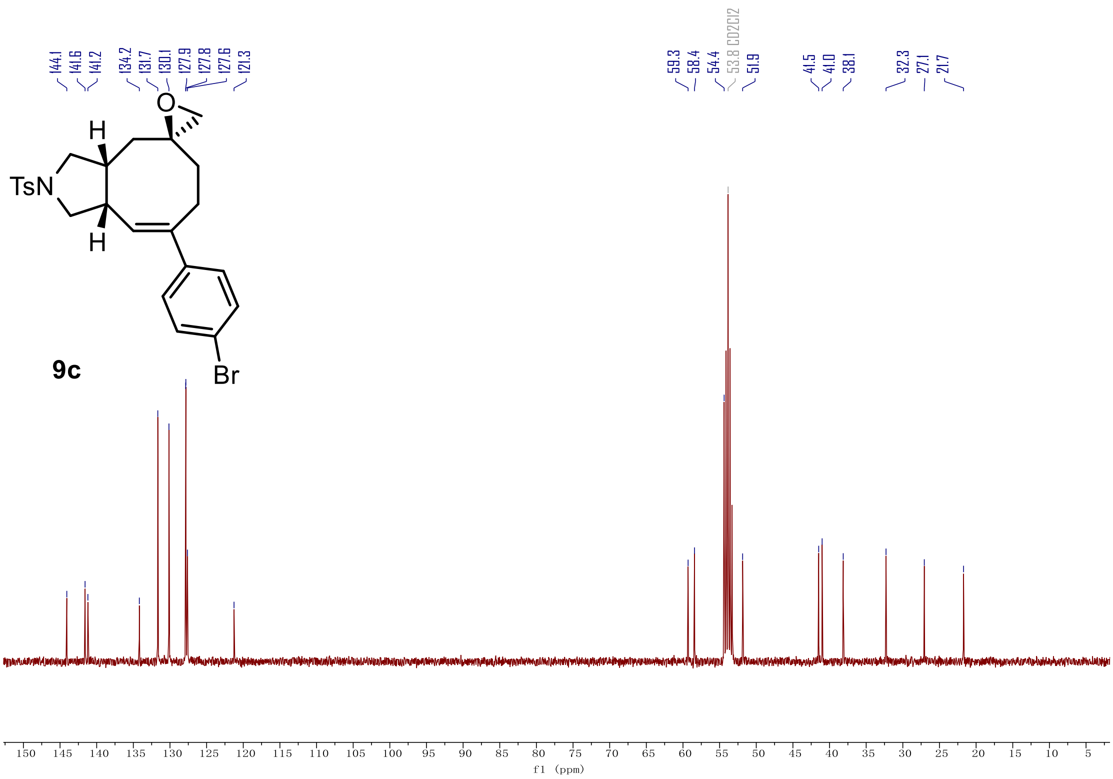
[13]C NMR in CD_2Cl_2, 101 MHz



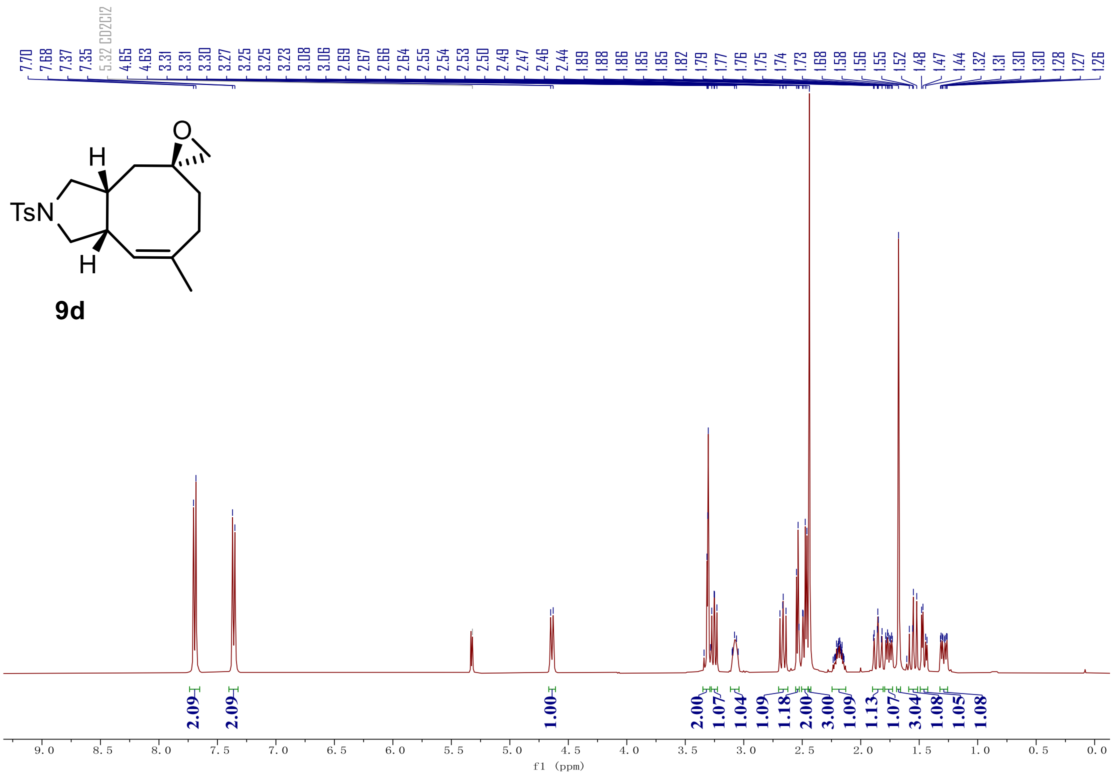
[1]H NMR in CD_2Cl_2, 400 MHz



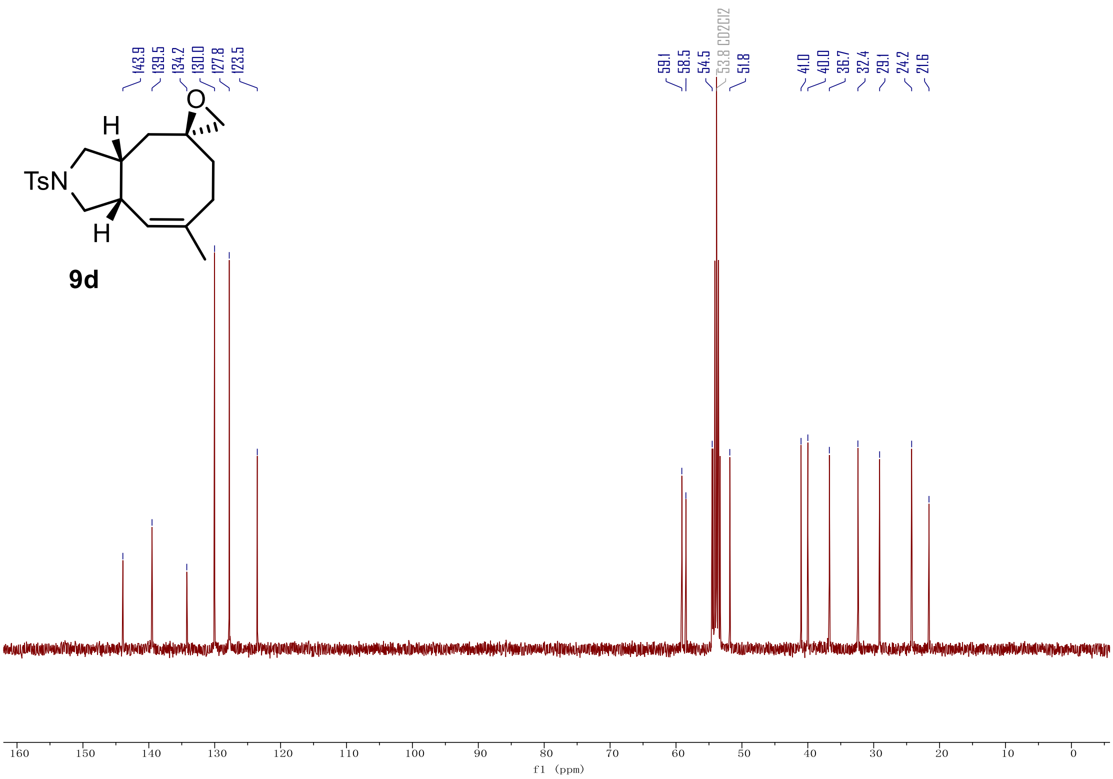
[13]C NMR in CD_2Cl_2, 101 MHz



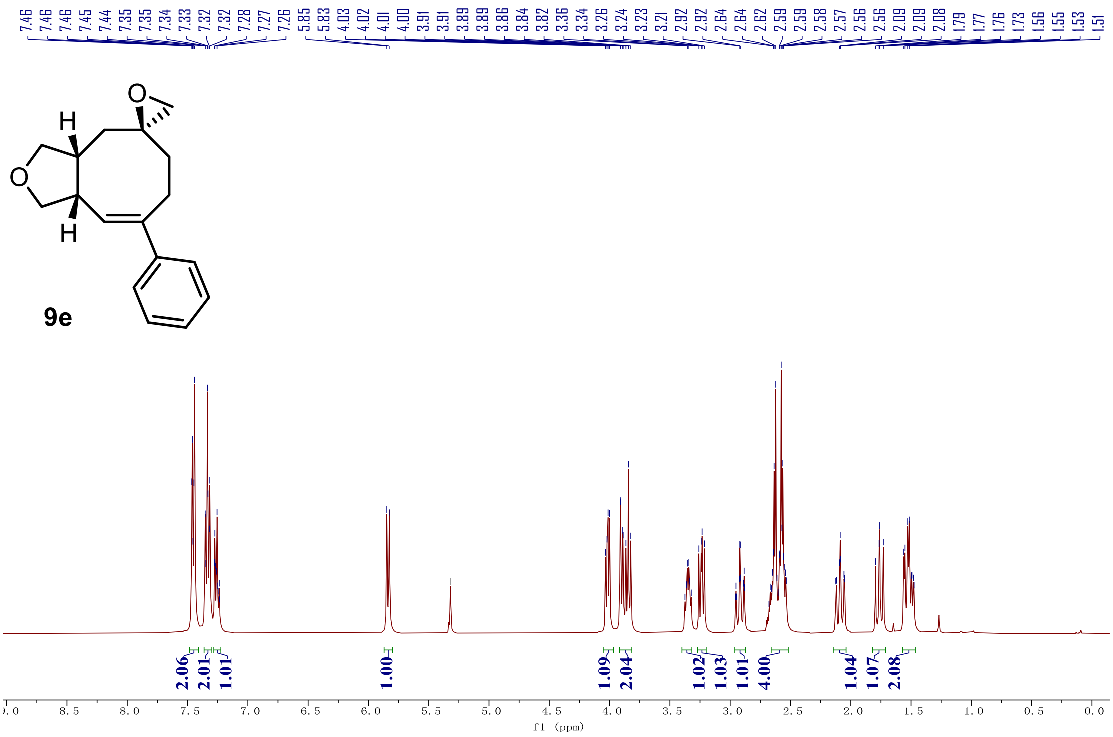
^{1}H NMR in CD_2Cl_2, 400 MHz



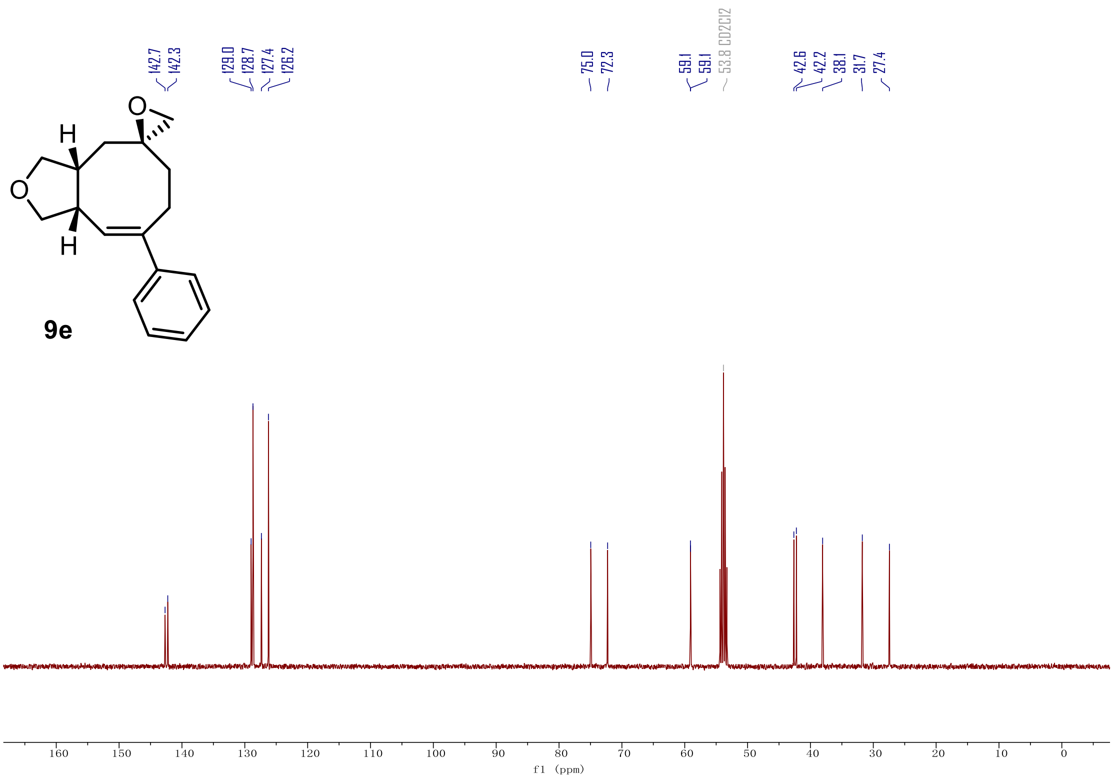
^{13}C NMR in CD_2Cl_2, 101 MHz



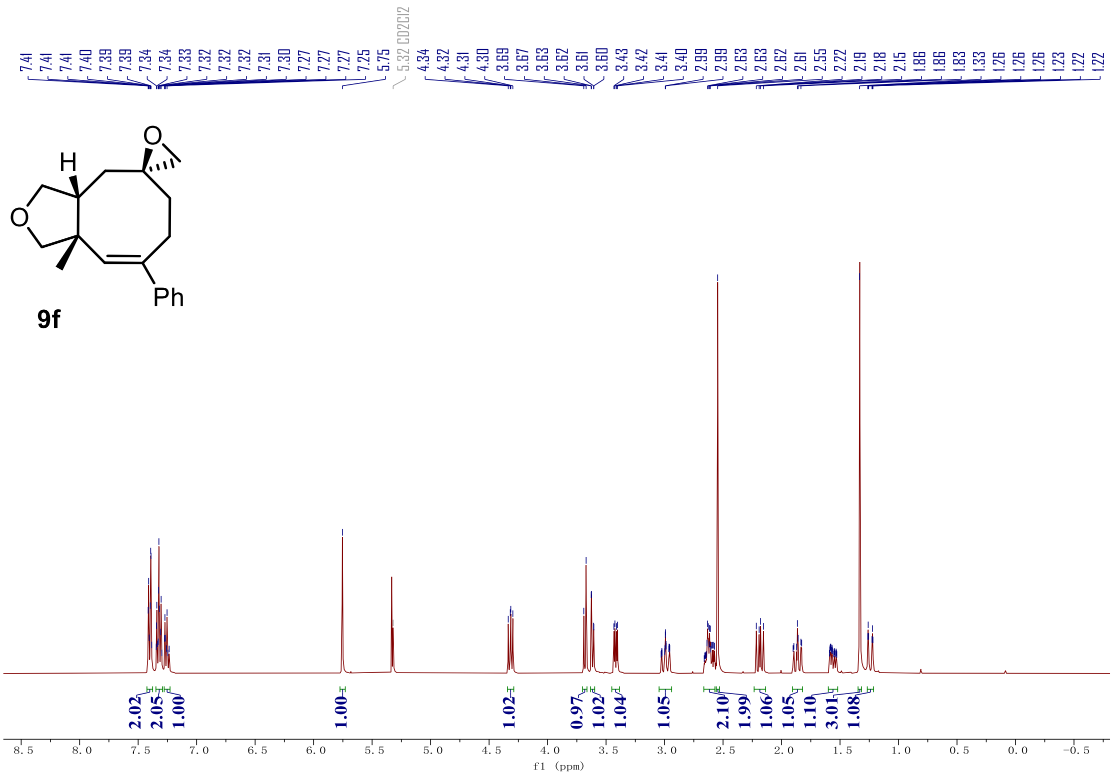
^{1}H NMR in CD_2Cl_2, 400 MHz



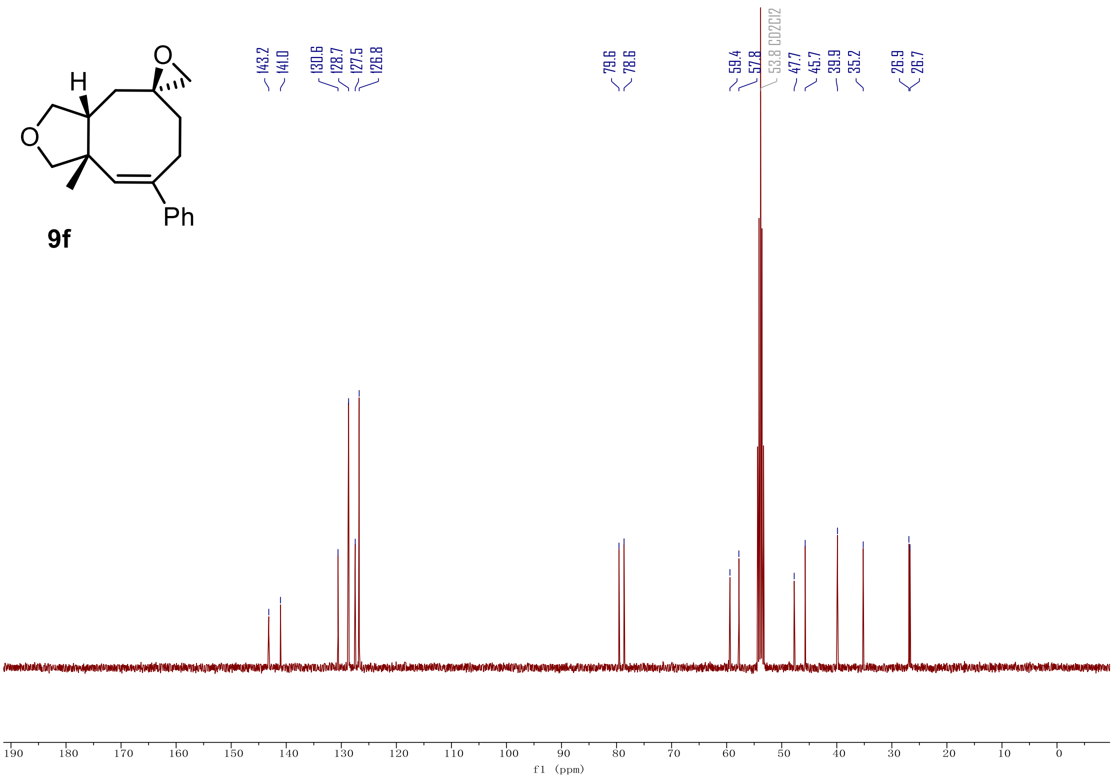
^{13}C NMR in CD_2Cl_2, 101 MHz



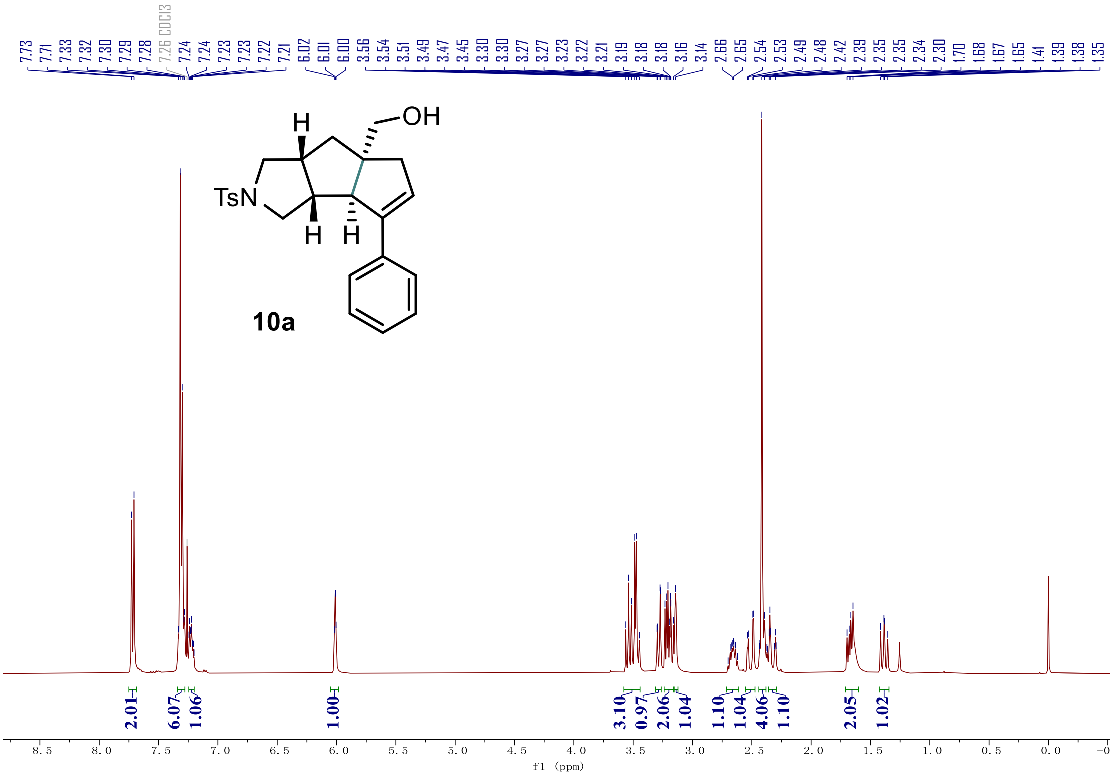
^{1}H NMR in CD_2Cl_2, 400 MHz



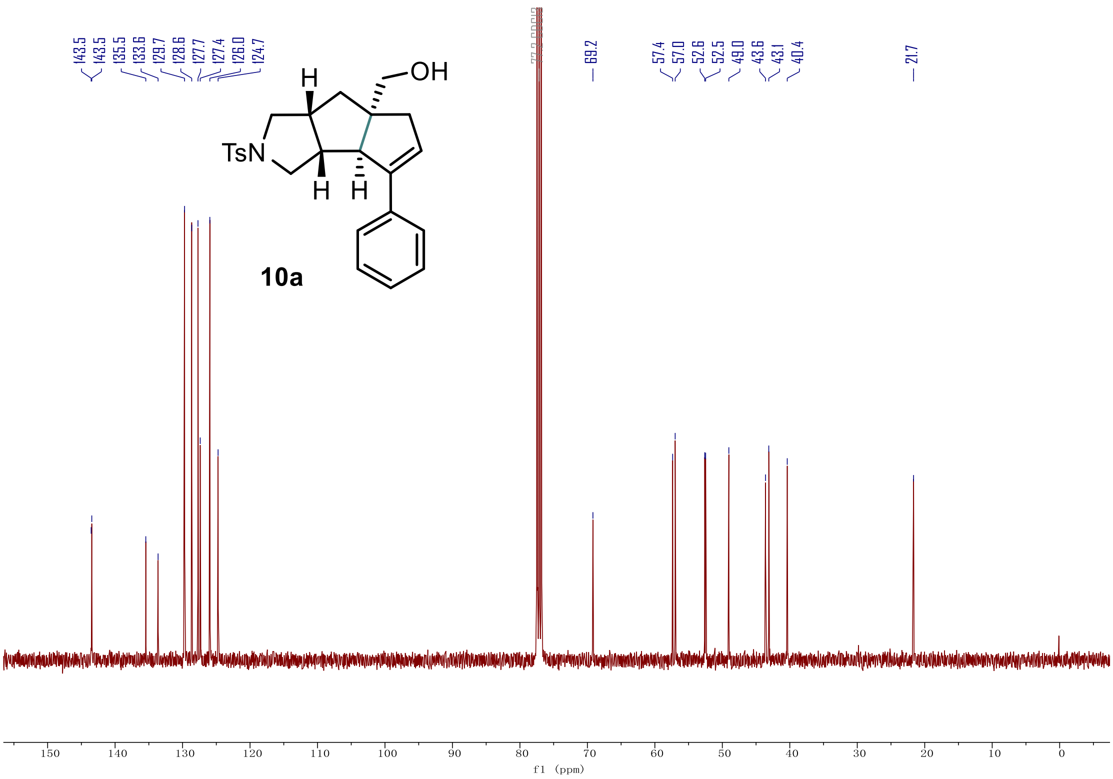
^{13}C NMR in CD_2Cl_2, 101 MHz



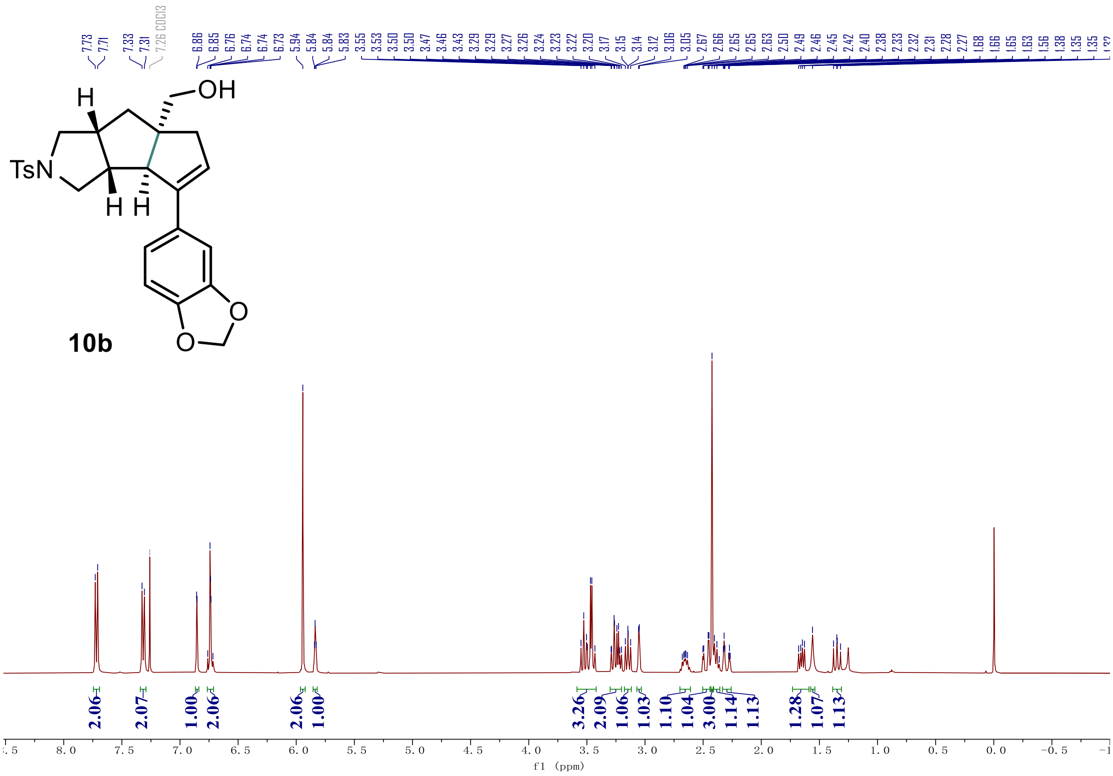
^{1}H NMR in $CDCl_3$, 400 MHz



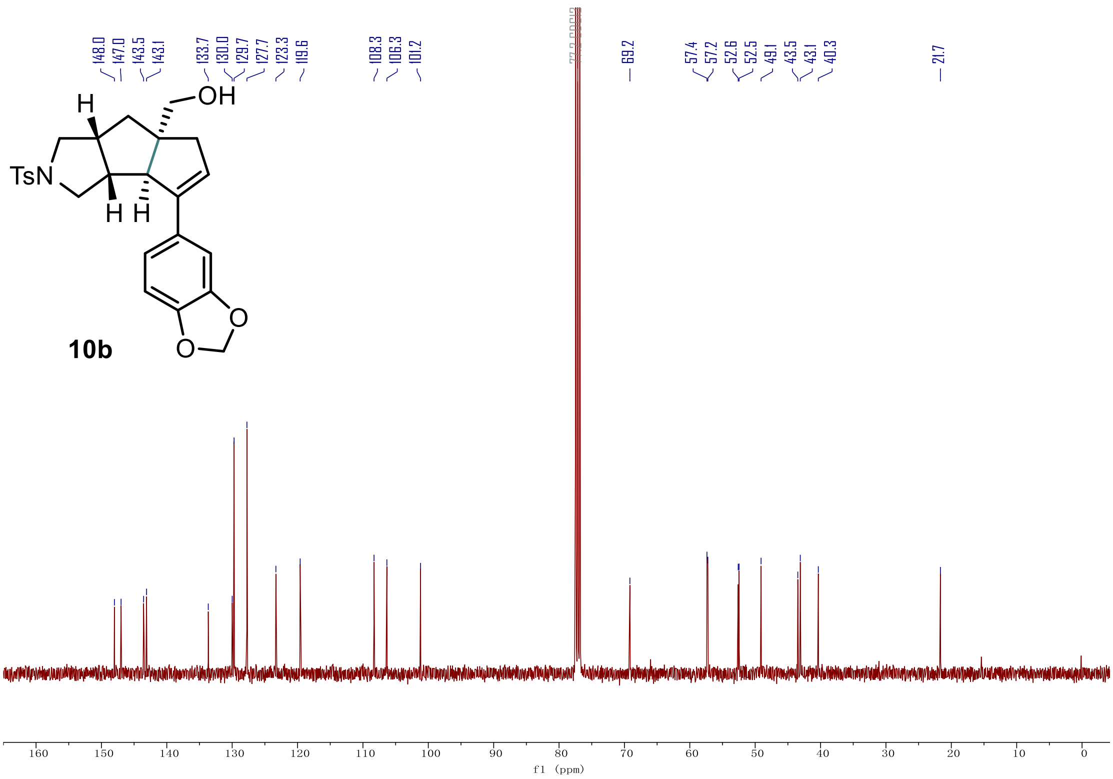
^{13}C NMR in $CDCl_3$, 101 MHz



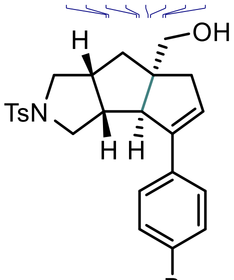
^{1}H NMR in $CDCl_3$, 400 MHz



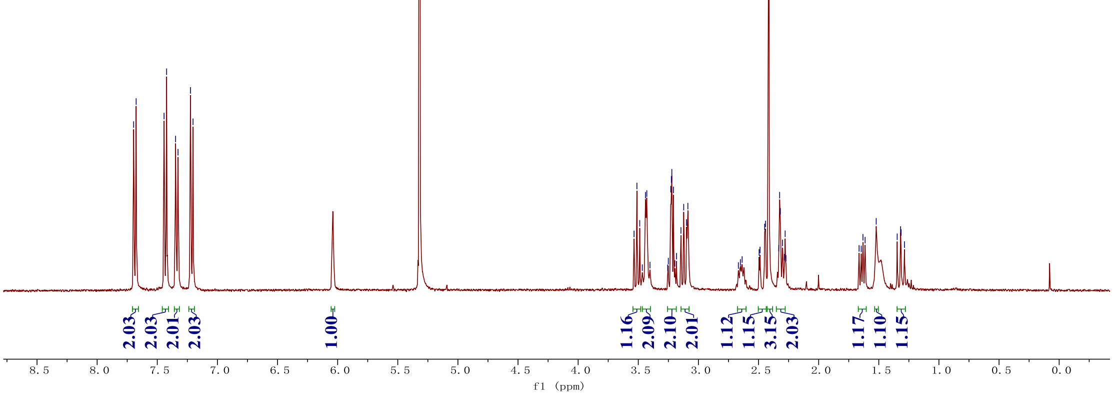
^{13}C NMR in $CDCl_3$, 101 MHz



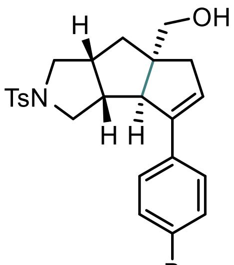
[1]H NMR in CD_2Cl_2, 400 MHz



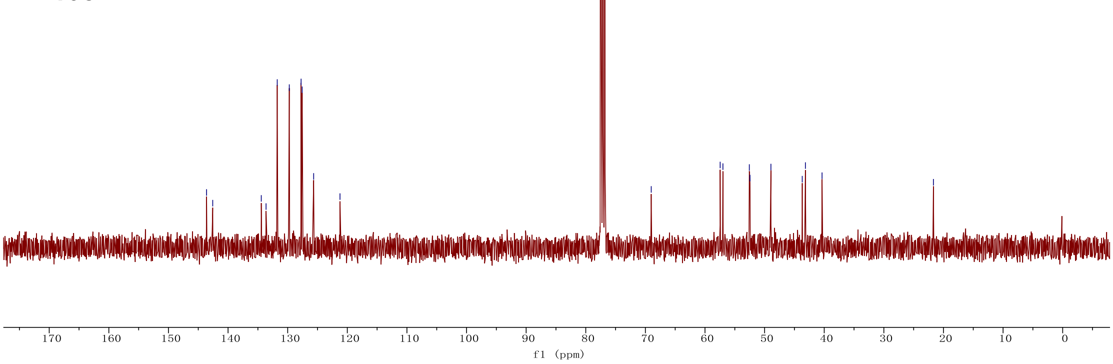
10c



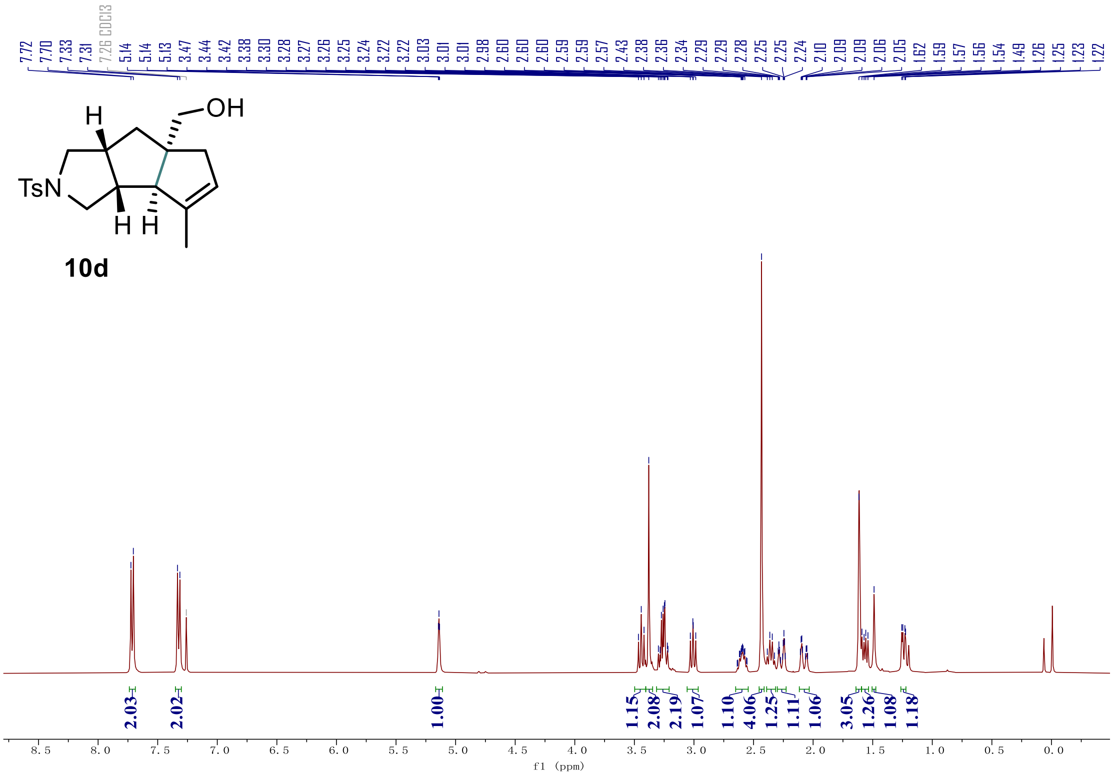
[13]C NMR in $CDCl_3$, 101 MHz



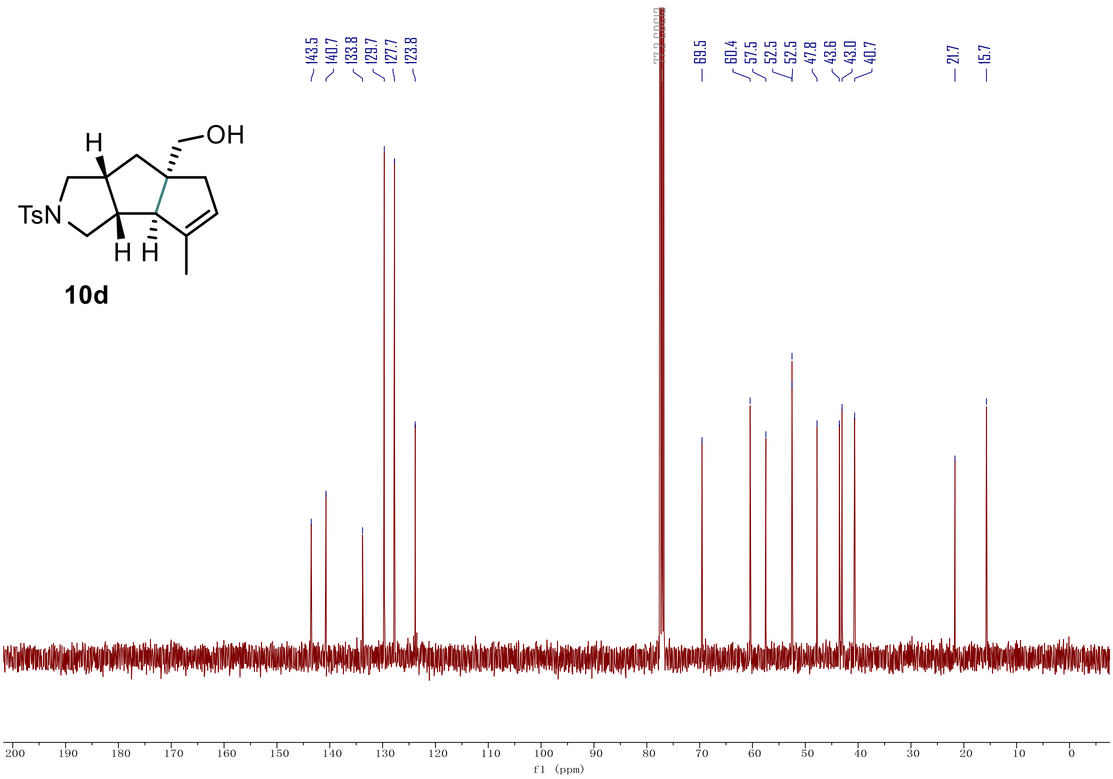
10c



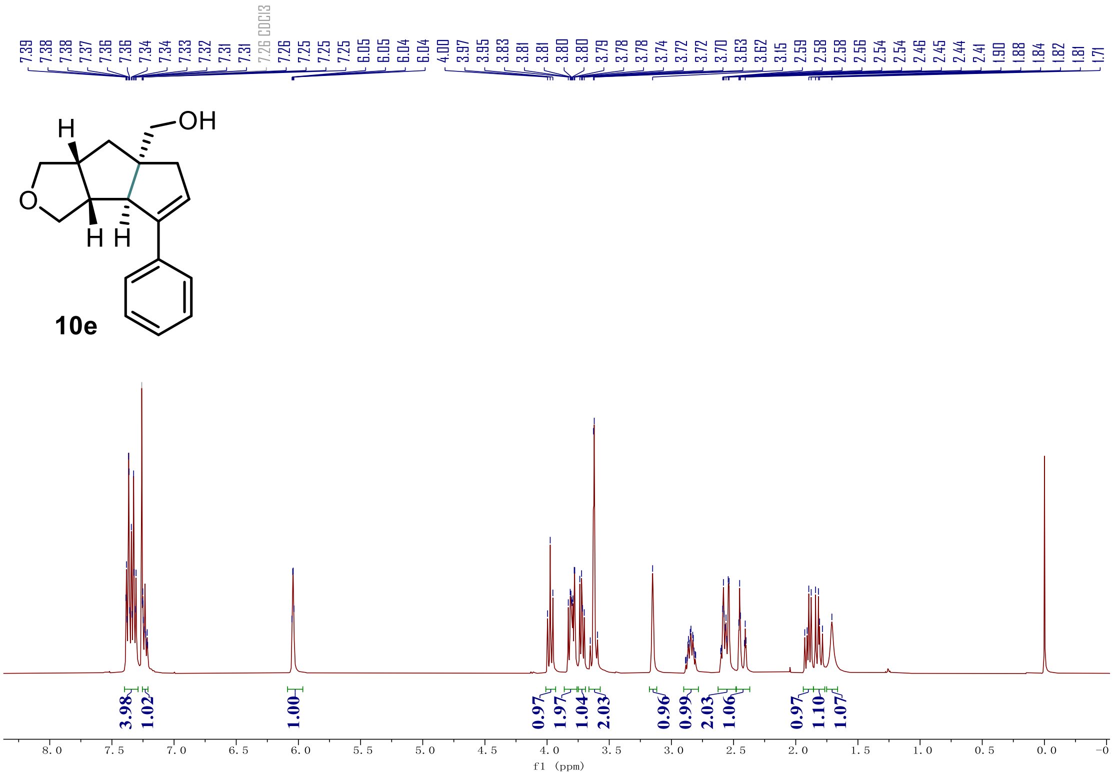
^{1}H NMR in $CDCl_3$, 400 MHz



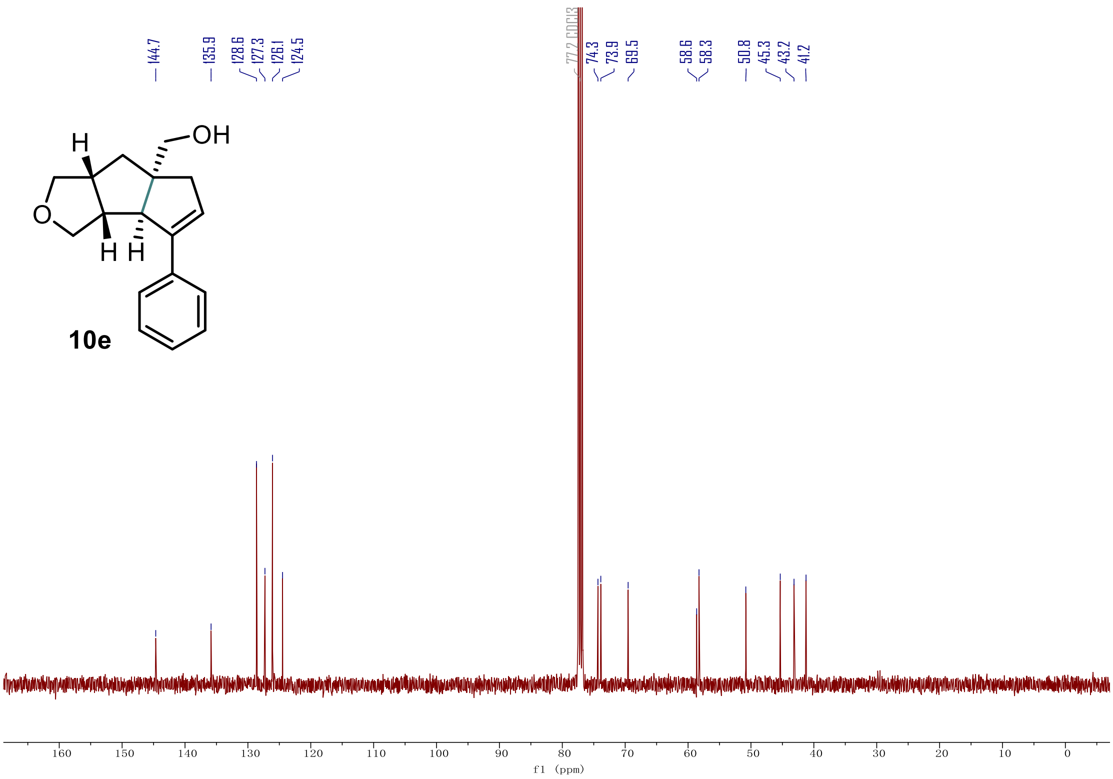
^{13}C NMR in $CDCl_3$, 101 MHz



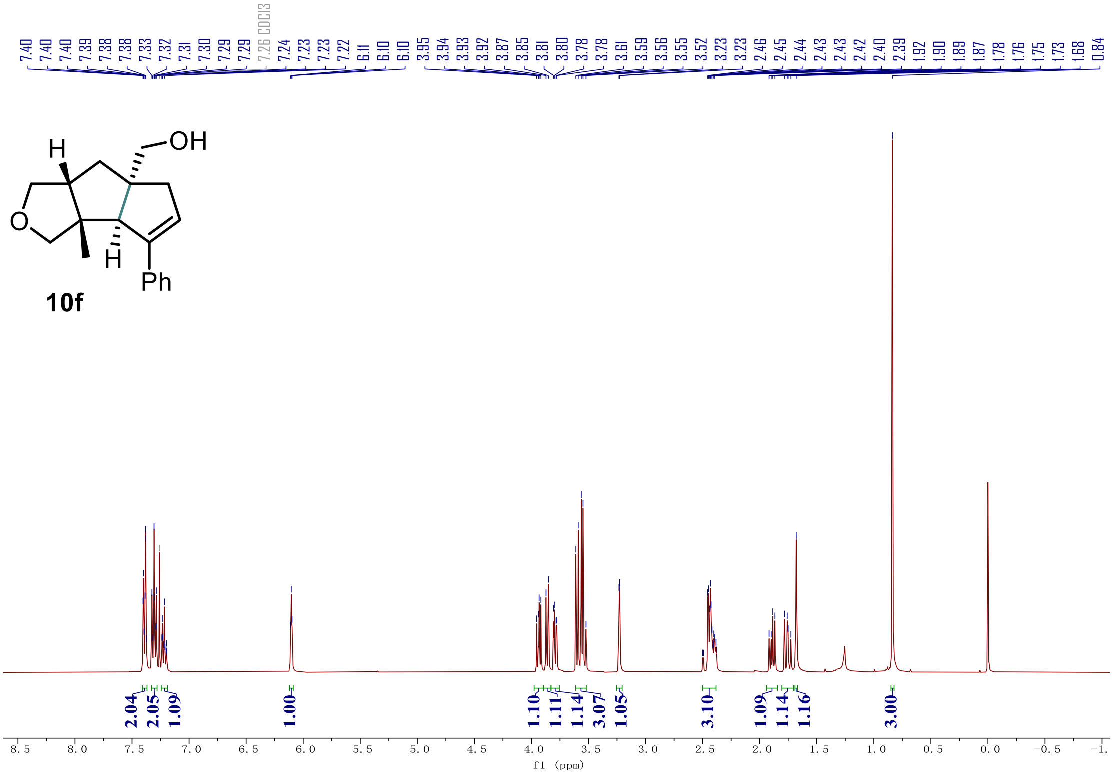
[1]H NMR in $CDCl_3$, 400 MHz



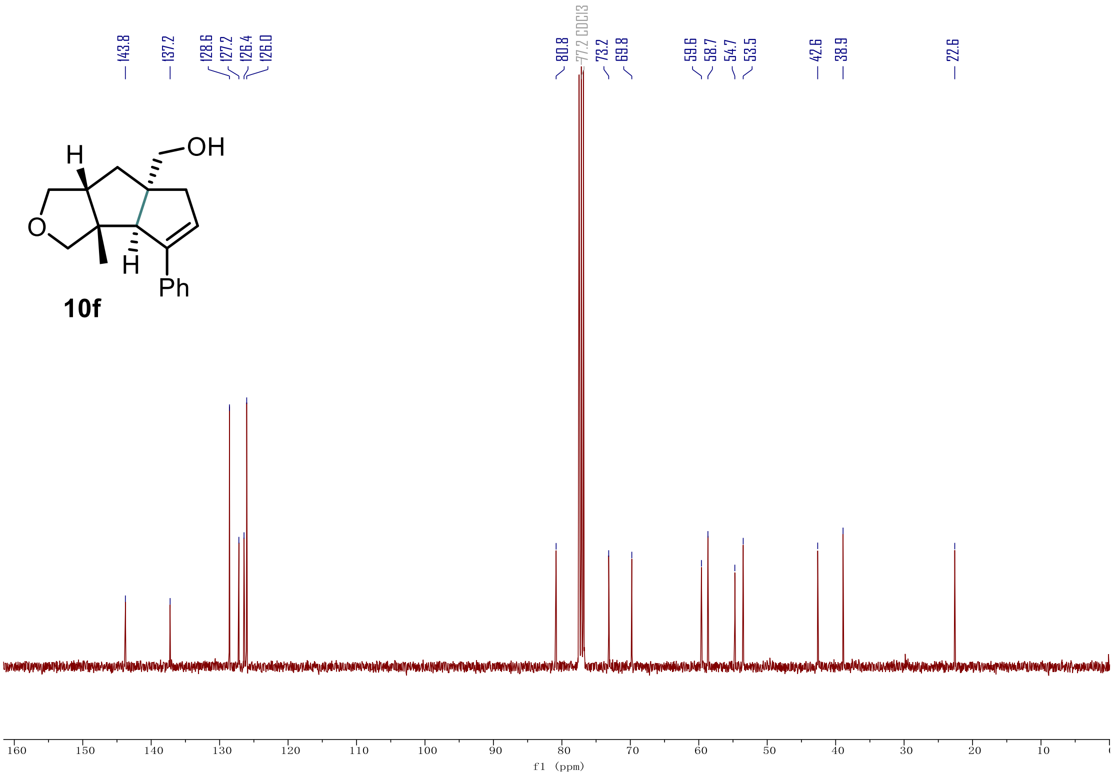
[13]C NMR in $CDCl_3$, 101 MHz



^{1}H NMR in $CDCl_3$, 400 MHz

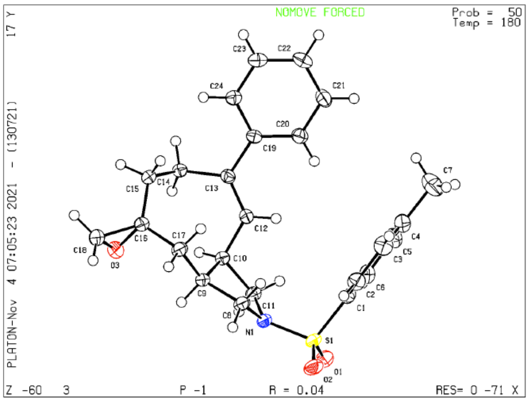


^{13}C NMR in $CDCl_3$, 101 MHz



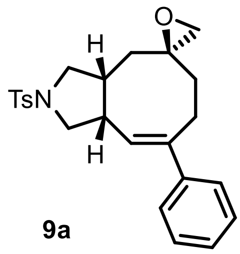
X-ray Crystal Analysis

Crystallographic Data of Compound **9a**



Ellipsoids are drawn at 50% probability

≡

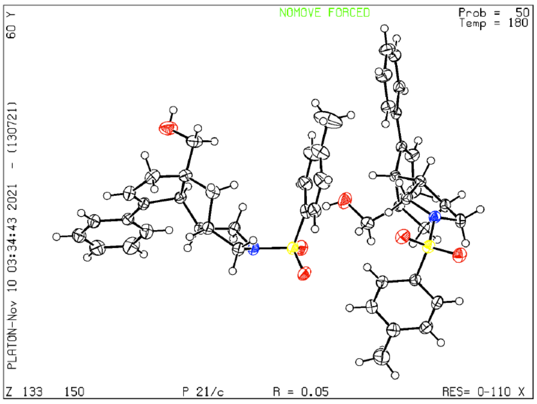


9a

CCDC number: 2130262

Table S3. Crystal data and structure refinement for 9a

Crystal data	
Chemical formula	$C_{24}H_{27}NO_3S$
M_r	409.52
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	180
a, b, c (Å)	10.1455 (4), 10.4127 (5), 10.7631 (4)
α, β, γ (°)	91.406 (4), 112.178 (4), 99.062 (4)
V (Å^3)	1035.38 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.56 × 0.12 × 0.08
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.110, 1.05
No. of reflections	5169
No. of parameters	263
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.37



Ellipsoids are drawn at 50% probability

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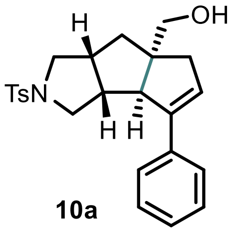

10a

CCDC number: 2130263

Table S4. Crystallographic Data of Compound 10a

Crystal data	
Chemical formula	$C_{24}H_{27}NO_3S$
M_r	409.52
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	180
a, b, c (Å)	23.8751 (7), 10.0099 (3), 19.2157 (6)
β (°)	113.616 (3)
V (Å^3)	4207.7 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.20 × 0.09 × 0.04
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.143, 1.06
No. of reflections	9622
No. of parameters	528
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.09, −0.48

7. Energy and Cartesian Coordinates for the Stationary Points

Table S2. Computed Energies for the Stationary Points.

Thermal corrections to Gibbs energies (TCGs), single-point energies (SPEs) in gas phase and solvent.

	Imaginary Frequencies (cm^{-1})	SPEs (in gas phase) (hartree)	TCGs (in gas phase) (hartree)	SPEs (under SMD model) (hartree)
8a'	none	-1338.586275	0.313382	-1338.618091
S1	none	-592.284351	0.077732	-592.299773
8a'-COM1	none	-1930.885341	0.41043	-1930.928275
8a'-COM2	none	-1930.879607	0.410027	-1930.922624
8a'-INT1	none	-1930.881312	0.415753	-1930.929056
8a'-INT2	none	-1930.873404	0.41386	-1930.921078
8a'-TS1	-188.20	-1930.876204	0.414165	-1930.919953
8a'-TS2	-213.66	-1930.868411	0.412959	-1930.913052
8a'-TS3	-445.54	-1930.848477	0.410184	-1930.911418
8a'-TS4	-426.79	-1930.839363	0.411518	-1930.904754
A	none	-2947.383927	0.331493	-2947.425904
B	none	-2947.380245	0.331402	-2947.422801
INT1	none	-2947.36202	0.334579	-2947.40109
TS1	-328.15	-2947.334715	0.332282	-2947.38079
TS2	-147.35	-2947.333671	0.330281	-2947.384224
TS3	-169.63	-2947.339634	0.332166	-2947.386822
TS4	-348.09	-2947.286444	0.333453	-2947.333943
TS5	-70.20	-2947.329918	0.331241	-2947.379338
TS6	-453.23	-2947.279875	0.332487	-2947.328804
C	none	-2487.008259	0.333409	-2487.121208
D	none	-2487.006717	0.333456	-2487.119803
INT2	none	-2487.025026	0.334511	-2487.124431
TS7	-415.74	-2486.992141	0.332316	-2487.097537
TS8	-19.55	-2486.980462	0.331651	-2487.096194
TS9	-107.77	-2487.024429	0.33492	-2487.121989
TS10	-320.60	-2486.945644	0.330796	-2487.051746
TS11	-20.30	-2486.985893	0.332979	-2487.096319
TS12	-307.44	-2486.945527	0.333313	-2487.049541

Cartesian coordinates for the stationary points

8a'

O	-0.73513400	4.27203600	-0.09235200
C	-1.05967200	3.20604300	0.38907100
C	-2.41686700	2.59539000	0.09161800
C	-2.32381700	1.54417600	-1.04480800

C	-1.65683100	0.23810900	-0.65313400
C	-0.32061900	0.10220800	-0.60938900
C	0.68069300	1.17995900	-0.92337600
C	2.02680800	0.58360400	-1.34971900
C	2.06072600	1.00625800	1.04978800
C	1.09732800	1.96694900	0.34646700
C	-0.07026000	2.41213800	1.23162300
H	-2.82209400	2.13057000	0.99812100
H	-3.07905300	3.40679800	-0.22367500
H	-3.33795400	1.33936700	-1.39988400
H	-1.79487500	2.00271900	-1.88829200
H	0.10303800	-0.84357000	-0.26962600
H	0.30068400	1.86932500	-1.68560300
H	2.61508500	1.31061700	-1.92038500
H	1.90980200	-0.32797000	-1.94261800
H	2.80558800	1.51835700	1.66325500
H	1.51269200	0.30534800	1.69016100
H	1.64024900	2.86180400	0.01766200
H	0.29919600	3.06472900	2.03082200
H	-0.55510900	1.54274300	1.68516400
N	2.72346100	0.29534500	-0.07434400
S	3.16504200	-1.28601900	0.22179100
O	3.45514900	-1.37065300	1.64633500
O	2.21416400	-2.21749600	-0.38376800
C	4.68835800	-1.42669300	-0.69224800
H	4.48786000	-1.20880000	-1.74284200
H	5.02945000	-2.45744700	-0.57819500
H	5.40736300	-0.72429600	-0.27141600
C	-2.54110700	-0.90151800	-0.27982600
C	-3.81280800	-0.67785000	0.26709100
C	-2.12714000	-2.23054700	-0.46010300
C	-4.63191300	-1.74022600	0.64419500
H	-4.17145800	0.33716700	0.41552300
C	-2.94473200	-3.29191300	-0.08620300
H	-1.16246500	-2.43682800	-0.91516500
C	-4.20082500	-3.05296800	0.47126600
H	-5.60878200	-1.53835800	1.07421500
H	-2.60193200	-4.31082000	-0.24094100
H	-4.83954700	-3.88237100	0.75986800

S1

S	-0.00007100	0.08772100	0.15959500
O	0.00267800	-0.51366400	1.52066300
C	1.41551200	-0.60981000	-0.69734300
H	1.32986800	-0.43024700	-1.76825800
H	2.29779400	-0.10723800	-0.29449300

H	1.45620100	-1.67268100	-0.45440900
C	-1.41361900	-0.61616800	-0.69538500
H	-2.29780900	-0.11916900	-0.28982100
H	-1.33130700	-0.43480900	-1.76625200
H	-1.44785200	-1.67956700	-0.45376000
C	-0.00434300	1.68702400	-0.23527000
H	-0.92971000	2.18873500	0.03696600
H	0.91722700	2.19448100	0.03919000

8a'-COM1

O	-2.08133800	-1.06367800	1.53985400
C	-1.66661100	-0.27156300	0.70816900
C	-1.90726800	1.21511600	0.86640800
C	-0.74077400	1.88875100	1.63414200
C	0.53002500	2.05567300	0.82075600
C	1.40148200	1.05014000	0.63336100
C	1.27216600	-0.33907800	1.19572400
C	2.64049400	-1.01733600	1.31819400
C	1.62363100	-1.66236200	-0.80687000
C	0.54222400	-1.30477900	0.22223500
C	-0.74274800	-0.75218900	-0.39856100
H	-2.03426100	1.67074000	-0.11975700
H	-2.83364700	1.34109700	1.43591900
H	-1.08050500	2.87175500	1.97349700
H	-0.54041200	1.30570500	2.54081800
H	2.25911300	1.21013400	-0.02119000
H	0.75795200	-0.32670600	2.16290400
H	2.58675500	-1.86386700	2.01992100
H	3.43880700	-0.34460700	1.63793200
H	1.52189500	-2.69055800	-1.17352400
H	1.60526500	-0.99497100	-1.67535300
H	0.28449900	-2.20173400	0.80033800
H	-1.25944400	-1.54239700	-0.95396100
H	-0.52024000	0.06170000	-1.09499400
N	2.88016800	-1.46130800	-0.06254100
S	4.21557400	-2.34748000	-0.43122200
O	4.25527600	-2.46107100	-1.88083500
O	5.31791100	-1.78190700	0.33170000
C	3.92354000	-3.99343800	0.21664100
H	3.81093400	-3.93420200	1.30040200
H	4.80015600	-4.59213300	-0.03853400
H	3.03304100	-4.41133200	-0.25624600
C	0.77138700	3.38527100	0.19425100
C	-0.29718900	4.18902900	-0.22810500

C	2.07392600	3.87297500	0.01277400
C	-0.07222700	5.42063200	-0.83902400
H	-1.32021700	3.84784000	-0.09423400
C	2.30075400	5.10413000	-0.59463300
H	2.91712200	3.29234900	0.37586900
C	1.22827400	5.88271900	-1.02814400
H	-0.91694100	6.01902700	-1.16792200
H	3.31885600	5.46197800	-0.71744300
H	1.40471700	6.84494700	-1.49936100
S	-5.00526300	-1.33043500	-0.57689700
O	-6.32635500	-1.72828300	-1.12930200
C	-4.05153500	-2.83088900	-0.35218800
H	-4.72962600	-3.58448200	0.05218500
H	-3.20956300	-2.63349200	0.31483400
H	-3.71337300	-3.13652200	-1.34532400
C	-5.27925900	-0.75353400	1.09708500
H	-5.70302600	0.25027200	1.01496000
H	-4.33284800	-0.74293100	1.64148000
H	-6.01022800	-1.42524600	1.55057100
C	-3.94943200	-0.23537900	-1.25341100
H	-4.38962700	0.76238300	-1.27348800
H	-3.60041600	-0.58275600	-2.22675300

8a’-COM2

O	-2.36557800	1.22733200	-0.79143300
C	-1.64251600	0.59518300	-0.03802300
C	-1.59574800	0.93488000	1.43702300
C	-0.57544300	2.07211200	1.69505900
C	0.71321600	2.03148100	0.88398300
C	1.44643500	0.92110500	0.71537200
C	1.10939400	-0.43036400	1.28414000
C	2.35820100	-1.31579700	1.36594400
C	1.07207400	-2.24798000	-0.40145500
C	0.14508100	-1.26465100	0.36154600
C	-0.69900300	-0.45008200	-0.61725300
H	-2.59157600	1.27765400	1.73337500
H	-1.37156400	0.04133200	2.02053500
H	-1.07387900	3.02392000	1.49542500
H	-0.32437500	2.08447800	2.76445400
H	2.32605400	0.96281400	0.07150600
H	0.67479400	-0.31523100	2.28176700
H	2.21230700	-2.11936500	2.10796300
H	3.27226800	-0.76788300	1.60305100
H	0.85580700	-3.28743100	-0.10975200

H	0.98374100	-2.17086400	-1.48717000
H	-0.53217700	-1.84078700	1.00275100
H	-1.32197100	-1.12851900	-1.21157800
H	-0.04860300	0.08131200	-1.32417100
N	2.42244200	-1.84342400	0.00509500
S	3.72292200	-2.74581000	-0.47480100
O	3.50376500	-3.06981200	-1.87538500
O	4.91091200	-2.03825700	-0.02381300
C	3.64728400	-4.28230800	0.44484800
H	3.72948600	-4.06524300	1.51112400
H	4.49997800	-4.87999500	0.11660100
H	2.71558200	-4.79940200	0.20961200
C	1.14961100	3.30538300	0.24818700
C	0.24278400	4.08162700	-0.48724900
C	2.47787500	3.73755300	0.34470600
C	0.65820200	5.25153400	-1.11736100
H	-0.78799000	3.75000600	-0.59405900
C	2.89255300	4.91119900	-0.28134100
H	3.18385300	3.15299300	0.92882200
C	1.98401100	5.67223100	-1.01428600
H	-0.05425200	5.83279200	-1.69563000
H	3.92565000	5.23391000	-0.18979600
H	2.30567600	6.58808000	-1.50124600
S	-4.83844900	-1.34504500	-0.10972600
O	-6.09617400	-2.13657100	-0.11775200
C	-5.26077800	0.32760700	0.37258900
H	-4.45178100	1.00536900	0.09237100
H	-5.41345200	0.31225000	1.45443000
H	-6.19829800	0.57524900	-0.12828400
C	-4.30915900	-1.16729100	-1.81200800
H	-3.88052400	-2.12774300	-2.10837600
H	-3.57628700	-0.36084000	-1.88781900
H	-5.20335400	-0.96679700	-2.40484500
C	-3.45938100	-1.72138600	0.74923000
H	-3.05484200	-2.67693100	0.40942600
H	-3.66046900	-1.69120400	1.82144800

8a'-INT1

O	-2.31718400	0.11813500	1.28069200
C	-1.98539300	0.74845500	0.13897800
C	-1.43649200	2.18880700	0.38192800
C	-0.23087100	2.27396100	1.33061900
C	1.11139600	1.95262100	0.70554300
C	1.54747800	0.68772100	0.59185900

C	0.78490200	-0.51489600	1.06945900
C	1.71780000	-1.70356000	1.31957800
C	0.79912900	-1.86873900	-0.93573900
C	-0.15364200	-1.08330800	-0.02184400
C	-1.01547800	-0.08489000	-0.78171100
H	-1.21666600	2.67937400	-0.57868000
H	-2.25437300	2.74567400	0.85913300
H	-0.18955600	3.28454100	1.75137800
H	-0.44428000	1.59744400	2.16514400
H	2.48470300	0.48428700	0.07211300
H	0.18911700	-0.28339000	1.95556000
H	1.23258600	-2.43837200	1.98019700
H	2.68176800	-1.42671100	1.75146800
H	0.32317000	-2.75204400	-1.37939100
H	1.18558000	-1.25430600	-1.75678400
H	-0.81555200	-1.79083500	0.49509400
H	-1.59213300	-0.66158700	-1.52193500
H	-0.37782400	0.58971800	-1.36848900
N	1.91186200	-2.23719900	-0.03986500
S	2.71165800	-3.65319500	-0.25958100
O	2.86973200	-3.83543000	-1.69520400
O	3.85140900	-3.64558700	0.64559200
C	1.60929900	-4.94969500	0.30970800
H	1.40929500	-4.80510100	1.37259900
H	2.12679800	-5.89744300	0.14900000
H	0.68978600	-4.91896900	-0.27767800
C	1.92854000	3.08727500	0.19217800
C	1.32217800	4.27090100	-0.25357200
C	3.32958500	3.01442800	0.14809500
C	2.08161300	5.32618300	-0.75529200
H	0.24101500	4.37041900	-0.21914000
C	4.09022000	4.06696700	-0.35092300
H	3.83087900	2.13199700	0.53488700
C	3.46980000	5.22845300	-0.81068800
H	1.58432600	6.22772500	-1.10214100
H	5.17331800	3.98486800	-0.36724700
H	4.06347100	6.05198600	-1.19637600
S	-4.56963100	-0.19000400	-0.38959200
O	-5.66373700	-0.17082300	-1.37910500
C	-3.84283700	-1.81442900	-0.27425000
H	-4.66068300	-2.48882300	-0.00817000
H	-3.05932600	-1.73799200	0.48711300
H	-3.45607000	-2.06303800	-1.26453000
C	-5.16114700	0.17339600	1.24962400

H	-5.68000000	1.13220700	1.17574700
H	-4.26093900	0.22383700	1.87606700
H	-5.86316800	-0.61908600	1.51919700
C	-3.29300700	1.01939700	-0.74316600
H	-3.78990200	1.96263600	-0.48450300
H	-3.17101100	0.97789700	-1.83189100

8a'-INT2

O	-2.80554500	0.09056000	-0.18059000
C	-1.87930000	-0.60258500	0.51945900
C	-1.63116600	0.01812200	1.91496300
C	-1.26571900	1.50997100	1.87260900
C	-0.13788800	2.00505900	0.97692100
C	1.03505100	1.38157000	0.79648200
C	1.34563500	0.01538100	1.33858900
C	2.84272800	-0.30356700	1.33418600
C	1.86574900	-1.35090300	-0.62847800
C	0.75147600	-1.10180900	0.41367900
C	-0.56355000	-0.77265000	-0.30234000
H	-2.58836300	-0.03938500	2.45205900
H	-0.91906000	-0.57903100	2.49740400
H	-2.17441700	2.03908000	1.57679600
H	-1.04505800	1.84304300	2.89795600
H	1.76194600	1.81062100	0.10483000
H	0.96851700	-0.07888800	2.35893200
H	3.06504500	-1.10640700	2.05613200
H	3.47269500	0.55847000	1.56311300
H	2.00308900	-2.42257500	-0.82578100
H	1.64385000	-0.86355700	-1.58288400
H	0.63816200	-2.00856900	1.02862300
H	-0.73042400	-1.55416700	-1.06024900
H	-0.44327300	0.15919500	-0.86130300
N	3.06948800	-0.73739600	-0.04664900
S	4.55854300	-1.24492500	-0.52331900
O	4.48723200	-1.46318800	-1.96027800
O	5.52879300	-0.33932700	0.07312400
C	4.81468200	-2.84991100	0.23618600
H	4.80280800	-2.73613800	1.32138600
H	5.79449100	-3.19991200	-0.09457400
H	4.03714000	-3.53637000	-0.10341500
C	-0.40926100	3.27263500	0.24379300
C	-1.58117100	3.38034700	-0.52097900
C	0.49362000	4.34056500	0.25961600
C	-1.83177100	4.53472900	-1.25781400

H	-2.26689000	2.53272900	-0.55467100
C	0.23538500	5.49798100	-0.47401700
H	1.39593400	4.26407900	0.86138000
C	-0.92796000	5.59829300	-1.23434500
H	-2.73462400	4.60369800	-1.85862500
H	0.94180500	6.32296000	-0.44642100
H	-1.13010600	6.49980700	-1.80575200
S	-3.73150600	-2.52213500	-0.31665200
O	-4.07765200	-3.95399400	-0.21856600
C	-5.13509900	-1.49523700	0.06970900
H	-4.76353800	-0.46422000	0.03880800
H	-5.46155500	-1.79864600	1.06748800
H	-5.90665100	-1.72878300	-0.66781100
C	-3.26353400	-2.10041500	-1.98602500
H	-2.42325600	-2.74716400	-2.24695100
H	-3.00268500	-1.03677100	-1.97271200
H	-4.12959000	-2.34423100	-2.60667400
C	-2.41945800	-2.07248100	0.82546000
H	-1.69877100	-2.89511500	0.73508900
H	-2.91952500	-2.16201400	1.79846300

8a’-TS1

O	-2.13631600	-0.78416300	1.36583400
C	-1.94313600	-0.06993900	0.33052400
C	-1.97271400	1.45753400	0.54380000
C	-0.83422000	1.97743400	1.44441100
C	0.50398300	2.10626900	0.74433900
C	1.32363400	1.05374900	0.58857800
C	1.04578500	-0.33053400	1.10216700
C	2.34429000	-1.11610000	1.31194000
C	1.44422600	-1.63906000	-0.89549300
C	0.31846800	-1.21446100	0.05899700
C	-0.87553700	-0.59627300	-0.66364500
H	-1.96121800	1.97596700	-0.42327300
H	-2.92425100	1.68568000	1.04004800
H	-1.12410100	2.95635600	1.84045200
H	-0.75904300	1.30631200	2.30683500
H	2.24108800	1.16955200	0.01007200
H	0.45448100	-0.30020300	2.02137700
H	2.17283400	-1.96281300	1.99419300
H	3.16785100	-0.51332800	1.70024000
H	1.28847200	-2.64454400	-1.30470900
H	1.55206100	-0.95012300	-1.74079100
H	-0.04066300	-2.09694800	0.60489400

H	-1.30591800	-1.38170000	-1.29687700
H	-0.55160700	0.21096300	-1.33318500
N	2.65375300	-1.56836400	-0.05423600
S	3.90244300	-2.60283700	-0.31534000
O	4.05159600	-2.73164300	-1.75729900
O	4.99892900	-2.16829200	0.53739600
C	3.37028300	-4.20214400	0.29865700
H	3.18061400	-4.12643200	1.37052400
H	4.18771100	-4.90054100	0.10899800
H	2.47599400	-4.51349100	-0.24420600
C	0.87057400	3.44038200	0.19250200
C	-0.11516100	4.34566600	-0.22688800
C	2.21231800	3.83693700	0.08333800
C	0.22606200	5.58468500	-0.76532500
H	-1.16533400	4.07993100	-0.14432000
C	2.55561800	5.07417800	-0.45238300
H	2.99524200	3.17821300	0.44775200
C	1.56371400	5.95406700	-0.88462100
H	-0.55784900	6.26249100	-1.09126700
H	3.60215000	5.35749800	-0.51917600
H	1.83104700	6.92147500	-1.29921900
S	-4.62969800	-1.31786800	-0.46365700
O	-5.83288100	-1.61058500	-1.27040000
C	-3.64605600	-2.79204600	-0.27749400
H	-4.31307000	-3.57583400	0.08724000
H	-2.83963200	-2.55443800	0.42755200
H	-3.27183400	-3.05139900	-1.27043800
C	-5.07157000	-0.88547200	1.20479300
H	-5.63636900	0.04784800	1.14523000
H	-4.13152500	-0.76853600	1.76198500
H	-5.70579500	-1.68584700	1.59108900
C	-3.51936300	-0.08872800	-0.92571500
H	-4.06430400	0.85810900	-0.87712500
H	-3.19499800	-0.29378600	-1.94941000

8a'-TS2

O	2.68420200	0.62766700	0.57799500
C	1.93387500	-0.09470100	-0.15863900
C	1.75916900	0.39760900	-1.60252600
C	1.08674000	1.78128100	-1.66394100
C	-0.20762300	2.01781100	-0.89751000
C	-1.20591700	1.13214100	-0.76649400
C	-1.17871000	-0.28108100	-1.27945400
C	-2.58151200	-0.88839800	-1.36672000

C	-1.56913400	-1.78963200	0.63160100
C	-0.44498200	-1.25384000	-0.29076300
C	0.67493700	-0.63882900	0.55100100
H	2.76407200	0.51327300	-2.02835800
H	1.24435800	-0.34546600	-2.21657300
H	1.82073200	2.50805900	-1.30625500
H	0.90667300	2.03700600	-2.71865600
H	-2.06995200	1.40493200	-0.15844500
H	-0.71722700	-0.31300400	-2.26873500
H	-2.58584000	-1.74337900	-2.06355300
H	-3.34946900	-0.17569600	-1.67425100
H	-1.53786900	-2.88655600	0.69960100
H	-1.49976500	-1.38947000	1.64660400
H	-0.05347300	-2.08945000	-0.88829500
H	0.99903600	-1.36470500	1.30856400
H	0.26863100	0.21166300	1.10920200
N	-2.81402200	-1.31008200	0.01403900
S	-4.25275700	-1.98185600	0.45075400
O	-4.19909600	-2.17816100	1.89124100
O	-5.29881800	-1.19365800	-0.18260400
C	-4.30335700	-3.60954100	-0.30048200
H	-4.27175000	-3.50203200	-1.38596700
H	-5.24787800	-4.06403500	0.00492100
H	-3.46554100	-4.20333400	0.06893000
C	-0.33773100	3.35358300	-0.24959500
C	0.67919000	3.82078500	0.59584300
C	-1.47692200	4.14412400	-0.43600100
C	0.55002100	5.04605700	1.24398300
H	1.55634100	3.19877600	0.76787200
C	-1.60184200	5.37419800	0.20809000
H	-2.26218600	3.79317500	-1.10079600
C	-0.58870800	5.82885400	1.04959300
H	1.33827300	5.38874900	1.90845000
H	-2.48984600	5.97895800	0.04735800
H	-0.68486900	6.78721100	1.55166000
S	4.30335100	-2.00025200	0.16717700
O	5.11738700	-3.22390100	0.00935300
C	5.21518500	-0.56346000	-0.35285100
H	4.59096100	0.30883300	-0.11485700
H	5.38662000	-0.67282800	-1.42631400
H	6.16614800	-0.57279100	0.18351400
C	3.95756300	-1.69685700	1.88667100
H	3.33161700	-2.52298200	2.23202700
H	3.44245900	-0.72815600	1.94177500

H	4.91393100	-1.70516500	2.41341000
C	2.77853500	-1.84845300	-0.62014200
H	2.16231200	-2.68678900	-0.28134600
H	2.97009300	-1.92597600	-1.69452100

8a'-TS3

O	-1.02573900	-1.69807200	2.20016000
C	-1.46790100	-1.19275500	1.03557600
C	-2.16236900	0.18864300	1.16516200
C	-1.28096700	1.26724200	1.81811800
C	-0.27494400	1.90959200	0.88387600
C	0.91173600	1.33739800	0.62235100
C	1.38784500	0.04472600	1.22123800
C	2.91650600	-0.04676800	1.20909000
C	2.03069700	-1.16415400	-0.77269200
C	0.99824800	-1.18403300	0.36242500
C	-0.43945800	-1.23873600	-0.13692100
H	-2.50940700	0.52885500	0.17634500
H	-3.04057000	0.04712900	1.81296800
H	-1.92342600	2.04773800	2.23929900
H	-0.77679200	0.78757700	2.66428600
H	1.57348200	1.79166500	-0.11660000
H	0.99230100	-0.09539600	2.23030900
H	3.25750300	-0.79006100	1.94533800
H	3.42043300	0.90107000	1.40967600
H	2.28728600	-2.17004200	-1.12514300
H	1.68381800	-0.58905100	-1.63865200
H	1.16821200	-2.06260400	0.99699600
H	-0.55875800	-2.17547600	-0.69945700
H	-0.62679200	-0.42923900	-0.85328700
N	3.19472600	-0.47971600	-0.17262800
S	4.71484000	-0.94700400	-0.58030800
O	4.72388800	-1.17446700	-2.01838600
O	5.63338200	-0.01146200	0.05345300
C	4.97937900	-2.54154100	0.19937100
H	4.91473100	-2.42334900	1.28211400
H	5.98091300	-2.86937900	-0.08564500
H	4.23244800	-3.24711700	-0.16880400
C	-0.66108700	3.18963700	0.22745600
C	-2.00631800	3.49768800	-0.02386600
C	0.30488000	4.13544300	-0.15027200
C	-2.37073500	4.68489600	-0.65598800
H	-2.78351300	2.79752300	0.27015400
C	-0.05560200	5.32188100	-0.78100000

H	1.35041500	3.94982300	0.07748400
C	-1.39664700	5.60228400	-1.04229300
H	-3.42028400	4.89301200	-0.84525700
H	0.71399300	6.03732200	-1.05662600
H	-1.67872800	6.53045400	-1.53044300
S	-3.77113500	-2.24470900	-0.69268200
O	-3.15169900	-1.90699800	-1.99388800
C	-4.67872100	-3.79404200	-0.82995900
H	-5.41111200	-3.69767100	-1.63549100
H	-5.16116700	-4.01815200	0.12438200
H	-3.94682700	-4.56513000	-1.07910000
C	-5.09673500	-1.09411600	-0.31805200
H	-4.64251800	-0.10802500	-0.20833700
H	-5.58748600	-1.39361600	0.61108600
H	-5.79380300	-1.10136900	-1.15927500
C	-2.52075500	-2.29928200	0.89442500
H	-2.06670700	-3.27849100	0.73276300
H	-3.25094800	-2.28861100	1.70615500

8a'-TS4

O	0.82055900	-2.95681100	1.05441800
C	-0.03929500	-2.23907200	0.31781600
C	0.29055500	-2.22911300	-1.18655200
C	1.71682900	-1.73165500	-1.47785300
C	2.20698800	-0.42885600	-0.85842700
C	1.48294200	0.69536300	-0.76137300
C	0.03164400	0.78642500	-1.13729000
C	-0.44497700	2.22674300	-1.33975500
C	-1.18827000	1.53497800	0.86350600
C	-0.89694000	0.27257200	0.01823900
C	-0.31608700	-0.83166600	0.91197600
H	0.25812400	-3.27240400	-1.52777200
H	-0.47709300	-1.69799600	-1.75806900
H	2.39660200	-2.52324000	-1.15401100
H	1.84541900	-1.65272300	-2.56767500
H	1.91713600	1.56499800	-0.26535100
H	-0.15300600	0.22256100	-2.05391200
H	-1.34589400	2.24510400	-1.97472200
H	0.31185200	2.87823200	-1.78147900
H	-2.25609100	1.61742900	1.11825300
H	-0.62509900	1.53899800	1.80118900
H	-1.82935700	-0.05869100	-0.46398800
H	-0.95694600	-0.95861600	1.79942700
H	0.64557800	-0.49150400	1.30792400

N	-0.73851800	2.65867000	0.02921000
S	-1.32047500	4.16959200	0.31536800
O	-1.41944300	4.31216000	1.76044200
O	-0.54553700	5.09143300	-0.50032600
C	-2.99555300	4.19799900	-0.32764900
H	-2.96752700	4.02622800	-1.40481900
H	-3.39456400	5.19183200	-0.11543700
H	-3.58956700	3.43851600	0.18384600
C	3.59256600	-0.45153400	-0.31295000
C	3.95578700	-1.45599600	0.59716600
C	4.52933700	0.52990700	-0.65335700
C	5.23095700	-1.46477200	1.15620400
H	3.21459400	-2.20198900	0.88612200
C	5.80793900	0.51315200	-0.09732800
H	4.25359500	1.30132700	-1.36829400
C	6.16206200	-0.48451000	0.80862500
H	5.49733700	-2.23763600	1.87192900
H	6.52808200	1.27718400	-0.37691900
H	7.15797100	-0.49886300	1.24245400
S	-3.04339600	-2.80246500	-0.07616600
O	-3.13310900	-2.20045400	-1.42648600
C	-4.10156900	-4.25681300	0.01015900
H	-4.05438300	-4.67902500	1.01668700
H	-3.71280600	-4.96783700	-0.72177800
H	-5.12044500	-3.96300300	-0.25458000
C	-3.81629600	-1.72511500	1.13358600
H	-3.21614800	-0.81427000	1.18456000
H	-3.83401400	-2.22207800	2.10640400
H	-4.82541800	-1.49836100	0.78188000
C	-1.20830600	-3.21526100	0.59539500
H	-1.04178900	-4.18669900	0.12569600
H	-1.41623800	-3.28948100	1.66550900

A

O	1.96676300	-0.10388400	1.22780200
C	0.86230100	0.66468300	1.76801200
C	0.64593300	2.00907800	1.10134800
C	-0.01137100	1.99816000	-0.28852900
C	-1.47955700	1.62636400	-0.32166500
C	-1.86119100	0.33821200	-0.35965300
C	-0.91424500	-0.82502500	-0.35294500
C	-1.55487200	-2.08269700	-0.94262700
C	-1.84609900	-2.14799900	1.45707000
C	-0.61113400	-1.30744300	1.08614800

C	-0.32882000	-0.21641000	2.11788000
H	0.04580600	2.61263100	1.80179400
H	1.62895200	2.49498400	1.00546900
H	0.12848800	2.99684000	-0.72421700
H	0.56269700	1.32519700	-0.94243000
H	-2.92695200	0.08914900	-0.34609700
H	0.01959100	-0.58978400	-0.88076400
H	-0.77835700	-2.81462000	-1.21419600
H	-2.17852700	-1.87204300	-1.82036700
H	-1.58396000	-3.00118600	2.09953300
H	-2.59765100	-1.54654400	1.98891900
H	0.27003900	-1.96539500	1.02127600
H	-0.15074800	-0.69647400	3.09193900
H	-1.21236200	0.42757500	2.23025900
N	-2.37844600	-2.60233500	0.15992600
S	-4.03380200	-2.64816400	-0.03152200
O	-4.61741500	-2.54614100	1.29466100
O	-4.43852100	-1.72691900	-1.08663100
C	-4.32459000	-4.29016300	-0.64448100
H	-3.77618600	-4.41266900	-1.58535300
H	-5.40498200	-4.37175800	-0.81340600
H	-3.98651800	-5.00254300	0.11489000
C	-2.48573000	2.72388900	-0.28577800
C	-2.15611700	3.98984900	0.22180800
C	-3.79696300	2.52437000	-0.75189200
C	-3.10315600	5.01141400	0.28573900
H	-1.14589300	4.18998900	0.58261800
C	-4.74061400	3.54392900	-0.69121300
H	-4.07853400	1.56406100	-1.18699200
C	-4.40076300	4.79287800	-0.16851800
H	-2.82046100	5.98396800	0.69157000
H	-5.74948000	3.36392000	-1.06556400
H	-5.14193300	5.59204700	-0.12481100
C	2.12193700	0.48087500	2.52089900
H	2.84883700	1.29739700	2.56584700
H	2.17019500	-0.25408500	3.32790400
In	3.42169800	-0.22478200	-0.45321400
Cl	2.32210500	-1.89321600	-1.70922400
Cl	5.21121700	-0.79214500	0.96843200
Cl	3.40834800	1.99138500	-1.27225100

B

C	0.75380700	-0.70709600	-0.46981300
C	0.79938000	0.75899000	-0.84516000

C	-0.34125300	1.19535100	-1.77717400
C	-1.68675300	1.32360400	-1.09603100
C	-2.54425300	0.29249400	-1.02416000
C	-2.25226700	-1.11190100	-1.47262400
C	-3.54114400	-1.92951900	-1.60220300
C	-2.64620200	-2.36248900	0.57946900
C	-1.51259600	-1.92022400	-0.37287800
C	-0.39081800	-1.21447700	0.38894300
H	0.79068200	1.36082700	0.07789800
H	1.75847700	0.94650300	-1.35272800
H	-0.05343200	2.16238400	-2.20720100
H	-0.40202100	0.49529000	-2.62363400
H	-3.51234200	0.46156600	-0.54193800
H	-1.67585700	-1.12210100	-2.40975500
H	-3.36003500	-2.86620000	-2.15223000
H	-4.36277200	-1.38841400	-2.08354800
H	-2.49341400	-3.39357300	0.93294600
H	-2.70310500	-1.70011700	1.45524100
H	-1.09894200	-2.81879000	-0.86025100
H	0.03869500	-1.92223300	1.11403000
H	-0.80436800	-0.37170000	0.96203900
N	-3.88402200	-2.25164700	-0.20802600
S	-5.17436400	-1.44666600	0.49853000
O	-4.69765700	-0.64373700	1.61761500
O	-5.94090600	-0.82605900	-0.56774500
C	-6.14028900	-2.77079500	1.18054300
H	-6.46384400	-3.41537400	0.35702000
H	-6.99722700	-2.30351500	1.68023900
H	-5.52220100	-3.31654400	1.90225200
C	-2.01855400	2.61459200	-0.42835700
C	-1.59456000	3.84834200	-0.94370100
C	-2.77446400	2.61662400	0.75698600
C	-1.92560000	5.04315700	-0.30745600
H	-1.01773300	3.89000600	-1.86845100
C	-3.10423300	3.81050600	1.39191200
H	-3.10309300	1.66963800	1.19162600
C	-2.68066800	5.02963800	0.86338400
H	-1.59173900	5.99068800	-0.73293600
H	-3.68904100	3.78503600	2.31249300
H	-2.93411500	5.96473300	1.36481100
O	2.04050900	-1.23040100	-0.03951000
C	1.51174100	-1.66631900	-1.29663400
H	1.23658200	-2.72404600	-1.30205200
H	2.07011800	-1.29661200	-2.16316500

In	4.01896400	-0.22912100	0.31044700
Cl	3.29717500	1.53114500	1.69681800
Cl	4.40359100	0.26985100	-1.98017400
Cl	5.25548400	-2.00415000	1.22346900

INT1

C	0.83959600	1.24499200	-0.44766000
C	-0.05534000	2.46855800	-0.62449100
C	-1.25451400	2.26491500	-1.56861400
C	-2.40466600	1.50762200	-0.94213000
C	-2.53093500	0.17826400	-1.07812800
C	-1.51843900	-0.71760400	-1.73334700
C	-2.09443500	-2.11555200	-1.98789100
C	-0.83361400	-2.27716400	0.02741700
C	-0.33089100	-1.05715000	-0.78831500
C	0.18595900	0.01101300	0.18194900
H	-0.43485900	2.77654600	0.36198000
H	0.57159400	3.29058700	-1.00166700
H	-1.59472400	3.26660000	-1.86153500
H	-0.93231200	1.77866900	-2.49953800
H	-3.40405800	-0.30264400	-0.62698100
H	-1.14837400	-0.27355400	-2.66971900
H	-1.45682900	-2.68016100	-2.68537500
H	-3.12203300	-2.11305800	-2.36720100
H	-0.06090600	-3.05871600	0.07588400
H	-1.09710100	-1.98728600	1.05412400
H	0.51495300	-1.38092600	-1.41258800
H	0.92494700	-0.50404800	0.81327500
H	-0.62034700	0.33857200	0.85635700
N	-2.03188100	-2.76471700	-0.67077100
S	-3.44583200	-2.86683600	0.22345000
O	-3.35887700	-2.01841800	1.40721800
O	-4.55759900	-2.70474200	-0.69839300
C	-3.42208200	-4.54951600	0.78786700
H	-3.44594700	-5.20251400	-0.09029200
H	-4.31639100	-4.68075900	1.40853000
H	-2.51346100	-4.70412200	1.38082600
C	-3.36429900	2.26492100	-0.08976600
C	-3.73706500	3.58568700	-0.38033600
C	-3.91748700	1.65441000	1.04986100
C	-4.64332300	4.26940200	0.42802600
H	-3.34015800	4.08750400	-1.26401700
C	-4.82262000	2.33896400	1.85616700
H	-3.62904900	0.63264700	1.31011500

C	-5.18940700	3.64944000	1.55012800
H	-4.92694200	5.29221000	0.17506700
H	-5.23705600	1.84494000	2.73619400
H	-5.89520700	4.18625000	2.18562000
O	2.58043300	-0.10765300	-1.50861100
C	1.68898100	0.93178900	-1.68319500
H	0.96629500	0.65506700	-2.47469500
H	2.17338600	1.87227300	-2.01259000
In	3.78461600	-0.11969000	0.12060800
Cl	5.93116400	0.81517100	0.08994400
Cl	3.30630900	-1.91178600	1.57505400
Cl	2.11845100	1.84259600	0.85686500

TS1

C	0.08832300	-0.56434000	0.24642500
C	-0.43411600	-0.42373900	1.65944500
C	0.07829200	0.94116800	2.15648800
C	1.18646000	1.34382700	1.19761800
C	2.14138400	0.42289500	0.87514800
C	2.49609900	-0.82579800	1.64367000
C	4.02412500	-1.04033800	1.64121600
C	3.20214100	-2.81725800	0.36187400
C	1.94623000	-2.11636700	0.94088200
C	0.93064100	-1.73395700	-0.13941400
H	-1.53092500	-0.46506500	1.66364100
H	-0.09160400	-1.25863400	2.28160300
H	-0.74001400	1.66876000	2.14532500
H	0.45085200	0.89481600	3.19127900
H	2.80169400	0.66406100	0.03640100
H	2.11979000	-0.75088300	2.67261800
H	4.32596600	-1.64131200	2.51220000
H	4.60676600	-0.11288500	1.63394000
H	3.48568900	-3.68298400	0.97690500
H	3.05688500	-3.15586200	-0.67148100
H	1.47786300	-2.77012900	1.68866000
H	0.21694900	-2.55323600	-0.33356900
H	1.43778200	-1.50881200	-1.08996900
N	4.28740400	-1.83283200	0.43957300
S	4.69818900	-1.01229600	-0.96729500
O	3.63636800	-1.17173100	-1.95221700
O	5.13429700	0.32138100	-0.57990200
C	6.10891100	-1.91488900	-1.54916500
H	6.89589900	-1.84233600	-0.79186300
H	6.41278800	-1.43751300	-2.48847200

H	5.80877000	-2.95430500	-1.72240400
C	1.17699800	2.67326700	0.54665400
C	-0.00674500	3.41893000	0.40546100
C	2.37868500	3.22326000	0.06101100
C	0.01170200	4.66445600	-0.21766600
H	-0.96559800	3.02351300	0.74645300
C	2.39251800	4.46977300	-0.55378400
H	3.31654600	2.67806100	0.18151400
C	1.20813600	5.19414500	-0.69695900
H	-0.92048000	5.21899200	-0.33043400
H	3.33501800	4.88107800	-0.91709400
H	1.21958100	6.17252500	-1.17952000
O	-1.57849700	-0.81007400	-1.00948100
C	-0.60366800	0.16598200	-0.85065700
In	-3.53905300	-0.57512200	-0.30598600
Cl	-3.69246000	-2.30572300	1.32568800
Cl	-3.27678700	1.55225900	0.83908400
Cl	-5.09164800	-0.56987800	-2.08056300
H	-0.98691300	1.15153900	-0.54038700
H	0.03863000	0.28222100	-1.74053600

TS2

O	2.20822800	-1.40782500	-0.89110100
C	0.32983800	-1.30807700	-2.06499700
C	-0.16148000	-2.55681100	-1.48162200
C	-0.60832100	-2.40147800	0.02303900
C	-1.86003900	-1.58477400	0.23462100
C	-1.80365900	-0.24140700	0.27806900
C	-0.55081400	0.56664000	0.10277100
C	-0.67749800	1.96313600	0.71227700
C	-1.29990900	2.12185300	-1.61773300
C	-0.33542000	0.94379200	-1.38012200
C	-0.57127600	-0.20787500	-2.40485600
H	-1.05160000	-2.86753300	-2.05499600
H	0.62940200	-3.31566800	-1.51487100
H	-0.75676100	-3.42725100	0.38204800
H	0.24885200	-1.98722400	0.56934200
H	-2.73133200	0.32722900	0.39427900
H	0.32186300	0.04035400	0.51055700
H	0.31656700	2.42814000	0.79664300
H	-1.16965800	1.95880400	1.69219600
H	-0.85758300	2.85830000	-2.30472100
H	-2.26185900	1.79674200	-2.03861400
H	0.69880000	1.29780200	-1.48393500

H	-0.27808900	0.18413700	-3.39556500
H	-1.62369100	-0.51485500	-2.40444600
N	-1.49382900	2.68900800	-0.27559300
S	-3.02841700	3.18878700	0.15286800
O	-3.82481100	3.19844400	-1.06230000
O	-3.47896800	2.44266900	1.32085800
C	-2.77730700	4.86704000	0.67352900
H	-2.07158500	4.86760100	1.51184500
H	-3.75709200	5.24351900	0.99094100
H	-2.39041900	5.43456300	-0.17895600
C	-3.16060100	-2.30091800	0.35388700
C	-3.33246600	-3.58461800	-0.18552100
C	-4.25765800	-1.70503300	0.99945400
C	-4.55976600	-4.24195500	-0.10689800
H	-2.50277400	-4.09004700	-0.68362300
C	-5.48033100	-2.36248500	1.08162500
H	-4.14804400	-0.72253600	1.46193700
C	-5.63988000	-3.63291100	0.52576500
H	-4.66758000	-5.23727300	-0.54043400
H	-6.31430600	-1.88136900	1.59453600
H	-6.59907300	-4.14757400	0.59495800
C	1.80931700	-1.13118400	-2.17455300
H	2.19427900	-1.85045200	-2.93273600
H	2.05764200	-0.11215500	-2.53151400
In	3.35066900	-0.19643700	0.37673400
Cl	5.59225800	-0.93230900	0.39696900
Cl	2.10134200	-0.40504300	2.40039900
Cl	3.00232700	1.94997500	-0.66581600

TS3

C	0.10665100	-0.75824600	0.17691600
C	-0.42287100	-0.67126000	1.58026900
C	-0.12366400	0.76566500	2.04290900
C	1.01612900	1.26546500	1.17039100
C	2.08717900	0.46131300	0.91017400
C	2.52930800	-0.77455400	1.64985200
C	4.07060000	-0.85376900	1.68977500
C	3.45422800	-2.66033100	0.34135600
C	2.12276700	-2.09232500	0.89466100
C	1.09540400	-1.79201800	-0.19840400
H	-1.50246400	-0.86824300	1.59290600
H	0.04897600	-1.42802000	2.21604900
H	-1.01671600	1.38324600	1.89973500
H	0.13748100	0.80953600	3.11152400

H	2.76500800	0.80181700	0.12018400
H	2.11827200	-0.76918800	2.66823100
H	4.40040400	-1.45004200	2.55364200
H	4.56792100	0.12158200	1.72492500
H	3.79599000	-3.51248300	0.94547000
H	3.37205800	-2.98570200	-0.70327800
H	1.69823900	-2.80432400	1.61484300
H	0.45004200	-2.67356200	-0.39654100
H	1.57807200	-1.51873100	-1.15062300
N	4.44312800	-1.58568300	0.47764200
S	4.78817900	-0.68526300	-0.89920400
O	3.72861800	-0.87262700	-1.88338900
O	5.14238500	0.65572800	-0.46126200
C	6.24574900	-1.47805300	-1.52350600
H	7.03353900	-1.38275100	-0.76962600
H	6.50994200	-0.94949100	-2.44729300
H	6.01043400	-2.52760000	-1.73240400
C	0.93533600	2.59237000	0.52172000
C	-0.29549700	3.15452000	0.14146900
C	2.11668100	3.31934500	0.27821100
C	-0.33609400	4.40717900	-0.46731200
H	-1.21469000	2.57937600	0.25513800
C	2.06764400	4.57245000	-0.32038500
H	3.08032300	2.90544500	0.58088000
C	0.83915800	5.12054900	-0.69397000
H	-1.29723000	4.82203800	-0.77304700
H	2.99134900	5.12675700	-0.49083300
H	0.80045100	6.10409500	-1.16475600
O	-1.76189400	0.58421700	-0.55822500
C	-0.62833800	-0.06644900	-0.92889800
In	-3.52092300	-0.48435100	-0.25386900
Cl	-5.19899300	-0.06774400	-1.85916100
Cl	-2.49852400	-2.69242800	-0.36481500
Cl	-4.00873400	0.06956800	2.02109000
H	0.11368500	0.61555000	-1.40499100
H	-0.77746600	-0.87147300	-1.68610700

TS4

C	0.24117100	-1.16626400	-0.09951500
C	-0.20038200	-2.56300600	-0.47924100
C	-1.03486600	-2.95365600	0.75531300
C	-2.00871500	-1.78533000	0.76099700
C	-1.58015500	-0.46025800	0.69981500
C	-0.74278500	0.69697400	1.24751900

C	-1.62584600	1.88077900	1.65605100
C	-0.92653800	2.33412200	-0.59820700
C	0.00573500	1.24528100	-0.01107000
C	0.28958600	0.05411300	-0.95578500
H	-0.83229300	-2.55562200	-1.37909600
H	0.68071200	-3.19391000	-0.66852700
H	-1.54186600	-3.91767500	0.66277700
H	-0.41946000	-3.00875200	1.66071700
H	-2.28867100	0.04497100	0.02267100
H	-0.04675700	0.43491200	2.04696200
H	-1.01756900	2.58698300	2.24297900
H	-2.51360100	1.61786500	2.24210500
H	-0.37708100	3.27575600	-0.73730200
H	-1.35951500	2.03651500	-1.56351000
H	0.95024900	1.69736200	0.30688300
H	1.27666400	0.14317400	-1.44095000
H	-0.45917700	-0.02133400	-1.75787200
N	-2.00591300	2.51232300	0.39090700
S	-3.58313800	2.40624500	-0.13145400
O	-3.66919300	1.54273500	-1.30436500
O	-4.40385100	2.10900200	1.03555000
C	-3.94124200	4.05933900	-0.66495200
H	-3.85507400	4.72192700	0.20213800
H	-4.96488600	4.04379100	-1.05747000
H	-3.23002000	4.33135200	-1.45343200
C	-3.38887600	-2.06762500	0.32328600
C	-3.73947600	-3.23788300	-0.37912700
C	-4.40295800	-1.13452000	0.61490900
C	-5.05235000	-3.45660800	-0.78055300
H	-2.98340700	-3.97360700	-0.65214700
C	-5.71555400	-1.36114000	0.22246900
H	-4.16955700	-0.22056800	1.16217400
C	-6.04384100	-2.52214500	-0.47795000
H	-5.30247600	-4.35916000	-1.33901800
H	-6.47860100	-0.62028100	0.46279500
H	-7.07336100	-2.69934800	-0.79261700
O	2.08167000	-0.16335000	1.19328300
C	1.24481600	-1.22295100	1.06977900
H	0.69043200	-1.40230700	2.01075000
H	1.77344200	-2.18105700	0.86153700
In	3.75907400	0.00476800	-0.02587700
Cl	5.78688500	-0.07593400	1.17957500
Cl	3.30646100	2.03583200	-1.21844100
Cl	3.28215400	-1.90361900	-1.44500800

TS5

C	-0.70680500	0.19091300	0.58472300
C	-0.54694200	1.62383700	0.50806000
C	0.63111900	1.77295200	1.57683300
C	1.99135400	1.46605300	1.00429500
C	2.55303900	0.24751200	1.09719600
C	1.91439500	-1.00097700	1.65165600
C	2.95817700	-2.11125300	1.82826800
C	1.86426200	-2.56675700	-0.23985600
C	0.94781200	-1.67487800	0.63313700
C	0.11325300	-0.71623600	-0.23372800
H	-0.19521100	1.99042000	-0.46367100
H	-1.43852600	2.15880000	0.86019800
H	0.55843000	2.82140100	1.89017500
H	0.42343800	1.17235700	2.47411000
H	3.56075300	0.13744500	0.68602200
H	1.38890500	-0.79304600	2.59751500
H	2.56250100	-2.92474200	2.45541400
H	3.90877000	-1.76644200	2.24921900
H	1.43709800	-3.57476400	-0.34492000
H	2.00573300	-2.14150100	-1.24257700
H	0.25298800	-2.31895000	1.19136500
H	-0.62095500	-1.30047500	-0.81480600
H	0.73649200	-0.15074200	-0.93854400
N	3.15211400	-2.62096500	0.46425200
S	4.51138700	-2.11681200	-0.38443100
O	4.10597700	-1.29991300	-1.52253000
O	5.45561200	-1.58875700	0.58547900
C	5.15572800	-3.63767300	-1.03062800
H	5.41786400	-4.28206900	-0.18547500
H	6.04157800	-3.37169300	-1.61966500
H	4.39117300	-4.09664600	-1.66755600
C	2.67485900	2.54755600	0.24039300
C	2.58848300	3.89351600	0.62489700
C	3.42379600	2.22496500	-0.90405700
C	3.23892400	4.88732900	-0.10326900
H	2.03253800	4.17856400	1.51993400
C	4.07269600	3.22018300	-1.63006600
H	3.49325200	1.18484800	-1.23342100
C	3.98215400	4.55424900	-1.23421000
H	3.16713900	5.92707500	0.21888700
H	4.64531300	2.94914700	-2.51802100
H	4.48659200	5.33313100	-1.80760600

O	-2.49379300	-1.22425900	0.90023000
C	-1.64165400	-0.40584200	1.60625700
H	-1.03601300	-0.97948200	2.34014600
H	-2.14509100	0.41027800	2.15894200
In	-3.95663200	-0.24102100	-0.23339800
Cl	-4.33118500	1.70607100	1.12083200
Cl	-5.75253800	-1.63579600	-0.82722100
Cl	-2.46198600	0.47523100	-2.00260400

TS6

C	-0.09514900	-1.00726500	0.02891400
C	0.25451300	-2.41425800	0.48638000
C	1.13703200	-2.91148900	-0.67974000
C	2.14372300	-1.78049200	-0.67480700
C	1.73087800	-0.45948300	-0.73234900
C	0.99215200	0.65424500	-1.47506200
C	1.97545800	1.76454600	-1.88658600
C	0.87144900	2.62141400	0.03773100
C	0.10316800	1.34372200	-0.36726500
C	-0.11277400	0.30398700	0.75823100
H	0.83215800	-2.41179200	1.42170800
H	-0.67154000	-2.98721300	0.62737100
H	1.59172000	-3.88395000	-0.47172900
H	0.56958400	-2.98441000	-1.61545600
H	2.41847100	0.09895600	-0.08000700
H	0.41853500	0.29568200	-2.33532300
H	1.50768000	2.39530200	-2.65876900
H	2.93936900	1.40038800	-2.25887200
H	0.32465000	3.51953500	-0.28191100
H	1.04113900	2.68204100	1.12029000
H	-0.86644900	1.63282800	-0.79333700
H	-1.06695900	0.44693000	1.29462800
H	0.69147200	0.34946600	1.50866200
N	2.15585400	2.56417000	-0.67608400
S	3.55849800	2.42307400	0.20887300
O	3.24812500	1.87816200	1.52992500
O	4.53665300	1.74629900	-0.62667100
C	4.06814200	4.10486200	0.44461400
H	4.26356700	4.54062700	-0.54048200
H	4.97875200	4.07138100	1.05439400
H	3.26905400	4.63889400	0.97119800
C	3.47433400	-2.10994800	-0.12120800
C	4.07386500	-3.31381600	-0.54187400
C	4.19523200	-1.26897200	0.74664100

C	5.36386600	-3.64555000	-0.14431800
H	3.54134500	-3.97915800	-1.22256700
C	5.47221900	-1.62402500	1.16719000
H	3.76820900	-0.34236300	1.13088000
C	6.06494600	-2.80400800	0.71874500
H	5.81990700	-4.56814900	-0.50488700
H	6.00692400	-0.96615700	1.85283100
H	7.07057200	-3.07101100	1.04645400
O	-2.24011600	-1.43406100	-0.19120400
C	-1.20688500	-1.10993700	-1.03765900
H	-1.37958400	-0.17733500	-1.59061300
H	-1.00879300	-1.90623300	-1.77565400
In	-3.85441800	-0.14726800	0.15299700
Cl	-3.41202300	1.55533700	-1.50321100
Cl	-3.45920400	0.73618700	2.34149500
Cl	-5.87080800	-1.34334400	-0.13633700

C

O	2.01106900	-1.97397600	-0.29095700
C	0.76769800	-1.99134500	-1.09121500
C	-0.27211500	-2.91624000	-0.49709700
C	-0.97131400	-2.42753300	0.78089700
C	-2.00046900	-1.33931500	0.55681400
C	-1.64098300	-0.04564900	0.49998600
C	-0.23919200	0.46791100	0.67723900
C	-0.22829500	1.94543200	1.09083300
C	-0.06633500	1.87265900	-1.30418300
C	0.47229600	0.55906500	-0.68896500
C	0.36753400	-0.62772100	-1.64509100
H	-1.01259500	-3.10179400	-1.29225000
H	0.22208900	-3.87613300	-0.28865900
H	-1.45604500	-3.29507700	1.24638200
H	-0.20496700	-2.09772600	1.49872300
H	-2.40259000	0.70754700	0.28374000
H	0.31951700	-0.15150900	1.39597000
H	0.76836400	2.24151600	1.46109200
H	-0.97069000	2.17743400	1.86264900
H	0.71452600	2.40211100	-1.87076300
H	-0.89797600	1.66033600	-1.99186800
H	1.56170200	0.80981400	-0.49746100
H	0.95738600	-0.40588700	-2.54773000
H	-0.68247600	-0.70319400	-1.96042100
N	-0.53751300	2.65302700	-0.15542900
S	-2.05878800	3.39082100	-0.29776400

O	-2.57036900	3.04951200	-1.61235100
O	-2.81719600	3.07289000	0.90074200
C	-1.68509800	5.12128000	-0.27005200
H	-1.20283300	5.35635400	0.68474300
H	-2.64664100	5.64170500	-0.35976100
H	-1.03682700	5.34890600	-1.12275800
C	-3.41966600	-1.74696200	0.36840300
C	-3.74902900	-3.04476800	-0.05154600
C	-4.46716400	-0.83905000	0.60005200
C	-5.07598600	-3.41783200	-0.25900900
H	-2.96841500	-3.78669100	-0.22980000
C	-5.79088400	-1.21343400	0.39787400
H	-4.25115500	0.16561800	0.96760600
C	-6.10164000	-2.50279900	-0.03686800
H	-5.30694900	-4.43042600	-0.59192000
H	-6.58808000	-0.49510900	0.59258400
H	-7.14098700	-2.79469500	-0.19138900
C	2.01009800	-2.60580900	-1.59472700
H	2.14492500	-3.68802500	-1.53523300
H	2.60852500	-2.07849400	-2.34403800
In	3.21313100	-0.30012400	0.33865000
Cl	2.93807000	0.09033000	2.58466400
Cl	4.60823500	0.00381200	-1.47234600

D

C	0.75490000	-1.29273000	-0.57404000
C	1.11678300	0.05449100	-1.16497000
C	0.11074000	0.56826900	-2.20739100
C	-1.10361100	1.14903600	-1.52523900
C	-2.22747400	0.43977800	-1.35315300
C	-2.43074700	-0.99945400	-1.75389100
C	-3.91667300	-1.39016200	-1.60163900
C	-2.85737000	-2.65951800	0.02582400
C	-1.70331100	-2.04057000	-0.82321700
C	-0.58003000	-1.52899600	0.09715700
H	1.15467800	0.80021400	-0.34429100
H	2.11364000	-0.03170100	-1.64516300
H	0.61115800	1.33396000	-2.81369400
H	-0.15483900	-0.25125900	-2.89067700
H	-3.06402300	0.93901800	-0.85713800
H	-2.10532700	-1.14701200	-2.79434500
H	-4.17378500	-2.24389500	-2.24555800
H	-4.61078900	-0.56897000	-1.81227400
H	-3.07831600	-3.68021600	-0.31685400

H	-2.61765500	-2.69827000	1.09561900
H	-1.28607600	-2.83591400	-1.46115600
H	-0.38896600	-2.31019200	0.84848800
H	-0.91019100	-0.63253600	0.64156600
N	-4.04197100	-1.83936200	-0.21175700
S	-4.33330900	-0.64246500	0.94468400
O	-3.08847200	-0.33991900	1.65273400
O	-5.06448100	0.42588800	0.28805600
C	-5.41548200	-1.46986800	2.07630600
H	-6.32821400	-1.73563900	1.53352200
H	-5.62302900	-0.75061200	2.87785100
H	-4.90776900	-2.35576300	2.47360800
C	-0.95333500	2.49841000	-0.91514400
C	-0.24225900	3.52511500	-1.55460300
C	-1.51967400	2.75565300	0.34504900
C	-0.11600200	4.77948300	-0.96130600
H	0.18794200	3.36488000	-2.54533400
C	-1.39022100	4.01028100	0.93606000
H	-2.06001700	1.95996900	0.86559800
C	-0.68866900	5.02541600	0.28607300
H	0.42297600	5.57245800	-1.48159100
H	-1.83764600	4.19385200	1.91376700
H	-0.58917300	6.00750900	0.75002400
O	1.88773400	-1.79785200	0.24581500
C	1.54912400	-2.45778400	-0.99938300
H	1.16227800	-3.46611900	-0.83388000
H	2.30368300	-2.35028000	-1.78554600
In	3.55284500	-0.46106400	0.55938700
Cl	5.05965900	-1.04816100	-1.07495000
Cl	3.12377700	0.84390200	2.38654200

INT2

C	0.61184900	-1.97108200	-0.81612400
C	0.27644800	-2.93649700	0.24591600
C	-0.12046300	-2.04390700	1.46740600
C	0.41062700	-0.62079000	1.31120600
C	1.73634000	-0.38655600	1.20633800
C	2.83208700	-1.41688200	1.18426000
C	4.19073000	-0.76293800	1.52567600
C	4.44964500	-1.40537300	-0.69180300
C	3.09624900	-2.03087700	-0.24556500
C	1.98985300	-1.75061500	-1.27368800
H	-0.60554200	-3.51128600	-0.07182900
H	1.11626100	-3.59917800	0.47812400

H	-1.20937700	-2.05154200	1.54685200
H	0.28830900	-2.50079900	2.37976700
H	2.06306100	0.65409100	1.15636700
H	2.59559900	-2.22620900	1.89183700
H	4.89334200	-1.50723600	1.92681900
H	4.11615000	0.06774900	2.23602300
H	5.26185200	-2.13809400	-0.59290200
H	4.43166600	-1.05143100	-1.73048900
H	3.22464000	-3.11646700	-0.13946200
H	2.10224200	-2.46407100	-2.11928700
H	2.08509500	-0.73983700	-1.70116700
N	4.71786000	-0.30779200	0.23713000
S	4.24417300	1.23074000	-0.27338100
O	3.21191300	1.10003800	-1.30464000
O	3.94728600	2.00743200	0.91820000
C	5.71190000	1.85759100	-1.03435500
H	6.48975100	1.91328900	-0.26591400
H	5.45432900	2.85316200	-1.41596300
H	5.99902800	1.19065600	-1.85499100
C	-0.53099300	0.53399600	1.27710000
C	-1.81993100	0.45637500	1.85458600
C	-0.15582900	1.75202900	0.68163300
C	-2.66738900	1.58065600	1.88387800
H	-2.14759100	-0.44996400	2.36951500
C	-0.99649300	2.86321800	0.72297900
H	0.80371200	1.83768200	0.16671800
C	-2.24984600	2.79079700	1.32964200
H	-3.64780700	1.49283200	2.35636900
H	-0.67317800	3.79232800	0.25270400
H	-2.90622700	3.66071900	1.35127700
O	-1.72178400	-1.54930000	-0.91670300
C	-0.51476700	-1.29993300	-1.48881400
In	-3.06940200	-0.08092200	-0.44419000
H	-0.24854700	-0.22636800	-1.62985200
H	-0.42482100	-1.71237300	-2.53174500
Cl	-2.68258400	1.65214600	-1.97128800
Cl	-4.99932500	-0.91452400	0.55977300

TS7

C	0.12791200	-0.26276900	0.66180000
C	-0.54567300	0.27714200	1.89545800
C	0.28701700	1.50234400	2.34975100
C	0.96740100	2.04300000	1.10215400
C	2.13906600	1.48376600	0.71076700

C	2.96767000	0.54945100	1.55429700
C	4.38693000	0.29795900	0.97495400
C	3.57941400	-1.81654300	1.50737100
C	2.36792100	-0.88729400	1.75024100
C	1.24240600	-1.23729700	0.75782000
H	-1.56658600	0.59346200	1.63388400
H	-0.59899500	-0.49338500	2.67825600
H	-0.35618000	2.24493500	2.83564100
H	1.03772200	1.19390900	3.08734100
H	2.54096100	1.72530100	-0.27667500
H	3.07639000	1.00233100	2.55186800
H	5.14757800	0.42404600	1.75729400
H	4.63203400	0.97432300	0.14734000
H	4.16417700	-1.93455600	2.43099800
H	3.31347400	-2.81105300	1.13096400
H	1.99292400	-1.00510800	2.77716300
H	0.77928800	-2.17868000	1.10276100
H	1.63369000	-1.42918000	-0.24810200
N	4.41658300	-1.10068300	0.54338900
S	4.07751400	-1.36594800	-1.08920800
O	3.48685400	-2.68981000	-1.19050900
O	3.34080400	-0.21852100	-1.61977600
C	5.68772600	-1.38106300	-1.82146300
H	6.17588400	-0.42018900	-1.62394900
H	5.53007500	-1.52163700	-2.89774200
H	6.24644300	-2.21625800	-1.38713700
C	0.24217800	3.03765700	0.27361600
C	-1.12153200	3.29981700	0.48991600
C	0.89255900	3.73664200	-0.75878800
C	-1.81810100	4.19916100	-0.31523100
H	-1.66781800	2.79661000	1.28915900
C	0.19958500	4.63945400	-1.55697200
H	1.96020600	3.59499800	-0.92676200
C	-1.16081400	4.87010900	-1.34357800
H	-2.87816100	4.37821100	-0.13110900
H	0.72752200	5.17638200	-2.34583500
H	-1.70167700	5.58063700	-1.96962600
O	-1.22119200	-1.20053400	-0.37582800
C	-0.47765300	-0.01863100	-0.65609400
In	-3.26410900	-1.24062600	-0.24746200
H	-1.08407500	0.89585800	-0.73933100
H	0.20292800	-0.14679200	-1.50845700
Cl	-4.30678400	-3.28468100	-0.16049100
Cl	-3.93783900	0.97879400	-0.05044300

TS8

O	-2.18780400	-1.19646300	-0.78173400
C	-0.75175500	0.00220400	-1.94828600
C	-0.97064800	1.33759300	-1.39101000
C	-0.52784200	1.47723900	0.11415000
C	0.96181700	1.41571700	0.33581000
C	1.58779900	0.22909400	0.43813500
C	0.93849400	-1.12551700	0.35999400
C	1.83820200	-2.20393600	0.98460700
C	2.22871600	-2.32195900	-1.36239000
C	0.85646300	-1.64335600	-1.10033200
C	0.57570100	-0.54480900	-2.18989900
H	-0.33764200	2.03935700	-1.96335500
H	-2.02806000	1.62491100	-1.48724600
H	-0.93096600	2.44113900	0.44887000
H	-1.02896300	0.68575700	0.69113600
H	2.67568100	0.23491200	0.53503900
H	-0.06460300	-1.12740700	0.81008500
H	1.27058500	-3.13076300	1.16132900
H	2.30688600	-1.88748800	1.92292600
H	2.07316300	-3.31140800	-1.81855700
H	2.87155900	-1.72895300	-2.02621200
H	0.05383700	-2.39177700	-1.15130400
H	0.56624000	-1.06915300	-3.16176000
H	1.36327900	0.21628900	-2.16359400
N	2.85144200	-2.44138400	-0.04567300
S	4.39386600	-1.78084600	0.16618600
O	4.72359700	-1.03711900	-1.03802200
O	4.40843700	-1.12297600	1.46326500
C	5.44704700	-3.20144200	0.25384700
H	5.13748100	-3.80626800	1.11256500
H	6.46597000	-2.81853700	0.38954400
H	5.36106000	-3.75564100	-0.68698900
C	1.71316700	2.70022900	0.37842800
C	1.17795300	3.87192700	-0.17842900
C	2.98839700	2.76763300	0.96542900
C	1.89755500	5.06605200	-0.17121900
H	0.18562100	3.87457500	-0.63499500
C	3.70294400	3.96003900	0.97665200
H	3.42280600	1.88596700	1.43985600
C	3.16351300	5.11392500	0.40542200
H	1.46230600	5.96194600	-0.61545100
H	4.68720000	3.99087700	1.44528500
H	3.72578800	6.04816900	0.41909400

C	-1.94800200	-0.88474400	-2.12359000
H	-2.76779800	-0.33547800	-2.62403300
H	-1.71507400	-1.79149000	-2.70333200
In	-3.72738600	-0.47483100	0.33592100
Cl	-3.82981000	-1.24564000	2.49837500
Cl	-4.82944800	1.11373100	-0.95545000

TS9

C	0.67556900	-1.82978700	-0.79219500
C	0.30440600	-2.91079200	0.17810900
C	-0.15125800	-2.13336300	1.43280100
C	0.37671200	-0.71388100	1.24453000
C	1.71002200	-0.49687900	1.07179500
C	2.83283600	-1.49023700	1.10385800
C	4.15118000	-0.78931000	1.51009500
C	4.50898500	-1.37588600	-0.71472200
C	3.15691700	-2.04110900	-0.33748800
C	2.04308400	-1.71400900	-1.33993900
H	-0.53000400	-3.48282100	-0.25310600
H	1.14905900	-3.57927600	0.37756300
H	-1.24173600	-2.14893700	1.49240700
H	0.24890300	-2.58284400	2.35276000
H	2.01998500	0.54104300	0.93496800
H	2.59334500	-2.31964500	1.78452100
H	4.85857700	-1.51897200	1.92936200
H	4.02030400	0.02588800	2.23016600
H	5.33537000	-2.09055300	-0.60186900
H	4.52040900	-0.99517100	-1.74384500
H	3.29236200	-3.12903000	-0.27611200
H	2.06451500	-2.45153300	-2.16897000
H	2.18304000	-0.71851200	-1.78858600
N	4.71089400	-0.29511300	0.25180100
S	4.25540400	1.25423400	-0.23718800
O	3.30415800	1.14766900	-1.34449500
O	3.85357600	1.97885700	0.95773600
C	5.76353800	1.93343000	-0.86101800
H	6.48210300	1.96989800	-0.03579100
H	5.51743900	2.93937700	-1.22246200
H	6.12078000	1.30291800	-1.68297900
C	-0.53915700	0.46187000	1.25822400
C	-1.80632800	0.38302200	1.87924100
C	-0.16465700	1.69095200	0.68557100
C	-2.63771700	1.51221900	1.96537400
H	-2.13224900	-0.53889100	2.36555400

C	-0.99297200	2.80853500	0.77944600
H	0.78068100	1.79075200	0.14804000
C	-2.22543100	2.73180200	1.42562800
H	-3.60334800	1.42317300	2.46676800
H	-0.67484000	3.74596600	0.32265600
H	-2.87160700	3.60733000	1.48985900
O	-1.66447700	-1.44896000	-0.94429800
C	-0.45015000	-1.16204600	-1.49715700
In	-3.09044000	-0.07498600	-0.47106200
H	-0.21023000	-0.08123100	-1.61266900
H	-0.34904700	-1.56688500	-2.53676000
Cl	-2.84868200	1.76987200	-1.88733200
Cl	-4.94452300	-1.00971800	0.58371400

TS10

C	-0.30452400	1.15803500	-0.72260400
C	0.24195800	2.55697400	-0.87014400
C	0.89432400	2.83105400	0.49770400
C	1.91551700	1.70540100	0.55141100
C	1.54374000	0.38054800	0.37791400
C	0.56850200	-0.73246200	0.72784800
C	1.30834300	-1.96912700	1.25797800
C	1.13135300	-2.25995100	-1.12333800
C	0.05364600	-1.24860900	-0.65344700
C	-0.15845100	-0.03097400	-1.60094200
H	1.00428700	2.59994500	-1.66031300
H	-0.56611800	3.26331400	-1.11828300
H	1.35514900	3.82072100	0.55524000
H	0.17733800	2.78153000	1.32675700
H	2.35751600	-0.11723700	-0.17233300
H	-0.24710800	-0.45581500	1.40150800
H	0.57064100	-2.67973600	1.66378700
H	2.05232900	-1.75861100	2.03383400
H	0.66096900	-3.17888600	-1.50107300
H	1.77435900	-1.84942800	-1.91492000
H	-0.89329400	-1.77229000	-0.49122100
H	-1.09749300	-0.15516200	-2.16962600
H	0.67250700	0.09992800	-2.30576100
N	1.94192400	-2.54356900	0.07103300
S	3.61321600	-2.46342100	-0.07103400
O	3.94886400	-1.62085800	-1.21251900
O	4.13112600	-2.12857600	1.24715800
C	4.08026000	-4.12565200	-0.46108800
H	3.78246600	-4.76772000	0.37422600

H	5.16972900	-4.11713600	-0.58740200
H	3.58601100	-4.41635100	-1.39506000
C	3.32453100	2.06643100	0.36114800
C	3.71890100	3.31281900	-0.17318400
C	4.33044600	1.14884900	0.73411900
C	5.06322700	3.62016400	-0.33701700
H	2.97974300	4.04446500	-0.49908500
C	5.67262000	1.46716900	0.58228800
H	4.06522900	0.18376100	1.16783200
C	6.04303300	2.70094700	0.04400700
H	5.35043000	4.58031000	-0.76616500
H	6.43142800	0.74644600	0.88766500
H	7.09828000	2.94869100	-0.07936700
O	-2.28517800	-0.00765700	0.11845100
C	-1.52539600	1.14158900	0.17940400
H	-1.22991000	1.37954300	1.21627200
H	-2.08818000	2.03990000	-0.16584900
In	-4.30432100	-0.00826000	0.10885700
Cl	-5.36013600	-2.05068900	0.25562300
Cl	-5.06516900	2.17549900	-0.13517500

TS11

C	0.60688900	-0.32597000	-0.57358800
C	0.66833400	1.09896100	-0.41894300
C	-0.40337500	1.38840800	-1.58941400
C	-1.79426900	1.44057400	-1.03129100
C	-2.64978500	0.41536400	-1.17174000
C	-2.36725800	-0.91239600	-1.83839500
C	-3.65092600	-1.77055200	-1.86333400
C	-2.27626000	-2.90842900	-0.37739000
C	-1.36696600	-1.83836100	-1.05670500
C	-0.47023300	-1.14711100	0.00377700
H	0.24416800	1.50503100	0.50798100
H	1.63732200	1.53769700	-0.68497500
H	-0.06857100	2.35317300	-1.99334700
H	-0.31814700	0.67027500	-2.42072900
H	-3.64894200	0.54745500	-0.74805800
H	-2.00050700	-0.74710500	-2.86330400
H	-3.60418600	-2.53595400	-2.65162500
H	-4.56777700	-1.18523300	-1.99497500
H	-2.15101000	-3.87863500	-0.87819400
H	-2.05108100	-3.03563800	0.68848700
H	-0.72156000	-2.34859100	-1.78526900
H	0.08207100	-1.94428900	0.53754300

H	-1.08401400	-0.59947000	0.73012900
N	-3.65277600	-2.46713000	-0.57326800
S	-4.34018400	-1.64142700	0.73345900
O	-3.26894300	-1.09996000	1.57147500
O	-5.35206100	-0.75041400	0.19592100
C	-5.13283700	-2.94452000	1.63121500
H	-5.90024700	-3.37942600	0.98283400
H	-5.57815100	-2.47436200	2.51652300
H	-4.38078000	-3.68556300	1.92410200
C	-2.14389700	2.62530900	-0.20275500
C	-1.73320600	3.91842100	-0.55813100
C	-2.88698100	2.44920700	0.97580300
C	-2.07091800	5.01227500	0.23540700
H	-1.17516500	4.08908800	-1.48156700
C	-3.22214500	3.54563900	1.76692800
H	-3.19167600	1.44319100	1.27670200
C	-2.81595100	4.82819100	1.39981700
H	-1.75905600	6.01413000	-0.06224600
H	-3.79937700	3.39489900	2.67993200
H	-3.07900800	5.68513500	2.02109200
O	2.50624000	-1.28300900	-0.18683100
C	1.72045600	-1.00673200	-1.31385900
H	1.41330700	-1.93817400	-1.81161900
H	2.19143600	-0.33002700	-2.04849900
In	4.27321300	-0.37232400	0.22619200
Cl	4.44172700	1.42195900	-1.25425800
Cl	5.55768300	-1.15864200	1.96039300

TS12

C	-0.49117800	-0.85420100	-0.08426300
C	-0.22168100	-2.32879100	0.05967700
C	0.70915800	-2.61114100	-1.13579600
C	1.86364900	-1.68251600	-0.82041600
C	1.64576800	-0.32162800	-0.69690600
C	0.91861500	0.86959500	-1.28815900
C	1.89666600	2.00748800	-1.62801300
C	1.10372500	2.48510800	0.58085900
C	0.12420200	1.47783900	-0.07747100
C	-0.34715000	0.30971800	0.83608500
H	0.28885400	-2.56285300	1.00394700
H	-1.17834300	-2.87018200	0.00968600
H	1.00030500	-3.66220100	-1.21699800
H	0.24425000	-2.33878700	-2.09357500
H	2.32410400	0.07886200	0.07134900

H	0.28973200	0.63391800	-2.15471500
H	1.37105300	2.76848600	-2.22692300
H	2.79061300	1.68726600	-2.17383800
H	0.62677400	3.46930800	0.68984900
H	1.44106900	2.15118500	1.57158600
H	-0.74699000	2.03486300	-0.44737800
H	-1.33067400	0.55523200	1.27753000
H	0.35455600	0.10182600	1.65433800
N	2.25294200	2.57251600	-0.32938000
S	3.78419900	2.27398800	0.29258600
O	3.65054000	1.49047300	1.51483900
O	4.58911300	1.76111700	-0.80623500
C	4.37801200	3.88194000	0.73299800
H	4.42825300	4.48735300	-0.17786300
H	5.37417800	3.73323900	1.16721300
H	3.69508200	4.31488900	1.47271700
C	3.07803800	-2.26781500	-0.24809000
C	3.10218600	-3.58825700	0.25266900
C	4.27054300	-1.51234400	-0.20961200
C	4.26915900	-4.12524400	0.78007700
H	2.20082900	-4.20082500	0.26152500
C	5.43717400	-2.06008000	0.30522400
H	4.29590100	-0.49667500	-0.60721800
C	5.43980400	-3.36454300	0.80387900
H	4.26780400	-5.14126400	1.17532900
H	6.35053900	-1.46502100	0.31355800
H	6.35734100	-3.79133500	1.21152000
O	-2.68747800	-1.15440300	-0.53980500
C	-1.56025700	-0.61487900	-1.16445100
H	-1.67427500	0.45387500	-1.39438900
H	-1.35108200	-1.15170000	-2.10149100
In	-4.26854900	-0.06209600	0.06944900
Cl	-3.56659800	2.17045800	0.09089300
Cl	-6.23897500	-1.05970100	0.70883700

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