Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Photoinduced Sulfonylation Cyclization to Medium-Sized Benzo[*b*]azocine and Mechanistic Insight

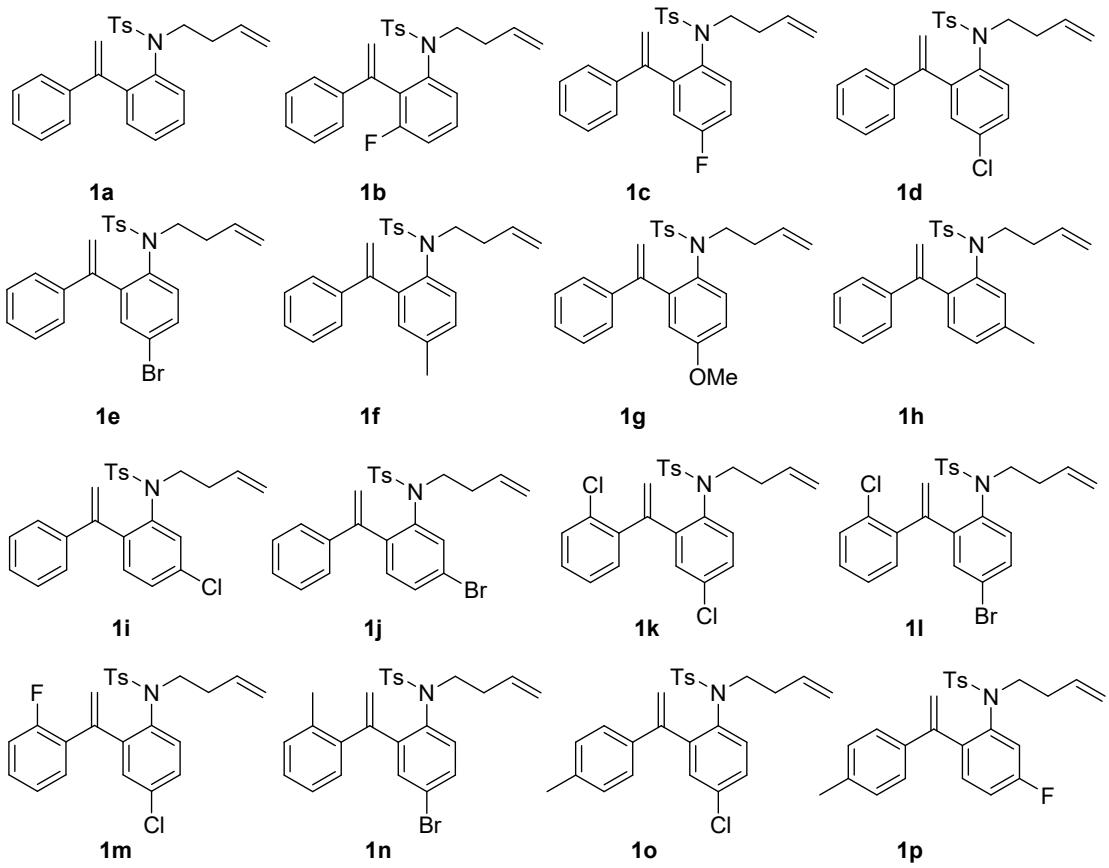
Table of Contents

1. General Conditions.

All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR, ^{13}C NMR spectra were recorded on a Bruker Ascend™ 400 or Bruker Ascend™ 500 spectrometer in deuterated solvents containing TMS as an internal reference standard. All high-resolution mass spectra (HRMS) were measured on a mass spectrometer by using electrospray ionization orthogonal acceleration time-of-flight (ESI-OA-TOF), and the purity of all samples used for HRMS (>95%) was confirmed by ^{1}H NMR and ^{13}C NMR spectroscopic analysis. Melting points were measured on a melting point apparatus equipped with a thermometer and were uncorrected. All the reactions were monitored by thin-layer chromatography (TLC) using GF254 silica gel-coated TLC plates. Purification by flash column chromatography was performed over SiO_2 (silica gel 200−300 mesh).

2. Typical Experimental Procedures.

Preparation of material 1.

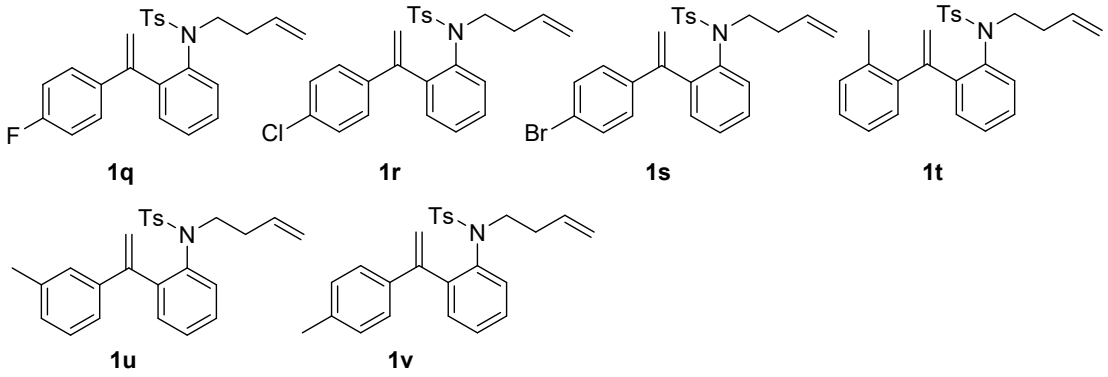


1a **1b** **1c** **1d**

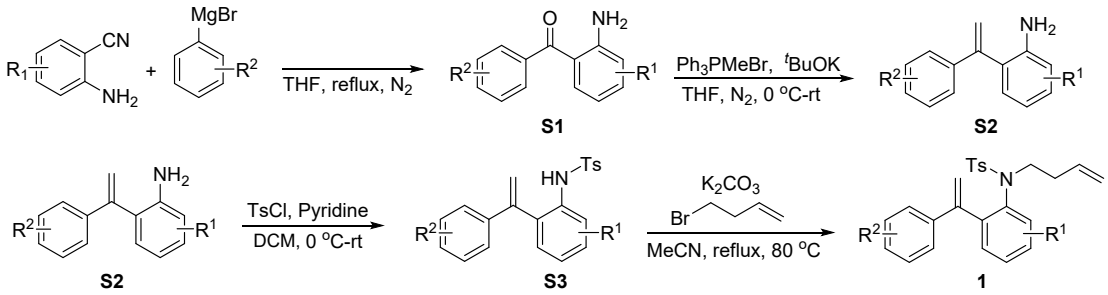
1e **1f** **1g** **1h**

1i **1j** **1k** **1l**

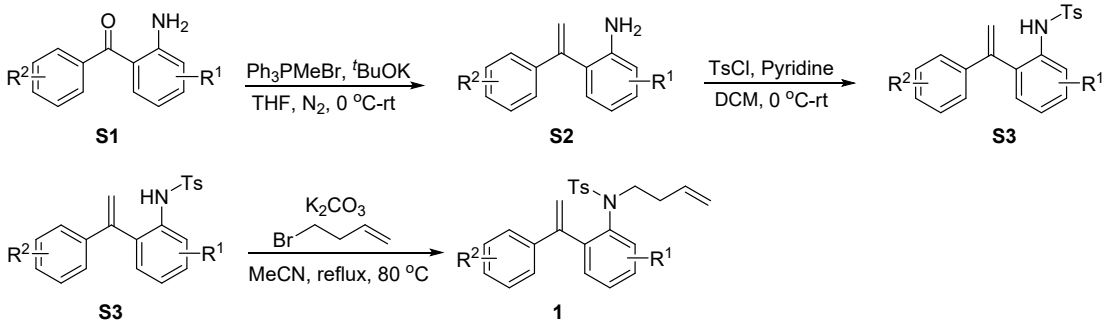
1m **1n** **1o** **1p**



2.1 The general procedure for the synthesis of 1.



1a, **1b**, **1c**, **1d**, **1i**, **1j**, **1k**, **1l**, **1m**, **1q**, **1r**, **1s** were prepared from (2-aminophenyl) (phenyl)methanone **S1**.



1e, **1f**, **1g**, **1h**, **1n**, **1o**, **1p**, **1t**, **1u**, **1v** were prepared from 2-aminobenzonitrile.

General Procedure for the synthesis of S1.

To a round-bottomed flask charged with 2-aminobenzonitrile (10 mmol, 1.0 equiv.) in dry THF (20 mL), arylmagnesium bromide (30 mmol, 3.0 equiv., 2.8 M in THF) was added dropwise *via* syringe at 0 °C in a nitrogen atmosphere. The reaction mixture was heated in oil bath at 65 °C for 4 h. Upon the reaction completed, the suspension was cooled to 0 °C, the reaction mixture was quenched by 3 M HCl, extracted with EtOAc (3×40 mL). The separated organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 100:1) to afford **S1**.

General Procedure for the synthesis of S2.

To a round-bottom flask, tetrahydrofuran (20 mL) solution containing Ph_3PMeBr (10.0 mmol, 1.5 equiv.) and potassium *tert*-butanol (7.5 mmol, 1.5 equiv.) were added in batches at 0 °C in a air atmosphere. Half an hour later, **S1** (5.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. The reaction mixture was warmed to room temperature and stirred for 4 h. Upon the reaction completed, the desired product **S2** was purified on silica gel column by flash column chromatography (eluent: petroleum ether/EtOAc = 100:1).

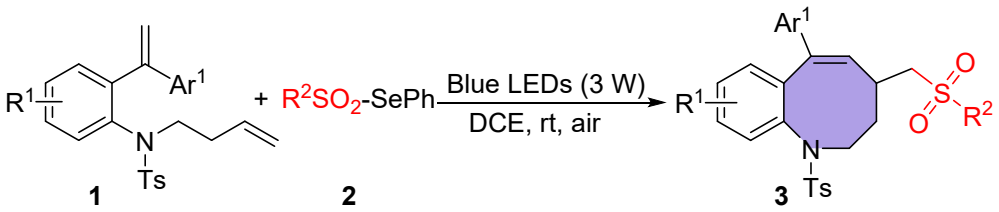
General Procedure for the synthesis of S3.

To a round-bottomed flask charged with dichloromethane (15 mL) solution dissolved with TsCl (2.4 mmol, 1.2 equiv.), **S2** (2.0 mmol, 1.0 equiv.) was added, and then pyridine (3.0 mmol, 1.5 equiv.) was dropped at 0 °C. The reaction mixture was warmed to room temperature and stirred for 12 h. Upon the reaction completed, the reaction mixture was extracted with EtOAc (3×15 mL). The separated organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 100:1) to afford **S3**.

General Procedure for the synthesis of 1.

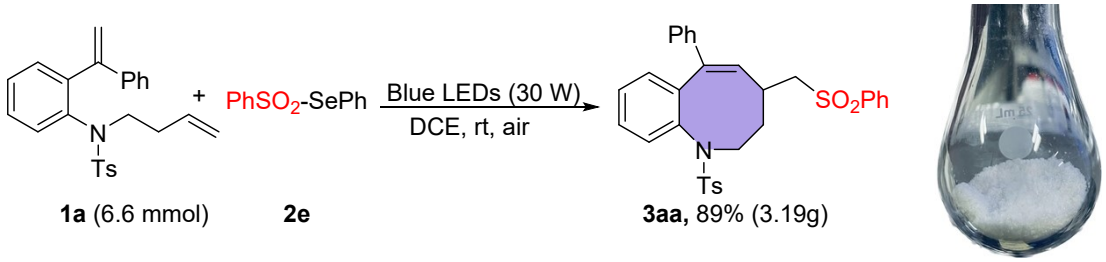
To a round bottom flask containing potassium carbonate (2.4 mmol, 2.0 equiv.), 4-Bromo-1-butene (2.4 mmol, 2.0 equiv.), **S3** (1.2 mmol, 1.0 equiv) and acetonitrile (10 mL) were added. The reaction mixture was stirred in oil bath at 80 °C for 4 h. Upon the reaction completed, the reaction mixture was concentrated in vacuo. The residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 100:1) to afford **1**.

2.2 The general procedure for the synthesis of 3.



Dienes **1** (0.30 mmol), selenosulfonates **2** (0.39 mmol) and DCE (3 mL) were placed in a 10 mL glass tube. The resulting mixture was allowed to stir at room temperature under 3 W blue LEDs irradiation for 12 hours under air and then monitored by TLC. After the completion of the reaction, the mixture was quenched by $NaHCO_3$ (sat. aq. 15 mL) and extracted with DCM (5 mL×3). Then the organic solvent was concentrated in vacuo. The residue was purified by flash column chromatography with ethyl acetate and petroleum ether as eluent (6:1)) to give 8-exo cyclization products **3**.

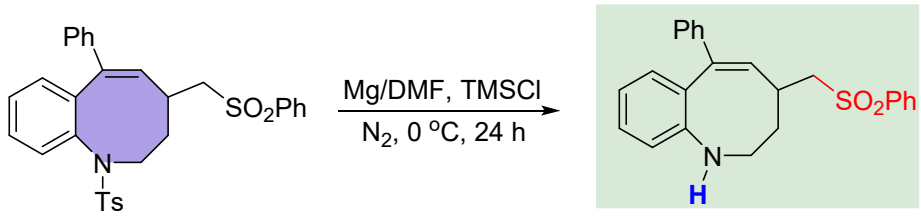
2.3 The gram-scale synthesis of compound 3aa.



1a (6.6 mmol) **2e** **3aa,** 89% (3.19g)

1a (6.6 mmol, 2.66 g), **2e** (8.58 mmol, 2.55 g) and DCE (10 mL) were placed in a 15 mL glass tube. The resulting mixture was allowed to stir at room temperature under 30 W blue LEDs irradiation for 14 hours under air and then monitored by TLC. After the completion of the reaction, the mixture was quenched by $NaHCO_3$ (sat. aq. 150 mL) and extracted with DCM (50 mL×3). Then the organic solvent was concentrated in vacuo. The residue was purified by flash column chromatography with ethyl acetate and petroleum ether as eluent to give **3aa** (3.19 g, 89%).

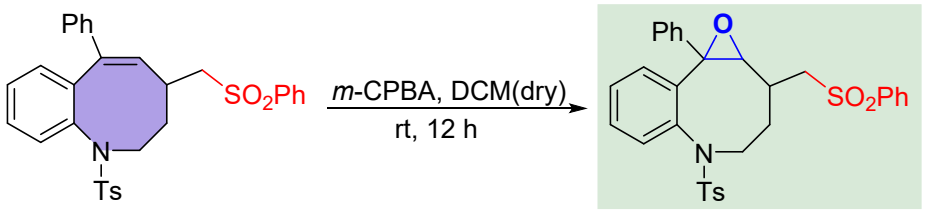
2.4 General procedure for the synthesis of 4.



3aa **4**

To a 10 mL dry Schlenk tube equipped with a magnetic stir bar, 3**aa** (0.3 mmol, 162.9 mg), TMSCl (1.5mmol, 162.9mg), Mg (0.9 mmol, 27.3 mg) and DMF (dry, 3 mL) were added. The tube was sealed and the reaction mixture was stirred at 0℃ for 24 h under N_2. Upon the reaction completed, H_2O was added to mixture and extracted with ethyl acetate. The combined organic layer was dried (anhydrous Na_2SO_4), filtered, and evaporated followed by a silica gel column chromatography (petroleum ether/ethyl acetate = 10：3) to afford desired product **4** (95.8 mg, 82%).

2.5 General procedure for the synthesis of 5.



3aa, 0.3 mmol **5**

To a 10 mL dry thick walled tube equipped with a magnetic stir bar, **3aa** (0.3 mmol, 162.9 mg) and DCM (dry, 1.5 mL) were added. Then, the *m*-CPBA (0.45 mmol, 77.6 mg) was dissolved in 1.5 mL of DCM (dry) was added. The tube was sealed and the reaction mixture was stirred at rt

for 12 h under N_2. Upon the reaction completed, the mixture was concentrated under reduced pressure. The resulting crude residue was purified via flash column chromatography (petroleum ether/ethyl acetate = 10:3) on silica gel to afford the desired product **5** (119.2 mg, 71%)**.**

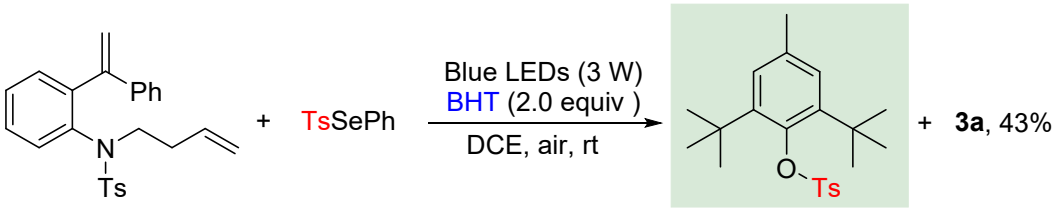
3. Control Experiments.

3.1 Control experiment in the presence of TEMPO.

1a **2a** **3a**, 0%

1a (0.20 mmol, 80.63 mg), TsSePh **2a** (0.26 mmol, 81.11 mg), TEMPO (0.40 mmol, 62.50 mg) and DCE (3mL) were placed in a 10 mL glass tube. The resulting mixture was allowed to stir at room temperature under 3 W blue LEDs irradiation for 12 hours and then monitored by TLC. No desired product **3a** was detected.

3.2 Control experiment in the presence of BHT.

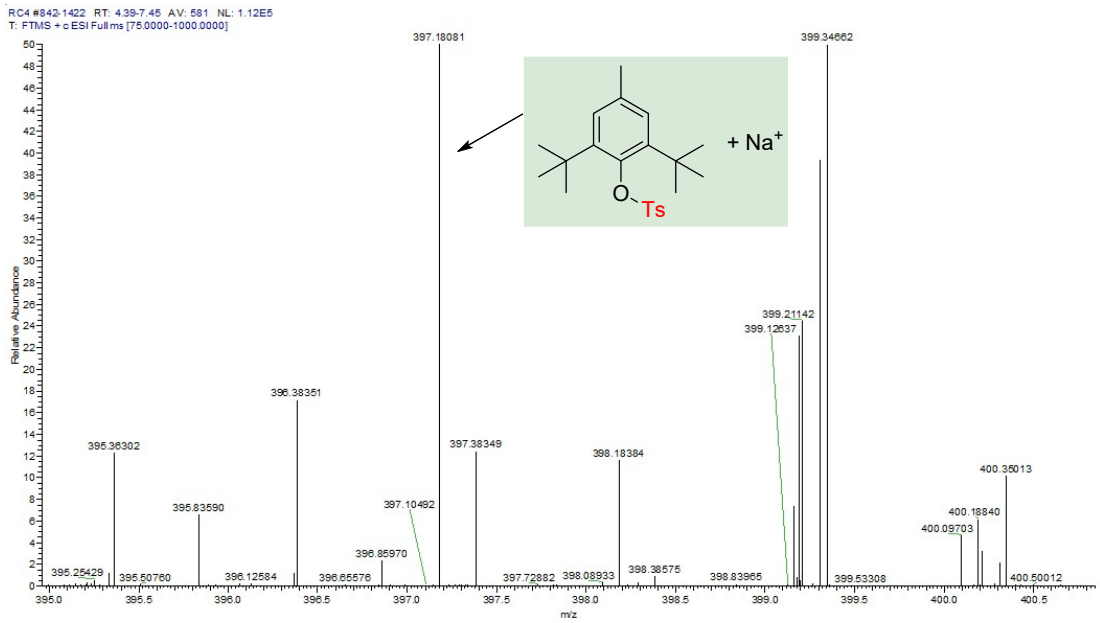


1a **2a** **6**

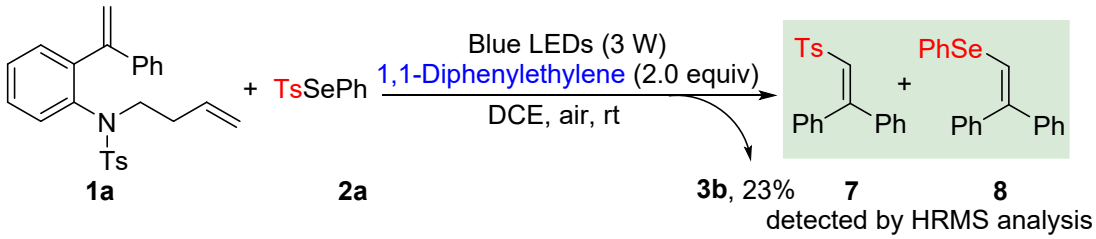
detected by HRMS analysis

1a (0.20 mmol, 80.63 mg), TsSePh **2a** (0.26 mmol, 81.11 mg), BHT (0.40 mmol, 62.50 mg) and DCE (3mL) were placed in a 10 mL glass tube. The resulting mixture was allowed to stir at room temperature under 3 W blue LEDs irradiation for 8 hours and then monitored by TLC. We successfully detected the adduct **6** by HRMS analysis. The residue was purified by column chromatography to give the corresponding product **3a** in 43% yield.

HRMS (ESI) calcd for adduct **6** $C_{22}H_{30}NaO_3S$ $[M+Na]^+$: 397.1808, found: 397.1808.



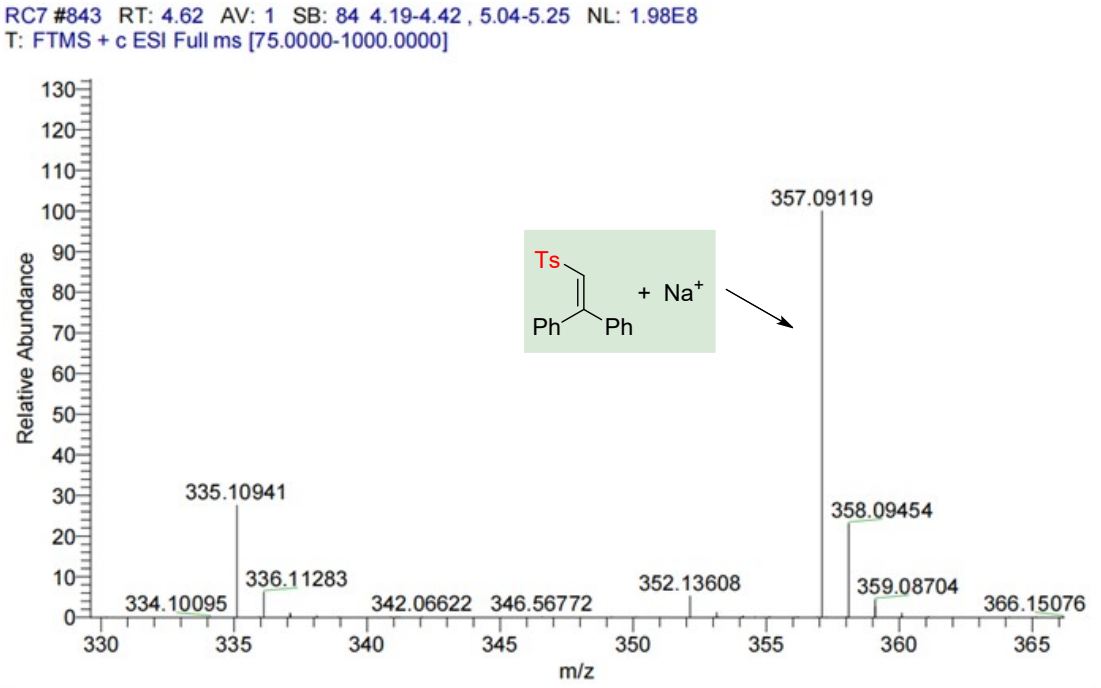
3.3 Control experiment in the presence of 1,1-Diphenylethylene.

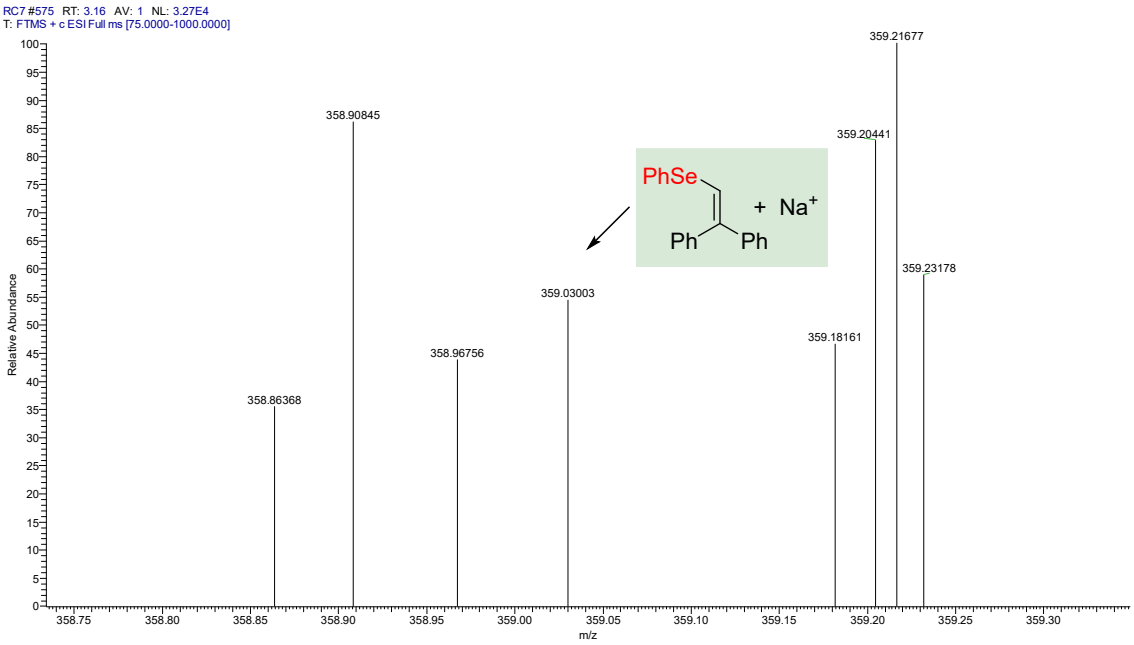


1a (0.20 mmol, 80.63 mg), TsSePh **2a** (0.26 mmol, 81.11 mg), 1,1-diphenylethylene (0.40 mmol, 108.2 mg) and DCE (3 mL) were placed in a 10 mL glass tube. The resulting mixture was allowed to stir at room temperature under 3 W blue LEDs irradiation for 12 hours and then monitored by TLC. We successfully detected the desired **7** and **8** by HRMS analysis. The residue was purified by column chromatography to give the corresponding product **3a** in 23% yield.

HRMS (ESI) calcd for $C_{21}H_{18}NaO_2S$ $[M+Na]^+$: 357.0920, found: 357.0912.

HRMS (ESI) calcd for $C_{20}H_{16}NaSe$ $[M+Na]^+$: 359.0309, found: 359.0300.





4. Effect of Visible Light Irradiation Experimental procedure.

In 10 mL glass tube equipped with a magnetic stir bar, **1a** (0.20 mmol), **2a** (0.26 mmol) and benzotrifluoride (0.20 mmol, as the internal standard) were added in DCE (2.0 mL). Then the mixture was stirred and irradiated by two 3 W blue LEDs at room temperature. After 1.0 h, the blue LEDs were turned off, and the glass tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The remaining mixture was stirred in the absence of light for an additional 1.0 h. Then, the glass tube was taken from the irradiation device and 0.2 mL of the mixture was taken out for analysis, and the blue LEDs were turned back on to irradiate the residual mixture. After an additional 1.0 h of irradiation, the blue LEDs were turned off, and the

glass tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The remaining mixture was stirred in the absence of light for an additional 1.0 h. Then, glass tube was removed for analysis, and the blue LEDs were turned back on to irradiate the residual mixture. After 1.0 h, the blue LEDs were turned off, and the glass tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The remaining mixture was stirred in the absence of light for an additional 1.0 h, and then it was analyzed. The yield was determined by ^{19}F NMR spectroscopy using benzotrifluoride as the internal standard.

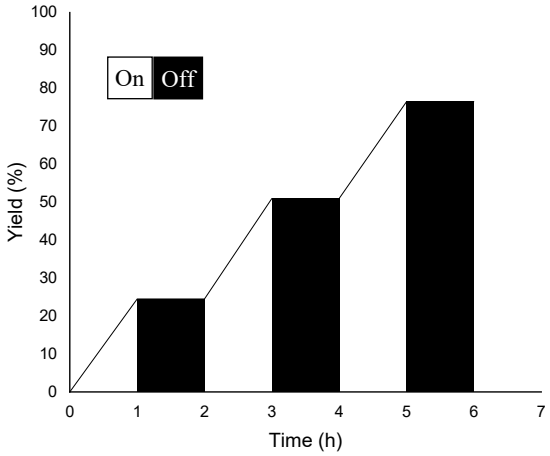


Fig 2. Light on/ off experiment

5. Calculation of apparent quantum efficiency (A. Q. E)

Experimental procedure:

In 25 mL glass tube equipped with a magnetic stir bar, **1a** (0.10 mmol), **2d** (0.26 mmol) and benzotrifluoride (0.20 mmol, as the internal standard) were added in DCE (1.0 mL). Then the mixture was stirred and irradiated by two 3 W blue LEDs at room temperature. After 1.0 h, the blue LEDs were turned off, and the glass tube was taken from the irradiation device and 0.2 ml of the mixture was taken out for analysis. The photon flux of the light source was determined by an optical power meter to be 162.03 mW (average of three experiments).

$$E_{photon} = \frac{hc}{\lambda_{inc\ (455\ nm)}} = \frac{6.63\ \times 10^{-34} J \cdot S \times 3 \times 10^{8} m \cdot s^{-1}}{455 \times 10^{-9} m} = 4.37 \times 10^{-19} J$$

$$E_{total} = P \cdot S \cdot t = 162.03 \times 10^{-3} W \cdot cm^{-3} \times 2.25\ cm^{2} \times 1.0 \times 3600\ s = 1.312 \times 10^{3} J$$

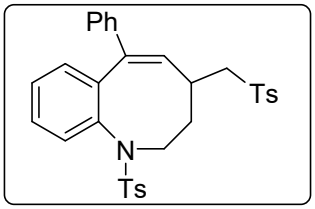
$$Number\ of\ incident\ photons = \frac{E_{total}}{E_{photon}} = 4.985\ mmol$$

$$A.Q.E(\%) = \frac{Number\ of\ product}{Number\ of\ incident\ photons} = \frac{0.0322\ mmol}{4.985\ mmol} = 0.65\% < 1$$

Where h (J·s) is Planck's constant, c ($m \cdot s^{-1}$) is the speed of light and λ_{inc} (m) is the wavelength of the incident light. P ($W \cdot cm^{-2}$) is the power density of the incident light, S (cm^2) is the irradiation area, and t (s) is the photoreaction time. The A.Q.E(%) result indicated that the reaction not involved radical chain pathway.

6. Products Characterization

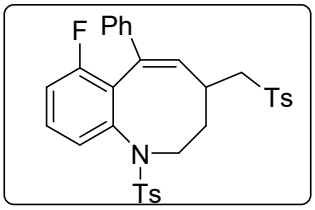
(*Z*)-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3a)



1a (0.30 mmol, 121.06 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3a** as a yellow solid (m. p. 93-94ºC) in 82% yield (137.20 mg).

R*f* (petroleum ether/ethyl acetate = 10:3): 0.10; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (t, J = 8.2 Hz, 4H), 7.29-7.25 (m, 2H), 7.23-7.17 (m, 9H), 7.11 (dd, J = 7.4, 1.6 Hz, 1H), 6.92 (d, J = 7.6 Hz, 1H), 5.85 (d, J = 8.5 Hz, 1H), 4.18 (dd, J = 14.7, 3.2 Hz, 1H), 3.36 (dd, J = 14.2, 8.9 Hz, 1H), 3.13 (dd, J = 14.3, 4.7 Hz, 1H), 2.96-2.87 (m, 1H), 2.37 (s, 3H), 2.33 (s, 3H), 2.29-2.25 (m, 1H), 1.84-1.77 (m, 1H), 1.59 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.76, 143.38, 141.56, 141.47, 140.19, 138.60, 137.55, 136.29, 130.86, 130.53, 129.93, 129.55, 129.25, 128.63, 128.59, 128.37, 128.10, 127.92, 127.66, 127.43, 62.93, 50.19, 34.36, 33.31, 21.61, 21.56; **HRMS** (ESI) calcd for $C_{32}H_{31}NNaO_4S_2[M+Na]^+$: 580.1587, found: 580.1579.

(*Z*)-7-fluoro-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (**3b**)

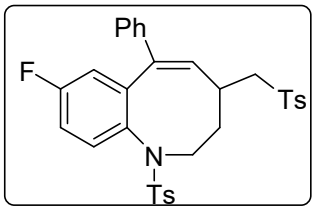


1b (0.30 mmol, 126.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3b** as a yellow solid (m. p. 102-103ºC) in 74% yield (127.81 mg).

R*f* (petroleum ether/ethyl acetate = 5:2): 0.37; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 (d, J = 8.1 Hz, 2H), 7.59 (d, J = 8.1 Hz, 2H), 7.33-7.14 (m, 8H), 7.13-7.05 (m, 3H), 6.84 (d, J = 8.0 Hz, 1H), 5.86 (d, J = 8.7 Hz, 1H), 4.16 (dd, J = 14.9, 3.4 Hz, 1H), 3.39 (dd, J = 14.3, 9.3 Hz, 1H), 3.13 (dd, J = 14.4, 4.3 Hz, 1H), 2.90 (dd, J = 19.9, 7.6 Hz, 1H), 2.37 (s, 3H), 2.36 (s, 3H), 2.29-2.22 (m, 1H),

1.72 (s, 1H), 1.56 (d, J = 13.7 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.48, 159.48, 144.83, 143.67, 142.26 (d, J = 5.9 Hz), 140.05, 137.16, 135.99, 133.90, 132.50, 130.12 (d, J = 9.7 Hz), 130.02, 129.60, 129.16 (d, J = 15.0 Hz), 128.15 (d, J = 38.0 Hz), 127.75, 127.53, 127.04, 124.65 (d, J = 3.0 Hz), 116.40, 62.75, 50.35, 34.70, 33.23, 21.63, 21.55; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -105.38; **HRMS** (ESI) calcd for $C_{32}H_{30}FNNaO_4S_2[M+Na]^+$: 598.1492, found: 598.1483.

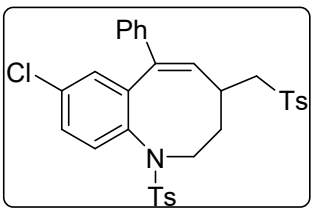
(*Z*)-8-fluoro-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (**3c**)



1c (0.30 mmol, 126.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3c** as a yellow solid (m. p. 151-152^{o}C) in 73% yield (125.8 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.17; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (dd, J = 19.2, 8.1 Hz, 4H), 7.28-7.19 (m, 9H), 6.98-6.87 (m, 2H), 6.78 (dd, J = 9.0, 2.8 Hz, 1H), 5.89 (d, J = 8.6 Hz, 1H), 4.20 (dd, J = 14.7, 3.3 Hz, 1H), 3.36 (dd, J = 14.2, 8.8 Hz, 1H), 3.15 (dd, J = 14.2, 4.9 Hz, 1H), 2.93-2.85 (m, 1H), 2.39 (s, 3H), 2.37 (s, 3H), 2.25-2.18 (m, 1H), 1.85-1.76 (m, 1H), 1.64 (d, J = 5.1 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.61, 160.62, 144.93, 143.78 (d, J = 8.6 Hz), 143.55, 140.70, 137.96, 137.27, 136.23 (d, J = 3.0 Hz), 136.10, 130.96, 130.35 (d, J = 9.0 Hz), 129.91, 129.61, 128.56, 128.08, 127.72, 127.62, 117.33 (d, J = 22.3 Hz), 116.28 (d, J = 22.7 Hz) 62.70, 50.19, 34.34, 33.06, 21.55; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -111.71; **HRMS (ESI)** calcd for $C_{32}H_{30}FNNaO_4S_2[M+Na]^+$: 598.1492, found: 598.1485.

(*Z*)-8-chloro-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3d)

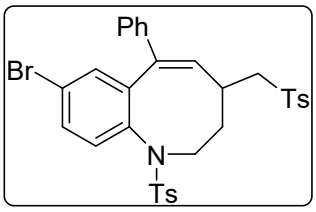


1d (0.30 mmol, 126.9 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether:

ethyl acetate = 10:3) to afford the compound **3d** as a yellow solid (m. p. 126-127°C) in 75% yield (133.24 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.17; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (dd, J = 14.2, 8.2 Hz, 4H), 7.29-7.17 (m, 10H), 7.09 (d, J = 2.4 Hz, 1H), 6.85 (d, J = 8.5 Hz, 1H), 5.94 (d, J = 8.6 Hz, 1H), 4.19 (dd, J = 14.7, 3.3 Hz, 1H), 3.36 (dd, J = 14.2, 9.0 Hz, 1H), 3.15 (dd, J = 14.2, 4.8 Hz, 1H), 2.91-2.81 (m, 1H), 2.39 (s, 3H), 2.38 (s, 3H), 2.14-2.08 (m, 1H), 1.83-1.75 (m, 1H), 1.62 (d, J = 15.7 Hz, 1H); **^{13}CNMR** (126 MHz, $CDCl_3$) δ 144.96, 143.62, 143.25, 140.73, 138.74, 137.70, 137.20, 135.82, 134.10, 131.22, 130.74, 129.98, 129.92, 129.63, 129.36, 128.61, 128.16, 128.12, 127.77, 127.63, 62.64, 50.11, 34.39, 32.98, 21.61, 21.56; **HRMS** (ESI) calcd for $C_{32}H_{30}ClNaO_4S_2[M+Na]^+$: 614.1197, found: 614.1189.

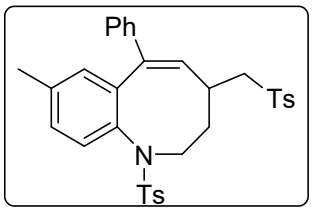
(*Z*)-8-bromo-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3e)



1e (0.30 mmol, 144.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3e** as a yellow solid (m. p. 122-123°C) in 80% yield (172.8 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.38; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (dd, J = 14.5, 8.2 Hz, 4H), 7.37 (dd, J = 8.5, 2.3 Hz, 1H), 7.26 (dd, J = 11.4, 6.4 Hz, 8H), 7.20 (d, J = 8.0 Hz, 2H), 6.79 (d, J = 8.5 Hz, 1H), 5.95 (d, J = 8.6 Hz, 1H), 4.19 (dd, J = 14.7, 3.4 Hz, 1H), 3.36 (dd, J = 14.2, 9.0 Hz, 1H), 3.14 (dd, J = 14.2, 4.8 Hz, 1H), 2.90-2.81 (m, 1H), 2.40 (s, 6H), 2.14-2.05 (m, 1H), 1.84-1.74 (m, 1H), 1.61 (s, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.99, 143.63, 143.56, 140.74, 139.26, 137.61, 137.19, 135.76, 133.70, 132.34, 131.30, 130.27, 129.94, 129.62, 128.61, 128.18, 128.13, 127.79, 127.64, 122.23, 62.65, 50.06, 34.40, 32.98, 21.66, 21.56; **HRMS (ESI)** calcd for $C_{32}H_{30}BrNNaO_4S_2[M+Na]^+$: 658.0692, found: 658.0684.

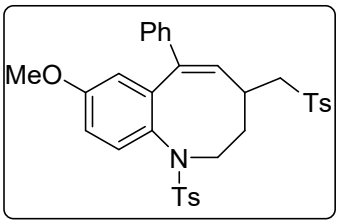
(*Z*)-8-methyl-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3f)



1f (0.30 mmol, 125.1 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3f** as a yellow solid (m. p. 84-85°C) in 75% yield (127.7 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.38; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, J = 15.3, 8.1 Hz, 4H), 7.24 (s, 4H), 7.19 (dd, J = 10.8, 8.3 Hz, 5H), 7.05 (dd, J = 8.1, 1.2 Hz, 1H), 6.91 (s, 1H), 6.79 (d, J = 8.1 Hz, 1H), 5.85 (d, J = 8.5 Hz, 1H), 4.17 (dd, J = 14.6, 3.3 Hz, 1H), 3.35 (dd, J = 14.2, 8.9 Hz, 1H), 3.13 (dd, J = 14.2, 4.8 Hz, 1H), 2.92-2.85 (m, 1H), 2.37 (s, 3H), 2.35 (s, 3H), 2.30 (s, 3H), 2.27-2.22 (m, 1H), 1.81-1.76 (m, 1H), 1.58 (d, J = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.70, 143.29, 141.62, 141.16, 138.66, 138.26, 137.69, 137.64, 136.30, 131.14, 130.46, 130.08, 129.86, 129.51, 128.67, 128.22, 128.17, 127.93, 127.65, 127.37, 62.88, 50.24, 34.30, 33.40, 21.63, 21.55, 21.23; **HRMS** (ESI) calcd for $C_{33}H_{33}NNaO_4S_2[M+Na]^+$: 594.1743, found: 594.1734.

(*Z*)-8-methoxy-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3g)

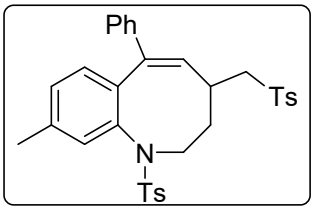


1g (0.30 mmol, 130.0 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3g** as a yellow solid (m. p. 84-85°C) in 72% yield (126.1 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.37; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, J = 20.6, 8.0 Hz, 4H), 7.25-7.17 (m, 9H), 6.83-6.76 (m, 2H), 6.58 (d, J = 2.4 Hz, 1H), 5.83 (d, J = 8.6 Hz, 1H), 4.19 (dd, J = 14.5, 3.2 Hz, 1H), 3.73 (s, 3H), 3.35 (dd, J = 14.1, 8.7 Hz, 1H), 3.14 (dd, J = 14.2, 4.8 Hz, 1H), 2.89 (t, J = 12.2 Hz, 1H), 2.38 (s, 3H), 2.35 (s, 3H), 2.30 (dd, J = 9.1, 4.8 Hz,

1H), 1.79 (td, J = 13.9, 4.5 Hz, 1H), 1.61 (d, J = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.91, 144.77, 143.25, 142.66, 141.18, 138.61, 137.61, 136.27, 133.11, 130.43, 129.88, 129.53, 129.49, 128.57, 128.15, 127.91, 127.62, 127.42, 115.60, 114.64, 62.91, 55.51, 50.35, 34.28, 33.42, 21.57, 21.54; **HRMS** (ESI) calcd for $C_{33}H_{33}NNaO_5S_2$[M+Na]$^+$: 610.1692, found: 610.1683.

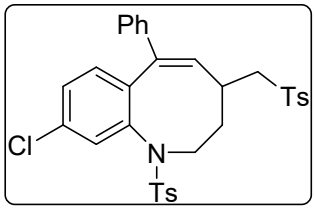
(*Z*)-9-methyl-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3h)



1h (0.30 mmol, 125.1 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3h** as a yellow solid (m. p. 117-118^{o}C) in 94% yield (161.2 mg).

R$_f$ (petroleum ether/ethyl acetate = 5:2): 0.34; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (dd, J = 15.5, 8.1 Hz, 4H), 7.23-7.16 (m, 9H), 7.11 (d, J = 7.7 Hz, 1H), 6.99 (d, J = 7.8 Hz, 1H), 6.75 (s, 1H), 5.77 (d, J = 8.5 Hz, 1H), 4.16 (dd, J = 14.6, 3.1 Hz, 1H), 3.35 (dd, J = 14.2, 8.8 Hz, 1H), 3.12 (dd, J = 14.2, 4.6 Hz, 1H), 2.97-2.88 (m, 1H), 2.37 (s, 3H), 2.34 (s, 3H), 2.28 (s, 4H), 1.74 (d, J = 12.6 Hz, 1H), 1.58 (d, J = 13.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.74, 143.35, 141.57, 139.98, 139.34, 138.62, 138.39, 137.57, 136.39, 130.53, 130.21, 129.92, 129.42, 129.28, 129.13, 128.55, 128.12, 127.89, 127.74, 127.36, 63.00, 50.03, 34.35, 33.42, 21.62, 21.55, 21.03; **HRMS** (ESI) calcd for $C_{33}H_{33}NNaO_4S_2$[M+Na]$^+$: 594.1743, found:594.1737.

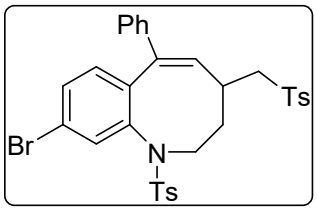
(*Z*)-9-chloro-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3i)



1i (0.30 mmol, 131.7 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3i** as a yellow solid (m. p. 62-63^{o}C) in 78% yield (138.6 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.15; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, J = 10.0, 8.4 Hz, 4H), 7.28 (dd, J = 8.3, 1.9 Hz, 1H), 7.26-7.18 (m, 9H), 7.06 (d, J = 8.3 Hz, 1H), 6.93 (d, J = 1.8 Hz, 1H), 5.87 (d, J = 8.6 Hz, 1H), 4.16 (dd, J = 14.7, 3.2 Hz, 1H), 3.35 (dd, J = 14.1, 8.8 Hz, 1H), 3.14 (dd, J = 14.2, 4.8 Hz, 1H), 2.93-85 (m, 1H), 2.40 (s, 3H), 2.37 (s, 3H), 2.27-2.21 (m, 1H), 1.84-1.74 (m, 1H), 1.61 (d, J = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.87, 143.77, 141.10, 141.00, 140.25, 137.74, 137.04, 136.30, 134.06, 131.88, 130.97, 129.94, 129.67, 128.87, 128.78, 128.56, 128.06, 128.02, 127.66, 62.71, 50.04, 34.35, 33.02, 21.62, 21.58; **HRMS (ESI)** calcd for $C_{32}H_{30}ClNNaO_4S_2[M+Na]^+$: 614.1197, found: 614.1190.

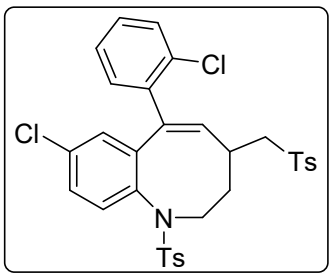
(*Z*)-9-bromo-6-phenyl-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3j)



1j (0.30 mmol, 145.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3j** as a yellow solid (m. p. 100-101^{o}C) in 75% yield (143.2 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, J = 10.5, 8.3 Hz, 4H), 7.43 (dd, J = 8.3, 1.7 Hz, 1H), 7.26-7.19 (m, 9H), 7.06 (d, J = 1.6 Hz, 1H), 7.00 (d, J = 8.3 Hz, 1H), 5.87 (d, J = 8.6 Hz, 1H), 4.16 (dd, J = 14.7, 3.2 Hz, 1H), 3.35 (dd, J = 14.1, 8.7 Hz, 1H), 3.14 (dd, J = 14.2, 4.8 Hz, 1H), 2.93-2.85 (m, 1H), 2.40 (s, 3H), 2.38 (s, 3H), 2.28-2.21 (m, 1H), 1.83-1.74 (m, 1H), 1.62 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.87, 143.78, 141.26, 140.92, 140.72, 137.80, 137.00, 136.29, 132.12, 131.82, 131.66, 130.95, 129.94, 129.66, 128.56, 128.06, 128.02, 127.67, 121.82, 62.71, 50.04, 34.35, 32.98, 21.63, 21.58; **HRMS** (ESI) calcd for $C_{32}H_{30}NNaO_4S_2[M+Na]^+$: 658.0692, found: 658.0687.

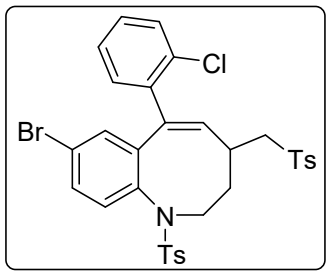
(*E*)-8-chloro-6-(2-chlorophenyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3k)



1k (0.30 mmol, 141.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3k** as a yellow solid (m. p. 104-105°C) in 77% yield (144.7 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.37; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 7.3 Hz, 2H), 7.54 (d, J = 15.6 Hz, 1H), 7.43-7.40 (m, 1H), 7.29 (dd, J = 28.2, 7.5 Hz, 5H), 7.18 (dd, J = 6.2, 2.5 Hz, 3H), 6.91 (d, J = 2.4 Hz, 1H), 6.78 (d, J = 8.5 Hz, 1H), 5.73 (d, J = 8.1 Hz, 1H), 4.22 (s, 1H), 3.33-3.18 (m, 2H), 2.94 (s, 1H), 2.44 (m, 7H), 2.14 (d, J = 13.8 Hz, 1H), 1.89-1.79 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.94, 143.87, 142.90, 139.81, 137.90, 137.00, 136.35, 136.20, 134.41, 132.88, 132.78, 132.57, 130.23, 129.94, 129.84, 129.73, 129.37, 129.27, 128.80, 127.79, 127.76, 127.03, 60.48, 50.49, 34.32, 31.11, 21.66, 21.61; **HRMS (ESI)** calcd for $C_{32}H_{29}Cl_2NNaO_4S_2[M+Na]^+$: 648.0807, found: 648.0809.

(*E*)-8-bromo-6-(2-chlorophenyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3l)

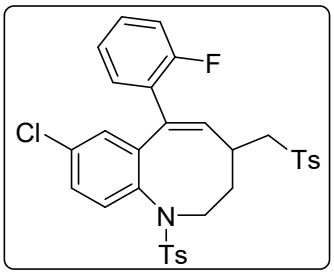


1l (0.30 mmol, 154.5 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3l** as a yellow solid (m. p. 113-114°C) in 71% yield 142.1 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.23; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73-7.54 (m, 5H), 7.43-7.39 (m, 1H), 7.29 (dd, J = 24.9, 8.6 Hz, 5H), 7.20-7.16 (m, 2H), 7.06 (d, J = 2.3 Hz, 1H),

6.71 (d, J = 8.5 Hz, 1H), 5.73 (d, J = 8.1 Hz, 1H), 4.22 (s, 1H), 3.32-3.18 (m, 2H), 2.93 (s, 1H), 2.45 (m, 7H), 2.14 (d, J = 13.8 Hz, 1H), 1.83 (d, J = 10.2 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.96, 143.89, 143.20, 139.78, 138.44, 136.98, 136.35, 136.30, 133.17, 132.88, 132.59, 132.27, 129.96, 129.85, 129.75, 129.66, 128.81, 127.79, 127.76, 127.04, 122.55, 60.52, 50.49, 34.28, 31.18, 21.71, 21.61; **HRMS (ESI)** calcd for $C_{32}H_{30}BrClNO_4S_2[M+H]^+$: 670.0483, found: 670.0480.

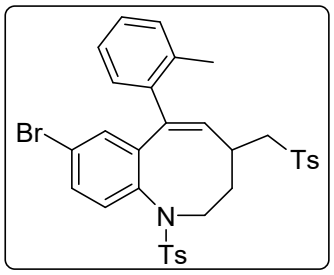
(*E*)-8-chloro-6-(2-fluorophenyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3m)



1m (0.30 mmol, 136.5 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3m** as a yellow solid (m. p. 103-104^{o}C) in 67% yield (122.3 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (t, J = 6.9 Hz, 4H), 7.26-7.20 (m, 7H), 7.08-6.99 (m, 3H), 6.84 (d, J = 8.5 Hz, 1H), 5.99 (d, J = 8.6 Hz, 1H), 4.21 (d, J = 13.5 Hz, 1H), 3.29-3.18 (m, 2H), 2.91 (t, J = 12.6 Hz, 1H), 2.41 (s, 3H), 2.39 (s, 3H), 2.31 (t, J = 15.0 Hz, 1H), 1.93 (d, J = 13.4 Hz, 1H), 1.83-1.75 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.29, 159.31, 144.91, 143.71, 142.92, 138.61, 137.14, 136.14, 135.37 (d, J = 6.5 Hz), 134.28, 132.59, 130.85, 130.32, 129.89, 129.69, 129.41, 129.12 (d, J = 8.5 Hz), 127.91, 127.66, 124.09 (d, J = 3.4 Hz), 115.85, 115.67, 61.81, 50.47, 34.25, 32.26, 21.62, 21.57; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -115.22; **HRMS** (ESI) calcd for $C_{32}H_{29}ClFNNaO_4S_2[M+Na]^+$: 632.1103, found: 632.1101.

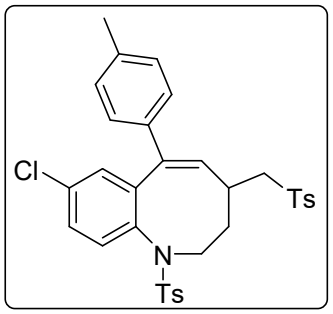
(*Z*)-8-bromo-6-(o-tolyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3n)



1n (0.30 mmol, 148.5 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3n** as a yellow solid (m. p. 124-125°C) in 62% yield (121.0 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.63 (d, J = 7.8 Hz, 2H), 7.39 (s, 1H), 7.35-7.09 (m, 9H), 7.01 (d, J = 1.9 Hz, 1H), 6.80 (d, J = 8.5 Hz, 1H), 5.57 (d, J = 7.8 Hz, 1H), 4.16 (s, 1H), 3.24 (s, 1H), 3.15 (dd, J = 14.1, 3.9 Hz, 1H), 2.92 (s, 1H), 2.43 (s, 3H), 2.41 (s, 3H), 2.35 (s, 3H), 1.92 (d, J = 13.3 Hz, 1H), 1.83-1.66 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.99, 143.94, 143.82, 141.22, 138.09, 136.85, 136.33, 135.58, 135.46, 134.46, 133.23, 132.08, 131.18, 130.56, 129.98, 129.83, 129.69, 127.97, 127.82, 127.48, 126.01, 122.41, 61.27, 50.22, 34.42, 31.29, 21.69, 21.61, 20.95; **HRMS** (ESI) calcd for $C_{33}H_{32}NNaO_4S_2[M+Na]^+$: 672.0848, found: 672.0845.

(*Z*)-8-chloro-6-(p-tolyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3o)

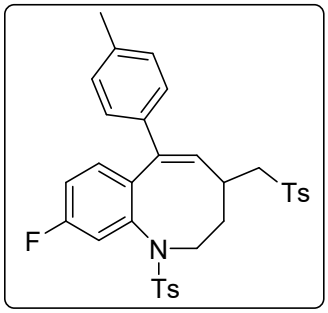


1o (0.30 mmol, 135.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3o** as a yellow solid (m. p. 124-125°C) in 73% yield (132.8 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.59 (dd, J = 11.3, 8.2 Hz, 4H), 7.24-7.14 (m, 7H), 7.08 (dd, J = 5.1, 2.4 Hz, 3H), 6.84 (d, J = 8.5 Hz, 1H), 5.90 (d, J = 8.6 Hz, 1H), 4.16 (dd, J = 14.7, 3.6 Hz, 1H), 3.34 (dd, J = 14.2, 9.0 Hz, 1H), 3.14 (dd, J = 14.2,

4.7 Hz, 1H), 2.88-2.80 (m, 1H), 2.39-2.32 (m, 9H), 2.06 (dd, *J* = 9.4, 4.7 Hz, 1H), 1.76 (d, *J* = 5.0 Hz, 1H), 1.57 (d, *J* = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.93, 143.61, 143.40, 138.73, 137.95, 137.55, 137.44, 137.22, 135.78, 134.01, 130.73, 130.42, 130.00, 129.91, 129.62, 129.28, 128.88, 128.47, 128.11, 127.62, 62.60, 50.12, 34.37, 32.97, 21.62, 21.55, 21.22; **HRMS** (ESI) calcd for $C_{33}H_{33}ClNO_4S_2[M+H]^+$:606.1534, found: 606.1532.

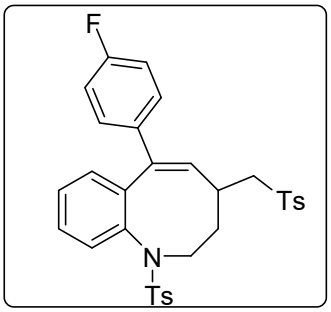
(*Z*)-9-fluoro-6-(p-tolyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3p)



1p (0.30 mmol, 131.1mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3p** as a yellow solid (m. p. 98-99^{o}C) in 61% yield (107.9 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.25; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 11.6, 8.2 Hz, 4H), 7.22 (t, *J* = 8.1 Hz, 4H), 7.11-7.00 (m, 6H), 6.67 (dd, *J* = 9.1, 2.4 Hz, 1H), 5.80 (d, *J* = 8.6 Hz, 1H), 4.16 (dd, *J* = 14.8, 3.2 Hz, 1H), 3.35 (dd, *J* = 14.2, 8.5 Hz, 1H), 3.14 (dd, *J* = 14.2, 5.0 Hz, 1H), 2.95-2.85 (m, 1H), 2.40 (s, 3H), 2.38 (s, 3H), 2.32 (s, 3H), 2.28-2.22 (m, 1H), 1.83-1.73 (m, 1H), 1.66 (s, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.12, 161.13, 144.79, 143.68, 141.22 (d, *J* = 9.2 Hz),138.38, 137.96 (d, *J* = 3.4 Hz), 137.67, 137.26 (d, *J* = 29.7 Hz), 136.40, 132.12 (d, *J* = 9.0 Hz), 129.91, 129.78, 129.65, 128.73, 128.37, 128.04, 127.66, 115.91 (d, *J* = 21.0 Hz), 115.50 (d, *J* = 21.1 Hz), 62.77, 50.06, 34.29, 33.21, 21.61, 21.55, 21.17; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -111.42; **HRMS (ESI)** calcd for $C_{33}H_{32}FNNaO_4S_2[M+Na]^+$: 612.1649, found: 612.1639.

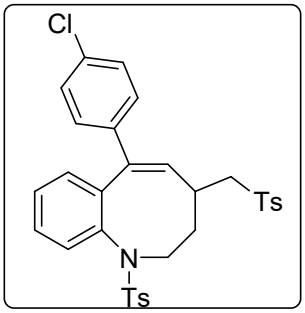
(*Z*)-6-(4-fluorophenyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (**3q**)



1q (0.30 mmol, 126.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3q** as a yellow solid (m. p. 88-89°C) in 73% yield (126.1 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.27; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (dd, J = 8.2, 2.6 Hz, 4H), 7.32-7.19 (m, 8H), 7.11 (dd, J = 7.6, 1.3 Hz, 1H), 6.94-6.86 (m, 3H), 5.85 (d, J = 8.5 Hz, 1H), 4.18 (dd, J = 14.7, 3.4 Hz, 1H), 3.38 (dd, J = 14.2, 9.3 Hz, 1H), 3.12 (dd, J = 14.2, 4.4 Hz, 1H), 2.95-2.86 (m, 1H), 2.39 (s, 3H), 2.34 (s, 3H), 2.28-2.21 (m, 1H), 1.86-1.81 (m, 1H), 1.57 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.38, 161.42, 144.77, 143.48, 141.51, 140.09, 137.76 (d, J = 2.8 Hz), 137.50 (d, J = 3.8 Hz), 136.23, 130.74, 130.59, 130.36 (d, J = 7.8 Hz), 129.92, 129.61, 129.37, 128.51 (d, J = 6.3 Hz), 127.96, 127.57, 124.17 (d, J = 954.9 Hz), 114.72 (d, J = 21.2 Hz), 62.88, 50.17, 34.34, 33.29, 21.59, 21.54; **HRMS** (ESI) calcd for $C_{32}H_{30}FNNaO_4S_2[M+Na]^+$: 598.1492, found: 598.1485.

(*Z*)-6-(4-chlorophenyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3r)

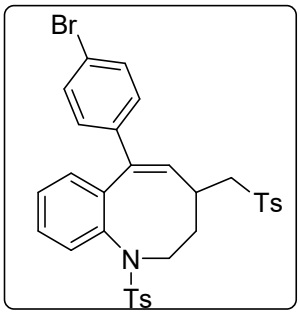


1r (0.30 mmol, 126.9 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3r** as a yellow solid (m. p. 88-89°C) in 71% yield (126.1 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.27; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (dd, J = 7.9,

6.2 Hz, 4H), 7.33-7.26 (m, 2H), 7.23-7.16 (m, 8H), 7.10 (dd, *J* = 7.5, 1.3 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 5.89 (d, *J* = 8.5 Hz, 1H), 4.18 (dd, *J* = 14.7, 3.5 Hz, 1H), 3.38 (dd, *J* = 14.2, 9.2 Hz, 1H), 3.12 (dd, *J* = 14.2, 4.4 Hz, 1H), 2.95-2.86 (m, 1H), 2.39 (s, 3H), 2.34 (s, 3H), 2.26 (dd, *J* = 10.5, 5.4 Hz, 1H), 1.90-1.81 (m, 1H), 1.58 (d, *J* = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.79, 143.49, 141.21, 140.17, 140.03, 137.46, 137.45, 136.25, 133.27, 131.14, 130.69, 129.96, 129.92, 129.60, 129.46, 128.61, 128.52, 128.06, 127.57, 62.83, 50.17, 34.37, 33.28, 21.61, 21.55; **HRMS** (ESI) calcd for $C_{32}H_{30}ClNNaO_4S_2[M+Na]^+$: 614.1197, found: 614.1191.

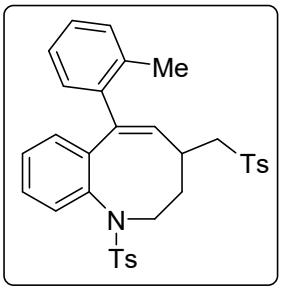
(*Z*)-6-(4-bromophenyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3s)



1s (0.30 mmol, 144.3 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3s** as a yellow solid (m. p. 82-83^{o}C) in 73% yield (139.4 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 13.3, 8.1 Hz, 4H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.34-7.25 (m, 2H), 7.25-7.21 (m, 4H), 7.10 (t, *J* = 9.0 Hz, 3H), 6.91 (d, *J* = 7.7 Hz, 1H), 5.88 (d, *J* = 8.5 Hz, 1H), 4.20 (dd, *J* = 14.6, 3.6 Hz, 1H), 3.37 (dd, *J* = 14.1, 9.1 Hz, 1H), 3.13 (dd, *J* = 14.1, 4.5 Hz, 1H), 2.92 (dd, *J* = 19.6, 7.5 Hz, 1H), 2.41 (s, 3H), 2.38 (s, 3H), 2.31 (dd, *J* = 9.8, 5.4 Hz, 1H), 1.92-1.82 (m, 1H), 1.60 (s, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.80, 143.46, 141.13, 140.37, 140.19, 137.66, 137.45, 136.36, 131.03, 130.71, 130.23, 129.92, 129.56, 129.47, 128.63, 128.52, 128.09, 127.60, 121.67, 62.88, 50.13, 34.34, 33.29, 21.63, 21.56.; **HRMS (ESI)** calcd for $C_{32}H_{30}BrNNaO_4S_2[M+Na]^+$: 658.0692, found:658.0684.

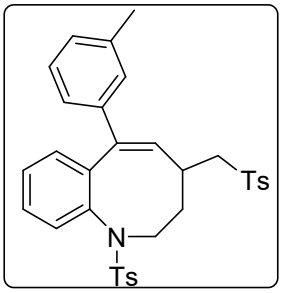
(*Z*)-6-(o-tolyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3t)



1t (0.30 mmol, 125.1 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3t** as a yellow solid (m. p. 100-101°C) in 63% yield (108.1 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, J = 8.1 Hz, 2H), 7.66 (d, J = 8.1 Hz, 2H), 7.38 (s, 1H), 7.31 (d, J = 8.1 Hz, 2H), 7.28-7.24 (m, 2H), 7.20 (dd, J = 6.3, 2.5 Hz, 3H), 7.15 (dd, J = 10.4, 4.2 Hz, 1H), 7.10 (t, J = 7.3 Hz, 1H), 6.95-6.89 (m, 2H), 5.54 (d, J = 7.5 Hz, 1H), 4.16 (s, 1H), 3.28 (s, 1H), 3.15 (dd, J = 14.1, 3.9 Hz, 1H), 2.99 (s, 1H), 2.66 (s, 1H), 2.46-2.36 (m, 9H), 1.93 (d, J = 13.6 Hz, 1H), 1.84-1.76 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.76, 143.63, 141.74, 137.22, 136.71, 136.46, 135.55, 133.34, 131.20, 130.57, 130.32, 129.96, 129.70, 128.88, 128.43, 128.02, 127.93, 127.78, 127.14, 125.86, 61.19, 50.06, 34.24, 31.03, 21.63, 21.59, 20.88; **HRMS** (ESI) calcd for $C_{33}H_{33}NNaO_4S_2[M+Na]^+$: 594.1743, found: 594.1740.

(*Z*)-6-(m-tolyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3u)

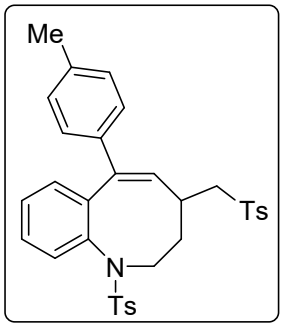


1u (0.30 mmol, 125.1 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3u** as a yellow solid (m. p. 83-84°C) in 89% yield (152.7 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.17; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65-7.60 (m, 4H),

7.31-7.25 (m, 3H), 7.21 (dd, J = 15.7, 8.0 Hz, 4H), 7.13-7.10 (m, 2H), 7.04 (d, J = 7.3 Hz, 1H), 7.01 (s, 1H), 6.96 (dd, J = 10.9, 4.4 Hz, 2H), 5.80 (d, J = 8.5 Hz, 1H), 4.19 (dd, J = 14.7, 3.0 Hz, 1H), 3.36 (dd, J = 14.2, 8.5 Hz, 1H), 3.14 (dd, J = 14.2, 4.9 Hz, 1H), 2.98-2.90 (m, 1H), 2.43 (dd, J = 11.1, 4.7 Hz, 1H), 2.39 (s, 3H), 2.36 (s, 3H), 2.30 (s, 3H), 1.84-1.75 (m, 1H), 1.63 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.72, 143.30, 141.58, 141.37, 140.16, 138.77, 137.56, 137.28, 136.38, 130.88, 130.27, 129.89, 129.48, 129.22, 128.98, 128.60, 128.33, 128.24, 128.14, 127.80, 127.72, 125.94, 63.00, 50.18, 34.30, 33.33, 21.62, 21.54, 21.52; **HRMS** (ESI) calcd for $C_{33}H_{33}NNaO_4S_2[M+Na]^+$: 594.1743, found:594.1733.

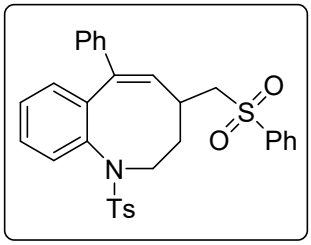
(*Z*)-6-(p-tolyl)-1-tosyl-4-(tosylmethyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (3v)



1v (0.30 mmol, 125.2 mg) was reacted with TsSePh **2a** (0.39 mmol, 121.67 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3v** as a yellow solid (m. p. 84-85^{o}C) in 70% yield (120.1 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.20; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dd, J = 11.4, 8.2 Hz, 4H), 7.30-7.18 (m, 7H), 7.12 (dd, J = 7.3, 1.7 Hz, 1H), 7.06 (q, J = 8.3 Hz, 4H), 6.93 (dd, J = 7.6, 1.0 Hz, 1H), 5.78 (d, J = 8.5 Hz, 1H), 4.19 (dd, J = 14.7, 3.2 Hz, 1H), 3.36 (dd, J = 14.2, 8.6 Hz, 1H), 3.13 (dd, J = 14.2, 4.9 Hz, 1H), 2.97-2.90 (m, 1H), 2.39 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H), 2.27 (dd, J = 9.0, 5.3 Hz, 1H), 1.83-1.75 (m, 1H), 1.61 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.70, 143.30, 141.68, 140.16, 138.58, 138.50, 137.59, 137.18, 136.37, 130.87, 129.90, 129.56, 129.49, 129.18, 128.64, 128.60, 128.43, 128.32, 128.11, 127.69, 62.98, 50.17, 34.28, 33.35, 21.62, 21.54, 21.19; **HRMS (ESI)** calcd for $C_{33}H_{33}NNaO_4S_2[M+Na]^+$: 594.1743, found: 594.1735.

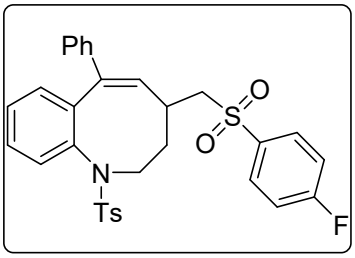
(*Z*)-6-phenyl-4-((phenylsulfonyl)methyl)-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine (3aa)



1a (0.30 mmol, 121.06 mg) was reacted with **2e** (0.39 mmol, 115.92 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3aa** as a white solid (m. p. 81-83°C) in 93% yield (151.7mg).

R_f (petroleum ether/ethyl acetate = 10:3): 0.11; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (t, J = 8.9 Hz, 2H), 7.62 (d, J = 8.1 Hz, 2H), 7.55 (t, J = 7.4 Hz, 1H), 7.43 (t, J = 7.7 Hz, 2H), 7.37-7.18 (m, 9H), 7.13 (dd, J = 7.4, 1.5 Hz, 1H), 6.94 (dd, J = 23.0, 7.0 Hz, 1H), 5.89 (d, J = 8.5 Hz, 1H), 4.20 (dd, J = 14.7, 3.1 Hz, 1H), 3.39 (dd, J = 14.2, 8.7 Hz, 1H), 3.16 (dd, J = 14.2, 5.0 Hz, 1H), 2.98-2.88 (m, 1H), 2.39 (s, 3H), 2.29 (dd, J = 9.6, 5.0 Hz, 1H), 1.88-1.79 (m, 1H), 1.63 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.36, 141.55, 141.49, 140.16, 139.26, 138.77, 137.55, 133.72, 130.92, 130.33, 129.53, 129.30, 128.67, 128.56, 128.44, 128.05, 127.97, 127.68, 127.49, 62.79, 50.18, 34.26, 33.24, 21.55; **HRMS** (ESI) calcd for $C_{31}H_{29}NNaO_4S_2[M+Na]^+$: 566.1430, found: 566.1424.

(*Z*)-4-(((4-fluorophenyl)sulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine (3ab)

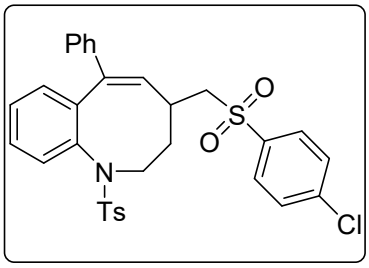


1a (0.30 mmol, 121.06 mg) was reacted with **2b** (0.33 mmol, 122.93 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3ab** as a yellow solid (m. p. 96-97°C) in 66% yield (111.2 mg).

R_f (petroleum ether/ethyl acetate = 10:3): 0.11; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (dd, J = 8.6, 5.0 Hz, 2H), 7.62 (d, J = 8.1 Hz, 2H), 7.33-7.20 (m, 9H), 7.14-7.07 (m, 3H), 6.92 (d, J = 7.6 Hz, 1H), 5.90 (d, J = 8.5 Hz, 1H), 4.21 (dd, J = 14.7, 3.2 Hz, 1H), 3.38 (dd, J = 14.2, 8.8 Hz, 1H), 3.15

(dd, *J* = 14.2, 4.9 Hz, 1H), 2.93 (t, *J* = 12.1 Hz, 1H), 2.40 (s, 3H), 2.25 (dd, *J* = 9.5, 4.9 Hz, 1H), 1.91-1.79 (m, 1H), 1.63 (s, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.78, 164.74, 143.40, 141.52, 141.33, 140.18, 138.84, 137.51, 135.23 (d, *J* = 3.1 Hz), 130.97 (d, *J* = 9.4 Hz), 130.81, 130.12, 129.55, 129.37, 128.62, 128.44, 128.03, 127.66, 127.59, 116.59 (d, *J* = 22.5 Hz), 62.89, 50.15, 34.35, 33.21, 21.55; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -103.32; **HRMS** (ESI) calcd for $C_{31}H_{28}FNNaO_4S_2[M+Na]^+$: 584.1336, found: 584.1327.

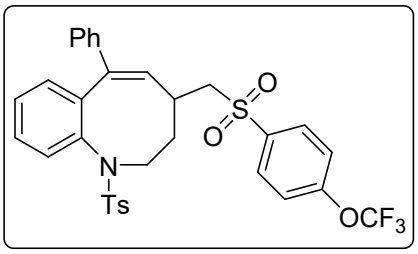
(*Z*)-4-(((4-chlorophenyl)sulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[b]azocine(3ac)



1a (0.30 mmol, 121.06 mg) was reacted with **2c** (0.39 mmol, 129.35 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3ac** as a yellow solid (m. p. 103-104^{o}C) in 75% yield (130.1 mg).

R_f (petroleum ether/ethyl acetate = 10:3): 0.11; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 35.7, 8.3 Hz, 4H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.32-7.19 (m, 9H), 7.13-7.08 (m, 1H), 6.92 (d, *J* = 7.5 Hz, 1H), 5.86 (d, *J* = 8.5 Hz, 1H), 4.21 (dd, *J* = 14.7, 3.2 Hz, 1H), 3.39 (dd, *J* = 14.2, 8.9 Hz, 1H), 3.16 (dd, *J* = 14.3, 4.7 Hz, 1H), 2.99-2.88 (m, 1H), 2.40 (s, 3H), 2.25 (dd, *J* = 9.5, 4.7 Hz, 1H), 1.92-1.78 (m, 1H), 1.62 (s, 1H).; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.39, 141.48, 141.22, 140.51, 140.17, 138.91, 137.63, 137.51, 130.76, 129.98, 129.62, 129.59, 129.55, 129.38, 128.61, 128.57, 128.46, 128.04, 127.66, 127.60, 62.83, 50.12, 34.36, 33.28, 21.55; **HRMS** (ESI) calcd for $C_{31}H_{28}ClNNaO_4S_2[M+Na]^+$: 600.1040, found: 600.1031.

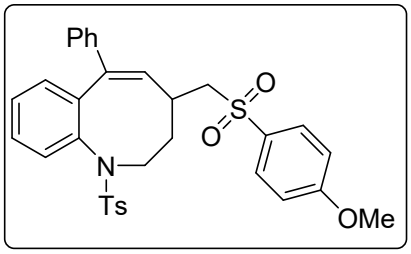
(*Z*)-6-phenyl-1-tosyl-4-(((4-(trifluoromethoxy)phenyl)sulfonyl)methyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine(3ad)



1a (0.30 mmol, 121.06 mg) was reacted with **2d** (0.39 mmol, 148.9 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3ad** as a yellow solid (m. p. 99-100°C) in 69% yield (129.9 mg).

R_f (petroleum ether/ethyl acetate = 10:3): 0.16; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 (d, J = 8.7 Hz, 2H), 7.61 (d, J = 8.1 Hz, 2H), 7.32-7.19 (m, 11H), 7.14-7.09 (m, 1H), 6.90 (d, J = 7.5 Hz, 1H), 5.93 (d, J = 8.5 Hz, 1H), 4.19 (dd, J = 14.7, 3.3 Hz, 1H), 3.40 (dd, J = 14.2, 9.1 Hz, 1H), 3.16 (dd, J = 14.3, 4.7 Hz, 1H), 2.94-2.85 (m, 1H), 2.38 (s, 3H), 2.26-2.16 (m, 1H), 1.89-1.79 (m, 1H), 1.59 (d, J = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.89, 143.44, 141.49, 141.34, 140.17, 138.81, 137.49, 137.25, 130.76, 130.44, 130.09, 129.58, 129.36, 128.62, 128.44, 128.05, 127.63, 127.60, 120.89, 120.14 (q, J = 259.9 Hz), 62.68, 50.14, 34.36, 33.17, 21.53; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -57.61; **HRMS** (ESI) calcd for $C_{32}H_{28}NNaO_5S_2[M+Na]^+$: 650.1253, found: 650.1243.

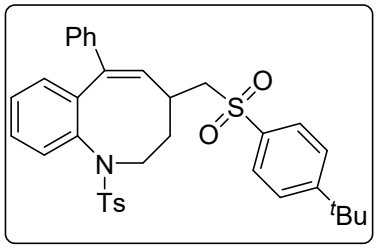
(*Z*)-4-(((4-methoxyphenyl)sulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine(3ae)



1a (0.30 mmol, 121.06 mg) was reacted with **2f** (0.39 mmol, 127.63 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3af** as a yellow solid (m. p. 97-98°C) in 77% yield (132.5 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (dd, J = 29.3, 8.4 Hz, 4H), 7.34-7.11 (m, 10H), 6.94 (d, J = 7.5 Hz, 1H), 6.87 (d, J = 8.8 Hz, 2H), 5.86 (d, J = 8.5 Hz, 1H), 4.20 (dd, J = 14.7, 3.2 Hz, 1H), 3.78 (s, 3H), 3.36 (dd, J = 14.2, 8.8 Hz, 1H), 3.13 (dd, J = 14.2, 4.7 Hz, 1H), 2.98-2.88 (m, 1H), 2.39 (s, 3H), 2.31-2.23 (m, 1H), 1.86-1.76 (m, 1H), 1.60 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.70, 143.36, 141.58, 141.41, 140.21, 138.60, 137.54, 130.87, 130.73, 130.52, 130.27, 129.52, 129.26, 128.61, 128.38, 127.92, 127.67, 127.45, 114.47, 63.16, 55.66, 50.17, 34.41, 33.29, 21.55; **HRMS** (ESI) calcd for $C_{32}H_{31}NNaO_5S_2[M+Na]^+$: 596.1936, found: 596.1929.

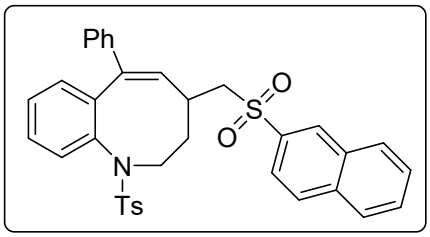
(*Z*)-4-(((4-(tert-butyl)phenyl)sulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine（3af）



1a (0.30 mmol, 121.06 mg) was reacted with **2g** (0.33 mmol, 116.82 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3ag** as a yellow solid (m. p. 98.6-99°C) in 70% yield (125.9 mg).

R$_f$ (petroleum ether/ethyl acetate = 10:3): 0.16; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (dd, J = 30.8, 8.3 Hz, 4H), 7.43 (d, J = 8.4 Hz, 2H), 7.30-7.18 (m, 9H), 7.13 (dd, J = 7.4, 1.4 Hz, 1H), 6.92 (d, J = 7.6 Hz, 1H), 5.91 (d, J = 8.5 Hz, 1H), 4.20 (dd, J = 14.7, 3.1 Hz, 1H), 3.37 (dd, J = 14.2, 8.8 Hz, 1H), 3.15 (dd, J = 14.2, 4.9 Hz, 1H), 2.97-2.88 (m, 1H), 2.38 (s, 3H), 2.28-2.20 (m, 1H), 1.86-1.77 (m, 1H), 1.62 (d, J = 13.6 Hz, 1H), 1.26 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.54, 143.35, 141.56, 141.53, 140.19, 138.63, 137.55, 136.08, 130.97, 130.50, 129.53, 129.19, 128.61, 128.59, 128.37, 128.01, 127.96, 127.69, 127.44, 126.30, 62.88, 50.17, 35.20, 34.30, 33.23, 31.02, 21.55; **HRMS** (ESI) calcd for $C_{35}H_{37}NNaO_4S_2[M+Na]^+$: 622.2056, found: 622.2048.

(*Z*)-4-((naphthalen-2-ylsulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine (3ag)

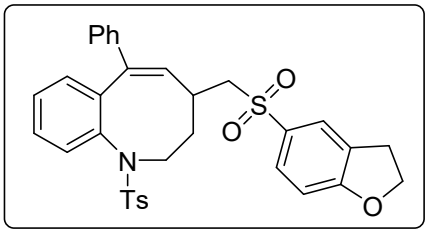


1a (0.30 mmol, 121.06 mg) was reacted with **2h** (0.39 mmol, 135.71 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3ag** as a yellow solid (m. p. 106-107°C) in 71% yield (126.5mg).

R$_f$ (petroleum ether/ethyl acetate = 10:3): 0.10; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.88-7.83 (m, 3H), 7.74-7.70 (m, 1H), 7.64-7.55 (m, 4H), 7.19-7.11 (m, 9H), 7.01-6.98 (m, 1H), 6.88 (d,

J = 7.7 Hz, 1H), 5.85 (d, *J* = 8.5 Hz, 1H), 4.18 (dd, *J* = 14.6, 3.3 Hz, 1H), 3.47 (dd, *J* = 14.3, 8.8 Hz, 1H), 3.24 (dd, *J* = 14.3, 4.8 Hz, 1H), 2.95-2.87 (m, 1H), 2.37 (s, 3H), 2.31 (dd, *J* = 9.5, 4.7 Hz, 1H), 1.88-1.77 (m, 1H), 1.62 (d, *J* = 13.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.35, 141.46, 141.32, 140.08, 138.77, 137.54, 136.14, 135.30, 132.13, 130.77, 130.25, 129.88, 129.65, 129.53, 129.44, 129.35, 129.21, 128.53, 128.49, 128.33, 127.99, 127.87, 127.72, 127.66, 127.38, 122.64, 62.87, 50.17, 34.35, 33.33, 21.55; **HRMS** (ESI) calcd for $C_{35}H_{31}NNaO_4S_2[M+Na]^+$: 616.1587, found: 616.1579.

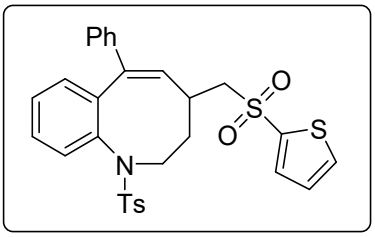
(*Z*)-4-(((2,3-dihydrobenzofuran-5-yl)sulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine(3ah)



1a (0.30 mmol, 121.06 mg) was reacted with **2i** (0.39 mmol, 132.31 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3ah** as a yellow solid (m. p. 101-102^{o}C) in 69% yield (121.2 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.36; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.34-7.16 (m, 9H), 7.12 (dd, *J* = 7.3, 1.5 Hz, 1H), 6.94 (d, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 8.2 Hz, 1H), 5.85 (d, *J* = 8.5 Hz, 1H), 4.62-52 (m, 2H), 4.20 (dd, *J* = 14.7, 3.2 Hz, 1H), 3.37 (dd, *J* = 14.2, 9.0 Hz, 1H), 3.12 (dd, *J* = 14.2, 4.7 Hz, 2H), 3.05-2.90 (m, 2H), 2.38 (s, 3H), 2.33-2.26 (m, 1H), 1.85-1.77 (m, 1H), 1.60 (d, *J* = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.69, 143.37, 141.60, 141.30, 140.27, 138.40, 137.54, 130.76, 130.72, 130.67, 129.84, 129.54, 129.28, 128.70, 128.65, 128.50, 128.41, 127.93, 127.65, 127.44, 125.38, 109.73, 72.41, 63.27, 50.18, 34.46, 33.33, 28.89, 21.55; **HRMS** (ESI) calcd for $C_{33}H_{32}O_5S_2[M+H]^+$: 586.1716, found: 586.1706.

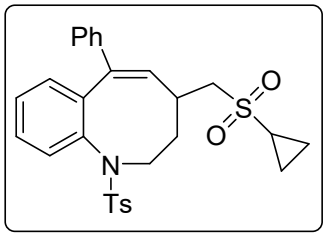
(*Z*)-6-phenyl-4-((thiophen-2-ylsulfonyl)methyl)-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine(3ai)



1a (0.30 mmol, 121.06 mg) was reacted with **2j** (0.39 mmol, 118.3 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3ai** as a yellow solid (m. p. 101-102°C) in 85% yield (164.9 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.38; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (d, J = 8.1 Hz, 2H), 7.57 (d, J = 4.8 Hz, 1H), 7.50 (d, J = 3.5 Hz, 1H), 7.34-7.18 (m, 9H), 7.12 (dd, J = 7.0, 1.9 Hz, 1H), 7.01-6.97 (m, 1H), 6.94-6.91 (m, 1H), 5.94 (d, J = 8.5 Hz, 1H), 4.21 (dd, J = 14.7, 3.3 Hz, 1H), 3.47 (dd, J = 14.2, 8.4 Hz, 1H), 3.27 (dd, J = 14.2, 5.1 Hz, 1H), 2.99-2.90 (m, 1H), 2.39 (s, 3H), 2.36-2.30 (m, 1H), 1.90-1.79 (m, 1H), 1.64 (d, J = 13.6 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.41, 141.53, 140.21, 140.18, 138.95, 137.53, 134.25, 134.20, 131.04, 130.06, 129.56, 129.31, 128.71, 128.54, 128.42, 128.01, 127.67, 127.52, 64.08, 50.23, 34.54, 33.14, 21.56; **HRMS** (ESI) calcd for $C_{29}H_{27}NNaO_4S_3[M+Na]^+$: 572.0994, found: 572.0988.

(Z)-4-((cyclopropylsulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine(3aj)

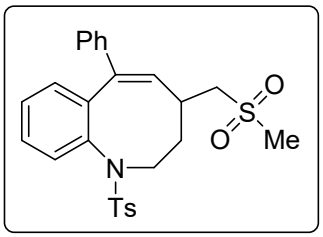


1a (0.30 mmol, 121.06 mg) was reacted with **2k** (0.39 mmol, 102.16 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 5:2) to afford the compound **3aj** as a yellow solid (m. p. 173-174°C) in 62% yield (94.4 mg).

R_f (petroleum ether/ethyl acetate = 5:2): 0.10; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (d, J = 8.0 Hz, 2H), 7.43-7.11 (m, 10H), 7.01-6.91 (m, 1H), 6.02 (d, J = 8.5 Hz, 1H), 4.24 (dd, J = 14.6, 3.1 Hz, 1H), 3.29 (dd, J = 13.9, 8.4 Hz, 1H), 3.12 (dd, J = 14.0, 5.5 Hz, 1H), 3.05-2.96 (m, 1H), 2.54 (dd, J = 15.8, 8.0 Hz, 1H), 2.39 (s, 3H), 2.25-2.20 (m, 1H), 1.91-1.81 (m, 1H), 1.74 (d, J = 12.2 Hz, 1H), 1.14-1.09 (m, 2H), 0.92-0.83 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.43, 141.64,

140.24, 138.66, 137.56, 130.87, 130.64, 129.59, 129.37, 128.66, 128.60, 128.08, 127.66, 127.51, 60.29, 50.31, 33.77, 33.09, 30.04, 21.57, 4.83, 4.60; **HRMS** (ESI) calcd for $C_{28}H_{29}NNaO_4S_2$[M+Na]$^+$: 530.1430, found: 530.1421.

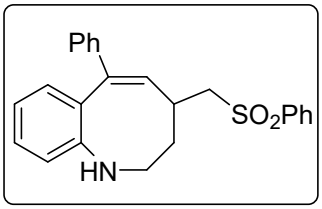
(*Z*)-4-((methylsulfonyl)methyl)-6-phenyl-1-tosyl-1,2,3,4-tetrahydrobenzo[*b*]azocine(3ak)



1a (0.30 mmol, 121.06 mg) was reacted with **2l** (0.39 mmol, 92.02 mg) according to General Procedure. The crude product was purified by column chromatography (petroleum ether: ethyl acetate = 10:3) to afford the compound **3ak** as a yellow solid (m. p. 173-174^{o}C) in 57% yield (82.4 mg).

R$_f$ (petroleum ether/ethyl acetate = 5:2): 0.10; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (d, J = 8.1 Hz, 2H), 7.39 (d, J = 7.0 Hz, 2H), 7.31-7.22 (m, 7H), 7.15 (dd, J = 6.3, 2.8 Hz, 1H), 6.94 (dd, J = 5.6, 3.3 Hz, 1H), 5.99 (d, J = 8.6 Hz, 1H), 4.25 (dd, J = 14.7, 3.1 Hz, 1H), 3.28 (dd, J = 13.9, 8.2 Hz, 1H), 3.10 (dd, J = 13.9, 5.6 Hz, 1H), 3.05-2.97 (m, 1H), 2.79 (s, 3H), 2.54-2.47 (m, 1H), 2.41 (s, 3H), 1.94-1.82 (m, 1H), 1.73 (d, J = 13.7 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.43, 141.54, 141.42, 140.23, 139.19, 137.54, 130.81, 130.00, 129.59, 129.47, 128.73, 128.63, 128.61, 128.11, 127.66, 61.06, 50.27, 41.72, 33.91, 33.09, 21.56; **HRMS** (ESI) calcd for $C_{26}H_{27}NNaO_4S_2$[M+Na]$^+$: 504.1274, found: 504.1266.

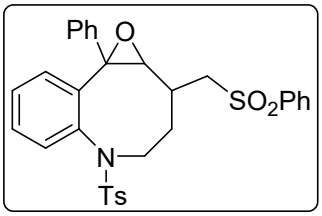
(*Z*)-6-phenyl-4-((phenylsulfonyl)methyl)-1,2,3,4-tetrahydrobenzo[*b*]azocine (4)



R$_f$ (petroleum ether/ethyl acetate = 5:2): 0.10; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (d, J = 7.4 Hz, 2H), 7.52 (t, J = 7.5 Hz, 1H), 7.36 (t, J = 7.8 Hz, 2H), 7.25 (dd, J = 9.3, 3.2 Hz, 3H), 7.17 (dd, J = 7.6, 1.7 Hz, 2H), 7.03-6.98 (m, 1H), 6.68 (dd, J = 7.8, 1.3 Hz, 1H), 6.57 (t, J = 7.3 Hz, 1H), 6.44 (d, J = 8.2 Hz, 1H), 5.28 (d, J = 9.4 Hz, 1H), 3.92-3.83 (m, 1H), 3.32 (dd, J = 14.3, 10.2 Hz, 1H), 3.20 (dd, J = 14.3, 3.3 Hz, 1H), 3.14-3.04 (m, 2H), 1.78-1.70 (m, 1H), 1.26 (s, 1H), 1.18 (t, J =

12.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 147.14, 143.83, 142.93, 138.49, 133.59, 133.51, 129.10, 128.73, 128.48, 128.19, 128.09, 128.05, 127.12, 121.14, 117.46, 116.64, 61.94, 40.91, 33.13, 31.10; **HRMS** (ESI) calcd for $C_{24}H_{24}NO_2S[M+H]^+$: 390.1522, found: 390.1515.

9b-phenyl-2-((phenylsulfonyl)methyl)-5-tosyl-1a,2,3,4,5,9b-hexahydrobenzo[*b*]oxireno[2,3-*d*]azocine (5)



R_f (petroleum ether/ethyl acetate = 5:2): 0.10; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (dd, J = 18.3, 7.9 Hz, 2H), 7.57 (t, J = 7.5 Hz, 1H), 7.47-7.39 (m, 7H), 7.28 (dd, J = 8.9, 3.7 Hz, 5H), 7.25-7.22 (m, 1H), 7.16 (d, J = 8.1 Hz, 2H), 4.11-4.03 (m, 1H), 3.40-3.33 (m, 1H), 3.25 (d, J = 8.6 Hz, 1H), 3.14-3.01 (m, 2H), 2.39 (s, 3H), 2.13 (d, J = 13.8 Hz, 1H), 1.71-1.57 (m, 2H).; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.92, 141.24, 139.29, 138.79, 137.62, 136.52, 133.78, 131.85, 130.30, 129.63, 129.49, 129.31, 128.50, 128.26, 128.20, 128.00, 127.71, 127.59, 68.92, 65.56, 58.37, 53.60, 36.29, 30.40, 21.55; **HRMS** (ESI) calcd for $C_{31}H_{29}NNaO_5S_2[M+Na]^+$: 582.1379, found: 582.1379.

7. DFT Caculations

AAll density functional theory (DFT) calculations were carried out with the Gaussian 16 programs[1] by using the hybrid density functional M06-2X[2], in combination with the Def2-SVP[3]

basis set for all atoms. All geometries have been fully optimized with no constraints of freedom. Vibrational analyses at the same theoretical level were performed to confirm each stationary point to be either a local minimum or a transition state (TS). The transition states were further verified by intrinsic reaction coordinate (IRC)[4] calculations. The solvent effect of dichloroethane (ε = 10.125) was simulated by performing the self-consistent reaction field (SCRF) of the SMD[5] method of Truhlar and Cramer at the same computational level. The energy unit of all structures was kcal/mol. All 3D structures were generated using CYLview.[6]

References:

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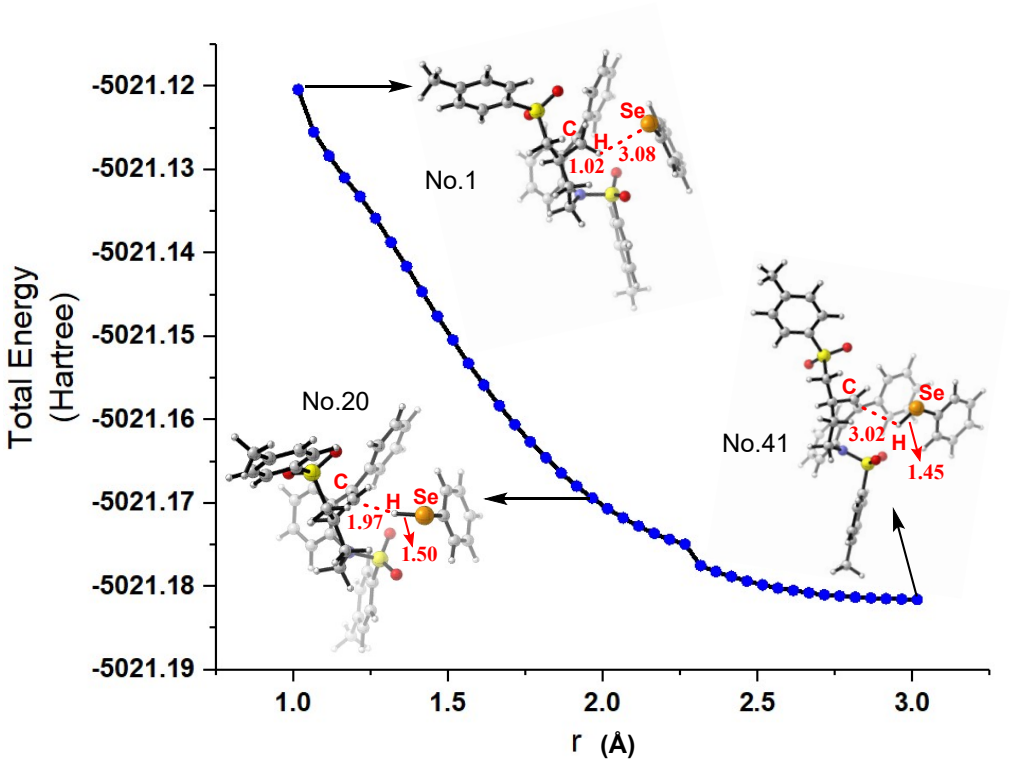


Figure S1. The energy profile (total energy) along the distance of C–H within the **INT-3** from a relaxed scan (41 points with 0.05 angstrom per step) in the deprotonation process using the $PhSe^-$.

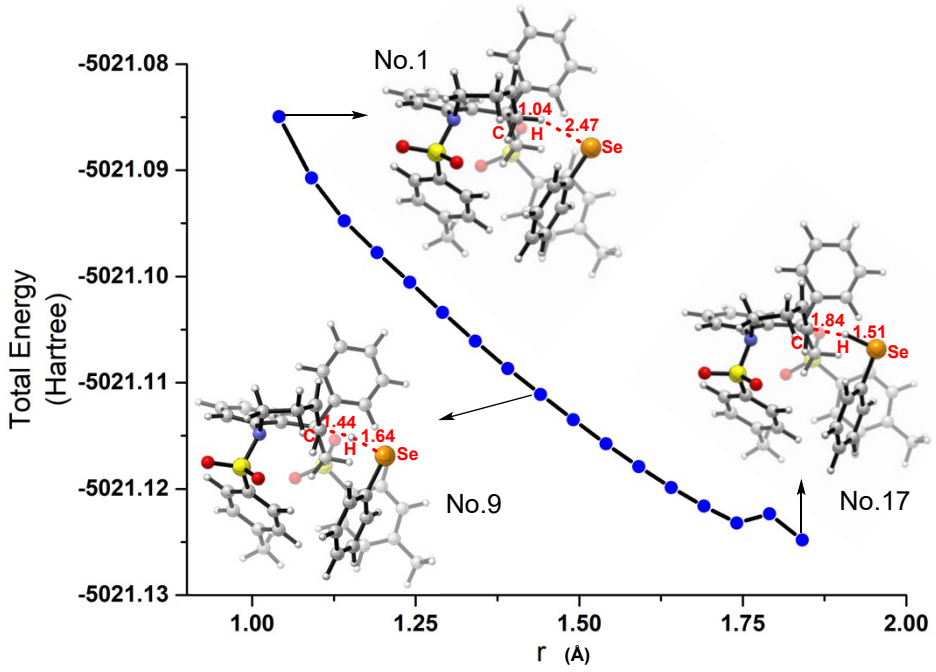


Figure S2. The energy profile (total energy) along the distance of C–H within the **INT-3'** from a relaxed scan (17 points with 0.05 angstrom per step) in the deprotonation process using the $PhSe^-$.

From the Figure S1 and S2, we can clearly see that the deprotonation process using the $PhSe^-$ is

barrierless.

Cartesian Coordinates and Thermochemical Data (Energies in Hartree)

1a

Number of imaginary frequencies: 0

C	-1.78685100	-2.69615800	2.44896700
C	-0.42848500	-2.42518700	2.62107600
C	0.22657500	-1.59534000	1.71605600
C	-0.45716500	-1.05812400	0.62033200
C	-1.82367200	-1.33688600	0.42857600
C	-2.47492200	-2.14562400	1.37125100
C	-2.58567900	-0.80035500	-0.73896600
C	-2.16695500	-1.04008400	-1.99053000
N	0.21773200	-0.16437700	-0.26378600
C	-0.03288300	1.27180000	-0.16425900
C	0.57132500	1.88957000	1.09858400
C	0.29209900	3.36151000	1.17301300
C	1.22629400	4.31170100	1.13224300
C	-3.80924500	-0.00027600	-0.44873200
C	-3.88943500	0.78207700	0.71471400
C	-5.01345700	1.56570500	0.97246300
C	-6.08451100	1.57180200	0.07858900
C	-6.02332600	0.78665600	-1.07397700
C	-4.89841300	0.00667000	-1.33422100
C	2.89430500	-0.36907900	-0.81252000
C	3.47330200	0.86190100	-1.11251900
C	4.72587200	1.16373400	-0.58003700
C	5.40526000	0.24922000	0.23435600
C	4.80207400	-0.98959900	0.50293600
C	3.55094700	-1.30712200	-0.01444400

C	6.76279500	0.56701500	0.79671900
S	1.26257600	-0.73196400	-1.41274300
O	1.06907600	0.05475900	-2.62311100
O	1.09739300	-2.17934200	-1.44482300
H	-2.31303900	-3.33695500	3.15833900
H	0.11600600	-2.84610200	3.46760800
H	1.28031000	-1.34380700	1.85112300
H	-3.53908900	-2.35428800	1.24007600
H	-2.69352500	-0.63137800	-2.85612300
H	-1.28483700	-1.65598900	-2.17772700
H	0.37788700	1.75236200	-1.06300300
H	-1.12324700	1.43732100	-0.19298400
H	1.65777300	1.70634500	1.11156500
H	0.13706100	1.38412100	1.97825800
H	-0.76390500	3.65058900	1.24320000
H	0.96537300	5.37181600	1.17676400
H	2.28876800	4.05783200	1.05726400
H	-3.05766100	0.78283200	1.42323900
H	-5.05209300	2.17337300	1.87829500
H	-6.96757300	2.17952100	0.28329400
H	-6.86267600	0.77309300	-1.77165800
H	-4.87099800	-0.62140100	-2.22666600
H	2.95405400	1.57129900	-1.75928800
H	5.18808300	2.12646900	-0.80756200
H	5.32695800	-1.71787400	1.12518500
H	3.08697100	-2.27414500	0.18712600
H	6.79006400	0.38409500	1.88059100
H	7.03770100	1.61294000	0.61021000
H	7.52944600	-0.07651200	0.33871000

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -1569.528467

Electronic Energy (0K) + ZPE = -1569.086209

Enthalpy (298K) = -1569.058137

Free Energy (298K) = -1569.148296

TS•

Number of imaginary frequencies: 0

C	-0.36268500	0.00115000	-0.10071800
C	0.30514000	1.22205500	-0.08096000
C	1.69626600	1.21124200	-0.01347900
C	2.41050900	0.00611200	0.01820300
C	1.69903200	-1.20367100	-0.01694200
C	0.31053200	-1.21950500	-0.08362900
C	3.91071600	-0.00229500	0.10492900
S	-2.14735200	-0.00207700	-0.23798400
O	-2.64930500	1.28104900	0.28639000
O	-2.64463400	-1.28474700	0.29213400
H	-0.25253400	2.15941000	-0.10402300
H	2.23860000	2.15837500	0.01439300
H	2.24540600	-2.14903900	0.00866900
H	-0.24463600	-2.15832200	-0.10818500
H	4.32695400	0.99806800	-0.06883700
H	4.23574100	-0.33844500	1.10182100
H	4.34255500	-0.69775800	-0.62870400

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -818.8804811

Electronic Energy (0K) + ZPE = -818.753395

Enthalpy (298K) = -818.743168

Free Energy (298K) =-818.789323

TS_1

Number of imaginary frequencies: 1

C	-5.46267800	0.23331200	-1.82900200
C	-4.65077000	1.34756300	-2.04663900
C	-3.45566300	1.47465600	-1.34460000
C	-3.07994400	0.51270000	-0.40065700
C	-3.89954500	-0.60646900	-0.16029200
C	-5.08057900	-0.73585900	-0.90538900
C	-3.55031800	-1.64309500	0.85759400
C	-3.32748600	-1.29485700	2.13362900
N	-1.82736200	0.63592100	0.27087900
C	-0.72491300	-0.24564400	-0.10179000
C	-0.19900900	0.04669400	-1.51512300
C	0.83706900	-0.94407800	-1.92397200
C	2.15877100	-0.62702500	-2.10997900
C	-3.45968000	-3.05603000	0.39195400
C	-3.03600800	-3.34968800	-0.91425000
C	-2.90470200	-4.66994600	-1.34277300
C	-3.20745800	-5.72168800	-0.47759400
C	-3.64445800	-5.44258200	0.81842800
C	-3.77175600	-4.12335900	1.24838300
C	-0.84467000	3.15389200	0.77130500
C	0.53589500	3.11800500	0.56433100
C	1.14652200	4.20982000	-0.04326100
C	0.40434800	5.33635400	-0.43272700
C	-0.97590100	5.34369700	-0.19832600
C	-1.61019800	4.25641400	0.40213400
C	1.09179900	6.51002600	-1.07344700
S	-1.63902300	1.73900500	1.49178100

O	-0.71280700	1.16547700	2.45684800
O	-2.97884500	2.13756900	1.90455900
H	-6.39631900	0.11755800	-2.38179800
H	-4.93912000	2.10806000	-2.77378500
H	-2.79017900	2.32155200	-1.52488500
H	-5.71497100	-1.60924200	-0.73816300
H	-3.04253200	-2.03617400	2.88388100
H	-3.42464200	-0.25580600	2.45558500
H	0.07488400	-0.13352400	0.64252000
H	-1.06951000	-1.29111400	-0.03278400
H	0.20558900	1.07053500	-1.55497300
H	-1.05162500	-0.00574700	-2.21562800
H	0.53506900	-1.99603300	-1.95784800
H	2.85374000	-1.38339500	-2.48630000
H	2.45552400	0.42013700	-2.23037800
H	-2.79848000	-2.53316400	-1.60031200
H	-2.56556100	-4.87704400	-2.35936300
H	-3.11122600	-6.75531100	-0.81434700
H	-3.89765000	-6.25852400	1.49776000
H	-4.13477700	-3.91527800	2.25659500
H	1.12811900	2.25115800	0.86733500
H	2.22563500	4.19127900	-0.21372400
H	-1.56497400	6.21659200	-0.48693900
H	-2.68503100	4.26346200	0.58948800
H	0.36914000	7.27377900	-1.38784900
H	1.66968700	6.19173500	-1.95345600
H	1.80001900	6.97389200	-0.37029100
C	4.68082800	-0.99887800	0.10572000
C	5.61003200	0.03037000	-0.02675100
C	6.96284100	-0.29753000	-0.08682600

C	7.38793700	-1.63125300	-0.02803800
C	6.42199100	-2.64303100	0.09542500
C	5.06702200	-2.33922600	0.15827000
C	8.84819900	-1.98368700	-0.08011000
S	2.94498500	-0.60908800	0.09701600
O	2.77850300	0.78771500	0.54506600
O	2.21805500	-1.67878000	0.79833100
H	5.27762500	1.06888800	-0.06585100
H	7.70454300	0.49840400	-0.17975400
H	6.74170100	-3.68622600	0.14558500
H	4.31558500	-3.12370300	0.26210800
H	9.46137600	-1.10946000	-0.33310500
H	9.18532200	-2.36841800	0.89469900
H	9.03481400	-2.77228100	-0.82312500

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4118704

Electronic Energy (0K) + ZPE = -2387.841521

Enthalpy (298K) = -2387.803400

Free Energy (298K) =-2387.919002

Int-1

Number of imaginary frequencies: 0

C	-5.21158800	0.79252100	-2.04347600
C	-4.23018300	1.77061900	-2.21009400
C	-3.08493600	1.73626200	-1.41989800
C	-2.92629700	0.75132900	-0.43863300
C	-3.91709000	-0.23133400	-0.25091200
C	-5.04525300	-0.20218300	-1.08364600
C	-3.80309200	-1.28853700	0.79916300
C	-3.61785800	-0.95498500	2.08513200

N	-1.72245100	0.70753800	0.32625600
C	-0.74033300	-0.33926700	0.05153000
C	-0.09000600	-0.19199900	-1.33382100
C	0.77881500	-1.35682000	-1.66083300
C	2.25228200	-1.27464800	-1.63346900
C	-3.90003700	-2.70795200	0.35460800
C	-3.43280500	-3.09111300	-0.91296300
C	-3.47641800	-4.42487400	-1.31690200
C	-4.00014600	-5.39888100	-0.46637300
C	-4.48226100	-5.02816200	0.79006200
C	-4.43507900	-3.69603200	1.19569800
C	-0.54276700	3.15842400	0.77178800
C	0.82075500	2.97999500	0.52800500
C	1.52651300	4.00783800	-0.08780300
C	0.89633300	5.20903200	-0.45159700
C	-0.46926900	5.35768800	-0.18250300
C	-1.19786900	4.33757500	0.42912200
C	1.68655000	6.31250100	-1.09861600
S	-1.45896600	1.83014000	1.51413200
O	-0.59881900	1.20707400	2.50869000
O	-2.76416900	2.35613700	1.89546100
H	-6.10829700	0.80196000	-2.66516400
H	-4.34739200	2.54856700	-2.96602900
H	-2.28966000	2.47140800	-1.56025100
H	-5.81169000	-0.97029400	-0.95763300
H	-3.50478100	-1.71826000	2.85865600
H	-3.57041400	0.09251900	2.39032200
H	0.02464600	-0.31054200	0.83863100
H	-1.24438600	-1.31731800	0.12666500
H	0.48460400	0.74715900	-1.36717000

H	-0.89900500	-0.11612900	-2.08286500
H	0.32194700	-2.34749700	-1.71459500
H	2.74219600	-2.17761800	-2.02158000
H	2.65818300	-0.37696500	-2.12608500
H	-3.02277000	-2.33589600	-1.58775800
H	-3.10006900	-4.70372100	-2.30279600
H	-4.04033200	-6.44209900	-0.78427100
H	-4.90750200	-5.78054600	1.45676300
H	-4.83402500	-3.41272400	2.17150100
H	1.32141100	2.04922100	0.80710000
H	2.59311900	3.87977600	-0.28732500
H	-0.97232000	6.28835200	-0.45303300
H	-2.26152400	4.45325000	0.64209800
H	1.03064900	7.11582200	-1.45779100
H	2.27170300	5.93046300	-1.94750100
H	2.39953300	6.74730800	-0.38136700
C	4.57342300	-1.33523900	0.05108500
C	5.38801100	-0.22158200	-0.13613000
C	6.76796500	-0.40503900	-0.19907800
C	7.33369000	-1.68033500	-0.07536700
C	6.48325600	-2.78110200	0.11615300
C	5.10412100	-2.61927400	0.18135600
C	8.82289700	-1.87767200	-0.12815400
S	2.81219500	-1.12405100	0.10066300
O	2.52840300	0.25064500	0.53416300
O	2.22599500	-2.23587000	0.85122200
H	4.94775300	0.77346000	-0.21973500
H	7.41932100	0.45940700	-0.34207800
H	6.91378000	-3.77939200	0.22114900
H	4.44162400	-3.47141000	0.34284100

H	9.34028700	-0.94828100	-0.39791300
H	9.20114100	-2.21090300	0.85030600
H	9.08854600	-2.65369000	-0.86050000

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4270668

Electronic Energy (0K) + ZPE = -2387.854749

Enthalpy (298K) = -2387.816910

Free Energy (298K) = -2387.930159

TS_2

Number of imaginary frequencies: 1

S	2.93357400	-1.30979600	0.95014600
S	-3.53843800	-0.10788900	0.15633400
O	2.91478600	-0.50909900	2.16624800
O	2.34500000	-2.64329100	0.93438000
N	2.14421100	-0.44074100	-0.22260600
C	2.44713100	0.95575300	-0.32988000
C	1.54653300	1.95034200	0.12300400
C	0.18190300	1.68366600	0.63566400
C	-0.87334400	2.70019400	0.36074700
C	-0.20820700	0.51465300	1.22897700
H	-1.21642100	0.44625300	1.64015700
C	3.65982900	1.31541100	-0.93087600
H	4.29938400	0.52422900	-1.32617000
C	1.97857700	3.28892800	0.01968000
H	1.32003800	4.07789500	0.38501300
C	-0.97320900	-0.75117500	-0.62611000
H	-1.05783800	0.11097200	-1.29579200
C	0.10516700	-1.74372800	-0.92782400
H	-0.22209100	-2.36224000	-1.78808900

H	0.23336900	-2.44119800	-0.08713000
C	4.62965600	-1.47570200	0.45476700
C	-1.84287500	3.00544000	1.32698400
H	-1.77967700	2.54073400	2.31234000
C	1.46148400	-1.15603600	-1.31024600
H	1.34120700	-0.42647200	-2.12366400
H	2.11010000	-1.95976000	-1.69361900
C	5.58405600	-0.60385100	0.97353100
H	5.29315400	0.14840700	1.70802400
C	-0.97533700	3.31680100	-0.89836400
H	-0.23684700	3.08852900	-1.67053600
C	4.05259900	2.64655900	-1.02909500
O	-3.46924100	0.90847500	-0.89475300
C	-2.87850200	3.89473000	1.04715800
H	-3.61893400	4.11966200	1.81729300
C	3.20886300	3.63638100	-0.52600000
H	3.50105600	4.68683600	-0.57173700
C	-2.27679800	-1.34890000	-0.20303200
H	-2.71261300	-1.95968900	-1.01626800
H	-2.19791600	-1.98389800	0.69309700
C	4.96961300	-2.45585000	-0.47957600
H	4.21278800	-3.14822000	-0.85208400
C	6.90150300	-0.70939200	0.53292700
H	7.65711700	-0.02996700	0.93248600
C	-2.96886200	4.49656700	-0.20732300
H	-3.78018400	5.19318500	-0.42660700
C	-7.46954300	-2.38021500	-0.32696800
C	-2.01223200	4.20250400	-1.18059600
H	-2.07681000	4.66223100	-2.16875500
C	-5.07225300	-0.99242800	-0.03056000

C	-5.70213800	-1.00175500	-1.27196700
H	-5.26340900	-0.46087400	-2.11216500
C	-6.90044200	-1.69941700	-1.41086000
H	-7.40730700	-1.71131000	-2.37783900
C	7.27248400	-1.67175300	-0.41519600
C	6.28900100	-2.54178800	-0.91133500
H	6.56699200	-3.30403700	-1.64244900
O	-3.44153600	0.28989700	1.56535400
C	-8.76354500	-3.13162600	-0.47298400
H	-9.52791500	-2.72170400	0.20389400
H	-9.14459500	-3.07564300	-1.50053600
H	-8.62960300	-4.19090900	-0.20801600
C	8.69859900	-1.79816900	-0.87357200
H	9.18271800	-2.65757900	-0.38384300
H	8.75113200	-1.96820900	-1.95794500
H	9.27817500	-0.89917200	-0.62724300
C	-6.81217300	-2.34450400	0.91271000
H	-7.25159000	-2.86361900	1.76744600
C	-5.61660400	-1.65186500	1.07134900
H	-5.11276300	-1.60944600	2.03836500
H	5.00599700	2.90471000	-1.49218200
H	0.51397600	-0.22804800	1.55849600

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4102725

Electronic Energy (0K) + ZPE = -2387.837462

Enthalpy (298K) = -2387.801081

Free Energy (298K) = -2387.909096

INT-2

Number of imaginary frequencies: 0

S	-2.96492100	-0.28883300	-1.20239400
S	3.52390800	0.00784300	-0.30904500
O	-3.00394800	1.16304400	-1.10843100
O	-2.58615000	-0.94320400	-2.44927000
N	-1.91096800	-0.83171200	-0.05244400
C	-1.72462300	-0.07663200	1.14264500
C	-0.84445900	1.03323900	1.15389400
C	-0.04084200	1.42620700	0.00387800
C	0.20794000	2.84982700	-0.22986600
C	0.47794700	0.42765100	-0.99867700
H	1.30438100	0.90314300	-1.54429000
C	-2.43466800	-0.45074500	2.28661300
H	-3.10463200	-1.31148800	2.22416900
C	-0.73944600	1.74744200	2.37101100
H	-0.05802800	2.59818800	2.42017000
C	0.93476400	-0.95303700	-0.45085600
H	0.91117100	-0.92275200	0.65029000
C	0.03807900	-2.10421800	-0.93231300
H	0.54264900	-3.07075400	-0.77810800
H	-0.13507000	-1.99382700	-2.01418500
C	-4.56216000	-0.90108300	-0.73082700
C	-0.79769200	3.80243400	0.04990200
H	-1.76026300	3.45781900	0.43185100
C	-1.29643500	-2.15489600	-0.19727700
H	-1.15285100	-2.54174700	0.82173600
H	-1.99596200	-2.83414100	-0.70637000
C	-5.32605200	-0.16848500	0.18110400
H	-4.96539200	0.79299200	0.55043700
C	1.42718400	3.32019700	-0.76303900
H	2.23962500	2.62035200	-0.96475600

C	-2.29984400	0.26432800	3.47338400
O	3.04077000	0.53701200	0.97069000
C	-0.59365900	5.15699600	-0.19037300
H	-1.39417900	5.86842300	0.02145000
C	-1.44738300	1.37245100	3.50510400
H	-1.32485000	1.94237400	4.42778800
C	2.37674500	-1.28093600	-0.84020200
H	2.71231900	-2.20645800	-0.35129800
H	2.52018200	-1.37445200	-1.92713000
C	-5.00947000	-2.11748300	-1.24123300
H	-4.40790800	-2.65866900	-1.97317900
C	-6.55097000	-0.68080600	0.59297400
H	-7.15871700	-0.11523000	1.30286800
C	0.62275400	5.60538900	-0.71137300
H	0.78397700	6.66850500	-0.89818500
C	7.46767600	-2.16167000	0.43747100
C	1.62873200	4.67909000	-0.99257300
H	2.58730300	5.01796700	-1.39030400
C	5.06188500	-0.83557400	-0.01832700
C	5.32704200	-1.34305100	1.25396300
H	4.60306400	-1.20826000	2.05937600
C	6.53011200	-2.00469400	1.47108400
H	6.75429400	-2.40350900	2.46295500
C	-7.02558200	-1.90891100	0.10495700
C	-6.24177300	-2.61284500	-0.81695300
H	-6.60470500	-3.56230400	-1.21561000
O	3.74040200	0.93794700	-1.42662400
C	8.76323600	-2.87836200	0.69757700
H	8.57604100	-3.90699100	1.03989400
H	9.38501900	-2.92011400	-0.20558100

H	9.33399000	-2.37127700	1.48969300
C	-8.35366800	-2.44183900	0.56597500
H	-9.15716800	-1.72141200	0.35291900
H	-8.59719200	-3.39057300	0.07113300
H	-8.34775800	-2.60925300	1.65349100
C	7.17260100	-1.63371900	-0.82545500
H	7.89761100	-1.74104900	-1.63472300
C	5.97220200	-0.96612800	-1.06303100
H	5.74823600	-0.54052700	-2.04252900
H	-2.85640500	-0.03525400	4.36239800
H	-0.29543900	0.26888000	-1.77212600

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4752678

Electronic Energy (0K) + ZPE = -2387.897872

Enthalpy (298K) = -2387.861831

Free Energy (298K) = -2387.969920

PhSe•

Number of imaginary frequencies: 0

C	-2.15995400	-1.20616600	-0.00001100
C	-0.76505800	-1.21346500	0.00002800
C	-0.06667700	-0.00010900	0.00003800
C	-0.76497100	1.21341900	0.00002000
C	-2.15977000	1.20626700	-0.00001200
C	-2.86135100	0.00005300	-0.00001500
H	-2.70121700	-2.15392600	-0.00001700
H	-0.22108200	-2.16041900	-0.00000300
H	-0.22075100	2.16023100	0.00001400
H	-2.70103700	2.15402500	-0.00000500

H	-3.95225500	0.00018200	-0.00002200
Se	1.83714800	-0.00000200	-0.00000700

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2632.6408929

Electronic Energy (0K) + ZPE = -2632.549798

Enthalpy (298K) = -2632.543181

Free Energy (298K) = -2632.581380

$PhSe^-$

Number of imaginary frequencies: 0

C	-2.18004000	-1.20201100	0.00002100
C	-0.78543200	-1.20229600	0.00001800
C	-0.05107100	-0.00002800	-0.00009200
C	-0.78541400	1.20228300	0.00000300
C	-2.17999700	1.20203800	0.00003600
C	-2.89066600	0.00001100	-0.00003200
H	-2.71683400	-2.15375500	0.00003300
H	-0.24495300	-2.15161100	0.00003700
H	-0.24486600	2.15155800	0.00002300
H	-2.71680300	2.15377500	0.00004800
H	-3.98207400	0.00004600	-0.00003900
Se	1.85709600	0.00000000	0.00000500

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -2632.8034562

Electronic Energy (0K) + ZPE = -2632.712891

Enthalpy (298K) = -2632.706249

Free Energy (298K) = -2632.743834

Int-3

Number of imaginary frequencies: 0

S	-2.94975800	-0.17343000	-1.13200800
S	3.41194400	0.02659200	-0.49642700
O	-2.84578100	1.24974500	-0.83224600
O	-2.66859400	-0.66847900	-2.47182000
N	-1.86639900	-0.93793700	-0.12798000
C	-1.53726200	-0.34364300	1.11692600
C	-0.67040000	0.77956300	1.16263000
C	-0.00856200	1.29351600	-0.02109400
C	0.17719300	2.71098100	-0.14556900
C	0.45270600	0.39415300	-1.10990200
H	1.21967300	0.92314500	-1.69298700
C	-2.09812000	-0.83476900	2.28854300
H	-2.78792700	-1.67853500	2.22948900
C	-0.38819400	1.37281000	2.41051600
H	0.30597200	2.21232900	2.45859800
C	0.89896100	-1.03824800	-0.72385700
H	0.88715700	-1.12294700	0.37334800
C	-0.02239900	-2.12008800	-1.30545000
H	0.48546600	-3.09588500	-1.29430400
H	-0.24978400	-1.88033000	-2.35510700
C	-4.55519900	-0.72753600	-0.64583800
C	-0.80925700	3.58461500	0.38237300
H	-1.70417800	3.16430200	0.84215100
C	-1.31302200	-2.24934000	-0.49944900
H	-1.12205700	-2.78407700	0.44154800
H	-2.07084800	-2.82142700	-1.05232400
C	-5.20738400	-0.07693600	0.40311500
H	-4.75319700	0.79185900	0.88265100
C	1.30376100	3.25628800	-0.81178300

H	2.10377000	2.60650600	-1.17004900
C	-1.78319200	-0.24950300	3.51948400
O	2.78995100	0.51519000	0.74410700
C	-0.67683000	4.95571500	0.23102900
H	-1.45254800	5.62283100	0.60766700
C	-0.92877800	0.84935700	3.58065900
H	-0.68029300	1.30155500	4.54098000
C	2.34604300	-1.28758600	-1.14456300
H	2.71410100	-2.23643100	-0.73093800
H	2.49487400	-1.28060000	-2.23419900
C	-5.12150800	-1.82413800	-1.29417100
H	-4.60050800	-2.30221300	-2.12506000
C	-6.45022100	-0.55034600	0.81069500
H	-6.97268100	-0.04997200	1.62856800
C	0.44967200	5.47777900	-0.41155200
H	0.55799800	6.55874500	-0.51779700
C	7.37352500	-1.97482200	0.51872600
C	1.44007900	4.63071800	-0.92125300
H	2.32404400	5.05044500	-1.40192500
C	4.95555200	-0.74476100	-0.09581700
C	5.14334900	-1.26599600	1.18486400
H	4.35606500	-1.17977100	1.93565300
C	6.35486300	-1.87943700	1.48081800
H	6.52080000	-2.28929100	2.47949600
C	-7.04814900	-1.65344700	0.18259200
C	-6.36737300	-2.27913700	-0.87089300
H	-6.82423900	-3.13447500	-1.37263500
O	3.65174300	0.99293300	-1.57815100
C	8.67744300	-2.63650100	0.86508800
H	8.50916100	-3.66010100	1.23056000

H	9.34596500	-2.68032400	-0.00380800
H	9.18824300	-2.08462400	1.66837800
C	-8.40864900	-2.12979900	0.60721100
H	-9.19068300	-1.57067700	0.06951200
H	-8.54639400	-3.19510800	0.38046400
H	-8.56857900	-1.96959200	1.68180600
C	7.15232000	-1.43414300	-0.75410600
H	7.94018700	-1.49502300	-1.50736300
C	5.94574400	-0.81383500	-1.07190800
H	5.77778500	-0.37985300	-2.05891600
H	-2.21889300	-0.65493700	4.43388500
H	-0.39745200	0.36541300	-1.82002800

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -2388.3081406

Electronic Energy (0K) + ZPE = -2387.729268

Enthalpy (298K) = -2387.693502

Free Energy (298K) = -2387.799154

PhSeH

Number of imaginary frequencies: 0

C	-2.20012400	-1.20200300	0.00001200
C	-0.80528700	-1.21827100	0.00001800
C	-0.09588900	-0.01255700	-0.00001000
C	-0.78903600	1.20356500	-0.00001100
C	-2.18338100	1.20868900	-0.00000900
C	-2.89463400	0.00802800	-0.00000400
H	-2.74587500	-2.14740300	0.00002300
H	-0.27011600	-2.16977300	0.00003400
H	-0.23964300	2.14762700	-0.00005200
H	-2.71599500	2.16149500	-0.00002900

H	-3.98567100	0.01536400	0.00000200
Se	1.81689100	0.04355200	0.00001500
H	1.99311800	-1.41277300	-0.00045700

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -2633.2645119

Electronic Energy (0K) + ZPE = -2633.165531

Enthalpy (298K) = -2633.158156

Free Energy (298K) = -2633.197160

3a

Number of imaginary frequencies: 0

S	-2.98064000	-0.19856000	-1.14721900
S	3.60599000	0.00823900	0.17650800
O	-3.14093300	1.22531000	-0.89175300
O	-2.55809200	-0.68252400	-2.45448300
N	-1.89685700	-0.77758500	-0.04497500
C	-1.69591500	-0.08078100	1.18421300
C	-0.80566900	1.00828800	1.25138600
C	-0.03836300	1.46097700	0.05966700
C	-0.08293300	2.91031900	-0.28030700
C	0.71175800	0.61314800	-0.66711100
H	1.20040900	1.00845100	-1.56414400
C	-2.39536400	-0.49893500	2.32142300
H	-3.07747200	-1.34745500	2.23463000
C	-0.65994600	1.66927700	2.47954400
H	0.02159800	2.52032300	2.54160200
C	1.03328900	-0.82157400	-0.33391600
H	0.92401200	-0.96940100	0.75289300
C	0.12273600	-1.83487300	-1.05639000
H	0.62727300	-2.81202600	-1.11391900

H	-0.06697300	-1.49599900	-2.08609900
C	-4.52605600	-0.98596500	-0.76199600
C	-1.26433200	3.65380100	-0.13440800
H	-2.16866600	3.15034600	0.21098400
C	-1.19822900	-2.03450400	-0.32798800
H	-1.02692300	-2.52462500	0.64176300
H	-1.86168200	-2.69122600	-0.90961300
C	-5.34535400	-0.42896400	0.22319600
H	-5.06060300	0.50534700	0.71016100
C	1.07456000	3.56004300	-0.73809500
H	2.00820400	2.99526100	-0.80484700
C	-2.22207500	0.15855800	3.53633500
O	3.20009500	0.04170000	1.58381600
C	-1.29236600	5.00789500	-0.46349000
H	-2.22133300	5.57116500	-0.35606500
C	-1.35238300	1.24797100	3.61180600
H	-1.21036600	1.77091200	4.55899100
C	2.49366500	-1.11989300	-0.68063000
H	2.77910000	-2.13017400	-0.35488300
H	2.70839100	-1.00820200	-1.75417600
C	-4.87979800	-2.16128400	-1.41993200
H	-4.23775800	-2.56228400	-2.20568700
C	-6.52849700	-1.07800600	0.55717600
H	-7.17949900	-0.64922100	1.32237900
C	-0.14081700	5.64270700	-0.93317500
H	-0.16423900	6.70422200	-1.18649200
C	7.67650600	-2.03886700	-0.09407200
C	1.04247900	4.91503900	-1.06643800
H	1.95178600	5.40817200	-1.41543700
C	5.19592500	-0.78335200	0.07526500

C	5.57710400	-1.67341400	1.07990500
H	4.91211500	-1.86213700	1.92455500
C	6.81648400	-2.29611300	0.98577900
H	7.13077200	-2.99220200	1.76666900
C	-6.90750100	-2.27076400	-0.07972500
C	-6.07117400	-2.79672700	-1.07114300
H	-6.35990800	-3.71564700	-1.58536400
O	3.69148800	1.26452800	-0.57662700
C	9.01334900	-2.72211800	-0.17128600
H	8.89168300	-3.81539500	-0.16370000
H	9.55587800	-2.43858800	-1.08206800
H	9.63338000	-2.45829100	0.69851700
C	-8.19045500	-2.95516400	0.30225400
H	-9.04321000	-2.26760500	0.20308000
H	-8.37704000	-3.83470400	-0.32685700
H	-8.15703100	-3.28175700	1.35261200
C	7.26615100	-1.13444500	-1.08125800
H	7.92944400	-0.91922000	-1.92136000
C	6.02758600	-0.49951500	-1.00407500
H	5.71222900	0.21616900	-1.76500100
H	-2.76782300	-0.17467700	4.42036300

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -2387.9031476

Electronic Energy (0K) + ZPE = -2387.336576

Enthalpy (298K) = -2387.300730

Free Energy (298K) = -2387.407681

$TS_{I'}$

Number of imaginary frequencies: 1

C	1.04110900	-0.20452700	3.36155900

C	-0.33973600	-0.01367400	3.29283700
C	-1.01031500	-0.24552300	2.09423500
C	-0.30544800	-0.62634700	0.94920600
C	1.09198700	-0.80060600	1.00144100
C	1.74475900	-0.60681200	2.22967300
C	1.90113400	-1.11932200	-0.20268200
C	1.80852500	-0.31705300	-1.30687400
N	-1.00362200	-0.92611700	-0.25849200
C	-1.18646700	-2.32636200	-0.64292100
C	-2.10961900	-3.08999300	0.30877000
C	-2.28552400	-4.51412000	-0.12847800
C	-3.44830600	-5.05680900	-0.48987400
C	2.90721100	-2.19499200	-0.11794200
C	2.68958100	-3.31439600	0.70530400
C	3.62282400	-4.34627800	0.76439300
C	4.79879500	-4.27225700	0.01591500
C	5.03501800	-3.15852300	-0.79252900
C	4.09994900	-2.12959600	-0.86098900
C	-3.42938200	0.33279900	-0.68548500
C	-4.32871500	-0.53976200	-1.29767800
C	-5.66120200	-0.52364600	-0.89366700
C	-6.10614900	0.35979200	0.09984500
C	-5.17991700	1.23618200	0.68358100
C	-3.84252900	1.23146600	0.29747000
C	-7.55252700	0.39532600	0.50766700
S	-1.71616300	0.27497300	-1.14823000
O	-1.66311000	-0.13961800	-2.54280200
O	-1.09237800	1.52301400	-0.72765100
H	1.57292200	-0.03812300	4.29971900
H	-0.89949400	0.29315500	4.17765000

H	-2.09597800	-0.14584500	2.03764900
H	2.82800000	-0.73531800	2.27034200
H	2.32775200	-0.57025000	-2.23463500
H	1.04032700	0.45796900	-1.36095500
H	-1.58187600	-2.34574600	-1.66740000
H	-0.19272500	-2.80399900	-0.68051400
H	-3.08728600	-2.58468000	0.35927700
H	-1.66973000	-3.06510600	1.32055600
H	-1.37562000	-5.12606500	-0.16041000
H	-3.51701800	-6.09935000	-0.80963500
H	-4.37484600	-4.47360400	-0.47348000
H	1.77153900	-3.37921000	1.29373100
H	3.43125700	-5.21295200	1.39934700
H	5.53352400	-5.07752000	0.06781400
H	5.95944700	-3.08558700	-1.36779600
H	4.31354800	-1.25416000	-1.47778200
H	-3.99128700	-1.21872400	-2.08305400
H	-6.37268400	-1.20604800	-1.36331100
H	-5.51465300	1.93683800	1.45145300
H	-3.12359200	1.91945700	0.74550900
H	-7.65688300	0.61177800	1.57948500
H	-8.05263100	-0.55670000	0.28697400
H	-8.08430300	1.18804200	-0.04192600
C	2.49277100	2.77234800	-0.26921800
C	1.95643700	2.86674200	1.01348600
C	1.07034300	3.90496400	1.28849500
C	0.70894000	4.82998500	0.29905000
C	1.26602600	4.69988300	-0.98224400
C	2.15270400	3.67005500	-1.28014100
C	-0.28193900	5.92173400	0.59141600

S	3.52551000	1.37622300	-0.66643800
O	4.14305300	0.88799000	0.58011200
O	4.37979200	1.72624500	-1.81836600
H	2.23900400	2.14502400	1.78200400
H	0.65034400	3.99917400	2.29222000
H	0.99861000	5.41923300	-1.75922600
H	2.58621100	3.56684100	-2.27623000
H	-0.31886500	6.15048700	1.66455800
H	-0.03643300	6.83957100	0.04012800
H	-1.29164800	5.60999500	0.28001300

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4184476

Electronic Energy (0K) + ZPE = -2387.848304

Enthalpy (298K) = -2387.809825

Free Energy (298K) = -2387.926134

INT-1'

Number of imaginary frequencies: 0

C	1.65241800	0.06573200	3.52568300
C	0.28376300	0.33994100	3.58188000
C	-0.50214600	0.15041900	2.45037300
C	0.06528500	-0.27053200	1.24361200
C	1.45260800	-0.54172600	1.16387700
C	2.21806800	-0.38257000	2.33958500
C	2.14547800	-0.92788200	-0.07351800
C	1.91359500	-0.17609600	-1.33387700
N	-0.76614800	-0.49375700	0.10956400
C	-0.89097200	-1.83321700	-0.47111300
C	-1.69277300	-2.78276200	0.42088600
C	-1.79174200	-4.15046300	-0.18685100

C	-2.93395500	-4.74117200	-0.53848400
C	3.17517700	-1.95207300	-0.04879800
C	3.12780900	-3.00222900	0.89884000
C	4.08217000	-4.01233600	0.89756700
C	5.11888900	-4.00397900	-0.03969400
C	5.18724600	-2.97203600	-0.97888900
C	4.23103700	-1.96268300	-0.98981400
C	-3.35870900	0.13293000	-0.45848000
C	-3.90761500	-0.54595600	-1.54490400
C	-5.19196600	-1.07109300	-1.42908700
C	-5.93377700	-0.91692700	-0.24944300
C	-5.36028300	-0.20980800	0.81776100
C	-4.07697800	0.31968700	0.72207000
C	-7.32911400	-1.46598900	-0.14638600
S	-1.68906200	0.72811200	-0.54828800
O	-1.34941000	0.82903000	-1.96526400
O	-1.54745800	1.88541300	0.31894100
H	2.27981300	0.20377200	4.40753900
H	-0.17560300	0.68117500	4.51068200
H	-1.57752600	0.32200800	2.49127200
H	3.29077600	-0.57825400	2.29028000
H	2.27611800	-0.70716300	-2.22417500
H	0.86969700	0.11774000	-1.50821600
H	-1.36469200	-1.73694600	-1.45916900
H	0.11606100	-2.24110000	-0.65454500
H	-2.69954800	-2.36910800	0.59251700
H	-1.18587200	-2.84592700	1.39935000
H	-0.84275100	-4.67380200	-0.35702100
H	-2.94656700	-5.73835600	-0.98502100
H	-3.89845000	-4.24627700	-0.38452000

H	2.31395700	-3.03130800	1.62589500
H	4.01420200	-4.81816200	1.63060100
H	5.86903400	-4.79638900	-0.03766500
H	5.99992000	-2.94840100	-1.70702700
H	4.32717600	-1.14882900	-1.70914100
H	-3.33658000	-0.65728700	-2.46799300
H	-5.62914600	-1.61030400	-2.27207300
H	-5.93129900	-0.07066900	1.73796300
H	-3.64149700	0.87960900	1.55169300
H	-7.61032600	-1.64452200	0.89969800
H	-7.42817000	-2.40509100	-0.70727700
H	-8.05177000	-0.75052700	-0.56965500
C	1.76795600	2.60619500	-0.65336700
C	1.84548900	2.84215900	0.71797600
C	0.99336700	3.78806100	1.28061300
C	0.08151900	4.49937300	0.49008300
C	0.04856800	4.25655800	-0.88920900
C	0.88108200	3.30684500	-1.46961700
C	-0.88427200	5.46554500	1.11455400
S	2.84101700	1.40190500	-1.39666300
O	4.03751300	1.27126600	-0.55993300
O	2.98710100	1.73427800	-2.81614100
H	2.56873300	2.29811800	1.32807100
H	1.03845700	3.97932000	2.35507100
H	-0.65172900	4.81313200	-1.51582800
H	0.85614100	3.11283800	-2.54278200
H	-0.50002600	5.86450000	2.06268900
H	-1.10839500	6.30261300	0.43949600
H	-1.83370600	4.94821100	1.32777600

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4408451

Electronic Energy (0K) + ZPE = -2387.868075

Enthalpy (298K) = -2387.830320

Free Energy (298K) = -2387.941376

$TS_{2'}$

Number of imaginary frequencies: 1

C	2.39899100	0.19317100	3.13658300
C	3.10351500	-0.96253400	2.80447700
C	3.13103300	-1.38186600	1.47939400
C	2.45119100	-0.67190200	0.47958300
C	1.77614800	0.53108900	0.78901600
C	1.76028900	0.92443000	2.14144800
C	1.01593200	1.40401600	-0.18072900
C	-0.33014200	0.85544400	-0.55813900
N	2.49958700	-1.15692400	-0.87436200
C	3.75967300	-0.90266600	-1.62087800
C	4.22086200	0.54050600	-1.54010900
C	3.23102800	1.56269900	-1.99076100
C	1.88506700	1.33150600	-2.15279800
C	1.15001900	2.86872700	0.00593300
C	2.37142200	3.41175100	0.45219700
C	2.56189000	4.78732500	0.55048100
C	1.53955300	5.66915800	0.19559300
C	0.32780900	5.15100800	-0.26222200
C	0.13649300	3.77409800	-0.35622700
C	0.43463300	-2.93295300	-0.37218000
C	0.37967200	-3.40934300	0.93866900
C	-0.86120200	-3.69498500	1.49233500
C	-2.03953300	-3.53466300	0.74966400

C	-1.94929500	-3.07231200	-0.56887000
C	-0.71627900	-2.77069800	-1.14041700
C	-3.37046900	-3.83779700	1.37823700
S	2.00089000	-2.74505700	-1.17014700
O	2.93267800	-3.69387900	-0.56246800
O	1.80269600	-2.81770800	-2.61398500
H	2.34817600	0.53283100	4.17227300
H	3.62708200	-1.53653200	3.57054800
H	3.67213400	-2.28584500	1.19679100
H	1.20601600	1.82474800	2.41001500
H	-0.83847600	1.44568700	-1.33242300
H	-0.26803400	-0.19241700	-0.88254400
H	4.56046800	-1.56132500	-1.24187600
H	3.56468500	-1.17095200	-2.66803800
H	5.14562600	0.62005700	-2.13516700
H	4.53052700	0.77841300	-0.50436800
H	3.59432600	2.59354200	-2.03100300
H	1.26614300	2.14568700	-2.53813600
H	1.51961300	0.32091200	-2.33320500
H	3.18961100	2.74064900	0.72036400
H	3.52036800	5.17300500	0.90310800
H	1.68675000	6.74761900	0.27284300
H	-0.48372400	5.82417200	-0.54487300
H	-0.82758600	3.41032300	-0.70982900
H	1.29687400	-3.57230700	1.50587100
H	-0.91969600	-4.06268500	2.51893300
H	-2.85794000	-2.96034400	-1.16432400
H	-0.64083500	-2.44140200	-2.17790800
H	-4.18479100	-3.78914100	0.64320400
H	-3.58352100	-3.11576800	2.18257200

H	-3.37069400	-4.83810000	1.83497800
C	-3.10178700	0.81491700	0.18097100
C	-3.86900700	-0.34315700	0.21126200
C	-5.16255200	-0.31247000	-0.31038300
C	-5.69084600	0.86219500	-0.85658300
C	-4.89655600	2.02157900	-0.85683700
C	-3.60918000	2.01029900	-0.33409500
C	-7.08070900	0.90021500	-1.42795800
S	-1.46226000	0.78441900	0.88213600
O	-1.27459600	-0.50773000	1.54498700
O	-1.30404300	2.01329700	1.66545600
H	-3.45397600	-1.24833600	0.65318400
H	-5.77463200	-1.21670000	-0.28624000
H	-5.30410400	2.94964600	-1.26369000
H	-3.01202400	2.92437600	-0.31165600
H	-7.59376700	-0.06074000	-1.29533000
H	-7.67905900	1.68586000	-0.94374700
H	-7.05058000	1.13118700	-2.50348900

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4073535

Electronic Energy (0K) + ZPE = -2387.833671

Enthalpy (298K) = -2387.797825

Free Energy (298K) = -2387.901203

INT-2'

Number of imaginary frequencies: 0

C	2.02655800	0.73356700	3.11136900
C	3.05654000	-0.18028300	2.89877700
C	3.32666300	-0.59930700	1.60232200
C	2.56979700	-0.13169000	0.51753000

C	1.55678700	0.83133300	0.70699700
C	1.30583800	1.23111800	2.03126400
C	0.67724500	1.45550700	-0.40044400
C	-0.63273400	0.64955000	-0.51873600
N	2.87998300	-0.62109400	-0.79679200
C	4.00972100	0.02556700	-1.49710000
C	3.87453700	1.54148300	-1.48648200
C	2.59429800	2.05768300	-2.05451800
C	1.26818800	1.39943400	-1.86362500
C	0.44840100	2.95541600	-0.14515500
C	1.51170400	3.75343000	0.30062000
C	1.37919500	5.13647000	0.41901300
C	0.17574200	5.75741800	0.08614200
C	-0.88652100	4.97861700	-0.36955700
C	-0.74894600	3.59477200	-0.48541300
C	1.30776000	-2.81274400	-0.37515100
C	1.25799800	-3.24461200	0.95170400
C	0.05596600	-3.72783900	1.45076700
C	-1.08551900	-3.80728100	0.63970100
C	-0.99666200	-3.38923800	-0.69386800
C	0.19791400	-2.89253300	-1.21256800
C	-2.37574100	-4.31981600	1.21442400
S	2.84827100	-2.28055800	-1.06185200
O	3.92585200	-2.94764000	-0.33387100
O	2.80544600	-2.44059100	-2.51136300
H	1.78624900	1.07248100	4.12030500
H	3.64576200	-0.56367800	3.73321600
H	4.12330900	-1.31756500	1.40432700
H	0.51223100	1.95484800	2.21687000
H	-1.27004400	1.05319800	-1.31708100

H	-0.40290800	-0.39762800	-0.76265100
H	4.96841400	-0.26604900	-1.03255300
H	3.99961700	-0.34425000	-2.53126200
H	4.72518800	1.95030300	-2.05295200
H	4.01683600	1.90383500	-0.44830200
H	2.60666800	3.06660500	-2.47096800
H	0.52660100	1.91445800	-2.49159200
H	1.29814100	0.34923200	-2.18452300
H	2.46174000	3.28592500	0.56646600
H	2.22420200	5.72975000	0.77312200
H	0.06688400	6.83919600	0.18067300
H	-1.83601800	5.44723600	-0.63479200
H	-1.60500700	3.02153600	-0.84260100
H	2.15195200	-3.21106000	1.57549700
H	-0.00027100	-4.05926200	2.48968900
H	-1.87250300	-3.46451500	-1.34220400
H	0.27530400	-2.58708700	-2.25738400
H	-3.14657200	-4.43310600	0.44061400
H	-2.74956300	-3.62372300	1.98170200
H	-2.22690400	-5.29283600	1.70465600
C	-3.30032900	0.19362400	0.23343100
C	-3.71402700	-1.11829400	0.03264100
C	-4.96949200	-1.35224300	-0.52707200
C	-5.80964600	-0.28953600	-0.88022100
C	-5.36712100	1.02407100	-0.65329600
C	-4.11912500	1.27557600	-0.09447300
C	-7.16750700	-0.53493300	-1.47673400
S	-1.69461100	0.50013500	0.94472300
O	-1.28958100	-0.69671400	1.68420500
O	-1.78161900	1.78149100	1.65140900

H	-3.06083200	-1.94087600	0.32383400
H	-5.30603700	-2.37900800	-0.68580700
H	-6.01975800	1.86082100	-0.91226300
H	-3.78526000	2.29616400	0.10256700
H	-7.34402500	-1.60532500	-1.64207300
H	-7.95637100	-0.15260700	-0.81159400
H	-7.27113200	-0.01069400	-2.43808600

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4374161

Electronic Energy (0K) + ZPE = -2387.861188

Enthalpy (298K) = -2387.825528

Free Energy (298K) = -2387.927906

INT-3'

Number of imaginary frequencies: 0

C	2.01331400	0.69543700	3.12333800
C	3.06109000	-0.19520900	2.89817200
C	3.34636100	-0.58544100	1.59643600
C	2.58440500	-0.10953400	0.52081400
C	1.55335100	0.83030200	0.72459400
C	1.28659000	1.20412600	2.05274600
C	0.66367600	1.45295100	-0.37082900
C	-0.63046900	0.62451300	-0.51493000
N	2.89733900	-0.56939900	-0.80342100
C	4.04488000	0.07252900	-1.45077100
C	3.80769800	1.55793700	-1.63297000
C	2.52679400	2.07804400	-1.97252500
C	1.24682100	1.38738700	-1.86231800
C	0.40973800	2.95533600	-0.12306800
C	1.41892900	3.76088900	0.42059700

C	1.25228500	5.14077800	0.53802300
C	0.06917400	5.74243600	0.11261700
C	-0.93969400	4.95160900	-0.43488200
C	-0.76881800	3.57267700	-0.55457500
C	1.33739400	-2.78188700	-0.39959600
C	1.32577400	-3.21613300	0.92832500
C	0.14068100	-3.70951300	1.45533500
C	-1.02021800	-3.79623200	0.67219300
C	-0.96862400	-3.37521800	-0.66265100
C	0.20887100	-2.87110200	-1.21151000
C	-2.28919400	-4.32589300	1.27610900
S	2.85278300	-2.23741800	-1.11839700
O	3.96110700	-2.89684000	-0.43828100
O	2.77007900	-2.33611400	-2.57043400
H	1.76249700	1.00914000	4.13749900
H	3.65113200	-0.58452500	3.72890000
H	4.15464300	-1.28822400	1.38763100
H	0.48131700	1.91102100	2.25174000
H	-1.26357000	1.01681000	-1.32156900
H	-0.37937100	-0.41947300	-0.74668400
H	4.97468100	-0.07062000	-0.87676400
H	4.17956200	-0.38163500	-2.44245400
H	4.62811500	2.09219200	-2.13437400
H	3.78868100	2.10361300	-0.62920800
H	2.50668400	3.14083000	-2.24405600
H	0.51174700	1.91959200	-2.47907800
H	1.34841000	0.33693800	-2.15511900
H	2.34884300	3.30817100	0.77166900
H	2.05202300	5.74404800	0.97056200
H	-0.06692400	6.82070100	0.20870900

H	-1.87261800	5.40711800	-0.77081000
H	-1.58111700	2.98770900	-0.98786100
H	2.23406300	-3.17921600	1.53083900
H	0.11342400	-4.04525200	2.49385100
H	-1.85996100	-3.45759900	-1.28842200
H	0.25731500	-2.56726700	-2.25848800
H	-3.08021700	-4.43706300	0.52291300
H	-2.64626400	-3.64316000	2.06298700
H	-2.11706000	-5.30309700	1.75007800
C	-3.28840600	0.15538900	0.23305700
C	-3.72272900	-1.16013800	0.11927200
C	-4.97354800	-1.40867200	-0.44470900
C	-5.78541400	-0.35785300	-0.88789100
C	-5.32094900	0.96085700	-0.74687400
C	-4.07862400	1.22833200	-0.18475200
C	-7.13500400	-0.61908000	-1.49514700
S	-1.69629200	0.48506900	0.95244300
O	-1.27283100	-0.69310500	1.70725500
O	-1.78364000	1.78143000	1.62825300
H	-3.09189400	-1.97213600	0.48069900
H	-5.32937500	-2.43715600	-0.53458900
H	-5.95313900	1.78861600	-1.07565700
H	-3.72763600	2.25408700	-0.05486300
H	-7.35652700	-1.69314200	-1.53001100
H	-7.92387900	-0.11898600	-0.91400200
H	-7.18331000	-0.21936100	-2.51897700

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -2388.2520438

Electronic Energy (0K) + ZPE = -2387.674759

Enthalpy (298K) = -2387.639445

Free Energy (298K) = -2387.739840

3a'

Number of imaginary frequencies: 0

C	2.07993100	0.73303300	3.11931900
C	2.82853700	-0.43243600	2.99156100
C	3.02307100	-0.97211300	1.72561100
C	2.45157700	-0.38386800	0.58851800
C	1.70766300	0.81216400	0.69651000
C	1.54135400	1.33850300	1.98825500
C	0.94742900	1.50932300	-0.45698700
C	-0.42554200	0.80473600	-0.59029500
N	2.72483700	-0.96061400	-0.70058500
C	4.00076800	-0.51028800	-1.29363200
C	3.97262000	1.00081500	-1.51092800
C	2.77196800	1.36674200	-2.32725100
C	1.51907900	1.47468800	-1.88071800
C	0.82791400	3.03503100	-0.22947700
C	1.96899900	3.75531000	0.15511800
C	1.94424700	5.14265600	0.26272800
C	0.77464700	5.84907600	-0.02589800
C	-0.35983100	5.14811600	-0.42490800
C	-0.33214400	3.75491600	-0.52600500
C	0.87242900	-2.95461700	-0.34944300
C	0.69350000	-3.47590800	0.93180500
C	-0.58204600	-3.86681300	1.32025200
C	-1.66910800	-3.76281000	0.44135500
C	-1.45573700	-3.23508700	-0.83923200
C	-0.18652300	-2.83352400	-1.24692800
C	-3.03591300	-4.21154200	0.87852900

S	2.50608600	-2.61554900	-0.93266100
O	3.44943200	-3.38814700	-0.12597800
O	2.53753000	-2.80973500	-2.37728600
H	1.91166500	1.18078800	4.09995400
H	3.26965800	-0.91451100	3.86529400
H	3.62713300	-1.87029200	1.59583300
H	0.94644600	2.24122100	2.11482000
H	-1.04277400	1.27176400	-1.36899200
H	-0.27185300	-0.24945300	-0.86123600
H	4.84754400	-0.78980400	-0.64328500
H	4.11292100	-1.02260100	-2.25797800
H	4.89916300	1.28555500	-2.02721400
H	3.97348400	1.51254500	-0.53804500
H	2.91915700	1.46547300	-3.40710700
H	0.74650600	1.70645700	-2.62186500
H	2.89442400	3.22033000	0.37806400
H	2.84573000	5.67514200	0.57109500
H	0.75138000	6.93688800	0.05774300
H	-1.28210400	5.68332500	-0.65810500
H	-1.24263800	3.24429300	-0.83762600
H	1.54574000	-3.59035100	1.60279600
H	-0.73788700	-4.27580900	2.32074900
H	-2.29434700	-3.15379000	-1.53427500
H	-0.01029400	-2.45285200	-2.25447600
H	-3.78029100	-4.06123200	0.08548800
H	-3.35813300	-3.65876200	1.77434200
H	-3.02597800	-5.27913000	1.14456800
C	-3.10750700	0.52834800	0.24250400
C	-3.67532300	-0.73853700	0.18132600
C	-4.97271800	-0.87502300	-0.31190300

C	-5.70196600	0.24113500	-0.73778500
C	-5.10680200	1.51040700	-0.64563700
C	-3.81675000	1.66468000	-0.15170400
C	-7.09600700	0.09893300	-1.28159500
S	-1.45965500	0.71117500	0.89905900
O	-1.11886700	-0.51822900	1.61567400
O	-1.43272300	1.99090900	1.61246200
H	-3.10521700	-1.59763600	0.53349300
H	-5.43059800	-1.86553000	-0.35749300
H	-5.67372000	2.39141200	-0.95458800
H	-3.37129400	2.65628200	-0.05086800
H	-7.47043900	-0.92514200	-1.15801900
H	-7.78590200	0.78884900	-0.77470200
H	-7.11810300	0.34617800	-2.35401300

SMD-M06-2X/Def2-SVP

Electronic Energy (0K) = -2387.8692893

Electronic Energy (0K) + ZPE = -2387.302550

Enthalpy (298K) = -2387.267285

Free Energy (298K) = -2387.369743

$TS_{1''}$

Number of imaginary frequencies: 1

S	2.83470500	-0.73114700	1.19793900
O	2.94976800	0.37564300	2.13777600
O	2.27128200	-2.00665600	1.61679200
N	1.88606900	-0.19647100	-0.06433900
C	1.94116300	1.19465600	-0.40501700
C	0.98176900	2.11833000	0.06916800
C	-0.22530700	1.76084400	0.87658100
C	-1.51176600	2.43161500	0.50937500

C	-0.21570100	0.88789700	1.89831900
H	-1.14312000	0.65138100	2.42586400
C	2.97068700	1.61934900	-1.25563100
H	3.67190000	0.87362900	-1.63688900
C	1.14613600	3.46461300	-0.30464500
H	0.42066000	4.19678700	0.05440900
C	-0.87959300	-0.65775500	-1.40864900
H	-0.51781400	0.36433300	-1.54981600
C	0.11580800	-1.68664200	-0.98263600
H	-0.01020000	-2.60271600	-1.58429500
H	-0.07121900	-1.97846400	0.06772100
C	4.45781100	-1.04622500	0.55182900
C	-2.42581800	2.79928300	1.50830600
H	-2.15107100	2.67277100	2.55718700
C	1.55598700	-1.20116800	-1.08874800
H	1.74516300	-0.75437100	-2.07630500
H	2.24072600	-2.05499000	-0.98992200
C	5.38119900	0.00176000	0.50052000
H	5.11200100	0.98810500	0.88160100
C	-1.86982300	2.65061700	-0.83049900
H	-1.16597600	2.40409500	-1.62863200
C	3.10705100	2.95657500	-1.61107800
C	-3.67403600	3.32474100	1.18038000
H	-4.36899500	3.60194700	1.97506600
C	2.19440600	3.88712900	-1.11490000
H	2.28921900	4.94376000	-1.37008700
C	-2.23285700	-0.90577700	-1.53652300
H	-2.86669500	-0.14922400	-2.00500200
H	-2.56916900	-1.94315800	-1.62716200
C	4.78701900	-2.32510000	0.10711900

H	4.06523100	-3.13875900	0.19352600
C	6.64247300	-0.24150700	-0.03015300
H	7.37292100	0.56951700	-0.07266500
C	-4.03269000	3.49965500	-0.15630800
H	-5.01158800	3.90717600	-0.41508800
C	-7.20424200	-2.83971100	-0.81559600
C	-3.12199400	3.16660300	-1.16055400
H	-3.38632000	3.31161300	-2.20974500
C	-4.85608400	-1.57591400	0.04744000
C	-5.88878400	-0.82863800	-0.53901800
H	-5.77053800	0.25096700	-0.65367600
C	-7.05590300	-1.45981200	-0.96775400
H	-7.85429600	-0.86975300	-1.42156500
C	6.99825200	-1.51503500	-0.50302500
C	6.05731300	-2.54828100	-0.42202700
H	6.32550200	-3.54764900	-0.77030500
C	8.37202300	-1.75543900	-1.06365200
H	9.13739500	-1.60341000	-0.28765500
H	8.47201000	-2.77713900	-1.45127000
H	8.58993000	-1.04867300	-1.87766200
C	-6.17937500	-3.58874800	-0.23440800
H	-6.29082900	-4.66781800	-0.11273800
C	-5.00923200	-2.96283700	0.19408300
H	-4.20724700	-3.54782400	0.64845700
H	3.92080900	3.26860000	-2.26728900
H	0.69808300	0.41991700	2.25530100
Se	-3.25996700	-0.70698500	0.62564300
H	-8.11911400	-3.33188900	-1.15019500

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -4202.170457

Electronic Energy (0K) + ZPE = -4201.636422

Enthalpy (298K) = -4201.602171

Free Energy (298K) = -4201.707075

INT-1''

Number of imaginary frequencies: 0

S	2.81917100	-0.71409100	1.22939100
O	2.94323000	0.39919200	2.16083900
O	2.26051900	-1.98664700	1.66300500
N	1.85963400	-0.18742300	-0.02748900
C	1.92238600	1.19936000	-0.38481500
C	0.96981900	2.13408100	0.07946900
C	-0.23474600	1.79121900	0.89561300
C	-1.52534500	2.44169500	0.50923000
C	-0.21470800	0.94462700	1.93885400
H	-1.13816100	0.70944700	2.47333400
C	2.95213500	1.60841700	-1.24316700
H	3.64861600	0.85487400	-1.61757700
C	1.13927300	3.47473600	-0.31144700
H	0.41753600	4.21441300	0.03994000
C	-0.89838600	-0.62699800	-1.43256300
H	-0.52980600	0.35335300	-1.74003500
C	0.07417600	-1.65490600	-0.96753700
H	-0.03924300	-2.57510500	-1.57201000
H	-0.13947700	-1.95545900	0.07618100
C	4.43827200	-1.03479100	0.57425400
C	-2.45804900	2.80185200	1.49357800
H	-2.19517800	2.68853500	2.54693800
C	1.52415000	-1.19619600	-1.04660800
H	1.73929100	-0.76479400	-2.03608300

H	2.19019600	-2.06157000	-0.92529100
C	5.36383500	0.00750100	0.51987800
H	5.10092000	0.99464000	0.90319400
C	-1.86969300	2.64596900	-0.83643900
H	-1.15133900	2.40505100	-1.62255000
C	3.09456800	2.94042000	-1.61538900
C	-3.71083600	3.30297100	1.14589400
H	-4.42034300	3.57444400	1.92968900
C	2.18760400	3.88195900	-1.12932300
H	2.28712700	4.93475700	-1.39827800
C	-2.34048300	-0.88081400	-1.42804100
H	-2.90383800	-0.16972600	-2.04382400
H	-2.58416700	-1.91392600	-1.71728700
C	4.76065300	-2.31609300	0.12320300
H	4.03564500	-3.12674500	0.21144400
C	6.62379300	-0.23928400	-0.01987600
H	7.35543900	0.56988300	-0.06606000
C	-4.05522000	3.46277000	-0.19674700
H	-5.03747800	3.85165400	-0.47106300
C	-7.23571200	-2.83822000	-0.58948400
C	-3.12550500	3.13947100	-1.18639800
H	-3.37818900	3.27330900	-2.23993900
C	-4.80458100	-1.59624700	0.01823100
C	-5.94511400	-0.82419000	-0.22912200
H	-5.87837800	0.26484600	-0.18681900
C	-7.15803900	-1.44643500	-0.52905700
H	-8.04486500	-0.83908000	-0.71916100
C	6.97133400	-1.51040700	-0.49639900
C	6.02426200	-2.54192900	-0.41313800
H	6.28673800	-3.54130500	-0.76699800

C	8.33876700	-1.78072500	-1.05917500
H	8.92625100	-2.39615700	-0.36041500
H	8.27151400	-2.33643600	-2.00519600
H	8.88902400	-0.84788600	-1.23642000
C	-6.09841700	-3.61000200	-0.34505200
H	-6.15548400	-4.69922800	-0.38772900
C	-4.88582100	-2.99286900	-0.03704200
H	-3.99767200	-3.59517600	0.16543400
H	3.90859600	3.23992600	-2.27709200
H	0.70590700	0.49518000	2.30267700
Se	-3.13779800	-0.73420800	0.43205600
H	-8.18447200	-3.32322600	-0.82583600

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -4202.1758349

Electronic Energy (0K) + ZPE = -4201.641637

Enthalpy (298K) = -4201.606857

Free Energy (298K) = -4201.714683

$TS_{2''}$

Number of imaginary frequencies: 1

S	2.87597000	-1.04514300	1.09706300
O	2.80267900	-0.06896700	2.17406300
O	2.39237200	-2.40558700	1.29787200
N	2.00875400	-0.43143900	-0.17673300
C	2.12442300	0.97106400	-0.44021500
C	1.13923500	1.89665500	-0.01314600
C	-0.15427100	1.52933700	0.60497600
C	-1.30896300	2.45411600	0.40810900
C	-0.43627200	0.32626800	1.19273800
H	-1.42809900	0.18100400	1.62795600

C	3.25103600	1.40430300	-1.14894100
H	3.96006400	0.65283900	-1.50249300
C	1.40650300	3.25946900	-0.26362000
H	0.68670700	4.00402700	0.07816300
C	-1.00936300	-1.00673000	-0.67856500
H	-1.02252200	-0.19557000	-1.41650800
C	0.12413300	-1.97859400	-0.78695500
H	-0.12149000	-2.72611800	-1.56794100
H	0.24056700	-2.54627000	0.14950800
C	4.57149400	-1.14981500	0.58588200
C	-2.15614800	2.77538300	1.47883100
H	-1.90788800	2.41570700	2.47980400
C	1.46559600	-1.36143200	-1.17644000
H	1.36245000	-0.78765300	-2.10852600
H	2.19586700	-2.16214200	-1.37252800
C	5.44060200	-0.10230800	0.88346700
H	5.08796700	0.75145700	1.46397400
C	-1.63914100	2.93519500	-0.87062700
H	-0.99342800	2.69426200	-1.71859100
C	3.47546000	2.75482900	-1.39742000
C	-3.30411000	3.54152300	1.27854400
H	-3.94910400	3.78116500	2.12602300
C	2.55086900	3.68697100	-0.92688900
H	2.71317500	4.75421200	-1.08701700
C	-2.33924700	-1.56425600	-0.29993200
H	-2.71894900	-2.23704100	-1.08954500
H	-2.28533300	-2.14224100	0.63510200
C	4.99621500	-2.26422400	-0.14072300
H	4.30811800	-3.08861900	-0.33456100
C	6.75582700	-0.16947600	0.42813000

H	7.44498500	0.64591800	0.65674200
C	-3.62825900	3.99938300	0.00128100
H	-4.52936300	4.59438500	-0.15741200
C	-7.53693800	-2.90498900	-0.19715900
C	-2.78924300	3.69491300	-1.07284400
H	-3.03683000	4.04456900	-2.07686800
C	-5.24914100	-1.29693500	-0.13888200
C	-5.54750500	-2.05304900	-1.27864100
H	-4.89304800	-2.00401100	-2.15190000
C	-6.68256300	-2.86267900	-1.30093800
H	-6.90687600	-3.45401200	-2.19058900
C	7.20876200	-1.26622500	-0.31610400
C	6.31161200	-2.31067800	-0.58966600
H	6.65571400	-3.17806600	-1.15733600
C	8.63122600	-1.34615600	-0.79600900
H	9.17786500	-2.12970400	-0.24904800
H	8.67094300	-1.60659500	-1.86338000
H	9.15754000	-0.39483400	-0.64630700
C	-7.24858100	-2.14022500	0.93273900
H	-7.91231900	-2.16880400	1.79882500
C	-6.10348200	-1.34191200	0.96705000
H	-5.86859900	-0.75563500	1.85735000
H	4.36378800	3.07309200	-1.94474600
H	0.33334200	-0.37515200	1.49930300
Se	-3.70330200	-0.15371000	-0.09345200
H	-8.42878900	-3.53360500	-0.21965500

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -4202.1611037

Electronic Energy (0K) + ZPE = -4201.626352

Enthalpy (298K) = -4201.592832

Free Energy (298K) = -4201.695748

INT-2''

Number of imaginary frequencies: 0

S	2.79496400	-1.26440400	0.91137300
O	2.57816100	-0.43514200	2.08987400
O	2.36046500	-2.65587400	0.89926800
N	2.03729100	-0.53641700	-0.36984400
C	2.20163100	0.87330500	-0.53863300
C	1.17805600	1.80320700	-0.17246600
C	-0.11704300	1.44476300	0.34349400
C	-1.21407700	2.44201000	0.33832100
C	-0.55465200	0.05399400	0.71471600
H	-1.40357100	0.14932300	1.40705600
C	3.39486000	1.31553700	-1.11434600
H	4.12407500	0.56607100	-1.42740900
C	1.49892100	3.18011000	-0.35386500
H	0.77265700	3.93021000	-0.04212800
C	-1.03036800	-0.75967100	-0.53192500
H	-1.12482400	-0.06610400	-1.38699100
C	-0.03605100	-1.85695700	-0.92151700
H	-0.45229300	-2.44040400	-1.75831300
H	0.09301200	-2.54895100	-0.07508800
C	4.53597000	-1.23826900	0.56999500
C	-1.97914700	2.66939700	1.49515900
H	-1.71385800	2.15523800	2.42187000
C	1.33264100	-1.35491700	-1.36760300
H	1.23328300	-0.71738500	-2.25793600
H	1.96445000	-2.21036900	-1.65040000
C	5.33359300	-0.25298800	1.14441700

H	4.89385900	0.47331600	1.82927100
C	-1.58077900	3.11119100	-0.84336400
H	-1.00633500	2.93734100	-1.75630900
C	3.66321100	2.67078200	-1.29379000
C	-3.06396400	3.54299700	1.47549200
H	-3.63829500	3.71234400	2.38811200
C	2.70451800	3.60374200	-0.88822100
H	2.89782100	4.67270200	-0.99371100
C	-2.40054600	-1.39414300	-0.30400600
H	-2.67507200	-2.02846300	-1.15698500
H	-2.40818000	-2.00402100	0.61123100
C	5.06664800	-2.18914500	-0.30412600
H	4.42871000	-2.96834000	-0.72512400
C	6.68987100	-0.21399900	0.82420400
H	7.32467400	0.55476700	1.26919500
C	-3.42156700	4.19234600	0.29265200
H	-4.27933300	4.86689900	0.27415100
C	-7.52593600	-2.95014800	-0.04996300
C	-2.67678400	3.97157700	-0.86695900
H	-2.95423900	4.46767900	-1.79884300
C	-5.31229000	-1.24002000	-0.10102700
C	-5.55187800	-2.11175700	-1.16988100
H	-4.88201800	-2.11459300	-2.03259900
C	-6.64958300	-2.97092900	-1.13686500
H	-6.82689200	-3.65236800	-1.97094300
C	7.25098700	-1.14484700	-0.05805900
C	6.42047800	-2.13187800	-0.61391100
H	6.84864500	-2.87092300	-1.29477600
C	8.71498200	-1.11158100	-0.39781200
H	9.21901000	-2.01388800	-0.01950000

H	8.86317800	-1.08944300	-1.48729400
H	9.20668700	-0.23394600	0.04061900
C	-7.29693400	-2.07062800	1.00778800
H	-7.97772300	-2.04928300	1.86076500
C	-6.18873600	-1.22146500	0.98848000
H	-5.99961200	-0.54602800	1.82488000
H	4.60574100	2.99114000	-1.73920300
H	0.22530900	-0.49264400	1.25502400
Se	-3.81694800	-0.03139300	-0.13186700
H	-8.38829400	-3.61869900	-0.02963800

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -4202.2177675

Electronic Energy (0K) + ZPE = -4201.678484

Enthalpy (298K) = -4201.645382

Free Energy (298K) = -4201.747789

$TS_{2'''}$

Number of imaginary frequencies: 1

C	0.56008700	-2.99534200	-2.29037400
C	-0.06574900	-1.76157200	-2.23444500
C	0.40476500	-0.77718700	-1.32264200
C	1.65070000	-1.00049100	-0.66802200
C	2.25437600	-2.25927000	-0.69159600
C	1.69380300	-3.25831900	-1.50936300
C	3.40407300	-2.58157700	0.20677300
C	3.31978700	-3.65386400	1.01052700
N	2.08432000	-0.03634200	0.28737900
C	1.34011000	-0.06584800	1.55248800
C	-0.16707200	0.10052800	1.35286600
C	-0.77571900	-0.92525700	0.43618100

C	-2.15938200	-0.68414300	-0.06200600
C	4.62170500	-1.72473900	0.18772800
C	5.09778300	-1.18849700	-1.01525700
C	6.27602700	-0.44324300	-1.04241800
C	6.98961100	-0.21304500	0.13316500
C	6.51368300	-0.72730900	1.34100500
C	5.33778000	-1.47305000	1.36785400
C	1.52558300	2.62714700	-0.26510700
C	1.22603300	3.37568600	0.87409100
C	0.17502000	4.28581300	0.82312400
C	-0.57162200	4.46758400	-0.35091800
C	-0.22743800	3.72339500	-1.48696000
C	0.81996500	2.80504000	-1.45331500
C	-1.71369600	5.44475500	-0.37722100
S	2.80027500	1.38559400	-0.19629800
O	3.70841000	1.78261200	0.86854900
O	3.27270700	1.16402500	-1.55510400
H	0.17770400	-3.76993700	-2.95799100
H	-0.94046300	-1.55075500	-2.85193100
H	0.05621500	0.25326800	-1.43150300
H	2.17359800	-4.23746100	-1.54995700
H	4.15287500	-3.94587700	1.65458600
H	2.41641600	-4.26817700	1.03935300
H	1.73982700	0.71743500	2.21155000
H	1.55422300	-1.03448300	2.03344800
H	-0.64679300	0.03031500	2.34683800
H	-0.39914200	1.11113600	0.97638200
H	-0.55867100	-1.97149300	0.68276800
H	-2.49637300	-1.47085700	-0.75279700
H	-2.28545200	0.30703900	-0.52669700

H	4.54031500	-1.35559300	-1.93871400
H	6.63520300	-0.03614700	-1.98952400
H	7.90831100	0.37603600	0.11174900
H	7.05523700	-0.53582400	2.26930300
H	4.95732800	-1.85496000	2.31771300
H	1.81260200	3.24744500	1.78536900
H	-0.07095900	4.87413300	1.71017600
H	-0.78214100	3.87169800	-2.41581500
H	1.09453700	2.23536100	-2.34284500
H	-2.13229300	5.54454500	-1.38684800
H	-2.51767200	5.11663600	0.29908300
H	-1.38668000	6.43743400	-0.03512200
C	-4.94882200	-0.73602100	0.55890500
C	-5.54305200	-1.96227200	0.25895700
C	-6.79708200	-1.96749500	-0.34106300
C	-7.46194000	-0.76772500	-0.64118300
C	-6.83883500	0.44553300	-0.32335800
C	-5.58285800	0.47165700	0.27946700
C	-8.81551700	-0.79934300	-1.29464500
S	-3.34016300	-0.71180400	1.31764500
O	-3.14632000	-1.97683700	2.03031100
O	-3.20949800	0.54980900	2.05359200
H	-5.03036800	-2.89330300	0.50739200
H	-7.27910900	-2.91942500	-0.57534200
H	-7.35022800	1.38495300	-0.54279800
H	-5.10301500	1.41566500	0.54358800
H	-9.51750300	-1.40970800	-0.70795900
H	-9.23396000	0.20987300	-1.39884700
H	-8.75065900	-1.25126000	-2.29604800

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4071295

Electronic Energy (0K) + ZPE = -2387.833857

Enthalpy (298K) = -2387.797889

Free Energy (298K) = -2387.902825

INT-2'''

Number of imaginary frequencies: 0

C	-0.63773500	-3.29282300	1.82993500
C	0.12804300	-2.16926100	1.75497200
C	-0.24908400	-1.02062900	0.87409900
C	-1.65138200	-1.12751100	0.35141600
C	-2.37211700	-2.30173500	0.38144300
C	-1.86203300	-3.40369600	1.11660100
C	-3.62731800	-2.47516700	-0.41658000
C	-3.68094800	-3.47100900	-1.31465100
N	-2.07980600	-0.03830300	-0.45883200
C	-1.24747700	0.12913200	-1.66022500
C	0.23754600	0.23208700	-1.31537100
C	0.71084600	-0.88011300	-0.36816300
C	2.13402600	-0.64975500	0.13729600
C	-4.78990500	-1.57826800	-0.17966700
C	-5.07363900	-1.11101800	1.10961200
C	-6.19723600	-0.32052300	1.34770300
C	-7.05121800	0.01972800	0.29945100
C	-6.77229500	-0.43199200	-0.99262400
C	-5.65011400	-1.22136800	-1.23028000
C	-1.39378900	2.53988700	0.34417600
C	-1.17464500	3.38708000	-0.74124500
C	-0.06602200	4.22863600	-0.72559100
C	0.81887900	4.24044800	0.36231100

C	0.54043000	3.41690400	1.46297600
C	-0.56124500	2.56571900	1.46248700
C	2.05012000	5.10165700	0.33782200
S	-2.70555400	1.34048200	0.26687900
O	-3.70583100	1.87690700	-0.64201000
O	-3.04298300	0.96569600	1.63320600
H	-0.31560000	-4.12767000	2.45567400
H	1.05406700	-2.09823300	2.32917500
H	-0.14271200	-0.07126900	1.43389600
H	-2.44128800	-4.32621300	1.15770700
H	-4.58684000	-3.66675500	-1.89322800
H	-2.81864400	-4.11937200	-1.48841700
H	-1.59308400	1.01133500	-2.21753300
H	-1.43474800	-0.74838300	-2.29783300
H	0.81302500	0.18139700	-2.25084100
H	0.46159400	1.20958400	-0.86107600
H	0.68414400	-1.84347900	-0.90323600
H	2.52439100	-1.53459400	0.65840800
H	2.20528100	0.22588200	0.80131500
H	-4.40241100	-1.36142200	1.93247600
H	-6.40166300	0.03591200	2.35892200
H	-7.92716600	0.64390600	0.48521700
H	-7.42631800	-0.15673600	-1.82208400
H	-5.42296800	-1.55080000	-2.24612000
H	-1.86298300	3.38162000	-1.58803800
H	0.11999600	4.88850800	-1.57550700
H	1.19851200	3.44427400	2.33415300
H	-0.77950400	1.92898500	2.32161900
H	2.38686700	5.34699800	1.35361200
H	2.86974400	4.56681100	-0.16830800

H	1.87365300	6.03411300	-0.21482700
C	4.89063900	-0.62194600	-0.47990200
C	5.43574600	-1.90558300	-0.52514200
C	6.68303500	-2.12227200	0.04903700
C	7.38989600	-1.07554200	0.66271700
C	6.81725700	0.20225700	0.68407500
C	5.56803100	0.43975200	0.11289000
C	8.73921200	-1.33420700	1.27287000
S	3.29134200	-0.33477000	-1.20302300
O	3.06531600	-1.35551600	-2.23079500
O	3.21629400	1.08204300	-1.57123700
H	4.89019100	-2.71432700	-1.01440500
H	7.12442600	-3.12092300	0.01814900
H	7.36090600	1.02607600	1.15079000
H	5.12735400	1.43813000	0.11608000
H	9.44820400	-1.68562400	0.50839700
H	9.14996300	-0.42789800	1.73537500
H	8.67428500	-2.11934500	2.04062000

SMD-UM06-2X/Def2-SVP

Electronic Energy (0K) = -2388.4322566

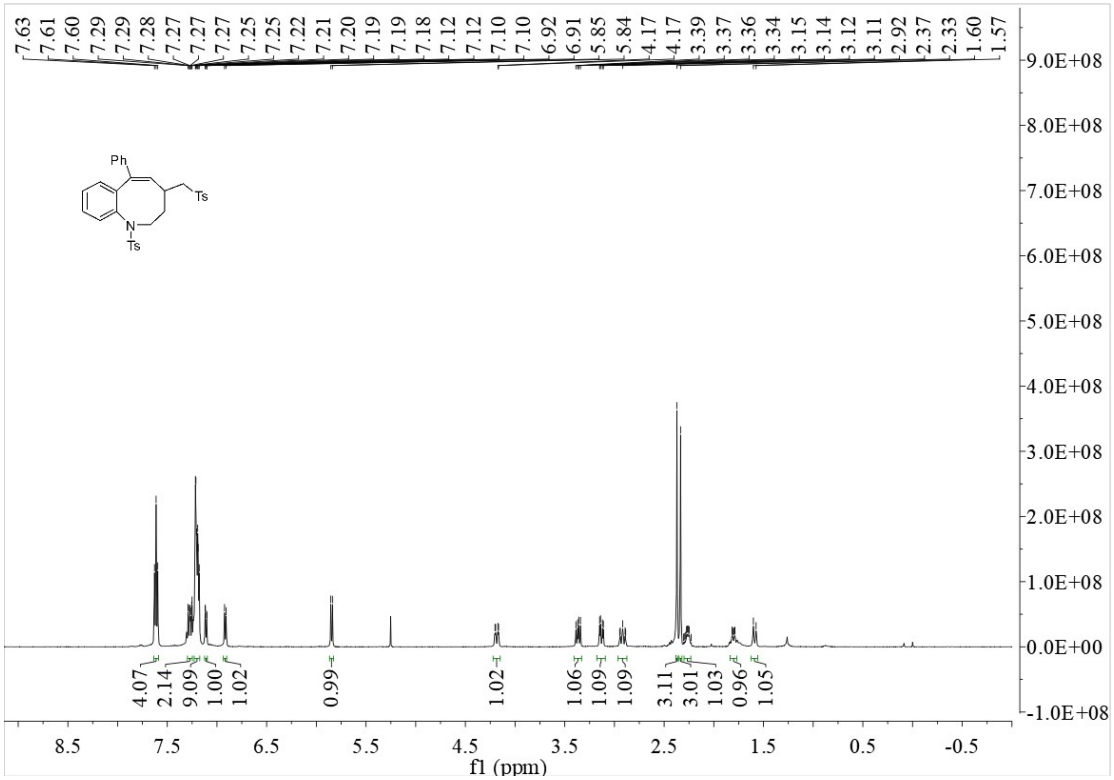
Electronic Energy (0K) + ZPE = -2387.857614

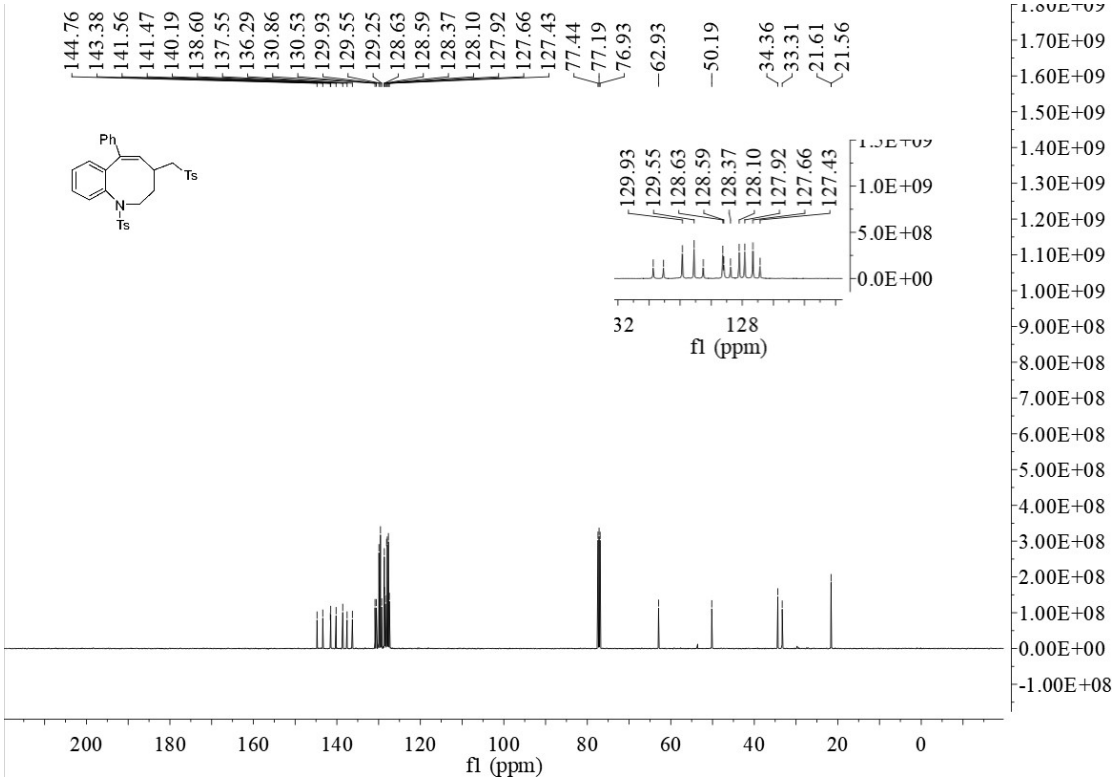
Enthalpy (298K) = -2387.821210

Free Energy (298K) = -2387.929980

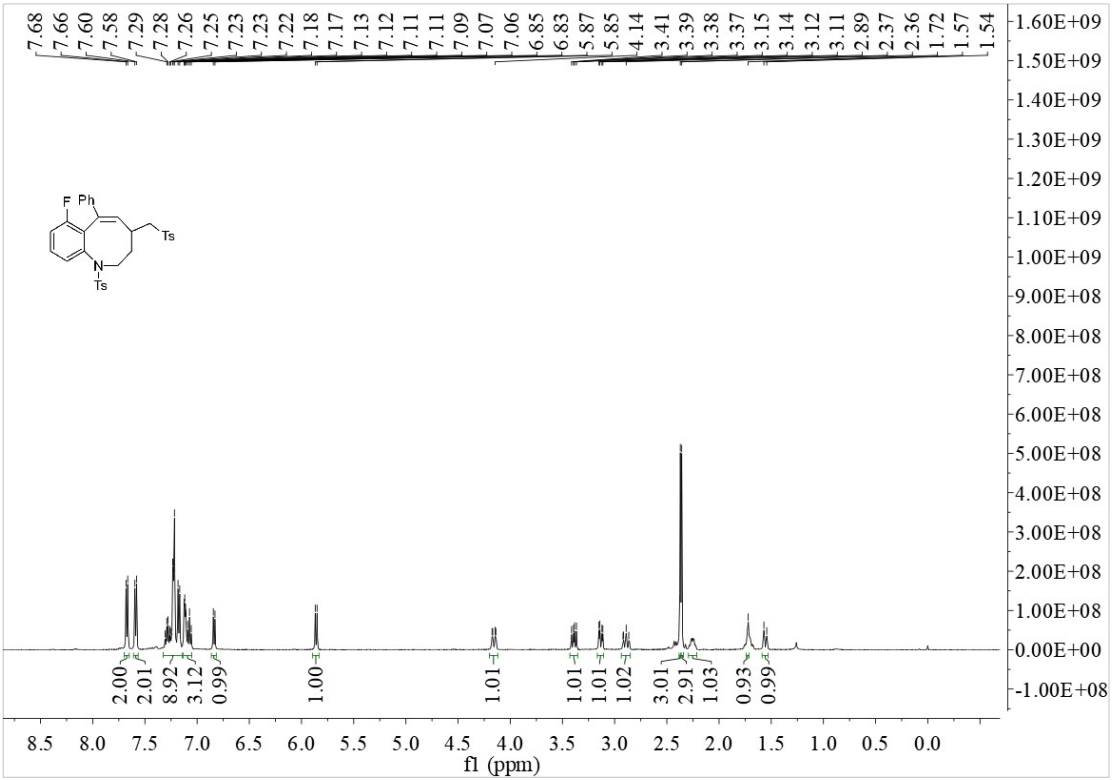
8. NMR Spectra of Products

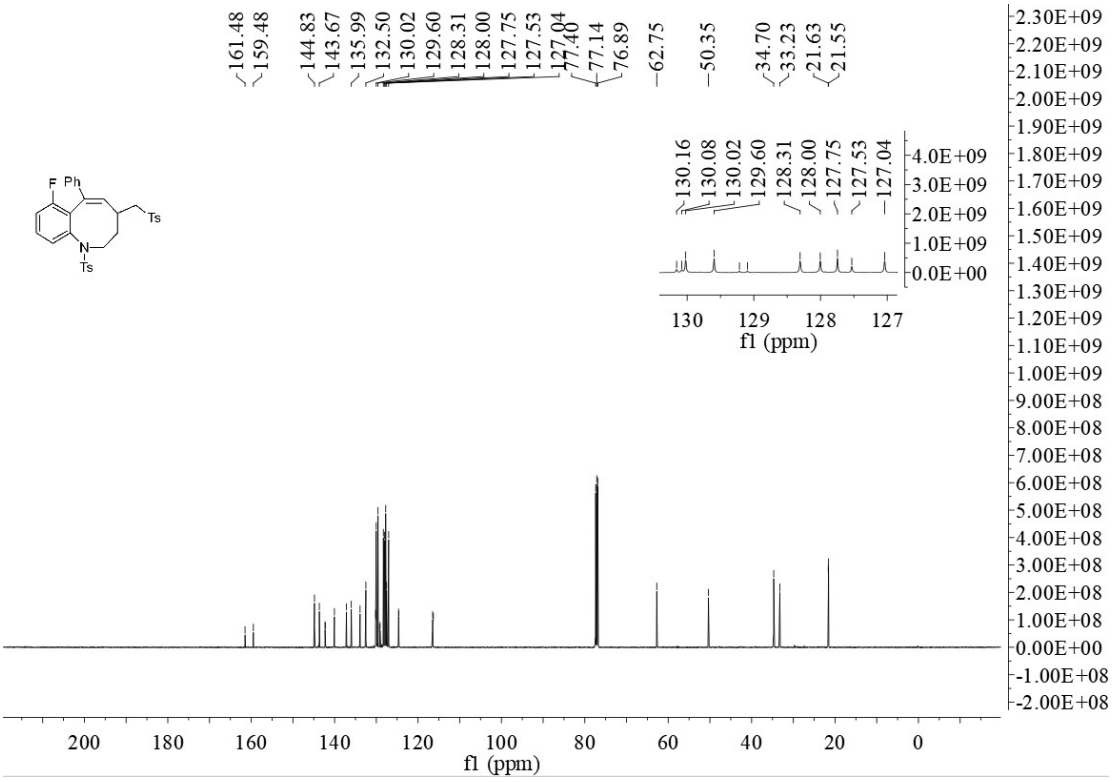
Compound 3a

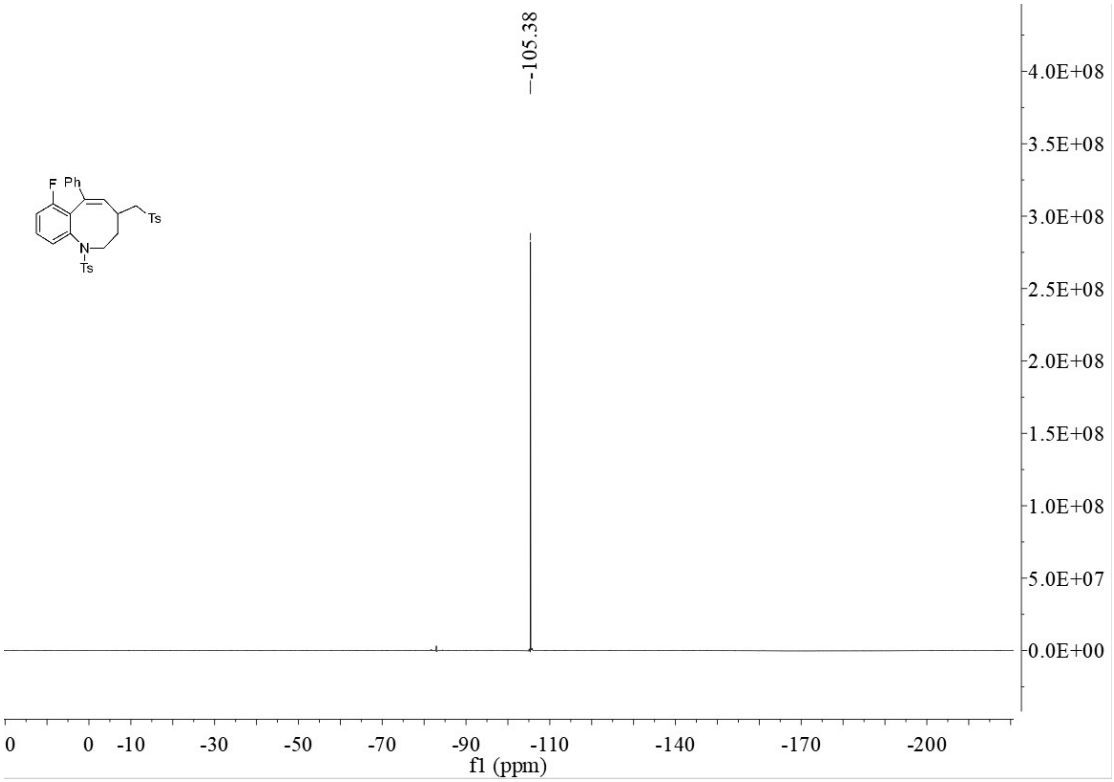




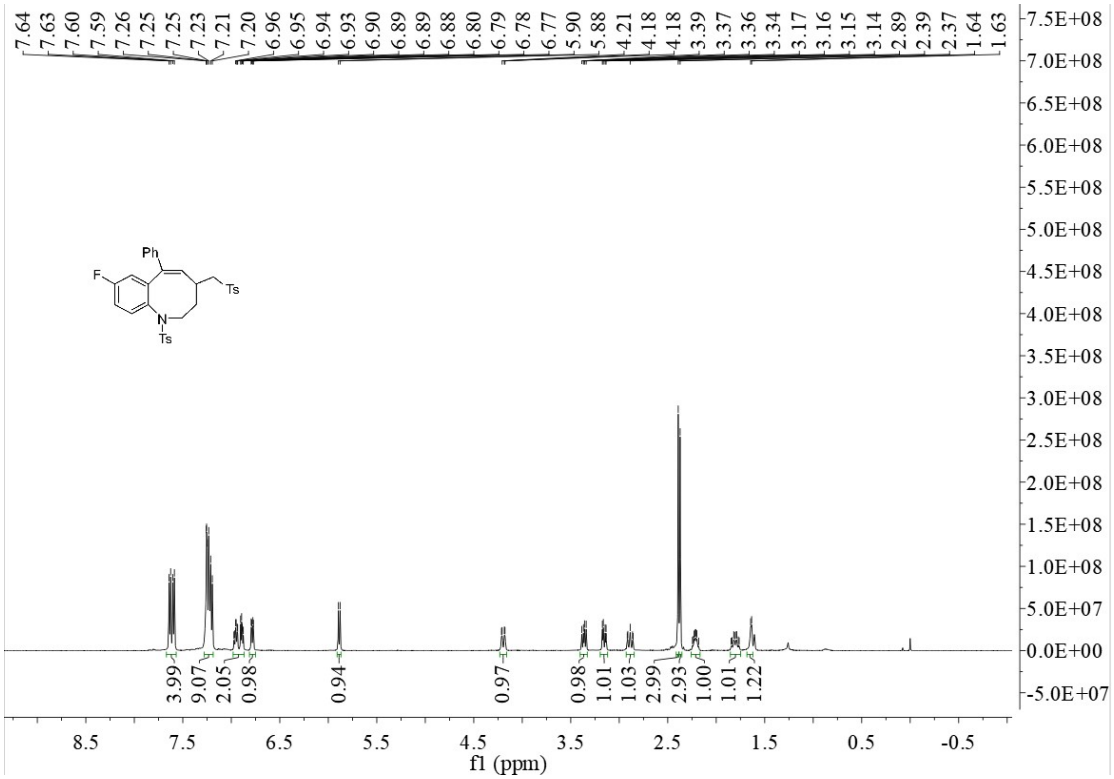
Compound 3b

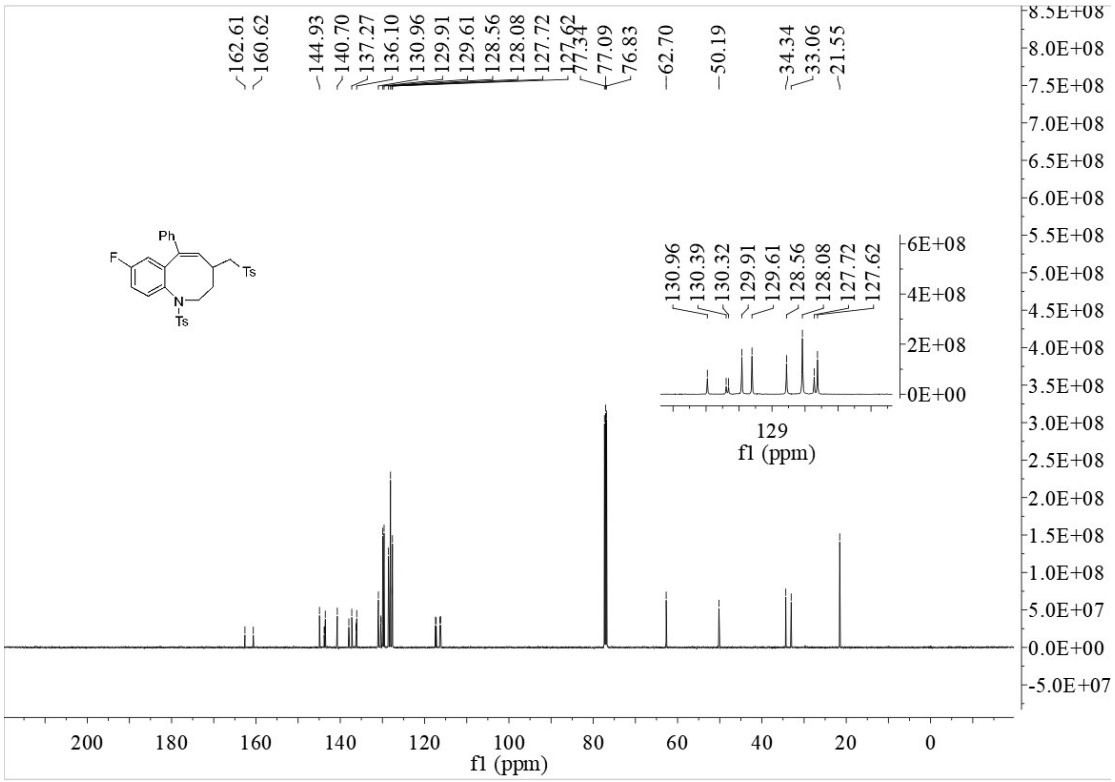

7.68 7.66 7.60 7.58 7.29 7.28 7.26 7.25 7.23 7.23 7.22 7.18 7.17 7.13 7.12 7.11 7.11 7.09 7.07 7.06 6.85 6.83 5.87 5.85 4.14 3.41 3.39 3.38 3.37 3.15 3.14 3.12 3.11 2.89 2.37 2.36 1.72 1.57 1.54
F Ph
Ts
N
Ts
2.00 2.01 8.92 3.12 0.99 1.00 1.01 1.01 1.01 1.02 3.01 2.91 1.03 0.93 0.99
fl (ppm)

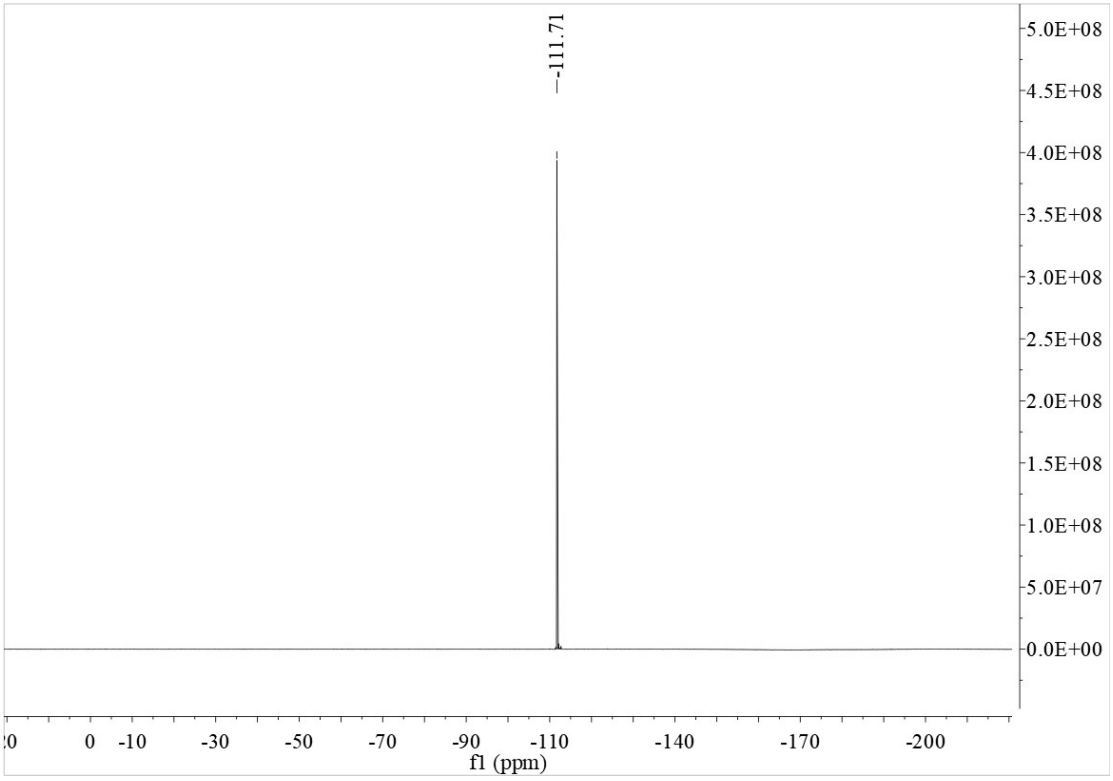

161.48 159.48 144.83 143.67 135.99 132.50 130.02 129.60 128.31 128.00 127.75 127.53 127.04 77.40 77.14 76.89 62.75 50.35 34.70 33.23 21.63 21.55
130.16 130.08 130.02 129.60 128.31 128.00 127.75 127.53 127.04
F Ph
Ts
N
Ts
fl (ppm)
fl (ppm)


-105.38
F
Ph
Ts
N
Ts
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
0 0 -10 -30 -50 -70 -90 -110 -140 -170 -200
f1 (ppm)

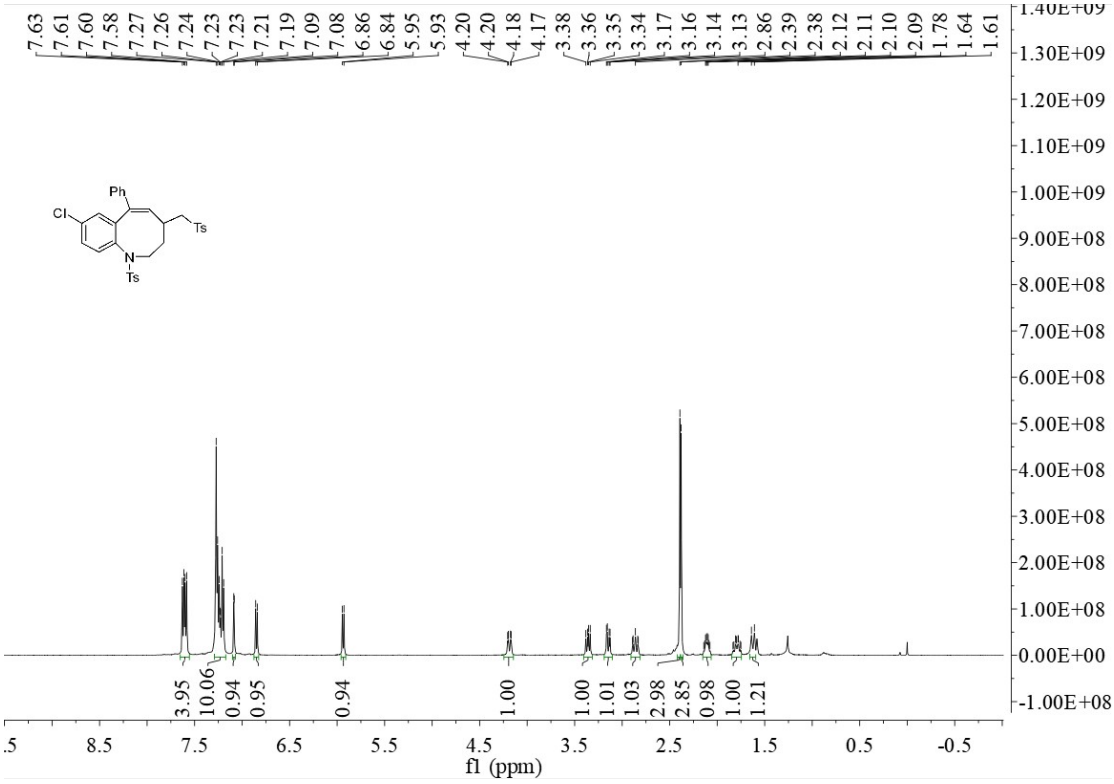
Compound 3c

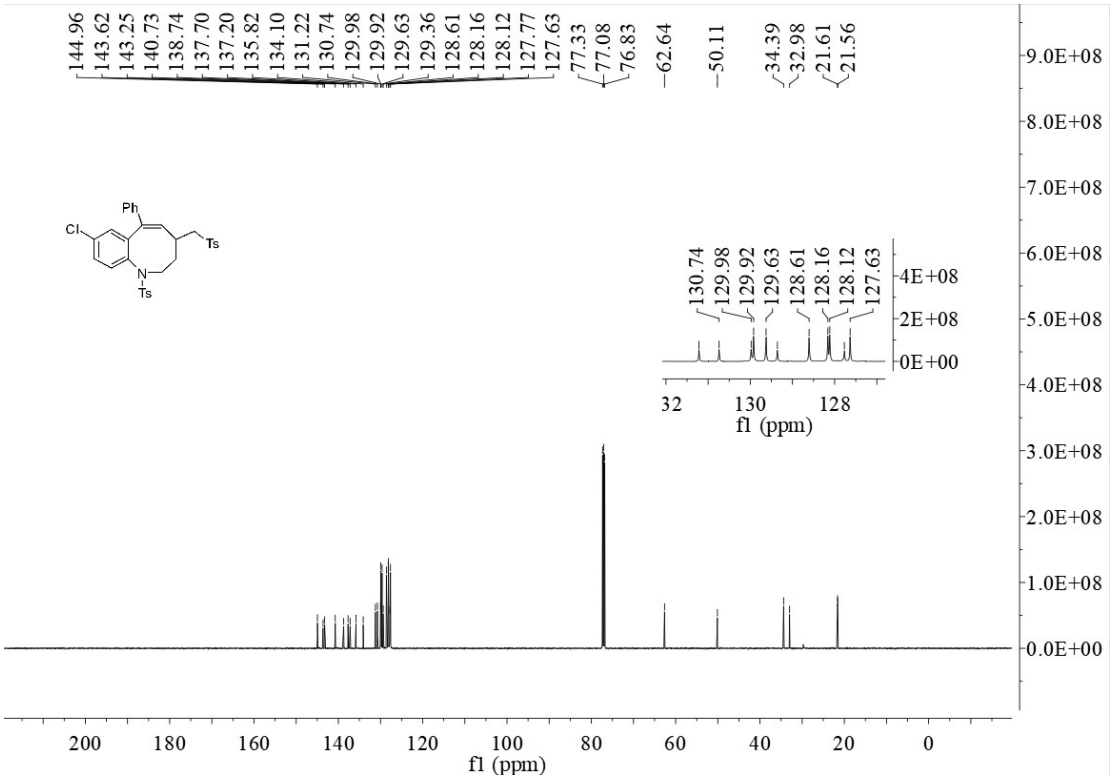

7.64 7.63 7.60 7.59 7.26 7.25 7.25 7.23 7.21 7.20 6.96 6.95 6.94 6.93 6.90 6.89 6.89 6.88 6.80 6.79 6.78 6.77 5.90 5.88 4.21 4.18 4.18 3.39 3.37 3.36 3.34 3.17 3.16 3.15 3.14 2.89 2.39 2.37 1.64 1.63
Ph
F
Ts
N
Ts
3.99 9.07 2.05 0.98 0.94 0.97 0.98 1.01 1.03 2.99 2.93 1.00 1.01 1.22
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)


162.61
160.62
144.93
140.70
137.27
136.10
130.96
129.91
129.61
128.56
128.08
127.72
127.62
77.34
77.09
76.83
62.70
50.19
34.34
33.06
21.55
Ph
F
Ts
N
Ts
130.96
130.39
130.32
129.91
129.61
128.56
128.08
127.72
127.62
6E+08
4E+08
2E+08
0E+00
129
f1 (ppm)
8.5E+08
8.0E+08
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

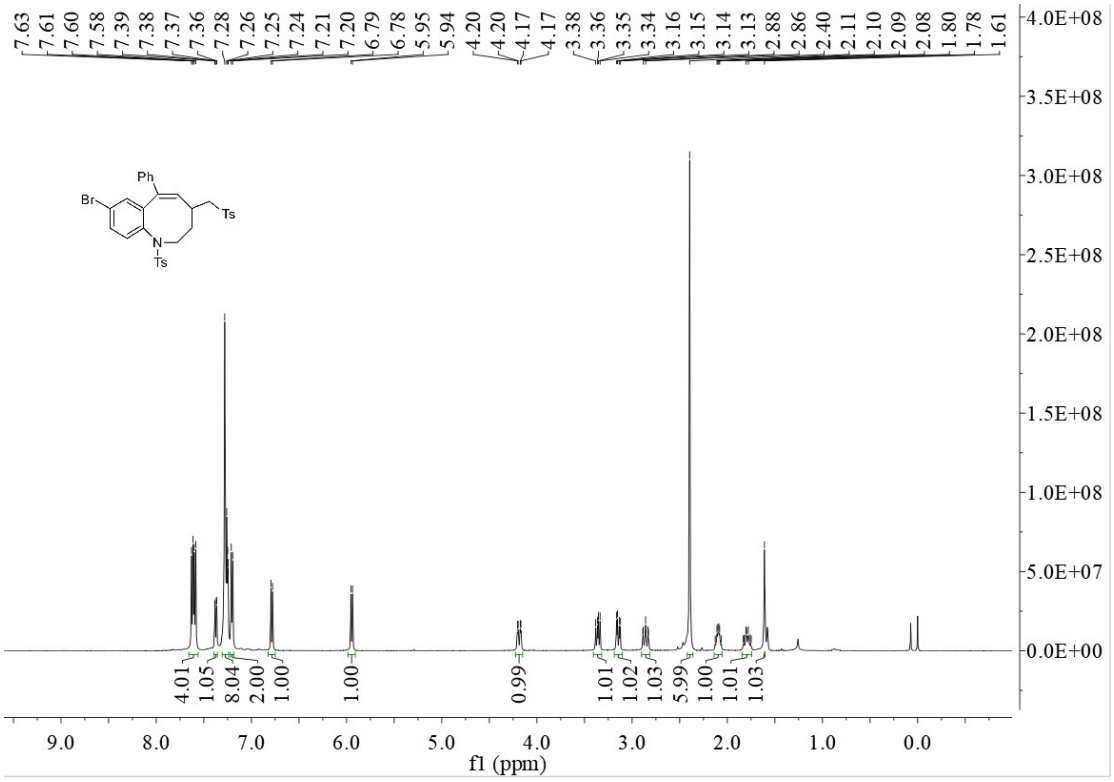

-111.71
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
0
-10
-30
-50
-70
-90
-110
-140
-170
-200
f1 (ppm)

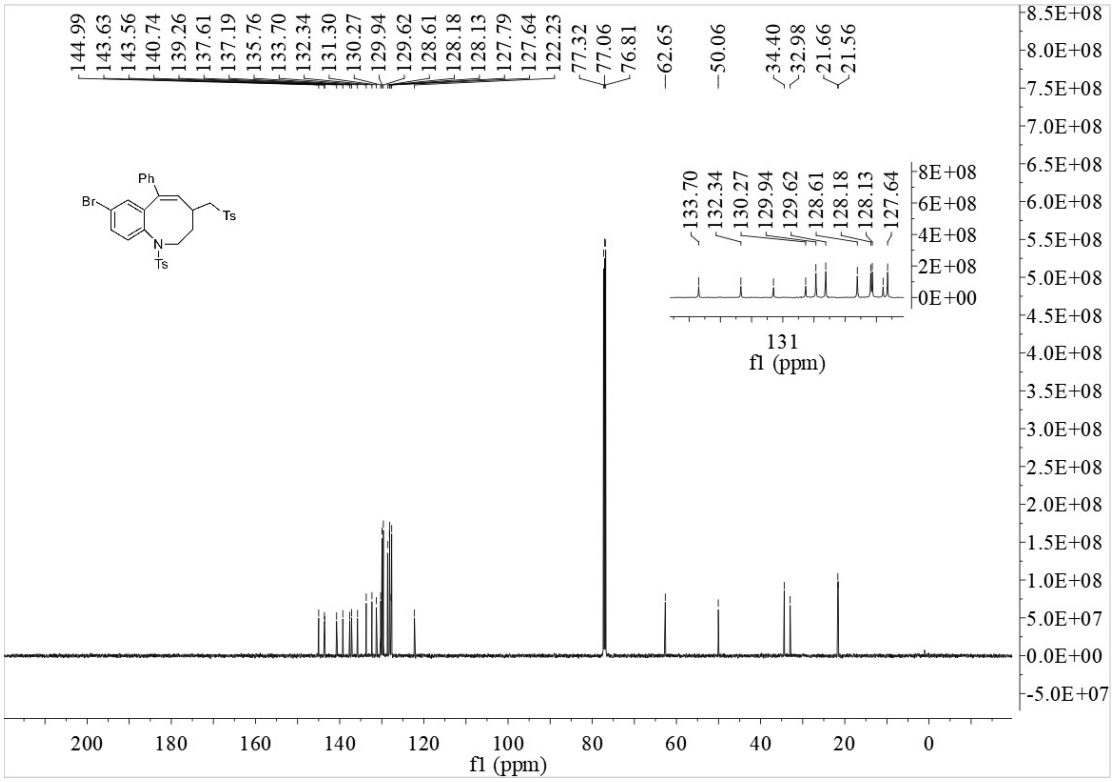
Compound 3d


7.63 7.61 7.60 7.58 7.27 7.26 7.24 7.23 7.23 7.21 7.19 7.09 7.08 6.86 6.84 5.95 5.93 4.20 4.20 4.18 4.17 3.38 3.36 3.35 3.34 3.17 3.16 3.14 3.13 2.86 2.39 2.38 2.12 2.11 2.10 2.09 1.78 1.64 1.61
Ph
Cl
Ts
N
Ts
3.95 10.06 0.94 0.95 0.94 1.00 1.00 1.01 1.03 2.98 2.85 0.98 1.00 1.21
fl (ppm)

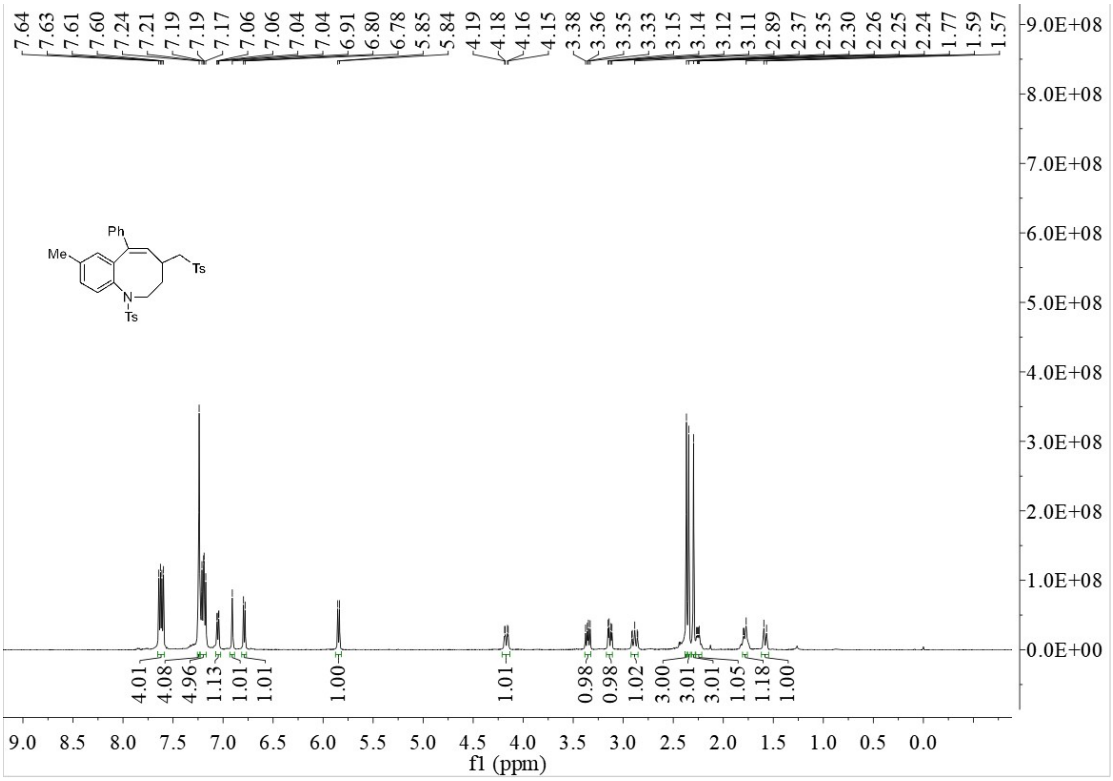

144.96 143.62 143.25 140.73 138.74 137.70 137.20 135.82 134.10 131.22 130.74 129.98 129.92 129.63 129.36 128.61 128.16 128.12 127.77 127.63 77.33 77.08 76.83 62.64 50.11 34.39 32.98 21.61 21.56
Ph
Cl
Ts
N
Ts
130.74 129.98 129.92 129.63 128.61 128.16 128.12 127.63
fl (ppm)
fl (ppm)

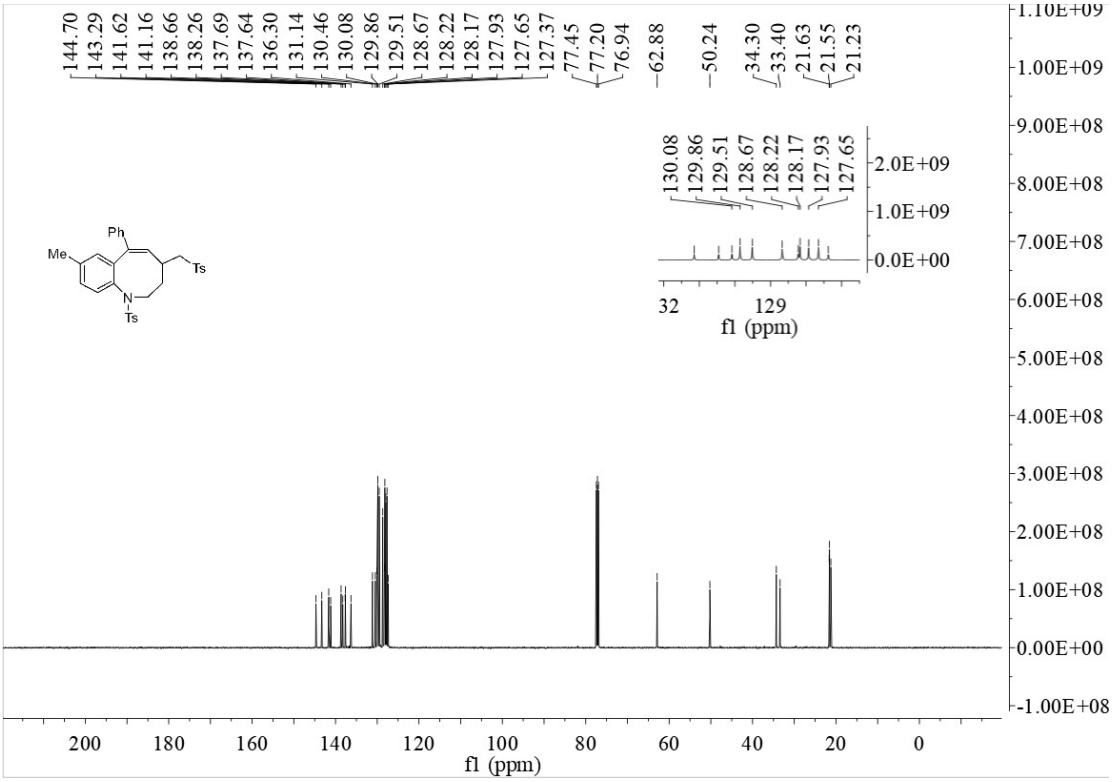
Compound 3e


7.63 7.61 7.60 7.58 7.39 7.38 7.37 7.36 7.28 7.26 7.25 7.24 7.21 7.20 6.79 6.78 5.95 5.94 4.20 4.20 4.17 4.17 3.38 3.36 3.35 3.34 3.16 3.15 3.14 3.13 2.88 2.86 2.40 2.11 2.10 2.09 2.08 1.80 1.78 1.61
Ph
Br
Ts
N
Ts
4.01 1.05 8.04 2.00 1.00 1.00 0.99 1.01 1.02 1.03 5.99 1.00 1.01 1.03
fl (ppm)

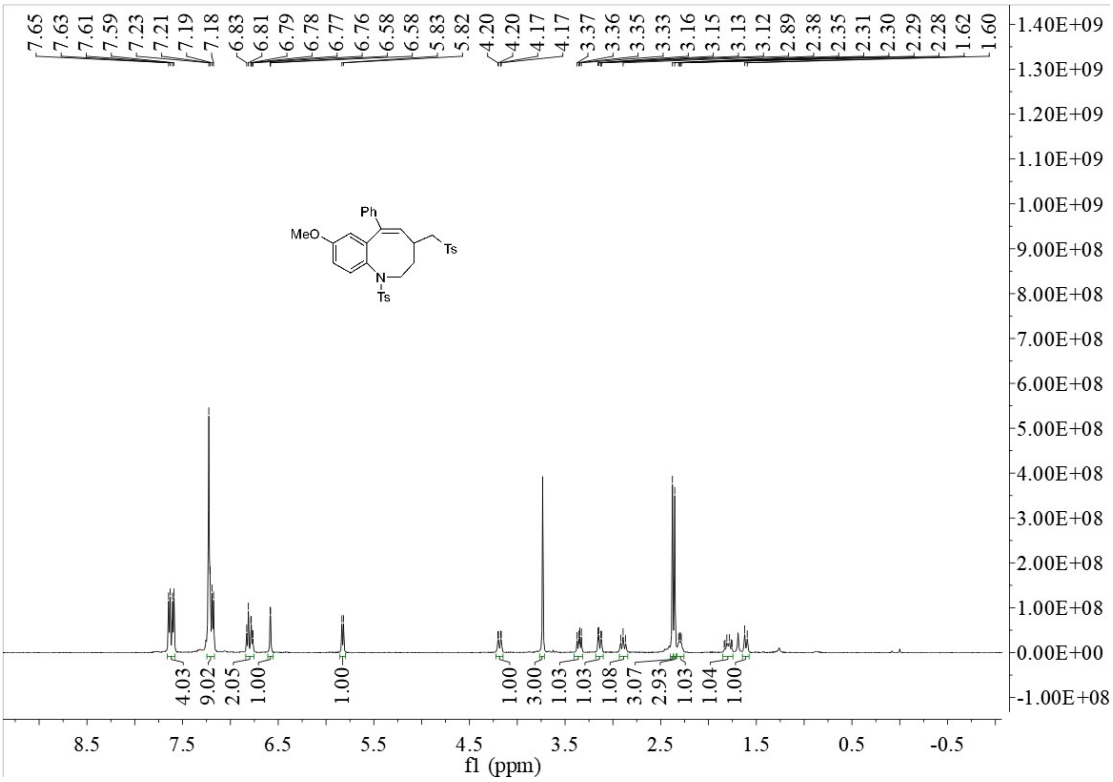

144.99 143.63 143.56 140.74 139.26 137.61 137.19 135.76 133.70 132.34 131.30 130.27 129.94 129.62 128.61 128.18 128.13 127.79 127.64 122.23 77.32 77.06 76.81 62.65 50.06 34.40 32.98 21.66 21.56
Ph
Br
Ts
N
Ts
133.70 132.34 130.27 129.94 129.62 128.61 128.18 128.13 127.64
131
fl (ppm)
fl (ppm)

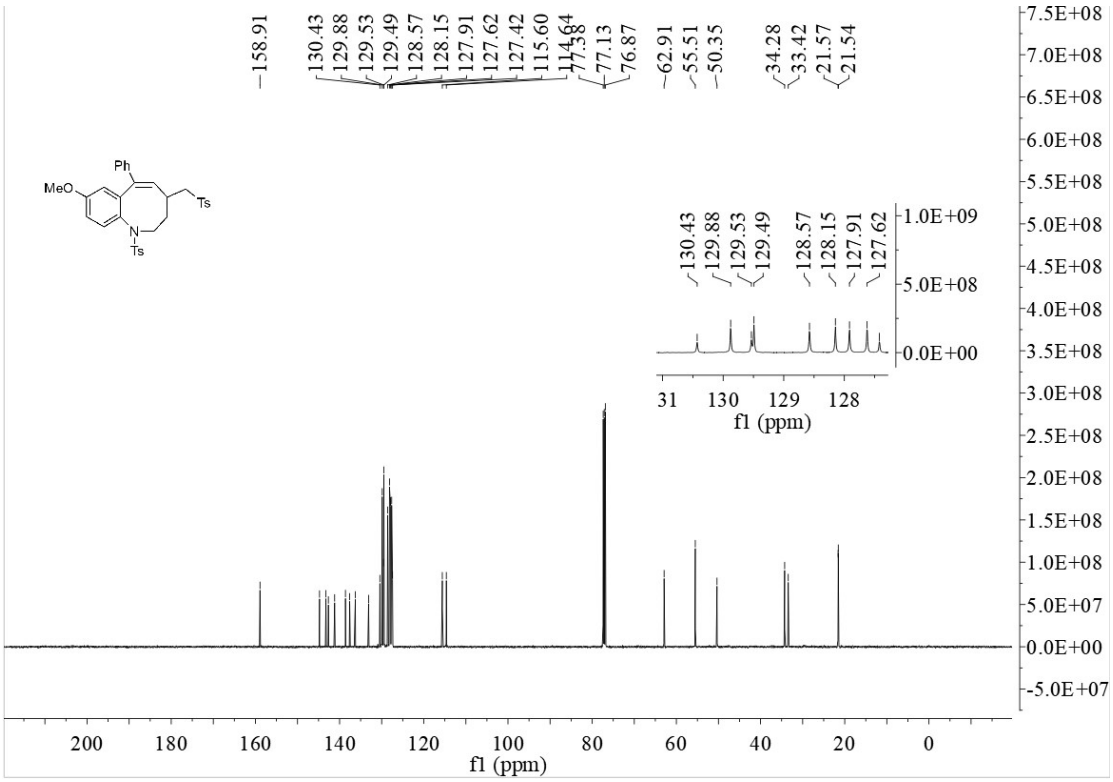
Compound 3f


7.64 7.63 7.61 7.60 7.24 7.21 7.19 7.19 7.17 7.06 7.06 7.04 7.04 6.91 6.80 6.78 5.85 5.84 4.19 4.18 4.16 4.15 3.38 3.36 3.35 3.33 3.15 3.14 3.12 3.11 2.89 2.37 2.35 2.30 2.26 2.25 2.24 1.77 1.59 1.57
Ph
Me
Ts
N
Ts
4.01 4.08 4.96 1.13 1.01 1.01 1.00 1.01 0.98 0.98 1.02 3.00 3.01 3.01 1.05 1.18 1.00
9.0E+08
8.0E+08
7.0E+08
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

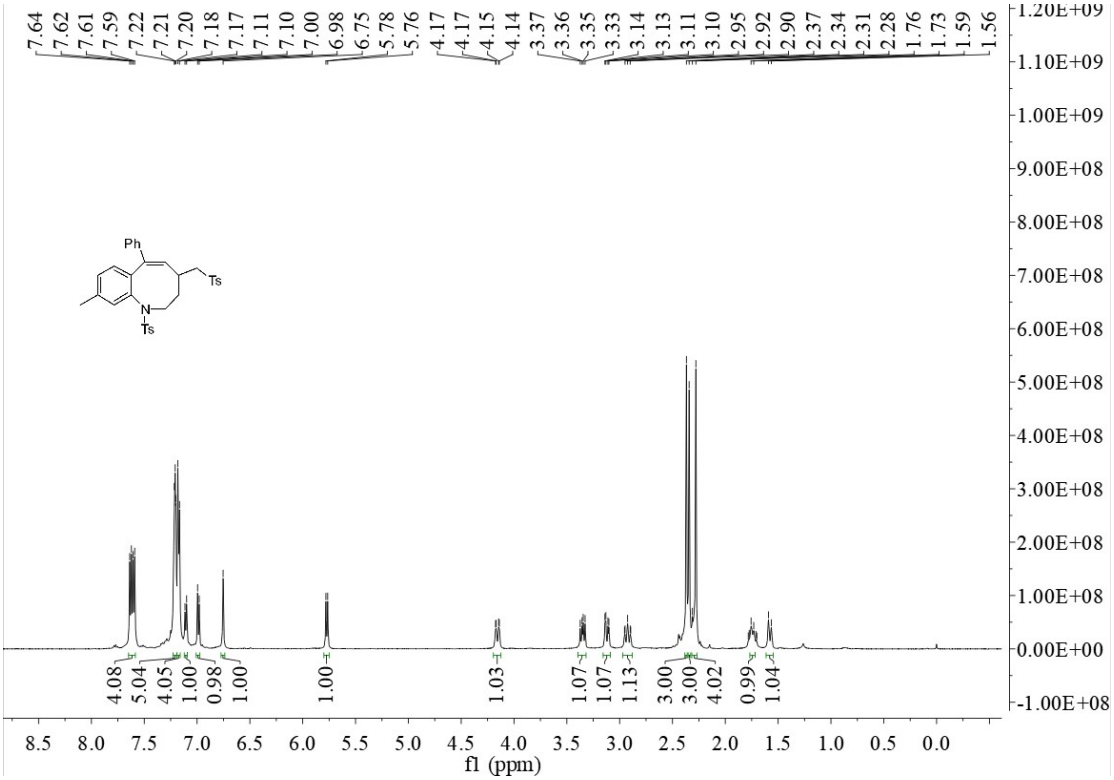

144.70 143.29 141.62 141.16 138.66 138.26 137.69 137.64 136.30 131.14 130.46 130.08 129.86 129.51 128.67 128.22 128.17 127.93 127.65 127.37 77.45 77.20 76.94 62.88 50.24 34.30 33.40 21.63 21.55 21.23
130.08 129.86 129.51 128.67 128.22 128.17 127.93 127.65
2.0E+09
1.0E+09
0.0E+00
32 129
f1 (ppm)
Ph
Me
Ts
N
Ts
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

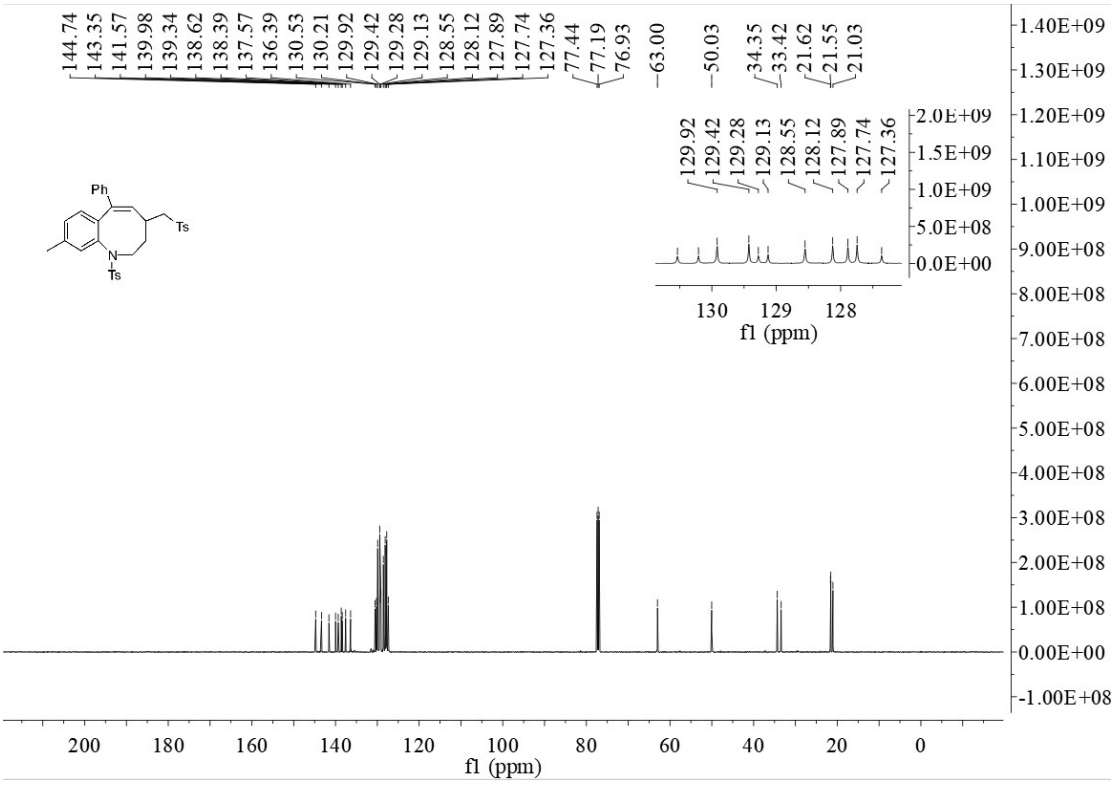
Compound 3g


7.65
7.63
7.61
7.59
7.23
7.21
7.19
7.18
6.83
6.81
6.79
6.78
6.77
6.76
6.58
6.58
5.83
5.82
4.20
4.20
4.17
4.17
3.37
3.36
3.35
3.33
3.16
3.15
3.13
3.12
2.89
2.38
2.35
2.31
2.30
2.29
2.28
1.62
1.60
Ph
MeO
Ts
N
Ts
4.03
9.02
2.05
1.00
1.00
1.00
3.00
1.03
1.03
1.08
3.07
2.93
1.03
1.04
1.00
fl (ppm)

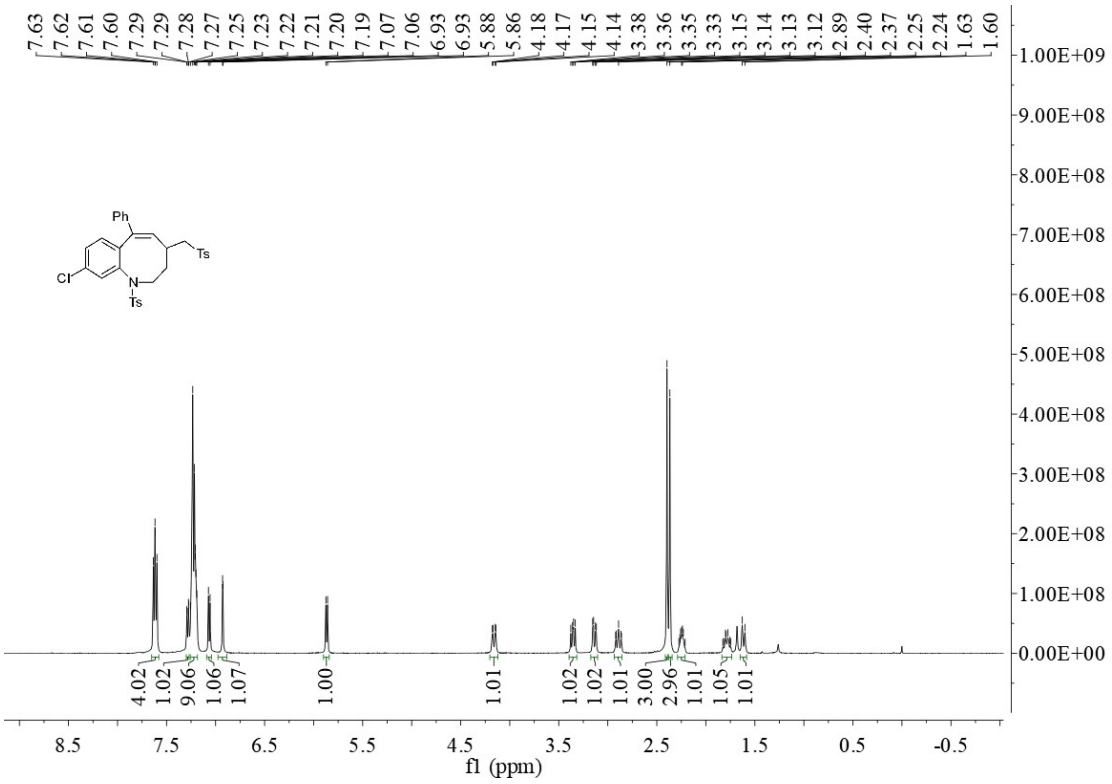

158.91
130.43
129.88
129.53
129.49
128.57
128.15
127.91
127.62
127.42
115.60
114.64
77.38
77.13
76.87
62.91
55.51
50.35
34.28
33.42
21.57
21.54
Ph
MeO
Ts
N
Ts
130.43
129.88
129.53
129.49
128.57
128.15
127.91
127.62
fl (ppm)
fl (ppm)

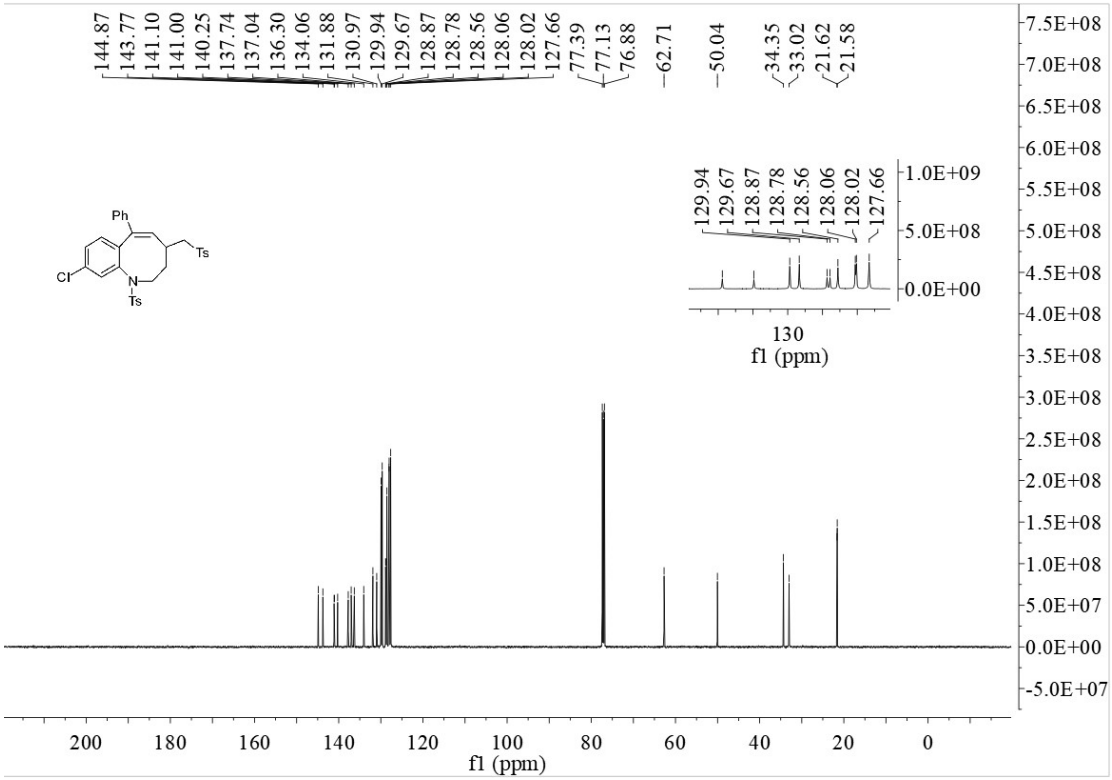
Compound 3h


7.64 7.62 7.61 7.59 7.22 7.21 7.20 7.18 7.17 7.11 7.10 7.00 6.98 6.75 5.78 5.76 4.17 4.17 4.15 4.14 3.37 3.36 3.35 3.33 3.14 3.13 3.11 3.10 2.95 2.92 2.90 2.37 2.34 2.31 2.28 1.76 1.73 1.59 1.56
Ph
Ts
N
Ts
4.08 5.04 4.05 1.00 0.98 1.00 1.00 1.03 1.07 1.07 1.13 3.00 3.00 4.02 0.99 1.04
fl (ppm)

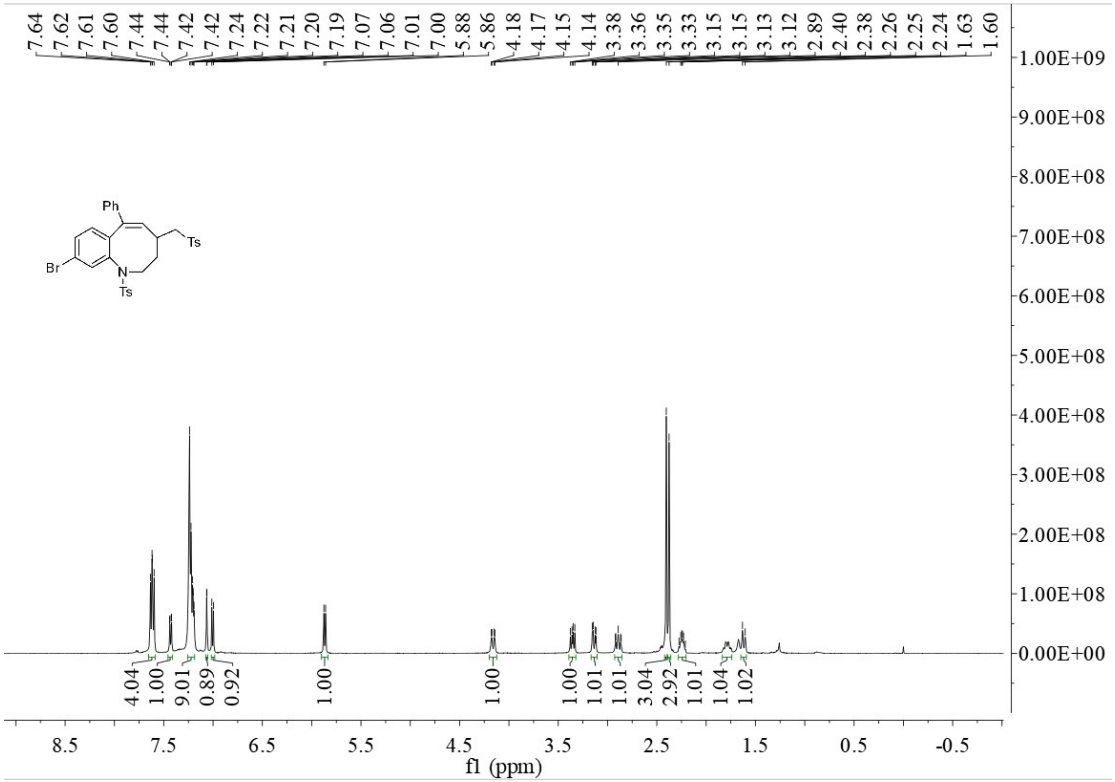

144.74 143.35 141.57 139.98 139.34 138.62 138.39 137.57 136.39 130.53 130.21 129.92 129.42 129.28 129.13 128.55 128.12 127.89 127.74 127.36 77.44 77.19 76.93 63.00 50.03 34.35 33.42 21.62 21.55 21.03
129.92 129.42 129.28 129.13 128.55 128.12 127.89 127.74 127.36
Ph
Ts
N
Ts
fl (ppm)
fl (ppm)

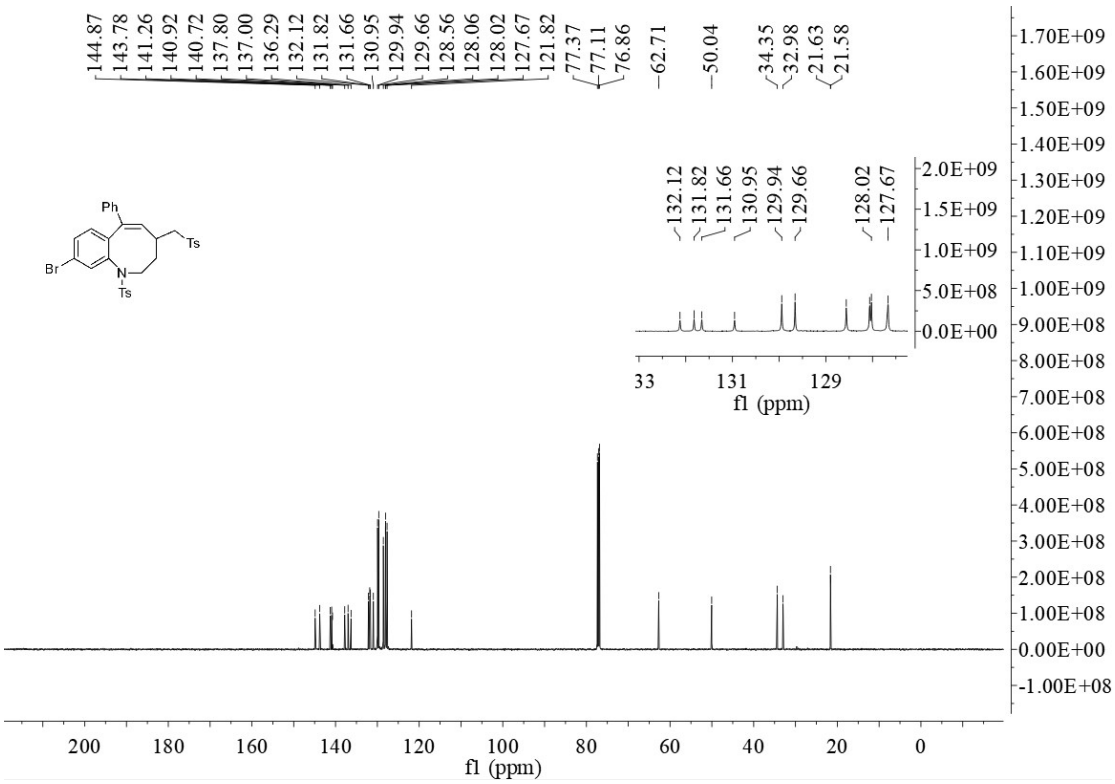
Compound 3i


7.63 7.62 7.61 7.60 7.29 7.29 7.28 7.27 7.25 7.23 7.22 7.21 7.20 7.19 7.07 7.06 6.93 6.93 5.88 5.86 4.18 4.17 4.15 4.14 3.38 3.36 3.35 3.33 3.15 3.14 3.13 3.12 2.89 2.40 2.37 2.25 2.24 1.63 1.60
Ph
Ts
Cl
N
Ts
4.02 1.02 9.06 1.06 1.07 1.00 1.01 1.02 1.02 1.01 3.00 2.96 1.01 1.05 1.01
fl (ppm)

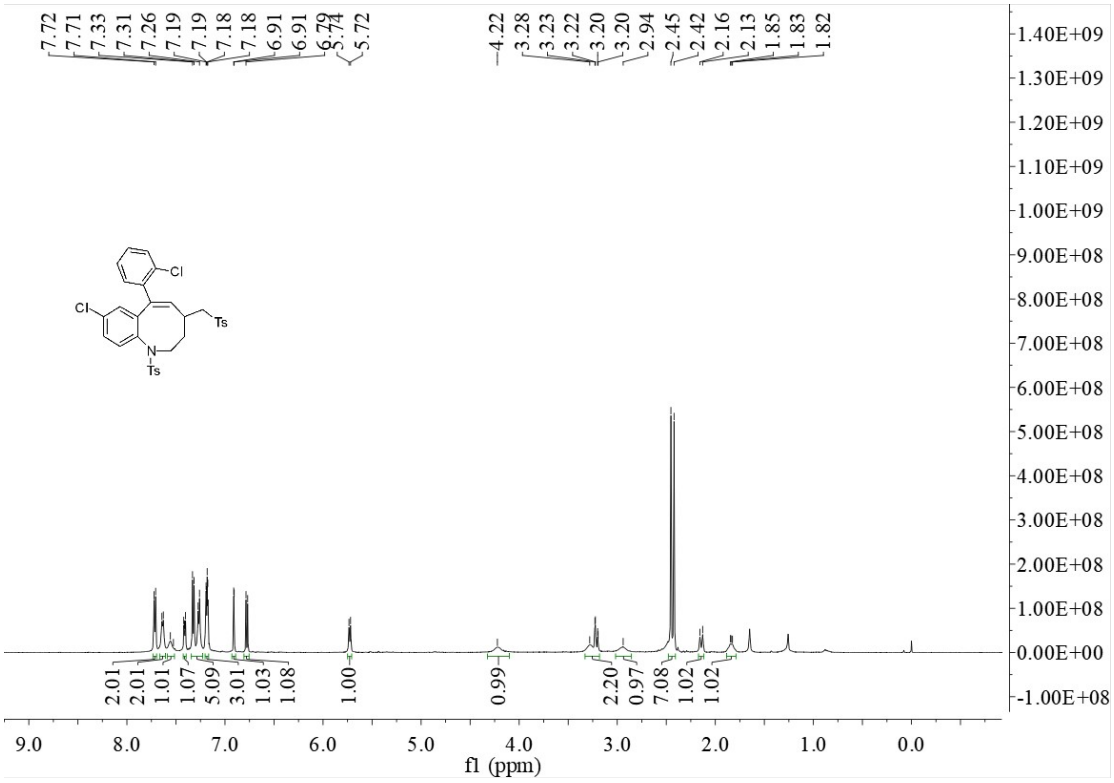

144.87 143.77 141.10 141.00 140.25 137.74 137.04 136.30 134.06 131.88 130.97 129.94 129.67 128.87 128.78 128.56 128.06 128.02 127.66 77.39 77.13 76.88 62.71 50.04 34.35 33.02 21.62 21.58
Ph
Ts
Cl
N
Ts
129.94 129.67 128.87 128.78 128.56 128.06 128.02 127.66
130
fl (ppm)
fl (ppm)

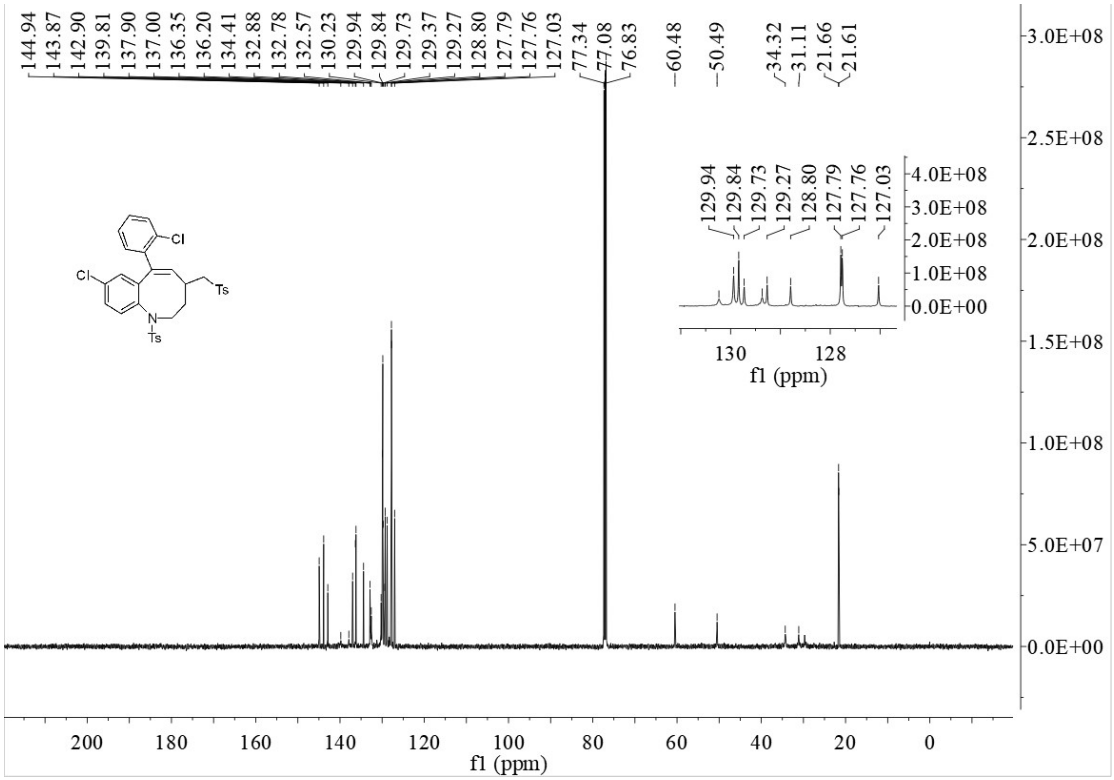
Compound 3j


7.64 7.62 7.61 7.60 7.44 7.44 7.42 7.42 7.24 7.22 7.21 7.20 7.19 7.07 7.06 7.01 7.00 5.88 5.86 4.18 4.17 4.15 4.14 3.38 3.36 3.35 3.33 3.15 3.15 3.13 3.12 2.89 2.40 2.38 2.26 2.25 2.24 1.63 1.60
Ph
Ts
Br
N
Ts
4.04 1.00 9.01 0.89 0.92 1.00 1.00 1.00 1.01 1.01 3.04 2.92 1.01 1.04 1.02
fl (ppm)

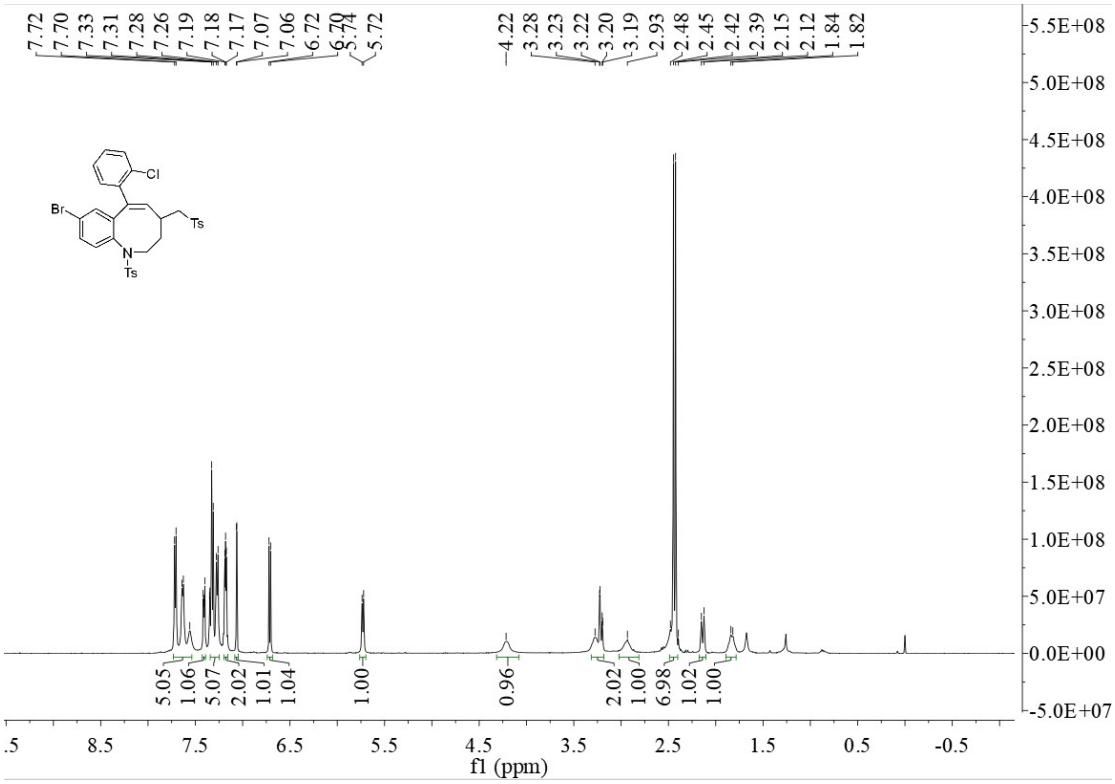

144.87 143.78 141.26 140.92 140.72 137.80 137.00 136.29 132.12 131.82 131.66 130.95 129.94 129.66 128.56 128.06 128.02 127.67 121.82 77.37 77.11 76.86 62.71 50.04 34.35 32.98 21.63 21.58
Ph
Ts
Br
N
Ts
132.12 131.82 131.66 130.95 129.94 129.66 128.02 127.67
fl (ppm)
fl (ppm)

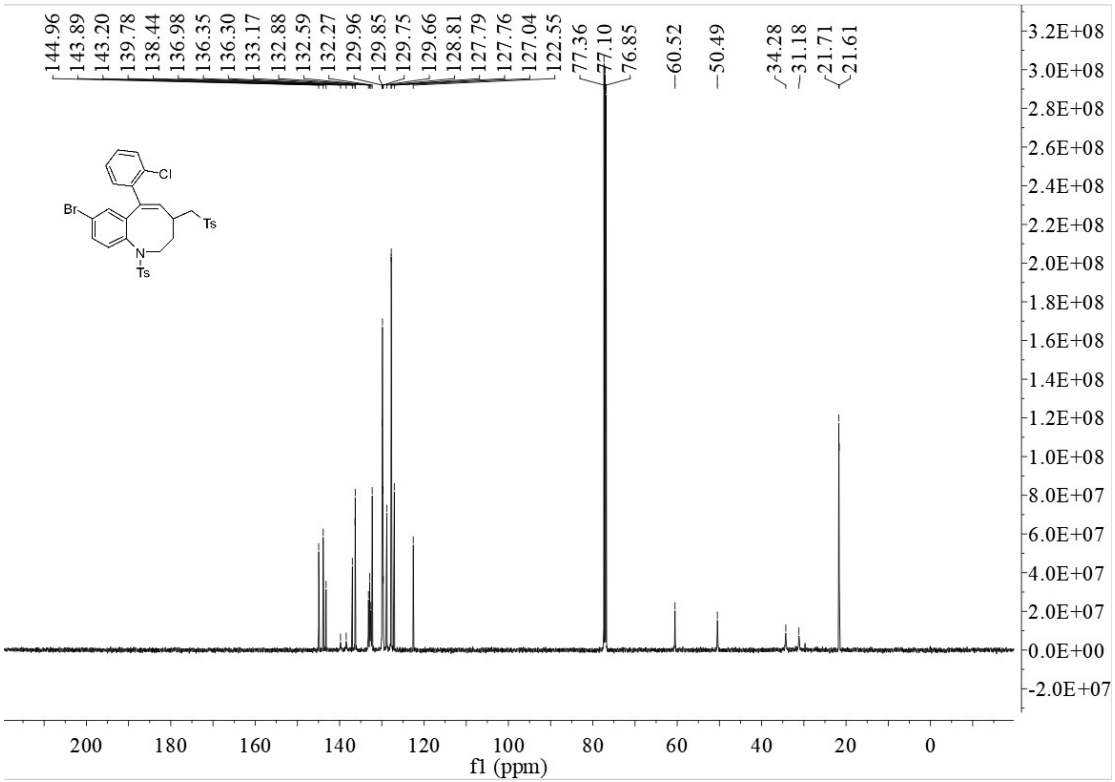
Compound 3k


7.72
7.71
7.33
7.31
7.26
7.19
7.19
7.18
7.18
6.91
6.91
6.79
5.74
5.72
4.22
3.28
3.23
3.22
3.20
3.20
2.94
2.45
2.42
2.16
2.13
1.85
1.83
1.82
Cl
Cl
Ts
N
Ts
2.01
2.01
1.01
1.07
5.09
3.01
1.03
1.08
1.00
0.99
2.20
0.97
7.08
1.02
1.02
1.40E+09
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

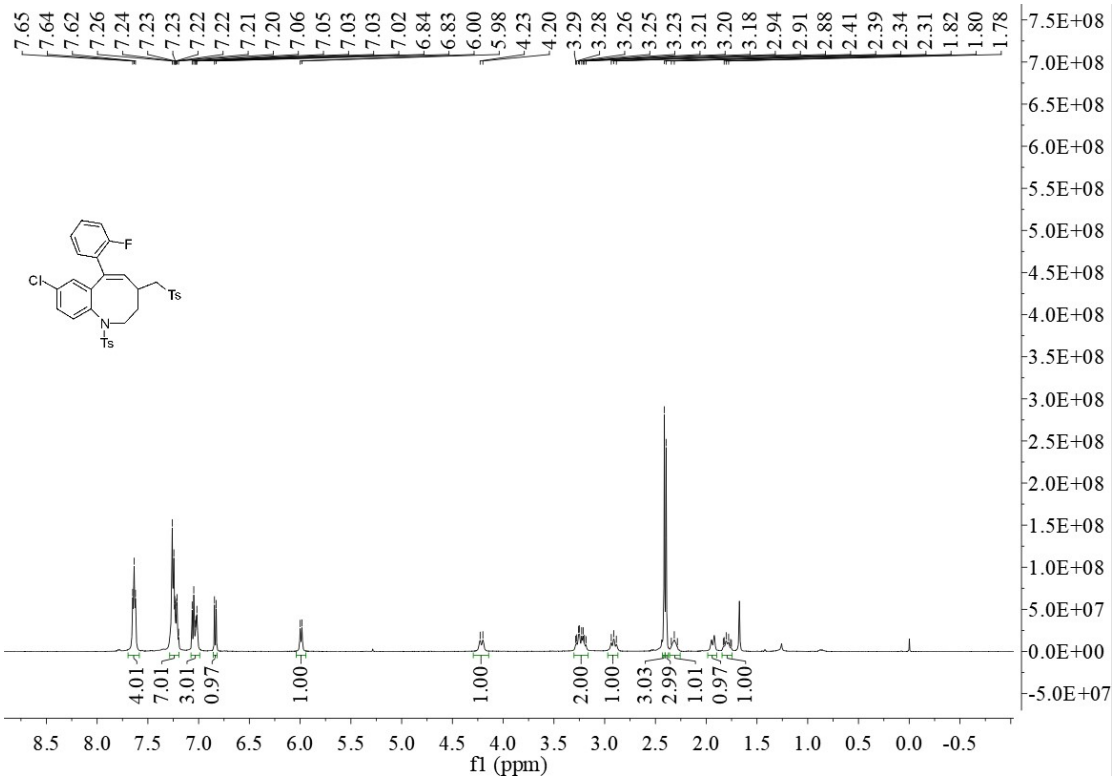

144.94
143.87
142.90
139.81
137.90
137.00
136.35
136.20
134.41
132.88
132.78
132.57
130.23
129.94
129.84
129.73
129.37
129.27
128.80
127.79
127.76
127.03
77.34
77.08
76.83
60.48
50.49
34.32
31.11
21.66
21.61
Cl
Cl
Ts
N
Ts
129.94
129.84
129.73
129.27
128.80
127.79
127.76
127.03
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
130
128
f1 (ppm)
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

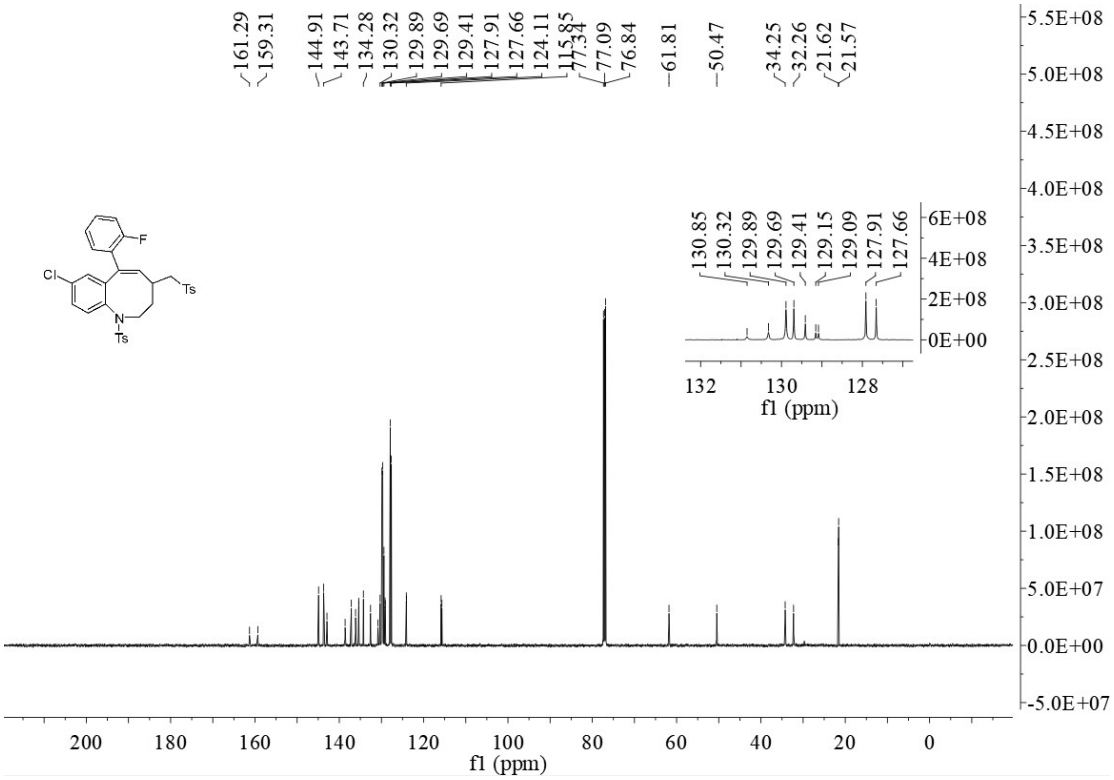
Compound 3l

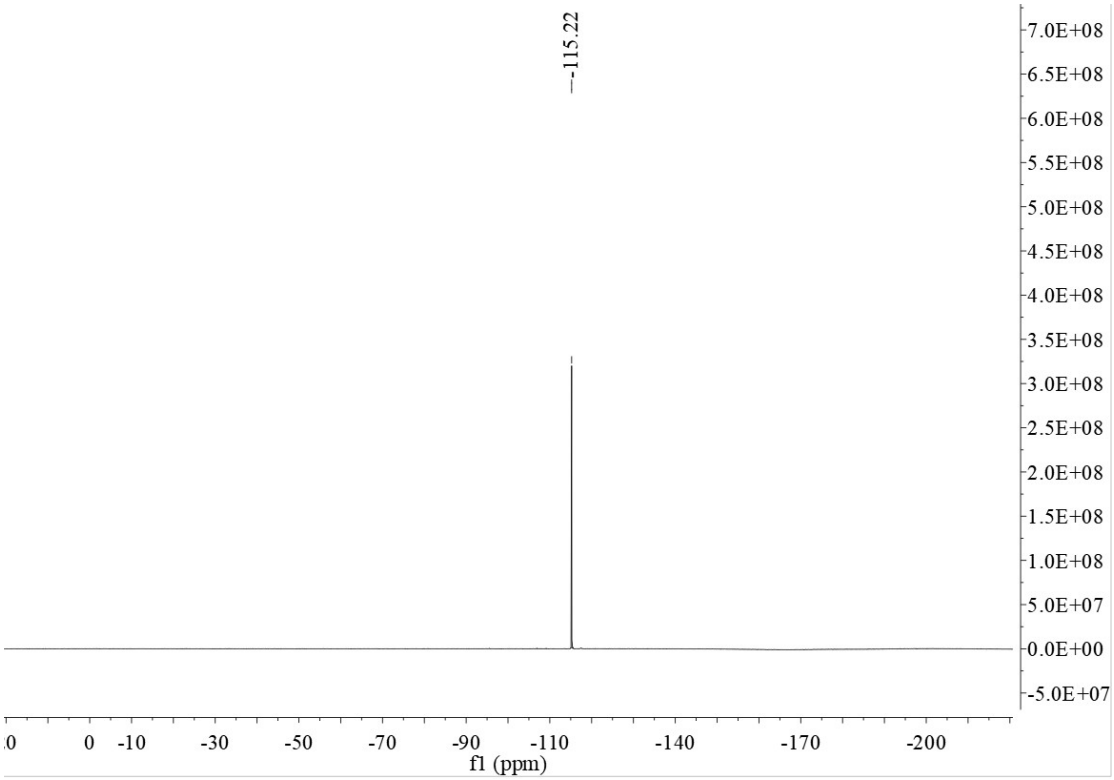

7.72
7.70
7.33
7.31
7.28
7.26
7.19
7.18
7.17
7.07
7.06
6.72
6.70
5.74
5.72
4.22
3.28
3.23
3.22
3.20
3.19
2.93
2.48
2.45
2.42
2.39
2.15
2.12
1.84
1.82
Cl
Br
Ts
N
Ts
5.05
1.06
5.07
2.02
1.01
1.04
1.00
0.96
2.02
1.00
6.98
1.02
1.00
f1 (ppm)


144.96
143.89
143.20
139.78
138.44
136.98
136.35
136.30
133.17
132.88
132.59
132.27
129.96
129.85
129.75
129.66
128.81
127.79
127.76
127.04
122.55
77.36
77.10
76.85
60.52
50.49
34.28
31.18
21.71
21.61
Cl
Br
Ts
N
Ts
f1 (ppm)

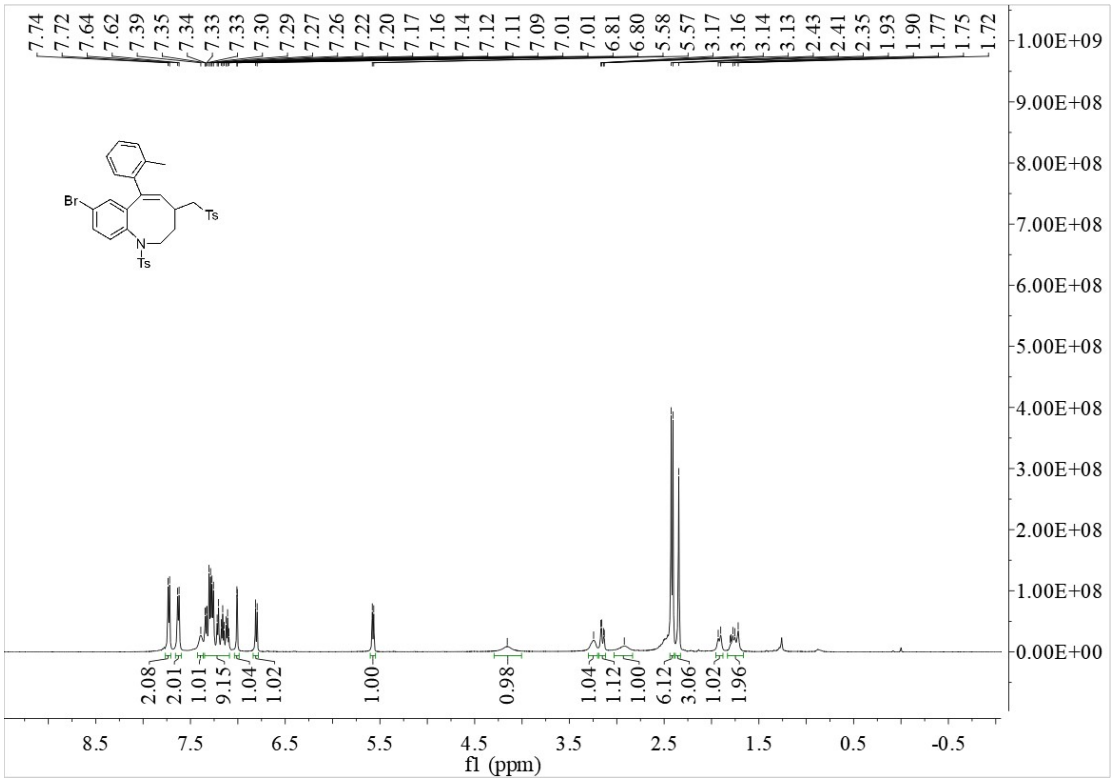
Compound 3m

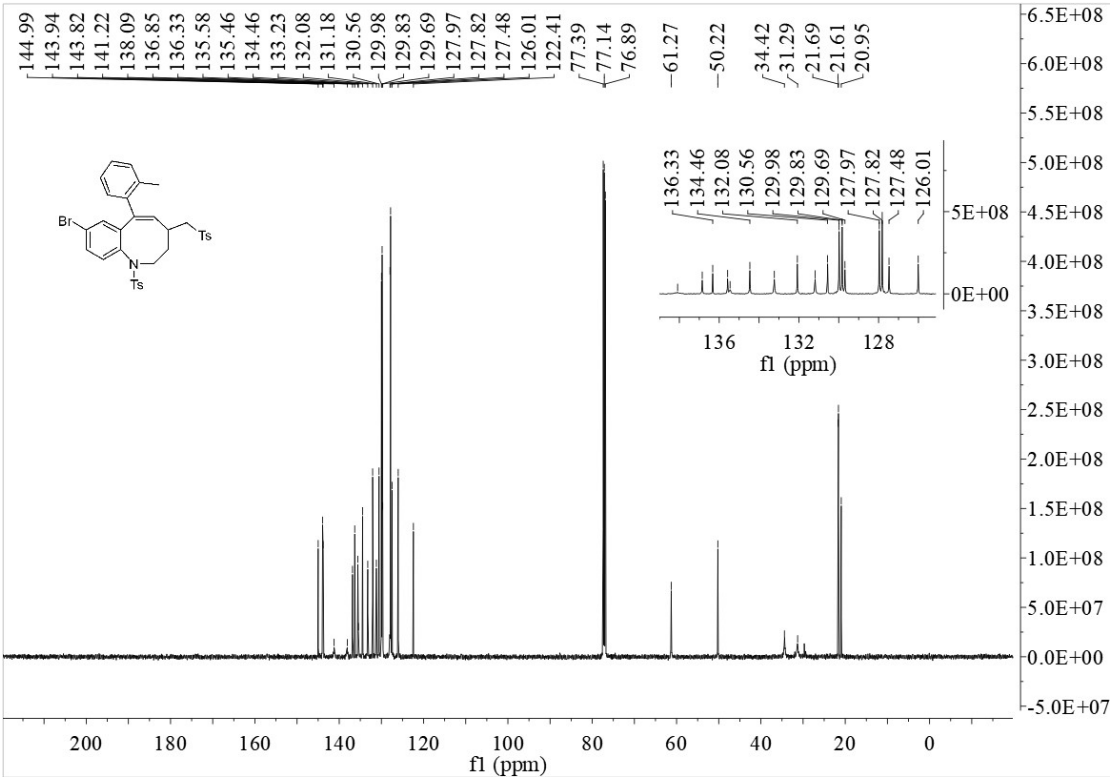

7.65 7.64 7.62 7.26 7.24 7.23 7.23 7.22 7.22 7.21 7.20 7.06 7.05 7.03 7.03 7.02 6.84 6.83 6.00 5.98 4.23 4.20 3.29 3.28 3.26 3.25 3.23 3.21 3.20 3.18 2.94 2.91 2.88 2.41 2.39 2.34 2.31 1.82 1.80 1.78
F
Cl
Ts
N
Ts
4.01 7.01 3.01 0.97 1.00 1.00 2.00 1.00 3.03 2.99 1.01 0.97 1.00
f1 (ppm)


161.29 159.31 144.91 143.71 134.28 130.32 129.89 129.69 129.41 127.91 127.66 124.11 115.85 77.34 77.09 76.84 61.81 50.47 34.25 32.26 21.62 21.57
F
Cl
Ts
N
Ts
130.85 130.32 129.89 129.69 129.41 129.15 129.09 127.91 127.66
f1 (ppm)
f1 (ppm)

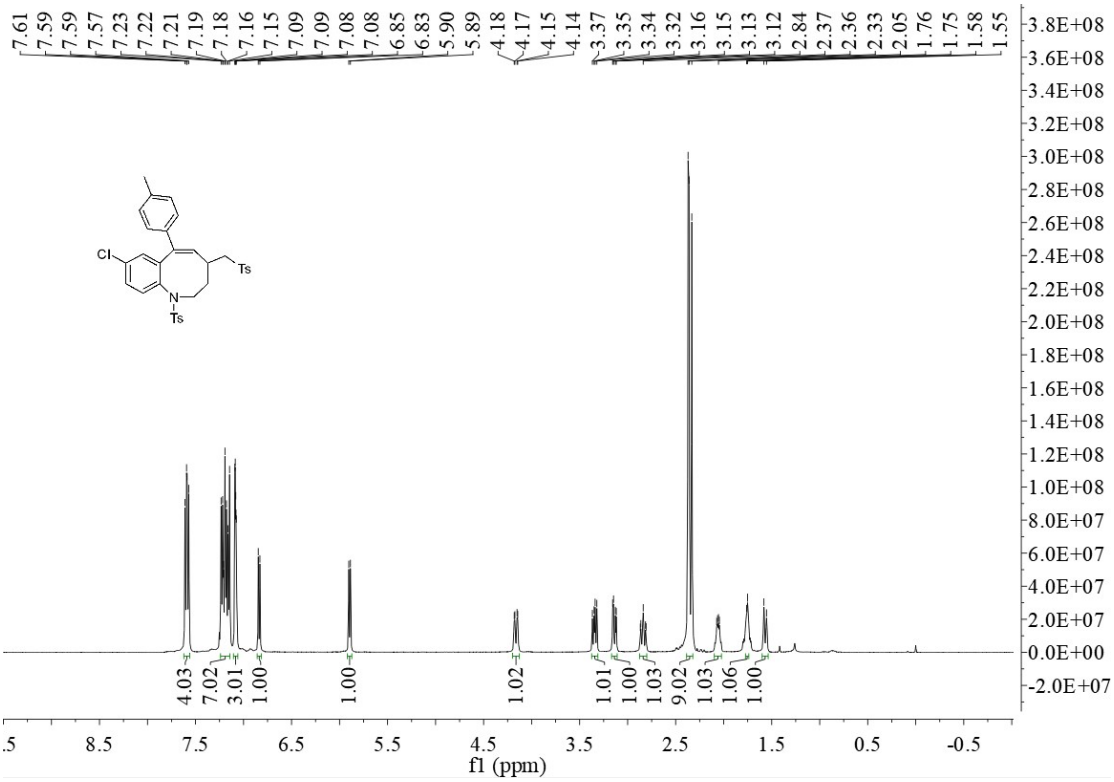

-115.22
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0 -10 -30 -50 -70 -90 -110 -140 -170 -200
f1 (ppm)

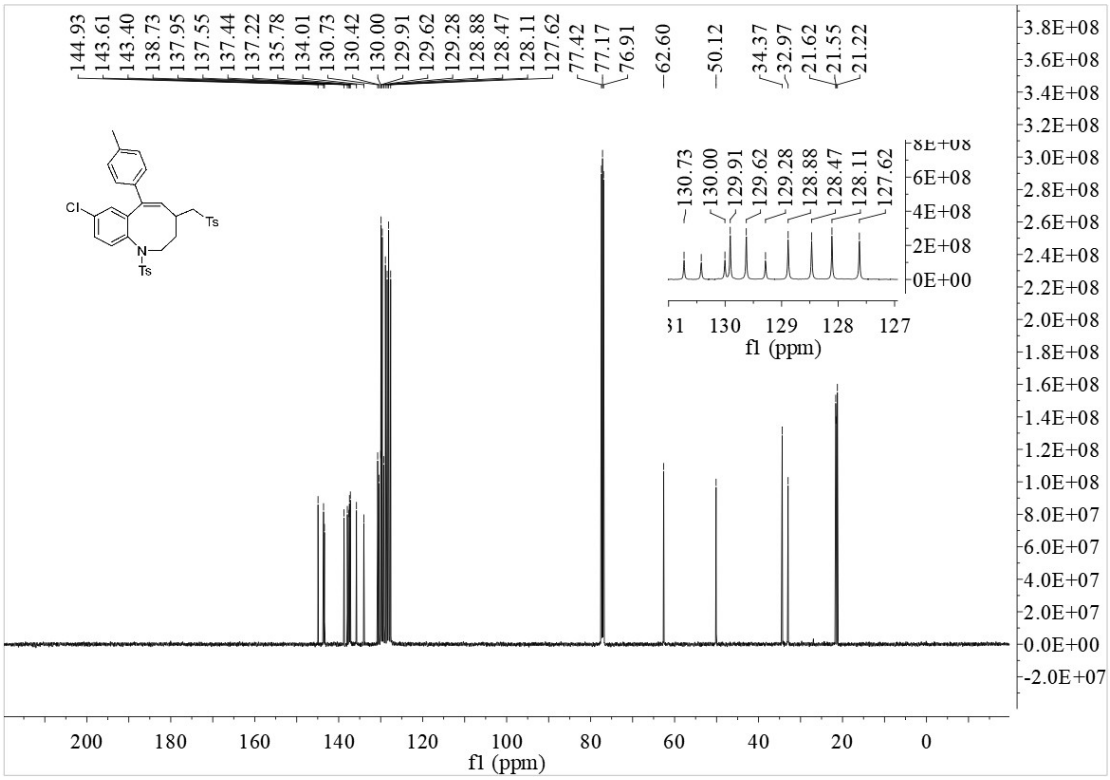
Compound 3n


7.74 7.72 7.64 7.62 7.39 7.35 7.34 7.33 7.33 7.30 7.29 7.27 7.26 7.22 7.20 7.17 7.16 7.14 7.12 7.11 7.09 7.01 7.01 6.81 6.80 5.58 5.57 3.17 3.16 3.14 3.13 2.43 2.41 2.35 1.93 1.90 1.77 1.75 1.72
Br
Ts
N
Ts
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
2.08 2.01 1.01 9.15 1.04 1.02 1.00 0.98 1.04 1.12 1.00 6.12 3.06 1.02 1.96
8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)

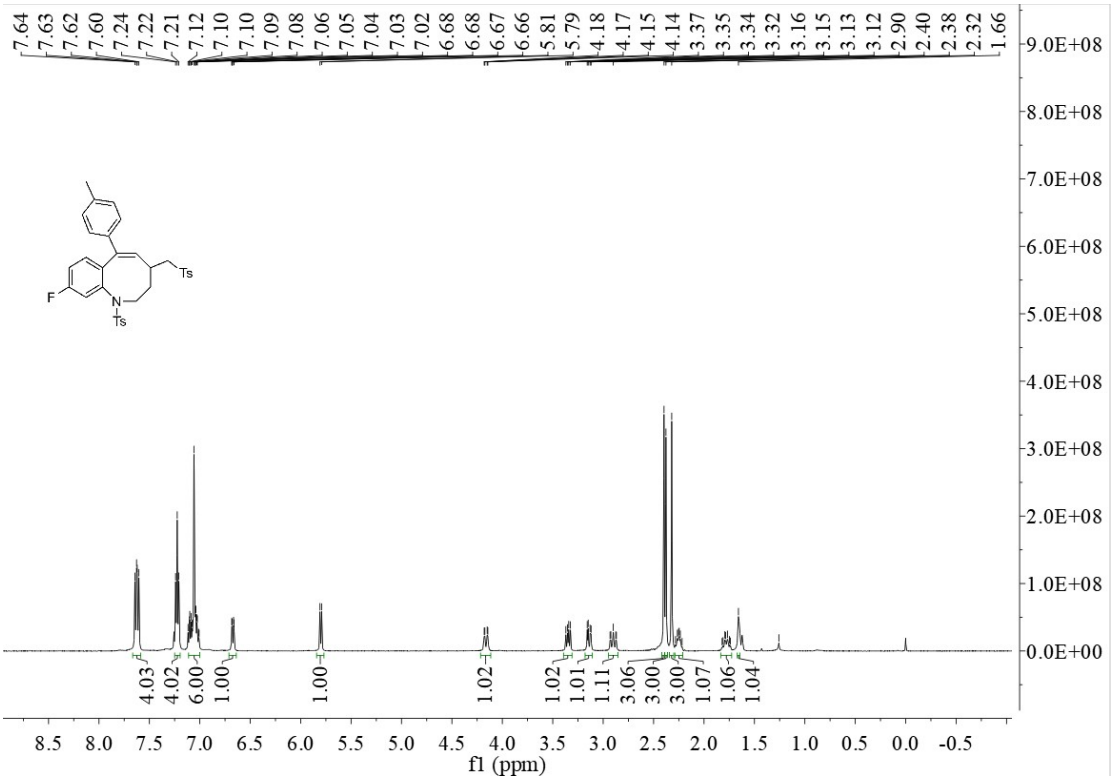

144.99
143.94
143.82
141.22
138.09
136.85
136.33
135.58
135.46
134.46
133.23
132.08
131.18
130.56
129.98
129.83
129.69
127.97
127.82
127.48
126.01
122.41
77.39
77.14
76.89
61.27
50.22
34.42
31.29
21.69
21.61
20.95
Br
Ts
N
Ts
136.33
134.46
132.08
130.56
129.98
129.83
129.69
127.97
127.82
127.48
126.01
5E+08
0E+00
136
132
128
f1 (ppm)
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

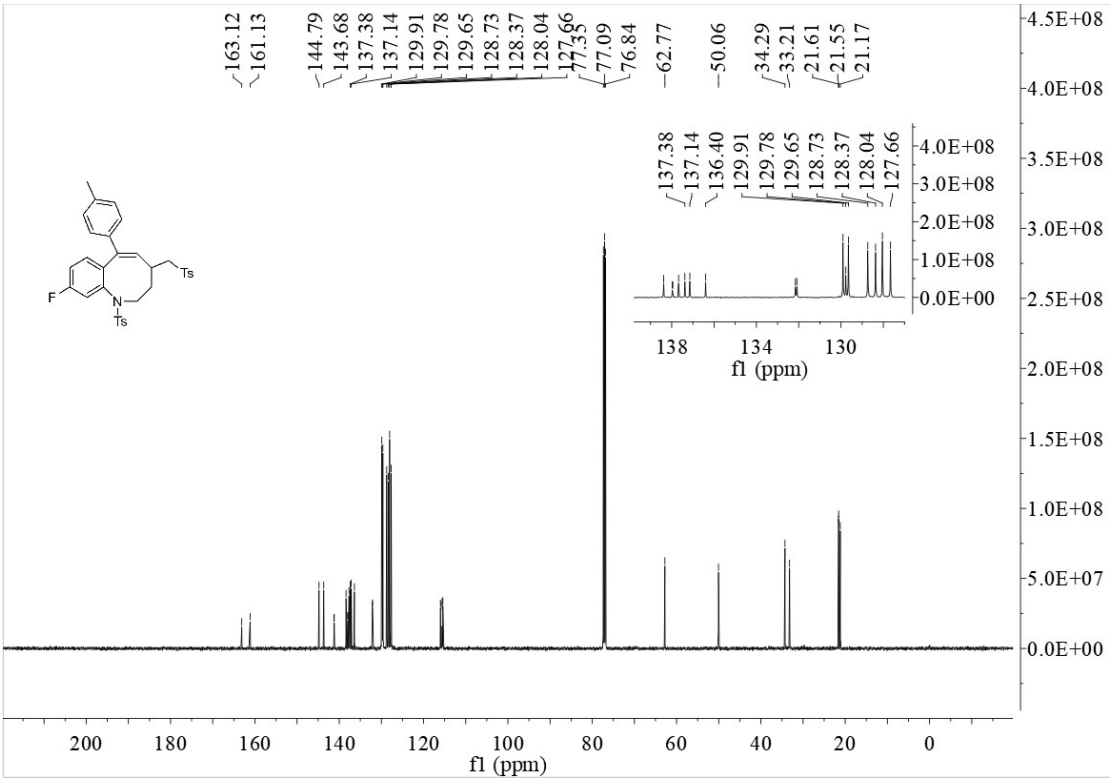
Compound 3o

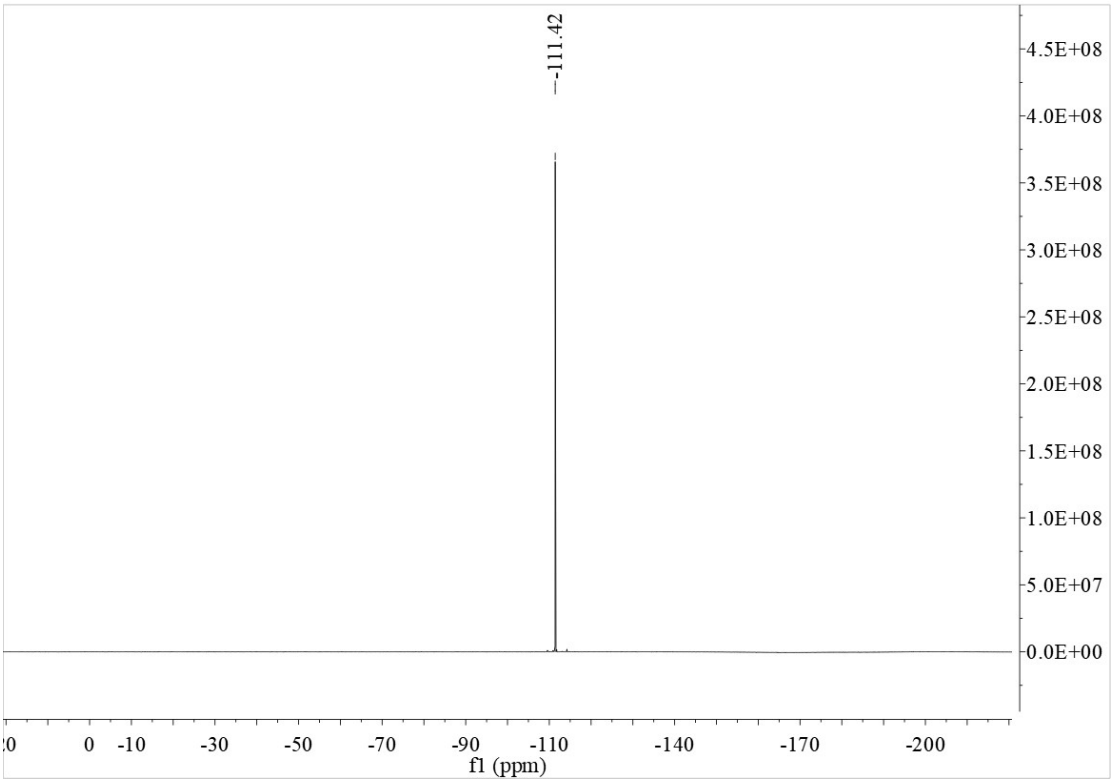

7.61
7.59
7.59
7.57
7.23
7.22
7.21
7.19
7.18
7.16
7.15
7.09
7.09
7.08
7.08
6.85
6.83
5.90
5.89
4.18
4.17
4.15
4.14
3.37
3.35
3.34
3.32
3.16
3.15
3.13
3.12
2.84
2.37
2.36
2.33
2.05
1.76
1.75
1.58
1.55
Cl
Ts
N
Ts
4.03
7.02
3.01
1.00
1.00
1.02
1.01
1.00
1.03
9.02
1.03
1.06
1.00
3.8E+08
3.6E+08
3.4E+08
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


144.93
143.61
143.40
138.73
137.95
137.55
137.44
137.22
135.78
134.01
130.73
130.42
130.00
129.91
129.62
129.28
128.88
128.47
128.11
127.62
77.42
77.17
76.91
62.60
50.12
34.37
32.97
21.62
21.55
21.22
Cl
Ts
N
Ts
fl (ppm)
fl (ppm)

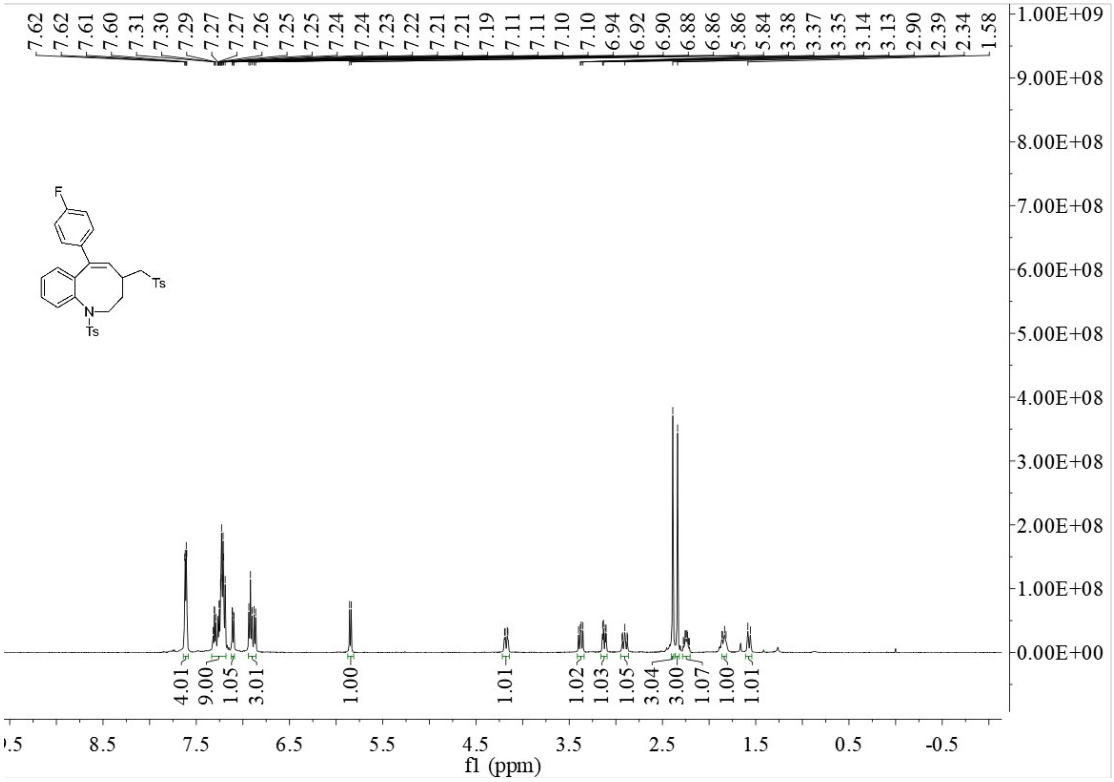
Compound 3p

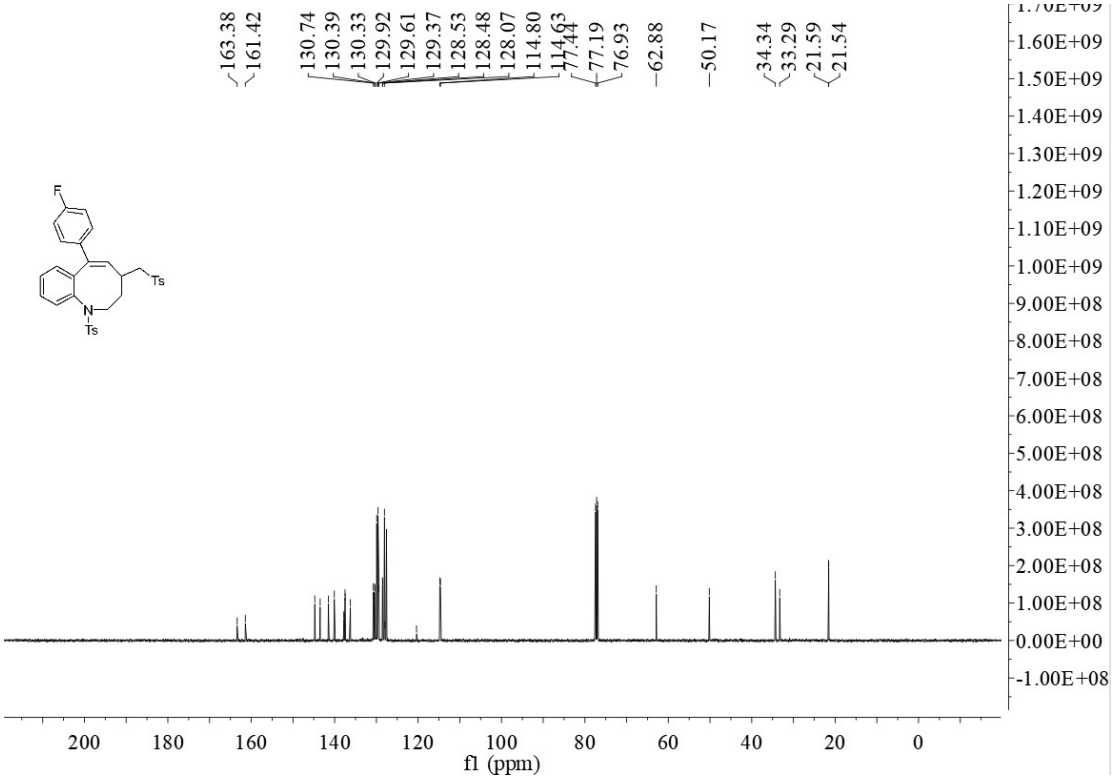

7.64
7.63
7.62
7.60
7.24
7.22
7.21
7.12
7.10
7.10
7.09
7.08
7.06
7.05
7.04
7.03
7.02
6.68
6.68
6.67
6.66
5.81
5.79
4.18
4.17
4.15
4.14
3.37
3.35
3.34
3.32
3.16
3.15
3.13
3.12
2.90
2.40
2.38
2.32
1.66
F
Ts
N
Ts
4.03
4.02
6.00
1.00
1.00
1.02
1.02
1.01
1.11
3.06
3.00
3.00
1.07
1.06
1.04
fl (ppm)


163.12
161.13
144.79
143.68
137.38
137.14
129.91
129.78
129.65
128.73
128.37
128.04
127.66
77.35
77.09
76.84
62.77
50.06
34.29
33.21
21.61
21.55
21.17
137.38
137.14
136.40
129.91
129.78
129.65
128.73
128.37
128.04
127.66
F
Ts
N
Ts
f1 (ppm)
f1 (ppm)

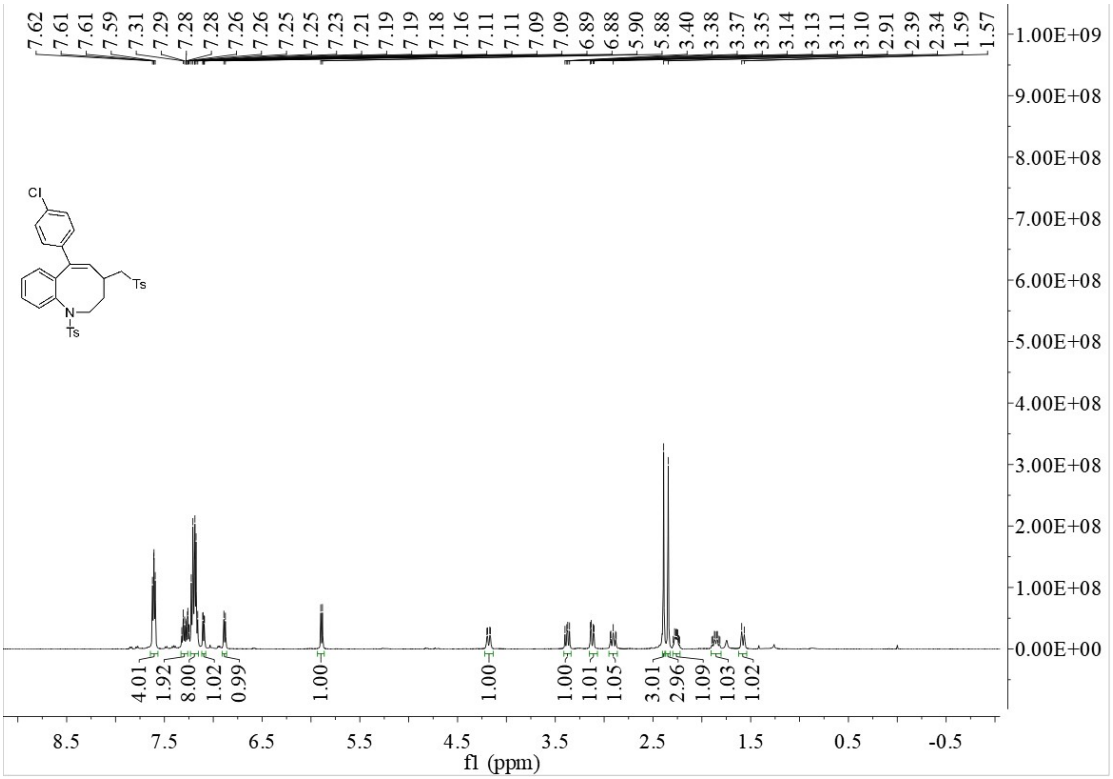

-111.42
f1 (ppm)

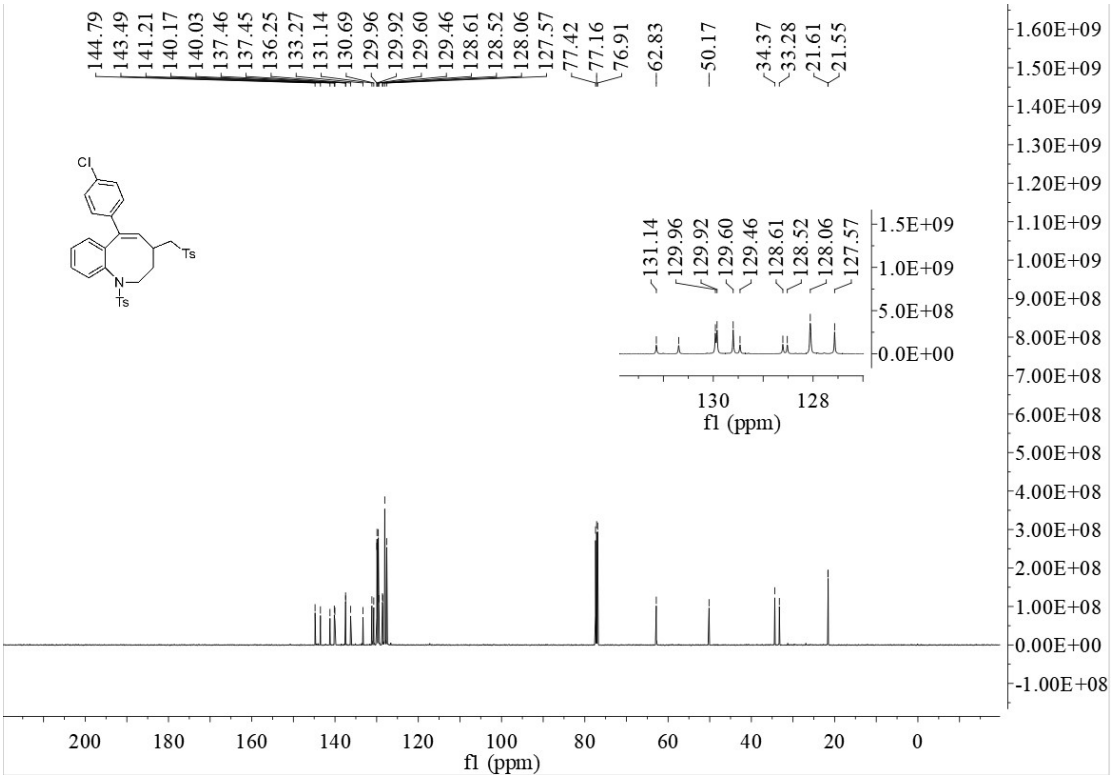
Compound 3q


7.62 7.62 7.61 7.60 7.31 7.30 7.29 7.27 7.27 7.26 7.25 7.25 7.24 7.24 7.23 7.22 7.21 7.21 7.19 7.11 7.11 7.10 7.10 6.94 6.92 6.90 6.88 6.86 5.86 5.84 3.38 3.37 3.35 3.14 3.13 2.90 2.39 2.34 1.58
4.01 9.00 1.05 3.01 1.00 1.01 1.02 1.03 1.05 3.04 3.00 1.07 1.00 1.01
f1 (ppm)

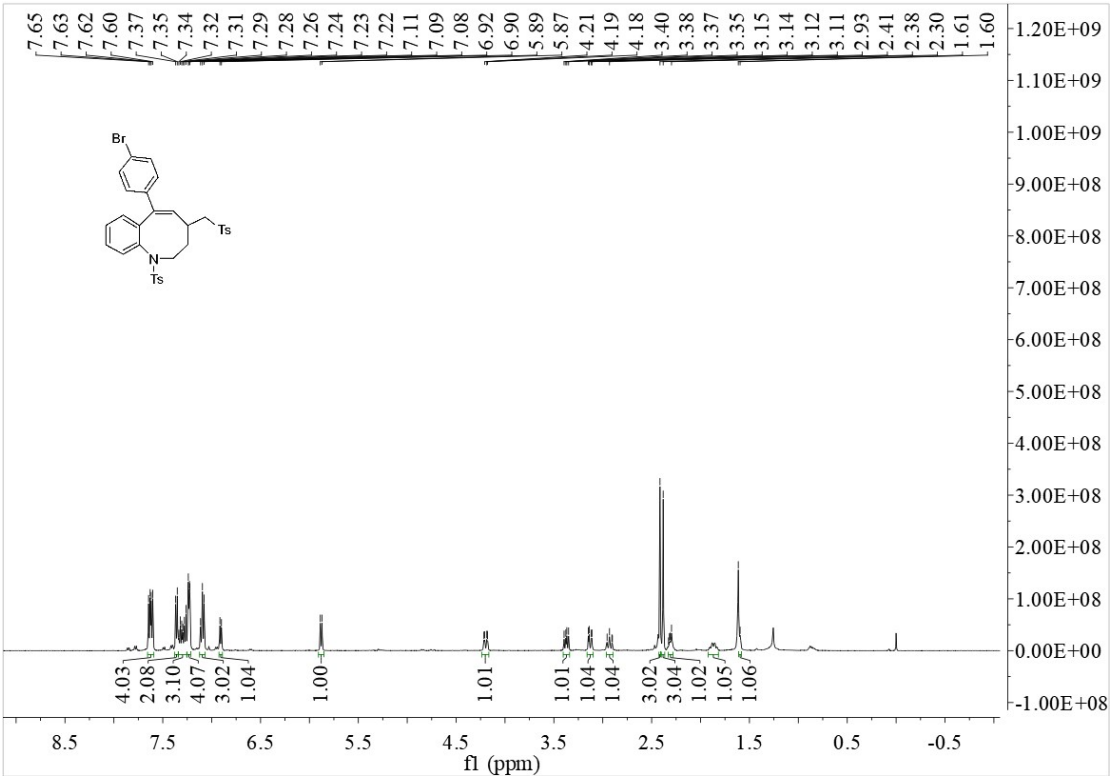

163.38 161.42 130.74 130.39 130.33 129.92 129.61 129.37 128.53 128.48 128.07 114.80 114.63 77.44 77.19 76.93 62.88 50.17 34.34 33.29 21.59 21.54
f1 (ppm)

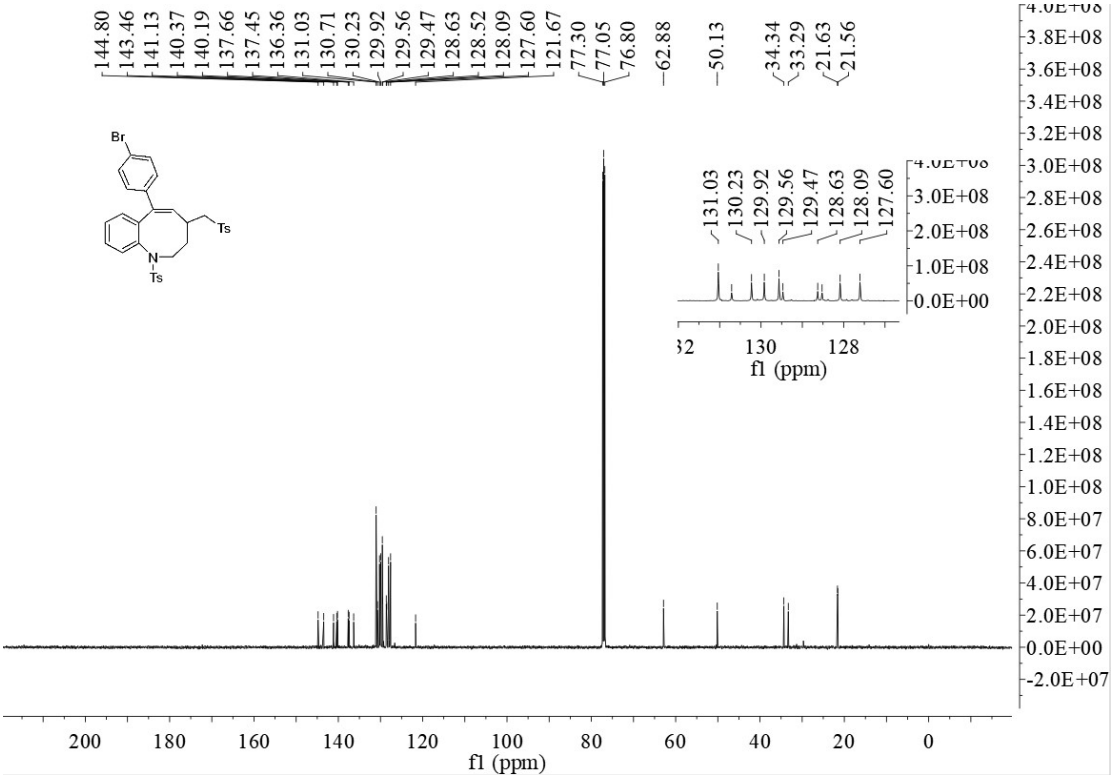
Compound 3r



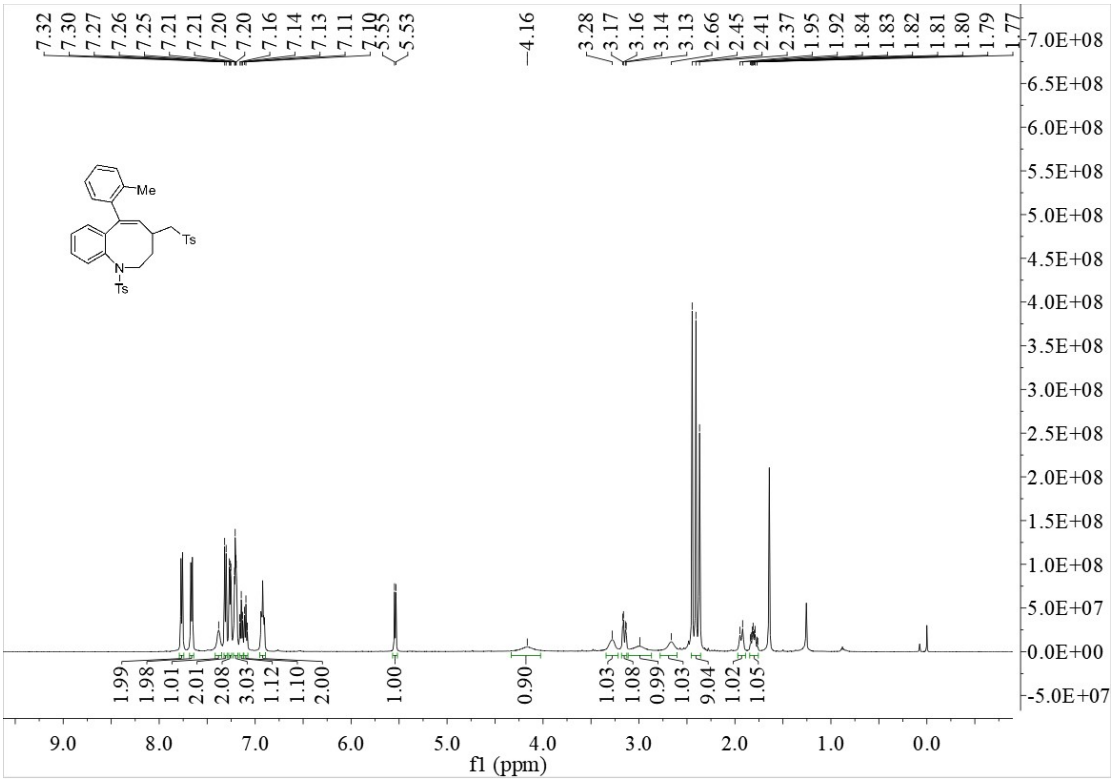


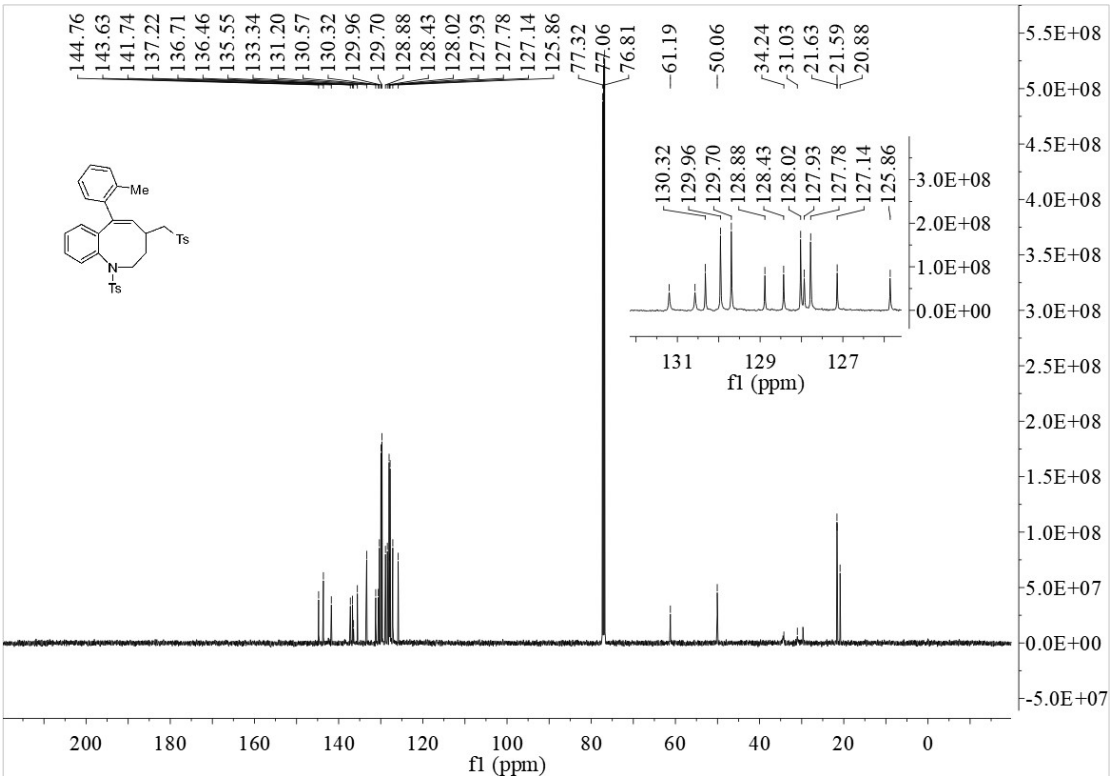
Compound 3s


7.65 7.63 7.62 7.60 7.37 7.35 7.34 7.32 7.31 7.29 7.28 7.26 7.24 7.23 7.22 7.11 7.09 7.08 6.92 6.90 5.89 5.87 4.21 4.19 4.18 3.40 3.38 3.37 3.35 3.15 3.14 3.12 3.11 2.93 2.41 2.38 2.30 1.61 1.60
Br
Ts
N
Ts
4.03 2.08 3.10 4.07 3.02 1.04 1.00 1.01 1.01 1.04 1.04 3.02 3.04 1.02 1.05 1.06
fl (ppm)

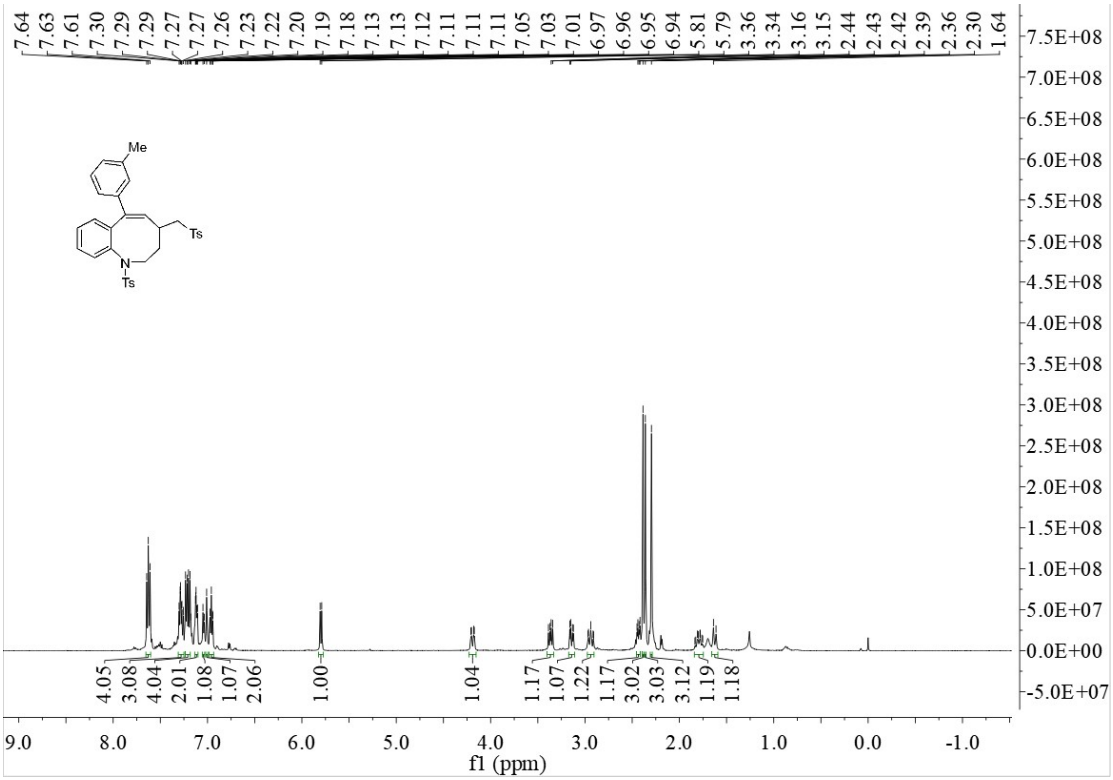

144.80 143.46 141.13 140.37 140.19 137.66 137.45 136.36 131.03 130.71 130.23 129.92 129.56 129.47 128.63 128.52 128.09 127.60 121.67 77.30 77.05 76.80 62.88 50.13 34.34 33.29 21.63 21.56
Br
Ts
N
Ts
131.03 130.23 129.92 129.56 129.47 128.63 128.09 127.60
130
128
fl (ppm)
200 180 160 140 120 100 80 60 40 20 0
fl (ppm)

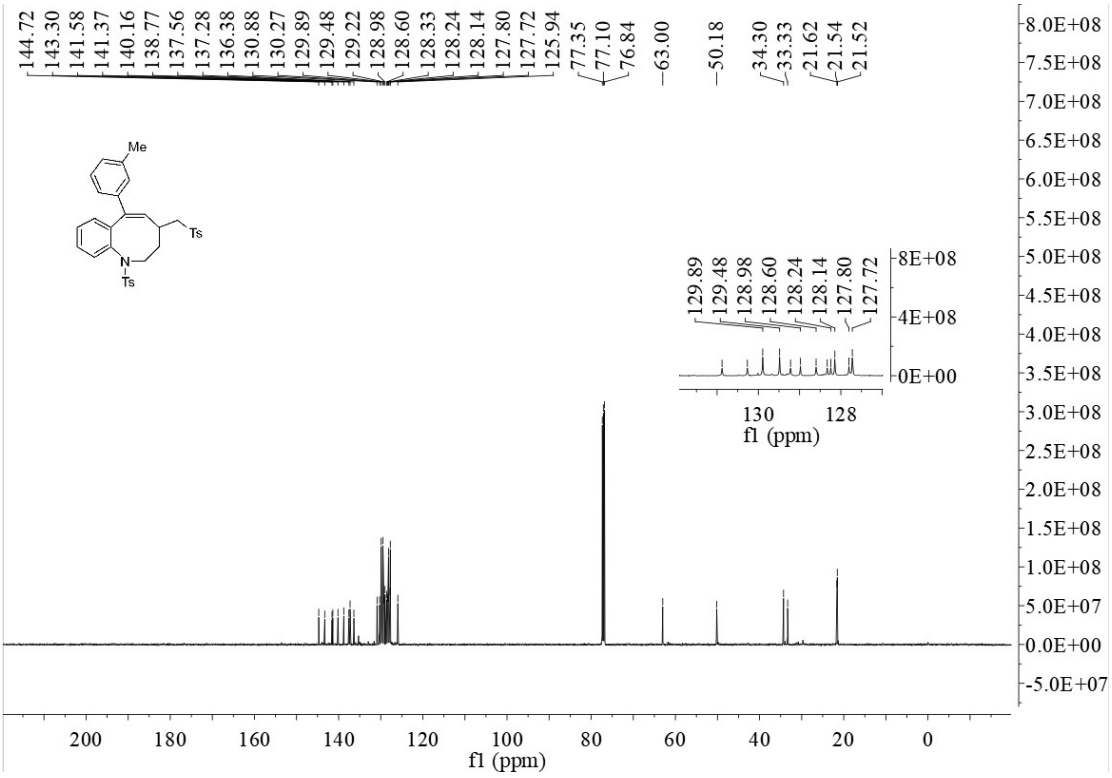
Compound 3t


7.32 7.30 7.27 7.26 7.25 7.21 7.21 7.20 7.20 7.16 7.14 7.13 7.11 7.10 5.55 5.53 4.16 3.28 3.17 3.16 3.14 3.13 2.66 2.45 2.41 2.37 1.95 1.92 1.84 1.83 1.82 1.81 1.80 1.79 1.77
Me
Ts
N
Ts
1.99 1.98 1.01 2.01 2.08 3.03 1.12 1.10 2.00 1.00 0.90 1.03 1.08 0.99 1.03 9.04 1.02 1.05
f1 (ppm)

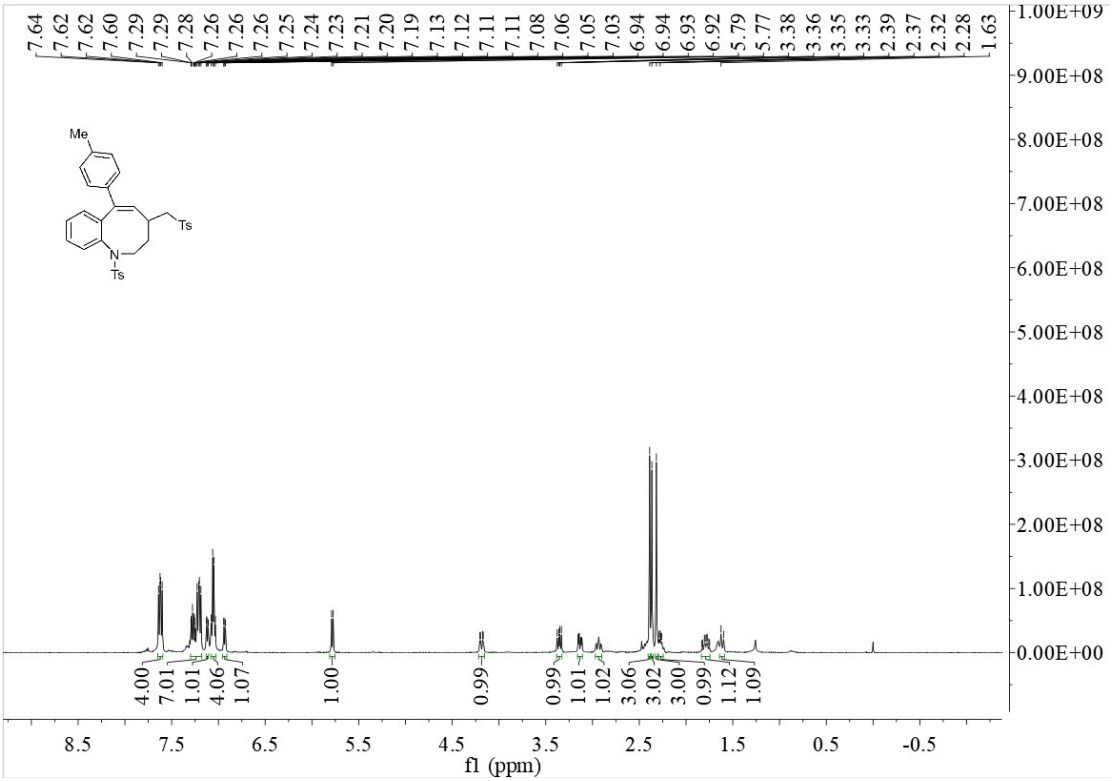

144.76 143.63 141.74 137.22 136.71 136.46 135.55 133.34 131.20 130.57 130.32 129.96 129.70 128.88 128.43 128.02 127.93 127.78 127.14 125.86 77.32 77.06 76.81 61.19 50.06 34.24 31.03 21.63 21.59 20.88
Me
Ts
N
Ts
130.32 129.96 129.70 128.88 128.43 128.02 127.93 127.78 127.14 125.86
131 129 127
f1 (ppm)
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

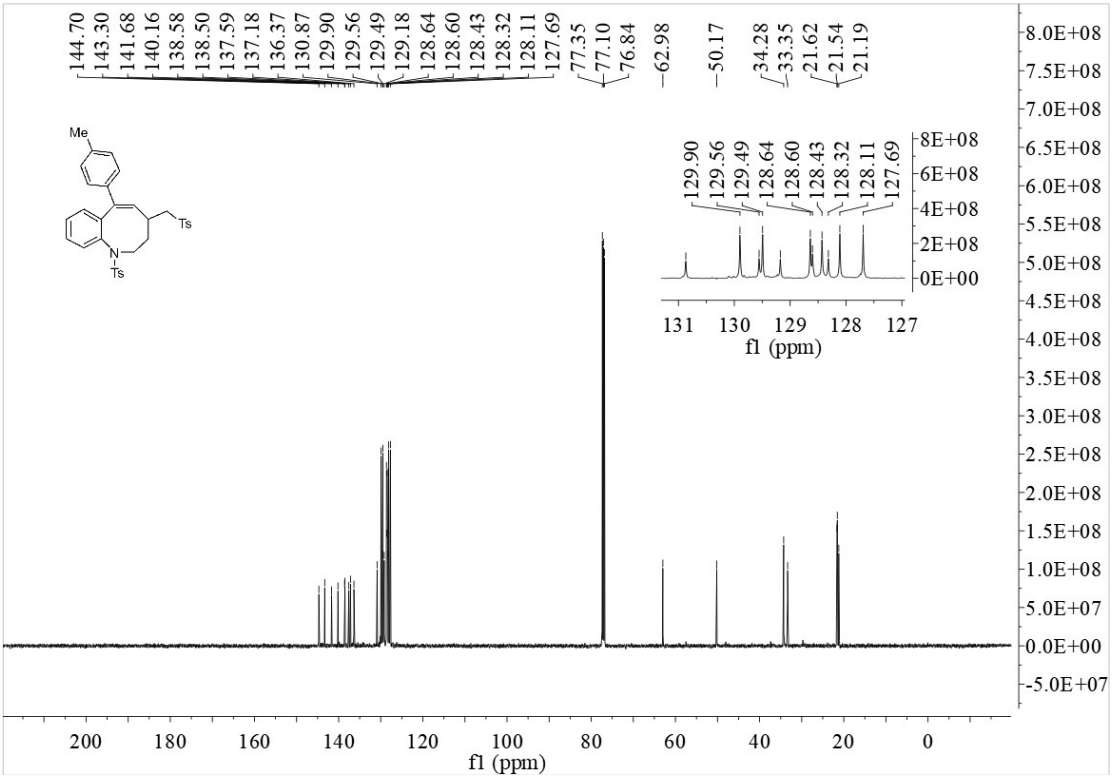
Compound 3u


7.64 7.63 7.61 7.30 7.29 7.29 7.27 7.27 7.26 7.23 7.22 7.20 7.19 7.18 7.13 7.13 7.12 7.11 7.11 7.11 7.05 7.03 7.01 6.97 6.96 6.95 6.94 5.81 5.79 3.36 3.34 3.16 3.15 2.44 2.43 2.42 2.39 2.36 2.30 1.64
Me
Ts
N
Ts
4.05 3.08 4.04 2.01 1.08 1.07 2.06 1.00 1.04 1.17 1.07 1.22 1.17 3.02 3.03 3.12 1.19 1.18
f1 (ppm)

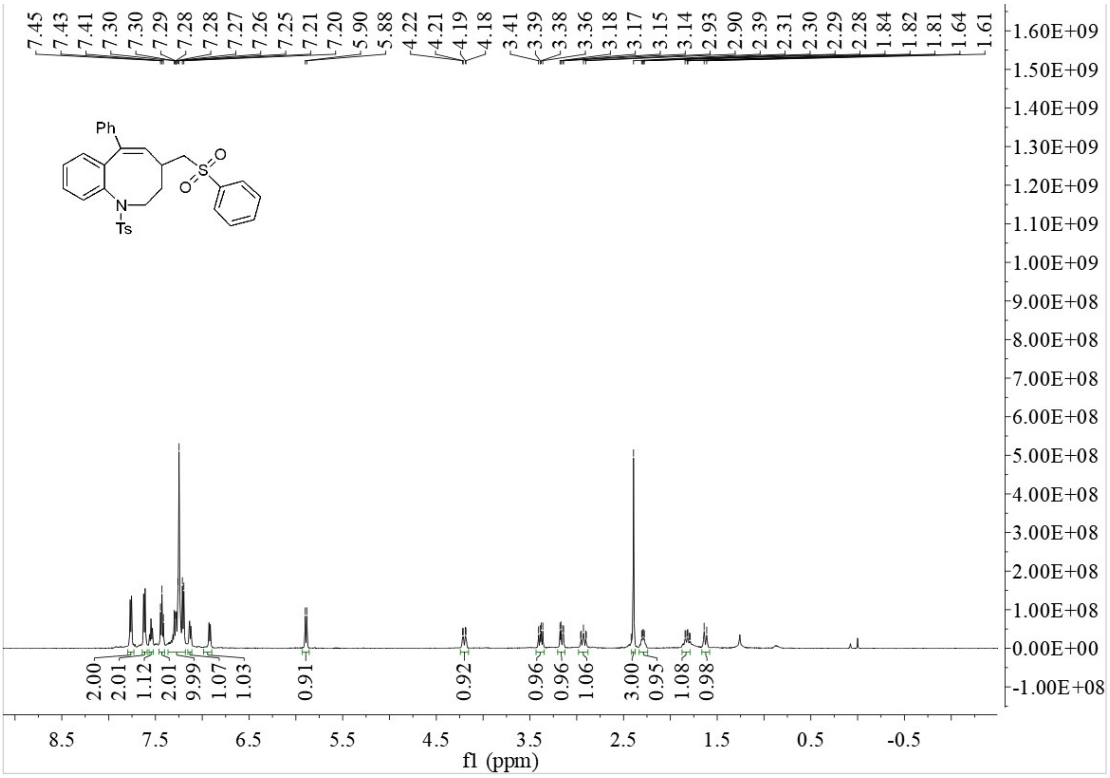

144.72 143.30 141.58 141.37 140.16 138.77 137.56 137.28 136.38 130.88 130.27 129.89 129.48 129.22 128.98 128.60 128.33 128.24 128.14 127.80 127.72 125.94 77.35 77.10 76.84 63.00 50.18 34.30 33.33 21.62 21.54 21.52
Me
Ts
N
Ts
129.89 129.48 128.98 128.60 128.24 128.14 127.80 127.72
f1 (ppm)
f1 (ppm)

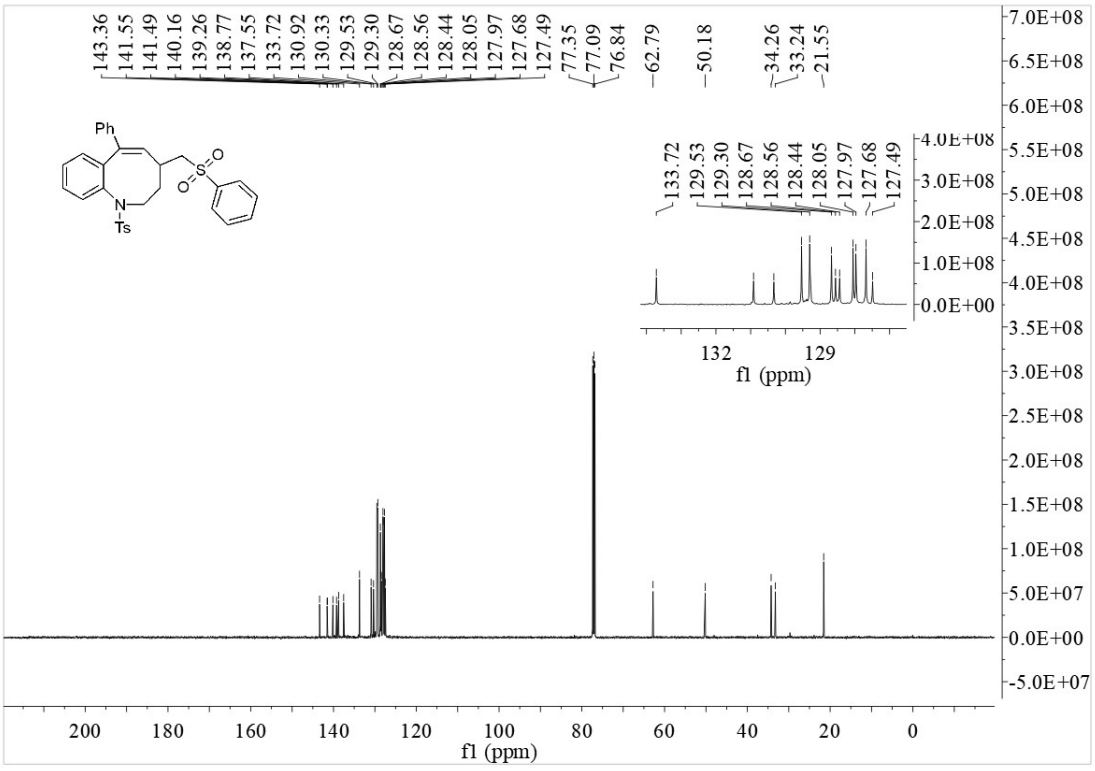
Compound 3v



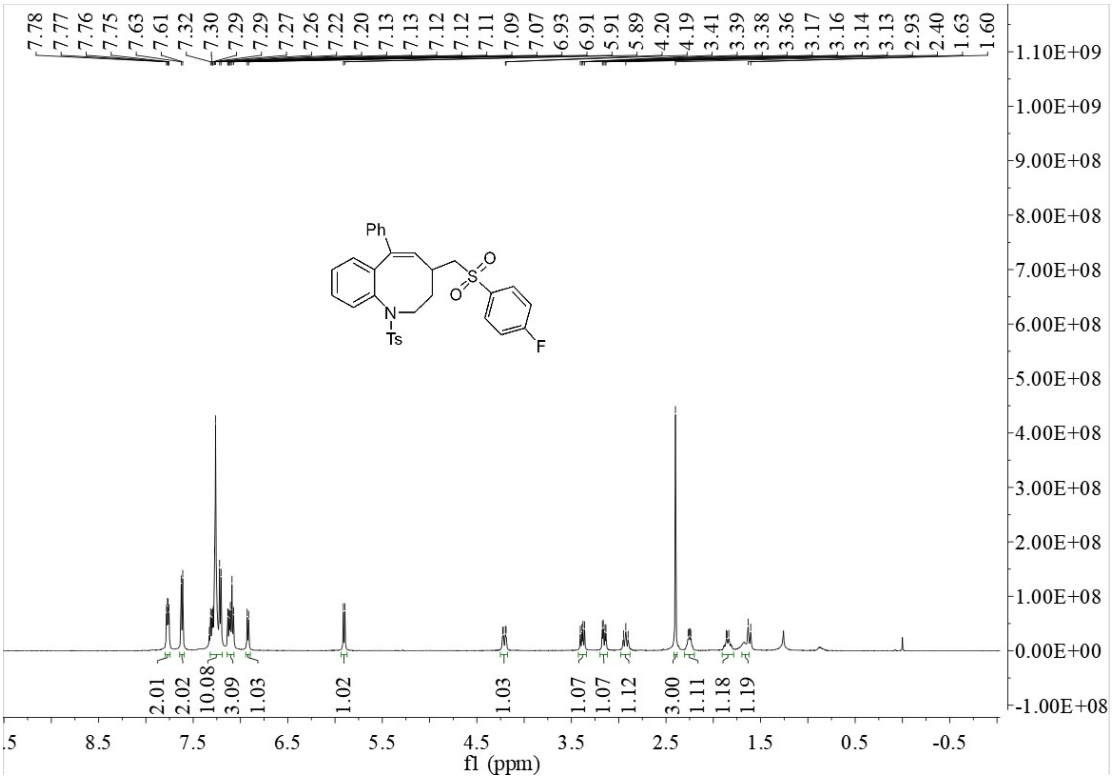


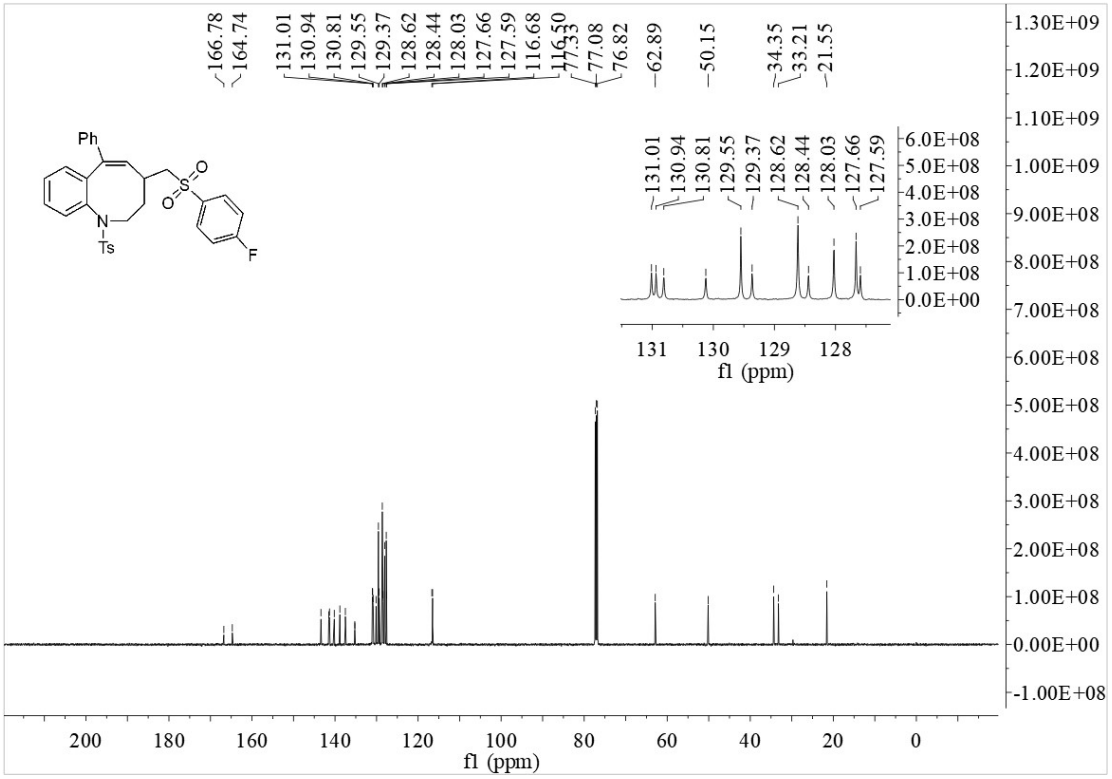
Compound 3aa

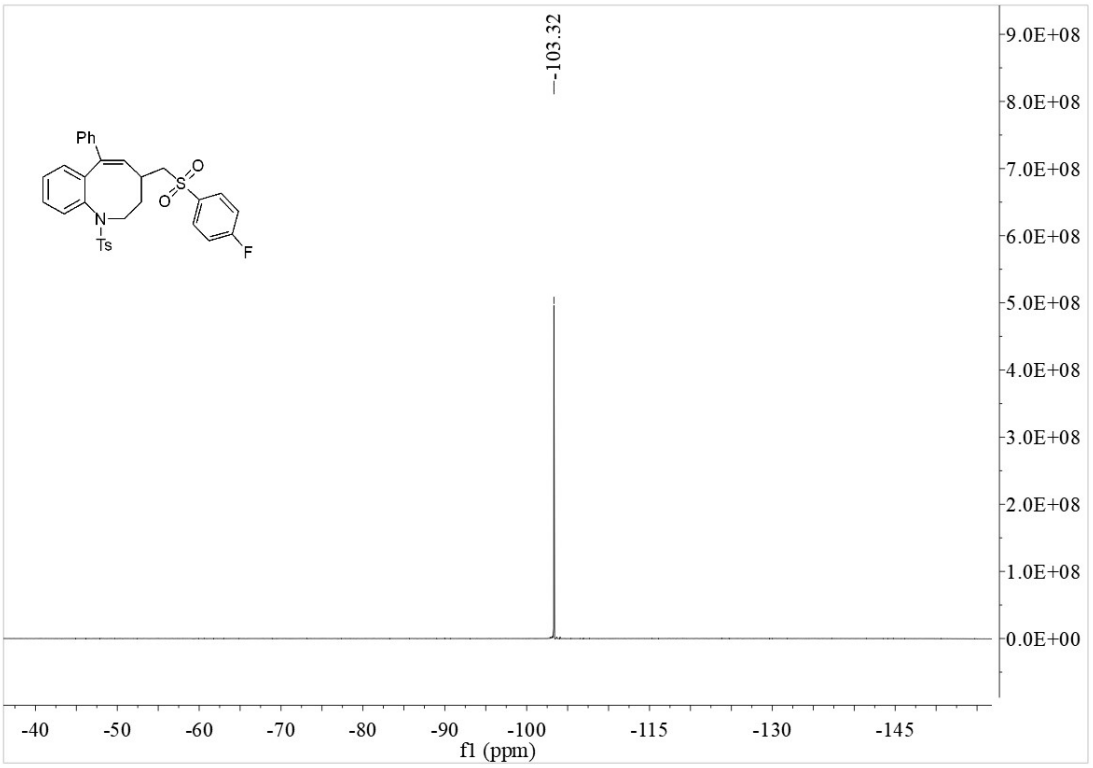




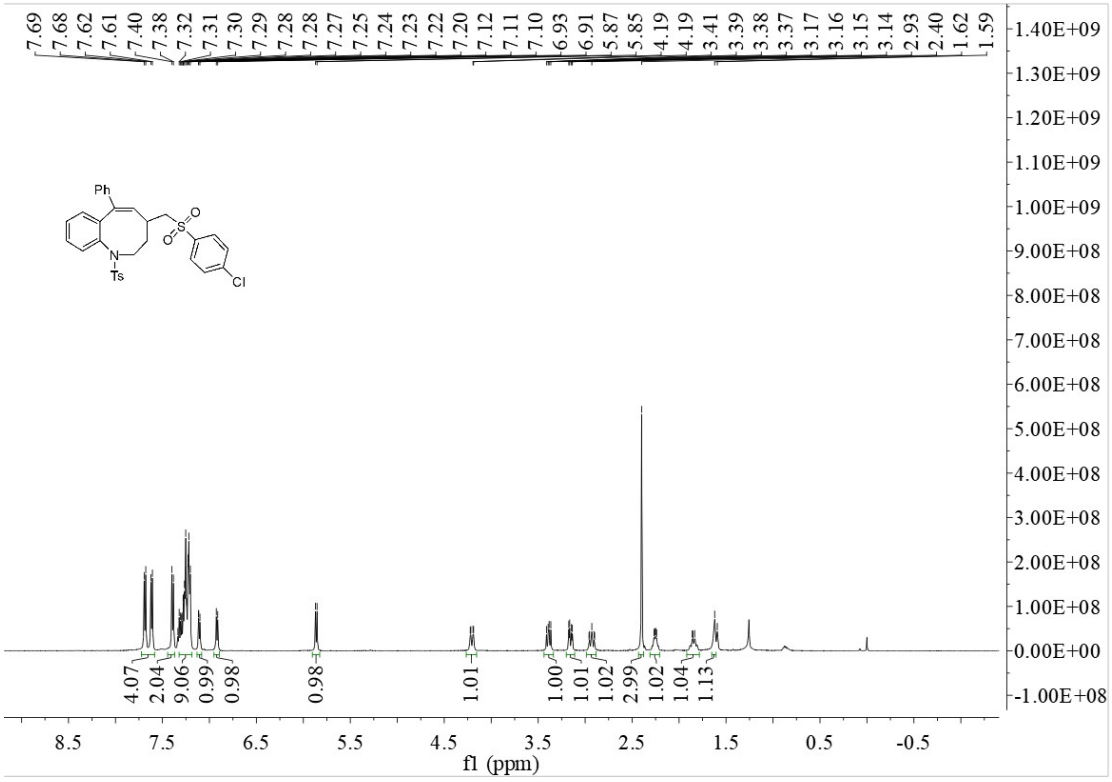
Compound 3ab

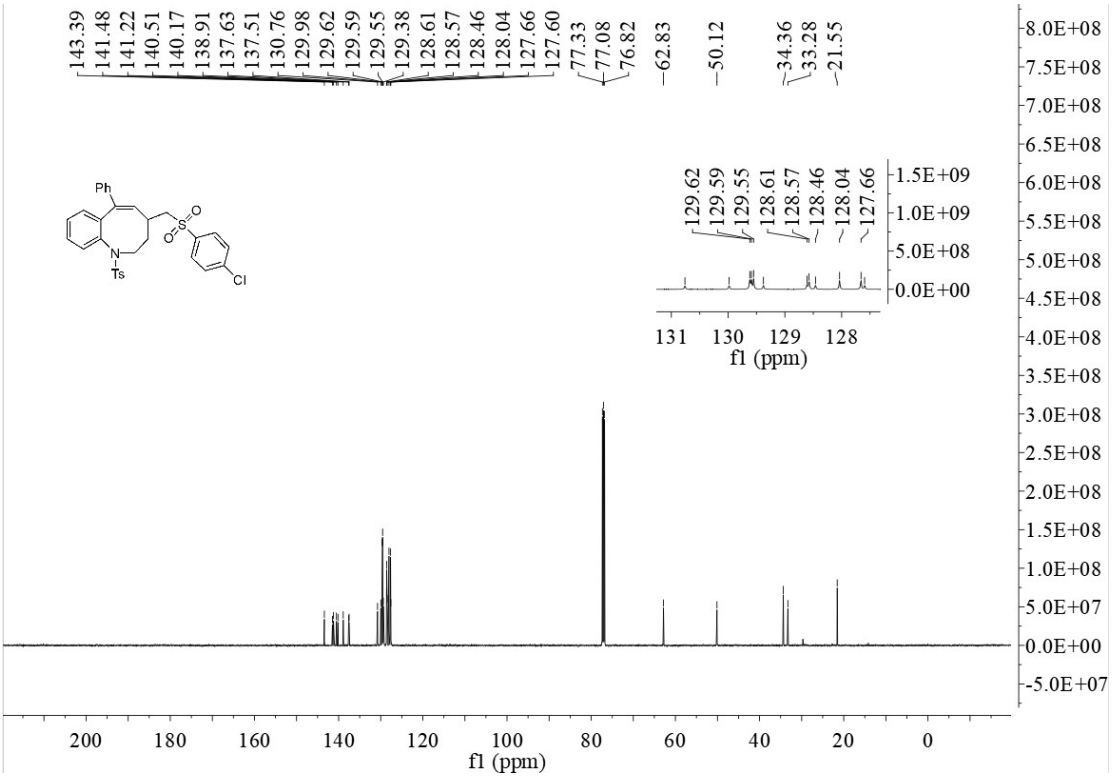

7.78 7.77 7.76 7.75 7.63 7.61 7.32 7.30 7.29 7.29 7.27 7.26 7.22 7.20 7.13 7.13 7.12 7.12 7.11 7.09 7.07 6.93 6.91 5.91 5.89 4.20 4.19 3.41 3.39 3.38 3.36 3.17 3.16 3.14 3.13 2.93 2.40 1.63 1.60
Ph
N
Ts
O
O
S
F
2.01 2.02 10.08 3.09 1.03 1.02 1.03 1.07 1.07 1.12 3.00 1.11 1.18 1.19
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)


166.78 164.74 131.01 130.94 130.81 129.55 129.37 128.62 128.44 128.03 127.66 127.59 116.68 116.50 77.33 77.08 76.82 62.89 50.15 34.35 33.21 21.55
Ph
N
Ts
O
O
S
F
131.01 130.94 130.81 129.55 129.37 128.62 128.44 128.03 127.66 127.59
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
131 130 129 128
f1 (ppm)
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

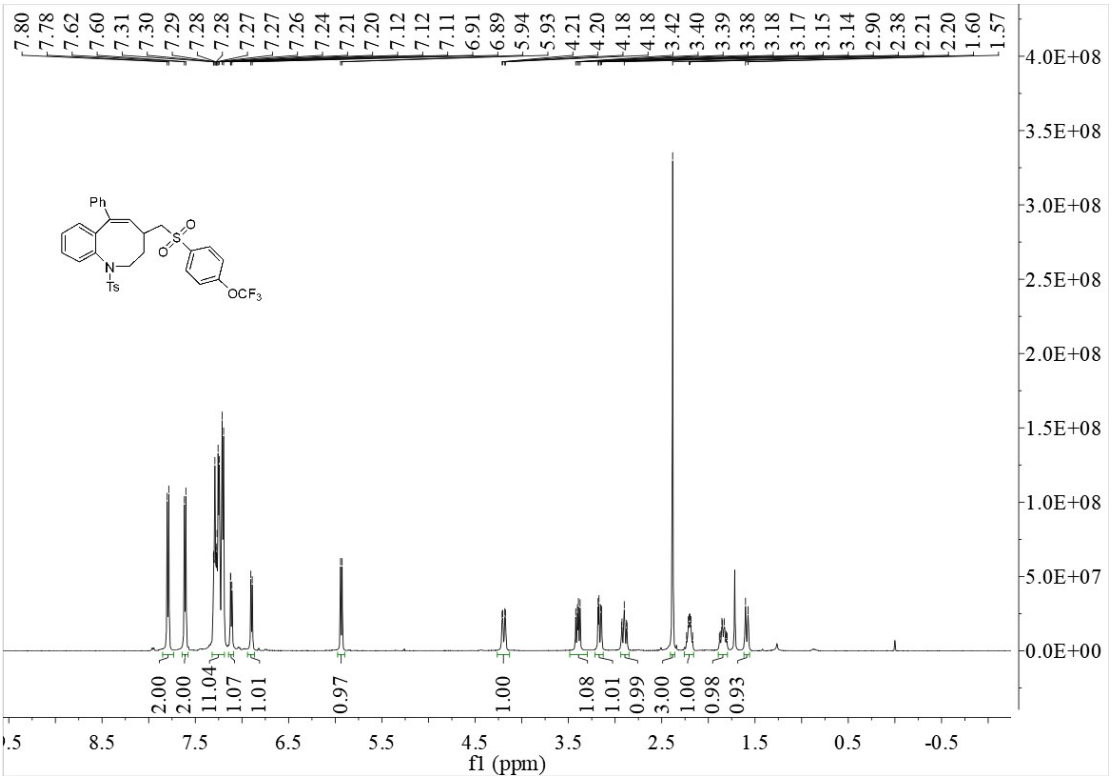


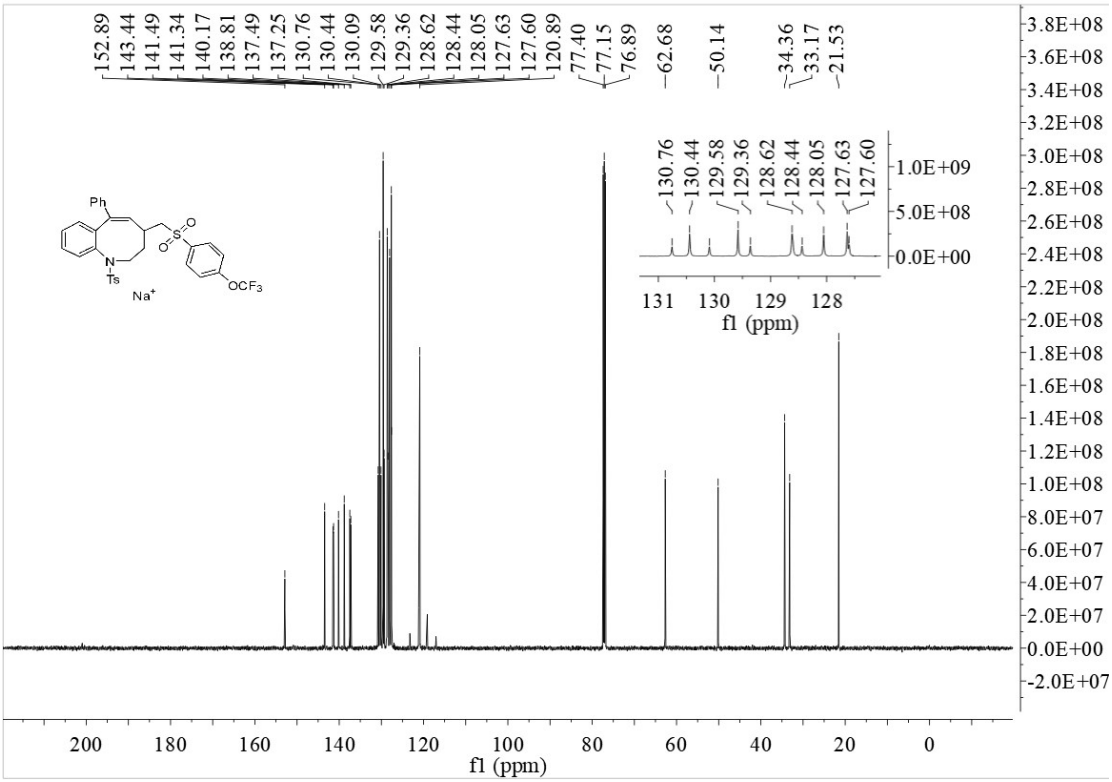
Compound 3ac

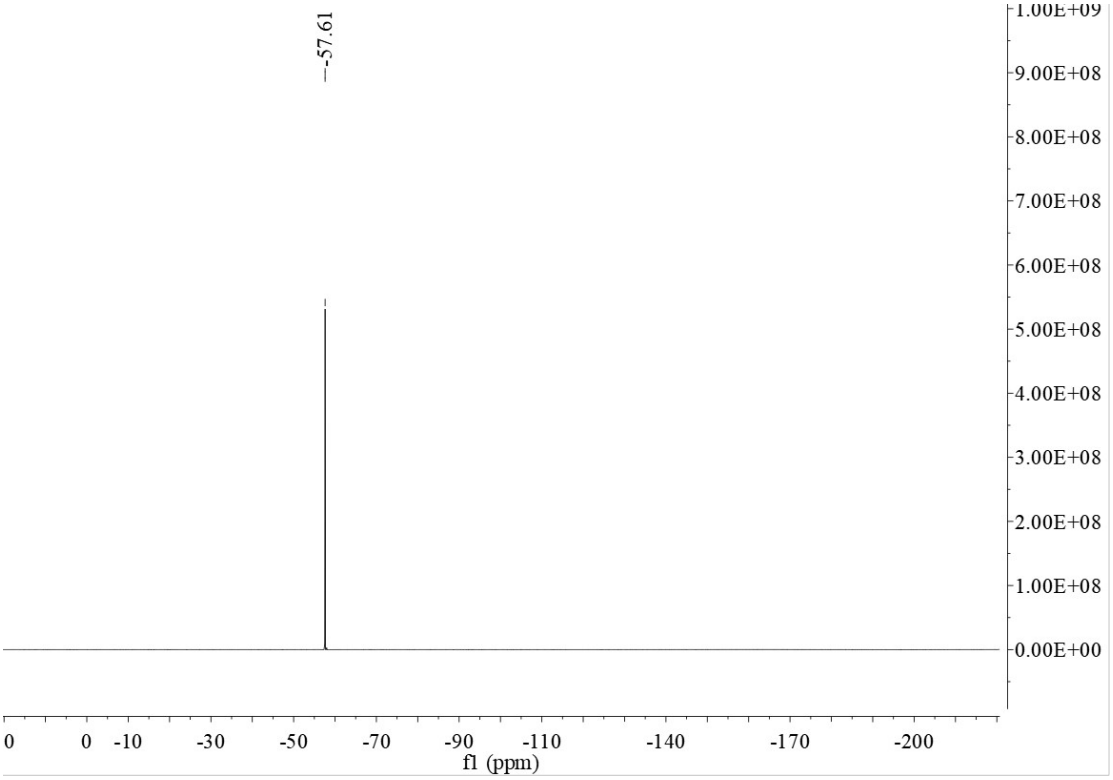




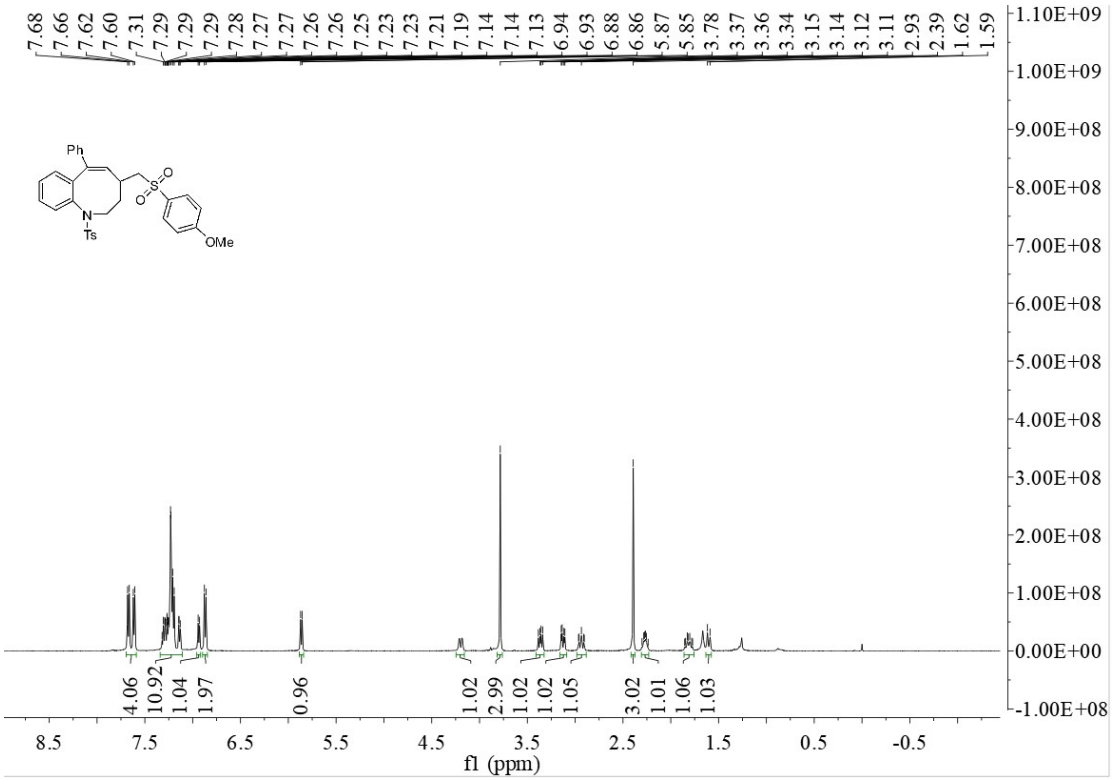
Compound 3ad

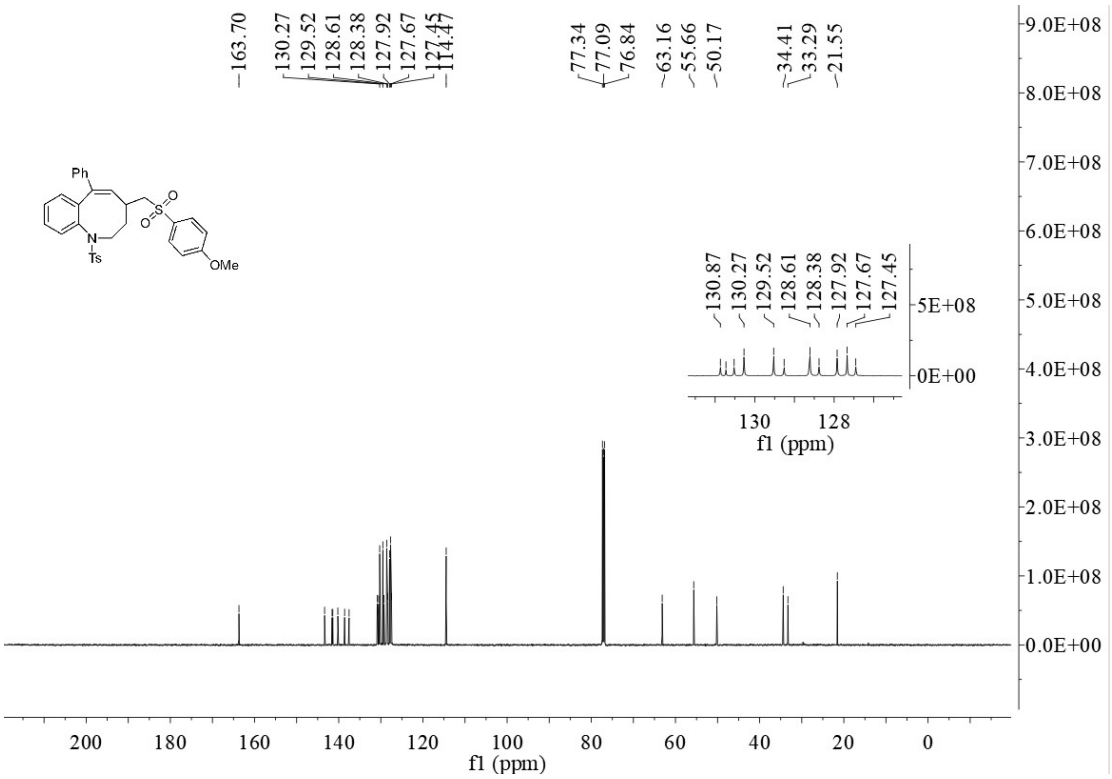



152.89
143.44
141.49
141.34
140.17
138.81
137.49
137.25
130.76
130.44
130.09
129.58
129.36
128.62
128.44
128.05
127.63
127.60
120.89
77.40
77.15
76.89
62.68
50.14
34.36
33.17
21.53
Ph
N
Ts
Na+
OCF3
fl (ppm)
f1 (ppm)

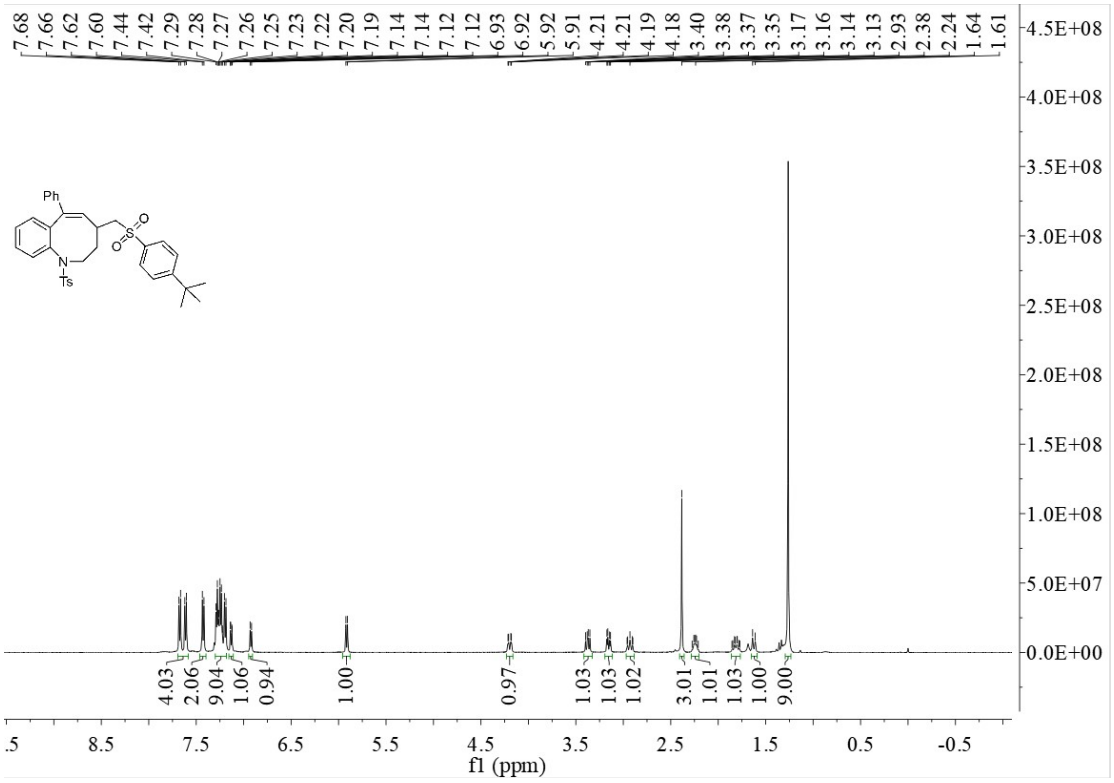

-57.61
f1 (ppm)

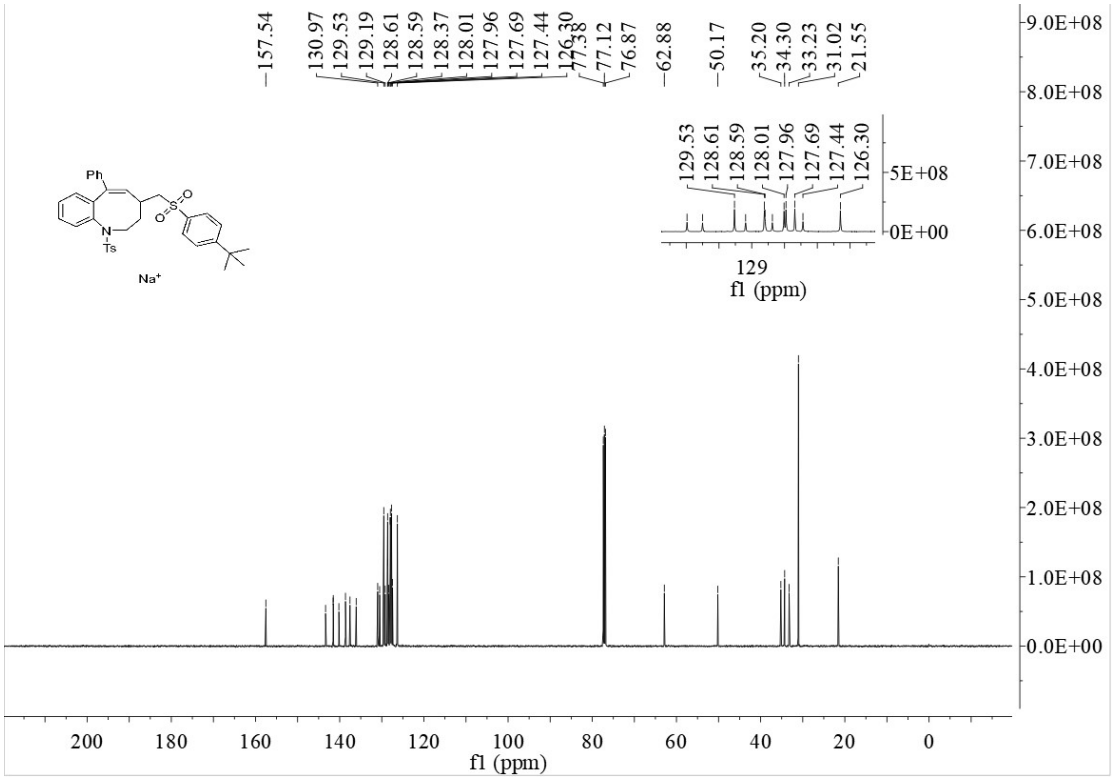
Compound 3ae



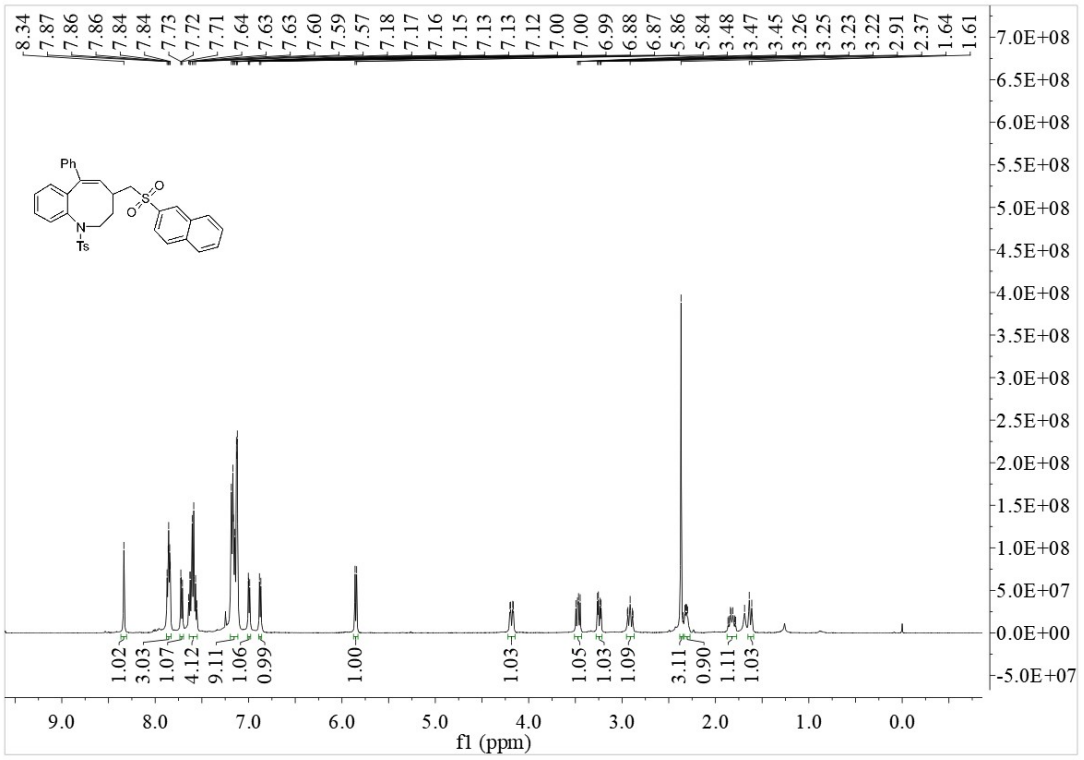


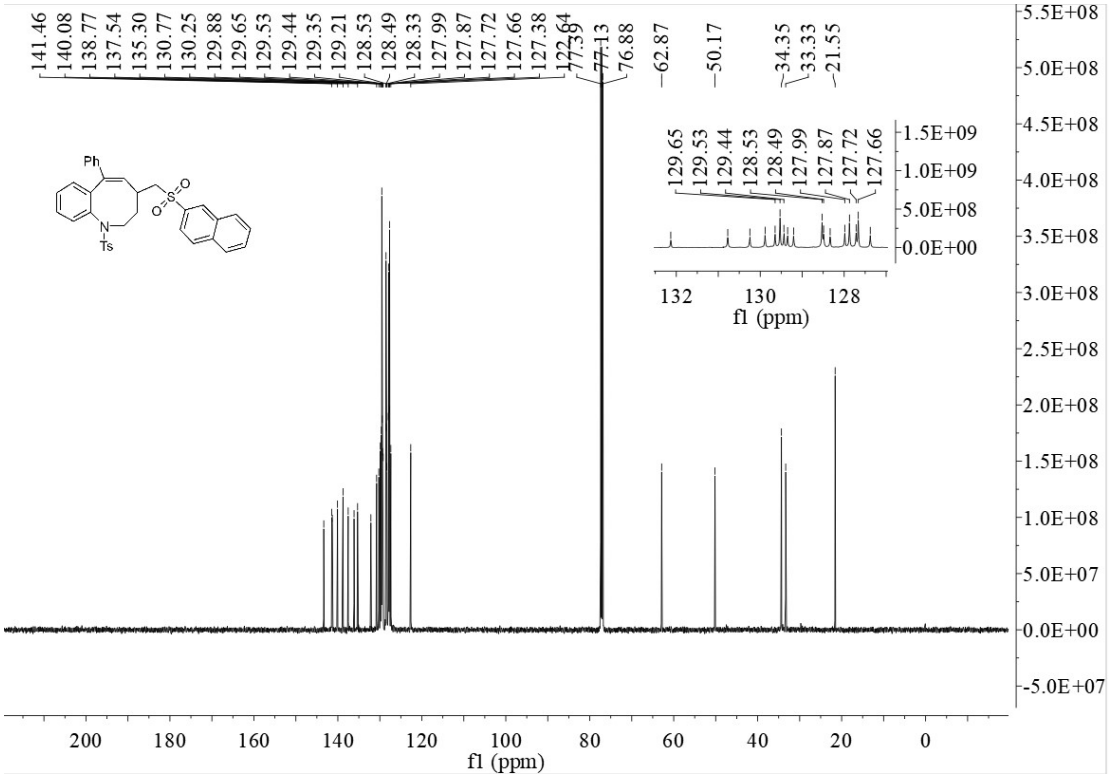
Compound 3af



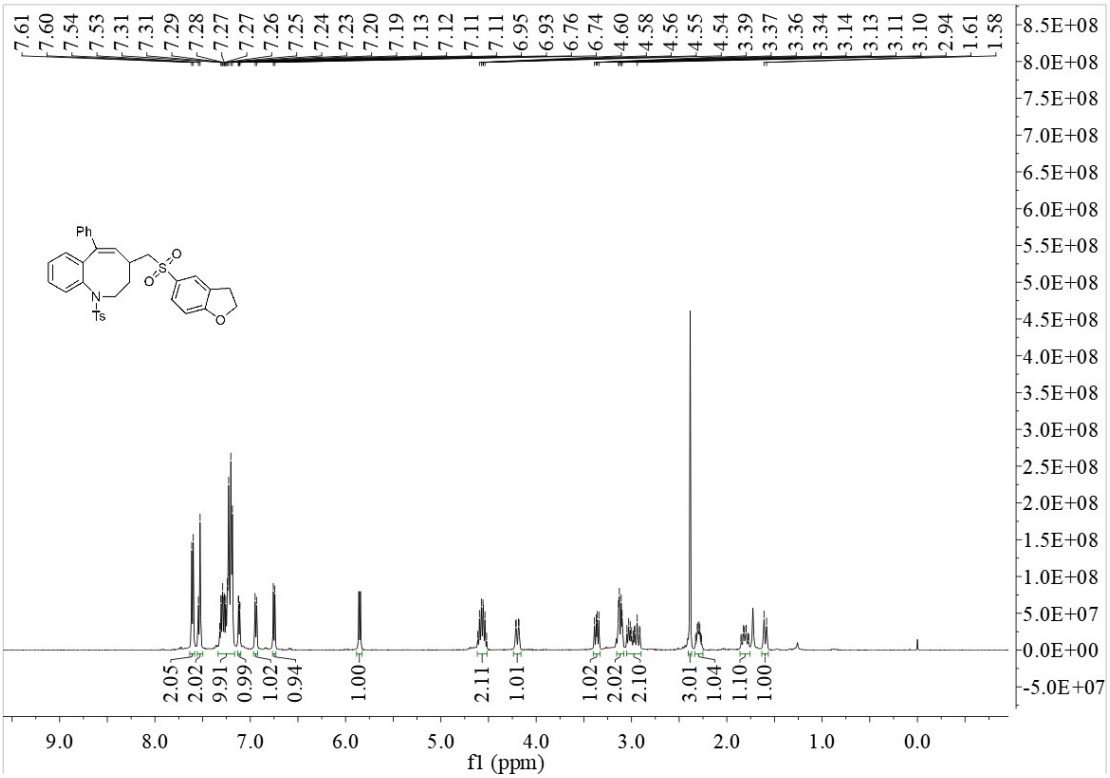


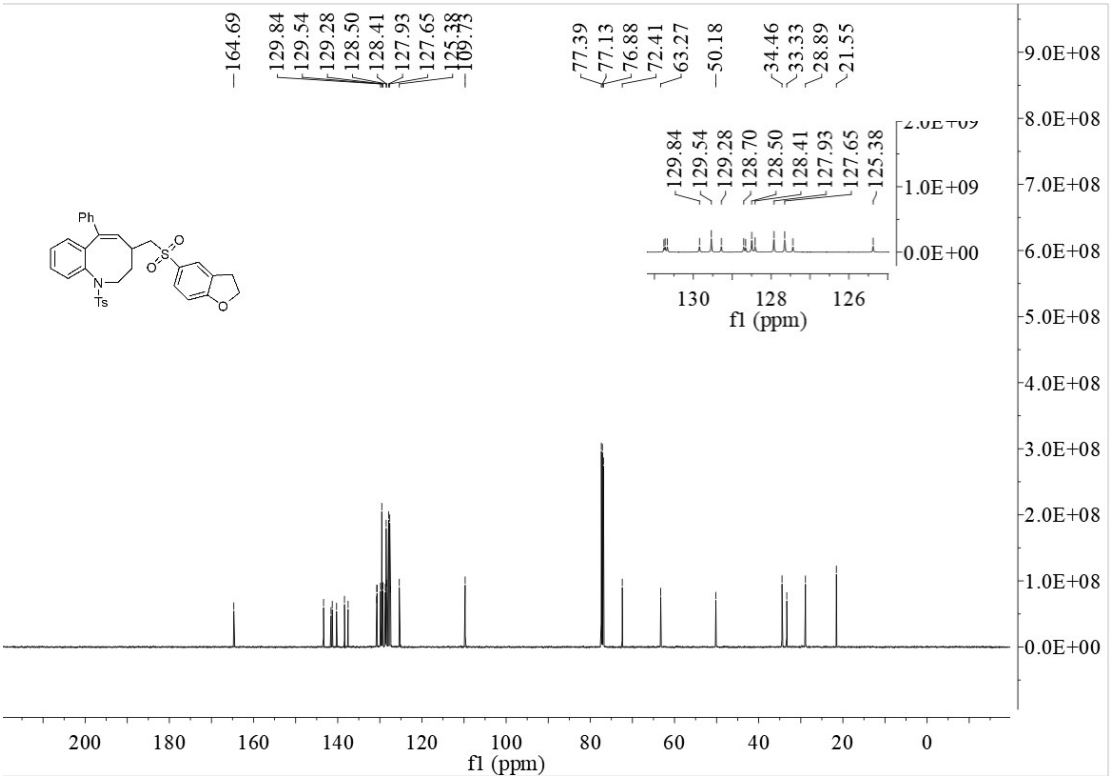
Compound 3ag



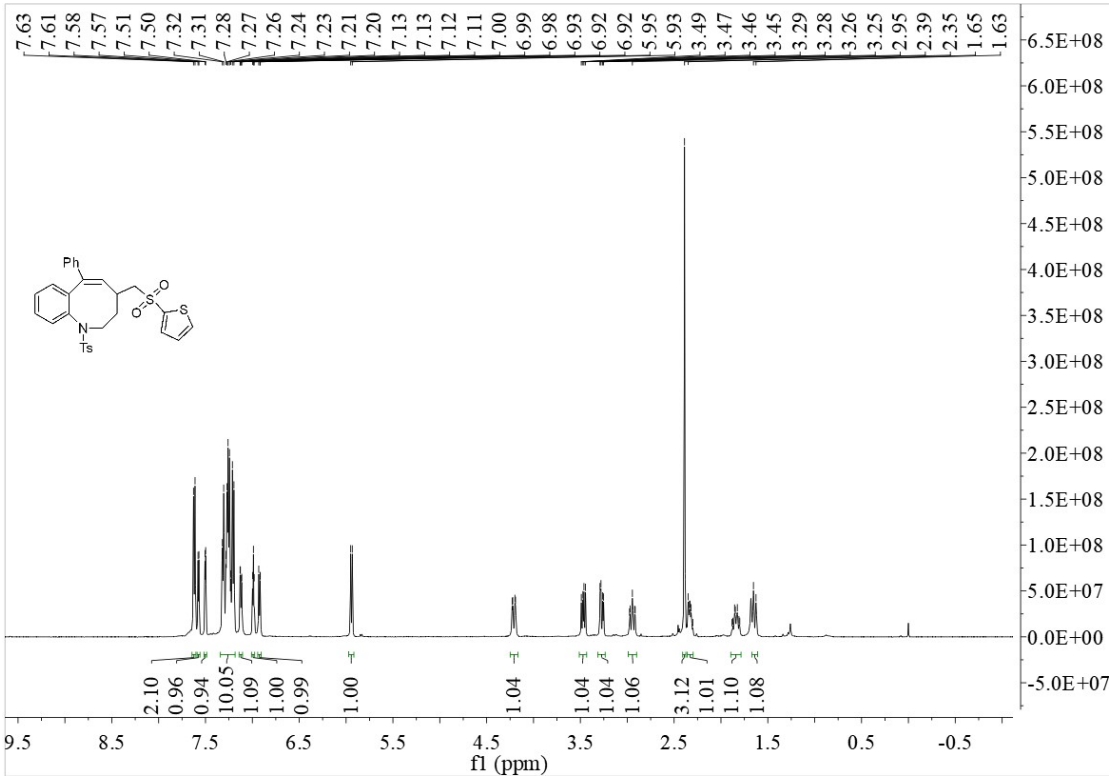


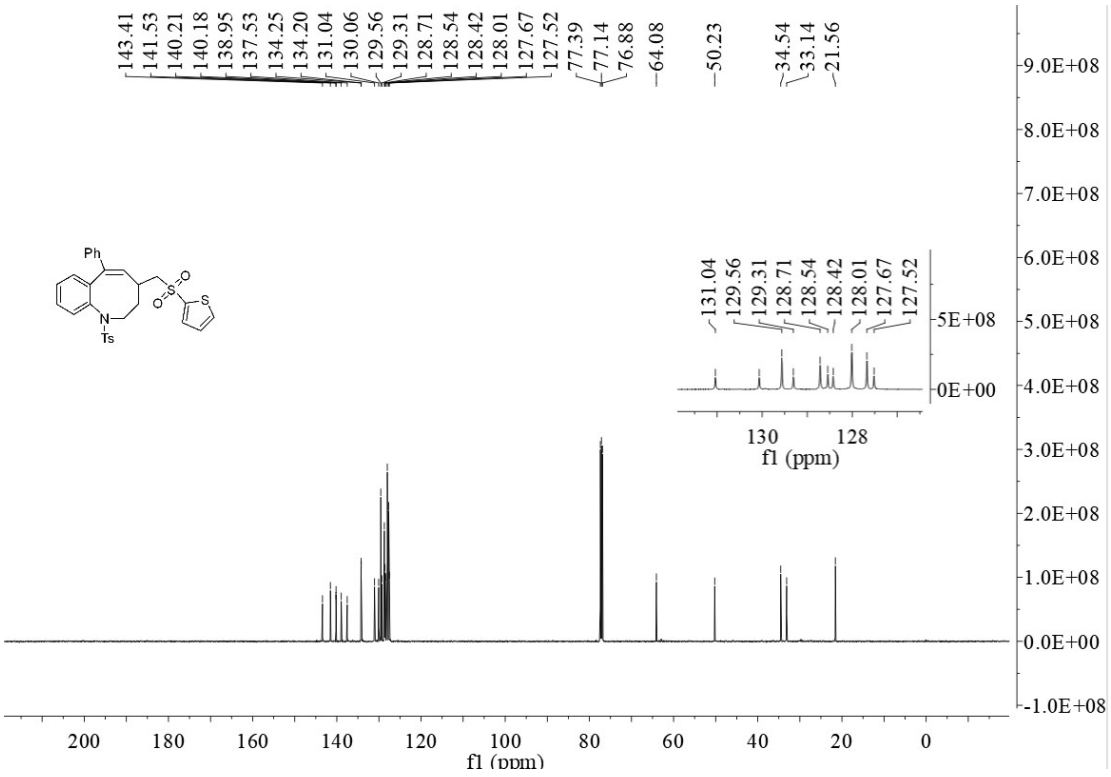
Compound 3ah



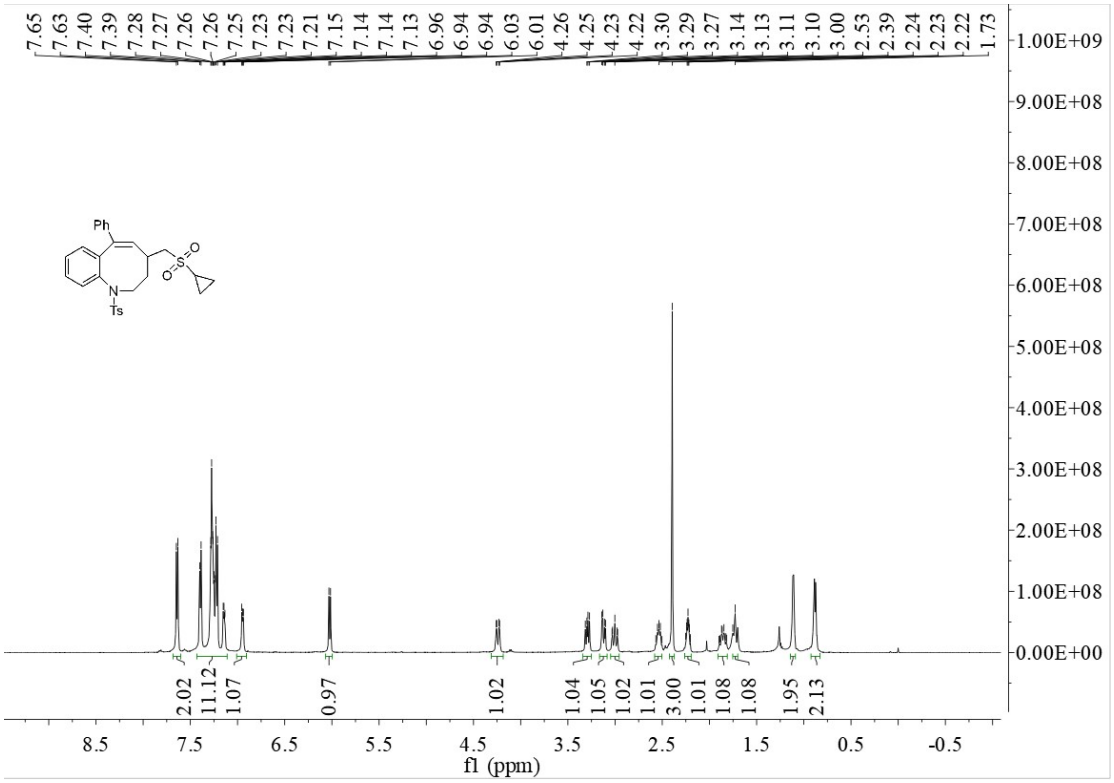


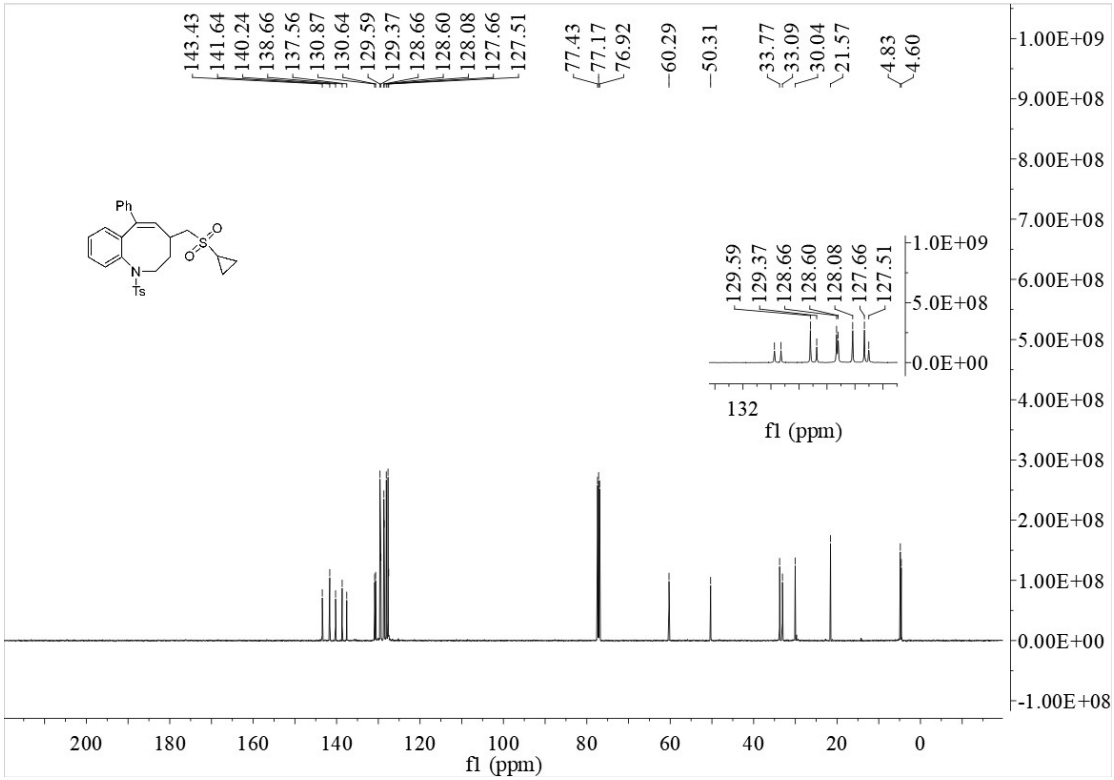
Compound 3ai



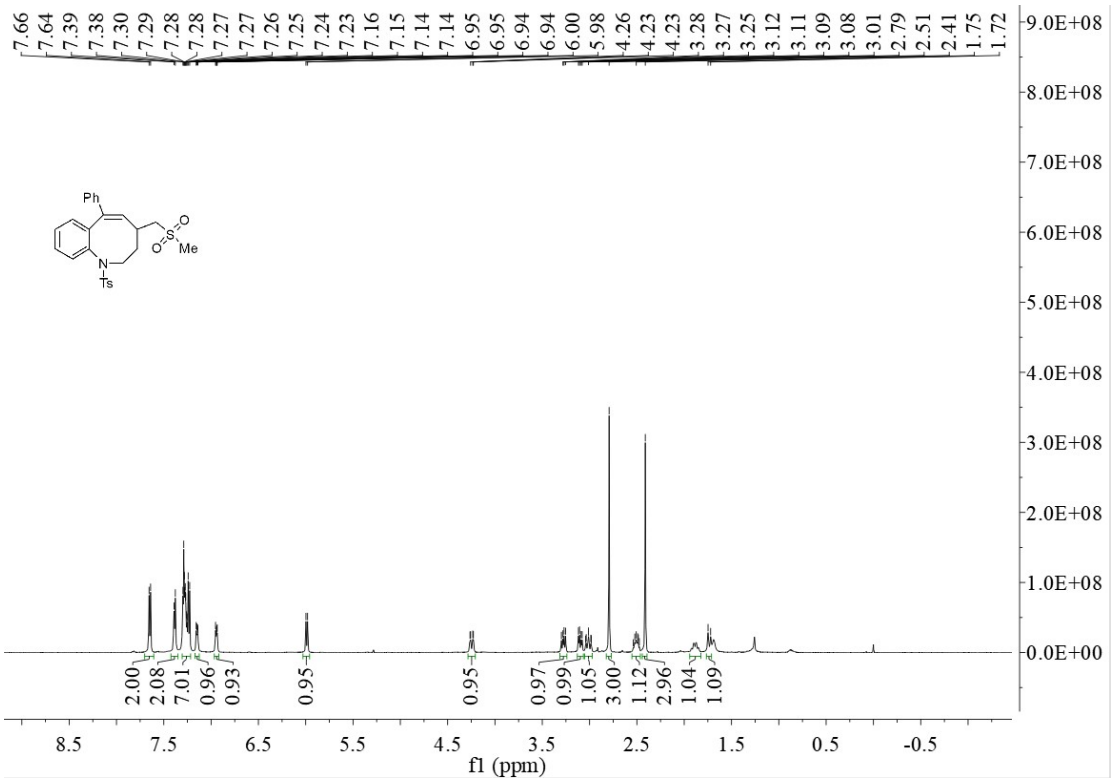


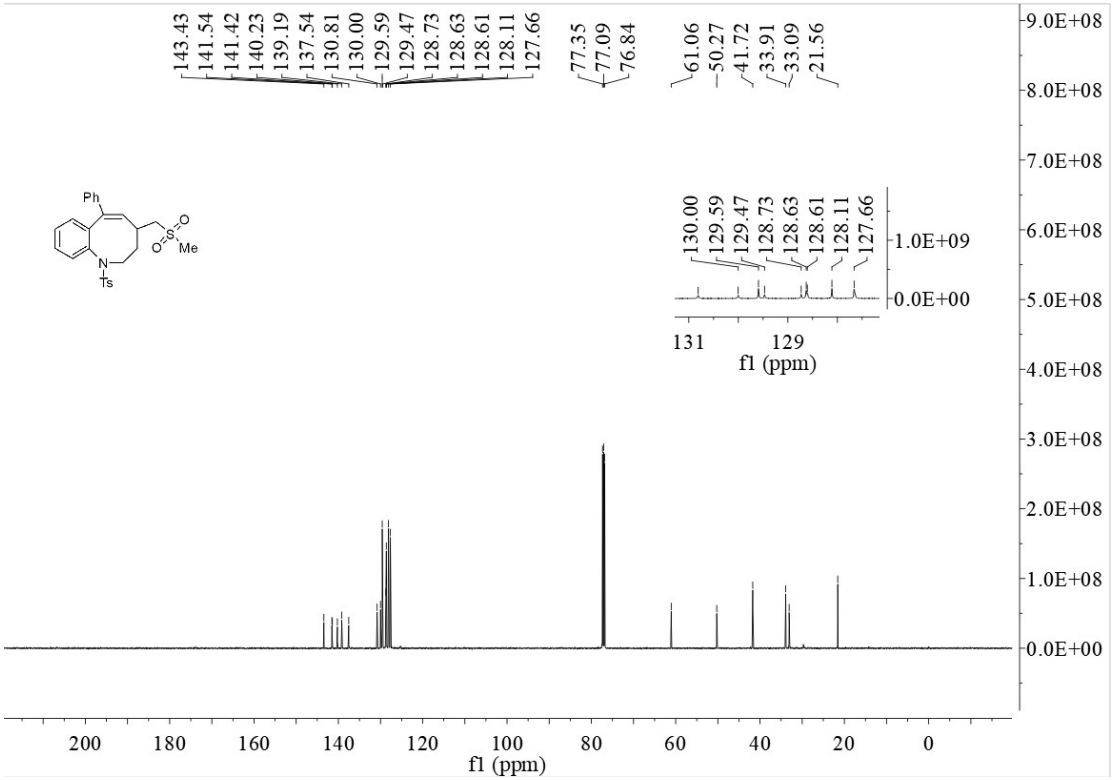
Compound 3aj



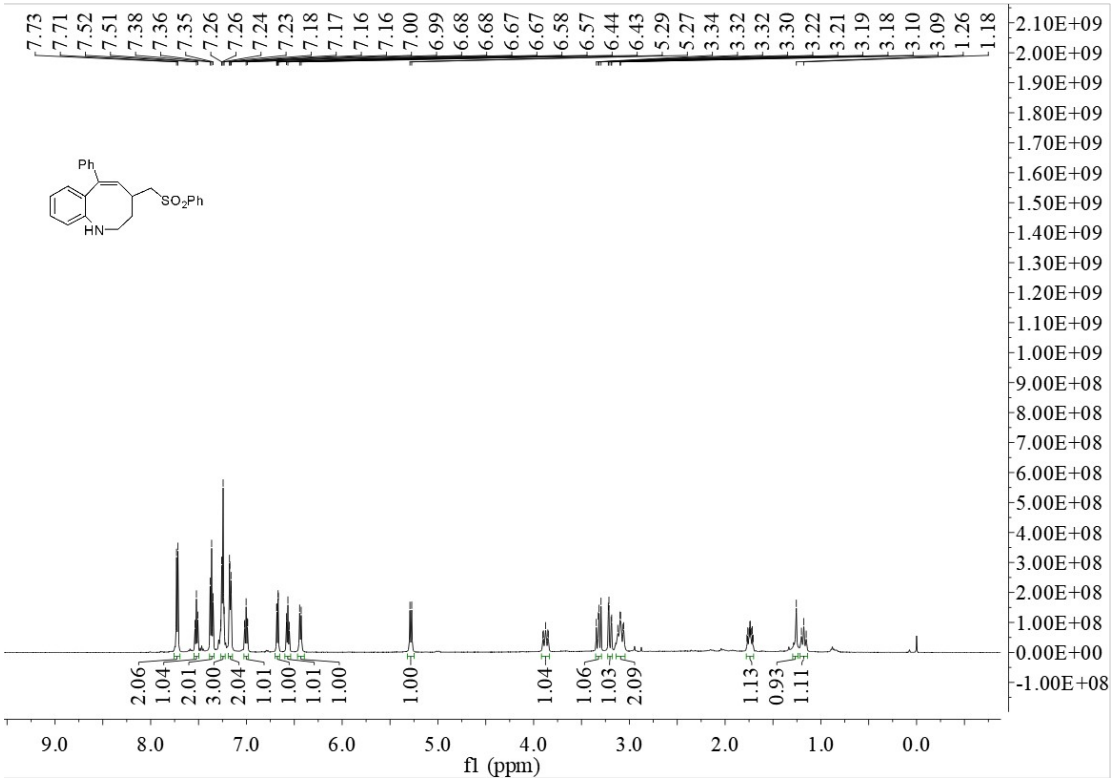


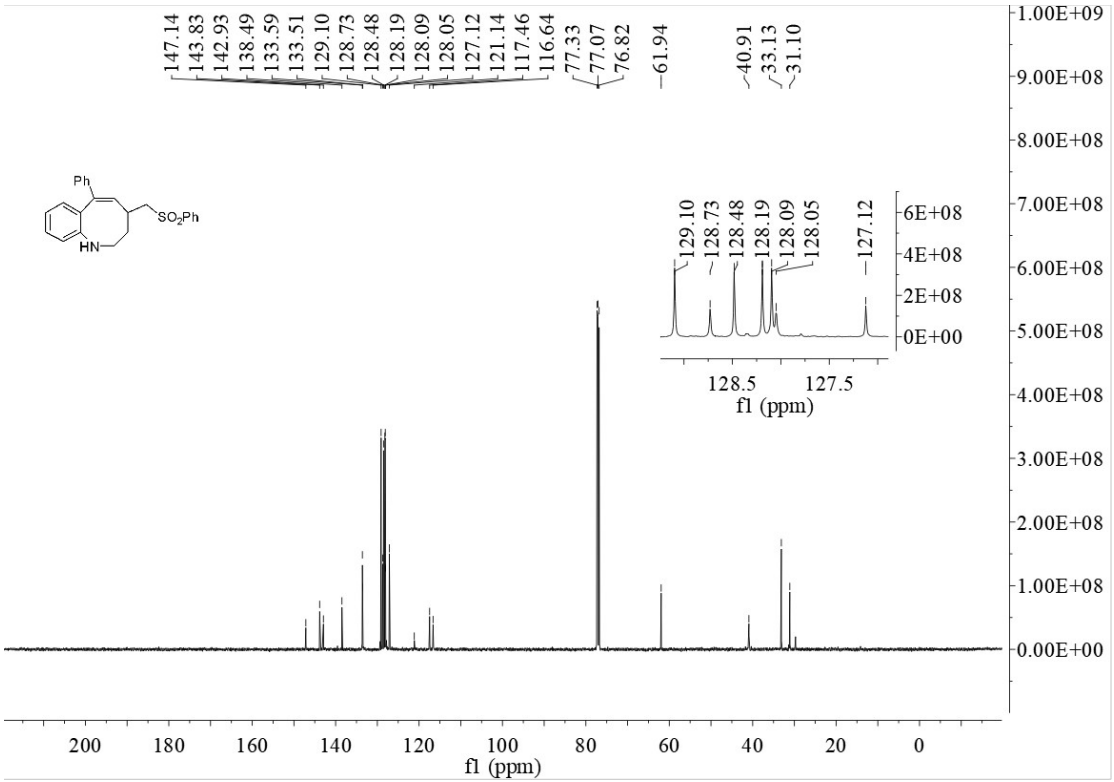
Compound 3ak



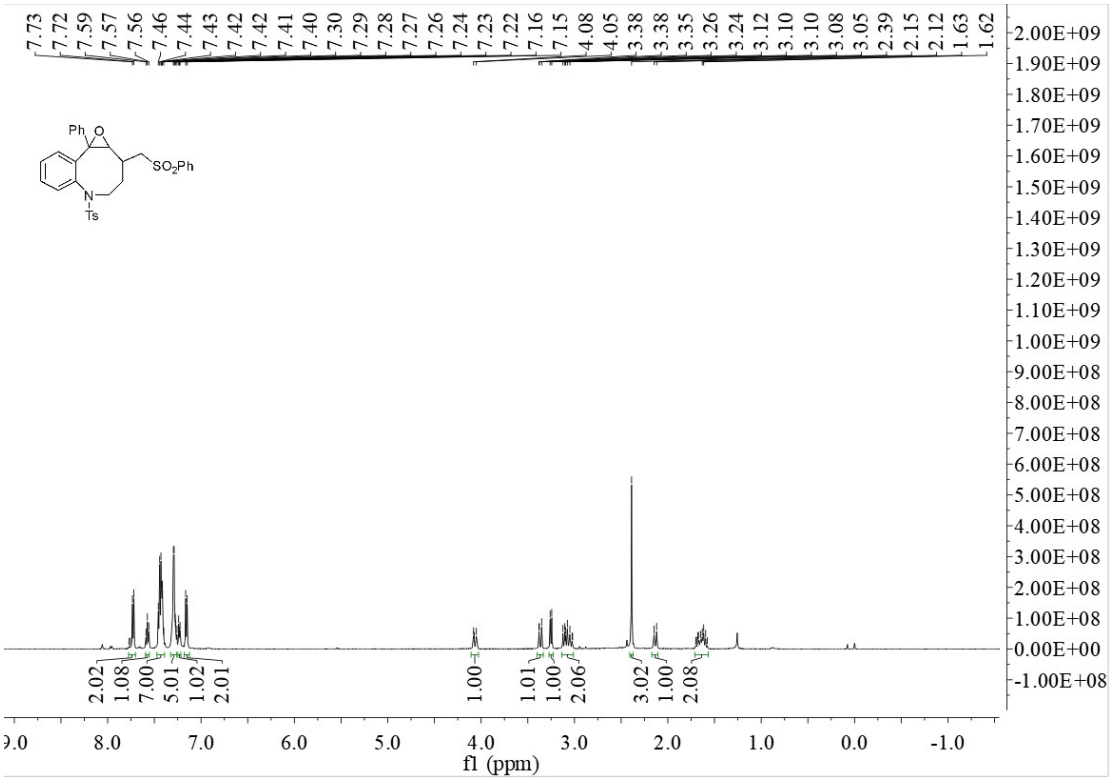


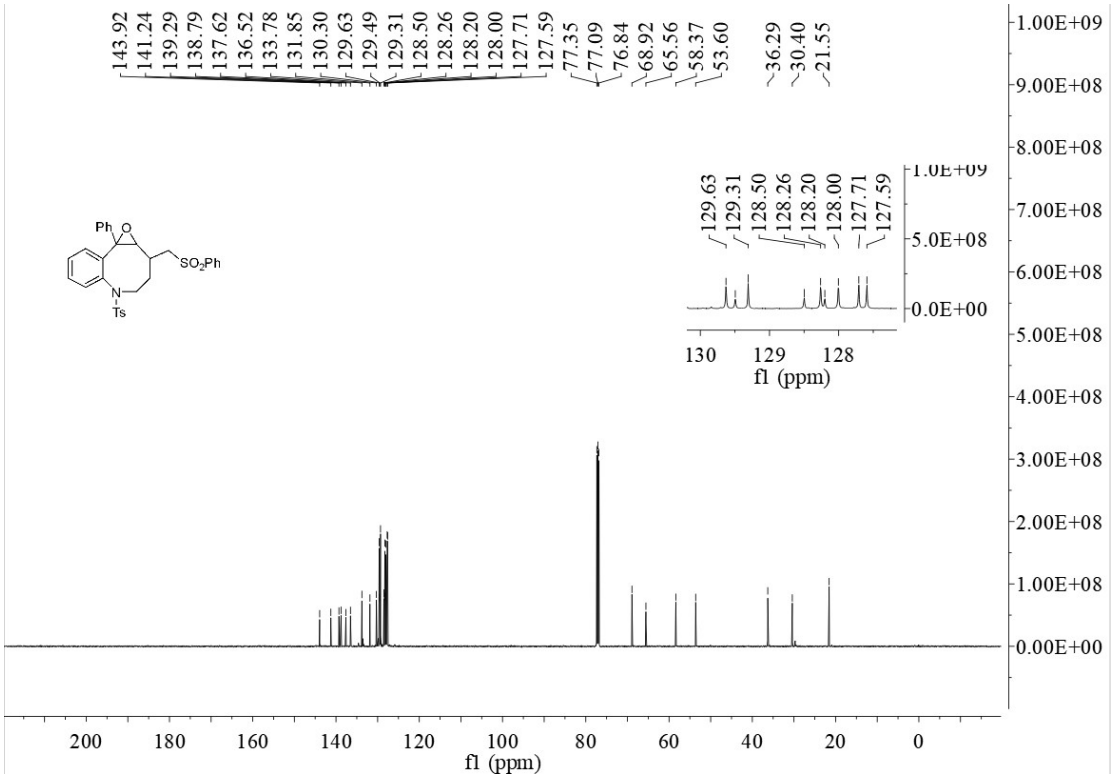
Compound 4


7.73 7.71 7.52 7.51 7.38 7.36 7.35 7.26 7.26 7.24 7.23 7.18 7.17 7.16 7.16 7.00 6.99 6.68 6.68 6.67 6.67 6.58 6.57 6.44 6.43 5.29 5.27 3.34 3.32 3.32 3.30 3.22 3.21 3.19 3.18 3.10 3.09 1.26 1.18
Ph
SO2Ph
HN
2.06 1.04 2.01 3.00 2.04 1.01 1.00 1.01 1.00 1.00 1.04 1.06 1.03 2.09 1.13 0.93 1.11
f1 (ppm)


147.14 143.83 142.93 138.49 133.59 133.51 129.10 128.73 128.48 128.19 128.09 128.05 127.12 121.14 117.46 116.64 77.33 77.07 76.82 61.94 40.91 33.13 31.10
Ph
SO2Ph
HN
129.10 128.73 128.48 128.19 128.09 128.05 127.12
128.5 127.5
f1 (ppm)
f1 (ppm)

Compound 5


7.73 7.72 7.59 7.57 7.56 7.46 7.44 7.43 7.42 7.42 7.41 7.40 7.30 7.29 7.28 7.27 7.26 7.24 7.23 7.22 7.16 7.15 4.08 4.05 3.38 3.38 3.35 3.26 3.24 3.12 3.10 3.10 3.08 3.05 2.39 2.15 2.12 1.63 1.62
Ph
O
SO2Ph
N
Ts
2.02 1.08 7.00 5.01 1.02 2.01 1.00 1.01 1.00 2.06 3.02 1.00 2.08
f1 (ppm)


143.92 141.24 139.29 138.79 137.62 136.52 133.78 131.85 130.30 129.63 129.49 129.31 128.50 128.26 128.20 128.00 127.71 127.59 77.35 77.09 76.84 68.92 65.56 58.37 53.60 36.29 30.40 21.55
129.63 129.31 128.50 128.26 128.20 128.00 127.71 127.59
Ph
O
SO2Ph
N
Ts
f1 (ppm)