Supporting Information

Au-Catalyzed 5C Reaction of Type II Diene-Ynenes toward Dihydrosemibullvalenes: Reaction Development and Mechanistic Study

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1. General Information

All reactions were carried out in oven-dried glassware. All chemicals were used as received without further purification. DCM (with molecular sieves, water ≤ 30 ppm) was purchased from *J&K*. Flash column chromatographies were performed using silica gel (200−300 mesh). Analytical thin layer chromatographies (TLCs) were performed with 0.2−0.3 mm silica gel HSGF254 plates.

Nuclear magnetic resonance (NMR) spectra were measured on Bruker AVANCE III 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz) and Bruker AVANCE III HD 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz) NMR spectrometers. Data for ^{1}H NMR spectra are reported as follows: chemical shift δ (ppm) referenced to either tetramethylsilane (TMS, 0.00 ppm), $CHCl_3$ (7.26 ppm) or $CHDCl_2$ (5.32 ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, dp = doublet of pentets, ddd = doublet of doublet of doublets, dtt = doublet of triplet of triplets), coupling constant *J* (Hz), and integration. Data for ^{13}C{^{1}H} NMR spectra are reported in terms of chemical shift *δ* (ppm) referenced to either $CDCl_3$ (77.16 ppm) or CD_2Cl_2 (53.84 ppm).

High-resolution mass spectrometry (HRMS) data were recorded on Bruker Apex IV and Bruker Solarix XR fourier transform ion cyclotron resonance (FTICR) mass spectrometers (ionization: ESI; mass analyzer: FT-ICR). Single crystals grown from vapor diffusion method in DCM/hexane were collected X-ray diffraction data on a XtaLAB PRO 007HF(Mo): Kappa single diffractometer at 180 K.

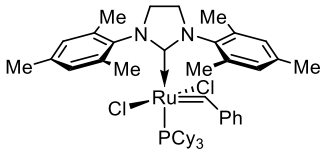
Abbreviations:

DCM: Dichloromethane

DIAD: Diisopropyl azodicarboxylate

EA: Ethyl acetate

Grubbs-II catalyst:



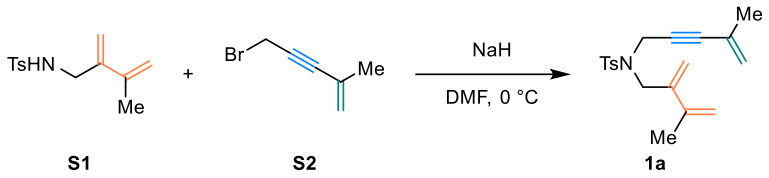
Benzylidene[1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene]
dichloro(tricyclohexylphosphine)ruthenium

ORTEP: Oak Ridge thermal ellipsoid plot

PE: Petroleum ether

2. Synthesis of Substrates

Synthesis of 1a:



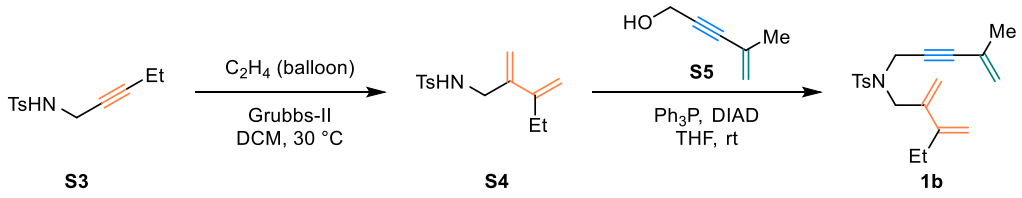
To a stirring DMF solution (25 mL) of sulfonamide **S1**[1] (0.8651g, 3.44 mmol) was added NaH (60 wt%, 0.2476 g, 6.19 mmol) under 0 ℃. After 15 minutes the bromide **S2**[2] was added to the mixture and the mixture was allowed to warm to room temperature and reacted for 2 hours. The reaction was quenched with saturated NH_4Cl. The aqueous phase was extracted with ether, and the combined organic phase was washed with brine and dried with anhydrous Na_2SO_4 before concentration on a rotary evaporator to give the crude product. The crude mixture was further purified by flash column chromatography (PE/EA = 20/1) to give **1a** (828.4 mg, 2.51 mmol, 73%) as a pale-yellow solid (m.p. 51 ~ 52 ℃, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 5.44 (s, 1H), 5.31 (s, 1H), 5.23 (s, 1H), 5.10 (s, 1H), 5.09 – 5.07 (m, 1H), 4.91 (s, 1H), 4.13 (s, 2H), 4.02 (s, 2H), 2.41 (s, 3H), 1.93 (s, 3H), 1.60 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.5, 141.1, 140.3, 135.7, 129.6, 128.1, 126.0, 122.0, 117.3, 115.3, 87.3, 80.8, 49.5, 36.5, 23.1, 21.6, 21.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{24}NO_2S$, 330.1522; found, 330.1515.

Synthesis of 1b:



Sulfonamide **S3**[3] (1.08 g, 4.54 mmol) and Grubbs-II catalyst (115.7 mg, 0.14 mmol) were dissolved in DCM (45 mL) under an ethylene atmosphere. The solution was bubbled with ethylene for 5 min, and then was stirred under 1 atm ethylene in 30 ℃ oil bath for 1.5 hours. The reaction mixture was concentrated on a rotary evaporator and purified by flash column chromatography (PE to PE/EA = 20/1) to afford sulfonamide **S4** (1.02 g, 3.86 mmol, 85%) as a pale-yellow solid.

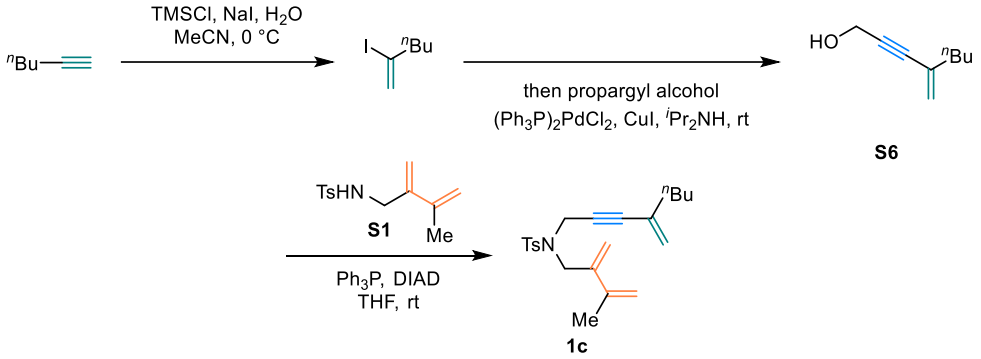
To the mixture of sulfonamide **S4** (930.0 mg, 3.50 mmol), **S5**[4] (556.9 mg, 5.79 mmol) and triphenylphosphine (1.84 g, 7.00 mmol) was added THF (35 mL) under argon. DIAD (1.42 g, 7.00 mmol) was added dropwise, and the mixture was stirred for 6 hours, before being quenched with silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 50/1) afforded **1b** (1.04 g, 3.01 mmol, 86%) as a white solid (m.p. 57 ~ 58 ℃, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 5.39 (s, 1H), 5.32 (s, 1H), 5.20 (s, 1H), 5.07 (d, J = 4.5 Hz, 2H), 4.90 (s, 1H), 4.12 (s, 2H), 3.99 (s, 2H), 2.40 (s, 3H), 2.29 (q, J = 7.4 Hz, 2H), 1.60 (s, 3H), 1.07 (t, J = 7.4 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 146.6, 143.5, 140.9, 135.7, 129.5, 128.1, 126.0, 122.0, 116.7, 113.1, 87.3, 80.7, 49.8, 36.4, 26.8, 23.1, 21.6, 13.1.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{26}NO_2S$, 344.1679; found, 344.1682.

Synthesis of 1c:



Under argon atmosphere a solution of NaI (3.60 g, 24.00 mmol) in acetonitrile (20 mL) was mixed with TMSCl (3.29 mL, 26.0 mmol) in an ice bath. To the mixture water (0.18 mL) was added, followed by 1-hexyne (1.67 g, 20.33 mmol). The mixture was stirred for 5 hours before being diluted with *n*-hexane (20 mL) and quenched with water. The organic phase was separated and washed with saturated $Na_2S_2O_3$, water and brine consequently. The crude product was dried with anhydrous Na_2SO_4 and carefully concentrated to give crude 2-iodohex-1-ene as a colorless liquid.

To the crude 2-iodohex-1-ene was added $(Ph_3P)_2PdCl_2$ (241.6 mg, 0.34 mmol), CuI (149.1 mg, 0.78 mmol) and $^{i}Pr_2NH$ (40 mL). The mixture was degassed by bubbling with argon for 3 minutes. Under argon atmosphere the mixture was added propargyl alcohol (726.2 mg, 12.95 mmol) and the mixtrue was stirred for 11 hours at room temperature. The crude mixture was diluted with ether and quenched with saturated NH_4Cl. The aqueous phase was extracted with ether and the combined organic phase was washed with 1 M HCl, water and brine, consequently. Volatiles were removed under vacuum and flash column chromatography (PE to PE/EA = 10/1) afforded **S6** (415.7 mg, 3.01 mmol, 23%, 2 steps) as a brown oil.

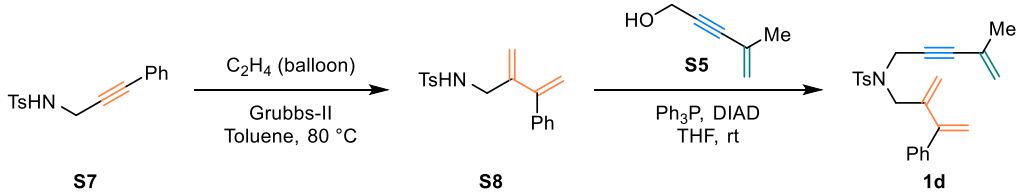
To the mixture of **S6** (407.5 mg, 2.95 mmol), **S1** (818.0 mg, 3.25 mmol) and triphenylphosphine (937.2 mg, 3.57 mmol) was added THF (30 mL) under argon. DIAD (713.9 mg, 3.53 mmol) was added dropwise, and the mixture was stirred for 12 hours, before being quenched by silica. Volatiles in the mixture was removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 50/1) afforded **1c** (534.3 mg, 1.44 mmol, 49%) as a pale-yellow oil (R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 8.3 Hz, 2H), 5.44 (s, 1H), 5.31 (s, 1H), 5.23 (s, 1H), 5.09 (s, 1H), 5.07 (s, 1H), 4.93 (s, 1H), 4.14 (d, J = 12.0 Hz, 2H), 4.02 (s, 2H), 2.40 (s, 3H), 1.93 (s, 3H), 1.87 (t, J = 7.0 Hz, 2H), 1.44 – 1.07 (m, 4H), 0.90 – 0.83 (m, 3H).

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 143.4, 141.0, 140.2, 135.6, 130.9, 129.5, 128.0, 121.2, 117.2, 115.2, 86.7, 81.2, 49.3, 36.5, 36.5, 30.1, 21.9, 21.6, 21.2, 13.9.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{30}NO_2S$, 372.1992; found, 372.1985.

Synthesis of 1d:



Sulfonamide **S7**[5] (564.9 mg, 1.98 mmol) and Grubbs-II catalyst (152.1 mg, 0.18 mmol) were dissolved in toluene (40 mL) under an ethylene atmosphere. The solution was bubbled with ethylene for 5 min, and then stirred under 1 atm ethylene in 80 °C oil bath for 20 hours. The reaction mixture was concentrated on a rotary evaporator and purified by flash column chromatography (PE to PE/EA = 10/1) to afford sulfonamide **S8** (276.9 mg, 0.88 mmol, 45%) as a brown oil.

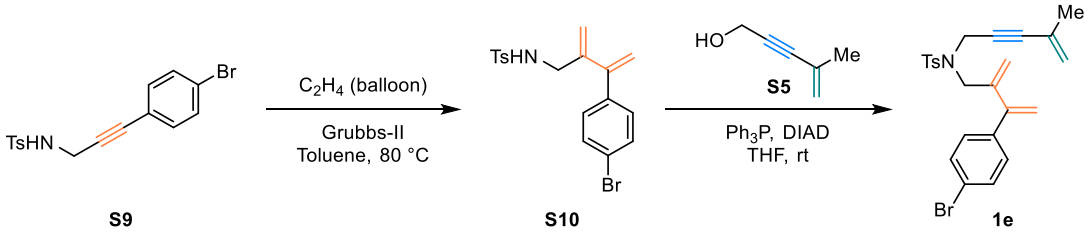
To the mixture of sulfonamide **S8** (714.6 mg, 2.28 mmol), **S5** (250.9 mg, 2.61 mmol) and triphenylphosphine (1.20 g, 4.56 mmol) was added THF (20 mL) under argon. DIAD (922.7 mg, 4.56 mmol) was added dropwise, and the mixture was stirred for 11 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 50/1) afforded **1d** (463.7 mg, 1.18 mmol, 52%) as a pale-yellow oil (R_f = 0.5 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.2 Hz, 2H), 7.34 – 7.27 (m, 7H), 5.60 (s, 1H), 5.38 (s, 1H), 5.29 (s, 1H), 5.19 (s, 1H), 5.08 (s, 1H), 4.92 (s, 1H), 4.24 (s, 2H), 4.04 (s, 2H), 2.40 (s, 3H), 1.59 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 147.6, 143.5, 141.7, 140.9, 135.8, 129.6, 128.4, 128.3, 128.0, 127.6, 126.0, 122.1, 120.3, 116.3, 87.3, 80.7, 49.7, 36.7, 23.1, 21.6.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{24}H_{26}NO_2S$, 392.1679; found, 392.1681.

Synthesis of 1e:



Sulfonamide **S9**[6] (2.49 g, 6.83 mmol) and Grubbs-II catalyst (1.16 g, 1.37 mmol) were dissolved in toluene (70 mL) under an ethylene atmosphere. The solution was bubbled with ethylene for 5 min, and then stirred under 1 atm ethylene in 80 °C oil bath for 18 hours. The reaction mixture was concentrated on a rotary evaporator and purified by flash column chromatography (PE to DCM) to afford sulfonamide **S10** (1.51 g, 3.84 mmol, 56%) as a brown oil.

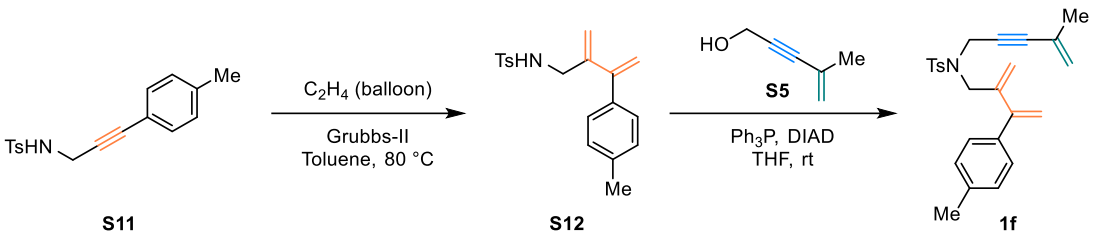
To the mixture of sulfonamide **S10** (1.51 g, 3.84 mmol), **S5** (409.2 mg, 4.26 mmol) and triphenylphosphine (1.22 g, 4.65 mmol) was added THF (40 mL) under argon. DIAD (933.8 mg, 4.56 mmol) was added dropwise, and the mixture was stirred for 12 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) and recrystallization with pentane/DCM afforded **1e** (592.6 mg, 1.26 mmol, 33%) as a pale-yellow solid (m.p. 68 ~ 70 °C, R_f = 0.5 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.2 Hz, 2H), 7.45 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 5.61 (s, 1H), 5.39 (s, 1H), 5.28 (s, 1H), 5.17 (s, 1H), 5.09 (s, 1H), 4.92 (s, 1H), 4.22 (s, 2H), 4.02 (s, 2H), 2.40 (s, 3H), 1.60 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 146.6, 143.6, 141.4, 139.8, 135.7, 131.4, 130.1, 129.6, 128.0, 125.9, 122.2, 121.7, 120.6, 116.8, 87.4, 80.6, 49.6, 36.7, 23.1, 21.6.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{24}H_{25}BrNO_2S$, 470.0784; found, 470.0785.

Synthesis of 1f:



Sulfonamide **S11**[6] (896.5 mg, 3.00 mmol) and Grubbs-II catalyst (503.9 mg, 0.59 mmol) were dissolved in toluene (50 mL) under an ethylene atmosphere. The solution was bubbled with ethylene for 5 min, and then stirred under 1 atm ethylene in 80 °C oil bath for 19 hours. The reaction mixture was concentrated on a rotary evaporator and purified by flash column chromatography (PE to DCM) to afford sulfonamide **S12** (668.4 mg, 2.04 mmol, 68%) as a brown oil.

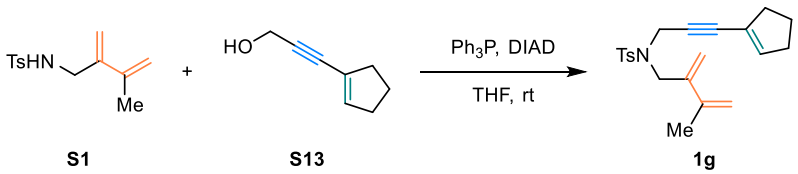
To the mixture of sulfonamide **S12** (668.4 mg, 2.04 mmol), **S5** (216.6 mg, 2.25 mmol) and triphenylphosphine (644.6 mg, 2.46 mmol) was added THF (20 mL) under argon. DIAD (512.4 mg, 2.53 mmol) was added dropwise, and the mixture was stirred for 17 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) and recrystallization with pentane/DCM afforded **1f** (439.8 mg, 1.08 mmol, 53%) as a pale-yellow solid (m.p. 44 ~ 46 °C, R_f = 0.5 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.71 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 7.21 – 7.13 (m, 4H), 5.50 (s, 1H), 5.37 (s, 1H), 5.27 (s, 1H), 5.20 (s, 1H), 5.10 (s, 1H), 4.93 (s, 1H), 4.21 (s, 2H), 4.02 (s, 2H), 2.40 (s, 3H), 2.35 (s, 3H), 1.60 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 148.2, 144.1, 142.6, 138.1, 137.8, 136.2, 129.9, 129.2, 128.4, 128.2, 126.4, 122.2, 120.1, 115.5, 87.5, 81.0, 50.0, 37.0, 23.1, 21.6, 21.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{25}H_{28}NO_2S$, 406.1835; found, 406.1839.

Synthesis of 1g:



To the mixture of sulfonamide **S1** (859.6 mg, 3.42 mmol), **S13**[7] (378.1 mg, 3.09 mmol) and triphenylphosphine (975.3 mg, 3.71 mmol) was added THF (30 mL) under argon. DIAD (757.6 mg, 3.75 mmol) was added dropwise, and the mixture was stirred for 15 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) and recrystallization with

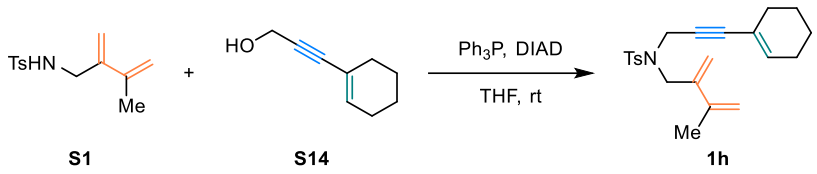
pentane/DCM afforded **1g** (593.1 mg, 1.67 mmol, 54%) as a white solid (m.p. 53 ~ 54 °C, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 5.74 – 5.68 (m, 1H), 5.43 (s, 1H), 5.31 (s, 1H), 5.24 (s, 1H), 5.09 (s, 1H), 4.15 (s, 2H), 4.02 (s, 2H), 2.42 (s, 3H), 2.38 – 2.29 (m, 2H), 2.17 – 2.09 (m, 2H), 1.93 (s, 3H), 1.87 – 1.76 (m, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.4, 141.1, 140.3, 138.1, 135.8, 129.5, 128.1, 123.8, 117.3, 115.3, 83.5, 82.8, 49.4, 36.7, 36.2, 33.2, 23.3, 21.6, 21.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{26}NO_2S$, 356.1679; found, 356.1680.

Synthesis of 1h:



S1 **S14** **1h**

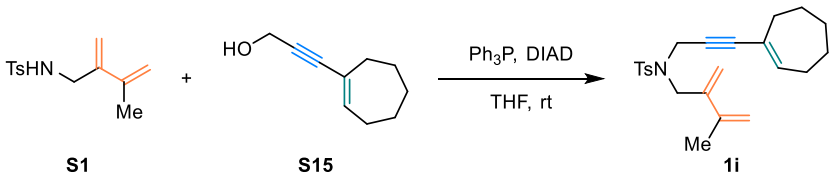
To the mixture of sulfonamide **S1** (904.3 mg, 3.60 mmol), **S14**[8] (563.4 mg, 4.14 mmol) and triphenylphosphine (942.5 mg, 3.59 mmol) was added THF (40 mL) under argon. DIAD (727.5 mg, 3.60 mmol) was added dropwise, and the mixture was stirred for 12 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 50/1) afforded **1h** (754.1 mg, 2.04 mmol, 56%) as a pale-yellow liquid (R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 5.74 – 5.68 (m, 1H), 5.43 (s, 1H), 5.30 (s, 1H), 5.24 (s, 1H), 5.09 (s, 1H), 4.11 (s, 2H), 4.01 (s, 2H), 2.41 (s, 3H), 2.01 (d, J = 10.7 Hz, 2H), 1.92 (s, 3H), 1.78 – 1.72 (m, 2H), 1.58 – 1.48 (m, 4H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.4, 141.1, 140.3, 135.8, 135.0, 129.5, 128.1, 119.9, 117.2, 115.2, 88.0, 78.8, 49.4, 36.6, 29.0, 25.6, 22.3, 21.6, 21.5, 21.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{28}NO_2S$, 370.1835; found, 370.1840.

Synthesis of 1i:



S1 **S15** **1i**

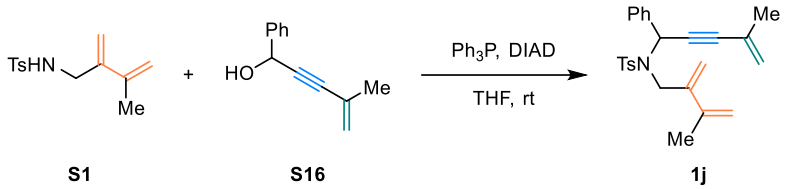
To the mixture of sulfonamide **S1** (827.9 mg, 3.29 mmol), **S15**[7] (450.7 mg, 3.00 mmol) and triphenylphosphine (1.57 g, 5.99 mmol) was added THF (30 mL) under argon. DIAD (1.21 g, 5.98 mmol) was added dropwise, and the mixture was stirred for 12 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 50/1) afforded **1i** (816.3 mg, 2.13 mmol, 65%) as a white solid (m.p. 69 ~ 70 °C, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 5.92 – 5.85 (m, 1H), 5.44 (s, 1H), 5.30 (d, J = 1.1 Hz, 1H), 5.24 (s, 1H), 5.09 (s, 1H), 4.12 (s, 2H), 4.02 (s, 2H), 2.42 (s, 3H), 2.13 – 2.04 (m, 2H), 2.02 – 1.95 (m, 2H), 1.93 (s, 3H), 1.74 – 1.64 (m, 2H), 1.49 – 1.36 (m, 4H).

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 143.3, 141.2, 140.3, 140.2, 135.9, 129.5, 128.1, 126.0, 117.2, 115.3, 89.6, 78.8, 49.4, 36.7, 33.9, 32.1, 29.2, 26.59, 26.56, 21.7, 21.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{23}H_{30}NO_2S$, 384.1992; found, 384.1992.

Synthesis of 1j:



S1 **S16** **1j**

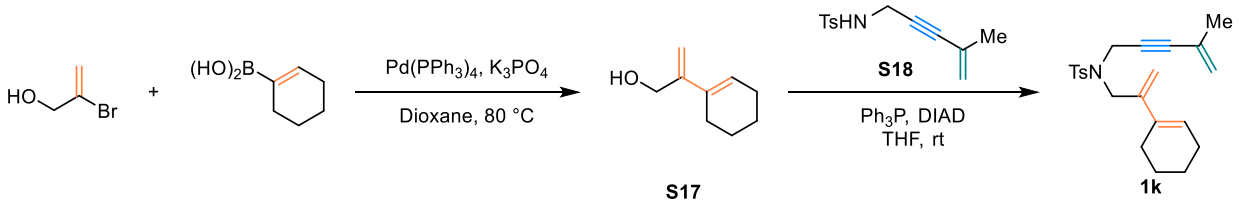
To the mixture of sulfonamide **S1** (552.5 mg, 2.20 mmol), **S16**[9] (344.1 mg, 2.00 mmol) and triphenylphosphine (631.0 mg, 2.39 mmol) was added THF (20 mL) under argon. DIAD (475.7 mg, 2.35 mmol) was added dropwise, and the mixture was stirred for 15 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) and recrystallization with pentane/DCM afforded **1j** (172.2 mg, 0.42 mmol, 21%) as a white solid (m.p. 99 ~ 100 °C, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.2 Hz, 2H), 7.56 – 7.42 (m, 2H), 7.34 (d, J = 8.2 Hz, 2H), 7.26 – 7.17 (m, 3H), 6.17 (s, 1H), 5.24 – 5.11 (m, 2H), 5.05 (s, 1H), 4.99 (s, 1H), 4.86 (s, 1H), 4.80 (s, 1H), 4.36 (d, J = 15.0 Hz, 1H), 3.76 (d, J = 15.0 Hz, 1H), 2.44 (s, 3H), 1.71 (d, J = 1.3 Hz, 3H), 1.42 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 143.6, 141.4, 140.8, 136.5, 135.6, 129.7, 128.5, 128.1, 128.0, 127.8, 125.9, 122.5, 117.0, 113.6, 90.5, 81.9, 54.3, 48.3, 23.2, 21.7, 21.0.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{25}H_{28}NO_2S$, 406.1835; found, 406.1835.

Synthesis of 1k:



S17 **1k**

To the mixture of 2-bromoprop-2-en-1-ol (660.8 mg, 4.82 mmol), 1-cyclohexenylboronic acid (1.27 g, 10.08 mmol), $Pd(PPh_3)_4$ (283.3 mg, 0.24 mmol) and anhydrous K_3PO_4 (4.27 g, 20.12 mmol) was added 1,4-dioxane (25 mL) under argon atmosphere. The mixture was stirred in an 80 °C oil bath for 10 hours and was the cooled and quenched with saturated NH_4Cl. The aqueous phase was extracted with ether and the combined organic phase was washed with brine and dried with anhydrous Na_2SO_4. After removal of volatiles on rotary evaporator, flash column chromatography (PE to PE/EA = 5/1) afforded **S17** (225.0 mg, 1.63 mmol, 34%) as a pale-yellow oil.

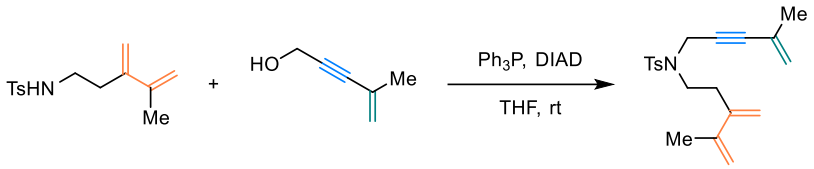
To the mixture of sulfonamide **S18**[10] (349.8 mg, 1.40 mmol), **S15** (225.0 mg, 1.63 mmol) and triphenylphosphine (446.7 mg, 1.70 mmol) was added THF (15 mL) under argon. DIAD (342.7 mg, 1.69 mmol) was added dropwise, and the mixture was stirred for 19 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 30/1) and recrystallization with pentane/DCM afforded **1k** (339.5 mg, 0.92 mmol, 65%) as a white solid (m.p. 95 ~ 96 °C, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 6.25 – 6.17 (m, 1H), 5.18 (s, 1H), 5.09 – 5.07 (m, 1H), 5.06 (s, 1H), 4.91 (s, 1H), 4.12 (s, 2H), 3.98 (s, 2H), 2.40 (s, 3H), 2.22 – 2.11 (m, 4H), 1.74 – 1.64 (m, 2H), 1.60 (s, 3H), 1.59 – 1.54 (m, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.5, 141.5, 135.7, 133.7, 129.5, 128.1, 127.1, 126.1, 121.9, 114.1, 87.3, 81.0, 49.6, 36.5, 26.0, 23.2, 22.9, 22.2, 21.6.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{28}NO_2S$, 370.1835; found, 370.1835.

Synthesis of 1l:



S19 **S5** **1l**

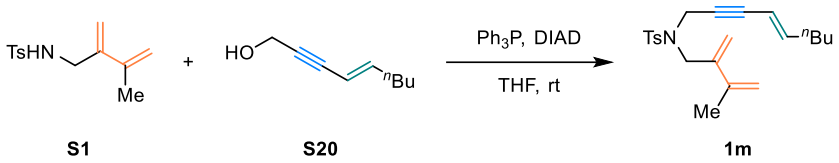
To the mixture of sulfonamide **S19**[1] (226.4 mg, 0.85 mmol), **S5** (99.7 mg, 1.04 mmol) and triphenylphosphine (269.6 mg, 1.03 mmol) was added THF (9 mL) under argon. DIAD (210.7 mg, 1.04 mmol) was added dropwise, and the mixture was stirred for 10 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) afforded **1l** (145.3 mg, 0.42 mmol, 50%) as a white solid (m.p. 45 ~ 46 °C, R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 5.16 (s, 1H), 5.16 (s, 1H), 5.12 (s, 1H), 5.05 (s, 1H), 5.02 (s, 1H), 5.00 (s, 1H), 4.27 (s, 2H), 3.35 – 3.23 (m, 2H), 2.66 – 2.56 (m, 2H), 2.40 (s, 3H), 1.90 (s, 3H), 1.66 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 144.5, 143.4, 141.9, 136.2, 129.6, 127.8, 126.0, 122.3, 114.7, 113.5, 86.9, 81.2, 46.7, 37.6, 33.0, 23.1, 21.6, 21.1.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{26}NO_2S$, 344.1679; found, 344.1679.

Synthesis of 1m:



S1 **S20** **1m**

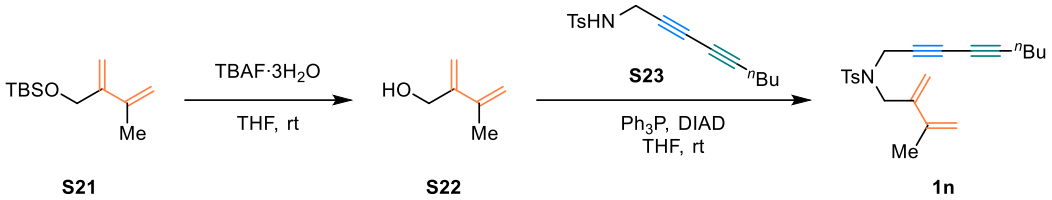
To the mixture of sulfonamide **S1** (352.4 mg, 1.40 mmol), **S20**[11] (175.6 mg, 1.27 mmol) and triphenylphosphine (666.4 mg, 2.54 mmol) was added THF (10 mL) under argon. DIAD (508.8 mg, 2.52 mmol) was added dropwise, and the mixture was stirred for 11 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) afforded **1m** (150.3 mg, 0.40 mmol, 32%) as a pale-yellow oil (R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 5.75 (dt, J = 15.8, 7.0 Hz, 1H), 5.42 (s, 1H), 5.30 (d, J = 1.1 Hz, 1H), 5.23 (s, 1H), 5.17 – 5.10 (m, 1H), 5.09 (d, J = 1.9 Hz, 1H), 4.11 (d, J = 2.1 Hz, 2H), 4.00 (s, 2H), 2.42 (s, 3H), 2.02 (td, J = 7.2, 5.5 Hz, 2H), 1.92 (d, J = 1.2 Hz, 3H), 1.38 – 1.26 (m, 4H), 0.95 – 0.84 (m, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 145.4, 143.3, 141.2, 140.3, 135.8, 129.5, 128.2, 117.2, 115.2, 108.6, 84.9, 80.0, 49.4, 36.7, 32.8, 30.9, 22.2, 21.6, 21.3, 14.0.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{30}NO_2S$, 372.1992; found, 372.1994.

Synthesis of 1n



S21 S22 1n

To the solution of **S21**[12] (2.12 g, 9.98 mmol) in THF (20 mL) was added TBAF·3H$_2$O (4.76 g, 15.08 mmol)under argon atmosphere. The mixture was stirred at room temperature for 4 hours, before being quenched with water. The aqueous phase was separated and extracted with ether. The combined organic phase was dried with anhydrous Na_2SO_4 and volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (pentane to pentane/ether = 5/1) afforded **S22** + TBSOH (649.6 mg, which contained 85.2 wt% **S22** judged on ^{1}H-NMR) as a colorless oil. Therefore, the reaction gave 5.64 mmol **S22** with a yield of 57%.

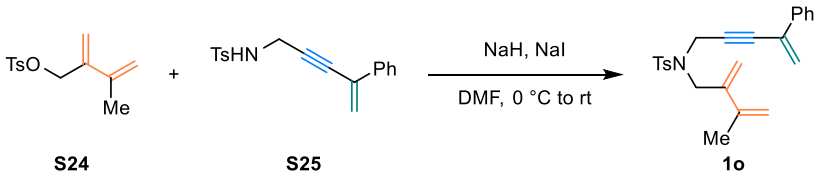
To the mixture of sulfonamide **S23**[13] (467.5 mg, 1.62 mmol), **S22** + TBSOH (192.9 mg, which contained 85.2 wt% **S22**, 1.67 mmol) and triphenylphosphine (508.1 mg, 1.94 mmol) was added THF (16 mL) under argon. DIAD (387.9 mg, 1.92 mmol) was added dropwise, and the mixture was stirred for 11 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) afforded **1n** (357.5 mg, 1.62 mmol, 60%) as a pale-yellow oil (R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 5.40 (s, 1H), 5.30 (s, 1H), 5.22 (s, 1H), 5.08 (s, 1H), 4.05 (s, 2H), 3.98 (s, 2H), 2.43 (s, 3H), 2.21 (t, J = 6.9 Hz, 2H), 1.91 (s, 3H), 1.52 – 1.32 (m, 4H), 0.91 (t, J = 7.2 Hz, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.8, 140.9, 140.1, 135.2, 129.6, 128.1, 117.5, 115.4, 80.4, 71.1, 68.3, 64.3, 49.7, 36.5, 30.3, 22.0, 21.7, 21.2, 18.9, 13.6.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{28}NO_2S$, 370.1835; found, 370.1835.

Synthesis of 1o:



S24 S25 1o

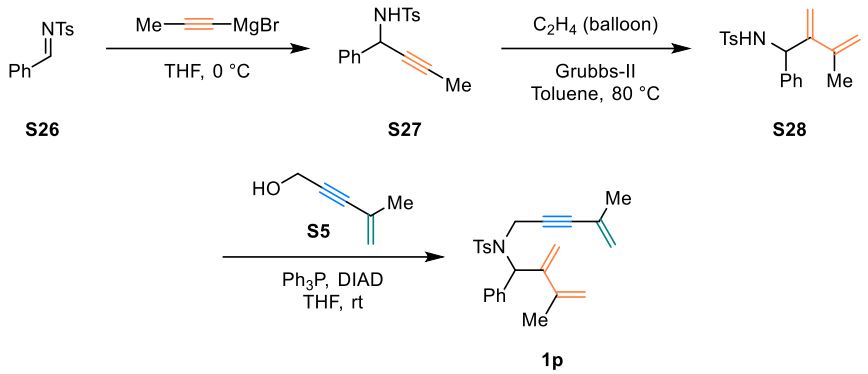
To a stirring DMF solution (10 mL) of sulfonamide **S25**[14] (170.0 mg, 0.55 mmol) was added NaH (60 wt%, 50.0 mg, 1.25 mmol) under 0 °C. After 15 minutes **S24**[15] (0.57 mol/L DMF solution, 1.0 mL, 0.57 mmol) and NaI (75.0 mg, 0.50 mmol) were added to the mixture and the mixture was allowed to warm to room temperature and reacted for 25 minutes. The reaction was quenched with saturated NH_4Cl. The aqueous phase was separated and extracted with ether, and the combined organic phase was washed with water and brine and dried with anhydrous Na_2SO_4 before concentration on a rotary evaporator to give the crude product. The crude mixture was further purified by flash column chromatography (PE/EA = 10/1) to give **1o** (18.0 mg, 0.046 mmol, 8%) as a pale-yellow oil (R_f = 0.5 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.2 Hz, 2H), 7.38 – 7.26 (m, 5H), 7.17 (d, J = 8.2 Hz, 2H), 5.77 (s, 1H), 5.45 (s, 1H), 5.33 (s, 1H), 5.28 (s, 1H), 5.26 (s, 1H), 5.11 (s, 1H), 4.26 (s, 2H), 4.08 (s, 2H), 2.26 (s, 3H), 1.94 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 143.7, 141.1, 140.3, 136.8, 135.6, 130.0, 129.6, 128.5, 128.4, 128.0, 125.9, 121.0, 117.4, 115.4, 85.3, 83.3, 49.7, 36.6, 21.6, 21.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{24}H_{26}NO_2S$, 392.1679; found, 392.1681.

Synthesis of 1p:



To the solution of **S26** (1.30 g, 5.00 mmol) in THF (15 mL) was added 1-propynylmagnesium bromide (0.5 M THF solution, 15 mL, 7.50 mmol) under argon atmosphere at 0 °C. The mixture was stirred at 0 °C for 4 hours, before being quenched with saturated NH_4Cl. The aqueous phase was separated and extracted with ether. The combined organic phase was washed with brine and dried with anhydrous Na_2SO_4 and volatiles in the mixture were removed via rotary evaporation, resulting in crude **S27** as a brownish powder which was directly used for the following step.

Crude sulfonamide **S27** and Grubbs-II catalyst (212.3 mg, 0.25 mmol) were dissolved in toluene (100 mL) under an ethylene atmosphere. The solution was bubbled with ethylene for 5 min, and then stirred under 1 atm ethylene in 80 °C oil bath for 22 hours. The reaction mixture was concentrated on a rotary evaporator. Flash column chromatography (PE/DCM = 5/1 to DCM) and recrystallization with hexane/DCM afforded sulfonamide **S28** (1.12 g, 3.43 mmol, 69%, 2 steps) as a white solid.

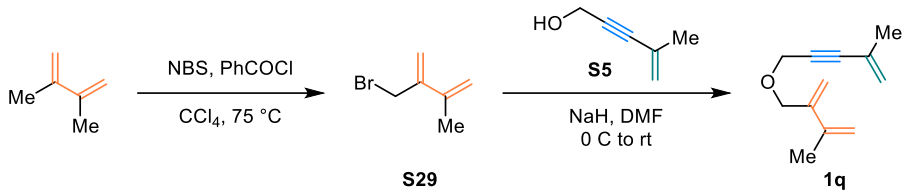
To the mixture of sulfonamide **S28** (491.6 mg, 1.50 mmol), **S5** (163.7 mg, 1.70 mmol) and triphenylphosphine (475.6 mg, 1.81 mmol) was added THF (15 mL) under argon. DIAD (369.6 mg, 1.82 mmol) was added dropwise, and the mixture was stirred for 18 hours, before being quenched by silica. Volatiles in the mixture were removed via rotary evaporation. Flash column chromatography (PE to PE/EA = 20/1) afforded **1p** (329.8 mg, 0.81 mmol, 54%) as a pale-yellow oil (R_f = 0.6 (PE/EA = 5/1)).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.4 Hz, 2H), 7.22 – 7.15 (m, 5H), 7.11 – 7.05 (m, 2H), 6.10 (s, 1H), 5.50 (s, 1H), 5.22 (s, 1H), 5.11 – 5.07 (m, 1H), 4.99 (s, 1H), 4.98 (s, 1H), 4.94 (s, 1H), 4.20 (d, J = 18.6 Hz, 1H), 4.06 (d, J = 18.5 Hz, 1H), 2.40 (s, 3H), 1.91 (d, J = 1.2 Hz, 3H), 1.65 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 145.5, 143.1, 141.2, 138.0, 137.7, 129.3, 129.2, 128.4, 127.9, 127.8, 126.4, 121.7, 117.2, 115.0, 85.1, 84.3, 63.3, 35.8, 23.1, 21.9, 21.6.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{25}H_{28}NO_2S$, 406.1835; found, 406.1835.

Synthesis of 1q:



To the solution of 2,3-dimethylbuta-1,3-diene (535.0 mg, 6.51 mmol), *N*-bromosuccinimide (534.9 mg, 3.01 mmol) in CCl_4 (6 mL) was added 1 drop of benzoyl chloride. The mixture was heated in a 75 °C oil bath for 1 hour, before being filtered and quenched with saturated $Na_2S_2O_3$. The organic phase was further washed with iced water and dried on anhydrous Na_2SO_4. Carefully removal of solvent on rotary evaporator gave crude bromide **S29**, which was directly used for the next step.

To the solution of NaH (60 wt%, 50.0 mg, 1.25 mmol) in DMF (5 mL) was added **S5** (92.8 mg, 0.97 mmol) under 0 °C. After 20 minutes crude **S29** was washed into to the mixture with DMF (5 mL) and the mixture was allowed to warm to room temperature and reacted for 15 hours. The reaction was quenched with saturated NH_4Cl. The aqueous phase was separated and extracted with ether, and the combined organic phase was washed with water and brine and dried with anhydrous Na_2SO_4 before concentration on a rotary evaporator to give the crude product. The crude mixture was further purified by flash column chromatography (PE to PE/EA = 20/1) to give **1q** (32.5 mg, 0.18 mmol, 19%) as a pale-yellow oil (R_f = 0.8 (PE/EA = 10/1)).

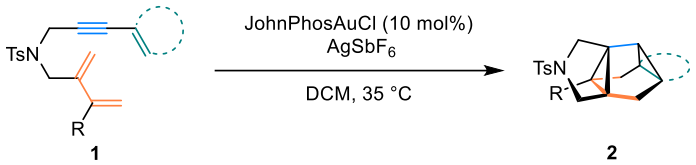
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.31 (s, 1H), 5.29 (s, 2H), 5.24 (s, 1H), 5.19 (s, 1H), 5.04 (s, 1H), 4.28 (s, 2H), 4.27 (s, 2H), 1.93 (d, J = 1.3 Hz, 3H), 1.90 (t, J = 1.3 Hz, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.5, 140.9, 126.5, 122.3, 115.4, 113.8, 87.7, 84.3, 70.8, 57.9, 23.5, 21.1.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{12}H_{17}O$, 177.1274; found, 177.1274.

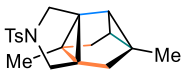
3. Details for the Gold-Catalyzed '5C' Reaction

General Procedure



DCM (1.0 mL) was added to the mixture of JohnPhosAuCl and $AgSbF_6$ (weighed in glove box) under argon atmosphere. The mixture was stirred for 15 minutes, before being transferred into the solution of **1** in DCM (1.0 mL). 2.0 mL DCM was utilized to rinse and transfer all the catalyst into the substrate solution. The combined solution was stirred in a 35 ℃ oil bath and monitored with TLC. After completion, volatiles were removed on a rotary evaporator and the residue was purified with flash column chromatography (PE to PE/EA = 30/1) to afford **2**. For each substrate, two individual runs were performed and the average yield was reported.

Synthesis of 2a



Run 1: Following the General Procedure, 79.0 mg of **1a**, 12.9 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 8 hours, affording 51.0 mg of **2a** (65%)

Run 2: Following the General Procedure, 79.2 mg of **1a**, 12.8 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 8 hours, affording 47.4 mg of **2a** (60%)

Average yield: 63%

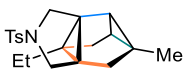
2a: white solid, m.p. 71 ~ 72 ℃, R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 3.60 (d, J = 9.4 Hz, 1H), 3.46 (d, J = 9.4 Hz, 1H), 3.28 (d, J = 9.6 Hz, 1H), 3.21 (s, 1H), 2.43 (s, 3H), 1.76 – 1.68 (m, 3H), 1.51 (d, J = 12.5 Hz, 1H), 1.37 (d, J = 6.7 Hz, 1H), 1.17 – 1.12 (m, 1H), 1.02 (s, 3H), 0.90 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.3, 134.9, 129.7, 127.4, 52.0, 48.1, 46.8, 45.6, 40.8, 39.0, 34.5, 33.3, 30.3, 30.1, 21.7, 19.9, 11.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{24}NO_2S$, 330.1522; found, 330.1530.

Synthesis of 2b



Run 1: Following the General Procedure, 49.8 mg of **1b**, 7.8 mg of JohnPhosAuCl and 5.7 mg of $AgSbF_6$ reacted for 4 hours, affording 26.8 mg of **2a** (54%)

Run 2: Following the General Procedure, 50.3 mg of **1b**, 7.7 mg of JohnPhosAuCl and 5.6 mg of $AgSbF_6$ reacted for 4 hours, affording 27.8 mg of **2a** (55%)

Average yield: 55%

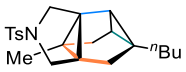
2b: pale-yellow oil, R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 3.62 (d, J = 9.5 Hz, 1H), 3.42 (d, J = 9.5 Hz, 1H), 3.24 (s, 2H), 2.43 (s, 3H), 1.79 – 1.67 (m, 3H), 1.52 (d, J = 12.5 Hz, 1H), 1.37 (d, J = 6.7 Hz, 1H), 1.22 – 1.12 (m, 2H), 1.08 (q, J = 7.3 Hz, 1H), 1.02 (s, 3H), 0.78 (t, J = 7.4 Hz, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.3, 134.8, 129.7, 127.4, 52.2, 48.5, 47.5, 46.8, 46.0, 39.1, 35.0, 30.4, 30.1, 30.0, 21.6, 19.9, 19.2, 12.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{26}NO_2S$, 344.1679; found, 344.1681.

Synthesis of 2c



Run 1: Following the General Procedure, 78.7 mg of **1c**, 11.7 mg of JohnPhosAuCl and 8.9 mg of $AgSbF_6$ reacted for 11.5 hours, affording 33.1 mg of **2c** (42%)

Run 2: Following the General Procedure, 77.4 mg of **1c**, 11.7 mg of JohnPhosAuCl and 8.9 mg of $AgSbF_6$ reacted for 11.5 hours, affording 32.9 mg of **2c** (43%)

Average yield: 42%,

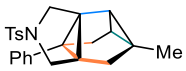
2c: pale-yellow oil R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 3.60 (d, J = 9.5 Hz, 1H), 3.45 (d, J = 9.5 Hz, 1H), 3.28 (d, J = 9.7 Hz, 1H), 3.21 (d, J = 9.7 Hz, 1H), 2.43 (s, 3H), 1.75 – 1.67 (m, 3H), 1.51 (d, J = 12.4 Hz, 1H), 1.38 (d, J = 6.7 Hz, 2H), 1.23 – 1.15 (m, 5H), 1.12 – 1.04 (m, 1H), 0.89 (s, 4H), 0.86 – 0.79 (m, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.3, 134.8, 129.7, 127.4, 52.0, 48.2, 46.4, 45.6, 43.8, 41.0, 34.2, 33.4, 32.1, 30.0, 29.4, 29.1, 22.9, 21.7, 14.2, 11.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{30}NO_2S$, 372.1992; found, 372.1992.

Synthesis of 2d



Run 1: Following the General Procedure, 73.9 mg of **1d**, 13.8 mg of JohnPhosAuCl and 7.4 mg of $AgSbF_6$ reacted for 16 hours, affording 20.9 mg of **2d** (28%)

Run 2: Following the General Procedure, 73.5 mg of **1d**, 10.0 mg of JohnPhosAuCl and 7.3 mg of $AgSbF_6$ reacted for 16 hours, affording 19.0 mg of **2d** (26%)

Average yield: 27%

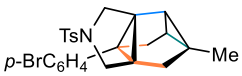
2d: white solid, m.p. 117 ~ 118 ℃, R_f = 0.4 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.18 (m, 3H), 7.13 – 7.01 (m, 6H), 3.75 (d, J = 9.3 Hz, 1H), 3.46 (d, J = 9.3 Hz, 1H), 3.31 (d, J = 9.4 Hz, 1H), 3.18 (d, J = 9.4 Hz, 1H), 2.37 (s, 3H), 2.06 (d, J = 13.1 Hz, 1H), 2.04 – 1.94 (m, 2H), 1.74 (d, J = 12.6 Hz, 1H), 1.61 (d, J = 6.6 Hz, 1H), 1.34 – 1.30 (m, 1H), 1.14 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 142.8, 137.4, 135.3, 129.5, 128.7, 128.7, 127.2, 126.6, 51.8, 49.3, 48.5, 47.8, 46.6, 40.0, 36.2, 34.3, 31.0, 29.9, 21.6, 20.1.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{24}H_{26}NO_2S$, 392.1679; found, 392.1682.

Synthesis of 2e



Run 1: Following the General Procedure, 94.7 mg of **1e**, 10.6 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 24 hours, affording 14.9 mg of **2e** (16%)

Run 2: Following the General Procedure, 92.3 mg of **1e**, 10.8 mg of JohnPhosAuCl and 8.3 mg of $AgSbF_6$ reacted for 24 hours, affording 15.4 mg of **2e** (17%)

Average yield: 16%

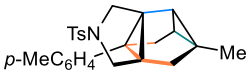
2e: pale-yellow foam, R_f = 0.4 (PE/EA = 5/1)

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.28 (d, *J* = 8.0 Hz, 2H), 7.21 – 7.12 (m, 4H), 6.91 (d, *J* = 8.0 Hz, 2H), 3.71 (d, *J* = 9.4 Hz, 1H), 3.41 (d, *J* = 9.5 Hz, 1H), 3.29 (d, *J* = 9.5 Hz, 1H), 3.13 (d, *J* = 9.5 Hz, 1H), 2.43 (s, 3H), 2.08 – 1.94 (m, 2H), 1.93 – 1.85 (m, 1H), 1.75 (d, *J* = 12.6 Hz, 1H), 1.63 (d, *J* = 6.7 Hz, 1H), 1.32 (s, 1H), 1.12 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 143.5, 136.9, 135.6, 131.9, 130.6, 129.8, 127.2, 120.8, 51.9, 48.9, 48.7, 47.9, 46.8, 40.2, 36.2, 34.3, 31.3, 30.0, 21.8, 20.0.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{24}H_{25}BrNO_2S$, 470.0784; found, 470.0780.

Synthesis of 2f



Run 1: Following the General Procedure, 80.8 mg of **1f**, 10.8 mg of JohnPhosAuCl and 8.3 mg of $AgSbF_6$ reacted for 24 hours, affording 20.9 mg of **2f** (26%)

Run 2: Following the General Procedure, 80.9 mg of **1f**, 10.8 mg of JohnPhosAuCl and 8.3 mg of $AgSbF_6$ reacted for 24 hours, affording 20.7 mg of **2f** (26%)

Average yield: 26%

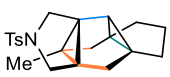
2f: pale-yellow foam, R_f = 0.4 (PE/EA = 5/1)

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.20 – 7.08 (m, 4H), 7.02 (d, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 7.6 Hz, 2H), 3.66 (d, *J* = 9.3 Hz, 1H), 3.45 (d, *J* = 9.3 Hz, 1H), 3.27 – 3.15 (m, 2H), 2.39 (s, 3H), 2.34 (s, 3H), 2.03 (d, *J* = 13.0 Hz, 1H), 1.97 (d, *J* = 12.5 Hz, 1H), 1.90 (dd, *J* = 13.1, 4.9 Hz, 1H), 1.71 (d, *J* = 12.6 Hz, 1H), 1.61 (d, *J* = 6.7 Hz, 1H), 1.30 (dd, *J* = 6.7, 4.9 Hz, 1H), 1.11 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 143.2, 136.4, 135.5, 134.8, 129.6, 129.5, 128.8, 127.4, 52.2, 49.2, 48.8, 48.2, 46.9, 40.0, 36.6, 34.5, 31.2, 30.2, 21.7, 21.4, 20.0.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{25}H_{28}NO_2S$, 406.1835; found, 406.1836.

Synthesis of 2g



Run 1: Following the General Procedure, 71.1 mg of **1g**, 10.6 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 4 hours, affording 33.7 mg of **2g** (47%)

Run 2: Following the General Procedure, 70.9 mg of **1g**, 10.8 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 4 hours, affording 36.8 mg of **2g** (52%)

Average yield: 50%

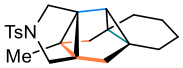
2g: pale-yellow foam, R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.66 (m, 2H), 7.31 (d, J = 8.0 Hz, 2H), 3.50 (d, J = 9.4 Hz, 1H), 3.46 (d, J = 9.4 Hz, 1H), 3.33 (d, J = 9.7 Hz, 1H), 3.19 (d, J = 9.7 Hz, 1H), 2.42 (s, 3H), 1.86 (d, J = 12.6 Hz, 1H), 1.78 – 1.43 (m, 8H), 1.31 – 1.19 (m, 1H), 0.95 (s, 3H), 0.92 – 0.83 (m, 1H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.2, 134.8, 129.7, 127.4, 52.2, 48.2, 47.9, 46.3, 43.3, 39.8, 37.9, 36.0, 31.6, 29.4, 29.3, 28.8, 22.7, 21.6, 11.6.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{26}NO_2S$, 356.1679; found, 356.1678.

Synthesis of 2h



Run 1: Following the General Procedure, 76.7 mg of **1h**, 11.6 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 4 hours, affording 40.3 mg of **2h** (53%)

Run 2: Following the General Procedure, 77.0 mg of **1h**, 11.1 mg of JohnPhosAuCl and 7.9 mg of $AgSbF_6$ reacted for 4 hours, affording 41.0 mg of **2h** (53%)

Average yield: 53%

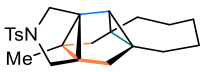
2h: pale-yellow oil, R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 3.56 (d, J = 9.4 Hz, 1H), 3.46 (d, J = 9.4 Hz, 1H), 3.26 (d, J = 9.6 Hz, 1H), 3.20 (d, J = 9.7 Hz, 1H), 2.43 (s, 3H), 1.83 – 1.66 (m, 4H), 1.62 – 1.56 (m, 4H), 1.24 – 1.16 (m, 2H), 1.15 (s, 1H), 1.10 – 0.99 (m, 2H), 0.89 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.2, 135.0, 129.7, 127.5, 51.7, 48.3, 47.9, 45.0, 43.5, 40.7, 39.5, 36.0, 34.2, 32.7, 27.0, 26.9, 22.5, 22.5, 21.7, 11.3.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{28}NO_2S$, 370.1835; found, 370.1843.

Synthesis of 2i



Run 1: Following the General Procedure, 76.4 mg of **1i**, 10.7 mg of JohnPhosAuCl and 8.2 mg of $AgSbF_6$ reacted for 24 hours, affording 36.9 mg of **2i** (48%)

Run 2: Following the General Procedure, 76.1 mg of **1i**, 10.8 mg of JohnPhosAuCl and 8.4 mg of $AgSbF_6$ reacted for 24 hours, affording 35.0 mg of **2i** (46%)

Average yield: 47%

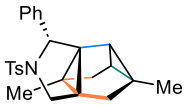
2i: white solid, m.p. 157 ~ 158 °C, R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 7.8 Hz, 2H), 7.31 (d, J = 7.8 Hz, 2H), 3.55 (d, J = 9.4 Hz, 1H), 3.45 (d, J = 9.4 Hz, 1H), 3.28 (d, J = 9.6 Hz, 1H), 3.21 (d, J = 9.6 Hz, 1H), 2.43 (s, 3H), 2.02 – 1.84 (m, 4H), 1.74 – 1.48 (m, 4H), 1.42 (d, J = 12.4 Hz, 1H), 1.34 – 1.17 (m, 6H), 0.91 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.2, 134.8, 129.7, 127.4, 51.6, 48.8, 48.1, 46.9, 45.3, 40.0, 39.7, 39.4, 37.6, 35.0, 34.3, 33.9, 32.0, 28.7, 28.4, 21.6, 11.2.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{23}H_{30}NO_2S$, 384.1992; found, 384.1991.

Synthesis of 2j



Run 1: Following the General Procedure, 80.7 mg of **1j**, 10.6 mg of JohnPhosAuCl and 8.3 mg of $AgSbF_6$ reacted for 24 hours, affording 44.4 mg of **2j** with impurities. Further recrystallization in hexane/DCM gave 24.5 mg pure **1j** (30%).

Run 2: Following the General Procedure, 81.2 mg of **1j**, 10.6 mg of JohnPhosAuCl and 8.2 mg of $AgSbF_6$ reacted for 24 hours, affording 53.0 mg of **2j** with impurities. Further recrystallization in hexane/DCM gave 22.3 mg pure **1j** (27%).

Average yield: 29%

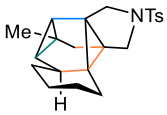
2j: white solid, m.p. 150 ~ 152 ℃, R_f = 0.4 (PE/EA = 5/1)

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.68 (d, J = 8.4 Hz, 2H), 7.44 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 7.9 Hz, 2H), 7.33 – 7.21 (m, 3H), 5.08 (s, 1H), 3.54 (d, J = 11.3 Hz, 1H), 3.39 (d, J = 11.3 Hz, 1H), 2.46 (s, 3H), 1.71 – 1.62 (m, 3H), 1.51 (d, J = 6.7 Hz, 1H), 1.16 (d, J = 12.3 Hz, 1H), 1.11 (dd, J = 6.8, 4.4 Hz, 1H), 1.03 (s, 3H), 0.92 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 144.2, 141.2, 134.1, 130.0, 128.4, 128.1, 127.4, 127.1, 66.6, 55.2, 54.4, 44.9, 42.7, 38.8, 34.9, 33.8, 31.5, 30.2, 21.7, 19.8, 14.0.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{25}H_{28}NO_2S$, 406.1835; found, 406.1835.

Synthesis of 2k



Run 1: Following the General Procedure, 73.6 mg of **1k**, 10.6 mg of JohnPhosAuCl and 8.3 mg of $AgSbF_6$ reacted for 13 hours, affording 17.6 mg of **2k** (24%)

Run 2: Following the General Procedure, 73.5 mg of **1k**, 10.7 mg of JohnPhosAuCl and 8.3 mg of $AgSbF_6$ reacted for 13 hours, affording 16.3 mg of **2k** (22%)

Average yield: 23%

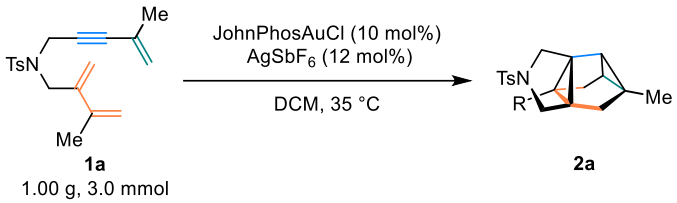
2k: pale-yellow foam, R_f = 0.5 (PE/EA = 5/1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 3.68 (d, J = 9.6 Hz, 1H), 3.43 (d, J = 9.6 Hz, 1H), 3.20 (s, 1H), 3.20 (s, 1H), 2.43 (s, 3H), 1.76 – 1.61 (m, 4H), 1.48 (s, 1H), 1.37 (d, J = 6.7 Hz, 1H), 1.32 – 1.21 (m, 3H), 1.19 – 1.06 (m, 1H), 1.01 (s, 3H), 0.93 – 0.82 (m, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 143.3, 134.8, 129.7, 127.4, 51.8, 48.8, 46.3, 45.7, 45.5, 39.1, 38.7, 36.6, 35.0, 32.5, 29.3, 25.7, 25.3, 21.8, 21.7, 20.1.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{28}NO_2S$, 370.1835; found, 370.1834.

Gram Scale Synthesis



1a
1.00 g, 3.0 mmol

2a

In the glove box, JohnPhosAuCl (0.30 mmol, 159.2 mg) and $AgSbF_6$ (0.36 mmol, 123.7 mg) were added into a 100 mL round-bottom flask. Then DCM (15 ml) was added, and the mixture was stirred at room temperature for 10 minutes. After adding DCM solution of **1a** (3.0 mmol, 1.00 g in 15 mL DCM), the reaction system was stirred at 35 ℃ for 4.5 h. After bringing the round-bottom flask to room temperature, the reaction mixture was filtered through a celite pad to get clear organic liquid. The liquid was concentrated under reduced pressure. Flash column chromatography (PE to PE/EA = 25/1 to 5/1) afforded **2a** (529.1 mg, 1.61 mmol, 53%) as a white solid.

4. Details for Single Point Energy Extrapolation

The extrapolation is done as the following procedure:

1. A DLPNO-CCSD(T1) calculation is performed with def2-TZVPP basis set and corresponding pseudo potential, along with def2-TZVPP/C auxiliary basis. The T_{CutPNO} value is set to 10^{-6}. The correlation energy is denoted as $E_{\mathrm{corr}}^{\mathrm{CC\text{-}largePNO/TZ}}$.
2. A following DLPNO-CCSD(T1) calculation is performed identical basis set, but the T_{CutPNO} value is set to 10^{-7}. The correlation energy is denoted as $E_{\mathrm{corr}}^{\mathrm{CC\text{-}smallPNO/TZ}}$.
3. A RI-MP2 calculation is performed with def2-TZVPP basis set and corresponding pseudo potential, along with def2-QZVPP/C auxiliary basis. The Hartree-Fock energy and the correlation energy is denoted as $E_{\mathrm{HF}}^{\mathrm{TZ}}$ and $E_{\mathrm{corr}}^{\mathrm{MP2/TZ}}$.
4. A following RI-MP2 calculation is performed with def2-QZVPP basis set and corresponding pseudo potential, along with def2-QZVPP/C auxiliary basis. The Hartree-Fock energy and the correlation energy is denoted as $E_{\mathrm{HF}}^{\mathrm{QZ}}$ and $E_{\mathrm{corr}}^{\mathrm{MP2/QZ}}$.

The DLPNO-CCSD(T1) with $T_{\mathrm{cutPNO}} = 0$ correlation energy is extrapolated as:[16,17]

$$E_{\mathrm{corr}}^{\mathrm{CC\text{-}0PNO/TZ}} = E_{\mathrm{corr}}^{\mathrm{CC\text{-}largePNO/TZ}} + F(E_{\mathrm{corr}}^{\mathrm{CC\text{-}smallPNO/TZ}} - E_{\mathrm{corr}}^{\mathrm{CC\text{-}largePNO/TZ}})$$

where $F = 1.5$.

The HF/CBS reference energy is extrapolated as:[18–21]

$$E_{\mathrm{ref}}^{\mathrm{HF/CBS}} = \frac{\mathrm{e}^{-\alpha\sqrt{Y}}E_{\mathrm{HF}}^{\mathrm{TZ}} - \mathrm{e}^{-\alpha\sqrt{X}}E_{\mathrm{HF}}^{\mathrm{QZ}}}{\mathrm{e}^{-\alpha\sqrt{Y}} - \mathrm{e}^{-\alpha\sqrt{X}}}$$

where $X = 3$, $Y = 4$ and $\alpha = 7.88$.

The MP2/CBS correlation energy is extrapolated as:

$$E_{\mathrm{corr}}^{\mathrm{MP2/CBS}} = \frac{X^{\beta}E_{\mathrm{corr}}^{\mathrm{MP2/TZ}} - Y^{\beta}E_{\mathrm{corr}}^{\mathrm{MP2/QZ}}}{X^{\beta} - Y^{\beta}}$$

where $X = 3$, $Y = 4$ and $\beta = 2.97$.

The final Gibbs free energy is computed as:

$$G = TCG + E_{\mathrm{ref}}^{\mathrm{HF/CBS}} + E_{\mathrm{corr}}^{\mathrm{CC\text{-}0PNO/TZ}} + E_{\mathrm{corr}}^{\mathrm{MP2/CBS}} - E_{\mathrm{corr}}^{\mathrm{MP2/TZ}} + G_{\mathrm{solv}}$$

where TCG is the quasi-RRHO thermal correction to Gibbs free energy and G_{solv} is the SMD solvation free energy.

5. Further Discussion on the Reaction Mechanism

Exo- vs. *endo*-cyclopropanation from IN0

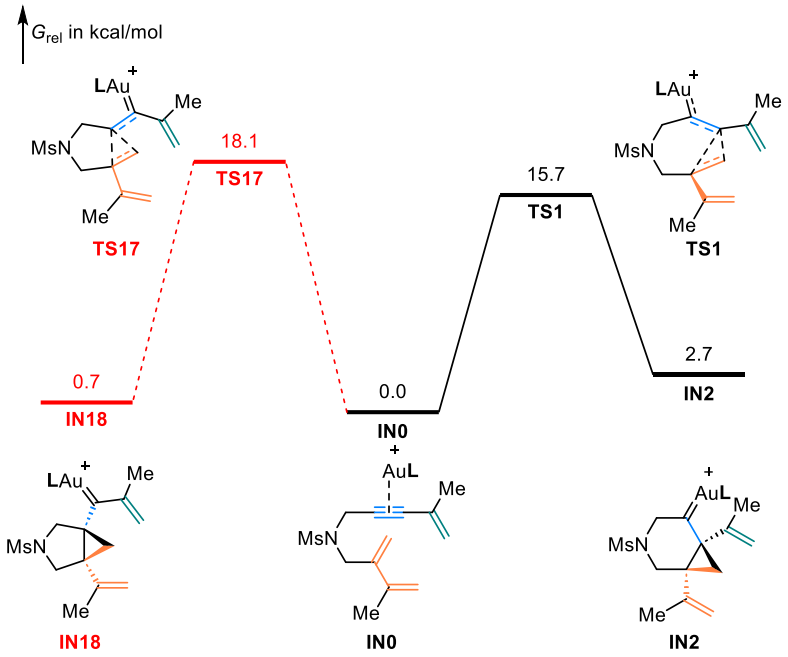


Figure S1. *Exo*- and *endo*-cyclopropanation from **IN0**. Free energy was calculated at SMD(DCM):DLPNO-CCSD(T1)/CBS//PBE0-D3BJ/def2-SVP/SMD(DCM) level.

From **IN0**, an *exo*-type cyclopropanation could take place via **TS19** to give the 5/3 cycle **IN20**. Such *exo*-cyclopropanation is disfavored for 2.4 kcal/mol and could not take place, for the *endo*-cyclopropanation through **TS1** is irreversible. Reason for such selectivity should be likewise to our previous paper.[22]

RDG Analysis on TS3 and TS11

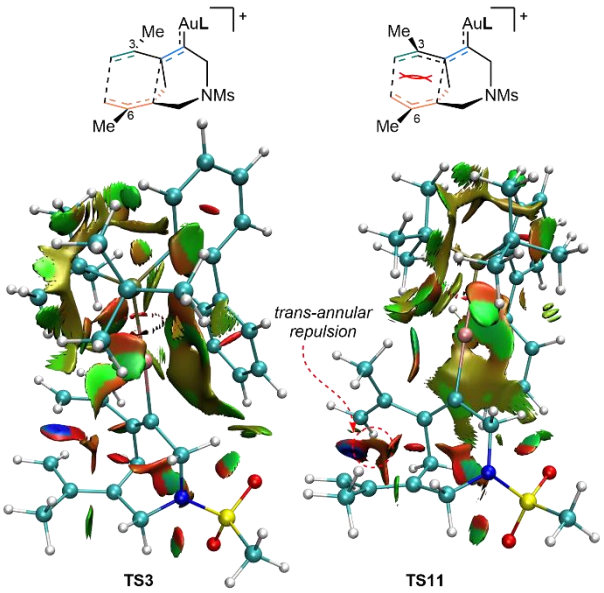


Figure S2. RDG analysis of **TS3** and **TS11**.

RDG anaylsis[23] was performed with Multiwfn 3.8(dev)[24] and was visualized with VMD 1.9.3,[25] on the PBE0/def2-SVP/SMD(DCM) orbitals.The selectivity between **TS3** and **TS11** could probably due to the steric and orbital repulsion[26] between C3 and C6, in **TS11**.

[1, 2]-H shift from IN12

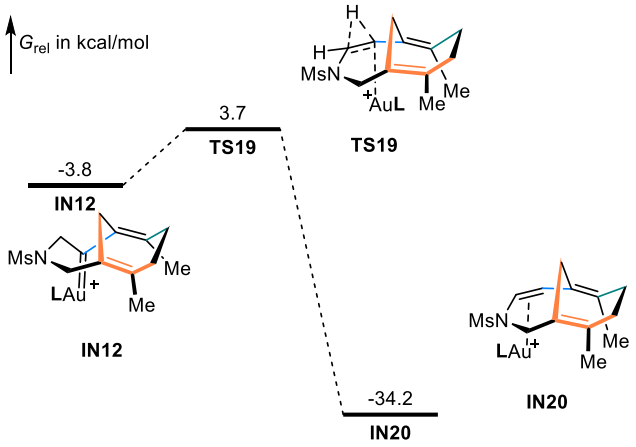


Figure S3. [1, 2]-H shift from **IN12**. Free energies calculated at SMD(DCM):DLPNO-CCSD(T1)/CBS//PBE0-D3BJ/def2-SVP/SMD(DCM) level are given relative to **IN0**.

From **IN12** a [1, 2]-H shift could easily take place through **TS17** to give **IN18**, which has the desired [4.4.1] bridged skeleton. However, since the formation of **IN12** is thermodynamically disfavored, such process cannot take place.

Uncatalyzed Diels-Alder Cycloaddition of 1a'

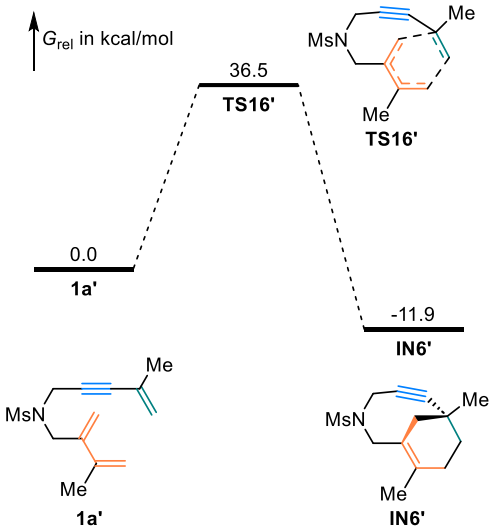


Figure S4. Uncatalyzed Diels-Alder Cycloaddition of **1a'**. Free energy was calculated at SMD(DCM):DLPNO-CCSD(T1)/CBS//PBE0-D3BJ/def2-SVP/SMD(DCM) level.

The uncatalyzed Diels-Adler [4 + 2] cycloaddition of the model substrate **1a'** was also investigated. Such process has a barrier of 36.5 kcal/mol and is exergonic by 11.9 kcal/mol. The high barrier made the process unable to take place at ambient temperature. It is noteworthy that coordination of alkyne to Au(I) significantly accelerates such process, probably by bending the alkyne to reduce strain as well as introducing polarity to the transition state.

6. Summary of Energies and Optimized Cartesian Coordinates

Summary of Energies

Table S1. Summary of Computed Energies in Hartree

	TCG	$E_{ref}^{HF/CBS}$	$E_{corr}^{CC\text{-}0PNO/TZ}$	$E_{corr}^{MP2/CBS}$	$E_{corr}^{MP2/TZ}$	E_{solv}^{PBE0}	E_{gas}^{PBE0}
1a'	0.247214	-1105.229920	-3.244728	-3.362530	-3.007800	-1108.473968	-1108.452668
2a'	0.260583	-1105.286107	-3.265529	-3.399298	-3.044675	-1108.593588	-1108.571393
IN0	0.636248	-2354.019194	-7.671820	-8.051673	-7.193205	-2362.264097	-2362.181546
TS1	0.637248	-2353.980394	-7.684540	-8.066300	-7.207051	-2362.241711	-2362.157889
IN2	0.638951	-2354.004125	-7.682112	-8.063753	-7.204883	-2362.276705	-2362.191351
TS3	0.642982	-2353.976320	-7.700642	-8.091145	-7.231986	-2362.269993	-2362.183035
IN4	0.644594	-2353.991175	-7.695712	-8.082421	-7.223034	-2362.288626	-2362.200332
TS5	0.644290	-2353.980368	-7.696955	-8.083957	-7.225035	-2362.281992	-2362.185473
IN6	0.645185	-2354.040919	-7.692534	-8.084005	-7.225497	-2362.323264	-2362.237024
TS7	0.645858	-2354.016556	-7.697357	-8.085415	-7.226977	-2362.310715	-2362.219134
IN8	0.648126	-2354.060254	-7.686491	-8.075234	-7.217032	-2362.352591	-2362.265711
TS9	0.645090	-2354.025980	-7.693487	-8.087096	-7.227791	-2362.333628	-2362.243474
IN10	0.647448	-2354.052930	-7.679735	-8.070060	-7.210674	-2362.353916	-2362.259360
TS11	0.642011	-2353.963901	-7.706311	-8.098255	-7.238930	-2362.263999	-2362.178140
IN12	0.646408	-2354.011318	-7.691629	-8.074787	-7.215843	-2362.307028	-2362.220649
TS13	0.644846	-2353.983465	-7.688619	-8.070987	-7.212311	-2362.283844	-2362.184163
TS14	0.637723	-2353.984519	-7.685625	-8.068690	-7.209984	-2362.262365	-2362.174619
IN15	0.641586	-2354.034653	-7.692626	-8.078345	-7.220552	-2362.320125	-2362.230177
TS16	0.638391	-2353.962904	-7.692609	-8.081818	-7.222113	-2362.240751	-2362.154749
TS17	0.643156	-2353.987716	-7.695617	-8.079349	-7.219615	-2362.286637	-2362.196702
IN18	0.647305	-2354.052017	-7.702996	-8.090463	-7.233136	-2362.352941	-2362.267675
TS19	0.639096	-2353.967496	-7.692598	-8.075223	-7.216854	-2362.239645	-2362.152096
IN20	0.642462	-2354.001867	-7.686153	-8.070245	-7.212938	-2362.279714	-2362.187976
TS16'	0.250329	-1105.121155	-3.427900	-3.072671	-3.293706	-1108.770091	-1108.519762
IN6'	0.258059	-1105.230880	-3.399324	-3.043968	-3.270932	-1108.857168	-1108.599109

Optimized Cartesian Coordinates in Angstrom

1a'

Charge = 0; Multiplicity = 1

N	0.62323451	0.48324750	-0.21147373
C	-0.12940439	-0.09598833	-1.31265925
C	0.78722951	-0.32190725	0.99514355
C	-1.51939431	-0.41446605	-0.98115609
H	0.39148413	-1.01340813	-1.63324676
H	-0.08375778	0.60053167	-2.16257583
S	0.62095152	2.13631611	-0.05155702
C	1.53557953	-1.60433481	0.71924118
H	-0.19601065	-0.56910493	1.43237148
H	1.33560477	0.29019548	1.72477237
C	-2.66765415	-0.67640990	-0.67488243
C	-0.90747192	2.59301500	0.72188035
O	1.69786108	2.46956907	0.88008717
O	0.62600245	2.69255879	-1.40053994
C	2.96250106	-1.54152143	0.33350384
C	0.87430644	-2.76942755	0.83752906
C	-4.01160128	-0.95150451	-0.26040465
H	-1.73843696	2.31114740	0.06223160
H	-0.87802261	3.68302912	0.86085915
H	-0.98397292	2.08771027	1.69389064
C	3.65907278	-2.83393641	0.01780922
C	3.62682560	-0.37281177	0.27136418
H	-0.18263068	-2.78364099	1.11925328
H	1.35351969	-3.73645496	0.66950504
C	-4.39339650	-0.44697898	1.10340965
C	-4.85885314	-1.62150713	-1.06161966
H	3.64837220	-3.52068134	0.88019384
H	4.70632883	-2.65500200	-0.26194551
H	3.16682265	-3.36200480	-0.81538879
H	4.68515688	-0.35589811	-0.00631574
H	3.15410597	0.59067007	0.47408899
H	-4.27297714	0.64698593	1.16255602
H	-5.43667180	-0.69894934	1.33936589
H	-3.74102192	-0.88355180	1.87708275
H	-5.88364703	-1.82632727	-0.73899101
H	-4.55208205	-1.97670494	-2.04870460

2a'

Charge = 0; Multiplicity = 1

C	1.21990718	2.14762040	0.24898378
C	0.55830066	0.86650787	-0.18732500
C	0.68675232	3.22674915	-0.66573614
C	0.11740179	3.08199702	0.72081012
H	2.22691565	2.16407062	0.67057467
C	0.95368308	-0.53529941	0.17850127
C	-0.34833692	1.15789113	-1.36947745
C	-0.93446347	1.03452223	0.02027783
C	-0.08361034	2.59146366	-1.80118893
H	1.28247968	4.12211112	-0.86693865
C	0.36514935	4.16733351	1.73081181
C	-1.19049624	2.30644420	0.79735652
N	-0.34180029	-1.20030279	0.34184427
H	1.55485228	-1.04290218	-0.59510769
H	1.53642009	-0.54185746	1.11495117
C	-0.66897400	0.16915741	-2.45684880
C	-1.49730115	-0.30262850	0.43783891
H	0.52409552	2.58675881	-2.72169859
H	-1.01908477	3.13059400	-2.03241418
H	-0.38593744	4.97026128	1.64383607
H	0.31679803	3.77453771	2.75998431
H	1.35683401	4.62399240	1.58990977
H	-2.03890136	2.89547440	0.40726578
H	-1.41838465	2.05984700	1.84795498
S	-0.45657757	-2.79873746	0.67811617
H	0.13078286	0.15817379	-3.21493561
H	-0.78029401	-0.85440241	-2.07459707
H	-1.60646140	0.44120828	-2.96915844
H	-2.31953058	-0.66172558	-0.20436521
H	-1.87827604	-0.24525784	1.47053730
C	-0.68297979	-3.61085801	-0.88253962

O	-1.67964234	-3.00148578	1.45334199	H	-7.35703318	-0.22704566	0.04440370
O	0.83446620	-3.23526293	1.20776942	H	-7.51577450	-1.31931023	1.42723882
H	0.18508077	-3.40272025	-1.52174795	H	-7.99145553	0.38771056	1.59492192
H	-0.75480592	-4.68836185	-0.67606286	H	-5.94650662	-2.19690686	0.02790881
H	-1.61151181	-3.24868785	-1.34287051	H	-4.10115525	-2.40197671	-0.11418832
				H	-4.66844574	1.34656057	2.82293208
IN0				H	-6.50574817	1.62516212	2.86139598
Charge = 1; Multiplicity = 1				Au	0.21732499	-0.56604240	-0.49516432
C	-2.78317294	0.52160662	-1.01741458	P	2.12532802	-0.26149443	0.80344767
C	-1.84868280	-0.57716033	-1.32184231	C	1.55422416	0.34497737	2.50510648
C	-1.37155889	-1.65654944	-1.70142131	C	2.99847125	-1.93379061	0.81402865
C	-0.99756095	-2.94819507	-2.21806622	C	3.36033379	0.93008951	0.16005559
C	-0.25999244	-2.97437566	-3.52275045	C	3.28011508	1.51730549	-1.12155696
C	-1.32317217	-4.04421678	-1.51056881	C	4.46402825	1.23713988	0.97549547
N	-2.89411017	0.78617911	0.39924510	C	4.31439615	2.36931413	-1.53985146
H	-3.76389187	0.23888845	-1.43877390	C	5.47273343	2.09271425	0.54850785
H	-2.44832438	1.43044914	-1.53614646	H	4.54530092	0.79860175	1.96900814
H	0.71016149	-2.46164554	-3.42870842	C	5.40052926	2.65872568	-0.72192626
H	-0.82776186	-2.44855840	-4.30616797	H	4.24754027	2.81787776	-2.53390783
H	-0.08281845	-4.00940953	-3.84429256	H	6.31437800	2.31140915	1.20965167
H	-1.06858599	-5.03954595	-1.88558583	H	6.18681029	3.32986021	-1.07608270
H	-1.84455480	-3.97363160	-0.55262107	C	2.16579664	1.32279883	-2.09240216
S	-2.43645395	2.27491881	0.96376556	C	2.31432696	0.44299219	-3.17237558
O	-1.28008328	2.72514608	0.18754896	C	1.00469674	2.10279367	-2.00451562
O	-2.33712916	2.16506149	2.41756588	C	1.31422382	0.33526846	-4.13873506
C	-3.76427612	3.37544641	0.57030887	H	3.22293926	-0.15863122	-3.25529159
H	-3.89668031	3.39524269	-0.51957187	C	0.01220575	2.00154100	-2.97919746
H	-4.67704155	3.02917732	1.07182141	H	0.87463993	2.79340261	-1.16961764
H	-3.46764307	4.36904656	0.93484269	C	0.16115592	1.11563260	-4.04594723
C	-3.32203480	-0.29176069	1.28474713	H	1.44188487	-0.35610494	-4.97528850
C	-4.74376575	-0.73273758	1.02784569	H	-0.88256231	2.62343237	-2.89803364
C	-5.86233733	0.06412916	1.57859582	H	-0.61762935	1.03639731	-4.80867071
C	-7.25422118	-0.28772196	1.14014313	C	2.48684104	-0.00409969	3.66292268
C	-4.94835337	-1.82816762	0.27408746	H	2.05449918	0.41750191	4.58505381
C	-5.65862134	1.06058295	2.46091117	H	2.57549978	-1.08968357	3.81008617
H	-3.17220411	0.04615727	2.31665675	H	3.49341947	0.42096245	3.55855371
H	-2.64519623	-1.14828376	1.13269994	C	1.38238553	1.86121888	2.38736559

H	0.72642748	2.13419443	1.54615470
H	0.90076683	2.23066883	3.30713949
H	2.34312839	2.38244480	2.27356580
C	0.18210583	-0.28028664	2.78074627
H	-0.16207258	0.05188887	3.77328711
H	-0.56234790	0.05459166	2.04572715
H	0.20695014	-1.37879280	2.78300277
C	4.34797664	-1.94043144	1.52926859
H	4.27914004	-1.63237168	2.58010455
H	4.73987974	-2.97063818	1.50956777
H	5.08452487	-1.30282471	1.02107852
C	2.05989277	-2.96075916	1.44769008
H	2.48853686	-3.96643093	1.30886332
H	1.93534210	-2.79820047	2.52760896
H	1.06408574	-2.95098020	0.97555239
C	3.22434860	-2.28326517	-0.66003861
H	3.86419456	-1.54130469	-1.16190726
H	3.73233249	-3.25945334	-0.72068893
H	2.27528680	-2.35664479	-1.21417596

TS1

Charge = 1; Multiplicity = 1

C	4.52012420	-0.35266435	-1.11185696
C	4.59959764	0.13050744	0.31883431
C	5.30328564	1.38448306	0.62391097
C	2.13906709	-0.98492244	-1.43708337
C	1.63839121	-0.12366448	-0.32895896
C	2.14034781	0.39495782	0.73455903
C	2.02907339	1.33186949	1.83269069
C	1.62636364	0.80665293	3.17764088
C	2.24711828	2.63573411	1.57683476
S	3.96224294	-2.97030435	-1.40958096
O	2.82503000	-3.77180952	-0.96217832
O	5.25654415	-3.09978427	-0.74831303
N	3.52264522	-1.37872164	-1.29693986
H	4.28794864	0.48017319	-1.79353899
H	5.51207025	-0.72979338	-1.40579534
H	1.98484656	-0.43577428	-2.38459299
H	1.51916522	-1.89032881	-1.48861695
H	1.59999372	1.61509942	3.92091888
H	2.31466849	0.02363325	3.53123863
H	0.62663666	0.34804927	3.11879352
H	2.15196217	3.38279625	2.37074065
H	2.51750122	2.98166000	0.57656436
C	4.19399416	-3.28727107	-3.13511189
H	4.49528922	-4.34004895	-3.23092897
H	3.24541658	-3.11218302	-3.66006322
H	4.98538263	-2.62730584	-3.51463023
C	4.04062616	-0.63405739	1.30259472
H	4.14960465	-0.36738599	2.35376300
H	3.64748874	-1.62638833	1.08138296
C	5.64489660	1.66990655	2.05759905
H	6.19512198	2.61651482	2.14489998
H	4.73989625	1.74401390	2.68023452
H	6.26586541	0.86495198	2.48285461
C	5.65447751	2.24390018	-0.35314869
H	5.42164952	2.07941575	-1.40708101
H	6.19704511	3.16230128	-0.11164193
Au	-0.38185143	0.45989618	-0.31750733
P	-2.57553697	1.23543557	-0.36097416
C	-2.59050144	2.77397041	0.73679995
C	-3.06795569	1.54995320	-2.16214708
C	-3.83829154	0.10981203	0.35338460
C	-3.96572266	3.38703329	0.99135463
C	-2.00356252	2.31678739	2.07674445
C	-1.66127052	3.81152385	0.10502581
C	-3.46755821	0.18752195	-2.73402654
C	-4.19386973	2.56171947	-2.36255958
C	-1.82486772	2.04606900	-2.91003276
C	-3.51801468	-1.12958418	0.95162105
C	-5.18336760	0.52001942	0.33554804
H	-4.60989078	2.71897739	1.57913606
H	-3.82636805	4.30741648	1.58202196
H	-4.49231817	3.66331991	0.06875815

H	-0.97074288	1.95065356	1.96663634
H	-1.99044232	3.17329757	2.77068049
H	-2.60815880	1.52133947	2.53963721
H	-0.67208408	3.38412162	-0.12550005
H	-2.08078562	4.23957544	-0.81688959
H	-1.51363871	4.63797123	0.81921892
H	-4.40704118	-0.18736380	-2.30340086
H	-3.60816246	0.28590683	-3.82282215
H	-2.68491065	-0.56970783	-2.56535719
H	-4.38251561	2.65931023	-3.44438504
H	-5.14015617	2.25218807	-1.90036584
H	-3.92482960	3.55806420	-1.98494739
H	-1.00915325	1.30715480	-2.87543350
H	-2.09250059	2.20857606	-3.96699925
H	-1.44327382	2.99667850	-2.51289432
C	-4.54660106	-1.88389813	1.53827525
C	-2.15985259	-1.74284488	0.98871876
C	-6.19128391	-0.24874242	0.90633239
H	-5.45821292	1.46435575	-0.13143416
C	-5.86900290	-1.45519357	1.52296302
H	-4.29038200	-2.83857248	2.00402339
C	-1.67272394	-2.44528200	-0.12414662
C	-1.40447013	-1.73484359	2.16769576
H	-7.22567588	0.10090890	0.87163627
H	-6.64701691	-2.06838296	1.98433515
C	-0.45363769	-3.11834719	-0.05715047
H	-2.26605198	-2.47316592	-1.04143517
C	-0.17846568	-2.39939676	2.22763744
H	-1.78325720	-1.20277689	3.04412430
C	0.30028030	-3.09237138	1.11669687
H	-0.08431515	-3.67068514	-0.92465172
H	0.40390032	-2.37787453	3.15212020
H	1.26081850	-3.61059687	1.15011666

IN2

Charge = 1; Multiplicity = 1

C	-4.27718229	0.63963054	-0.25973002
C	-3.94971743	-0.66428965	-0.96745954
C	-4.40516188	-0.76495645	-2.38514570
C	-2.30257945	0.48345418	1.18514266
C	-1.65280109	-0.38161851	0.18189450
C	-2.41152881	-1.16748135	-0.71893605
C	-1.71727674	-1.86057957	-1.86043080
C	-1.83425112	-3.34759751	-1.97810817
C	-0.96993731	-1.13837417	-2.70651564
S	-4.70692264	0.41932483	2.39860612
O	-3.97588772	-0.44303325	3.32709699
O	-6.01992091	0.01433408	1.90743067
N	-3.73287472	0.65856256	1.07245703
H	-3.89134775	1.49734836	-0.83226386
H	-5.37103499	0.73146007	-0.20412390
H	-1.77477952	1.45726544	1.14676704
H	-2.05017269	0.06817359	2.17844219
H	-1.59417877	-3.84023295	-1.02120625
H	-1.15399107	-3.73174162	-2.75062737
H	-2.85743801	-3.65393082	-2.25248100
H	-0.41706224	-1.61711759	-3.51979963
H	-0.88698444	-0.05287718	-2.61318393
C	-4.85422035	2.01465974	3.14217547
H	-3.85236675	2.37002747	3.41784840
H	-5.33187005	2.69193240	2.42220397
H	-5.48020007	1.89731796	4.03808767
C	-3.71136290	-1.82955038	-0.14762693
H	-3.87425607	-2.82104497	-0.57196522
H	-3.84229056	-1.77034523	0.93386016
C	-4.10128612	0.40262746	-3.27522478
H	-4.71078636	1.28010735	-3.00253998
H	-3.04559895	0.70332942	-3.19396939
H	-4.31504993	0.16120428	-4.32531782
C	-5.09937018	-1.83147766	-2.80456905
H	-5.36028263	-2.65369009	-2.13392559
H	-5.44560839	-1.90008835	-3.83999156
Au	0.38071770	-0.35511074	0.14972743
P	2.72195179	-0.62116472	0.24368127

C	3.19884859	-0.88621641	2.04899525	H	7.00569013	1.55512626	-0.94881724
C	3.15082913	-2.07098262	-0.90131260	H	5.98686808	3.77946862	-1.49194825
C	3.71936920	0.81565847	-0.31809099	C	-0.44824840	2.72041022	-1.64614294
C	2.52738916	-2.17221236	2.53301433	H	1.26969911	1.79264008	-2.57337786
C	4.69969061	-0.94172234	2.32303438	C	-0.13976231	3.48336006	0.62132202
C	2.60517182	0.31290283	2.79484268	H	1.81608126	3.15390392	1.47496235
C	4.47774123	-2.77189700	-0.61823612	C	-0.95297792	3.34106365	-0.50408686
C	2.02418199	-3.10656213	-0.79298284	H	-1.07636020	2.60933343	-2.53370555
C	3.14123934	-1.49627024	-2.32096573	H	-0.52714443	3.97017372	1.52003052
C	3.14752650	2.06903324	-0.62632601	H	-1.97913236	3.71715602	-0.49091391
C	5.11206059	0.66552377	-0.44303353				
H	2.98253581	-3.06814326	2.08702420	**TS3**			
H	2.64612991	-2.24716398	3.62627127	Charge = 1; Multiplicity = 1			
H	1.44863927	-2.18016020	2.30835399	C	-4.48860364	0.31984830	1.29352067
H	4.84514722	-1.12637337	3.40030314	C	-4.23877766	1.16572589	0.07332371
H	5.20750479	-1.74953792	1.77990587	C	-4.16040621	2.56708321	0.14819938
H	5.19627681	0.00949994	2.08654754	C	-2.31915599	-0.85967113	1.21505392
H	1.51146385	0.36392626	2.67485268	C	-1.68245205	0.03470850	0.19687562
H	2.83003111	0.21459435	3.86951775	C	-2.34689422	0.58021627	-0.86707186
H	3.03735363	1.26438124	2.44822443	C	-1.79622573	1.63877732	-1.71196790
H	5.34776860	-2.10959343	-0.71124941	C	-1.78860709	1.47034307	-3.19585502
H	4.49345129	-3.23548186	0.37802037	C	-1.48878915	2.83720452	-1.12765209
H	4.60697848	-3.57888152	-1.35825828	S	-4.56006208	-2.36696742	1.05019666
H	1.92533554	-3.52175289	0.21942265	O	-3.66700910	-3.28306993	0.34414361
H	1.05246015	-2.68423163	-1.08980890	O	-5.88275468	-2.07062895	0.50276000
H	2.25203997	-3.94239809	-1.47483619	N	-3.76984796	-0.92601709	1.20632114
H	2.21166320	-0.94085281	-2.52857533	H	-4.22149523	0.85178778	2.21981834
H	3.99242174	-0.82638278	-2.50793004	H	-5.57157779	0.11161947	1.33269126
H	3.19886839	-2.32802143	-3.04195757	H	-1.96945810	-0.53518123	2.21334457
C	3.98657601	3.11510741	-1.04259976	H	-1.92424692	-1.87783351	1.07193914
C	1.69622525	2.40702822	-0.54719786	H	-0.96768558	0.78752364	-3.47296403
C	5.92783471	1.71036148	-0.86149584	H	-1.63280103	2.42518409	-3.71650107
H	5.57854407	-0.28982724	-0.20885131	H	-2.71428331	1.00467271	-3.56934172
C	5.36107365	2.94622277	-1.16296369	H	-1.13292912	3.68045219	-1.72801466
H	3.53541803	4.08215867	-1.27758132	H	-1.40514162	2.91786442	-0.04108005
C	0.86808190	2.25664699	-1.66916465	C	-4.77536335	-2.98657596	2.69349648
C	1.17602878	3.02215699	0.59943282	H	-5.29947820	-3.94936737	2.61189341

H	-3.78671835	-3.12570597	3.15113666
H	-5.37805975	-2.26855764	3.26532856
C	-3.86885978	0.40971430	-1.13195295
H	-4.15776152	0.88141356	-2.07583929
H	-4.20390542	-0.63060068	-1.12065715
C	-4.21953628	3.26576239	1.47798187
H	-4.14950814	4.35400612	1.34847804
H	-5.16116311	3.05444910	2.00735129
H	-3.39429350	2.94612009	2.13719371
C	-3.80352765	3.28214332	-0.99046282
H	-3.98294160	2.90004724	-1.99545079
H	-3.63457615	4.36045898	-0.92171367
Au	0.35253356	0.26394948	0.35286104
P	2.66577174	0.66102062	0.51859761
C	3.01851281	2.23364461	-0.46882739
C	3.12208413	0.78454196	2.35563828
C	3.76626736	-0.61827488	-0.21358432
C	4.48976388	2.61678816	-0.61086331
C	2.44853763	1.96033211	-1.86526087
C	2.24250935	3.38020548	0.18140782
C	3.23049081	-0.65977070	2.85213762
C	4.39856680	1.55682936	2.67909837
C	1.95233715	1.45989108	3.08246340
C	3.27487832	-1.73878000	-0.92003418
C	5.15789286	-0.47049245	-0.07741783
H	4.99470673	2.75363266	0.35411900
H	5.05072801	1.87997076	-1.20200407
H	4.54438945	3.57582142	-1.15253338
H	1.36826265	1.74800791	-1.83146326
H	2.60427045	2.85079456	-2.49657330
H	2.95464386	1.11274570	-2.35306279
H	2.67877092	3.67846556	1.14563092
H	2.27493453	4.25806351	-0.48471938
H	1.18511808	3.11665260	0.34227139
H	3.31832098	-0.65518331	3.95100986
H	2.33365177	-1.24522760	2.59111774
H	4.11047392	-1.17722907	2.44401071
H	4.54909290	1.53637470	3.77132185
H	5.29808710	1.12135882	2.22494989
H	4.32656944	2.61173037	2.37917228
H	1.01289745	0.90189706	2.94817025
H	2.18043840	1.49236922	4.16066269
H	1.78807785	2.49275174	2.74567362
C	4.19091122	-2.64794798	-1.47303145
C	1.83362245	-2.06872513	-1.11919662
C	6.05094905	-1.38586599	-0.62291765
H	5.56079681	0.38152007	0.46692267
C	5.56389869	-2.48085108	-1.33225256
H	3.80209704	-3.50971825	-2.02098037
C	1.16121522	-1.68243871	-2.28589028
C	1.16785402	-2.88290285	-0.19158738
H	7.12580332	-1.23812307	-0.49416567
H	6.25078595	-3.20810663	-1.77219189
C	-0.15579038	-2.08594543	-2.50970092
H	1.67653333	-1.06222627	-3.02354707
C	-0.14713259	-3.28701356	-0.41978331
H	1.69285137	-3.20581043	0.71110493
C	-0.81524259	-2.88487876	-1.57627728
H	-0.67014042	-1.77288640	-3.42183404
H	-0.65810782	-3.92041144	0.30964128
H	-1.85204249	-3.18919231	-1.73534770

IN4

Charge = 1; Multiplicity = 1

Au	0.25620916	0.43012396	0.14329779
P	2.39349095	1.42383819	0.10762590
C	2.47156166	2.56102074	-1.39845374
C	2.63496910	2.31506561	1.76509063
C	3.81939956	0.27685396	-0.07363444
C	1.40393881	3.64201265	-1.22666994
C	2.10716665	1.66247475	-2.58507614
C	3.82625390	3.20826930	-1.67340134
C	3.00016040	1.21966288	2.77086419
C	1.28678263	2.91857643	2.17670508

C	3.68486400	3.42324768	1.78212746	H	0.10727613	-2.95388876	-2.66798985
C	3.66322068	-1.11323034	-0.27070661	H	-0.92702362	-3.91659214	-0.60480689
C	5.12207653	0.80080204	0.00305538	C	-1.65255237	-0.31473745	0.21979653
H	0.42236193	3.20912834	-0.97629906	C	-2.11888250	-0.76947728	1.57011354
H	1.67608318	4.36645747	-0.44593030	C	-2.38273923	-0.48239395	-0.92569116
H	1.29893453	4.19645089	-2.17369144	N	-3.47496257	-1.27671260	1.69093143
H	1.10614295	1.21853689	-2.46721458	H	-1.42691028	-1.54154396	1.94032288
H	2.11175322	2.26428051	-3.50882425	H	-1.99399136	0.08863452	2.25744107
H	2.83320086	0.84471653	-2.71412427	C	-2.19013168	0.24251317	-2.13336733
H	4.59178150	2.46583216	-1.93765323	C	-4.58696530	-0.39216832	1.37465176
H	3.71826841	3.88449060	-2.53768286	S	-3.75249925	-2.87368785	2.01194384
H	4.19291453	3.80756259	-0.83009428	C	-2.28768741	-0.38890181	-3.45906197
H	2.98161496	1.64630959	3.78708436	C	-2.33299132	1.68490281	-2.01157639
H	2.27676214	0.38822022	2.74417198	C	-3.87795201	-0.92775517	-0.95611031
H	4.00411743	0.80795289	2.59457040	C	-4.41005561	0.12594816	-0.03327375
H	0.50151015	2.15042839	2.24949583	H	-4.64263417	0.41811895	2.11562935
H	0.94126346	3.69417710	1.47983186	H	-5.51764526	-0.97585517	1.44411740
H	1.40089943	3.38759576	3.16785378	C	-4.23590392	-2.93918429	3.71287364
H	4.69581914	3.06723681	1.54503214	O	-4.90106053	-3.30898819	1.21545519
H	3.72562982	3.84575877	2.79994231	O	-2.47674888	-3.57442900	1.87869860
H	3.42810095	4.24476551	1.09818057	H	-3.00364961	0.13149556	-4.11758668
C	4.80936696	-1.91552089	-0.38793904	H	-1.29447341	-0.25267530	-3.92968574
C	2.35628056	-1.82657826	-0.35951465	H	-2.50127727	-1.46398713	-3.41239518
C	6.24644389	-0.00907773	-0.11008301	C	-3.91443592	1.86564044	-1.74565052
H	5.26903081	1.86857463	0.15580945	H	-1.80466607	2.07881487	-1.12981138
C	6.08936822	-1.37851597	-0.30913359	H	-2.08229747	2.24004978	-2.92570217
H	4.67920472	-2.98956966	-0.54141869	H	-4.03996424	-1.94642735	-0.58594238
C	1.77916594	-2.38991204	0.78755525	H	-4.29737374	-0.86196048	-1.96721207
C	1.74616458	-2.04442535	-1.60181274	C	-4.38608170	1.44138429	-0.38879346
H	7.24310810	0.43333074	-0.04234603	H	-5.13949060	-2.33068969	3.85196576
H	6.96166536	-2.03034259	-0.40096513	H	-4.44548895	-3.99206961	3.94888742
C	0.60778201	-3.14136878	0.69434712	H	-3.40721671	-2.56248368	4.32655778
H	2.25854031	-2.23845874	1.75829150	H	-4.08617641	2.94199964	-1.88280108
C	0.57466128	-2.79647681	-1.69236304	H	-4.44169692	1.34438728	-2.55854306
H	2.19793831	-1.62296595	-2.50312598	C	-4.67591675	2.56973272	0.55099927
C	0.00014744	-3.34232009	-0.54476089	H	-4.95341176	2.24785125	1.56193966
H	0.15290968	-3.56635443	1.59167592	H	-5.49623692	3.19608297	0.16350608

H	-3.79163788	3.22756733	0.62717962

TS5

Charge = 1; Multiplicity = 1

Au	0.19171269	-0.12829838	0.05221322
P	2.39470301	0.22387429	0.75888763
C	2.74813112	2.08263593	0.60106910
C	2.55012737	-0.44444065	2.51882683
C	3.69375458	-0.62734673	-0.22549273
C	1.46705434	2.84041653	0.97207396
C	3.03523069	2.32660253	-0.88338213
C	3.89347554	2.61586239	1.45763675
C	1.61354359	0.36008067	3.42144291
C	3.96262416	-0.44199994	3.09919830
C	2.05715250	-1.89226104	2.44162786
C	3.39394375	-1.48750523	-1.30622585
C	5.04431860	-0.36518408	0.06633042
H	1.65153674	3.92069918	0.85161204
H	0.63059330	2.56074126	0.31339041
H	1.15711187	2.66923854	2.01202899
H	3.07500596	3.41313337	-1.06528684
H	3.99494544	1.89461258	-1.20040355
H	2.24089041	1.90873503	-1.52386368
H	4.85974782	2.14841467	1.22703584
H	4.00326507	3.69493442	1.25889920
H	3.69247645	2.49960748	2.53196288
H	1.95279573	1.39801280	3.55096395
H	0.58012097	0.36383623	3.04263362
H	1.59430701	-0.11008327	4.41824487
H	4.41620409	0.55748415	3.12951539
H	4.63369442	-1.11834114	2.55196701
H	3.90685784	-0.81052864	4.13683567
H	1.01674139	-1.94897305	2.08589917
H	2.09817833	-2.33815215	3.44892718
H	2.68905497	-2.50365200	1.77897055
C	4.45086354	-2.03017604	-2.05490285
C	2.02451421	-1.89012734	-1.73902697
C	6.07834493	-0.91845975	-0.68029740
H	5.30305681	0.29307930	0.89365256
C	5.77952792	-1.75446433	-1.75320239
H	4.21012935	-2.69215724	-2.89024390
C	1.32631697	-2.90482148	-1.06932651
C	1.47034308	-1.34559492	-2.90561910
H	7.11553903	-0.69110577	-0.42308329
H	6.57885221	-2.19542194	-2.35388231
C	0.09958784	-3.35981963	-1.55294663
H	1.75657807	-3.34962622	-0.16959843
C	0.24110146	-1.79788777	-3.38451685
H	2.01285306	-0.56317671	-3.44268218
C	-0.44663043	-2.80743953	-2.71128761
H	-0.42919714	-4.15451375	-1.02057135
H	-0.17698575	-1.36289947	-4.29588561
H	-1.40652832	-3.16624115	-3.09128865
C	-1.81894094	-0.32470723	-0.35588351
C	-2.68302564	-1.21449513	0.52368154
C	-2.36917718	0.42156236	-1.28717311
N	-3.57846346	-0.47591879	1.40349448
H	-3.31617506	-1.87081500	-0.09839508
H	-2.06446415	-1.87019973	1.14593708
C	-2.51696404	1.44515103	-2.20370031
C	-4.81961965	0.07062736	0.85811027
S	-2.95326714	0.16581261	2.80011338
C	-2.36847700	1.20565189	-3.66673678
C	-2.72910787	2.85646879	-1.72842019
C	-4.08431622	0.45597464	-1.52955050
C	-4.60562846	1.04332070	-0.27543495
H	-5.37953715	0.52101427	1.68488544
H	-5.41537356	-0.78628085	0.50320650
C	-2.08929248	1.66518799	2.40969713
O	-4.09273934	0.53141737	3.63916784
O	-1.96356281	-0.79216148	3.28980080
H	-2.48441851	0.14690118	-3.93104016
H	-3.05999296	1.83093016	-4.25088033
H	-1.34029481	1.51323000	-3.92612139

C	-4.20399611	3.18830724	-1.38153782
H	-2.10727749	3.03523555	-0.83917372
H	-2.39786899	3.53171743	-2.53033100
H	-4.17578524	-0.63392759	-1.64796558
H	-4.52662790	0.88237307	-2.44106776
C	-4.69333046	2.39233807	-0.20487632
H	-2.79385258	2.38226145	1.97306908
H	-1.70026697	2.04873294	3.36337435
H	-1.26815614	1.43270067	1.71819975
H	-4.26788232	4.26436053	-1.16983813
H	-4.81962274	3.00402321	-2.27917552
C	-5.13561028	3.16777172	0.99217038
H	-5.32761206	2.54680220	1.87628891
H	-6.05459757	3.73241535	0.75898490
H	-4.37527015	3.92117077	1.25832774

IN6

Charge = 1; Multiplicity = 1

Au	-0.26798716	0.19666752	0.07188236
P	-2.54817742	0.67526349	0.35110334
C	-2.88783010	2.33790269	-0.48959032
C	-2.85525935	0.64117269	2.21211331
C	-3.69890003	-0.55279506	-0.37608388
C	-4.13094159	3.06892709	0.01130084
C	-1.66688983	3.24093441	-0.28060926
C	-3.01397284	2.02685523	-1.98342960
C	-4.31903279	0.77007584	2.62723392
C	-2.32935716	-0.71944253	2.68138979
C	-2.03271961	1.76438832	2.84432695
C	-3.26335144	-1.74273081	-1.00036591
C	-5.07956319	-0.29768889	-0.30051961
H	-5.05640134	2.49695344	-0.13664187
H	-4.23559691	4.00435671	-0.56258462
H	-4.04694170	3.34318080	1.07245879
H	-1.84573546	4.19282958	-0.80654046
H	-0.74726721	2.79767660	-0.69199259
H	-1.48883264	3.47547164	0.77727733
H	-3.06296103	2.97676953	-2.53988641
H	-3.91953539	1.44905842	-2.21674111
H	-2.14036254	1.46803270	-2.35760757
H	-4.79287422	1.68547538	2.24928872
H	-4.35984670	0.80622030	3.72831735
H	-4.91566698	-0.09553359	2.30825242
H	-2.48358207	-0.80517722	3.76932426
H	-2.86544684	-1.55207876	2.20030536
H	-1.25278179	-0.83706402	2.47861715
H	-2.45370229	2.75490327	2.62001946
H	-2.04159500	1.63837960	3.93907553
H	-0.98296907	1.74736223	2.51158448
C	-4.22378805	-2.63256365	-1.50583473
C	-1.83965243	-2.14502890	-1.19189906
C	-6.01624726	-1.18688200	-0.81463025
H	-5.43864579	0.61540564	0.17155804
C	-5.58551741	-2.36608053	-1.41746135
H	-3.88004199	-3.55215392	-1.98543173
C	-1.21850168	-3.01981809	-0.29047929
C	-1.14363646	-1.75143956	-2.34413554
H	-7.08137089	-0.95587853	-0.74004879
H	-6.30821350	-3.07806555	-1.82353702
C	0.07523133	-3.48305120	-0.53128243
H	-1.75837973	-3.34425250	0.60247129
C	0.14880452	-2.21930537	-2.58425324
H	-1.62771963	-1.08476770	-3.06229160
C	0.76121264	-3.08569097	-1.67874319
H	0.54552299	-4.16743130	0.17913921
H	0.67599290	-1.90899667	-3.48992191
H	1.77313263	-3.45303422	-1.86728289
C	1.77689112	0.00606007	-0.59422728
C	2.51750765	0.32789951	-1.83505945
C	1.80730956	-0.20284475	0.63216175
N	3.73102517	1.04268241	-1.48625989
H	1.91093797	0.91044070	-2.53817454
H	2.79670287	-0.61004944	-2.34011611
C	2.52777336	-0.42790100	1.90176387

C	4.85026334	0.30976925	-0.87385987	C	-3.64270030	-0.55210144	-0.44282080
S	3.59526018	2.69024293	-1.25309274	C	2.53365849	-0.70555731	2.08284815
C	1.88326334	0.29922014	3.07461911	C	2.26176176	-0.49751107	-0.36182334
C	2.67023662	-1.94651072	2.16457531	C	-1.25163309	3.00142944	-0.47880779
C	3.92700128	0.16225617	1.54784381	C	-2.57037749	1.75989238	-2.17675780
C	4.46978286	-0.52883159	0.32128520	C	-3.73841049	3.12789983	-0.42601516
H	5.31425570	-0.30878948	-1.65423650	C	-2.78774110	-0.50757377	2.78362141
H	5.59263669	1.06511529	-0.57799933	C	-2.15999001	1.91406673	2.76194032
C	4.34518812	3.39394774	-2.69135846	C	-4.51870093	1.21030424	2.30880536
O	4.40789566	3.07510447	-0.10001380	C	-3.23744241	-1.81209412	-0.93476652
O	2.17061604	3.02059704	-1.28173502	C	-4.99580918	-0.18721387	-0.56044488
H	2.53044333	0.21984799	3.96088184	C	1.78905537	-0.21562105	3.31356176
H	0.90666609	-0.14329670	3.32377820	C	2.88626399	-2.19855532	2.19695294
H	1.73513708	1.36562617	2.84705327	C	3.84117166	0.09042152	1.83928228
C	3.97890188	-2.53464867	1.61102945	C	2.70693829	0.04555320	-1.64298175
H	1.80370933	-2.46990057	1.73360987	H	-1.09988517	3.26797507	0.57650675
H	2.63212539	-2.11902592	3.25074614	H	-1.29685931	3.93940301	-1.05628840
H	3.84544559	1.24715526	1.39235425	H	-0.37272164	2.44127028	-0.82984331
H	4.58186502	0.00345169	2.42357289	H	-3.52155598	1.28234918	-2.45111110
C	4.46391815	-1.87824930	0.34090496	H	-1.75261027	1.05383482	-2.39445093
H	5.39470699	3.07449999	-2.73584173	H	-2.43020596	2.63948318	-2.82581941
H	4.27971456	4.48621103	-2.58542034	H	-3.69750803	3.98278232	-1.12099203
H	3.79185435	3.05752441	-3.57775938	H	-3.70713391	3.53379689	0.59480305
H	3.86600183	-3.61911745	1.46467995	H	-4.70694639	2.63407683	-0.57994087
H	4.76531237	-2.41414893	2.37745004	H	-3.08932861	-0.44827990	3.84207822
C	4.87696041	-2.79337819	-0.76589845	H	-1.72226222	-0.78490245	2.74807892
H	4.02782412	-3.43270690	-1.06397408	H	-3.37283113	-1.31340022	2.31392968
H	5.24614274	-2.27660441	-1.66082525	H	-2.35249253	1.93173515	3.84696450
H	5.66956853	-3.47944481	-0.42138732	H	-1.09017337	1.69669982	2.61094340
				H	-2.37075525	2.91933248	2.36971184
TS7				H	-4.69728782	1.35893145	3.38649138
Charge = 1; Multiplicity = 1				H	-4.80277027	2.13844627	1.79716467
Au	-0.26176791	-0.07608551	0.47362506	H	-5.18735964	0.40392067	1.97833928
P	-2.47830251	0.63699393	0.32971665	C	-4.20292663	-2.66233330	-1.49663576
C	1.75128770	-0.51129643	0.80271441	C	-1.83848496	-2.33121731	-0.94487090
C	-2.54704784	2.21805746	-0.71619405	C	-5.93695809	-1.03929941	-1.12652876
C	-3.04788788	0.84812245	2.11777482	H	-5.32979223	0.78683165	-0.20720297

H	1.47338046	0.83240969	3.19640307
H	0.89231499	-0.82602963	3.49916704
H	2.43723789	-0.28244053	4.20080290
C	4.07464736	-2.61579098	1.31138437
H	1.99397452	-2.79215395	1.94749187
H	3.12494315	-2.41383396	3.24937169
C	4.41757955	-0.30029955	0.50443120
H	3.64200657	1.16985688	1.88264238
H	4.54546606	-0.14282643	2.65793461
N	3.66070336	1.10945027	-1.37978724
H	1.84682165	0.45182584	-2.19630034
H	3.16101114	-0.72410700	-2.28523781
C	-5.53903082	-2.29010086	-1.59181927
H	-3.88265069	-3.63701839	-1.87250383
C	-1.36862283	-3.15453286	0.08788652
C	-1.02314974	-2.11829329	-2.06556722
H	-6.97956248	-0.72202524	-1.20242756
C	4.49658062	-1.64003489	0.24435505
H	3.88826933	-3.59651482	0.85043431
H	4.96497961	-2.76005553	1.94983397
C	4.80108804	0.75058065	-0.51099563
S	3.11878940	2.68354691	-1.40498449
H	-6.26591081	-2.97451548	-2.03603989
C	-0.11090517	-3.75248955	-0.00077547
H	-2.00220709	-3.33868581	0.95903807
C	0.23420133	-2.71562777	-2.15105364
H	-1.38870979	-1.49226571	-2.88347800
C	5.02535181	-2.25159484	-1.00836955
H	5.15502973	1.66315410	-0.01222747
H	5.62649557	0.40301269	-1.14798025
C	2.39924404	3.06025452	0.17222641
O	2.04989954	2.72312771	-2.40164849
O	4.30123240	3.52260043	-1.55414703
C	0.69120988	-3.53815838	-1.12116522
H	0.23758460	-4.39981166	0.80781453
H	0.85381729	-2.54660527	-3.03555194
H	5.46708754	-1.53541156	-1.71081363
H	5.78917079	-3.00487786	-0.75304693
H	4.22015967	-2.79913592	-1.52797104
H	1.99655777	4.07947912	0.08587428
H	3.18187761	3.02974356	0.94042875
H	1.59565802	2.34439927	0.38916941
H	1.67037068	-4.01767781	-1.19493450

IN8

Charge = 1; Multiplicity = 1

Au	-0.14651832	0.28504136	-0.90815164
P	-2.41518369	0.95070270	-1.00329295
C	1.83994555	-0.02671723	-0.84405751
C	-3.01649329	0.80778974	-2.78393743
C	-2.46457666	2.71695220	-0.30486878
C	-3.56477258	-0.03764499	0.03281748
C	2.70927285	-0.72529553	-1.85913617
C	2.64754485	0.36397784	0.23459062
C	-2.17310781	1.75277203	-3.64045801
C	-2.72688229	-0.63944567	-3.19238559
C	-4.50253024	1.08519362	-2.99788198
C	-2.40651825	2.56522495	1.21796944
C	-1.19565402	3.44574957	-0.76490781
C	-3.67508098	3.55566183	-0.70847680
C	-3.15020521	-1.16977715	0.77050002
C	-4.89229807	0.40524916	0.17082783
C	1.96797192	-1.54353532	-2.89877275
C	3.47794580	0.45050162	-2.51460916
C	3.66195087	-1.55479340	-0.97117664
C	2.19368102	0.61270595	1.64446739
C	3.86221667	-0.66471712	0.23704142
H	-2.38700699	1.55640856	-4.70371117
H	-1.09435295	1.59542982	-3.47944749
H	-2.40555391	2.80897497	-3.44438231
H	-3.31454105	-1.35419043	-2.59660496
H	-1.65956566	-0.88990666	-3.08575513
H	-3.00730861	-0.77500032	-4.24979782
H	-4.80498158	2.09045634	-2.67710838

H	-5.13475058	0.34642642	-2.48585181	H	3.64920998	-2.23109251	1.68661534
H	-4.71649037	1.00381899	-4.07650940	C	4.84539152	1.63369676	0.90974274
H	-1.56520641	1.92621342	1.53356808	H	-6.06427205	-1.82987189	2.44857763
H	-3.33262244	2.14220770	1.63155523	C	0.26736739	-2.47032344	1.77690571
H	-2.25609251	3.55999190	1.66823104	H	-1.15492154	-1.09088869	2.62776899
H	-0.28451303	2.92832814	-0.42676568	C	-0.30329262	-3.39317791	-0.37774621
H	-1.14111145	3.55526123	-1.85656020	H	-2.18729906	-2.75484809	-1.21205433
H	-1.19610752	4.45764695	-0.32763488	C	3.84997216	0.27850513	4.92892919
H	-4.63055528	3.12022220	-0.38885686	O	2.95041426	-2.06931968	4.22285198
H	-3.59163276	4.54001650	-0.21879993	O	1.34605895	-0.10637896	4.26477056
H	-3.71173332	3.73192674	-1.79265945	H	4.49041110	2.66764301	0.79048877
C	-4.06895171	-1.78555762	1.63609671	H	5.92597306	1.62532877	0.69697407
C	-1.80865468	-1.81749590	0.69641483	H	4.70788277	1.32811818	1.95349801
C	-5.79205296	-0.22699226	1.02112825	C	0.57569531	-3.30363016	0.70213100
H	-5.23661921	1.27324180	-0.38884450	H	0.94428100	-2.40580804	2.63073309
H	1.32710423	-2.29952571	-2.42294631	H	-0.07720196	-4.05515442	-1.21738317
H	1.33363442	-0.89754691	-3.52483371	H	3.70531385	1.34653118	4.72040236
H	2.68442459	-2.05985363	-3.55627526	H	3.65463173	0.06491453	5.98954974
C	4.47116007	1.05677172	-1.53198711	H	4.86220264	-0.04801009	4.65592337
H	3.97879706	0.07274927	-3.41908752	H	1.49472316	-3.89510702	0.71323597
H	2.74889878	1.20726952	-2.84914952				
H	3.17345263	-2.49277847	-0.67104206	**TS9**			
H	4.60594657	-1.80209003	-1.48164658	Charge = 1; Multiplicity = 1			
N	3.00642947	-0.33471989	2.41079641	C	-2.37086100	-1.93845680	-1.87008135
H	2.36298527	1.64880243	1.97939310	C	-3.57895969	-2.32594866	-1.06397639
H	1.12187801	0.38796535	1.72992969	C	-3.83276528	-1.21443190	-0.06131295
C	3.94513564	-1.17208584	1.65628585	C	-3.94395578	0.15609489	-0.65749323
C	4.17243544	0.72328173	-0.08147291	C	-3.70795121	0.23466751	-2.14632000
C	-5.37406812	-1.32560706	1.76781873	C	-2.37596580	-0.48458570	-2.35561561
H	-3.74090888	-2.65766486	2.20685093	C	-4.52685750	1.27568207	0.17137820
C	-0.91583488	-1.73099699	1.77473842	N	-3.66647736	1.31390912	1.35844100
C	-1.48756538	-2.65720673	-0.38005131	S	-4.22940964	1.83322826	2.81535315
H	-6.81543238	0.14643835	1.10317427	C	-3.87225410	3.56558525	2.87185436
H	4.51666861	2.14986450	-1.63912655	C	-4.58992778	-1.62701068	1.17270947
H	5.48626899	0.67724063	-1.73200459	C	-1.62238935	-0.45921548	-1.06641595
S	2.67372341	-0.65168852	3.99036363	C	-1.66002062	-0.22822924	-3.65737513
H	4.96733577	-1.08729401	2.06329892	C	-2.63565159	-0.25849755	0.00348702

C	-2.41286972	0.56615632	1.24448482	H	5.49811124	0.15768510	-1.68360005
O	-3.43100456	1.17777830	3.84901882	H	2.15562986	-1.08960456	-2.81139668
O	-5.68449027	1.68662904	2.81636941	H	3.67302687	-0.94692468	-3.73962494
H	-4.47596852	2.21856464	-0.40022015	H	3.71108446	-1.56407613	-2.07190215
H	-5.57105541	1.11347253	0.47658048	H	1.61299000	1.40417423	-3.17167684
H	-4.03431531	-2.39981562	1.72602099	H	2.90335576	2.61793695	-2.93192750
H	-4.79025890	-0.79457316	1.85621415	H	3.05349006	1.40352510	-4.22035295
H	-5.56078027	-2.05830299	0.88203340	H	4.64275553	2.87142783	0.41374477
H	-4.51581015	-0.21461086	-2.74564238	H	3.92605799	3.48882949	-1.10051949
H	-3.60060257	1.28337554	-2.46331732	H	3.56114062	4.26944185	0.45056292
H	-4.44702059	-2.45842137	-1.73066353	H	1.19356744	4.13287714	0.02513507
H	-3.41015700	-3.27855122	-0.54136637	H	1.39454138	3.29126958	-1.52571948
H	-1.54373785	1.23099672	1.10124246	H	0.35634716	2.58495745	-0.26412527
H	-2.24493025	-0.02764229	2.15396764	H	3.10056925	1.80762218	2.19709052
H	-1.44025673	0.84471159	-3.76766901	H	1.99788907	3.20326221	2.12227888
H	-2.28094883	-0.54171358	-4.51085997	H	1.37060205	1.56139586	1.84277283
H	-0.70933354	-0.77944842	-3.70198694	C	4.03868250	-2.19029030	2.05074428
H	-1.92384913	-2.64033476	-2.58725334	C	1.85704623	-2.14873828	0.93824116
H	-1.47193400	-1.94159355	-1.07755304	C	5.76031058	-0.53980350	1.75451210
H	-4.39294521	4.06254713	2.04252189	H	5.30209848	1.06376682	0.42492621
H	-4.24453246	3.94064909	3.83569715	C	5.31077149	-1.71609004	2.34931463
H	-2.78559177	3.70506972	2.79841172	H	3.68124285	-3.11441886	2.51129429
Au	0.38277420	-0.06906801	-0.81378026	C	0.82671400	-1.97272063	1.87307017
P	2.59055406	0.68157136	-0.56859309	C	1.65950307	-3.03688629	-0.12801082
C	3.43328290	0.60273755	-2.25564552	H	6.75706456	-0.15021312	1.97400452
C	2.49907484	2.42541165	0.17405814	H	5.94924056	-2.26616533	3.04495066
C	3.63810693	-0.31617722	0.56345947	C	-0.37410768	-2.66998333	1.74456013
C	4.92884858	0.90690546	-2.25084677	H	0.97513968	-1.29102433	2.71432089
C	3.22486586	-0.83548258	-2.73864671	C	0.45961881	-3.73666268	-0.25366684
C	2.70242771	1.56800478	-3.18857169	H	2.46104178	-3.19118589	-0.85388355
C	3.73559761	3.29531169	-0.03553134	C	-0.55869660	-3.55810403	0.68415524
C	1.29052877	3.13953904	-0.44295744	H	-1.16477778	-2.52720321	2.48542555
C	2.23232233	2.22642997	1.66880487	H	0.32461507	-4.43440199	-1.08416290
C	3.18792630	-1.51284681	1.16295841	H	-1.49263914	-4.11831965	0.59532384
C	4.92979524	0.14508736	0.87490454				
H	5.29099695	0.87270573	-3.29161335	**IN10**			
H	5.16414358	1.90293122	-1.85344037	Charge = 1; Multiplicity = 1			

Au	0.91507238	0.14519027	0.13385306	C	2.38755336	-2.54956124	1.38978301
P	2.88213568	1.29384940	0.02759489	C	2.51810865	-2.39270224	-1.01700201
C	2.88597739	2.54435956	1.45163045	H	7.70679145	0.57905186	0.72762540
C	3.03508750	2.05298112	-1.69085872	H	7.55071481	-1.91161162	0.95724252
C	4.33402334	0.19783063	0.26022066	C	1.29807042	-3.41305594	1.27361383
C	3.87667469	3.69810809	1.30040148	H	2.77113163	-2.28139346	2.37744567
C	1.47576374	3.13325550	1.57493395	C	1.43209786	-3.26029353	-1.13099628
C	3.19167319	1.73722414	2.71644882	H	3.00661547	-2.00976272	-1.91510377
C	4.41042661	2.64928878	-1.98619672	C	0.81798885	-3.77135598	0.01325048
C	1.95103394	3.11927719	-1.84536057	H	0.82610180	-3.81352151	2.17446444
C	2.77732071	0.91138070	-2.67718799	H	1.06753653	-3.54317715	-2.12165786
C	4.24790114	-1.20835558	0.37568894	H	-0.03119799	-4.45305486	-0.07744694
C	5.59409140	0.80869705	0.38771621	C	-2.45961427	-1.42378555	0.80233293
H	4.92298781	3.37122519	1.24638983	C	-3.67860895	-1.11094885	-0.01701517
H	3.78859254	4.34122943	2.19122515	C	-1.27820391	-0.77497114	0.05983503
H	3.65331415	4.32263578	0.42404789	C	-1.89356203	-0.14226321	1.31870477
H	1.46407143	3.82522700	2.43251901	H	-2.32802499	-2.37375901	1.32257055
H	0.72079485	2.35377878	1.75912004	C	-5.03487105	-1.74967653	0.09968265
H	1.17310847	3.70166119	0.68573478	C	-3.27906110	-0.29886778	-1.23356561
H	4.22815433	1.37227462	2.74036500	C	-3.83276475	0.39614814	-0.00980622
H	2.51739085	0.87130875	2.82022431	C	-1.76194664	-0.29714471	-1.29820044
H	3.03938312	2.38599269	3.59402488	H	-0.39222508	-1.45292628	0.11847753
H	4.37765005	3.09597175	-2.99327108	C	-1.13653954	-0.08317903	2.61734404
H	5.19742869	1.88254254	-1.99610961	C	-2.85348839	0.99252720	0.97939914
H	4.69629009	3.44252831	-1.28400445	N	-5.93376451	-0.61966046	-0.13731809
H	0.95071808	2.72716122	-1.60278383	H	-5.22846197	-2.53949517	-0.63996050
H	2.14564597	4.00069907	-1.21821981	H	-5.16694149	-2.18072566	1.10842540
H	1.93373219	3.45395772	-2.89500384	C	-4.00130305	-0.30745543	-2.55379024
H	3.51782035	0.10443862	-2.56934164	C	-5.31403376	0.69702600	0.02675768
H	1.77035941	0.48300450	-2.55430596	H	-1.42462422	-1.00154884	-2.07543647
H	2.85938990	1.30518133	-3.70312975	H	-1.37460625	0.69921628	-1.56893512
C	5.42094434	-1.93624566	0.63074471	H	-0.51841233	0.82563156	2.68260258
C	3.00534497	-2.02358349	0.24528749	H	-1.84188932	-0.07275349	3.46380489
C	6.74530693	0.06951584	0.63232554	H	-0.47510373	-0.95412840	2.73740415
H	5.68377922	1.89052538	0.30476620	H	-2.31957318	1.87835985	0.59652710
C	6.65742937	-1.31420959	0.75948649	H	-3.38611321	1.29870596	1.89427395
H	5.34781818	-3.02249164	0.72249391	S	-7.43495866	-0.80605224	-0.77394816

H	-3.72561721	0.57987243	-3.14627416
H	-3.72277404	-1.19832203	-3.13902963
H	-5.09243880	-0.30656995	-2.44292299
H	-5.66277670	1.37066334	-0.77000027
H	-5.57159258	1.15248666	0.99957344
C	-8.55290460	-0.72043229	0.59717151
O	-7.51170142	-2.15645889	-1.32674894
O	-7.70669578	0.34868211	-1.62997958
H	-8.31967682	-1.53757914	1.29260899
H	-8.44332173	0.25734633	1.08509948
H	-9.57010191	-0.83503747	0.19655294

TS11

Charge = 1; Multiplicity = 1

Au	0.31849337	-0.45337932	0.36174911
P	2.57768700	-0.90607100	0.84860289
C	-1.64624874	-0.07095836	-0.11381686
C	2.94616912	-2.67692765	0.27607869
C	2.84387218	-0.62571259	2.69657524
C	3.80180485	0.17928168	0.00759768
C	-2.10042198	-0.84107735	-1.31302240
C	-2.39481439	0.92177414	0.49489229
C	4.13653686	-3.36072746	0.94542966
C	1.69401861	-3.52200246	0.54135358
C	3.16034367	-2.59042421	-1.23762537
C	4.29174716	-0.72292643	3.17059228
C	2.33846222	0.79636401	2.96048074
C	1.97448668	-1.62619690	3.45979925
C	3.43345206	1.29896637	-0.77049594
C	5.16769496	-0.13482427	0.12379486
N	-3.46932866	-0.68703619	-1.77186692
H	-1.91184639	-1.90585282	-1.07084086
H	-1.42200723	-0.61350975	-2.15135000
C	-3.59043688	1.54383334	-0.27133068
C	-2.26755280	1.28822138	1.89152775
H	5.09042197	-2.84559818	0.77344659
H	4.23839005	-4.37271432	0.51951550
H	3.98758891	-3.47571009	2.02796458
H	1.87626880	-4.54508993	0.17337217
H	0.81408607	-3.12182370	0.01457491
H	1.45013600	-3.59207750	1.61039147
H	4.10365945	-2.09019300	-1.49858162
H	2.33682631	-2.05143541	-1.73455118
H	3.19137209	-3.61094898	-1.65314151
H	4.30639280	-0.57729295	4.26354288
H	4.92189049	0.06270766	2.73111553
H	4.74827158	-1.69898321	2.96248056
H	2.92444540	1.54621911	2.40745637
H	1.27915106	0.91415593	2.68497455
H	2.44025733	1.01842739	4.03559838
H	0.93277782	-1.61889444	3.10235374
H	2.36220003	-2.65225083	3.38455820
H	1.96654703	-1.35101968	4.52718918
C	4.43999995	2.04667948	-1.40283656
C	2.04046490	1.78781905	-0.98539489
C	6.15125805	0.61648890	-0.50891781
H	5.47757943	-0.99085208	0.72019017
C	-4.53483870	-0.73310617	-0.79962795
S	-3.78792321	-0.22664111	-3.33038917
C	-4.50509477	0.45943173	0.11811244
H	-3.84102522	2.53552706	0.10956490
H	-3.39724196	1.61401167	-1.34291310
C	-1.74398887	0.28026363	2.86361647
C	-2.91234904	2.39460049	2.39324042
C	5.78459045	1.71608542	-1.28085435
H	4.14542498	2.91089406	-2.00313792
C	1.48107945	2.73128800	-0.11345824
C	1.32472119	1.41729127	-2.13283059
H	7.20207855	0.33932462	-0.39684729
H	-4.48298436	-1.67816995	-0.23387509
H	-5.50398130	-0.73476285	-1.32506335
C	-3.99627635	-1.73103692	-4.23587905
O	-5.06731028	0.47810006	-3.32040238
O	-2.59322452	0.44039660	-3.84633320

C	-5.12020799	0.44880978	1.37551410
H	-1.58042042	0.72115699	3.85590079
H	-2.46082204	-0.55348708	2.96136907
H	-0.80161608	-0.16582203	2.50492233
H	-2.87925979	2.59321806	3.46779071
H	-3.17276051	3.24007686	1.75705065
H	6.54347311	2.31798202	-1.78685611
C	0.23243904	3.29063918	-0.38211744
H	2.03748782	3.03591587	0.77588445
C	0.07382475	1.97481691	-2.39904434
H	1.75844644	0.69044894	-2.82464608
H	-3.06819284	-2.31421882	-4.17055478
H	-4.20437172	-1.45466501	-5.27933999
H	-4.84242889	-2.28519885	-3.80871038
C	-5.65801299	-0.82874461	1.95973487
C	-5.10160347	1.62181444	2.13445906
C	-0.47224232	2.91495580	-1.52541434
H	-0.19038353	4.02569375	0.30756881
H	-0.48727694	1.66595949	-3.28402198
H	-5.96386871	-0.68033049	3.00414033
H	-6.54514600	-1.17326790	1.40385065
H	-4.91855011	-1.64498148	1.92701789
H	-5.43931706	1.59312383	3.17472287
H	-5.15668573	2.59282996	1.64604013
H	-1.45039548	3.35337010	-1.73776757

IN12

Charge = 1; Multiplicity = 1

Au	0.27489780	-0.08792546	0.14256518
P	2.48006345	-0.10230468	-0.70092562
C	-1.65240682	0.04789150	0.77651325
C	2.48295044	0.92983261	-2.29254961
C	3.03743005	-1.88786827	-0.95044354
C	3.71925779	0.64472725	0.43277083
C	-2.26959619	1.42409723	0.54546635
C	-2.51839375	-0.90042573	1.35182242
C	3.62995155	0.65755197	-3.26366356
C	1.15916327	0.66753633	-3.02246231
C	2.50046081	2.39249293	-1.83991884
C	4.48597308	-2.05967743	-1.40101599
C	2.87333040	-2.56343737	0.41336000
C	2.09201453	-2.53296357	-1.96475338
C	3.41604400	1.02896894	1.75800229
C	5.02602977	0.85258554	-0.04299149
N	-3.40584367	1.39582869	-0.37066976
H	-1.53418524	2.12593856	0.13880352
H	-2.61656478	1.84661514	1.50377804
C	-3.85829391	-0.44724609	1.87977711
C	-2.38954052	-2.28039207	1.14407838
H	4.62391195	0.83005727	-2.83120041
H	3.52707355	1.34983848	-4.11551641
H	3.59324874	-0.36360268	-3.66811174
H	1.02631759	-0.38880085	-3.29487273
H	1.15674115	1.25257546	-3.95694833
H	0.29135808	0.99354201	-2.43110981
H	1.71239754	2.59572254	-1.09635760
H	2.30663702	3.03724218	-2.71256528
H	3.46751198	2.68649477	-1.40797719
H	4.67818655	-3.13682131	-1.53738453
H	5.19585152	-1.69741503	-0.64451731
H	4.70311567	-1.56345826	-2.35464286
H	1.84093812	-2.49591371	0.78668361
H	3.13157191	-3.63072568	0.31669893
H	3.54401589	-2.12428501	1.16730500
H	2.28653960	-3.61732535	-1.99838575
H	1.03464737	-2.38705894	-1.69207082
H	2.24486122	-2.13571533	-2.97826964
C	4.42735510	1.60140786	2.54605503
C	2.08672779	0.88952731	2.42172668
C	6.01539174	1.42020590	0.75161439
H	5.28210322	0.57245141	-1.06317573
C	-4.75680083	1.03275527	0.08559834
S	-3.05946407	1.34221164	-1.99594013
C	-4.75507301	-0.35146585	0.67237436

H	-4.25412432	-1.13722689	2.63266397	H	-6.98836052	-2.04826241	-0.97228633
H	-3.77397196	0.52524139	2.37961914	H	-1.24256744	0.67019436	4.44571563
C	-1.21344451	-2.98723354	0.60851408				
C	-3.59251257	-3.12515264	1.41913140	**TS13**			
C	5.71417638	1.79685626	2.05795304	Charge = 1; Multiplicity = 1			
H	4.18473320	1.89583046	3.56997952	Au	0.22113189	-0.33362918	0.37188812
C	1.73604202	-0.29052792	3.09191180	P	2.23966117	0.73902232	-0.19367772
C	1.22276117	1.99174512	2.49558498	C	2.26386206	0.96997498	-2.07917679
H	7.01907678	1.56730898	0.34609446	C	2.34304791	2.35912518	0.77233824
H	-5.42920136	1.15132752	-0.77019880	C	3.77444973	-0.19475020	0.21114043
H	-5.05020922	1.77926814	0.84233888	C	0.83882026	1.31144868	-2.52946929
C	-2.61524235	-0.32390351	-2.41214963	C	2.63336754	-0.39913025	-2.65771807
O	-1.87409693	2.17332834	-2.19790801	C	3.20950765	2.04397219	-2.61104522
O	-4.29653939	1.65750375	-2.70312984	C	1.20955931	3.26872393	0.29643458
C	-5.20465866	-1.46703806	0.06568009	C	3.67485254	3.09981817	0.67771226
H	-0.31249030	-2.36662494	0.54198567	C	2.09886139	1.97019604	2.23368192
H	-1.02376376	-3.87555714	1.23424732	C	3.76550736	-1.44884576	0.86264530
H	-1.45609807	-3.38211658	-0.39511929	C	5.00965188	0.33003524	-0.20936512
C	-4.82751198	-2.86430259	0.51389167	H	0.48653613	2.27143602	-2.12835465
H	-3.32884954	-4.18585020	1.31234821	H	0.82399092	1.38330801	-3.62947681
H	-3.86705190	-2.97556271	2.47613495	H	0.12437248	0.53114907	-2.22622463
H	6.47864054	2.24438408	2.69785183	H	2.49251128	-0.37692357	-3.75094380
C	0.54284852	-0.37008876	3.81008768	H	3.67939174	-0.67061862	-2.45640107
H	2.41180700	-1.14768939	3.05941344	H	1.98760568	-1.19550089	-2.25164644
C	0.03244309	1.91194192	3.21917700	H	2.94462113	3.04419086	-2.24054283
H	1.49410813	2.92147843	1.98904061	H	4.26331132	1.84836669	-2.37422947
H	-3.46545380	-0.98199334	-2.19493354	H	3.12687443	2.06745938	-3.71042033
H	-2.39367223	-0.32422886	-3.48890996	H	1.38755175	3.65634202	-0.71710042
H	-1.72556116	-0.61424277	-1.83571909	H	0.23734394	2.75313660	0.31053960
C	-6.07082681	-1.46417682	-1.15796150	H	1.13843697	4.13330057	0.97648367
H	-4.67016011	-3.44042594	-0.41347658	H	3.58492689	4.04354175	1.24102310
H	-5.69260801	-3.34741513	1.00012490	H	3.95114846	3.35789528	-0.35329267
C	-0.31135513	0.73072579	3.87667961	H	4.49628388	2.52867097	1.13158566
H	0.28434063	-1.29721188	4.32801469	H	2.87670213	1.28801295	2.60960095
H	-0.62702950	2.78195057	3.27134412	H	1.11635533	1.49254239	2.37151438
H	-6.37271180	-0.45876660	-1.47637740	H	2.12445328	2.88056759	2.85499392
H	-5.56218360	-1.95541682	-2.00559551	C	4.98148048	-2.12840553	1.04313421

C	2.55999710	-2.13851676	1.40505560	H	-1.98168934	-3.33174921	-3.08654369
C	6.20520749	-0.35196214	-0.01400758	C	-4.66129613	-1.01070196	-2.00220623
H	5.04438933	1.29564664	-0.70985277	H	-2.74798792	0.00759992	-2.05716291
C	6.19081741	-1.59559167	0.61241428	H	-2.96171437	-1.21801418	-3.36022279
H	4.96469022	-3.09829497	1.54612425	H	-3.69396959	-2.94591131	1.19851742
C	2.01932324	-1.76526326	2.64348617	H	-4.18754376	-3.02880521	-0.48851609
C	2.03622305	-3.26067076	0.74860158	C	-5.04320632	-0.46753304	-0.65338601
H	7.14410021	0.08965107	-0.35614377	H	-2.41095055	3.15568006	0.85199528
H	7.11948273	-2.14923576	0.77144096	H	-1.75728755	1.54093409	0.35722367
C	0.97607398	-2.49661723	3.21017568	H	-3.51303011	1.93608473	0.11971898
H	2.43388956	-0.90502392	3.17313118	H	-5.10282688	-0.39482453	-2.79675533
C	0.98663299	-3.98545907	1.31242920	H	-5.02566175	-2.03827441	-2.15426272
H	2.46203735	-3.56787140	-0.21025093	C	-5.78832846	0.82805303	-0.66428785
C	0.45524675	-3.60672231	2.54521053	H	-5.95000151	1.25189818	0.33470740
H	0.57104311	-2.19683306	4.17990365	H	-6.77362224	0.69488454	-1.14279324
H	0.58836537	-4.85850972	0.78886968	H	-5.25297430	1.57550295	-1.27494901
H	-0.36128029	-4.18009470	2.99120452				
C	-1.57924063	-1.19559101	0.84762740	**TS14**			
C	-2.15351073	-1.04708262	2.25029740	Charge = 1; Multiplicity = 1			
C	-2.36448534	-1.81051143	-0.05006597	C	-4.55688738	0.20518790	-0.18154925
N	-3.29453486	-0.13133770	2.31199900	C	-3.92328925	1.58487597	-0.16591253
H	-2.50548838	-2.01357086	2.65060751	C	-4.63640537	2.53644315	0.75301946
H	-1.39891680	-0.67563921	2.95187588	C	-2.39192675	-0.74761290	-0.83733599
C	-2.33045066	-1.94841431	-1.47538037	C	-1.64586749	0.39220572	-0.48988851
C	-4.61752106	-0.57975524	1.86714490	C	-2.38095299	1.63545772	-0.18477310
S	-2.98013724	1.49273772	2.38564075	C	-1.66713502	2.66304039	0.65216607
C	-1.60279825	-3.04511546	-2.09631477	C	-1.54843911	4.06259694	0.13622152
C	-3.11440912	-1.00754472	-2.29334599	C	-1.11000855	2.28403997	1.81084827
C	-3.79336334	-2.34840911	0.28097897	S	-4.54193030	-2.13768239	-1.53728885
C	-4.61068918	-1.11411164	0.45431719	O	-3.53002112	-2.84885059	-2.30621658
H	-5.31503903	0.25473756	2.00017412	O	-5.76862835	-1.67329730	-2.16290790
H	-4.93825633	-1.37705719	2.55805123	N	-3.77102234	-0.75427361	-0.93927430
C	-2.62868414	2.08315422	0.75003207	H	-4.66819142	-0.15007039	0.85762787
O	-4.21351361	2.14661964	2.82011300	H	-5.55600834	0.26579383	-0.63547413
O	-1.75797788	1.64903614	3.17311253	H	-1.91378288	-0.73247115	0.34851133
H	-0.59343462	-2.59210616	-2.24434683	H	-1.89300712	-1.61909771	-1.27099259
H	-1.44542873	-3.89447800	-1.41850394	H	-0.94112171	4.67948739	0.81304491

H	-2.53539247	4.54098666	0.03108016	H	1.46674304	-1.28172862	-2.55970996
H	-1.07907158	4.07190553	-0.86173936	H	2.76851342	-1.62345275	-3.73227251
H	-0.55589256	2.99351513	2.43223763	H	2.97836313	-2.06824076	-2.02220945
H	-1.18158047	1.25412483	2.17137431	H	4.60622082	2.80614902	-1.78069940
C	-4.95776729	-3.09422086	-0.11147524	H	4.76885993	3.76399020	-0.29674855
H	-4.03616219	-3.37025099	0.41726754	H	5.43442807	2.12655717	-0.35123466
H	-5.63433625	-2.51418447	0.52967812	H	2.41377153	4.24604716	-0.30278126
H	-5.47007303	-3.99259761	-0.48512632	H	2.06349884	3.25506445	-1.73436735
C	-3.23783355	2.07174819	-1.37996001	H	1.17158206	2.97307078	-0.21641933
H	-3.24534912	3.14020324	-1.59776028	H	2.27058299	1.89361839	1.76893565
H	-3.22338424	1.42722518	-2.26305901	H	4.03848205	1.63934670	1.79603853
C	-4.73867559	2.13201565	2.19518023	H	3.37221513	3.28932710	1.73414876
H	-5.46074797	1.31010312	2.33332161	C	3.91216260	-2.49414823	1.92799054
H	-3.76841366	1.78179009	2.57972891	C	1.62851361	-1.82630767	1.35882191
H	-5.07529166	2.97360680	2.81631579	C	5.90213595	-1.42197463	1.11203723
C	-5.17331676	3.67225480	0.29162931	H	5.60327143	0.19366852	-0.24863463
H	-5.12629600	3.94709220	-0.76523390	C	5.29882625	-2.40122964	1.89711283
H	-5.68589493	4.36438757	0.96646108	H	3.43269051	-3.25245027	2.55166937
Au	0.41762991	0.35331334	-0.49656214	C	0.95470445	-1.16834500	2.39780699
P	2.74472845	0.51130035	-0.68122387	C	0.93931995	-2.78886231	0.60700339
C	3.19165488	0.06955903	-2.46053907	H	6.98976747	-1.32443756	1.08085629
C	3.24274017	2.26319513	-0.15806257	H	5.90541526	-3.08916418	2.49117451
C	3.70660121	-0.64841219	0.36807378	C	-0.37634749	-1.47118665	2.68313566
C	2.53476864	1.10208094	-3.37778377	H	1.48722588	-0.42637696	2.99793731
C	4.68510279	-0.02359681	-2.76514594	C	-0.39151092	-3.09032322	0.89228414
C	2.55916654	-1.30595394	-2.69761151	H	1.45886702	-3.31700667	-0.19603733
C	4.59201239	2.74673698	-0.68338881	C	-1.05244682	-2.43567149	1.93427933
C	2.15382088	3.22911089	-0.64000334	H	-0.88296758	-0.96098202	3.50614558
C	3.23328813	2.25706371	1.37324191	H	-0.91159647	-3.84921572	0.30173367
C	3.09723572	-1.62795152	1.18157720	H	-2.08794193	-2.69039335	2.17548549
C	5.11018493	-0.56283085	0.35893823				
H	1.46248886	1.22345214	-3.15522511	**IN15**			
H	3.02041651	2.08584275	-3.30440239	Charge = 1; Multiplicity = 1			
H	2.62675127	0.76162522	-4.42203474	C	-2.89566988	-1.39065781	0.76300347
H	4.80350548	-0.22088727	-3.84342597	C	-3.23315401	-1.42735026	-0.72207549
H	5.23073690	0.90114885	-2.53713919	C	-4.65779064	-1.80199492	-0.99779025
H	5.16217456	-0.85606239	-2.22989400	C	-2.10273014	0.89093674	0.58042698

C	-1.79124978	0.68931727	-0.75789164	C	1.73497244	0.96510153	3.31823502
C	-2.55560188	-0.32753984	-1.55884062	C	4.16471326	0.99925152	2.70292821
C	-3.32379737	0.28623515	-2.70488219	C	2.53858095	2.36467764	1.40989513
C	-3.50106364	-0.50983918	-3.96257116	C	0.91728600	-2.26746121	2.29133972
C	-3.82203909	1.52781363	-2.60207329	C	2.41475005	-3.00671242	0.44670867
S	-3.29090006	0.28134379	2.88218869	C	3.36319000	-2.36662471	2.68338716
O	-4.57030981	-0.38849441	3.05592329	C	3.48904200	0.24489028	-1.63126734
O	-3.16448956	1.71998531	3.05699130	C	4.95532929	-0.67028881	0.06672292
N	-2.81210718	-0.03180673	1.28220955	H	0.69759503	0.97185510	2.94892760
H	-3.65419647	-1.93352006	1.34002305	H	1.88514063	0.06903527	3.93734614
H	-1.91925251	-1.87718202	0.93290435	H	1.86362738	1.84560603	3.96810238
H	-1.44853340	1.57495257	-1.30323370	H	4.90617446	1.18237459	1.91317758
H	-1.89128734	1.83302091	1.09419715	H	4.27861755	1.80201015	3.44974262
H	-2.52898804	-0.80270947	-4.39017183	H	4.40420833	0.04996306	3.19838429
H	-4.04820904	0.07370211	-4.71581837	H	1.50429930	2.47901444	1.04915850
H	-4.06286957	-1.43823249	-3.77738475	H	2.75994199	3.20363181	2.08943273
H	-4.37358442	1.97883457	-3.43194523	H	3.21688902	2.44431707	0.54666000
H	-3.71047517	2.12925964	-1.69601682	H	0.74307670	-1.58590362	3.13476997
C	-2.08561680	-0.53846532	3.87655724	H	0.10064770	-2.13449364	1.56572830
H	-1.10638767	-0.08022345	3.69241250	H	0.86339027	-3.29789336	2.67807285
H	-2.39543262	-0.37916489	4.91967945	H	1.67116723	-2.77979138	-0.33485903
H	-2.08946275	-1.61058331	3.64130358	H	3.41358697	-2.97329947	-0.01028552
C	-2.11331370	-1.76378236	-1.65265741	H	2.23253344	-4.03773708	0.79048576
H	-2.34968048	-2.30469309	-2.57023421	H	4.38530678	-2.28733716	2.29261773
H	-1.14888017	-2.01712362	-1.20311206	H	3.27429743	-1.72604988	3.57155206
C	-5.68498417	-0.87481794	-0.42018605	H	3.22839500	-3.40884775	3.01619677
H	-5.58417263	0.13121054	-0.85892324	C	4.59280676	0.28827967	-2.49798483
H	-6.70550702	-1.23716284	-0.60785846	C	2.20084909	0.72246682	-2.21280942
H	-5.55669727	-0.75557909	0.66840603	C	6.03527345	-0.62626238	-0.80687083
C	-4.97715816	-2.90704999	-1.68216836	H	5.12264642	-1.04708488	1.07396417
H	-4.21013502	-3.57388030	-2.08614736	C	5.85364702	-0.13975837	-2.09902177
H	-6.02234316	-3.17715872	-1.86112209	H	4.44406502	0.66806869	-3.51163511
Au	0.20193687	0.16003690	0.05839103	C	1.38401148	-0.16583655	-2.92900315
P	2.32235299	-0.30710460	0.91935769	C	1.87213726	2.08520552	-2.20091778
C	2.73579665	1.04826319	2.16679892	H	7.01707847	-0.96964132	-0.47296647
C	2.28957113	-2.05836286	1.64182313	H	6.69193961	-0.09435218	-2.79851799
C	3.67295858	-0.24133311	-0.31912316	C	0.27064677	0.30255156	-3.62541467

H	1.64472952	-1.22668228	-2.96261547
C	0.75276853	2.54883300	-2.89202069
H	2.51133495	2.78792332	-1.66161152
C	-0.04690669	1.66044337	-3.61159061
H	-0.34719841	-0.39989732	-4.18849427
H	0.51215829	3.61487658	-2.87819464
H	-0.91895469	2.02501565	-4.15929745

TS16

Charge = 1; Multiplicity = 1

Au	-0.37531786	0.45478561	0.35615641
P	-2.52554171	1.30220685	0.65142709
C	-2.54699126	3.00983625	-0.15570466
C	-2.88857071	1.29103022	2.51061808
C	-3.87563189	0.35549352	-0.16101525
C	-3.90794752	3.70114861	-0.20542722
C	-1.54070402	3.89680272	0.57836145
C	-2.06653547	2.77064533	-1.59145568
C	-3.24681662	-0.15850111	2.85053055
C	-1.59736815	1.65770663	3.25158727
C	-3.99730778	2.23650231	2.96625093
C	-3.64171920	-0.77549326	-0.97494904
C	-5.20204774	0.78443434	0.02545299
H	-4.61862170	3.16505538	-0.84900736
H	-3.76676180	4.70337994	-0.64276187
H	-4.35988712	3.83564579	0.78600032
H	-0.55732768	3.40920326	0.67650254
H	-1.89432181	4.18115567	1.57990247
H	-1.39991486	4.82536651	0.00128805
H	-2.73160669	2.08199272	-2.13562544
H	-1.04543433	2.35874218	-1.61597688
H	-2.06300200	3.73088693	-2.13263111
H	-3.31276059	-0.26151288	3.94589265
H	-2.47494895	-0.86055921	2.49471275
H	-4.21276573	-0.46191372	2.42241083
H	-1.25055852	2.67385091	3.02078865
H	-1.79015597	1.60828051	4.33582331
H	-0.78189575	0.95565687	3.01739596
H	-4.12826322	2.11932317	4.05463032
H	-3.74089400	3.28876138	2.77791931
H	-4.96802517	2.02022280	2.50110551
C	-4.73589554	-1.41542156	-1.57799910
C	-2.30615323	-1.38263525	-1.24274451
C	-6.27466851	0.13206111	-0.57181952
H	-5.41123640	1.65098812	0.64988326
C	-6.03988417	-0.97393432	-1.38471055
H	-4.54500050	-2.28780014	-2.20761042
C	-1.60015586	-1.07382920	-2.41231788
C	-1.79591624	-2.36453481	-0.38088899
H	-7.29168757	0.49321958	-0.40222487
H	-6.87037996	-1.49647348	-1.86570720
C	-0.39710045	-1.71843993	-2.70225414
H	-1.99864524	-0.32233290	-3.09858408
C	-0.59471637	-3.00851967	-0.67488707
H	-2.35343979	-2.62716769	0.52191337
C	0.11213990	-2.68192736	-1.83238489
H	0.14527087	-1.46378444	-3.61602903
H	-0.19790041	-3.76916342	0.00150969
H	1.06248367	-3.17820180	-2.04034614
C	1.60101863	-0.26294375	0.23302581
C	2.06585975	-1.34464766	1.15235719
C	2.07574125	0.42558195	-0.72531852
N	3.41500246	-1.80655917	0.90290947
H	1.97284126	-0.97494209	2.18969504
H	1.38448750	-2.20050119	1.05600553
C	2.45168098	1.34437362	-1.70332330
C	4.52051980	-0.88786625	1.08452085
S	3.70997060	-3.42214242	0.70563583
C	2.25463459	1.03785122	-3.16380497
C	3.01649387	2.53397085	-1.26699014
C	4.78540899	-0.03819895	-0.14729250
H	4.29699814	-0.25645888	1.95679159
H	5.43203905	-1.45350248	1.33434038
C	3.90545311	-4.09389778	2.33270582

O	2.51065964	-4.01850154	0.12186054
O	4.99300323	-3.53873767	0.01857416
H	2.41507939	-0.02578988	-3.38545784
H	2.94240118	1.63380557	-3.78142431
H	1.22677304	1.29056471	-3.47347942
H	3.21250130	3.33153636	-1.98962477
H	2.91711736	2.83405045	-0.22264426
C	5.22341345	1.33220383	0.01205804
C	4.47802168	-0.55536350	-1.36570444
H	4.12008992	-5.16557909	2.21443358
H	4.74571404	-3.59048007	2.82908916
H	2.97138209	-3.95047841	2.89211151
C	5.46327918	1.87496656	1.38755411
C	5.22758297	2.19259768	-1.06126513
H	4.09258557	-1.57219531	-1.45412498
H	4.70334036	-0.03272227	-2.29526125
H	4.53029257	1.88888041	1.97833654
H	6.18342068	1.25740171	1.94697572
H	5.85164715	2.90105727	1.34450114
H	5.54175622	3.22914701	-0.91233161
H	5.24274727	1.83550356	-2.09134732

TS17

Charge = 1; Multiplicity = 1

Au	0.44538614	0.79028165	-0.05880946
C	-1.62397587	0.93621877	-0.10041628
P	2.78236420	0.71865556	-0.02847915
C	-2.23282568	0.26129314	-1.20318579
C	-2.43168781	1.67604375	0.85105971
H	-1.84451397	1.42506615	-1.47345693
C	3.38000208	2.04933003	1.18632344
C	3.40255555	0.95997281	-1.79443647
C	3.49291508	-0.87942313	0.54040298
N	-3.54327152	-0.12048903	-1.50427965
H	-1.53435683	-0.29600264	-1.83176267
C	-3.77701808	2.13340413	0.35587429
C	-2.23196853	1.64721556	2.20123184
C	2.41816473	3.24035026	1.08136465
C	3.24572351	1.44235239	2.58528794
C	4.80179377	2.56094534	0.96046558
C	2.97294197	2.35097528	-2.26248325
C	4.90770073	0.78243669	-1.97949007
C	2.68033558	-0.10358097	-2.62643903
C	2.71153940	-2.02717782	0.80424002
C	4.88039133	-0.94951578	0.75825656
C	-4.83655247	0.28134964	-0.89802558
S	-3.74081320	-0.94234303	-2.99063626
C	-4.63776916	0.90229037	0.44086175
H	-4.16798229	2.97121954	0.94316050
H	-3.71264490	2.49075256	-0.68271936
C	-1.03540823	1.14674361	2.93455313
C	-3.42522628	1.98491283	3.05865857
H	2.40272492	3.68335555	0.07638286
H	2.75006956	4.02090419	1.78550855
H	1.38744206	2.96034508	1.34652705
H	3.39984448	2.23676864	3.33371137
H	3.98611362	0.65197081	2.77199713
H	2.24100070	1.02030475	2.75035831
H	4.90510951	3.07245163	-0.00694057
H	5.56598817	1.77555438	1.02474562
H	5.03180024	3.29827437	1.74725154
H	3.17113608	2.44061716	-3.34296705
H	3.53264256	3.14966864	-1.75504865
H	1.89627570	2.52103061	-2.10221698
H	5.50185009	1.47665078	-1.37159046
H	5.22959598	-0.24474599	-1.75811282
H	5.15070012	0.97792836	-3.03705632
H	2.95435954	-1.12152087	-2.31008463
H	1.58563677	-0.00144849	-2.56214786
H	2.97432192	0.00887017	-3.68279395
C	3.34832329	-3.18549017	1.27856760
C	1.23432919	-2.13821711	0.62303793
C	5.49431090	-2.10589890	1.22515406
H	5.50260189	-0.07704857	0.56741045

H	-5.47458804	-0.60965359	-0.85023528
H	-5.32113331	1.00046719	-1.57802382
C	-4.24602779	-2.56630483	-2.51208901
O	-2.42630219	-1.02907341	-3.61836688
O	-4.84303825	-0.30494672	-3.69633203
C	-4.95724147	0.34159050	1.62472662
H	-0.18728304	0.89636446	2.28380741
H	-0.71305128	1.90934116	3.66368040
H	-1.29129596	0.24884128	3.52194047
C	-4.53871295	0.91558656	2.96427458
H	-3.11974181	2.04861307	4.11323824
H	-3.82836023	2.97404359	2.79767448
C	4.72145950	-3.23374912	1.48922936
H	2.73705905	-4.06826896	1.48118511
C	0.68923859	-2.48152772	-0.62219505
C	0.37952152	-2.03451261	1.72914239
H	6.57503335	-2.12042937	1.38415247
H	-5.18107199	-2.51209914	-1.94072814
H	-4.41538750	-3.10848913	-3.45346639
H	-3.44440055	-3.03896986	-1.93195182
C	-5.69587811	-0.95583594	1.76359650
H	-4.23073450	0.04735767	3.57382913
H	-5.43547306	1.30788647	3.47619678
H	5.18548009	-4.15152129	1.85868108
C	-0.68073674	-2.69812318	-0.76023386
H	1.34743561	-2.58656186	-1.48700925
C	-0.99259270	-2.24430332	1.58710300
H	0.79690713	-1.78722375	2.70843163
H	-6.51598717	-0.85489805	2.49363090
H	-5.02298189	-1.73650216	2.16018088
H	-6.12941938	-1.32336395	0.82497552
C	-1.52640202	-2.57415495	0.34254363
H	-1.08727117	-2.95642220	-1.74131561
H	-1.64830748	-2.15225563	2.45663146
H	-2.60224895	-2.73230025	0.23413779

IN18

Charge = 1; Multiplicity = 1

Au	-0.03026498	-0.15541467	0.49039428
C	-1.87735073	0.13099375	1.76953138
P	1.78304280	-0.67386251	-0.86700838
C	-1.97221443	1.15760019	0.83078202
C	-2.76117341	-1.04701158	1.78088357
H	-1.33689669	0.42344348	2.67712614
C	1.38970974	0.09615274	-2.54595273
C	1.99167689	-2.55395598	-0.82346827
C	3.39059661	0.03673127	-0.34368746
N	-2.71452103	1.28987814	-0.32339846
H	-1.44890103	2.08608881	1.07710059
C	-4.06486260	-0.80745417	1.07510839
C	-2.40013717	-2.32017904	2.05504673
C	1.22169339	1.59266971	-2.26380833
C	2.45824935	-0.08748557	-3.62026122
C	0.06175519	-0.48662903	-3.03076533
C	2.94931069	-3.14386339	-1.85499534
C	2.50111112	-2.85054676	0.59087294
C	0.61484775	-3.19815784	-1.00541698
C	3.54067711	0.85250577	0.79977038
C	4.53063369	-0.26474171	-1.10991079
C	-3.48615445	0.28638043	-1.10616781
S	-2.50378515	2.76797710	-1.16928154
C	-3.68981019	-0.99706226	-0.36899136
H	-4.85069160	-1.50140043	1.39357716
H	-4.43840942	0.21024827	1.25714883
C	-1.08113403	-2.72274305	2.62710837
C	-3.32682191	-3.40513475	1.56590117
H	0.42597712	1.79501581	-1.53180684
H	0.94439685	2.10018007	-3.20178898
H	2.15499750	2.04796670	-1.89881308
H	2.08188198	0.35918431	-4.55513885
H	2.68055957	-1.14309267	-3.82580240
H	3.39325437	0.43098778	-3.36908530
H	-0.70309279	-0.46679388	-2.23897543
H	0.17127981	-1.52124513	-3.38446803

H	-0.30765051	0.11844765	-3.87387511
H	2.96419019	-4.23813244	-1.72234619
H	3.98170478	-2.79325341	-1.73006436
H	2.62515527	-2.94466597	-2.88577750
H	1.82816326	-2.44074211	1.36099963
H	2.54524108	-3.94271139	0.73187106
H	3.51008558	-2.44676057	0.76136802
H	0.24238994	-3.09213678	-2.03276527
H	0.70107086	-4.27618067	-0.79353890
H	-0.13381914	-2.77536029	-0.31802273
C	4.82077111	1.31856240	1.13612446
C	2.43411430	1.28469663	1.70162177
C	5.79117336	0.20829973	-0.76233681
H	4.44022964	-0.88220132	-2.00167416
H	-2.96824865	0.13813550	-2.06044529
H	-4.46466890	0.74878975	-1.32764894
C	-4.01460818	3.62895973	-0.87505036
O	-1.41797939	3.49302692	-0.51857518
O	-2.41075411	2.43736866	-2.58410484
C	-3.39242593	-2.22567822	-0.84286147
H	-0.43966768	-1.86257137	2.86610840
H	-1.22588379	-3.30963112	3.55076134
H	-0.53270234	-3.37934828	1.93034326
C	-3.39280362	-3.48067519	0.01665173
H	-2.98882676	-4.38754191	1.92882057
H	-4.33883697	-3.26687330	1.97603911
C	5.93847096	1.00282448	0.37137352
H	4.92890539	1.94786114	2.02274926
C	2.16881728	0.58451853	2.88684776
C	1.72685355	2.46559678	1.43786619
H	6.65524837	-0.04686897	-1.38021834
H	-4.85349854	3.03493064	-1.26001108
H	-3.93615538	4.57669059	-1.42724905
H	-4.10913030	3.81239880	0.20302463
C	-2.99965893	-2.49801835	-2.26350479
H	-2.52126931	-4.06327826	-0.33106356
H	-4.26397620	-4.10128448	-0.26116896
H	6.92195719	1.38135662	0.66040824
C	1.21097211	1.05318540	3.78584233
H	2.72480489	-0.33050599	3.10646522
C	0.77072960	2.93375301	2.33888076
H	1.93200174	3.02337370	0.52133186
H	-3.00041857	-1.60559963	-2.90139970
H	-3.70029960	-3.22297200	-2.71243220
H	-2.00229532	-2.96340888	-2.31397270
C	0.51064767	2.22978582	3.51534082
H	1.01494892	0.49764106	4.70654026
H	0.22978930	3.85702017	2.11754768
H	-0.23403398	2.60065916	4.22406230

TS19

Charge = 1; Multiplicity = 1

Au	0.31536315	0.19452571	-0.49640221
P	2.41297887	-0.80056043	-0.47830973
C	-1.62462509	1.03552932	-0.82367251
C	3.00513736	-0.79158828	-2.27024603
C	2.25515592	-2.52799625	0.28693415
C	3.68573632	0.09464678	0.49606340
C	-1.85964533	1.54349390	-2.17285932
C	-2.21090908	0.90216795	0.29997332
C	4.43904690	-1.27437724	-2.47800574
C	2.03534639	-1.64550857	-3.08803755
C	2.91037302	0.66726528	-2.72666155
C	3.32800928	-3.52531002	-0.14366010
C	0.87962639	-3.08527704	-0.09584769
C	2.28647916	-2.33068980	1.80447160
C	4.95086848	-0.50405594	0.63594649
C	3.44165756	1.32069390	1.15406018
C	-1.92961104	0.50092303	-3.24990432
C	-1.99245822	2.86018857	-2.39866102
C	-2.24845533	0.33697444	1.67634531
H	4.60613422	-2.29707292	-2.11678574
H	5.16949626	-0.60646977	-2.00069568
H	4.64957756	-1.26722554	-3.56006427

H	2.26184101	-1.51531186	-4.15873841	C	0.16194992	2.88197860	2.22835681
H	2.12510673	-2.71647134	-2.85620241	H	1.50997723	1.40629628	3.04918650
H	0.98960789	-1.33840902	-2.92410252	C	-4.80537588	0.75950196	0.45735615
H	3.56652371	1.32436876	-2.13555242	H	-4.77231752	0.74240071	2.60266593
H	1.88046515	1.05218689	-2.66012562	H	-5.42541444	-0.75451910	1.92217169
H	3.23233509	0.73197285	-3.77876901	C	-2.86569932	-2.40966566	-0.18208021
H	3.29078381	-3.73105440	-1.22230557	O	-4.34232335	-2.86359236	1.94050491
H	4.34533450	-3.20762205	0.11842824	O	-1.84432765	-2.54119843	2.21501967
H	3.14192474	-4.47702524	0.38047589	C	-0.10812534	3.73918212	1.16143881
H	0.72104234	-3.13136890	-1.18208654	H	0.55902548	4.44912131	-0.76837974
H	0.79575126	-4.11115120	0.29866058	H	-0.50644320	2.85455187	3.09274570
H	0.07155322	-2.49489232	0.35739725	C	-4.12321701	1.94348845	0.34812686
H	2.00395312	-3.27889253	2.28980192	C	-5.51996010	0.16905728	-0.68092304
H	1.56364550	-1.56507347	2.13029702	H	-2.68937869	-3.48446747	-0.33084934
H	3.28207175	-2.04332192	2.17002543	H	-1.99103158	-1.83108728	-0.50465135
C	5.95551993	0.07672231	1.40102605	H	-3.77079551	-2.09068072	-0.71381305
H	5.16183028	-1.45346253	0.14575761	H	-0.99164906	4.38227927	1.18409962
C	4.46708081	1.88892903	1.92688163	H	-4.11599461	2.51802607	-0.57902989
C	2.16694227	2.09365869	1.10950509	H	-3.79038455	2.46859976	1.24803138
H	-2.16448139	0.95439850	-4.22269171	C	-5.61285985	0.96911804	-1.94731926
H	-0.97232566	-0.03961082	-3.33361782	C	-6.11232324	-1.03982328	-0.58558908
H	-2.69980924	-0.25180859	-3.01494673	H	-4.61661209	1.20033932	-2.35440790
H	-2.16472411	3.23362767	-3.41225961	H	-6.11488646	1.93372976	-1.76920416
H	-1.91872354	3.59062752	-1.58957514	H	-6.17951165	0.42282182	-2.71280080
N	-3.34799728	-0.57294168	1.87609653	H	-6.66160225	-1.45208078	-1.43660264
H	-2.32184843	1.14845642	2.41714434	H	-6.06677097	-1.66020461	0.31204079
H	-1.30081175	-0.18775397	1.86283212				
C	5.71133031	1.28245047	2.05365125	**IN20**			
H	6.92540111	-0.41833244	1.48835692	Charge = 1; Multiplicity = 1			
H	4.27088063	2.83616220	2.43499289	Au	0.16603907	-0.01948924	0.55320516
C	1.88933351	2.96058313	0.04304642	P	2.28347726	0.41031046	-0.39735632
C	1.29350915	2.06708563	2.20577381	C	-1.70249788	-0.11162953	1.38238128
C	-4.67492374	0.02696508	1.77160461	C	3.10639794	1.74885059	0.66604547
S	-3.10263883	-2.19390386	1.56103681	C	2.03292331	0.90831878	-2.20111042
H	6.48803990	1.75204411	2.66213803	C	3.43060153	-1.02398927	-0.41927105
C	0.75912552	3.77696728	0.06944504	C	-1.79891307	-0.15117234	2.82824451
H	2.57479204	3.00247586	-0.80599316	C	-2.85188749	-0.05455579	0.55486906

C	2.01556090	2.72850721	1.11639285	H	-3.27965888	-1.69891074	2.78620248
C	3.64798047	1.02383458	1.90145365	N	-3.63143682	0.64174021	-1.53813740
C	4.21980631	2.54648705	-0.00983577	H	-3.04680317	-1.34541547	-1.18504770
C	3.31477778	1.09972383	-3.00797718	H	-1.67891136	-0.18742223	-1.23434269
C	1.20017623	2.19069473	-2.22777643	C	5.31871014	-3.11510085	-0.39407473
C	1.23303218	-0.23644400	-2.82850707	H	6.72258114	-1.64574037	-1.13915987
C	4.76040443	-0.81678588	-0.82597942	H	3.70349565	-4.33675562	0.33799473
C	3.04650087	-2.31647172	0.00251973	C	1.40364663	-2.85778848	1.81921318
C	-0.81261772	0.63177069	3.64643844	C	0.69204154	-3.06176424	-0.47889275
C	-2.60989603	-1.07935739	3.38649068	C	-3.67723017	1.86776620	-0.77134356
C	-2.73267180	-0.32327234	-0.92987930	S	-3.87322926	0.64922727	-3.17160472
H	1.54052421	3.24970282	0.27423302	H	6.04248618	-3.93370105	-0.37796195
H	2.47648514	3.49292915	1.76321105	C	0.16635277	-3.34018883	2.24484247
H	1.22828287	2.22335004	1.69596603	H	2.17249209	-2.59993393	2.55197436
H	2.87483026	0.40187944	2.38144995	C	-0.54496493	-3.54549332	-0.05059168
H	4.50665592	0.38030681	1.66347758	H	0.90296560	-2.97276317	-1.54668667
H	3.97777912	1.77421773	2.63827788	C	-3.60997983	1.41837231	0.67437228
H	5.05808775	1.92398680	-0.34868491	H	-4.61830560	2.40658664	-0.95978248
H	4.62683649	3.26014823	0.72546698	H	-2.83369883	2.54408988	-0.99603501
H	3.84848020	3.13250151	-0.86247834	C	-2.39170903	1.30993772	-3.89018152
H	3.87817986	0.16195948	-3.11079904	O	-4.95769912	1.58930587	-3.42634745
H	3.03702809	1.42493693	-4.02417674	O	-3.98213909	-0.74702841	-3.57637744
H	3.97778095	1.86530964	-2.58614784	C	-0.81029779	-3.68744151	1.31124659
H	0.28180335	2.09618173	-1.62598282	H	-0.03425460	-3.44789423	3.31375594
H	1.76699184	3.05838458	-1.86132139	H	-1.30138008	-3.82345447	-0.78902997
H	0.90348115	2.40286922	-3.26795684	C	-4.28748941	0.16501317	1.01769946
H	1.79138502	-1.18442080	-2.80325739	C	-3.22065389	2.41984107	1.70034717
H	1.03081710	0.00364626	-3.88513783	H	-2.23615119	2.33220539	-3.52095798
H	0.26960169	-0.38854320	-2.31830229	H	-2.54741085	1.32100676	-4.97821748
C	5.69742465	-1.84362223	-0.81767879	H	-1.54614306	0.65738847	-3.63692998
H	5.07950113	0.17158304	-1.15225779	H	-1.77725305	-4.07151113	1.64525526
C	4.00738603	-3.34004887	0.00910524	H	-4.51002048	-0.00368792	2.06879971
C	1.67920910	-2.70878450	0.45198232	H	-5.03009942	-0.22026631	0.31324523
H	0.20569825	0.23646728	3.49839404	C	-2.05999190	3.31222991	1.37986695
H	-0.79806884	1.69041426	3.35099717	C	-3.88467923	2.49254341	2.86294202
H	-1.05993430	0.57070685	4.71513815	H	-2.28952234	4.01209874	0.56075658
H	-2.54667227	-1.29922344	4.45712104	H	-1.19096650	2.71155210	1.05821748

H	-1.76939897	3.90882774	2.25503099
H	-3.60093451	3.22751350	3.62146725
H	-4.73509025	1.84466408	3.08814751

TS16’

Charge = 0; Multiplicity = 1

C	-0.84492852	1.04228519	-0.28372476
C	0.52886411	1.20153863	0.35981757
C	1.47348125	2.11247189	-0.22450238
C	1.10497866	2.93571876	-1.42290872
C	0.88834532	0.36903157	1.37759400
C	2.81566928	2.02734373	0.14590362
C	-0.88098149	-1.16716222	-1.48623113
C	0.56938557	-1.37451780	-1.44348794
C	1.64411001	-1.17063784	-0.88166217
C	2.83129264	-0.79497744	-0.22044954
C	3.38701740	-1.63796869	0.89578667
C	3.51033739	0.33992262	-0.68789757
S	-2.54561046	-0.83582041	0.60693881
O	-2.46666901	-0.06601886	1.84688576
O	-2.50251236	-2.29522749	0.65081014
N	-1.31518039	-0.32947512	-0.36584298
H	-1.57769035	1.63050088	0.28991223
H	-0.84403474	1.45513058	-1.30259648
H	0.89326928	2.30171000	-2.30373208
H	0.20324789	3.54370826	-1.24700693
H	1.92116661	3.61865823	-1.69583936
H	1.80595511	0.50389401	1.94861455
H	0.19727816	-0.40184912	1.72523902
H	3.08441149	1.71631880	1.15777488
H	3.50943963	2.75183991	-0.29259793
H	-1.41646943	-2.12532095	-1.41830792
H	-1.17988927	-0.69554734	-2.44016643
H	3.95596520	-1.01833037	1.60670157
H	4.08261052	-2.40324231	0.50670564
H	2.59693772	-2.16399653	1.44980715
H	4.53806218	0.48603893	-0.33756143
H	3.33368998	0.65495961	-1.71932361
C	-4.05137627	-0.37284262	-0.20920537
H	-4.10177217	-0.88440451	-1.17969736
H	-4.88209138	-0.69429205	0.43497155
H	-4.06913609	0.71760645	-0.33788158

IN6’

Charge = 0; Multiplicity = 1

C	-0.38703668	-0.00922996	1.19663944
C	0.98695346	0.56301515	0.90403867
C	1.21056620	1.62754000	0.10765263
C	0.16293297	2.49697450	-0.50471585
C	2.21498748	-0.22180249	1.30029795
C	2.64669566	1.87212207	-0.28145855
C	-0.79264933	-1.64067253	-0.72387724
C	0.65511279	-1.66755052	-0.89513765
C	1.81310052	-1.36959071	-0.67826343
C	2.92984862	-0.67732604	-0.01102128
C	4.12290907	-1.58401211	0.26662879
C	3.34064080	0.59649583	-0.79944043
S	-2.75363891	0.00709946	-0.06498289
O	-3.20376282	-0.21921086	-1.43503505
O	-2.89405853	1.33427298	0.53334929
N	-1.14696727	-0.40543248	-0.00401920
H	-0.28514601	-0.87696254	1.87147360
H	-1.00769954	0.73320396	1.71783790
H	0.13809370	2.34837321	-1.59934797
H	-0.84547497	2.30242208	-0.11988570
H	0.40359775	3.56182941	-0.34309335
H	2.92284064	0.38805580	1.88921674
H	1.95652642	-1.10421077	1.90396675
H	3.20509029	2.23929485	0.59797724
H	2.71505010	2.66759400	-1.03863577
H	-1.11310207	-2.54186897	-0.16412084
H	-1.33191321	-1.63909493	-1.68138507
H	4.86467513	-1.05160923	0.88198659
H	4.61311271	-1.88902076	-0.67084240

H	3.81541412	-2.49390461	0.80448414	H	-3.23502863	-1.04775376	2.00596510
H	4.43129472	0.72703852	-0.72254695	H	-4.68204136	-0.85579342	0.94764687
H	3.11422601	0.45437474	-1.86636953	H	-3.48498486	-2.15358501	0.59277601
C	-3.61957903	-1.13516817	0.98102391				

7. Single Crystal X-Ray Diffraction Data

SXRD Data of 2a

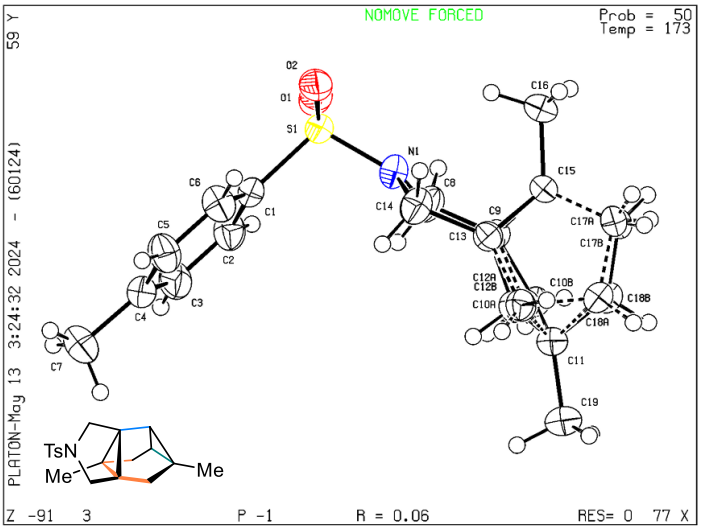


Figure S5. ORTEP of **2a**, the 50% probability ellipsoid is shown.
CCDC Deposition Number: 2354908

Crystal data	
Chemical formula	$C_{19}H_{23}NO_2S$
M_r	329.44
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	173
a, b, c (Å)	6.1952(12), 7.8941(16), 17.917(4)
α, β, γ (°)	102.21(3), 93.06(3), 99.06(3)
V (Å^3)	842.3(3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.15 × 0.13 × 0.10
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.160, 1.07
No. of reflections	3799
No. of parameters	224
No. of restraints	5
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.28

SXRD data of 2j

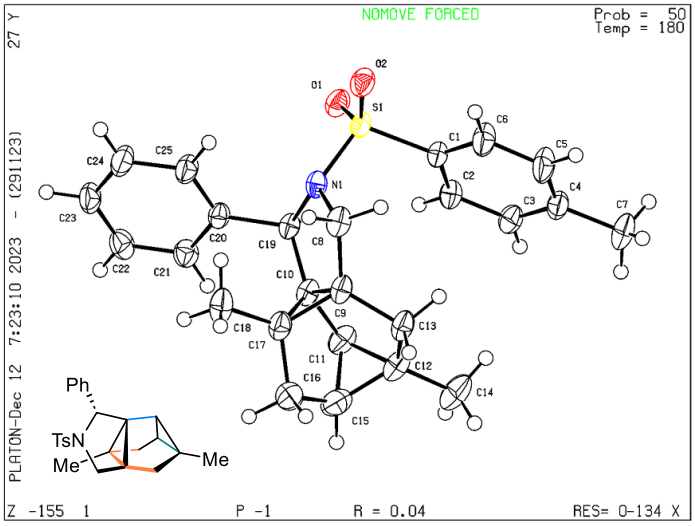
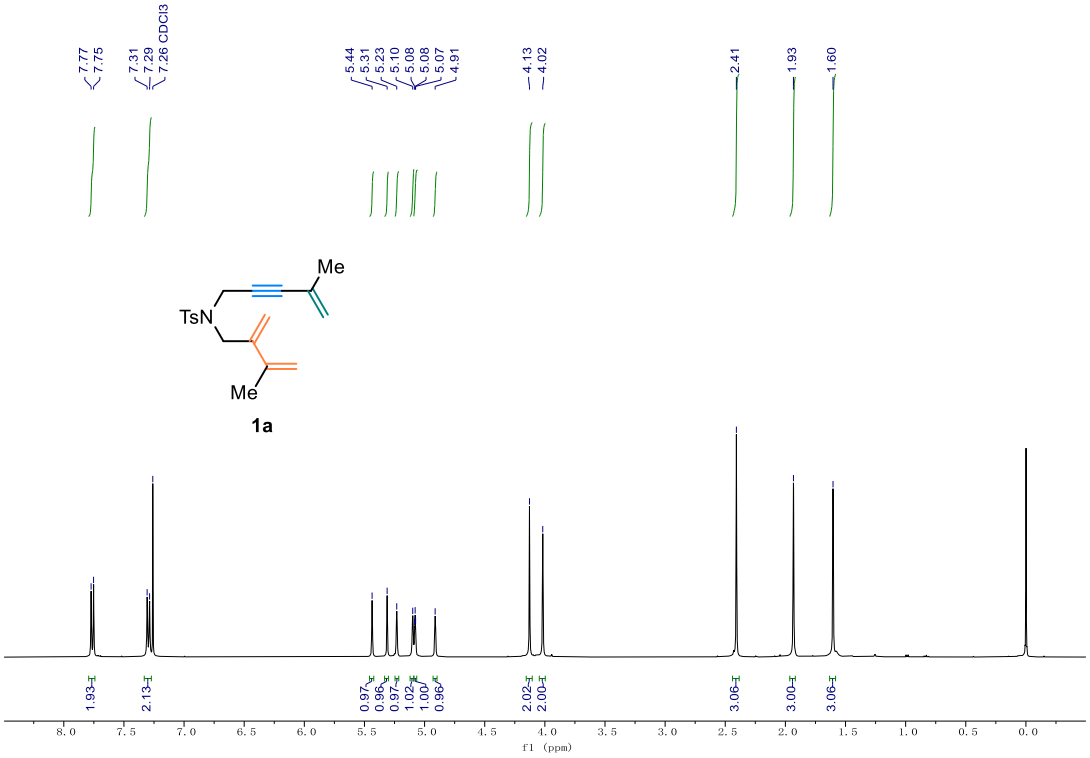


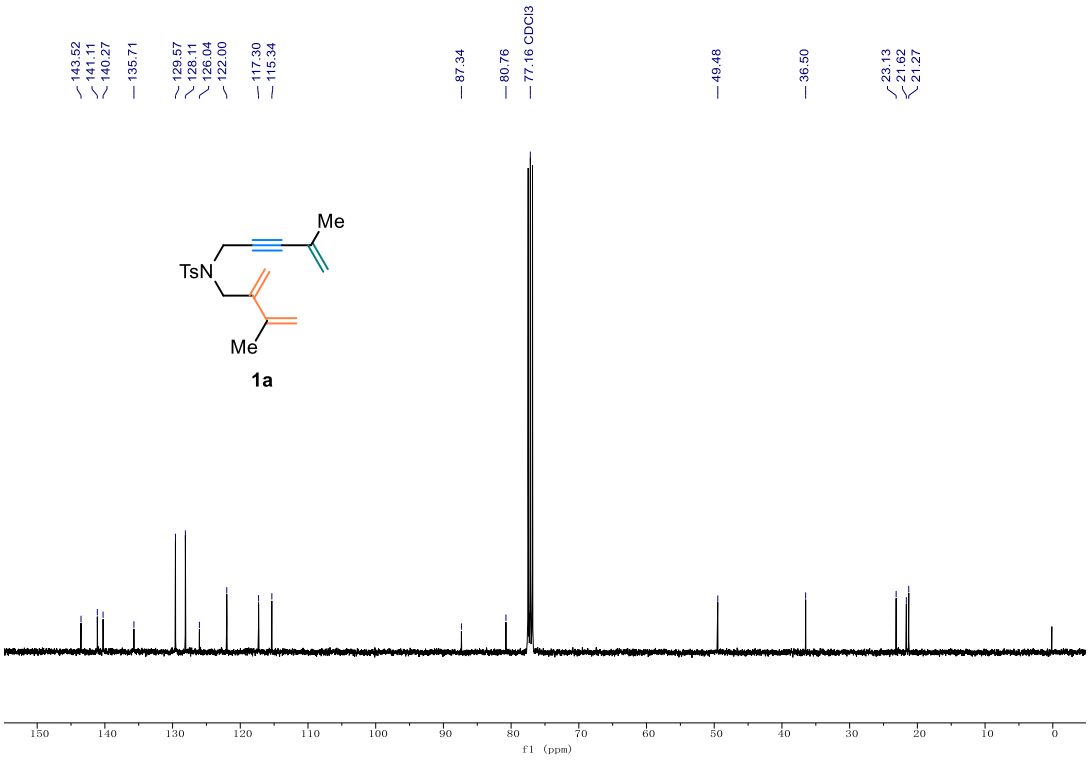
Figure S6. ORTEP of **2j**, the 50% probability ellipsoid is shown.
CCDC Deposition Number: 2354907

Crystal data	
Chemical formula	$C_{25}H_{27}NO_2S$
M_r	405.53
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	180
a, b, c (Å)	9.5601(4), 10.0808(4), 12.4359(4)
α, β, γ (°)	109.297(3), 107.249(3), 97.920(3)
V (Å^3)	1042.67(7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.15 × 0.15 × 0.03
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.126, 1.04
No. of reflections	5224
No. of parameters	265
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, -0.30

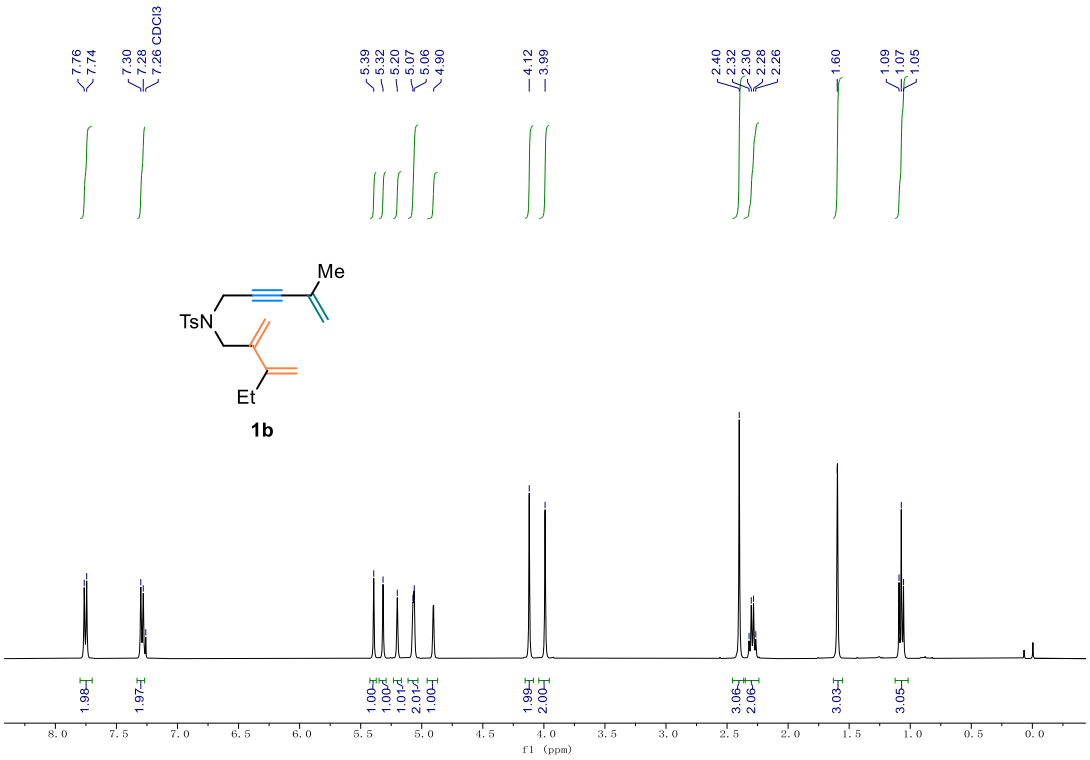
8. Copies of NMR Spectra



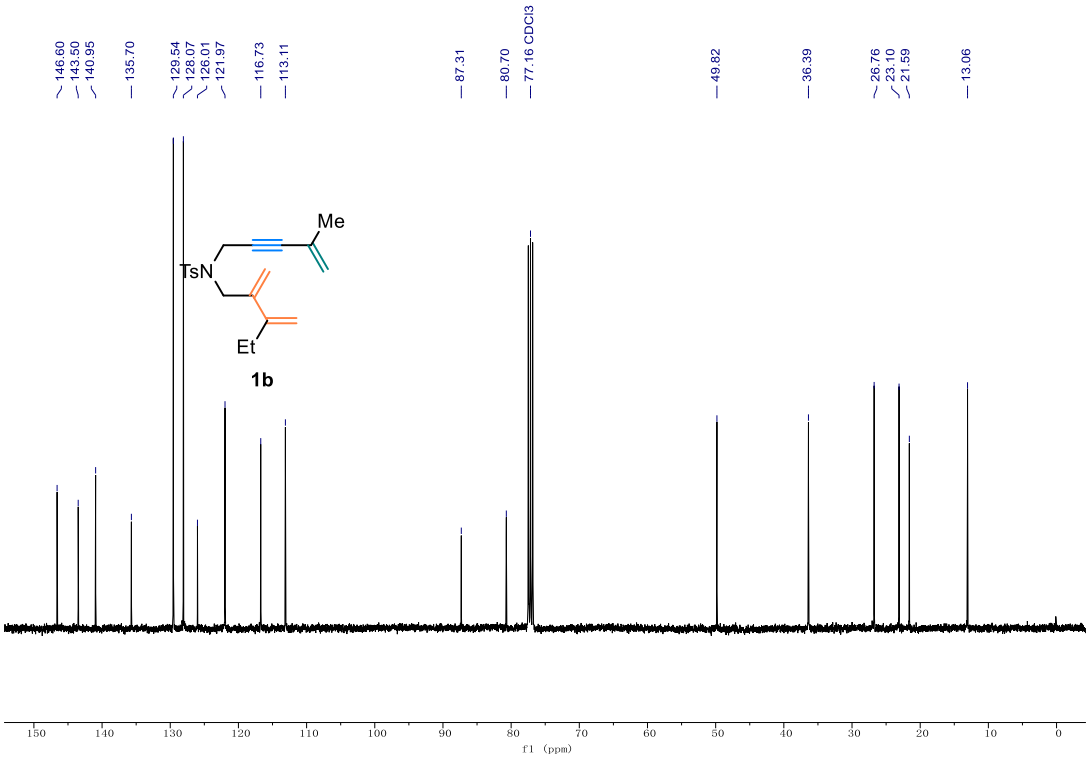
^{1}H NMR of **1a** (400 MHz, $CDCl_3$)



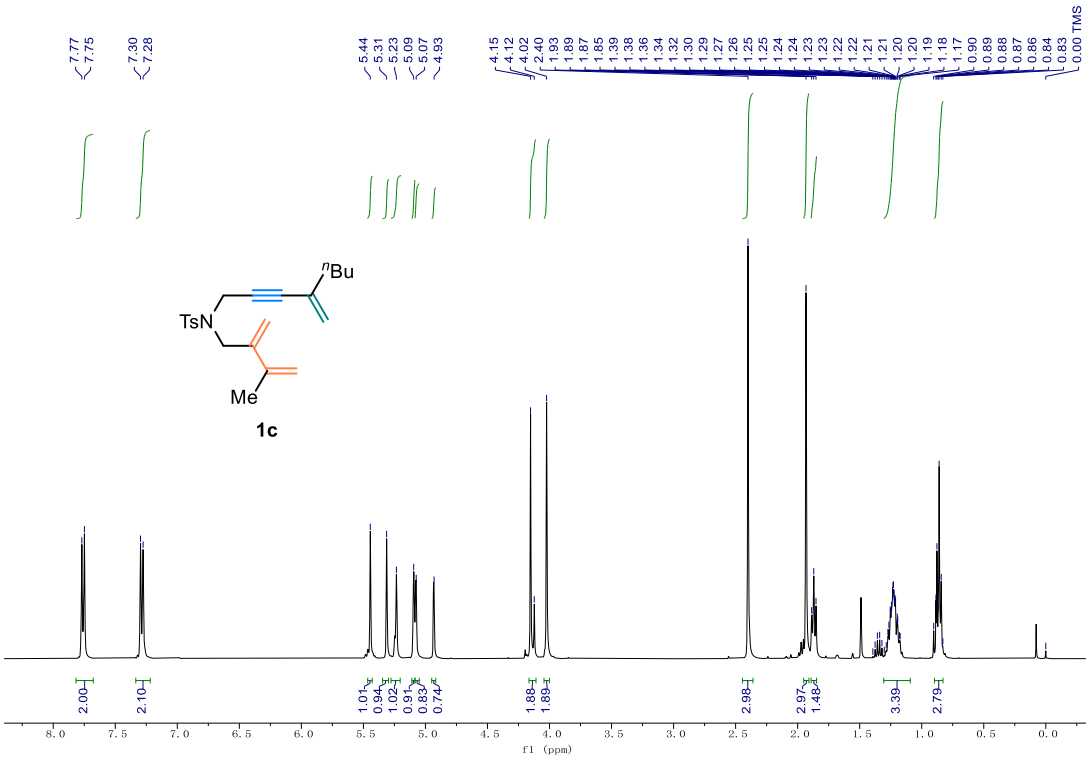
^{13}C{^{1}H} NMR of **1a** (101 MHz, $CDCl_3$)



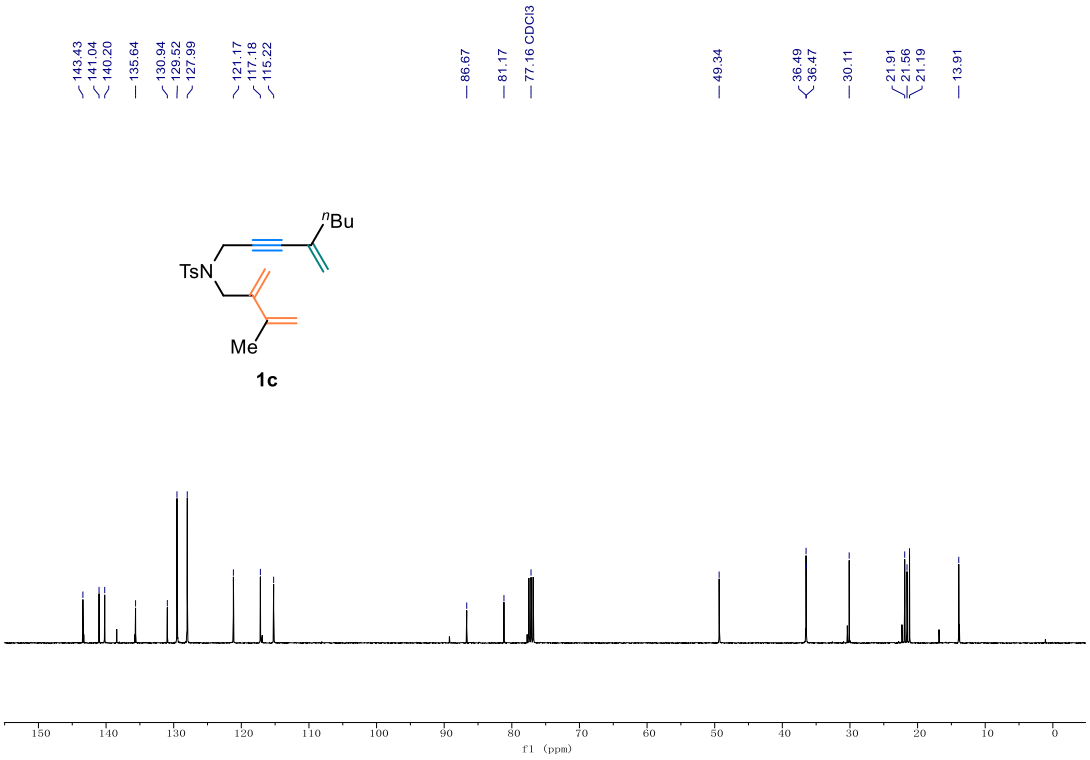
^{1}H NMR of **1b** (400 MHz, $CDCl_3$)



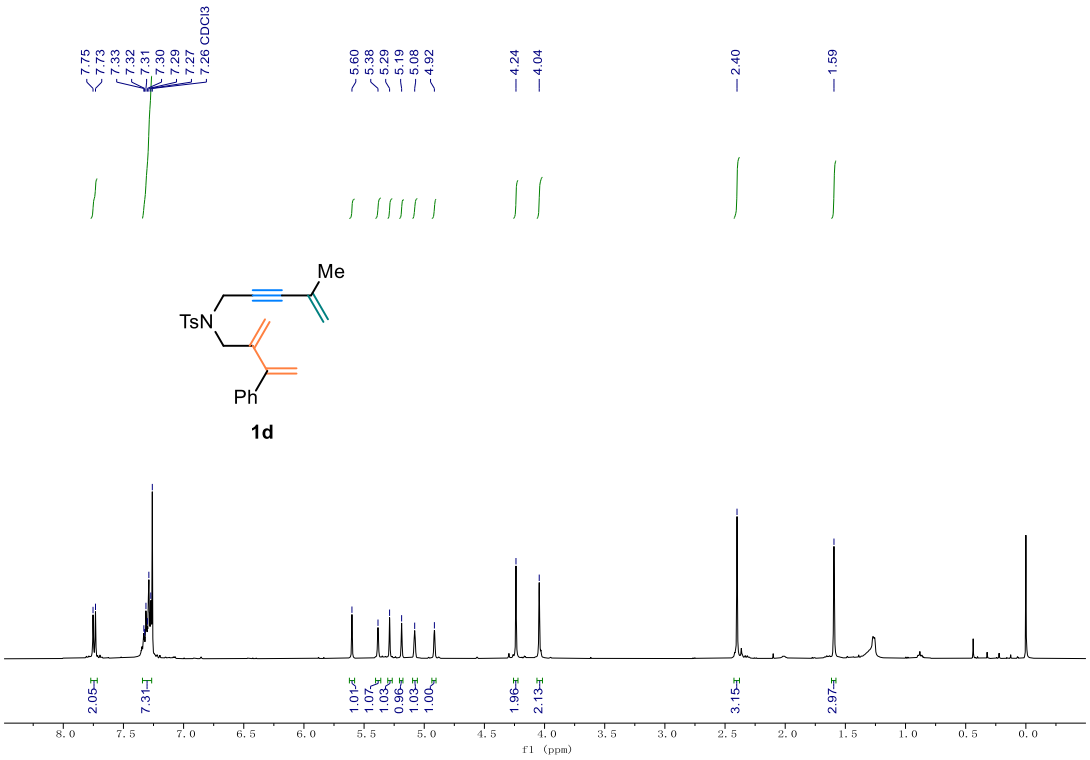
^{13}C{^{1}H} NMR of **1b** (101 MHz, $CDCl_3$)



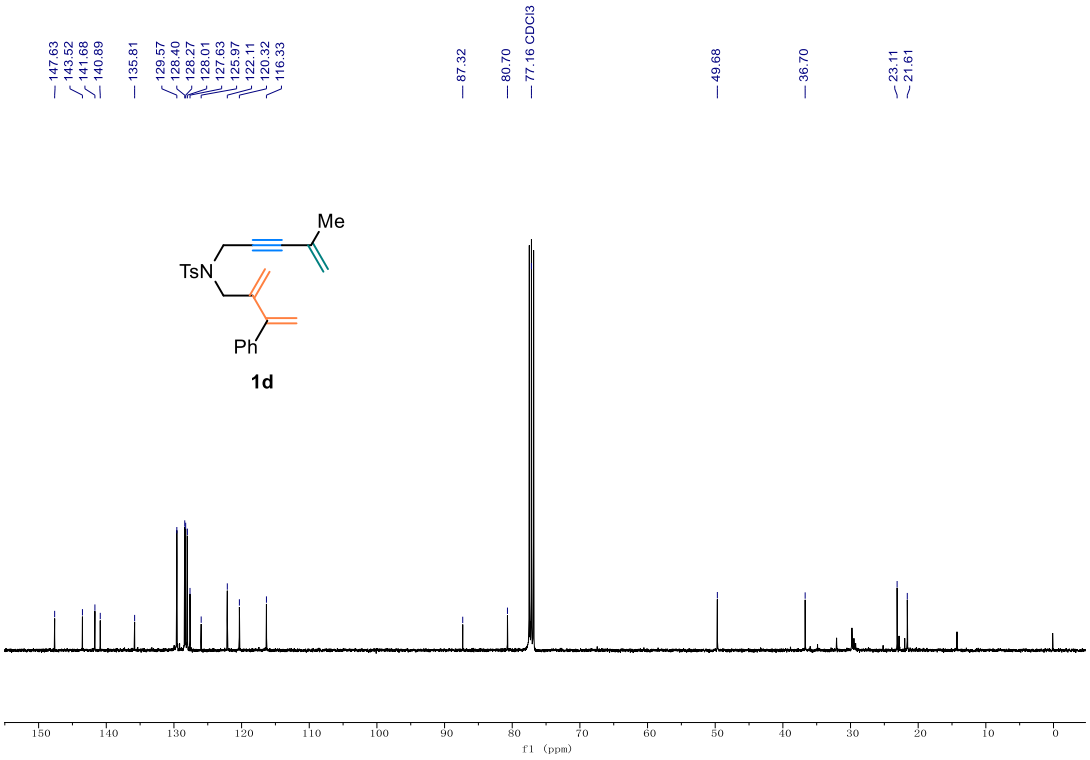
^{1}H NMR of **1c** (400 MHz, $CDCl_3$)



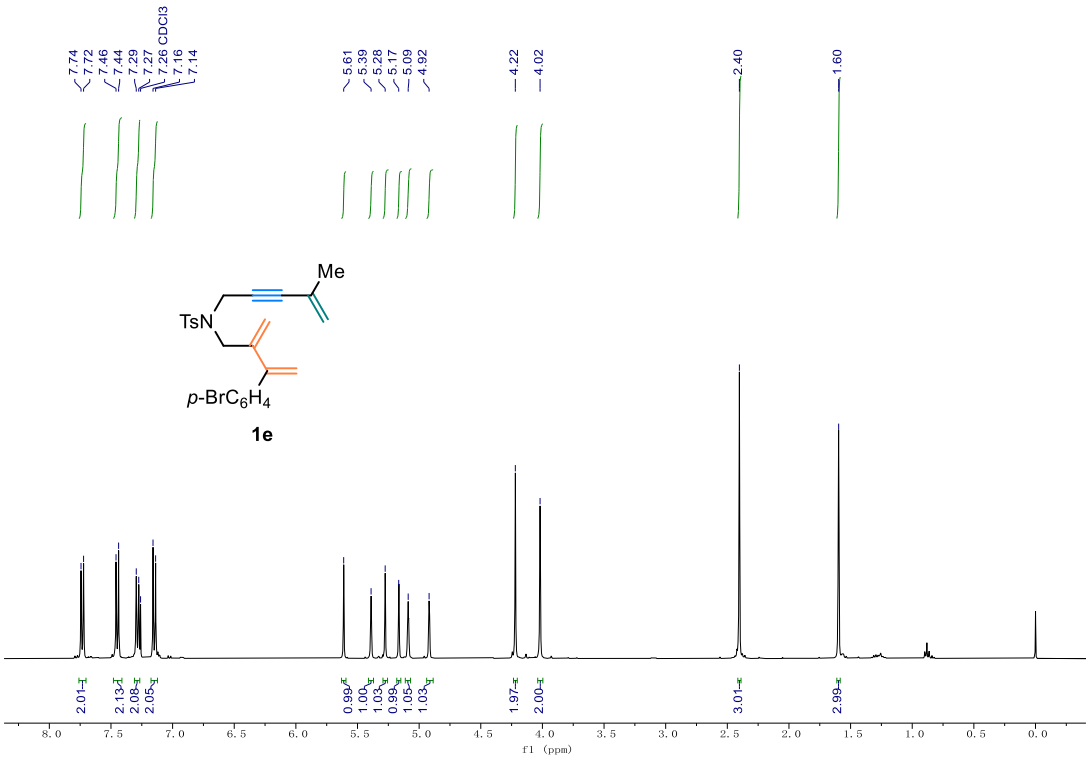
^{13}C{^{1}H} NMR of **1c** (101 MHz, $CDCl_3$)



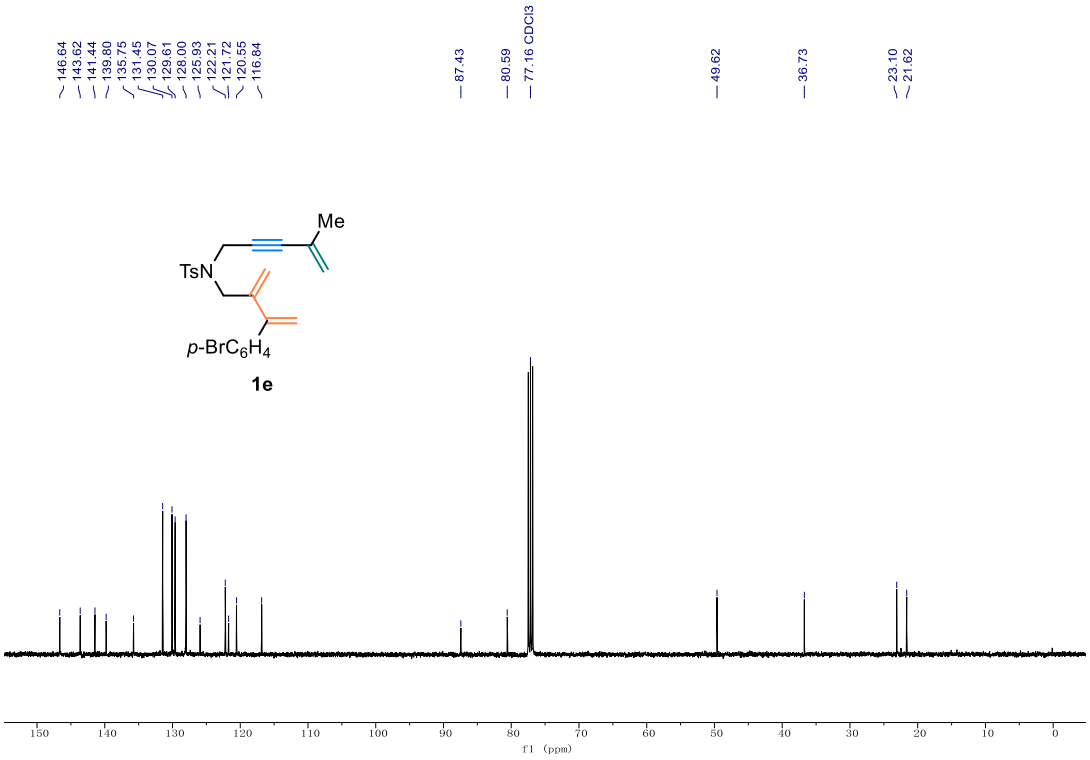
^{1}H NMR of **1d** (400 MHz, $CDCl_3$)



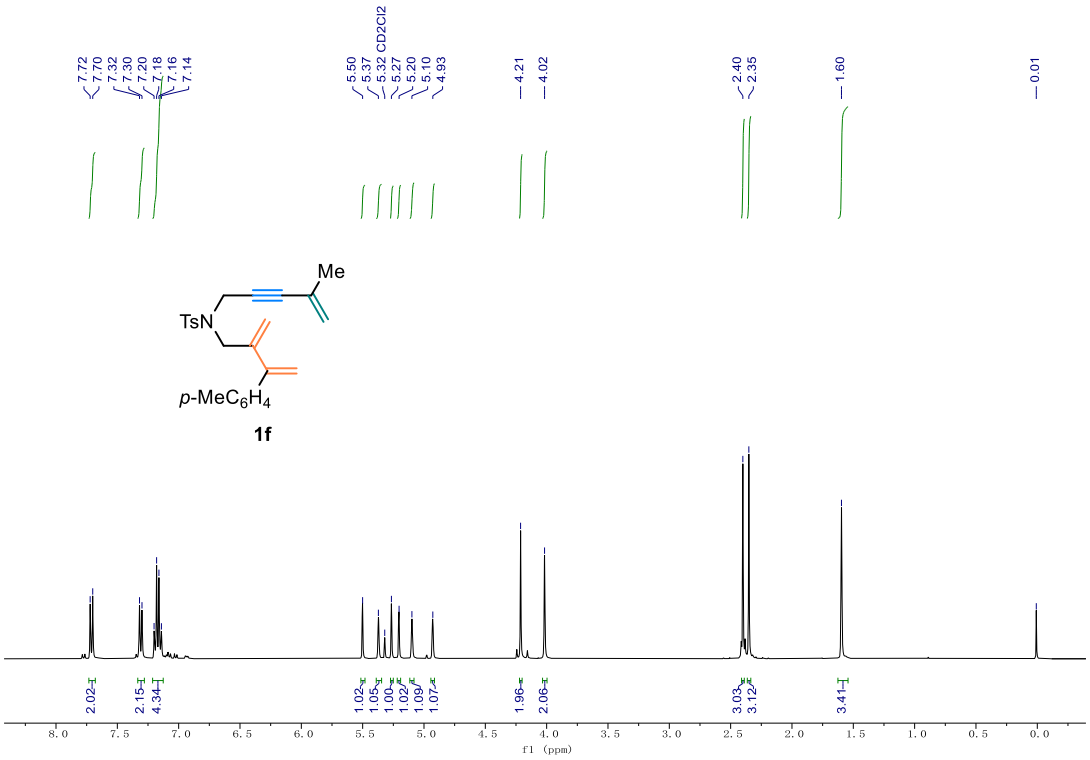
^{13}C{^{1}H} NMR of **1d** (101 MHz, $CDCl_3$)



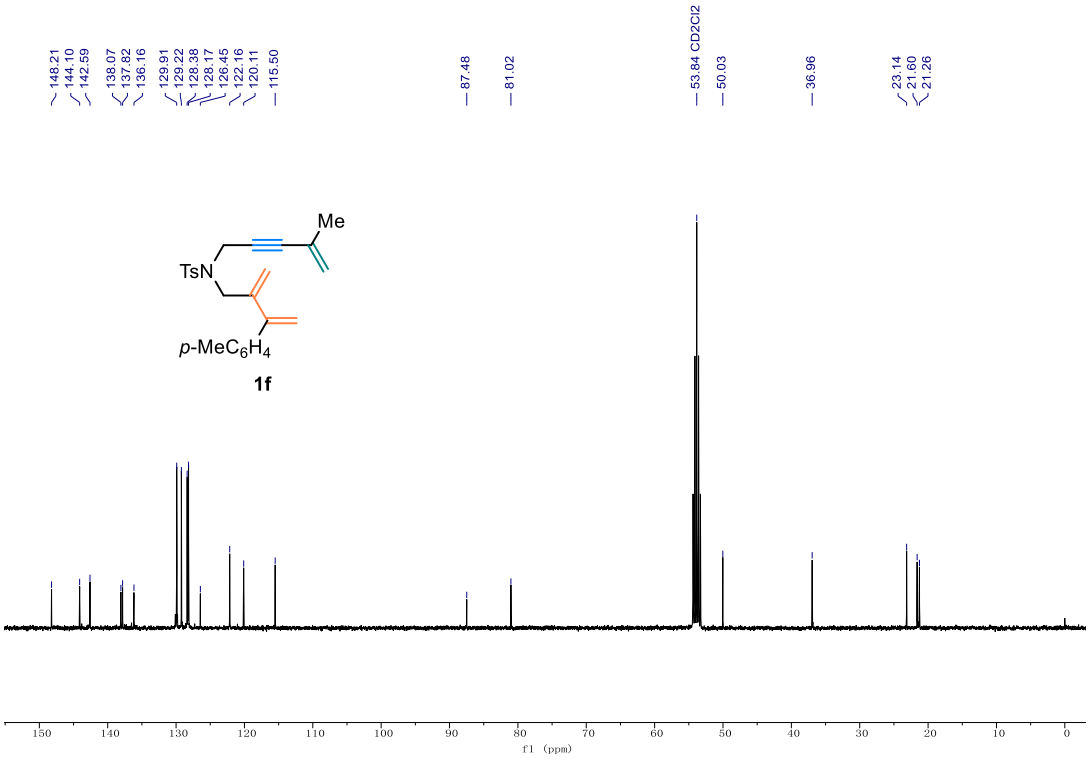
^{1}H NMR of **1e** (400 MHz, $CDCl_3$)



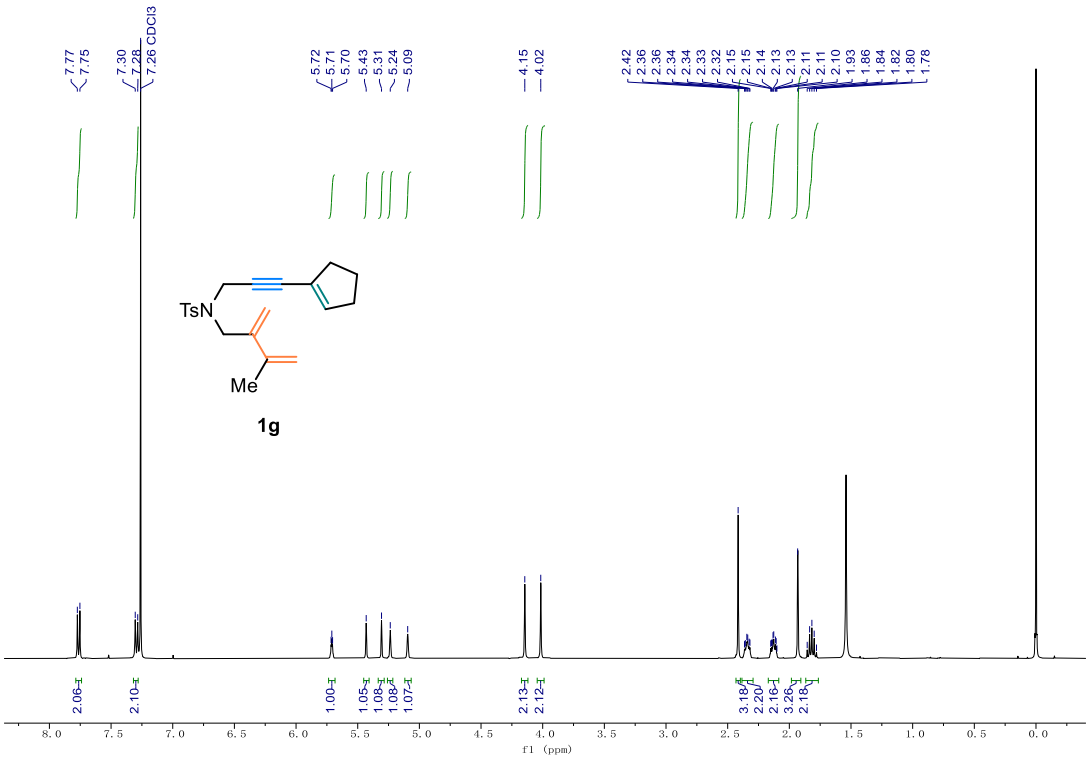
^{13}C{^{1}H} NMR of **1e** (101 MHz, $CDCl_3$)



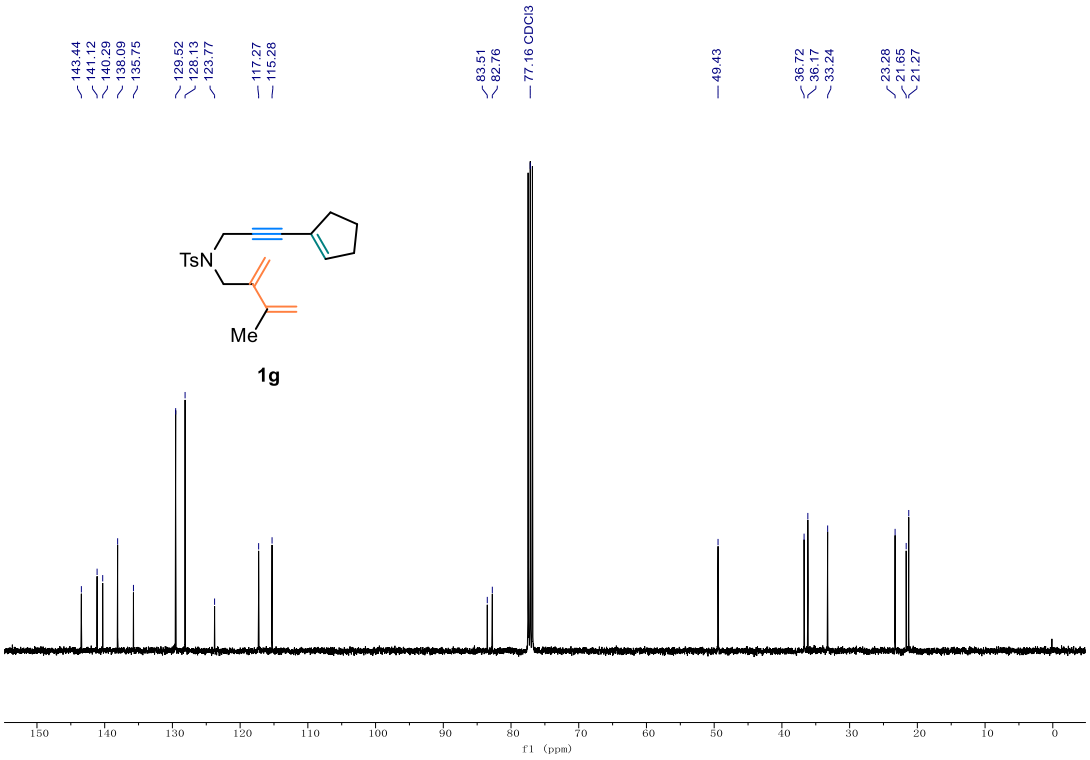
^{1}H NMR of **1f** (400 MHz, CD_2Cl_2)



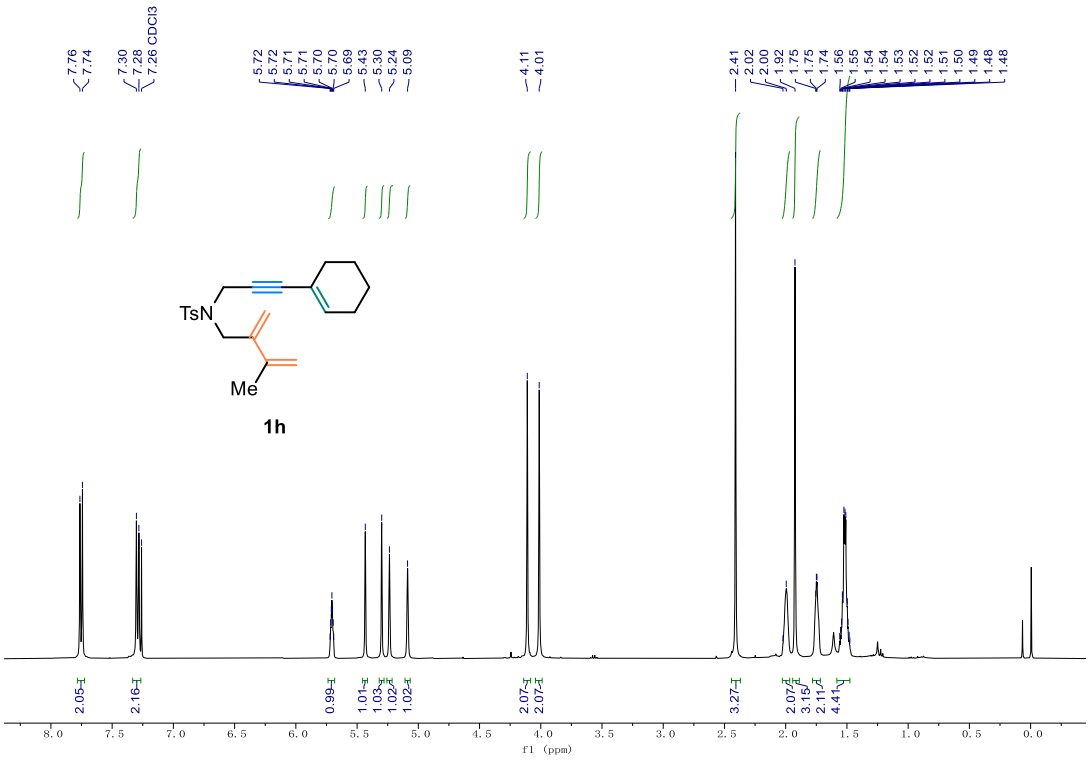
^{13}C{^{1}H} NMR of **1f** (101 MHz, CD_2Cl_2)



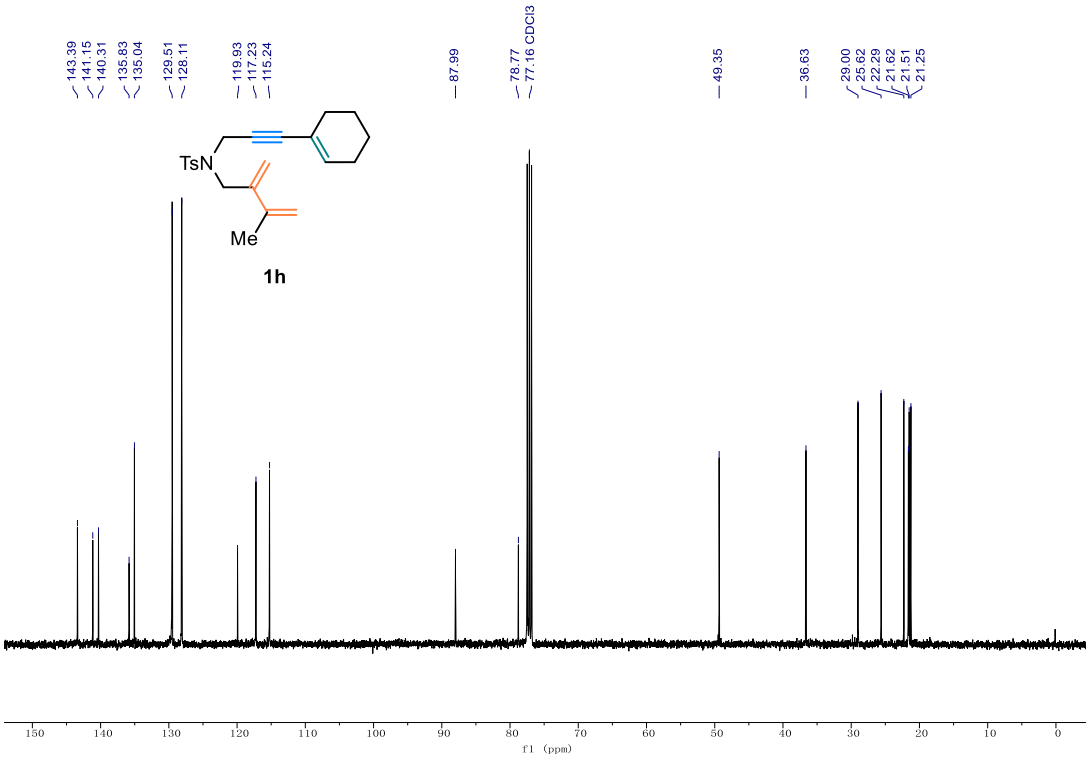
^{1}H NMR of **1g** (400 MHz, $CDCl_3$)



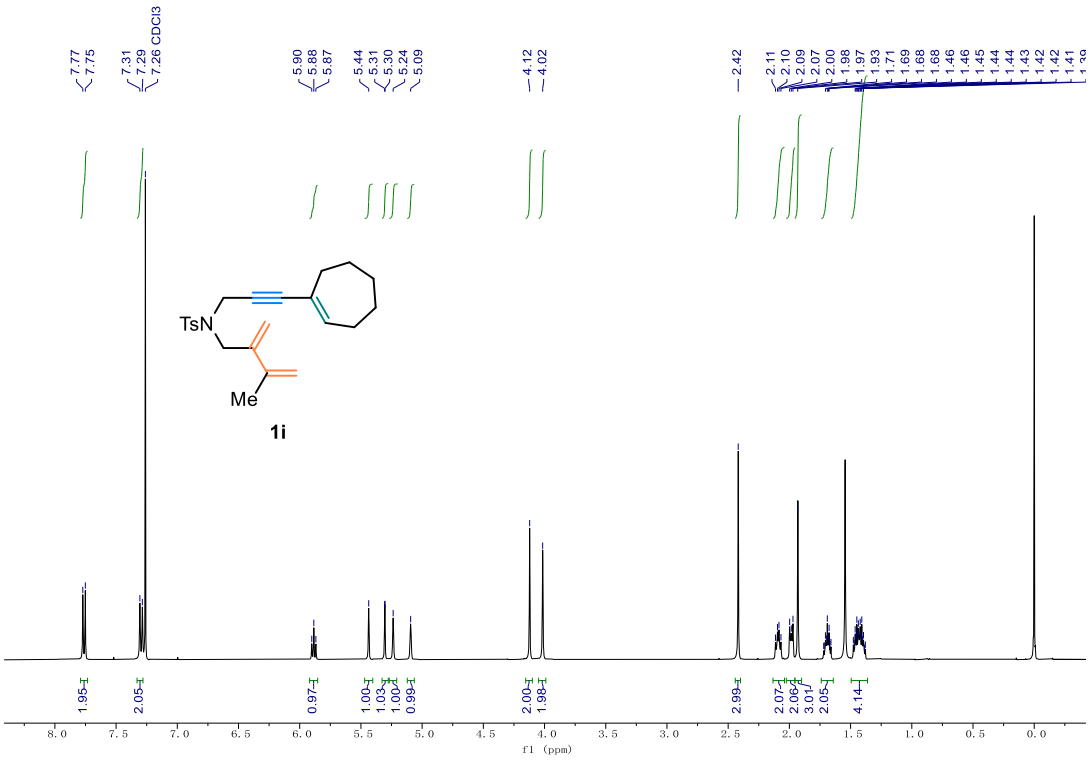
^{13}C{^{1}H} NMR of **1g** (101 MHz, $CDCl_3$)



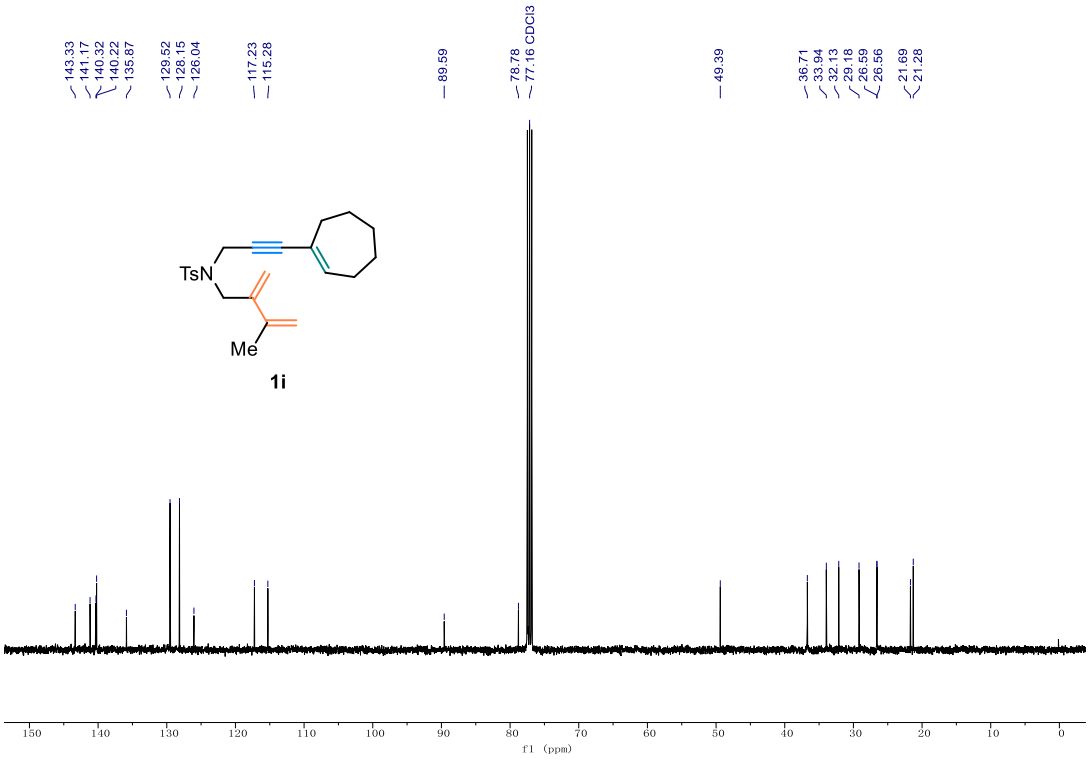
^{1}H NMR of **1h** (400 MHz, $CDCl_3$)



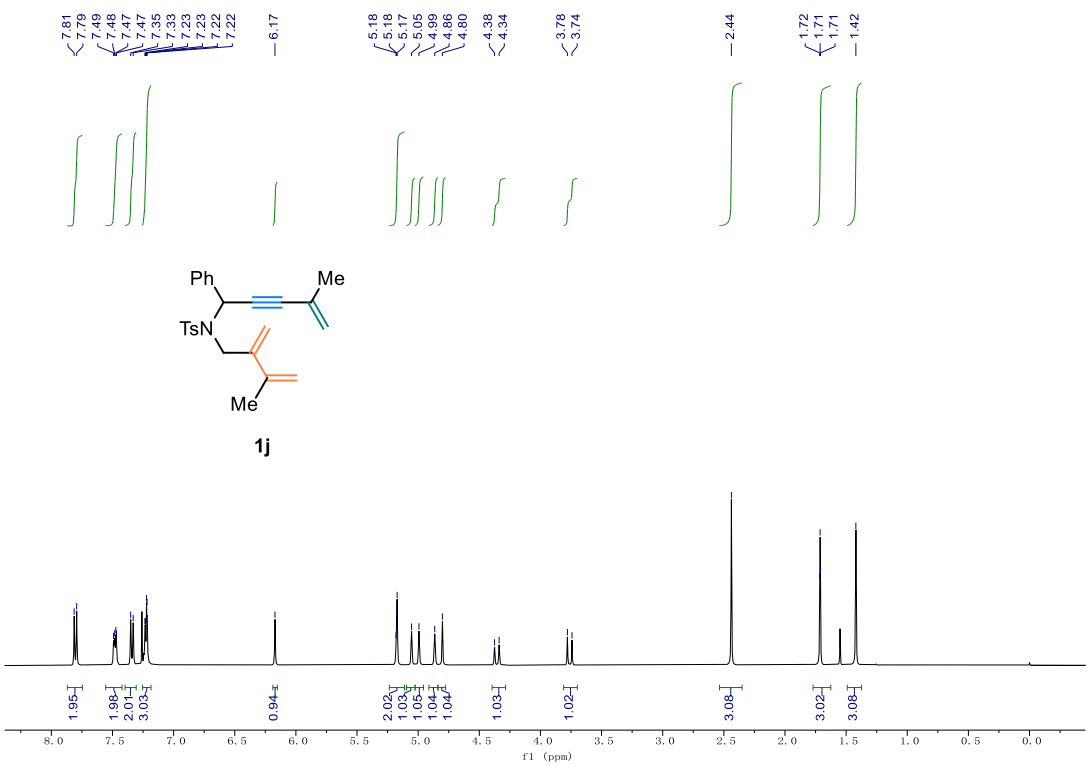
^{13}C{^{1}H} NMR of **1h** (101 MHz, $CDCl_3$)



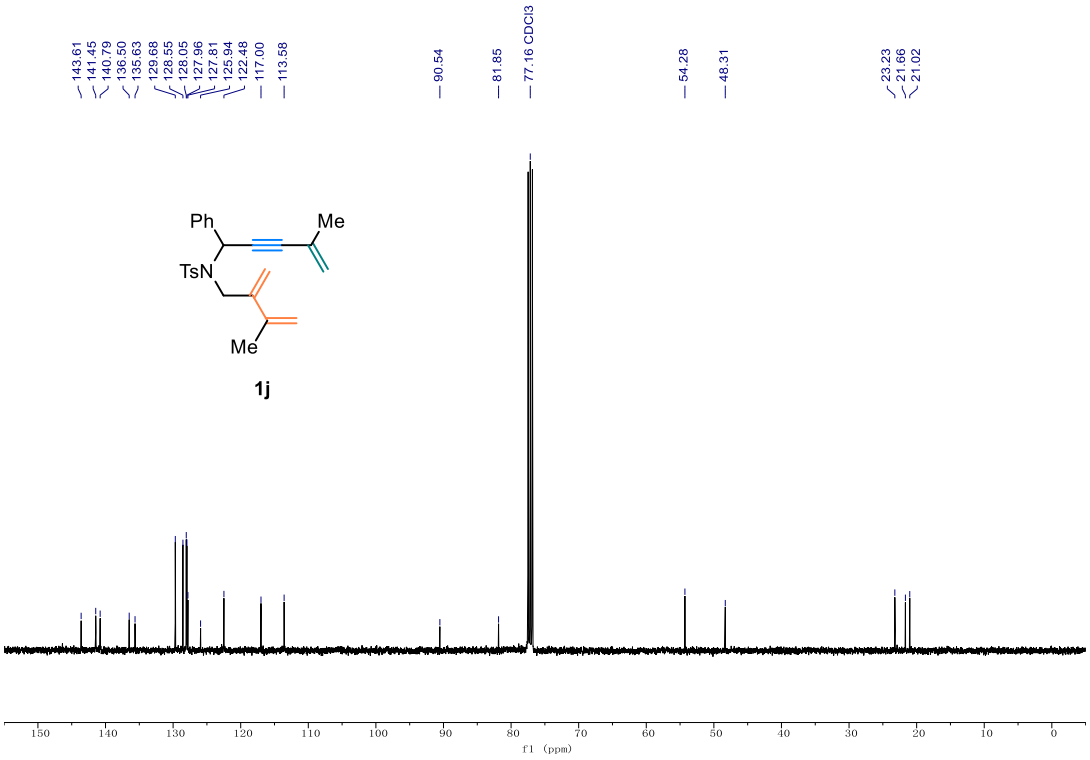
^{1}H NMR of **1i** (400 MHz, $CDCl_3$)



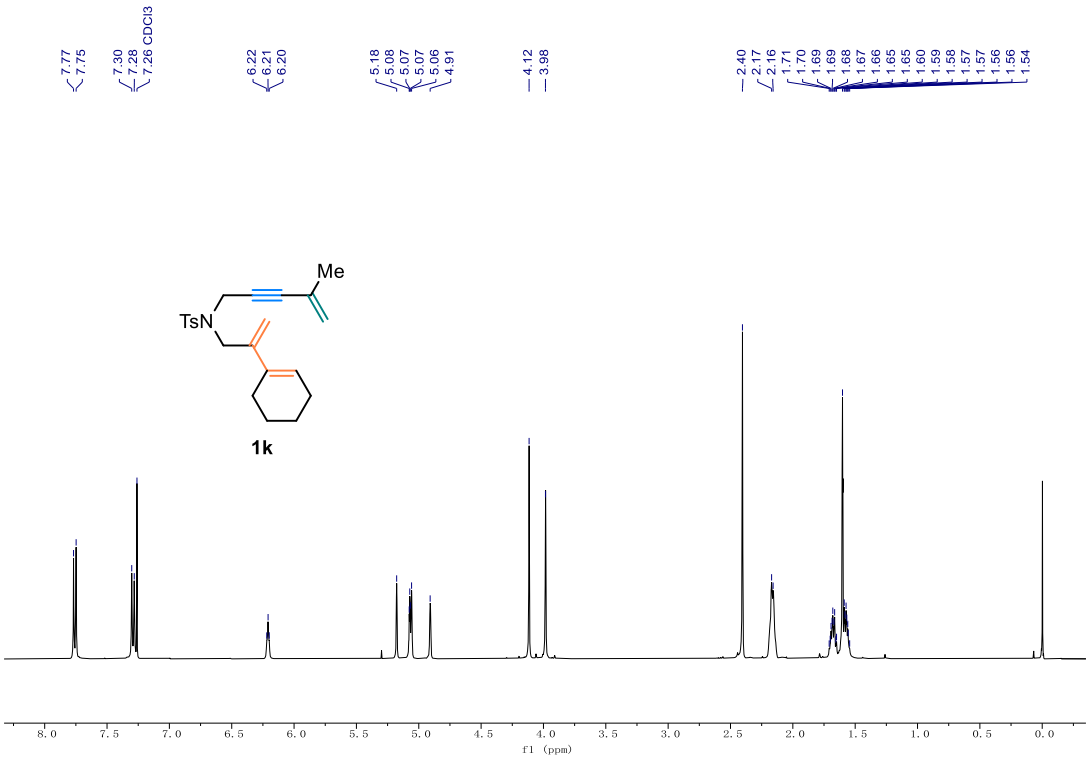
^{13}C{^{1}H} NMR of **1i** (101 MHz, $CDCl_3$)



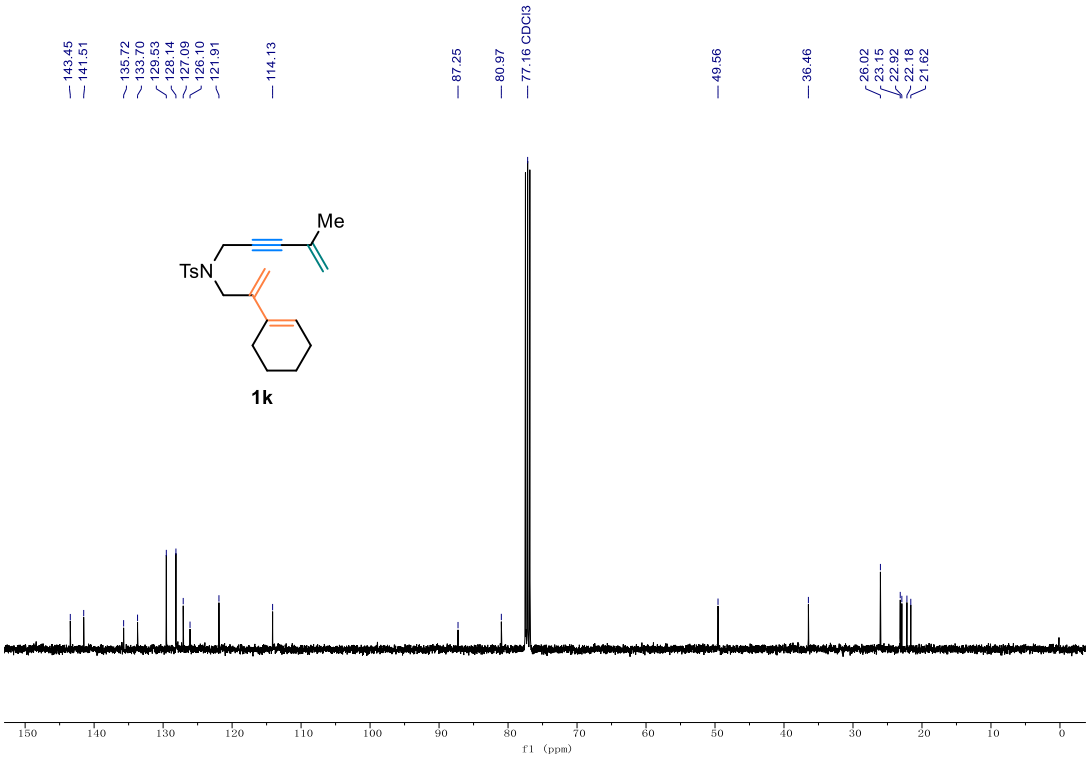
^{1}H NMR of **1j** (400 MHz, $CDCl_3$)



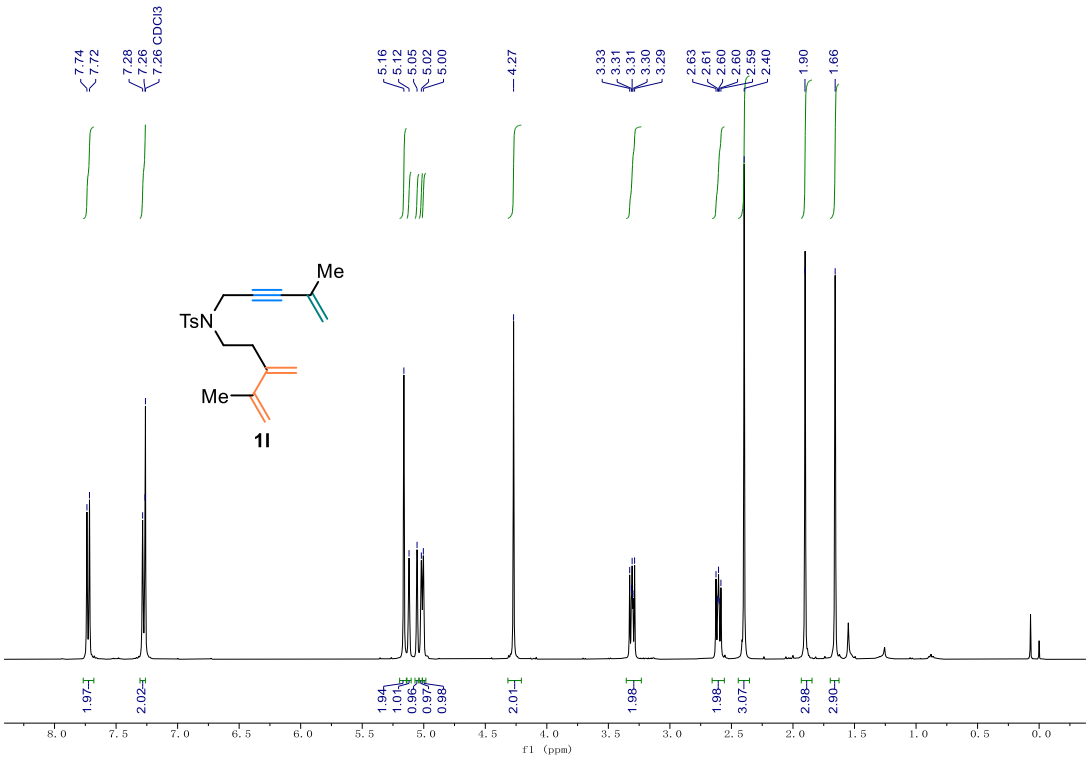
^{13}C{^{1}H} NMR of **1j** (101 MHz, $CDCl_3$)



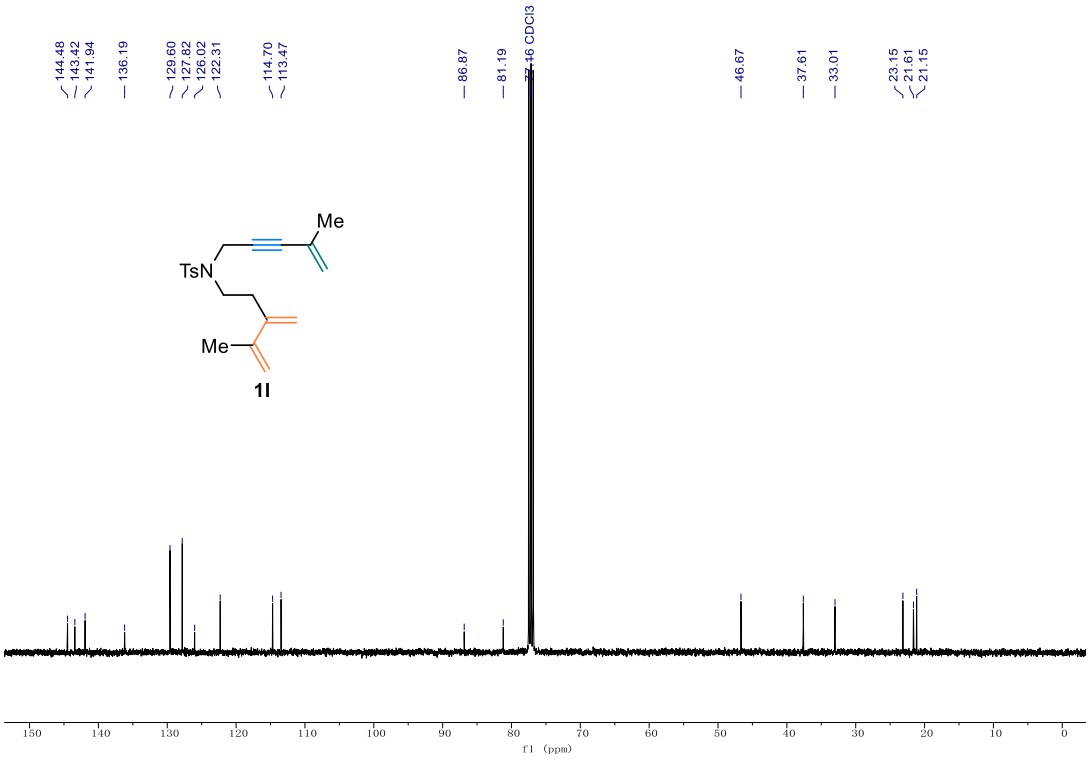
^{1}H NMR of **1k** (400 MHz, $CDCl_3$)



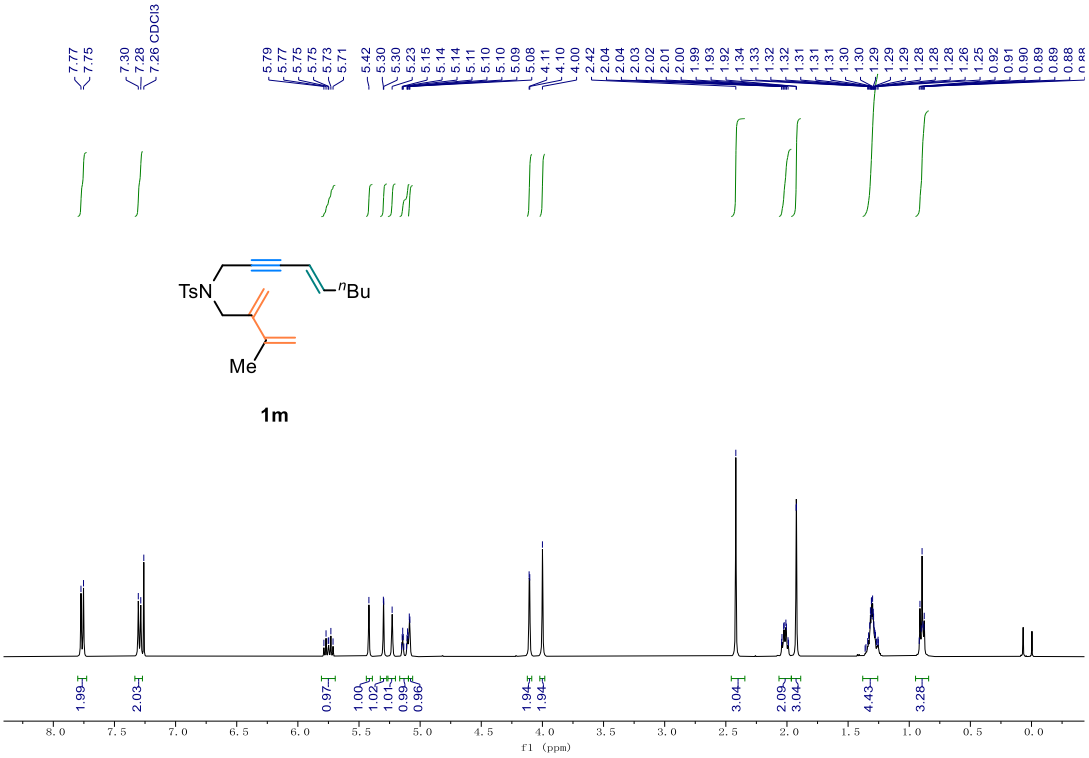
^{13}C{^{1}H} NMR of **1k** (101 MHz, $CDCl_3$)



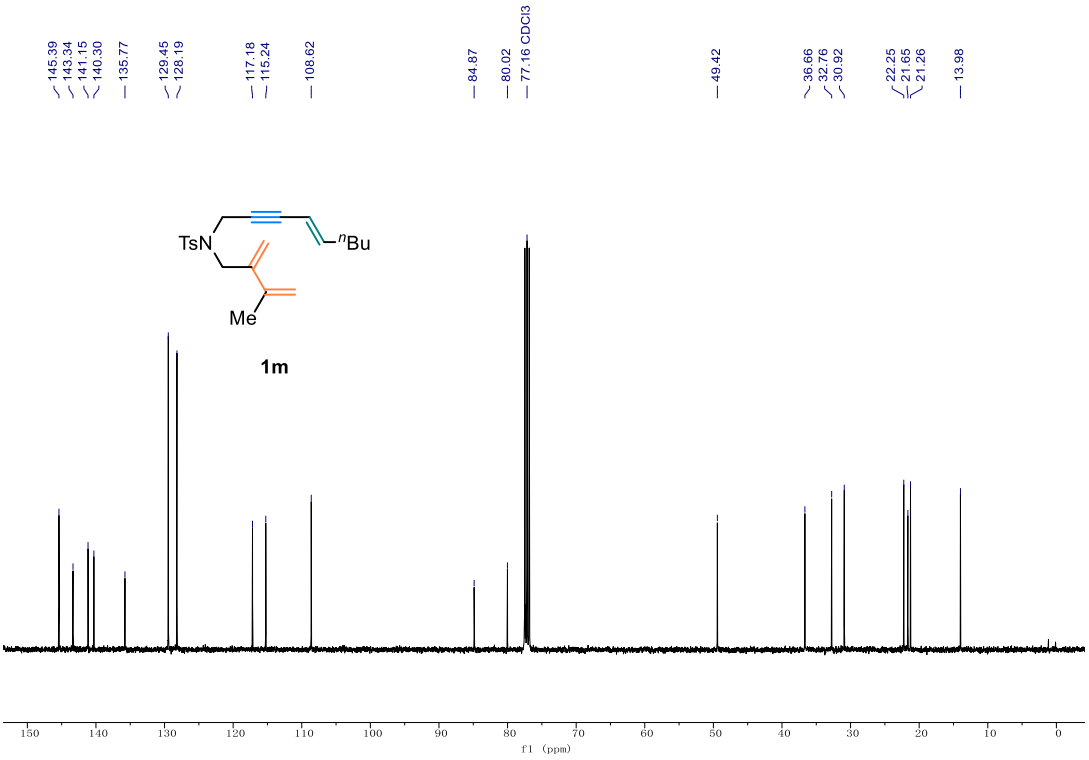
^{1}H NMR of **1l** (400 MHz, $CDCl_3$)



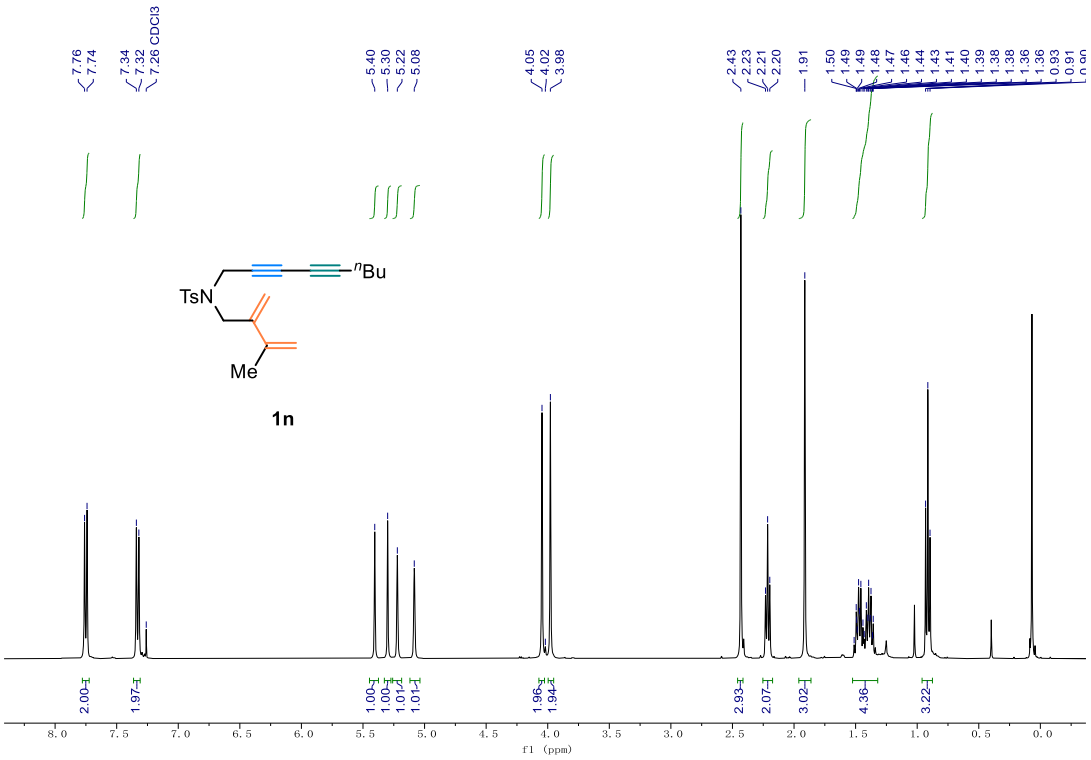
^{13}C{^{1}H} NMR of **1l** (101 MHz, $CDCl_3$)



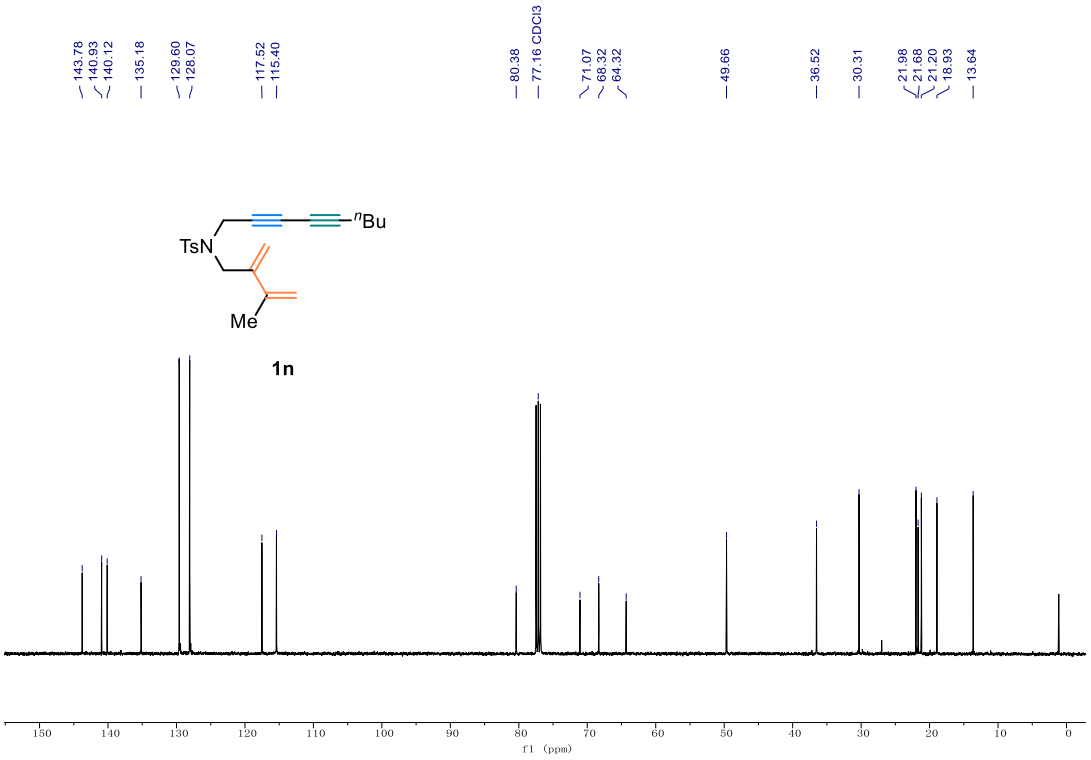
^{1}H NMR of **1m** (400 MHz, $CDCl_3$)



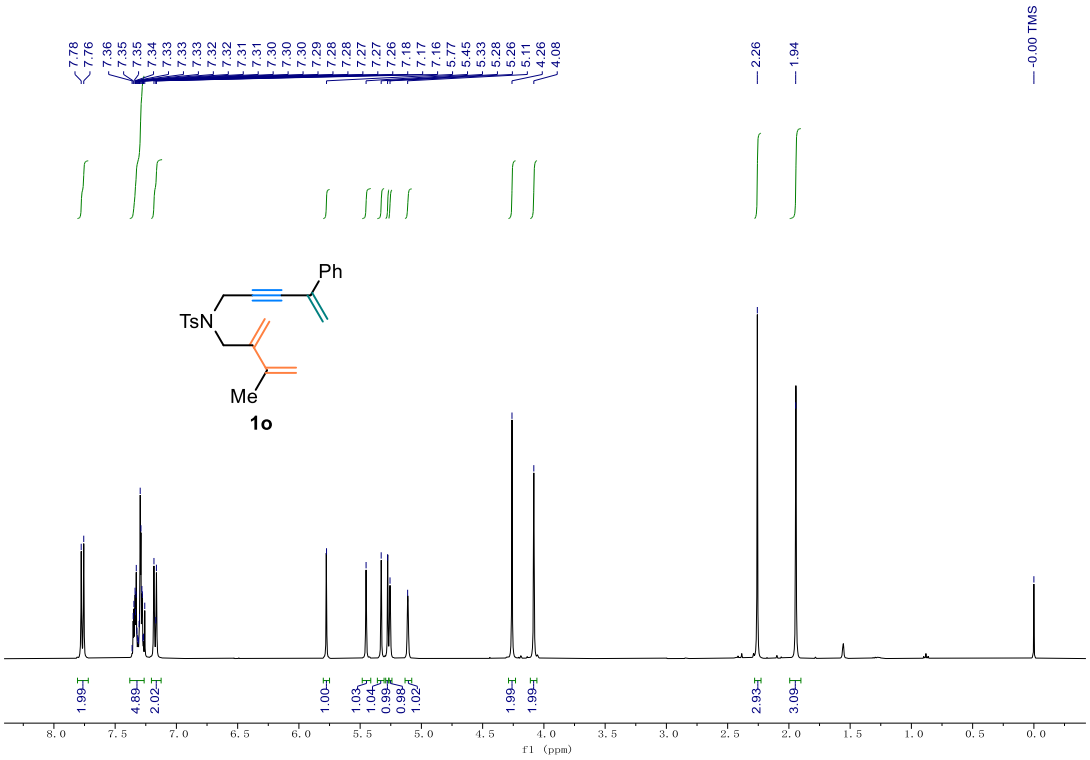
^{13}C{^{1}H} NMR of **1m** (101 MHz, $CDCl_3$)



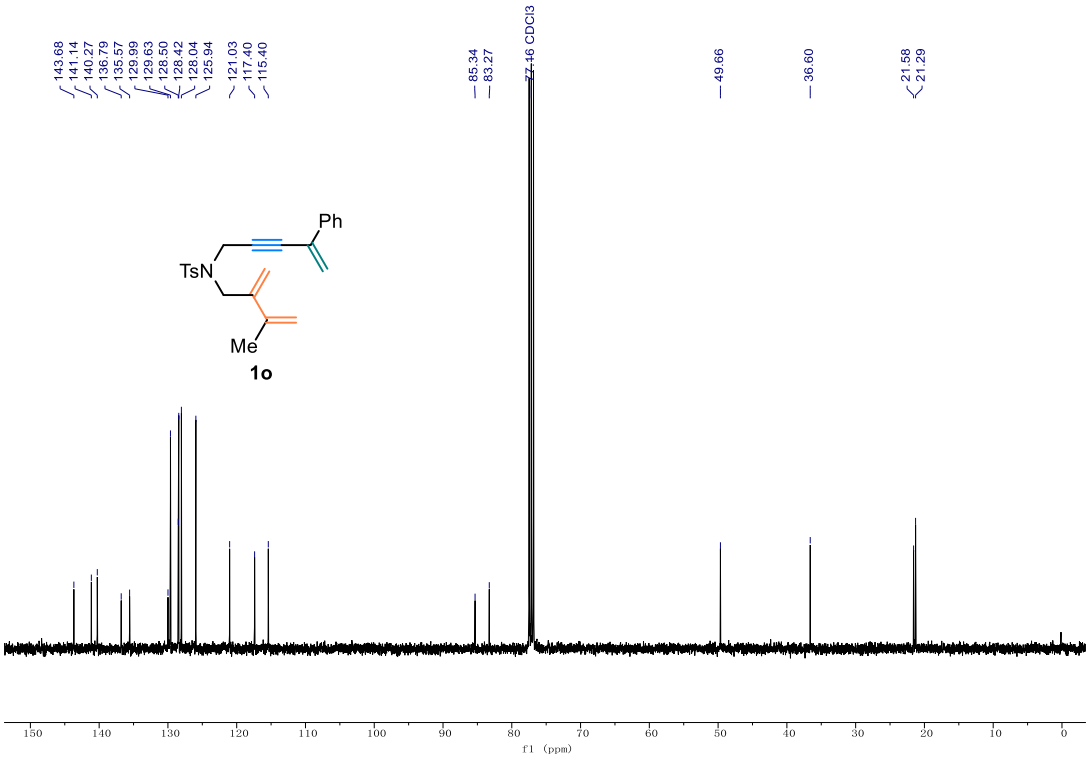
^{1}H NMR of **1n** (400 MHz, $CDCl_3$)



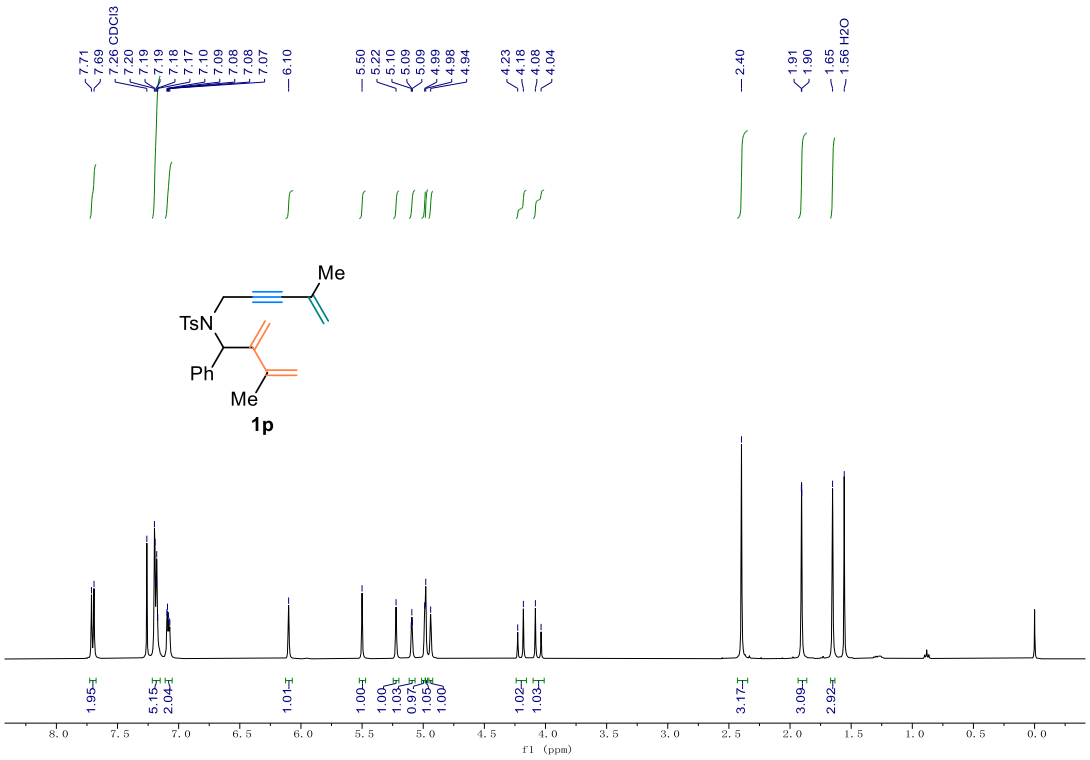
^{13}C{^{1}H} NMR of **1n** (101 MHz, $CDCl_3$)



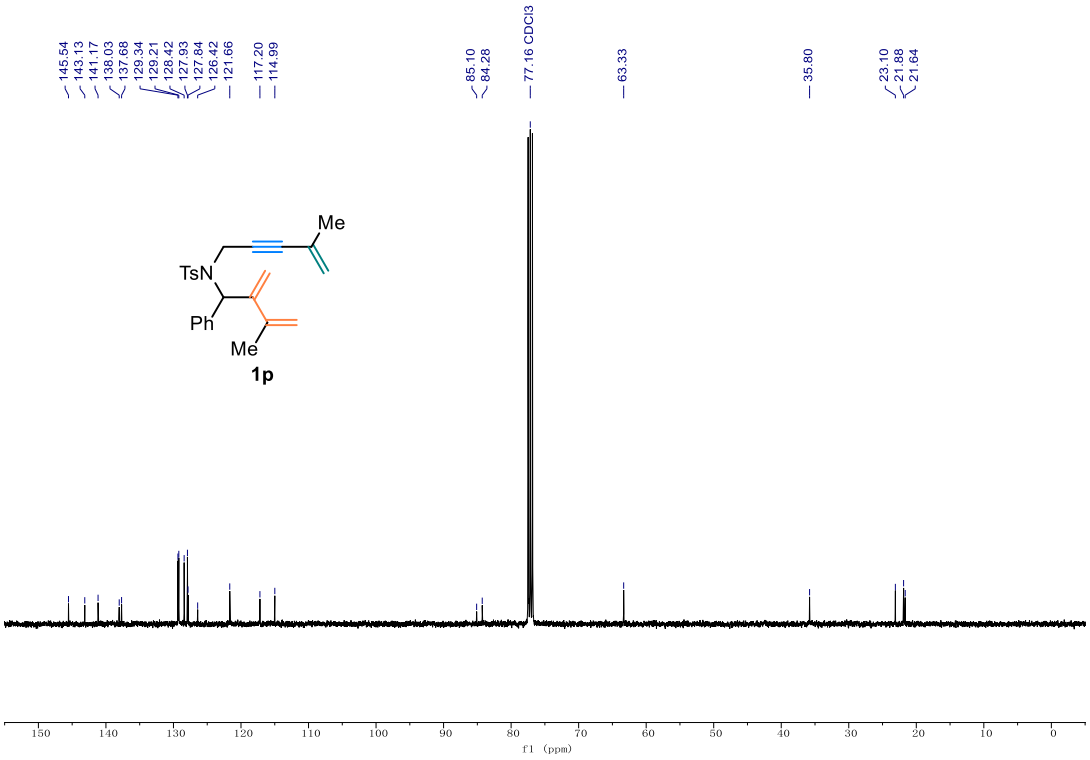
^{1}H NMR of **1o** (400 MHz, $CDCl_3$)



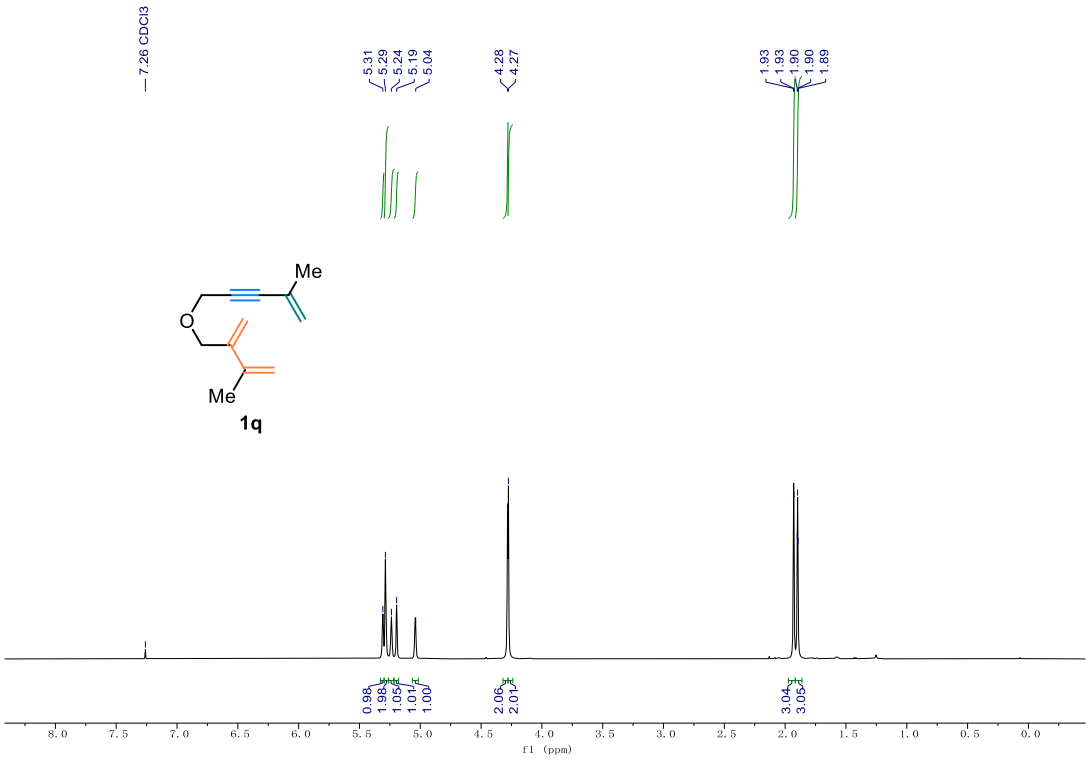
^{13}C{^{1}H} NMR of **1o** (101 MHz, $CDCl_3$)



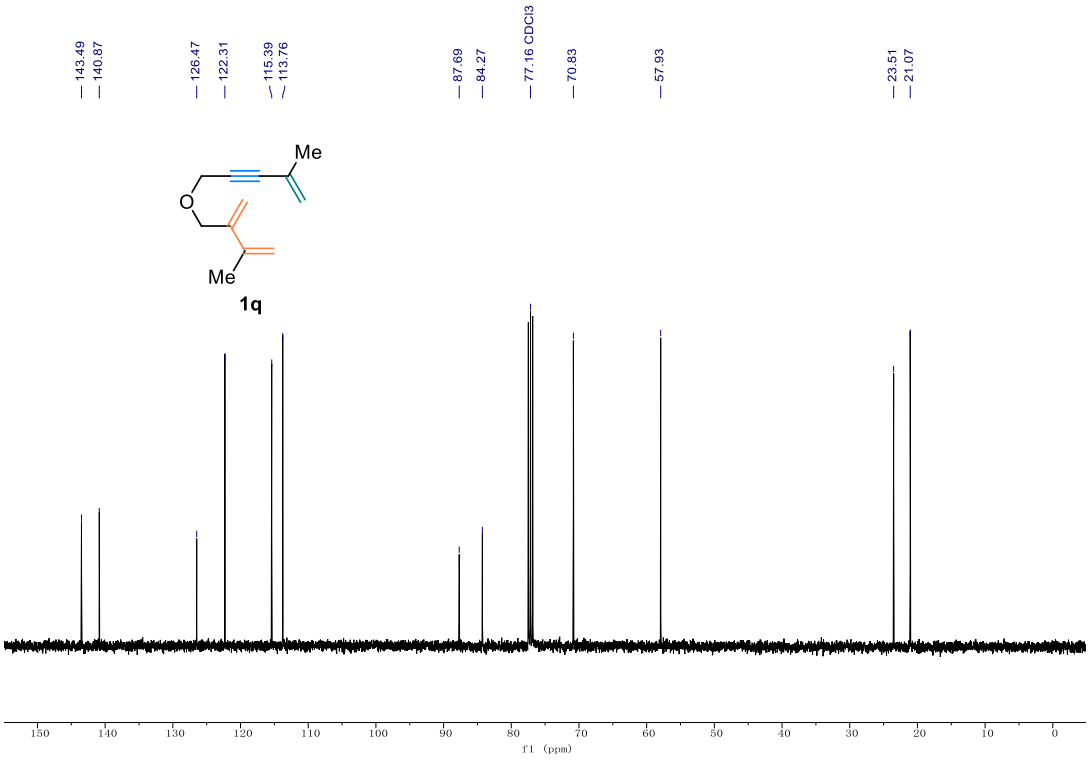
^{1}H NMR of **1p** (400 MHz, $CDCl_3$)



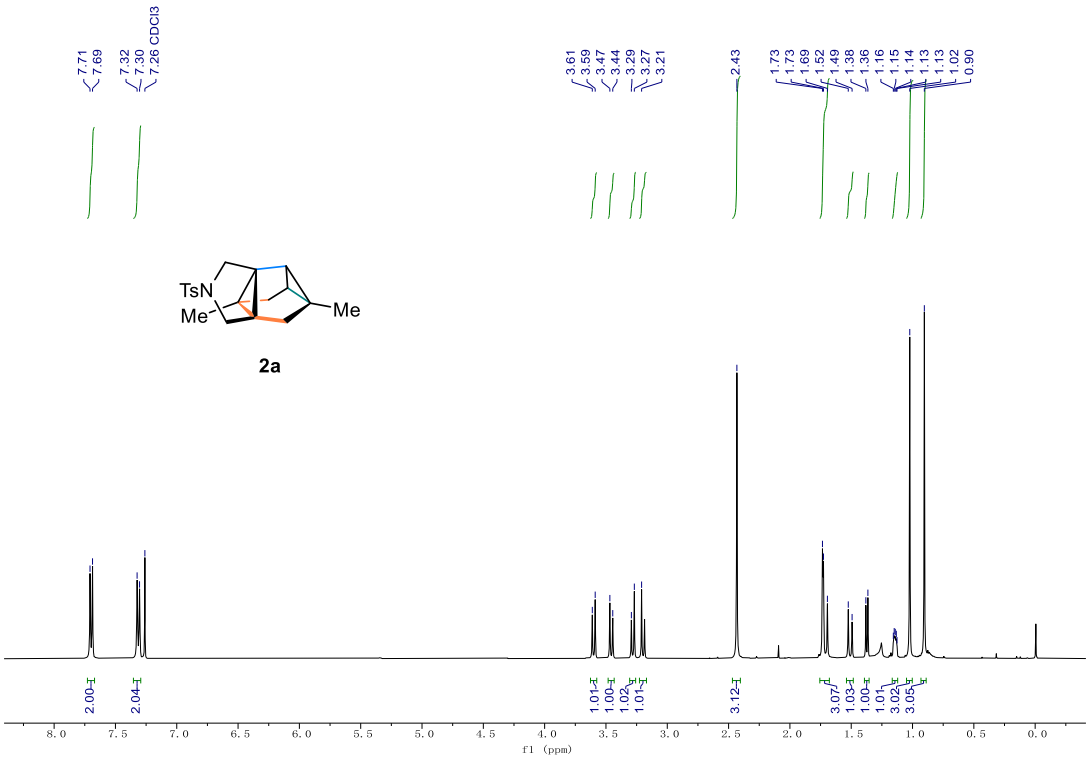
^{13}C{^{1}H} NMR of **1p** (101 MHz, $CDCl_3$)



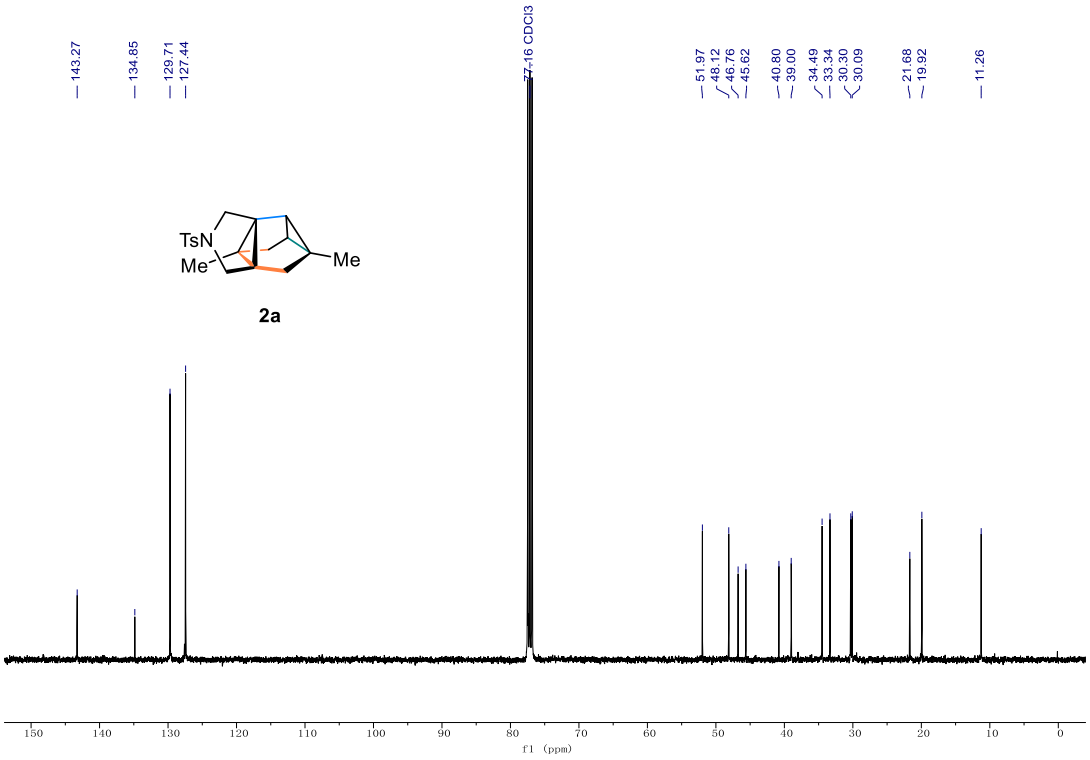
^{1}H NMR of **1q** (400 MHz, $CDCl_3$)



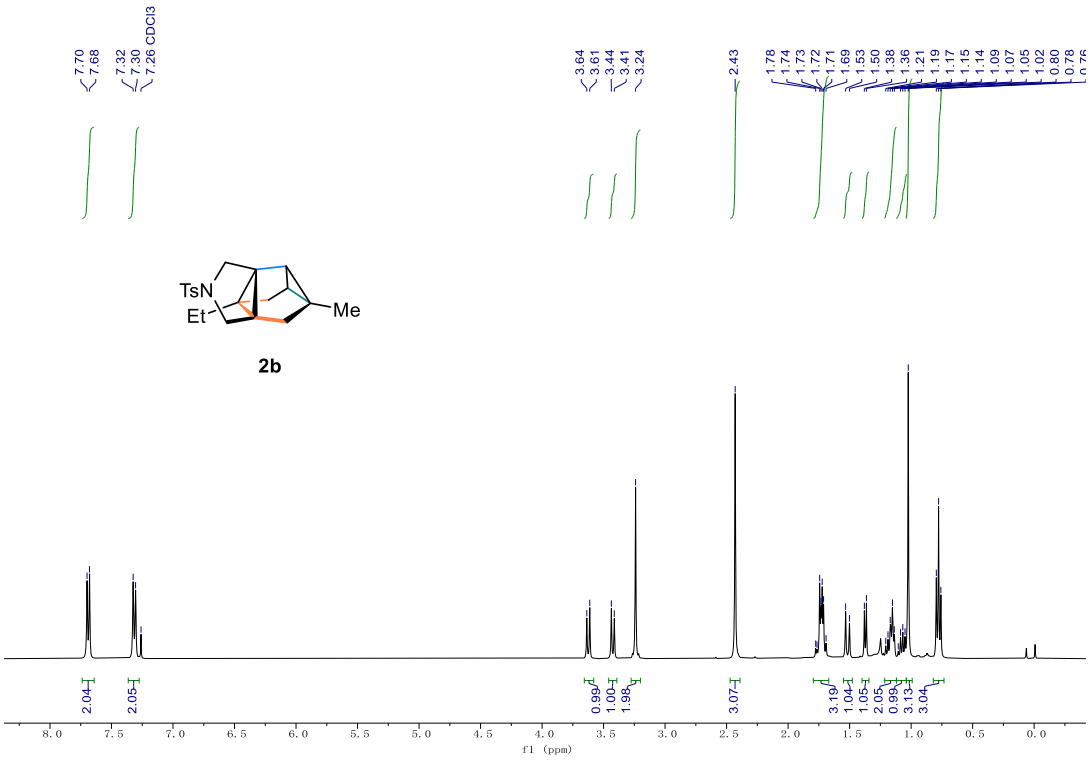
^{13}C{^{1}H} NMR of **1q** (101 MHz, $CDCl_3$)



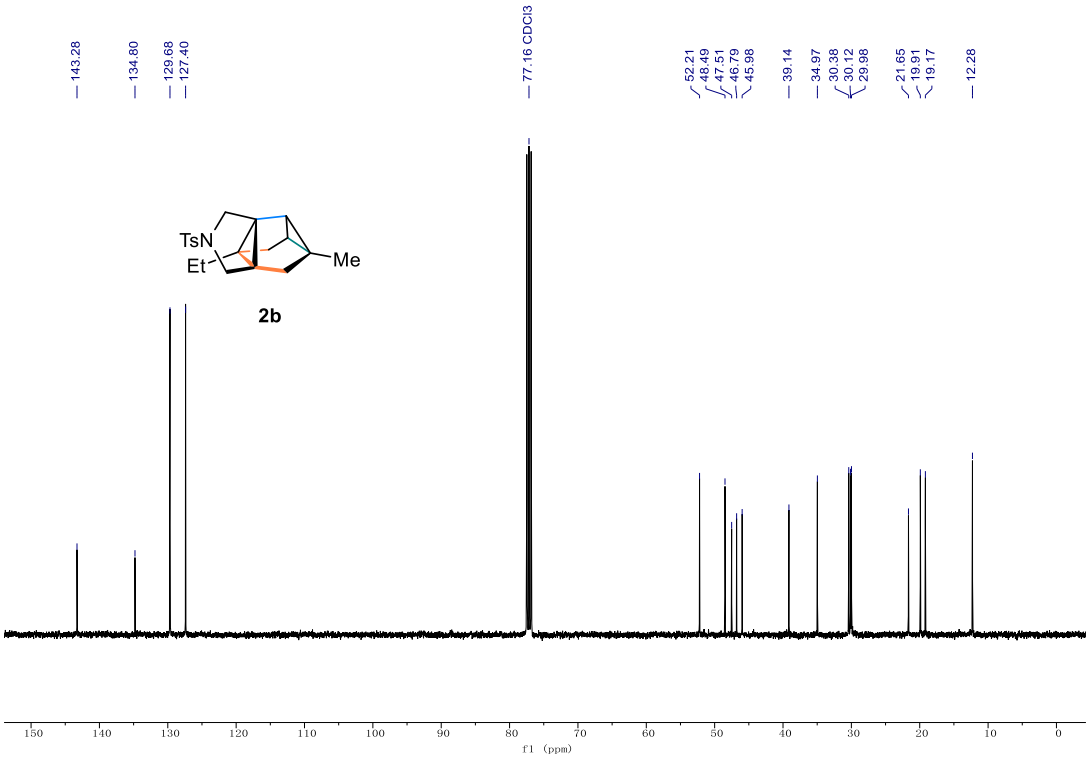
^{1}H NMR of **2a** (400 MHz, $CDCl_3$)



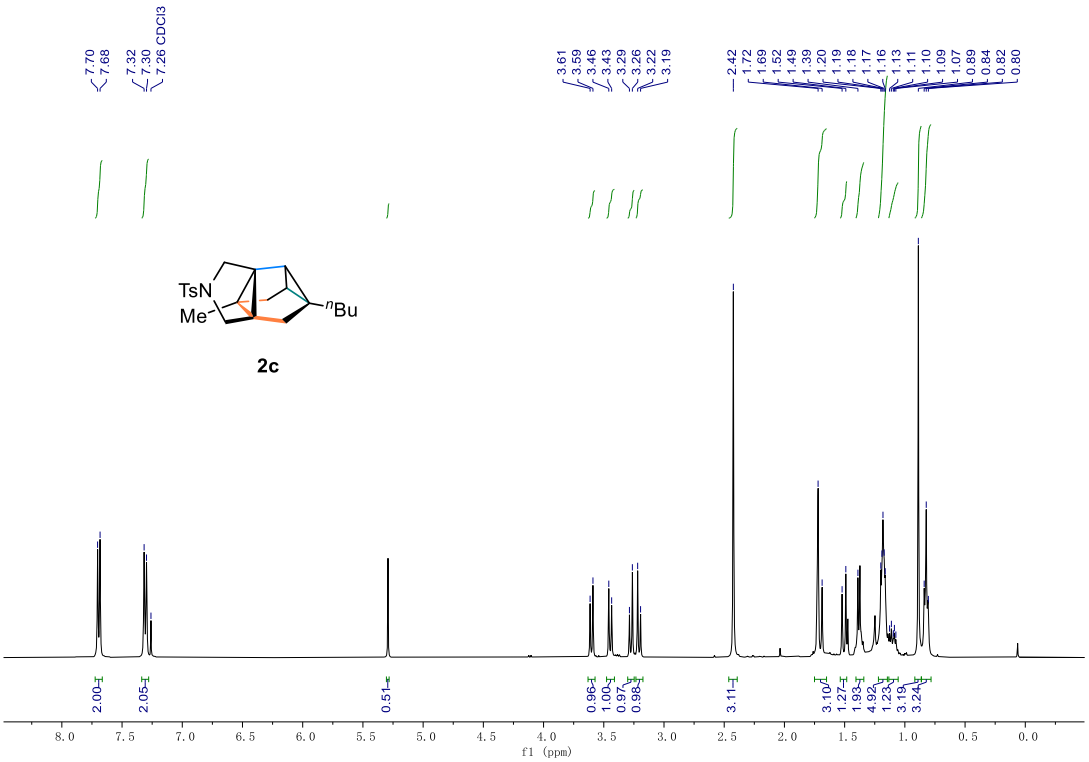
^{13}C{^{1}H} NMR of **2a** (101 MHz, $CDCl_3$)



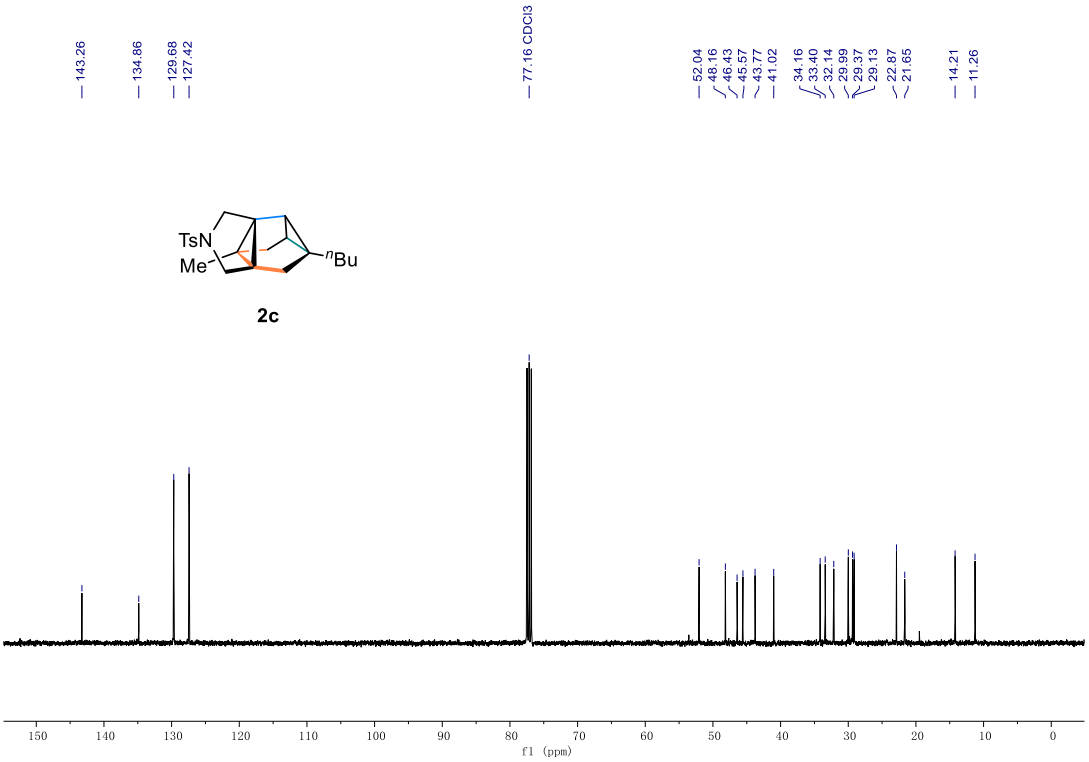
^{1}H NMR of **2b** (400 MHz, $CDCl_3$)



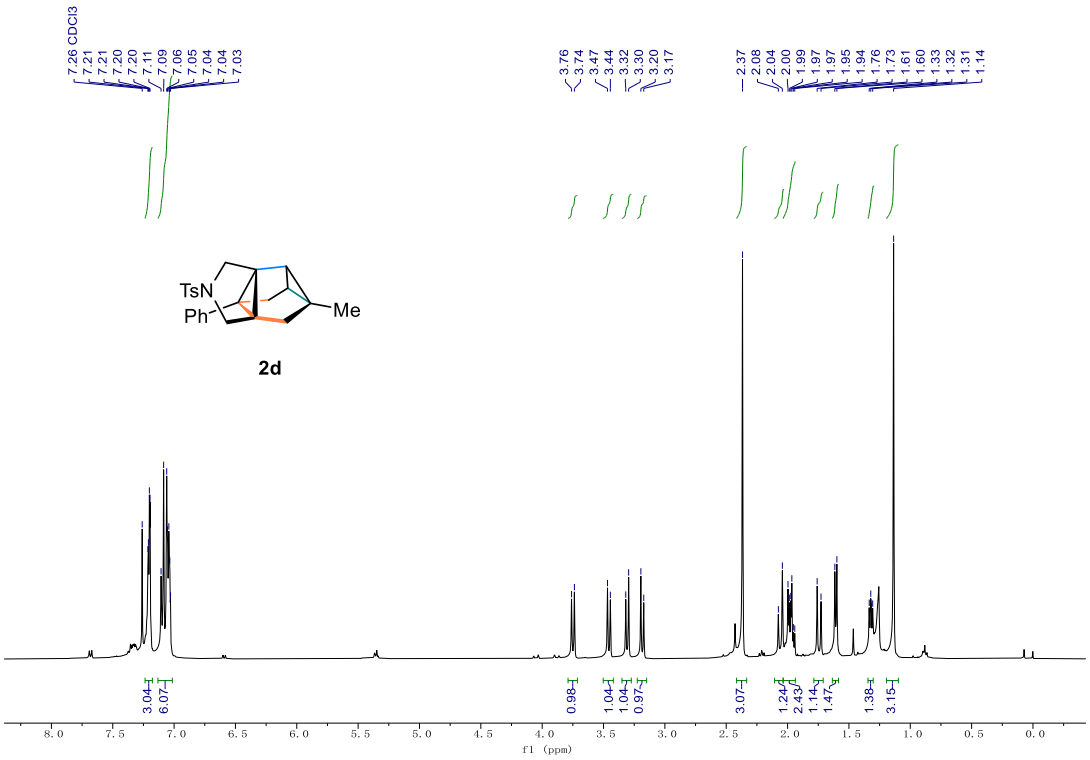
^{13}C{^{1}H} NMR of **2b** (101 MHz, $CDCl_3$)



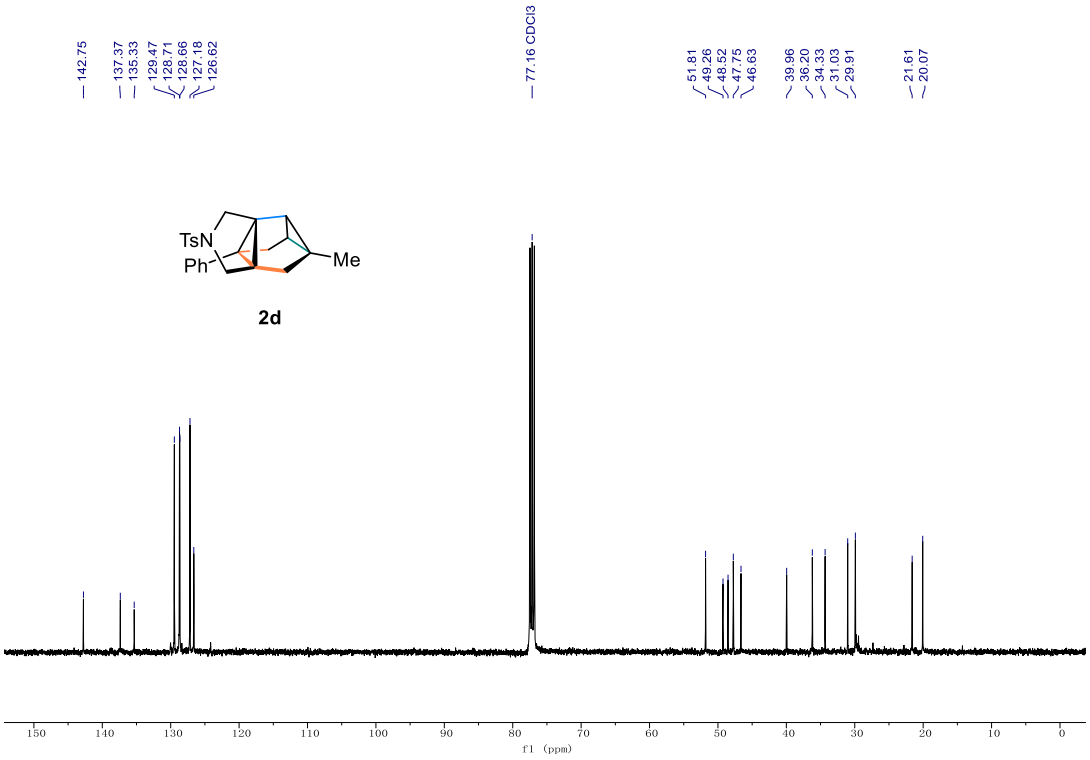
^{1}H NMR of **2c** (400 MHz, $CDCl_3$)



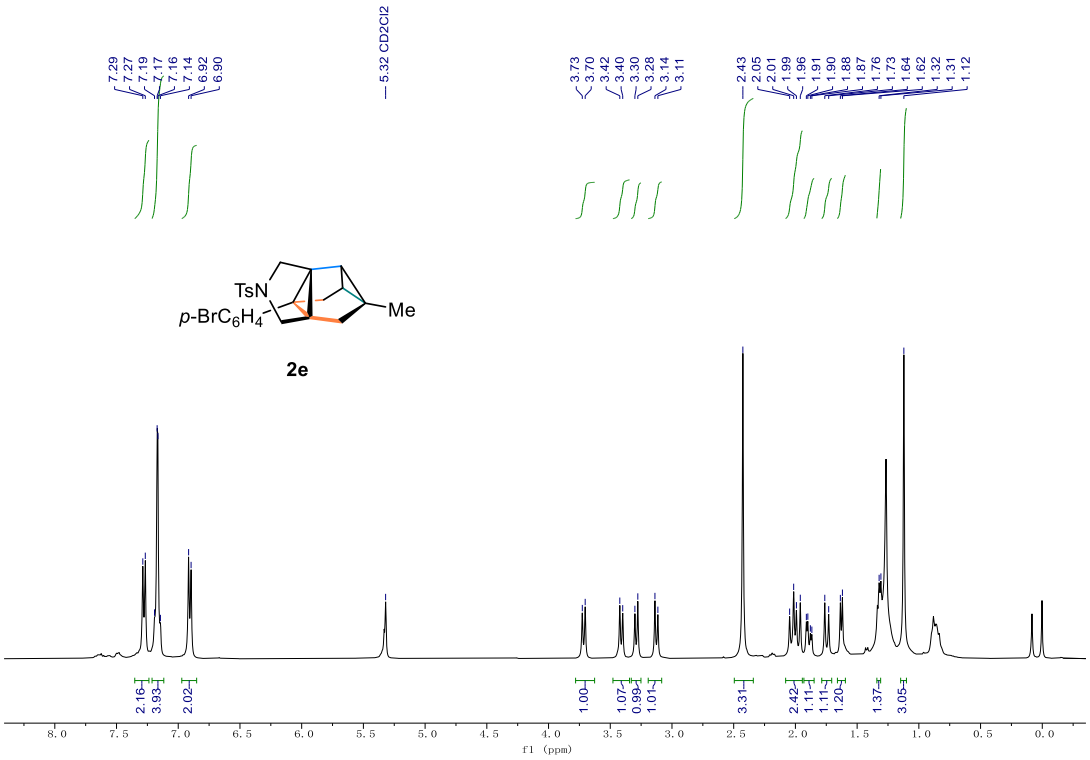
^{13}C{^{1}H} NMR of **2c** (101 MHz, $CDCl_3$)



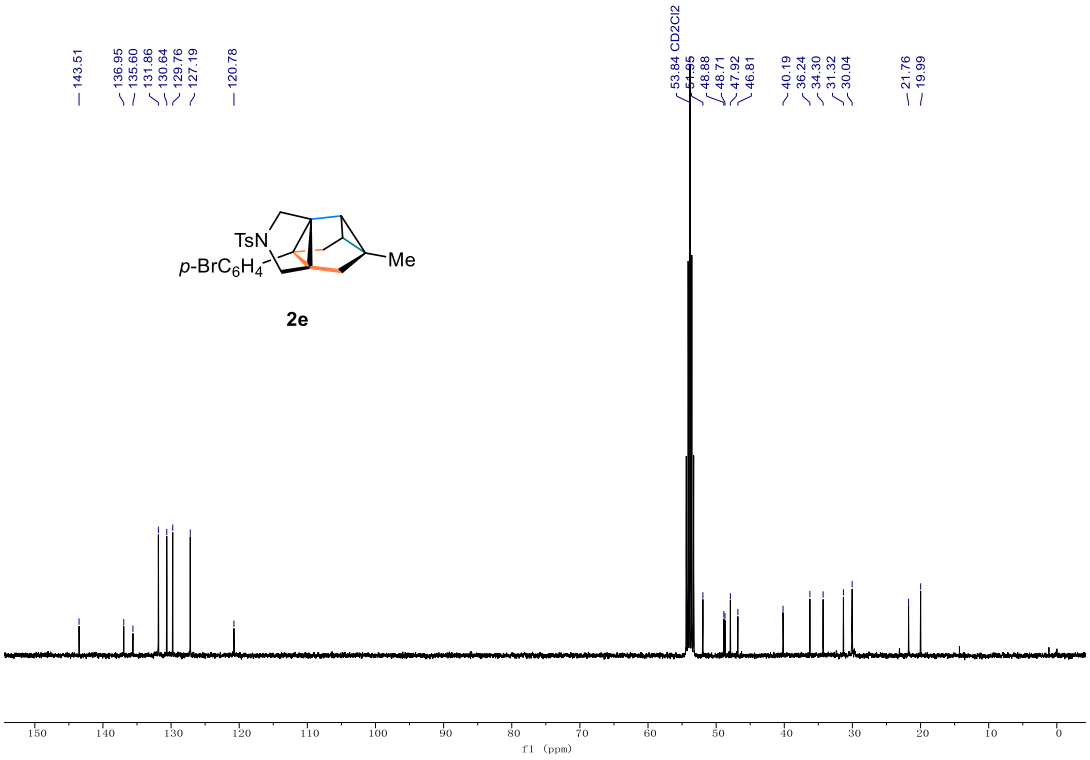
^{1}H NMR of **2d** (400 MHz, $CDCl_3$)



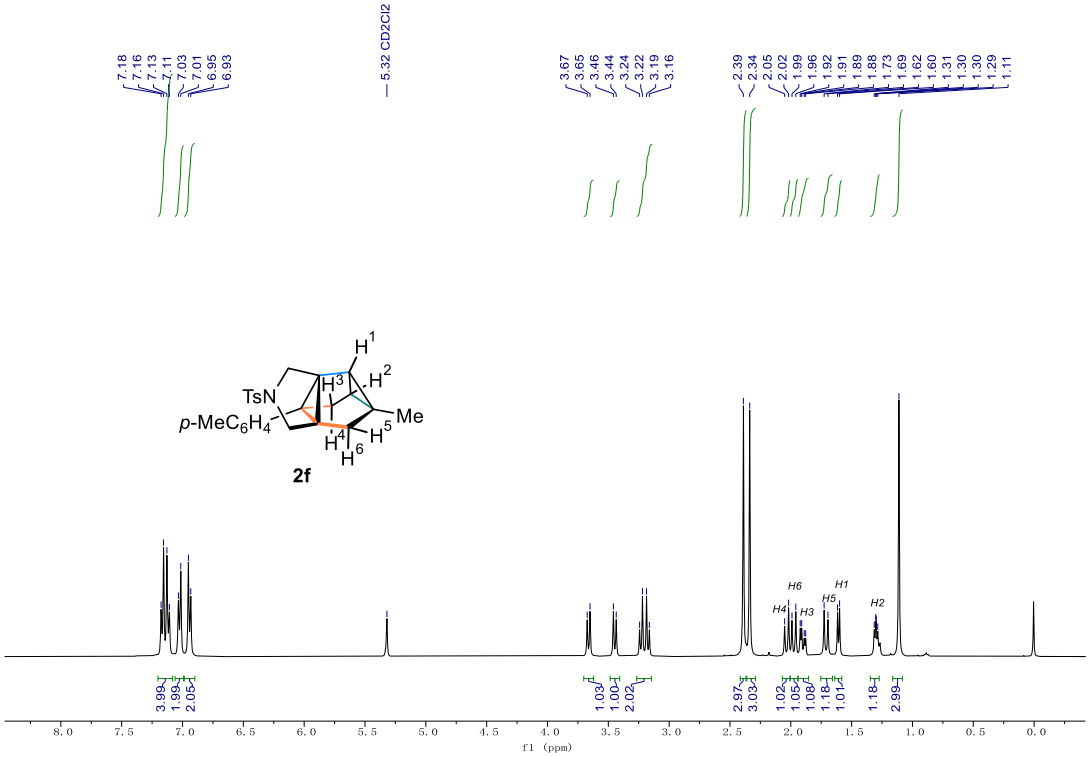
^{13}C{^{1}H} NMR of **2d** (101 MHz, $CDCl_3$)



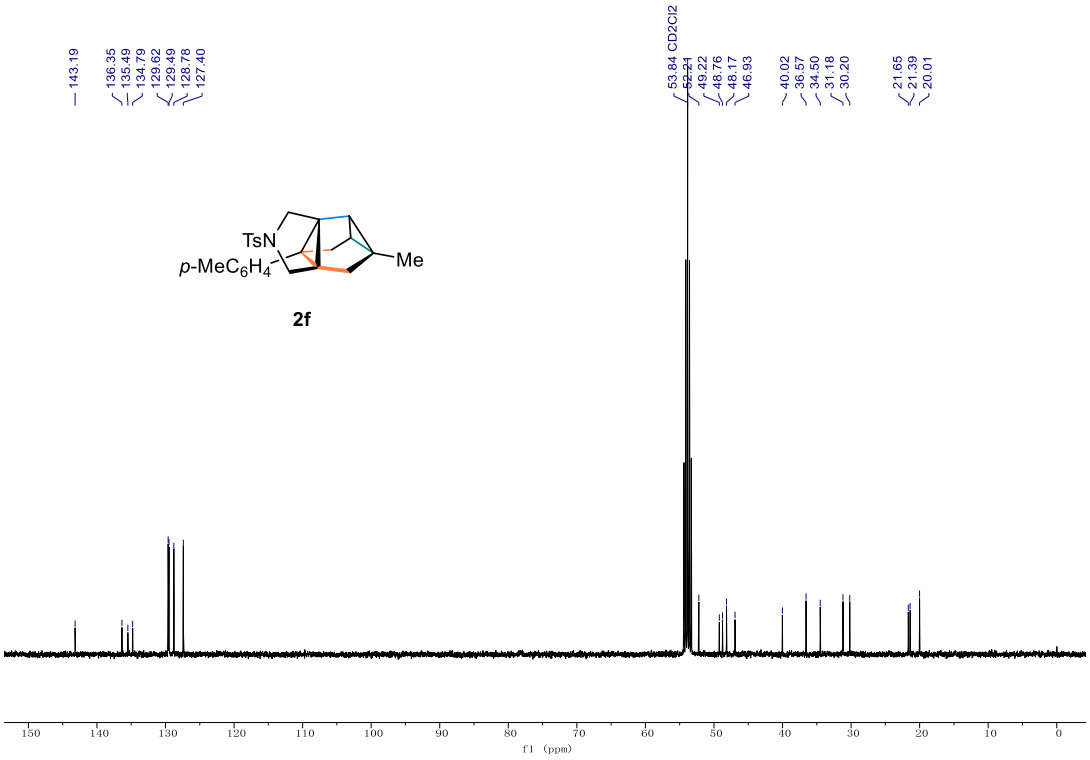
^{1}H NMR of **2e** (400 MHz, CD_2Cl_2)



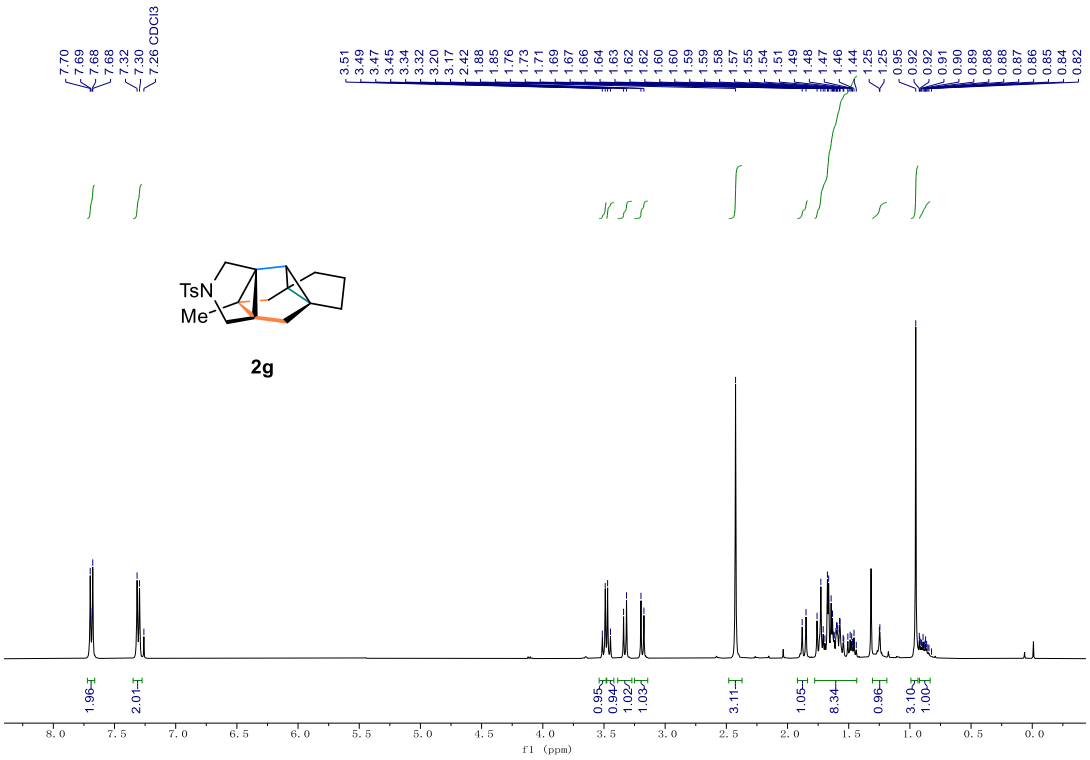
^{13}C{^{1}H} NMR of **2e** (101 MHz, CD_2Cl_2)



^{1}H NMR of **2f** (400 MHz, CD_2Cl_2)

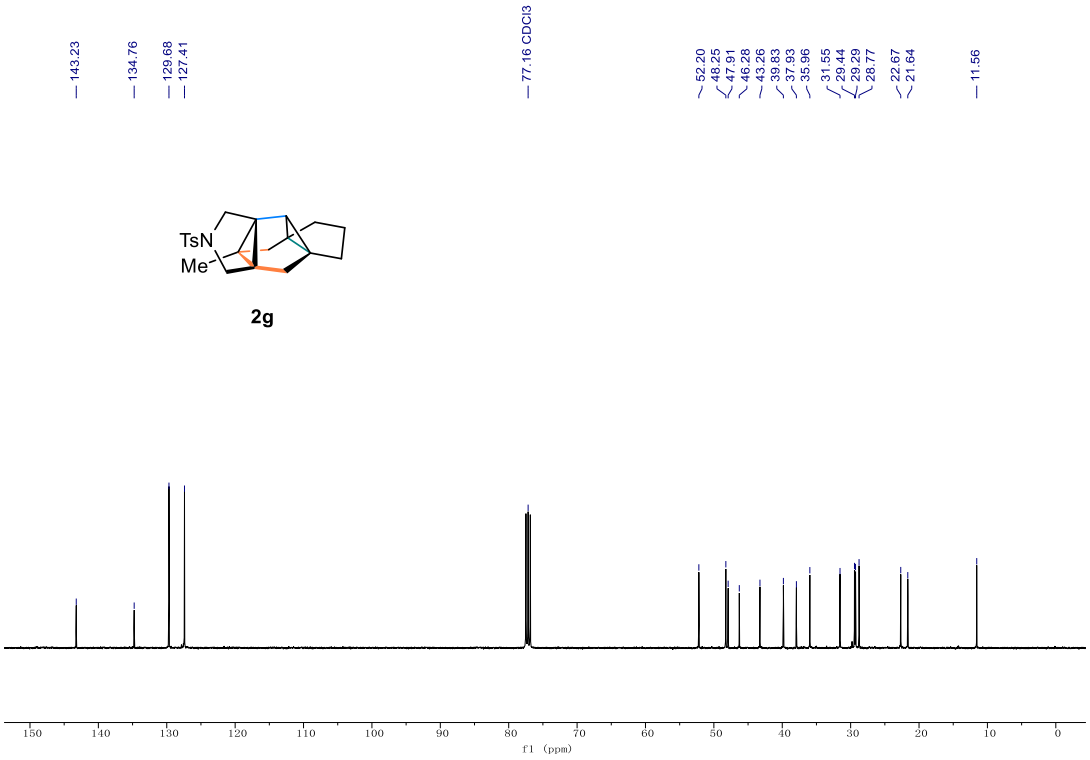


^{13}C{^{1}H} NMR of **2f** (101 MHz, CD_2Cl_2)



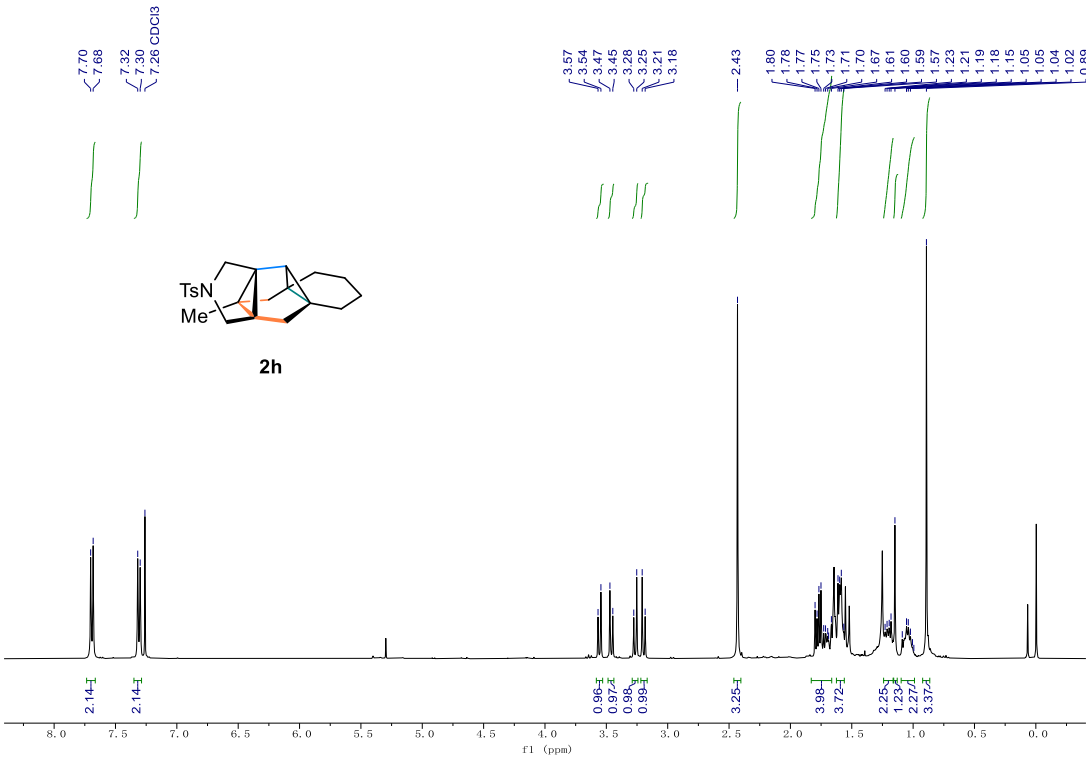
2g

^{1}H NMR of **2g** (400 MHz, $CDCl_3$)

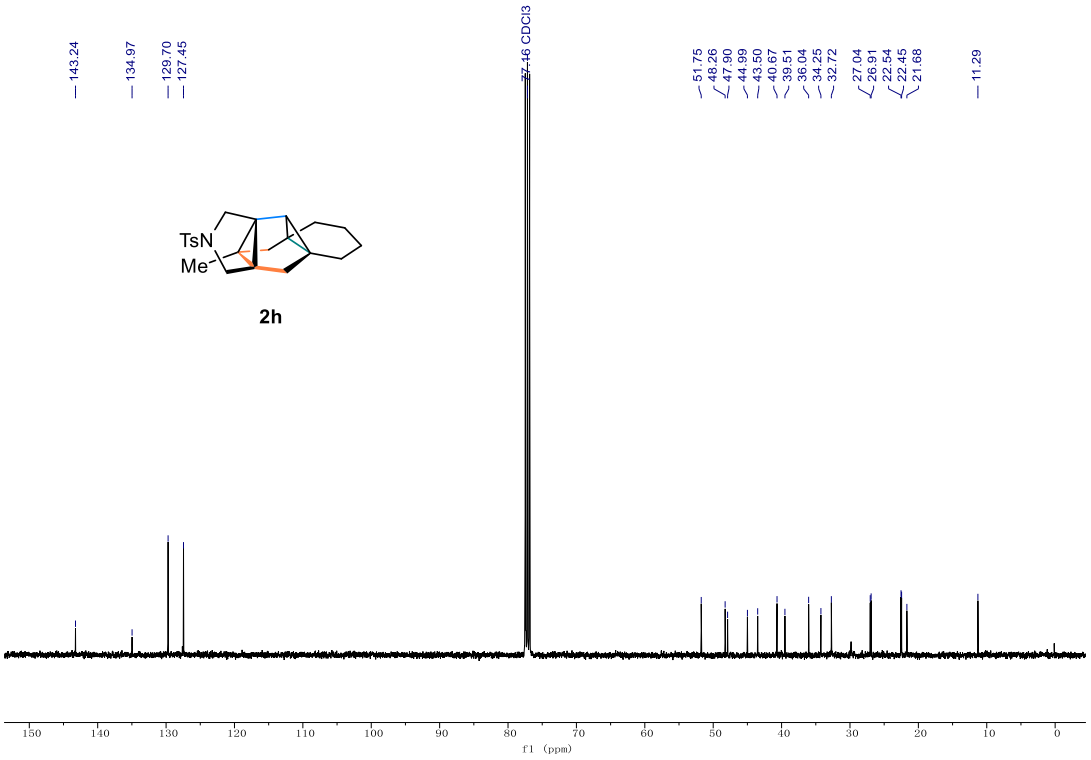


2g

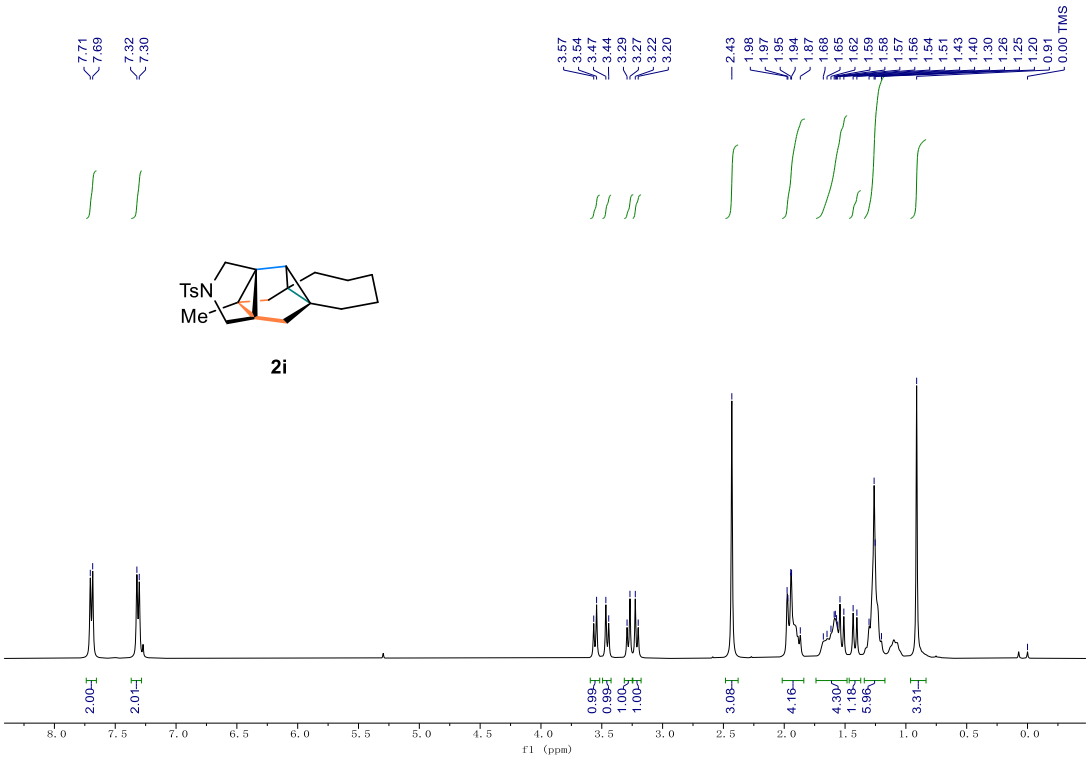
^{13}C{^{1}H} NMR of **2g** (101 MHz, $CDCl_3$)



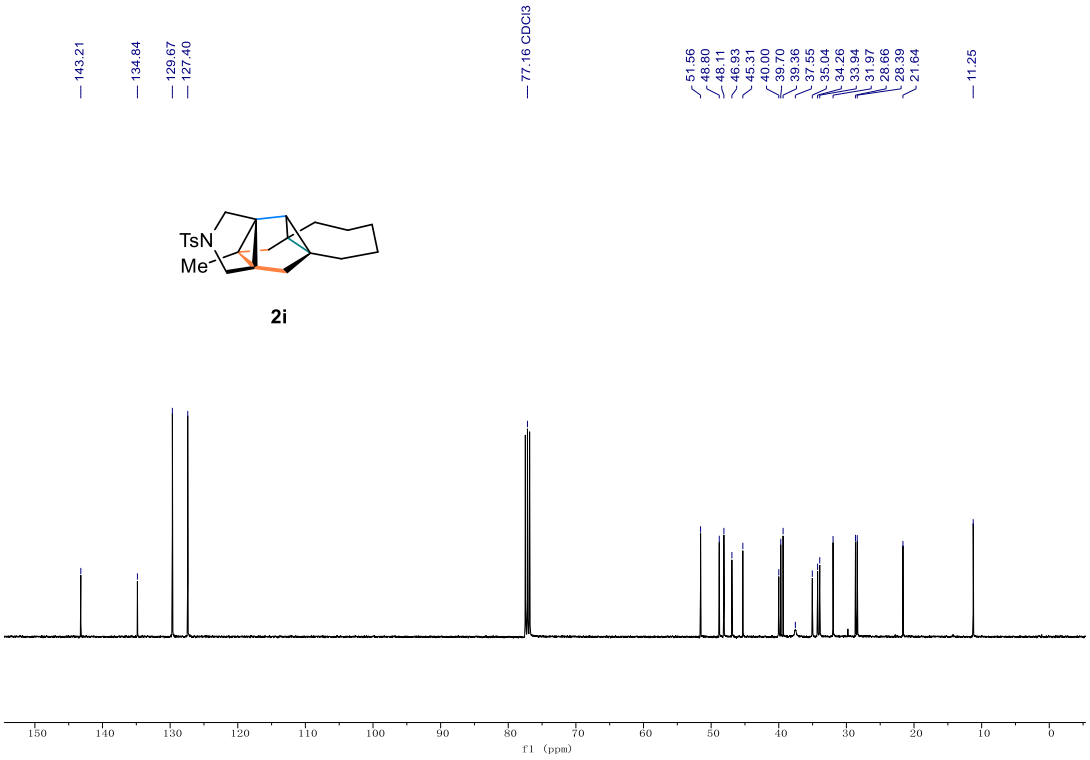
^{1}H NMR of **2h** (400 MHz, $CDCl_3$)



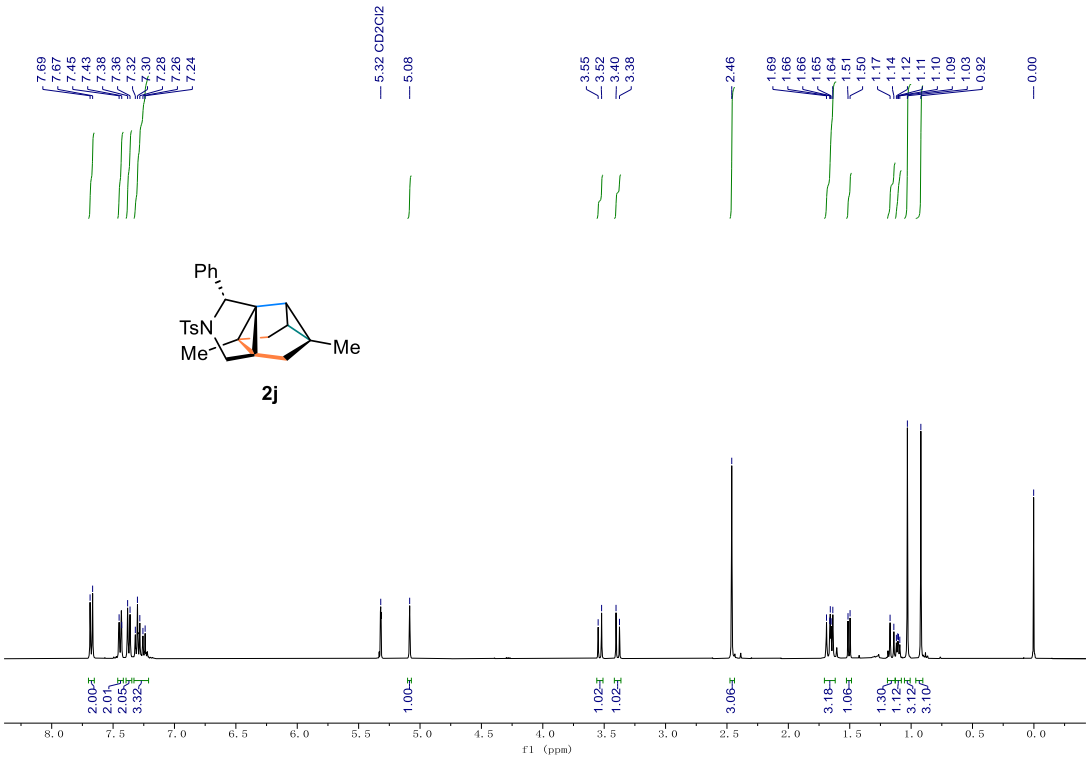
^{13}C{^{1}H} NMR of **2h** (101 MHz, $CDCl_3$)



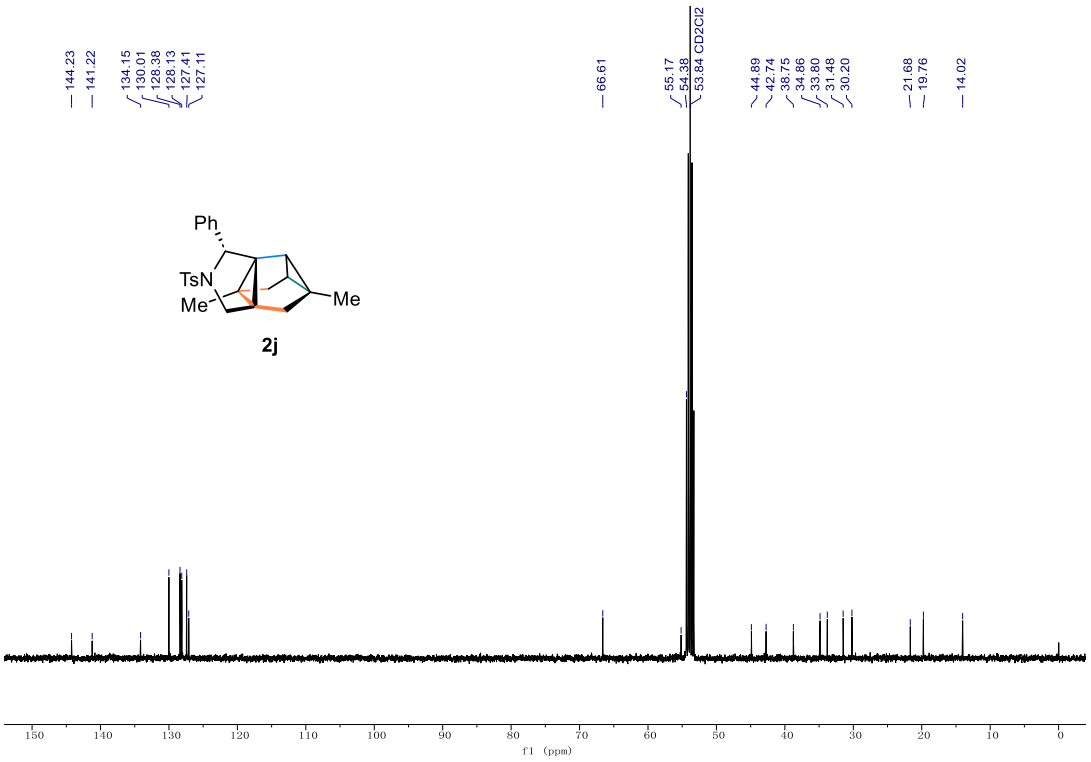
^{1}H NMR of **2i** (400 MHz, $CDCl_3$)



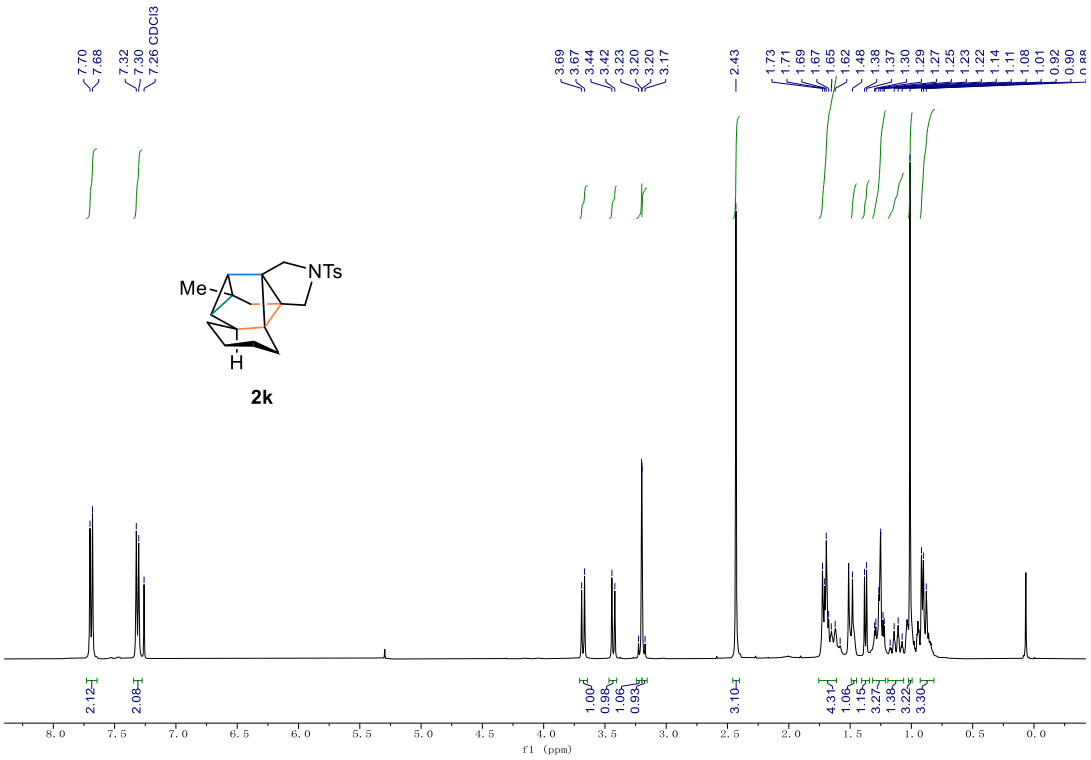
^{13}C{^{1}H} NMR of **2i** (101 MHz, $CDCl_3$)



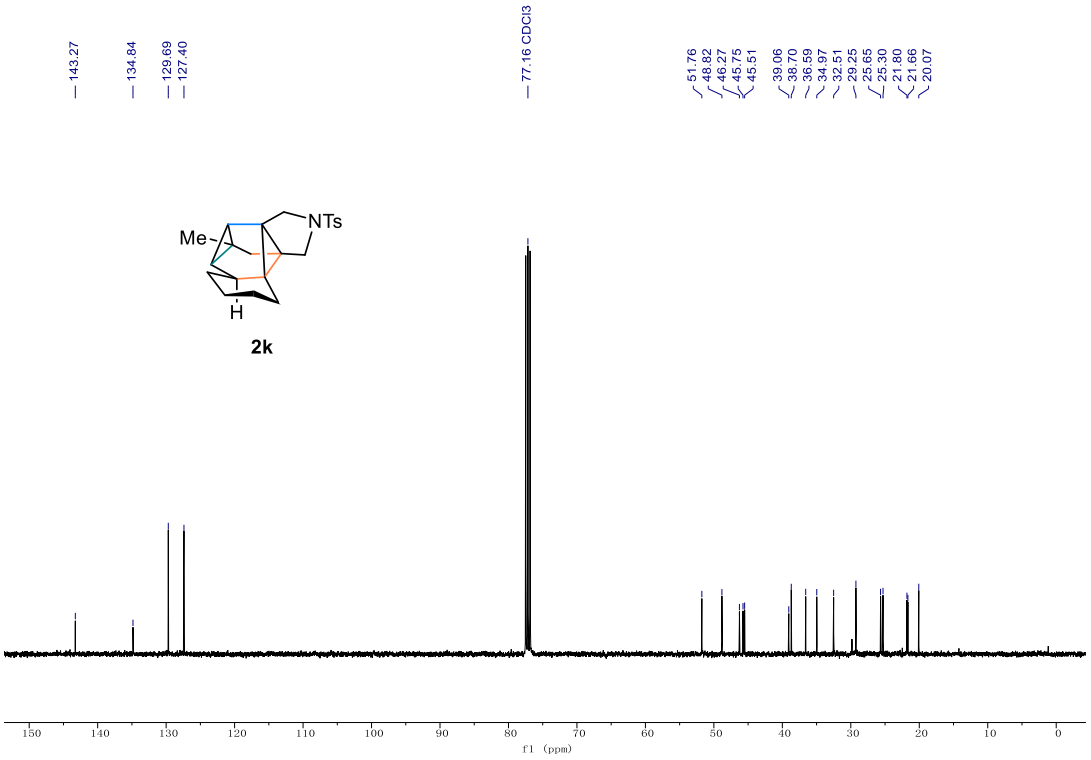
^{1}H NMR of **2j** (400 MHz, CD_2Cl_2)



^{13}C{^{1}H} NMR of **2j** (101 MHz, CD_2Cl_2)



^{1}H NMR of **2k** (400 MHz, $CDCl_3$)

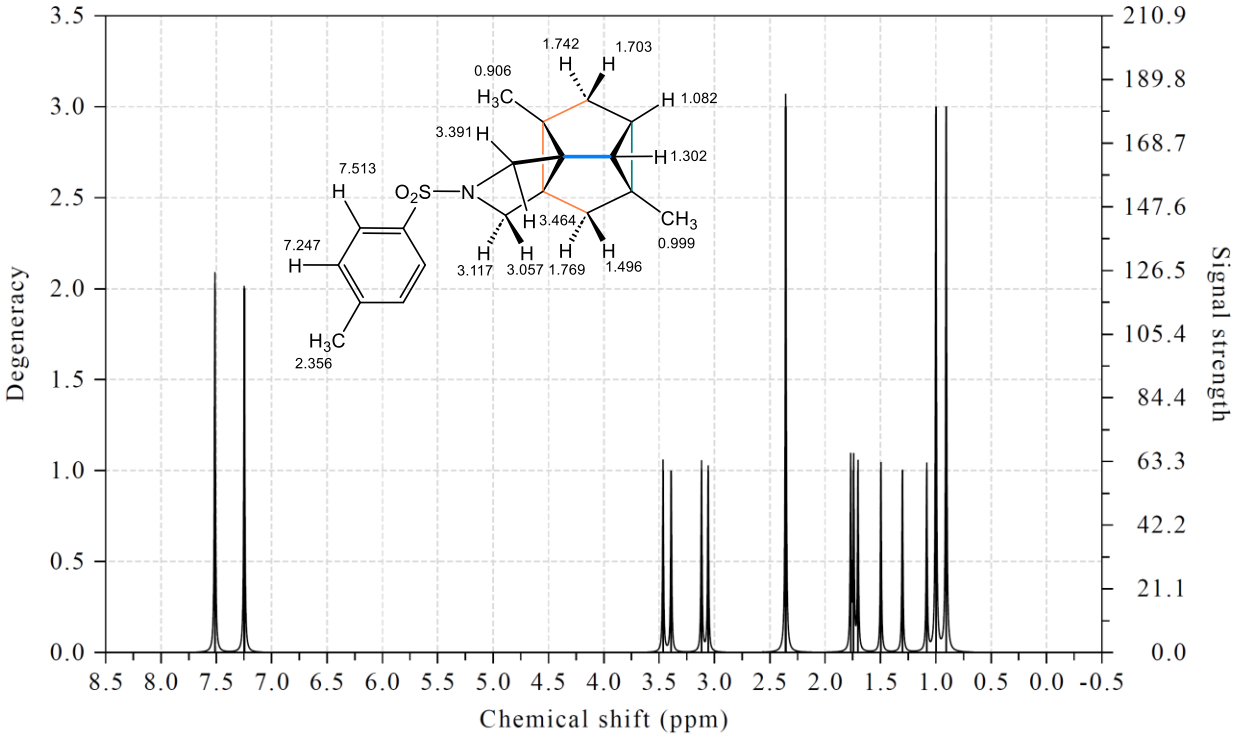


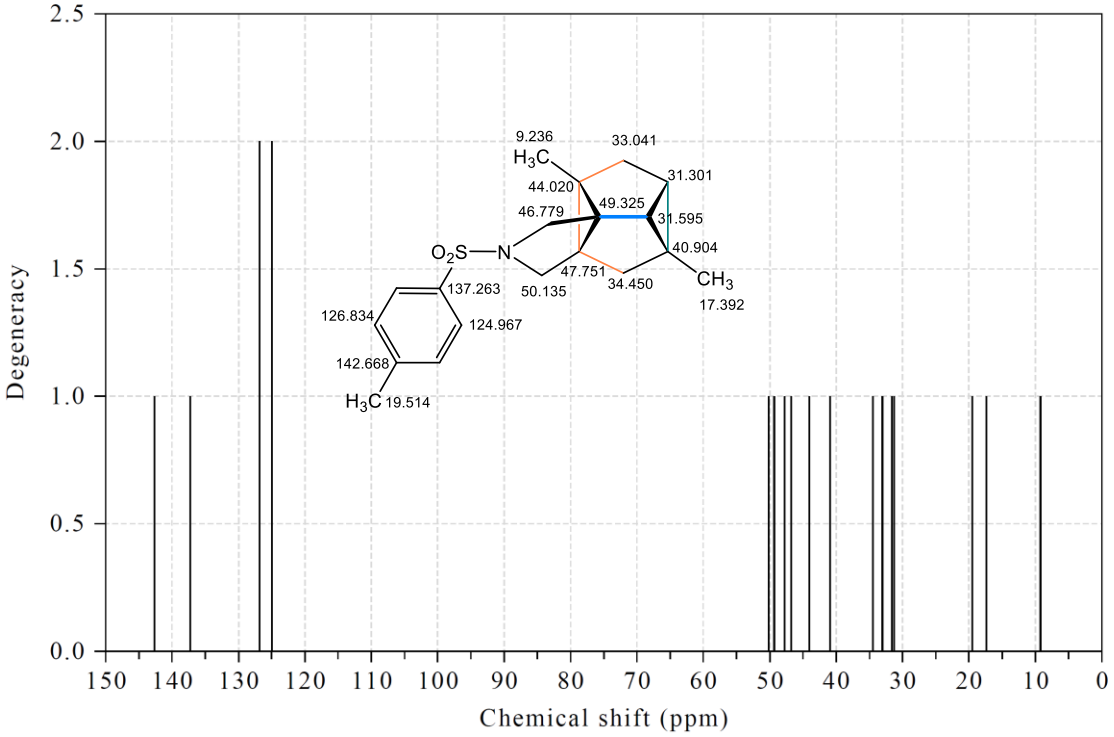
^{13}C{^{1}H} NMR of **2k** (101 MHz, $CDCl_3$)

9. Assignment of NMR Signals

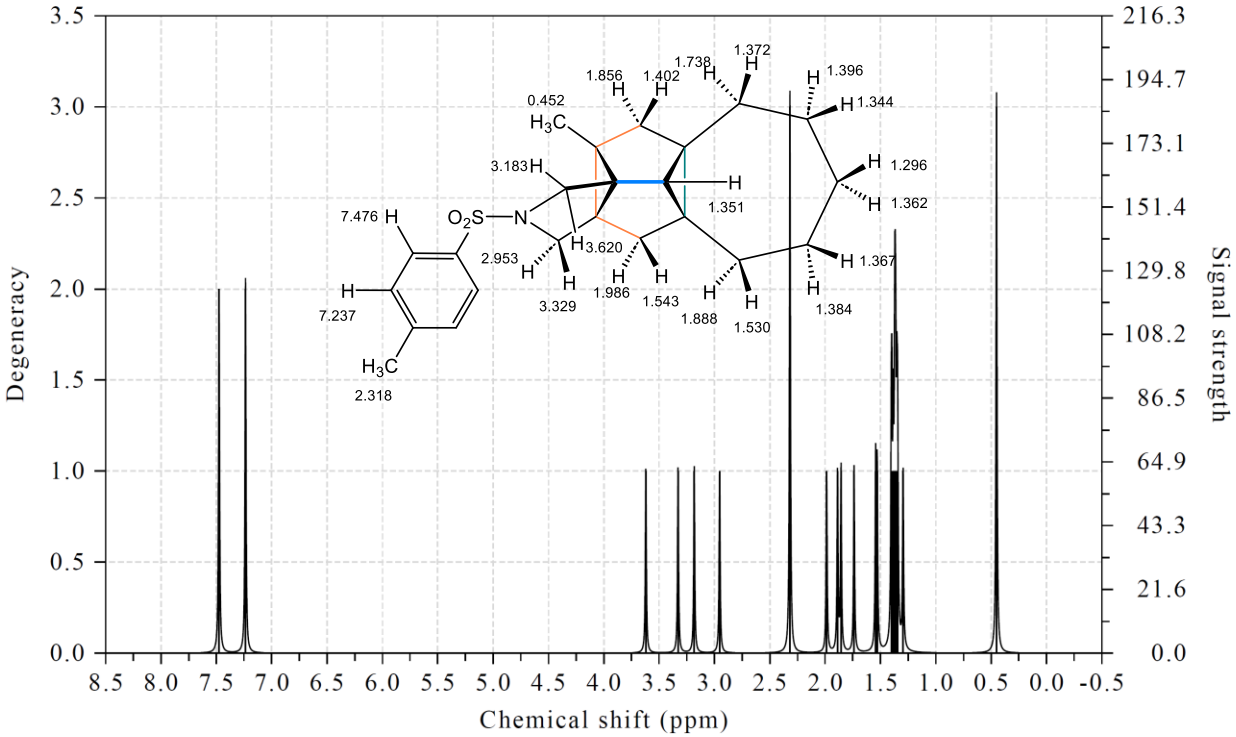
To assign the NMR signals, DFT calculations were performed for **2a** and **2i**.

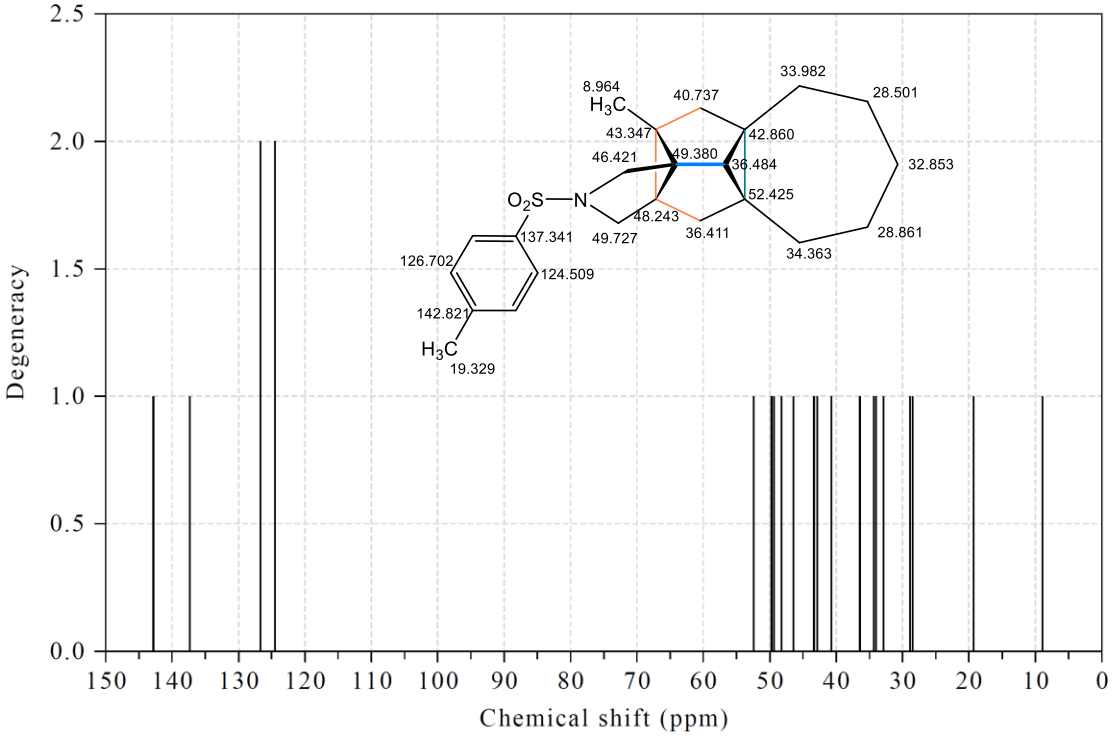
A scaling factor method was used to give ^{1}H- and ^{13}C-NMR chemical shifts comparable with experiment. According to literature,[27] the structures of discussed molecules were optimized at B3LYP/6-311+G(2d,p) level. These gas phase geometries were then subjected to GIAO-NMR calculations[28–30] at B3LYP/6-311+G(2d,p)/SMD($CHCl_3$) level using *Gaussian* 09 E.01. To account for conformation effect, conformation search was performed using *crest*-3.0.1 at GFN-xTB2/ALPB($CHCl_3$) level. After optimization of each conformer at B3LYP/6-311+G(2d,p) level, ωB97M-V/def2-QZVP/SMD($CHCl_3$) single point energy calculations were performed with *ORCA*-5.0.4 to give accurate Gibbs energy for Boltzmann distribution. The averaged chemical shifts for conformers (< 2.0 kcal/mol) were computed with the help of *Multiwfn*-3.8(dev). The ^{1}H-NMR spectra were broadened with Gaussian function with a FWHM of 0.01 ppm. The ^{13}C NMR chemical shifts calculated matched the experimental results, and ^{1}H NMR chemical shifts of several characteristic protons also agreed with the experimental results.





^{1}H- and ^{13}C-NMR chemical shifts prediction for **2a**





^{1}H- and ^{13}C-NMR chemical shifts prediction for **2i**

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