Supporting information

For

Formal Hydrogenation of Arynes with Silyl C_β–H Bonds as an Active Hydride Source

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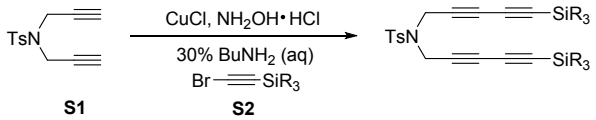
General information

All reactions were carried out in oven or flame-dried glassware unless otherwise noted. Compounds were purchased from Aldrich, Acros or Gelest unless otherwise noted. Toluene and dichloromethane (CH_2Cl_2) were distilled over calcium hydride (CaH_2) and THF was distilled over sodium and benzophenone under nitrogen atmosphere. Flash

column chromatography was performed by using silica gel 60 Å (32−63 mesh) purchased from Silicycle Inc. Analytical thin layer chromatography (TLC) was performed on 0.25 mm E. Merck pre-coated silica gel 60 (particle size 0.040−0.063 mm). Yields refer to chromatographically and spectroscopically pure compounds unless otherwise stated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AV-500 spectrometer. Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), qn (quintet), m (multiplet), br s (broad single), and app (apparent). ^{1}H NMR signals that fall within a ca. 0.3 ppm range are generally reported as a multiplet, with a single chemical shift value corresponding to the center of the peak. Coupling constants, *J*, are reported in Hz (Hertz). Electrospray ionization (ESI) mass spectra were recorded on a Waters Micromass Q-Tof Ultima in the University of Illinois at Urbana-Champaign. Electron impact (EI) mass spectra and Chemical Ionization (CI) mass spectra were obtained using a Micromass 70-VSE in the University of Illinois at Urbana–Champaign.

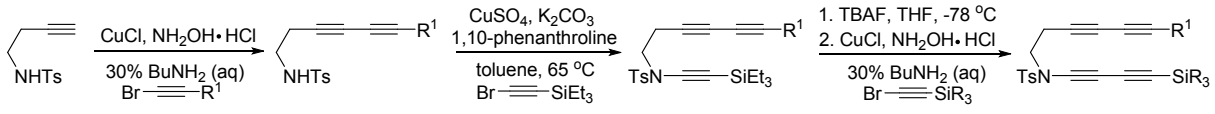
Experimental Details

General procedure for symmetric bis-1,3-diyne synthesis:



Symmetrical bis-1,3-diyne substrates were prepared in one step using the Cadiot-Chodkiewicz coupling reaction. To a 30% *n*-$BuNH_2$ (3 mL/1 mmol of substrate) aqueous solution containing CuCl (2 equiv), and $NH_2OH{\cdot}HCl$ (0.2 equiv) was added diyne **S1** dissolved in CH_2Cl_2 at 0 °C. Bromoalkyne **S2** (dissolved in CH_2Cl_2) (3 – 4 equiv) was then added drop wise over 5 min and the reaction mixture was stirred at 0 °C for additional 5 min. After aqueous work up, the crude product was purified by column chromatography on silica gel to afford bis-1,3-diynes in moderate to good yields.

General procedure for unsymmetric bis-1,3-diyne synthesis



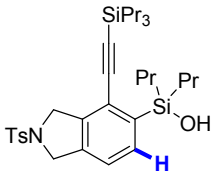
Unsymmetrical bis-1,3-diyne substrates were synthesized in four steps involving the first Cadiot-Chodkiewicz coupling reaction, *N*-alkynalation of tosylamide, desilylation and the second Cadiot-Chodkiewicz coupling reaction sequence. Tosylamide **S3** was coupled with bromoalkyne **S4** (1.5 equiv) under the typical Cadiot-Chodkiewicz reaction conditions described above gave diyne **S5**. *N*-alkynylation of **S5** with bromoalkyne **S6** (1.1 equiv) in the presence of catalytic amount of $CuSO_4{\cdot}5H_2O$ (0.1 equiv), 1, 10-phenanthroline (0.2 equiv) and K_2CO_3

(2 equiv) in toluene at 65 °C for 8 h afforded triyne **S7**. Desilylaton of **S7** using TBAF (1.1 equiv) at -78 °C and subsequent aqueous workup provided terminal alkyne and then subsequent coupling reaction with bromoalkyne **S8** (1.5 equiv) generated unsymmetrical bis-1,3-diynes in moderate to good yields.

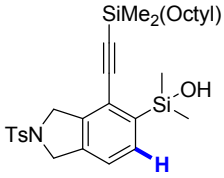
Characterization Data

General Procedure for Formal Hydrogenation Reaction

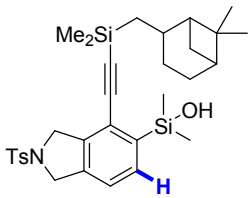
In a glove box, bis-1,3-diyne **1a** (50 mg, 0.082 mmol) and $AgSbF_6$ (2.8 mg, 10 mol %) were dissolved in 5 mL of dry toluene in a thick-walled 25 mL Schlenk tube equipped with a magnetic stirring bar. The reaction tube was brought out of the glove box and stirred in an oil bath at 90 °C for 4 h. The reaction mixture was cooled to room temperature. Solvents were removed under reduced pressure and the crude product was purified by flash column chromatography (SiO_2, gradient elution, hexanes:EtOAc = 5: 1) to afford **3a** (38 mg, 80%) as a gummy material.



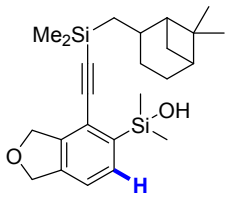
3a: (80% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.5 Hz, 1H), 4.65 (s, 2H), 4.63 (s, 2H), 2.46 (bs, 1H), 2.41 (s, 3H), 1.48 (m, 6H), 1.37 (m, 4H), 1.03 (t, *J* = 7.26 Hz, 9H), 0.92 (m, 10H), 0.70 (m, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.7, 140.0, 139.9, 137.2, 133.8, 133.5, 129.8, 127.6, 122.4, 121.8, 104.2, 101.1, 54.3, 53.9, 21.5, 18.2, 18.1, 17.8, 17.6, 16.6, 15.9; **HRMS** (ESI) calcd for $C_{32}H_{50}NO_3SSi_2$ $[M+H]^+$: 584.3044, found 584.3048.



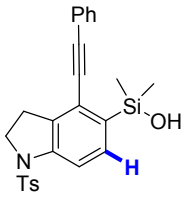
3b: (80% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.12 (d, *J* = 7.5 Hz, 1H), 4.66 (s, 2H), 4.63 (s, 2H), 2.43-2.42 (bs, 1H), 2.41 (s, 3H), 1.36 (m, 12H), 0.88 (dd, *J* = 8.51, 5.01 Hz, 3H), 0.71 (m, 2H), 0.43 (s, 6H), 0.24 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.7, 141.6, 139.4, 137.4, 133.8, 133.0, 129.8, 127.5, 122.1, 122.0, 103.2, 102.4, 54.2, 53.8, 33.3, 31.9, 29.3, 23.8, 22.7, 21.5, 15.9, 14.1, 0.1, -1.8; **HRMS** (ESI) calcd for $C_{29}H_{44}NO_3SSi_2$ $[M+H]^+$: 542.2575, found 542.2582.



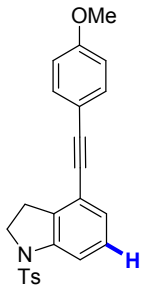
3c: (66% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 7.5 Hz, 1H), 4.65 (s, 2H), 4.62 (s, 2H), 2.41 (s, 3H), 2.20 (m,1H), 2.04 (m, 1H), 1.87 (dd, *J* = 9.5, 4.8 Hz, 1H), 1.76 (dt, *J* = 11.4, 11.0, 4.6 Hz, 3H), 1.68 (t, *J* = 5.5 Hz, 1H), 1.38 (d, *J* = 9.9 Hz, 1H), 1.31 (m, 1H), 1.26 (t, *J* = 7.1 Hz, 1H), 1.19 (s, 1H), 0.82- 0.65(m, 6H), 0.44 (s, 6H), 0.21 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.6, 141.6, 139.5, 137.2, 133.9, 133.5, 129.8, 127.6, 122.4, 121.7, 103.0, 103.0, 54.2, 53.9, 49.1, 40.6, 39.6, 31.3, 26.9, 25.3, 24.7, 24.0, 23.0, 21.5, 20.1, 1.3, -0.8; **HRMS** (ESI) calcd for $C_{31}H_{44}NO_3SSi_2$ $[M+H]^+$: 566.2575, found 566.2575.



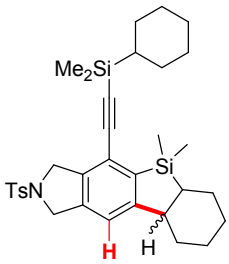
3d: (91% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.4 Hz, 1H), 7.20 (d, *J* = 7.4 Hz, 1H), 5.16 (s, 2H), 5.15 (s, 2H), 2.64 (bs, 1H), 2.23 (m, 1H), 2.04 (dd, *J* = 10.4, 5.3 Hz, 1H), 1.86 (m, 1H), 1.74 (m, 4H), 1.38 (d, *J* = 10.0 Hz, 1H), 1.33 (m, 1H), 1.19 (s, 3H), 0.84 (s, 3H), 0.73 (m, 2H), 0.49 (s, 6H), 0.25 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.6, 140.8, 140.5, 132.7, 120.6, 104.1, 101.8, 74.2, 73.8, 49.1, 40.7, 39.6, 31.3, 26.9, 25.3, 24.7, 24.1, 23.0, 20.1, 0.3, -.8, -0.8; **HRMS** (ESI) calcd for $C_{24}H_{37}O_2Si_2$ $[M+H]^+$: 413.2327.



3e: (64% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.46 (m, 3H), 7.35 (m, 3H), 7.25 (d, *J* = 7.3 Hz, 2H), 3.95 (t, *J* = 8.5 Hz, 2H), 3.11 (t, *J* = 8.5 Hz, 2H), 2.38 (s, 3H), 0.49 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 144.3, 143.2, 135.7, 134.5, 133.8, 131.2, 129.8, 128.8, 128.5, 127.3, 124.2, 122.5, 113.6, 96.2, 87.7, 49.5, 27.8, 21.5, 0.4; **HRMS** (ESI) calcd for $C_{25}H_{26}NO_3SSi$ $[M+H]^+$: 448.1397, found 448.1400.



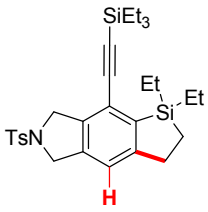
3f: (75% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.7 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.17 (t, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.7 Hz, 2H), 3.95 (t, *J* = 8.5 Hz, 2H), 3.82 (s, 3H), 3.04 (t, *J* = 8.5 Hz, 2H), 2.38 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.8, 144.2, 142.0, 134.0, 133.9, 133.0, 129.7, 127.9, 127.3, 126.3, 120.7, 114.9, 114.5, 114.0, 93.3, 85.2, 55.3, 49.7, 27.8, 21.5; **HRMS** (ESI) calcd for $C_{24}H_{22}NO_3S$ $[M+H]^+$: 404.1315, found 404.1320.



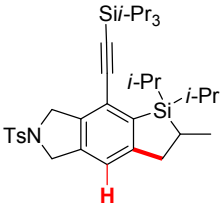
2i (10:1 mixture of diastereomers): (94% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 6.95 (s, 1H), 4.61 (m, 4H), 2.41 (m,, 4H), 1.92 (m, 2H), 1.78 (m, 6H), 1.42 (m, 2H), 1.23 (m, 6H), (0.74 (dd, *J* = 17.0, 7.12 Hz, 2H), 0.38 (s, 3H), 0.18 (s, 6H), 0.15 (s, 3H), **minor isomer** δ 6.96 (s, 1H), 3.0 (m, 1H), 0.37 (s, 3H), 0.27 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) **mixture of isomers** δ 155.4, 143.6, 142.6, 137.4, 136.2, 133.7, 129.8, 127.6, 121.9, 118.6, 116.4, 103.2, 98.2, 54.3, 54.2, 53.5, 53.5, 46.4, 44.2, 37.5, 32.5, 31.1, 28.8, 27.8, 27.8, 27.3, 26.8, 26.5, 26.3, 25.7, 25.5, 24.2, 24.0, 21.5, -2.8, -3.5, -3.6; **HRMS** (ESI) calcd for $C_{33}H_{46}NO_2SSi_2$ $[M+H]^+$: 576.2782, found 576.2791.

General Procedure for C–H insertion Reaction

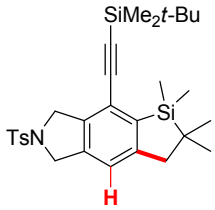
In a glove box, bis-1,3-diyne **1j** (50 mg, 0.095 mmol) and AgOTf (2.4 mg, 10 mol %) were dissolved in 5 mL of dry toluene in a thick-walled 25 mL Schlenk tube equipped with a magnetic stirring bar. The reaction tube was brought out of the glove box and stirred in an oil bath at 90 °C for 4 h. The reaction mixture was cooled to room temperature and the solvents was removed under reduced pressure. The crude was purified by flash column chromatography (SiO_2, gradient elution, hexanes:EtOAc = 10:1) to afford **2j** (47 mg, 95%) as a gummy material.



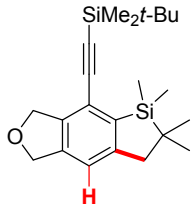
2j: (95% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.5 Hz, 2H) 7.32 (d, *J* = 8.5 Hz, 2H), 6.95 (s, 1H), 4.62 (s, 2H), 4.59 (s, 2H), 2.97 (t, *J* = 7.5 Hz, 2H), 2.40 (s, 3H), 1.07 (t, *J* = 7.5 Hz, 9H), 0.98 (t, *J* = 7.5 Hz, 2H), 0.92 (t, *J* = 4 Hz, 6H), 0.87 (q, *J* = 8 Hz, 4H), 0.24 (q, *J* = 7.5 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.3, 143.5, 140.2, 137.7, 136.7, 133.8, 129.7, 127.5, 121.9, 119.5, 103.9, 96.7, 54.0, 53.4, 31.6, 21.4, 7.5, 7.4, 6.9, 4.7,4.3; **HRMS** (ESI) calcd for $C_{29}H_{42}NO_2SSi_2$ $[M+H]^+$: 524.2469, found 524.2479.



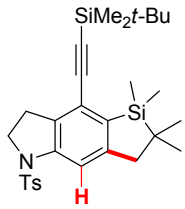
2k: (92% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.5 Hz, 2H) 7.31 (d, *J* = 8.5 Hz, 2H), 6.94 (s, 1H), 4.65 (m, 4H), 3.31 (dd, *J* = 16.5, 9 Hz, 1H), 2.61 (dd, *J* = 16.5, 10 Hz, 1H), 2.40 (s, 3H), 1.59 (m, 1H), 1.52 (m, 1H), 1.33 (m, 1H), 1.24 (d, *J* = 7.5 Hz, 3H), 1.14 (s, 18H), 1.14 (m, 3H), 1.12 (d, *J* = 7.5 Hz, 3H), 1.09 (d, *J* = 7.5 Hz, 3H), 0.94 (d, *J* = 7.5 Hz, 3H), 0.92 (d, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.4, 143.5, 129.3, 137.7, 137.4, 133.8, 129.7, 127.5, 122.5, 119.4, 105.4, 95.8, 54.2, 53.9, 42.2, 21.4, 18.9, 18.5, 18.4, 17.6, 17.5, 15.7, 11.6, 11.3, 10.6; **HRMS** (ESI) calcd for $C_{35}H_{54}NO_2SSi_2$ $[M+H]^+$: 608.3408, found 608.3418.



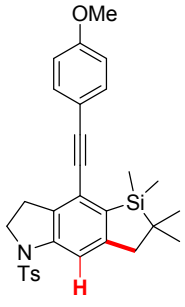
2l: (89% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.5 Hz, 2H) 7.30 (d, *J* = 8.5 Hz, 2H), 6.90 (s, 1H), 4.62 (s, 2H), 4.58 (s, 2H), 2.64 (s, 2H), 2.40 (s, 3H), 1.02 (s, 6H). 1.00 (s, 9H), 0.25 (s, 6H), 0.20 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.3, 143.5, 141.8, 137.7, 136.5, 133.8, 129.7, 127.5, 122.1, 120.0, 103.1, 97.8, 54.1, 53.4, 49.5, 26.1, 25.0, 23.7, 21.4, 16.6; **HRMS** (ESI) calcd for $C_{29}H_{42}NO_2SSi_2$ $[M+H]^+$: 524.2469, found 524.2473.



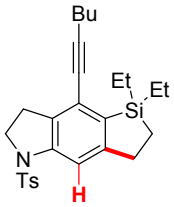
2m: (95% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.0 (s, 1H), 5.14 (s, 2H), 5.09 (s, 2H), 2.71 (s, 2H), 1.07 (s, 6H), 1.0 (s, 9H), 0.31 (s, 6H), 0.2 (s,6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.1, 141.2, 141.2, 140.0, 120.6, 118.6, 103.9, 96.8, 74.1, 73.5, 49.6, 26.2, 25.2, 23.9, 16.6, -4.5, -5.2; **HRMS** (ESI) calcd for $C_{22}H_{33}OSi_2$ $[M-H]^+$: 369.2064, found 369.2058.



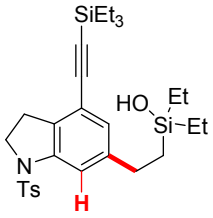
2n: (87% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.41 (s, 1H), 7.24 (d, *J* = 8.2 Hz, 2H), 3.91 (t, *J* = 8.4 Hz, 2H), 2.96 (t, *J* = 8.4 Hz, 2H), 2.70 (s, 2H), 2.39 (s, 3H), 1.05 (s, 6H), 0.96 (s, 9H), 0.24 (s, 6H), 0.15 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.0, 144.1, 143.5, 136.2, 134.1, 132.4, 129.7, 127.3, 112.2, 103.9, 96.9, 50.1, 49.9, 27.3, 26.1, 25.2, 23.9, 21.5, 16.5, -4.6, -5.2; **HRMS** (ESI) calcd for $C_{29}H_{42}NO_2SSi_2$ $[M+H]^+$: 524.2469, found 524.2467.



2o: (85% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.40 (d, *J* = 7.8Hz, 2H), 7.38 (s, 1H), 7.25 (d, *J* = *8*.1 Hz, 2H), 6.8 (d, *J* = 7.8 Hz, 2H), 3.93 (t, *J* = 8.4 Hz, 2H), 3.82 (s, 3H), 3.02 (t, *J* = 8.4 Hz, 2H), 2.74 (s, 2H), 2.38 (s, 3H), 1.07 (s, 6H), 0.29 (s, 6H)); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.8, 152.0, 144.1, 143.5, 136.0, 134.1, 132.8, 131.5, 129.7, 127.3, 124.2, 115.2, 114.1, 111.8, 93.5, 86.4, 55.3, 50.1, 50.0, 27.3, 25.2, 23.8, 21.5, -4.9; **HRMS** (ESI) calcd for $C_{30}H_{34}NO_3SSi$ $[M+H]^+$: 516.2023, found 516.2031.

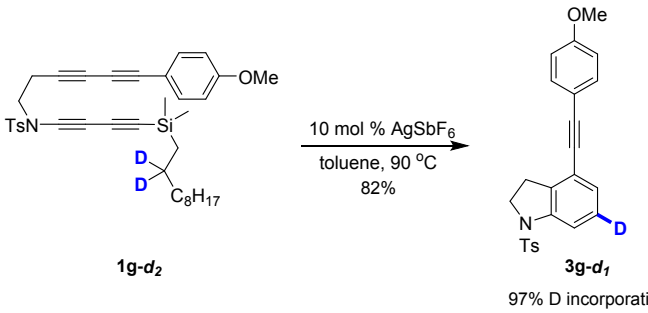


2p: (81% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.8 Hz, 2H), 7.40 (s, 1H), 7.23 (d, *J* = 7.8 Hz, 2H), 3.90 (t, *J* = 8.2 Hz, 2H), 3.02 (t, *J* = 7.1 Hz, 2H), 2.93 (t, *J* = 8.2 Hz, 2H), 2.37 (m, 5H), 1.54 (m, 2H), 1.44 (m, 2H), 1.0- 0.82 (m, 15H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 154.8, 144.0, 143.4, 134.7, 134.2, 131.7, 129.6, 127.3, 124.5, 110.9, 94.4, 79.4, 50.0, 32.2, 30.8, 27.3, 22.0, 21.5, 19.1, 13.6, 7.7, 7.1, 5.1; **HRMS** (ESI) calcd for $C_{27}H_{36}NO_2SSi_2$ $[M+H]^+$: 466.2231



2q: (81% yield) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.46 (s, 1H), 7.20 (d, *J* =8.1 Hz, 2H), 6.92 (s, 1H), 3.92 (t, *J* = 8.4 Hz, 2H), 2.93 (t, *J* = 8.3 Hz, 2H), 2.62 (m, 2H), 2.35 (s, 3H), 1.05- 0.88 (m, 14H), 0.63 (m, 8H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 145.8, 144.2, 142.1, 133.9, 132.1, 129.7, 127.3, 126.0, 120.0, 114.6, 103.6, 95.4, 50.0, 29.6, 27.5, 21.5, 17.4, 7.5, 7.4, 6.9, 4.4, 4.2; **HRMS** (ESI) calcd for $C_{29}H_{44}NO_3SSi_2$ $[M+H]^+$: 542.2575, found 542.2536.

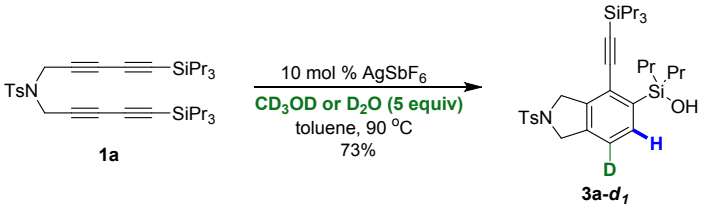
Deuterium labeling studies



1g-*d*$_2$ **3g-*d*$_1$**

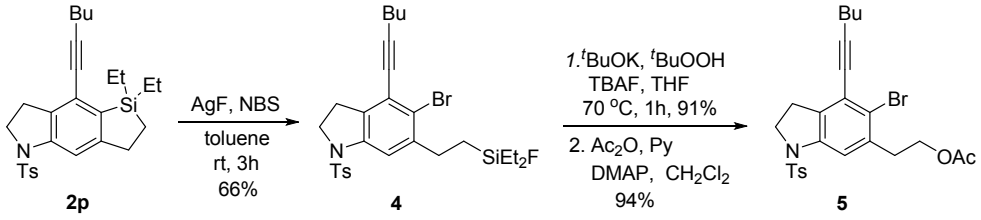
97% D incorporation

3g-*d*$_1$(Reaction was run by using described procedure above): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.60 (s, 1H), 7.39 (d, *J* = *7*.3 Hz, 2H), 7.24 (d, *J* = *8*.2 Hz, 2H), 7.11 (s, 1H), 6.86 (d, *J* = *7.3* Hz, 2H), 3.95 (t, *J* = 8.5 Hz, 2H), 3.83 (s, 3H), 3.04 (t, *J* = 8.5 Hz, 2H), 2.37 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.8, 144.1, 142.0, 134.0, 133.8, 133.0, 129.7, 127.3, 126.2, 120.6, 114.9, 114.4, 93.3, 85.2, 55.3, 49.6, 27.7, 21.5; **HRMS** (ESI) calcd for $C_{24}H_{21}DNO_3S$ $[M+H]^+$: 405.1378, found 405.1375.



General Procedure: In a glove box, bis-1,3-diyne **1a** (50 mg, 0.082 mmol) and $AgSbF_6$ (2.8 mg, 10 mol %) were dissolved in 5 mL of dry toluene and then added CD_3OD (16.6 µL, 0.42 mmol) in a thick-walled 25 mL Schlenk tube equipped with a magnetic stirring bar. The reaction tube was brought out of the glove box and stirred in an oil bath at 90 °C for 4 h. The reaction mixture was cooled to room temperature and the solvents were removed under reduced pressure. The crude was purified by flash column chromatography (SiO_2, gradient elution, hexanes:EtOAc = 10:1) to afford **3a-*d*$_1$** (35 mg, 73%) as a gummy material. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.41 (s, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 4.65 (s, 2H), 4.63 (s, 2H), 2.46 (bs, 1H), 2.41 (s, 3H), 1.48 (m, 6H), 1.37 (m, 4H), 1.03 (t, *J* = 7.26 Hz, 9H), 0.92 (m, 10H), 0.70 (m, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.7, 140.0, 139.9, 136.7, 134.3, 133.9, 129.8, 127.6, 123.7, 104.2, 101.1, 54.3, 53.9, 21.5, 18.2, 18.1, 17.8, 17.6, 16.6, 15.9; **HRMS** (ESI) calcd for $C_{32}H_{49}DNO_3SSi_2$ $[M+H]^+$: 585.3107, found 585.3113.

Synthetic transformations of the C–H insertion product



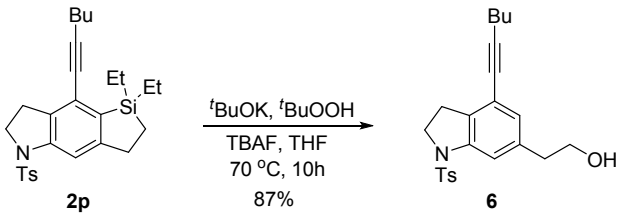
Halogenative ring opening: To the solution of **2p** (100 mg, 0.21 mmoles) in 3 mL of dry toluene was added AgF (32.5 mg, 1.2 equiv) and NBS (51 mg, 1.3 equiv), and the reaction mixture was stirred vigorously for 3 h in the dark. After the reaction was completed (monitored by TLC), the reaction mixture was filtered through a pad of silica gel and washed with hexanes/EtOAc mixture (5:1). Evaporation of the solvent gave **4** (80 mg, 66%) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.5 Hz, 2H), 7.46 (s, 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 3.89 (t, *J* = 8.3 Hz, 2H), 2.91 (t, *J* = 8.3 Hz, 2H), 2.80 (m, 2H), 2.43 (t, *J* = 6.5 Hz, 2H), 2.38 (s, 3H), 1.57 (m, 2H), 1.48 (m, 2H), 1.03 (t, *J* = 7.9 Hz, 5H), 0.93 (m, 7H), 0.68 (m, 4H); **^{13}C NMR** (125 MHz, $CDCl_3$) 144.4, 144.3, 141.0, 133.6, 133.6, 129.7, 127.3, 123.4, 120.2, 114.7, 99.3, 77.5, 49.9, 31.1, 30.6, 28.2, 21.9, 21.5, 19.3, 15.2, 13.6, 6.6, 6.2; **HRMS** (ESI) calcd for $C_{27}H_{36}BrFNO_2SSi$ $[M+H]^+$: 564.1398, found

Tamao-Fleming Oxidation: *tert*-Butyl hydroperoxide (0.05 mL, 5.5 M in decane over MS, 3 equiv) was added to an ice-cooled (0 °C) stirred solution of ^{t}BuOK (29.8 mg, 3 equiv) in 2.0 mL of THF under the N_2 atmosphere. After 10 min, a solution of **4** (50 mg, 0.08 mmol) in 1.0 mL of THF was added to the resultant mixture followed by the addition of TBAF (0.26 mL, 1.0 M solution in THF, 3 equiv). The mixture was stirred at 70 °C for 1h and then cooled down in an ice bath. 0.5 g of $Na_2S_2O_3 \cdot 5H_2O$ in 2.0 mL of water was added and the mixture was stirred for 30 min. After this time, 5 mL of saturated NH_4Cl was added. The resulted solution was extracted with ether (3 x 20 mL). The combined organic fractions were washed with 5% citric acid, $NaHCO_3$ (sat.) and brine. The solution was dried over anhydrous $MgSO_4$, and concentrated. The crude material was purified by flash column chromatography (SiO_2, gradient elution, hexane: EtOAc 5:1) to afford the alcohol product (38 mg, 91%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.49 (s, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 3.89 (m, 4H), 3.05 (t, *J* = 6.6 Hz, 2H), 2.94 (t, *J* = 8.5 Hz, 2H), 2.44 (t, *J* = 6.9 Hz, 2H), 2.38 (s, 3H), 1.57 (m, 2H), 1.47 (m, 3H), 0.92 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 144.5, 141.0, 137.9, 134.5, 133.5, 129.8, 127.4, 116.1, 99.7, 62.1, 50.0, 40.5, 30.6, 28.3, 28.1, 21.9, 21.6, 19.3, 13.6.

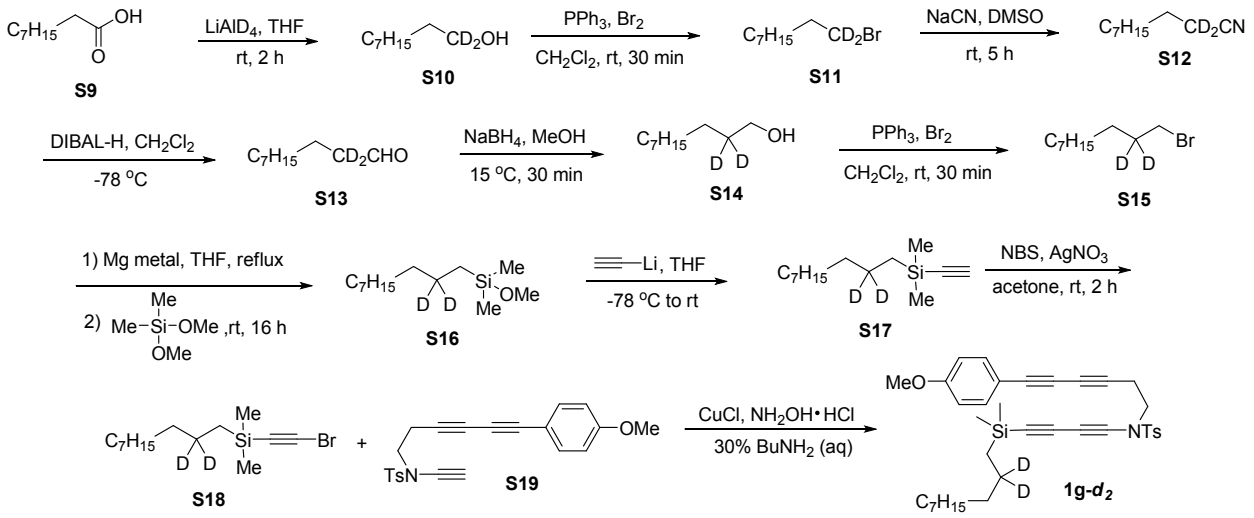
To a solution of alcohol (33 mg, 0.069 mmoles) in CH_2Cl_2 (2 mL) was added pyridine (11 mg, 2.0 equiv), Ac_2O (8.4 mg, 1.2 equiv) and DMAP (cat.) at room temperature and the reaction mixture was stirred for 15 min. After the completion of the reaction (conformed by TLC), the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (SiO_2, gradient elution, hexane: EtOAc, 10:1) to afford the compound **5** (34 mg, 94%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.8 Hz, 2H), 7.49 (s, 1H), 7.25 (d, *J* = 7.8 Hz, 2H), 4.30 (t, *J* = 6.5 Hz, 2H), 3.89 (t, *J* = 8.3 Hz, 2H), 3.11 (t, *J* = 6.4 Hz, 2H), 2.94 (t, *J* = 8.3 Hz, 2H), 2.44 (t, *J* = 6.4 Hz, 2H), 2.39 (s, 3H), 2.08 (s, 3H), 1.56 (m, 2H), 1.47 (s, 2H), 0.92 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.0, 144.5, 141.1, 137.5, 134.8, 133.7, 129.8, 127.3, 123.7, 121.0, 116.1, 99.8, 77.3, 63.4, 49.9, 36.4, 30.6, 28.3, 21.9, 21.6, 21.0, 19.3, 13.6; **HRMS** (ESI) calcd for $C_{25}H_{29}BrNO_4S$ $[M+Na]^+$: 540.0815, found 540.0820.

Direct Tamao-Fleming oxidation of 2p



To an ice-cooled (0°C) stirred solution of ^{t}BuOK (72 mg, 0.6 mmol, 6 equiv) in 2.0 mL of THF under the N_2 atmosphere, *tert*-butyl hydroperoxide (0.11 mL, 5.5 M in decane over MS, 6 equiv) was added. After 10 min, a solution of **2p** (50 mg, 0.1 mmol) in 1.0 mL of THF was added to the reaction mixture which was then followed by the addition of TBAF (0.64 mL, 1.0 M solution in THF, 6 equiv). The mixture was stirred overnight at 70 ^{o}C and, the reaction mixture was cooled down with an ice bath and 1.0 g of $Na_2S_2O_3 \cdot 5H_2O$ in 5.0 mL of water was added. The mixture was stirred for 30 min and 10 mL of saturated NH_4Cl was added. To the resulting solution was extracted with ether (3 x 20 mL). The combined organic fractions were washed with 5 % citric acid, $NaHCO_3$ (sat.), brine, dried over $MgSO_4$, and concentrated. The crude material was purified by flash silica gel column chromatography (hexane/EtoAc 5:1)to afford compound **6** (37 mg, 87%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.43 (s, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 6.86 (s, 1H), 3.91 (t, *J* = 8.4 Hz, 2H), 3.84 (t, *J* = 6.4 Hz, 2H), 2.91 (t, *J* = 8.4 Hz, 2H), 2.82 (t, *J* = 6.4 Hz, 1H), 2.37 (m, 5H), 1.53 (m, 2H), 1.43 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** δ (125 MHz, $CDCl_3$) 144.2, 142.2, 138.6, 133.7, 132.3, 129.7, 127.3, 121.0, 114.6, 94.6, 77.8, 63.6, 50.0, 39.1, 30.7, 27.3, 21.9, 21.5, 19.1, 13.6; **HRMS** (ESI) calcd for $C_{23}H_{28}NO_3S$ $[M+H]^+$: 398. 1784, found 398.1789.

Preparation of deuterated substrate (1g-*d_2*)



Preparation of S10: To a cooled solution of **S9** (2 g, 13.86 mmol) in 25 ml of THF was added $LiAlD_4$ (0.58 g, 13.86 mmol) portionwise over 15 min. After the addition, the reaction mixture was stirred at room temperature for an additional 2 h. The reaction mixture was quenched carefully by using sat. $Na_2SO_{4(aq)}$ solution and diluted with Et_2O (60 mL). The crude product was filtered through a pad of silica, and the solvent was removed under reduced pressure to afford **S10** (1.7 g, quantative) which was used for next step without further purification. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 2.40 (bs, 1H), 1.50 (t, *J* = 6.5 Hz, 2H), 1.24 (m, 12H), 0.84 (t, *J* = 6.7 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 62.0 (m), 32.5, 31.8, 29.6, 29.4, 29.2, 25.7, 22.6, 14.0; **HRMS** (ESI) calcd for $C_9H_{19}D_2O$ $[M+H]^+$: 147.1712, found 147.1710.

Preparation of S11: To a solution of PPh_3 (4.35 g, 16.62 mmol) in CH_2Cl_2 (30 mL) was added Br_2 (2.6 g, 16.62 mmol) dropwise at 0 °C. The mixture was stirred for 15 min and the alcohol **S10** (1.7 g, 13.85 mmol) in 10 ml of CH_2Cl_2 was added. The reaction mixture was stirred for an additional 15 min at room temperature. After completion of the reaction, the solvent was removed under reduced pressure, and hexane (100 ml) was added. The suspension was stirred and filtered through a pad of silica. The filtrates were concentrated and purified by flash column chromatography (SiO_2, gradient elution hexanes:EtOAc = 50:1) to afford **S11** (2.8 g, 96 %) as a pale yellow liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.84 (t, *J* = 7.3 Hz, 2H), 1.41 (dd, *J* = 13.4, 6.5 Hz, 2H), 1.28 (m, 9H), 0.88 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 32.6, 31.8, 29.4, 29.2, 28.8, 28.1, 22.6, 14.1.

Preparation of S12: To a solution of **S11** (2.8 g, 13.3 mmol) in 20 mL of DMSO was added NaCN (0.72 g, 14.5 mmol) and stirred for 5 h at 60 °C. The reaction mixture was cooled down to room temperature adn diluted with H_2O (50 mL). The solution mixture was extracted with Et_2O (3 x 40 mL) and the organic layer was washed with NaCl (30 wt. %, 20 mL), dried over $MgSO_4$ and the solvent was removed under reduce pressure. The crude product was purified by flash column chromatography (SiO_2, gradient elution hexanes:EtOAc = 50:1) to afford **S12** (2.0 g, 93 %) as a colorless liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.62 (t, *J* = 7.4 Hz, 2H), 1.41 (m, 2H), 1.26 (m, 9H), 0.86

(t, J = 6.7 Hz, 3H);); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 119.8, 31.8, 29.2, 29.1, 28.7, 28.6, 25.2, 22.6, 16.6 (m), 14.0; **HRMS** (ESI) calcd for $C_{10}H_{18}D_2N$ $[M+H]^+$: 156.1716, found

Preparation of S13: DIBAL-H (14.1 mL, 1 M in toluene, 14.1 mmol) was added to a solution of **S12** (2.0 g, 12.9 mmol) in 20 mL of CH_2Cl_2 at -78 ^oC The reaction mixture was stirred at -78 ^oC for an additional 30 min. After consuming all of the starting material, the reaction was added ether (100 mL) and Rochelle's salt solution (10 wt. %, 60 mL) which was stirred vigorously for additional 30 min until two distinct layers were formed. The ether layer was separated, washed with NaCl (30 wt. %, 20 mL), dried over $MgSO_4$ and the solvent was removed under reduce pressure to afford **S13** (1.8 g, 89 %) as a colorless oil which was used for next step without further characterization.

Preparation of S14: To the solution of **S13** (1.8 g, 11.4 mmol) in MeOH (15 mL), was added $NaBH_4$ (0.43 g, 12.0 mmol) at 0 ^oC and the resulted mixture was stirred at room temperature for an additional 30 min. The Reaction was quenched with sat. NH_4Cl solution and the solvents were removed under reduce pressure. 50 mL of ether was then added to the crude material. The organic layer washed with water (35 mL), NaCl (30 wt. %, 20 mL), dried over $MgSO_4$ and the solvent was removed under reduce pressure. The Crude material was purified by flash column chromatography (SiO_2, gradient elution; hexanes:EtOAc = 15:1)) to afford **S14** (1.7 g, 94 %) as a colorless liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.57 (s, 2H), 1.26 (m, 14H), 0.85 (t, J = 6.6 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 62.7, 31.8, 29.6, 29.5, 29.4, 29.3, 25.5, 22.6, 14.0; ; **HRMS** (ESI) calcd for $C_{10}H_{21}D_2O$ $[M+H]^+$: 161.1869, found

Preparation of S15: Alkyl bromide **S15** (2.3 g, 97%) was prepared from **S14** by using same procedure mentioned above. **^{1}H NMR** (400 MHz, CDCl3) δ ppm 3.38 (s, 2H), 1.40 (m, 2H), 1.27 (m, 12H), 0.88 (t, J = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 33.7, 31.8, 29.5, 29.4, 29.2, 28.7, 28.0, 22.6, 14.0.

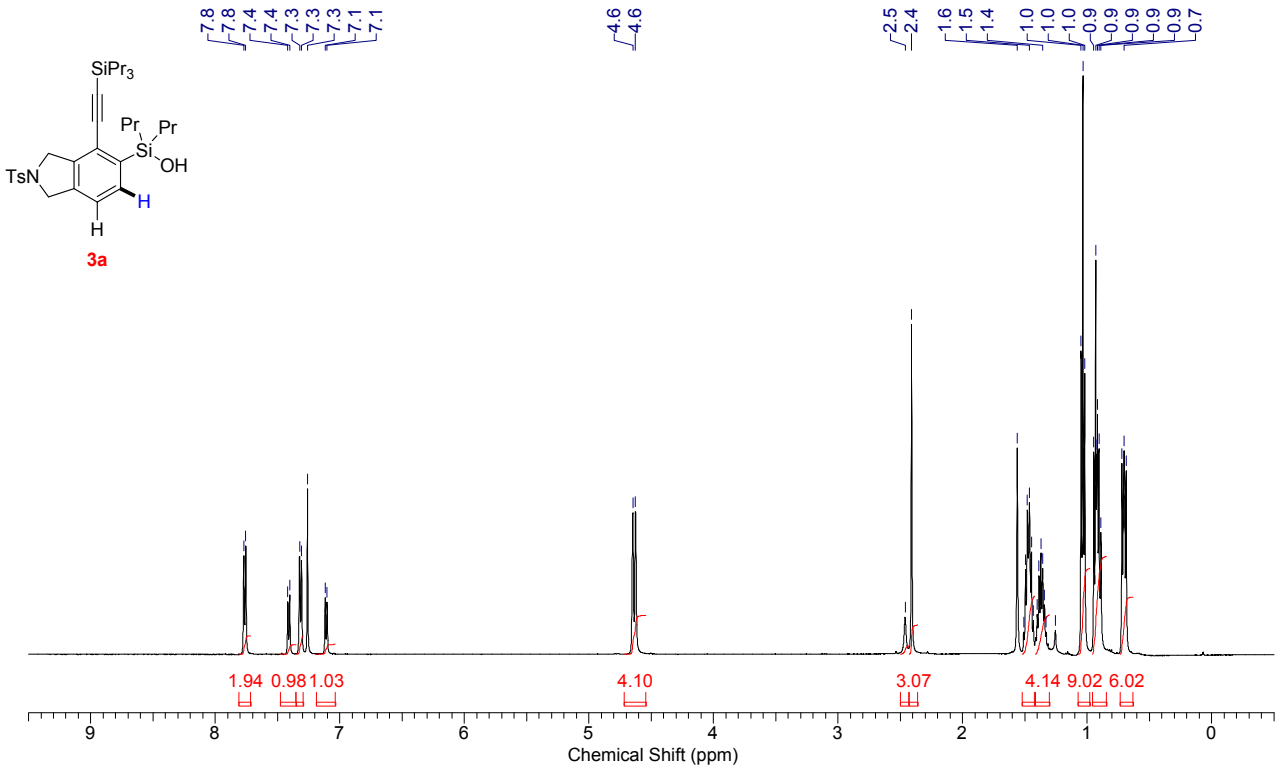
Preparation of S16: Oven dried magnesium turnings were taken in a dry flask and added 5 mL of dry THF followed by a pinch of Iodine. The violet colored liquid was heated to 70 ^oC in oil bath and then slowly added small amount of **S15** (2.3 g, 10.3 mmol) THF solution. After the initiation of the reaction, the remaining alkyl halide was added dropwisely and at the same temperature for additional 15 min. Dimethoxy dimethyl silane (1.2 mL, 20.6 mmol) in THF was then added to this in situ generated Grignard reagent at 0 ^oC. The reaction mixture was then stirred overnight at room temperature. The reaction was quenched with aq. NH_4Cl and water, extracted with ether (2 x 50 mL). The organic layer was washed with NaCl (30 wt. %, 20 mL), dried over $MgSO_4$, and the solvent was removed under reduce pressure. The crude material was purified by using flash column chromatography (SiO_2, gradient elution hexanes:EtOAc = 25:1) to afford **S16** (1.05g, 64 %) as a colorless liquid and proceeded further without further characterization.

Preparation of S17: Acetylene gas was passed through a *n*-BuLi (2 mL, 2.5 M in hexanes, 12.2 mmol) THF solution at -78 ^oC with a vent needle for 15 min. **S16** (1.05 g, 6.1 mmol) THF solution was then added to the reaction mixture. The resulted solution was slowly warmed to room temperature and stirred for overnight at the

same temperature. The reaction mixture was quenched with aq.NH_4Cl and water (30 mL), extracted with ether (2 x 50 mL) and combined organic layers were washed with NaCl (30 wt. %, 20 mL), dried over $MgSO_4$. Filtrate was concentrated under reduced pressure and purified by using flash column chromatography (SiO_2, gradient elution hexanes:EtOAc 25:1) to afford **S17** (820 mg, 76.5 %) as a colorless liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.37 (s, 1H), 1.30 (m, 14H), 0.88 (t, *J* = 6.6 Hz, 3H), 0.61 (s, 2H), 0.16 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 93.2, 89.5, 33.0, 31.9, 29.6, 29.6, 29.3, 29.2, 22.7, 15.6, 14.1, -1.9.

Preparation of S18: NBS (753 mg, 4.24 mmol) and $AgNO_3$ (72 mg, 0.4 mmol) were added to a degassed solution of **S17** (800 mg, 3.53 mmol) in acetone (10 mL) The resulting solution was stirred at room temperature for 2 h. Solvent was removed under reduce pressure and the crude product was purified by using flash column chromatography (SiO_2, gradient elution, hexanes:EtOAc = 30:1) to afford **S18** (760 mg, 70.5 %) as a colorless liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.29 (m, 12H), 0.8 (t, *J* = 6.8 Hz, 2H), 0.60 (s, 2H), 0.15 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 86.4, 61.4, 33.0, 31.9, 29.7, 29.6, 29.3, 29.2, 22.7, 15.7, 14.1, -1.8.

Preparation of 1g-*d_2*: Compound **S20** was synthesized from **S18** and **S19** by using the procedure described above. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm 7.81 (d, *J* = 8.26 Hz, 1H), 7.41 (d, *J* = 8.80 Hz, 1H), 7.37 (d, *J* = 8.07 Hz, 1H), 6.83 (d, *J* = 8.79 Hz, 1H), 3.81 (s, 1H), 3.55 (t, *J* = 7.54 Hz, 1H), 2.68 (t, *J* = 7.53 Hz, 1H), 2.43 (s, 1H), 1.28 (d, *J* = 15.44 Hz, 1H), 0.97 (t, *J* = 7.96 Hz, 1H), 0.61 (s, 1H), 0.16 (s, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.3, 145.4, 134.2, 134.2, 130.1, 127.6, 114.1, 113.5, 90.4, 87.5, 78.1, 76.1, 72.6, 68.1, 67.7, 59.9, 55.3, 49.7, 33.2, 33.1, 29.7, 29.6, 29.3, 22.7, 21.7, 19.6, 15.7, 14.1, -2.0, ; **HRMS** (ESI) calcd for $C_{36}H_{44}D_2NO_3SSi$ $[M+H]^+$: 602.3088, found 602.3090.


SiPr3
Pr
Pr
Si
OH
TsN
H
H
3a
7.8
7.8
7.4
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7.3
7.3
7.3
7.1
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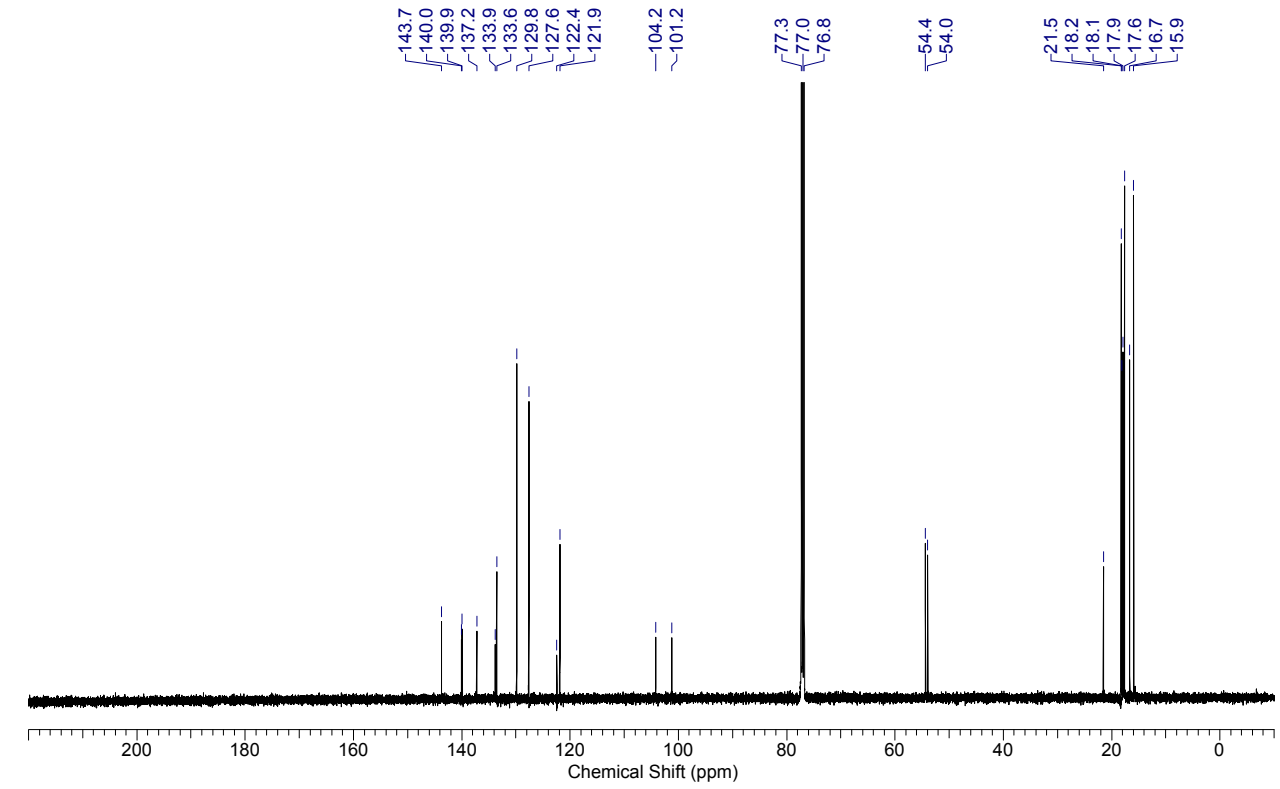
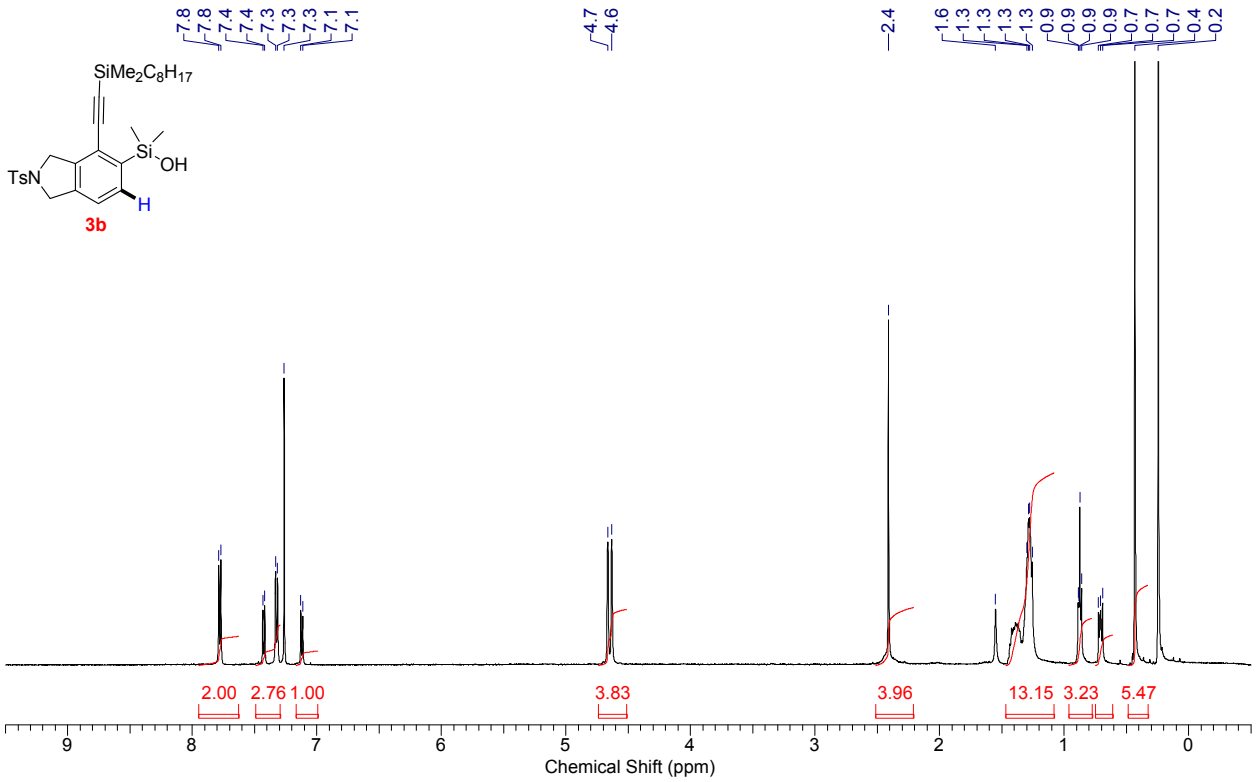
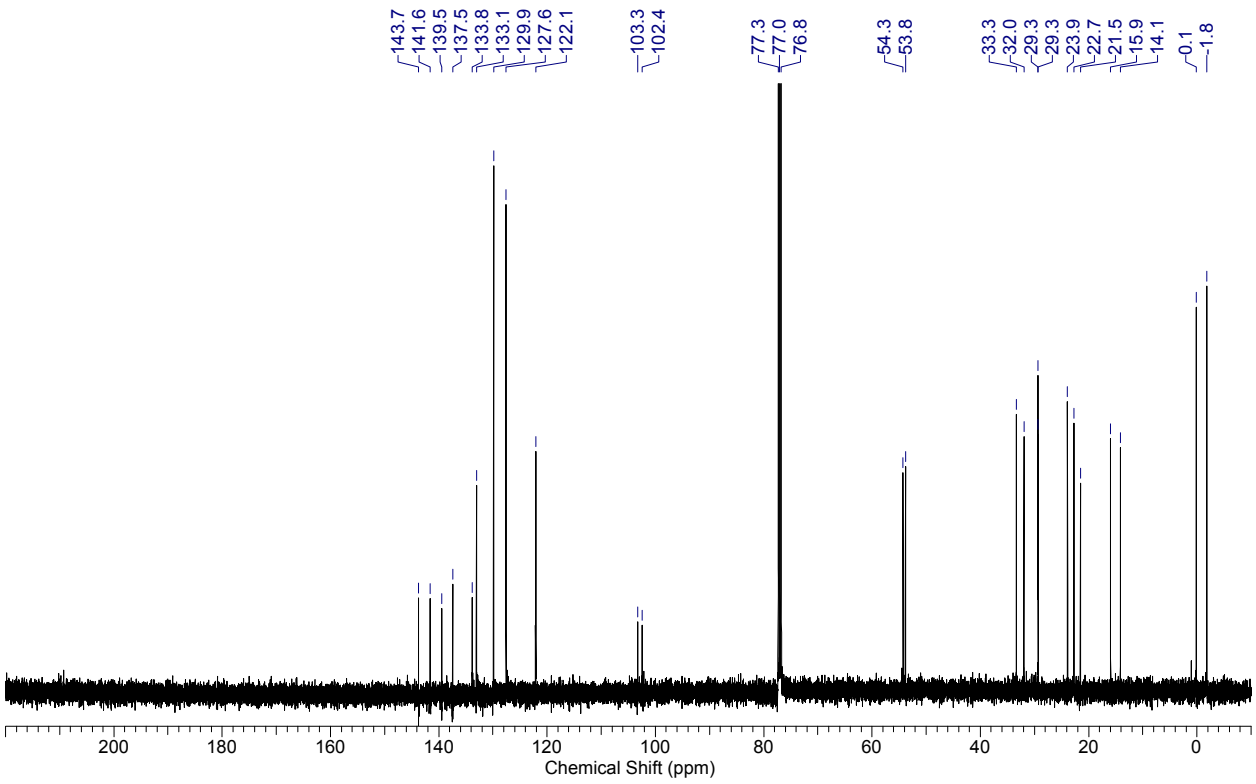
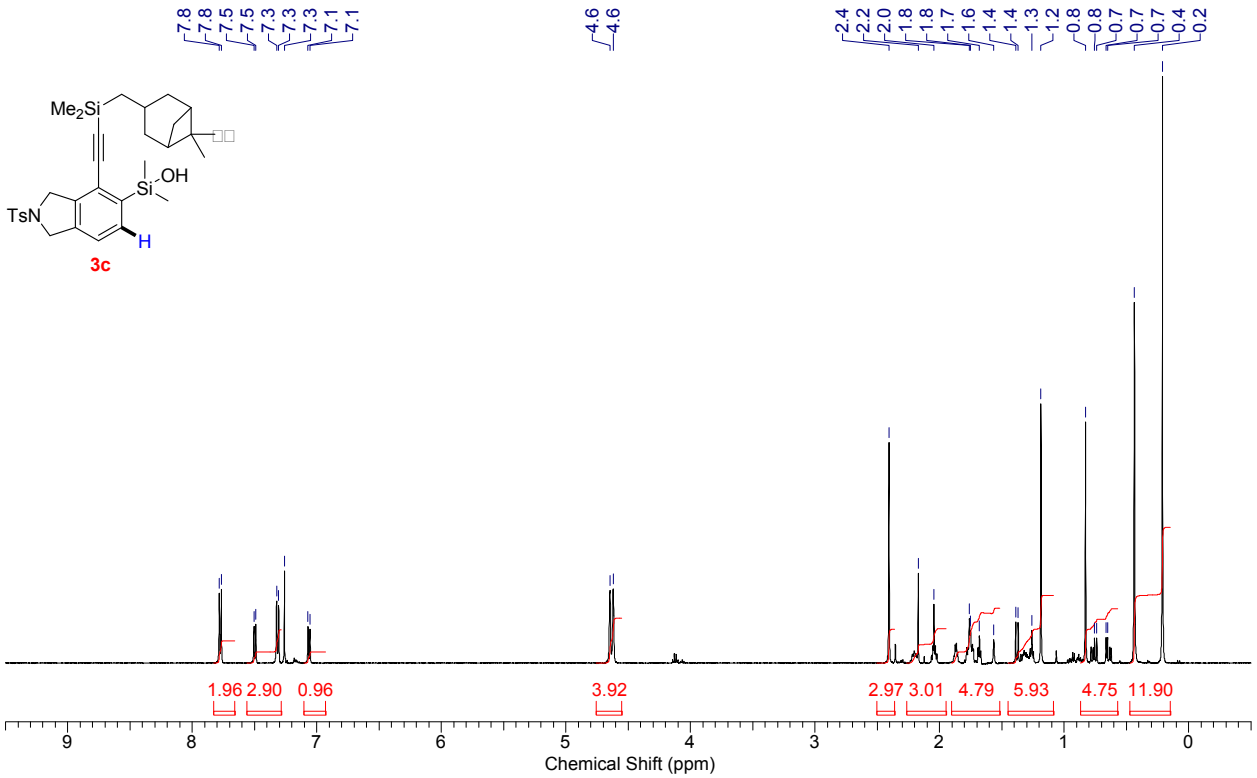
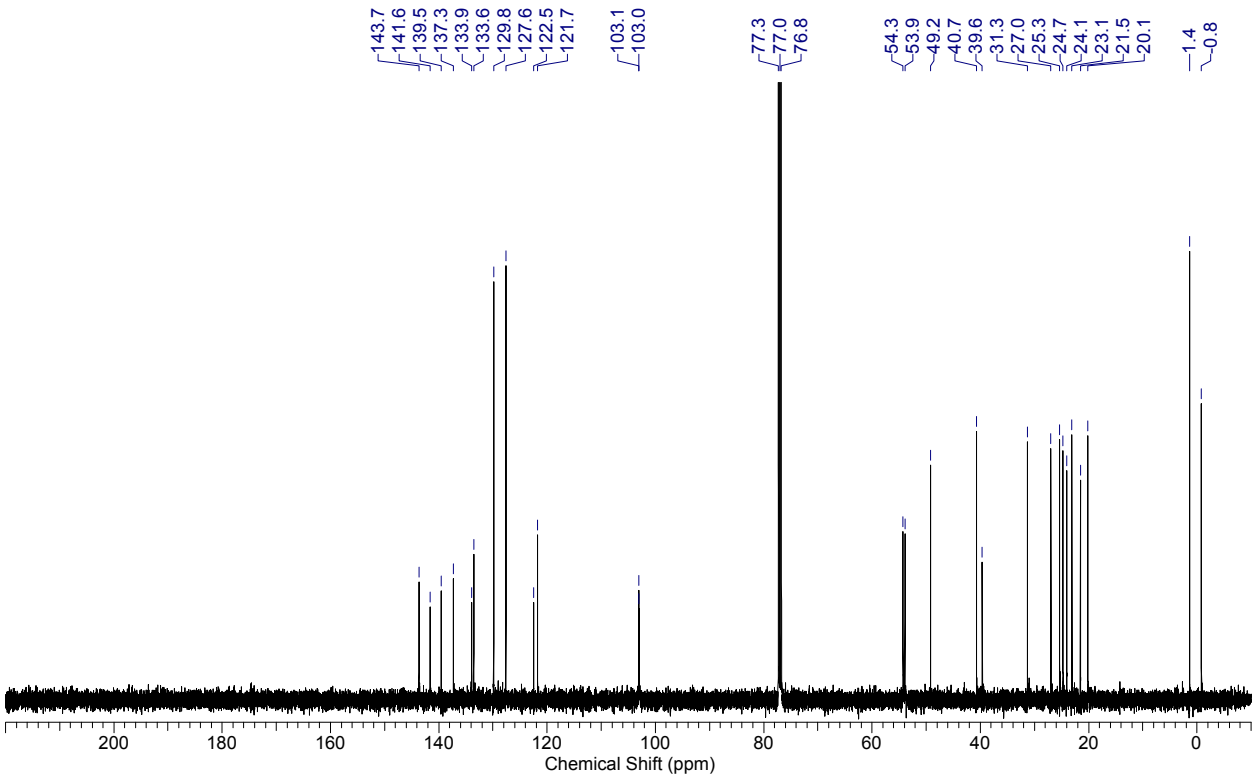
4.6
2.5
2.4
1.6
1.5
1.4
1.0
1.0
1.0
0.9
0.9
0.9
0.9
0.9
0.7
1.94
0.98
1.03
4.10
3.07
4.14
9.02
6.02
Chemical Shift (ppm)

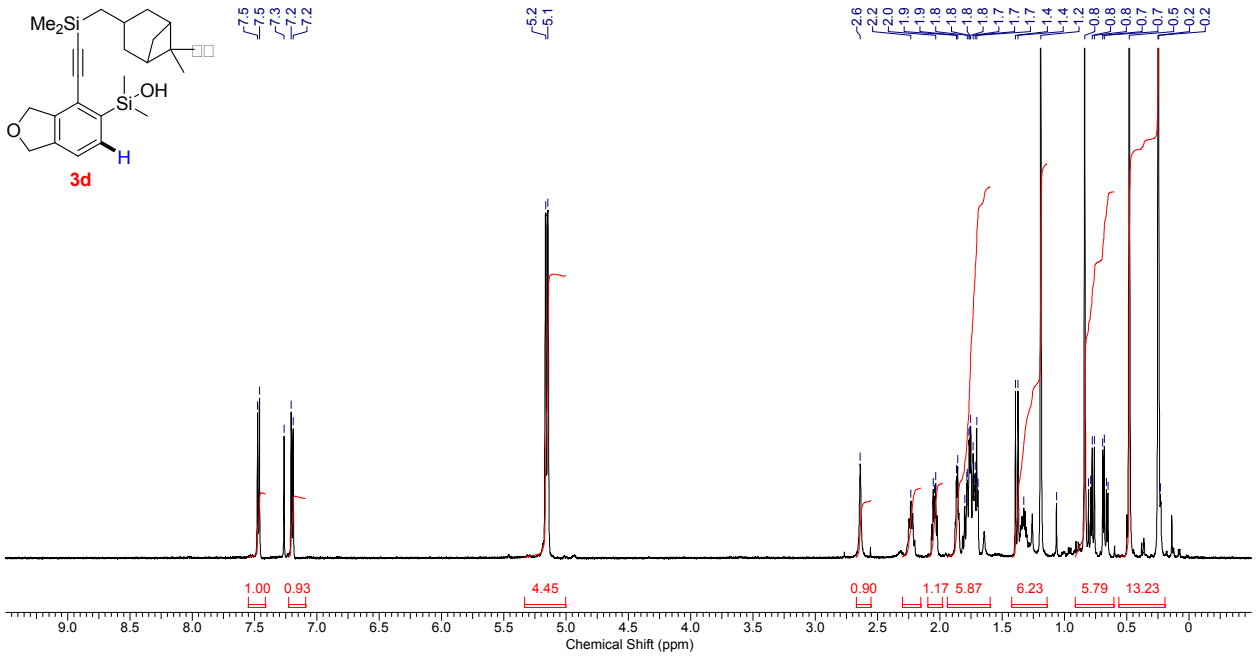

143.7
140.0
139.9
137.2
133.9
133.6
129.8
127.6
122.4
121.9
104.2
101.2
77.3
77.0
76.8
54.4
54.0
21.5
18.2
18.1
17.9
17.6
16.7
15.9
Chemical Shift (ppm)

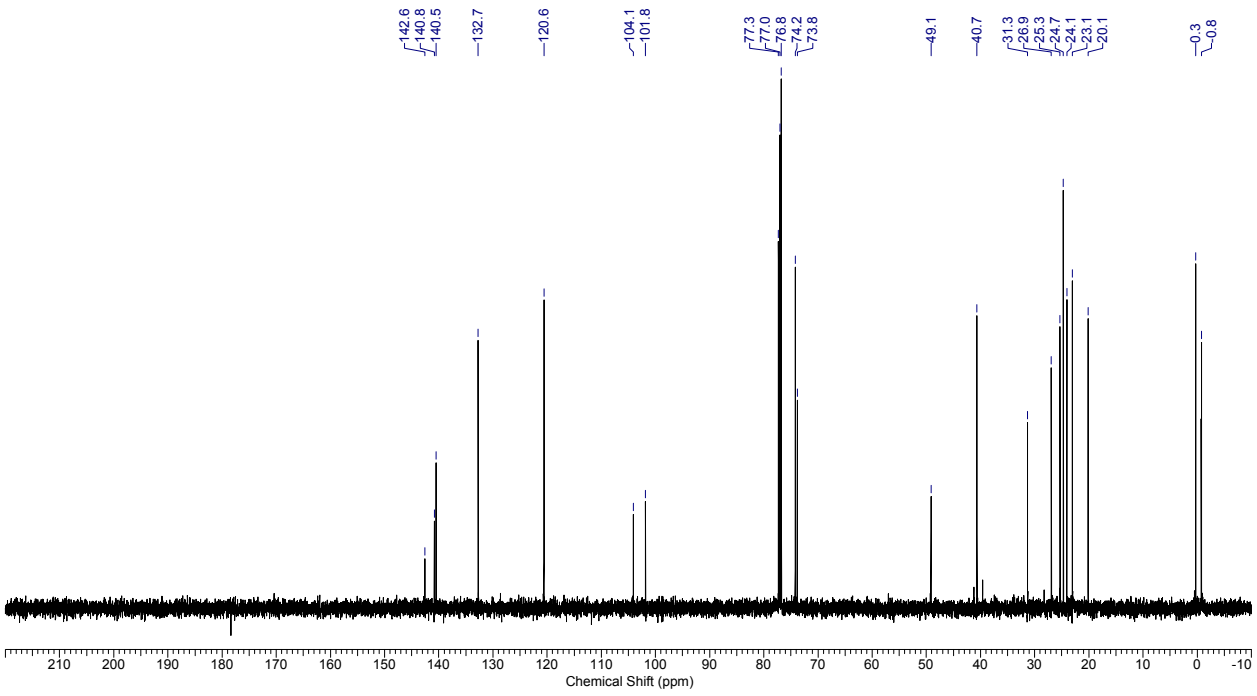

7.8
7.8
7.4
7.4
7.3
7.3
7.3
7.1
7.1
4.7
4.6
2.4
1.6
1.3
1.3
1.3
1.3
0.9
0.9
0.9
0.9
0.7
0.7
0.7
0.4
0.2
SiMe2C8H17
Si
OH
TsN
H
3b
2.00
2.76
1.00
3.83
3.96
13.15
3.23
5.47
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

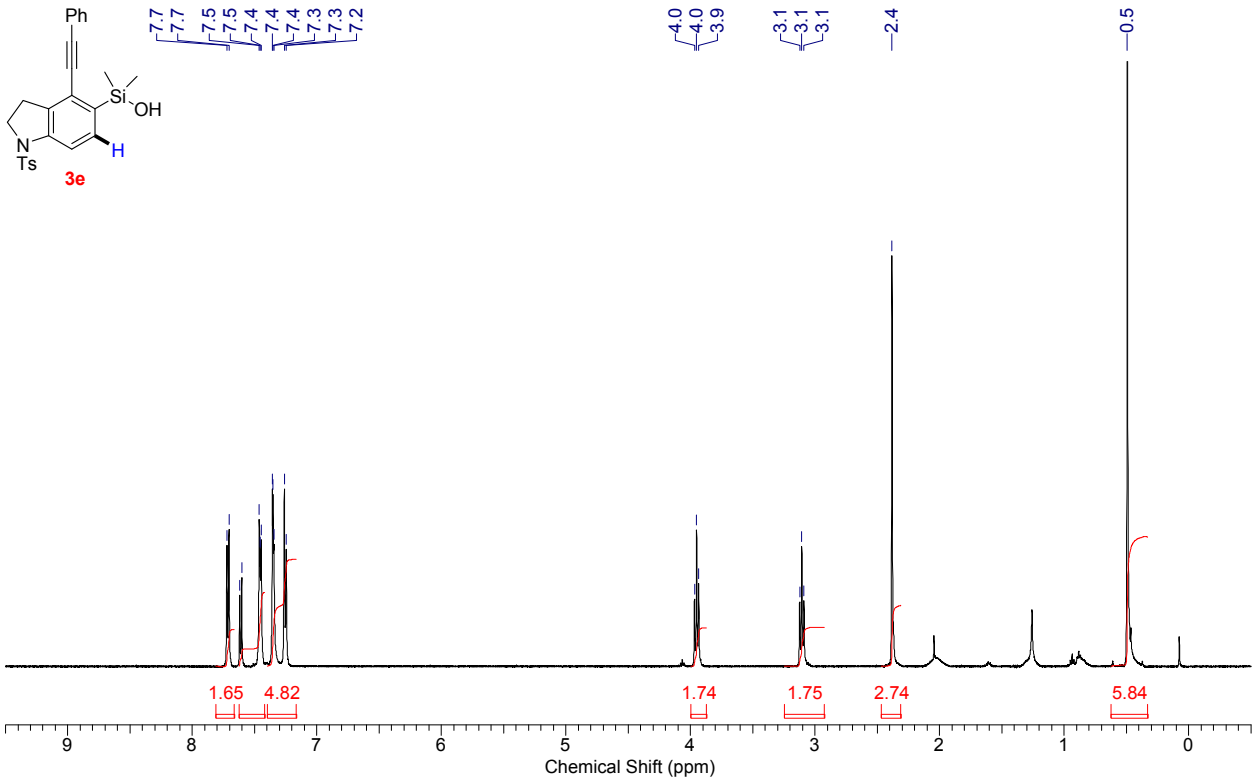

143.7
141.6
139.5
137.5
133.8
133.1
129.9
127.6
122.1
103.3
102.4
77.3
77.0
76.8
54.3
53.8
33.3
32.0
29.3
29.3
23.9
22.7
21.5
15.9
14.1
0.1
-1.8
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

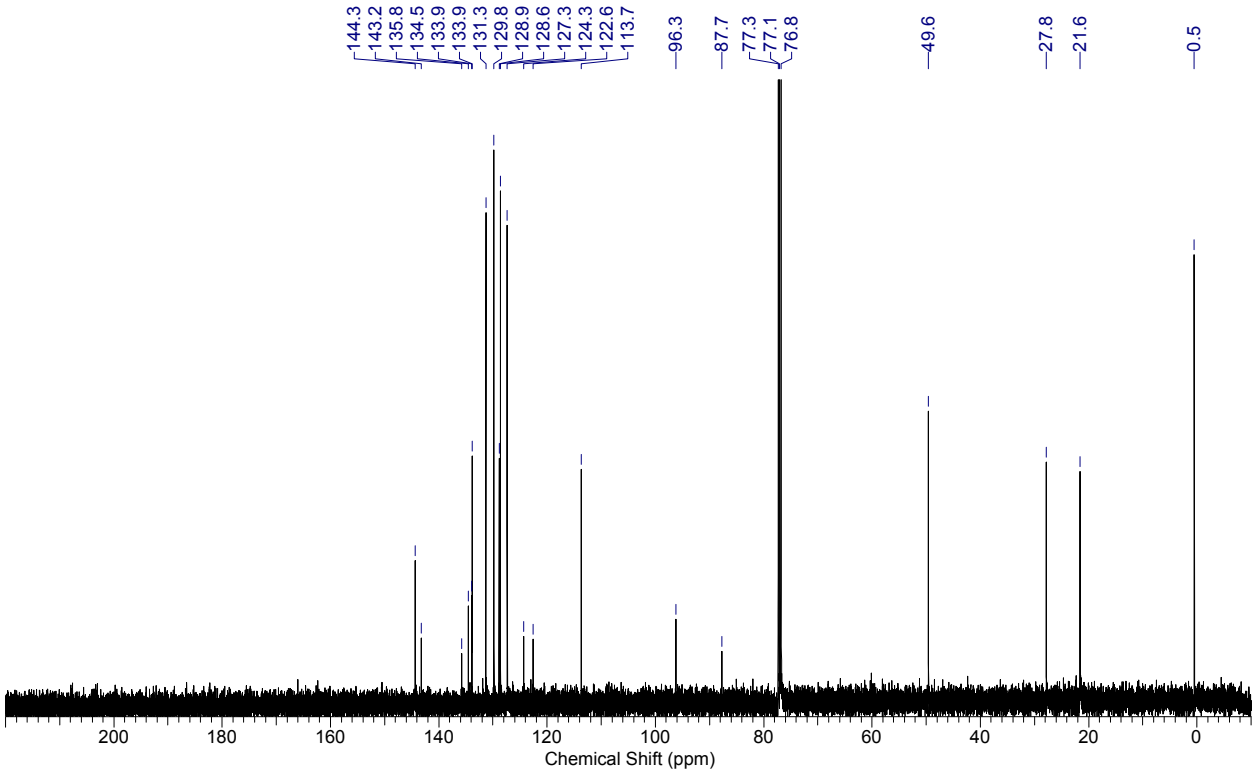

7.8
7.8
7.5
7.5
7.3
7.3
7.3
7.1
7.1
4.6
4.6
2.4
2.2
2.0
1.8
1.8
1.7
1.6
1.4
1.4
1.3
1.2
0.8
0.8
0.7
0.7
0.7
0.4
0.2
Me2Si
OH
Si
TsN
H
3c
1.96 2.90 0.96
3.92
2.97 3.01 4.79 5.93 4.75 11.90
Chemical Shift (ppm)

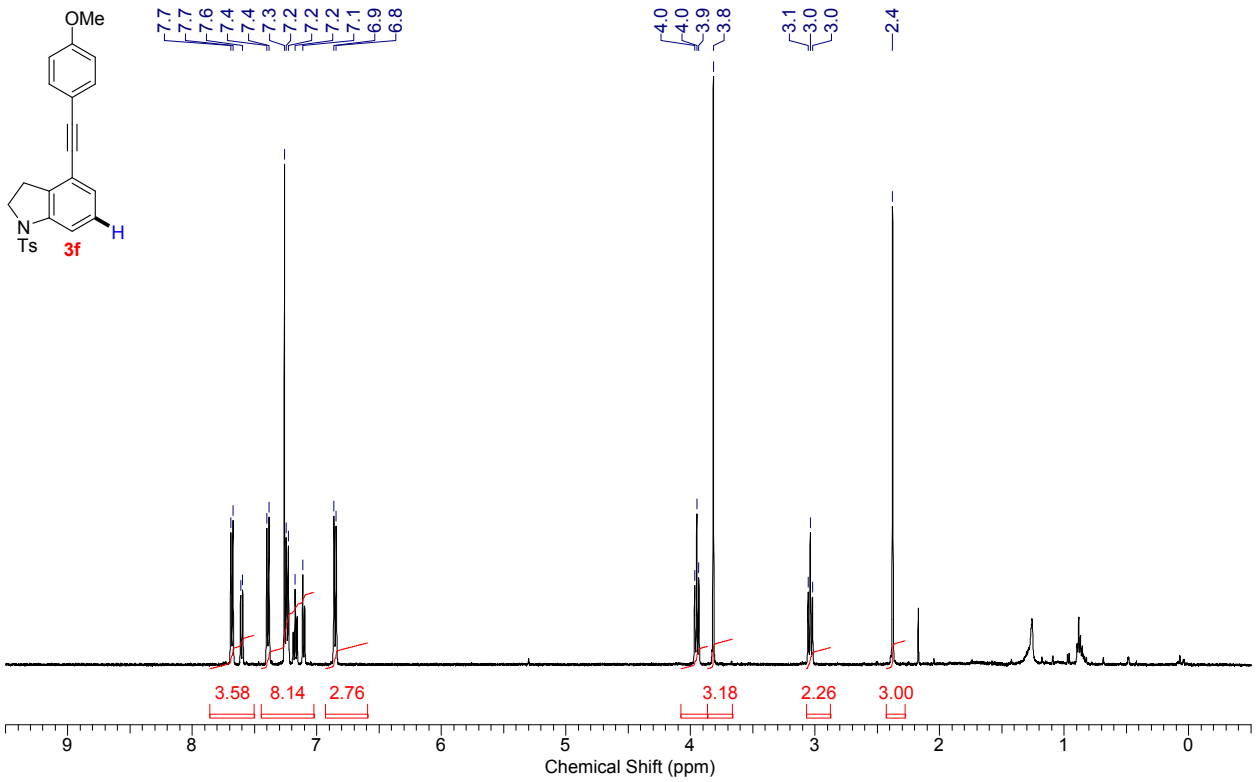

143.7
141.6
139.5
137.3
133.9
133.6
129.8
127.6
122.5
121.7
103.1
103.0
77.3
77.0
76.8
54.3
53.9
49.2
40.7
39.6
31.3
27.0
25.3
24.7
24.1
23.1
21.5
20.1
1.4
0.8
Chemical Shift (ppm)

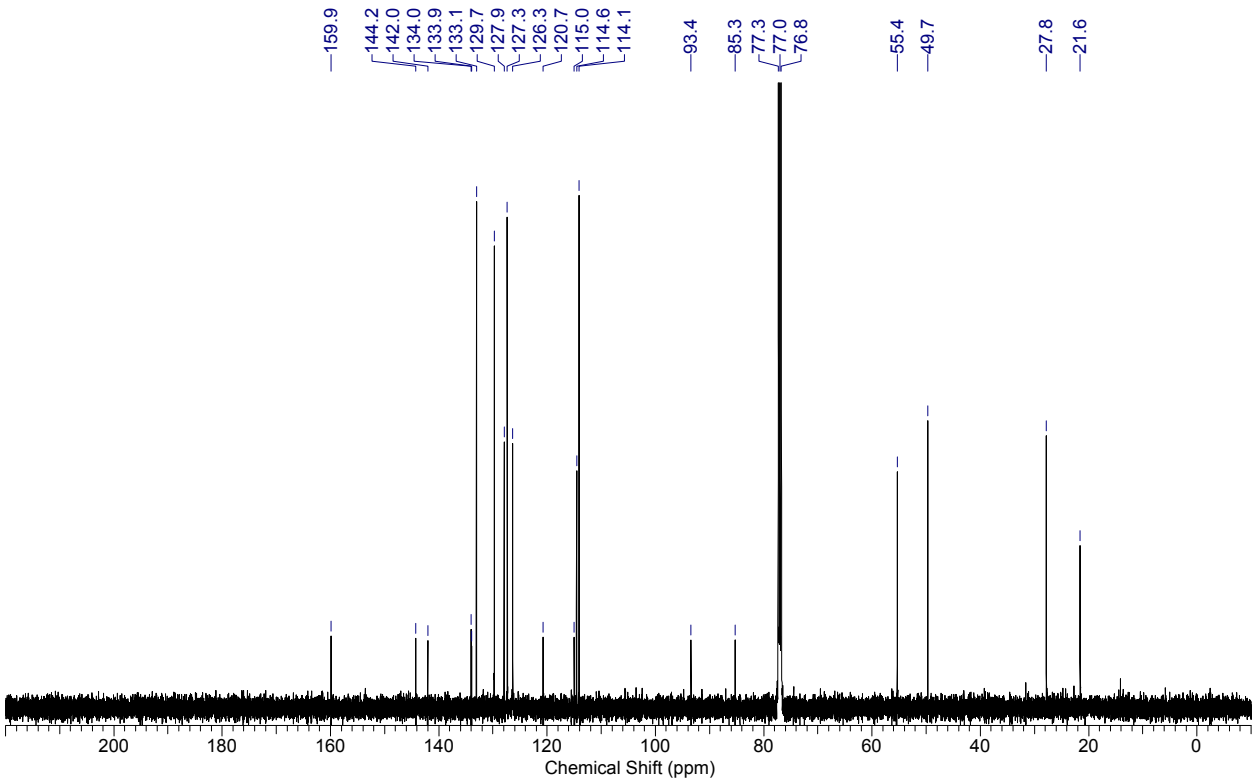

Me2Si
OH
Si
O
H
3d
7.5
7.5
7.3
7.2
7.2
5.2
5.1
2.6
2.2
2.0
1.9
1.9
1.8
1.8
1.8
1.7
1.7
1.7
1.4
1.4
1.2
0.8
0.8
0.8
0.7
0.7
0.5
0.2
0.2
1.00
0.93
4.45
0.90
1.17
5.87
6.23
5.79
13.23
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

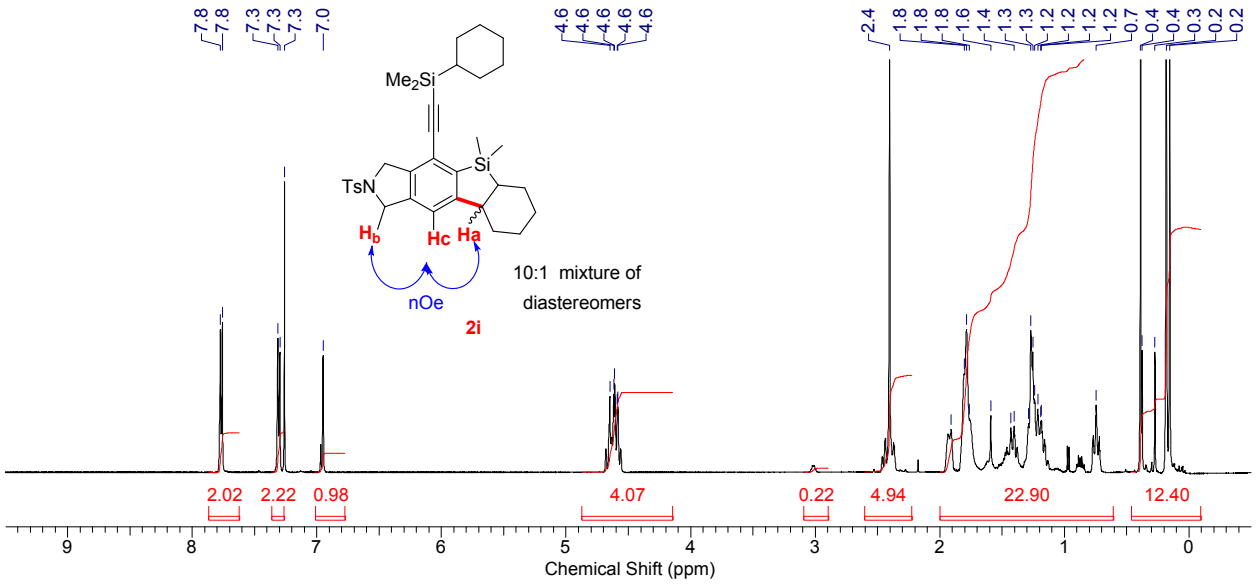

142.6
140.8
140.5
132.7
120.6
104.1
101.8
77.3
77.0
76.8
74.2
73.8
49.1
40.7
31.3
26.9
25.3
24.7
24.1
23.1
20.1
0.3
0.8
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
Chemical Shift (ppm)

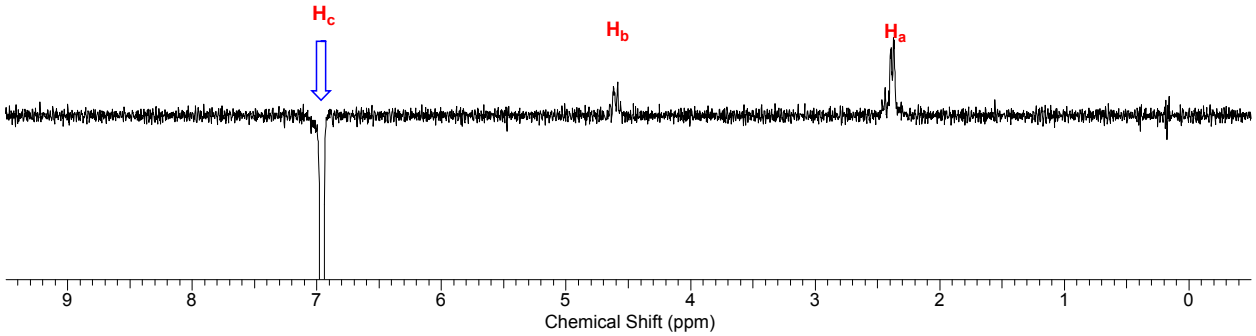

Ph
Si
OH
N
Ts
H
3e
7.7
7.7
7.5
7.5
7.4
7.4
7.4
7.3
7.3
7.2
4.0
4.0
3.9
3.1
3.1
3.1
2.4
0.5
1.65
4.82
1.74
1.75
2.74
5.84
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

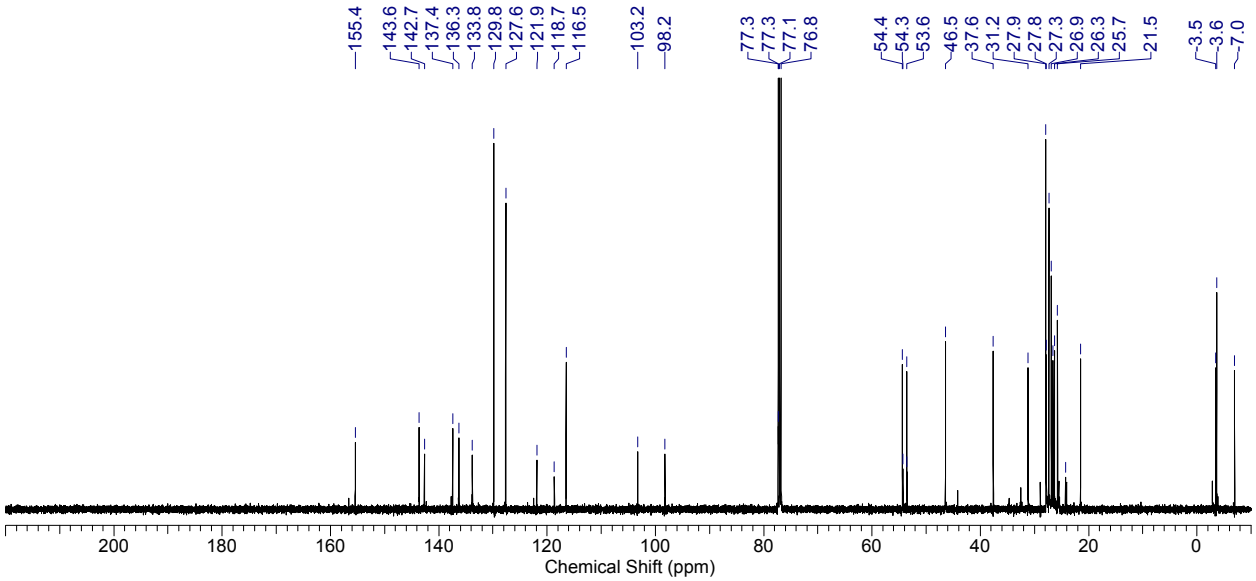

144.3
143.2
135.8
134.5
133.9
133.9
131.3
129.8
128.9
128.6
127.3
124.3
122.6
113.7
96.3
87.7
77.3
77.1
76.8
49.6
27.8
21.6
0.5
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

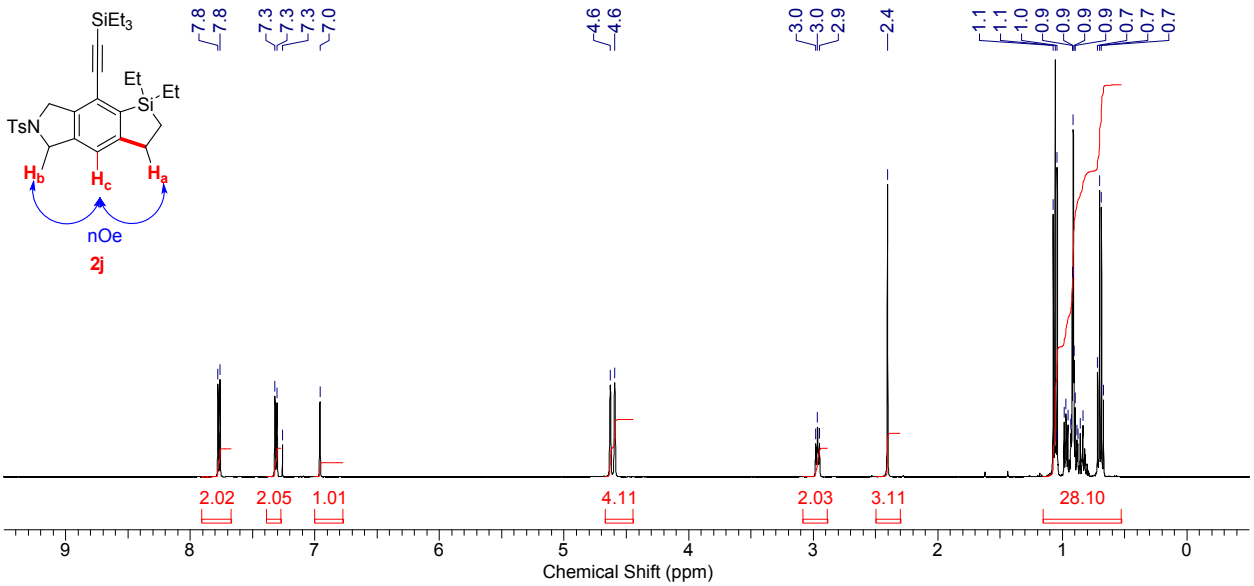

OMe
N
Ts
H
3f
7.7
7.7
7.6
7.4
7.4
7.3
7.2
7.2
7.2
7.1
6.9
6.8
4.0
4.0
3.9
3.8
3.1
3.0
3.0
2.4
3.58
8.14
2.76
3.18
2.26
3.00
Chemical Shift (ppm)

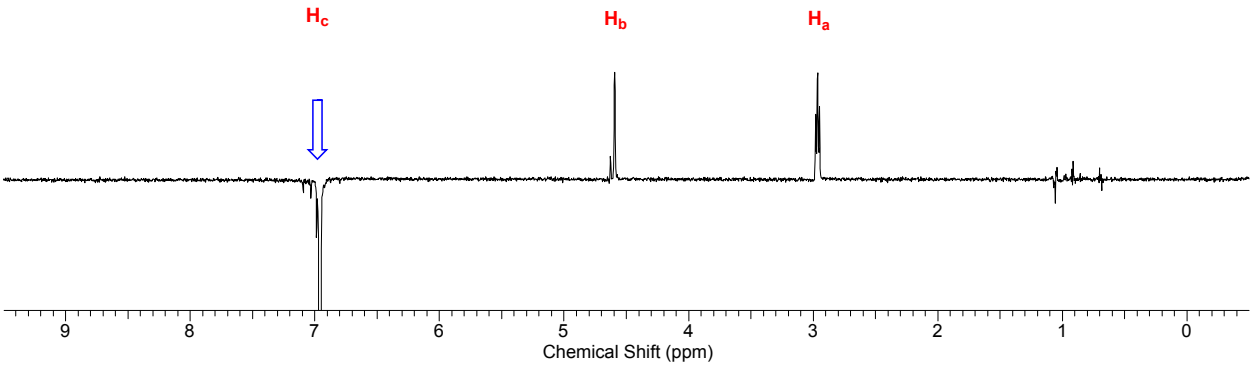

159.9
144.2
142.0
134.0
133.9
133.1
129.7
127.9
127.3
126.3
120.7
115.0
114.6
114.1
93.4
85.3
77.3
77.0
76.8
55.4
49.7
27.8
21.6
Chemical Shift (ppm)

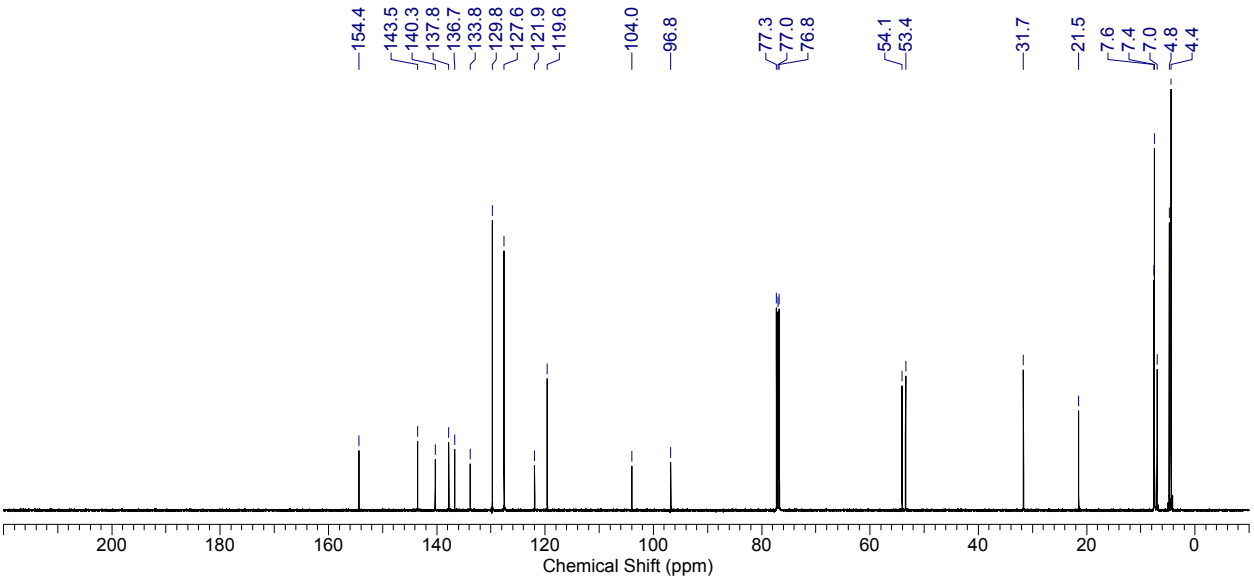

7.8
7.8
7.3
7.3
7.3
7.0
4.6
4.6
4.6
4.6
4.6
2.4
1.8
1.8
1.8
1.6
1.4
1.3
1.3
1.2
1.2
1.2
1.2
0.7
0.4
0.4
0.3
0.2
0.2
Me2Si
Si
TsN
Hb
Hc
Ha
nOe
2i
10:1 mixture of
diastereomers
2.02
2.22
0.98
4.07
0.22
4.94
22.90
12.40
Chemical Shift (ppm)

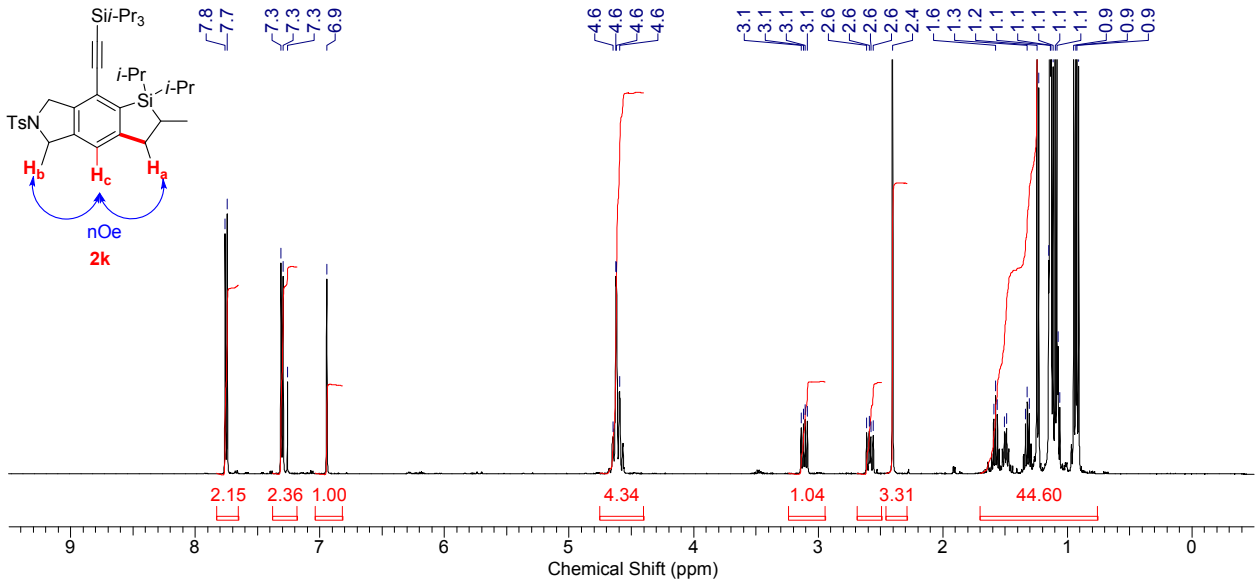

Hc
Hb
Ha
Chemical Shift (ppm)

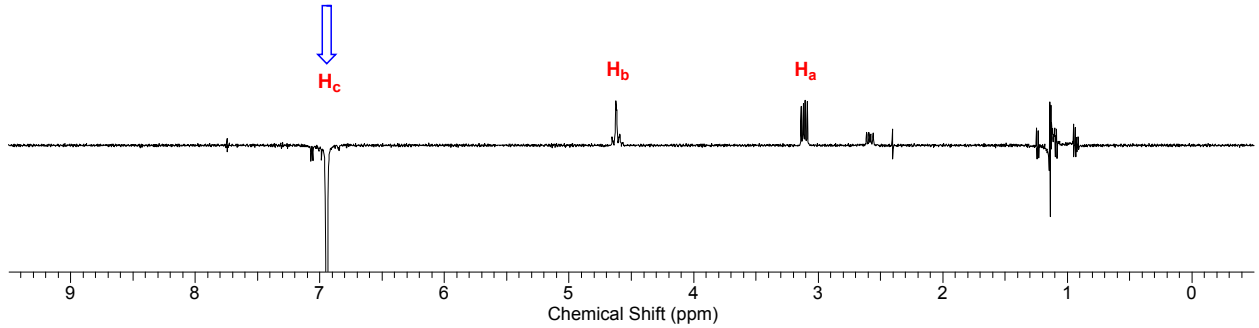

155.4
143.6
142.7
137.4
136.3
133.8
129.8
127.6
121.9
118.7
116.5
103.2
98.2
77.3
77.3
77.1
76.8
54.4
54.3
53.6
46.5
37.6
31.2
27.9
27.8
27.3
26.9
26.3
25.7
21.5
3.5
3.6
7.0
Chemical Shift (ppm)

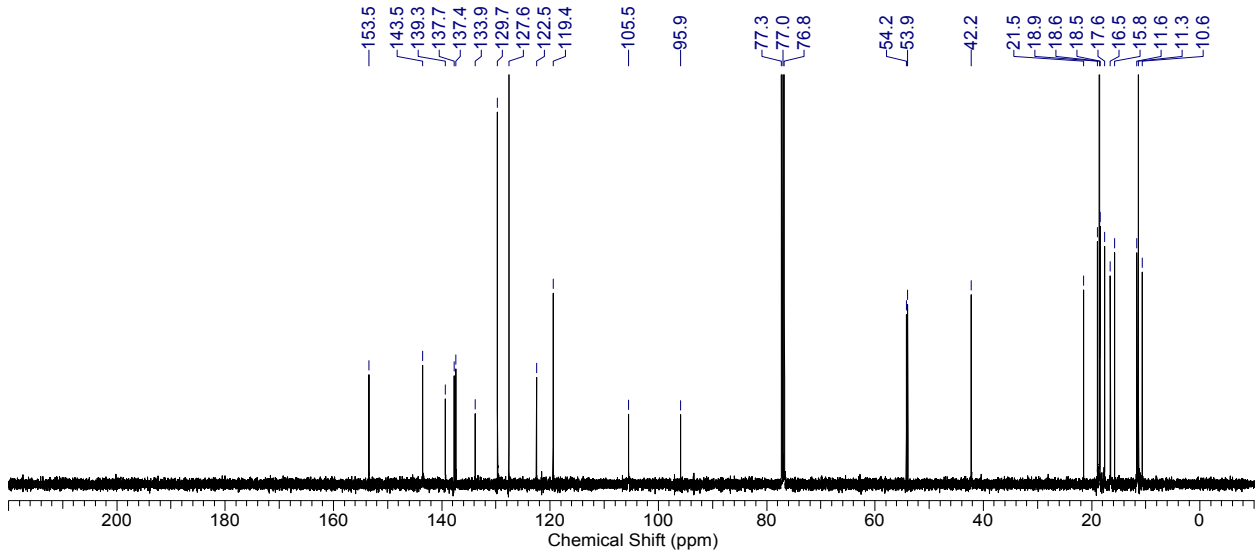

SiEt3
Et
Et
Si
TsN
Hb
Hc
Ha
nOe
2j
7.8
7.8
7.3
7.3
7.3
7.0
4.6
4.6
3.0
3.0
2.9
2.4
1.1
1.1
1.0
0.9
0.9
0.9
0.9
0.7
0.7
0.7
2.02
2.05
1.01
4.11
2.03
3.11
28.10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

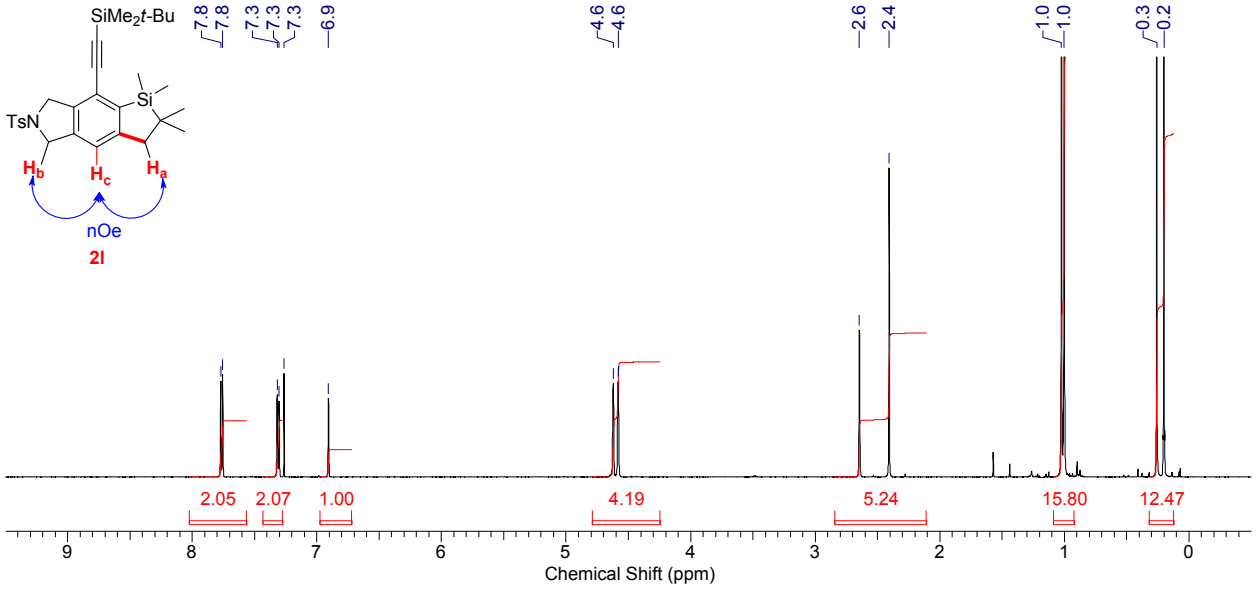

Hc
Hb
Ha
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

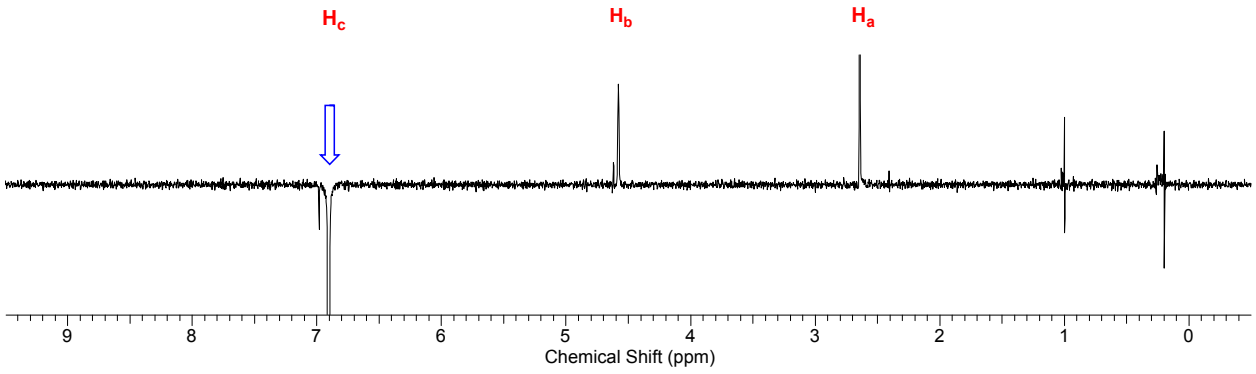

154.4
143.5
140.3
137.8
136.7
133.8
129.8
127.6
121.9
119.6
104.0
96.8
77.3
77.0
76.8
54.1
53.4
31.7
21.5
7.6
7.4
7.0
4.8
4.4
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

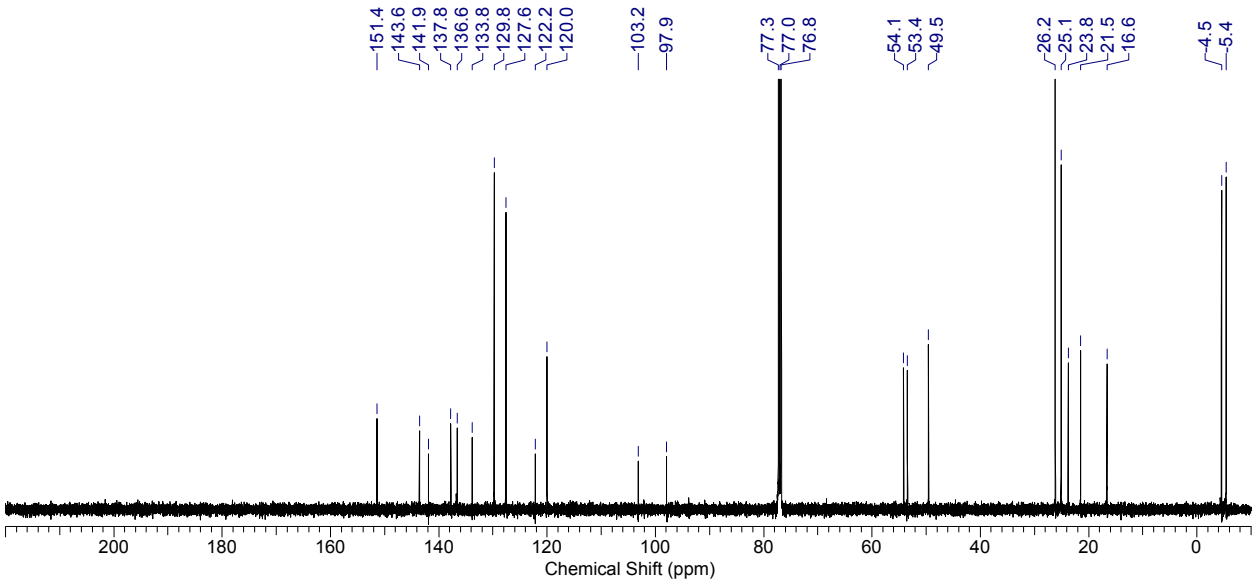

Si*i*-Pr3
i-Pr
i-Pr
Si
TsN
Hb
Hc
Ha
nOe
2k
7.8
7.7
7.3
7.3
7.3
6.9
4.6
4.6
4.6
4.6
3.1
3.1
3.1
3.1
2.6
2.6
2.6
2.6
2.4
1.6
1.3
1.2
1.1
1.1
1.1
1.1
1.1
0.9
0.9
0.9
2.15
2.36
1.00
4.34
1.04
3.31
44.60
Chemical Shift (ppm)

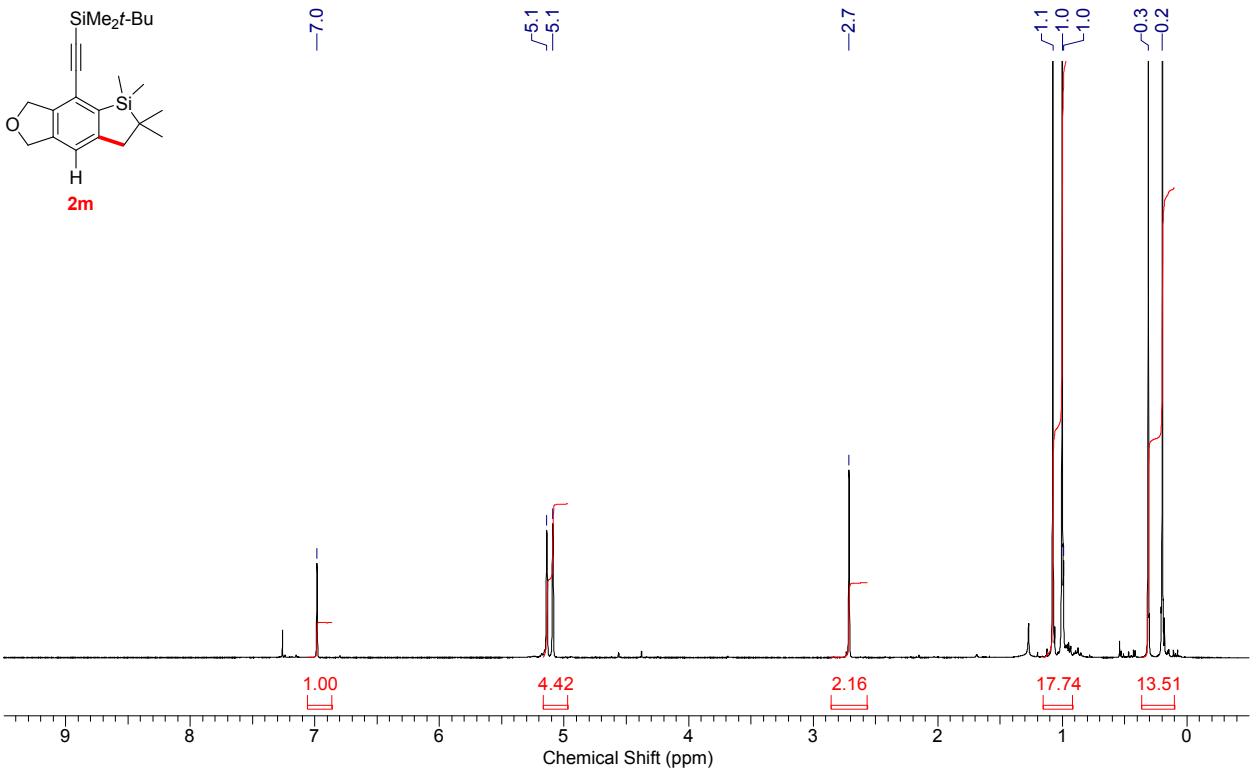

Hc
Hb
Ha
Chemical Shift (ppm)

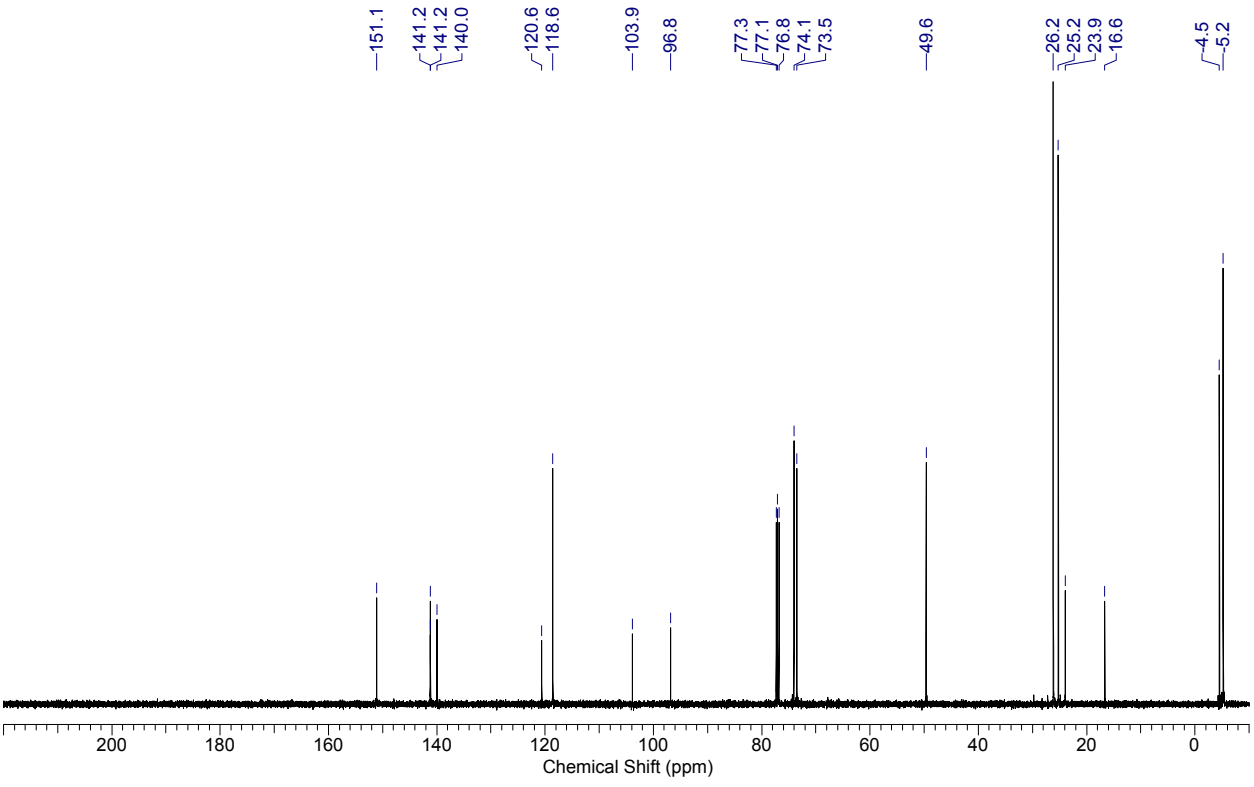

153.5
143.5
139.3
137.7
137.4
133.9
129.7
127.6
122.5
119.4
105.5
95.9
77.3
77.0
76.8
54.2
53.9
42.2
21.5
18.9
18.6
18.5
17.6
16.5
15.8
11.6
11.3
10.6
Chemical Shift (ppm)

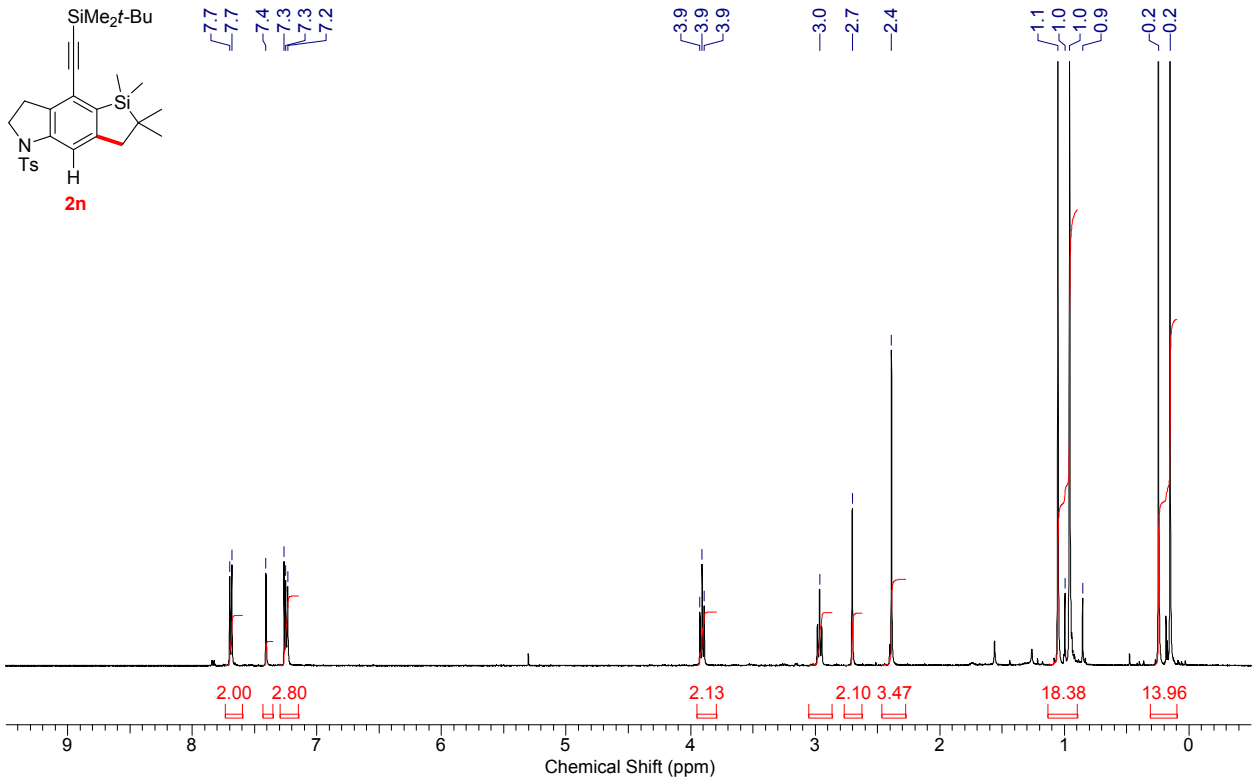

SiMe2t-Bu
TsN
Si
Hb
Hc
Ha
nOe
2l
7.8
7.8
7.3
7.3
7.3
6.9
4.6
4.6
2.6
2.4
1.0
1.0
0.3
0.2
2.05
2.07
1.00
4.19
5.24
15.80
12.47
Chemical Shift (ppm)

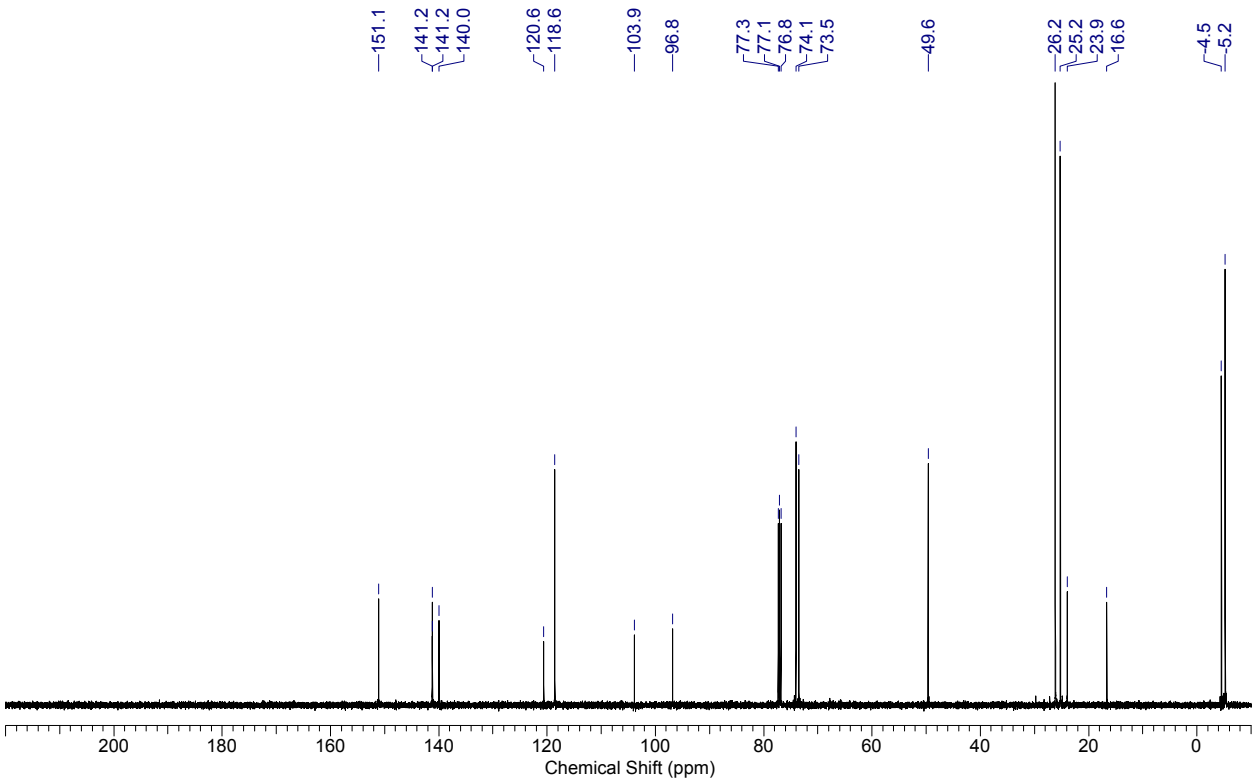

Hc
Hb
Ha
Chemical Shift (ppm)

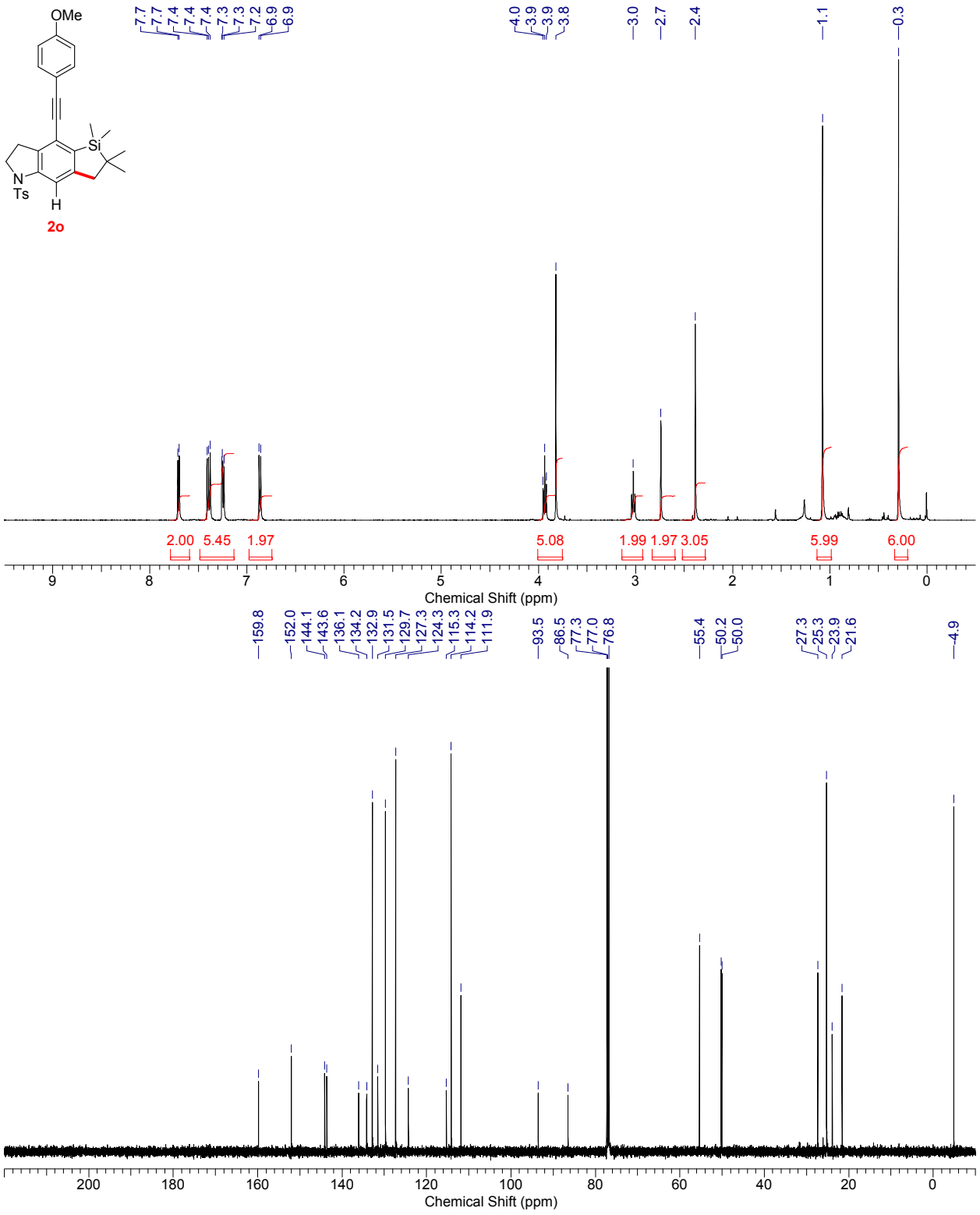

151.4
143.6
141.9
137.8
136.6
133.8
129.8
127.6
122.2
120.0
103.2
97.9
77.3
77.0
76.8
54.1
53.4
49.5
26.2
25.1
23.8
21.5
16.6
4.5
5.4
Chemical Shift (ppm)

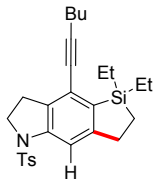

SiMe2t-Bu
Si
O
H
2m
7.0
5.1
5.1
2.7
1.1
1.0
1.0
0.3
0.2
1.00
4.42
2.16
17.74
13.51
Chemical Shift (ppm)


151.1
141.2
141.2
140.0
120.6
118.6
103.9
96.8
77.3
77.1
76.8
74.1
73.5
49.6
26.2
25.2
23.9
16.6
4.5
5.2
Chemical Shift (ppm)


SiMe2t-Bu
Si
N
Ts
H
2n
7.7
7.7
7.4
7.3
7.3
7.2
3.9
3.9
3.9
3.0
2.7
2.4
1.1
1.0
1.0
0.9
0.2
0.2
2.00
2.80
2.13
2.10
3.47
18.38
13.96
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

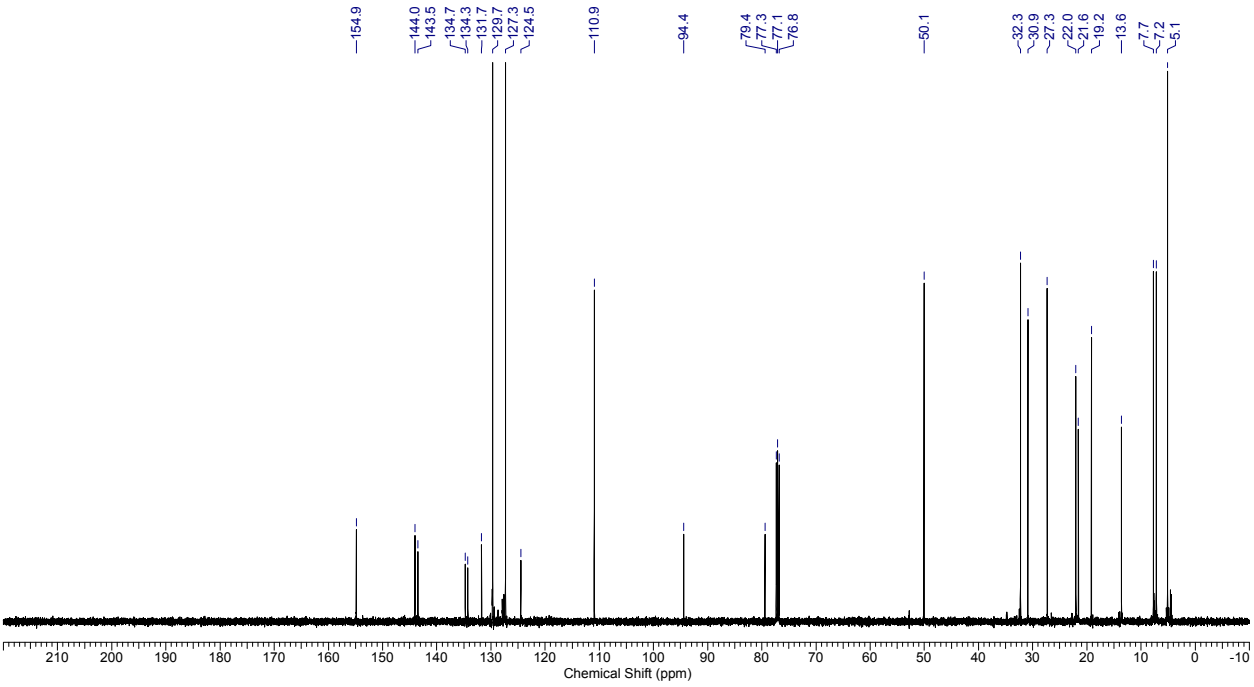

151.1
141.2
141.2
140.0
120.6
118.6
103.9
96.8
77.3
77.1
76.8
74.1
73.5
49.6
26.2
25.2
23.9
16.6
4.5
5.2
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

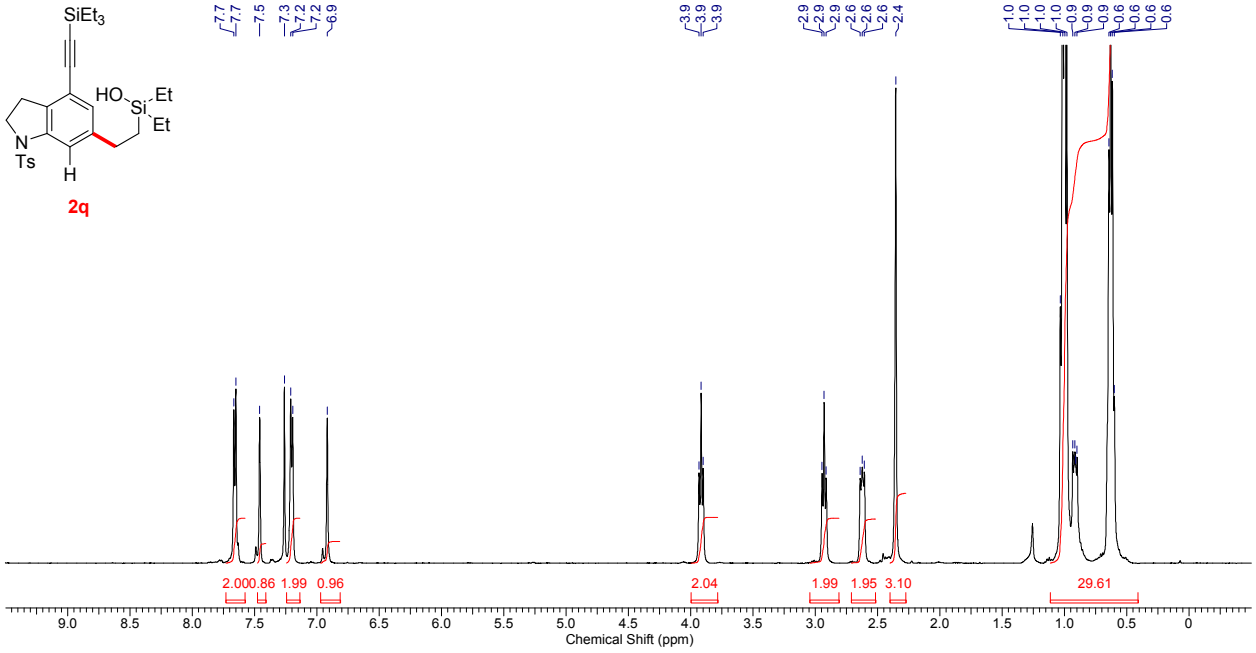

OMe
Si
N
Ts
H
2o
7.7
7.7
7.4
7.4
7.4
7.3
7.3
7.2
6.9
6.9
4.0
3.9
3.9
3.8
3.0
2.7
2.4
1.1
0.3
2.00
5.45
1.97
5.08
1.99
1.97
3.05
5.99
6.00
Chemical Shift (ppm)
159.8
152.0
144.1
143.6
136.1
134.2
132.9
131.5
129.7
127.3
124.3
115.3
114.2
111.9
93.5
86.5
77.3
77.0
76.8
55.4
50.2
50.0
27.3
25.3
23.9
21.6
4.9
Chemical Shift (ppm)

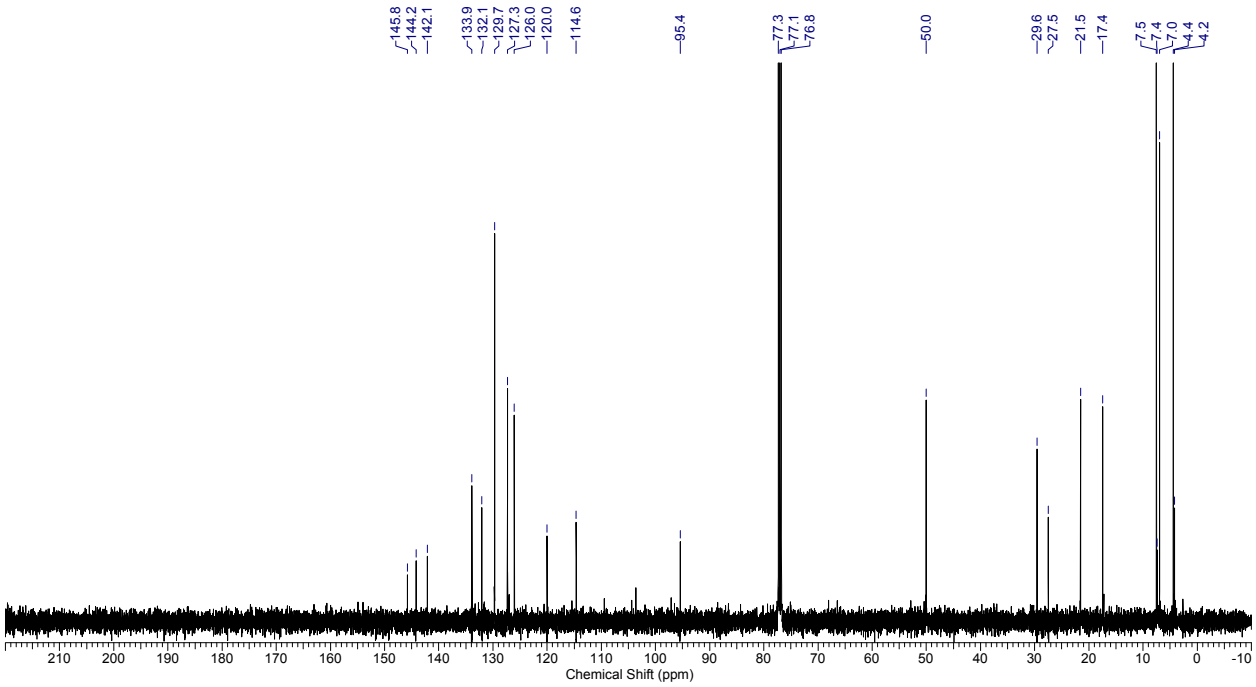

Bu
Et
Si
Et
N
Ts
H

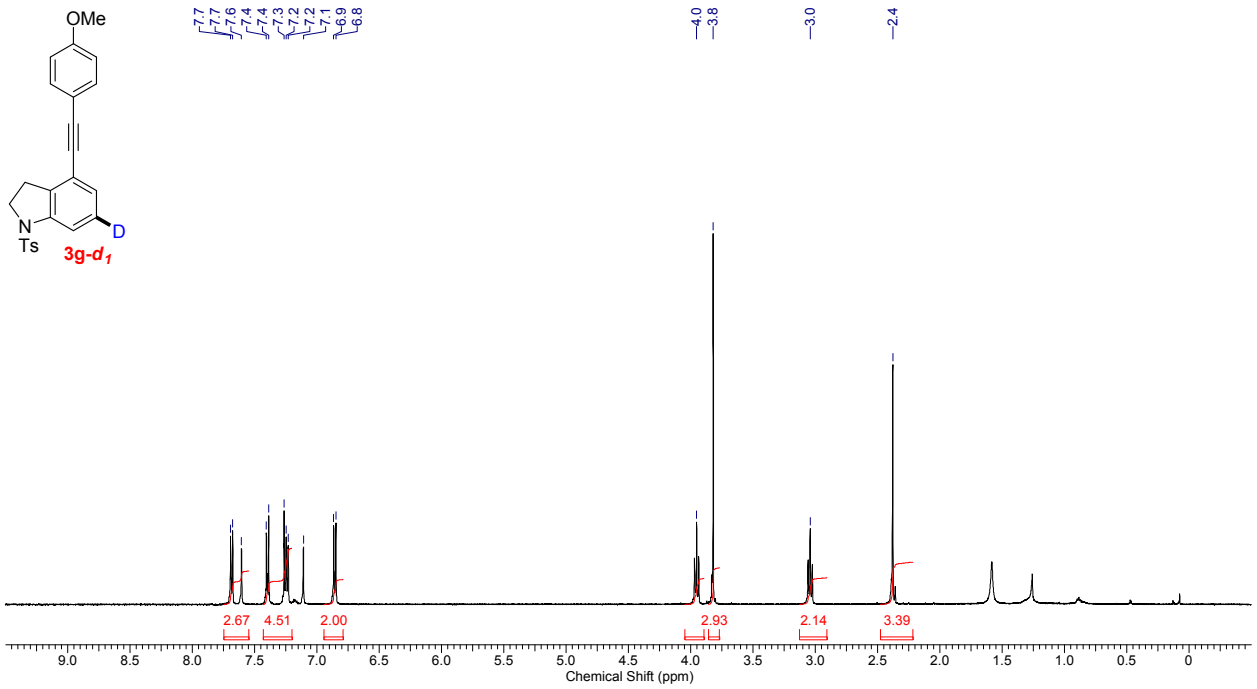
2p

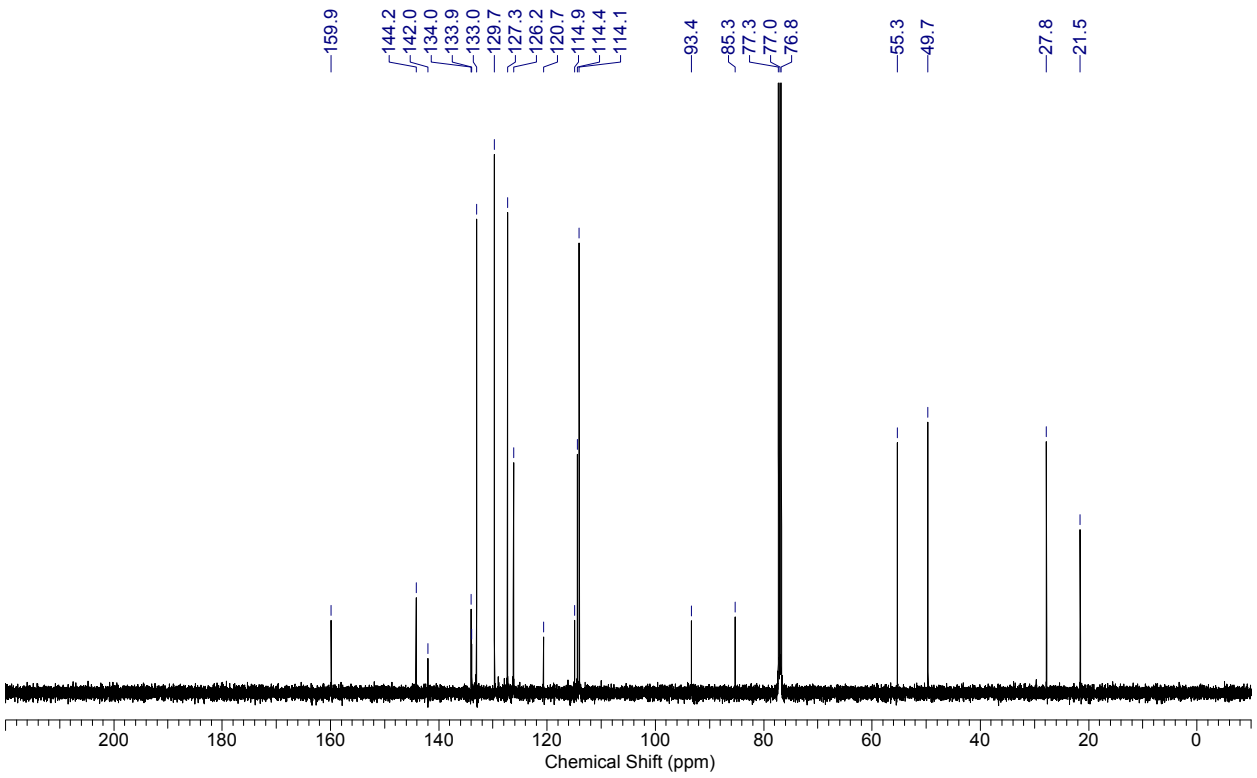
7.7
7.7
7.4
7.2
7.2
3.9
3.9
3.9
3.0
3.0
3.0
2.9
2.9
2.9
2.4
2.4
2.4
1.5
1.5
1.4
1.0
1.0
0.9
0.9
0.9
0.8
0.8
0.8
2.00
2.34
2.13
4.20
5.42
4.51
16.55
Chemical Shift (ppm)

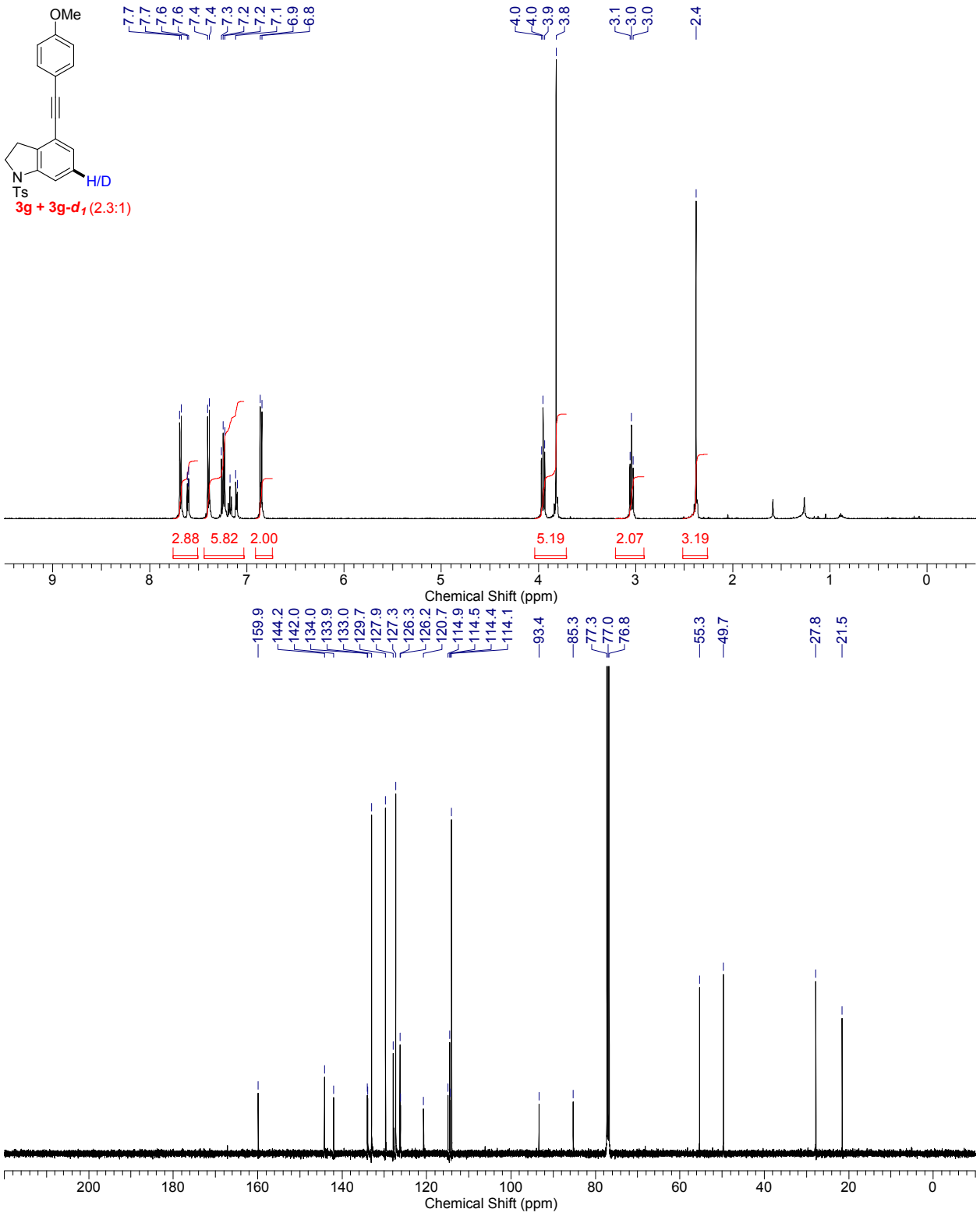

154.9
144.0
143.5
134.7
134.3
131.7
129.7
127.3
124.5
110.9
94.4
79.4
77.3
77.1
76.8
50.1
32.3
30.9
27.3
22.0
21.6
19.2
13.6
7.7
7.2
5.1
Chemical Shift (ppm)

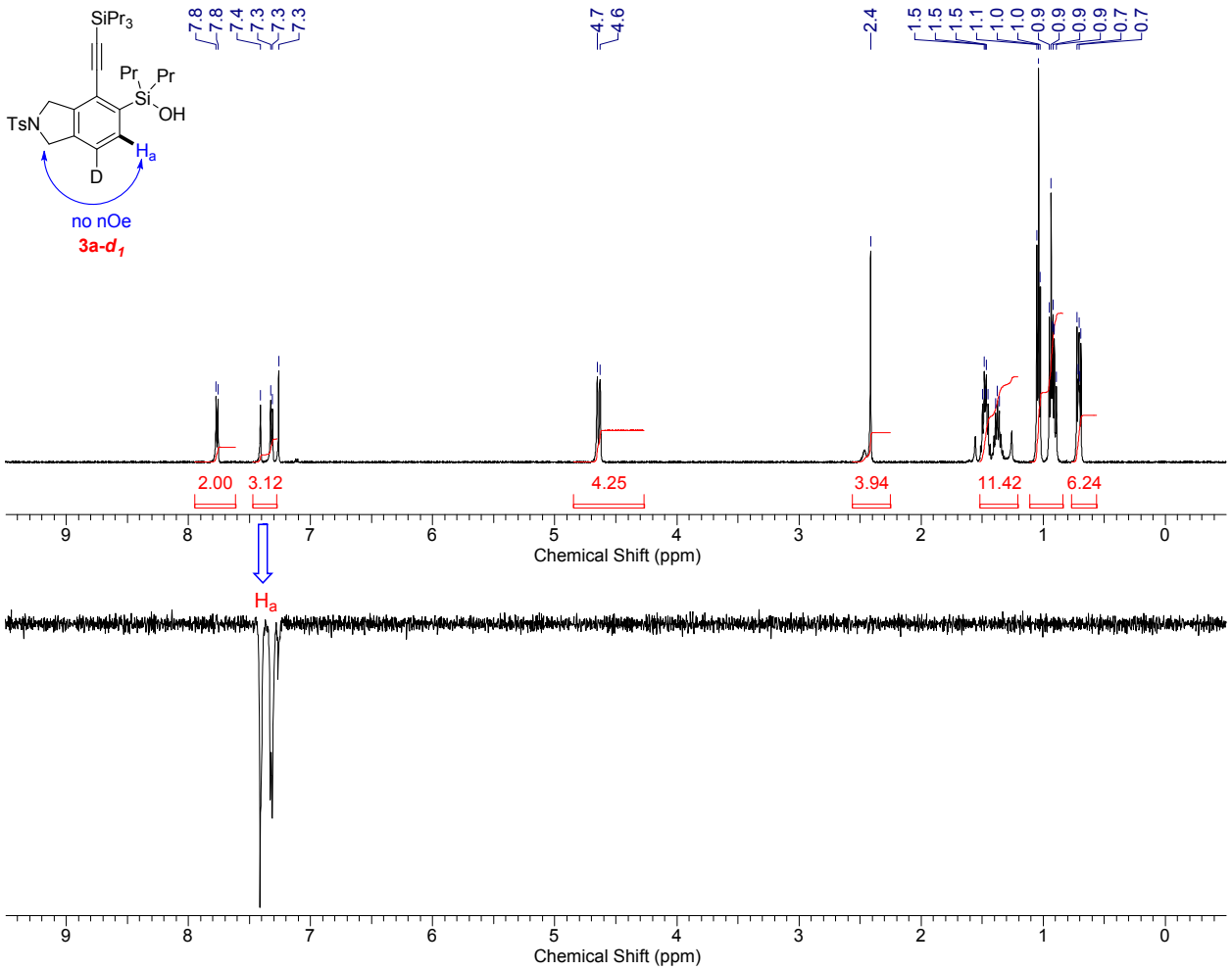

SiEt3
HO
Si
Et
Et
N
Ts
H
2q
7.7
7.7
7.5
7.3
7.2
7.2
6.9
3.9
3.9
3.9
2.9
2.9
2.9
2.6
2.6
2.6
2.4
1.0
1.0
1.0
1.0
0.9
0.9
0.9
0.6
0.6
0.6
0.6
2.00
0.86
1.99
0.96
2.04
1.99
1.95
3.10
29.61
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

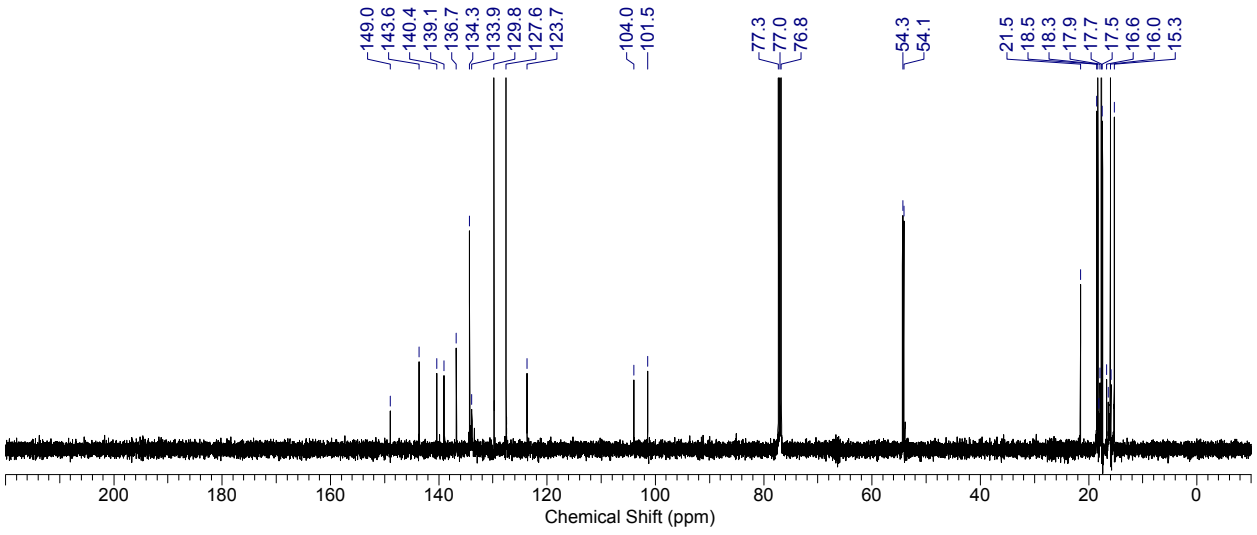

145.8
144.2
142.1
133.9
132.1
129.7
127.3
126.0
120.0
114.6
95.4
77.3
77.1
76.8
50.0
29.6
27.5
21.5
17.4
7.5
7.4
7.0
4.4
4.2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
Chemical Shift (ppm)

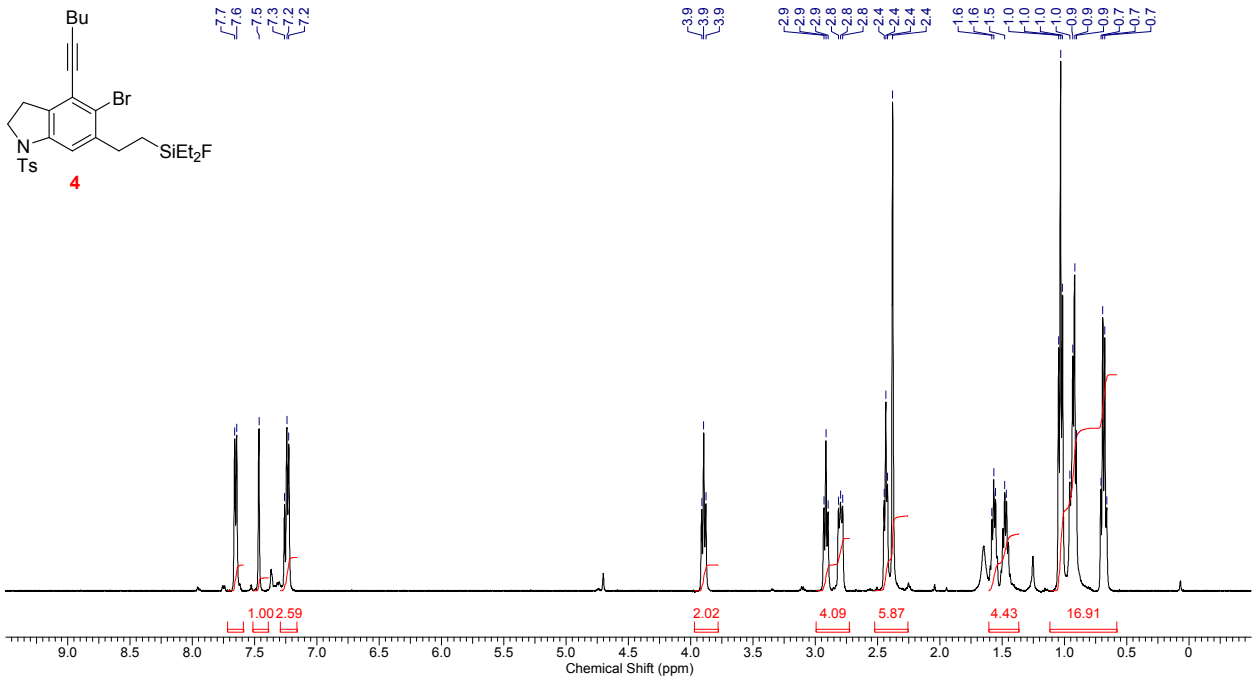

OMe
N
Ts
D
3g-d_1
7.7
7.7
7.6
7.4
7.4
7.3
7.2
7.2
7.1
6.9
6.8
4.0
3.8
3.0
2.4
2.67
4.51
2.00
2.93
2.14
3.39
Chemical Shift (ppm)

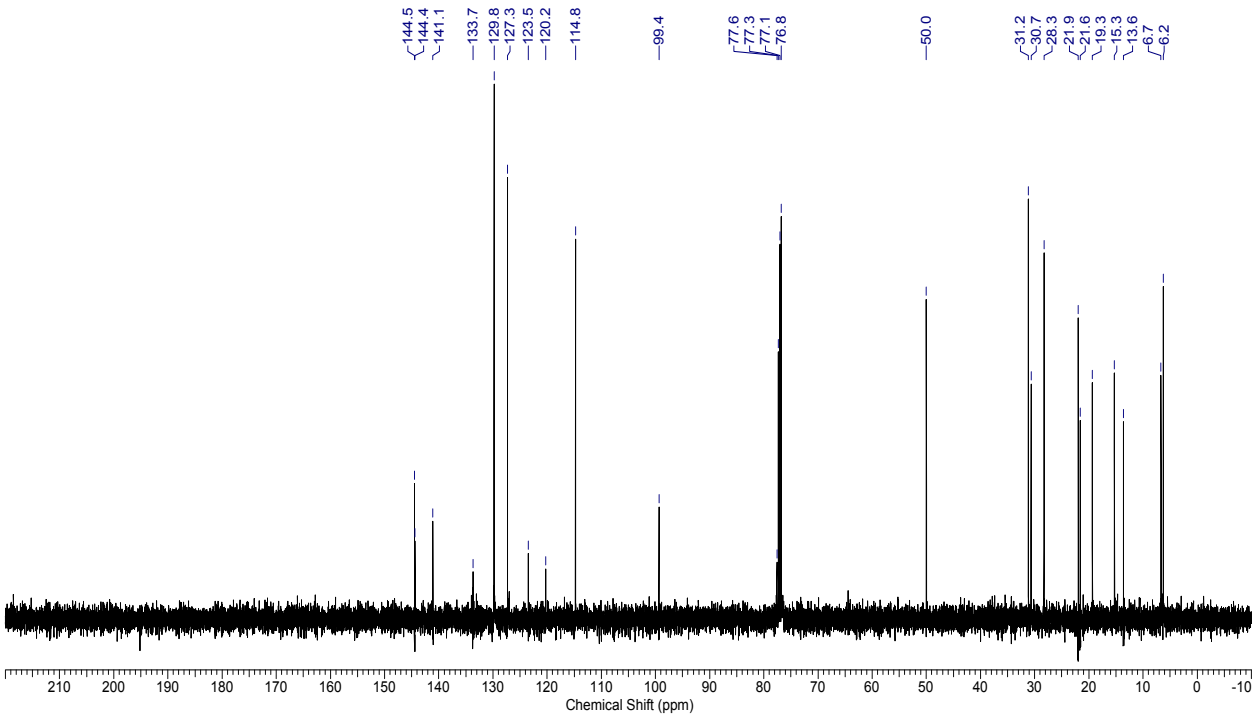

159.9
144.2
142.0
134.0
133.9
133.0
129.7
127.3
126.2
120.7
114.9
114.4
114.1
93.4
85.3
77.3
77.0
76.8
55.3
49.7
27.8
21.5
Chemical Shift (ppm)

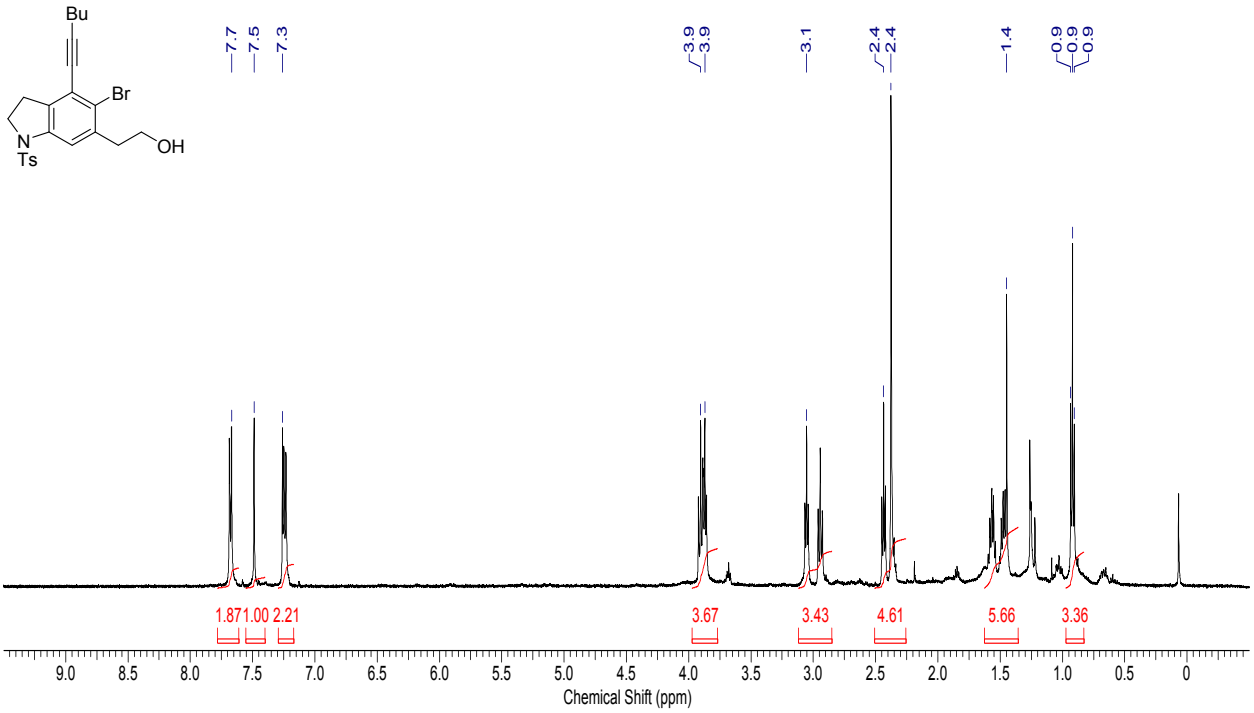

OMe
N
Ts
H/D
3g + 3g-d1 (2.3:1)
7.7
7.7
7.6
7.6
7.4
7.4
7.3
7.2
7.2
7.1
6.9
6.8
4.0
4.0
3.9
3.8
3.1
3.0
3.0
2.4
2.88
5.82
2.00
5.19
2.07
3.19
Chemical Shift (ppm)
159.9
144.2
142.0
134.0
133.9
133.0
129.7
127.9
127.3
126.3
126.2
120.7
114.9
114.5
114.4
114.1
93.4
85.3
77.3
77.0
76.8
55.3
49.7
27.8
21.5
Chemical Shift (ppm)

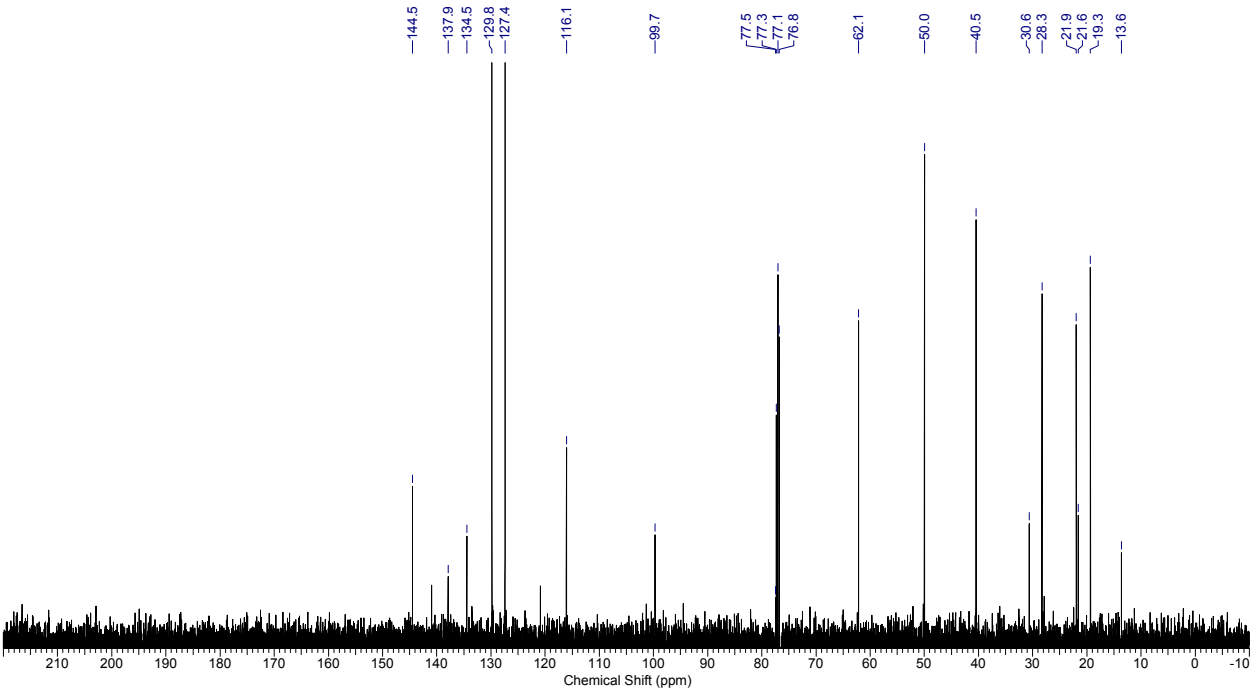

SiPr3
Pr
Pr
Si
OH
TsN
Ha
D
no nOe
3a-d1
7.8
7.8
7.4
7.3
7.3
7.3
4.7
4.6
2.4
1.5
1.5
1.5
1.1
1.0
1.0
0.9
0.9
0.9
0.9
0.7
0.7
2.00
3.12
4.25
3.94
11.42
6.24
Chemical Shift (ppm)
Ha
Chemical Shift (ppm)

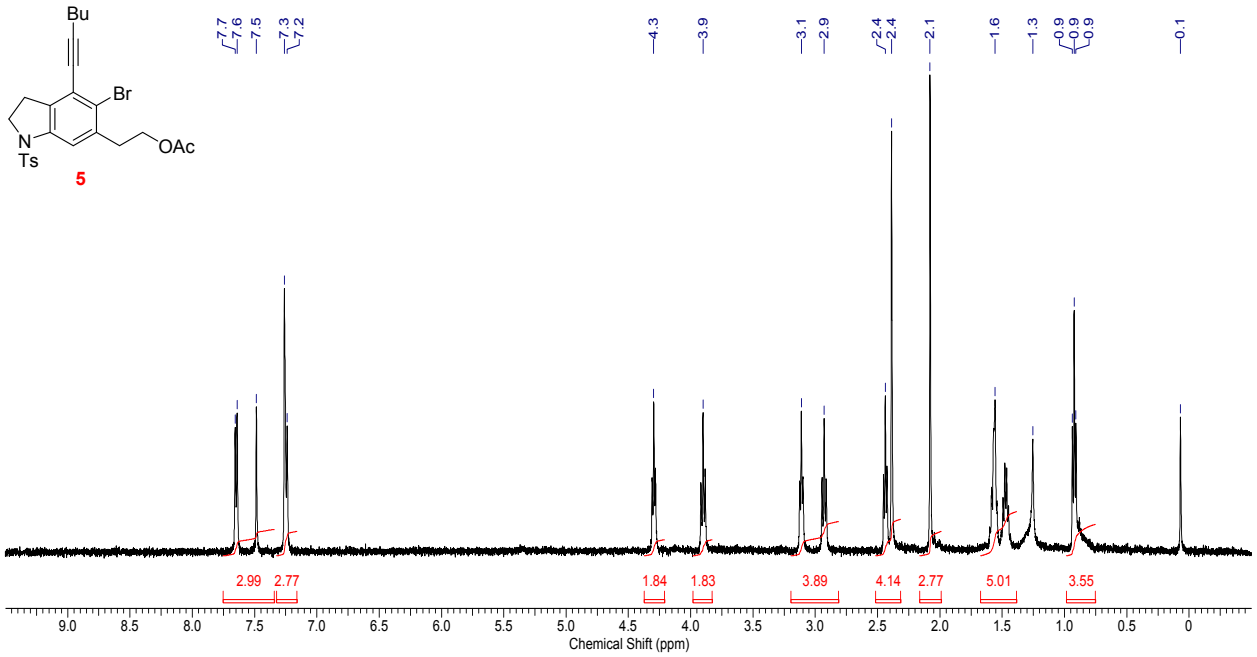

149.0
143.6
140.4
139.1
136.7
134.3
133.9
129.8
127.6
123.7
104.0
101.5
77.3
77.0
76.8
54.3
54.1
21.5
18.5
18.3
17.9
17.7
17.5
16.6
16.0
15.3
Chemical Shift (ppm)

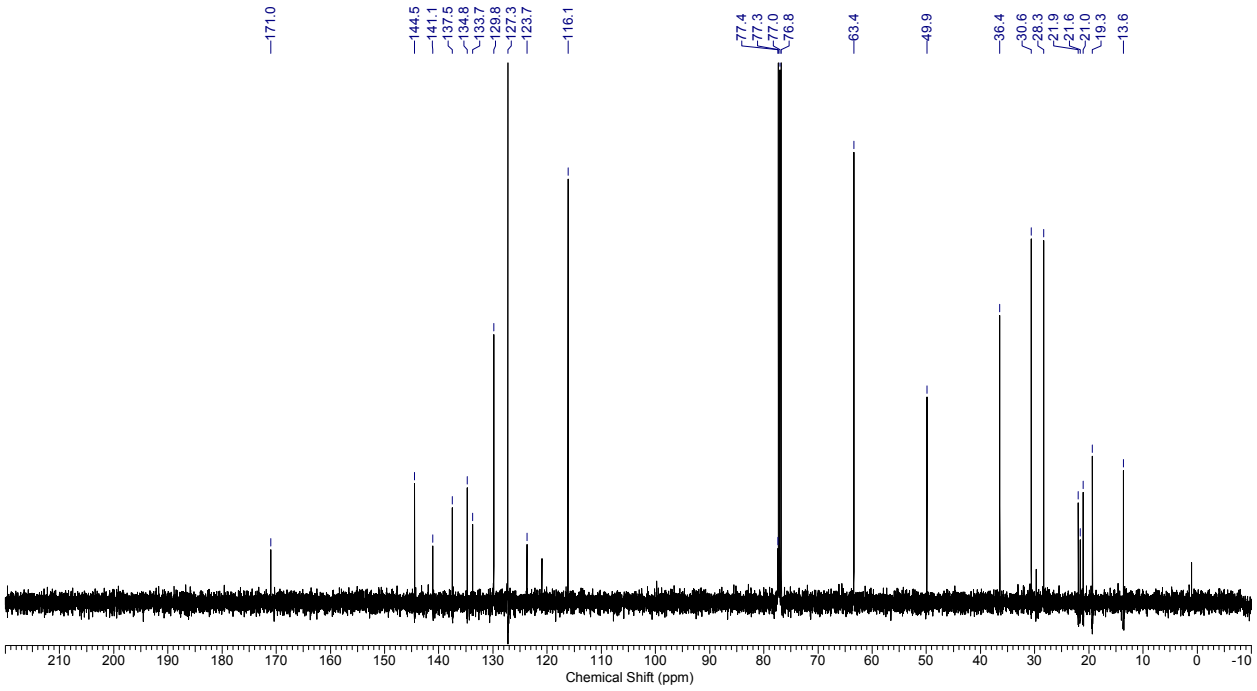

Bu
Br
N
Ts
SiEt2F
4
7.7
7.6
7.5
7.3
7.2
7.2
3.9
3.9
3.9
2.9
2.9
2.9
2.8
2.8
2.8
2.4
2.4
2.4
2.4
1.6
1.6
1.5
1.0
1.0
1.0
1.0
0.9
0.9
0.9
0.7
0.7
0.7
1.00
2.59
2.02
4.09
5.87
4.43
16.91
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

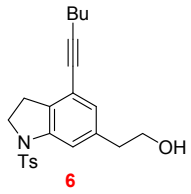

144.5
144.4
141.1
133.7
129.8
127.3
123.5
120.2
114.8
99.4
77.6
77.3
77.1
76.8
50.0
31.2
30.7
28.3
21.9
21.6
19.3
15.3
13.6
6.7
6.2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
Chemical Shift (ppm)


Bu
Br
N
Ts
OH
7.7
7.5
7.3
3.9
3.9
3.1
2.4
2.4
1.4
0.9
0.9
0.9
1.87
1.00
2.21
3.67
3.43
4.61
5.66
3.36
Chemical Shift (ppm)


144.5
137.9
134.5
129.8
127.4
116.1
99.7
77.5
77.3
77.1
76.8
62.1
50.0
40.5
30.6
28.3
21.9
21.6
19.3
13.6
Chemical Shift (ppm)

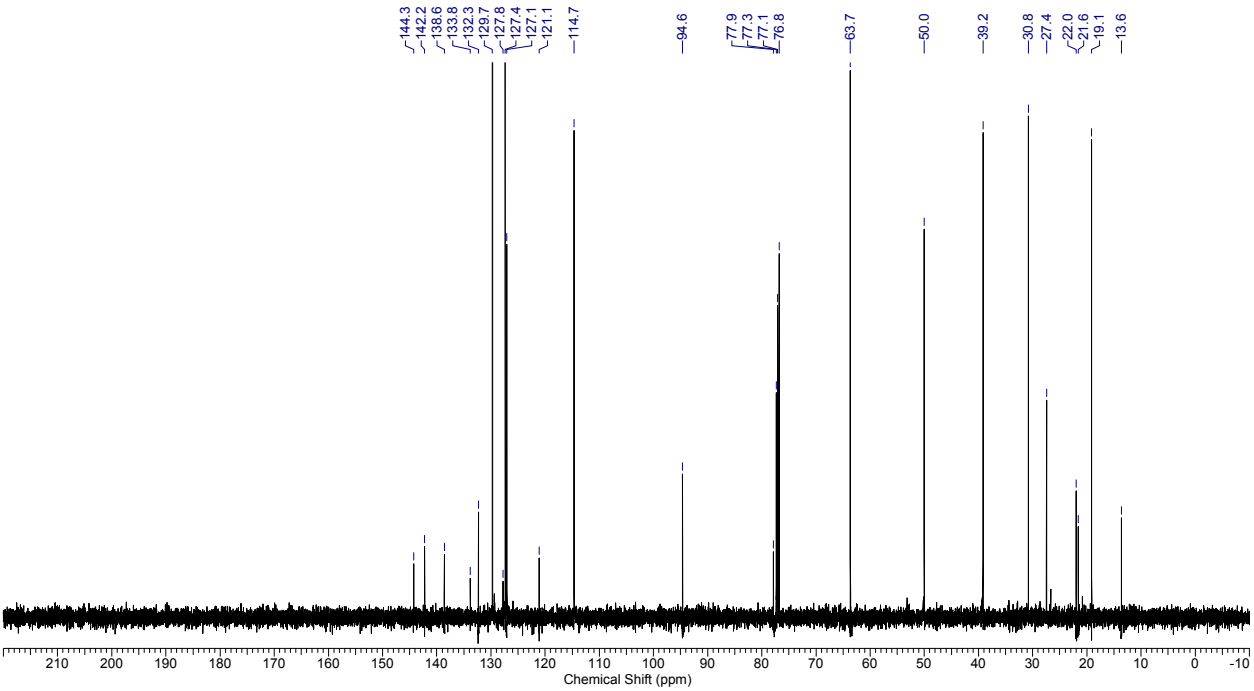

Bu
Br
N
Ts
OAc
5
7.7
7.6
7.5
7.3
7.2
4.3
3.9
3.1
2.9
2.4
2.4
2.1
1.6
1.3
0.9
0.9
0.9
0.1
2.99
2.77
1.84
1.83
3.89
4.14
2.77
5.01
3.55
Chemical Shift (ppm)

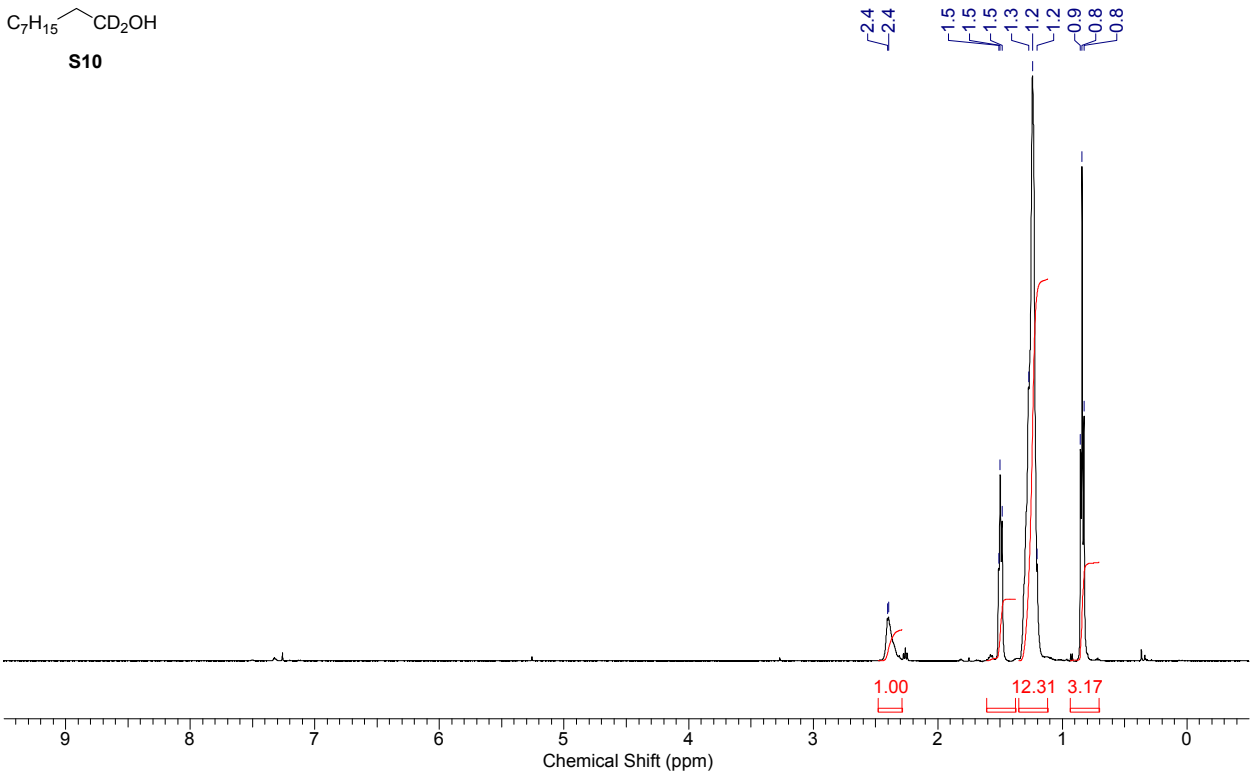

171.0
144.5
141.1
137.5
134.8
133.7
129.8
127.3
123.7
116.1
77.4
77.3
77.0
76.8
63.4
49.9
36.4
30.6
28.3
21.9
21.6
21.0
19.3
13.6
Chemical Shift (ppm)

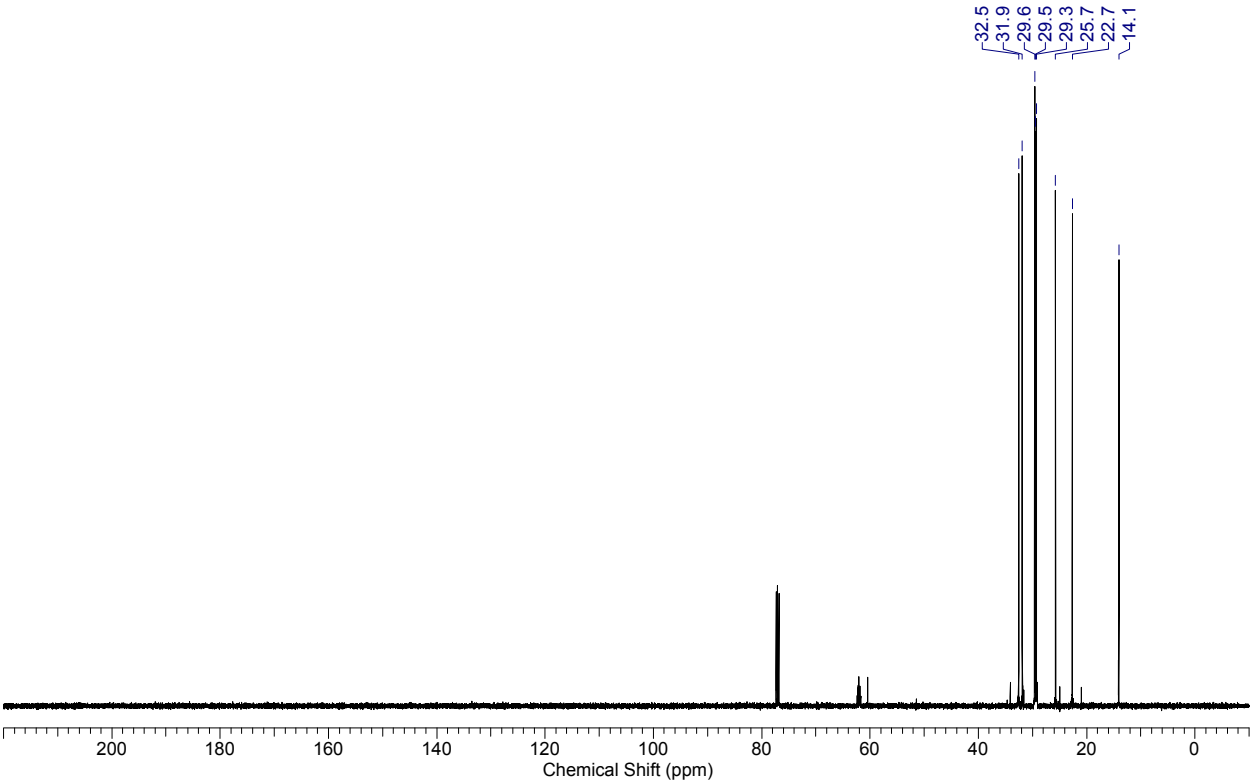

Bu
N
Ts
OH

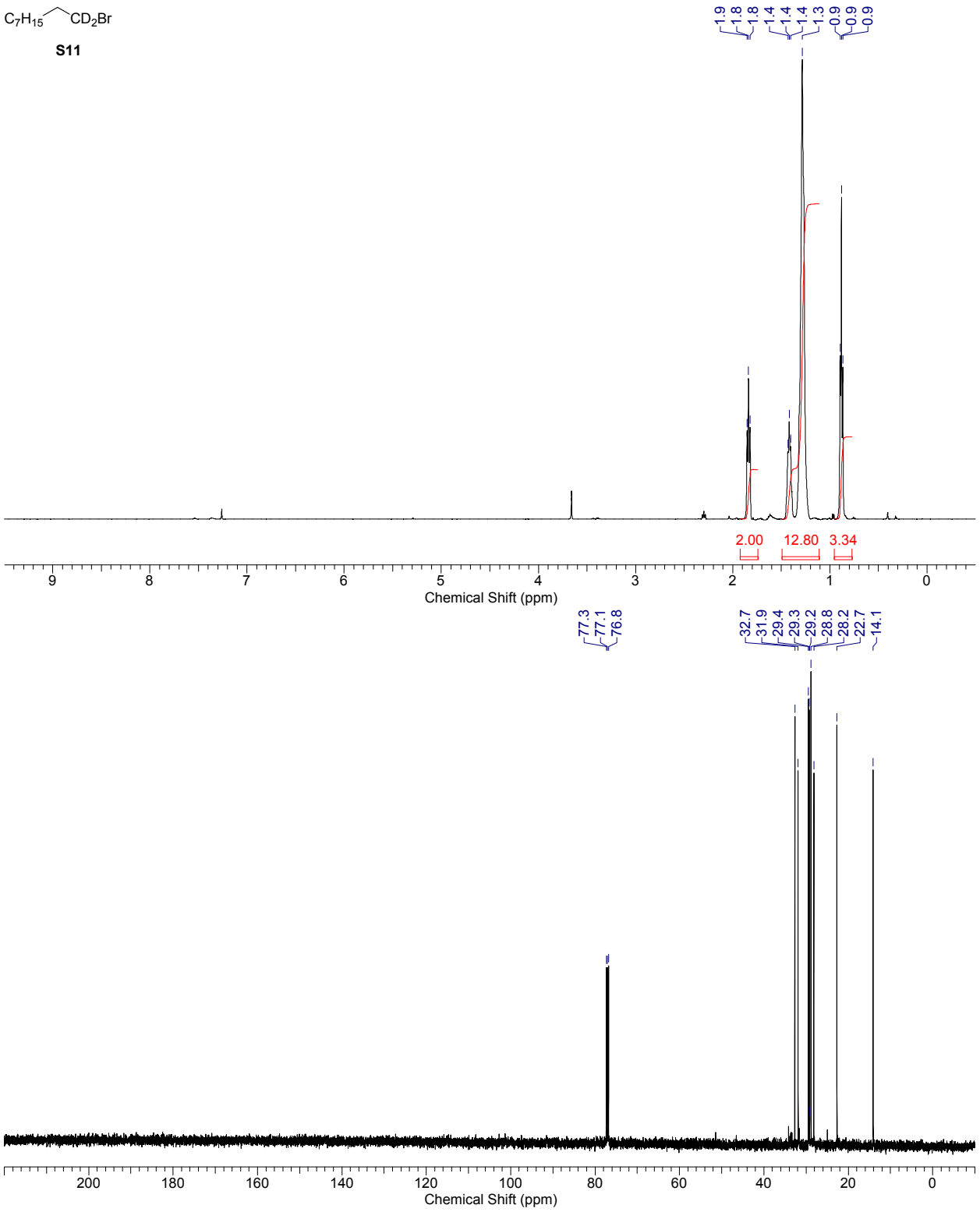
6

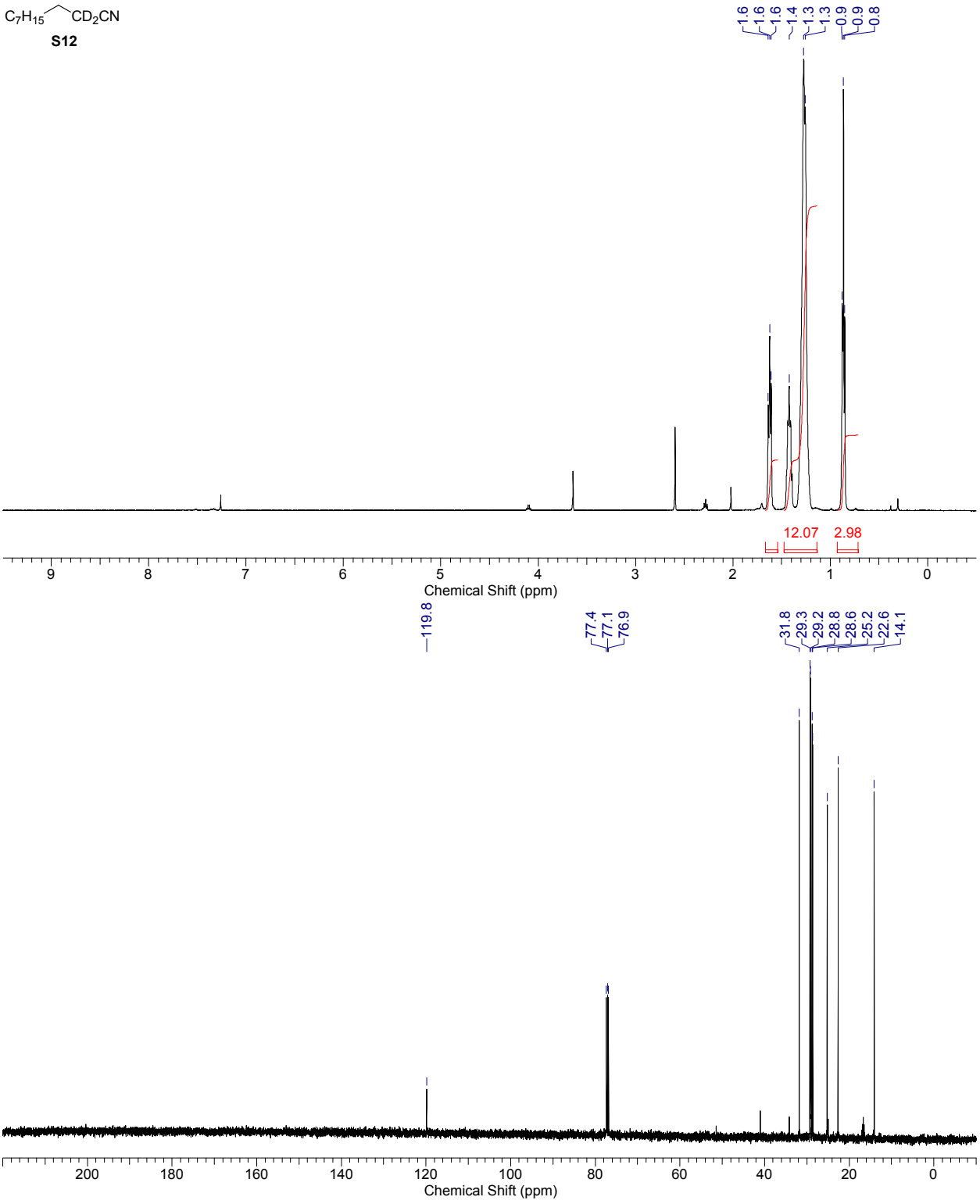
2.14
1.03
2.58
1.00
4.62
4.37
5.67
5.06
3.98
Chemical Shift (ppm)

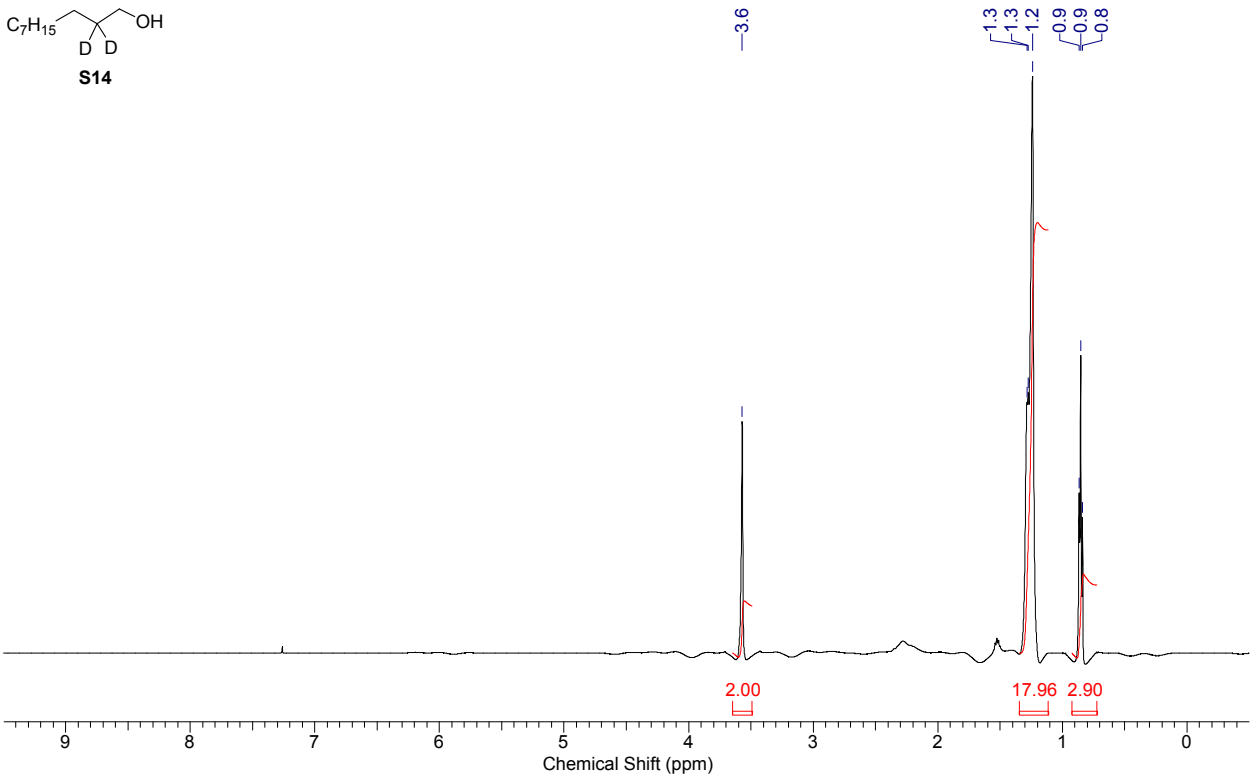

144.3
142.2
138.6
133.8
132.3
129.7
127.8
127.4
127.1
121.1
114.7
94.6
77.9
77.3
77.1
76.8
63.7
50.0
39.2
30.8
27.4
22.0
21.6
19.1
13.6
Chemical Shift (ppm)

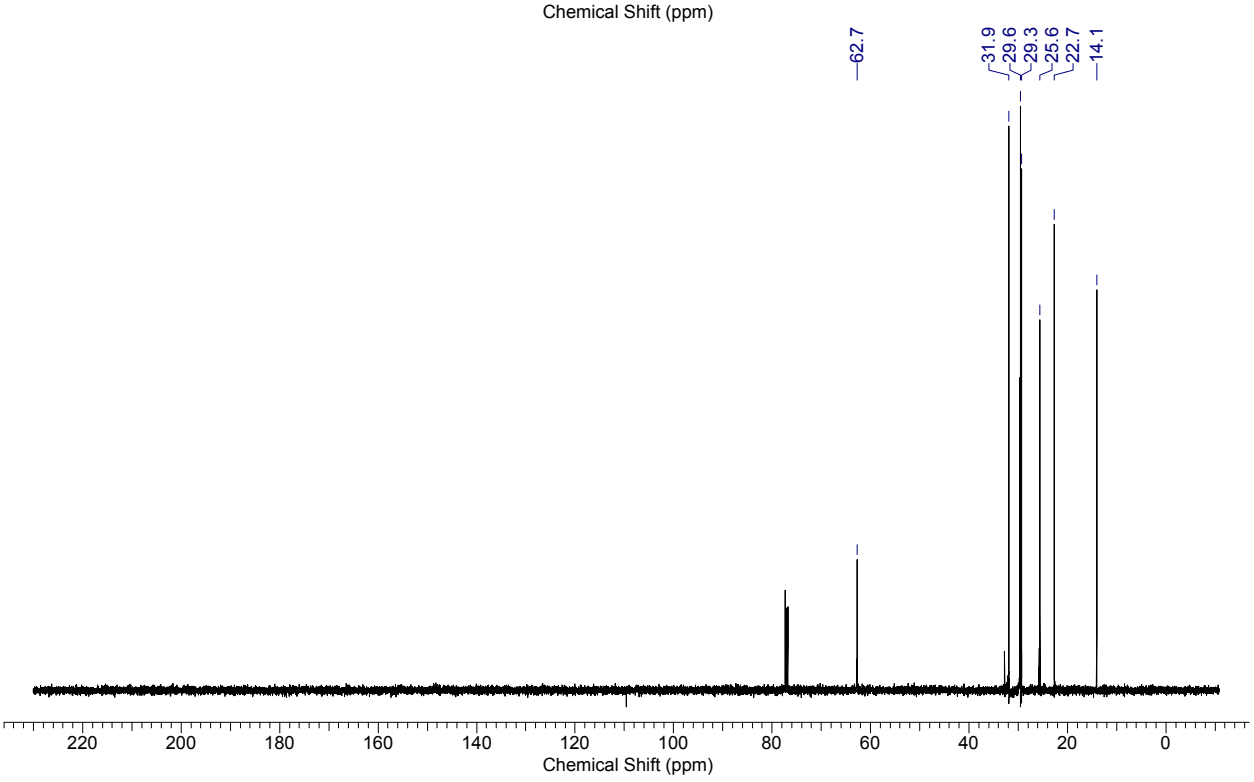

C7H15 CD2OH
S10
2.4
2.4
1.5
1.5
1.5
1.3
1.2
1.2
0.9
0.8
0.8
1.00
12.31
3.17
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

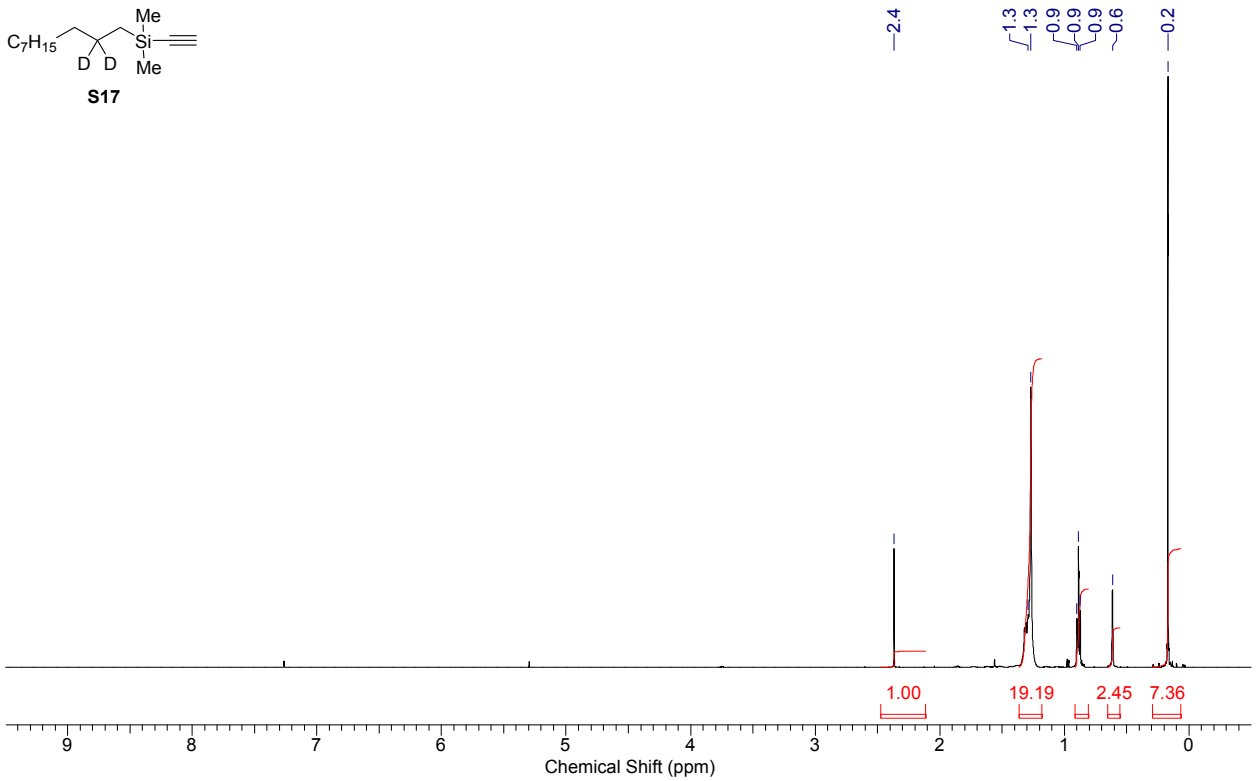

32.5
31.9
29.6
29.5
29.3
25.7
22.7
14.1
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

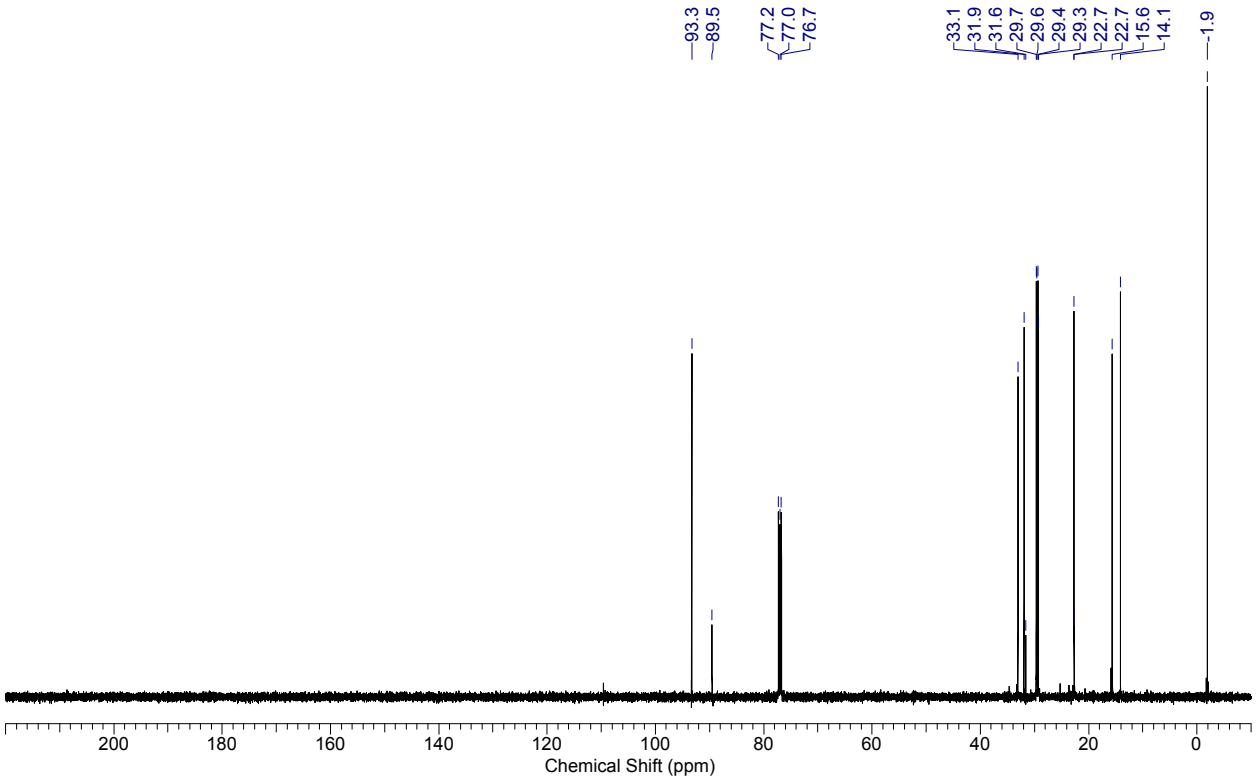

C7H15
CD2Br
S11
1.9
1.8
1.8
1.4
1.4
1.4
1.3
0.9
0.9
0.9
2.00
12.80
3.34
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)
77.3
77.1
76.8
32.7
31.9
29.4
29.3
29.2
28.8
28.2
22.7
14.1
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

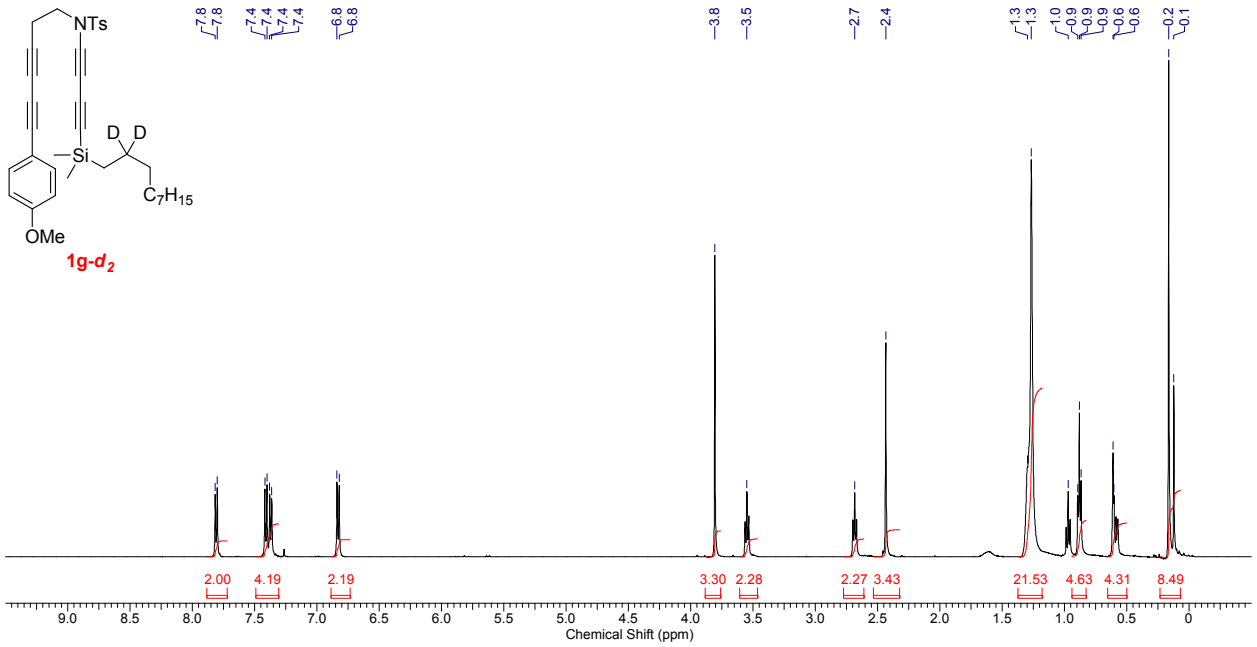

C7H15 CD2CN
S12
1.6
1.6
1.6
1.4
1.3
1.3
0.9
0.9
0.8
12.07
2.98
Chemical Shift (ppm)
119.8
77.4
77.1
76.9
31.8
29.3
29.2
28.8
28.6
25.2
22.6
14.1
Chemical Shift (ppm)

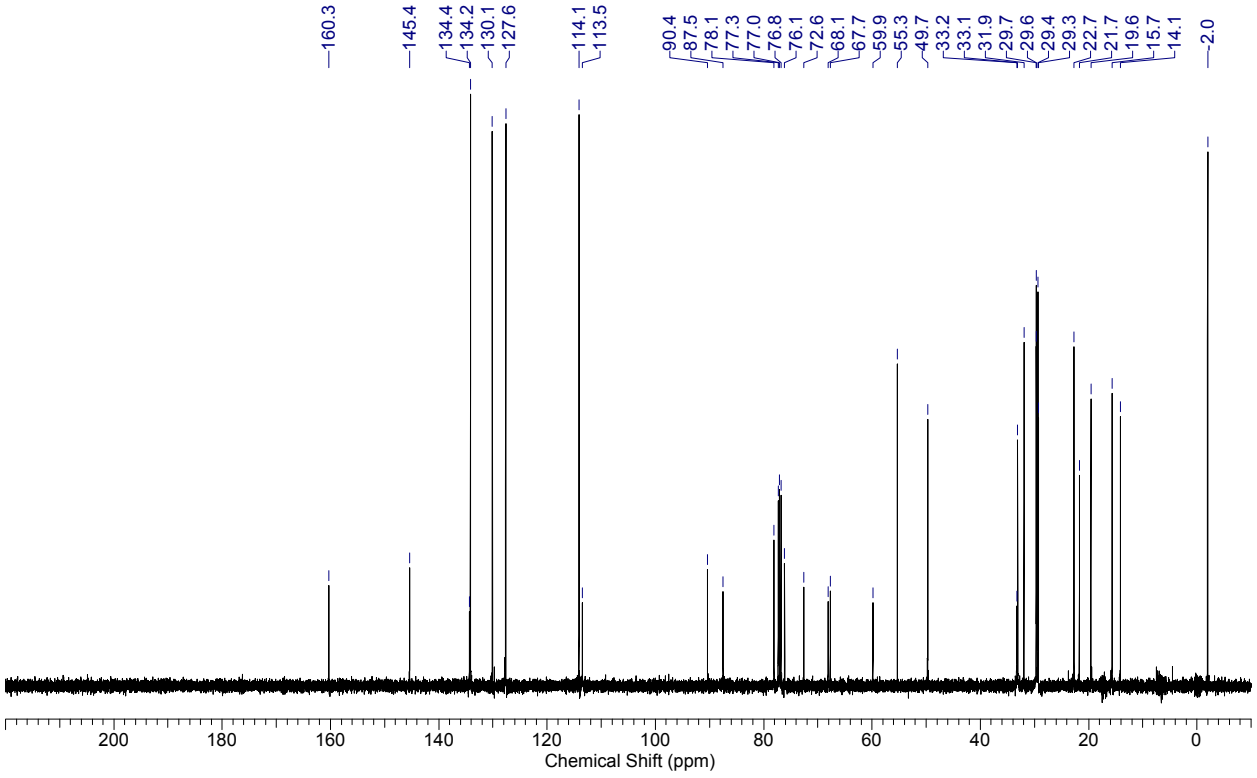

C7H15
OH
D D
S14
3.6
1.3
1.3
1.2
0.9
0.9
0.8
2.00
17.96
2.90
Chemical Shift (ppm)


62.7
31.9
29.6
29.3
25.6
22.7
14.1
Chemical Shift (ppm)


Me
C7H15
Si
D D
Me
Me
S17
2.4
1.3
1.3
0.9
0.9
0.9
0.6
0.2
1.00
19.19
2.45
7.36
9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)


93.3
89.5
77.2
77.0
76.7
33.1
31.9
31.6
29.7
29.6
29.4
29.3
22.7
22.7
15.6
14.1
1.9
200 180 160 140 120 100 80 60 40 20 0
Chemical Shift (ppm)


NTs
D D
Si
C7H15
OMe
1g-d2
7.8 7.8 7.4 7.4 7.4 7.4 6.8 6.8
3.8 3.5 2.7 2.4
1.3 1.3 1.0 0.9 0.9 0.9 0.6 0.6 0.2 0.1
2.00 4.19 2.19 3.30 2.28 2.27 3.43 21.53 4.63 4.31 8.49
Chemical Shift (ppm)


160.3 145.4 134.4 134.2 130.1 127.6 114.1 113.5
90.4 87.5 78.1 77.3 77.0 76.8 76.1 72.6 68.1 67.7 59.9 55.3 49.7 33.2 33.1 31.9 29.7 29.6 29.4 29.3 22.7 21.7 19.6 15.7 14.1 2.0
Chemical Shift (ppm)

Computational Details

All DFT calculations were carried out with the Gaussian 09 suite of computational programs.[1] The geometries of all stationary points were optimized using the M06 hybrid functional[2] at the basis set level of 6-31G(d) for all atoms except for Ag, which was described by the LANL2DZ.[3] Frequencies were analytically computed at the same level of theory to obtain the gas phase free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC)[4] calculations. The effect of solvent was examined by performing single-point self-consistent reaction field (SCRF) calculations based on the polarizable continuum model (PCM)[5] for gas-phase optimized structures. Toluene was used as the solvent according to the experimental condition, and the default UFF atomic radii was used in all PCM calculations. All the energies discussed in the main text are relative solvation free energies (ΔG_{sol}), which were obtained by adding the solvation corrections to the computed gas phase relative free energies (ΔG_{298}).

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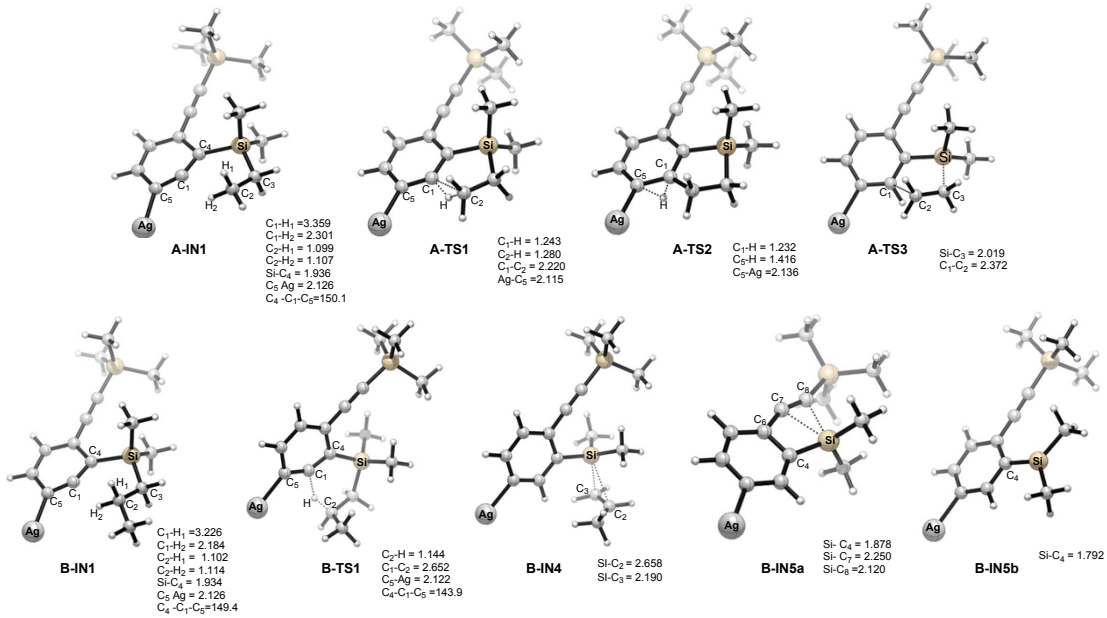

Figure S1. Geometric Structures for the Transition States and Intermediates in Figures 1 and 2 (Distances and angles are in angstrom and degree, respectively.)

Table S1. Energies (in Hartree) Calculated at the M06/6-31G(d)-LANL2DZ Level

Species	E_0[a]	H_{298}[b]	G_{298}[c]	E[d]	G_{Sol}[e]
A-IN1	-1308.456480	-1308.430015	-1308.514307	-1308.774457	-1308.822081
A-TS1	-1308.452502	-1308.427347	-1308.507174	-1308.768749	-1308.813872
A-IN2	-1308.489795	-1308.464856	-1308.544485	-1308.810535	-1308.854612
A-TS2	-1308.484108	-1308.459395	-1308.538575	-1308.801958	-1308.846996
A-IN3	-1308.554970	-1308.530866	-1308.608474	-1308.877148	-1308.929008
A-TS3	-1308.451852	-1308.426776	-1308.506798	-1308.770658	-1308.81372
A-IN4	-1308.472106	-1308.445949	-1308.527792	-1308.791862	-1308.834461
B-IN1	-1347.708252	-1347.680771	-1347.766497	-1348.055273	-1348.102333
B-TS1	-1347.709462	-1347.682897	-1347.766050	-1348.055158	-1348.100978
B-IN4	-1347.737323	-1347.710176	-1347.794259	-1348.085708	-1348.127906
B-IN5a	-1230.005642	-1229.983629	-1230.056018	-1230.272027	-1230.312559
B-IN5b	-1229.984749	-1229.962026	-1230.037514	-1230.250455	-1230.29403
Propene	-117.712937	-117.708419	-117.737533	-117.7919573	-117.792514
B-IN2	-1347.744622	-1347.718539	-1347.800016	-1348.093644	-1348.137405
B-TS2	-1347.738597	-1347.712679	-1347.793563	-1348.084842	-1348.129448
B-IN3	-1347.812851	-1347.786688	-1347.869149	-1348.163316	-1348.212903

[a] Sum of electronic and zero-point energies

[b] Sum of electronic and thermal enthalpies
[c] Sum of electronic and thermal free energies
[d] Electronic energies

Cartesian Coordinates for All Species

A-IN1

C	-2.57102800	-2.85794600	0.25832000
C	-1.33643600	-2.44437500	0.12359300
C	-0.46630100	-1.45777500	-0.00347000
C	-1.30938000	-0.27504000	0.04305300
C	-2.70469200	-0.40368300	0.17495300
C	-3.33016100	-1.64233200	0.27670500
H	-3.30370200	0.50360000	0.20251600
H	-4.41263900	-1.69819300	0.37693200
C	-0.68731200	0.99714500	-0.01533700
C	-0.12119100	2.07921300	-0.04062100
Si	0.82520400	3.68880500	-0.02455700
C	1.18584900	4.07556700	1.77284000
H	1.76195900	3.27194500	2.24941700
H	1.77536800	4.99835700	1.85230500
H	0.26345000	4.21842900	2.34858600
C	-0.23315700	5.00398400	-0.83035900
H	0.29582900	5.96592300	-0.83153800
H	-0.46896100	4.75312700	-1.87166200
H	-1.17846500	5.14592700	-0.29274300
C	2.40745000	3.36928900	-0.97990100
H	2.98541400	2.55078400	-0.52946500
H	2.20560700	3.10881600	-2.02674300
H	3.04399900	4.26367300	-0.97711600
Si	1.46188900	-1.45882700	-0.17423700
C	2.10761000	-0.63034400	1.37221300
H	1.86917400	-1.20682100	2.27508700
H	3.19986300	-0.53040100	1.31688100
H	1.68181800	0.37488500	1.48781200
C	1.89254500	-0.56350900	-1.75443500
H	2.98331500	-0.46609400	-1.84031300
H	1.53773700	-1.11468700	-2.63414400
H	1.46474800	0.44520100	-1.78436200
C	1.92241300	-3.28211000	-0.26508700
H	1.80255800	-3.63282500	-1.30101900
H	3.00197400	-3.34270600	-0.05635500
C	1.16556400	-4.18978100	0.69426200
H	1.24752800	-3.85746100	1.73818400
H	0.08700200	-4.22344300	0.44742200

Ag	-3.23708100	-4.87235900	0.39537700
H	1.51778800	-5.22797200	0.64863300

A-TS1

C	-1.73512500	-1.75938900	3.14117700
C	-0.61041600	-1.81556600	2.36448000
C	-0.13828000	-1.02216600	1.35170300
C	-1.03809200	0.00532300	0.97962000
C	-2.25613500	0.12701100	1.66852800
C	-2.59458600	-0.72431000	2.71593500
H	-2.93589600	0.92801400	1.38372600
H	-3.54751900	-0.57036000	3.21978200
C	-0.66689500	0.90327200	-0.05941200
C	-0.28089600	1.64401400	-0.95020400
Si	0.37003100	2.75135600	-2.29886800
C	2.22674200	2.85343600	-2.03654300
H	2.68910400	1.85689200	-2.05754600
H	2.69643800	3.45087900	-2.82881700
H	2.47419300	3.32432500	-1.07643700
C	-0.44554400	4.42716400	-2.13229900
H	-0.06117700	5.11527000	-2.89648600
H	-1.53263700	4.36036800	-2.26117100
H	-0.24763000	4.87523100	-1.15092400
C	-0.02991800	1.93466600	-3.93755100
H	0.44648600	0.94946500	-4.02362000
H	-1.11031700	1.80086100	-4.07022000
H	0.33437800	2.55194700	-4.76925300
Si	1.59959400	-1.26306900	0.64962700
C	2.66084000	0.20827000	1.08771900
H	2.72147800	0.35630200	2.17400700
H	3.68194500	0.08815100	0.70268900
H	2.24179800	1.12284100	0.64789700
C	1.61046900	-1.69390100	-1.16288800
H	2.63559200	-1.77811900	-1.54555400
H	1.09141600	-2.63903300	-1.36321100
H	1.10284500	-0.90445700	-1.73308500
C	2.10115100	-2.78039900	1.74648500
H	2.12735600	-3.70189000	1.15362200
H	3.12302200	-2.56092400	2.08976500
C	1.22961500	-2.91883800	2.93307500
H	0.02836800	-2.87402500	2.49240700
Ag	-2.24549900	-3.02176700	4.75997100
H	1.03715400	-3.91950800	3.34534600
H	1.35289600	-2.18174100	3.72935800

A-IN2

C	-1.10565100	-1.01839600	1.68026900
C	0.08711400	-1.24591600	0.85028700
C	0.42923700	-0.28343200	-0.21728400
C	-0.46985200	0.70868800	-0.56271000
C	-1.66876900	0.81335500	0.18690200
C	-1.97241400	-0.01574900	1.27187900
H	-2.37058300	1.60290800	-0.08622000
H	-2.90269200	0.16969500	1.80596900
C	-0.16101200	1.63298000	-1.60116500
C	0.16290100	2.40598700	-2.48812700
Si	0.75764300	3.56543700	-3.82423000
C	2.60969000	3.72094800	-3.56540100
H	3.10545200	2.74399000	-3.64439900
H	3.05355600	4.37933100	-4.32340100
H	2.84442100	4.14520000	-2.58067800
C	-0.11758300	5.20534200	-3.61199000
H	0.23159000	5.92042900	-4.36828200
H	-1.20315500	5.10232400	-3.72936200
H	0.07796600	5.64358400	-2.62575600
C	0.36459900	2.76694300	-5.47256500
H	0.85326500	1.78951500	-5.57274400
H	-0.71429900	2.62179100	-5.60571900
H	0.71923900	3.40089900	-6.29575800
Si	2.20612100	-0.61703300	-0.83440300
C	3.24262500	0.87291700	-0.37409300
H	3.18188000	1.10197200	0.69750100
H	4.29774300	0.69409600	-0.61807300
H	2.91154600	1.75893500	-0.93183200
C	2.27088300	-1.02427700	-2.65537900
H	3.30111900	-1.22986700	-2.97222400
H	1.66268000	-1.90235700	-2.90437100
H	1.90024000	-0.17635100	-3.24684300
C	2.39734700	-2.07268300	0.37256900
H	2.14895600	-3.01496100	-0.13959600
H	3.41054800	-2.18645000	0.77428200
C	1.38250200	-1.79625400	1.48765900
H	-0.30318800	-2.10257200	0.22901200
Ag	-1.50078500	-2.25414900	3.36039900
H	1.14998800	-2.68910900	2.08743900
H	1.76761500	-1.03588000	2.18414700

A-TS2

C	-1.07887800	-0.96821100	1.70337100
C	0.16628200	-1.06534100	0.97146800
C	0.47047600	-0.17944800	-0.12460000
C	-0.46635200	0.76995000	-0.50526900
C	-1.71219200	0.83725300	0.18071800
C	-2.01289900	-0.00852000	1.22373900
H	-2.44093500	1.57923300	-0.14369700
H	-2.98276600	0.07925500	1.70902400
C	-0.16616600	1.67271900	-1.56015900
C	0.15386700	2.42986300	-2.46282600
Si	0.73564500	3.54337500	-3.84419800
C	2.58138700	3.75155300	-3.58449000
H	3.10197900	2.78550800	-3.62749400
H	3.01216900	4.39394700	-4.36347900
H	2.80085000	4.21500500	-2.61427100
C	-0.17595500	5.17162600	-3.70912900
H	0.16475900	5.86283900	-4.49098600
H	-1.25829700	5.04169000	-3.82934900
H	0.00303800	5.65285300	-2.73990200
C	0.36569300	2.65123000	-5.44910200
H	0.87238800	1.67856500	-5.49473900
H	-0.70971500	2.47944700	-5.57822600
H	0.71300400	3.24654300	-6.30360900
Si	2.21863200	-0.55024000	-0.78509600
C	3.37862000	0.80750300	-0.22378300
H	3.35308100	0.94351600	0.86516200
H	4.41394900	0.58105100	-0.50862500
H	3.10522200	1.76369600	-0.68939300
C	2.26733200	-0.83382000	-2.63048900
H	3.26487000	-1.16907500	-2.94231700
H	1.54504400	-1.59680600	-2.94580200
H	2.04063100	0.09192100	-3.17515300
C	2.31566400	-2.12967900	0.27209200
H	1.98080200	-2.98591600	-0.33246100
H	3.32217800	-2.37002600	0.63204600
C	1.34935800	-1.89645500	1.43954600
H	-0.74735100	-1.81114400	0.61523700
Ag	-1.44764500	-2.20059500	3.40825900
H	1.00502100	-2.82934000	1.91396900
H	1.84408500	-1.31388200	2.23346800

A-IN3

C	-1.10328200	-1.19004300	1.49908800
C	0.17965800	-1.17402800	0.88846300
C	0.45559300	-0.26742500	-0.13901600
C	-0.53201600	0.65416500	-0.55231700
C	-1.80964900	0.64132100	0.03776700
C	-2.10316100	-0.28294400	1.03458300
H	-2.57178900	1.33302400	-0.31463300
H	-3.11685500	-0.36146800	1.42686400
C	-0.21125600	1.59205300	-1.56810000
C	0.12970700	2.38328800	-2.43424700
Si	0.73607200	3.52874400	-3.77652000
C	2.58129700	3.71712000	-3.49631800
H	3.09522500	2.74788900	-3.54908600
H	3.02446800	4.36759500	-4.26158300
H	2.79608200	4.16450100	-2.51748800
C	-0.16077200	5.16284700	-3.60816100
H	0.19007900	5.86744400	-4.37345800
H	-1.24360400	5.04534100	-3.73654900
H	0.01795600	5.62221200	-2.62826900
C	0.37261400	2.68615900	-5.40920900
H	0.86996700	1.71017100	-5.47697000
H	-0.70323500	2.52840900	-5.55179000
H	0.73340000	3.30202100	-6.24334700
Si	2.21599400	-0.55605800	-0.79570900
C	3.35525500	0.78572100	-0.14791400
H	3.31715900	0.86316200	0.94726100
H	4.39813600	0.59197800	-0.42894700
H	3.07434400	1.76132200	-0.56785700
C	2.31478500	-0.71902500	-2.65532400
H	3.29300200	-1.11577200	-2.95649100
H	1.54560400	-1.39758000	-3.04462100
H	2.18492700	0.25516500	-3.14406400
C	2.32708600	-2.20451900	0.14178800
H	2.04250000	-3.00923500	-0.55156800
H	3.32387300	-2.45424900	0.52163200
C	1.29820100	-2.11521100	1.28112300
H	-1.38944900	-2.02267000	2.14768700
Ag	-0.70861900	0.43932100	3.06568000
H	0.89386300	-3.09750200	1.56725400
H	1.78876600	-1.72357100	2.18849700

A-TS3

C	-1.33968100	-1.34838800	1.34620200
C	-0.14837200	-1.48960000	0.60486700
C	0.33901400	-0.48765700	-0.26507200
C	-0.47428900	0.62512700	-0.52435200
C	-1.67680300	0.76710000	0.19157400
C	-2.07564400	-0.17912900	1.13332000
H	-2.28510900	1.65329400	0.01578500
H	-2.99849700	0.00294200	1.68190800
C	-0.07676600	1.58990400	-1.49525300
C	0.27920700	2.36751300	-2.36731100
Si	0.82684100	3.52952100	-3.71519300
C	2.70283500	3.44949200	-3.76177300
H	3.05822600	2.42122100	-3.91445900
H	3.09041400	4.05742500	-4.58968500
H	3.14961600	3.83328000	-2.83548400
C	0.22516400	5.25023900	-3.29027700
H	0.53513800	5.96374400	-4.06497200
H	-0.86868400	5.28898000	-3.22131400
H	0.63711100	5.59712900	-2.33472000
C	0.09365900	2.90681100	-5.32257500
H	0.44089400	1.89198300	-5.55456000
H	-1.00225200	2.88840800	-5.28663600
H	0.38975300	3.55859900	-6.15499700
Si	2.13388800	-0.56601900	-0.81419700
C	3.05808600	1.00345900	-0.40297900
H	2.91464300	1.29956600	0.64502400
H	4.13412500	0.87443600	-0.58033300
H	2.70603500	1.83367700	-1.02565000
C	2.49147600	-1.25094100	-2.50503800
H	3.56874200	-1.32883500	-2.69647200
H	2.03607700	-2.23581600	-2.66104900
H	2.06743400	-0.56544900	-3.25345500
C	2.81156800	-1.83016700	0.60655000
H	2.93880100	-2.85640000	0.25089900
H	3.77073300	-1.31325900	0.75536700
C	1.94312500	-1.66360800	1.71119400
H	0.27444300	-2.49320600	0.50814700
Ag	-2.08009100	-2.84501500	2.63759200
H	1.46585300	-2.49079100	2.23234700
H	1.90330400	-0.70922400	2.23925400

A-IN4

C	-2.52148100	-3.01241200	2.05488100
C	-1.28027000	-2.99183200	1.40881000
C	-0.73804300	-1.81291800	0.88112600
C	-1.47010300	-0.60812500	1.00742600
C	-2.70916200	-0.61517100	1.65260000
C	-3.21940200	-1.80234000	2.16499900
H	-3.26443500	0.31650100	1.74585400
H	-4.18818100	-1.77126300	2.66152100
C	-0.90687500	0.58403200	0.46236300
C	-0.35645000	1.55916300	-0.03060900
Si	0.47831400	3.05254400	-0.76743800
C	1.37283800	3.94932600	0.61194100
H	2.13469000	3.31773800	1.08682400
H	1.88008200	4.84018100	0.21874200
H	0.67629100	4.28014900	1.39174600
C	-0.83427800	4.12027800	-1.56493800
H	-0.37709300	5.01066200	-2.01611300
H	-1.36581900	3.57962100	-2.35749800
H	-1.57584000	4.46210000	-0.83291200
C	1.69595200	2.40621600	-2.04698500
H	2.42156800	1.70438600	-1.61233100
H	1.18264200	1.90065000	-2.87595800
H	2.26786900	3.23813000	-2.47860800
Si	0.87650800	-1.59353700	-0.00578000
C	2.27755600	-0.73871100	0.88193800
H	2.40893700	-1.09492200	1.90982100
H	3.22648600	-0.83546200	0.33943400
H	2.02317500	0.32853800	0.93368300
C	0.84923800	-1.31876500	-1.84993000
H	1.85332200	-1.37659800	-2.28871100
H	0.18090500	-2.00997600	-2.37524800
H	0.46894500	-0.30133200	-2.01242500
C	1.33391800	-3.88607600	-0.53045700
H	0.28976700	-4.19899600	-0.59050000
H	1.89234700	-3.86565600	-1.46549400
C	1.93872600	-3.63800200	0.65079400
H	-0.72631600	-3.92931200	1.32001600
H	1.41216100	-3.73787300	1.60217900
Ag	-3.34830400	-4.78588700	2.84295100
H	3.00284000	-3.41084700	0.70242900

B-IN1

C	-2.40897300	-2.92587000	0.42151300
C	-1.18107700	-2.48350500	0.30092600
C	-0.34570400	-1.46824500	0.15058900
C	-1.22533400	-0.31462000	0.11932300
C	-2.61870900	-0.48370800	0.22170800
C	-3.20590800	-1.73682100	0.36410500
H	-3.24707400	0.40354800	0.19428800
H	-4.28844300	-1.82332600	0.43961300
C	-0.64319500	0.97358500	0.01490700
C	-0.10985700	2.07041000	-0.05134500
Si	0.78181600	3.70992400	-0.09596500
C	1.04117400	4.22076600	1.68793000
H	1.62471700	3.47047800	2.23705900
H	1.59067500	5.16990700	1.73744000
H	0.08789600	4.35871600	2.21219100
C	-0.27734200	4.92930800	-1.03971100
H	0.22082400	5.90627000	-1.08916600
H	-0.45604700	4.59507400	-2.06893300
H	-1.25096800	5.07675900	-0.55686600
C	2.42113200	3.38975300	-0.95024500
H	2.99089800	2.60349800	-0.43616000
H	2.28448300	3.08369200	-1.99522100
H	3.03713900	4.29846400	-0.94874900
Si	1.58393300	-1.41644000	0.03164200
C	2.16922400	-0.52009400	1.56426400
H	1.92611300	-1.07815200	2.47757700
H	3.25949900	-0.39241700	1.53036900
H	1.71516300	0.47614000	1.64240500
C	2.03805200	-0.57096000	-1.56932600
H	3.12771400	-0.44369900	-1.62511200
H	1.72806400	-1.16747700	-2.43633200
H	1.58136500	0.42178800	-1.65234600
C	2.09297500	-3.23017700	0.02452700
H	2.06557300	-3.61387300	-1.00790700
H	3.15317400	-3.26652800	0.32587700
C	1.28294400	-4.14285800	0.93684400
H	1.27364600	-3.75133700	1.96718000
H	0.21992300	-4.13040200	0.60547700
C	1.76393400	-5.58461900	0.93025600
H	2.79760500	-5.64677200	1.29426100
H	1.14960000	-6.22724300	1.57338900

H	1.74908600	-6.00100300	-0.08571100
Ag	-3.02807500	-4.94897500	0.63499800

B-TS1

C	-2.91000600	-3.24393300	-1.03297500
C	-1.65740500	-2.81933800	-0.93466000
C	-0.89602300	-1.73956500	-0.73088400
C	-1.79015100	-0.62112500	-0.60000600
C	-3.17823000	-0.82397000	-0.69407400
C	-3.72933200	-2.08369900	-0.90113500
H	-3.83353700	0.03812200	-0.59089200
H	-4.81133900	-2.18926900	-0.95976500
C	-1.24034100	0.66599700	-0.36576400
C	-0.72305400	1.75327400	-0.16193000
Si	0.15263100	3.37659800	0.11445300
C	1.79120300	2.94954300	0.92425000
H	2.39952700	2.29934800	0.28074800
H	2.37309900	3.86079800	1.11504400
H	1.64846600	2.44209000	1.88709100
C	-0.91497900	4.44195600	1.22109200
H	-0.43689700	5.41648500	1.38546600
H	-1.89993500	4.62610600	0.77525500
H	-1.06848400	3.97666100	2.20243600
C	0.41511000	4.14572500	-1.57371900
H	1.02675800	3.49940100	-2.21664600
H	-0.53656800	4.33018400	-2.08660400
H	0.93535300	5.10784600	-1.47871600
Si	1.01226700	-1.66527700	-0.55876000
C	1.40649100	-1.11181300	1.18189000
H	1.06755800	-1.82605800	1.94211400
H	2.49022100	-0.98017800	1.30231100
H	0.93057000	-0.14348100	1.38598100
C	1.71719200	-0.51603600	-1.84996700
H	2.81079000	-0.47120900	-1.75858500
H	1.47922700	-0.85047100	-2.86725100
H	1.32802400	0.50251100	-1.72592000
C	1.47968900	-3.47202600	-0.93166000
H	1.82191100	-3.51348800	-1.97539900
H	2.35041400	-3.72705300	-0.30696300
C	0.38707500	-4.49205600	-0.69501700
H	-0.57851400	-4.08168900	-1.14986200
Ag	-3.61211800	-5.22862100	-1.29830600
C	0.13055900	-4.84399400	0.75404100
H	-0.72382800	-5.52462100	0.86460300
H	1.00801400	-5.34556100	1.18188100

H	-0.07188800	-3.95215600	1.36200600
H	0.52881900	-5.39916200	-1.30337700

B-IN4

C	-2.30862100	-1.33834300	-0.25966200
C	-0.91780800	-1.25772800	-0.38778700
C	-0.20832000	-0.08270400	-0.10528400
C	-0.93118800	1.06366900	0.30317800
C	-2.32046400	0.99493000	0.43775600
C	-2.99127700	-0.19105800	0.16424600
H	-2.86664500	1.88254800	0.75253300
H	-4.07406400	-0.20730400	0.28041400
C	-0.22323600	2.27746600	0.54831300
C	0.43346700	3.29249000	0.73152100
Si	1.43004400	4.83216300	1.04008700
C	1.76366100	4.93466400	2.88154500
H	2.33280300	4.06590000	3.23737200
H	2.34932300	5.83327100	3.11606900
H	0.83163300	4.98402100	3.45747700
C	0.45285900	6.30180400	0.41930700
H	1.01677700	7.22992600	0.58006300
H	0.24178800	6.21990700	-0.65386700
H	-0.50477300	6.39865800	0.94489100
C	3.03943700	4.62977300	0.08871000
H	3.59386500	3.73615900	0.40796100
H	2.86606200	4.55977800	-0.99306800
H	3.69355000	5.49499900	0.25902400
Si	1.62819000	0.17211500	-0.24958500
C	2.59244500	0.51011600	1.30967500
H	2.18731000	-0.02107200	2.17938500
H	3.65738900	0.26661800	1.19935700
H	2.51938200	1.58289500	1.52660600
C	2.23655400	1.12334200	-1.73398000
H	3.33191500	1.17903000	-1.76307100
H	1.87022200	0.69957700	-2.67607200
H	1.84574700	2.14653500	-1.64822900
C	2.31455600	-1.74575600	-1.03258400
H	1.47446000	-1.84613600	-1.72640600
H	3.28187700	-1.49616900	-1.47701100
C	2.28116900	-2.38002800	0.17724400
H	-0.37768400	-2.14260700	-0.73234100
Ag	-3.39136300	-3.09106000	-0.70697200
C	3.44980300	-2.62170400	1.03944400
H	3.27421200	-2.28564700	2.06959600
H	3.59258500	-3.71214600	1.10659000

H	4.37061200	-2.17772500	0.64719200
H	1.31387200	-2.73192300	0.55220500

B-IN5a

C	-1.88795500	-1.52266100	-0.15374900
C	-0.54189400	-1.15001400	-0.00383000
C	-0.19987100	0.18715700	0.16847000
C	-1.23044500	1.15508900	0.19739100
C	-2.57252300	0.82474300	0.06197200
C	-2.87588800	-0.52309600	-0.11503600
H	-3.35291600	1.58165400	0.09036400
H	-3.92453400	-0.79432400	-0.22621600
C	-0.53725600	2.38418300	0.38500400
C	0.46977100	3.10513400	0.53385700
Si	1.46126900	4.74141500	0.61822400
C	2.97183700	4.44732600	1.67891100
H	3.67045500	3.72658400	1.23361400
H	3.52019200	5.39172700	1.79341800
H	2.70599800	4.10310700	2.68644600
C	0.26309800	5.94693100	1.38827900
H	0.72779700	6.93888800	1.46279300
H	-0.64760100	6.05051300	0.78616700
H	-0.02717700	5.63829200	2.39969400
C	1.89938800	5.15820100	-1.14999100
H	2.61701900	4.44831000	-1.58060200
H	1.01010900	5.17749700	-1.79160700
H	2.35988900	6.15421100	-1.19321800
Si	1.36542400	1.18504100	0.45120800
C	2.11916100	0.96945500	2.13395600
H	2.47127600	-0.06580800	2.23930600
H	2.97260700	1.63543300	2.30252500
H	1.37215200	1.14496500	2.91773200
C	2.51913200	1.35821300	-0.99400400
H	3.33250900	2.06499700	-0.78980300
H	2.97474900	0.38356100	-1.21532800
H	1.98020000	1.68556100	-1.89133200
H	0.24305800	-1.90610900	-0.02525800
Ag	-2.43004800	-3.54569900	-0.44378300

B-IN5b

C	-1.99767700	-1.41744200	-0.10878300
C	-0.61365000	-1.30830100	-0.03608200
C	0.04571500	-0.06190900	0.12987500
C	-0.73505700	1.13014100	0.22545900
C	-2.12490200	1.01965500	0.15062400
C	-2.73187100	-0.22201600	-0.01134000
H	-2.72677300	1.92361600	0.21974500
H	-3.81980500	-0.24822600	-0.06283400
C	-0.14800900	2.41224700	0.38850100
C	0.32432900	3.53086000	0.52763100
Si	1.05957900	5.23363300	0.73264600
C	2.40501700	5.09553700	2.03367100
H	3.22194300	4.43949900	1.70416500
H	2.84221600	6.08334800	2.23016900
H	2.01665200	4.71184600	2.98534200
C	-0.30758700	6.39251600	1.26610700
H	0.08976600	7.40582600	1.40953000
H	-1.10250000	6.45039800	0.51286800
H	-0.75999600	6.07513300	2.21341500
C	1.78786000	5.71870200	-0.92559600
H	2.56546200	5.01484900	-1.25044700
H	1.02137400	5.76196500	-1.70875800
H	2.25127300	6.71180500	-0.85858900
Si	1.83626100	-0.08121800	0.20833300
C	2.89641000	1.40587000	0.44985900
H	2.61925400	1.91570600	1.38320600
H	3.95748500	1.13537100	0.47686700
H	2.71995000	2.13685200	-0.35137200
C	2.68547100	-1.71555400	0.03948800
H	3.76940700	-1.61022500	0.15373100
H	2.32583700	-2.43149300	0.79026500
H	2.48630900	-2.15941100	-0.94561000
H	-0.00476300	-2.21101500	-0.10701800
Ag	-2.97232000	-3.27641200	-0.35304500

B-IN2

C	-1.15981600	-1.12108700	1.55657900
C	0.09876600	-1.24540200	0.80672900
C	0.46241700	-0.21435800	-0.18645700
C	-0.45979700	0.75112500	-0.54582700
C	-1.69805900	0.78007900	0.14396600
C	-2.03392100	-0.12035800	1.16111100
H	-2.41373300	1.55681000	-0.13001500
H	-3.00272700	-0.00121300	1.64325400
C	-0.14956800	1.69986000	-1.56189400
C	0.17107300	2.47076900	-2.45181900
Si	0.73796700	3.57395400	-3.84612200
C	2.61280500	3.50635200	-3.82136900
H	2.97578000	2.47402600	-3.91950900
H	3.03186200	4.08348600	-4.65588900
H	3.02050500	3.92609100	-2.89275300
C	0.09936600	5.30425800	-3.53114400
H	0.41646300	5.97774700	-4.33800500
H	-0.99606200	5.33155400	-3.48742400
H	0.48702700	5.70988600	-2.58859000
C	0.05828700	2.83874500	-5.42901500
H	0.42145900	1.81371700	-5.57838100
H	-1.03800000	2.81270200	-5.42795000
H	0.37719000	3.43367200	-6.29484400
Si	2.25950400	-0.49648500	-0.77038300
C	3.29985000	1.02236000	-0.43112500
H	3.27924300	1.33066700	0.62082700
H	4.34602100	0.82519100	-0.69968300
H	2.95091900	1.86556600	-1.04162000
C	2.29481900	-0.97140400	-2.57895800
H	3.32126600	-1.17605800	-2.90906200
H	1.69287500	-1.86503200	-2.78572400
H	1.90288600	-0.14820800	-3.19219600
C	2.46694100	-1.94006200	0.45371300
H	2.32207300	-2.88566300	-0.09139600
H	3.45940700	-1.99426500	0.91834300
C	1.37279700	-1.77157900	1.52277500
H	-0.19693500	-2.08641000	0.11666000
Ag	-1.62996400	-2.52437000	3.08102400
C	1.78767800	-0.80964900	2.62861800
H	1.00027100	-0.69348100	3.38614300
H	2.69115100	-1.16975900	3.13507500

H	2.00895200	0.19198800	2.23218900
H	1.12016600	-2.74511700	1.97758900

B-TS2

C	-1.10334200	-0.87708800	1.72711600
C	0.16981800	-0.94560100	1.04228200
C	0.47940800	-0.07194900	-0.06105500
C	-0.47255200	0.84172000	-0.48923600
C	-1.73784900	0.89084300	0.16118900
C	-2.04811500	0.04995600	1.20533500
H	-2.47612700	1.60747700	-0.19699200
H	-3.03534700	0.11567600	1.65801900
C	-0.16829500	1.71316900	-1.56923900
C	0.16173200	2.43238700	-2.49889000
Si	0.76754300	3.46445000	-3.93208400
C	2.63335700	3.53875200	-3.75027000
H	3.07505100	2.53429900	-3.80349500
H	3.07866900	4.13715800	-4.55567400
H	2.93095700	3.99331000	-2.79659700
C	-0.02125500	5.15678400	-3.81663500
H	0.32650100	5.79382700	-4.64024800
H	-1.11440600	5.09725800	-3.88197000
H	0.23629500	5.65929500	-2.87646000
C	0.27838200	2.55236200	-5.49330500
H	0.72431200	1.54967900	-5.52454600
H	-0.80939300	2.44251300	-5.57814600
H	0.62878500	3.09892400	-6.37858100
Si	2.22051300	-0.45356200	-0.72906200
C	3.39079200	0.97205400	-0.40907500
H	3.41818300	1.27560900	0.64439200
H	4.41338200	0.70791500	-0.70792300
H	3.08645000	1.84421600	-1.00390700
C	2.17366100	-0.90867100	-2.54288900
H	3.16184500	-1.24090700	-2.88639300
H	1.46082000	-1.71807400	-2.74388400
H	1.88145100	-0.04279300	-3.15206400
C	2.36323800	-1.95696400	0.43324600
H	2.08577800	-2.85222900	-0.14388900
H	3.37101800	-2.13745700	0.82698400
C	1.36349700	-1.73076000	1.58149400
H	-0.71169500	-1.72429600	0.66926900
Ag	-1.49922300	-2.10991600	3.42620100
C	1.99086700	-0.93345100	2.72397700
H	2.84133100	-1.47876200	3.14954800
H	2.36187800	0.03925500	2.37115600

H	1.27102900	-0.73794700	3.53129600
H	0.99902600	-2.69138400	1.98752300

B-IN3

C	-1.11312700	-0.96725000	1.57254300
C	0.16988000	-1.00212200	0.95908100
C	0.46211800	-0.13731100	-0.10037800
C	-0.51240300	0.77984700	-0.55153600
C	-1.78506700	0.81617800	0.04738600
C	-2.08912600	-0.05503900	1.08638000
H	-2.53392100	1.51142800	-0.32598400
H	-3.09574200	-0.08019700	1.50166300
C	-0.17974900	1.66419500	-1.61192400
C	0.16839100	2.40446500	-2.51929600
Si	0.75050600	3.47064100	-3.93581600
C	2.60099900	3.68135200	-3.71112000
H	3.11306000	2.71017000	-3.68067600
H	3.02789400	4.25456700	-4.54435100
H	2.83669600	4.21929100	-2.78402000
C	-0.14935100	5.10964300	-3.84470500
H	0.17300100	5.76493800	-4.66441100
H	-1.23512100	4.98069800	-3.93059900
H	0.05785600	5.63105700	-2.90216600
C	0.35647000	2.53414000	-5.50928700
H	0.86162200	1.56011000	-5.53532500
H	-0.72080800	2.35949300	-5.61698900
H	0.69133300	3.10568800	-6.38483400
Si	2.21946000	-0.45232300	-0.73943200
C	3.34643500	0.97336100	-0.27340900
H	3.40512900	1.12496700	0.81260100
H	4.36782800	0.80898100	-0.63965500
H	2.97886900	1.90481600	-0.72596400
C	2.28937600	-0.81303000	-2.57266400
H	3.30076400	-1.12117500	-2.86791100
H	1.59925300	-1.61880600	-2.85190200
H	2.02499800	0.07535000	-3.16080100
C	2.36783500	-2.01172900	0.34092600
H	2.17644900	-2.88076700	-0.30453700
H	3.35809200	-2.17012200	0.78597700
C	1.27874300	-1.92509600	1.43181500
H	-1.40968900	-1.75597500	2.27005700
Ag	-0.40721300	0.64769000	3.06221500
C	1.86786300	-1.40545400	2.74806700
H	2.67005600	-2.05562200	3.11883600
H	2.30544600	-0.40225700	2.60468200

H	1.10686100	-1.36729100	3.54894200
H	0.84793900	-2.91944400	1.63323700

Propene

6	0.000031395	-0.000021204	-0.000000125
1	0.000024973	0.000013662	-0.000000016
1	0.000013706	0.000008401	0.000000026
6	-0.000016837	-0.000014099	-0.000000035
1	-0.000025416	-0.000029660	0.000000141
6	0.000016975	-0.000004510	-0.000000135
1	-0.000025918	0.000012636	-0.000000029
1	-0.000009420	0.000017474	-0.000001717
1	-0.000009459	0.000017301	0.000001890